SUPPORTING INFORMATION

For

Highly Selective Direct Oxidative Arylation with Arylsilanes *via* Rhodium-Catalyzed C—C Bond Cleavage of Secondary Benzyl Alcohols Directed by Pyridinyl Group

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General Experimental Section

Analytic methods. ^{1}H NMR and ^{13}C NMR data were obtained on Varian 300 M and Bruker 400 M nuclear resonance spectrometers unless otherwise specified, respectively. $CDCl_3$ as solvent and tetramethylsilane (TMS) as the internal standard were employed. Chemical shifts were reported in units (ppm) by assigning TMS resonance in the ^{1}H NMR spectrum as 0.00 ppm. The data of ^{1}H NMR was reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m =multiplet and br = broad), coupling constant (*J* values) in Hz and integration. Chemical shifts for ^{13}C NMR spectra were recorded in ppm from TMS using the central peak of $CDCl_3$ (77.0 ppm) as the internal standard. Flash chromatography was performed using 200-300 mesh silica gel with the indicated solvent system according to standard techniques. Analytical thin-layer chromatography (TLC) was performed on pre-coated, glass-backed silica gel plates. Visualization of the developed chromatogram was performed by UV absorbance (254 nm). HRMS (ESI) analysis was performed by Analytical Instrumentation Center, Peking University.

Source of Chemicals. $[Cp^{*}Rh(CH_3CN)_3][SbF_6]_2$ was prepared from $[Cp^{*}RhCl_2]_2$ (Sinocompound Technology Co., Ltd.) and $AgSbF_6$ (Alfa Aesar)[1]. AgF, Trimethoxyphenyl silane and Triethoxyphenyl silane was purchased from Alfar Aesar. Other arylsilanes were prepared from corresponding Grignard reagents and tetraethoxylsilane (Alfa Aesar)[2]. Alcohol substrates were synthesized by the reported method[3]. All the solvents were freshly distilled before used, and all the other reagents were directly used from purchased without any further purification unless otherwise specified.

General Experimental Procedure

General Procedure for Rh(III)-catalyzed oxidative arylation with arylsilanes via C—C Bond Cleavage of Secondary Benzyl Alcohols:

Under N_2 atmosphere, an oven-dried Schlenk tube containing a stir bar was charged with 1-phenyl-(4-methyl-2-(pyridin-2-yl))benzyl alcohol (**1a**) (55.1 mg, 0.20 mmol), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (8.3 mg, 0.01 mmol) and AgF (101.5 mg , 0.80 mmol). Then THF (0.50 mL), $PhSi(OMe)_3$ (**2a**) (158.6 mg, 0.80 mmol) and *t*-BuOH (0.50 mL) were injected sequently by syringe. The tube was placed on the parallel reactor and stirred at 90 °C for 16 hours. Then the mixture was cooled to room temperature and evaporated in vacuum. Further purification by flash chromatography on silica gel (hexane/EtOAc/CH_2Cl_2 50:1:1 to 20:1:1 gradually) afforded the product **3a** as a white solid (41.2 mg, 84%).

Procedure for the deuterium labeling experiment:

Under N_2 atmosphere, an oven-dried Schlenk tube containing a stir bar was charged with 1-phenyl-(3,4,5,6-4*D*-2-(pyridin-2-yl))benzyl alcohol (**7**) (26.5 mg, 0.10 mmol), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (4.2mg, 0.005 mmol) and AgF (50.7 mg , 0.40 mmol). Then THF (0.50 mL), $PhSi(OMe)_3$ (**2a**) (79.3mg, 0.40 mmol) and *t*-BuOH (0.50 mL) were injected sequently by syringe. The tube was placed on the parallel reactor and stirred at 90 °C for 16 hours. Then the mixture was cooled to room temperature and evaporated in vacuum. Further purification by flash chromatography on silica gel (hexane/EtOAc/CH_2Cl_2 50:1:1 to 20:1:1 gradually) afforded a mixture of monoaryl (**3ba-*d*$_4$**) and diaryl product (**3ba'-*d*$_4$**). (13.2 mg, 49% for **3ba-*d*$_4$** 9:1 in ^{1}H NMR). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.63 (d, J = 4.0 Hz, 1H), 8.30 (d, J = 4.0 Hz, 0.11H), 7.70 (s, 0.97H), 7.38 (td, J = 8.4, 1.6 Hz, 1H), 7.22 (m, 3H), 7.17-7.08 (m, 4H), 6.89 (d, J = 8.0 Hz, 1.23H). HRMS: m/z: $[M + H]^+$ calculated for $C_{17}H_{11}D_3N$: 235.13091; found 235.13070 and $C_{23}H_{15}D_3N$: 311.16221; found: 311.16156. 97% H/D crossover was observed.

Procedure for the competition experiment of C—C cleavage versus C—H activation:

Under N_2 atmosphere, 1-phenyl-(4-methyl-2-(pyridin-2-yl))benzyl alcohol (**1a**) (55.1 mg, 0.20 mmol), 2-(3-ethylphenyl)pyridine (**8**) (36.6 mg, 0.20 mmol), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (8.3 mg, 0.01 mmol) and AgF (101.5 mg , 0.80 mmol) were charged into an oven-dried Schlenk tube. Then THF (0.50 mL), $PhSi(OMe)_3$ (**2a**) (79.3mg, 0.40 mmol) and *t*-BuOH (0.50 mL) were injected sequently by syringe. The tube was placed on the parallel reactor and stirred at 90 °C for 2 h. Then the mixture was cooled to room temperature and evaporated in vacuum. Further purification by flash chromatography on silica gel (hexane/EtOAc/CH_2Cl_2 50:1:1 to 20:1:1 gradually) afforded the mixture of 2-(3-ethylphenyl)pyridine (**8**) and 2-(3-ethylphmnyl)pyridine (**5**) (25.5 mg), mixture of 2-(4-methylbiphenyl-2-yl)pyridine (**3aa**) and 2-(4-ethylbiphenyl-2-yl)pyridine (**3ja**) (31.6 mg), respectively.

^{1}H NMR (400 MHz, $CDCl_3$)of mixture **5** and **8**: δ = 8.69 (m, 1.23 H), 7.87-7.84 (m, 1.25H), 7.76- 7.13 (m, 3.79H), 7.40-7.34 (m, 1.28H), 7.26-7.19 (m, 2.62H), 2.74 (q, J = 7.2 Hz, 2H), 2.43 (s, 0.81H), 1.29 (t, J = 7.6 Hz, 3H).

The ratio of **5** and **8** = 1 : 3.7, the yield of **5** was 15%, and 56% **8** was recovered.

^{1}H NMR (400 MHz, $CDCl_3$) of mixture **3aa** and **3ja**: δ = 8.64-8.63 (m, 1.13H), 7.54-7.53 (m,

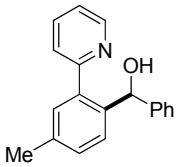
1.12H), 7.37-7.32 (m, 2.41H), 7.28-7.25 (m, 1.23H), 7.21-7.19 (m, 3.38H), 7.15-7.12 (m, 2.30), 7.09-7.06 (m, 1.17H), 2.75 (q, *J* = 7.6 Hz, 0.31H), 2.44 (s, 3H), 1.31 (t, *J* = 7.6 Hz, 0.53H).

The ratio of **3aa** and **3ja** = 6.4 : 1, theyield of **3aa** and **3ja** was 55% and 9% respectively.

Procedure for the Rh(III) catalyzed directed C—H arylation:

Under N_2 atmosphere, 2-(3-ethylphmnyl)pyridine (**5**) (33.8 mg, 0.20 mmol), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (4.2 mg, 0.005 mmol) and AgF (50.7 mg , 0.40 mmol) were charged into an oven-dried Schlenk tube. Then THF (0.50 mL), $PhSi(OMe)_3$ (**2a**) (79.3mg, 0.40 mmol) and *t*-BuOH (0.50 mL) were injected sequently by syringe. The tube was placed on the parallel reactor and stirred at 90 °C for 16 h. Then the mixture was cooled to room temperature and evaporated in vacuum. Further purification by flash chromatography on silica gel (hexane/EtOAc/CH_2Cl_2 50:1:1 to 20:1:1 gradually) afforded the product **3aa** (30.6 mg, 62%). For 2-phenylpyridine (**5'**), a mixture of monoaryl (**3ba**) and diaryl product (**3ba'**) was obtained (24.5 mg, 44% for **3ba** , **3ba** : **3ba'** = 6.6 : 1 by ^1H NMR)

Characterization of alcohol substrates 1



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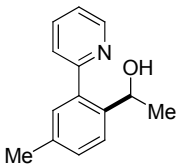

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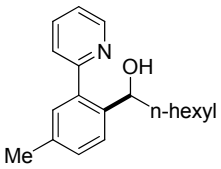

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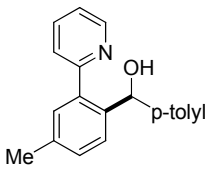

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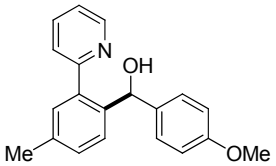

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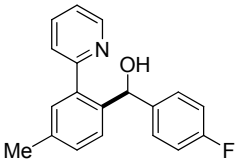

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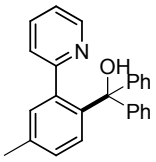

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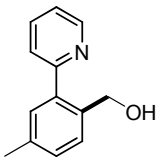

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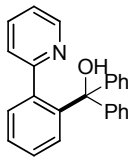

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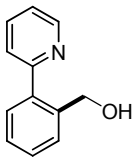

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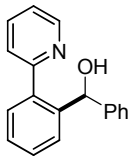

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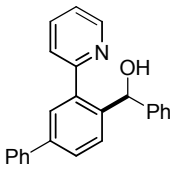

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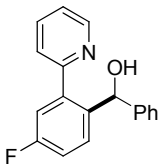

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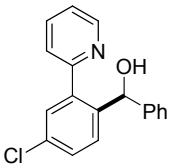

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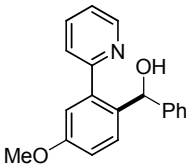

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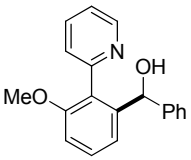

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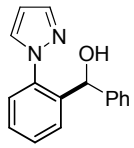

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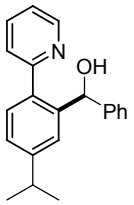
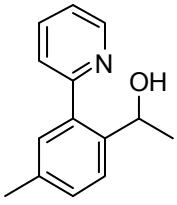


1r

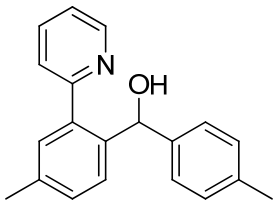
All the alcohol substrates were prepared by the methods reported in in reference 3 except **1h**, which was obtained from the reduction of ethyl 4-methyl-2-(pyridin-2-yl)benzoate(see ref 4). Among the alcohol substrates, **1b**, **1d**, **1e, 1f, 1g, 1h, 1o** and **1p** have not been reported. The rest ones were all characterized in reference 3.



1b

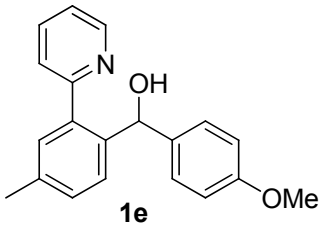
1-(4-methyl-2-(pyridin-2-yl)phenyl)ethanol (1b). Yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$): 8.62 (d, J = 3.9 Hz, 1H), 7.83 (t, J = 7.5, 1H), 7.58-7.48 (m, 2H), 7.33-7.28 (m, 3H), 6.37 (br,

1H), 4.76-4.69 (q, J = 6.6 Hz, 1H), 2.40 (s, 3H), 1.49 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): 159.9, 147.8, 140.5, 139.4, 137.4, 137.1, 131.3 (2C), 129.7, 126.4, 124.1, 122.0. 66.5, 21.0, 20.4. HRMS: m/z: $[M + H]^+$ calculated for $C_{14}H_{16}NO$: 212.12264; found: 212.12242.



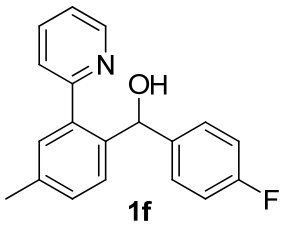
1d

(4-methyl-2-(pyridin-2-yl)phenyl)(p-tolyl)methanol (1d). Slabby oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.58 (d, 1H, *J* = 4.5 Hz), 7.75 (td, *J* = 7.8, 1.2 Hz, 1H,), 7.49-7.46 (d, J = 7.8 Hz, 1H), 7.27-7.23 (m, 2H), 7.18-7.15 (m, 3H), 7.08-7.01 (m, 3H), 5.75 (s, 1H), 2.38 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.8, 147.6, 141.2, 139.9, 139.5, 137.4, 137.3, 135.8, 131.4, 129.8, 129.6, 128.3, 126.3, 124.1, 122.0. 21.0. HRMS: m/z: $[M + H]^+$ calculated for $C_{20}H_{20}NO$: 290.15394; found:290.15390.



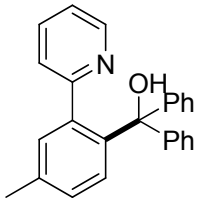
1e

(4-methoxyphenyl)(4-methyl-2-(pyridin-2-yl)phenyl)methanol (1e). Slabby oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.50-8.49 (m, 1H), 7.64 (td, *J* = 7.8, 1.8 Hz, 1H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.22-7.06 (m, 7H), 6.72 (d, *J* = 8.7 Hz, 2H), 5.73 (s, 1H), 3.67 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.5, 157.9, 147.3, 141.0, 139.4, 137.1, 137.0, 135.1, 131.1, 129.4, 129.3, 127.2, 123.9, 121.8, 112.9, 73.0, 54.9. 20.8. HRMS: m/z: $[M + H]^+$ calculated for $C_{20}H_{20}NO_2$: 306.14940; found: 306.14886.



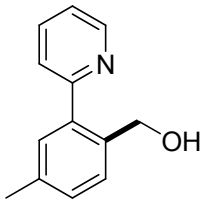
1f

4-fluorophenyl)(4-methyl-2-(pyridin-2-yl)phenyl)methanol (1f). White solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.56-8.54 (dt, *J* = 5.1, 0.9 Hz, 1H), 7.74 (t, *J* = 7.8 Hz, 1H), 7.45-7.42 (dd, J = 0.9, 7.8 Hz, 1H), 7.27-7.16 (m, 5H), 7.09-7.07 (d, *J*= 7.8 Hz, 1H), 6.86 (t, *J*= 8.4 Hz, 2H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.5 (d, *J* = 242.5 Hz), 159.7, 147.4, 140.8, 139.5, 138.9 (d, *J* = 2.8 Hz), 137.6, 137.5, 131.6, 130.0, 129.7, 127.8 (2C), 124.1, 122.1, 114.3 (d, *J* = 21.1Hz), 73.5, 21.0. HRMS: m/z: $[M + H]^+$ calculated for $C_{19}H_{17}FNO$: 294.12887; found 294.12883.



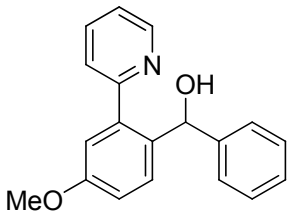
1g

(4-methyl-2-(pyridin-2-yl)phenyl)diphenylmethanol (1g). White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.13 (s, 1H), 8.28 (d, J = 4.4 Hz, 1H), 7.47 (td, J = 7.6, 1.6 Hz, 1H), 7.33-7.31 (m, 4H), 7.20 (s, 1H), 7.13-7.09 (m, 5H), 7.06-7.03 (m, 3H), 6.94(m, 1H), 6.74 (d, J = 8.0 Hz，1H)。 ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.4，147.2，146.3，144.9，140.1, 137.1(2C), 133.1, 130.3, 128.7, 127.6, 127.3, 126.2, 125.0, 121.4, 81.3, 20.8.



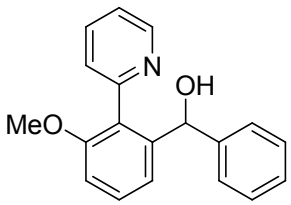
1h

(4-methyl-2-(pyridin-2-yl)phenyl)methanol (1h). Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.62 (d, J = 3.6 Hz, 1H), 7.83 (t, J = 7.2 Hz, 1H), 7.61 (d, J = 7.6 Hz, 1H), 7.38-7.21 (m, 4H), 6.30 (br, 1H), 4.43 (s, 2H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.3, 147.9, 139.7, 137.7, 137.5, 137.4, 131.1, 130.8, 129.8, 123.7, 122.1, 64.2, 21.1. HRMS: m/z: $[M + H]^+$ calculated for $C_{13}H_{14}NO$: 200.10699; found: 200.10674.



1o

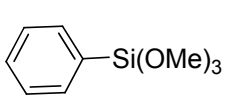
(4-methoxy-2-(pyridin-2-yl)phenyl)(phenyl)methanol (1o). White solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.59-8.57 (m, 1H), 7.74 (td, J = 7.5, 1.8 Hz, 1H), 7.43 (dt, J = 8.1, 0.9 Hz, 1H), 7.26-7.11 (m, 7H), 7.00-6.98 (m, 2H), 6.89-6.86 (dd, J = 2.7, 8.4 Hz), 5.76 (s, 1H), 3.84 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.4, 158.8, 147.6, 143.2, 141.0, 137.4, 136.3, 131.3, 127.6, 126.3, 124.0, 122.2, 116.7, 113.5, 73.4, 55.4. HRMS: m/z: $[M + H]^+$ calculated for $C_{19}H_{18}NO_2$: 292.13320; found: 292.13274.



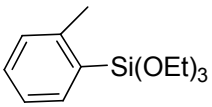
1p

(3-methoxy-2-(pyridin-2-yl)phenyl)(phenyl)methanol (1p). slight pink solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.54-8.52 (m, 1H), 7.54 (td, J = 12.3, 1.8 Hz, 1H), 7.27 (t, J = 7.5 Hz, 2H), 7.19-7.07 (m, 6H), 6.88 (dd, J = 2.1, 6.3 Hz, 2H), 5.56 (s, 1H), 3.66 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 156.5, 155.4, 147.7, 145.0, 142.8, 135.4, 129.3, 128.3, 127.2, 126.9, 126.0, 125.8, 121.6, 121.1, 110.2, 73.1, 55.3. HRMS: m/z: $[M + H]^+$ calculated for $C_{19}H_{18}NO_2$: 292.13375; found: 292.13270.

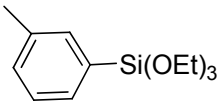
Characterization of Arylsilanes 2



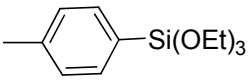
2a



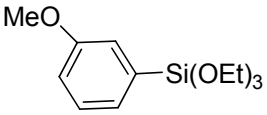
2b



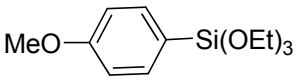
2c



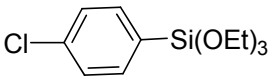
2d



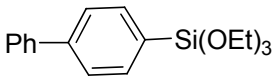
2e



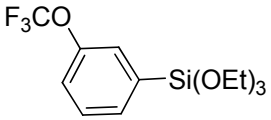
2f



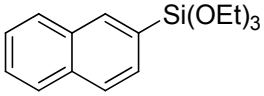
2g



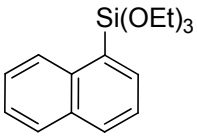
2h



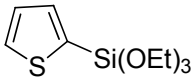
2i



2j

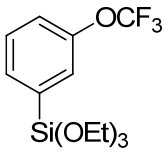


2k



2l

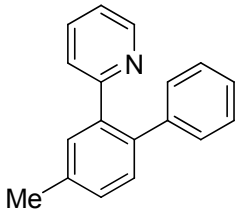
All the arylsines except triethoxyl(3-(trifluoromethoxy)phenyl)silane **(2i)** in this work were known compounds (**2a-2f** in ref. 2, **2g** and **2h** in ref. 4, **2j** in ref. 5, **2k** in ref. 6, **2l** in ref 7). The spectral data match those reported previously.



2i

triethoxyl(3-(trifluoromethoxy)phenyl)silane (2i). Yellow liquid. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.60-7.57 (td, J = 0.9, 7.2 Hz, 1H), 7.50 (m, 1H), 7.41 (t, J = 8.1 Hz, 1H), 7.29-7.25 (m, 1H), 3.88 (q, J = 6.9 Hz, 6H), 1.25 (t, J = 6.9 Hz, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): 149.1 (d, J =1.6 Hz), 134,2, 133.0, 129.4, 126.9, 122.7, 120.5 (q, J = 255.3 Hz), 58.9, 18.1. HRMS: m/z: $[M + Na]^+$ calculated for $C_{13}H_{20}F_3O_4SiNa$: 347.08969; found 347.08941.

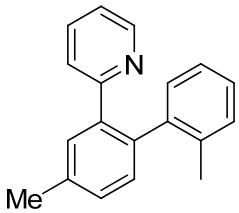
Characterization of Products 3



3aa

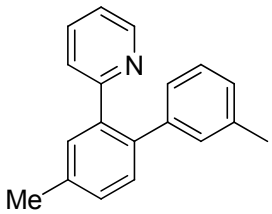
2-(4-methylbiphenyl-2-yl)pyridine (3aa). White solid (41.2mg, 84%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.63 (dt, J = 4.8, 0.9 Hz), 7.53 (s, 1H), 7.37-7.07 (m, 9H), 6.85 (dd, J = 0.9, 8.1 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 159.3, 149.3, 141.2, 139.2, 137.7, 137.3, 135.0, 131.0, 130.4, 129.7, 129.2, 127.9, 126.4, 125.4, 121.2, 21.0.

For the reaction between **1a** and $PhSi(OEt)_3$ (**2a'**): **3aa** (37.7 mg, 77%)
For the reaction between **1b** and **2a**: 42.9 mg (0.20 mmol) **1b** was used. **3aa** (30.1 mg, 61%).
For the reaction between **1c** and **2a**: 50.9 mg (0.20 mmol) **1c** was used. **3aa** (23.3 mg, 47%).
For the reaction between **1d** and **2a**: 55.5 mg (0.19 mmol) **1d** was used. **3aa** (25.7 mg, 55%).
For the reaction between **1e** and **2a**: 47.4 mg (0.16 mmol) **1e** was ussd. **3aa** (32.1 mg, 84%).
For the reaction between **1f** and **2a**: 58.7 mg (0.20 mmol) **1f** was ussd. **3aa** (34.3 mg, 70%).

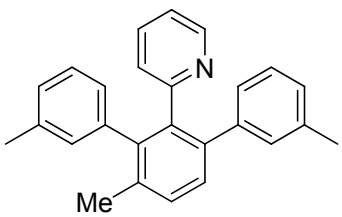


3ab

2-(2',4-dimethylbiphenyl-2-yl)pyridine (3ab). White solid (41.2 mg, 79%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.61 (d, J = 4.8Hz, 1H), 7.63 (s, 1H), 7.30-7.24 (m, 2H), 7.19 (s, 1H), 7.17-7.12 (m, 3H), 7.07-7.00 (m, 2H), 6.85 (td, J = 8.1, 0.9 Hz), 2.46(s, 3H), 1.88(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 158.8, 149.3, 141.1, 139.5, 137.3 (2C), 136.0, 135.0, 130.5 (3C), 129.8, 129.0, 127.1, 125.5, 124.5, 121.2, 21.1, 19.9. HRMS: m/z: $[M + H]^+$ calculated for $C_{19}H_{18}N$:260.14338; found: 260.14309.



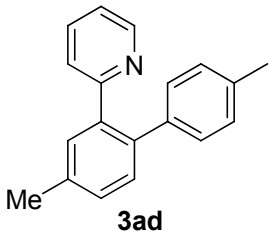
3ac



3ac'

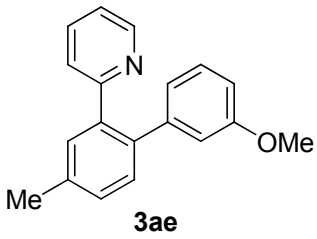
2-(3',4-dimethylbiphenyl-2-yl)pyridine (3ac). White solid (50.1 mg, 82%, **3ac** : **3ac**' = 7.7 : 1 by ^{1}H NMR). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.63 (d, J = 4.2, 1H), 7.51 (s, 1H), 7.39-7.25 (m, 3H), 7.10-7.05 (m, 2H), 7.00 (m, 2H), 2.43 (s, 3H), 2.24 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.4, 149.2, 141.2, 139.2, 137.9, 137.5, 137.2, 135.0, 131.0, 130.4 (2C), 129.2,

127.8, 127.2, 126.8, 125.4, 121.2, 21.3, 21.1. HRMS: m/z: $[M + H]^+$ and calculated for **3ac** $C_{19}H_{18}N$: 260.14338; found 260.14345 and **3ac**' $[M + H]^+$ calculated for $C_{26}H_{24}N$: 350.10933; found 350.19018.



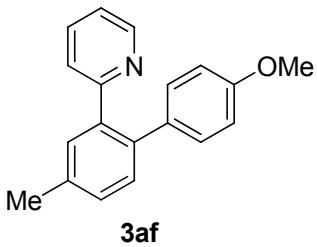
3ad

2-(4,4'-dimethylbiphenyl-2-yl)pyridine (3ad). White solid (46.0 mg, 89%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.65(d, J = 4.2 Hz, 1H), 7.52 (s, 1H), 7.38 (td, J =7.8, 1.8 Hz, 1H), 7.33-7.25 (m, 2H), 7.11 (ddd, J =7.5, 5.1, 1.2 Hz, 1H), 7.02(s, 4H), 6.88 (d, J =7.8, 1H), 2.43 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.5, 149.3, 139.2, 138.3, 137.7, 137.1, 136.1, 135.0, 131.0, 130.4, 129.5, 129.2, 128.7, 125.4, 121.1, 21.0 (2C). HRMS: m/z: $[M + H]^+$ calculated for $C_{19}H_{18}N$: 260.14338; found: 260.14312.



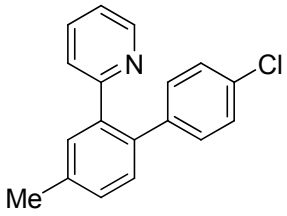
3ae

2-(3'-methoxy-4-methylbiphenyl-2-yl)pyridine (3ae). Colorless oil (39.6 mg, 72%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.63 (m, 1H), 7.52 (m, 1H), 7.40-7.33 (m, 2H), 7.28-7.25 (m, 1H), 7.15-7.07 (m, 2H), 6.89 (d, J = 5.1 Hz, 1H), 6.77-6.73 (m, 2H), 6.66 (m, 1H), 3.62 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.4, 159.2, 149.3, 142.7, 139.3, 137.7, 137.5, 135.2, 131.0, 130.3, 129.3, 129.0,125.4, 122.2, 121.3, 115.0, 112,7, 55.0, 21.0. HRMS: m/z: $[M + H]^+$ calculated for $C_{19}H_{18}NO$:276.13829; found: 276.13819.

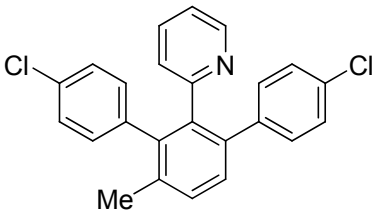


3af

2-(4'-methoxy-4-methylbiphenyl-2-yl)pyridine (3af). White solid (53.1 mg, 96%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.66 (d, J = 4.8, 1H), 7.53 (s, 1H), 7.39 (td, J = 7.8, 1.5Hz, 1H), 7.34-7.28 (m, 2H), 7.13-7.06 (m,3 H), 6.89 (d, J =7.8, 1H), 6.80-6.77 (m, 2H), 3.79 (s, 3H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.5, 158.4, 149.3, 139.1, 137.4, 136.9, 135.1, 133.7, 131.0, 130.7, 130.3, 129.2, 125.4, 121.1, 113.5, 55.1, 21.0. HRMS: m/z: $[M + H]^+$ calculated for $C_{19}H_{18}NO$: 276.13829; found: 276.13805.

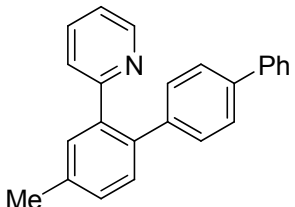


3ag



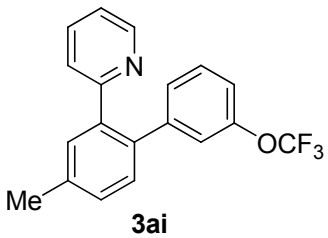
3ag'

2-(4'-chloro-4-methylbiphenyl-2-yl)pyridine (3ag). White solid (54.9 mg, 67%, **3ag** : **3ag**'= 7.7 : 1 by ^{1}H NMR). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.63 (d, J = 4.8, 1H), 7.49 (s, 1H), 7.42 (td, J = 7.5, 1.8 Hz, 1H), 7.27-7.25(m, 2H), 7.19-7.16 (m, 2H), 7.12 (dd, J =7.5, 4.8Hz, 1H), 7.07-7.03 (m, 2H), 6.88 (d, J = 7.8 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.1, 149.4, 139.8, 139.2, 137.7, 136.5, 135.3, 132.6, 131.1, 130.9, 130.2, 129.3, 128.2, 125.3, 121.4, 21.0. HRMS: m/z: $[M + H]^+$ calculated for $C_{18}H_{15}ClN$: 280.08875; found: 280.08862. and **3ag**': $[M + H]^+$ calculated for $C_{24}H_{18}Cl_2N$: 390.08108; found: 390.08089.



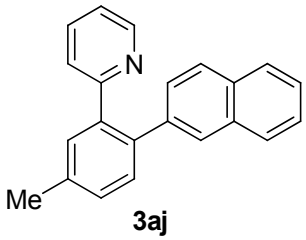
3ah

2-(4'-phenyl-4-methylbiphenyl-2-yl)pyridine (3ah). White solid (51.8 mg, 81%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.64 (d, J = 4.8 Hz, 1H), 7.59-7.54 (m, 3H), 7.48-7.29 (m, 8H), 7.22-7.19 (m, 2H), 7.08 (ddd, J = 7.5, 5.1, 1.2Hz, 1H), 6.93 (d, J = 7.8 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.4, 149.4, 140.6, 140.3, 139.3, 139.2, 137.5, 137.3, 135.2, 131.2, 130.4, 130.1, 129.3, 128.7, 127.2, 126.9, 126.7, 125.5, 121.3, 21.1. HRMS: m/z: $[M + H]^+$ calculated for $C_{24}H_{20}N$: 322.15903; found:322.15884.



3ai

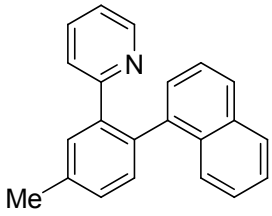
2-(4-methyl-3'-(trifluoromethoxy)biphenyl-2-yl)pyridine (3ai). Colorless oil (60.4 mg, 92%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.61 (m, 1H), 7.51 (s, 1H), 7.40 (td, J = 7.8, 1.8 Hz), 7.34-7.22 (m, 3H), 7.13-7.02 (m, 3H), 6.94-6.87 (m, 2H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 158.9, 149.5, 148.8 (d, J = 1.7), 143.4, 139.4, 138.1, 136.2, 135.4, 131.3, 130.2, 129.4 (d, J = 5.1 Hz), 128.0, 125.2, 122.3, 122.0, 121.5, 120.3 (q, J = 255.6), 119.0, 21.1. HRMS: m/z: $[M + H]^+$ calculated for $C_{19}H_{15}F_3NO$: 330.11003; found: 330.11011.



3aj

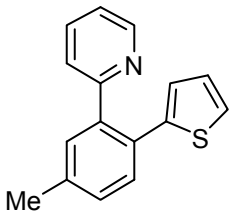
,

2-(5-methyl-2-(naphthalen-2-yl)phenyl)pyridine (3aj). Yellow solid (54.2 mg, 92%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.64 (d, J = 5.1 Hz, 1H), 7.77-7.73 (m, 3H), 7.63-7.57 (m, 2H), 7.44-7.40 (m, 3H), 7.32-7.23 (m, 2H), 7.14 (dd, J = 1.8, 8.4, 1H), 7.04 (ddd, J = 7.5, 1.8, 0.9, 1H), 6.87 (d, J = 7.8 Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.2, 149.4, 139.3, 139.0, 137.6, 137.5, 135.2, 133.4, 132.0, 131.1, 130.8, 129.3, 128.3, 128.1, 127.5, 127.2, 125.9, 125.7, 125.4, 121.3, 21.1. HRMS: m/z: $[M + H]^+$ calculated for $C_{22}H_{18}N$: 296.14338; found: 296.14333.



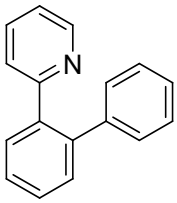
3ak

2-(5-methyl-2-(naphthalen-1-yl)phenyl)pyridine (3ak). Yellow oil (44.7 mg, 76%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.53 (d, J = 4.8Hz, 1H), 7.78 (d, J = 7.8Hz, 1H), 7.74 (d, J = 8.1Hz, 1H), 7.70-7.67 (m, 2H), 7.39-7.24 (m, 6H), 7.03 (td, J = 7.5, 1.8Hz, 1H), 6.87 (ddd, J = 7.5, 5.1, 1.2Hz, 1H), 6.65 (d, J = 7.8Hz, 1H), 2.51 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$): δ = 158.7, 149.2, 140.4, 139.3, 137.7, 135.9, 134.8, 133.5, 132.1, 131.5, 130.8, 129.0, 128.0, 127.9, 127.3, 126.2, 125.8, 125.5, 125.1, 124.2, 121.1, 21.2. HRMS: m/z: $[M + H]^+$ calculated for $C_{22}H_{18}N$: 296.14338; found: 296.14318

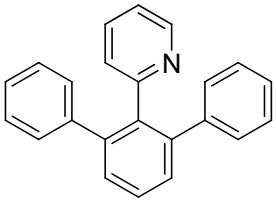


3al

2-(5-methyl-2-(thiophen-2-yl)phenyl)pyridine (3al). Yellow solid (43.2 mg, 86%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.65 (d, J = 4.8 Hz, 1H), 7.50-7.41 (m, 3H), 7.25-7.07 (m, 4H), 6.85 (dd, J = 3.6, 5.1 Hz, 1H), 6.65 (d, J = 2.7 Hz, 1H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 159.3, 149.3, 142.9, 139.6, 137.9, 135.4, 131.1, 130.6, 130.2, 129.2, 127.0, 126.7, 125.3, 124.9, 121.6, 21.0. HRMS: m/z: $[M + H]^+$ calculated for $C_{16}H_{14}NS$: 252.08415; found: 252.08401.



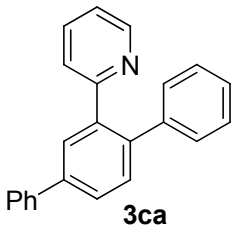
3ba



3ba'

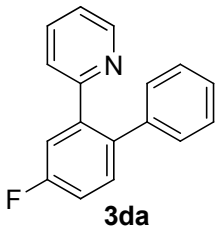
2-(biphenyl-2-yl)pyridine (3ba). White solid (36.0 mg, 68% , **3ba : 3ba'** = 8.3 : 1 by ^{1}H NMR).^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.63 (d, J = 4.2 Hz, 1H), 7.71-6.68 (m, 1H), 7.48-7.43 (m, 3H), 7.37 (td, J = 7.8, 1.8 Hz, 1H), 7.24-7.21 (m, 3H), 7.17-7.14 (m, 2H), 9.09 (dd, J = 6.6, 5.1Hz, 1H), 6.88(d, J = 8.1, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.3, 149.4, 141.4, 140.7, 139.5, 135.1, 130.5(2C), 129.7, 128.5, 128.0, 127.6, 126.7, 125.4, 121.3. HRMS: m/z: $[M + H]^+$ calculated for **3ba'** $C_{23}H_{18}N$: 308.14338; found: 308.14339.

For the reaction between **1g** and **2a**: 67.5 mg **1g** was used (47.5 mg, 88%, **3ba : 3ba'** = 8.3 : 1 by ^{1}H NMR).
For the reaction between **1h** and **2a**: 37.9 mg **1h** was used. (7.6 mg, 16%, trace **3ba'** was obseved).



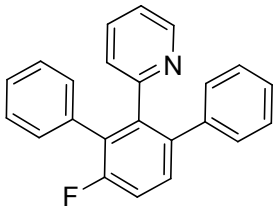
3ca

2-(4-phenylbiphenyl-2-yl)pyridine (3ca). White solid (52.4 mg, 85%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.66 (ddd, J = 5.1, 1.8, 1.2 Hz, 1H), 7.94 (d, J =2.1Hz, 1H), 7.72-7.69 (m, 3H), 7.52 (d, J = 7.8 Hz, 1H), 7.48-7.42 (m, 2H), 7.40-7.32 (m, 2H), 7.26-7.18 (m, 5H), 7.12 (ddd, J = 7.5, 4.8, 1.6Hz, 1H), 6.94 (dt, J = 7.8, 0.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ =159.2, 149.4, 141.0, 140.5, 140.4, 139.8, 139.6, 135.2, 131.0 , 129.6, 129.3 , 128.7, 128.0, 127.4, 127.1, 127.0, 126.7, 125.4, 121.4. HRMS: m/z: $[M + H]^+$ calculated for $C_{23}H_{18}N$: 308.14338; found 308.14304.



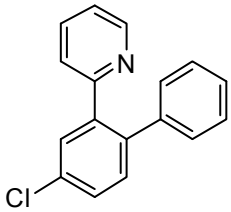
3da

2-(4-fluorobiphenyl-2-yl)pyridine (3da). White solid (28.3, mg 57%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.64 (ddd, J = 4.8, 1.8, 0.9 Hz, 1H), 7.46-7.36 (m, 3H), 7.26-7.18 (m, 4H), 7.17-7.10 (m, 4H), 6.86 (d, J = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.3(d, J = 245.4 Hz), 158.0, 149.5, 141.3 (d, J = 7.6 Hz), 140.5, 136.7 (d, J = 3.2 Hz), 135.3, 132.1 (d, J = 7.9 Hz), 129.7, 128.1, 126.8, 125.3, 121.8, 117.2 (d, J = 22.3 Hz), 115.4 (d, J = 21.1 Hz).



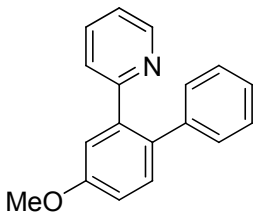
3da'

2-(3-phenyl-4-fluorobiphenyl-2-yl)pyridine (3da'). White solid (7.4 mg, 11%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.27 (d, J = 6.4 Hz, 1H), 7.42 (dd, J = 5.2, 8.4 Hz, 1H), 7.29-7.25 (m, 2H), 7.19-7.10 (m, 8H), 7.08-7.06 (m, 2H), 6.89-6.86 (m, 1H), 6.83 (d, J = 7.6 Hz, 1H).^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.2 (d, J = 244.6 Hz), 157.7 (d, J = 2.6 Hz), 148.5, 140.9 (d, J = 2.7 Hz), 140.8, 137.7 (d, J = 3.6 Hz), 134.9, 134.2, 130.7, 130.5, 129.6, 129.2 (d, J = 16.1), 127.7, 127.5, 126.9, 126.5, 126.4, 121.1, 115.4 (d, J = 23.1 Hz). ^{1}H RMS: m/z: $[M + H]^+$ calculated for $C_{23}H_{17}FN$: 326.13395; found: 326.13398.

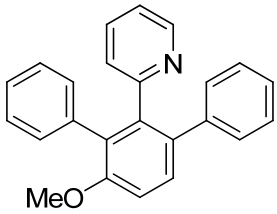


3ea

2-(4-chlorobiphenyl-2-yl)pyridine (3ea). White solid (25.2 mg, 47%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.63 (d, J = 4.2 Hz, 1H), 7.80 (d, J = 7.8Hz, 1H), 7.67-7.59 (m, 3H), 7.57-7.49 (m, 4H), 7.39 (td, J = 7.8, 1.8 Hz, 1H), 7.28-7.10 (m, 5H), 7.11 (ddd, J = 7.5, 5.1, 1.2 Hz, 1H), 6.90 (d, J=7.8Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.9, 149.5, 140.9, 140.2, 139.0, 135.3, 133.6, 131.8, 130.4, 129.5, 128.5, 128.2, 127.0, 125.2, 121.8. HRMS: m/z: $[M + H]^+$ calculated for $C_{17}H_{12}ClN$: 266.07310; found: 266.07289.

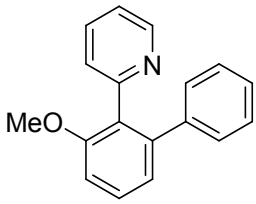


3fa



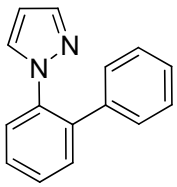
3fa'

2-(4-methoxybiphenyl-2-yl)pyridine (3fa). 49.4 mg(0.17 mmol) **1l** was used. White solid (44.6 mg, 61%, **3fa : 3fa'** = 2 : 1). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.63 (d, J = 4.5, 1H), 7.37-7.33 (m, 2H), 7.25-7.17 (m, 4H), 7.12-7.08 (m, 3H), 6.86 (d, J = 7.8 Hz, 1H), 3.89 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 159.1 (2C), 149.4, 141.1, 140.5, 135.2, 133,3, 131.7,129.8, 128.0, 126.3, 125.4, 121.4, 115.0 (2C), 55.5. HRMS: m/z: $[M + H]^+$ calculated for $C_{18}H_{16}NO$: 262.12264; found: 262.12238. and **3fa'**: $[M + H]^+$ calculated for $C_{24}H_{20}NO$: 338.15394; found: 338.15374.

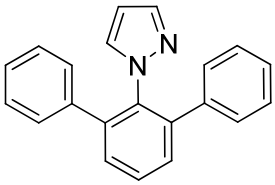


3ga

2-(3-methoxybiphenyl-2-yl)pyridine (3ga). 67.5 mg(0.23 mmol) **1m** was used. White solid. (37.9 mg, 63%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.57 (d, J = 4.8 Hz, 1H), 7.50-7.39 (m, 2H), 7.14-6.99 (m, 9H), 3.78 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.2, 156.8, 148.7, 142.7, 141.0, 135.3, 129.5, 129.1, 127.5, 126.3, 126.2, 122.4, 121.2, 110.0, 55.9.

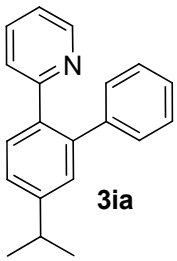


3ha

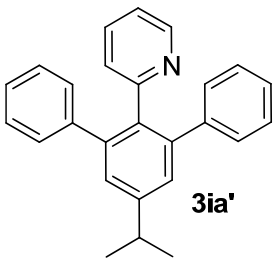


3ha'

1-(biphenyl-2-yl)-*1H*-pyrazole (3ha). White solid (23.8 mg, 46% , **3ha : 3ha'** = 8.3 : 1). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.63-7.60 (m, 2H), 7.48-7.46 (m, 3H), 7.29-7.25 (m, 3H), 7.12-7.09 (m, 2H), 7.07 (dd, J = 2.4, 0.6 Hz, 1H), 6.18 (dd, J = 2.4, 2.1 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): 140.2, 138.6, 136.7, 131.2, 131.0, 128.5, 128.4, 128.3, 128.2, 127.4, 126.5, 106.3. HRMS: m/z: $[M + H]^+$ calculated for **3ha'**: $[M + H]^+$ calculated for $C_{21}H_{17}N_2$: 297.13862; found: 297.13844.



3ia



3ia'

2-(5-isopropylbiphenyl-2-yl)pyridine (3ia). 58.4 mg(0.19 mmol) **1p** was used. White solid (25.4 mg, 41%, **3ia : 3ia'** = 9.1 : 1). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.61 (d, J = 4.8Hz, 1H), 7.63 (d, J=7.8, 1H), 7.39-7.32 (m, 2H), 7.28 (d, J=1.8, 1H), 7.25-7.21 (m, 3H), 7.19-7.15 (m, 2H), 7.07 (ddd, J=7.5, 5.1, 1.2Hz, 1H), 6.86 (d, J = 7.8Hz, 1H), 3.0(m, 1H), 1.33(s, 3H), 1.31(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.3, 149.3 (2C), 141.7, 140.5, 137.1, 135.0, 130.5, 129.7, 128.6, 128.0 , 126.5, 125.7, 125.3, 121.0, 33.9, 23.9. HRMS: m/z: $[M + H]^+$ calculated for $C_{20}H_{20}N$: 274.15903; found 274.15872. and **3ia'** $[M + H]^+$ calculated for $C_{26}H_{24}N$: 350.19033; found: 350.19009.

References:

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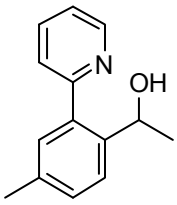
NMR Spectra of Alcohol Substrates 1



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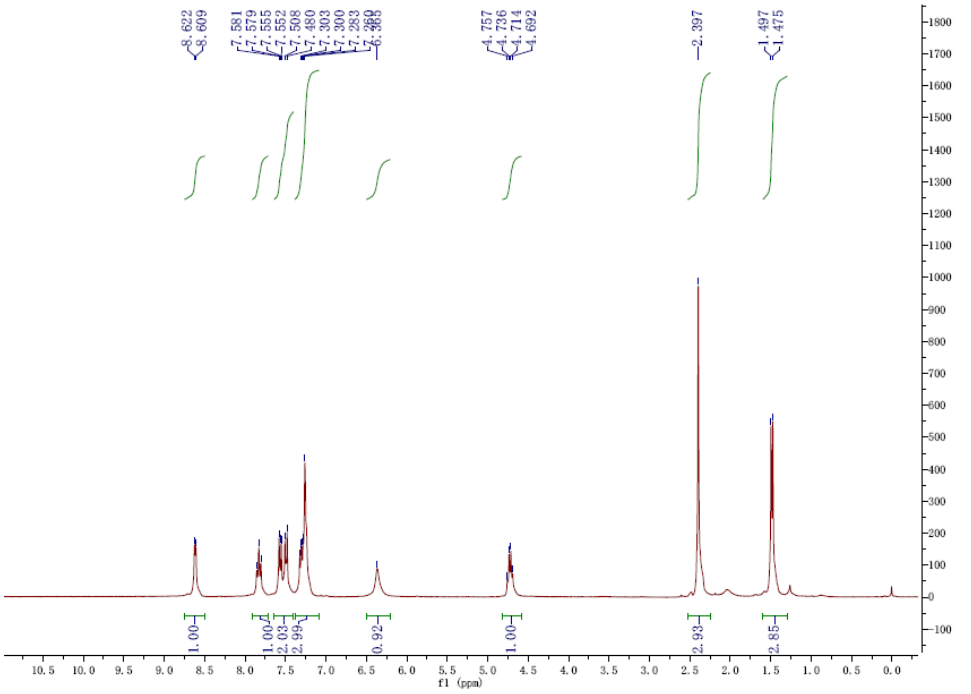

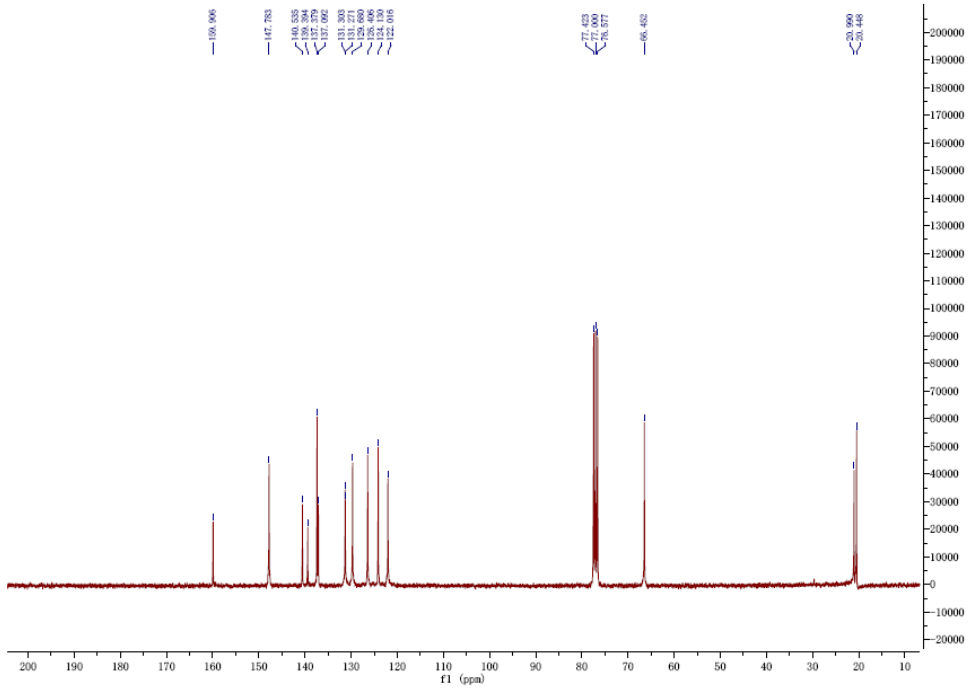

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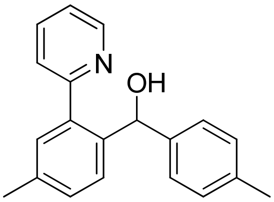

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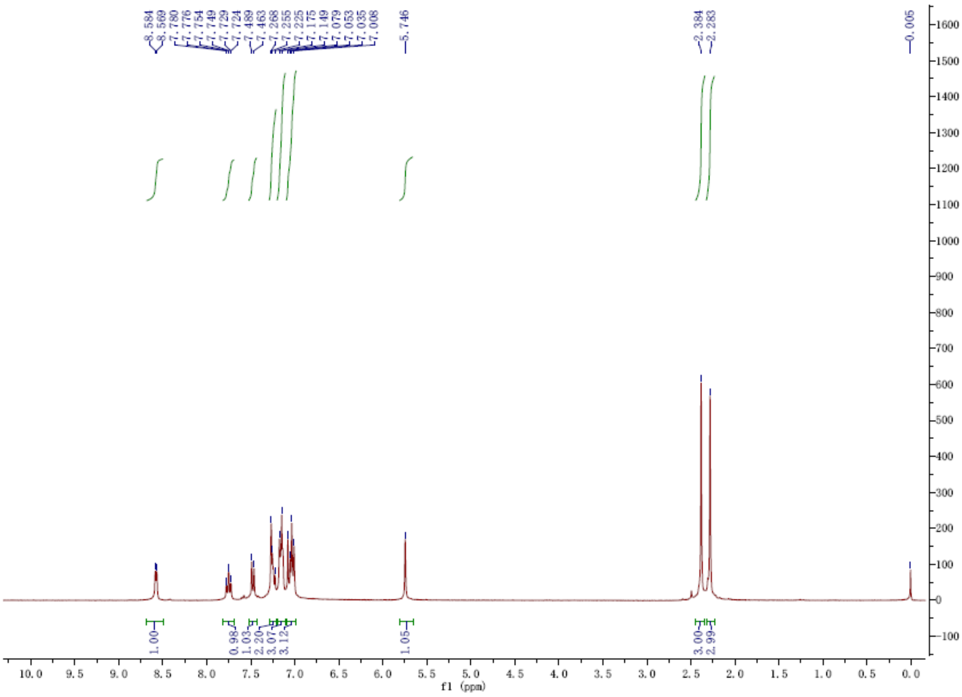

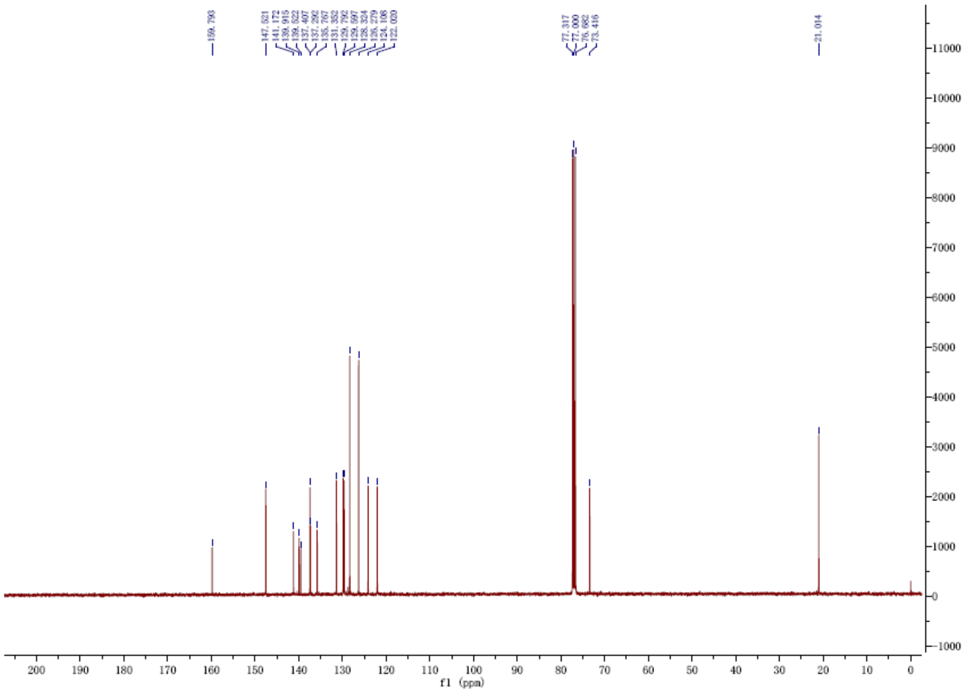

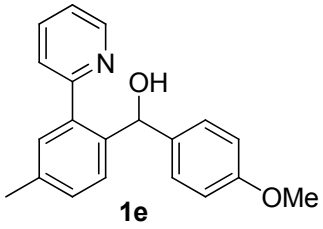
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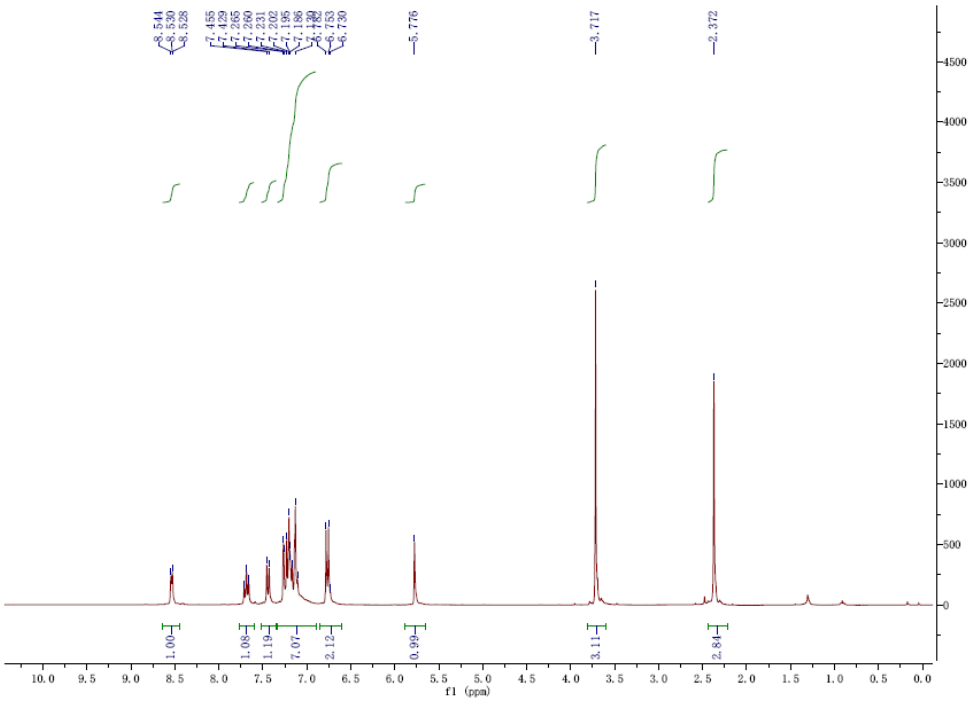
OMe

1e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1.08
1.19
7.07
2.12
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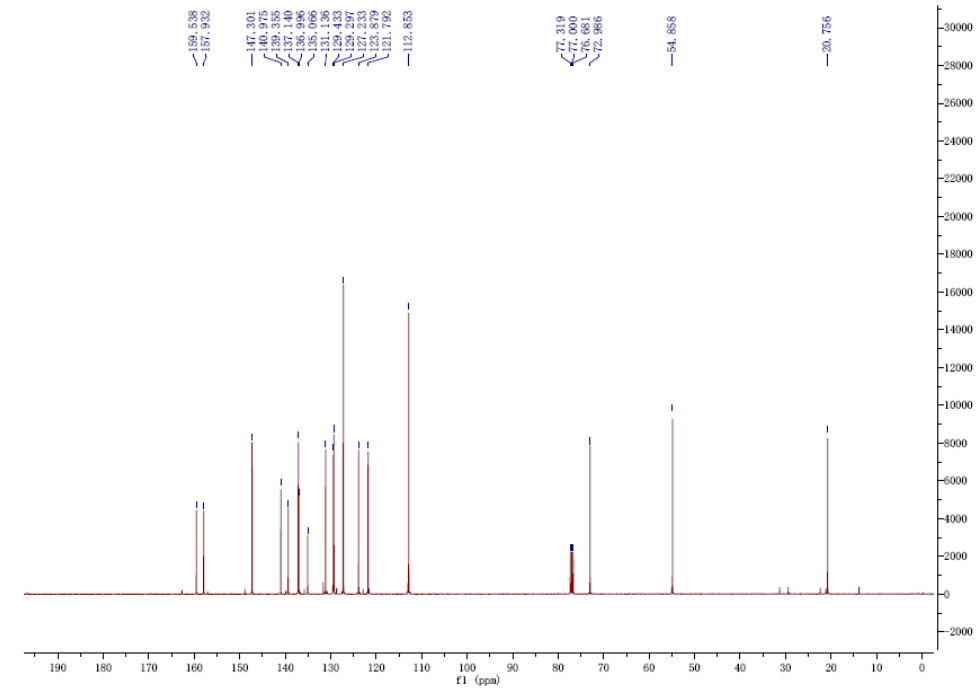
2.84
f1 (ppm)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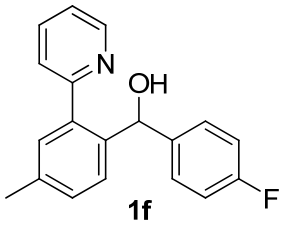

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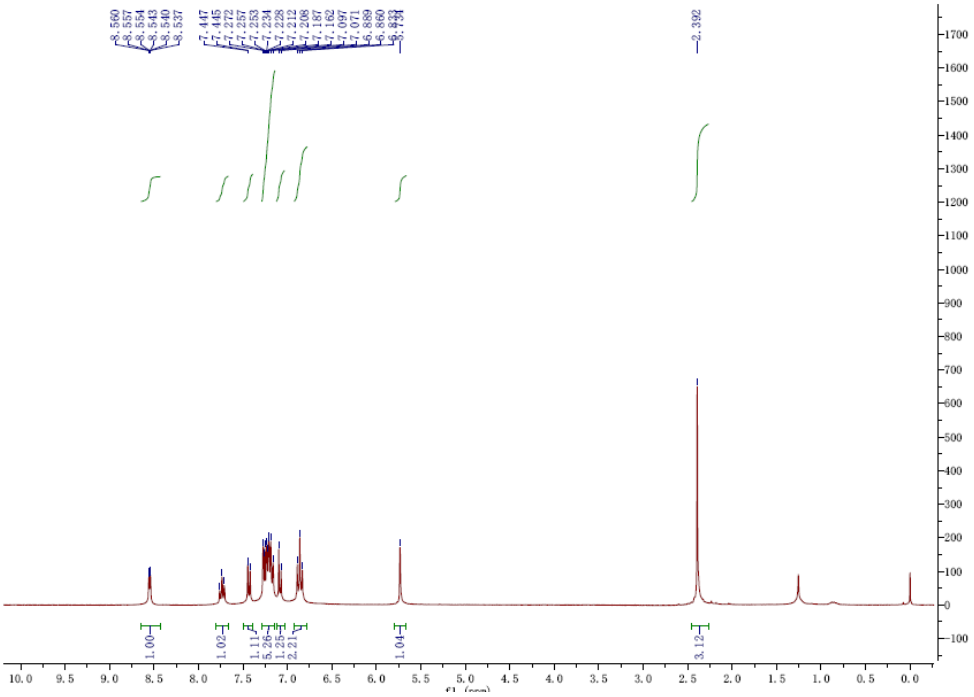

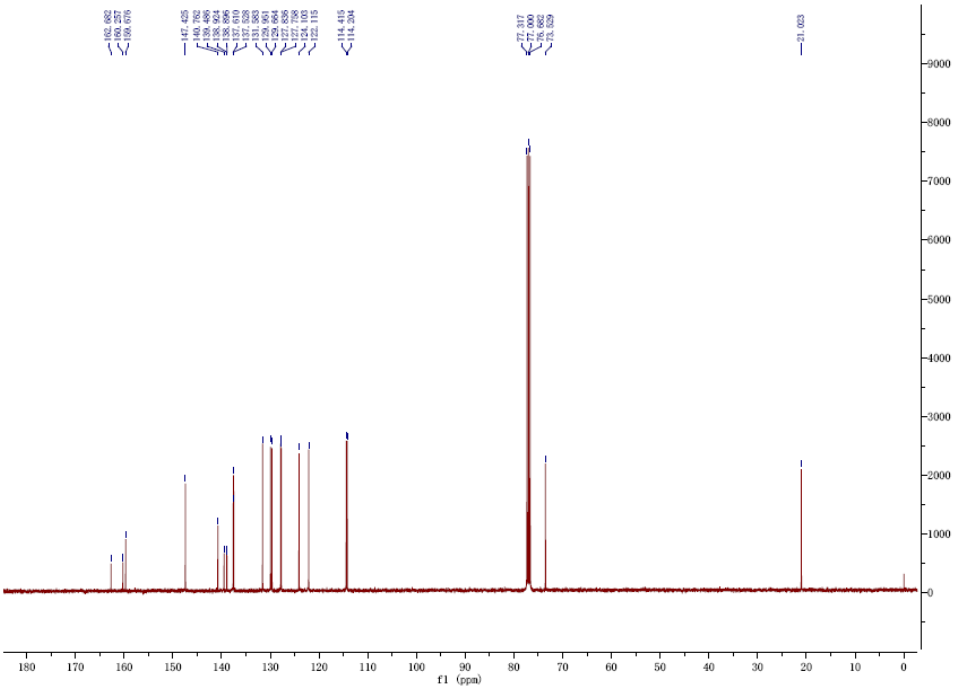

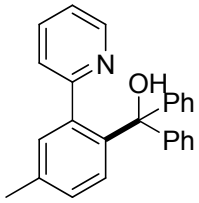
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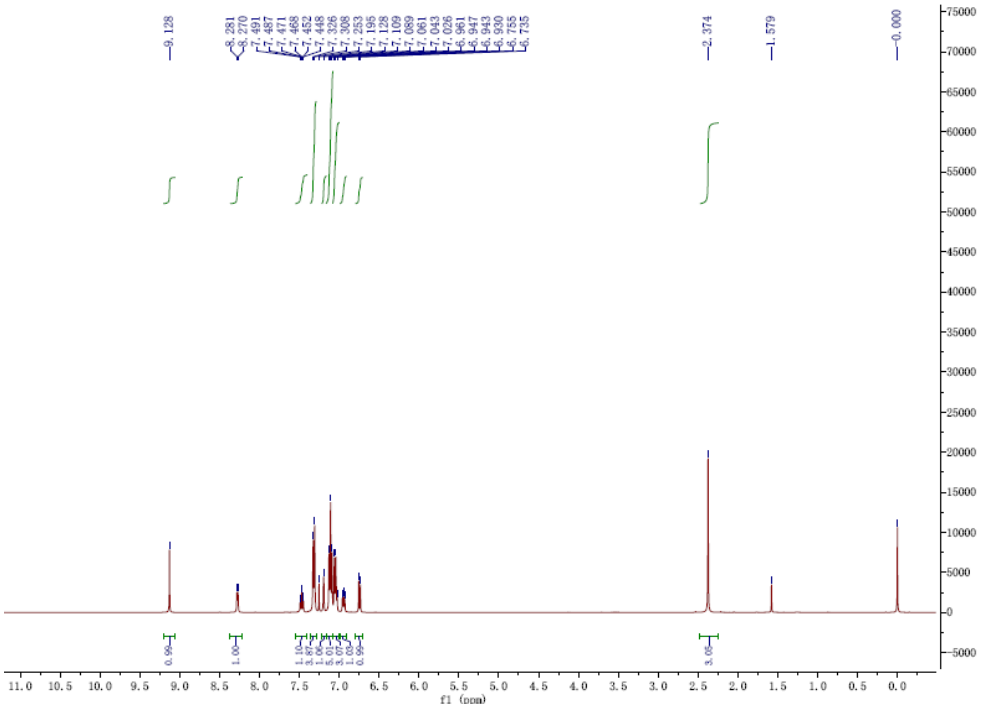
Ph

1g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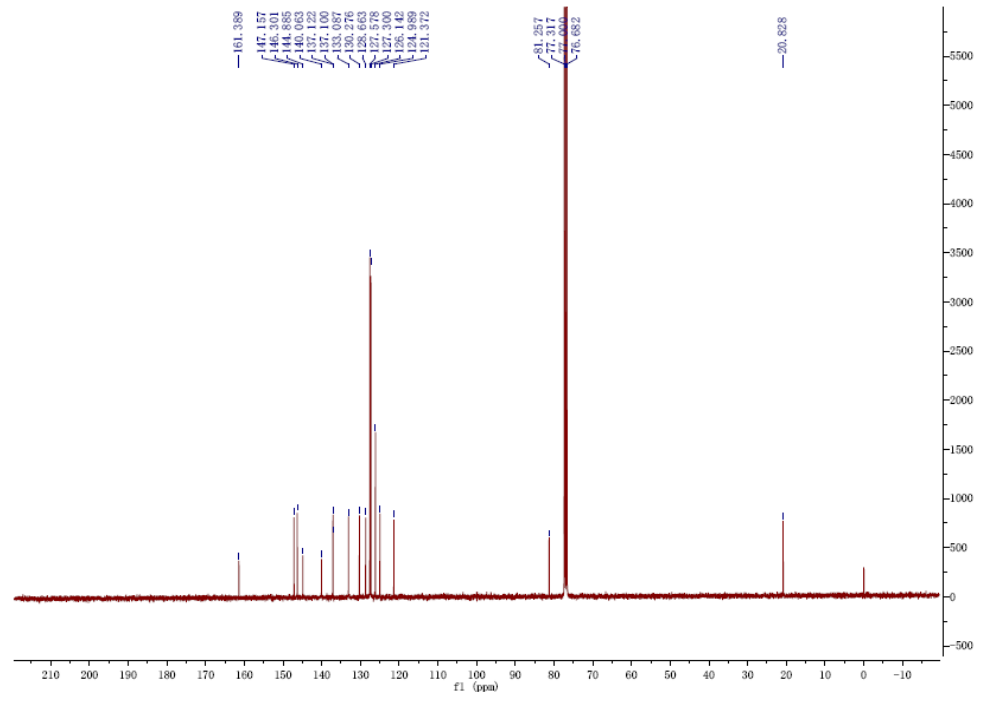
f1 (ppm)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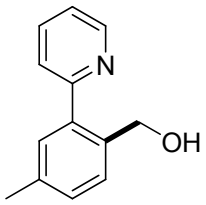
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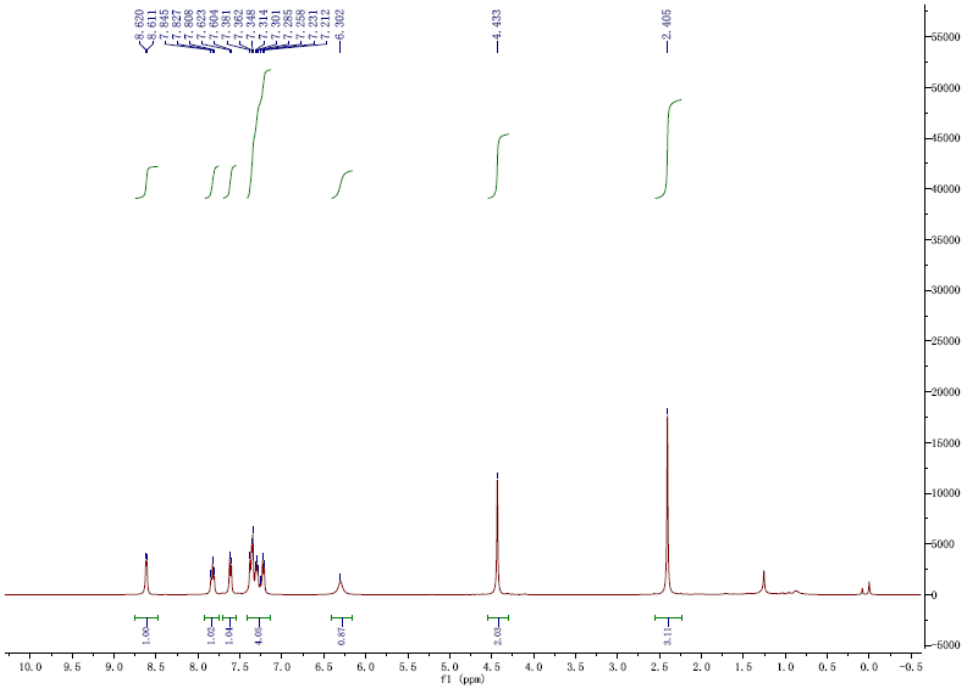
OH

1h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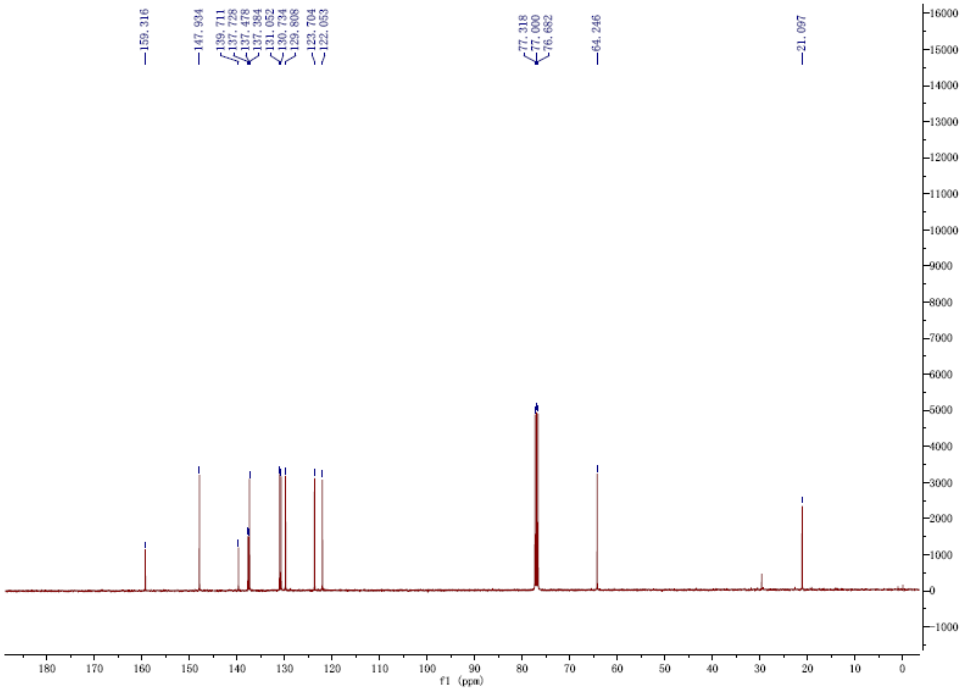
3.11
f1 (ppm)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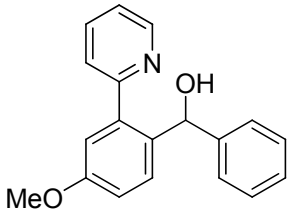
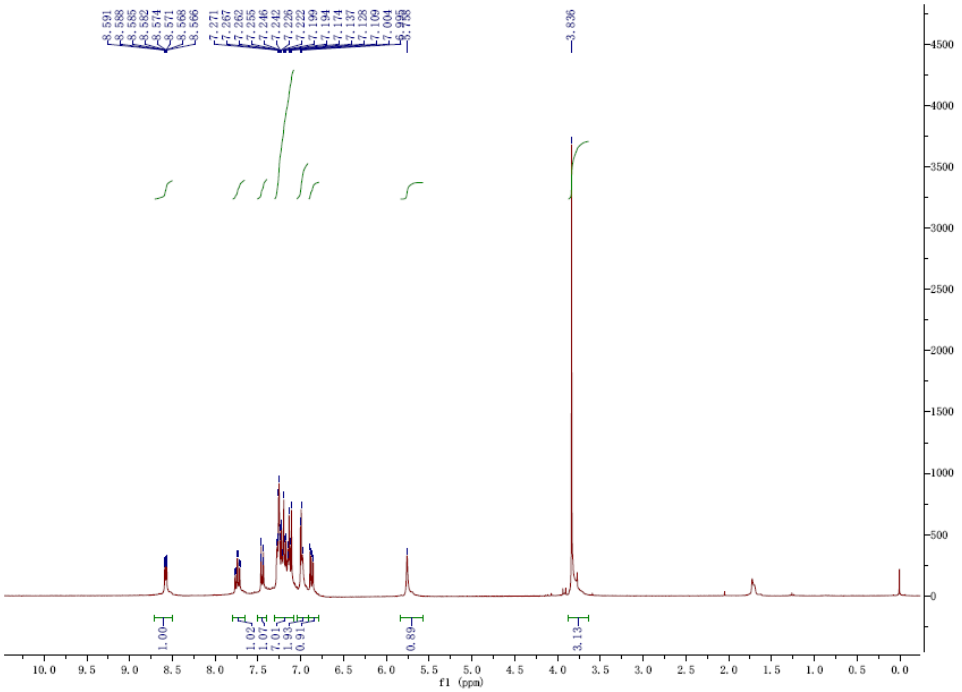
147.934
139.711
137.726
137.478
137.384
131.052
130.734
129.808
123.704
122.053
77.318
77.000
76.682
64.246
21.097
f1 (ppm)


N
OH
MeO

1o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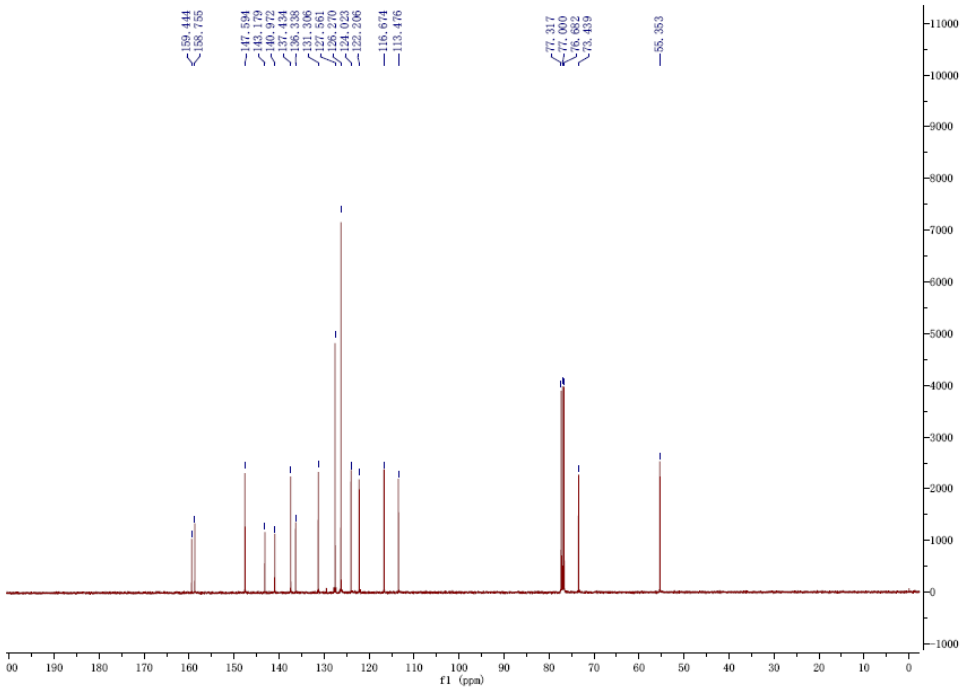
8.588
8.585
8.582
8.574
8.571
8.568
8.566
7.271
7.267
7.262
7.255
7.246
7.242
7.226
7.222
7.199
7.194
7.174
7.137
7.128
7.109
7.004
6.998
6.988
3.836
1.00
1.02
1.07
7.01
1.93
0.91
0.89
3.13
f1 (ppm)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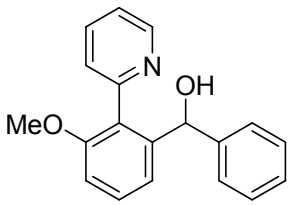
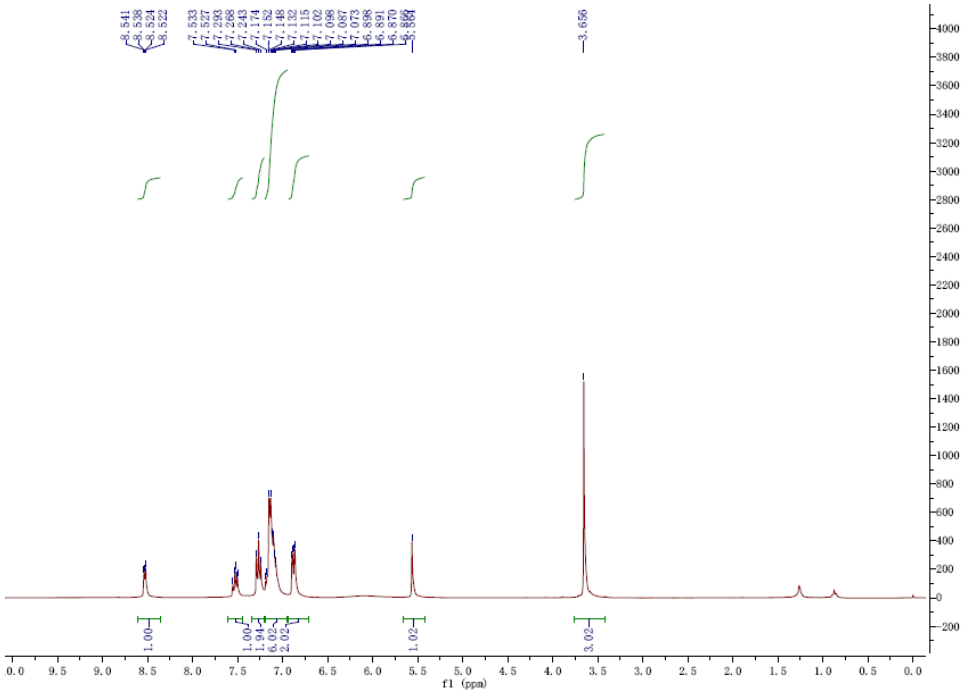
136.338
131.306
127.561
126.270
124.023
122.206
116.674
113.476
77.317
77.000
76.682
73.439
55.353
f1 (ppm)


N
OH
MeO

1p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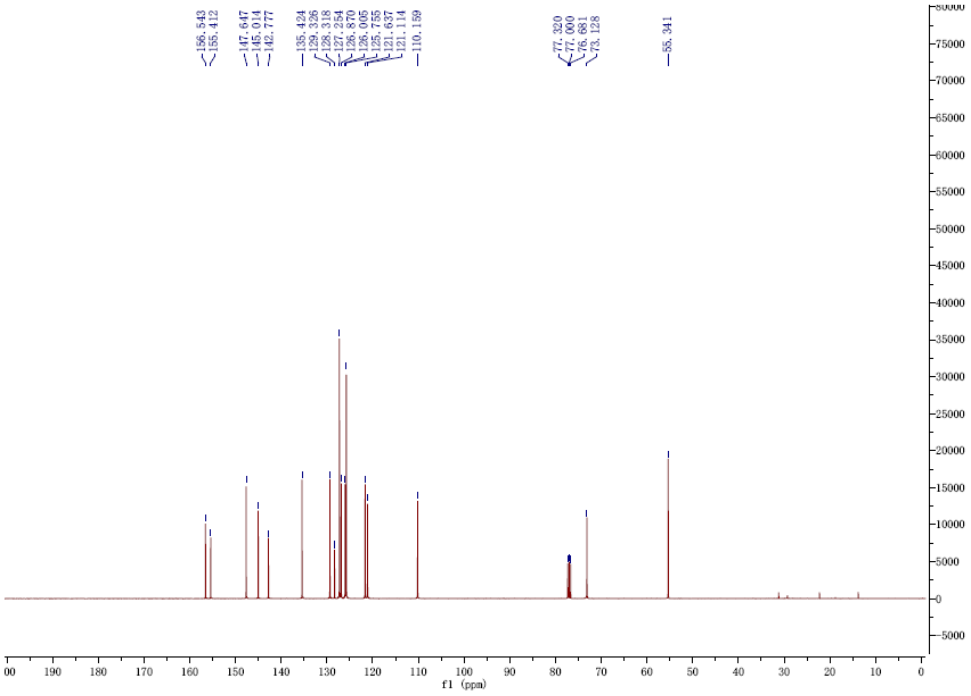
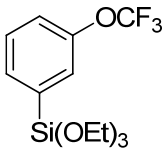
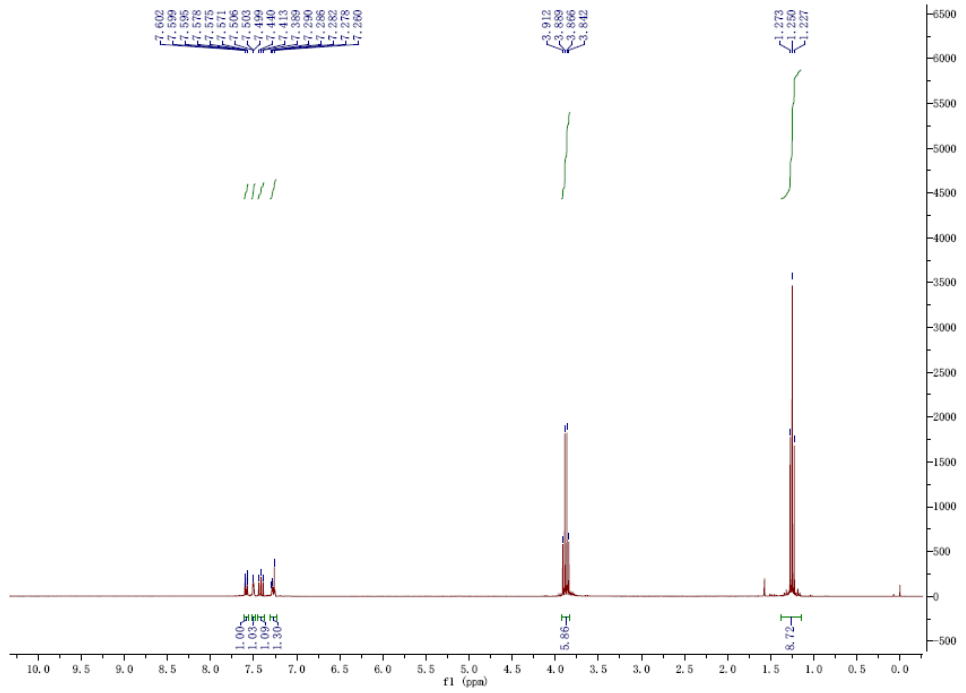
8.538
8.524
8.522
7.533
7.527
7.293
7.268
7.243
7.174
7.152
7.148
7.132
7.115
7.102
7.098
7.087
7.073
6.898
6.891
6.870
6.866
3.656
1.00
1.00
1.94
6.02
2.02
1.02
3.02
f1 (ppm)

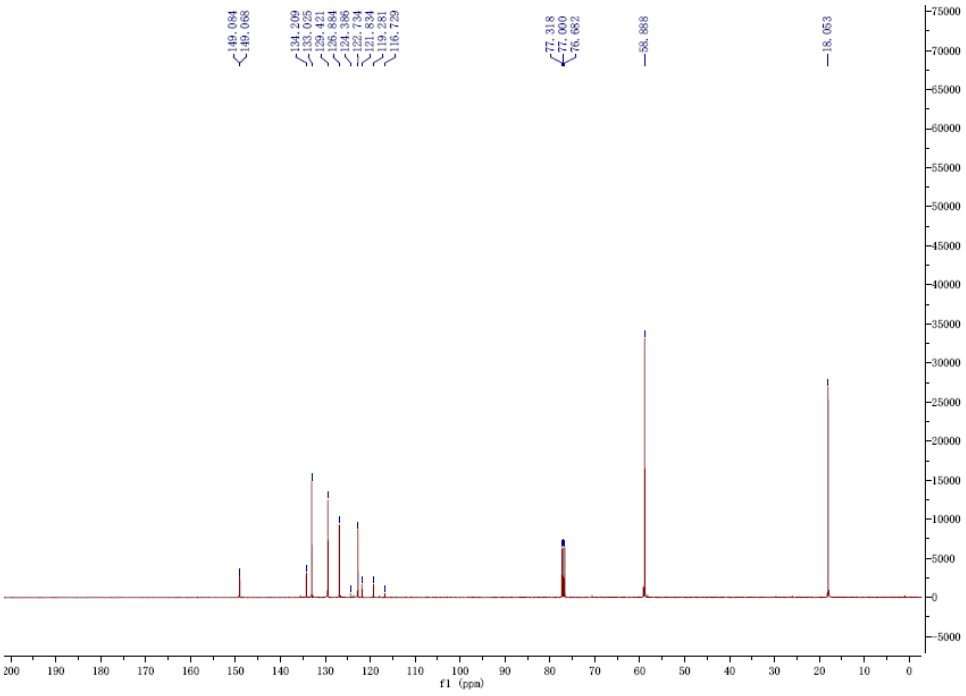

156.543
155.412
147.647
145.014
142.777
135.424
129.326
128.318
127.254
126.870
126.065
125.755
121.637
121.114
110.159
77.320
77.000
76.681
73.128
55.341
f1 (ppm)

NMR Spectra of Arylsilane 2

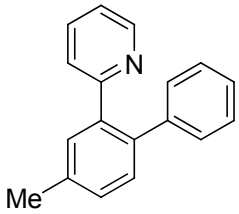


2i





NMR Spectra of Product 3



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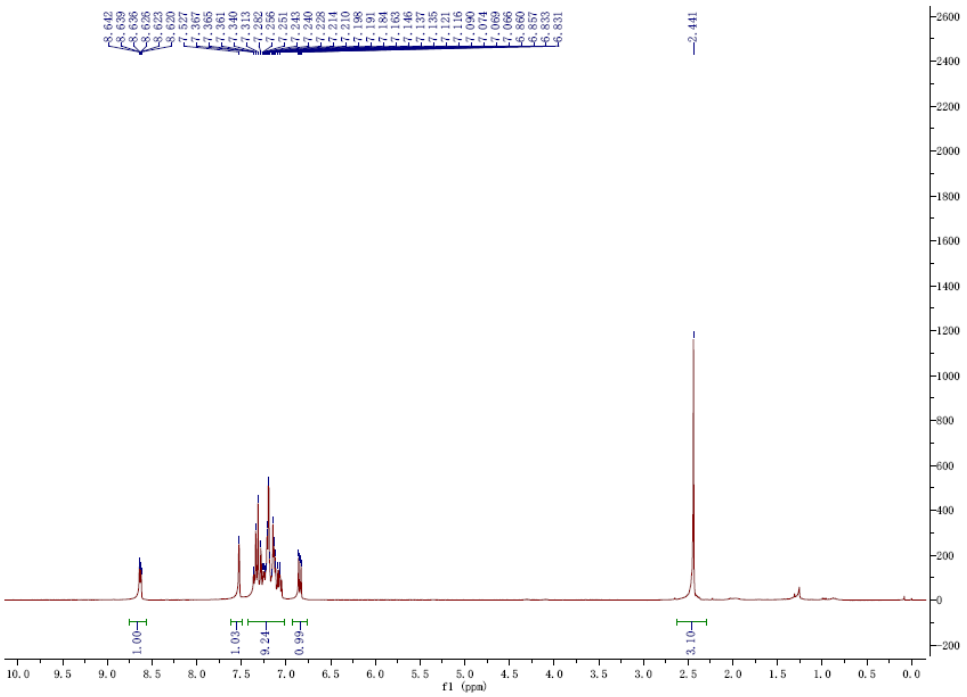

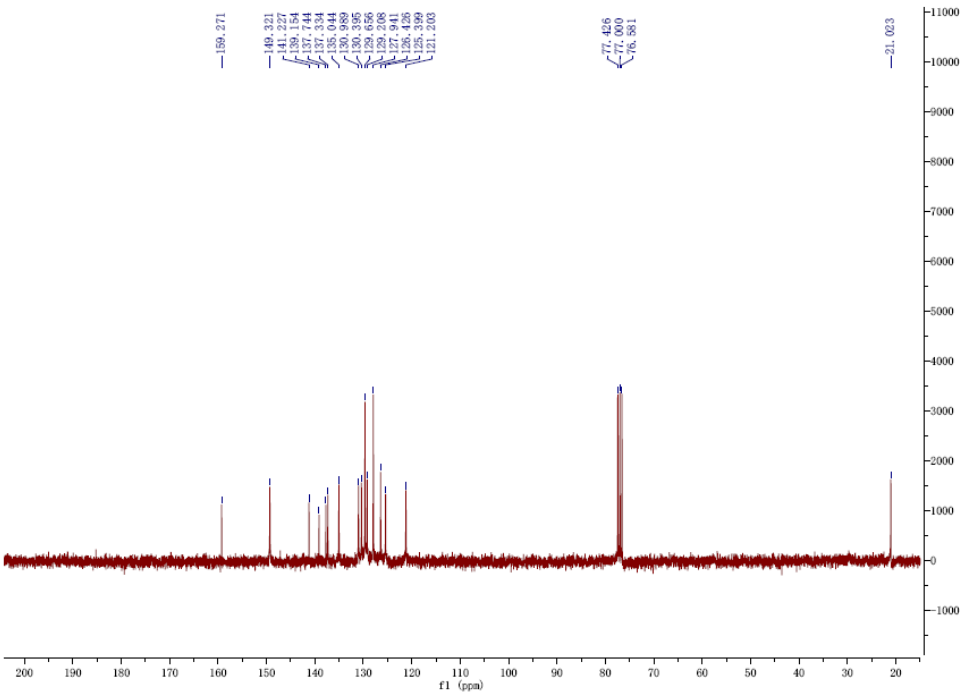

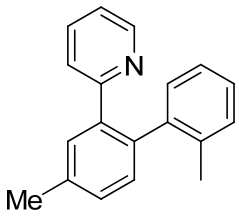

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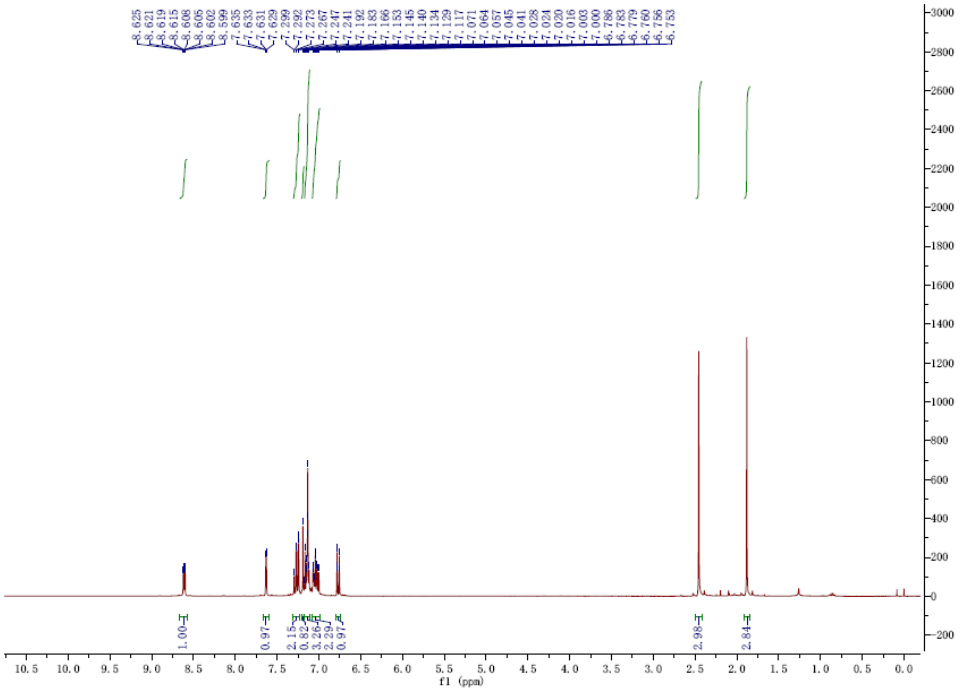
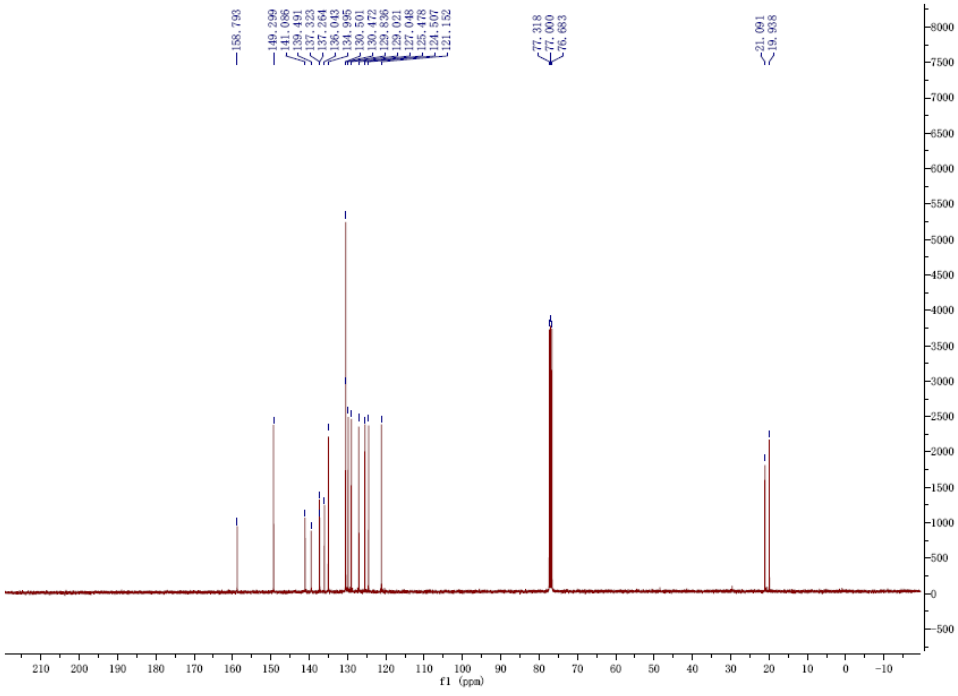
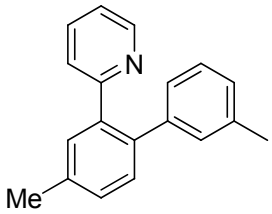
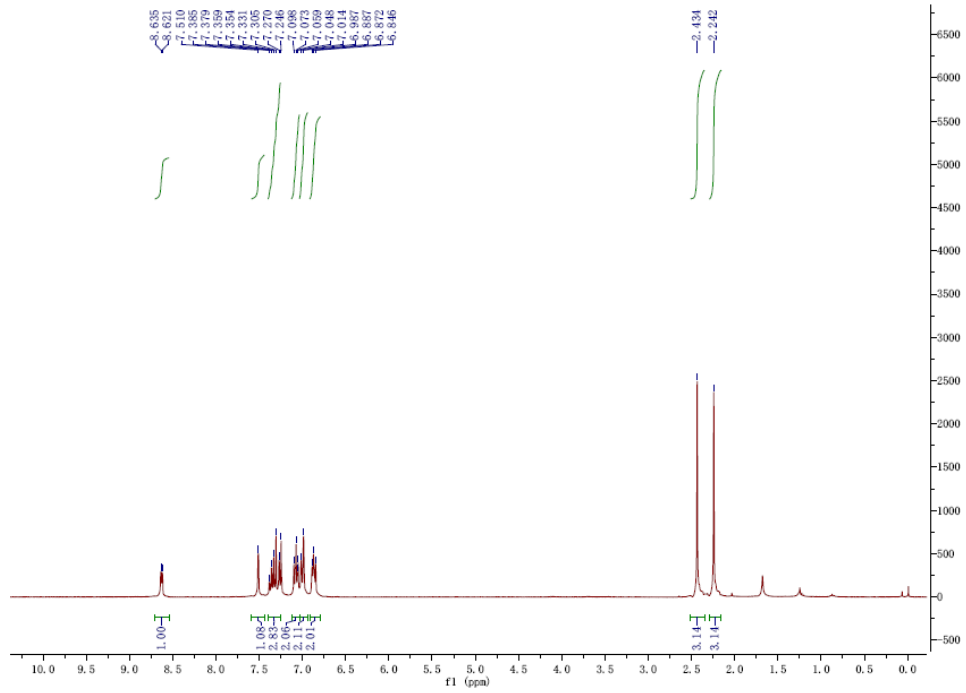





N
Me

3ac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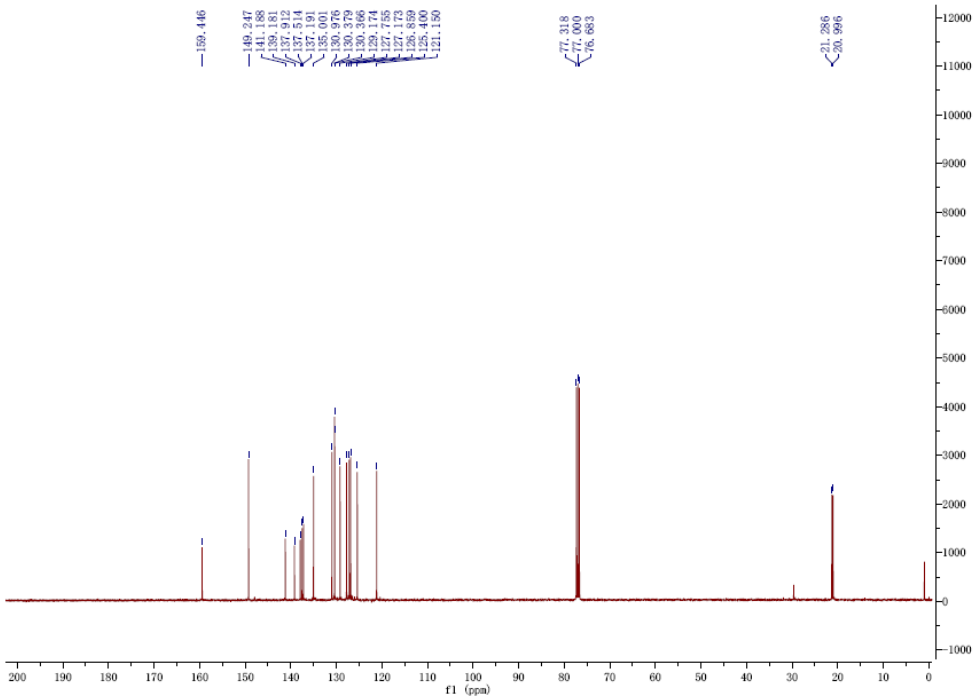
7.385
7.379
7.369
7.354
7.331
7.305
7.270
7.246
7.098
7.073
7.069
7.048
7.014
6.987
6.887
6.872
6.846
2.434
2.242
1.00
1.08
1.83
2.06
2.11
2.01
3.14
3.14
f1 (ppm)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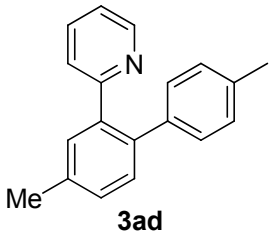
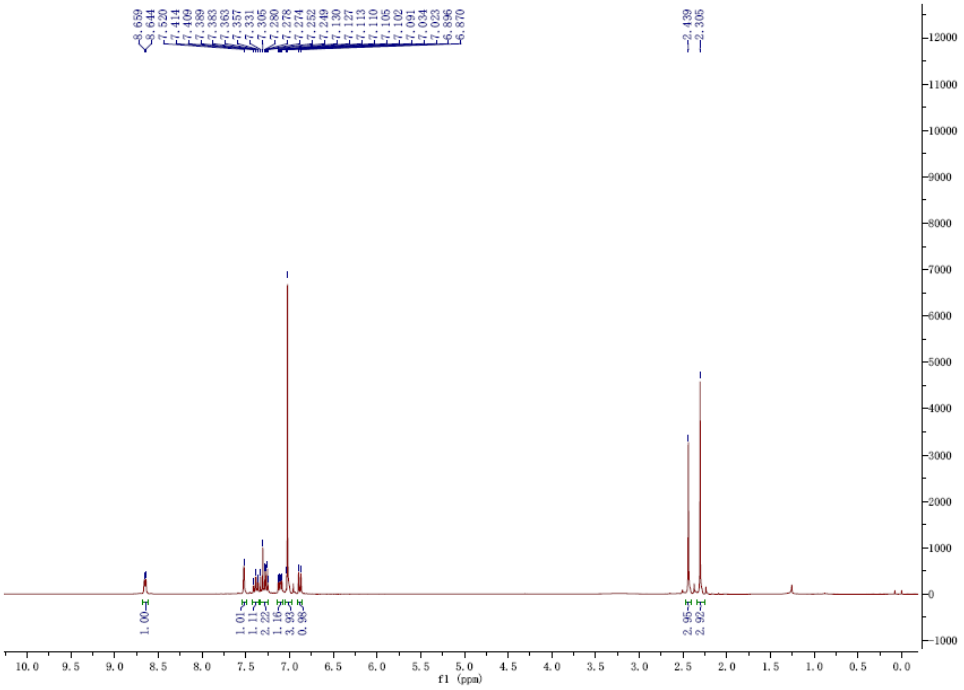
149.247
141.188
139.181
137.912
137.514
137.191
135.001
130.976
130.379
130.366
129.174
127.755
127.173
126.859
125.400
121.150
77.318
77.000
76.683
21.286
20.996
f1 (ppm)


N
Me

3ad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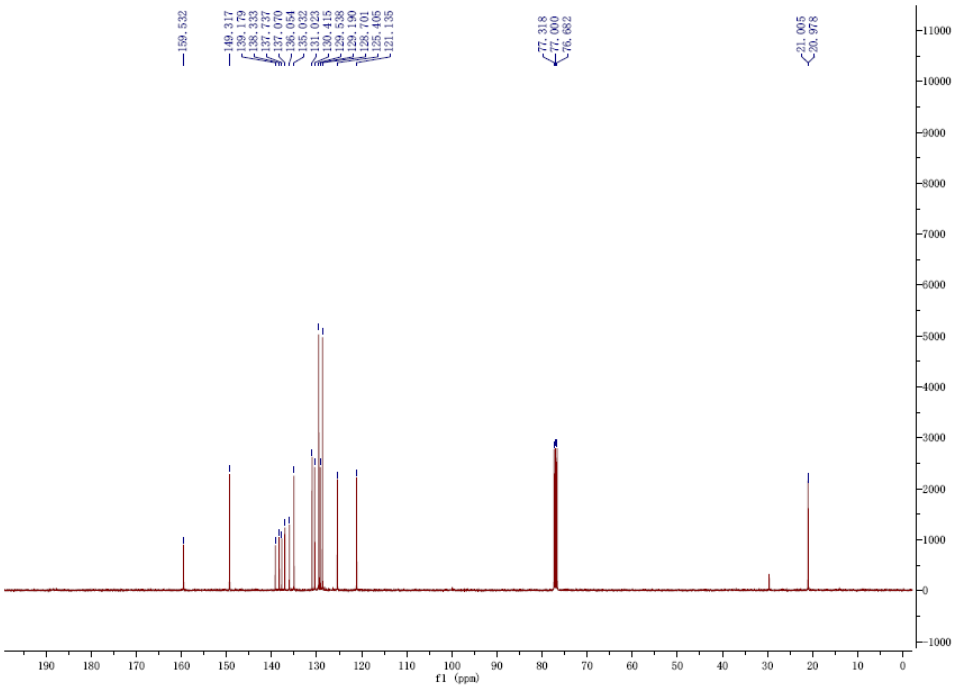
7.414
7.409
7.389
7.383
7.363
7.357
7.331
7.305
7.280
7.278
7.274
7.252
7.249
7.139
7.137
7.115
7.110
7.105
7.102
7.091
7.034
7.023
6.996
6.870
2.439
2.305
1.00
1.01
1.11
2.22
2.16
3.93
0.98
2.95
2.92
f1 (ppm)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139.179
138.333
137.737
137.070
136.054
135.032
131.023
130.115
129.538
129.190
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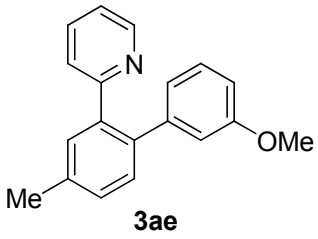
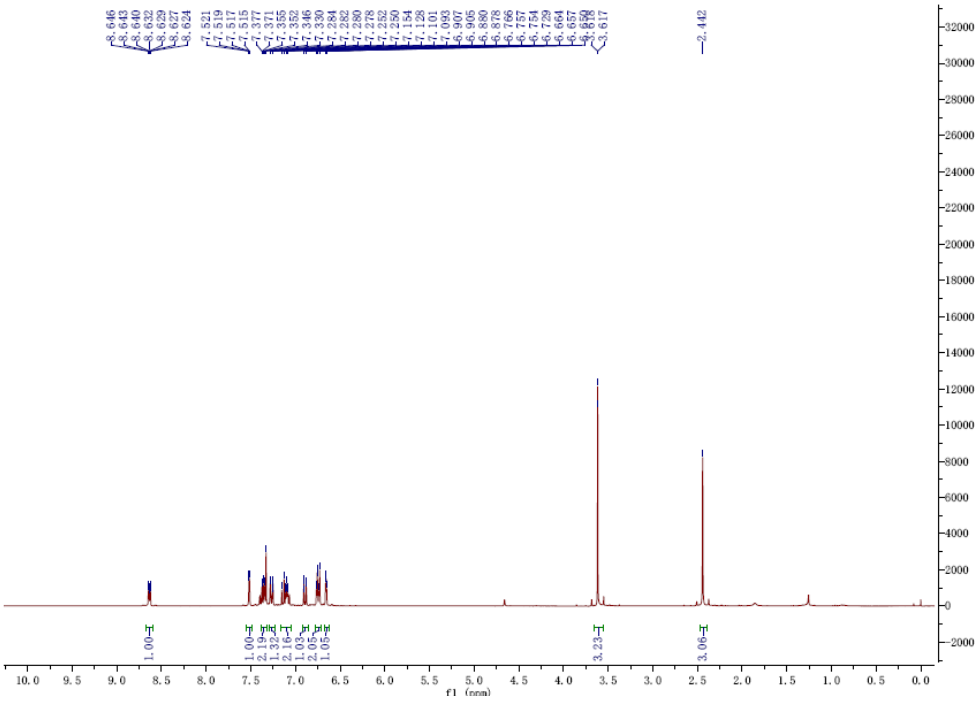
77.000
76.682
21.005
20.978
f1 (ppm)


N
OMe
Me

3ae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7.515
7.377
7.371
7.355
7.352
7.346
7.330
7.284
7.282
7.280
7.278
7.252
7.250
7.154
7.128
7.101
7.093
6.907
6.905
6.886
6.878
6.766
6.757
6.754
6.729
6.664
6.657
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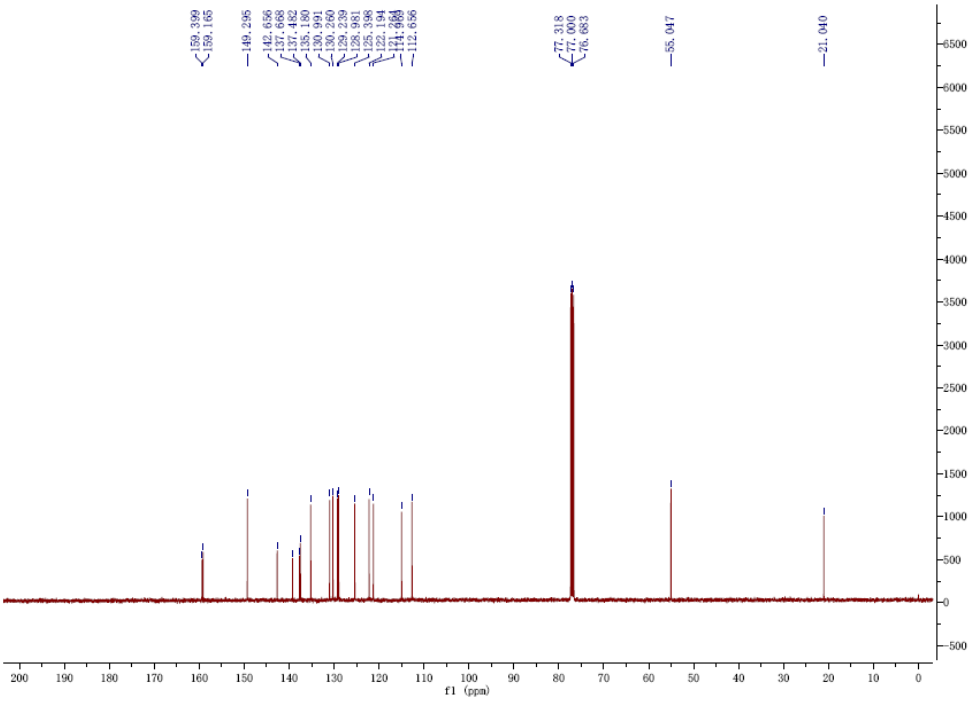
2.05
1.05
3.23
3.06
f1 (ppm)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142.656
137.668
137.482
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125.396
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112.656
77.318
77.000
76.683
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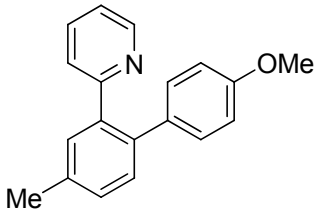
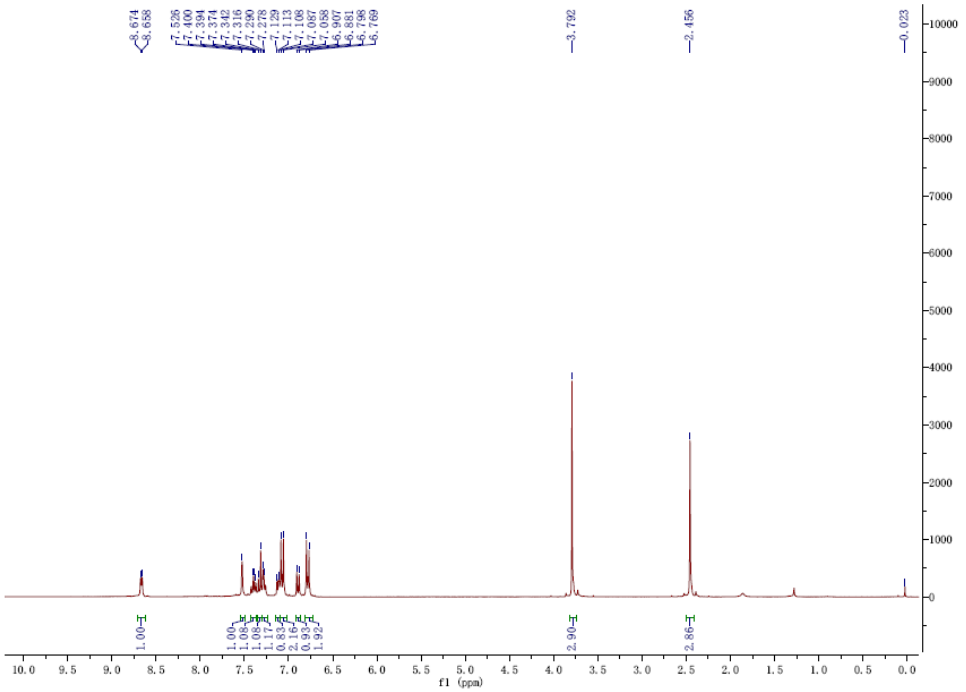
21.040
f1 (ppm)


N
OMe
Me

3af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7.278
7.129
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7.108
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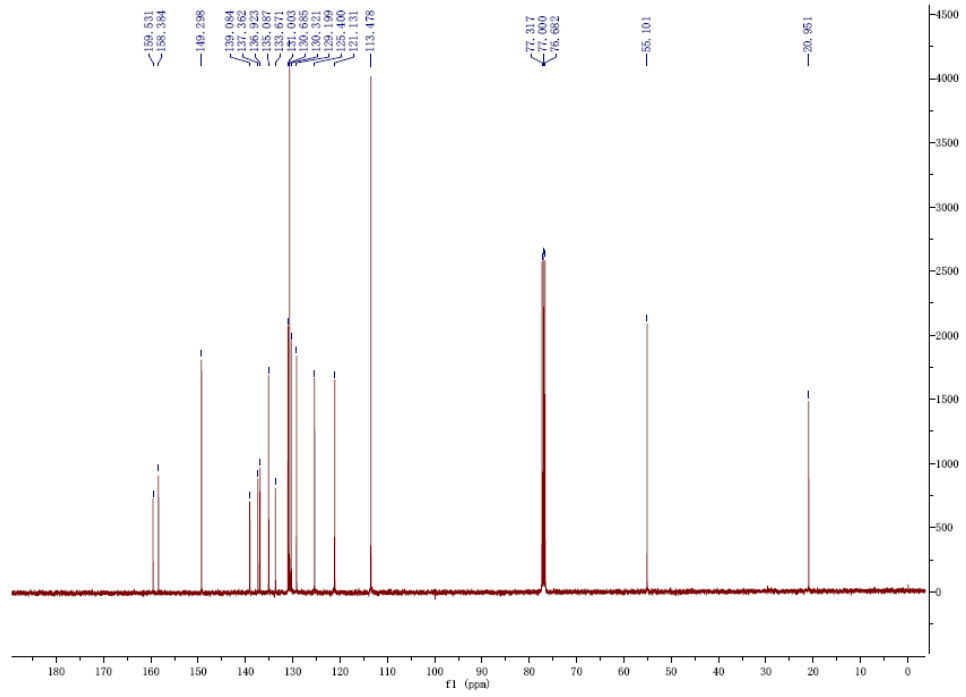
7.058
6.907
6.881
6.798
6.769
3.792
2.456
0.023
f1 (ppm)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139.084
137.362
136.923
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133.671
131.003
130.655
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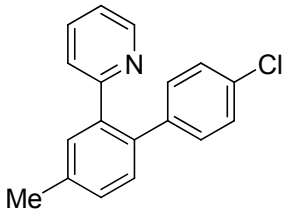
129.149
125.400
121.131
113.478
77.317
77.000
76.682
55.101
20.951
f1 (ppm)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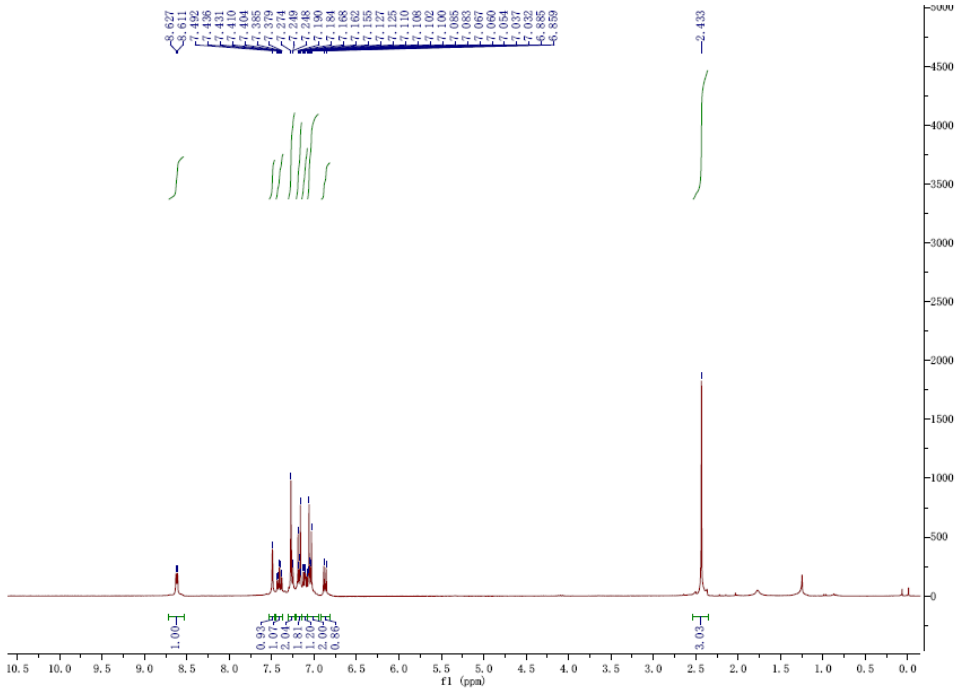
Cl
Me

3ag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7.274
7.249
7.248
7.190
7.184
7.168
7.162
7.155
7.127
7.125
7.110
7.106
7.102
7.100
7.085
7.083
7.066
7.060
7.054
7.037
7.032
6.885
6.859
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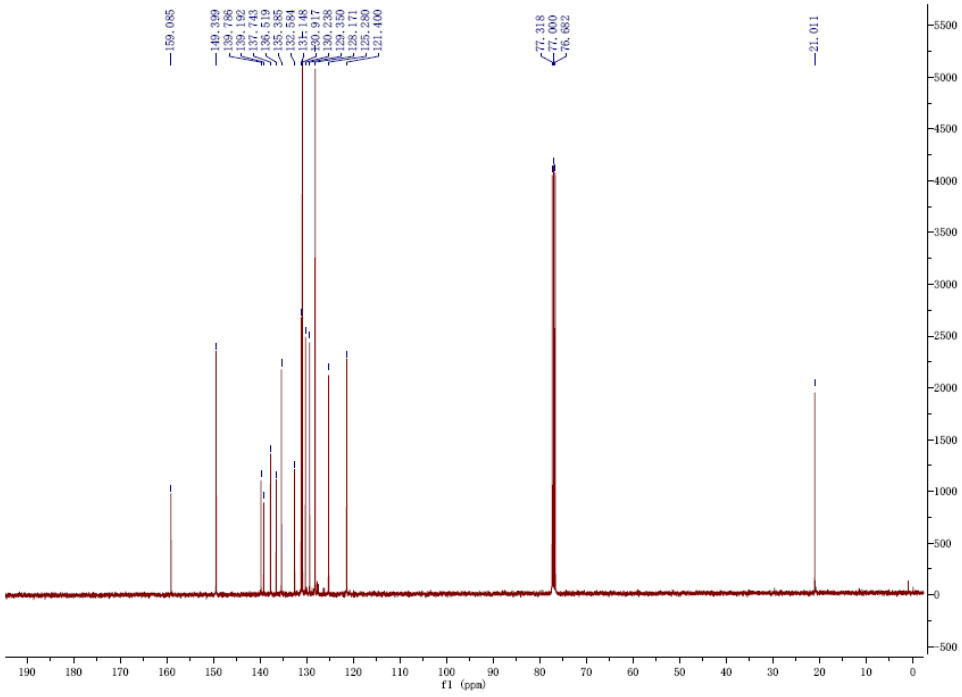
1.07
2.04
5.81
1.20
2.06
0.86
3.03
f1 (ppm)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137.743
136.519
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132.584
131.148
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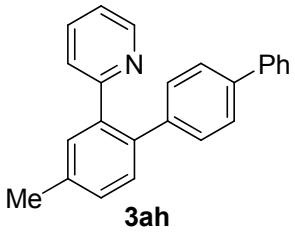
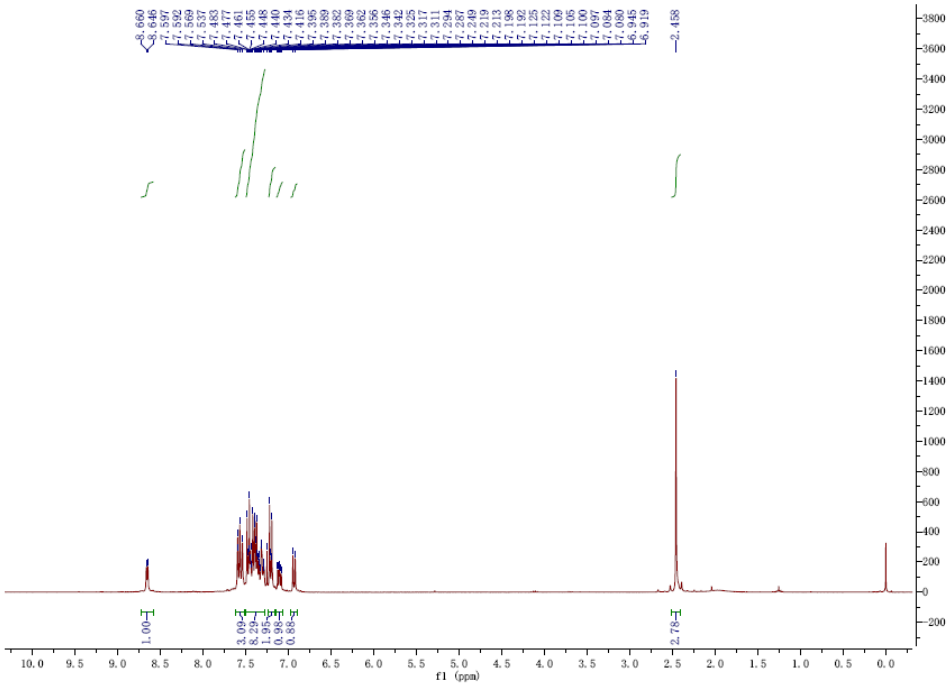
129.350
128.171
125.280
121.400
77.318
77.000
76.682
21.011
f1 (ppm)


N
Ph
Me

3ah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7.434
7.416
7.395
7.389
7.382
7.369
7.362
7.356
7.346
7.342
7.325
7.317
7.311
7.294
7.287
7.249
7.219
7.213
7.198
7.192
7.125
7.122
7.109
7.105
7.100
7.097
7.084
7.080
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3.09
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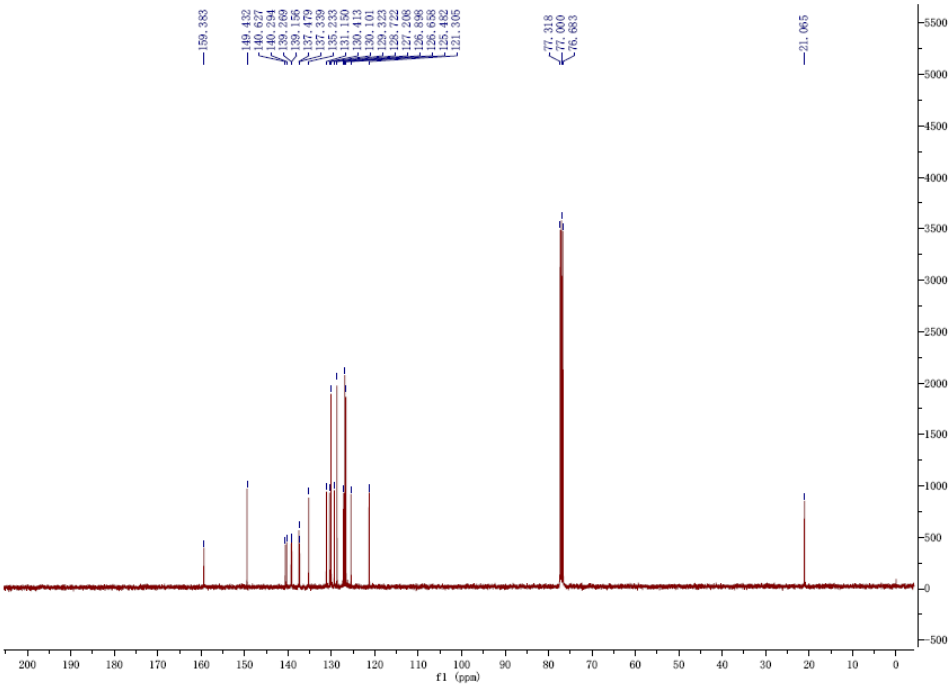
2.78
f1 (ppm)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139.156
137.479
137.339
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131.150
130.413
130.101
129.323
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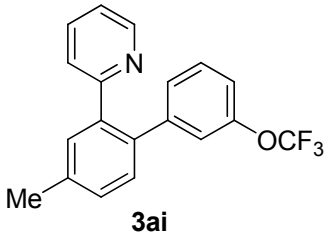
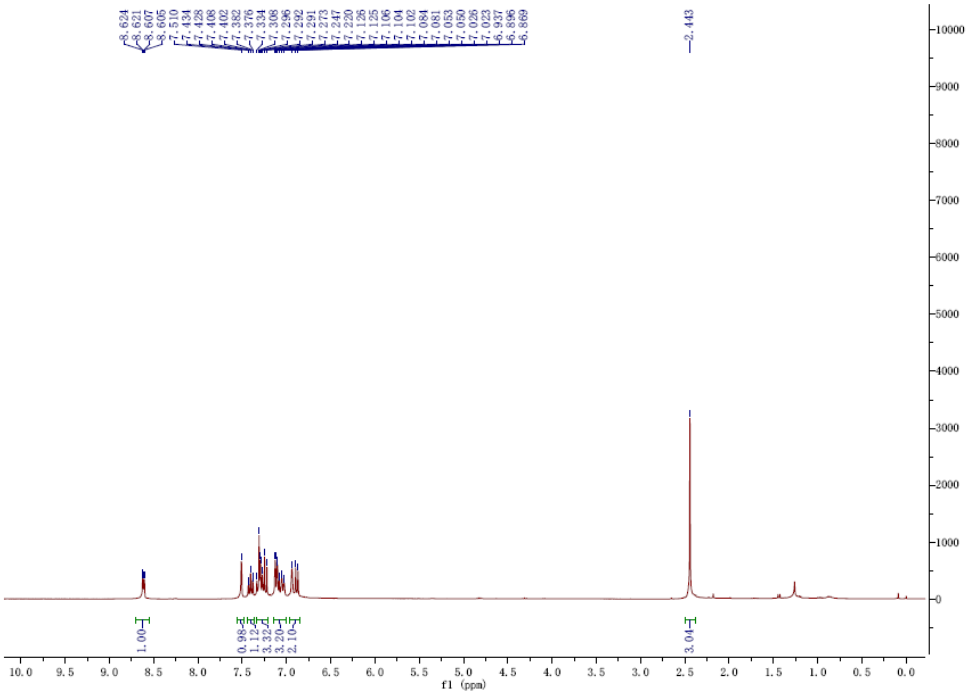
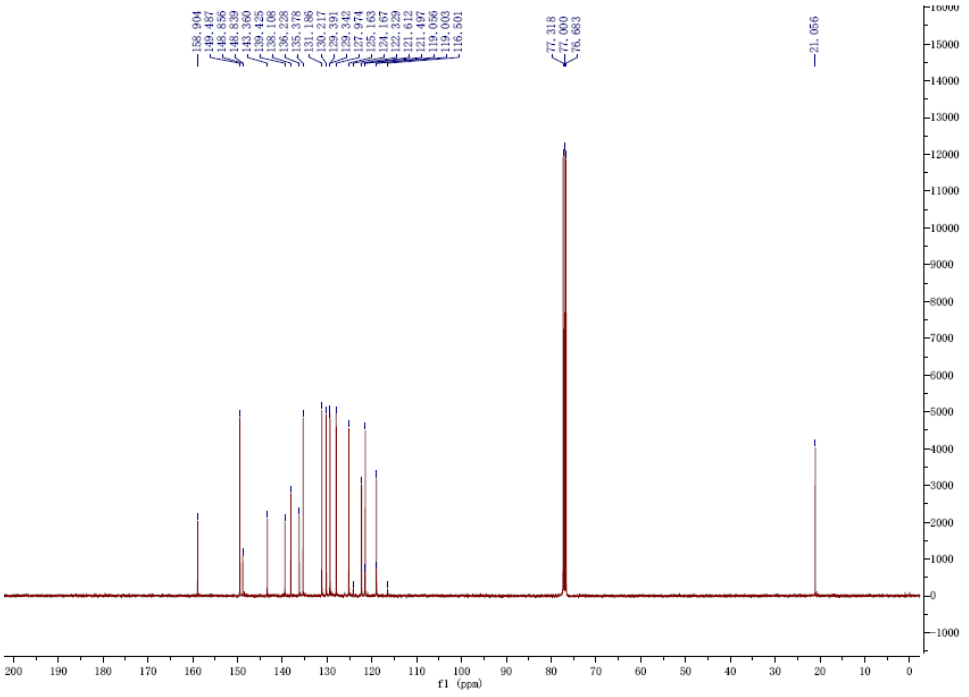
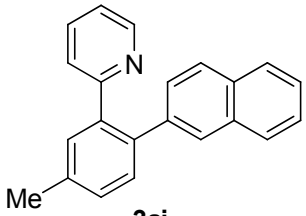
126.898
126.658
125.482
121.305
77.318
77.000
76.683
21.065
f1 (ppm)



3ai







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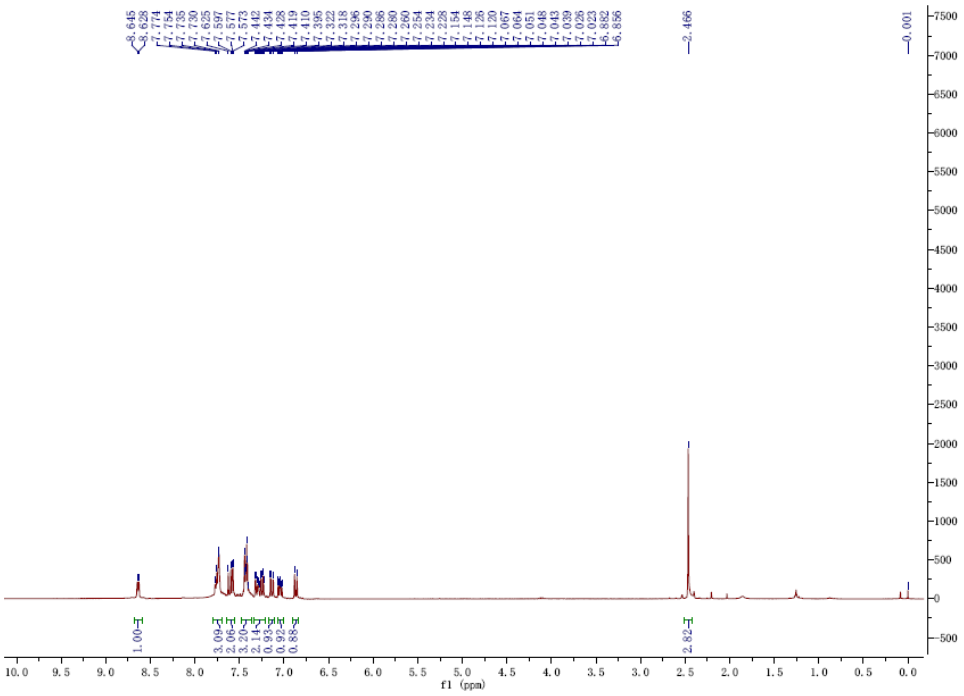

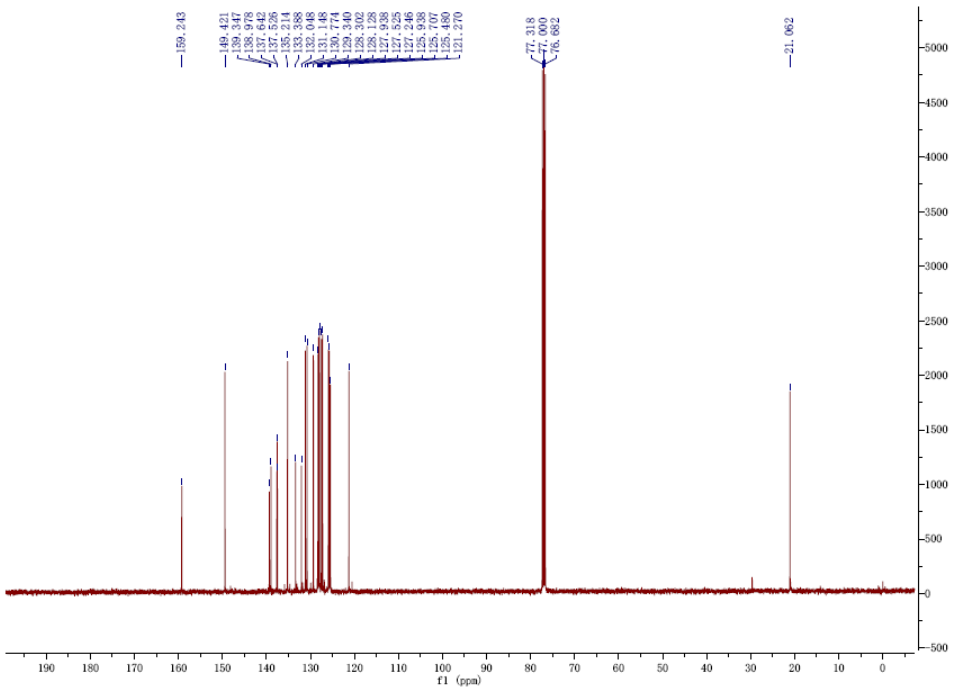

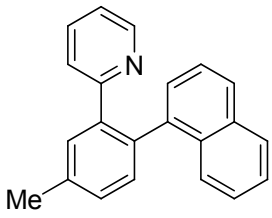

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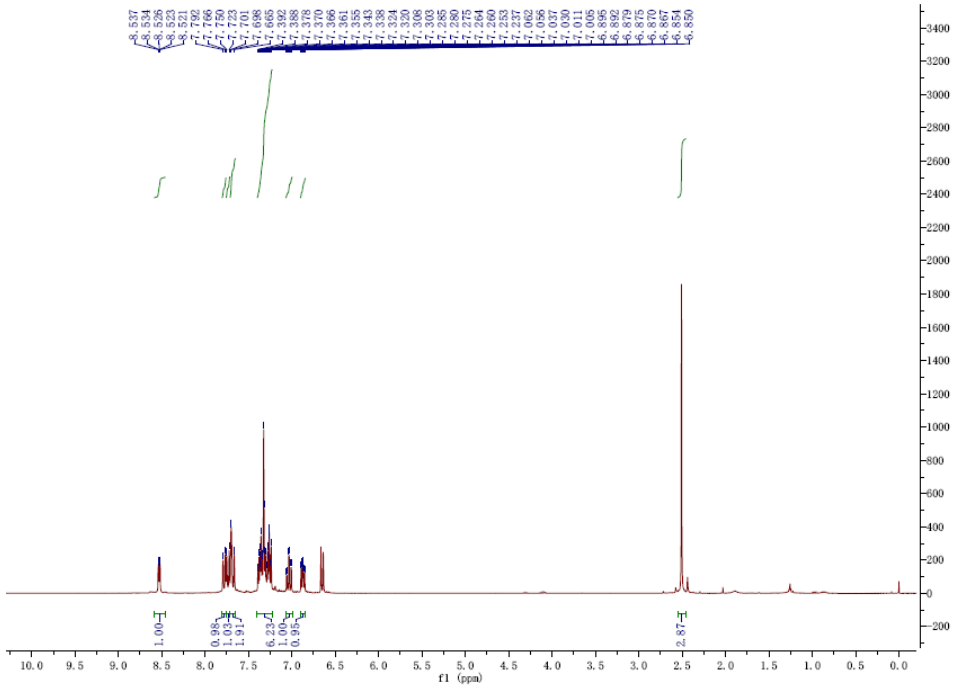
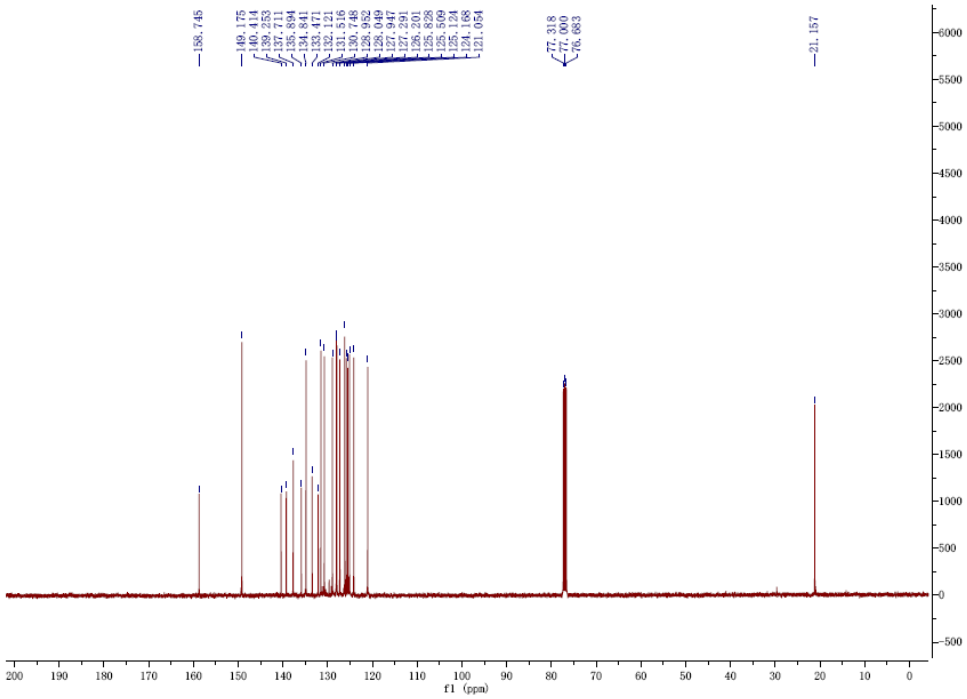
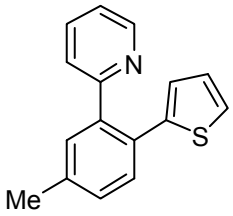
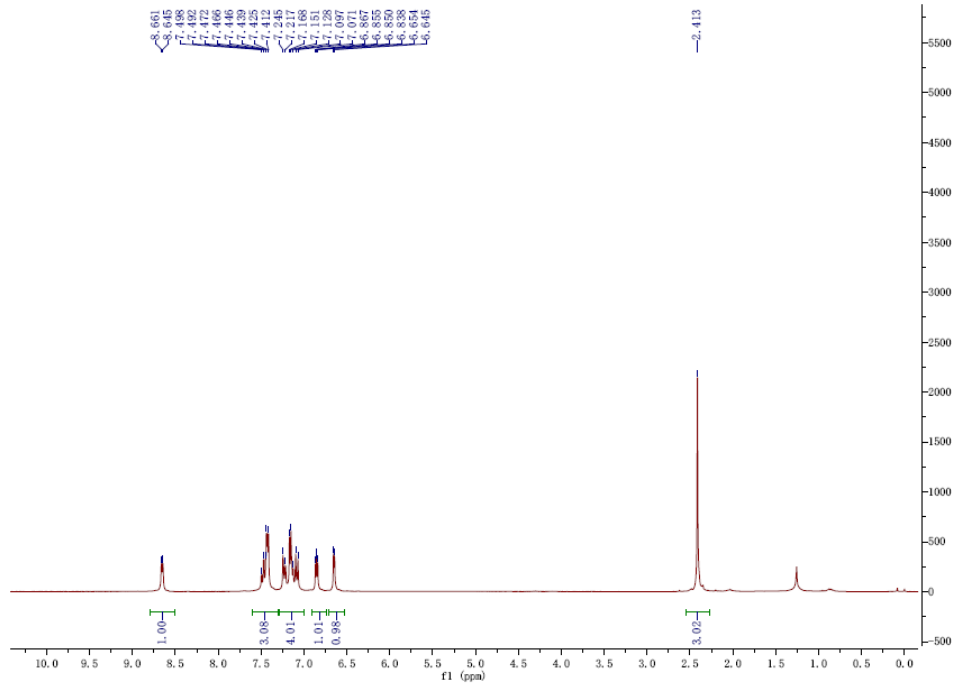





N
S
Me

3al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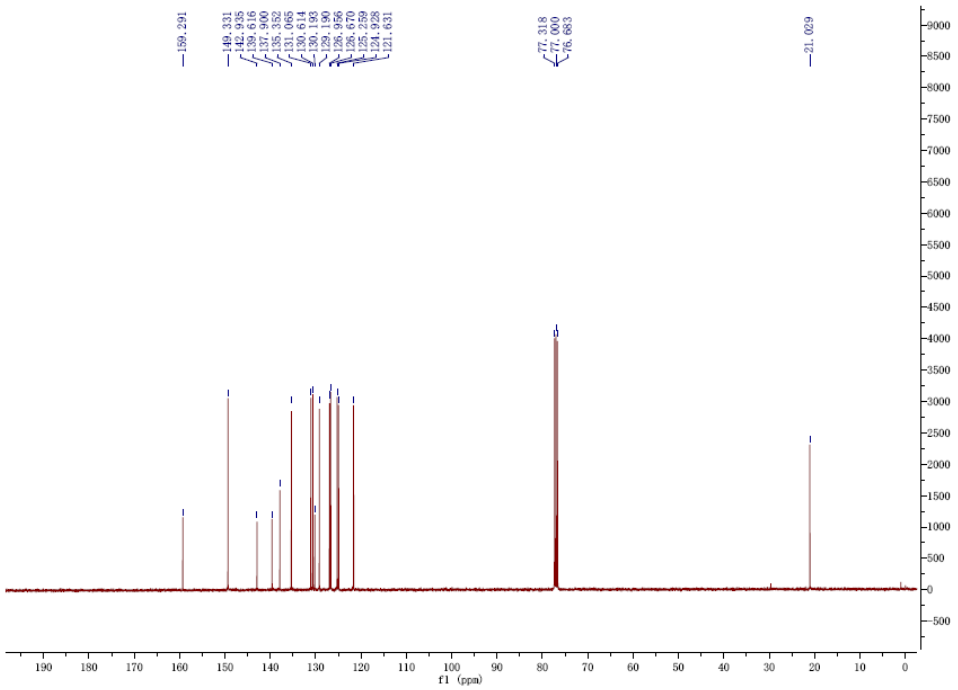
8.645
7.498
7.492
7.472
7.466
7.446
7.439
7.425
7.412
7.245
7.217
7.168
7.151
7.128
7.097
7.071
6.867
6.855
6.850
6.838
6.654
6.645
2.413
1.00
3.08
4.01
1.01
0.98
3.02
f1 (ppm)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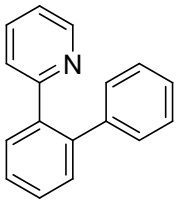
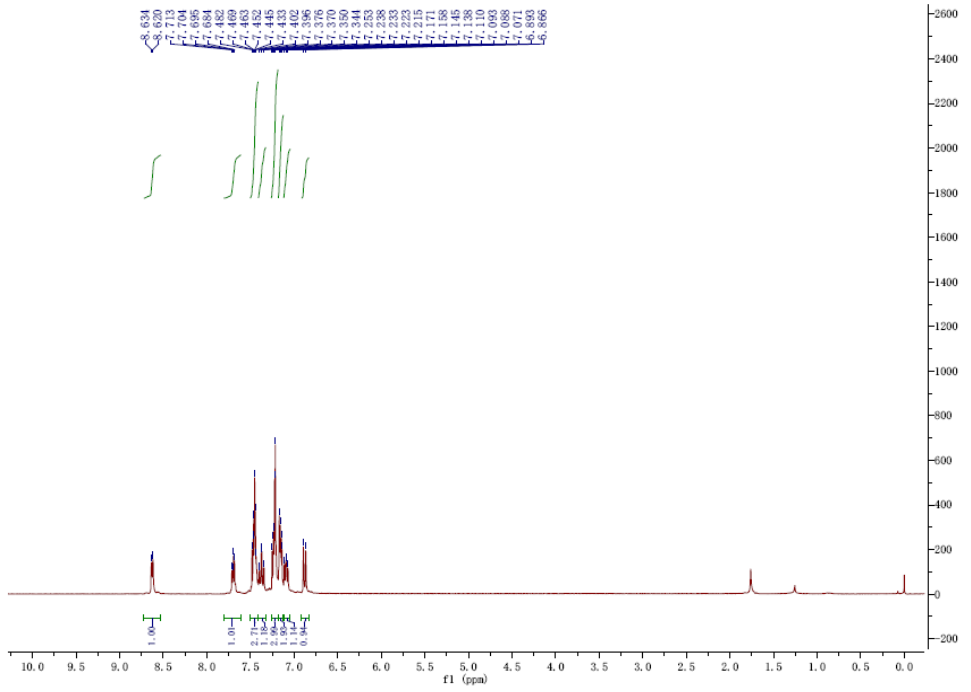
149.331
142.935
139.616
137.900
135.352
131.065
130.614
130.193
129.190
126.956
126.670
125.259
124.928
121.631
77.318
77.000
76.683
21.029
f1 (ppm)



3ba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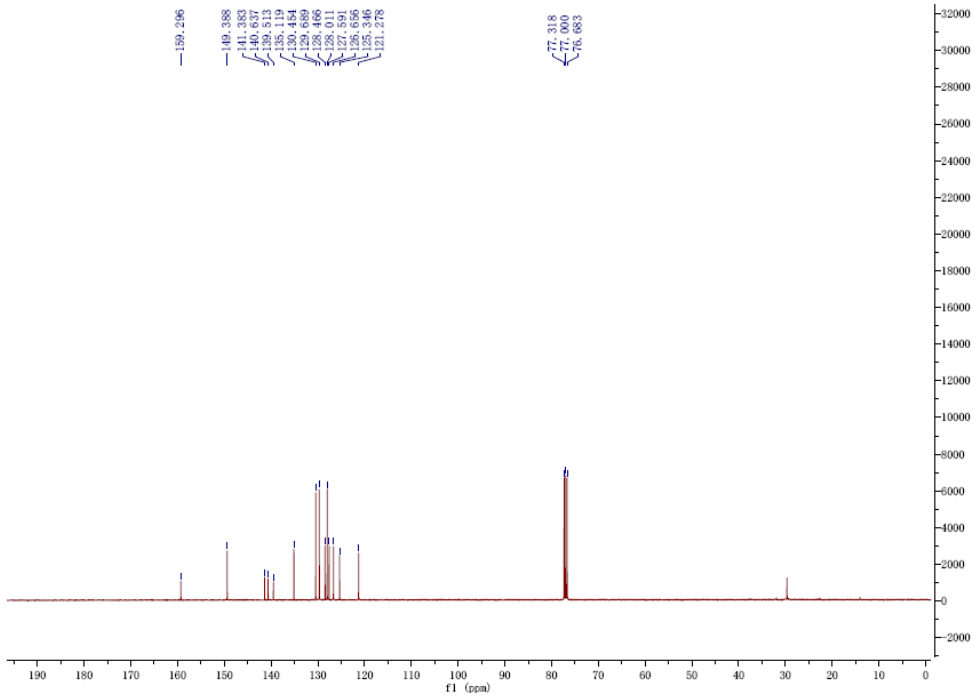
8.630
7.713
7.704
7.695
7.684
7.482
7.469
7.463
7.452
7.445
7.433
7.402
7.396
7.376
7.370
7.350
7.344
7.233
7.228
7.223
7.215
7.171
7.158
7.145
7.138
7.110
7.098
7.088
7.071
6.893
6.866
1.00
1.01
2.71
1.18
2.06
1.06
1.14
0.94
f1 (ppm)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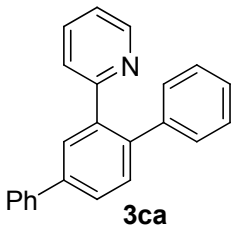
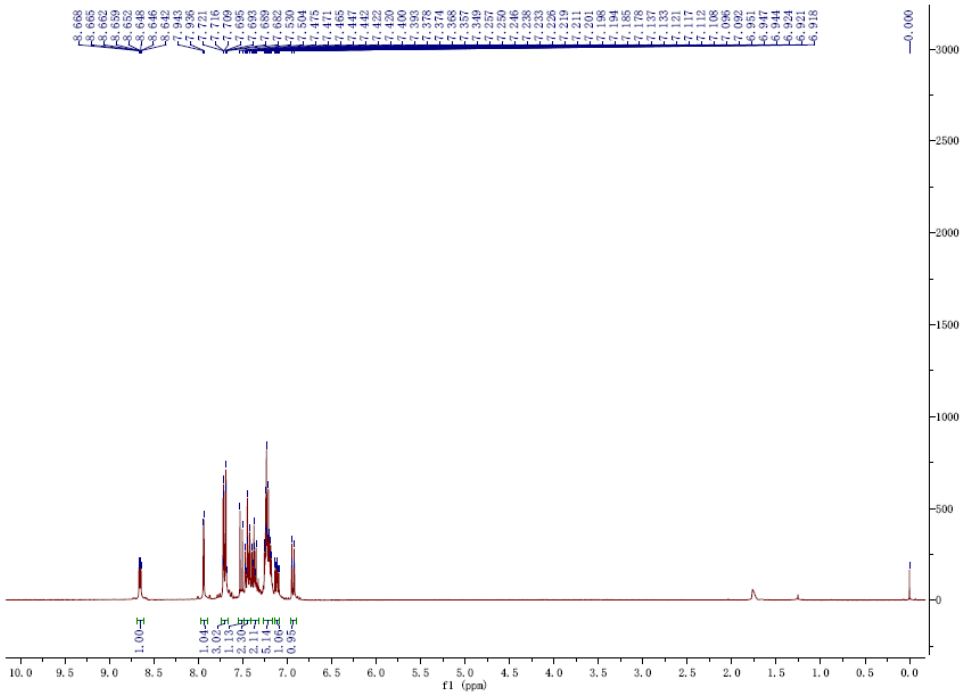
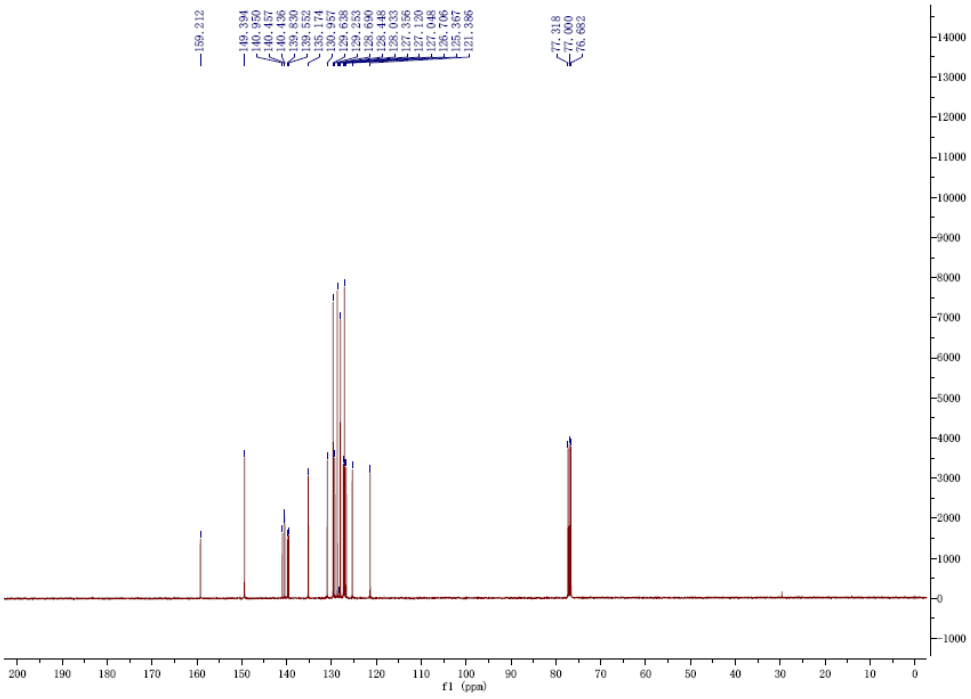
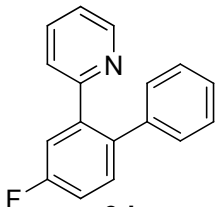
149.388
141.383
140.637
139.513
135.119
130.454
129.689
128.466
128.011
127.591
126.656
125.346
121.278
77.318
77.000
76.683
f1 (ppm)



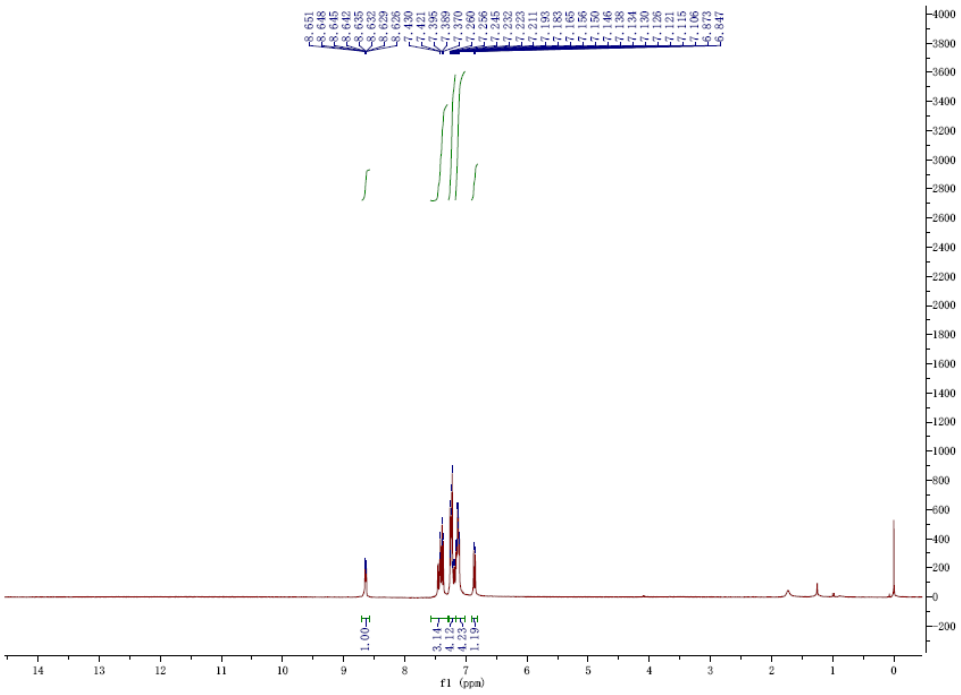
3ca






N
F

3da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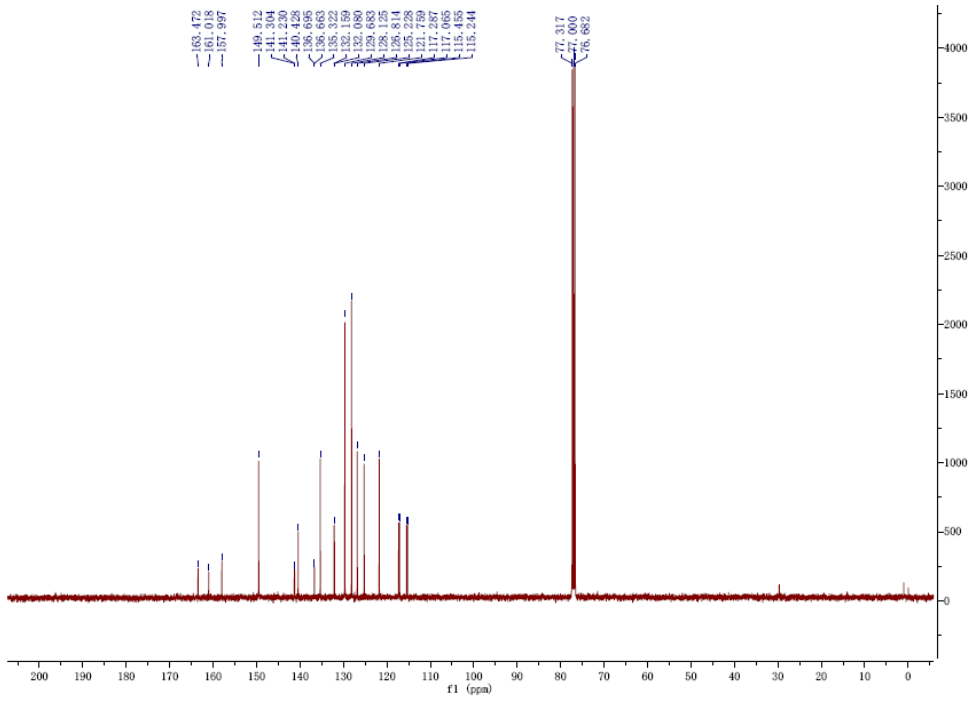
8.648
8.645
8.642
8.635
8.632
8.629
8.626
7.430
7.421
7.395
7.389
7.370
7.260
7.256
7.245
7.232
7.223
7.211
7.193
7.183
7.165
7.156
7.150
7.146
7.138
7.134
7.130
7.126
7.121
7.115
7.106
6.873
6.847
1.00
3.14
4.12
4.23
1.19
f1 (ppm)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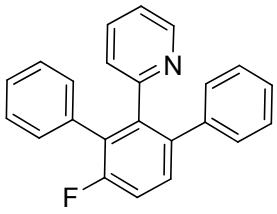
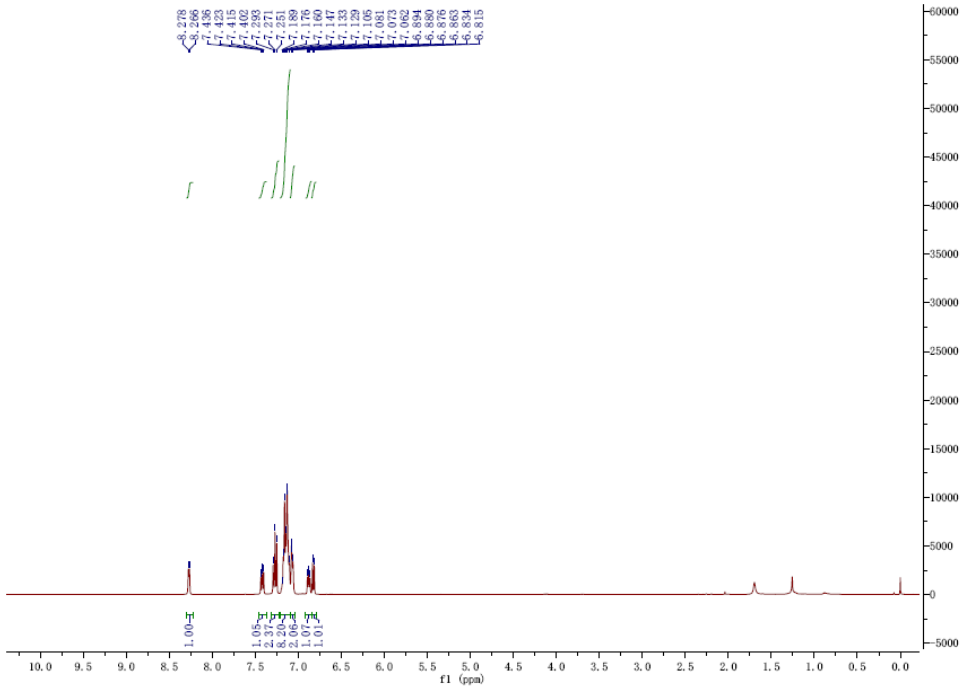
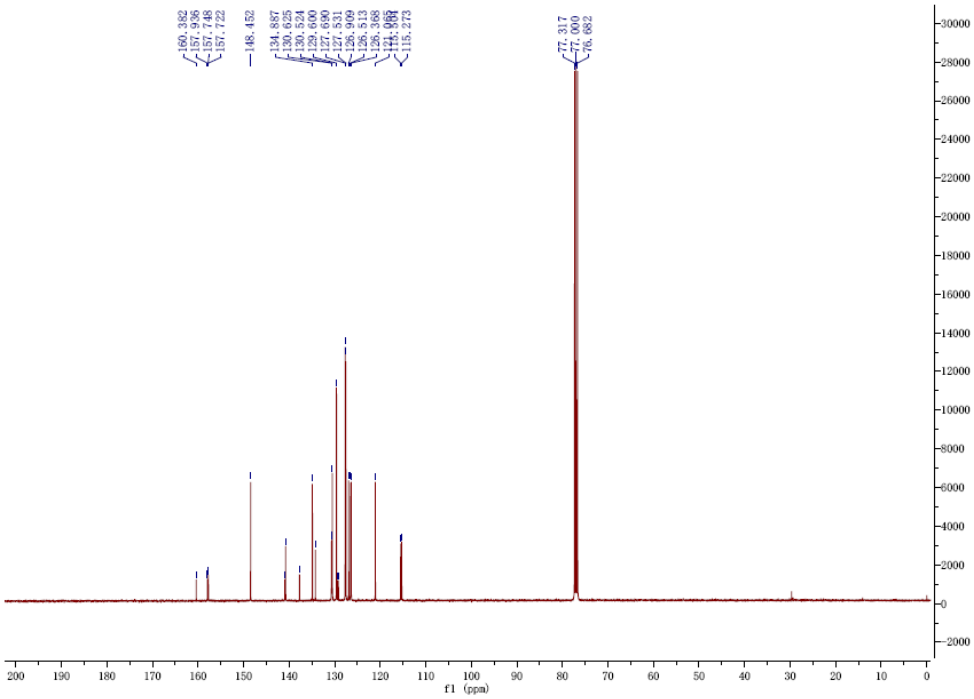
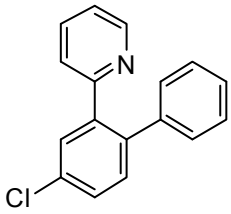
161.018
157.997
149.512
141.304
141.230
140.428
136.695
136.663
135.322
132.159
132.080
128.685
128.125
126.814
125.228
121.789
117.287
117.066
115.455
115.244
77.317
77.000
76.682
f1 (ppm)



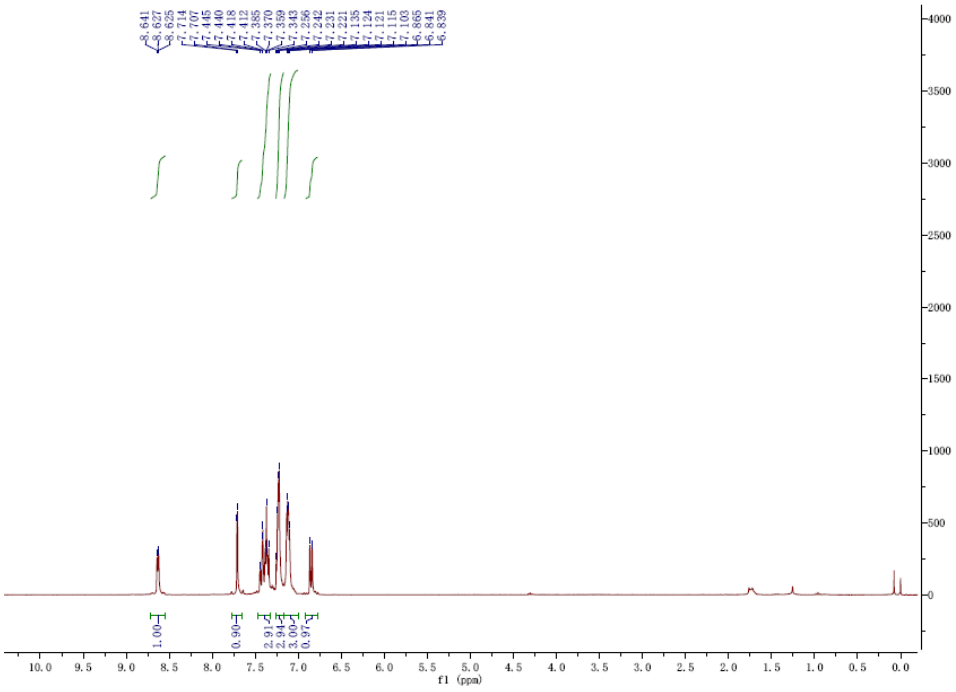
3da'






N
Cl

3ea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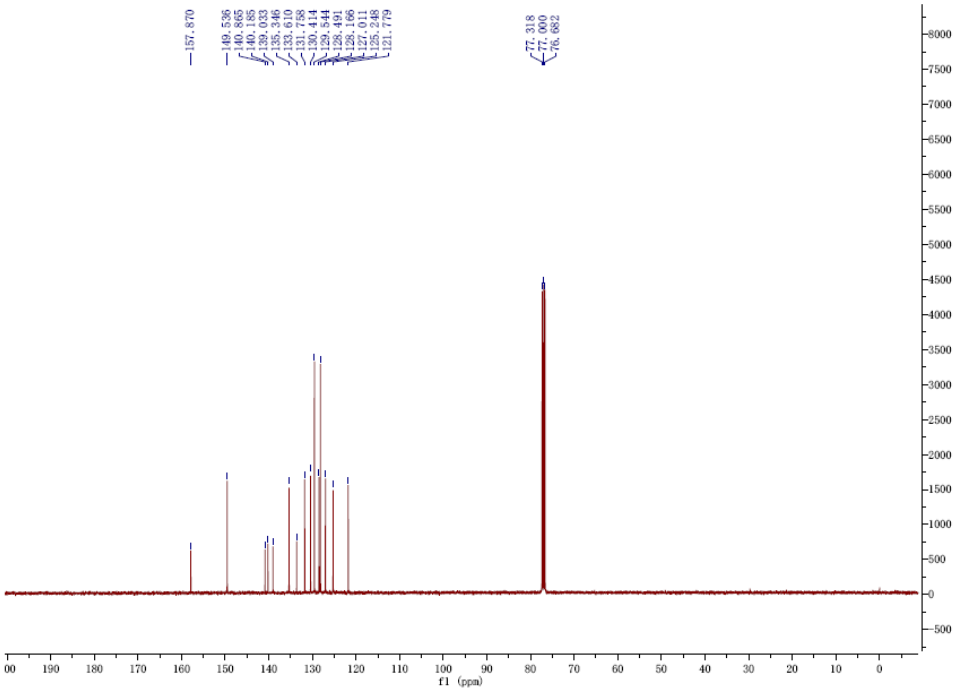
7.714
7.707
7.445
7.440
7.418
7.412
7.385
7.370
7.359
7.343
7.256
7.242
7.231
7.221
7.135
7.124
7.121
7.115
7.103
6.865
6.841
6.839
1.00
0.90
2.91
2.94
3.00
0.97
f1 (ppm)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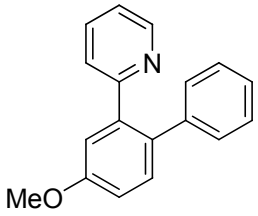
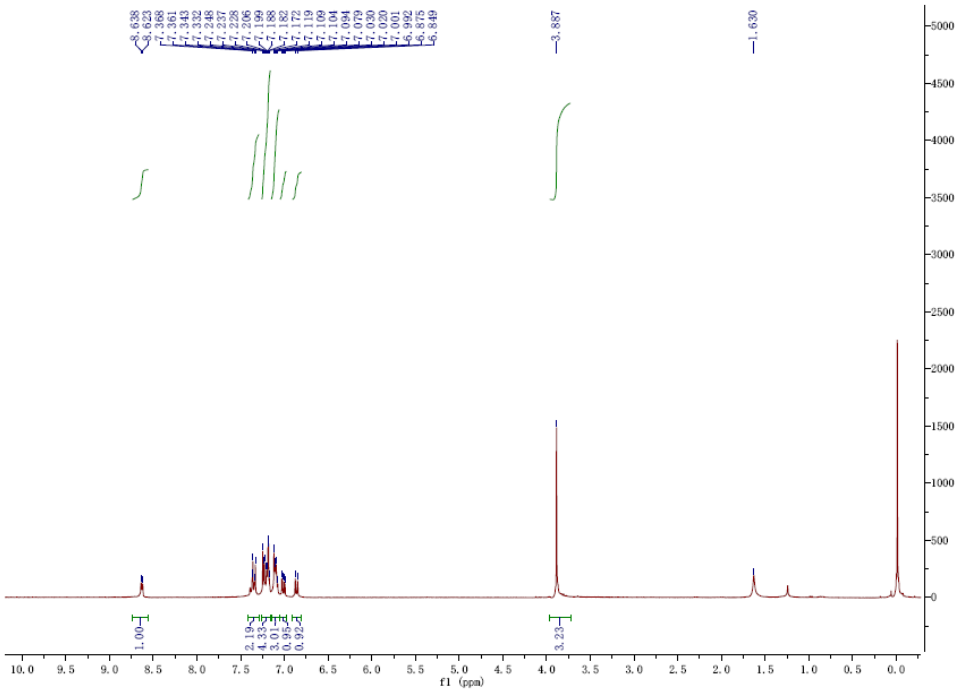
140.185
139.093
135.946
133.610
131.758
130.414
129.544
128.491
128.166
127.911
125.248
121.779
77.318
77.000
76.682
f1 (ppm)


N
MeO

3fa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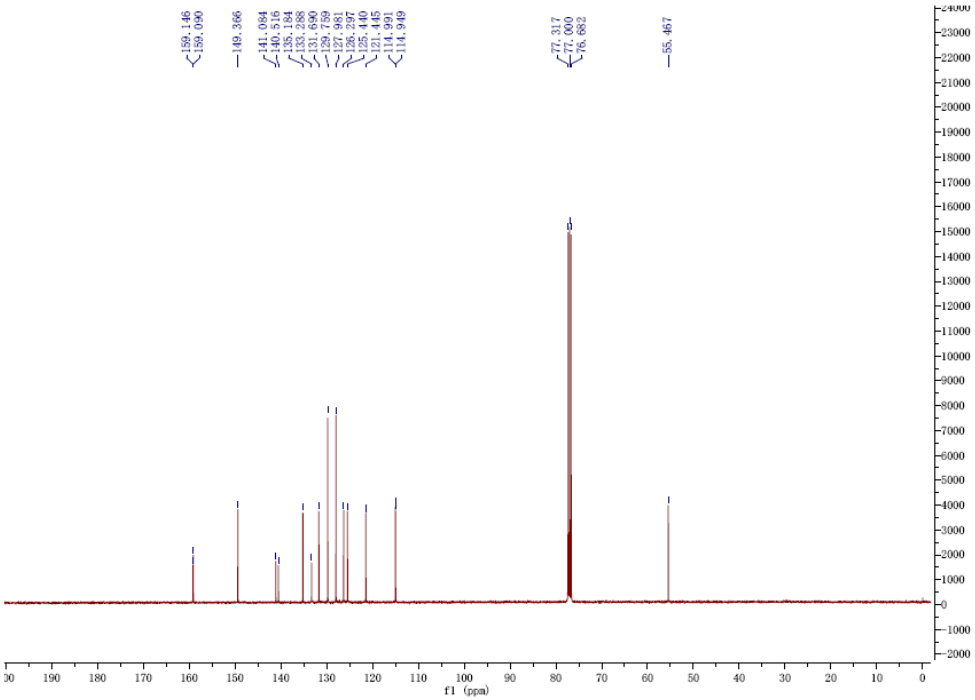
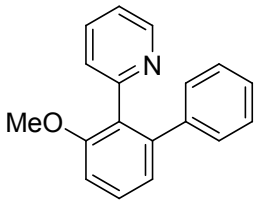
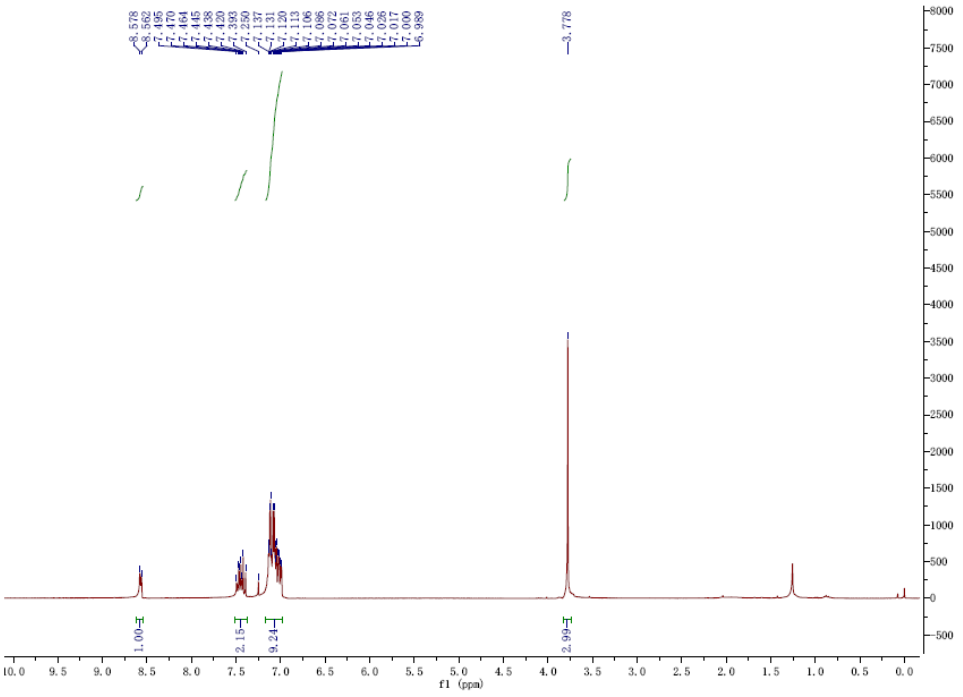
8.623
7.368
7.361
7.343
7.332
7.248
7.237
7.228
7.206
7.199
7.188
7.182
7.172
7.119
7.109
7.104
7.094
7.079
7.030
7.020
7.001
6.992
6.875
6.849
3.887
1.630
1.00
2.19
4.33
3.01
0.95
0.92
3.23
f1 (ppm)


159.146
159.090
149.366
141.084
140.516
135.184
133.288
131.690
129.759
127.981
126.297
125.440
121.445
114.991
114.949
77.317
77.000
76.682
55.467
f1 (ppm)


N
MeO

3ga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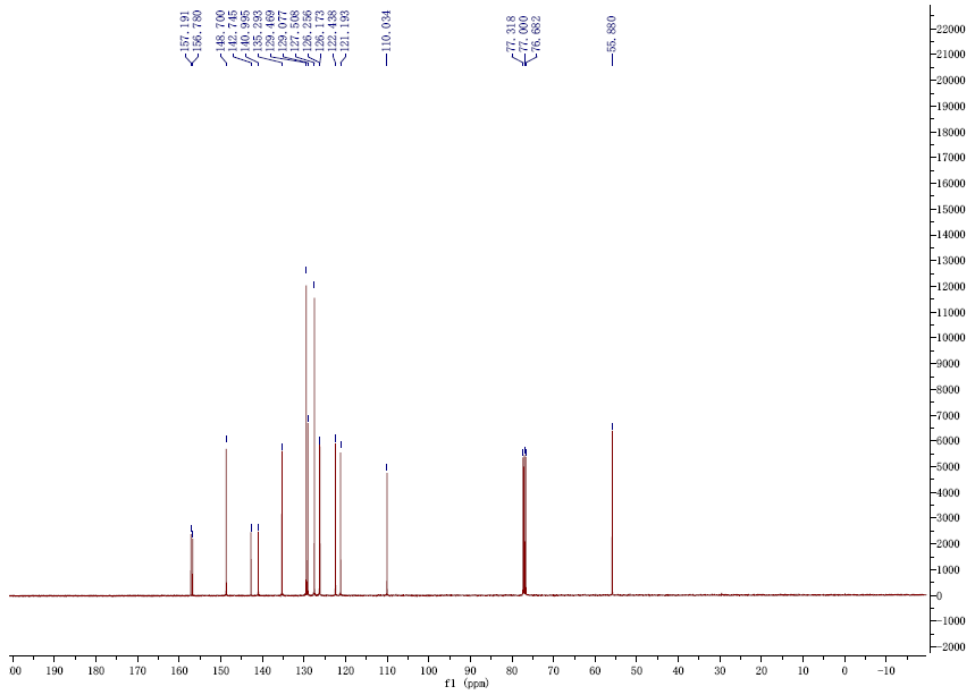
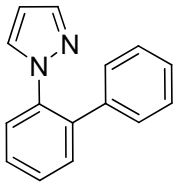
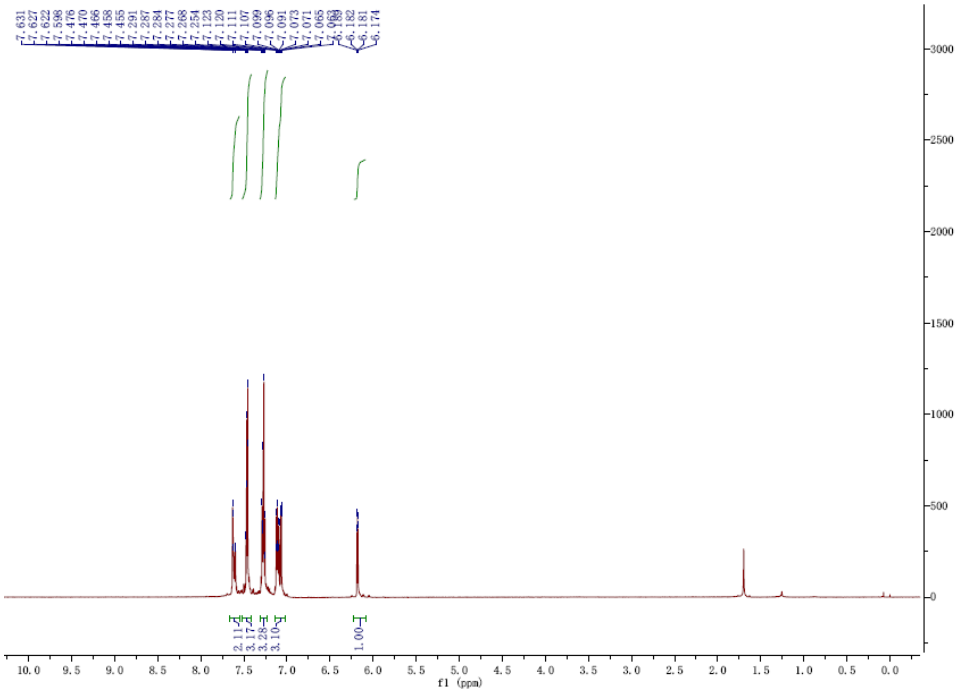
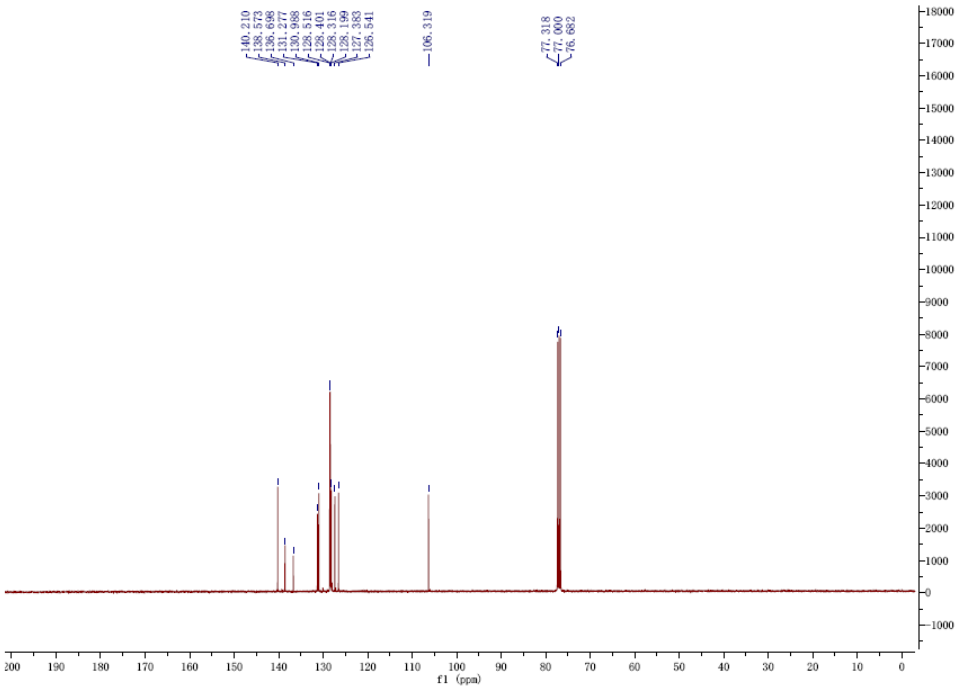
8.485
7.470
7.464
7.445
7.438
7.420
7.393
7.250
7.137
7.131
7.120
7.113
7.106
7.098
7.072
7.061
7.053
7.046
7.036
7.017
7.000
6.989
3.778
1.00
2.15
9.24
2.99
f1 (ppm)

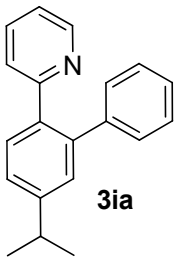

157.191
156.780
148.700
142.745
140.995
135.293
134.469
129.077
127.508
126.256
126.173
122.438
121.193
110.034
77.318
77.000
76.682
55.880
f1 (ppm)



3ha







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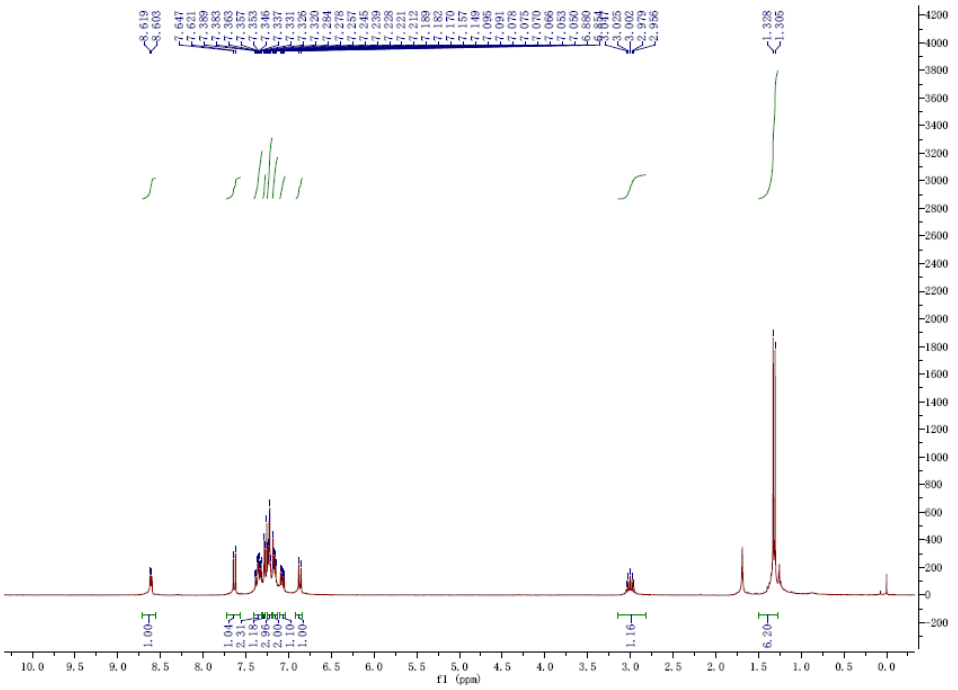
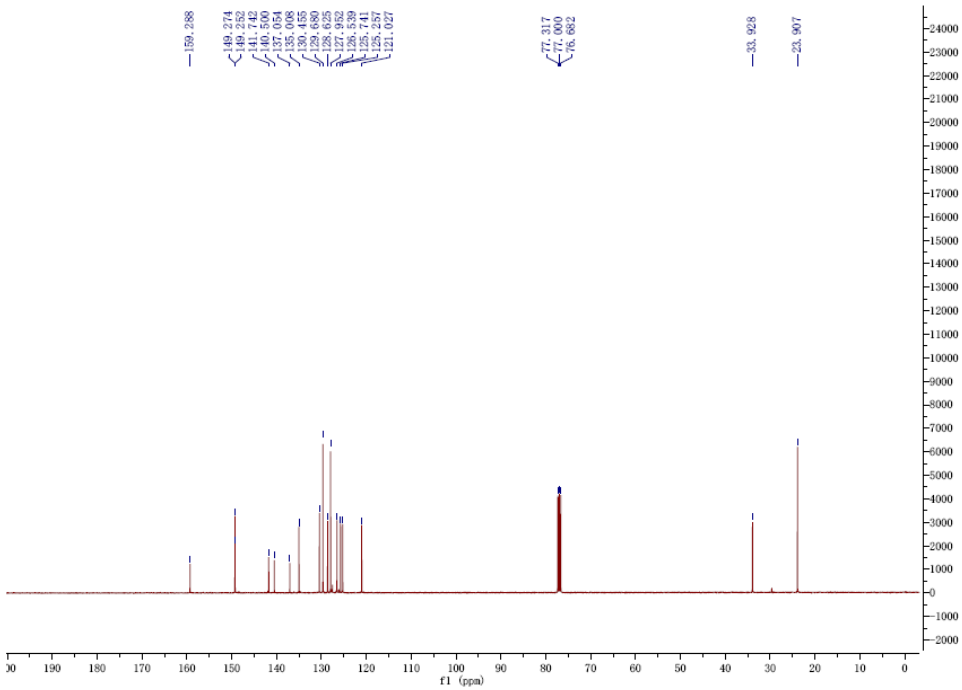
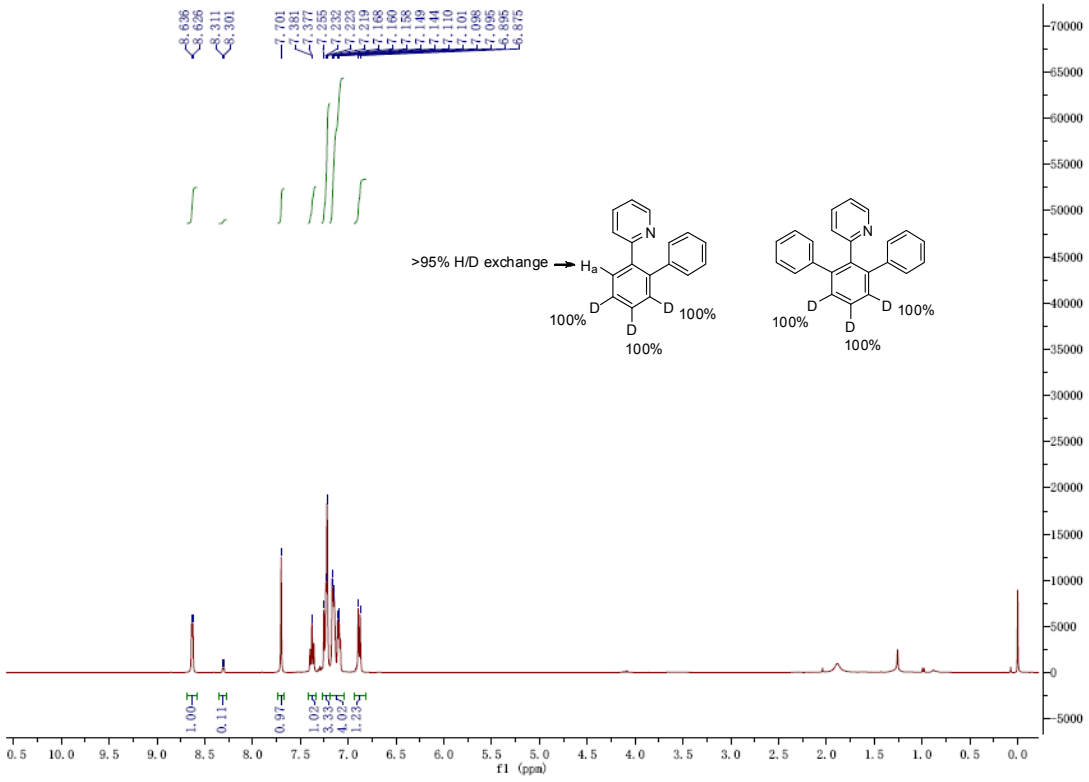
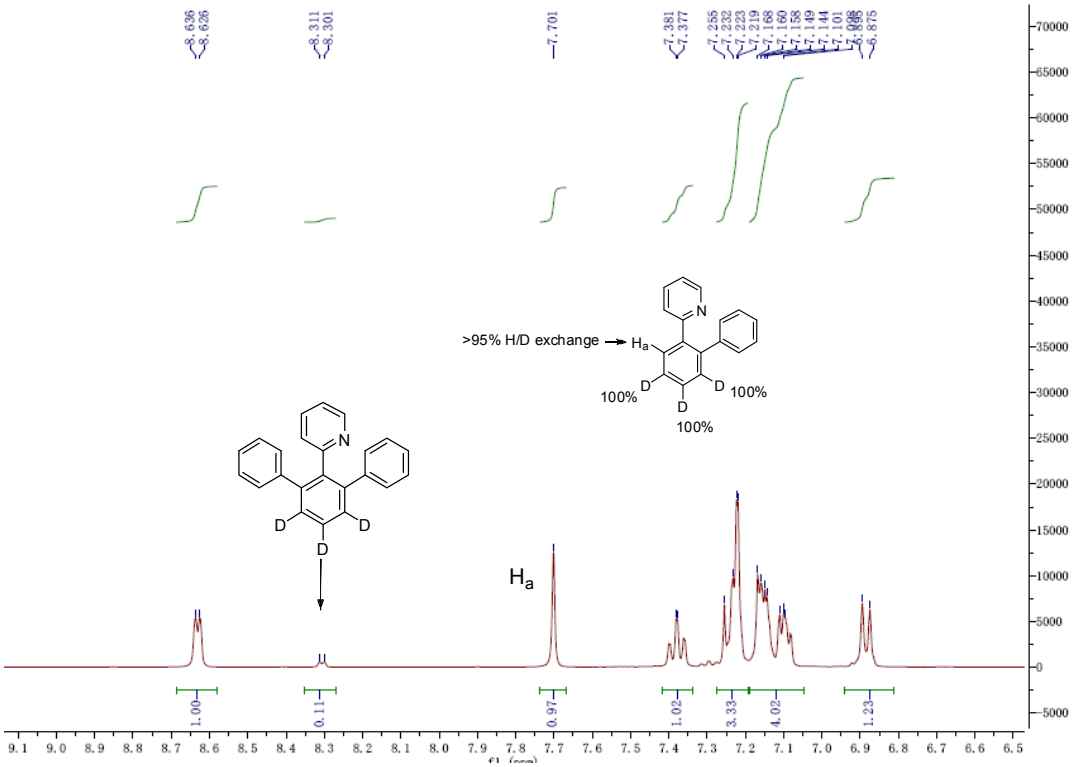




NMR Spectra of Deuterium Labeling Experiment





NMR Spectra of the competition experiment of C—C cleavage versus C—H activation