Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.


# Supporting Information

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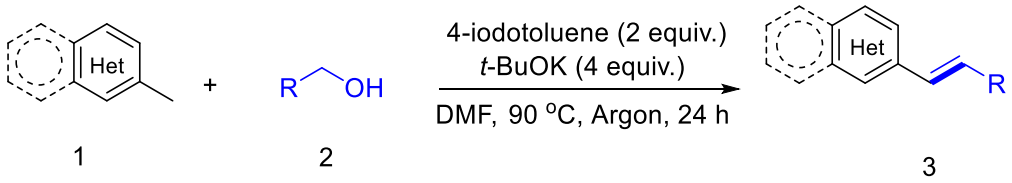
## 1. General information

All reactions were carried out under argon atmosphere, using flame-dried schlenk or vial and vacuum line techniques. Column chromatography was performed on silica gel (100-200 mesh) by using a gradient of hexane/ethyl acetate or hexane/ethyl acetate/triethylamine as mobile phase, based on Merck aluminium TLC plate (silica gel 60 F254). KO$^t$Bu (98%) from Sigma-Aldrich, and sublimate twice then kept under argon in a Schlenk tube. All other commercial reagents were purchased from Sigma-Aldrich, Alfa Aesar, TCI, Fluorochem and Acros and used as received, without further purification. All reagents were weighed in the air.

$^1$H and $^{13}$C NMR spectra were recorded on a Varian Inova 400 MHz spectrometer or on a Bruker Avance 400 MHz spectrometer in $CDCl_3$. For $^1$H NMR (400 MHz), $CDCl_3$ served as internal standard ($\delta$ = 7.26 ppm and 0 ppm) and datas are reported as follows: chemical shift (in ppm), multiplicity (s = singlet, br s = broad singlet, d = doublet, t = triplet, m = multiplet), coupling constant (in Hz). For $^{13}$C NMR (100 MHz), $CDCl_3$ was used as internal standard ($\delta$ = 77.16 ppm) and spectra were obtained with complete proton decoupling. Gas chromatography – mass spectra (GC-MS) were recorded on a ThermoFisher Scientific Trace GC Ultra instrument with a ThermoFisher Scientific ITQ 900 Ionic Trap and an Agilent DB-5MS 30 m x 0,25 mm capillary apolar column (Stationary phase: 0,25 µm film). Column chromatography was performed by using a gradient of hexane/ethyl acetate or hexane/ethyl acetate/triethylamine as mobile phase, based on Merck aluminium TLC plate (silica gel 60 F254).

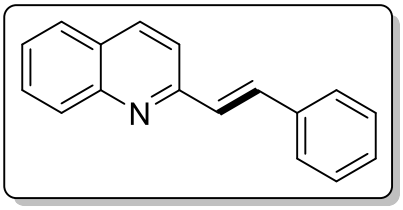
## 2. General procedure for the alkenylation reaction of methyl substituted N-heteroaromatics with alcohols



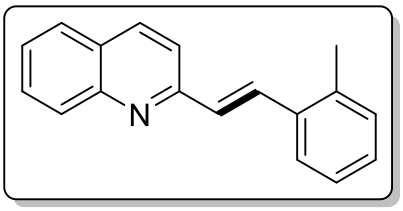

1 2 3

A flame-dried Schlenk flask equipped with a stirring bar under argon was charged with KO$^t$Bu (1.0 mmol, 4.0 equiv, 112 mg) and 4-iodotoluene (0.5 mmol, 2.0 equiv). The flask was evacuated and back-filled with argon 3 times. Then DMF (2 mL), followed by N-heteroaromatic **1** (0.25 mmol, 1.0 equiv) and alcohol **2** (1 mmol, 4.0 equiv) were successively added. The reaction mixture was stirred and heated at 90 °C for 24 hours. After allowing the reaction to cool down to room temperature, the reaction mixture was diluted with water (10 mL) and extracted with ethyl acetate (3 x 5 mL). The organic layer was washed with brine (3 x 5 mL), dried over anhydrous $MgSO_4$, and filtered. Then the solvent was evaporated under reduced pressure to give the crude product **3,** which was purified by chromatography on silica gel (eluent: hexane/ethyl acetate or hexane/ethyl acetate/triethylamine) to afford the desired product.

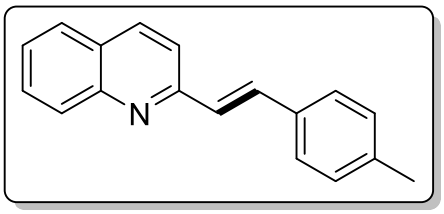
## 3. Characterization data for all compounds



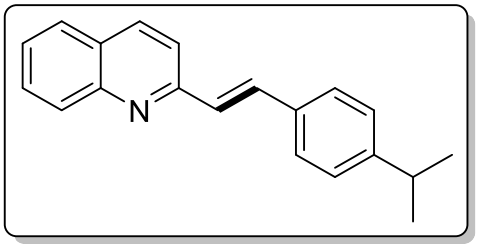
**(E)-2-Styrylquinoline (3aa)**: [1] $R_f$ = 0.3 (Hexane/EtOAc = 15:1), white solid, 76% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.11 (dd, *J* = 8.5, 1.9 Hz, 2H), 7.78 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.75-7.63 (m, 5H), 7.50 (ddd, *J* = 8.0, 6.9, 1.1 Hz, 1H), 7.46-7.39 (m, 3H), 7.36-7.32 (m, 1H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 155.86, 148.14, 136.40, 136.23, 134.32, 129.64, 129.08, 128.90, 128.69, 128.53, 127.40, 127.23, 127.16, 126.06, 119.15.



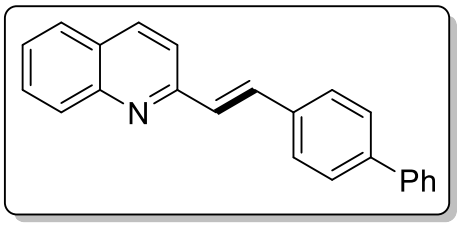
**(E)-2-(2-Methylstyryl)quinoline (3ab)**: [1] $R_f$ = 0.3 (Hexane/EtOAc = 10:1), yellow oil, 75% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.43 (d, *J* = 6.3 Hz, 2H), 8.27 (d, *J* = 15.7 Hz, 1H), 8.03 (ddd, *J* = 29.4, 11.9, 4.4 Hz, 4H), 7.82 (d, *J* = 6.7 Hz, 1H), 7.65 (d, *J* = 15.8 Hz, 1H), 7.56 (d, *J* = 8.7 Hz, 3H), 2.84 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 150.61, 142.57, 131.29, 131.08, 129.95, 126.82, 125.22, 124.54, 124.50, 123.68, 123.17, 122.25, 121.84, 120.98, 120.92, 120.44, 114.06, 14.77.



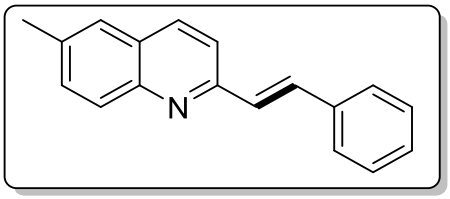
**(E)-2-(4-Methylstyryl)quinoline (3ac)**: [1] $R_f$ = 0.3 (Hexane/EtOAc = 15:1), white solid, 70% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.13-8.08 (m, 2H), 7.78 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.73-7.67 (m, 2H), 7.65 (d, *J* = 1.5 Hz, 1H), 7.58-7.52 (m, 2H), 7.49 (ddd, *J* = 8.1, 6.9, 1.2 Hz, 1H), 7.39 (d, *J* = 16.3 Hz, 1H), 7.22 (d, *J* = 7.7 Hz, 2H), 2.39 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 156.19, 148.15, 138.82, 136.40, 134.61, 133.76, 129.79, 129.57, 129.07, 127.92, 127.52, 127.30, 127.28, 126.12, 119.20, 21.42.



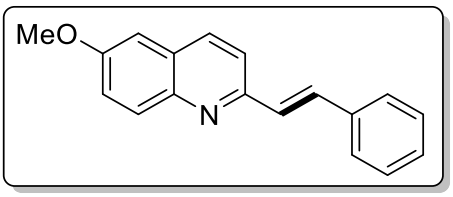
**(E)-2-(4-Isopropylstyryl)quinoline (3ae):** [1] $R_f$ = 0.3 (Hexane/EtOAc = 15:1), white solid, 82% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.38 (d, *J* = 7.5 Hz, 2H), 8.05 (d, *J* = 7.2 Hz, 1H), 7.97 (dd, *J* = 18.1, 7.8 Hz, 3H), 7.87 (d, *J* = 7.0 Hz, 2H), 7.77 (t, *J* = 6.7 Hz, 1H), 7.68 (d, *J* = 15.8 Hz, 1H), 7.56 (d, *J* = 6.9 Hz, 2H), 3.29 – 3.15 (m, 1H), 1.57 (d, *J* = 6.3 Hz, 6H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 150.86, 144.42, 142.82, 131.34, 129.30, 128.79, 124.63, 123.80, 122.75, 122.43, 122.13, 121.97, 121.70, 120.98, 114.10, 28.74, 18.75.



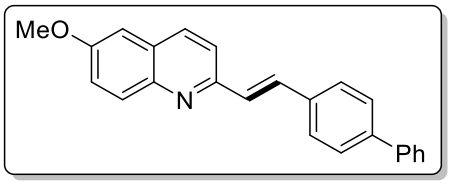
**(E)-2-(2-([1,1'-Biphenyl]-4-yl)vinyl)quinoline (3af):** [2] $R_f$ = 0.24 (Hexane/EtOAc = 40:1), yellow solid, 75% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.18 – 8.07 (m, 2H), 7.79 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.77 – 7.67 (m, 5H), 7.68 – 7.62 (m, 4H), 7.55 – 7.41 (m, 4H), 7.40 – 7.33 (m, 1H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 156.09, 148.41, 141.43, 140.60, 136.46, 135.66, 134.05, 129.88, 129.32, 129.11, 128.96, 127.84, 127.79, 127.63, 127.57, 127.47, 127.08, 126.29, 119.44.



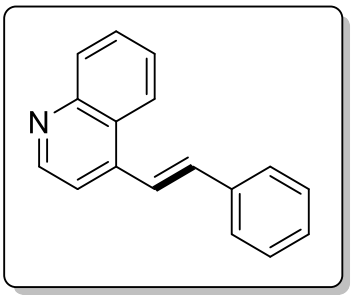

**(E)-6-Methyl-2-styrylquinoline (3ba)**: [3] $R_f$ = 0.15 (Hexane/ EtOAc = 90:1), white solid, 80 % isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.03 (dd, *J* = 8.6, 0.7 Hz, 1H), 8.00-7.96 (m, 1H), 7.68-7.61 (m, 4H), 7.57-7.50 (m, 2H), 7.44-7.37 (m, 3H), 7.36-7.29 (m, 1H), 2.53 (s, 1H). **$^{13}$C NMR (101 MHz, 400 MHz, $CDCl_3$)** δ 155.28, 146.96, 136.77, 136.22, 135.80, 133.98, 132.13, 129.28, 129.02, 128.90, 128.63, 127.50, 127.32, 126.57, 119.38, 21.72.



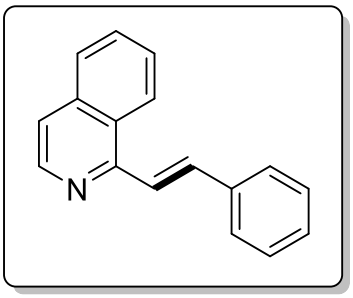

**(E)-6-Methoxy-2-styrylquinoline (3ca)**: [3] $R_f$ = 0.25 (Hexane/ EtOAc = 10:1), white solid, 82% isolated yield (83% in NMR). **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.03 - 7.96 (m, 2H), 7.65 - 7.58 (m, 4H), 7.42 - 7.35 (m, 4H), 7.33 - 7.29 (m, 1H), 7.05 (d, *J* = 2.8 Hz, 1H), 3.93 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 157.76, 153.82, 144.41, 136.83, 135.20, 133.32, 130.78, 129.19, 128.88, 128.50, 128.42, 127.24, 122.43, 119.68, 105.38, 55.66.



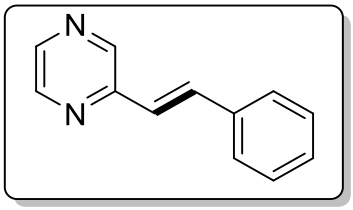

**(E)-2-(2-([1,1'-Biphenyl]-4-yl)vinyl)-6-methoxyquinoline (STB-8) (3cf)**: [1] $R_f$ = 0.2 (Hexane/EtOAc = 40:1), yellow solid, 40% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.04 (d, *J* = 8.6 Hz, 1H), 8.00 (d, *J* = 9.2 Hz, 1H), 7.74 – 7.66 (m, 3H), 7.64 (dd, *J* = 6.9, 1.4 Hz, 5H), 7.50 – 7.40 (m, 3H), 7.40 – 7.31 (m, 2H), 7.07 (d, *J* = 2.8 Hz, 1H), 3.94 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 157.80, 153.85, 144.47, 141.22, 140.70, 135.90, 135.23, 132.86, 130.81, 129.21, 128.97, 128.45, 127.71, 127.59, 127.57, 127.10, 122.48, 119.78, 105.42, 55.70.



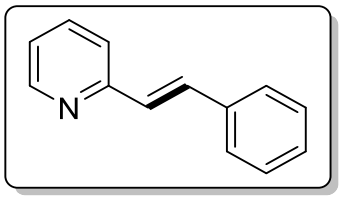

**(E)-4-Styrylquinoline (3da)**: [1] $R_f$ = 0.15 (Hexane/EtOAc = 30:1), white solid, 45% isolated yield (50% in $^1$H NMR). **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.90 (d, *J* = 4.6 Hz, 1H), 8.22 (d, *J* = 8.3 Hz, 1H), 8.15 (d, *J* = 8.3 Hz, 1H), 7.82 (d, *J* = 16.1 Hz, 1H), 7.78 – 7.71 (m, 1H), 7.68 – 7.53 (m, 4H), 7.45 – 7.42, (m, 2H), 7.35 (dd, *J* = 15.2, 7.7 Hz, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 150.37, 148.84, 143.10, 136.70, 135.28, 130.28, 129.46, 129.05, 128.94, 127.27, 126.66, 126.56, 123.62, 123.06, 117.22.



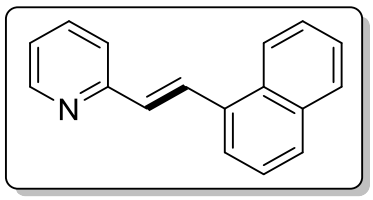

**(E)-1-Styrylisoquinoline (3ea):** [1] $R_f$ = 0.3 (Hexane/EtOAc = 15:1), white solid, 40% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.57 (d, *J* = 5.6 Hz, 1H), 8.39 (d, *J* = 8.5 Hz, 1H), 8.01 (s, 2H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.72 – 7.62 (m, 4H), 7.58 (d, *J* = 5.6 Hz, 1H), 7.44 – 7.41 (m, 4H), 7.36 – 7.33 (m, 4H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 154.70, 142.63, 137.08, 136.89, 135.99, 130.05, 128.91, 128.75, 127.59, 127.47, 127.34, 126.91, 124.61, 122.99, 120.10.



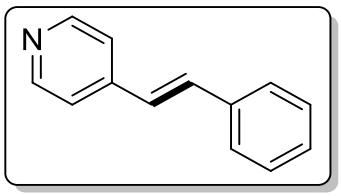
**(E)-2-Styrylpyrazine (3fa)**: [2] $R_f$ = 0.4 (Hexane/EtOAc = 2:1, one drop of $Et_3N$ in 100 ml eluent), white solid, 46% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.64 (s, 1H), 8.54 (s, 1H), 8.41 (d, *J* = 2.1 Hz, 1H), 7.75 (d, *J* = 16.1 Hz, 1H), 7.60 (d, *J* = 7.3 Hz, 2H), 7.42 – 7.32 (m, 3H), 7.16 (d, *J* = 16.1 Hz, 1H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 151.40, 144.46, 143.88, 142.87, 136.16, 135.32, 129.11, 128.97, 127.45, 124.15.



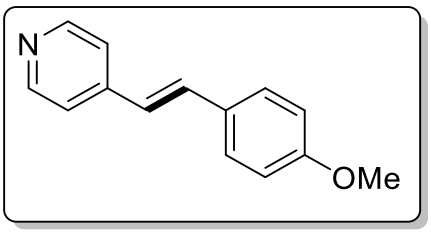
**(E)-2-Styrylpyridine (3ga):** [4] $R_f$ = 0.5 (Hexane/EtOAc = 5:1, one drop of $Et_3N$ in 100 ml eluent), light yellow solid, 45 % isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.61 (dt, *J* = 4.8, 1.4 Hz, 1H), 7.67-7.62 (m, 2H), 7.60-7.57 (m, 2H), 7.40-7.35 (m, 3H), 7.32-7.28 (m, 1H), 7.20-7.12 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 155.68, 149.70, 136.72, 136.65, 132.86, 128.82, 128.43, 127.99, 127.20, 122.20, 122.15.



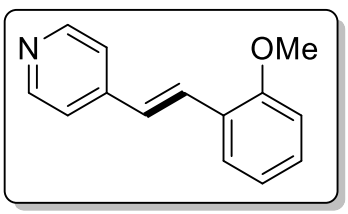
**(E)-2-(2-(Naphthalen-1-yl)vinyl)pyridine (3gg):** [5] $R_f$ = 0.45 (Hexane/EtOAc = 5:1, one drop of $Et_3N$ in 100 ml eluent), white solid, 46 % isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.67 (ddd, *J* = 4.8, 1.9, 0.9 Hz, 1H), 8.47 (d, *J* = 15.8 Hz, 1H), 8.35-8.30 (m, 1H), 7.88 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.85-7.81 (m, 2H), 7.72-7.68 (m, 1H), 7.58-7.50 (m, 3H), 7.46-7.44 (m, 1H), 7.23 (d, *J* = 15.7 Hz, 1H), 7.21-7.17 (m, 1H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 155.85, 149.92, 136.74, 134.47, 133.88, 131.68, 130.98, 129.95, 128.80, 128.72, 126.36, 126.06, 125.78, 124.10, 124.07, 122.51, 122.35.



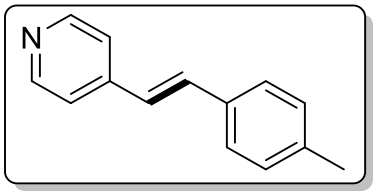
**(E)-4-Styrylpyridine (3ha)**: [2] $R_f$ = 0.5 (Hexane/EtOAc = 5:1, one drop of $Et_3N$ in 100 ml eluent), white solid, 72% isolated yield (80% in $^1$H NMR). **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.62 - 8.49 (m, 2H), 7.58 - 7.50 (m, 2H), 7.42 - 7.27 (m, 6H), 7.01 (dd, *J* = 16.4, 1.7 Hz, 1H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 149.97, 144.35, 135.90, 132.92, 128.62, 128.53, 126.79, 125.75, 120.62.



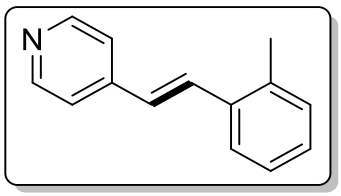
**(E)-4-(4-Methoxystyryl)pyridine (3hh)** : [6] $R_f$ = 0.5 (Hexane/ EtOAc = 5:1, one drop of $Et_3N$ in 100 ml eluent), light yellow solide, 77% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.57 - 8.52 (m, 2H), 7.50 - 7.45 (m, 2H), 7.35 - 7.31 (m, 2H), 7.25 (d, *J* = 16.3 Hz, 1H), 6.94 - 6.84 (m, 3H), 3.84 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 160.25, 150.25, 145.06, 132.79, 129.01, 128.50, 123.85, 120.74, 114.39, 55.48.



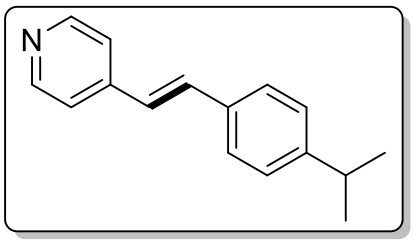
**(E)-4-(2-Methoxystyryl)pyridine (3hi)**: [6] $R_f$ = 0.5 (Hexane/ EtOAc = 5:1, one drop of $Et_3N$ in 100 ml eluent), light yellow oil, 62% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.57-8.53 (m, 2H), 7.68 (d, *J* = 16.5 Hz, 1H), 7.59 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.38 (ddd, *J* = 4.5, 1.7, 0.5 Hz, 2H), 7.33 - 7.28 (m, 1H), 7.05 - 6.97 (m, 2H), 6.92 (dd, *J* = 8.3, 1.0 Hz, 1H), 3.90 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 157.39, 150.15, 145.41, 129.99, 128.26, 127.07, 126.38, 125.27, 121.03, 120.90, 111.12, 55.62.



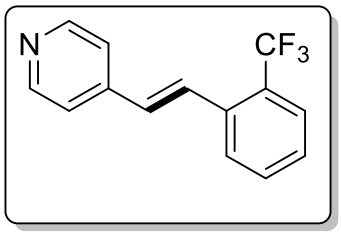
**(E)-4-(4-Methylstyryl)pyridine (3hc)**: [7] $R_f$ = 0.5 (Hexane/ EtOAc = 5:1, one drop of $Et_3N$ in 100 ml eluent), white solid, 52% isolated yield (78% in $^1$H NMR). **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.59 - 8.53 (m, 2H), 7.46 - 7.41 (m, 2H), 7.36 - 7.32 (m, 2H), 7.27 (d, *J* = 16.3 Hz, 1H), 7.22 - 7.17 (m, 2H), 6.96 (d, *J* = 16.3 Hz, 1H), 2.38 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 150.28, 144.92, 139.00, 133.50, 133.22, 129.69, 127.08, 125.08, 120.87, 21.47.



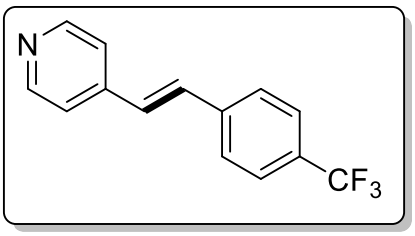
**(E)-4-(2-Methylstyryl)pyridine (3hb)**: [7] $R_f$ = 0.5 (Hexane/ EtOAc = 5:1, one drop of $Et_3N$ in 100 ml eluent), white solid, 41% isolated yield (70% in $^1$H NMR). **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.61 - 8.54 (m, 2H), 7.60 (dt, *J* = 4.8, 3.5 Hz, 1H), 7.54 (d, *J* = 16.1 Hz, 1H), 7.38 - 7.34 (m, 2H), 7.25 - 7.20 (m, 3H), 6.91 (d, *J* = 16.2 Hz, 1H), 2.44 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 150.33, 145.02, 136.46, 135.37, 131.08, 130.74, 128.72, 127.44, 126.48, 125.81, 121.04, 19.98.



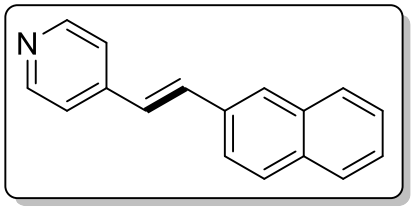
**(E)-4-(4-Isopropylstyryl)pyridine (3he)**: [7] $R_f$ = 0.5 (Hexane/ EtOAc = 5:1, one drop of $Et_3N$ in 100 ml eluent), light yellow solid, 68% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.61 - 8.54 (m, 2H), 7.51 - 7.46 (m, 2H), 7.38 - 7.34 (m, 2H), 7.33 - 7.25 (m, 3H), 6.98 (d, *J* = 16.3 Hz, 1H), 2.94 (p, *J* = 6.9 Hz, 1H), 1.29 (s, 3H), 1.27 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 150.28, 150.27, 144.93, 133.90, 133.21, 127.18, 127.07, 125.18, 120.89, 34.11, 24.00.



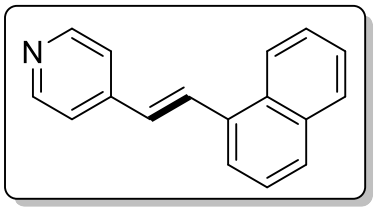
**(E)-4-(2-(Trifluoromethyl)styryl)pyridine (3hj)**: $R_f$ = 0.22 (Hexane/ EtOAc = 5:1, one drop of $Et_3N$ in 100 ml eluent), white solid, 50% isolated yield. (55% yield in $^1$H NMR). **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.62 (d, *J* = 5.5 Hz, 2H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.68 (dd, *J* = 19.3, 4.7 Hz, 2H), 7.60 – 7.56 (m, 1H), 7.42 (dd, *J* = 17.2, 6.7 Hz, 3H), 7.00 (d, *J* = 16.1 Hz, 1H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 150.06, 144.61, 135.27, 132.23, 130.06, 129.34, 128.50, 128.21(q, *J* = 30.0 Hz), 127.48, 126.28(q, *J* = 5.7 Hz), 124.39(q, *J* = 275.1 Hz), 121.41. **$^{19}$F NMR (377 MHz, $CDCl_3$)** δ -59.14. **HRMS**, calculated [M+H] 250.0844, Found 250.0833.



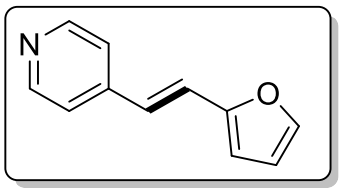
**(E)-4-(4-(Trifluoromethyl)styryl)pyridine (3hk)**: [8] $R_f$ = 0.5 (Hexane/ EtOAc = 5:1, one drop of $Et_3N$ in 100 ml eluent), white solid, 72% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.49 (d, *J* = 5.8 Hz, 2H), 7.52 (s, 3H), 7.27 (dd, *J* = 4.7, 1.4 Hz, 2H), 7.21 – 7.14 (m, 1H), 6.98 (d, *J* = 16.4 Hz, 1H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 150.27, 144.23, 139.66, 131.86, 130.54(q, *J* = 32.7 Hz), 128.59, 127.29, 125.95(q, *J* = 3.6 Hz), 124.00(q, *J* =273.3 Hz) 121.20. **$^{19}$F NMR (377 MHz, $CDCl_3$)** δ -62.63.



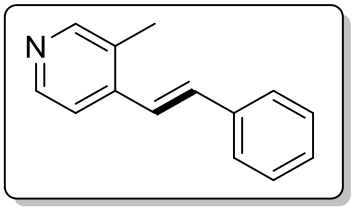
**(E)-4-(2-(Naphthalen-2-yl)vinyl)pyridine (3hl)**: [9] $R_f$ = 0.2 (Hexane/ EtOAc = 5:1, one drop of $Et_3N$ in 100 ml eluent), white solid, 75% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.64 - 8.57 (m, 2H), 7.91 - 7.89 (m, 1H), 7.87 - 7.82 (m, 3H), 7.74 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.52 - 7.39 (m, 5H), 7.13 (d, *J* = 16.3 Hz, 1H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 150.37, 144.76, 133.75, 133.66, 133.64, 133.37, 128.70, 128.33, 127.98, 127.89, 126.72, 126.67, 126.37, 123.46, 120.97.



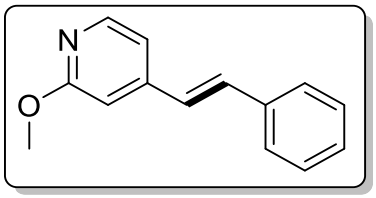
**(E)-4-(2-(Naphthalen-1-yl)vinyl)pyridine (3hg)**: [10] $R_f$ = 0.2 (Hexane/ EtOAc = 5:1, one drop of $Et_3N$ in 100 ml eluent), white solid, 72% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.63 (d, *J* = 6.0 Hz, 2H), 8.19 (d, *J* = 8.2 Hz, 1H), 8.11 (d, *J* = 16.0 Hz, 1H), 7.94 – 7.83 (m, 2H), 7.77 (d, *J* = 7.2 Hz, 1H), 7.64 – 7.43 (m, 5H), 7.08 (d, *J* = 16.0 Hz, 1H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 150.39, 144.85, 133.89, 133.81, 131.41, 130.38, 129.20, 129.12, 128.87, 126.58, 126.17, 125.73, 124.29, 123.55, 121.11.



**(E)-4-(2-(Furan-2-yl)vinyl)pyridine (3hm)**: [10] $R_f$ = 0.2 (Hexane/ EtOAc = 10:4, one drop of $Et_3N$ in 100 ml eluent), white solid, m.p = 84.5 ℃, 61% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.55 (d, *J* = 6.0 Hz, 2H), 7.45 (s, 1H), 7.30 (d, *J* = 6.1 Hz, 2H), 7.08 (d, *J* = 16.2 Hz, 1H), 6.93 (d, *J* = 16.2 Hz, 1H), 6.48 – 6.45 (m, 2H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 152.39, 150.31, 144.46, 143.38, 124.29, 120.71, 120.57, 112.09, 111.10.



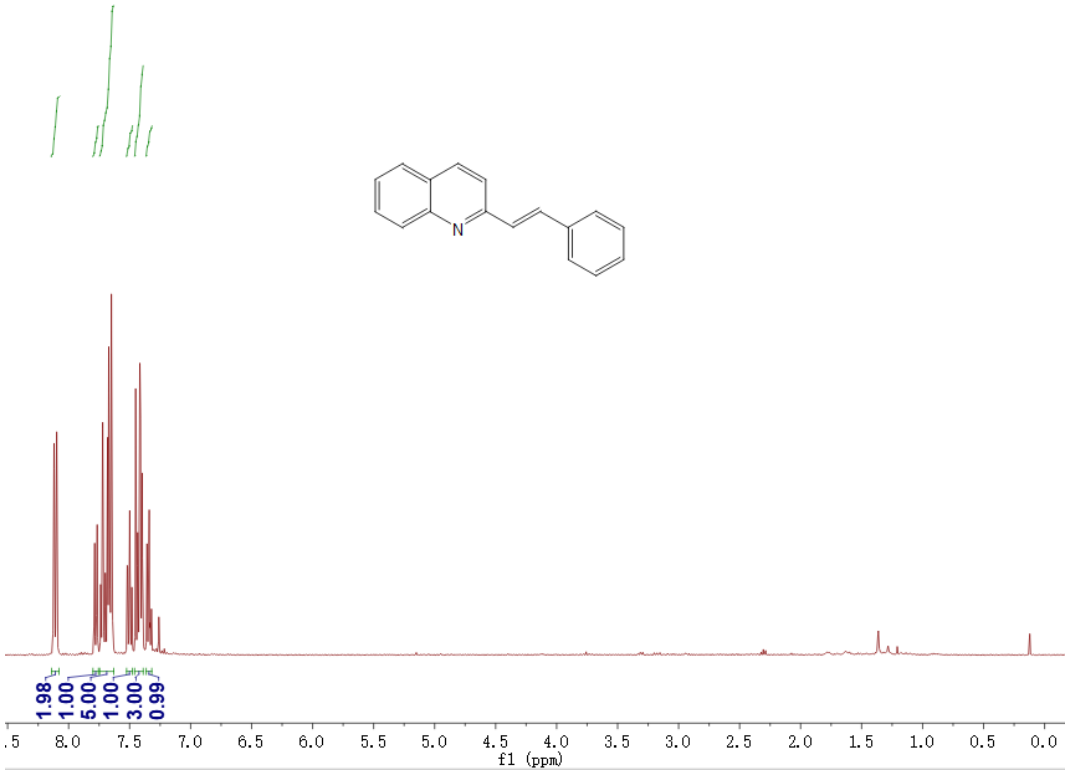
**(E)-3-Methyl-4-styrylpyridine (3ia)**: [11] $R_f$ = 0.2, Hexane/ EtOAc = 5:1, yellow solid, m.p =81.2 ℃, 68% isolated yield. **$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.45 - 8.39 (m, 2H), 7.57 - 7.53 (m, 2H), 7.44 - 7.38 (m, 3H), 7.35 - 7.30 (m, 1H), 7.20 (d, *J* = 4.1 Hz, 2H), 2.40 (s, 3H). **$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 151.49, 147.81, 143.62, 136.66, 133.81, 130.48, 128.96, 128.76, 127.11, 123.83, 119.02, 16.74.



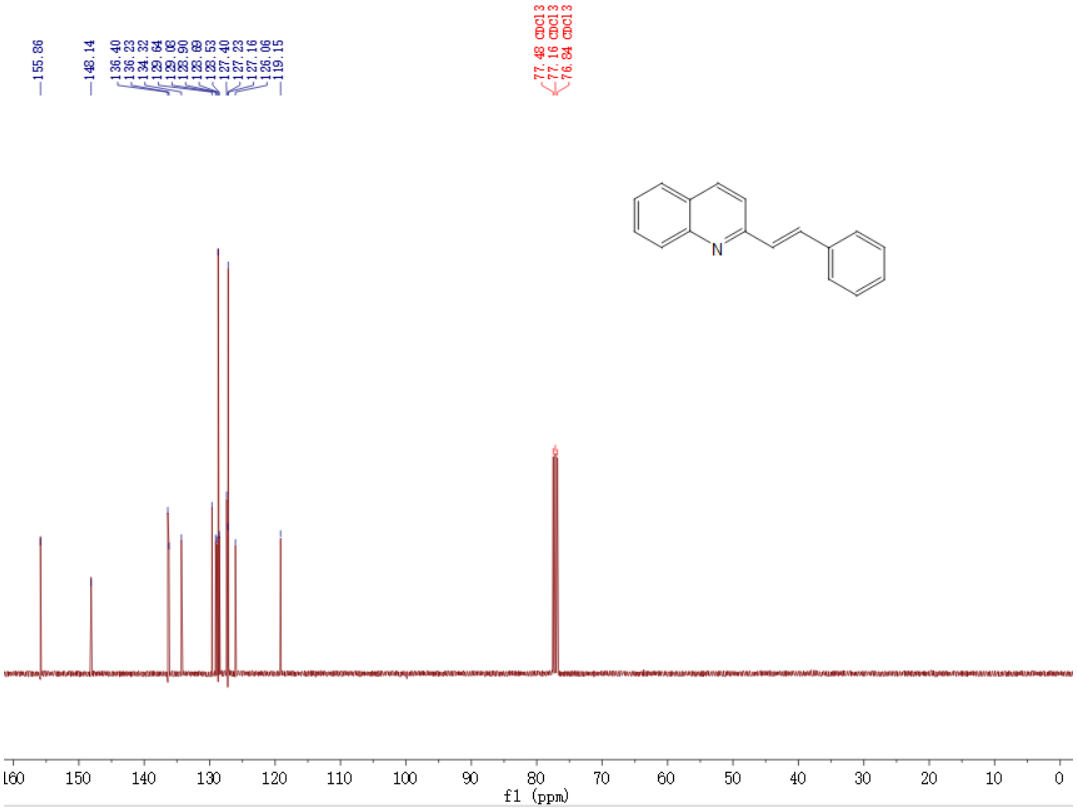
**(E)-2-Methoxy-4-styrylpyridine (3ja)**: $R_f$ = 0.2, Hexane/ EtOAc = 90:1, yellow solid, m.p = 53.6 ℃, 48% isolated yield (52% in $^1$H NMR).**$^1$H NMR (400 MHz, $CDCl_3$)** δ 8.13 (d, *J* = 5.4 Hz, 1H), 7.54 – 7.51 (m, 2H), 7.43 – 7.35 (m, 2H), 7.34 – 7.29 (m, 1H), 7.26 (d, *J* = 16.3 Hz, 1H), 7.03 (dd, *J* = 5.4, 1.2 Hz, 1H), 6.98 (d, *J* = 16.3 Hz, 1H), 6.82 – 6.77 (m, 1H), 3.97 (s, 3H).**$^{13}$C NMR (101 MHz, $CDCl_3$)** δ 165.13, 147.57, 147.14, 136.37, 133.05, 128.95, 128.77, 127.13, 126.25, 114.29, 108.28, 53.62. **HRMS**, calculated [M+H] 212.1075, Found 212.1073.

## 4. $^{1}H$ and $^{13}C$ NMR spectra for all compounds

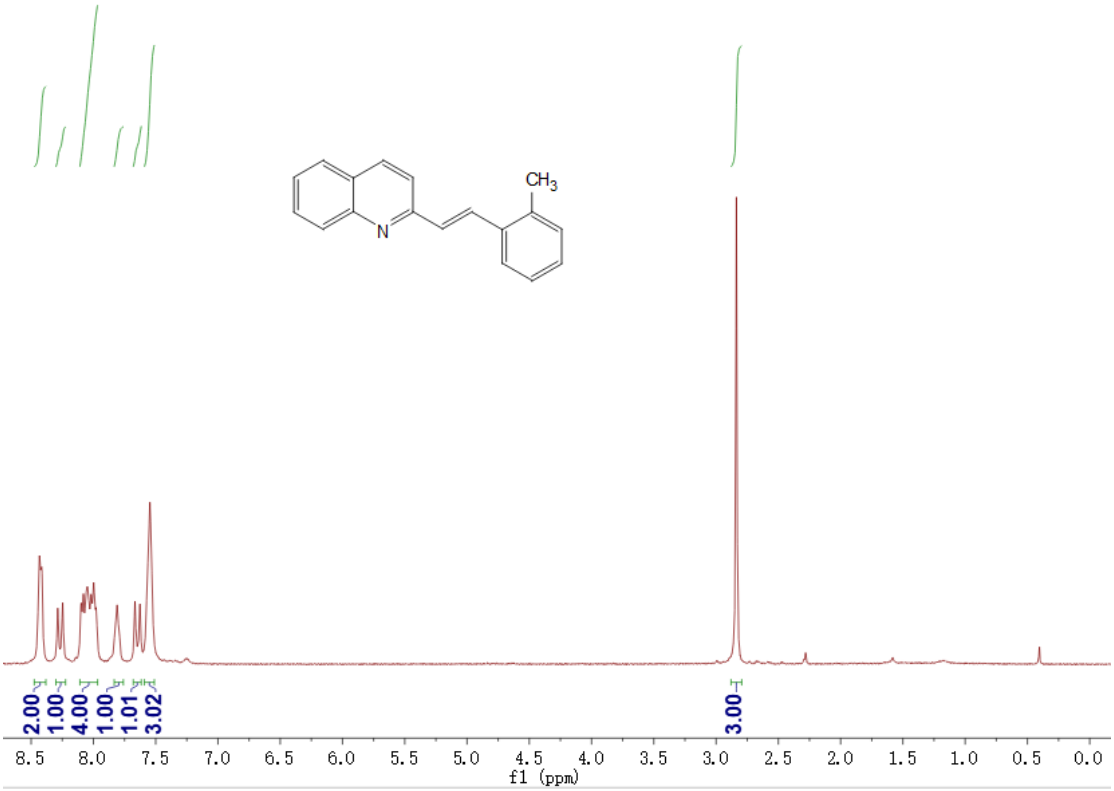
**(E)-2-Styrylquinoline (3aa), $^{1}H$ NMR (400 MHz, $CDCl_3$)**



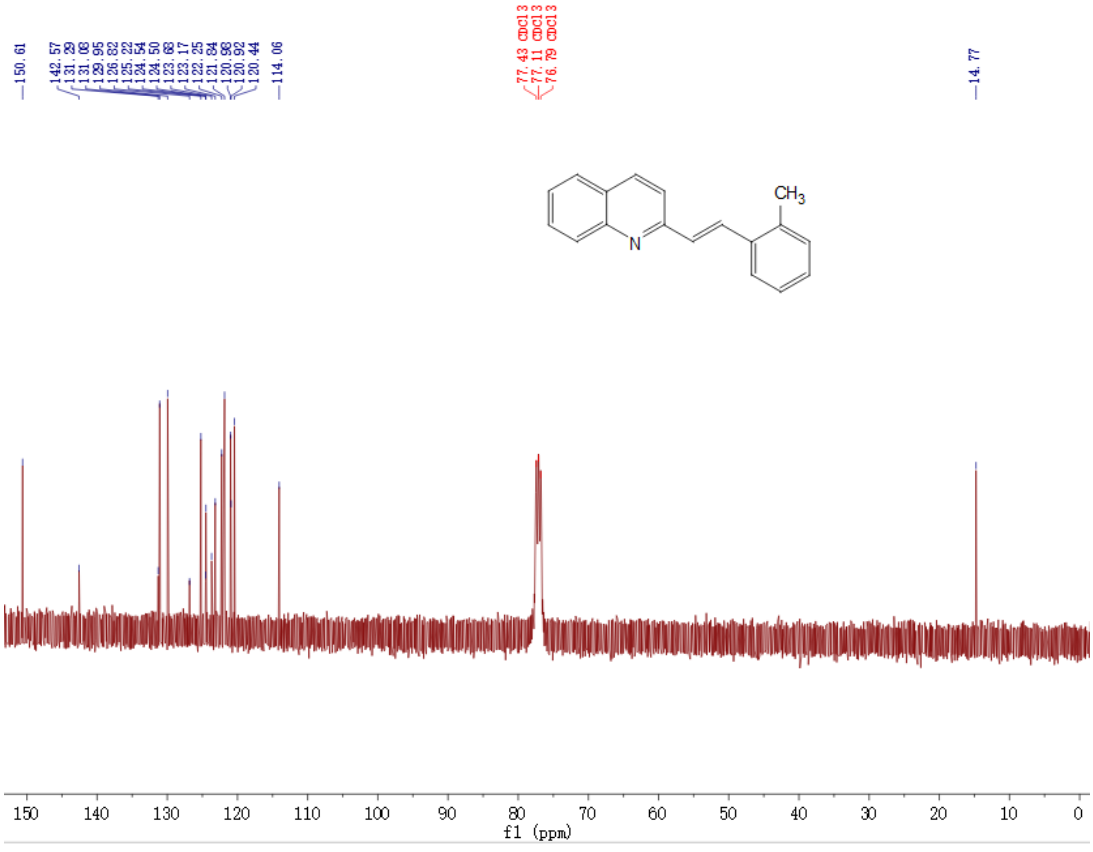

**(E)-2-Styrylquinoline (3aa), $^{13}C$ NMR (101 MHz, $CDCl_3$)**



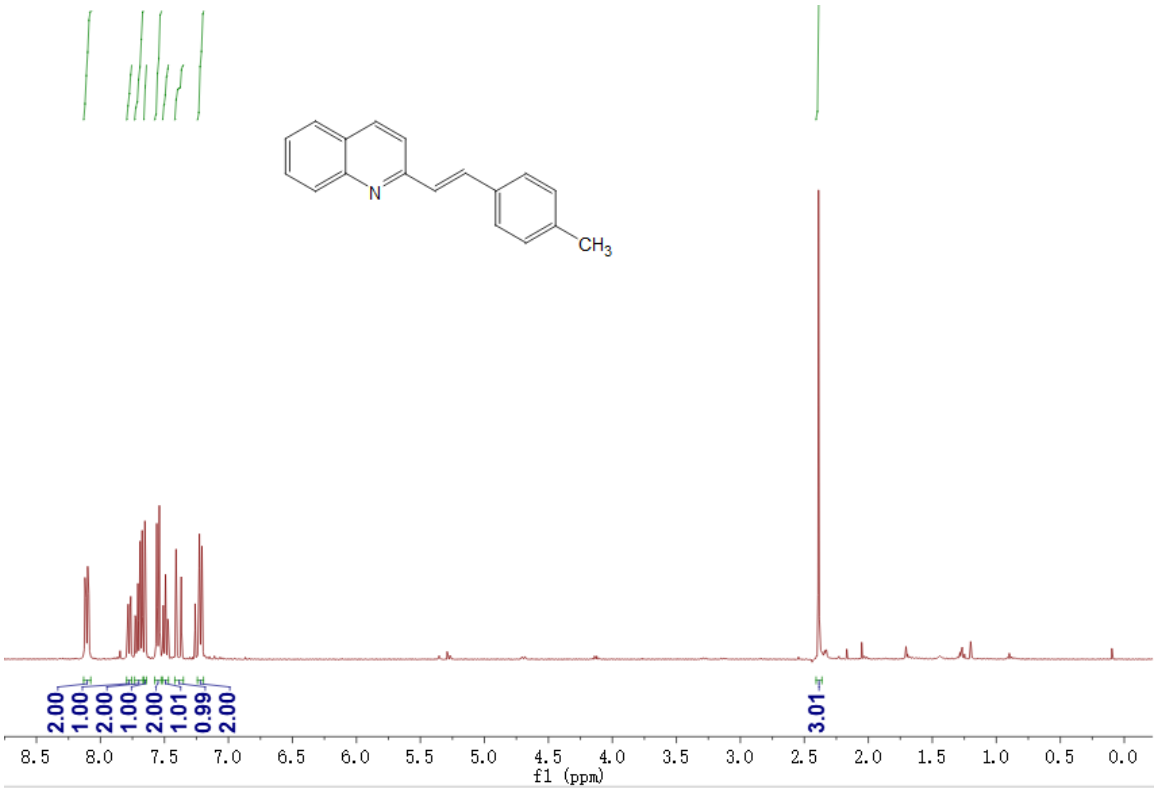
**(E)-2-(2-Methylstyryl)quinoline (3ab), $^{1}$H NMR (400 MHz, $CDCl_3$)**



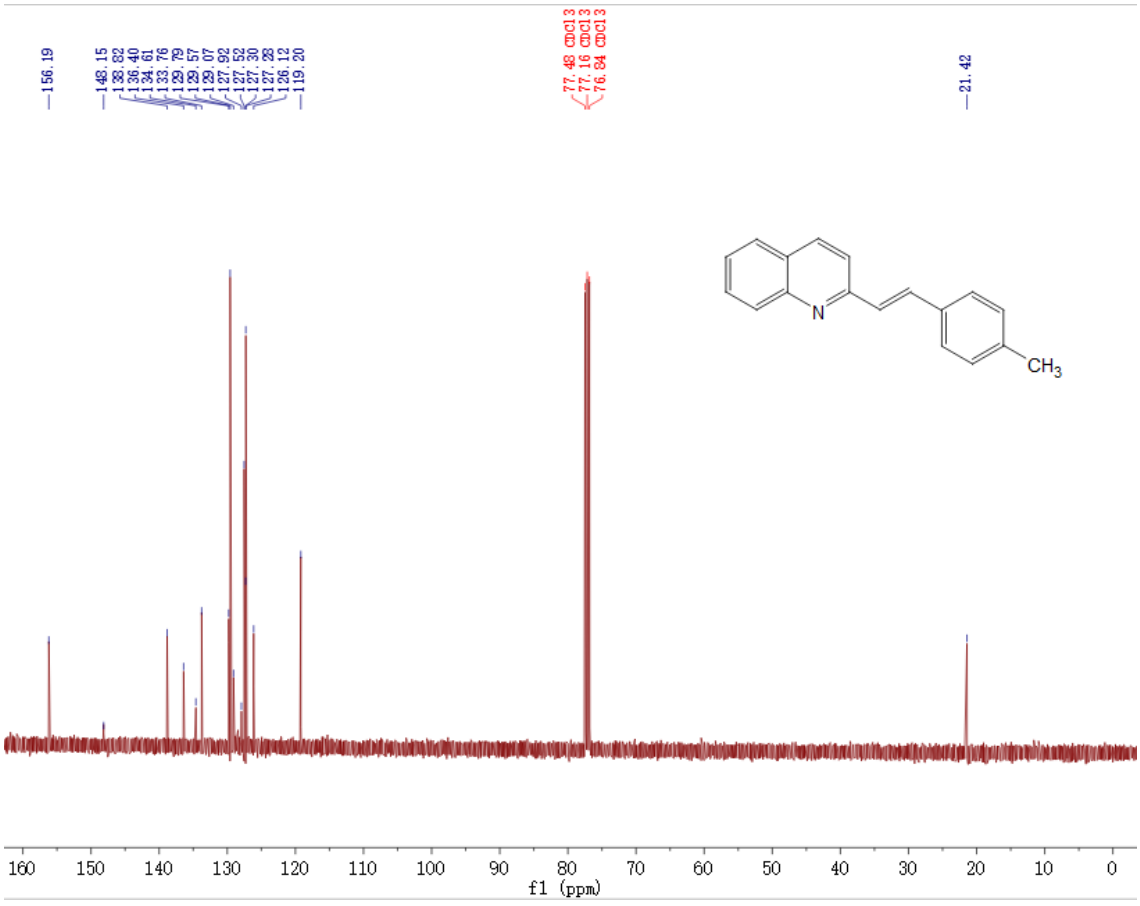

**(E)-2-(2-Methylstyryl)quinoline (3ab), $^{13}$C NMR (101 MHz, $CDCl_3$)**



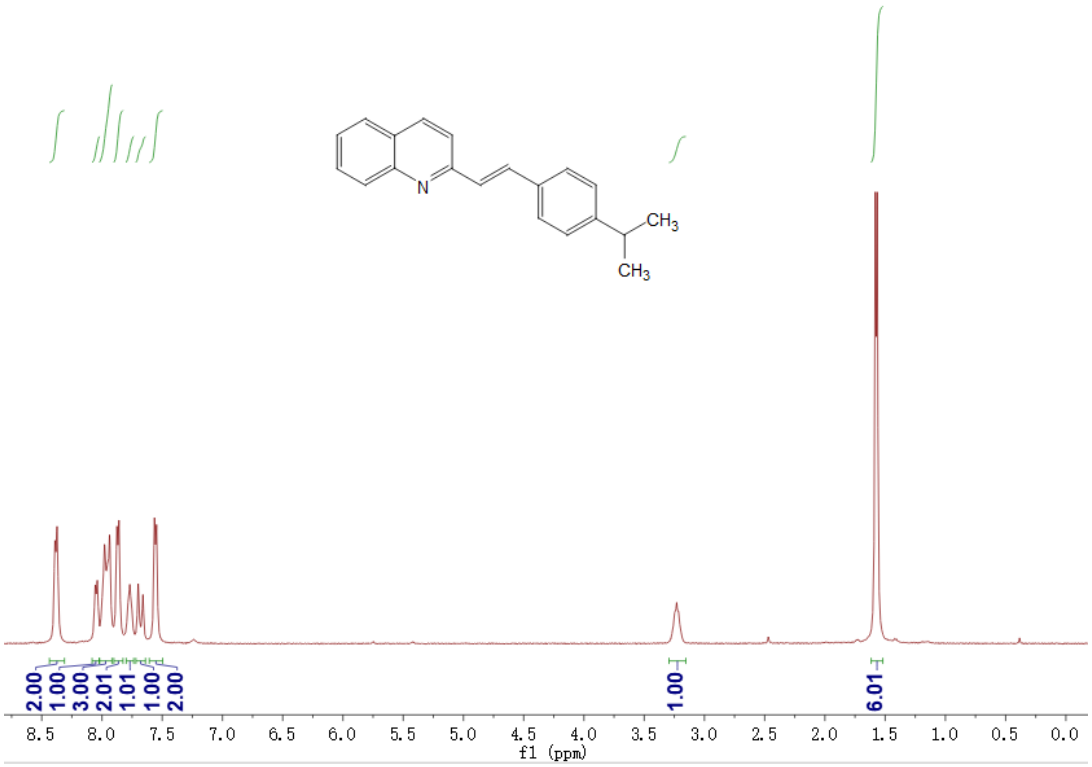
**(E)-2-(4-Methylstyryl)quinoline (3ac), $^{1}$H NMR (400 MHz, $CDCl_3$)**



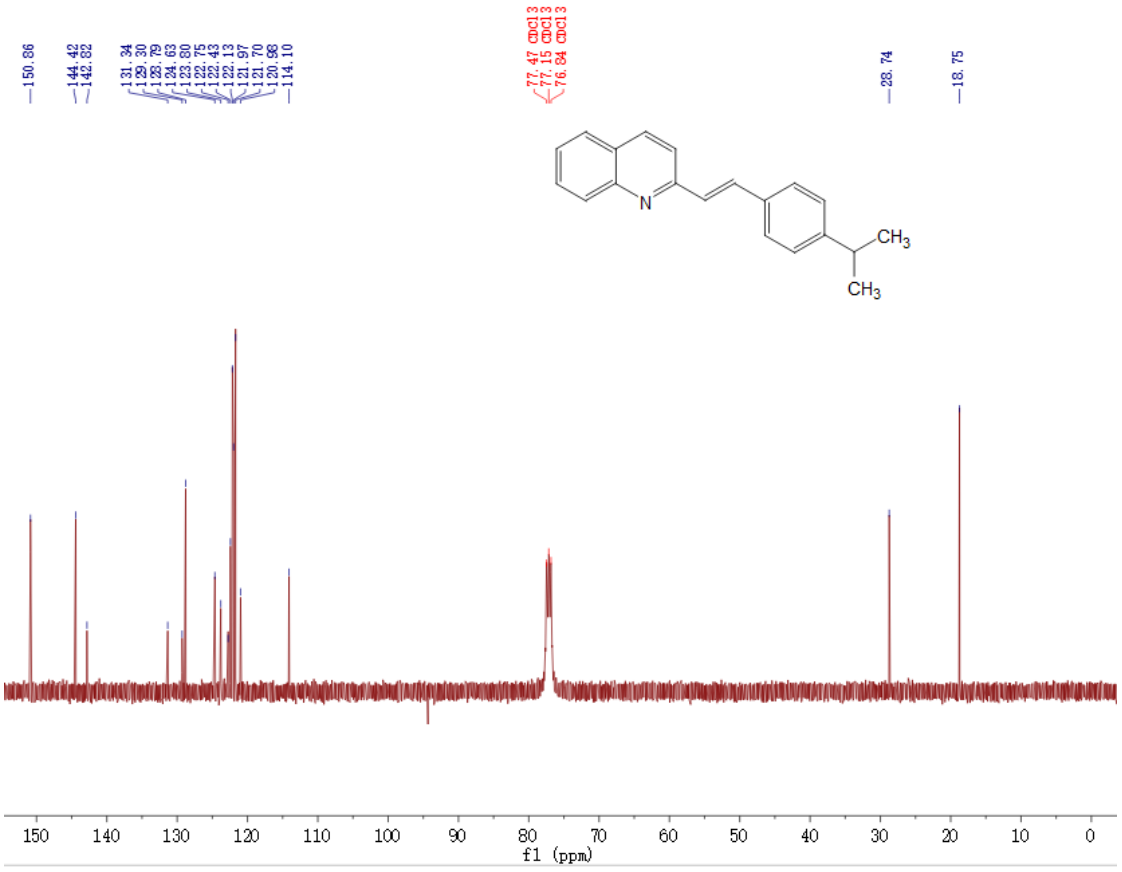

**(E)-2-(4-Methylstyryl)quinoline (3ac), $^{13}$C NMR (101 MHz, $CDCl_3$)**



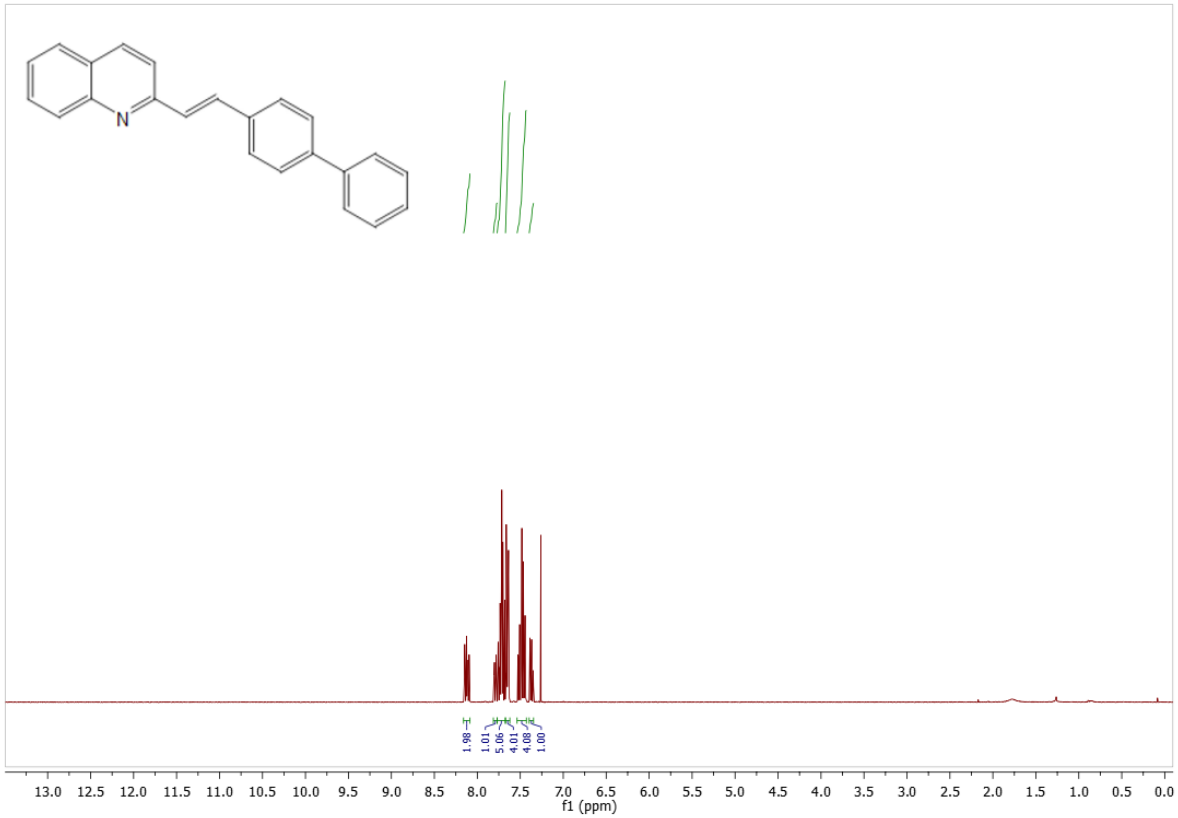
**(E)-2-(4-Isopropylstyryl)quinoline (3ae), $^{1}$H NMR (400 MHz, $CDCl_3$)**



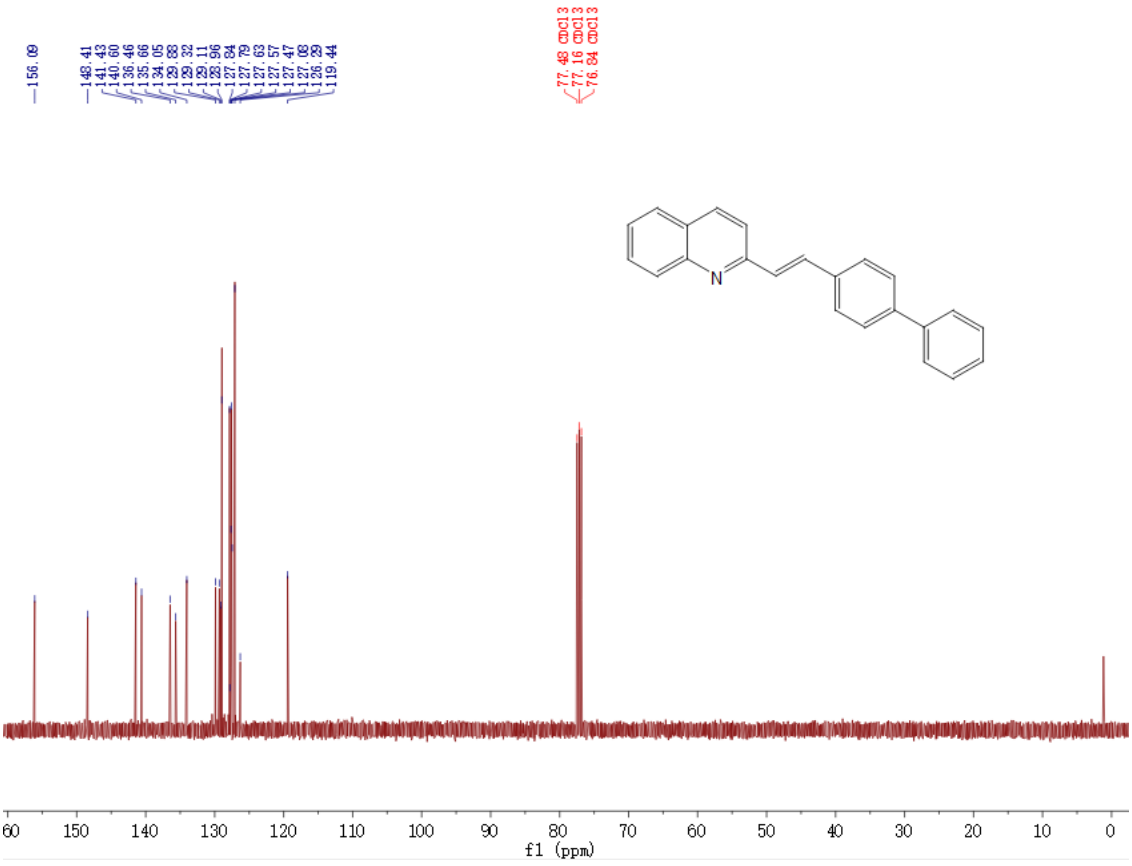

**(E)-2-(4-Isopropylstyryl)quinoline (3ae), $^{13}$C NMR (101 MHz, $CDCl_3$)**



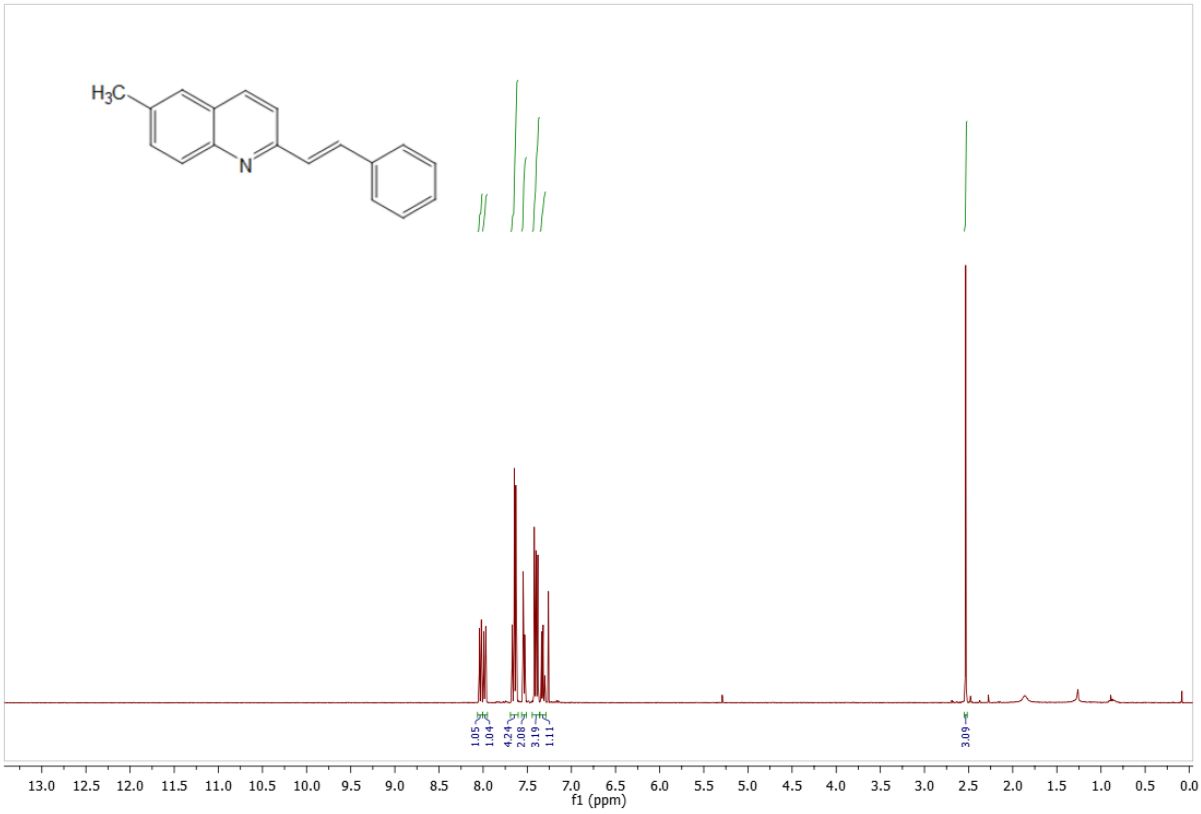
**(E)-2-(2-([1,1'-Biphenyl]-4-yl)vinyl)quinoline (3af), $^{1}$H NMR (400 MHz, $CDCl_3$)**



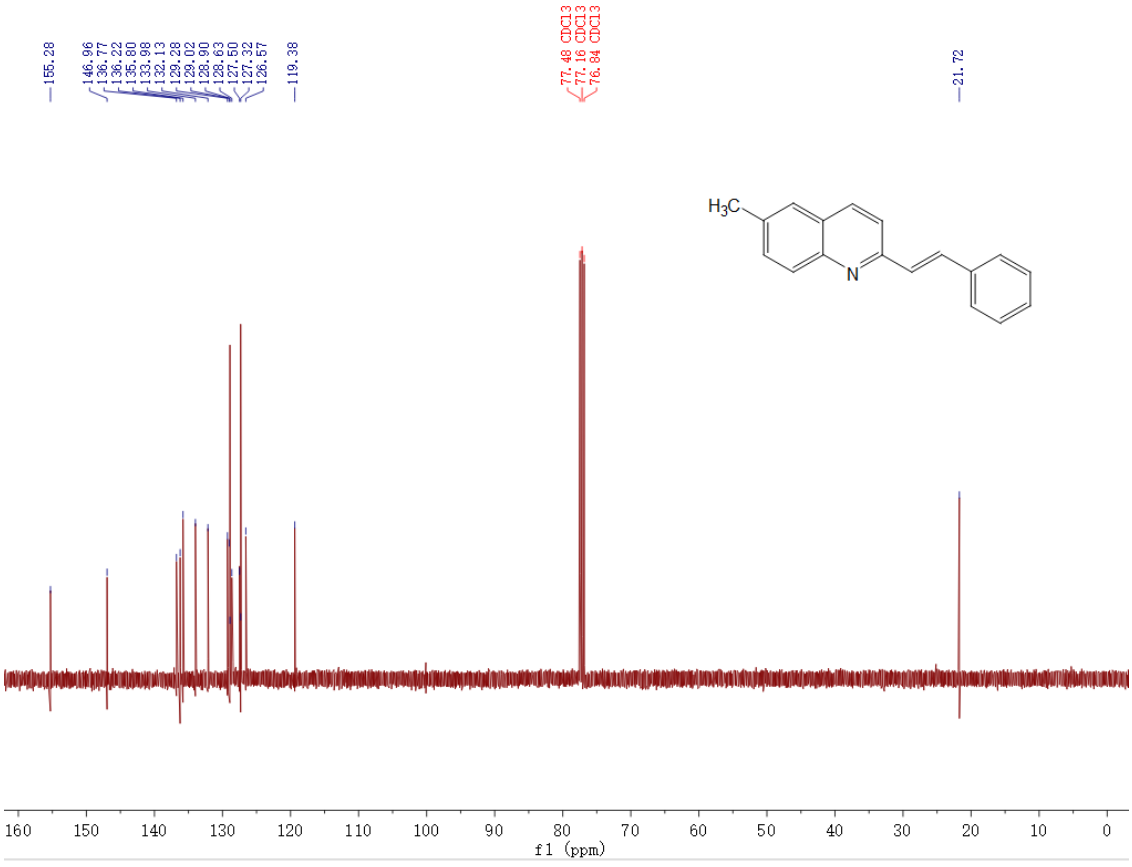

**(E)-2-(2-([1,1'-Biphenyl]-4-yl)vinyl)quinoline (3af), $^{13}$C NMR (101 MHz, $CDCl_3$)**



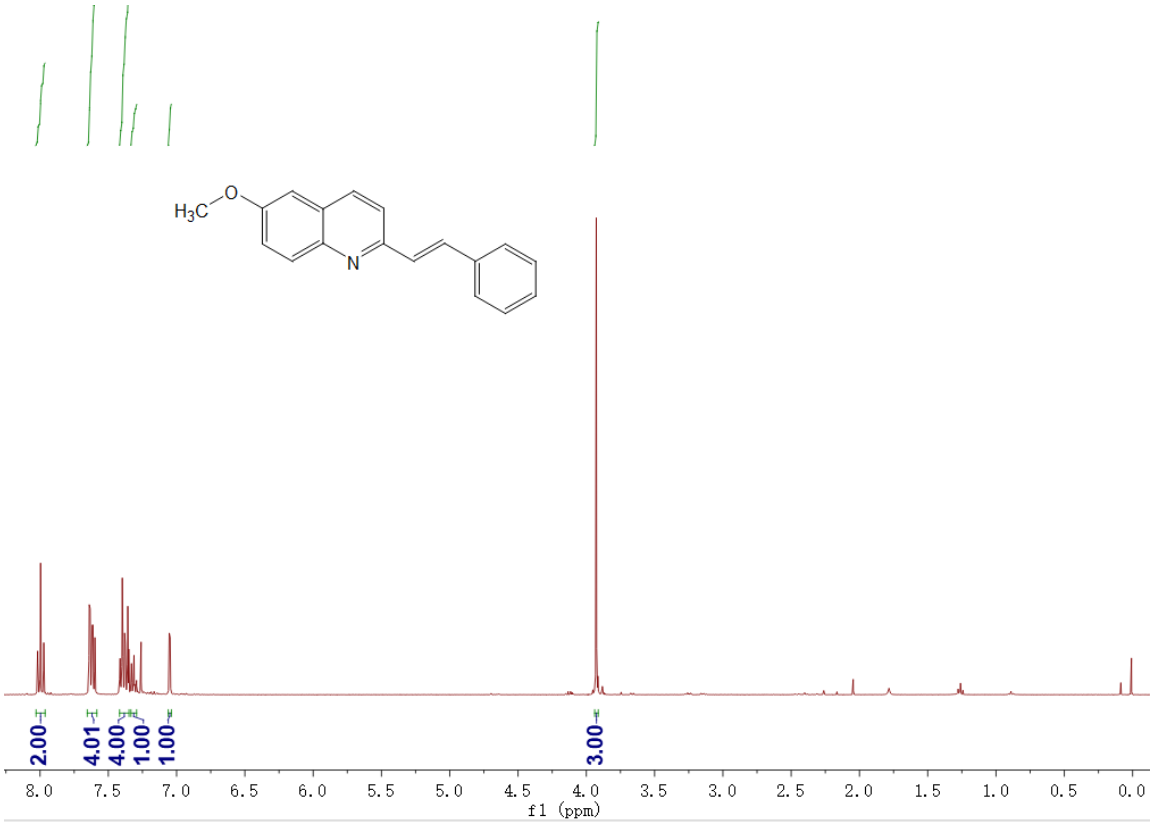
**(E)-6-Methyl-2-styrylquinoline (3ba), $^{1}$H NMR (400 MHz, $CDCl_3$)**



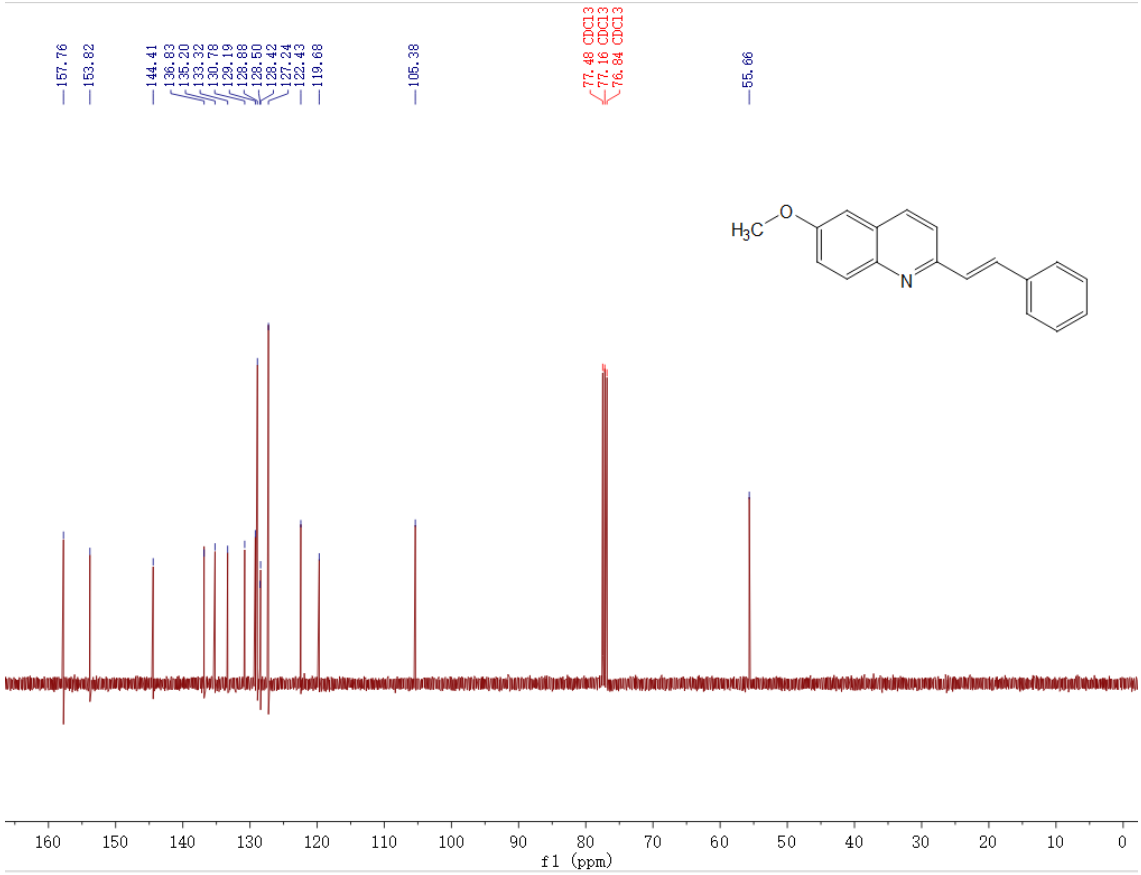

**(E)-6-Methyl-2-styrylquinoline (3ba), $^{13}$C NMR (101 MHz, 400 MHz, $CDCl_3$)**



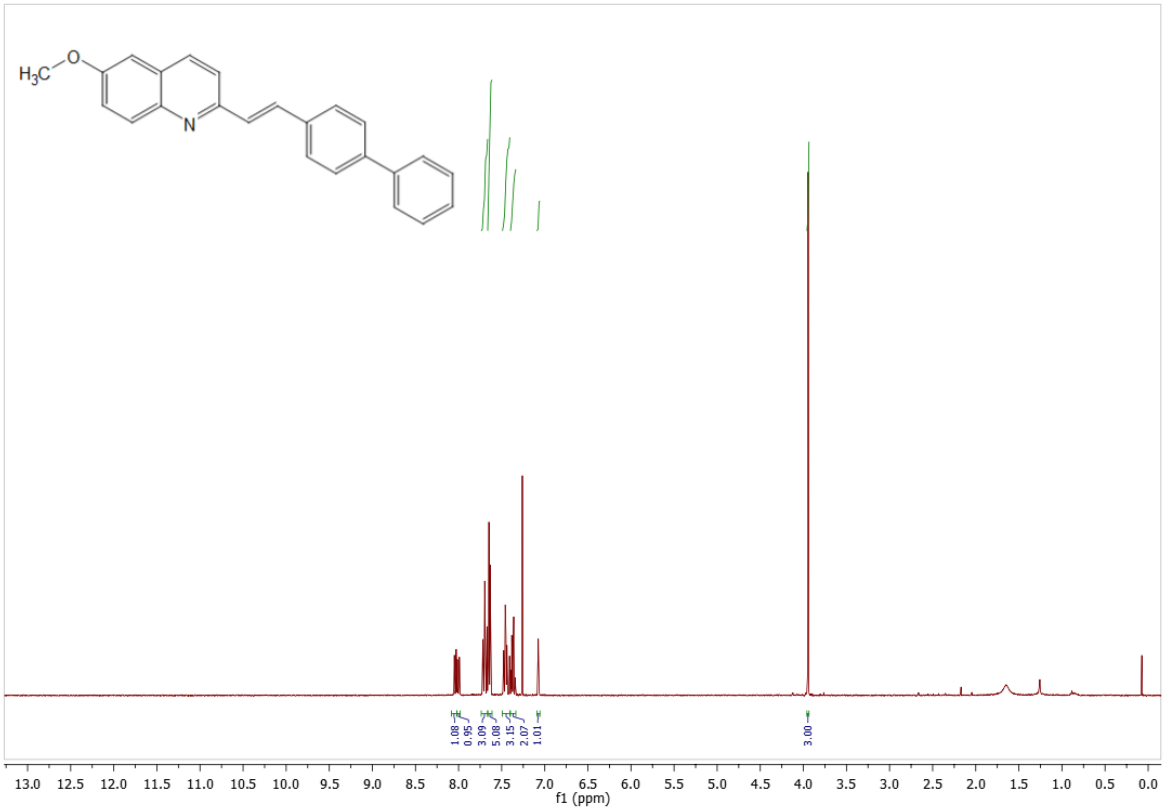
**(E)-6-Methoxy-2-styrylquinoline (3ca), $^{1}$H NMR (400 MHz, $CDCl_3$)**



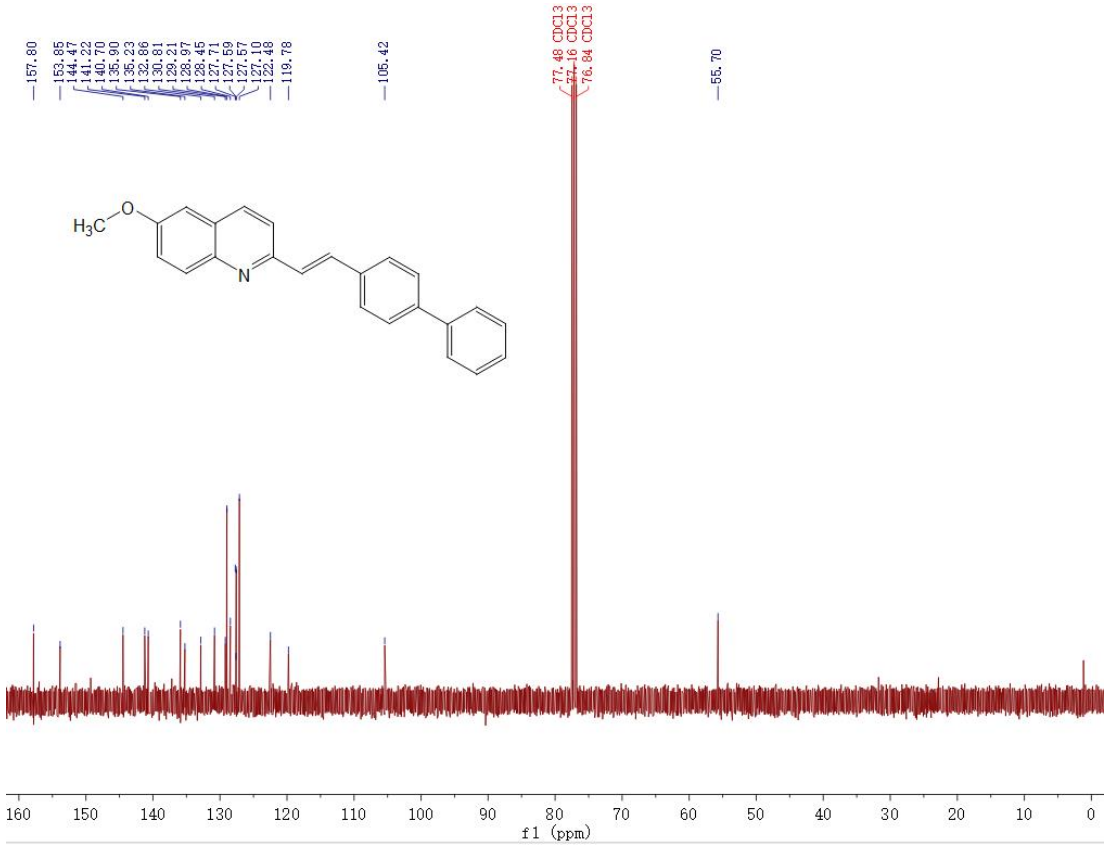

**(E)-6-Methoxy-2-styrylquinoline (3ca), $^{13}$C NMR (101 MHz, $CDCl_3$)**



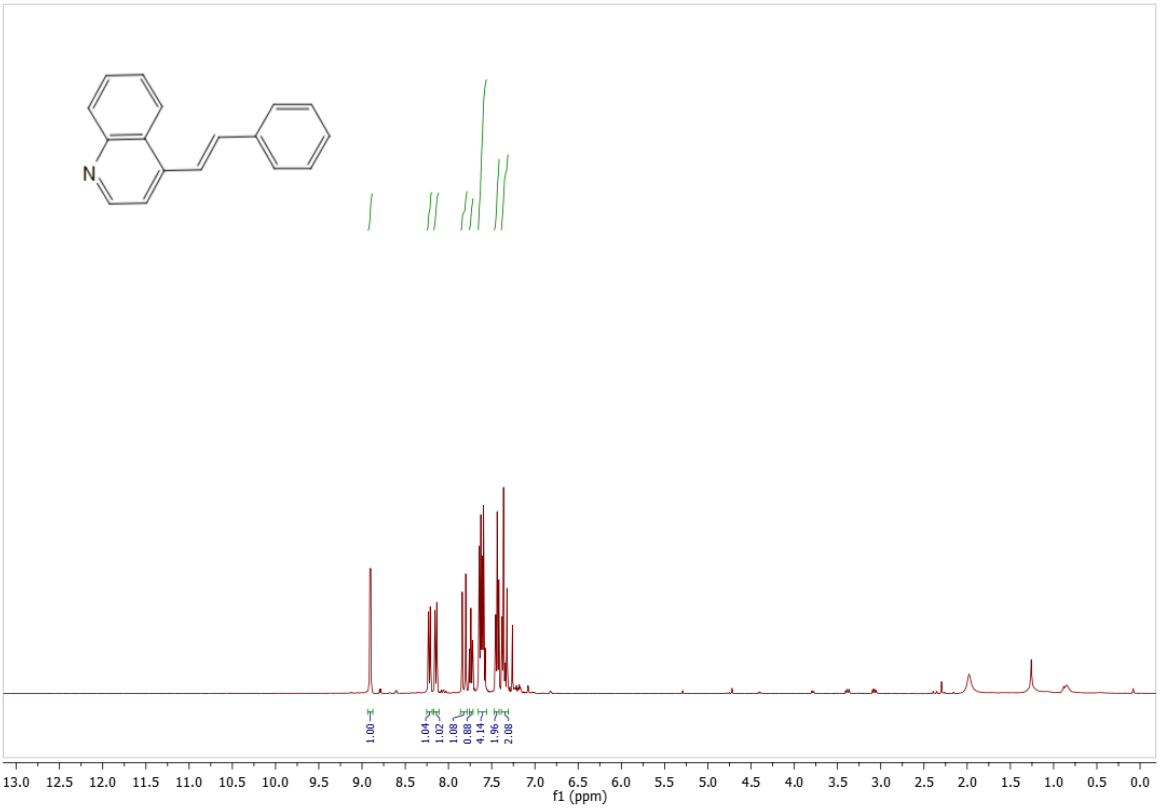
**(E)-2-(2-([1,1'-Biphenyl]-4-yl)vinyl)-6-methoxyquinoline (3cf), $^{1}$H NMR (400 MHz, $CDCl_3$)**



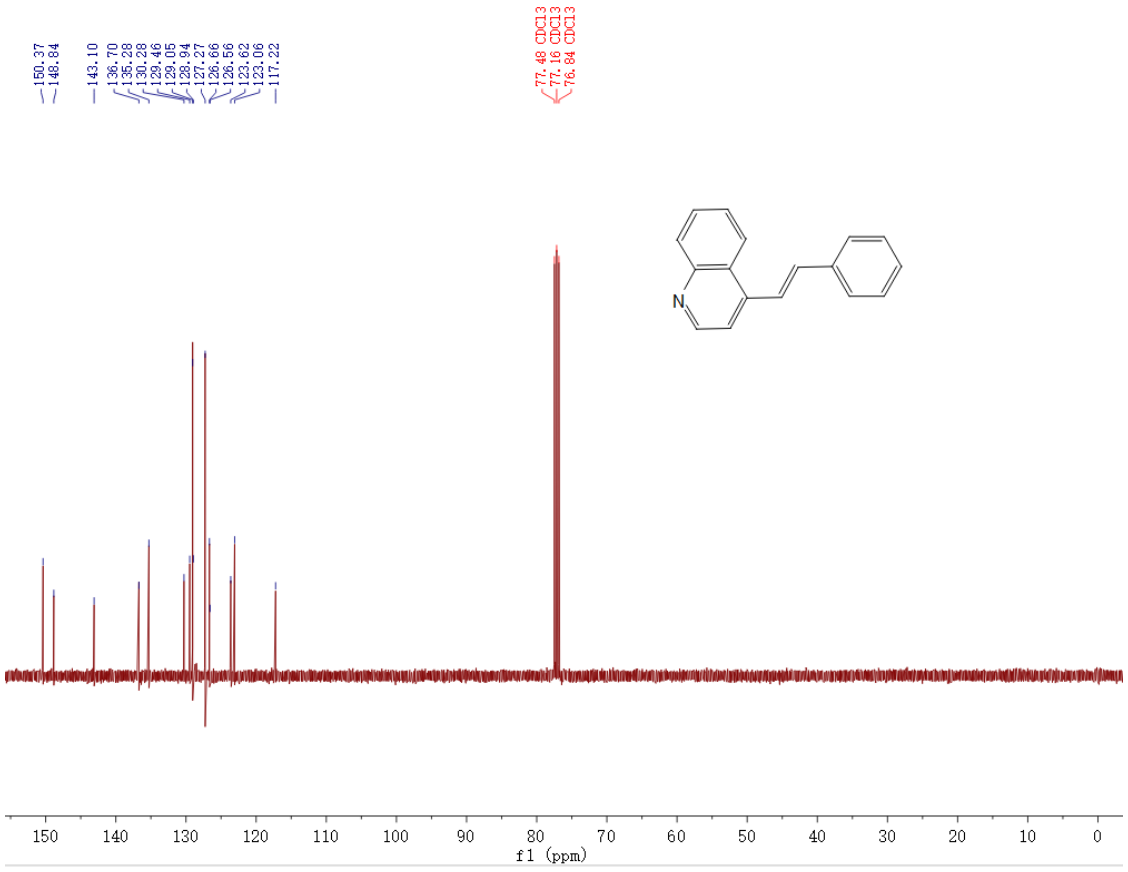

**(E)-2-(2-([1,1'-Biphenyl]-4-yl)vinyl)-6-methoxyquinoline (3cf), $^{13}$C NMR (101 MHz, $CDCl_3$)**



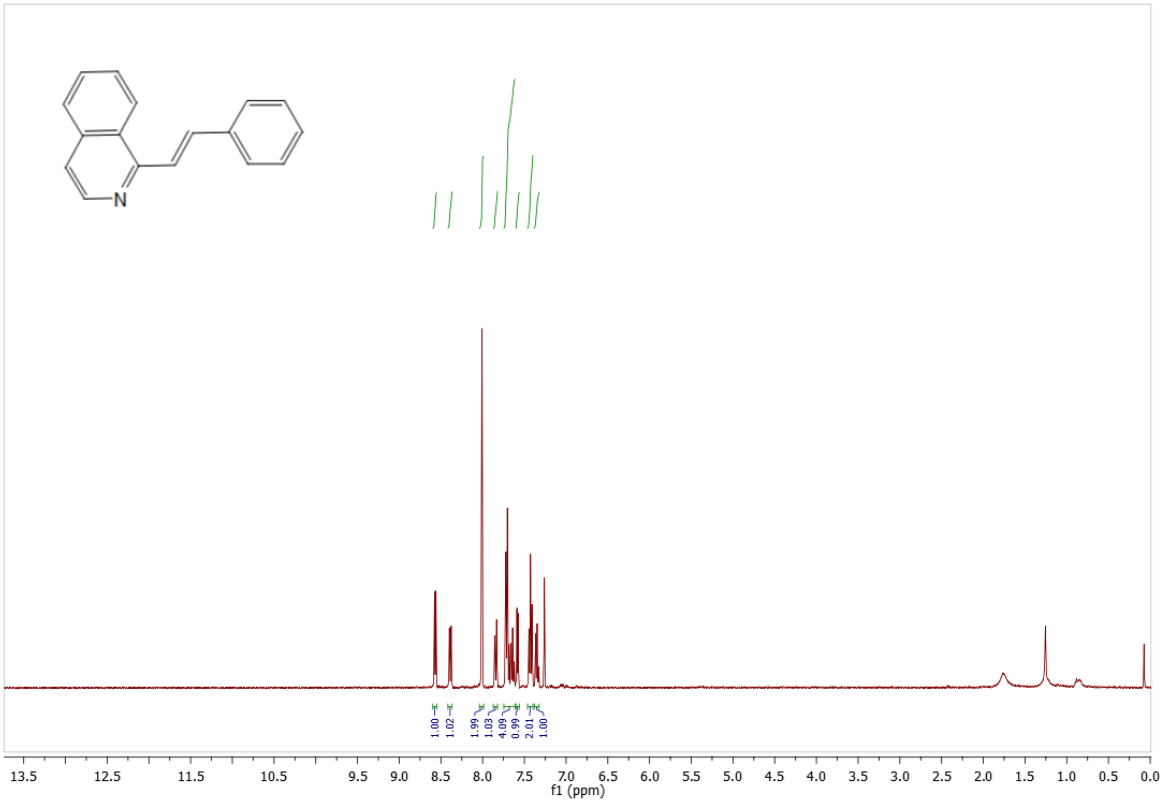
**(E)-4-Styrylquinoline (3da), $^{1}$H NMR (400 MHz, $CDCl_3$)**



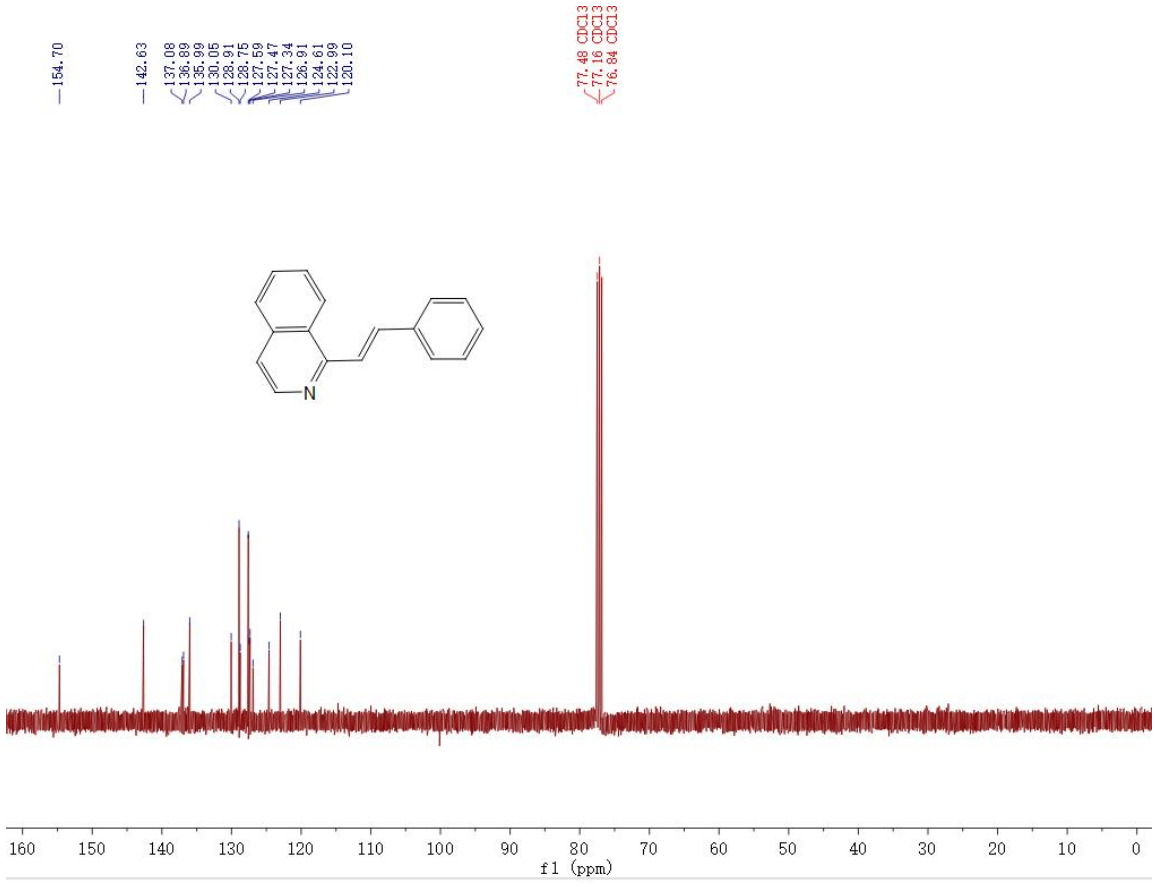

**(E)-4-Styrylquinoline (3da), $^{13}$C NMR (101 MHz, $CDCl_3$)**



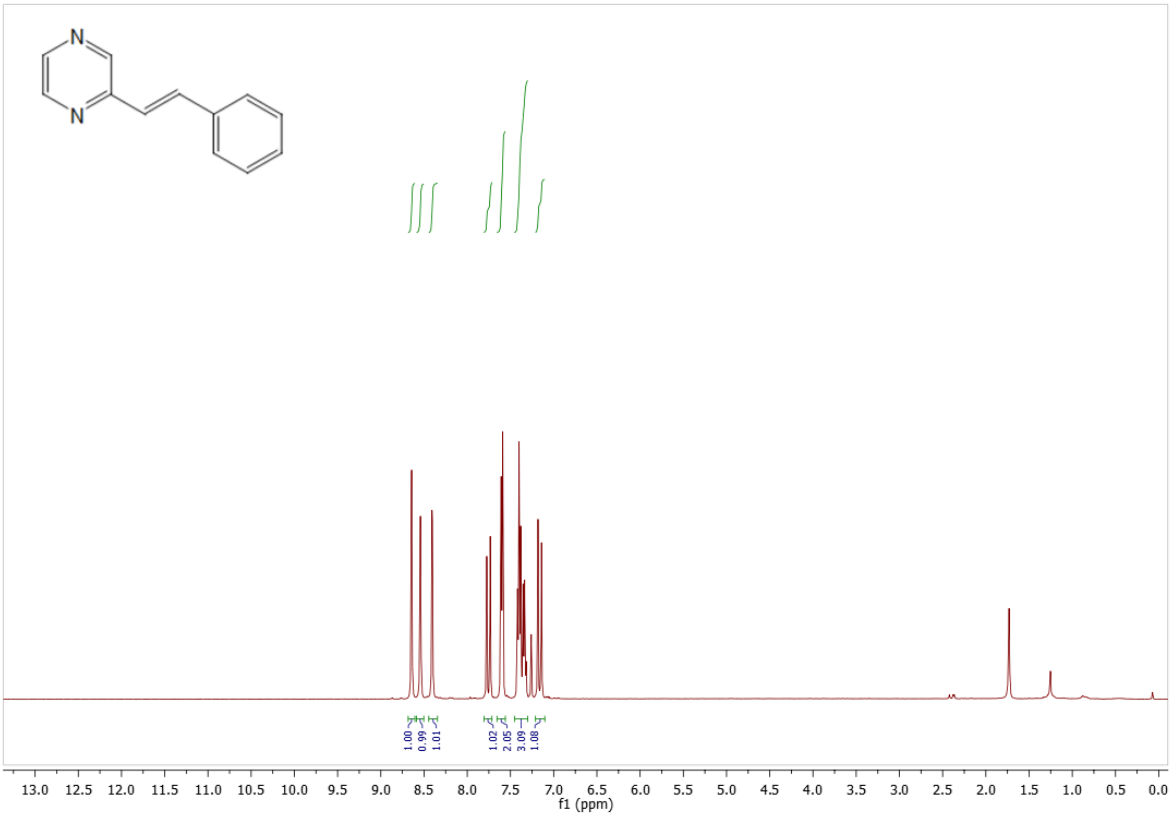
**(E)-1-Styrylisoquinoline (3ea), $^{1}$H NMR (400 MHz, $CDCl_3$)**



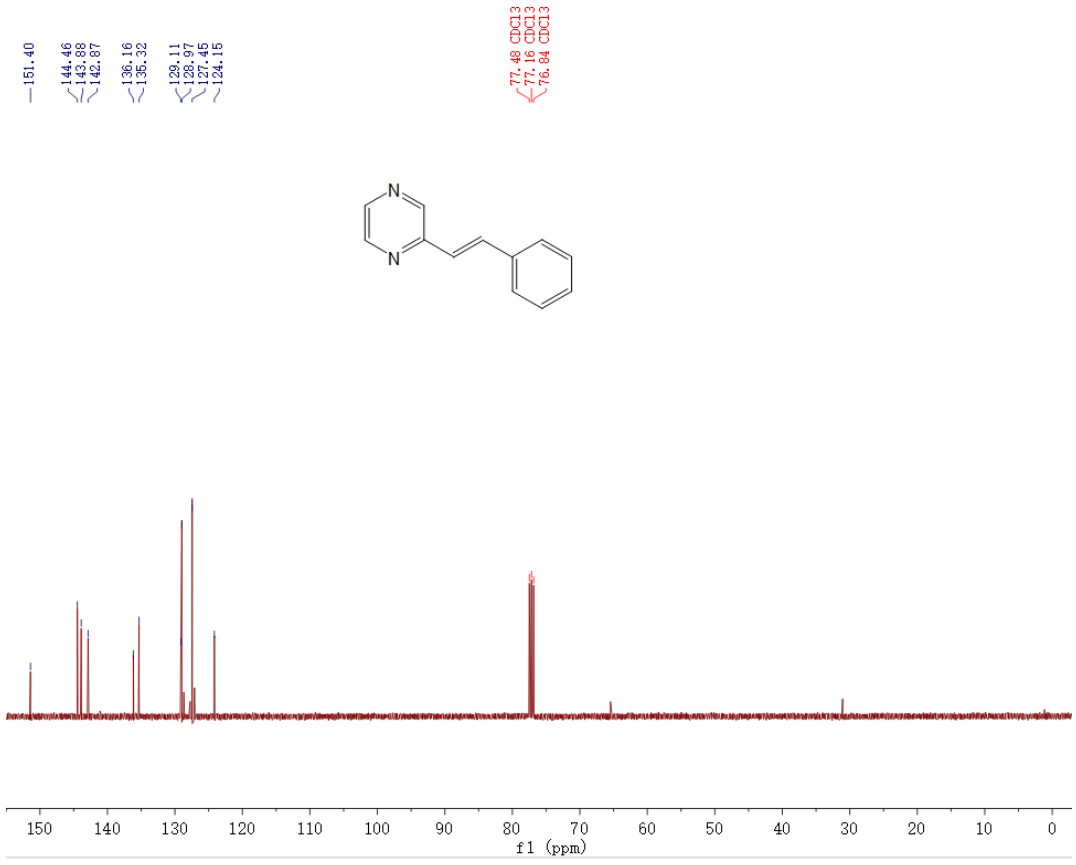

**(E)-1-Styrylisoquinoline (3ea), $^{13}$C NMR (101 MHz, $CDCl_3$)**



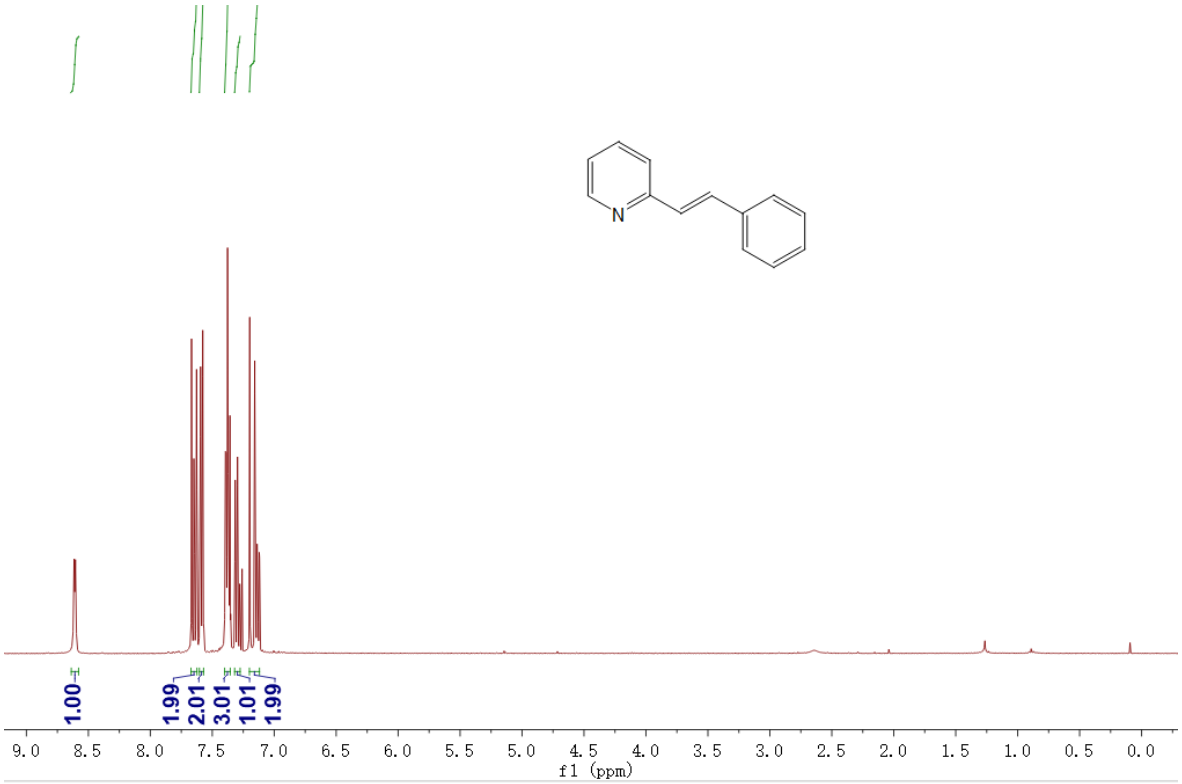
**(E)-2-Styrylpyrazine (3fa), $^{1}$H NMR (400 MHz, $CDCl_3$)**



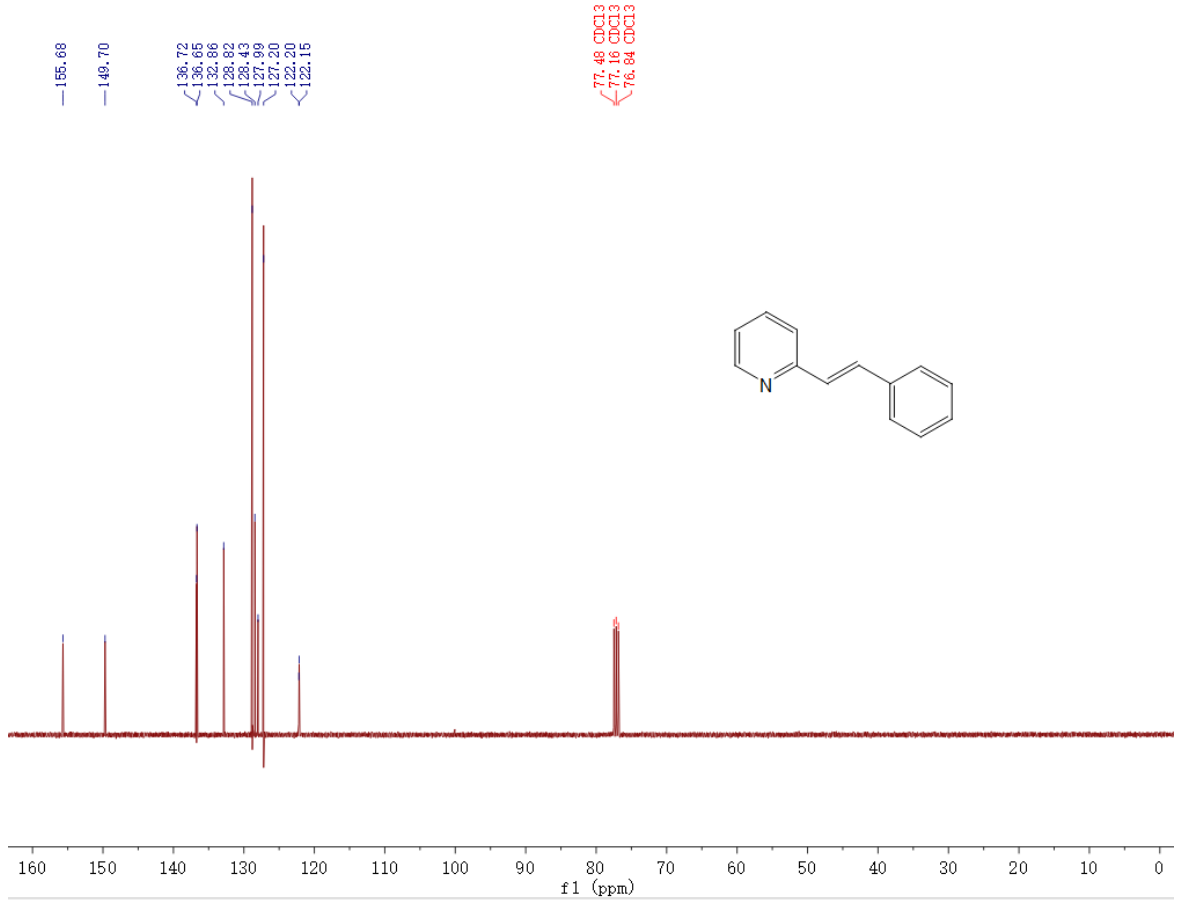

**(E)-2-Styrylpyrazine (3fa), $^{13}$C NMR (101 MHz, $CDCl_3$)**



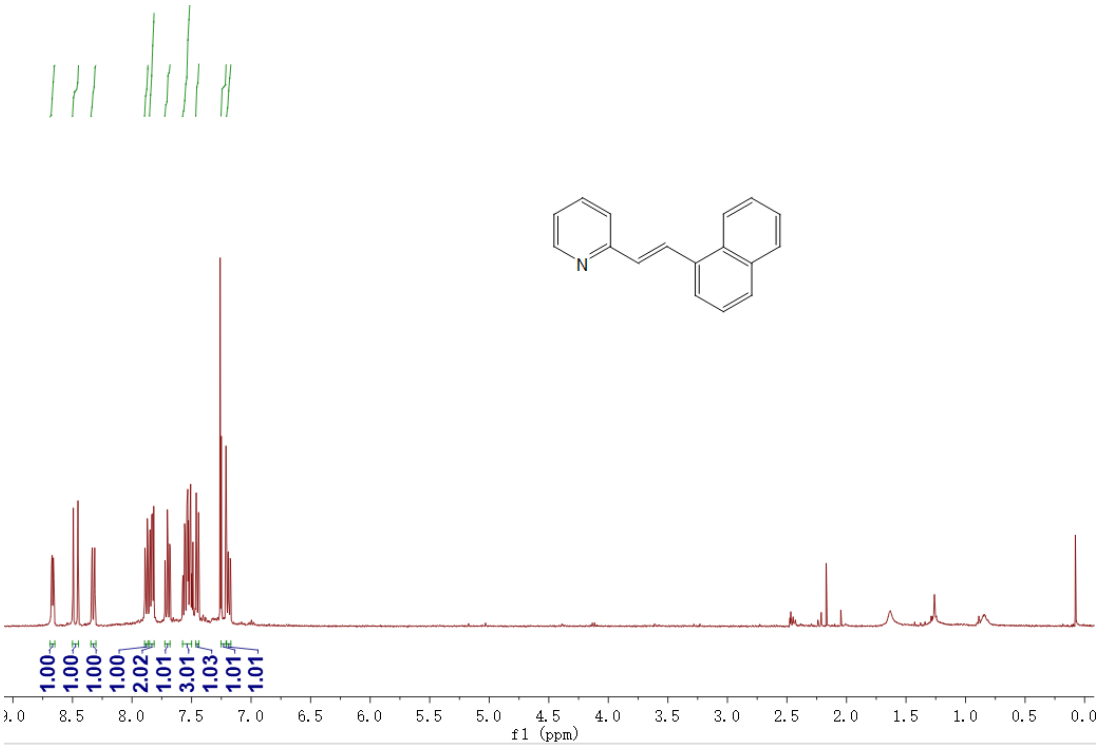
**4(E)-2-Styrylpyridine (3ga), $^{1}$H NMR (400 MHz, $CDCl_3$)**



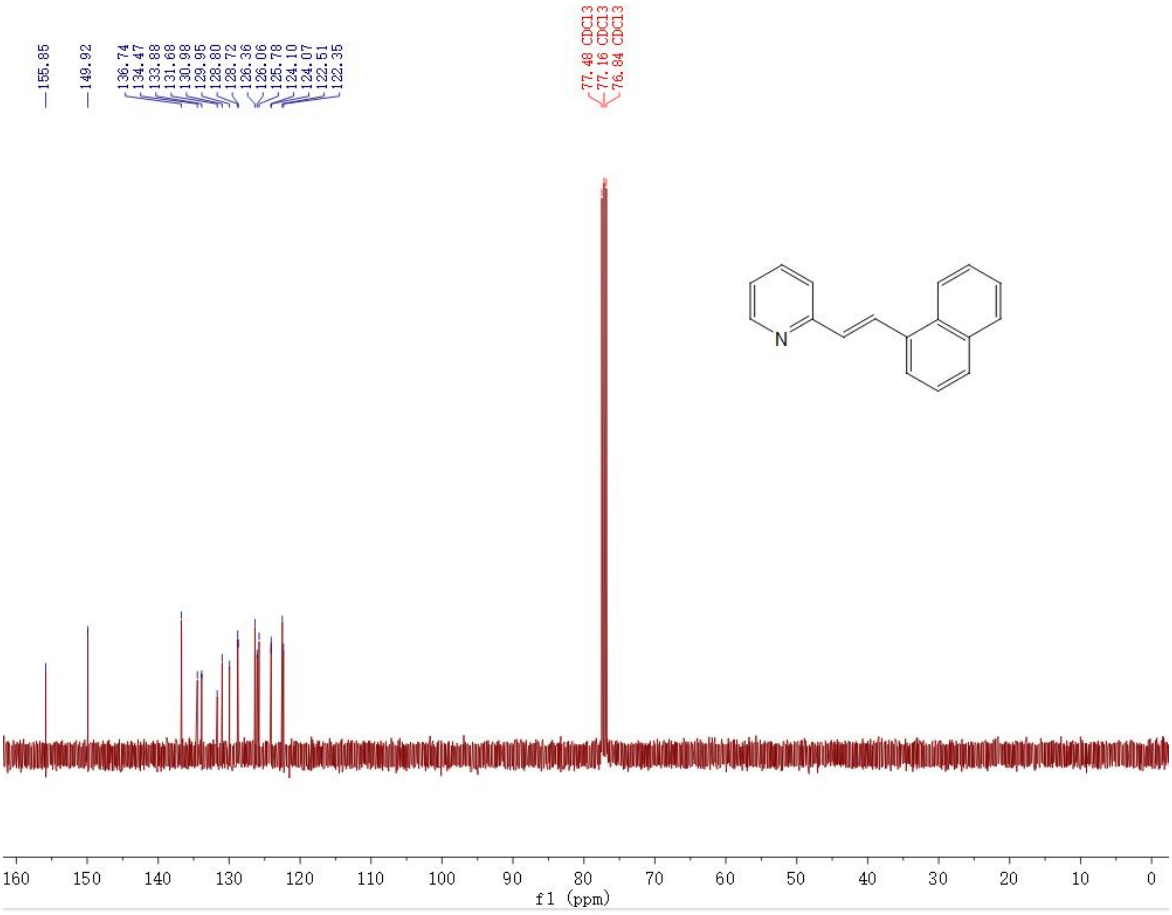

**(E)-2-Styrylpyridine (3ga), $^{13}$C NMR (101 MHz, $CDCl_3$)**



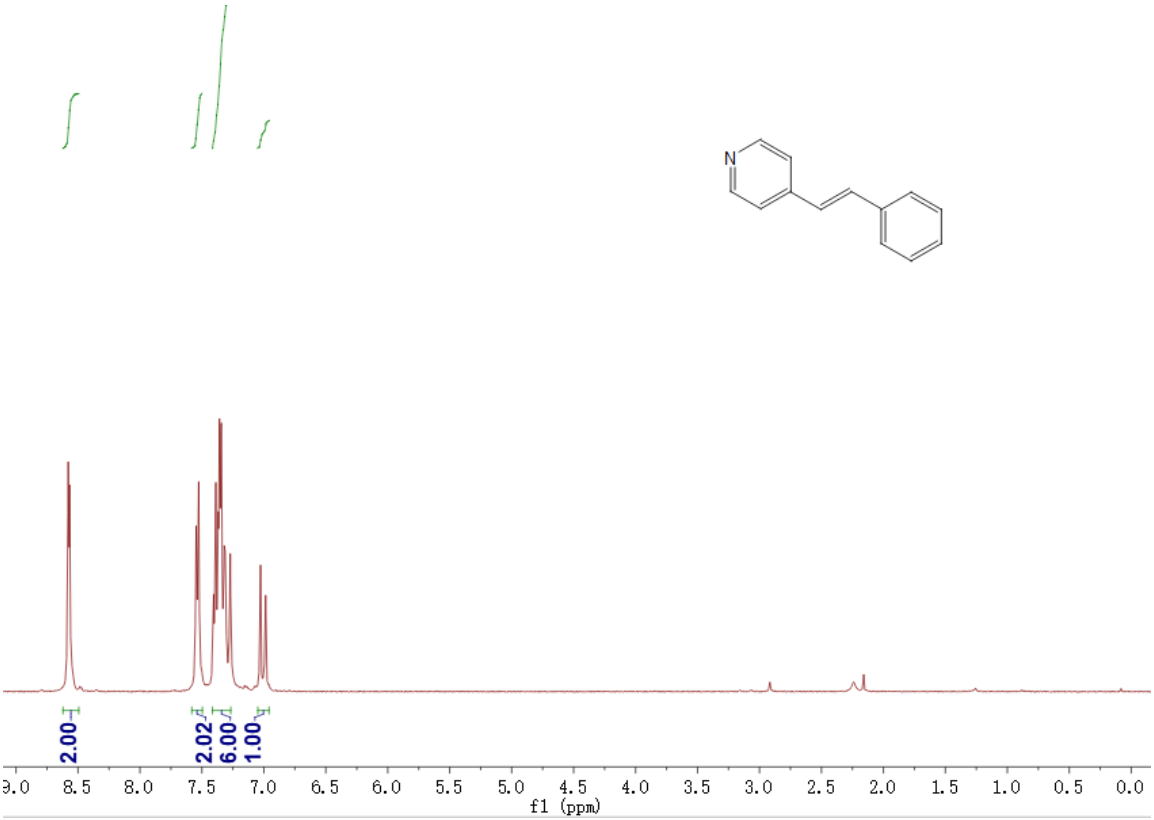
**(E)-2-(2-(Naphthalen-1-yl)vinyl)pyridine (3gg), $^{1}$H NMR (400 MHz, $CDCl_3$)**



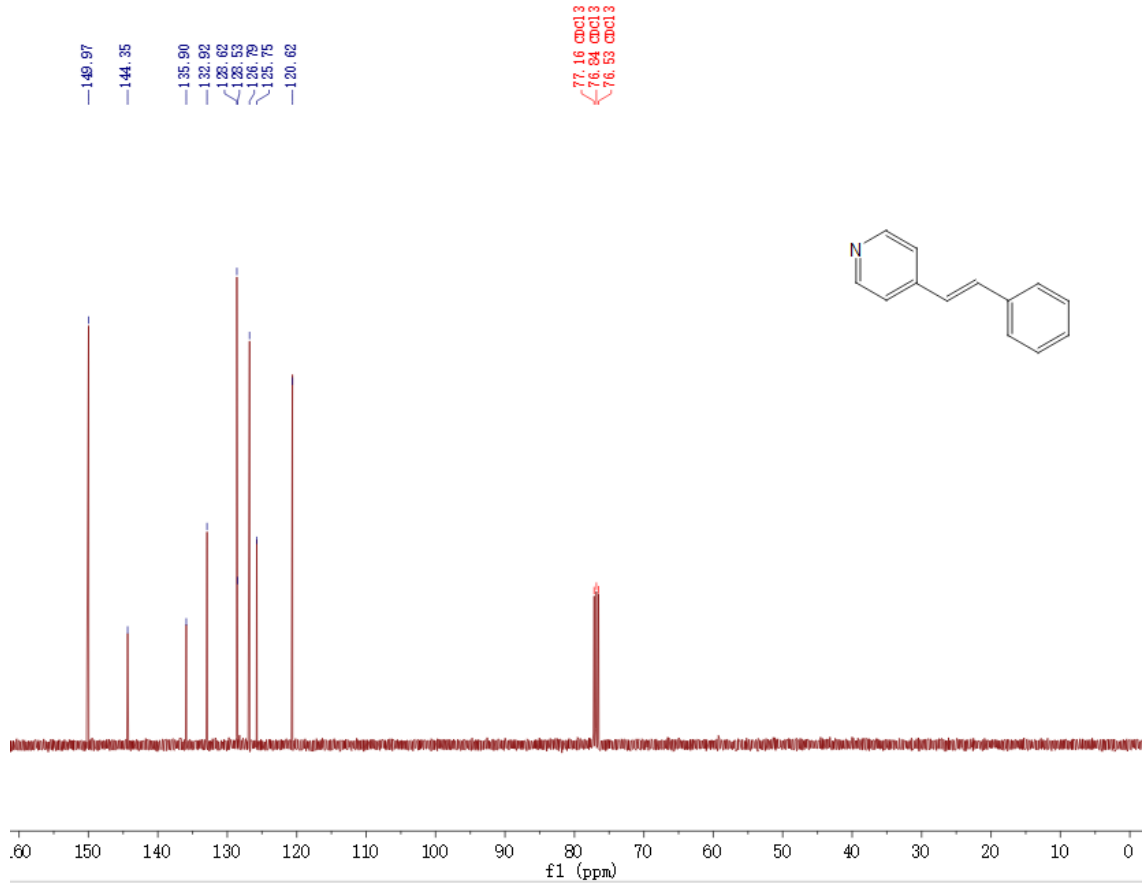

**(E)-2-(2-(Naphthalen-1-yl)vinyl)pyridine (3gg), $^{13}$C NMR (101 MHz, $CDCl_3$)**



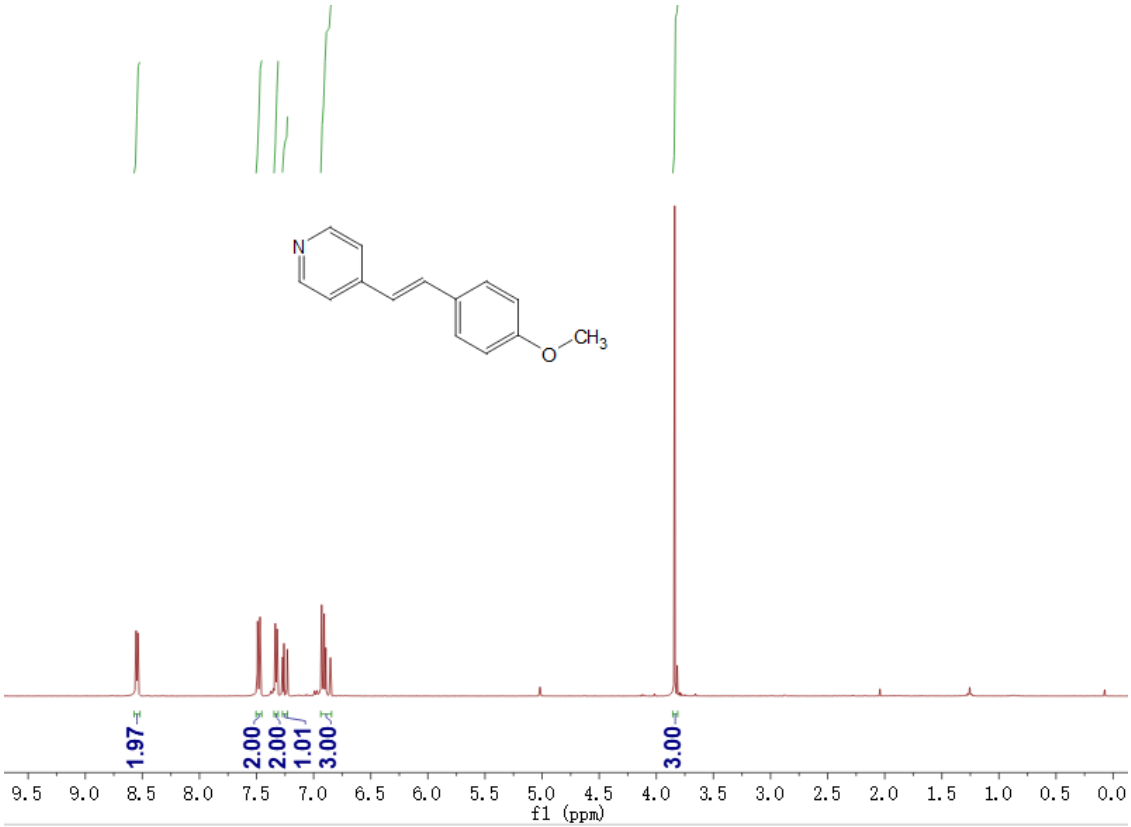
**(E)-4-Styrylpyridine (3ha), $^{1}$H NMR (400 MHz, $CDCl_3$)**



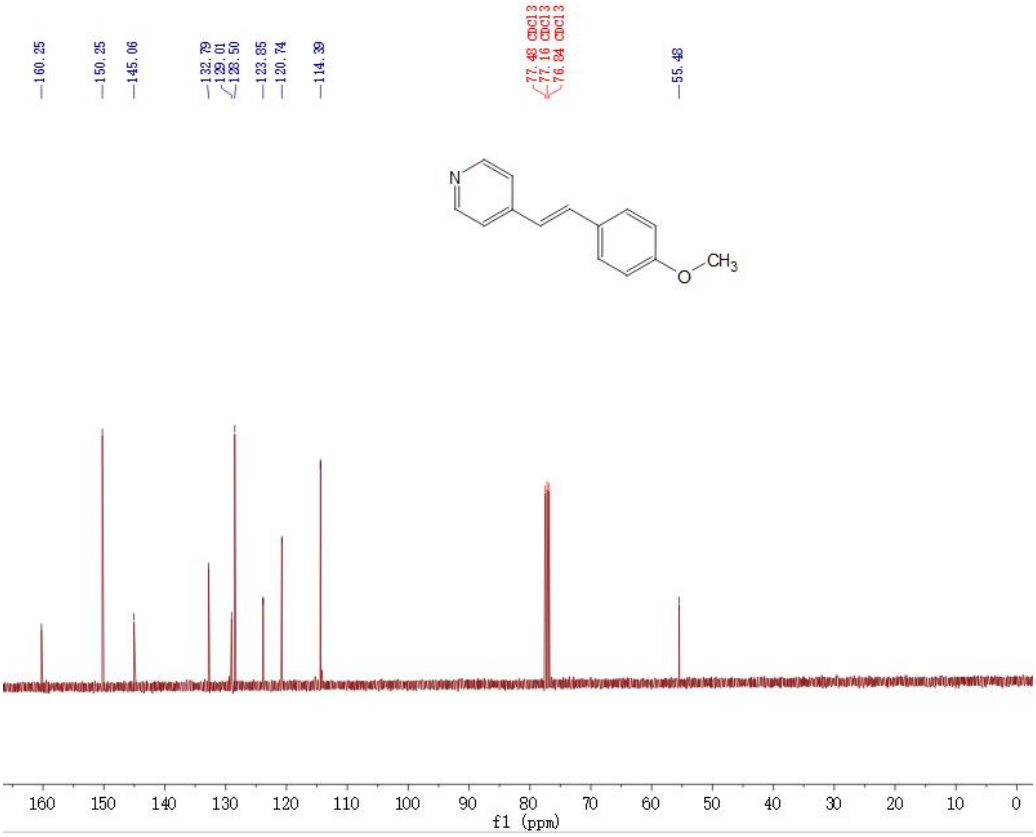

**(E)-4-Styrylpyridine (3ha), $^{13}$C NMR (101 MHz, $CDCl_3$)**



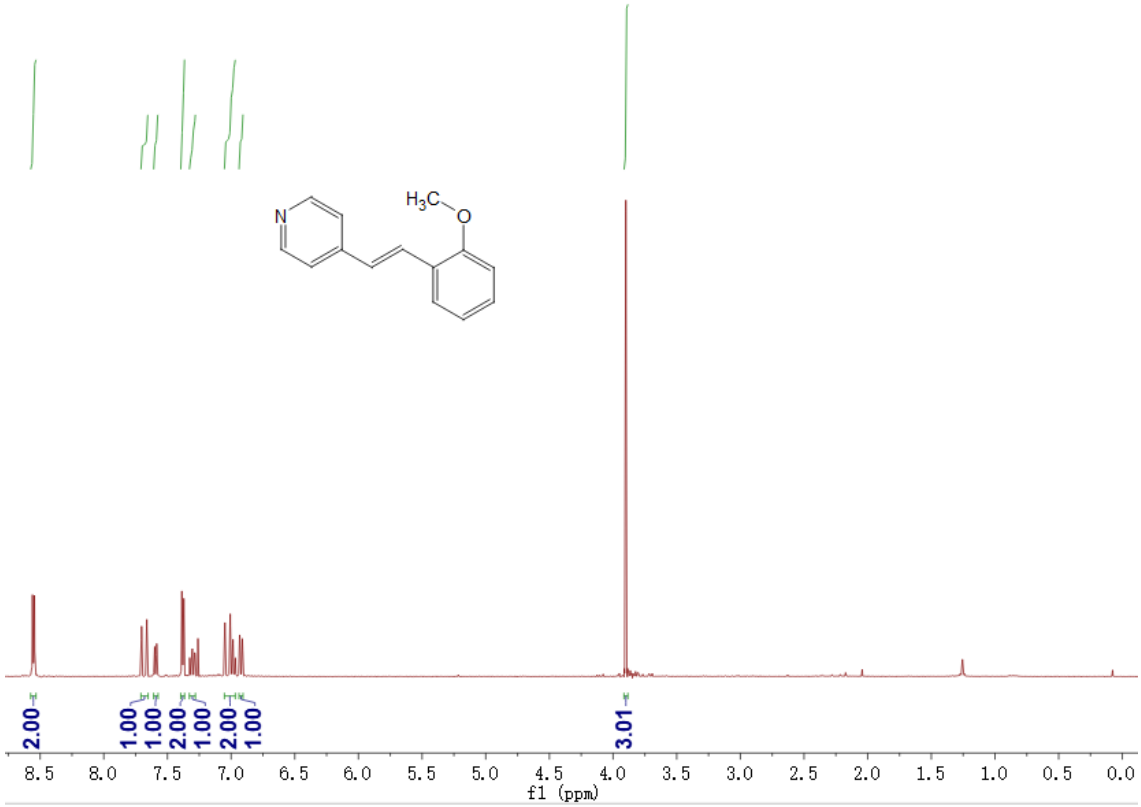
**(E)-4-(4-Methoxystyryl)pyridine (3hh), $^{1}$H NMR (400 MHz, $CDCl_3$)**



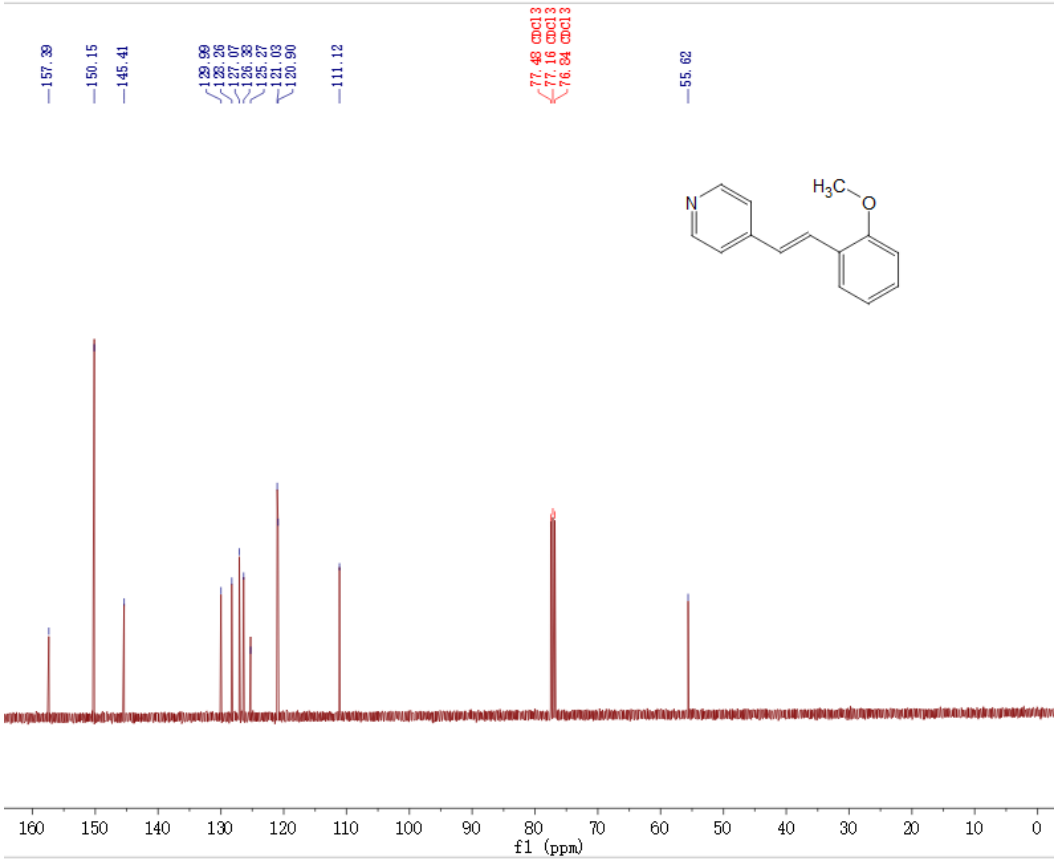

**(E)-4-(4-Methoxystyryl)pyridine (3hh), $^{13}$C NMR (101 MHz, $CDCl_3$)**



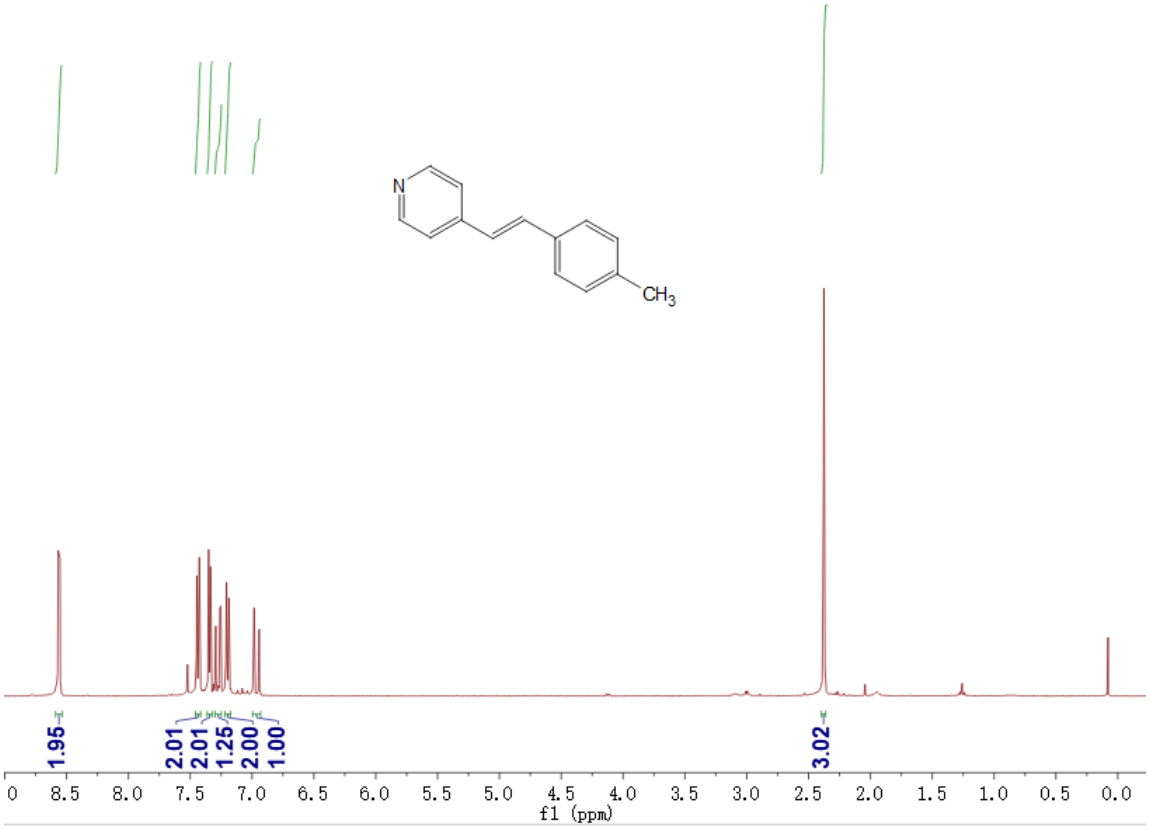
**(E)-4-(2-Methoxystyryl)pyridine (3hi), $^{1}$H NMR (400 MHz, $CDCl_3$)**



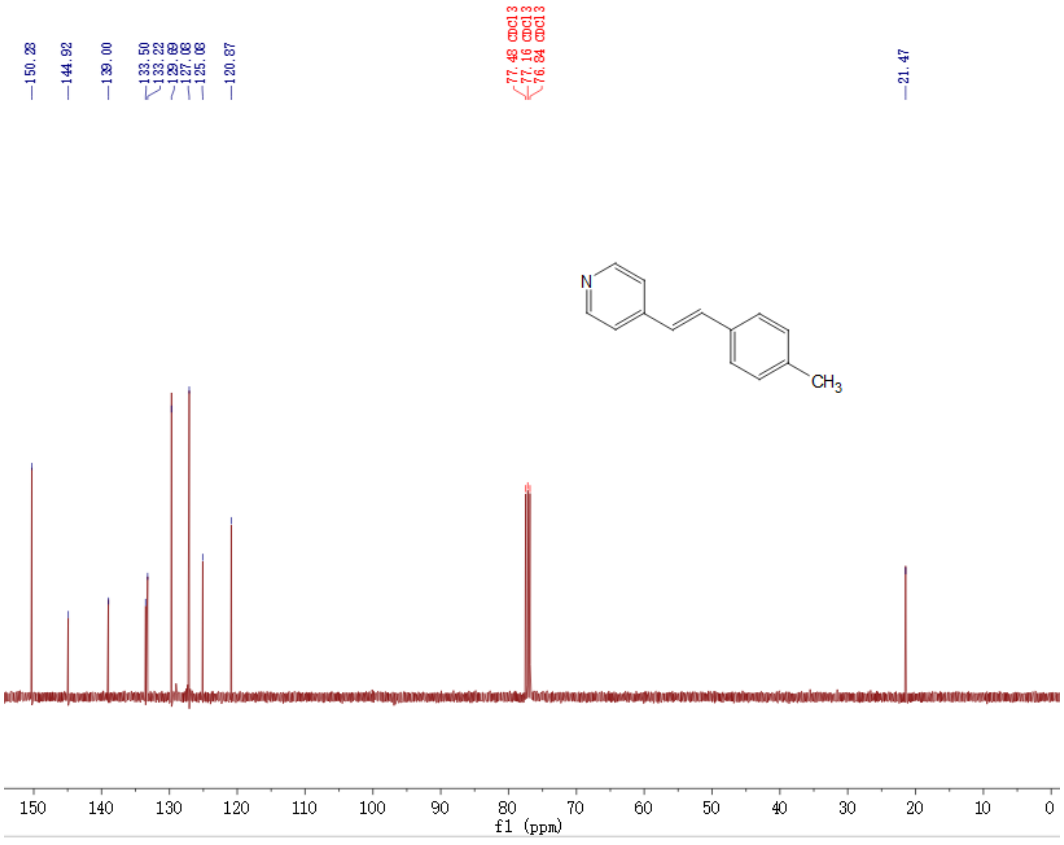

**(E)-4-(2-Methoxystyryl)pyridine (3hi), $^{13}$C NMR (101 MHz, $CDCl_3$)**



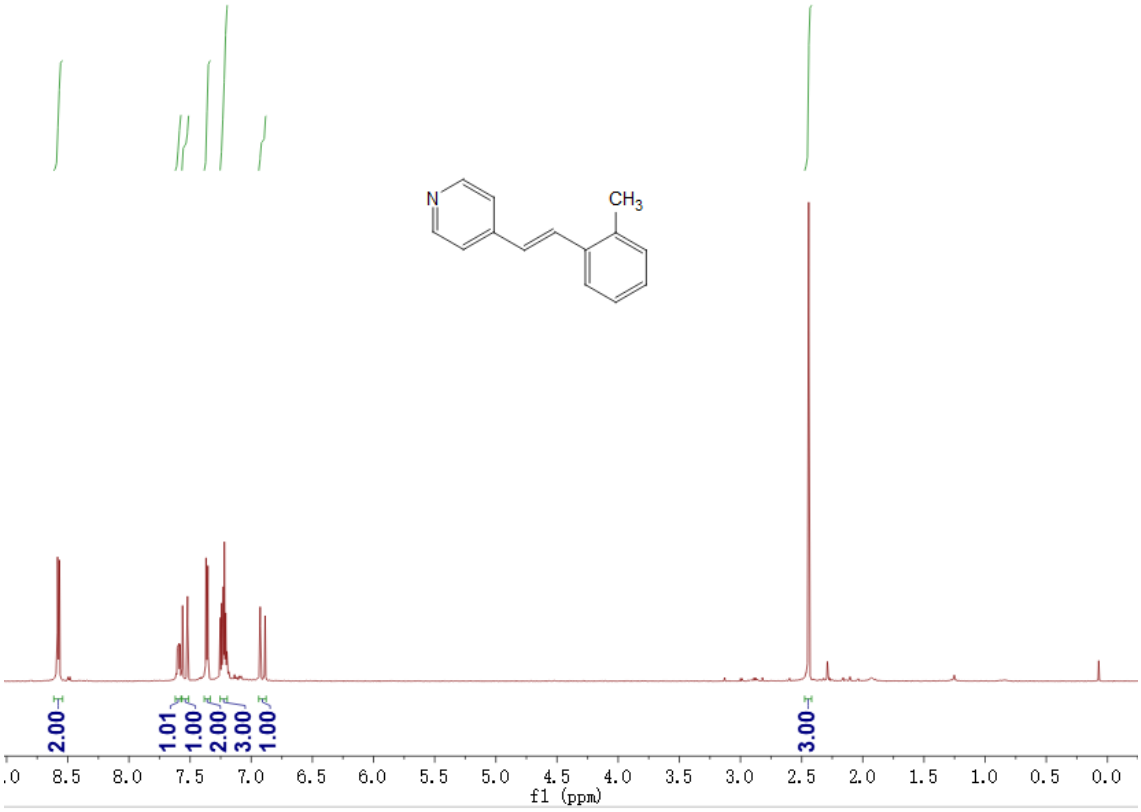
**(E)-4-(4-Methylstyryl)pyridine (3hc), $^{1}$H NMR (400 MHz, $CDCl_3$)**



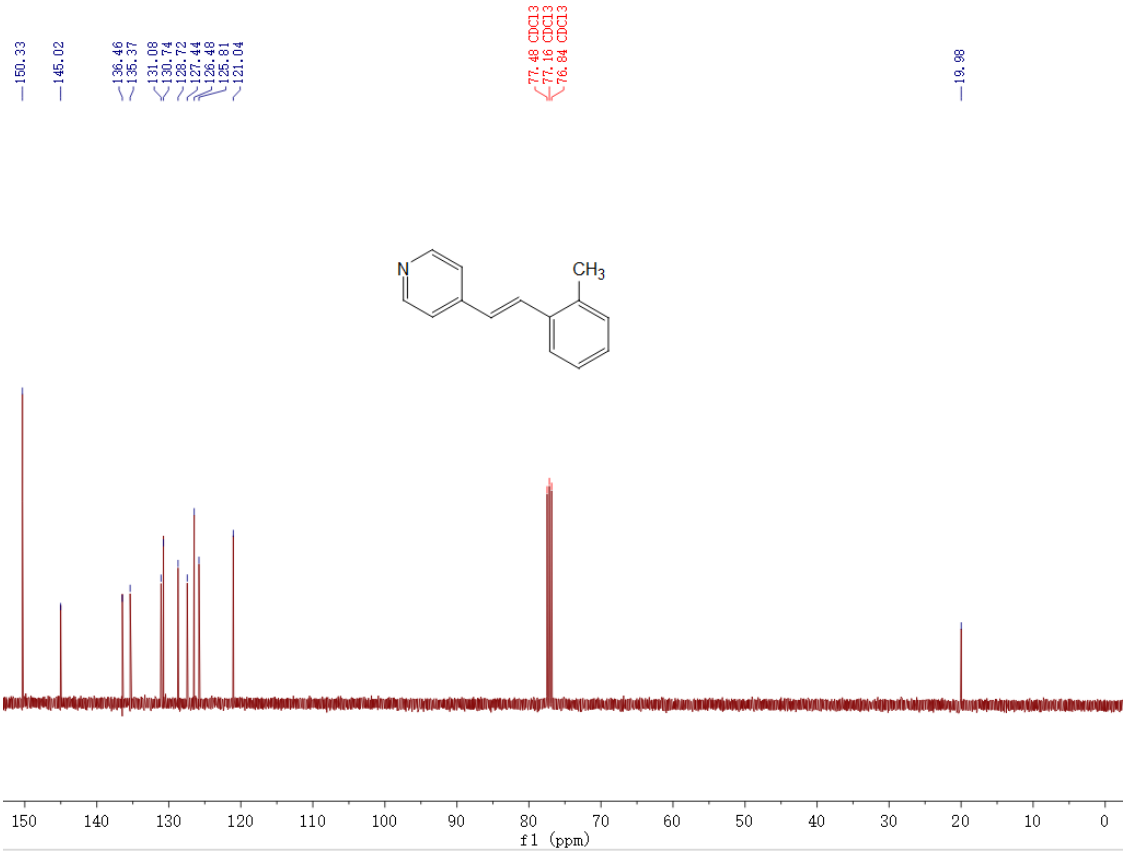

**(E)-4-(4-Methylstyryl)pyridine (3hc), $^{13}$C NMR (101 MHz, $CDCl_3$)**



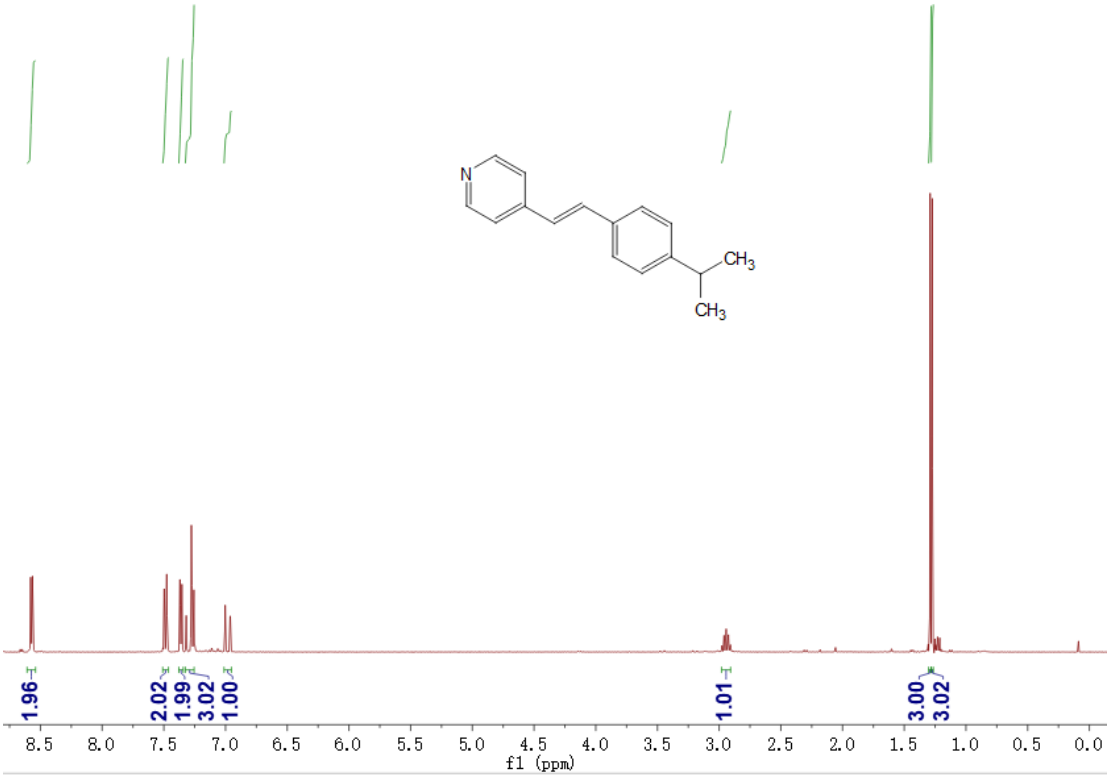
**(E)-4-(2-Methylstyryl)pyridine (3hb), $^{1}$H NMR (400 MHz, $CDCl_3$)**



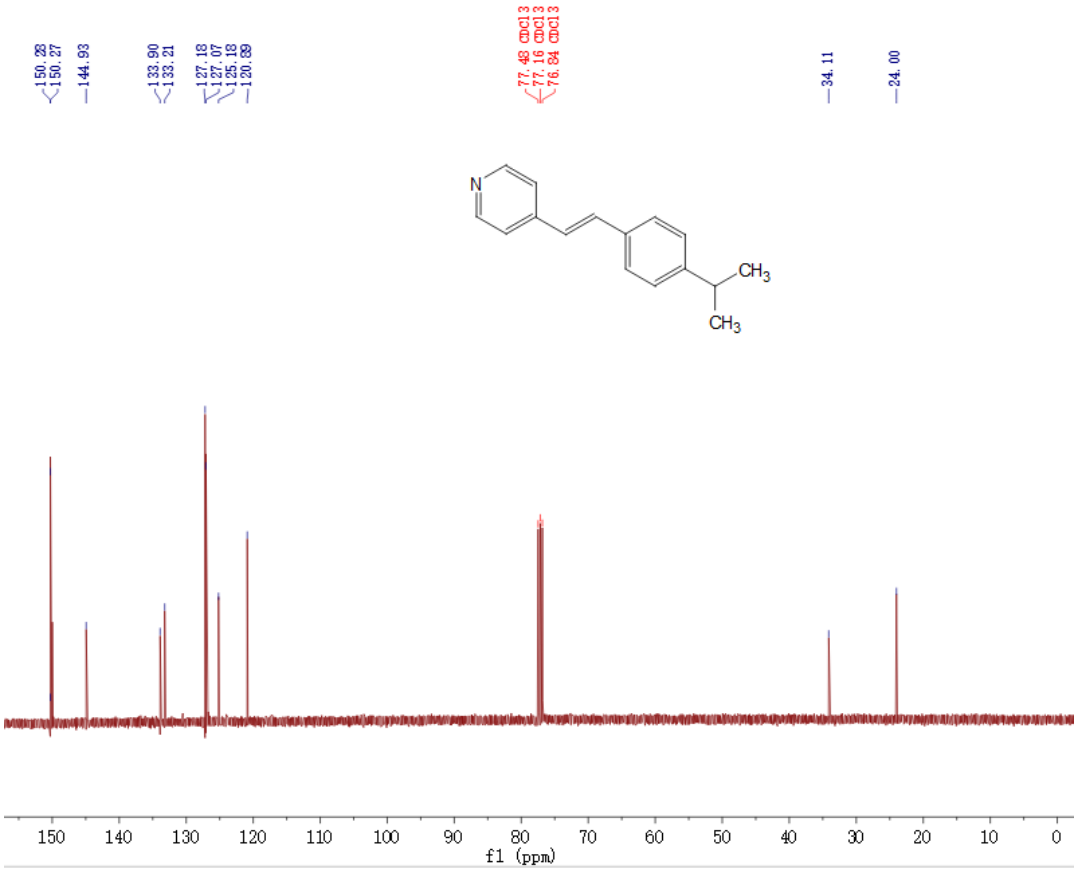

**(E)-4-(2-Methylstyryl)pyridine (3hb), $^{13}$C NMR (101 MHz, $CDCl_3$)**



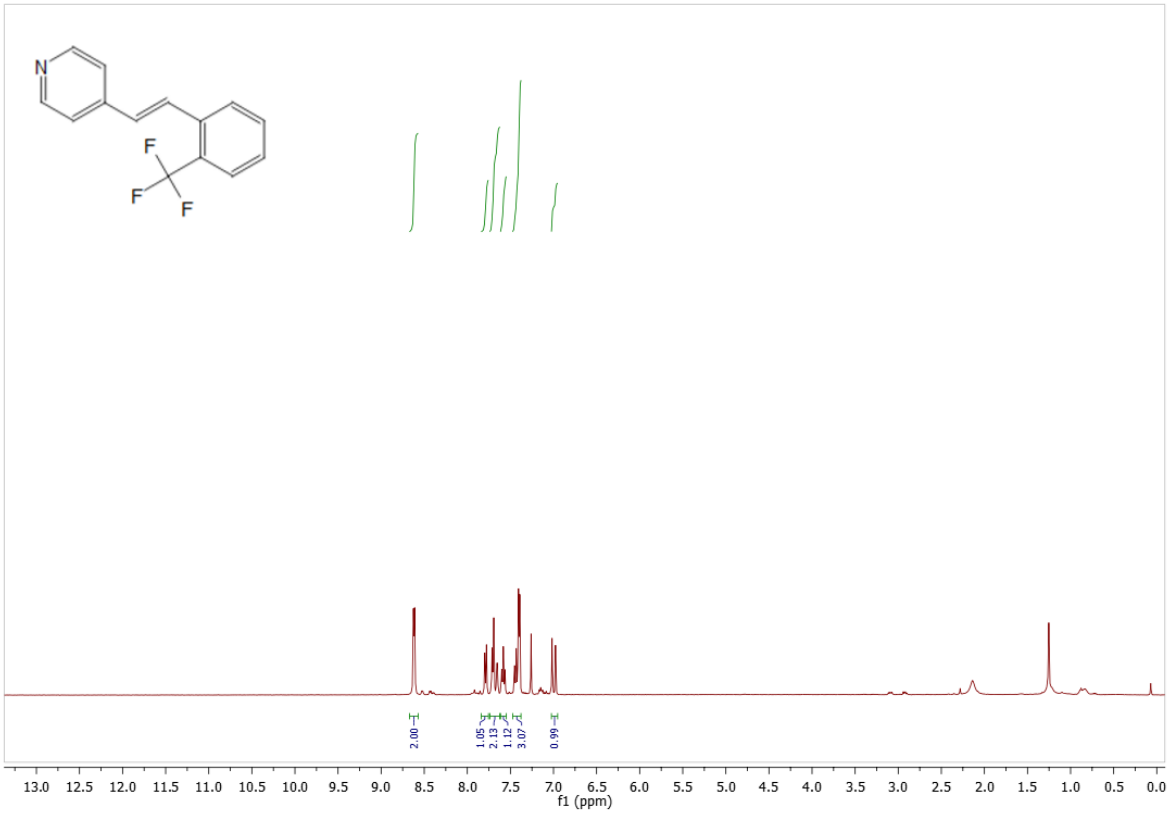
**(E)-4-(4-Isopropylstyryl)pyridine (3he), $^{1}$H NMR (400 MHz, $CDCl_3$)**



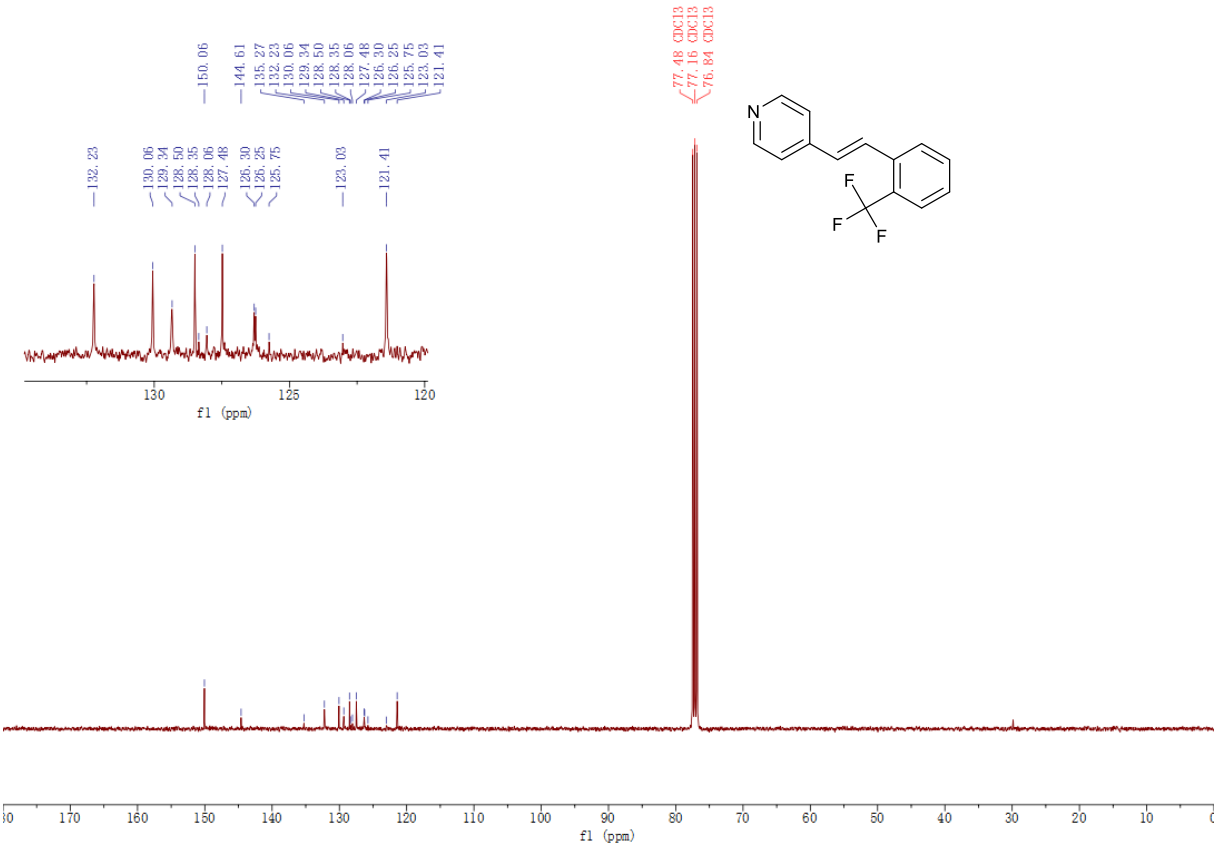

**(E)-4-(4-Isopropylstyryl)pyridine (3he), $^{13}$C NMR (101 MHz, $CDCl_3$)**



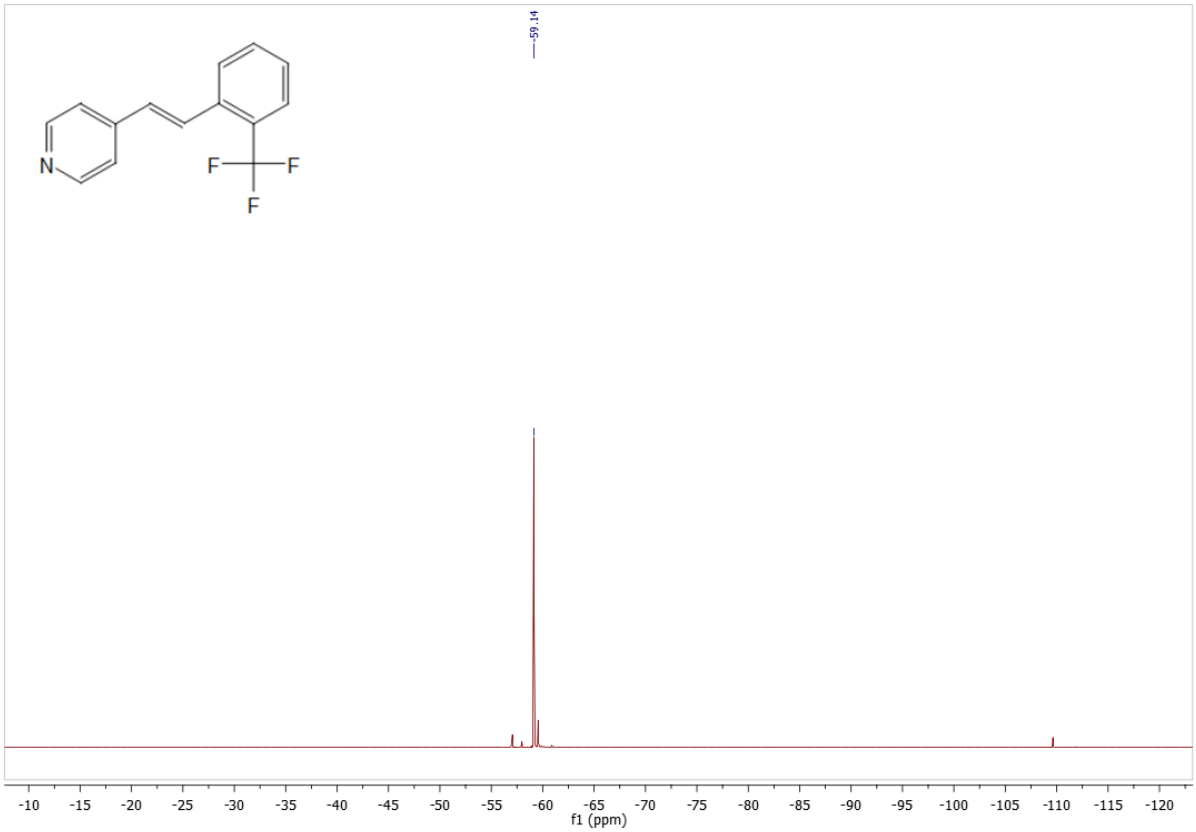
**(E)-4-(2-(Trifluoromethyl)styryl)pyridine (3hj), $^{1}$H NMR (400 MHz, $CDCl_3$)**



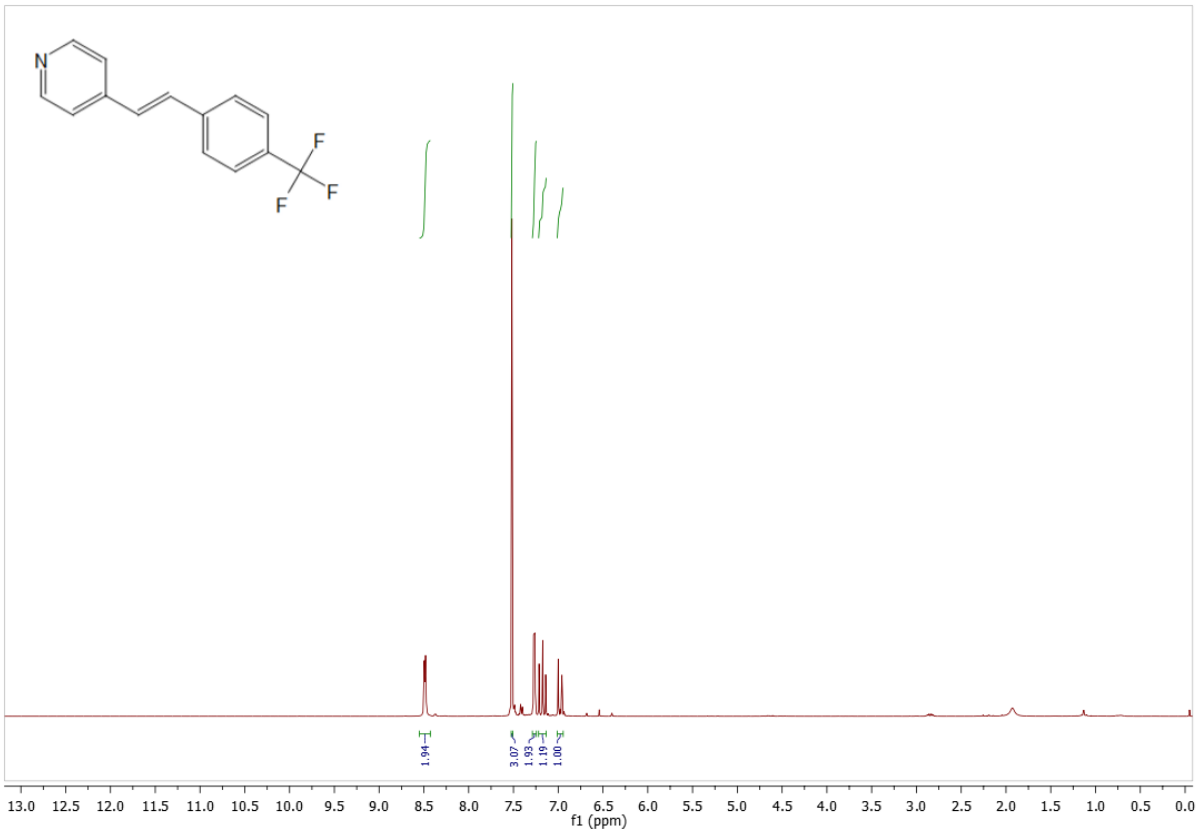

**(E)-4-(2-(Trifluoromethyl)styryl)pyridine (3hj), $^{13}$C NMR (101 MHz, $CDCl_3$)**



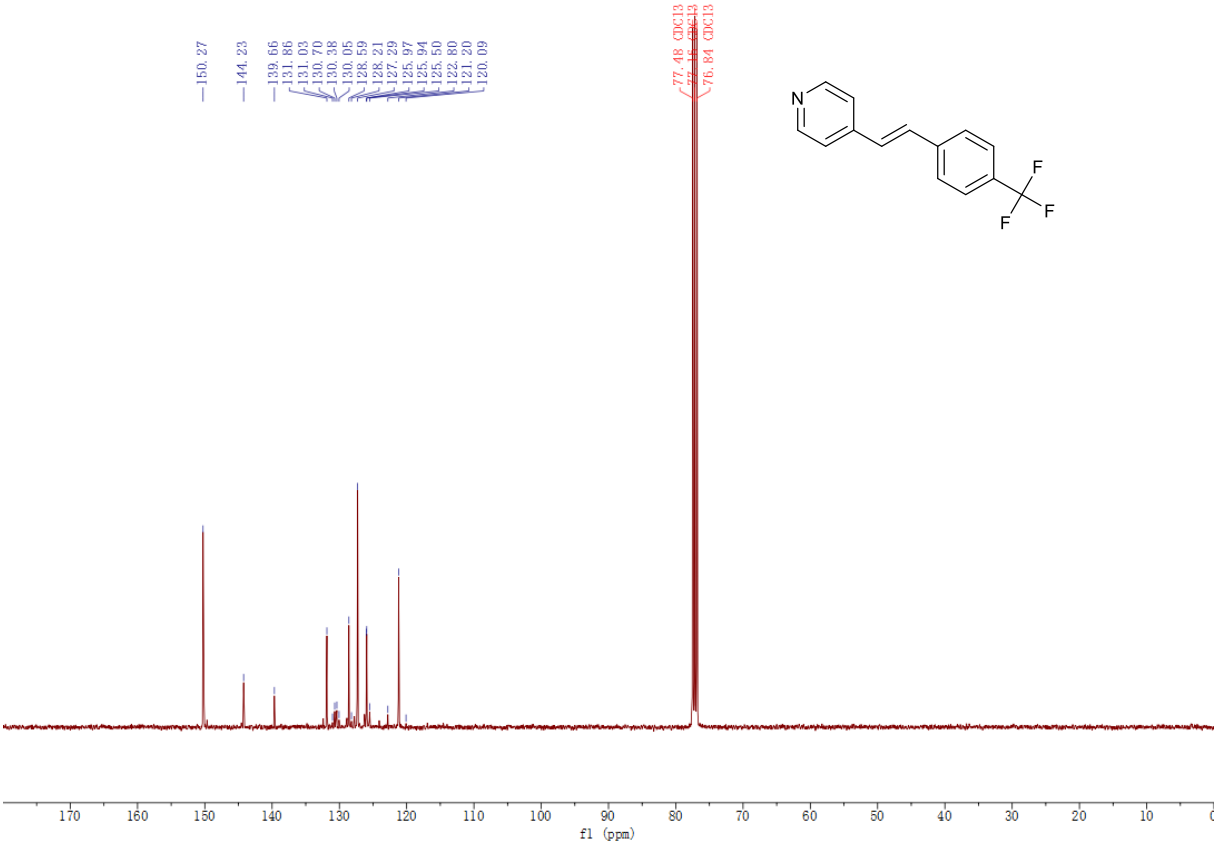
**(E)-4-(2-(Trifluoromethyl)styryl)pyridine (3hj), $^{19}F$ NMR (377 MHz, $CDCl_3$)**



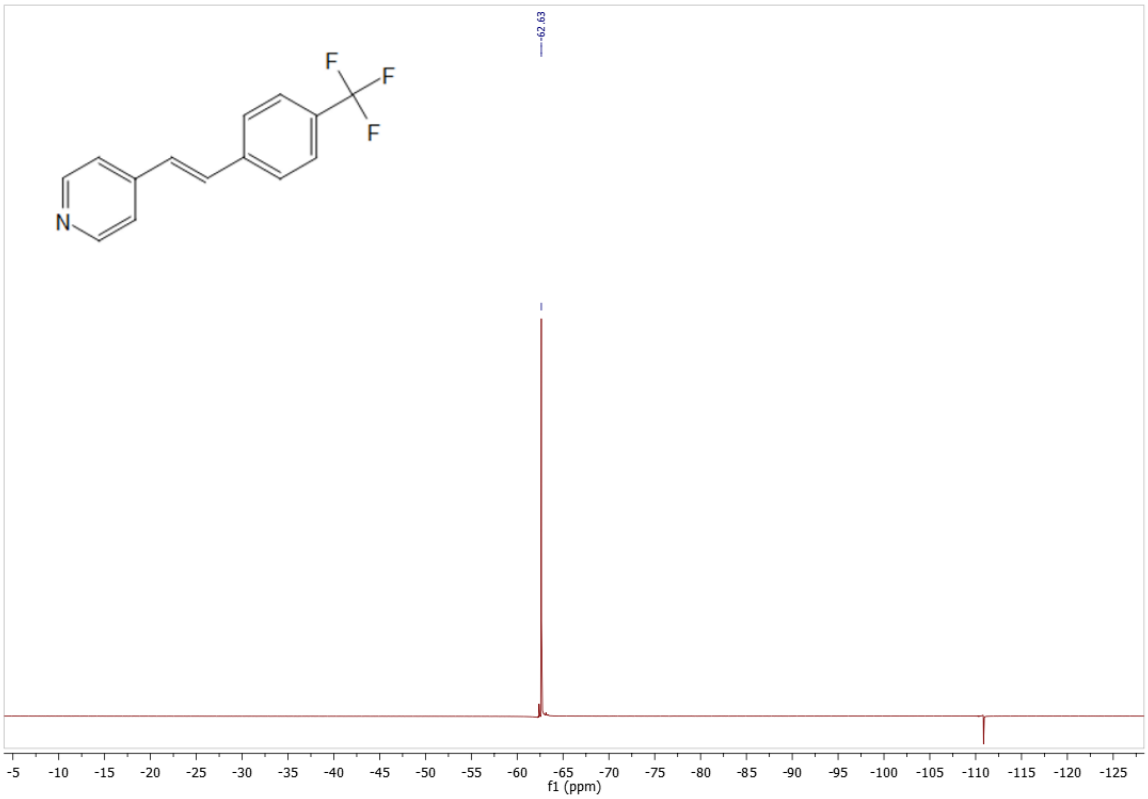

**(E)-4-(4-(Trifluoromethyl)styryl)pyridine (3hk), $^{1}H$ NMR (400 MHz, $CDCl_3$)**



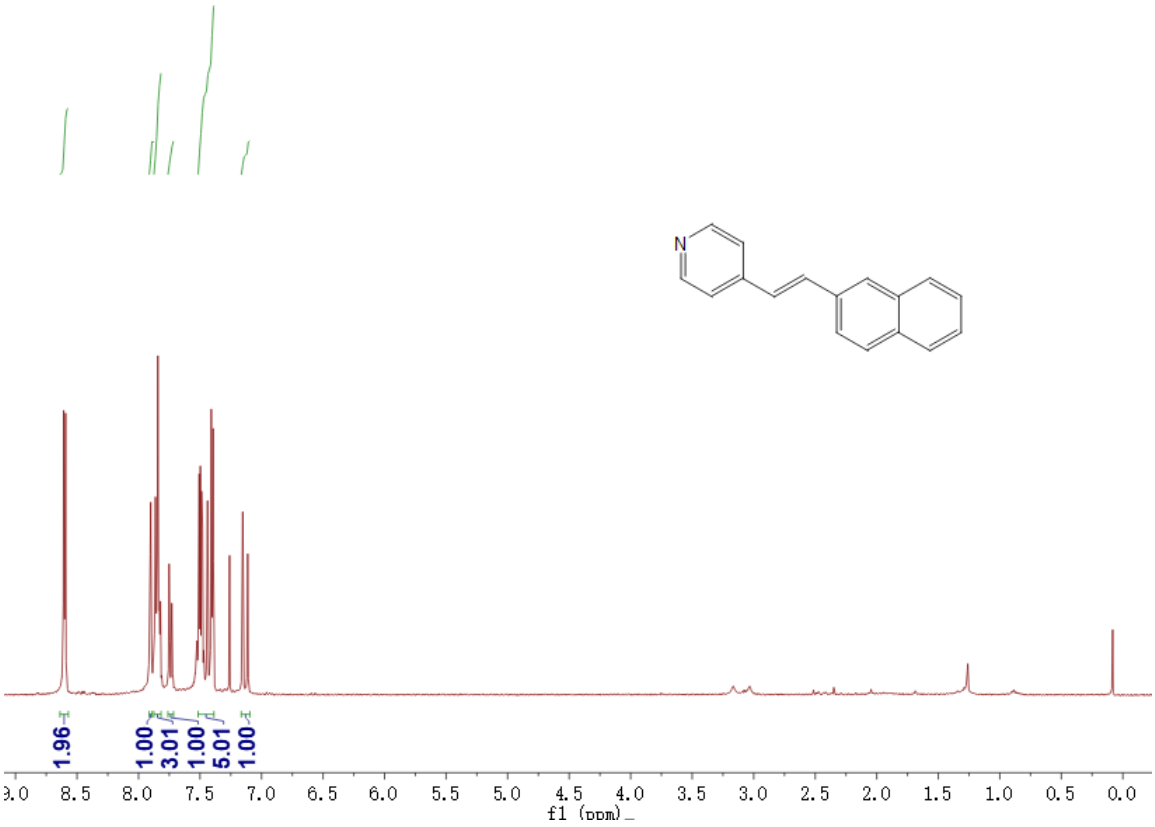
**(E)-4-(4-(Trifluoromethyl)styryl)pyridine (3hk), $^{13}$C NMR (101 MHz, $CDCl_3$)**



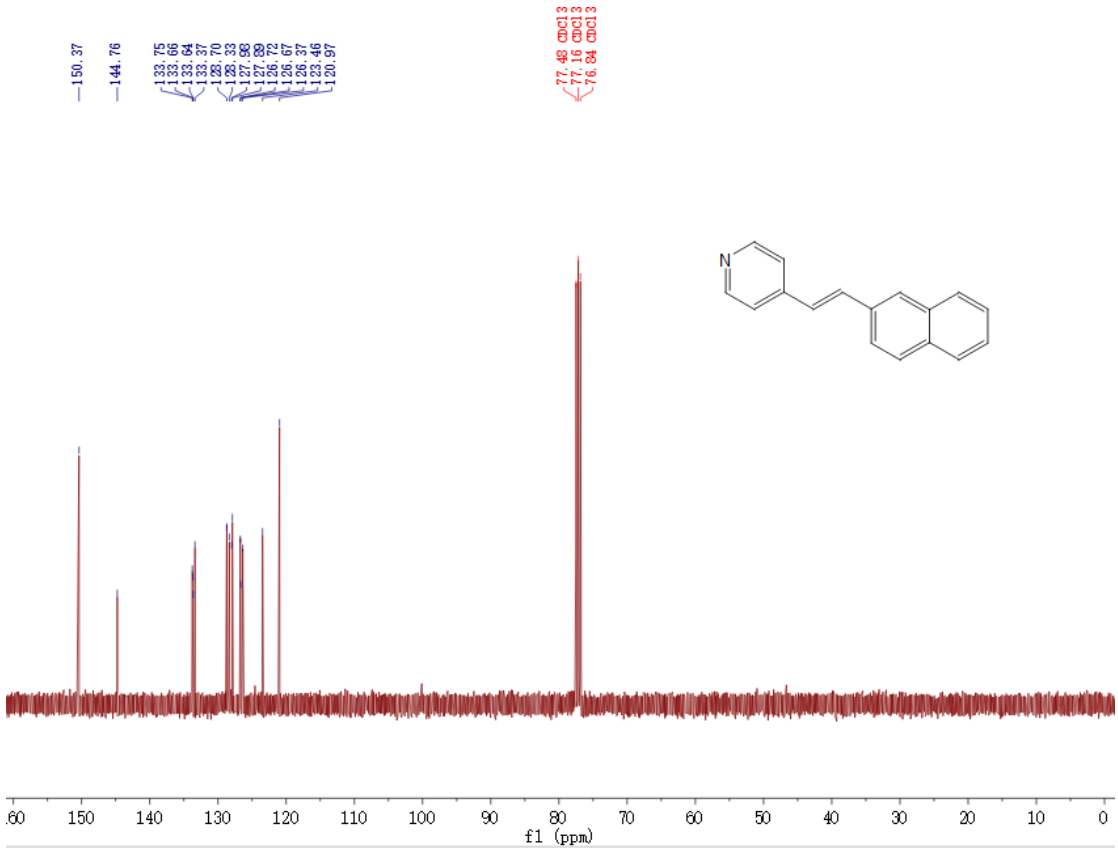

**(E)-4-(4-(Trifluoromethyl)styryl)pyridine (3fn), $^{19}$F NMR (377 MHz, $CDCl_3$)**



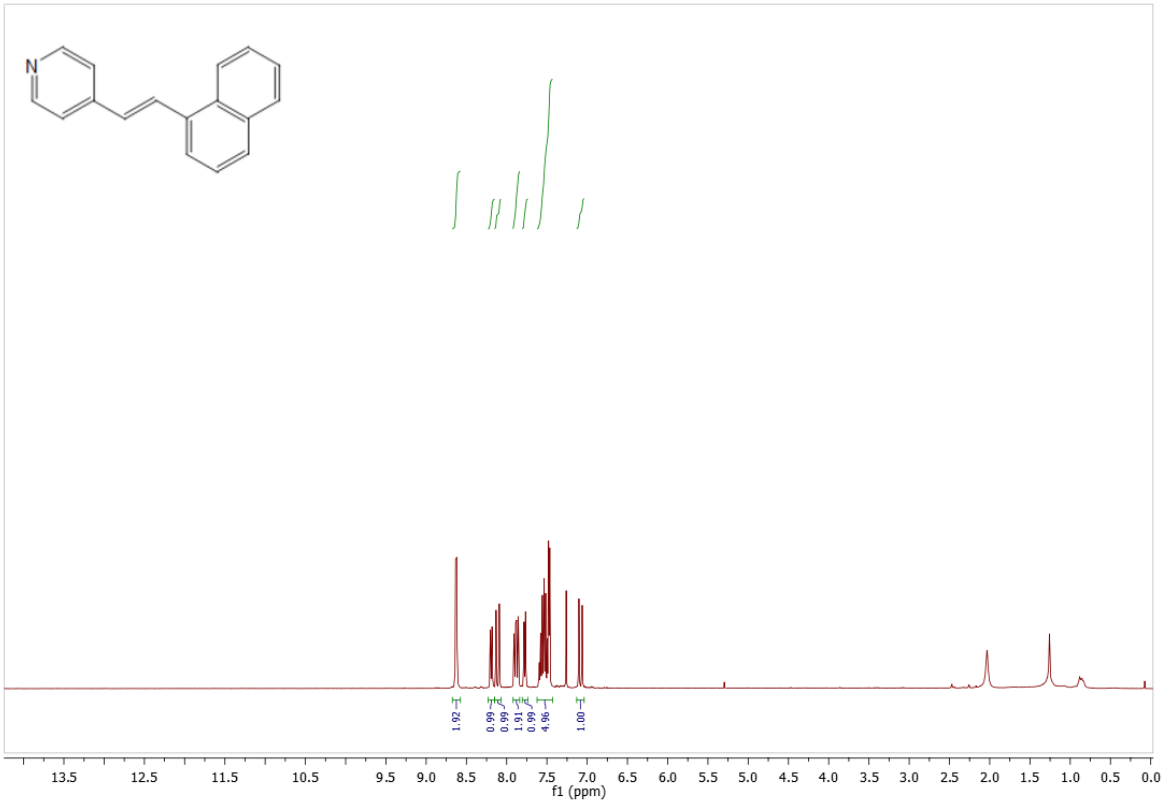
**(E)-4-(2-(naphthalen-2-yl)vinyl)pyridine (3hl), $^{1}$H NMR (400 MHz, $CDCl_3$)**



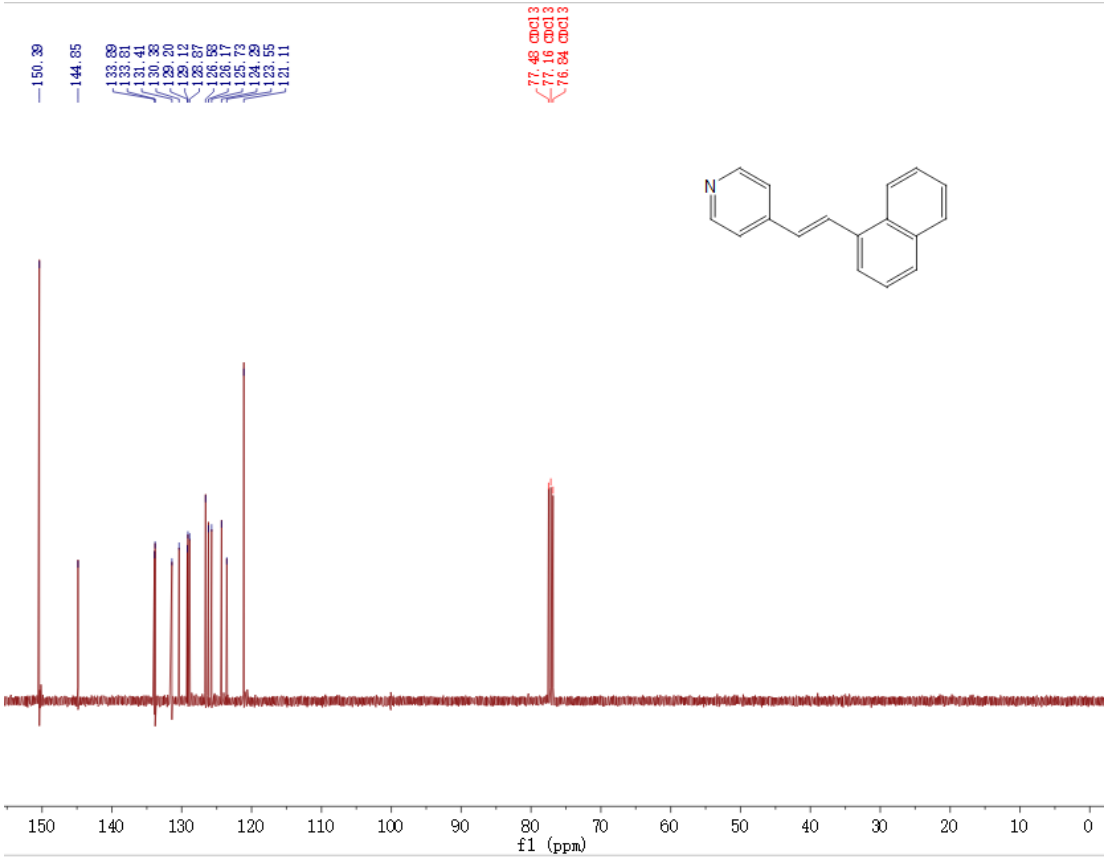

**(E)-4-(2-(Naphthalen-2-yl)vinyl)pyridine (3hl), $^{13}$C NMR (101 MHz, $CDCl_3$)**



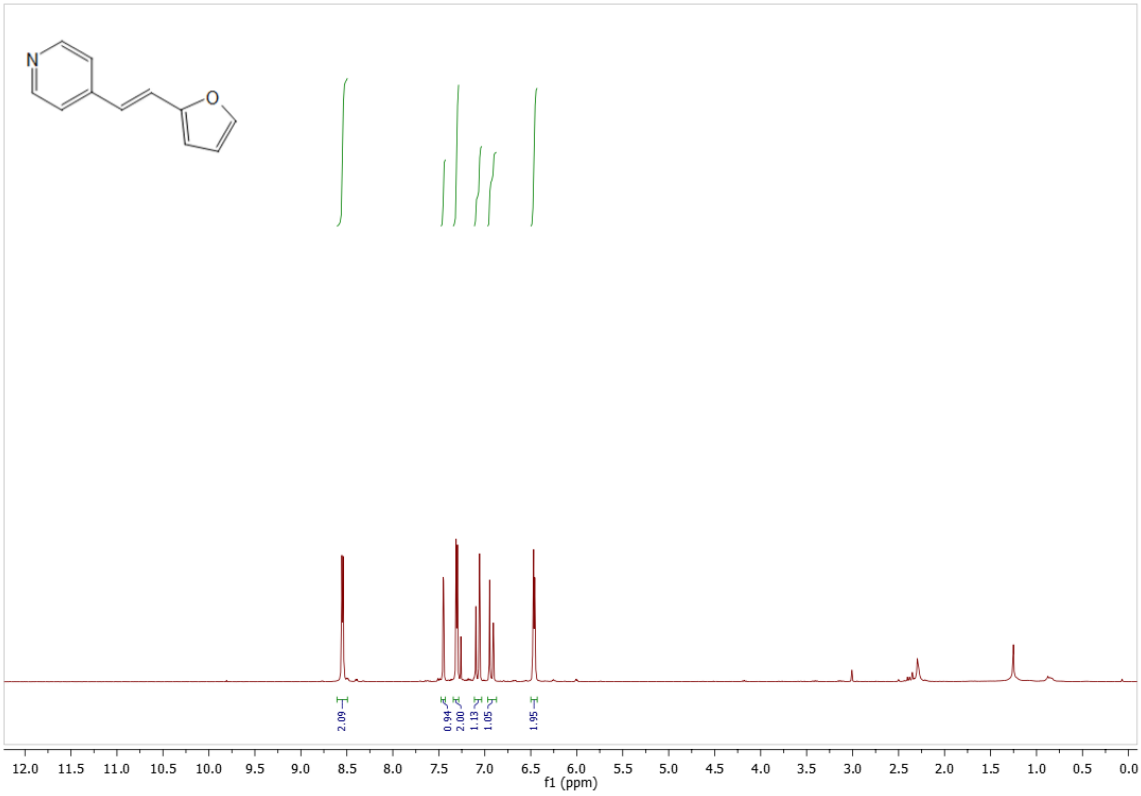
**(E)-4-(2-(Naphthalen-1-yl)vinyl)pyridine (3hg), $^{1}$H NMR (400 MHz, $CDCl_3$)**



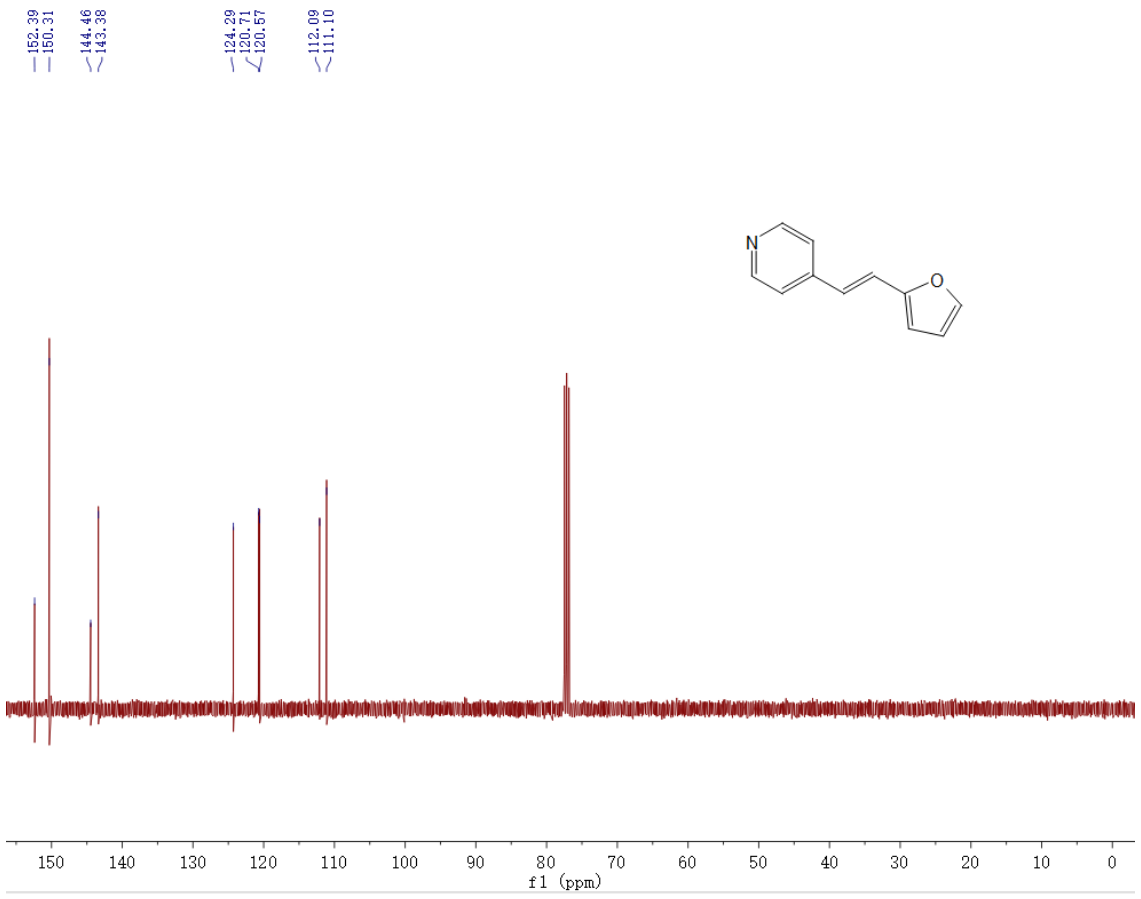

**(E)-4-(2-(Naphthalen-1-yl)vinyl)pyridine (3hg), $^{13}$C NMR (101 MHz, $CDCl_3$)**



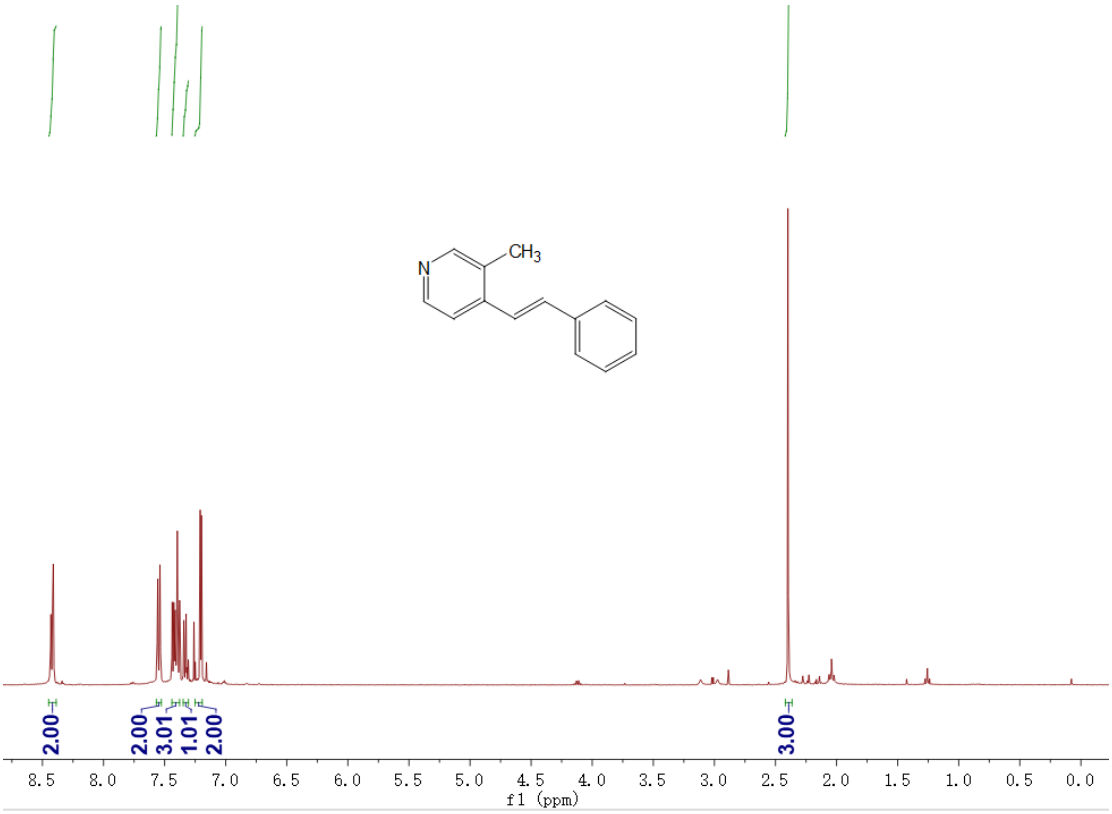
**(E)-4-(2-(Furan-2-yl)vinyl)pyridine (3hm), $^{1}$H NMR (400 MHz, $CDCl_3$)**



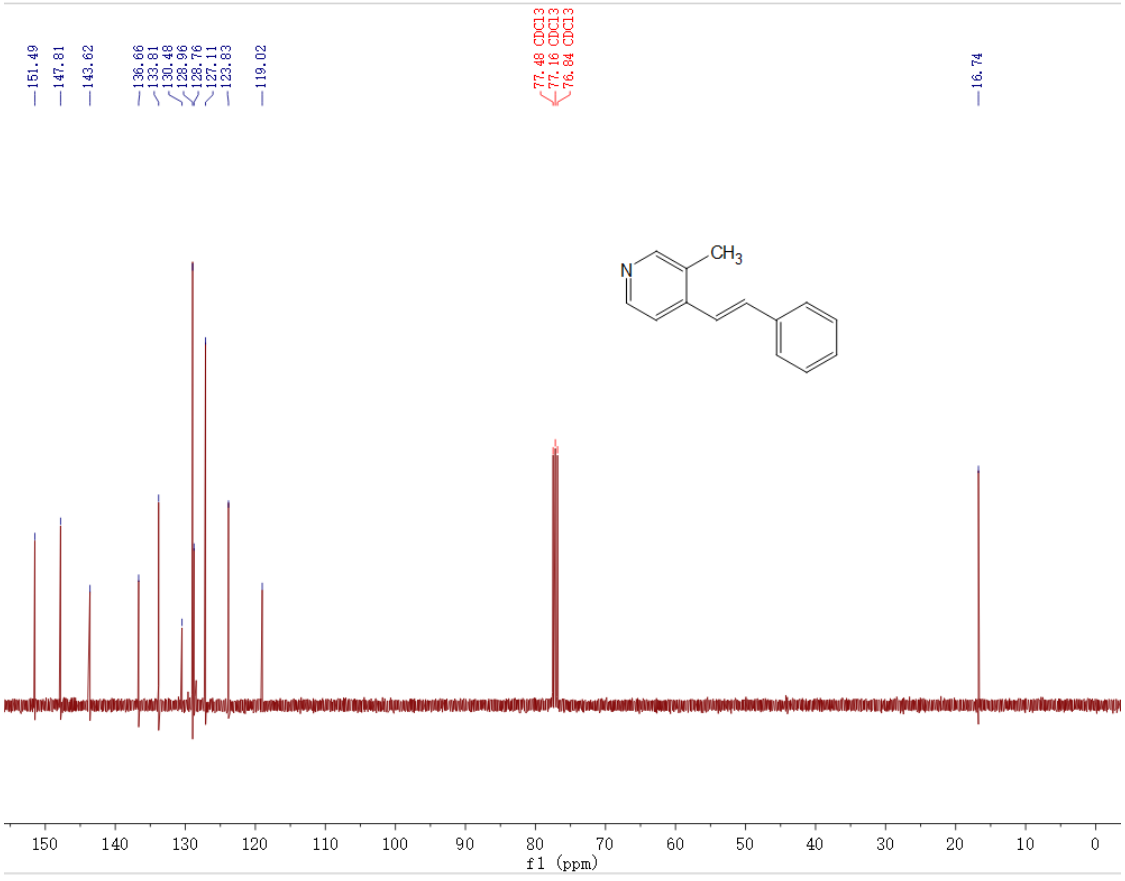

**(E)-4-(2-(Furan-2-yl)vinyl)pyridine (3hm), $^{13}$C NMR (101 MHz, $CDCl_3$)**



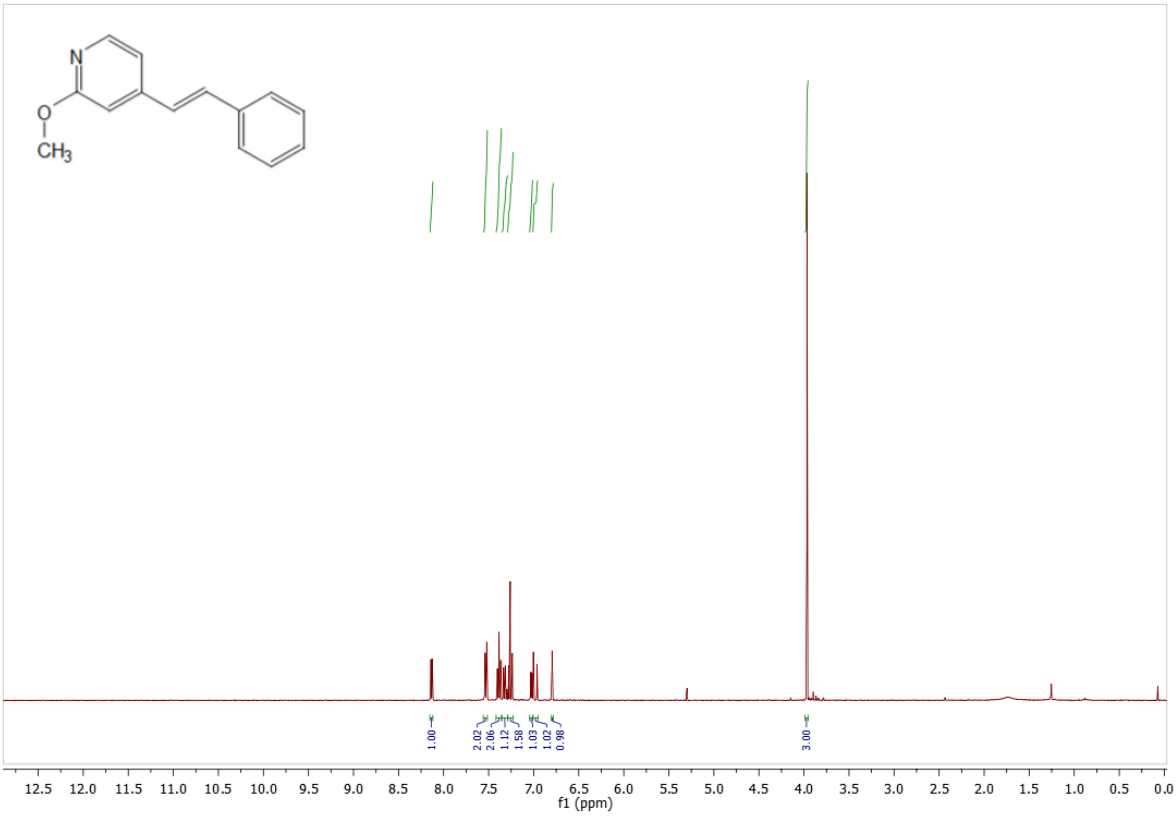
**(E)-3-Methyl-4-styrylpyridine (3ia), $^{1}$H NMR (400 MHz, $CDCl_3$)**



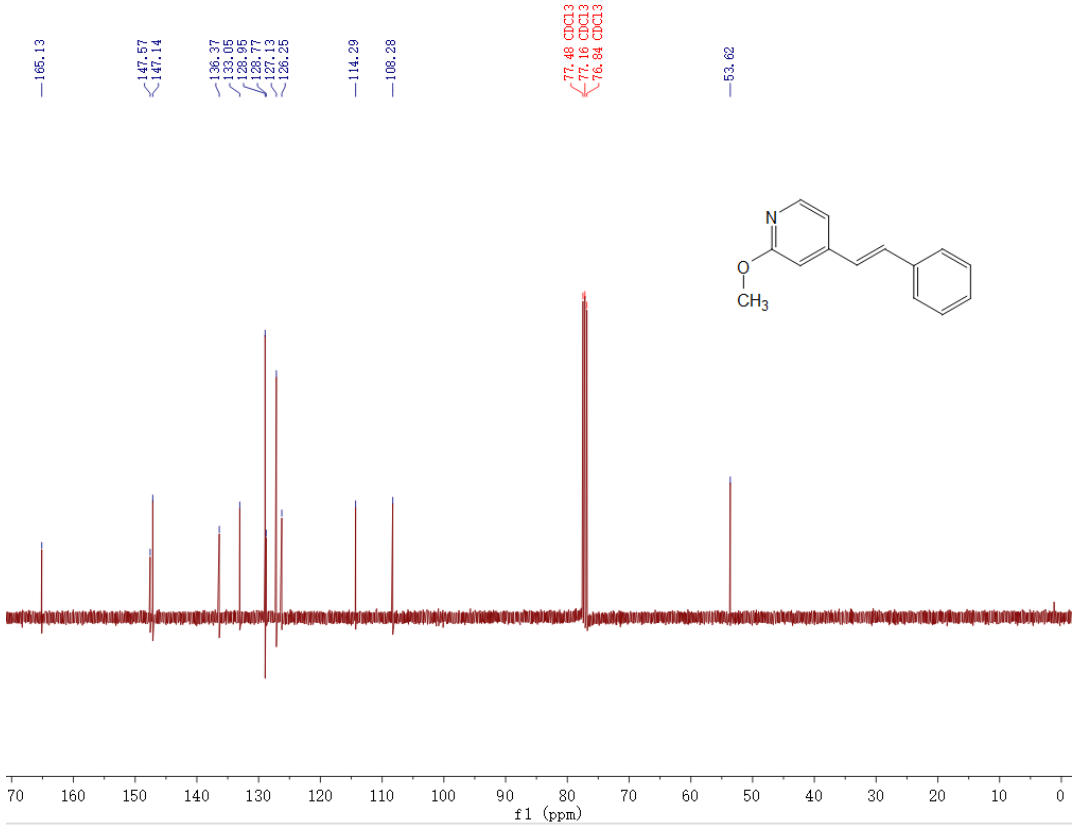

**(E)-3-Methyl-4-styrylpyridine (3ia), $^{13}$C NMR (101 MHz, $CDCl_3$)**



**(E)-2-Methoxy-4-styrylpyridine (3ja), $^{1}$H NMR (400 MHz, $CDCl_3$)**




**(E)-2-Methoxy-4-styrylpyridine (3ja), $^{13}$C NMR (101 MHz, $CDCl_3$)**

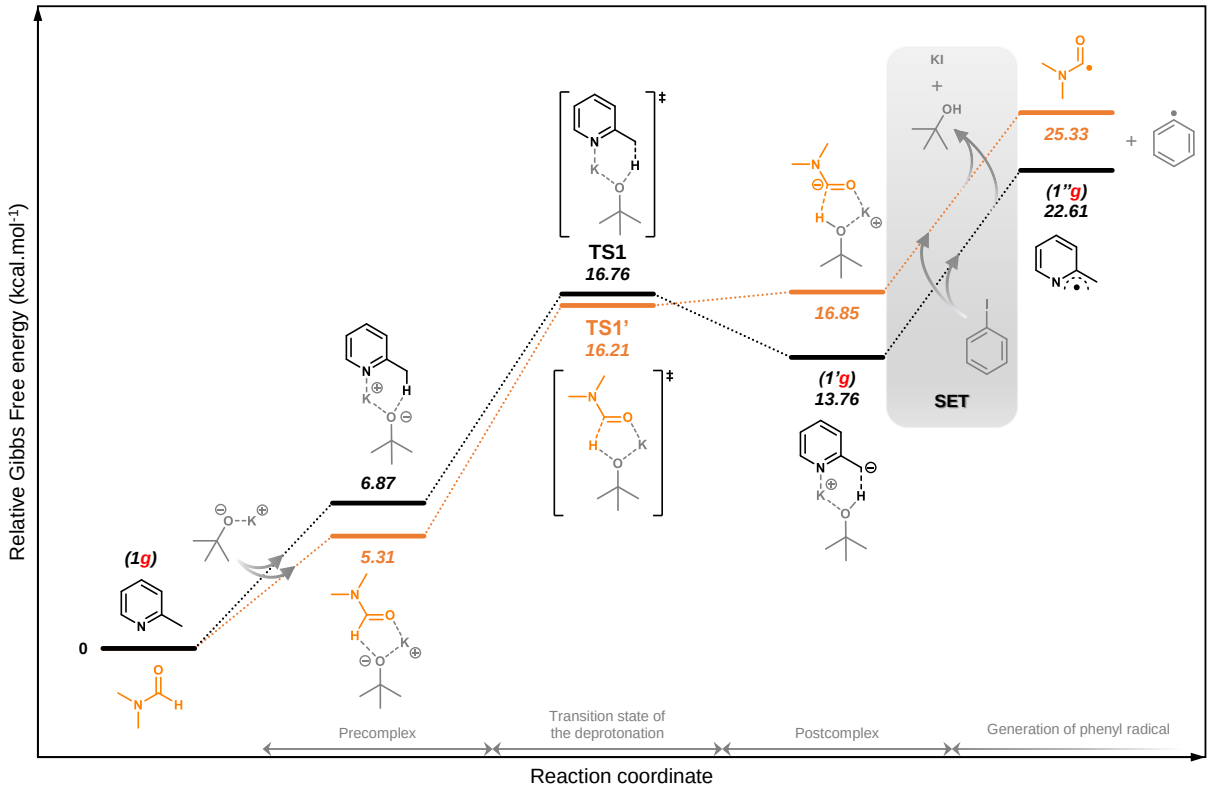


## 5- Computational details

All calculations were carried out using the density functional theory (DFT) [12,13] with the Gaussian 16 package[14]. The M062X[15] hybrid functional was combined to the 6-311++G(d,p)[16,17] triple-ζ basis set to describe C, N, H and O atoms whereas the relativistic Electron Core Potential (ECP) SDDAll[18,19] basis set was used for the iodide atom. Geometry optimizations were carried out without any symmetry restrictions. To model solvation effect in dimethylformamide, Conductor-like Polarizable Continuum Model (CPCM)[20,21] was considered for all optimized structures. The nature of all stationary points was fully characterized *via* subsequent analytical frequency calculations either as *minima* (all frequency positives) or as first order transition states (one imaginary frequency). Intrinsic Reaction Coordinate (IRC)[22,23] calculations were carried out to confirm *minimas* are linked to their corresponding transition states. The converge criteria was reduced by using the "Tight" SCF option available in Gaussian 16 combined with an ultrafine grid ("Int=UltraFine"). Chemcraft[24] software was used to plot the geometric structures of minima and transition states below.

It is to note that the phenyl radical formation mechanism from DMF/*t*BuOK (below) is a particular case. Indeed, the optimized geometries of the precomplex, the transition state and the postcomplex were retrieved from a previous article[25] and submitted to calculations at our level of theory. The aim was to get the Gibbs Free energies and the right order of magnitude to be able to compare these values with those obtained for the mechanism involving **1g** rather than DMF.

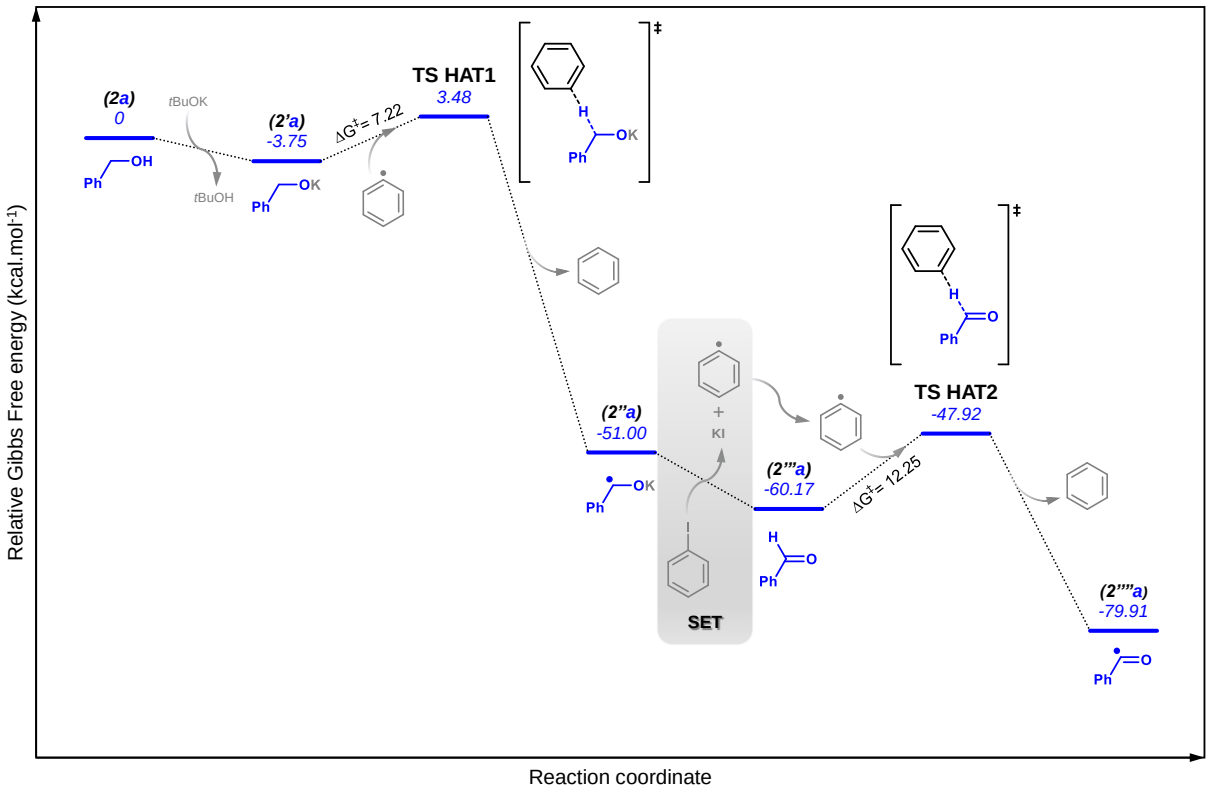
## More reaction pathways (DFT-CPCM)



Energy profiles (ΔG in kcal.mol$^{-1}$) for the phenyl radical generation from DMF (orange) or **1g** (black) in presence of tBuOK and PhI. Computed at the CPCM(DMF)-M062X/6-311++G(d,p), SDDAll(I) level of theory.

As a reminder, the salt 1'g can be generated through the deprotonation of 1g in presence of *t*BuOK. This endergonic process is achievable with an activation barrier of 16.76 kcal. mol$^{-1}$ by going through the formation of a precomplex at 6.87 kcal. mol$^{-1}$. For very similar results the carbamoyl anion could be obtained from DMF with a transition state of deprotonation requiring an activation barrier of 16.21 kcal. mol$^{-1}$. Then phenyl iodine (used as additive for the modelling) can react with the carbamoyl anion or 1'g through an endergonic SET to be converted into phenyl radical and the corresponding radical species at □G= 25.33 kcal. mol$^{-1}$ or □G= 22.61 kcal. mol$^{-1}$ for 1''g, respectively.

It is to note that from the reactants to the formation of the radical species, the only truly remarkable difference lies between the relative Gibbs Free energies of the postcomplexes because the carbamoyl anion and 1'g are slightly destabilized and more stabilized, respectively, compared with their corresponding transition states. Thus, here the generation of phenyl radical from 1g seems possible and even slightly more favorable than from DMF. However, according to the experimental conditions at 90°C and the small energy differences between the two processes, we can assume that they coexist.



Energy profiles (ΔG in kcal.mol$^{-1}$) for the benzoyl radical **2''''a** formation from the benzyl alcohol **2a** in presence of tBuOK, phenyl radical and PhI. Computed at the CPCM(DMF)-M062X/6-311++G(d,p), SDDAll(I) level of theory.

As already mentioned in the article, another possible way is the formation of the benzoyl radical intermediate 2''''a from 2"a. More precisely a SET can occur between the latter and phenyl iodine to give phenyl radical and the thermodynamically stabilized benzaldehyde product 2"a at ΔG= -60.17 kcal. mol$^{-1}$. The resulting products would easily react together to lead the benzoyl radical 2''''a (ΔG= -79.91 kcal. mol$^{-1}$) *via* a favorable exergonic HAT owing an achievable activation barrier of ΔG$^{‡}$= 12.25 kcal. mol$^{-1}$.

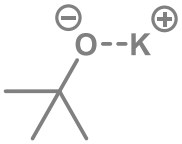
## Cartesian coordinates for the optimized structures (CPCM)

At CPCM(DMF)-M062X/6-311++G(d,p), SDDAll(I) level of theory, E and G correspond to the electronic and the Gibbs free energies.

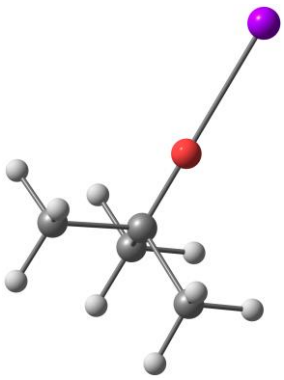
**Potassium tert-butoxide (*t*BuOK)**

E = -832.888908 Hartree

G = -832.922787 Hartree



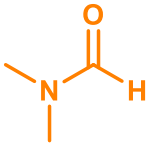

| | | | |
|---|---|---|---|
| C | -6.379488000 | 0.612242000 | -0.120248000 |
| O | -6.130343000 | 1.577387000 | 0.830030000 |
| K | -5.788721000 | 3.265257000 | 2.506431000 |
| C | -5.696355000 | -0.720224000 | 0.254378000 |
| H | -6.075623000 | -1.071300000 | 1.219064000 |
| H | -5.869928000 | -1.504428000 | -0.490640000 |
| H | -4.617052000 | -0.564830000 | 0.348272000 |
| C | -7.894908000 | 0.350880000 | -0.254026000 |
| H | -8.297842000 | 0.028851000 | 0.711102000 |
| H | -8.402985000 | 1.275771000 | -0.544073000 |
| H | -8.124535000 | -0.418388000 | -0.999421000 |
| C | -5.846553000 | 1.046579000 | -1.502230000 |
| H | -4.767331000 | 1.219690000 | -1.443220000 |
| H | -6.034341000 | 0.296313000 | -2.278112000 |
| H | -6.326670000 | 1.982571000 | -1.804230000 |



**Dimethylformamide (DMF)**

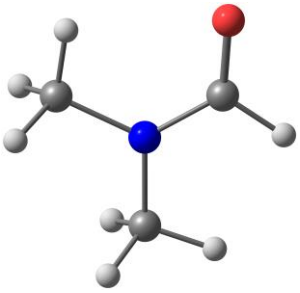
E = -248.377559 Hartree

G = -248.406870 Hartree




| | | | |
|---|---|---|---|
| N | 0.333999000 | -0.023270000 | -0.000135000 |
| C | 1.581006000 | -0.767204000 | 0.000018000 |
| H | 1.372159000 | -1.836226000 | -0.000293000 |

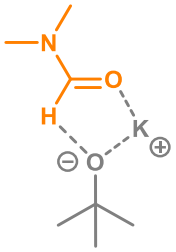
| | | | |
|---|---|---|---|
| H | 2.167285000 | -0.519775000 | -0.888028000 |
| H | 2.166853000 | -0.520196000 | 0.888472000 |
| C | 0.434519000 | 1.425598000 | 0.000092000 |
| H | 0.975541000 | 1.761900000 | -0.887641000 |
| H | -0.565980000 | 1.850485000 | -0.000567000 |
| H | 0.974294000 | 1.761777000 | 0.888642000 |
| C | -0.858518000 | -0.641360000 | 0.000007000 |
| H | -0.767055000 | -1.737987000 | -0.000265000 |
| O | -1.950391000 | -0.087412000 | -0.000011000 |



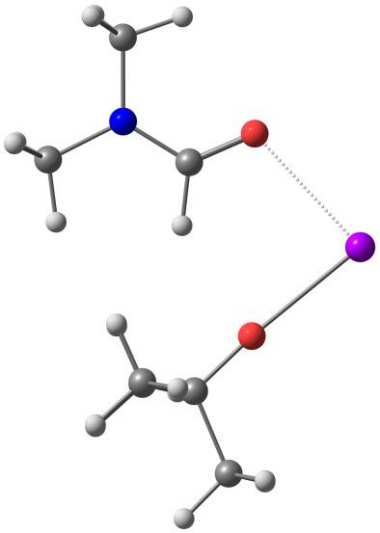
**Precomplex of *t*BuOK/DMF**

E = -1081.275399 Hartree

G = -1081.321202 Hartree




| | | | |
|---|---|---|---|
| O | -1.833970000 | 1.428288000 | 0.011929000 |
| N | -2.636858000 | -0.706590000 | 0.001204000 |
| C | -2.345449000 | -2.129060000 | -0.023556000 |
| H | -2.756639000 | -2.614056000 | 0.864959000 |
| H | -2.785911000 | -2.589283000 | -0.911280000 |
| H | -1.267133000 | -2.281475000 | -0.043465000 |
| C | -4.037874000 | -0.324838000 | 0.030367000 |
| H | -4.109070000 | 0.759418000 | 0.052031000 |
| H | -4.547399000 | -0.707761000 | -0.857107000 |
| H | -4.518953000 | -0.741563000 | 0.918435000 |
| C | 2.178925000 | -0.755658000 | -0.004997000 |
| O | 1.524536000 | 0.454986000 | -0.024158000 |
| C | 1.820868000 | -1.592738000 | -1.252305000 |
| H | 2.316332000 | -2.569710000 | -1.261719000 |
| H | 0.738882000 | -1.754739000 | -1.293190000 |
| H | 2.112383000 | -1.046842000 | -2.154960000 |
| C | 3.709139000 | -0.558111000 | 0.011935000 |
| H | 4.256340000 | -1.507257000 | 0.025847000 |
| H | 4.014803000 | 0.005393000 | -0.875029000 |
| H | 3.993413000 | 0.018764000 | 0.897342000 |
| C | 1.790863000 | -1.569506000 | 1.248723000 |
| H | 0.708542000 | -1.733574000 | 1.265791000 |
| H | 2.287745000 | -2.544980000 | 1.289151000 |
| H | 2.058960000 | -1.005671000 | 2.147596000 |
| K | 0.538194000 | 2.666503000 | -0.030060000 |
| C | -1.656946000 | 0.207613000 | -0.005400000 |

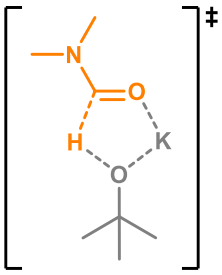


| | | | |
|---|---|---|---|
| H | -0.634302000 | -0.201939000 | -0.027071000 |

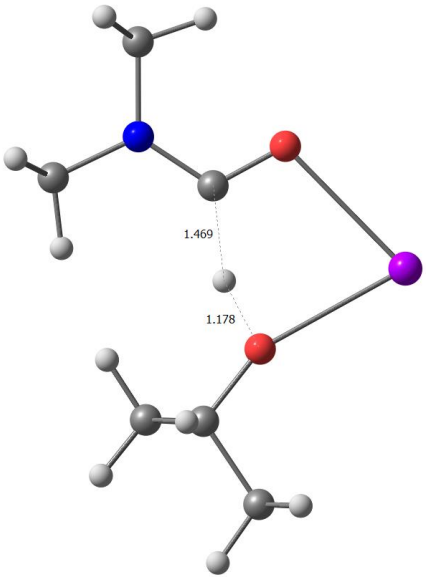
**TS1'**

E = -1081.258641 Hartree

G = -1081.303822 Hartree



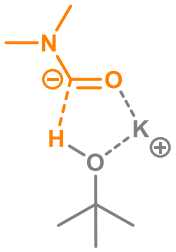

| | | | |
|---|---|---|---|
| C | -1.441852000 | 0.213845000 | -0.002946000 |
| O | -1.747857000 | 1.437280000 | -0.000353000 |
| H | 0.013175000 | 0.012008000 | -0.003500000 |
| N | -2.456952000 | -0.700547000 | -0.003023000 |
| C | -2.177747000 | -2.119573000 | -0.001254000 |
| H | -2.595403000 | -2.600806000 | 0.890167000 |
| H | -2.610540000 | -2.605316000 | -0.882846000 |
| H | -1.099607000 | -2.269060000 | -0.010137000 |
| C | -3.863731000 | -0.338934000 | 0.003446000 |
| H | -3.945704000 | 0.745350000 | -0.002848000 |
| H | -4.369370000 | -0.747826000 | -0.877469000 |
| H | -4.359038000 | -0.736393000 | 0.895515000 |
| C | 2.011986000 | -0.836792000 | 0.000832000 |
| O | 1.159698000 | 0.281129000 | -0.001968000 |
| C | 1.773472000 | -1.684969000 | -1.256650000 |
| H | 2.425691000 | -2.563013000 | -1.278516000 |
| H | 0.735533000 | -2.025892000 | -1.296570000 |
| H | 1.968212000 | -1.085071000 | -2.149865000 |
| C | 3.457965000 | -0.337283000 | 0.006240000 |
| H | 4.167308000 | -1.170275000 | 0.008546000 |
| H | 3.645018000 | 0.275313000 | -0.879928000 |
| H | 3.638521000 | 0.274666000 | 0.894198000 |
| C | 1.764526000 | -1.685908000 | 1.256015000 |
| H | 0.726509000 | -2.027363000 | 1.288092000 |
| H | 2.417061000 | -2.563602000 | 1.281966000 |
| H | 1.952377000 | -1.086540000 | 2.151064000 |
| K | 0.528621000 | 2.740280000 | 0.002126000 |




**Postcomplex of *t*BuOK/DMF**

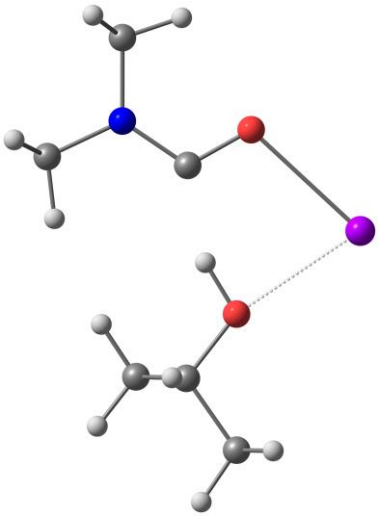
E = -1081.256636 Hartree

G = -1081.302801 Hartree




| | | | |
|---|---|---|---|
| C | -1.476560000 | 0.175542000 | 0.000249000 |
| O | -1.778850000 | 1.405456000 | 0.000072000 |
| H | 0.237275000 | 0.017471000 | 0.000706000 |
| N | -2.526129000 | -0.713417000 | -0.000015000 |

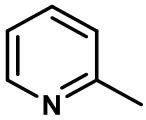
| | | | |
|---|---|---|---|
| C | -2.280666000 | -2.137188000 | 0.000172000 |
| H | -2.716029000 | -2.614203000 | 0.886117000 |
| H | -2.715513000 | -2.614348000 | -0.885948000 |
| H | -1.204589000 | -2.306517000 | 0.000500000 |
| C | -3.924669000 | -0.321478000 | -0.000439000 |
| H | -3.981076000 | 0.764783000 | -0.000547000 |
| H | -4.437098000 | -0.711713000 | -0.886549000 |
| H | -4.437595000 | -0.711562000 | 0.885450000 |
| C | 2.087822000 | -0.841918000 | 0.001505000 |
| O | 1.244365000 | 0.299179000 | 0.000935000 |
| C | 1.826015000 | -1.679046000 | -1.254408000 |
| H | 2.475214000 | -2.558270000 | -1.283035000 |
| H | 0.786158000 | -2.015146000 | -1.276912000 |
| H | 2.011755000 | -1.078681000 | -2.148571000 |
| C | 3.526887000 | -0.335854000 | 0.001942000 |
| H | 4.232910000 | -1.170286000 | 0.002384000 |
| H | 3.710663000 | 0.275108000 | -0.885385000 |
| H | 3.709993000 | 0.275482000 | 0.889149000 |
| C | 1.825059000 | -1.678505000 | 1.257579000 |
| H | 0.785191000 | -2.014613000 | 1.279425000 |
| H | 2.474253000 | -2.557703000 | 1.287089000 |
| H | 2.010097000 | -1.077747000 | 2.151624000 |
| K | 0.428661000 | 2.761391000 | 0.000278000 |



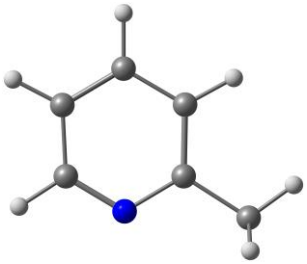
**1g**

E = -287.436938 Hartree

G = -287.466944 Hartree




| | | | |
|---|---|---|---|
| C | 0.875260000 | 0.003534000 | 0.000001000 |
| C | 0.161506000 | 1.203586000 | -0.000001000 |
| C | -1.227071000 | 1.168572000 | -0.000001000 |
| C | -1.865610000 | -0.065138000 | 0.000001000 |
| C | -1.074435000 | -1.208786000 | 0.000002000 |
| H | 0.693359000 | 2.147148000 | -0.000003000 |
| H | -1.799737000 | 2.088655000 | -0.000001000 |
| H | -2.944835000 | -0.146470000 | 0.000006000 |
| H | -1.535859000 | -2.191714000 | -0.000008000 |
| C | 2.378616000 | -0.016722000 | 0.000003000 |
| H | 2.790708000 | 0.991934000 | 0.000132000 |
| H | 2.745804000 | -0.547549000 | 0.880796000 |
| N | 0.259307000 | -1.186425000 | -0.000002000 |

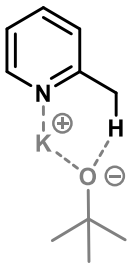


| | | | |
|---|---|---|---|
| H | 2.745813000 | -0.547310000 | -0.880933000 |

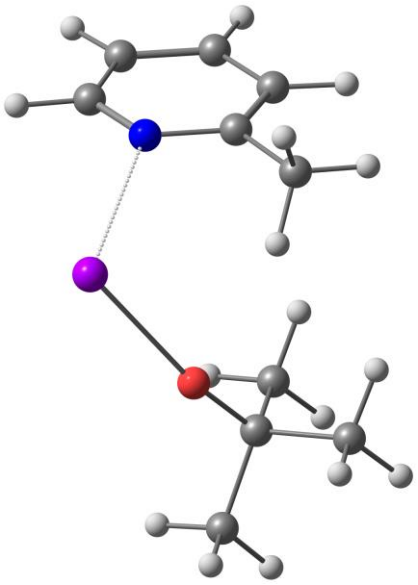
**Precomplex of *t*BuOK/Pyr**

E = -1120.333708 Hartree

G = -1120.378780 Hartree




| | | | |
|---|---|---|---|
| C | -0.392221000 | 0.703884000 | 1.726487000 |
| C | 0.464471000 | 1.438185000 | 2.548841000 |
| C | 0.536665000 | 2.816818000 | 2.398776000 |
| C | -0.249199000 | 3.429299000 | 1.430003000 |
| C | -1.071629000 | 2.622830000 | 0.652880000 |
| H | 1.062825000 | 0.927490000 | 3.293404000 |
| H | 1.195667000 | 3.403589000 | 3.028020000 |
| H | -0.228784000 | 4.500063000 | 1.274894000 |
| H | -1.698976000 | 3.061186000 | -0.117347000 |
| N | -1.146933000 | 1.296712000 | 0.788531000 |
| K | -2.037067000 | -0.436946000 | -1.268073000 |
| C | 1.491495000 | -1.790467000 | -1.384960000 |
| C | -0.508065000 | -0.789771000 | 1.830622000 |
| H | 0.166332000 | -1.189188000 | 2.588622000 |
| H | -0.263206000 | -1.236389000 | 0.859396000 |
| H | -1.532059000 | -1.068759000 | 2.093299000 |
| O | 0.169131000 | -1.415537000 | -1.467010000 |
| C | 2.328579000 | -0.698092000 | -0.682343000 |
| H | 2.250510000 | 0.239342000 | -1.242394000 |
| H | 1.937963000 | -0.524276000 | 0.325480000 |
| H | 3.387923000 | -0.966294000 | -0.602405000 |
| C | 2.090352000 | -2.022401000 | -2.788227000 |
| H | 3.143132000 | -2.323719000 | -2.750987000 |
| H | 1.524704000 | -2.805075000 | -3.303552000 |
| H | 2.015200000 | -1.103322000 | -3.377521000 |
| C | 1.645584000 | -3.099971000 | -0.580546000 |
| H | 1.073572000 | -3.897088000 | -1.065519000 |
| H | 2.689672000 | -3.422345000 | -0.501165000 |
| H | 1.249150000 | -2.962090000 | 0.429953000 |



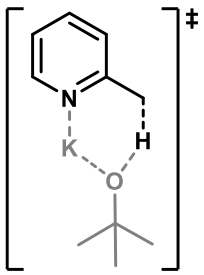
**TS1**

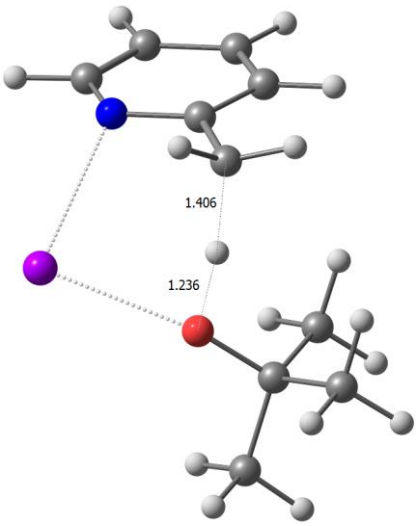
E = -1120.318927 Hartree

G = -1120.363023 Hartree

| | | | |
|---|---|---|---|
| C | -0.034645000 | -2.253844000 | -0.082874000 |
| C | 1.044449000 | -1.583223000 | 0.545856000 |

| | | | |
|---|---|---|---|
| C | 1.140851000 | -0.209025000 | 0.481835000 |
| C | 0.163125000 | 0.517101000 | -0.207295000 |
| C | -0.860361000 | -0.204146000 | -0.800697000 |
| H | 1.783363000 | -2.165851000 | 1.084036000 |
| H | 1.963796000 | 0.303308000 | 0.968715000 |
| H | 0.194693000 | 1.596085000 | -0.279707000 |
| H | -1.641769000 | 0.314931000 | -1.350264000 |
| N | -0.969773000 | -1.536366000 | -0.756248000 |
| K | -1.686959000 | -3.175993000 | -2.904792000 |
| C | 1.944584000 | -4.592914000 | -2.754549000 |
| C | -0.124389000 | -3.702005000 | -0.127049000 |
| H | 0.499172000 | -4.198537000 | 0.617356000 |
| H | 0.327486000 | -4.050663000 | -1.411939000 |
| H | -1.155136000 | -4.062151000 | -0.078154000 |
| O | 0.586797000 | -4.269858000 | -2.600084000 |
| C | 2.822864000 | -3.505565000 | -2.115758000 |
| H | 2.605902000 | -2.536213000 | -2.574278000 |
| H | 2.612097000 | -3.429741000 | -1.045660000 |
| H | 3.887078000 | -3.722871000 | -2.247087000 |
| C | 2.260231000 | -4.686615000 | -4.249499000 |
| H | 3.310348000 | -4.942716000 | -4.420382000 |
| H | 1.635817000 | -5.453447000 | -4.716097000 |
| H | 2.052688000 | -3.729525000 | -4.735814000 |
| C | 2.242661000 | -5.942208000 | -2.083395000 |
| H | 1.629408000 | -6.726380000 | -2.535870000 |
| H | 3.295595000 | -6.220753000 | -2.187685000 |
| H | 2.001740000 | -5.888607000 | -1.018014000 |



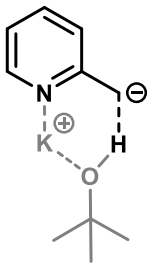




**Postcomplex of *t*BuOK/Pyr (1'g)**

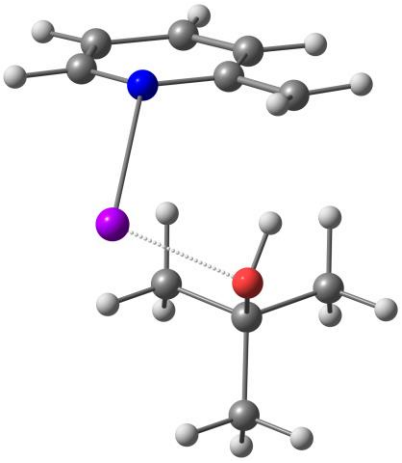
E = -1120.324525 Hartree

G = -1120.367802 Hartree

| | | | |
|---|---|---|---|
| C | -0.545397000 | 0.219706000 | 1.613480000 |
| C | 0.646719000 | 0.576840000 | 2.350634000 |
| C | 1.224134000 | 1.806096000 | 2.193224000 |
| C | 0.661109000 | 2.743606000 | 1.297073000 |
| C | -0.473318000 | 2.338275000 | 0.614055000 |



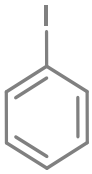
| | | | |
|---|---|---|---|
| H | 1.066757000 | -0.149770000 | 3.038354000 |
| H | 2.115515000 | 2.059896000 | 2.759056000 |
| H | 1.086096000 | 3.726263000 | 1.144794000 |
| H | -0.940234000 | 3.021939000 | -0.094661000 |
| N | -1.071261000 | 1.149485000 | 0.733309000 |
| K | -2.006307000 | 0.033938000 | -1.590415000 |
| C | 1.397095000 | -1.473070000 | -1.176057000 |
| C | -1.133369000 | -1.033593000 | 1.729195000 |
| H | -0.766788000 | -1.738724000 | 2.465217000 |
| H | -0.227430000 | -1.522271000 | -0.024957000 |
| H | -2.106447000 | -1.219659000 | 1.287368000 |
| O | -0.011945000 | -1.659662000 | -0.977980000 |
| C | 1.701597000 | 0.021975000 | -1.275190000 |
| H | 1.150454000 | 0.464947000 | -2.109949000 |
| H | 1.412622000 | 0.532707000 | -0.353117000 |
| H | 2.768598000 | 0.187714000 | -1.446479000 |
| C | 1.738555000 | -2.179366000 | -2.481804000 |
| H | 2.797929000 | -2.057300000 | -2.718401000 |
| H | 1.516980000 | -3.246206000 | -2.404208000 |
| H | 1.149634000 | -1.759704000 | -3.301262000 |
| C | 2.158348000 | -2.092644000 | -0.005683000 |
| H | 1.911995000 | -3.153290000 | 0.087522000 |
| H | 3.236336000 | -1.996555000 | -0.155329000 |
| H | 1.892375000 | -1.585005000 | 0.926691000 |



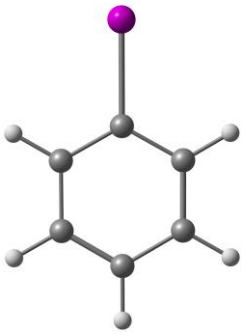
**Phenyl Iodide (PhI)**

E = -242.884012 Hartree

G = -242.915722 Hartree



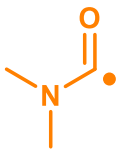
| | | | |
|---|---|---|---|
| C | 3.001250000 | -0.940236000 | -0.192134000 |
| C | 2.385898000 | -0.892236000 | 1.055023000 |
| C | 1.271698000 | -0.082604000 | 1.261578000 |
| C | 0.783192000 | 0.677082000 | 0.203442000 |
| C | 1.387082000 | 0.641005000 | -1.049282000 |
| C | 2.500380000 | -0.173726000 | -1.240039000 |
| H | 3.867213000 | -1.572181000 | -0.346781000 |
| H | 2.769436000 | -1.485582000 | 1.876478000 |
| H | 0.795572000 | -0.047924000 | 2.233436000 |
| H | 1.000578000 | 1.236129000 | -1.867110000 |
| H | 2.973528000 | -0.205076000 | -2.214264000 |
| I | -0.909195000 | 1.908199000 | 0.505003000 |



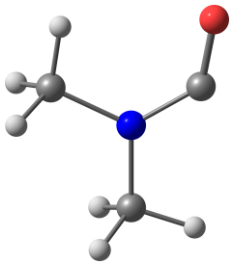
**DMF_Rad**

E = -247.731080 Hartree

G = -247.760944 Hartree



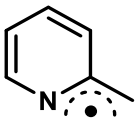

| | | | |
|---|---|---|---|
| N | 0.312250000 | -0.047982000 | -0.000116000 |
| C | 1.548043000 | -0.818134000 | 0.000032000 |
| H | 1.305682000 | -1.878788000 | -0.000211000 |
| H | 2.135385000 | -0.578590000 | -0.888847000 |
| H | 2.135003000 | -0.578911000 | 0.889254000 |
| C | 0.435476000 | 1.410655000 | 0.000119000 |
| H | 0.980698000 | 1.733052000 | -0.889102000 |
| H | -0.558942000 | 1.850804000 | -0.000504000 |
| H | 0.979532000 | 1.732928000 | 0.890104000 |
| C | -0.866589000 | -0.645825000 | -0.000079000 |
| O | -1.983086000 | -0.203100000 | -0.000040000 |



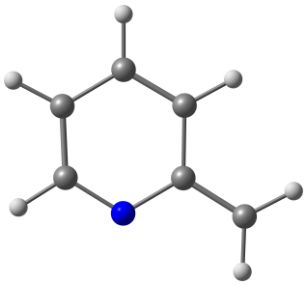
**1''g**

E = -286.795761 Hartree

G = -286.825364 Hartree




| | | | |
|---|---|---|---|
| C | -0.948268000 | -0.009262000 | 0.000005000 |
| C | -0.226917000 | 1.209638000 | 0.000004000 |
| C | 1.154425000 | 1.181451000 | -0.000001000 |
| C | 1.802011000 | -0.052604000 | -0.000003000 |
| C | 1.017870000 | -1.209480000 | -0.000001000 |
| H | -0.768620000 | 2.147740000 | 0.000006000 |
| H | 1.722826000 | 2.103908000 | -0.000002000 |
| H | 2.881464000 | -0.126883000 | -0.000009000 |
| H | 1.497054000 | -2.184356000 | -0.000004000 |
| N | -0.307037000 | -1.211536000 | 0.000005000 |
| C | -2.361091000 | -0.020141000 | -0.000005000 |
| H | -2.920629000 | 0.904878000 | -0.000011000 |
| H | -2.891013000 | -0.962149000 | -0.000008000 |



**Potassium iodide (KI)**

E = -611.431938 Hartree

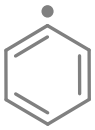
G = -611.457972 Hartree

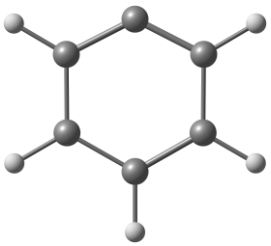

| | | | |
|---|---|---|---|
| K | -1.654663000 | 0.164886000 | 0.000000000 |
| I | -5.078041000 | 0.164886000 | 0.000000000 |

**Phenyl_Rad**

E = -231.42814 Hartree

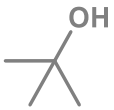
G = -231.456172 Hartree





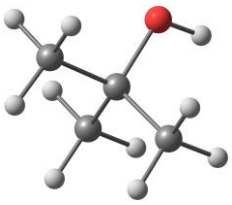
| | | | |
|---|---|---|---|
| C | 2.995229000 | -0.935460000 | -0.190949000 |
| C | 2.385539000 | -0.894468000 | 1.061710000 |
| C | 1.265568000 | -0.082140000 | 1.272558000 |
| C | 0.821517000 | 0.648728000 | 0.196589000 |
| C | 1.381878000 | 0.647740000 | -1.058405000 |
| C | 2.500677000 | -0.171629000 | -1.246746000 |
| H | 3.861734000 | -1.567102000 | -0.345529000 |
| H | 2.776480000 | -1.491695000 | 1.877669000 |
| H | 0.780712000 | -0.039720000 | 2.240975000 |
| H | 0.985927000 | 1.247382000 | -1.869792000 |
| H | 2.980863000 | -0.209322000 | -2.217990000 |

**tert-Butanol (*t*BuOH)**



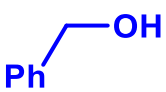

E = -233.500998 Hartree

G = -233.529920 Hartree



| | | | |
|---|---|---|---|
| C | -6.283638000 | 0.470007000 | -0.033862000 |
| O | -5.833097000 | 1.203312000 | 1.116351000 |
| C | -5.697985000 | -0.926120000 | 0.123785000 |
| H | -6.057153000 | -1.384170000 | 1.047944000 |
| H | -5.992244000 | -1.558153000 | -0.716366000 |
| H | -4.607499000 | -0.876115000 | 0.158175000 |
| C | -7.809923000 | 0.421265000 | -0.039899000 |
| H | -8.175521000 | -0.036485000 | 0.881832000 |
| H | -8.226445000 | 1.429743000 | -0.117583000 |
| H | -8.173495000 | -0.162337000 | -0.888724000 |
| C | -5.757853000 | 1.139628000 | -1.301572000 |
| H | -4.666931000 | 1.186309000 | -1.278440000 |
| H | -6.065589000 | 0.581021000 | -2.188441000 |
| H | -6.148644000 | 2.157629000 | -1.388546000 |
| H | -6.180426000 | 2.099625000 | 1.057672000 |

**2a**

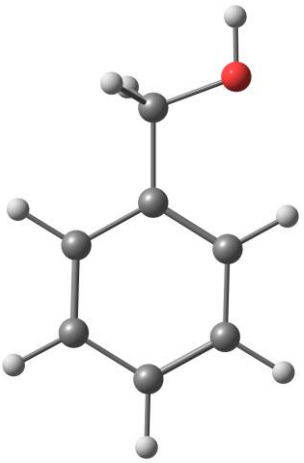



E = -346.592435 Hartree

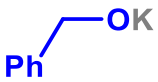
G = -346.625052 Hartree

| | | | |
|---|---|---|---|
| C | 3.032948000 | -0.890484000 | -0.153527000 |
| C | 2.226150000 | -1.047437000 | 0.967937000 |
| C | 1.059034000 | -0.296571000 | 1.107810000 |
| C | 0.690260000 | 0.617124000 | 0.123517000 |

| | | | |
|---|---|---|---|
| C | 1.501982000 | 0.768032000 | -1.003538000 |
| C | 2.666588000 | 0.022586000 | -1.141763000 |
| H | 3.939129000 | -1.474883000 | -0.260582000 |
| H | 2.502494000 | -1.756735000 | 1.739671000 |
| H | 0.430691000 | -0.419172000 | 1.980803000 |
| H | 1.217560000 | 1.474729000 | -1.777282000 |
| H | 3.287005000 | 0.149688000 | -2.021277000 |
| C | -0.552970000 | 1.462588000 | 0.246997000 |
| H | -0.260188000 | 2.509912000 | 0.386213000 |
| H | -1.123814000 | 1.399831000 | -0.686201000 |
| O | -1.333047000 | 1.016993000 | 1.343147000 |
| H | -2.080327000 | 1.612524000 | 1.444501000 |



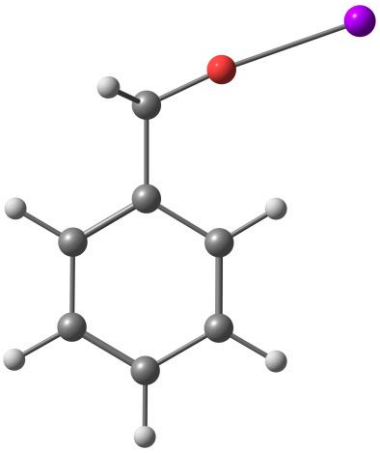
**2'a**




E = -945.987796 Hartree

G = -946.023890 Hartree

| | | | |
|---|---|---|---|
| C | 1.134019000 | 0.977174000 | 0.627279000 |
| C | 0.544668000 | 2.096352000 | 1.226500000 |
| C | 0.635012000 | 3.354391000 | 0.642266000 |
| C | 1.322421000 | 3.518056000 | -0.562188000 |
| C | 1.913368000 | 2.412748000 | -1.165672000 |
| C | 1.818973000 | 1.152384000 | -0.572309000 |
| H | 0.007765000 | 1.974131000 | 2.164111000 |
| H | 0.171324000 | 4.209683000 | 1.121576000 |
| H | 1.393981000 | 4.497337000 | -1.021306000 |
| H | 2.449422000 | 2.530744000 | -2.101410000 |
| H | 2.273759000 | 0.282075000 | -1.031540000 |
| C | 1.022679000 | -0.403523000 | 1.280629000 |
| H | 1.409820000 | -0.267105000 | 2.314841000 |
| H | -0.068297000 | -0.569847000 | 1.422513000 |
| O | 1.635831000 | -1.415725000 | 0.608200000 |
| K | 2.821869000 | -3.023439000 | -0.723111000 |



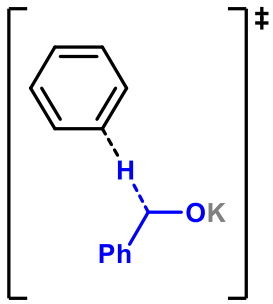
**TS_HAT1**

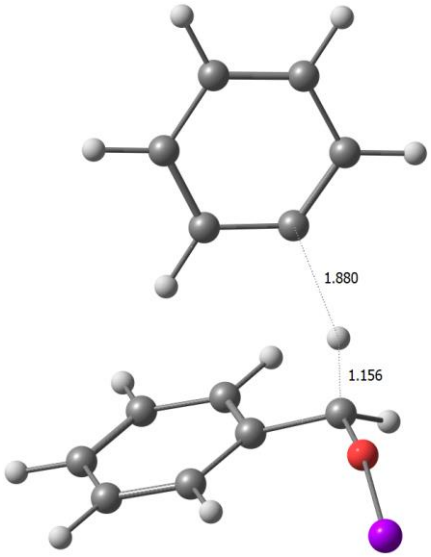
E = -1177.419993 Hartree

G = -1177.468552 Hartree

| | | | |
|---|---|---|---|
| C | -3.193389000 | 0.367484000 | -1.205208000 |
| C | -1.964067000 | 0.341331000 | -0.538388000 |

| | | | |
|---|---|---|---|
| C | -1.858636000 | -0.454591000 | 0.584314000 |
| C | -4.115508000 | -1.185638000 | 0.404396000 |
| C | -4.262175000 | -0.393058000 | -0.732628000 |
| H | -3.314194000 | 0.981666000 | -2.091023000 |
| H | -1.123813000 | 0.931090000 | -0.893257000 |
| H | -4.950333000 | -1.775700000 | 0.766817000 |
| H | -5.212585000 | -0.368183000 | -1.252687000 |
| C | 1.240806000 | 0.931589000 | 0.587718000 |
| C | 0.666241000 | 2.049167000 | 1.203491000 |
| C | 0.754218000 | 3.309352000 | 0.624514000 |
| C | 1.425063000 | 3.475711000 | -0.589158000 |
| C | 2.006420000 | 2.372081000 | -1.205657000 |
| C | 1.914145000 | 1.108980000 | -0.618721000 |
| H | 0.134095000 | 1.920346000 | 2.142867000 |
| H | 0.300893000 | 4.164449000 | 1.113883000 |
| H | 1.493910000 | 4.456962000 | -1.044421000 |
| H | 2.532333000 | 2.493866000 | -2.146564000 |
| H | 2.359308000 | 0.240056000 | -1.090256000 |
| C | 1.069818000 | -0.453646000 | 1.198656000 |
| H | 1.275363000 | -0.357408000 | 2.287302000 |
| H | -0.077345000 | -0.590509000 | 1.170768000 |
| O | 1.726200000 | -1.459318000 | 0.593431000 |
| K | 2.964889000 | -3.089509000 | -0.688379000 |
| C | -2.891292000 | -1.223598000 | 1.080958000 |
| H | -2.771152000 | -1.840281000 | 1.965335000 |



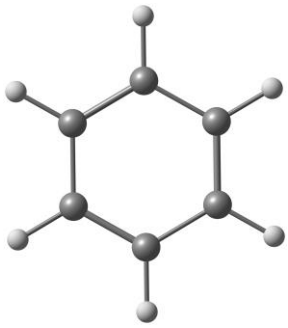

**Benzene (PhH)**

E = -232.100787 Hartree

G = -232.128244 Hartree

| | | | |
|---|---|---|---|
| C | 3.000568000 | -0.939332000 | -0.191891000 |
| C | 2.386215000 | -0.893400000 | 1.057121000 |
| C | 1.272193000 | -0.081475000 | 1.255770000 |
| C | 0.772579000 | 0.684465000 | 0.205312000 |
| C | 1.386922000 | 0.638554000 | -1.043718000 |
| C | 2.500940000 | -0.173384000 | -1.242326000 |

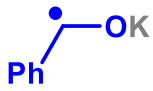
| | | | |
|---|---|---|---|
| H | 3.867364000 | -1.571187000 | -0.346490000 |
| H | 2.774982000 | -1.489418000 | 1.874477000 |
| H | 0.794036000 | -0.045586000 | 2.227636000 |
| H | 0.998084000 | 1.234606000 | -1.861009000 |
| H | 2.979033000 | -0.209212000 | -2.214232000 |
| H | -0.094209000 | 1.316320000 | 0.359909000 |



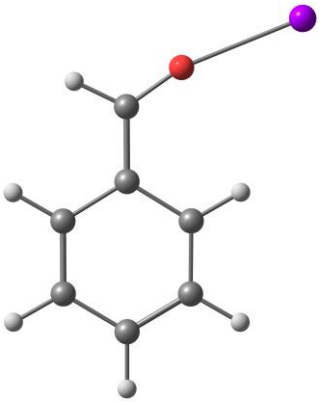
**2''a**

E = -945.390250 Hartree

G = -945.427120 Hartree



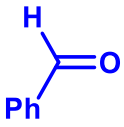

| | | | |
|---|---|---|---|
| C | 1.245965000 | 0.880754000 | 0.691327000 |
| C | 0.656644000 | 1.990792000 | 1.369308000 |
| C | 0.480006000 | 3.205578000 | 0.740042000 |
| C | 0.877287000 | 3.393356000 | -0.597462000 |
| C | 1.457794000 | 2.316029000 | -1.280462000 |
| C | 1.642591000 | 1.089708000 | -0.665514000 |
| H | 0.343773000 | 1.865697000 | 2.402368000 |
| H | 0.028567000 | 4.027967000 | 1.285897000 |
| H | 0.736869000 | 4.349016000 | -1.087209000 |
| H | 1.769495000 | 2.444320000 | -2.312709000 |
| H | 2.092294000 | 0.265145000 | -1.207271000 |
| C | 1.425845000 | -0.367670000 | 1.341320000 |
| H | 1.087875000 | -0.423294000 | 2.387789000 |
| O | 1.943370000 | -1.407754000 | 0.801029000 |
| K | 2.900178000 | -3.107367000 | -0.729403000 |



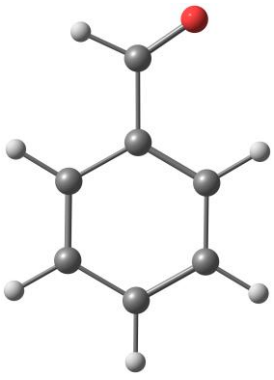
**2'''a**

E = -345.412710 Hartree

G = -345.443309 Hartree




| | | | |
|---|---|---|---|
| C | 3.036914000 | -0.890347000 | -0.175256000 |
| C | 2.366422000 | -0.915273000 | 1.049494000 |
| C | 1.195990000 | -0.189430000 | 1.212272000 |
| C | 0.694536000 | 0.563742000 | 0.146598000 |
| C | 1.365632000 | 0.587527000 | -1.076101000 |
| C | 2.539645000 | -0.141034000 | -1.237664000 |
| H | 3.951209000 | -1.458816000 | -0.298842000 |
| H | 2.761378000 | -1.501335000 | 1.870399000 |
| H | 0.659994000 | -0.194870000 | 2.154227000 |

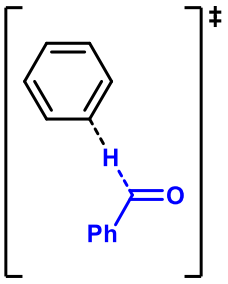


| | | | |
|---|---|---|---|
| H | 0.967472000 | 1.176218000 | -1.896252000 |
| H | 3.063886000 | -0.125371000 | -2.185203000 |
| C | -0.552053000 | 1.345936000 | 0.295834000 |
| H | -0.865329000 | 1.905244000 | -0.604213000 |
| O | -1.209244000 | 1.396451000 | 1.309896000 |

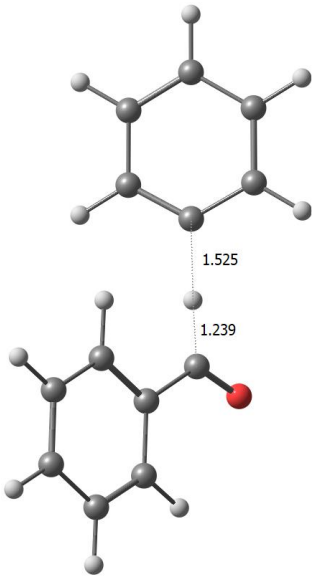
**TS_HAT2**

E = -576.836902 Hartree

G = -576.879964 Hartree



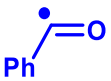

| | | | |
|---|---|---|---|
| C | -4.128268000 | -0.936920000 | -1.311027000 |
| C | -2.742672000 | -0.775539000 | -1.397855000 |
| C | -2.057116000 | -0.428835000 | -0.248934000 |
| C | -4.056496000 | -0.399333000 | 1.046796000 |
| C | -4.778524000 | -0.748637000 | -0.092883000 |
| H | -4.695856000 | -1.208846000 | -2.193999000 |
| H | -2.228622000 | -0.919937000 | -2.342291000 |
| H | -4.568295000 | -0.254972000 | 1.991761000 |
| H | -5.852969000 | -0.874910000 | -0.031393000 |
| C | 1.263584000 | 1.087827000 | -0.093702000 |
| C | 0.407064000 | 2.117428000 | 0.296246000 |
| C | 0.933423000 | 3.357915000 | 0.640994000 |
| C | 2.309802000 | 3.560158000 | 0.595211000 |
| C | 3.166942000 | 2.528988000 | 0.205113000 |
| C | 2.646903000 | 1.291048000 | -0.140514000 |
| H | -0.663569000 | 1.944674000 | 0.325178000 |
| H | 0.274908000 | 4.162454000 | 0.943831000 |
| H | 2.720585000 | 4.526132000 | 0.864365000 |
| H | 4.236517000 | 2.696919000 | 0.172942000 |
| H | 3.293220000 | 0.476590000 | -0.446291000 |
| C | 0.690722000 | -0.226520000 | -0.457242000 |
| H | -0.541802000 | -0.287832000 | -0.348996000 |
| O | 1.299456000 | -1.188438000 | -0.829541000 |
| C | -2.670439000 | -0.234613000 | 0.974747000 |
| H | -2.100873000 | 0.036075000 | 1.857927000 |




**2''''a**

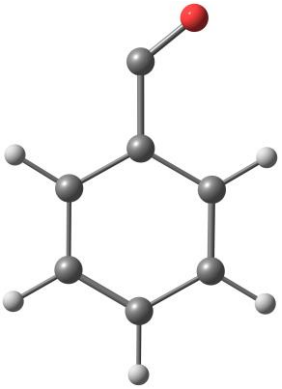
E = -344.771394 Hartree

G = -344.802698 Hartree

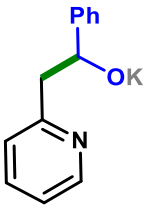



| | | | |
|---|---|---|---|
| C | 3.041815000 | -0.878518000 | -0.171928000 |
| C | 2.381376000 | -0.902227000 | 1.057702000 |

| | | | |
|---|---|---|---|
| C | 1.201261000 | -0.192589000 | 1.222849000 |
| C | 0.687263000 | 0.540901000 | 0.146786000 |
| C | 1.345229000 | 0.564945000 | -1.082210000 |
| C | 2.528059000 | -0.148195000 | -1.240315000 |
| H | 3.963804000 | -1.434351000 | -0.295355000 |
| H | 2.790103000 | -1.473784000 | 1.881991000 |
| H | 0.672892000 | -0.197369000 | 2.169058000 |
| H | 0.925346000 | 1.141169000 | -1.898618000 |
| H | 3.047169000 | -0.135727000 | -2.190499000 |
| C | -0.569541000 | 1.305246000 | 0.301705000 |
| O | -1.266697000 | 1.408293000 | 1.249562000 |



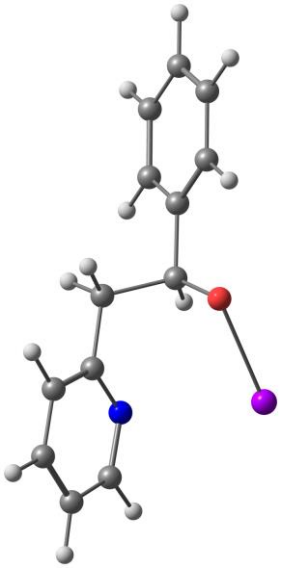
**3ga**




E = -1232.259569 Hartree

G = -1232.303729 Hartree

| | | | |
|---|---|---|---|
| C | 1.608708000 | -0.996833000 | -0.070913000 |
| C | 2.377657000 | -1.873729000 | 0.700695000 |
| C | 3.762140000 | -1.788567000 | 0.664474000 |
| C | 4.353194000 | -0.823535000 | -0.143133000 |
| C | 3.516497000 | 0.016426000 | -0.866168000 |
| H | 1.883793000 | -2.614621000 | 1.317770000 |
| H | 4.370191000 | -2.462600000 | 1.256712000 |
| H | 5.428008000 | -0.716013000 | -0.209434000 |
| H | 3.937967000 | 0.791643000 | -1.500219000 |
| N | 2.181938000 | -0.054570000 | -0.834664000 |
| C | 0.106517000 | -1.104375000 | -0.090487000 |
| H | -0.192035000 | -1.625357000 | -1.008837000 |
| H | -0.219069000 | -1.719257000 | 0.754595000 |
| C | -2.113448000 | 0.002143000 | -0.050934000 |
| C | -2.893505000 | 0.126640000 | 1.096971000 |
| C | -4.260980000 | -0.146230000 | 1.065314000 |
| C | -4.869669000 | -0.543496000 | -0.121999000 |
| C | -4.099888000 | -0.664958000 | -1.278815000 |
| C | -2.735563000 | -0.393842000 | -1.239026000 |
| H | -2.406718000 | 0.450443000 | 2.009364000 |
| H | -4.853813000 | -0.043823000 | 1.967956000 |
| H | -5.933142000 | -0.751282000 | -0.149804000 |
| H | -4.565749000 | -0.965596000 | -2.210865000 |
| H | -2.143154000 | -0.483140000 | -2.146126000 |
| C | -0.604461000 | 0.274102000 | 0.004480000 |

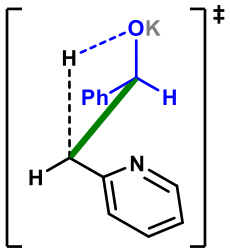


| | | | |
|---|---|---|---|
| H | -0.376800000 | 0.783026000 | -0.964380000 |
| O | -0.197736000 | 0.987275000 | 1.087463000 |
| K | 1.394507000 | 2.596731000 | 0.000182000 |

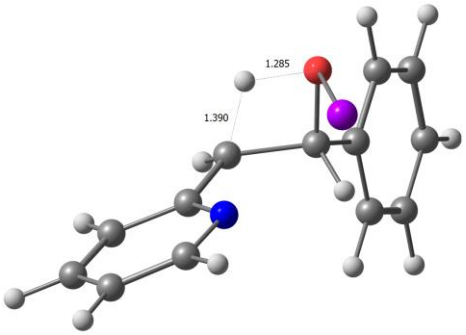
**TS2**

E = -1232.207752 Hartree

G = -1232.251276 Hartree




| | | | |
|---|---|---|---|
| C | 1.617161000 | 0.017754000 | 0.727681000 |
| C | 2.948562000 | -0.288492000 | 1.103869000 |
| C | 3.882473000 | -0.616834000 | 0.145314000 |
| C | 3.500013000 | -0.647948000 | -1.200726000 |
| C | 2.181755000 | -0.341398000 | -1.491793000 |
| H | 3.215812000 | -0.264631000 | 2.154083000 |
| H | 4.900491000 | -0.855665000 | 0.433361000 |
| H | 4.195800000 | -0.903790000 | -1.988634000 |
| H | 1.839287000 | -0.356314000 | -2.523994000 |
| N | 1.259048000 | -0.015637000 | -0.577583000 |
| C | 0.641572000 | 0.434258000 | 1.724453000 |
| H | 0.914035000 | 0.171938000 | 2.745082000 |
| H | 0.159538000 | 1.698081000 | 1.403944000 |
| C | -1.710996000 | -0.033782000 | 2.535775000 |
| C | -2.427077000 | 0.914183000 | 3.263401000 |
| C | -3.196461000 | 0.533132000 | 4.363548000 |
| C | -3.260578000 | -0.802422000 | 4.746602000 |
| C | -2.549978000 | -1.759348000 | 4.020557000 |
| C | -1.784079000 | -1.375424000 | 2.926175000 |
| H | -2.377280000 | 1.949987000 | 2.950837000 |
| H | -3.748894000 | 1.282425000 | 4.919841000 |
| H | -3.859519000 | -1.099210000 | 5.599715000 |
| H | -2.596826000 | -2.803574000 | 4.308709000 |
| H | -1.231329000 | -2.122571000 | 2.363489000 |
| C | -0.840595000 | 0.363068000 | 1.361790000 |
| H | -1.026416000 | -0.354528000 | 0.546568000 |
| O | -1.033374000 | 1.710419000 | 0.926520000 |
| K | -0.877123000 | 1.467520000 | -1.639558000 |



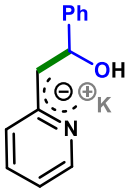

**3''ga**

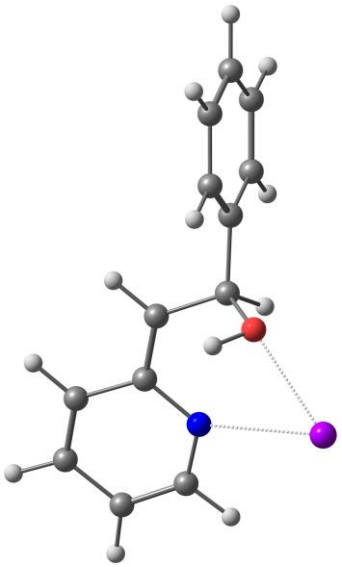
E = -1232.243506 Hartree

G = -1232.288063 Hartree

| | | | |
|---|---|---|---|
| C | 1.524681000 | -0.982985000 | 0.180782000 |

| | | | |
|---|---|---|---|
| C | 2.257732000 | -2.202052000 | 0.436494000 |
| C | 3.597014000 | -2.278870000 | 0.181690000 |
| C | 4.281980000 | -1.154191000 | -0.338119000 |
| C | 3.526585000 | -0.016097000 | -0.548854000 |
| H | 1.716209000 | -3.056921000 | 0.827599000 |
| H | 4.132815000 | -3.203250000 | 0.374424000 |
| H | 5.341260000 | -1.171617000 | -0.555022000 |
| H | 4.015155000 | 0.876223000 | -0.941002000 |
| N | 2.215720000 | 0.110407000 | -0.304950000 |
| C | 0.154091000 | -0.902468000 | 0.412586000 |
| H | -0.374241000 | -1.777443000 | 0.772113000 |
| H | -0.129492000 | 0.974523000 | 1.843553000 |
| C | -2.105112000 | 0.004347000 | -0.054118000 |
| C | -2.927627000 | -0.060651000 | 1.071265000 |
| C | -4.270925000 | -0.408637000 | 0.949084000 |
| C | -4.810930000 | -0.690595000 | -0.303221000 |
| C | -3.998255000 | -0.621075000 | -1.432836000 |
| C | -2.655931000 | -0.275467000 | -1.305684000 |
| H | -2.515312000 | 0.169261000 | 2.047581000 |
| H | -4.897647000 | -0.456135000 | 1.832470000 |
| H | -5.857010000 | -0.956883000 | -0.399051000 |
| H | -4.411110000 | -0.831773000 | -2.412798000 |
| H | -2.024450000 | -0.222835000 | -2.187478000 |
| C | -0.628241000 | 0.311347000 | 0.074868000 |
| H | -0.285014000 | 0.735009000 | -0.878737000 |
| O | -0.428426000 | 1.402445000 | 1.033008000 |
| K | 1.554517000 | 2.768094000 | -0.126141000 |



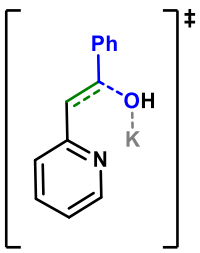



**TS3**

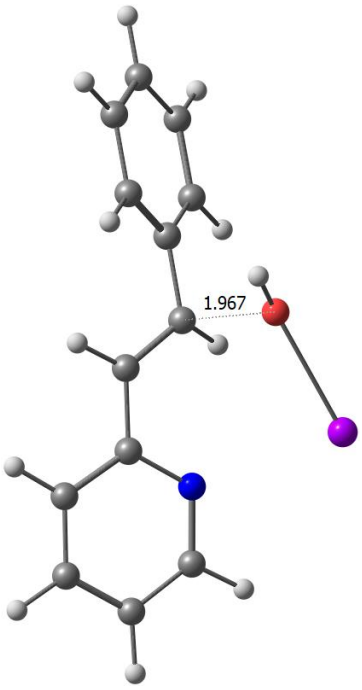
E = -1232.228116 Hartree

G = -1232.272161 Hartree

| | | | |
|---|---|---|---|
| C | 1.711319000 | -0.164552000 | 0.775113000 |
| C | 3.066544000 | -0.175395000 | 1.200308000 |
| C | 4.063421000 | -0.555455000 | 0.330600000 |
| C | 3.726655000 | -0.930523000 | -0.976592000 |
| C | 2.386911000 | -0.879664000 | -1.324294000 |
| H | 3.298074000 | 0.109428000 | 2.220258000 |
| H | 5.097599000 | -0.567423000 | 0.656998000 |



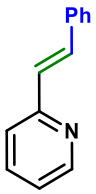
| | | | |
|---|---|---|---|
| H | 4.473610000 | -1.239151000 | -1.695596000 |
| H | 2.083326000 | -1.149780000 | -2.333420000 |
| N | 1.400673000 | -0.501953000 | -0.502739000 |
| C | 0.670222000 | 0.194480000 | 1.694568000 |
| H | 0.982265000 | 0.590117000 | 2.654446000 |
| H | -1.436692000 | 2.265858000 | 0.954290000 |
| C | -1.689444000 | 0.182789000 | 2.475617000 |
| C | -1.561891000 | 1.102808000 | 3.523523000 |
| C | -2.512731000 | 1.164021000 | 4.535473000 |
| C | -3.611060000 | 0.305148000 | 4.521756000 |
| C | -3.751364000 | -0.609651000 | 3.481992000 |
| C | -2.800955000 | -0.664864000 | 2.466282000 |
| H | -0.718172000 | 1.784371000 | 3.538389000 |
| H | -2.399742000 | 1.885811000 | 5.336342000 |
| H | -4.351721000 | 0.353421000 | 5.311192000 |
| H | -4.603236000 | -1.279632000 | 3.459245000 |
| H | -2.918593000 | -1.375344000 | 1.654557000 |
| C | -0.676572000 | 0.090287000 | 1.394031000 |
| H | -0.950032000 | -0.584723000 | 0.589242000 |
| O | -1.345602000 | 1.575611000 | 0.292287000 |
| K | -0.656897000 | 0.724102000 | -1.943930000 |




**3ga** still in interaction with **KOH**

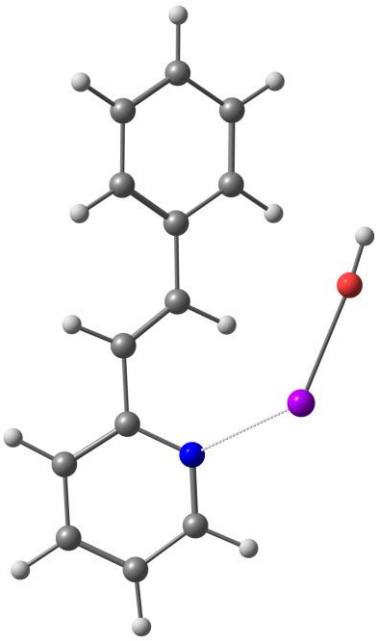
E = -1232.249745 Hartree

G = -1232.297197 Hartree




| | | | |
|---|---|---|---|
| C | 2.083242000 | -0.431797000 | -0.091581000 |
| C | 3.420994000 | -0.521938000 | 0.307088000 |
| C | 4.389724000 | -0.835354000 | -0.635475000 |
| C | 4.000528000 | -1.045051000 | -1.952657000 |
| C | 2.650608000 | -0.915555000 | -2.264756000 |
| H | 3.684253000 | -0.355745000 | 1.344553000 |
| H | 5.430840000 | -0.914968000 | -0.346355000 |
| H | 4.717519000 | -1.291621000 | -2.724538000 |
| H | 2.311296000 | -1.053202000 | -3.287060000 |
| N | 1.710561000 | -0.612457000 | -1.370149000 |
| C | 1.043696000 | -0.142464000 | 0.908544000 |
| H | 1.404668000 | 0.229021000 | 1.862711000 |
| H | -3.294067000 | 2.016322000 | -1.334876000 |
| C | -1.339699000 | -0.118325000 | 1.679578000 |
| C | -1.156281000 | 0.641528000 | 2.843408000 |

| | | | |
|---|---|---|---|
| C | -2.204056000 | 0.834978000 | 3.733380000 |
| C | -3.457415000 | 0.278897000 | 3.478051000 |
| C | -3.655810000 | -0.468450000 | 2.321272000 |
| C | -2.606219000 | -0.660829000 | 1.429258000 |
| H | -0.194876000 | 1.097110000 | 3.049828000 |
| H | -2.046542000 | 1.427806000 | 4.626699000 |
| H | -4.273378000 | 0.434510000 | 4.173651000 |
| H | -4.627614000 | -0.899196000 | 2.111123000 |
| H | -2.764081000 | -1.239972000 | 0.525416000 |
| C | -0.262121000 | -0.365797000 | 0.711705000 |
| H | -0.570610000 | -0.807438000 | -0.233232000 |
| O | -2.430680000 | 1.838932000 | -1.711641000 |
| K | -0.215073000 | 1.210434000 | -2.429757000 |



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