Supporting Information

Table of Contents

1. General information S-1

2. General Procedure for the C-Alkylation S-2

3. Characterization data for all compounds S-3

4. ^{1}H and ^{13}C NMR spectra for all compounds S-9

5. Computational details S-39

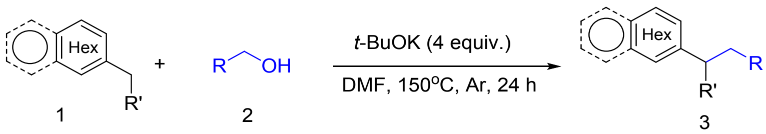
6. References S-49

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 under argon then kept in a Schenck tube. All other commercial reagents were purchased from Sigma-Aldrich, Alfa Aesar, TCI, and Acros and used as received, without further purification. All reagents were weighed in the air.

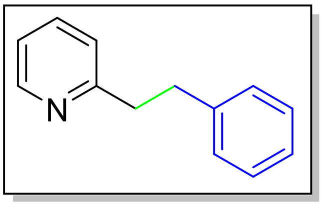
^{1}H and ^{13}C NMR spectra were recorded on a Varian Inova 400 MHz spectrometer or on a Bruker Avance 400 MHz spectrometer in $CDCl_3$. For ^{1}H NMR (400 MHz), $CDCl_3$ served as internal standard (δ = 7.27 ppm and 0 ppm) and data are reported as follows: chemical shift (in ppm), multiplicity (s = 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 (δ = 77.2 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 Alkylation reaction of methyl substituted N-heteroaromatics with alcohols

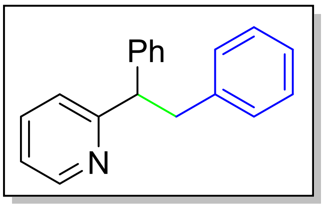


A flame-dried Schlenk flask was equipped with a stirring bar under argon was charged with KO*t*Bu (2.0 mmol, 4.0 equiv, 224 mg). The flask was evacuated and back-filled with argon 3 times. Then, the N-heteroaromatics **1** (0.5 mmol, 1.0 equiv), the alcohol **2** (2 mmol, 4.0 equiv), the solvent (2 mL) was successively added. The reaction mixture was stirred and heated at the required temperature for a fixed reaction time. After allowing the reaction to cool to room temperature, the reaction mixture was diluted with water (10 mL) and stirring was continued for additional 0.5 h. After extraction with ethyl acetate (3 x 5 mL), the organic layer washed with brine (3 x 5 mL), dried over anhydrous $MgSO_4$, and filtered. The solvent was evaporated under reduced pressure to give crude product **3-5**. Conversions were measured by comparing the relative integrations (^{1}H NMR as well as GC-MS) of the internal standard with the expected product. The crude product **3** was purified by chromatography on silica gel (eluent: hexane/ethyl acetate or hexane/ethyl acetate/triethylamine) to afford the desired product. In addition, two paralleled scale-up (5 mmol scale) reaction were performed under the optimal conditions: quinaldine (**1d,** 5 mmol), benzyl alcohol (**2a**, 20 mmol) were used as experimental reagents, and both of them can give excellent yield of **3da** in 75% (standard conditions) or 80% (using mixture solvent: 1.6 mL DMF + 14 mL toluene).

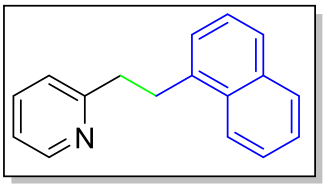
3. Characterization data for all compounds



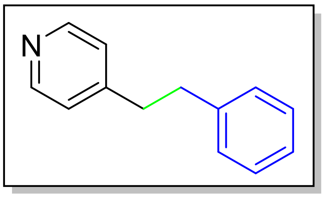
2-phenethylpyridine (3aa):[1]
Eluent: Hexane/EtOAc = 10:2 (yellow oil). 70 % isolated yield (78% in NMR). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.56 (ddd, *J* = 4.9, 1.9, 0.9 Hz, 1H), 7.56 (td, *J* = 7.7, 1.9 Hz, 1H), 7.30-7.25 (m, 2H), 7.20 (dt, *J* = 8.0, 2.0 Hz, 3H), 7.13-7.04 (m, 2H), 3.12-3.03 (m, 4H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 161.28, 149.39, 141.64, 136.43, 128.57, 128.46, 126.04, 123.10, 121.29, 40.36, 36.15.



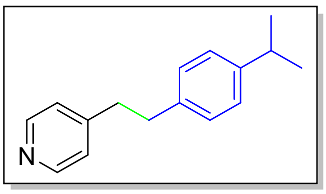
2-(1,2-diphenylethyl)pyridine (3ba):[2]
Eluent: Hexane/EtOAc = 10:2 (yellow oil). 28 % isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.62-8.58 (m, 1H), 7.52 (td, *J* = 7.7, 1.9 Hz, 1H), 7.36-7.24 (m, 4H), 7.20-7.04 (m, 8H), 4.38 (t, *J* = 7.8 Hz, 1H), 3.67 (dd, *J* = 13.7, 8.0 Hz, 1H), 3.37 (dd, *J* = 13.7, 7.5 Hz, 1H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 163.03, 149.27, 143.38, 140.48, 136.55, 129.19, 128.53, 128.28, 128.18, 126.60, 125.96, 123.41, 121.53, 55.52, 41.39.



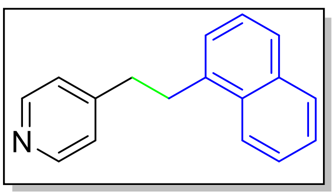
2-(2-(naphthalen-1-yl)ethyl)pyridine (3ab):[3]
Eluent: Hexane/EtOAc = 10:4 (yellow oil). 70 % isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.63 (ddd, *J* = 4.9, 1.9, 0.9 Hz, 1H), 8.19-8.14 (m, 1H), 7.90-7.86 (m, 1H), 7.74 (dt, *J* = 8.2, 1.1 Hz, 1H), 7.57-7.48 (m, 3H), 7.39 (dd, *J* = 8.1, 7.0 Hz, 1H), 7.35-7.31 (m, 1H), 7.13 (ddd, *J* = 7.5, 4.9, 1.2 Hz, 1H), 7.07 (dt, *J* = 7.7, 1.1 Hz, 1H), 3.57-3.52 (m, 2H), 3.27-3.23 (m, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 161.45, 149.49, 137.73, 136.36, 133.95, 131.90, 128.86, 126.86, 126.15, 125.97, 125.62, 125.55, 123.83, 123.06, 121.28, 39.53, 33.27.



4-phenethylpyridine (3ca):[3]
Eluent: Hexane/EtOAc = 1:1 (yellow oil), 70 % isolated yield (75% in NMR). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.41 (d, *J* = 5.1 Hz, 2H), 7.23-7.18 (m, 2H), 7.15-7.11 (m, 1H), 7.09-7.06 (m, 2H), 7.02-7.00 (m, 2H), 2.86 (s, 4H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 150.80, 149.62, 140.73, 128.59, 128.45, 126.37, 124.12, 37.19, 36.67.

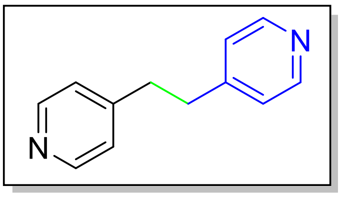


4-(4-isopropylphenethyl)pyridine (3cc):
Eluent: Hexane/EtOAc/NEt_3 = 10:3:1 (yellow oil), 66 % isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.51-8.47 (m, 2H), 7.17-7.14 (m, 2H), 7.11-7.08 (m, 4H), 2.91 (m, 5H), 1.25 (s, 3H), 1.23 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 150.80, 149.82, 146.96, 138.17, 128.40, 126.67, 124.05, 37.22, 36.26, 33.83, 24.18. **HRMS:** m/z $[M+H]^+$ calculated for C20H19N: 226.1590; measured: 226.1595.

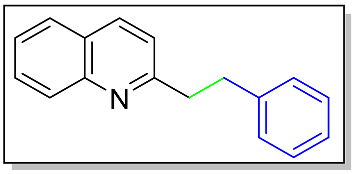


4-(2-(naphthalen-1-yl)ethyl)pyridine (3cb):[4]
Eluent: Hexane/EtOAc = 1:3 (yellow oil), 90 % isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.56-8.46 (m, 2H), 8.05 (dq, *J* = 8.6, 0.9 Hz, 1H), 7.89 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.75 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.57-7.49 (m, 2H), 7.37 (dd, *J* = 8.3, 7.0 Hz, 1H), 7.23 (dd, *J* = 6.9, 1.2 Hz, 1H), 7.14-7.09 (m, 2H), 3.42-3.36 (m, 2H), 3.09-3.03 (m, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 150.79, 149.83, 136.73, 134.03, 131.70, 129.09, 127.23, 126.30, 126.18, 125.72,

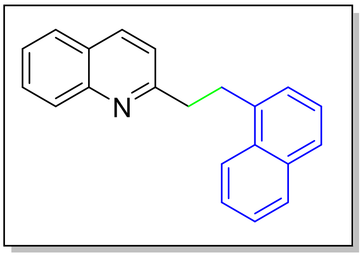
125.61, 124.05, 123.43, 36.30, 33.86.



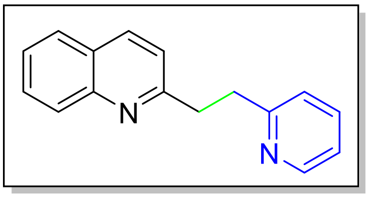
1,2-di(pyridin-4-yl)ethane (3cd): [5]
Eluent: CH_3COCH_3/MeOH = 5:1 (yellow oil), 90 % isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.49-8.45 (m, 4H), 7.06-7.03 (m, 4H), 2.91 (s, 4H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 149.92, 149.52, 123.88, 35.75.



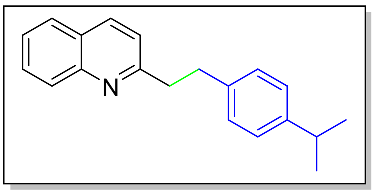
2-phenethylquinoline (3da):[6]
Eluent: Hexane/EtOAc = 10:2 (yellow oil), 76 % isolated yield (80% in NMR). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.06 (d, J = 8.5 Hz, 1H), 8.02 (d, J = 8.4 Hz, 1H), 7.75 (dd, J = 8.1, 1.4 Hz, 1H), 7.68 (ddd, J = 8.4, 6.8, 1.5 Hz, 1H), 7.47 (ddd, J = 8.0, 6.8, 1.1 Hz, 1H), 7.28 – 7.16 (m, 6H), 3.30 – 3.24 (m, 2H), 3.16 – 3.10 (m, 2H). **^{13}C NMR (101 MHz, 400 MHz, $CDCl_3$)** δ 161.89, 147.93, 141.56, 136.45, 129.59, 128.85, 128.63, 128.51, 127.65, 126.89, 126.12, 125.96, 121.69, 41.07, 36.09.



2-(2-(naphthalen-1-yl)ethyl)quinoline (3db):[7]
Eluent: Hexane/EtOAc = 10:1 (light brown solid), 81% isolated yield (83% in NMR). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.22 (dd, J = 8.4, 1.3 Hz, 1H), 8.17 (dd, J = 8.4, 1.0 Hz, 1H), 8.03 (d, J = 8.4 Hz, 1H), 7.90 (dd, J = 7.8, 1.6 Hz, 1H), 7.80 (dd, J = 8.1, 1.4 Hz, 1H), 7.75 (ddt, J = 8.5, 6.8, 1.8 Hz, 2H), 7.59 – 7.50 (m, 3H), 7.42 – 7.36 (m, 2H), 7.21 (d, J = 8.4 Hz, 1H), 3.69 – 3.63 (m, 2H), 3.49 – 3.43 (m, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 161.97, 148.04, 137.60, 136.35, 133.94, 131.88, 129.54, 128.93, 128.90, 127.64, 126.92, 126.89, 126.20, 126.02, 125.92, 125.66, 125.60, 123.83, 121.68, 40.11, 33.08.

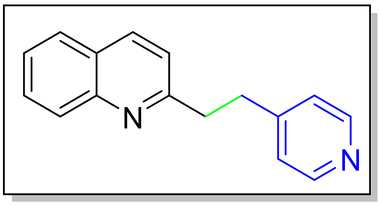


2-(2-(pyridin-2-yl)ethyl)quinoline (3de):[8]
Eluent: EtOAc/MeOH = 30:1 (brown solid), 80% isolated yield (82% in NMR) , **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.47 (ddd, J = 4.9, 1.9, 0.9 Hz, 1H), 7.98 (dq, J = 8.5, 0.9 Hz, 1H), 7.93 (dd, J = 8.4, 0.8 Hz, 1H), 7.68-7.65 (m, 1H), 7.59 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H), 7.45 (td, J = 7.6, 1.8 Hz, 1H), 7.38 (ddd, J = 8.1, 6.9, 1.2 Hz, 1H), 7.17 (s, 1H), 7.08 (dt, J = 7.8, 1.1 Hz, 1H), 7.00 (ddd, J = 7.5, 4.9, 1.2 Hz, 1H), 3.35 (ddd, J = 8.9, 6.3, 1.2 Hz, 2H), 3.28-3.23 (m, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 161.72, 161.07, 149.32, 147.94, 136.42, 136.35, 129.44, 128.86, 127.59, 126.86, 125.86, 123.19, 121.66, 121.27, 38.85, 38.03.

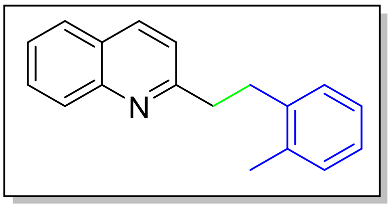


2-(4-isopropylphenethyl)quinoline (3dc):[7]
Eluent: Hexane/EtOAc = 10:1 (yellow oil), 60% isolated yield (75% in NMR). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.02 – 7.95 (m, 2H), 7.70 (dd, J = 8.1, 1.4 Hz, 1H), 7.62 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H), 7.41 (ddd, J = 8.1, 6.8, 1.2 Hz, 1H), 7.18 (d, J = 8.4 Hz, 1H), 7.12 (d, J = 5.8 Hz, 2H), 7.07 (d, J = 8.2 Hz, 2H), 3.23-3.18 (m, 2H), 3.07-3.01 (m, 2H), 2.80 (p, J = 6.9 Hz, 1H), 1.17 (s, 3H), 1.16 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 162.13, 148.08, 146.65, 138.97, 136.36, 129.51, 128.98, 128.52, 127.65, 126.92, 126.56, 125.89,

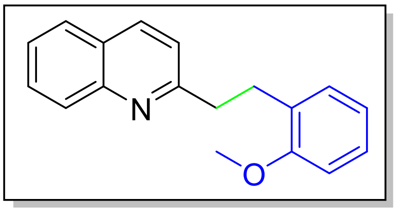
121.68, 41.23, 35.69, 33.83, 24.20.



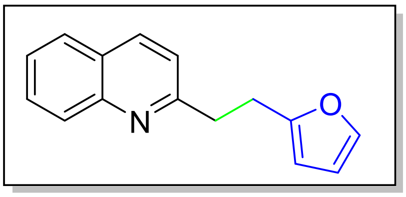
2-(2-(pyridin-4-yl)ethyl)quinoline (3dd):
Eluent: EtOAc/MeOH = 20:1 (brown solid), 70% isolated yield (84% in NMR). **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.44 (s, 2H), 8.01 (dd, J = 9.9, 8.3 Hz, 2H), 7.73 (dd, J = 8.2, 1.4 Hz, 1H), 7.66 (ddd, J = 8.4, 6.8, 1.5 Hz, 1H), 7.45 (td, J = 7.5, 6.8, 1.1 Hz, 1H), 7.16 (d, J = 8.4 Hz, 1H), 7.11 (d, J = 5.2 Hz, 2H), 3.27-.21 (m, 2H), 3.16-3.09 (m, 2H). **^{13}C NMR (101 MHz, CDCl$_3$)** δ 160.62, 150.48, 149.67, 147.91, 136.46, 129.59, 128.80, 127.58, 126.83, 126.01, 123.99, 121.40, 39.36, 34.77. **HRMS:** m/z [M+H]$^+$ calculated for C16H15N2: 235.1230; measured: 235.1238



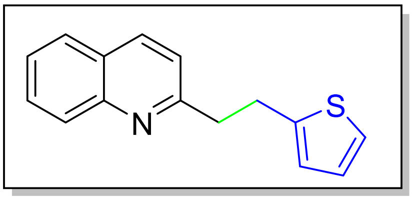
2-(2-methylphenethyl)quinoline (**3df**):[7]
Eluent: Hexane/EtOAc = 10:1 (yellow oil), 73% isolated yield (76% in NMR). **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.12 (dd, J = 8.5, 1.0 Hz, 1H), 8.06 (d, J = 8.3 Hz, 1H), 7.79 (dd, J = 8.1, 1.4 Hz, 1H), 7.72 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H), 7.51 (ddd, J = 8.1, 6.8, 1.2 Hz, 1H), 7.25-7.20 (m, 2H), 7.19-7.13 (m, 3H), 3.30-3.25 (m, 2H), 3.18-3.13 (m, 2H), 2.36 (s, 3H). **^{13}C NMR (101 MHz, CDCl$_3$)** δ 162.05,148.00, 139.75, 136.40, 136.13, 130.31, 129.56, 128.96, 128.93, 127.64, 126.90, 126.27, 126.14, 125.94, 121.62, 39.74, 33.37, 19.49.



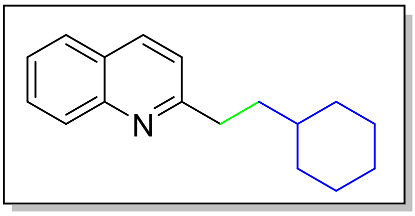
2-(2-methoxyphenethyl)quinoline (**3dg**):[5]
Eluent: Hexane/EtOAc = 10:2 (yellow oil), 65% isolated yield (70% in NMR). **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.11 (dq, J = 8.5, 0.9 Hz, 1H), 8.03 (dd, J = 8.5, 0.8 Hz, 1H), 7.79 – 7.76 (m, 1H), 7.70 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H), 7.49 (ddd, J = 8.1, 6.9, 1.2 Hz, 1H), 7.26 (d, J = 2.6 Hz, 1H), 7.23 – 7.16 (m, 2H), 6.88 (t, J = 7.2 Hz, 2H), 3.82 (s, 3H), 3.32 – 3.27 (m, 2H), 3.20 – 3.15 (m, 2H). **^{13}C NMR (101 MHz, CDCl$_3$)** δ 162.58, 157.56, 147.93, 136.13, 130.06, 129.86, 129.36, 128.88, 127.55, 127.37, 126.84, 125.74, 121.70, 120.46, 110.25, 55.28, 39.32, 30.73.



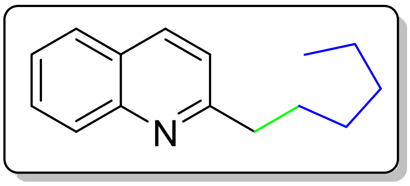
2-(2-(furan-2-yl)ethyl)quinoline (**3dh**):[7]
Eluent: Hexane/EtOAc = 10:2 (yellow oil), 63% isolated yield (78% in NMR). **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.08 (dq, J = 8.5, 0.9 Hz, 1H), 8.02 (dd, J = 8.4, 0.8 Hz, 1H), 7.77-7.73 (m, 1H), 7.68 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H), 7.48 (ddd, J = 8.2, 6.9, 1.2 Hz, 1H), 7.32 (dd, J = 1.9, 0.9 Hz, 1H), 7.20 (s, 1H), 6.26 (dd, J = 3.2, 1.9 Hz, 1H), 6.00 (dt, J = 3.2, 0.9 Hz, 1H), 3.363.31 (m, 2H), 3.23-3.17 (m, 2H). **^{13}C NMR (101 MHz, CDCl$_3$)** δ 161.23, 155.13, 147.89, 141.02, 136.39, 129.51, 128.85, 127.57, 126.87, 125.92, 121.37, 110.22, 105.46, 37.40, 27.95.



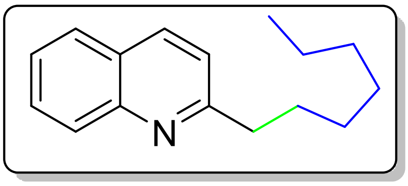
2-(2-(thiophen-2-yl)ethyl)quinoline (**3di**):[7]
Eluent: Hexane/EtOAc = 10:2 (yellow oil), 23% isolated yield (32% in NMR). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.13-8.07 (m, 2H), 7.80 (dd, J = 8.1, 1.4 Hz, 1H), 7.72 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H), 7.52 (ddd, J = 8.2, 6.9, 1.2 Hz, 1H), 7.28 (s, 1H), 7.11 (dd, J = 5.1, 1.2 Hz, 1H), 6.90 (dd, J = 5.1, 3.4 Hz, 1H), 6.82 (dt, J = 3.4, 1.0 Hz, 1H), 3.44-3.35 (m, 4H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 161.12, 144.22, 129.81, 127.69, 127.01, 126.88, 126.63, 126.19, 124.77, 123.38, 122.26, 121.69, 100.12, 40.95, 29.87.



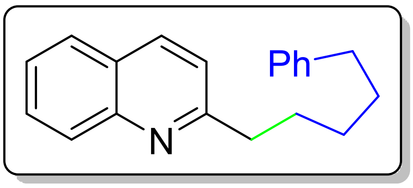
2-(2-cyclohexylethyl)quinoline (**3dj**): [6]
Eluent: Hexane/EtOAc = 10:2 (colorless liquid), 50% isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.96 (dd, J = 8.5, 5.3 Hz, 2H), 7.67 (dd, J = 8.1, 1.4 Hz, 1H), 7.61-7.56 (m, 1H), 7.38 (dd, J = 8.1, 6.8 Hz, 1H), 7.19 (s, 1H), 3.01 – 2.86 (m, 2H), 1.73 (dd, J = 12.7, 3.6 Hz, 2H), 1.67-1.53 (m, 5H), 1.26 (tp, J = 10.8, 3.2 Hz, 1H), 1.19-1.04 (m, 3H), 0.89 (qd, J = 12.0, 3.3 Hz, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 163.53, 147.92, 136.30, 129.40, 128.84, 127.55, 126.76, 125.70, 121.44, 37.86, 37.82, 36.94, 33.37, 26.75, 26.45.



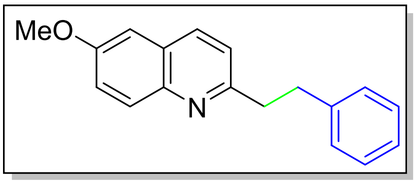
2-hexylquinoline (**3dk**):[9]
Eluent: Hexane/EtOAc = 10:1(light yellow oil), 56% isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.06-8.03 (m, 2H), 7.77-7.74 (m, 1H), 7.69-7.65 (m, 1H), 7.49-7.44 (m, 1H), 7.28 (d, J = 8.4 Hz, 1H), 2.99-2.94 (m, 2H), 1.85-1.77 (m, 2H), 1.45-1.39 (m, 2H), 1.36-1.29 (m, 4H), 0.90-0.86 (m, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 163.23, 148.04, 136.24, 129.39, 128.95, 127.57, 126.82, 125.71, 121.46, 39.52, 31.86, 30.15, 29.36, 22.69, 14.19.



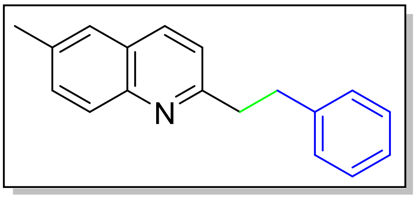
2-heptylquinoline (**3dl**):[7]
Eluent: Hexane/EtOAc = 10:1(light yellow oil), 66% isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.04 (d, J = 8.4 Hz, 2H), 7.76 (dd, J = 8.1, 1.6 Hz, 1H), 7.69-7.65 (m, 1H), 7.49-7.45 (m, 1H), 7.27 (s, 1H), 2.99-2.94 (m, 2H), 1.85-1.77 (m, 2H), 1.42-1.34 (m, 4H), 1.28 (td, J = 4.4, 2.6 Hz, 4H), 0.90-0.86 (m, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 163.25, 148.06, 136.24, 129.39, 128.98, 127.58, 126.82, 125.71, 121.47, 39.54, 31.90, 30.21, 29.67, 29.33, 22.77, 14.20.



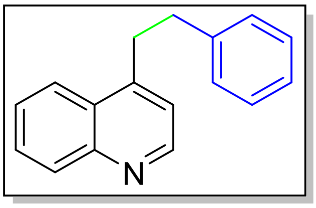
2-(5-phenylpentyl)quinoline (**3dm**) **:**
Eluent: Hexane/EtOAc = 10:1(light yellow oil), 56% isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.09-8.04 (m, 2H), 7.78 (dd, J = 8.1, 1.4 Hz, 1H), 7.69 (ddd, J = 8.4, 6.8, 1.5 Hz, 1H), 7.49 (ddd, J = 8.1, 6.9, 1.2 Hz, 1H), 7.30-7.25 (m, 3H), 7.21-7.16 (m, 3H), 3.02-2.96 (m, 2H), 2.66-2.61 (m, 2H), 1.92-1.84 (m, 2H), 1.71 (ddd, J = 15.4, 8.4, 6.8 Hz, 2H), 1.53-1.45 (m, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 163.01, 148.02, 142.76, 136.28, 129.42, 128.93, 128.48, 128.32, 127.57, 126.81, 125.74, 125.69, 121.45, 39.36, 35.91, 31.43, 29.98, 29.25. **HRMS:** m/z $[M+H]^+$ calculated for C20H22N: 276.1747; measured: 276.1752



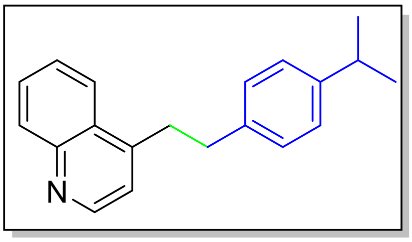
6-methoxy-2-phenethylquinoline (**3ea**):[6]
Eluent: Hexane/EtOAc = 10:2 (yellow oil), 31% isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.96-7.88 (m, 2H), 7.32 (dd, *J* = 9.2, 2.8 Hz, 1H), 7.26-7.19 (m, 4H), 7.18-7.12 (m, 2H), 7.00 (d, *J* = 2.8 Hz, 1H), 3.87 (s, 3H), 3.25-3.19 (m, 2H), 3.13-3.07 (m, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 159.28, 157.36, 143.93, 141.66, 135.30, 130.21, 128.63, 128.49, 127.76, 126.08, 122.13, 121.92, 105.25, 55.62, 40.78, 36.21.



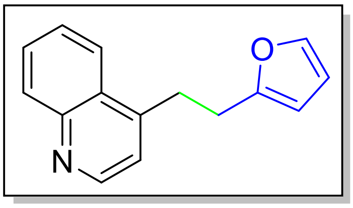
6-methyl-2-phenethylquinoline (**3fa**):[7]
Eluent: Hexane/EtOAc = 10:2 (yellow oil), 75 % isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.98 (ddd, *J* = 17.2, 8.7, 0.8 Hz, 2H), 7.56-7.52 (m, 2H), 7.31-7.25 (m, 4H), 7.23-7.18 (m, 2H), 3.32-3.26 (m, 2H), 3.19-3.14 (m, 2H), 2.53 (d, *J* = 0.9 Hz, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 160.89, 146.51, 141.64, 135.78, 135.68, 131.80, 128.61, 128.52, 128.47, 126.91, 126.51, 126.07, 121.62, 40.93, 36.10, 21.59.



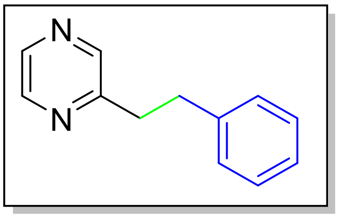
4-phenethylquinoline (**3ga**): [6]
Eluent: Hexane/EtOAc = 10:4 (yellow oil), 61 % isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.70 (d, *J* = 4.4 Hz, 1H), 8.06 (dt, *J* = 8.5, 0.8 Hz, 1H), 7.99 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.63 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.49 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 1H), 7.22 (dd, *J* = 8.0, 6.5 Hz, 2H), 7.17-7.14 (m, 1H), 7.14-7.11 (m, 2H), 7.09 (d, *J* = 4.4 Hz, 1H), 3.32-3.27 (m, 2H), 3.01-2.96 (m, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 150.22, 148.33, 147.59, 141.03, 130.34, 129.22, 128.65, 128.47, 127.51, 126.57, 126.43, 123.47, 120.97, 36.24, 34.18.



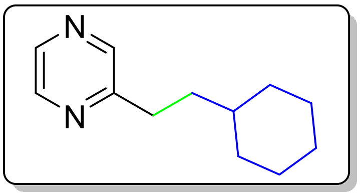
4-(4-isopropylphenethyl)quinoline (**3gc**): [6]
Eluent: Hexane/EtOAc = 10:4 (yellow oil), 78 % isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.80 (d, *J* = 4.4 Hz, 1H), 8.15 (ddd, *J* = 8.3, 1.3, 0.6 Hz, 1H), 8.07 (ddd, *J* = 8.5, 1.5, 0.6 Hz, 1H), 7.72 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.57 (ddd, *J* = 8.3, 6.8, 1.4 Hz, 1H), 7.22-7.15 (m, 5H), 3.41-3.35 (m, 2H), 3.08-3.02 (m, 2H), 2.92 (td, *J* = 6.9, 2.4 Hz, 1H), 1.28 (s, 3H), 1.26 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 150.28, 148.39, 147.74, 147.03, 138.40, 130.35, 129.14, 128.35, 127.55, 126.67, 126.49, 123.50, 120.89, 35.84, 34.18, 33.84, 24.18.



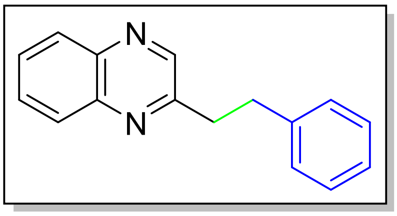
4-(2-(furan-2-yl)ethyl)quinoline (**3gh**): [6] Eluent: Hexane/EtOAc = 10:6 (yellow oil), 36 % isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.80 (d, *J* = 4.4 Hz, 1H), 8.13 (dd, *J* = 8.6, 1.3 Hz, 1H), 8.04 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.71 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.56 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 1H), 7.35 (dd, *J* = 1.9, 0.8 Hz, 1H), 7.19 (d, *J* = 4.4 Hz, 1H), 6.28 (dd, *J* = 3.2, 1.9 Hz, 1H), 5.99 (dt, *J* = 3.2, 0.9 Hz, 1H), 3.44-3.40 (m, 2H), 3.11-3.06 (m, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 154.42, 150.29, 148.43, 147.01, 141.35, 130.41, 129.20, 127.47, 126.59, 123.38, 120.87, 110.36, 105.80, 30.76, 28.50.



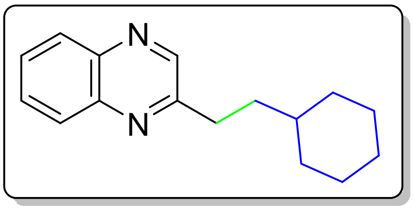
2-phenethylpyrazine (**3ha**): [6] Eluent: Hexane/EtOAc = 10:7 (yellow oil), 60 % isolated yield (80% in NMR).**^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.51 (dd, J = 2.6, 1.6 Hz, 1H), 8.39 (d, J = 2.6 Hz, 1H), 8.35 (d, J = 1.6 Hz, 1H), 7.29-7.24 (m, 2H), 7.21-7.15 (m, 3H), 3.15-3.10 (m, 2H), 3.09-3.04 (m, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 156.80, 144.75, 144.16, 142.39, 140.81, 128.57, 128.47, 126.30, 37.28, 35.44.



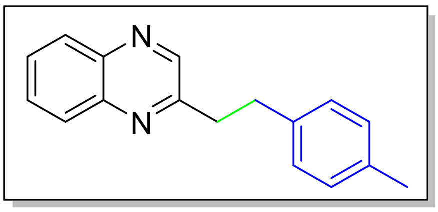
2-(2-cyclohexylethyl)pyrazine (**3hj**):[4]
Eluent: Hexane/EtOAc=10:4 (colorless oil), 35% isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.46 (dd, J = 2.5, 1.6 Hz, 1H), 8.43 (d, J = 1.6 Hz, 1H), 8.36 (d, J = 2.5 Hz, 1H), 2.83-2.77 (m, 2H), 1.78-1.59 (m, 7H), 1.30-1.14 (m, 4H), 0.98-0.88 (m, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 158.48, 144.67, 144.09, 142.09, 37.52, 37.22, 33.28, 33.10, 26.69, 26.39.



2-phenethylquinoxaline (**3ia**):[6]
Eluent: Hexane/EtOAc = 10:2 (yellow oil), 57 % isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.52 (s, 1H), 8.00-7.95 (m, 2H), 7.67-7.58 (m, 2H), 7.21-7.16 (m, 2H), 7.14-7.08 (m, 3H), 3.23 (dd, J = 9.4, 6.4 Hz, 2H), 3.08 (dd, J = 9.4, 6.4 Hz, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 156.46, 145.87, 142.24, 141.32, 140.79, 130.06, 129.27, 129.15, 128.91, 128.61, 128.52, 126.35, 38.17, 35.34.



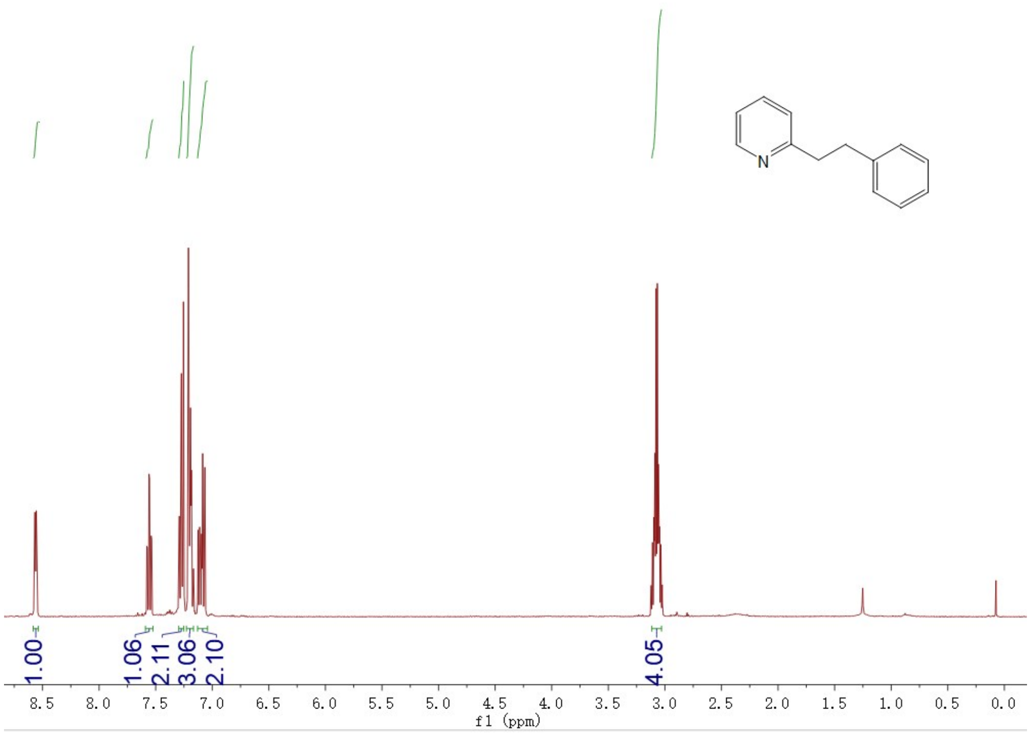
2-(2-cyclohexylethyl)quinoxaline (**3ij**):[4]
Eluent: Hexane/EtOAc = 10:4(red oil), 55% isolated yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.72 (s, 1H), 8.07-8.01 (m, 2H), 7.74-7.66 (m, 2H), 3.03-2.98 (m, 2H), 1.80 (ddt, J = 10.4, 3.7, 1.6 Hz, 2H), 1.74-1.68 (m, 4H), 1.66-1.62 (m, 1H), 1.37-1.31 (m, 1H), 1.25-1.14 (m, 3H), 1.02-0.93 (m, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 158.15, 145.96, 142.31, 141.27, 129.97, 129.26, 128.95, 128.94, 37.74, 37.24, 34.15, 33.31, 26.69, 26.39.



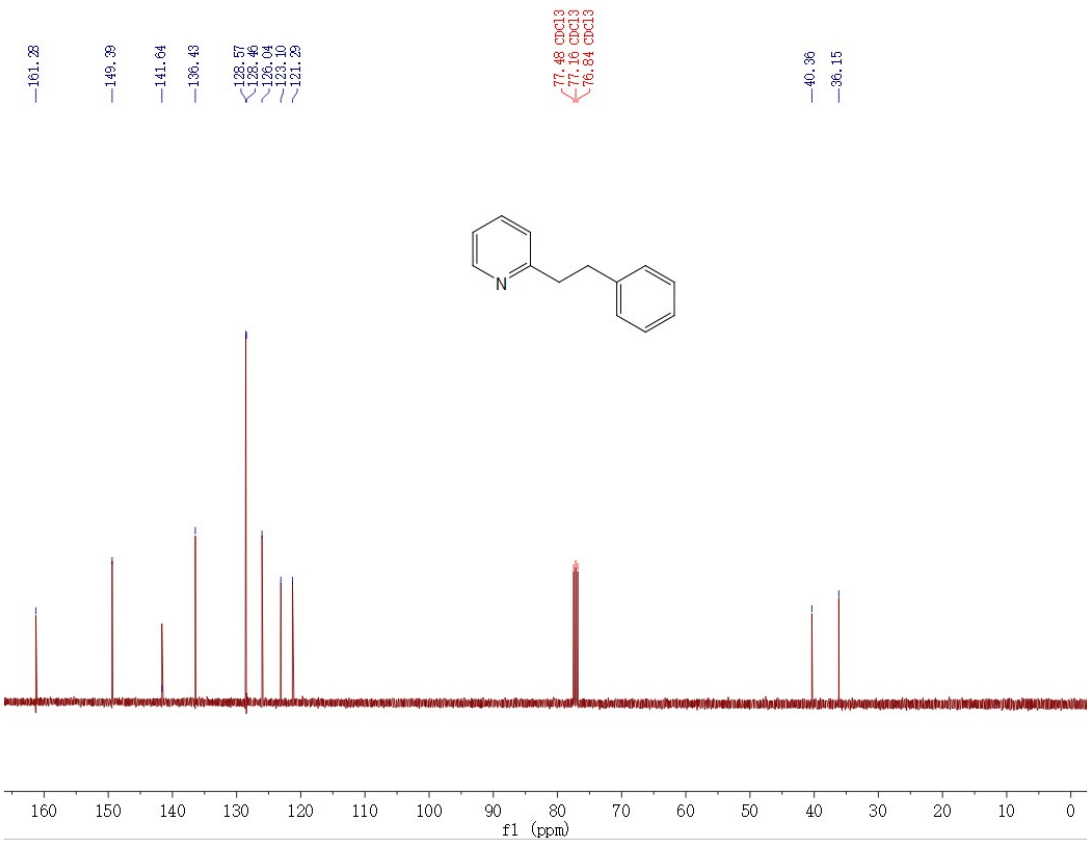
2-(4-methylphenethyl)quinoxaline (**3in**):[7]
Eluent: Hexane/EtOAc = 10:2 (yellow oil), 69% isolated yield (76% in NMR). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.61 (s, 1H), 8.10-8.05 (m, 2H), 7.77-7.68 (m, 2H), 7.14-7.08 (m, 4H), 3.31 (dd, J = 9.2, 6.4 Hz, 2H), 3.15 (dd, J = 9.4, 6.5 Hz, 2H), 2.31 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 156.59, 145.90, 142.24, 141.29, 137.66, 135.80, 130.03, 129.28, 129.25, 129.11, 128.90, 128.39, 38.33, 34.97, 21.10.

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

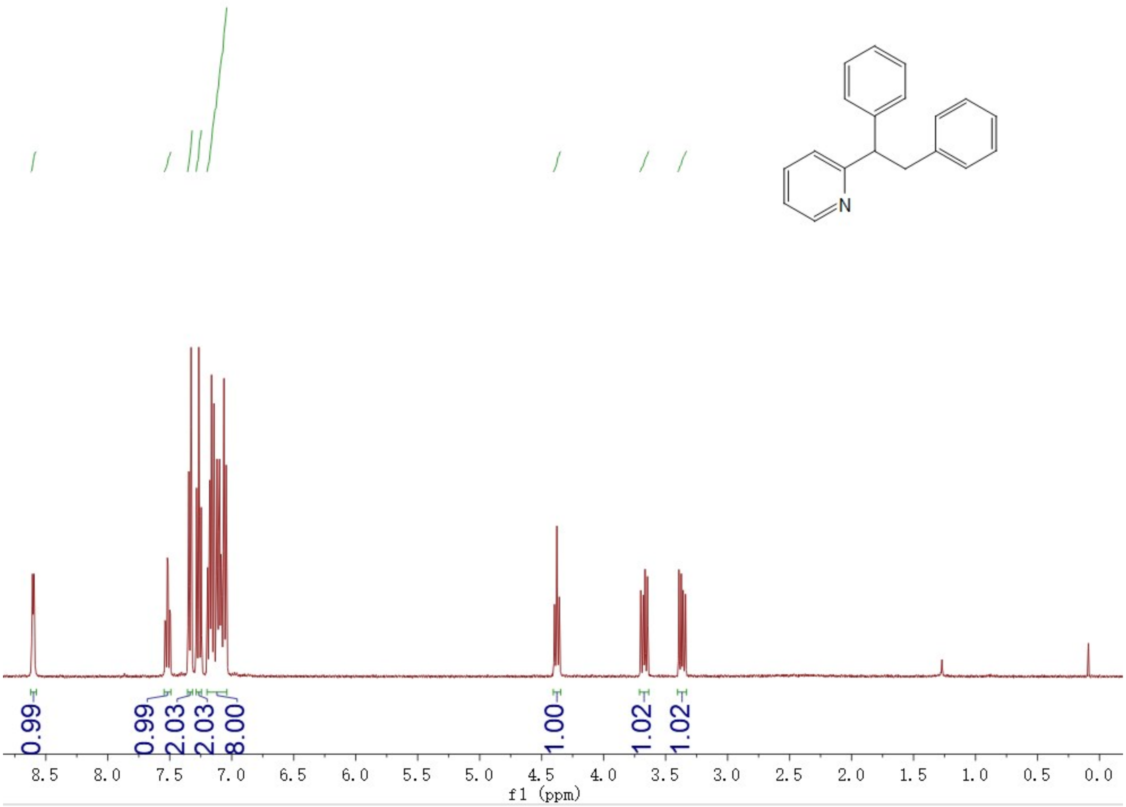
2-phenethylpyridine (3aa), ^{1}H NMR (400 MHz, $CDCl_3$)



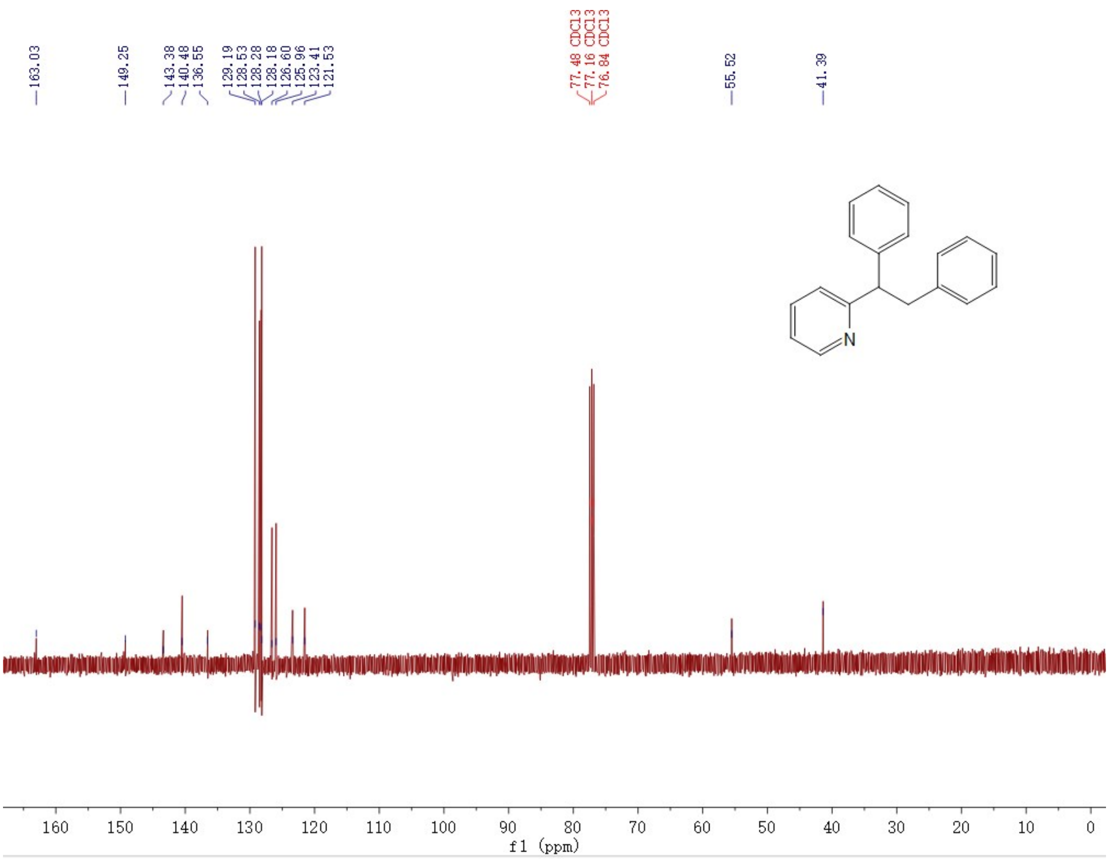
2-phenethylpyridine (3aa), ^{13}C NMR (101 MHz, $CDCl_3$)



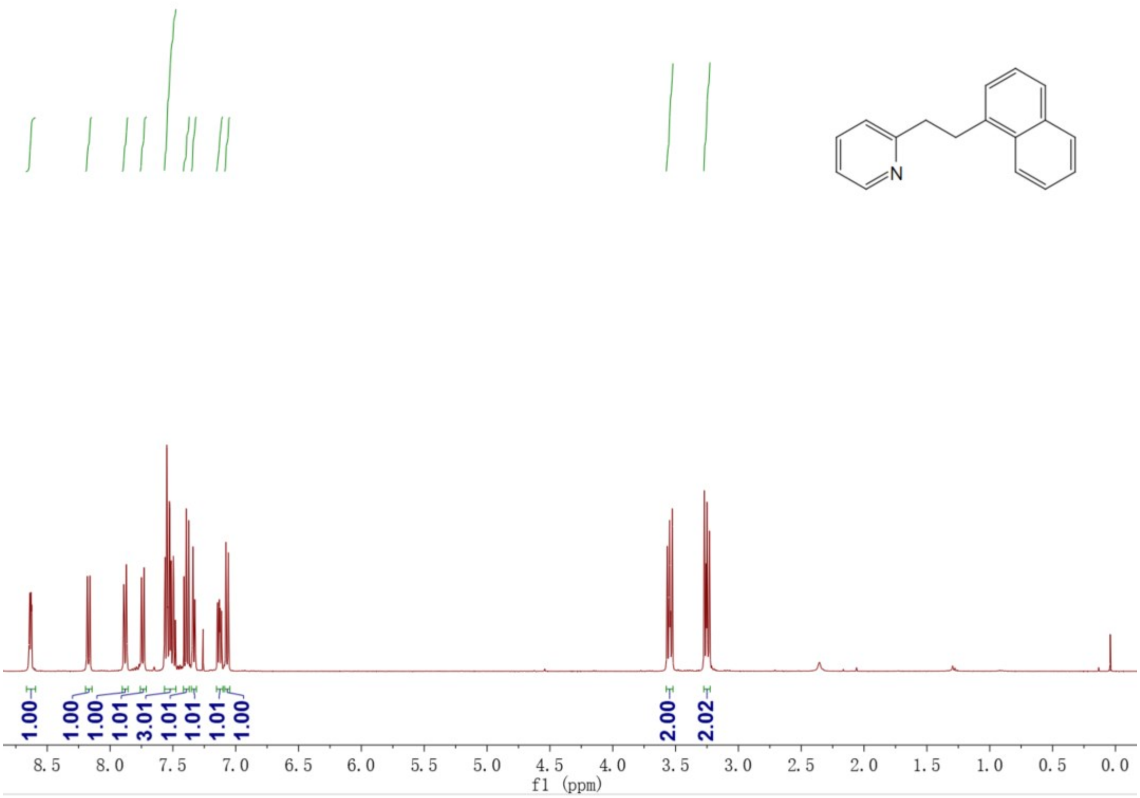
2-(1,2-diphenylethyl)pyridine (3ba), ^{1}H NMR (400 MHz, CDCl$_3$)



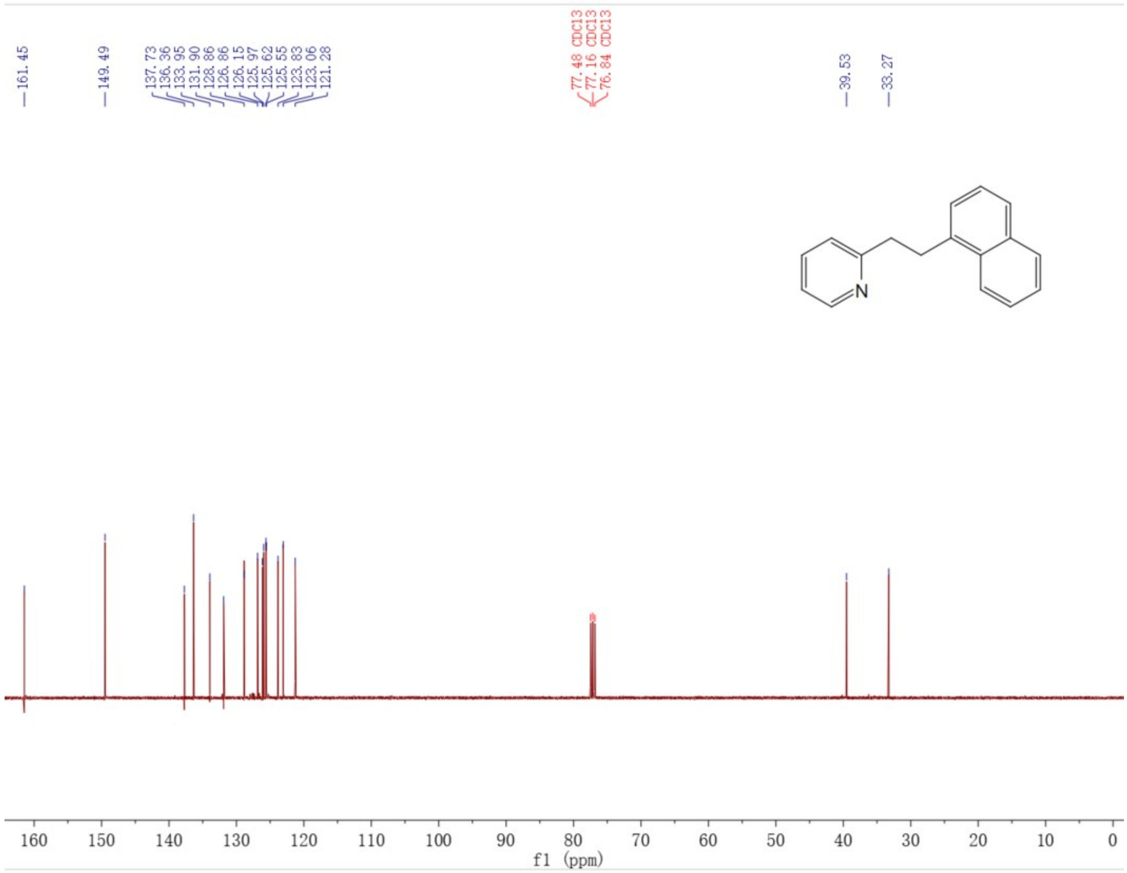
2-(1,2-diphenylethyl)pyridine (3ba), ^{13}C NMR (101 MHz, CDCl$_3$)



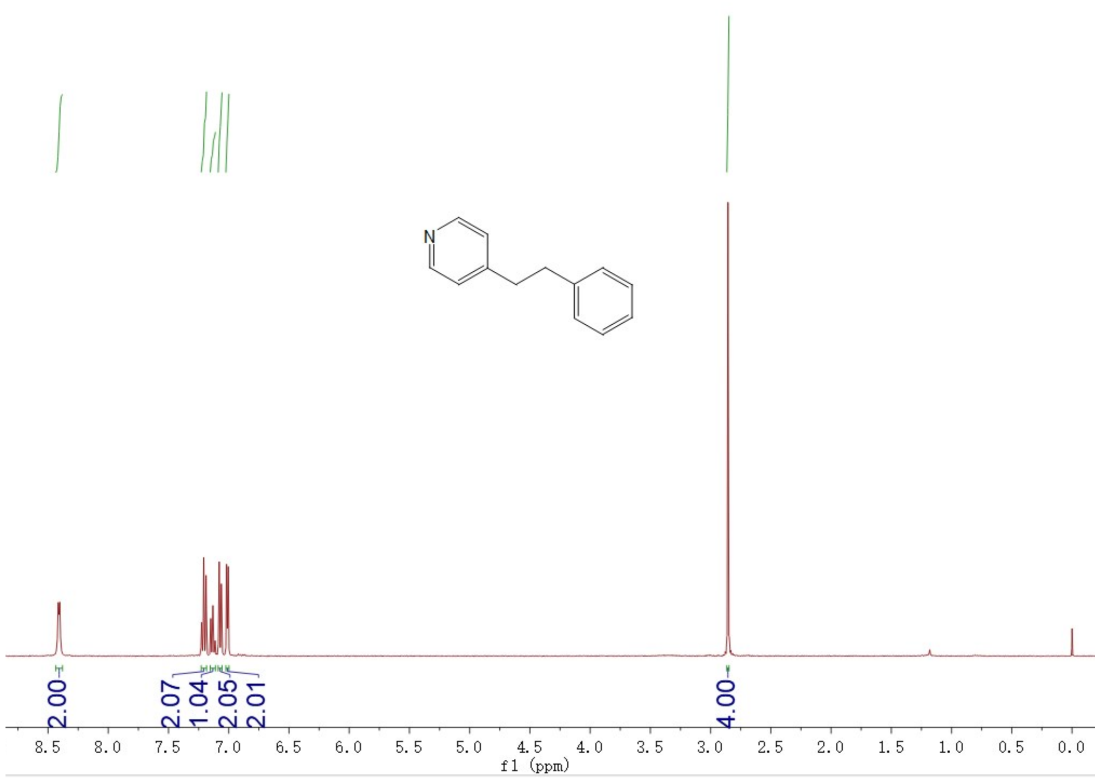
2-(2-(naphthalen-1-yl)ethyl)pyridine (3ab), ^{1}H NMR (400 MHz, $CDCl_3$)



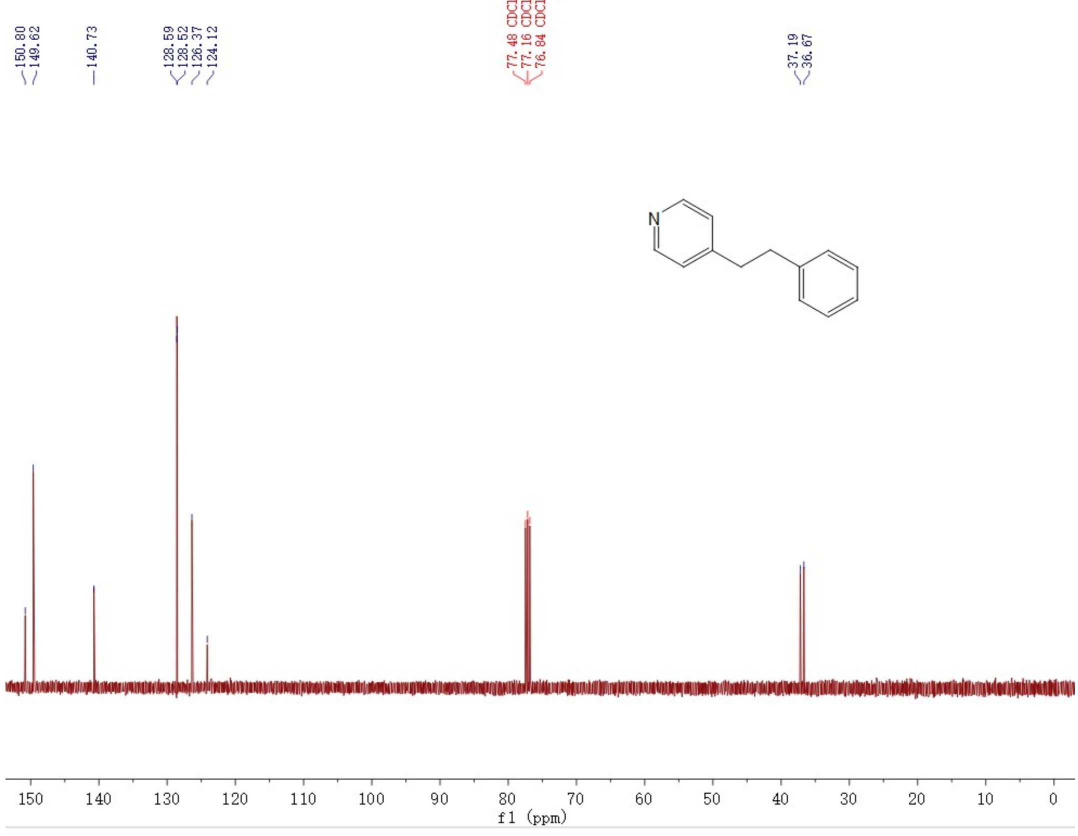
2-(2-(naphthalen-1-yl)ethyl)pyridine (3ab), ^{13}C NMR (101 MHz, $CDCl_3$)



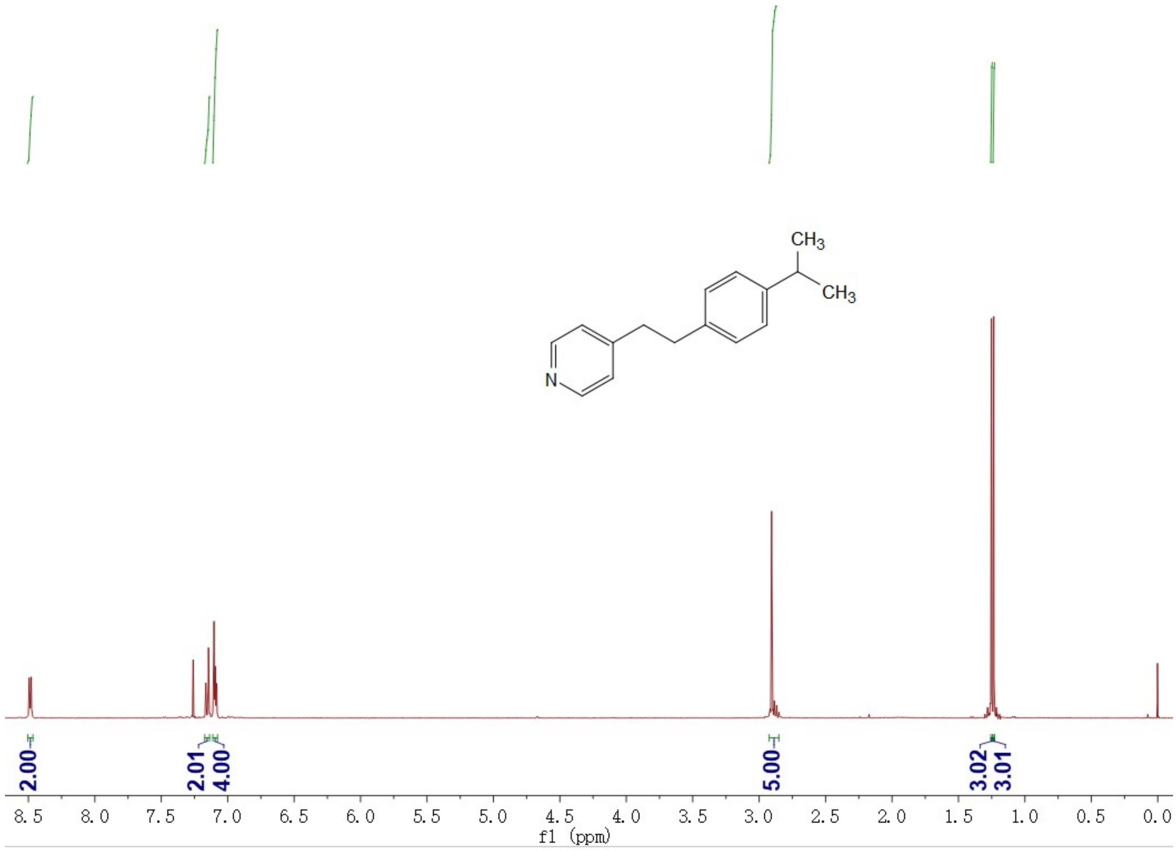
4-phenethylpyridine (3ca), ^{1}H NMR (400 MHz, CDCl$_3$)



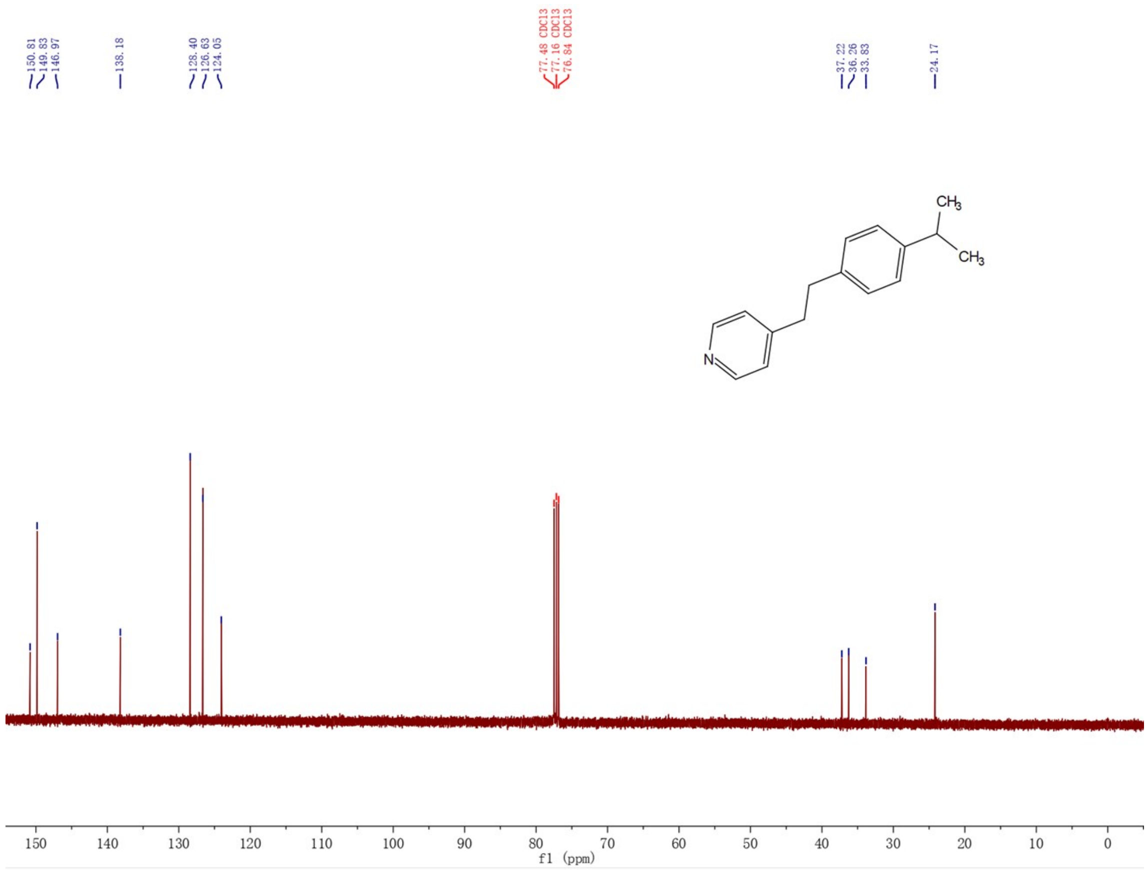
4-phenethylpyridine (3ca), ^{13}C NMR (101 MHz, CDCl$_3$)



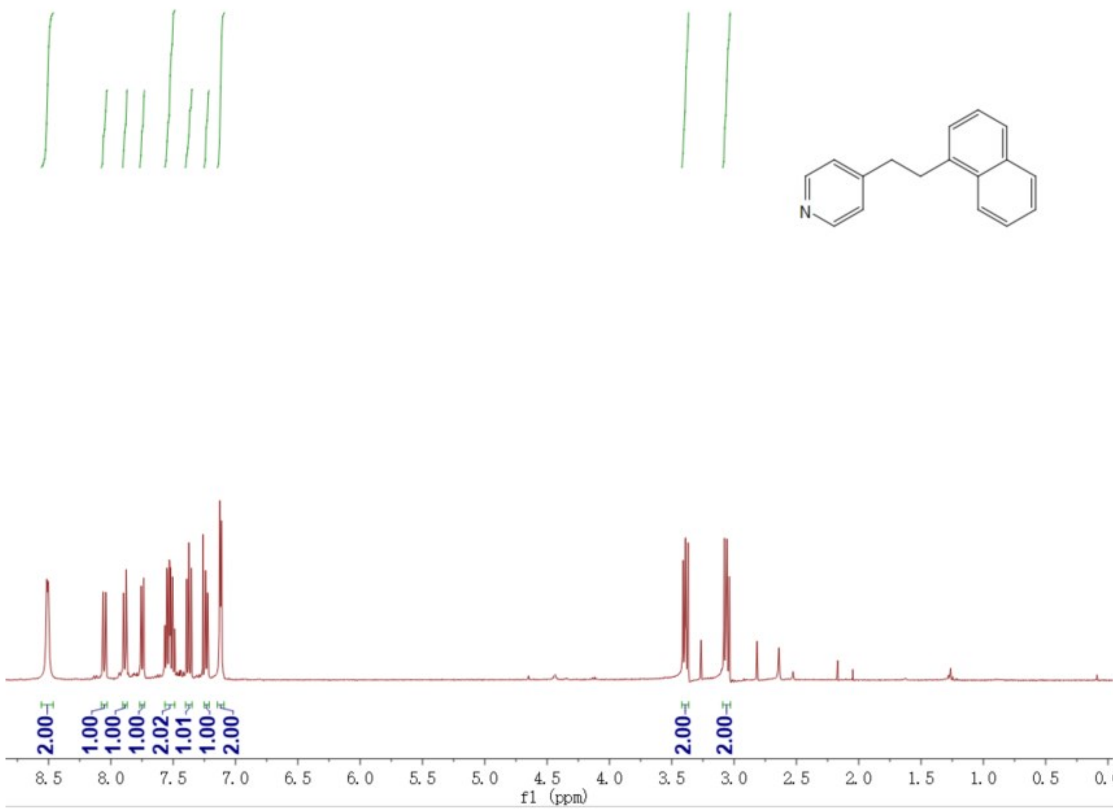
4-(4-isopropylphenethyl)pyridine (3cc), ^{1}H NMR (400 MHz, CDCl$_3$)



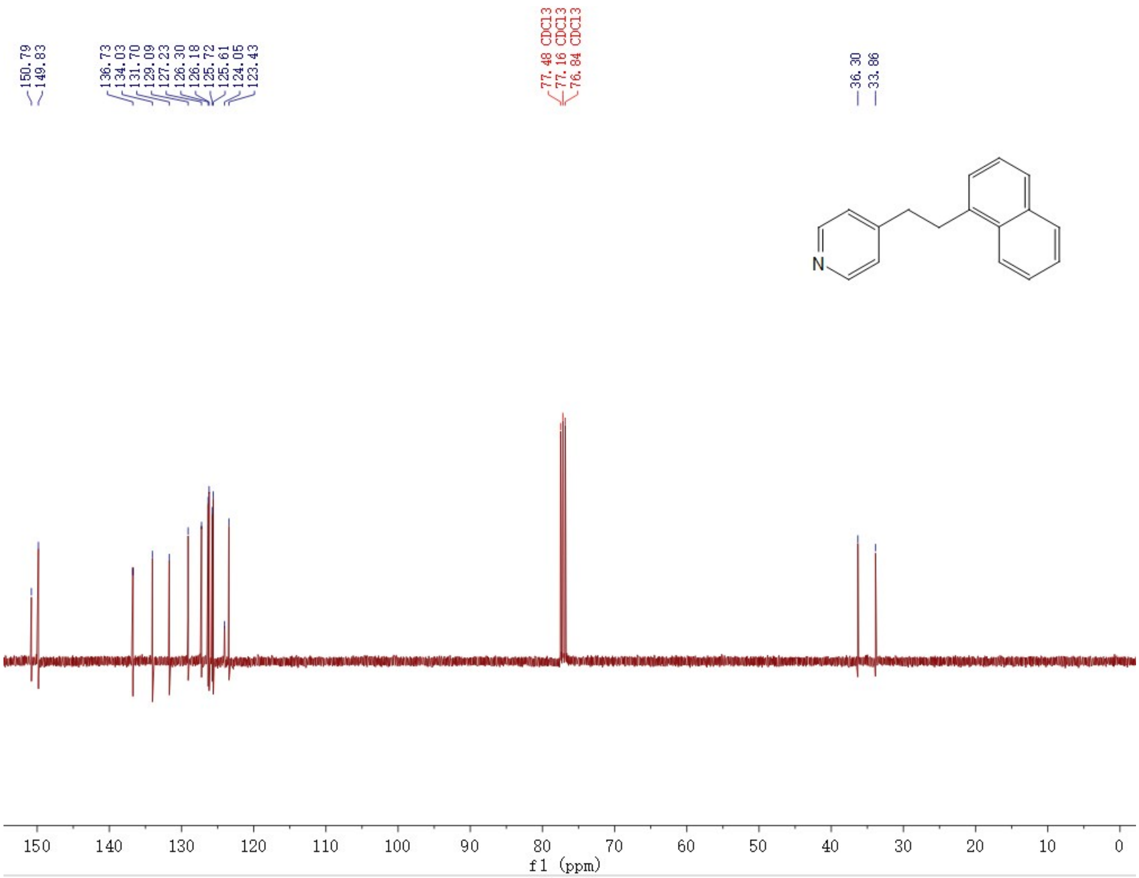
4-(4-isopropylphenethyl)pyridine (3cc), ^{13}C NMR (101 MHz, CDCl$_3$)



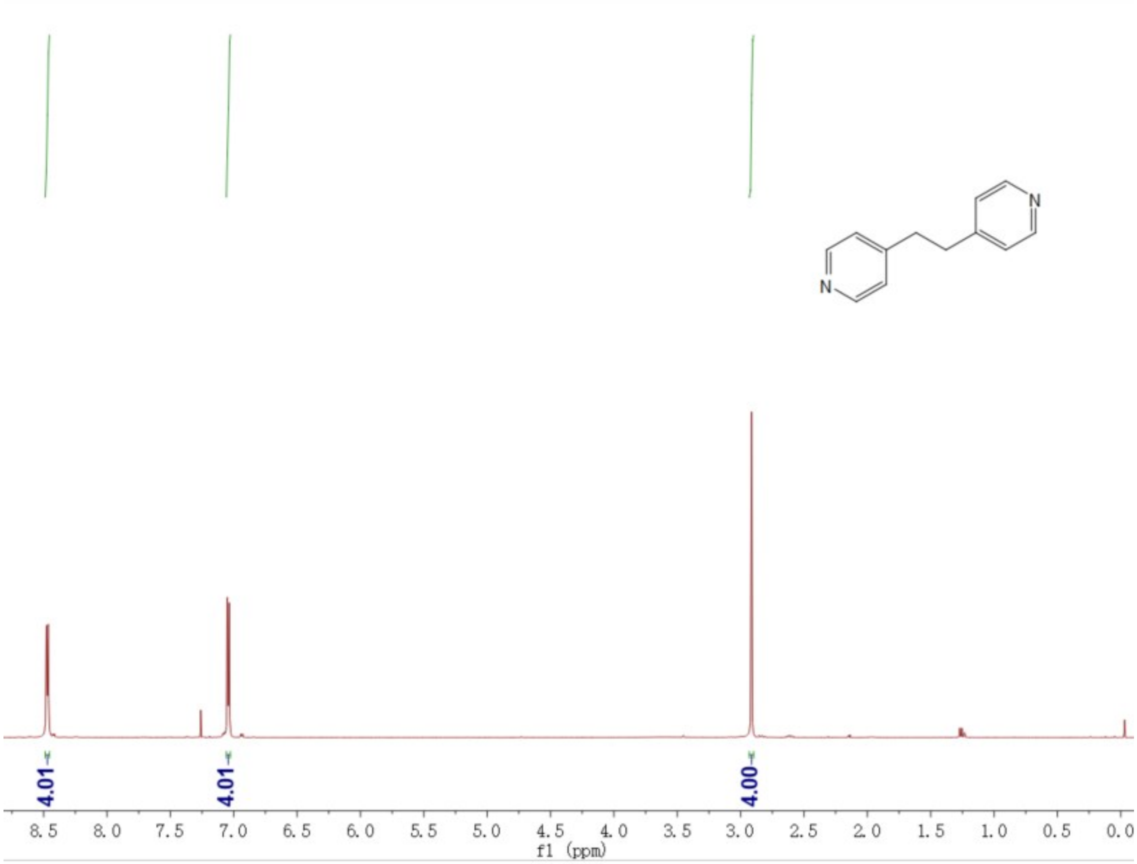
4-(2-(naphthalen-1-yl)ethyl)pyridine (3cb), ^{1}H NMR (400 MHz, CDCl$_3$)



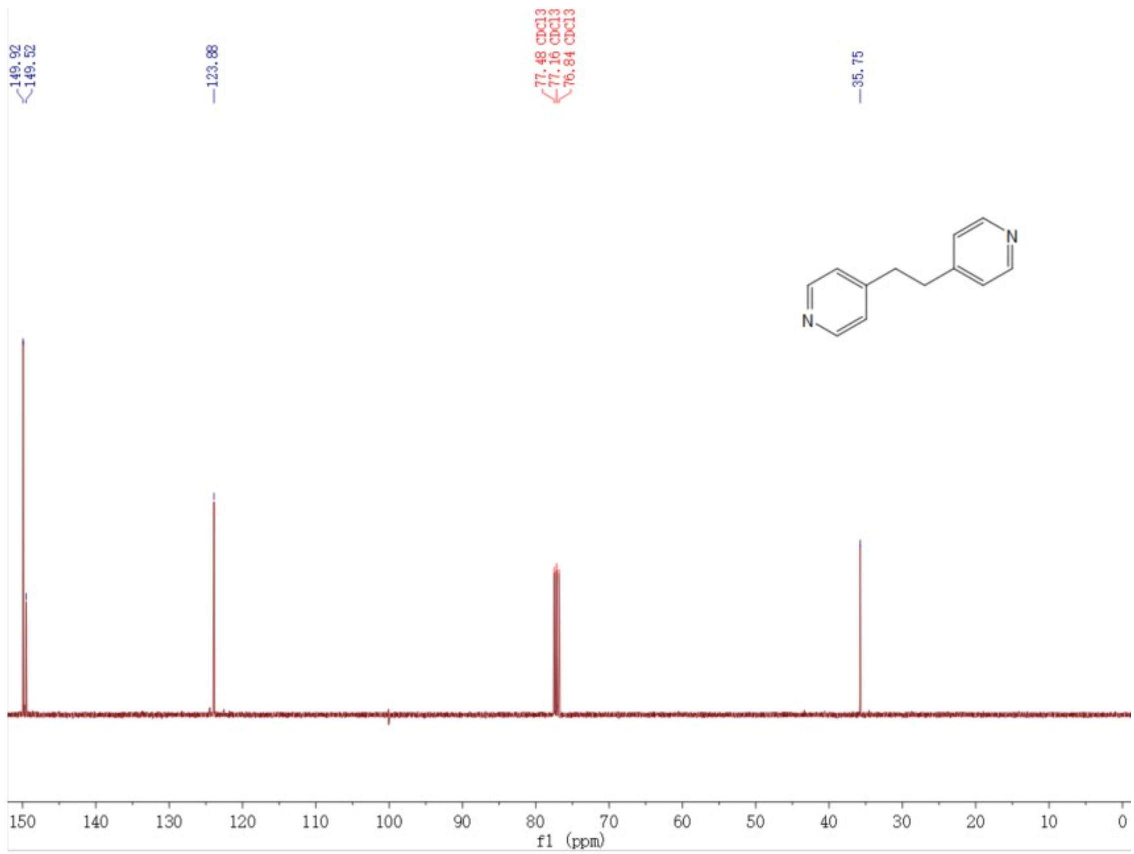
4-(2-(naphthalen-1-yl)ethyl)pyridine (3cb), ^{13}C NMR (101 MHz, CDCl$_3$)



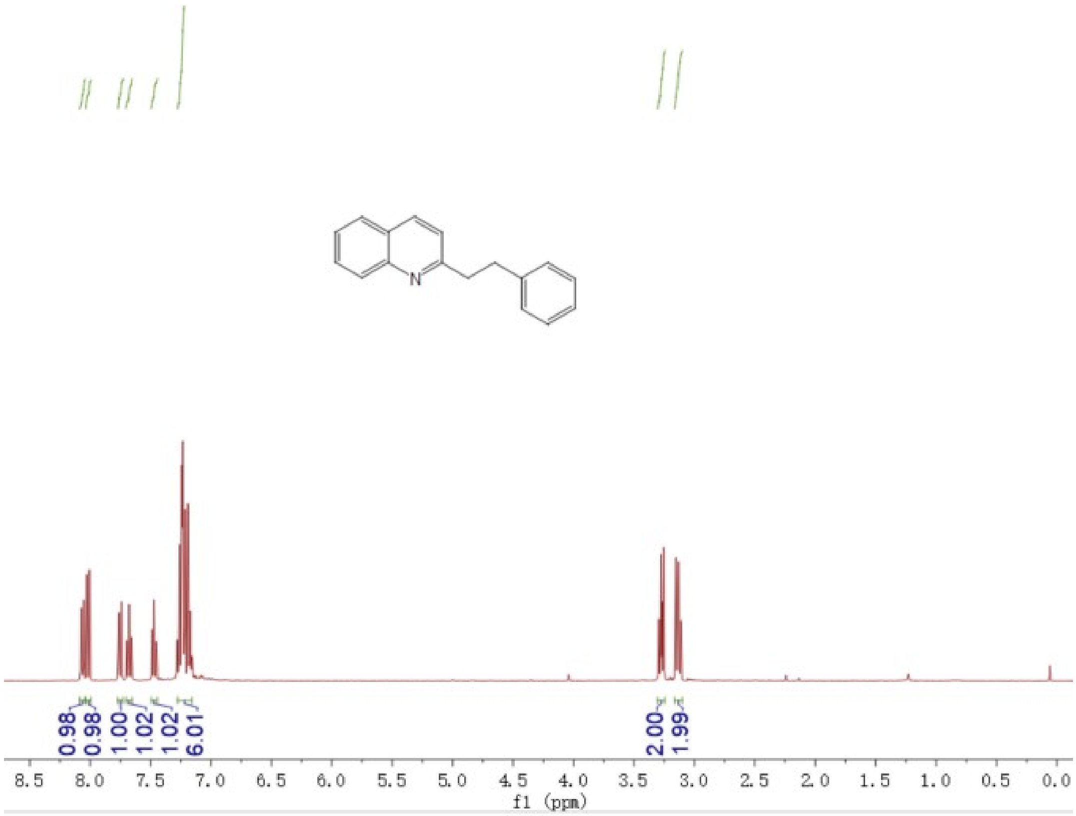
1,2-di(pyridin-4-yl)ethane (3cd), ^{1}H NMR (400 MHz, $CDCl_3$)



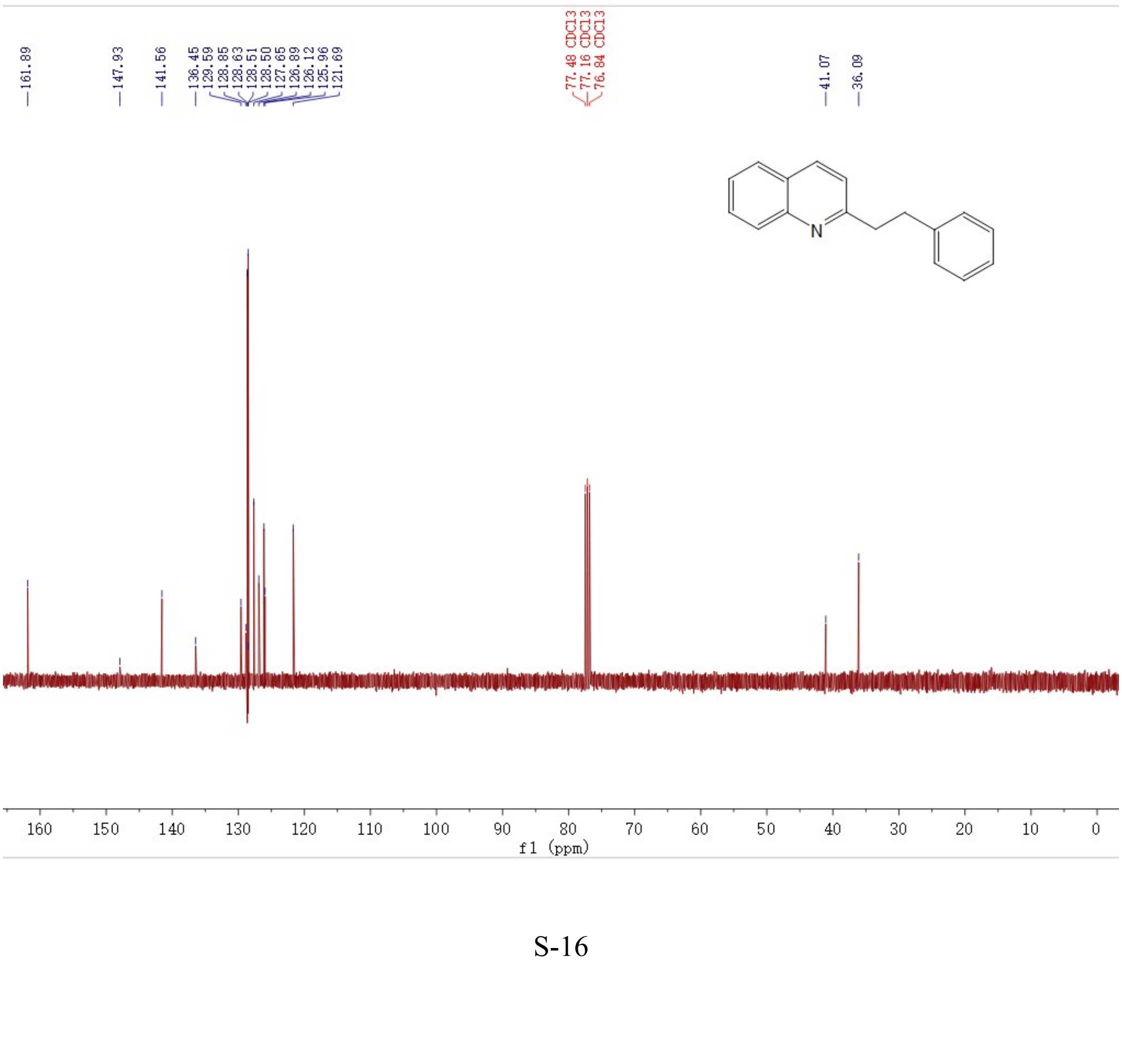
1,2-di(pyridin-4-yl)ethane (3cd), ^{13}C NMR (101 MHz, $CDCl_3$)



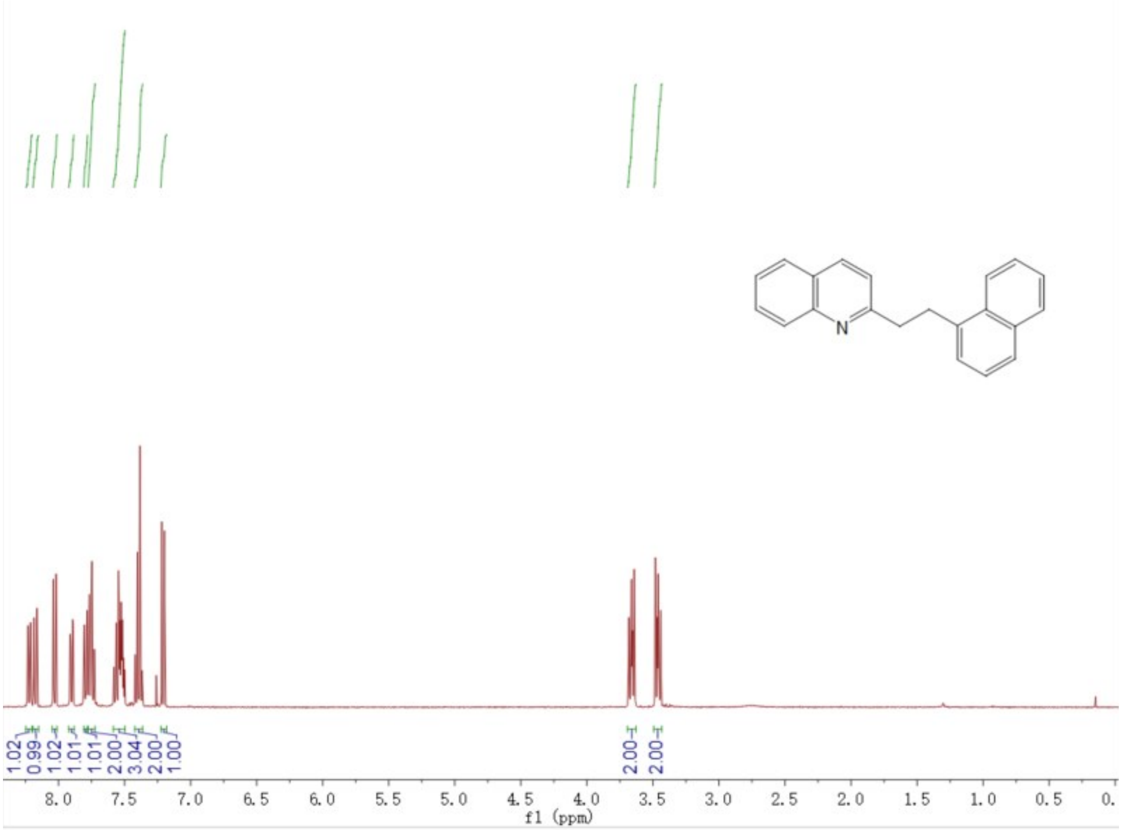
2-phenethylquinoline (3da), ^{1}H NMR (400 MHz, $CDCl_3$)



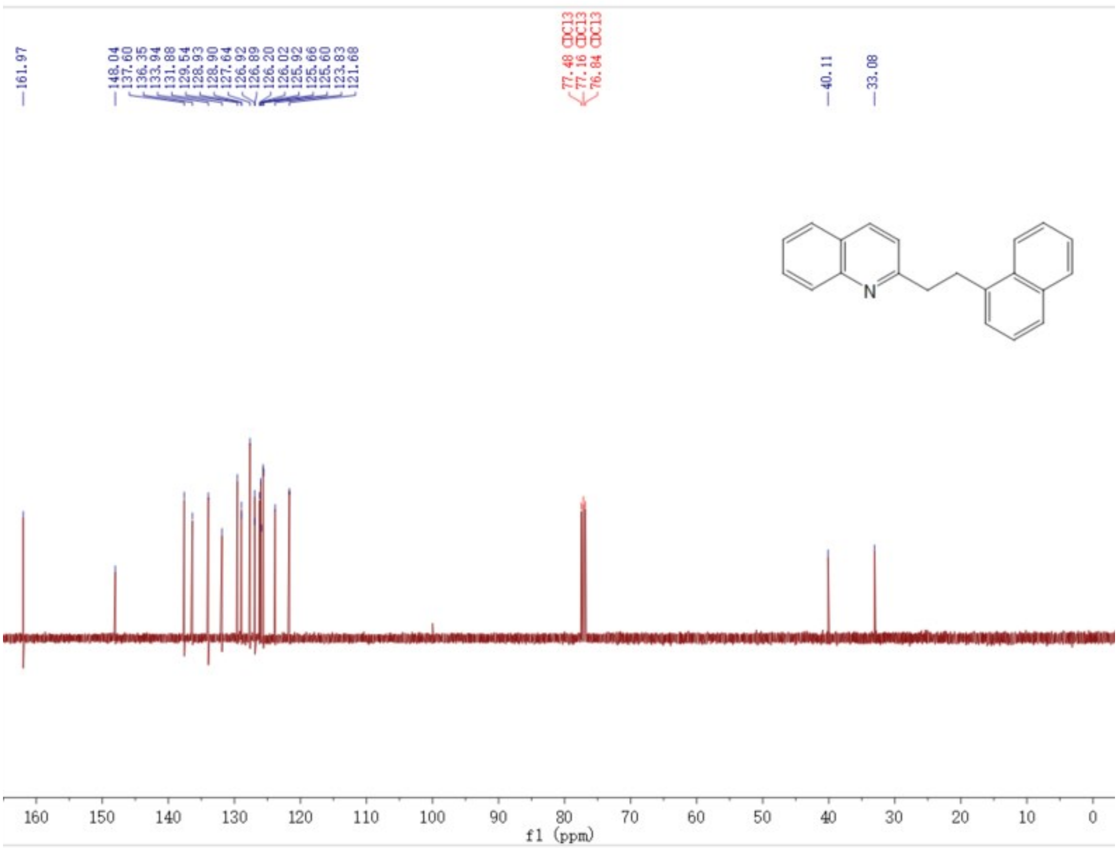
2-phenethylquinoline (3da), ^{13}C NMR (101 MHz, 400 MHz, $CDCl_3$)



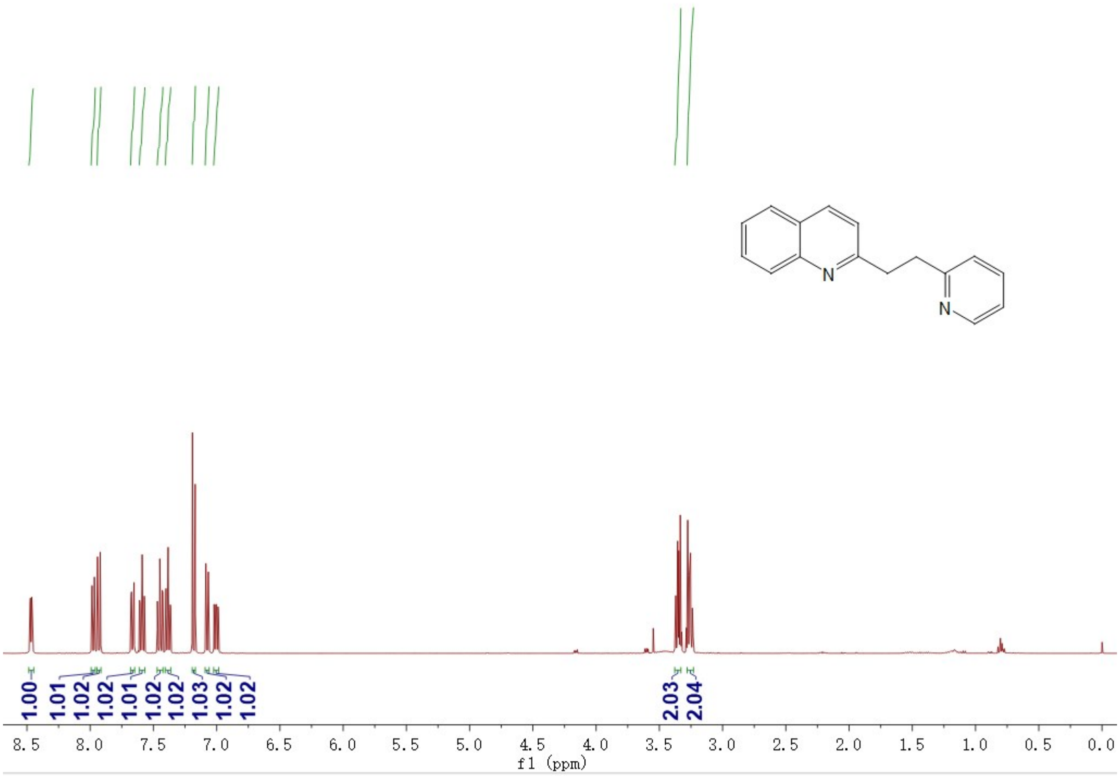
2-(2-(naphthalen-1-yl)ethyl)quinoline (3db), ^{1}H NMR (400 MHz, $CDCl_3$)



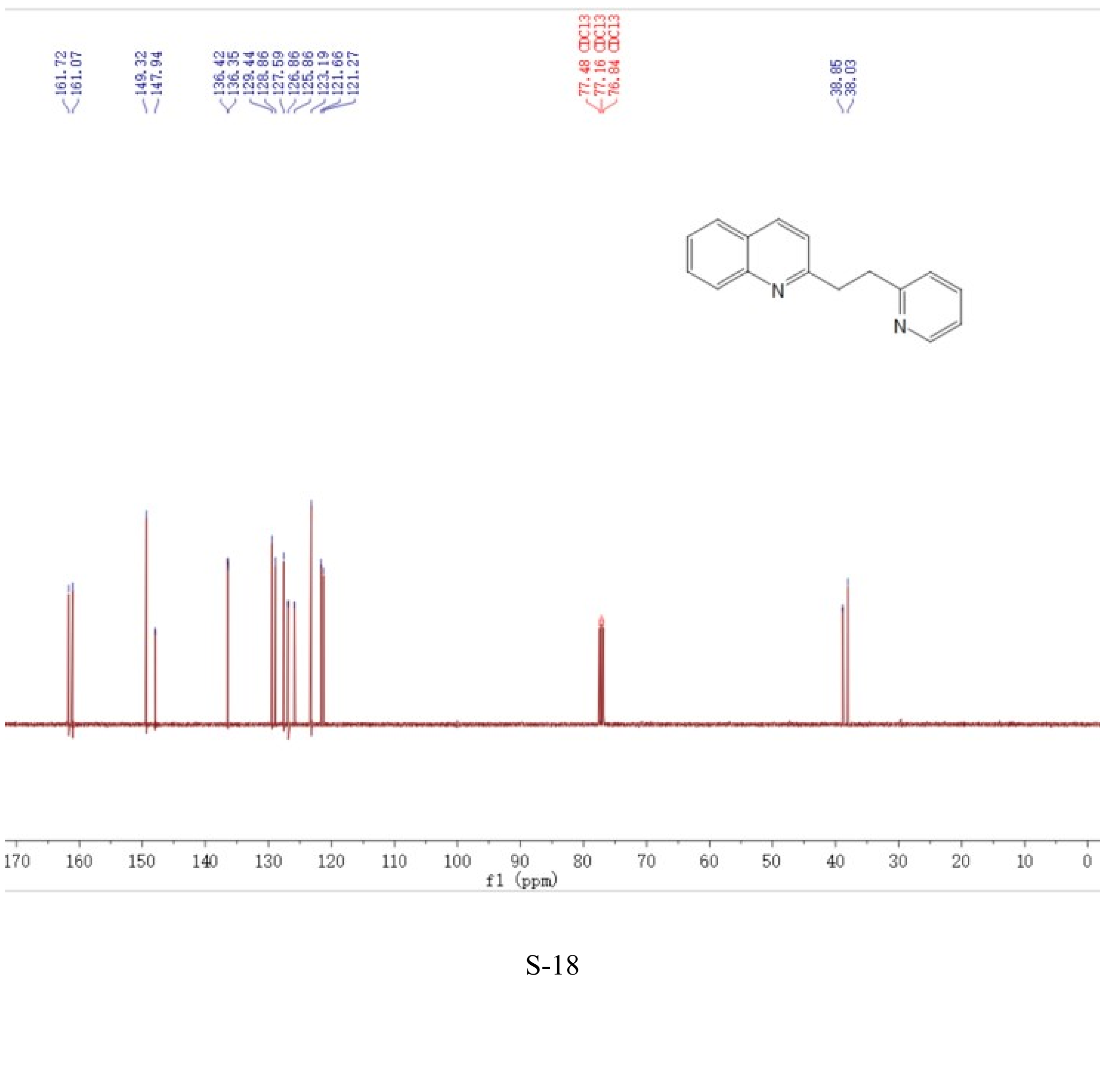
2-(2-(naphthalen-1-yl)ethyl)quinoline (3db), ^{13}C NMR (101 MHz, $CDCl_3$)



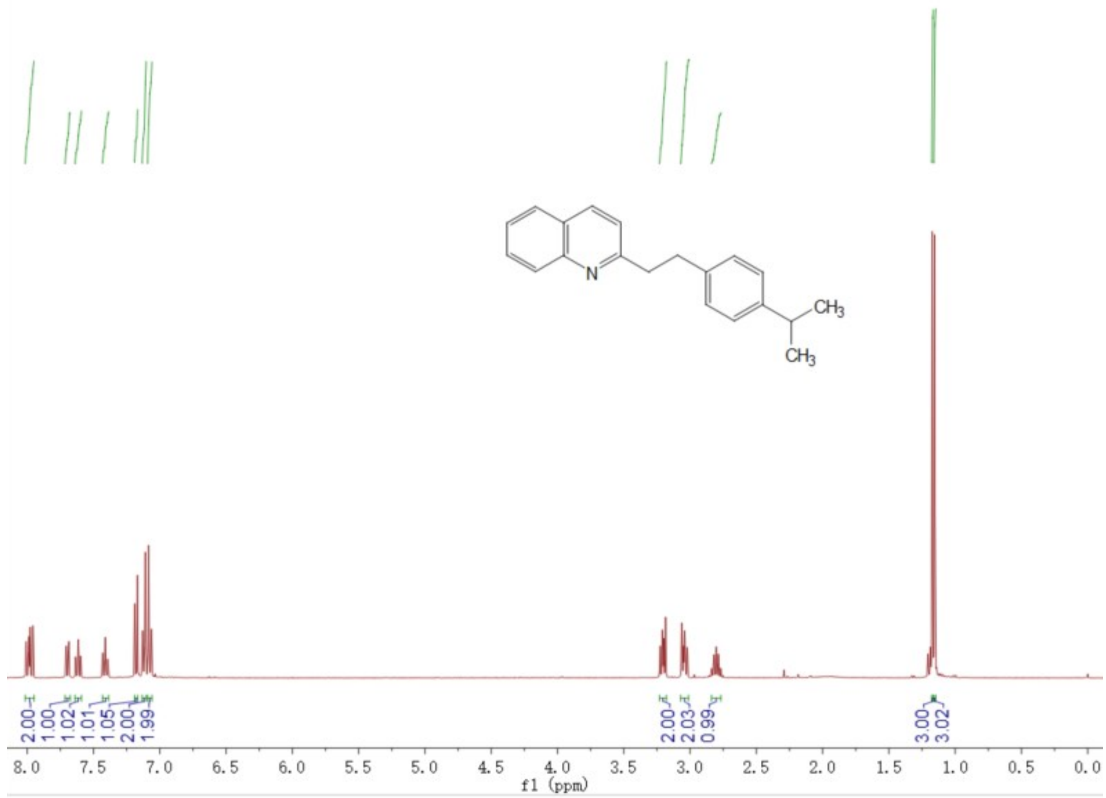
2-(2-(pyridin-2-yl)ethyl)quinoline (3de), ^{1}H NMR (400 MHz, $CDCl_3$)



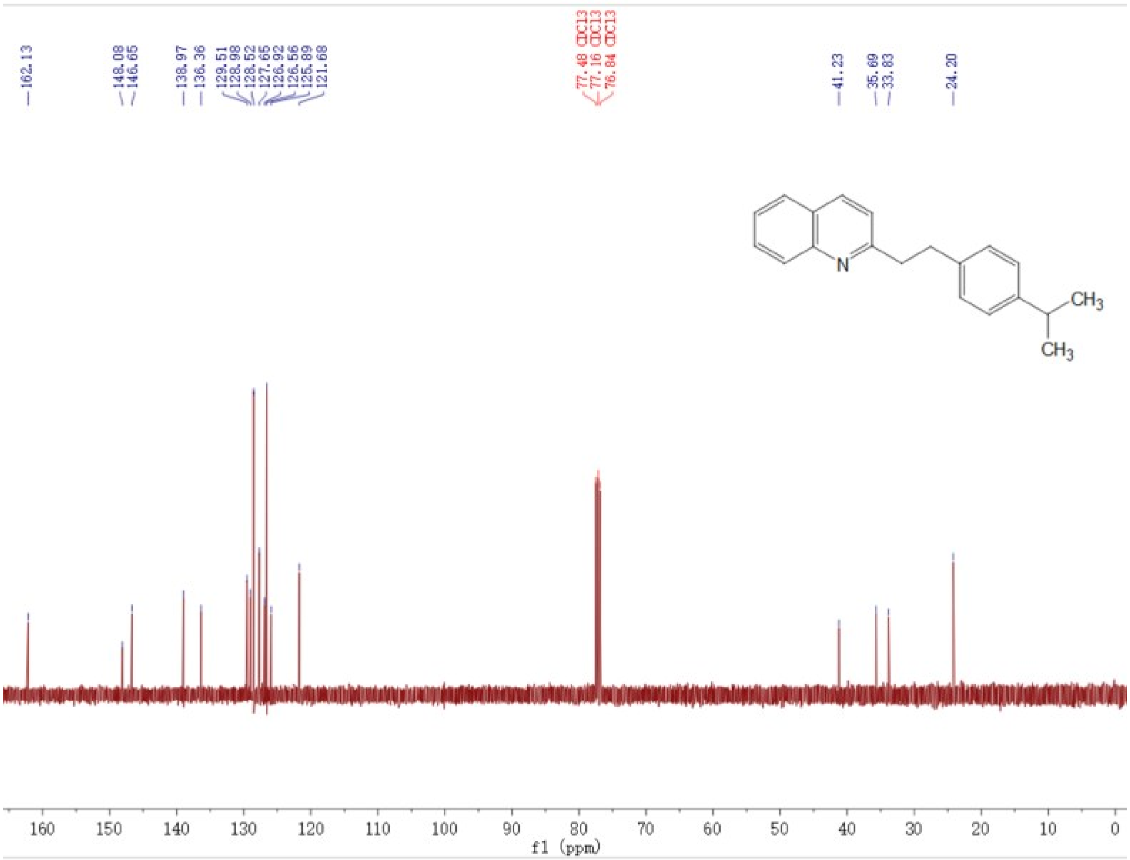
2-(2-(pyridin-2-yl)ethyl)quinoline (3de), ^{13}C NMR (101 MHz, $CDCl_3$)



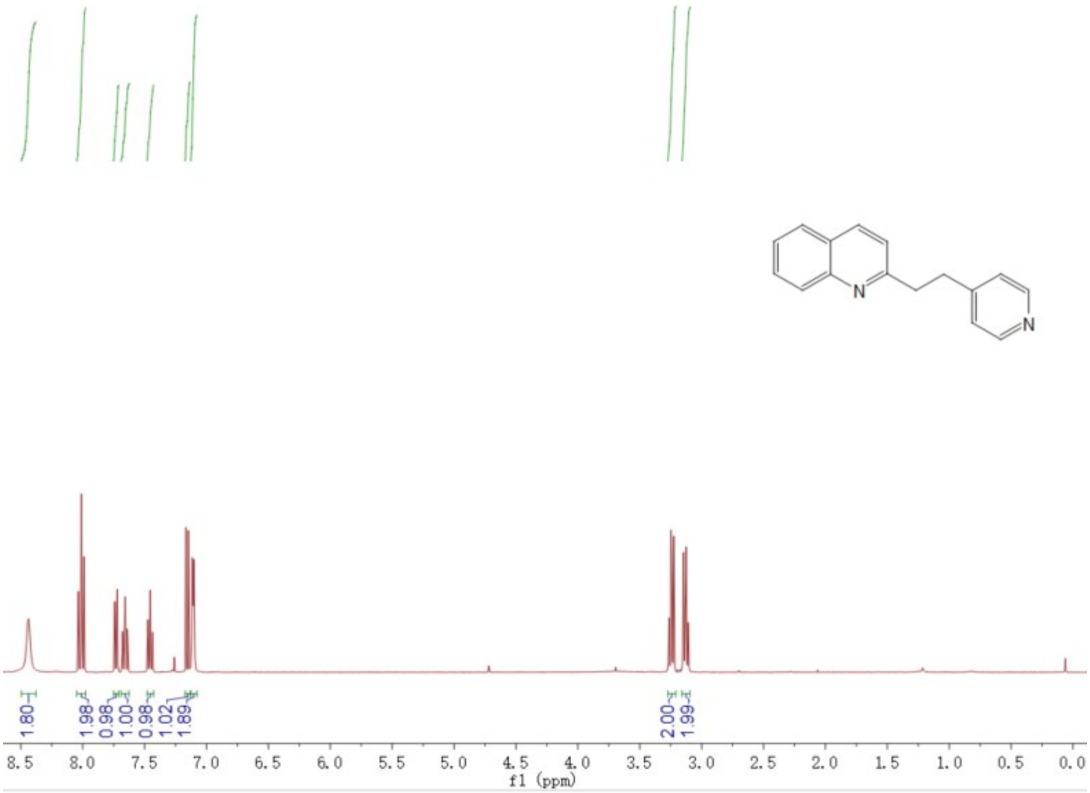
2-(4-isopropylphenethyl)quinoline (3dc), [1]H NMR (400 MHz, CDCl$_3$)



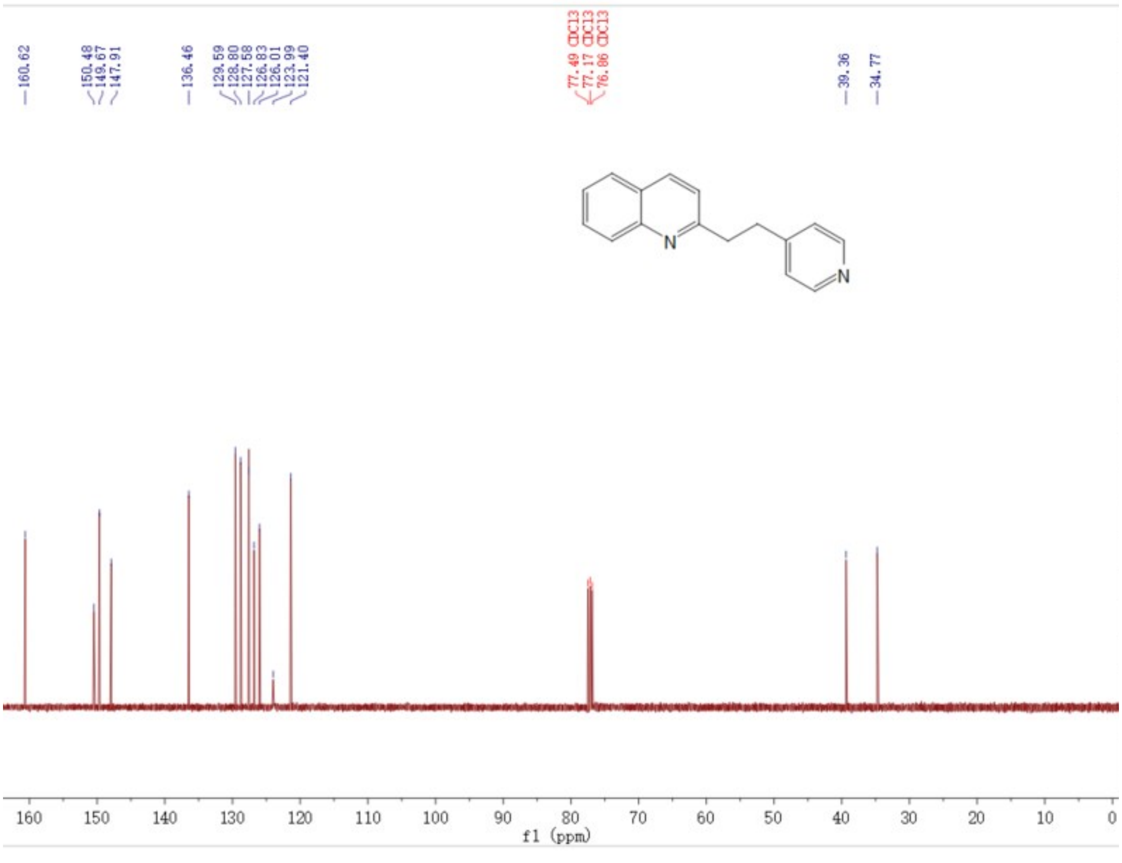
2-(4-isopropylphenethyl)quinoline (3dc), [13]C NMR (101 MHz, CDCl$_3$)



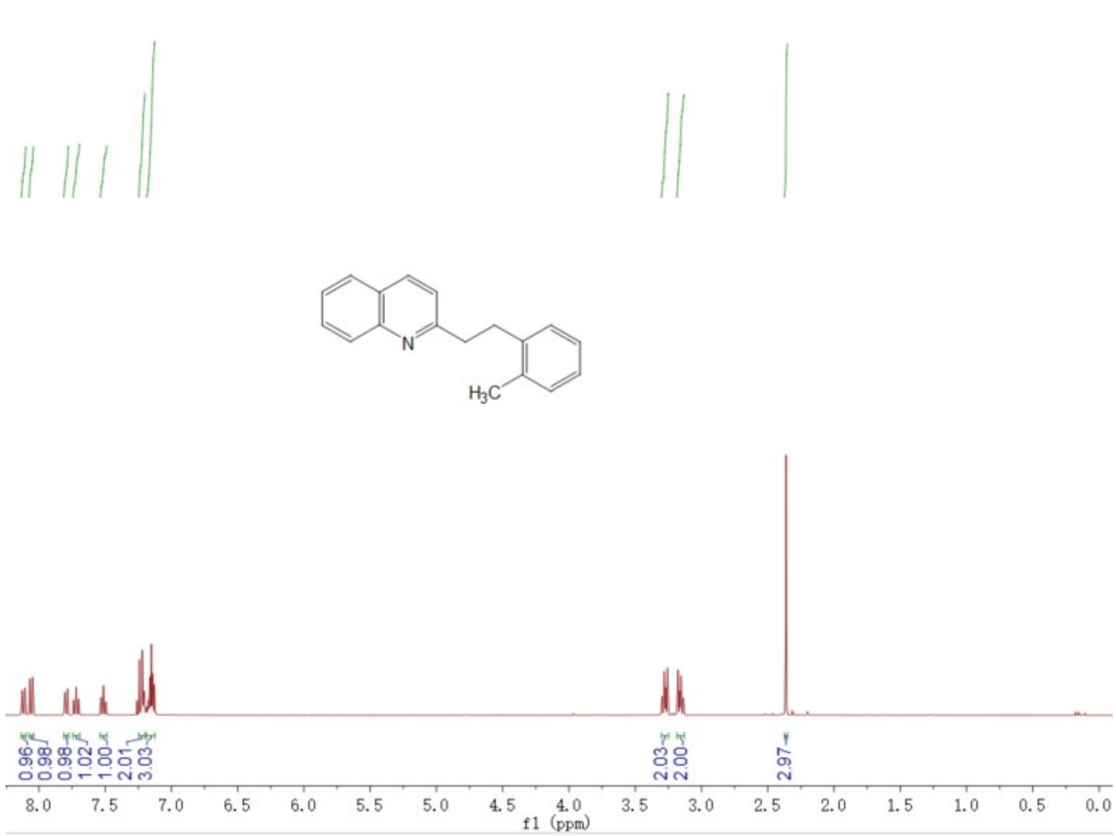
2-(2-(pyridin-4-yl)ethyl)quinoline (3dd), ^{1}H NMR (400 MHz, $CDCl_3$)



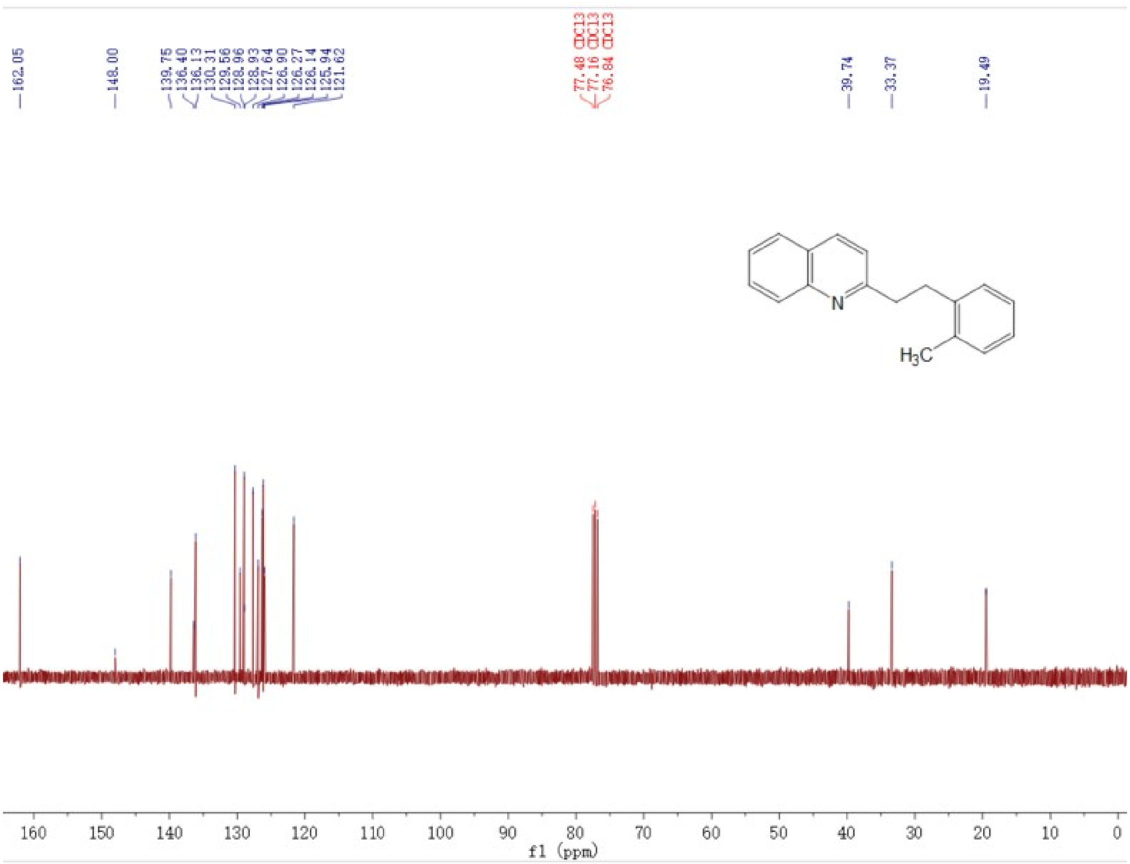
2-(2-(pyridin-4-yl)ethyl)quinoline (3dd), ^{13}C NMR (101 MHz, $CDCl_3$)



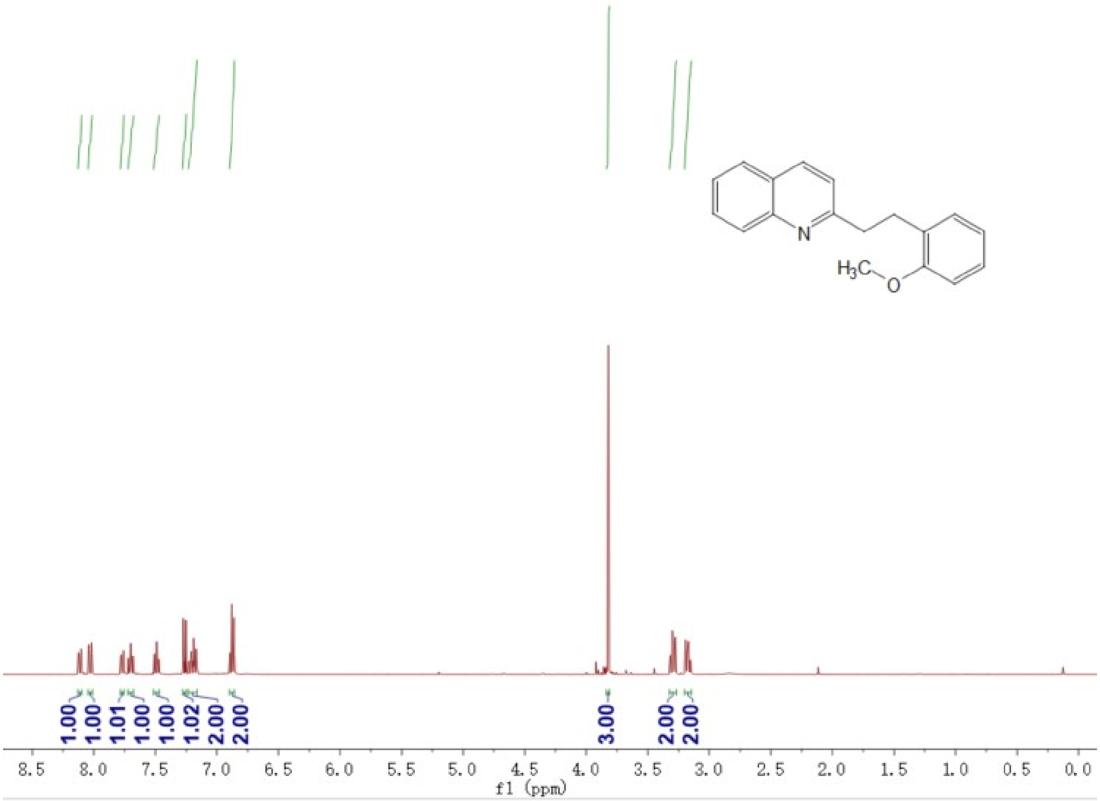
2-(2-methylphenethyl)quinoline (3df), ^{1}H NMR (400 MHz, $CDCl_3$)



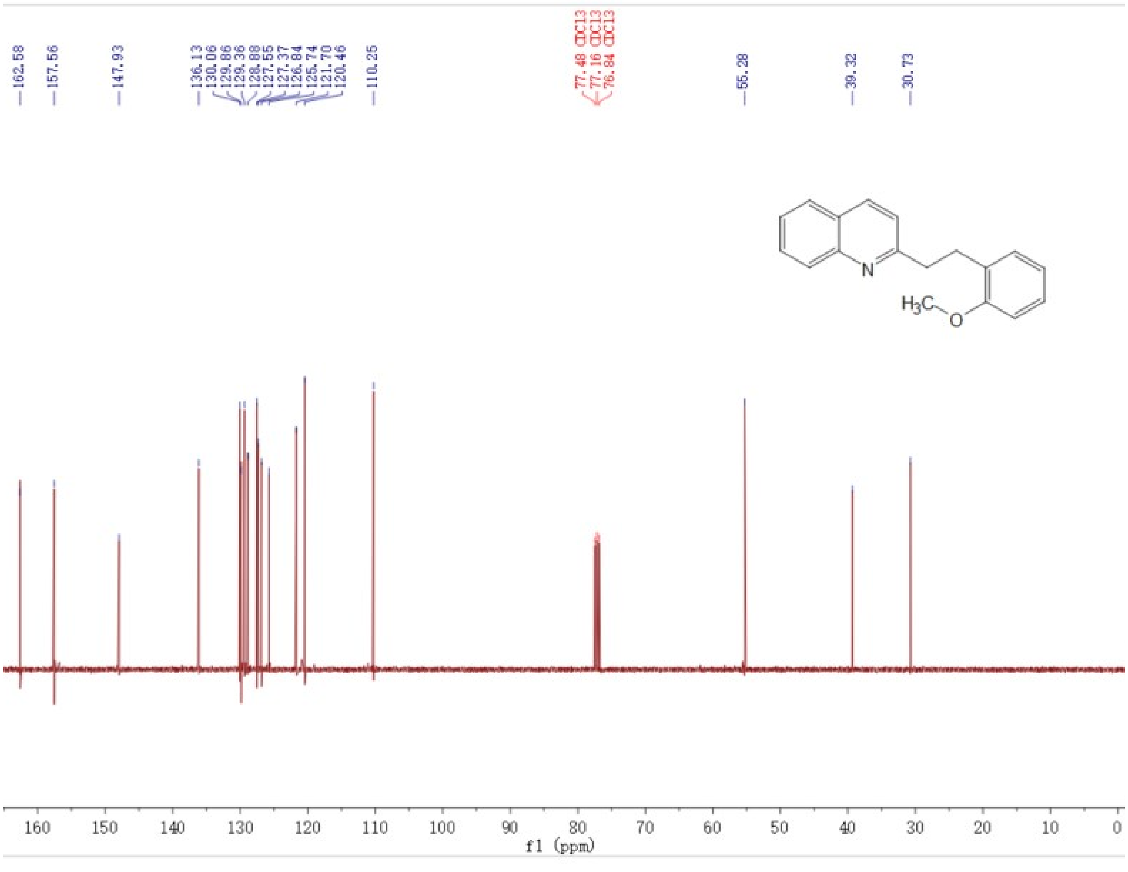
2-(2-methylphenethyl)quinoline (3df), ^{13}C NMR (101 MHz, $CDCl_3$)



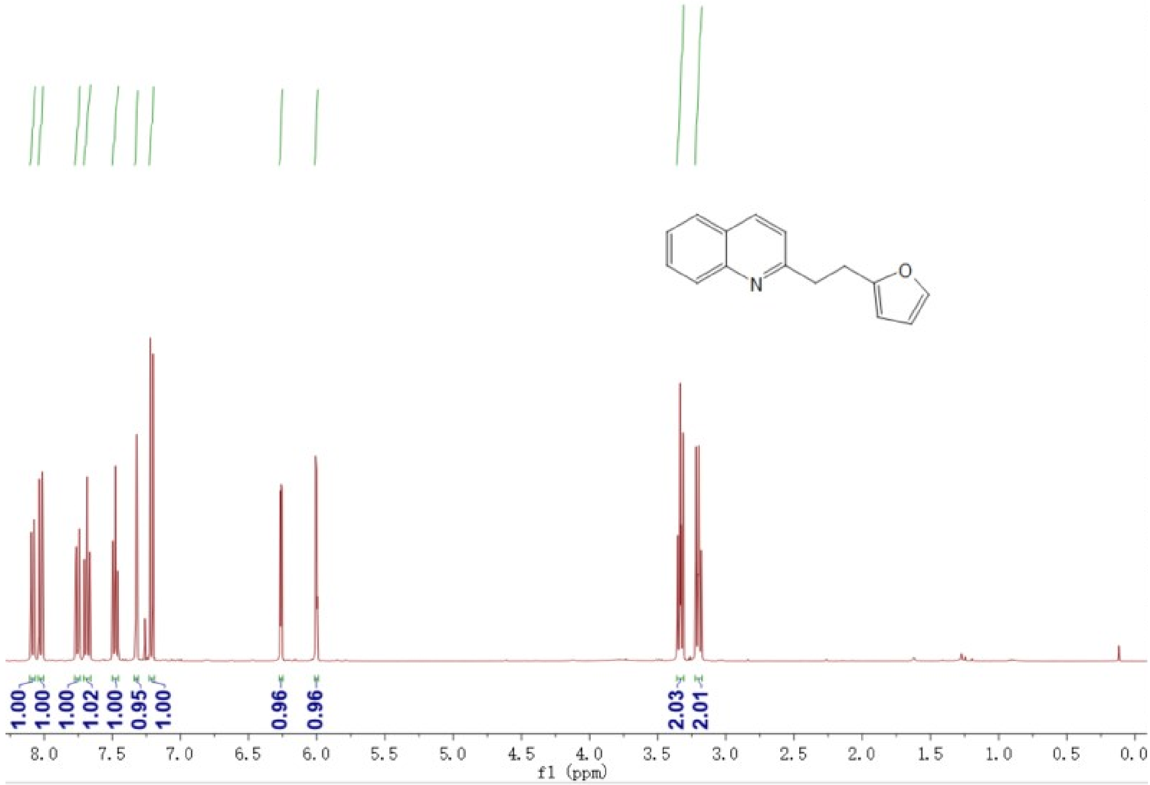
2-(2-methoxyphenethyl)quinoline (3dg), ^{1}H NMR (400 MHz, $CDCl_3$)



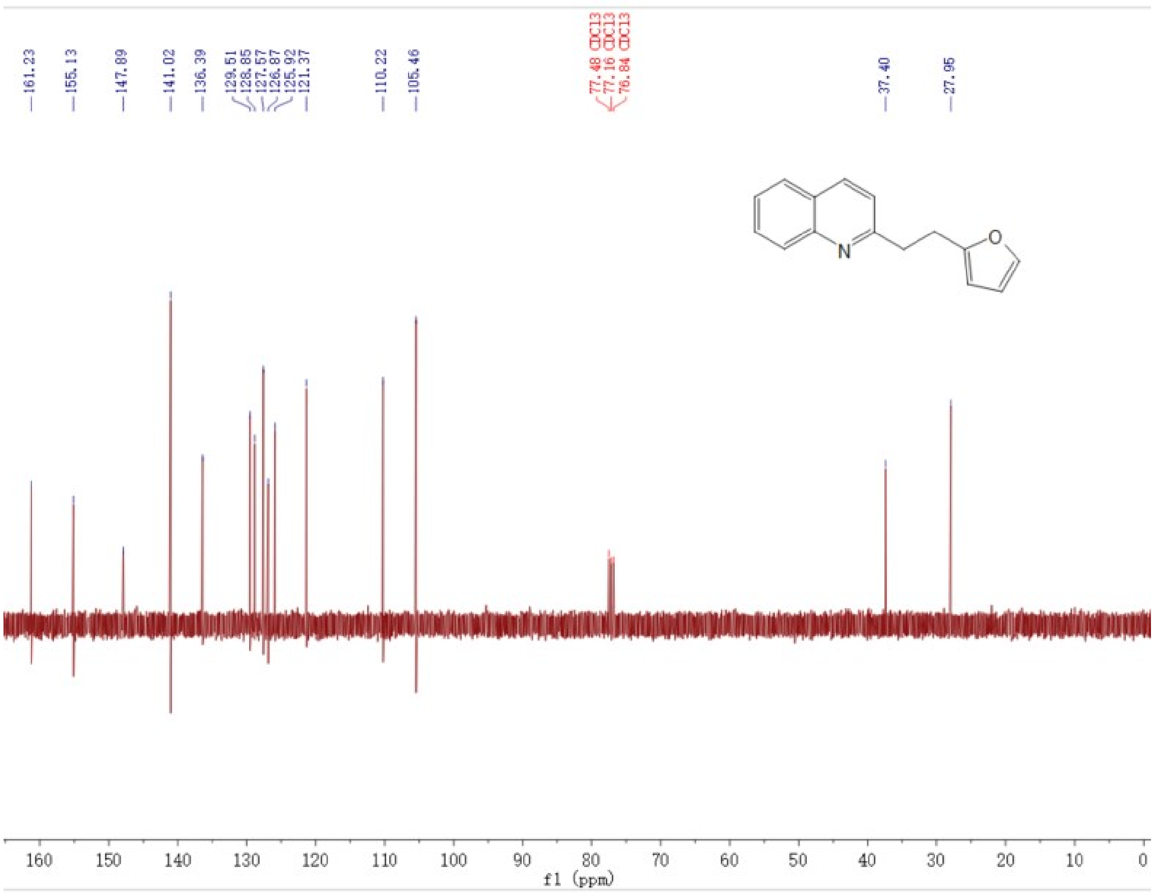
2-(2-methoxyphenethyl)quinoline (3dg), ^{13}C NMR (101 MHz, $CDCl_3$)



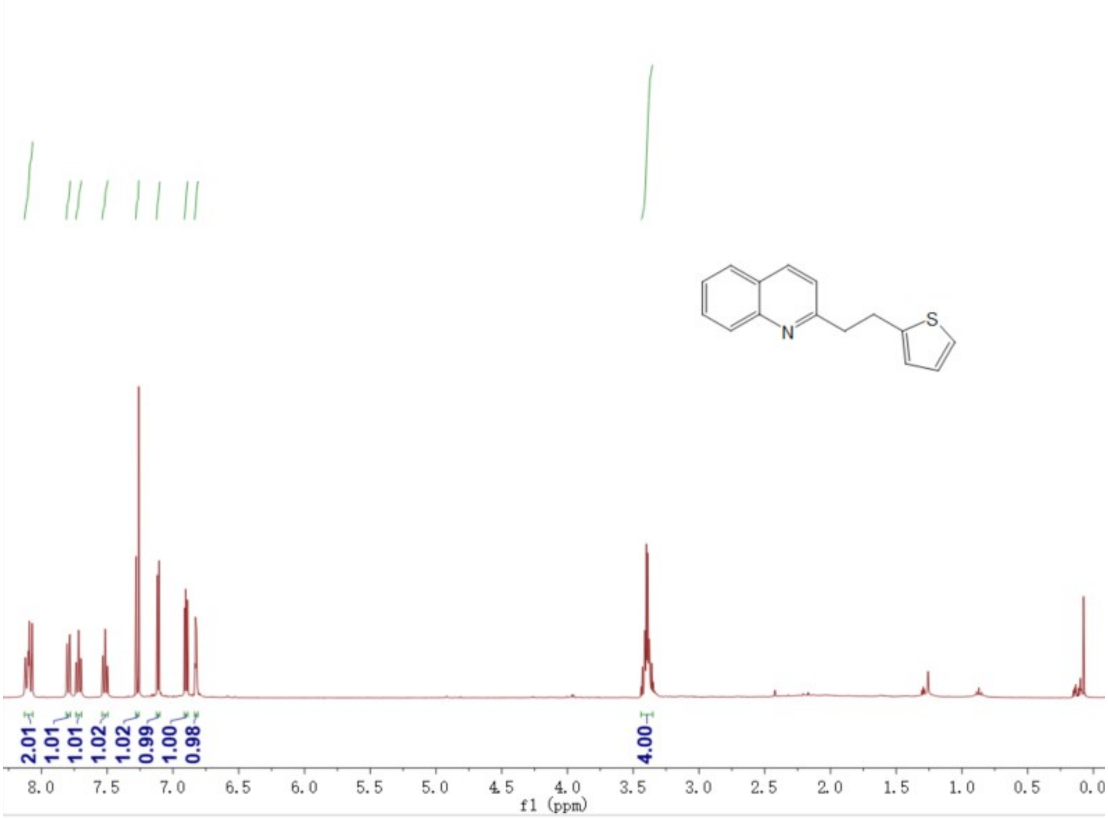
2-(2-(furan-2-yl)ethyl)quinoline (3dh), ^{1}H NMR (400 MHz, $CDCl_3$)



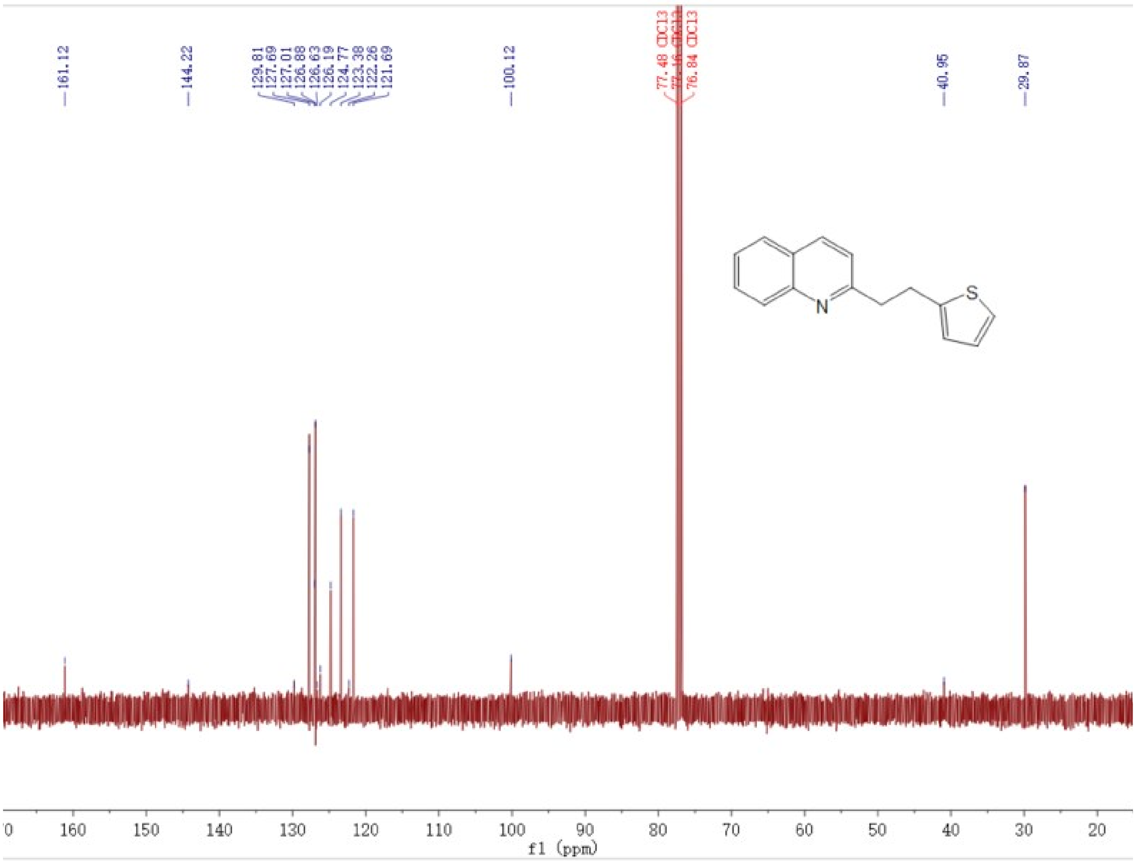
2-(2-(furan-2-yl)ethyl)quinoline (3dh), ^{13}C NMR (101 MHz, $CDCl_3$)



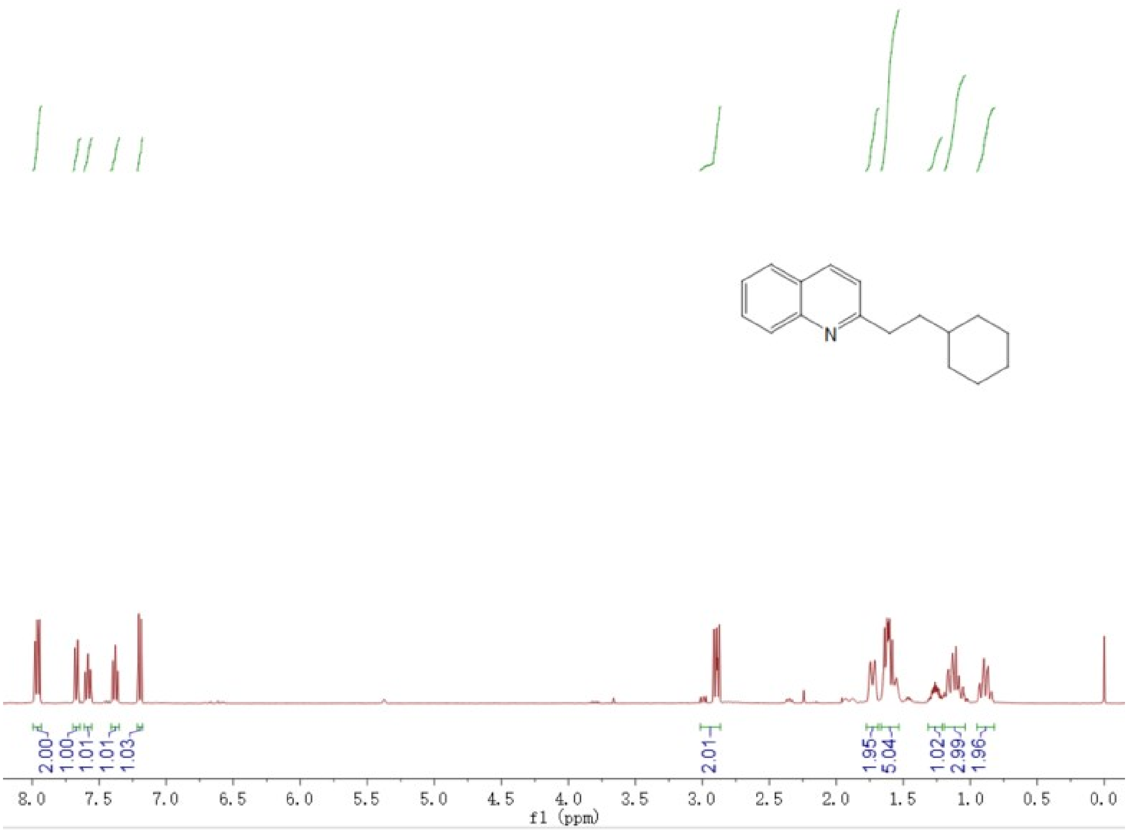
2-(2-(thiophen-2-yl)ethyl)quinoline (3di), ^{1}H NMR (400 MHz, $CDCl_3$)



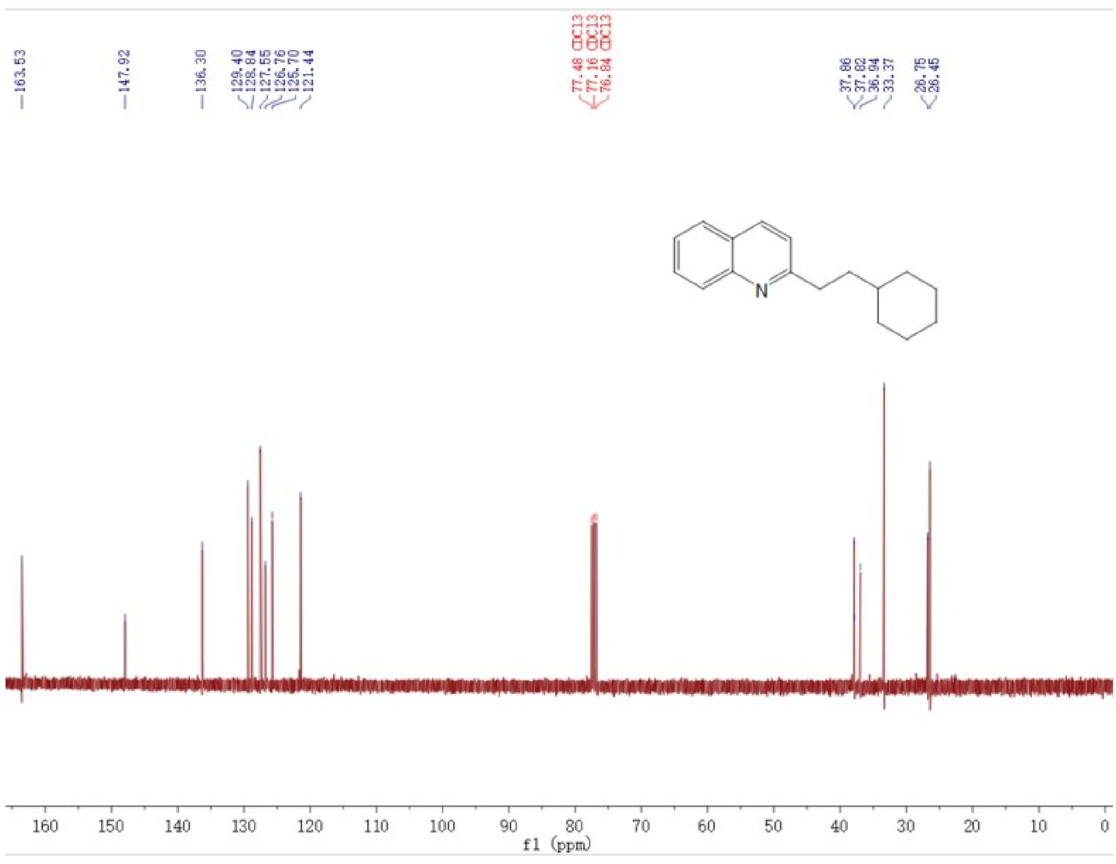
2-(2-(thiophen-2-yl)ethyl)quinoline (3di), ^{13}C NMR (101 MHz, $CDCl_3$)



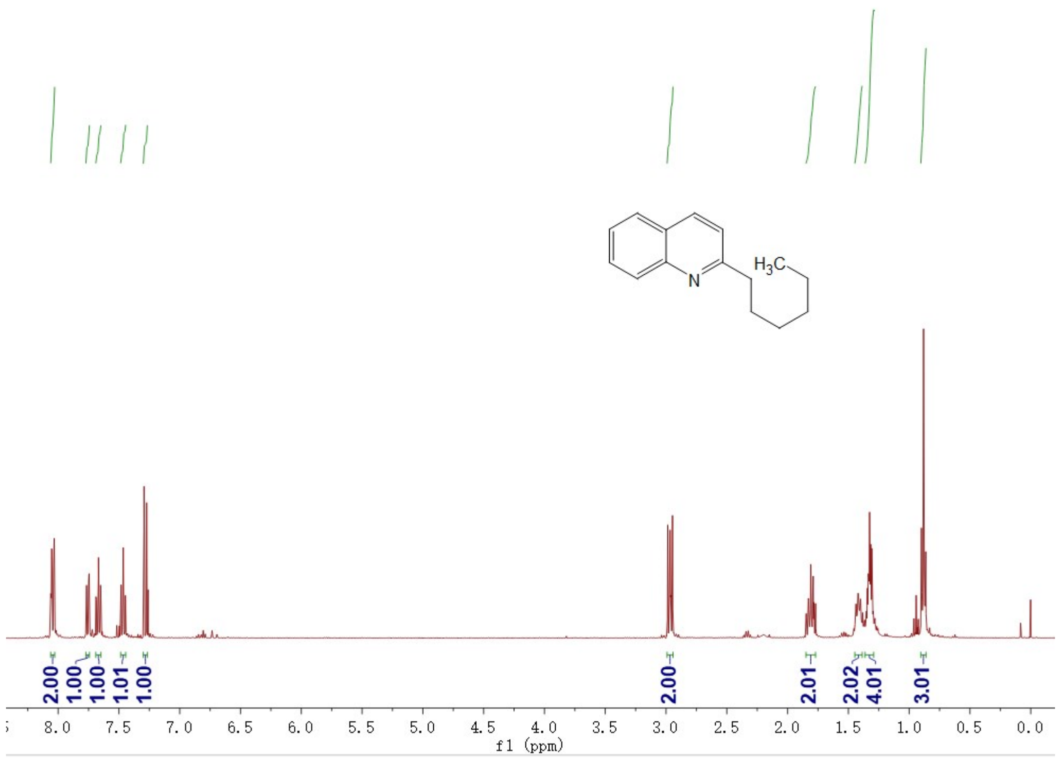
2-(2-cyclohexylethyl)quinoline (3dj), ^{1}H NMR (400 MHz, CDCl$_3$)



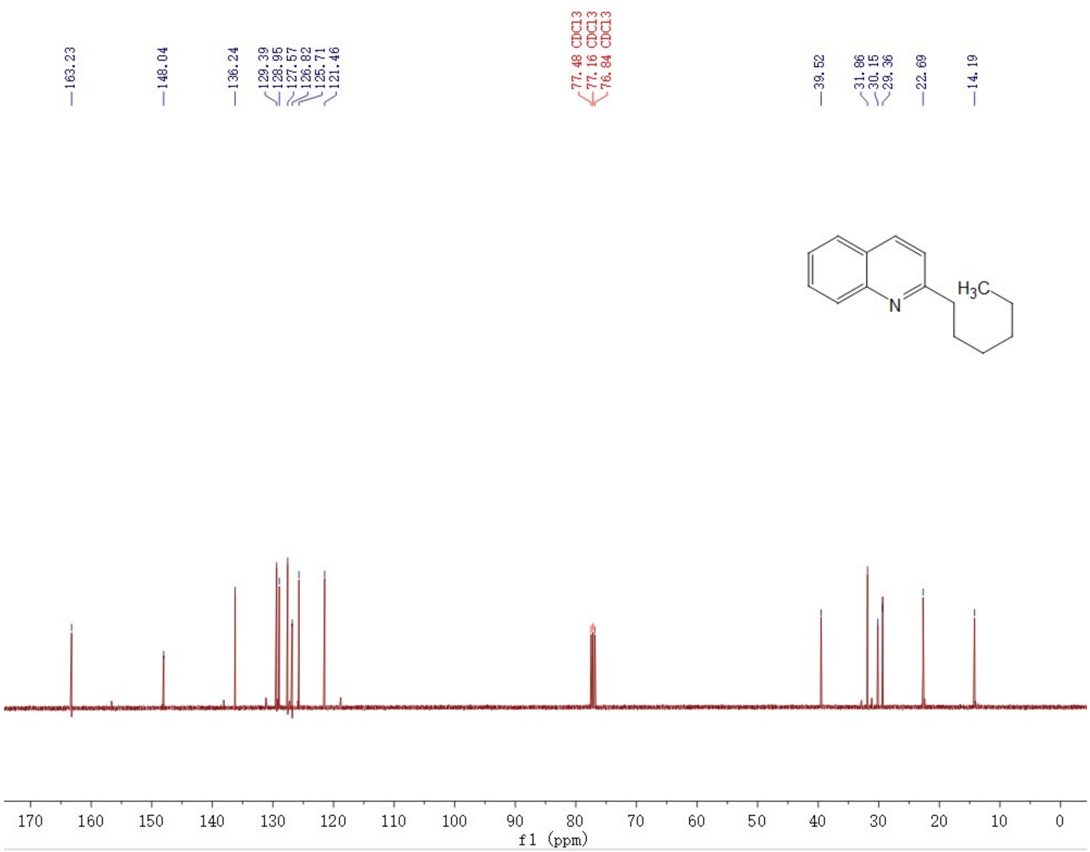
2-(2-cyclohexylethyl)quinoline (3dj), ^{13}C NMR (101 MHz, CDCl$_3$)



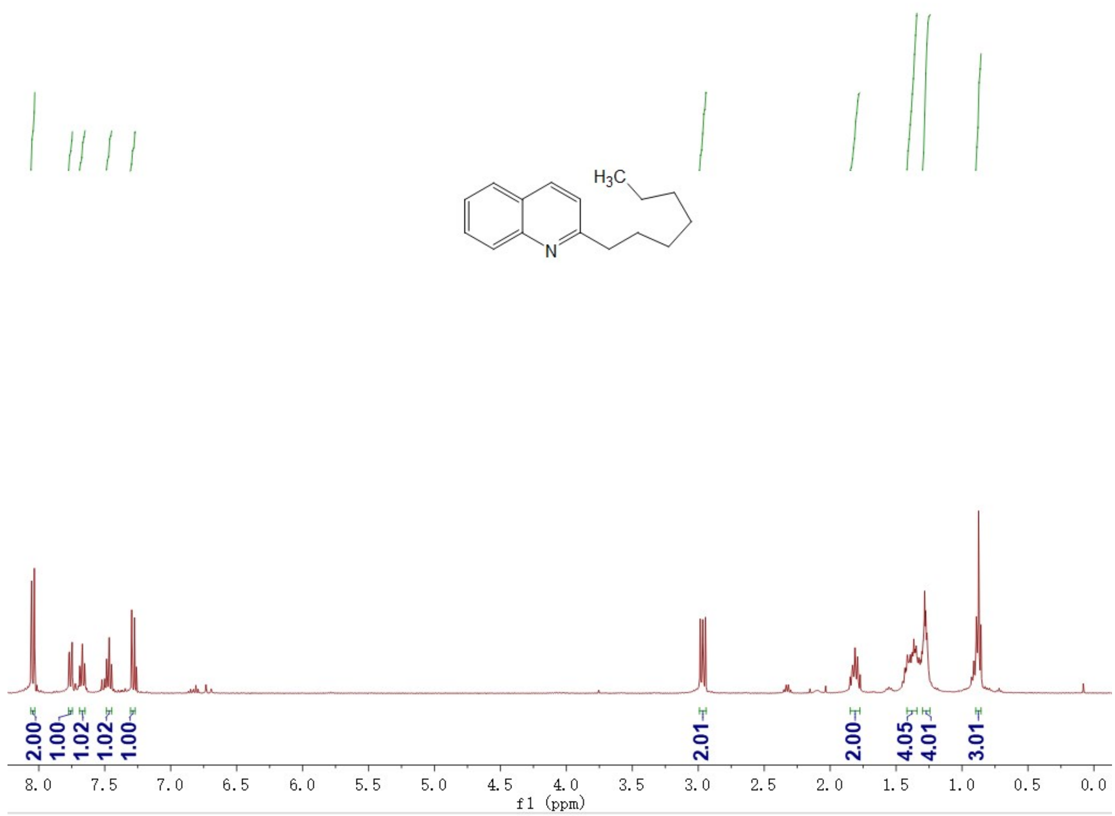
2-hexylquinoline (3dk), ^{1}H NMR (400 MHz, $CDCl_3$)



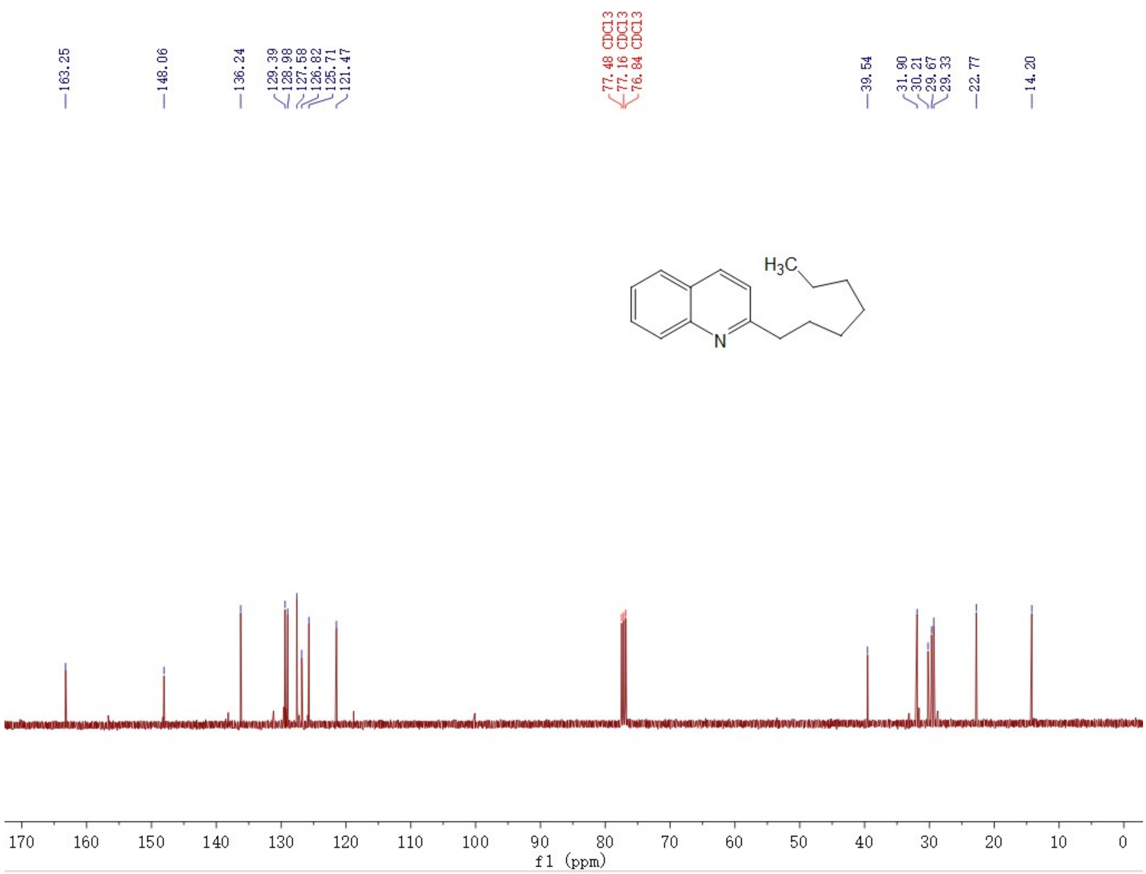
2-hexylquinoline (3dk), ^{13}C NMR (101 MHz, $CDCl_3$)



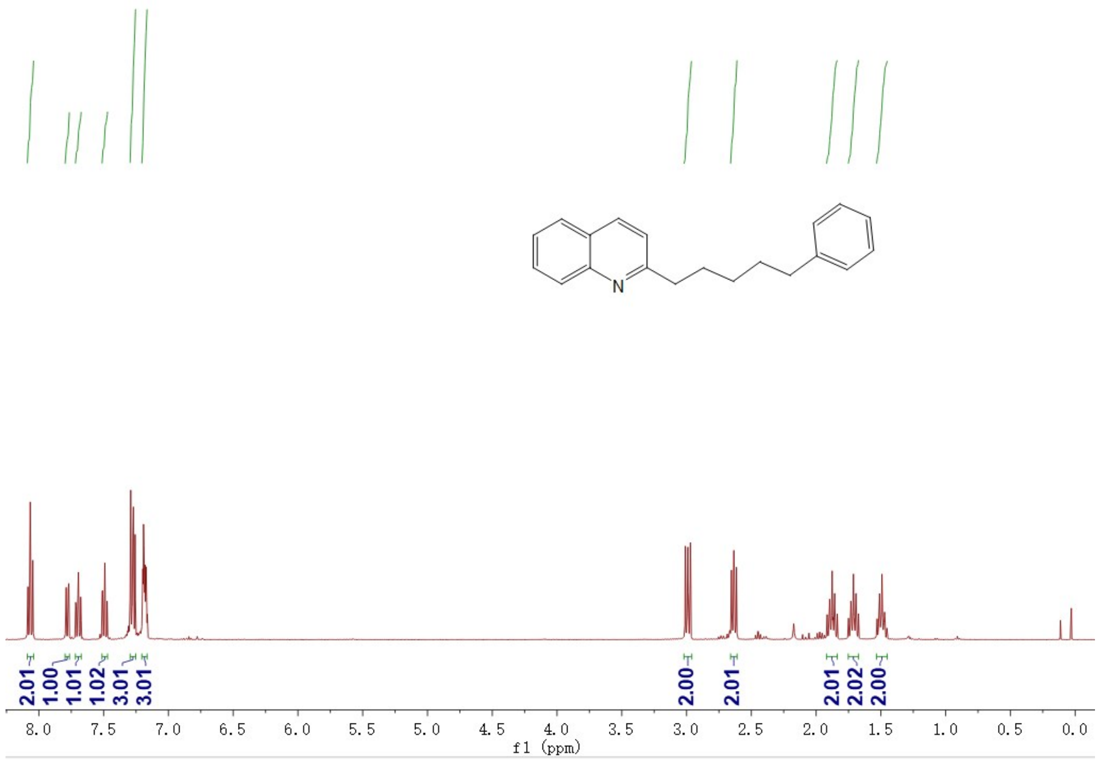
2-heptylquinoline (3dl), ^{1}H NMR (400 MHz, $CDCl_3$)



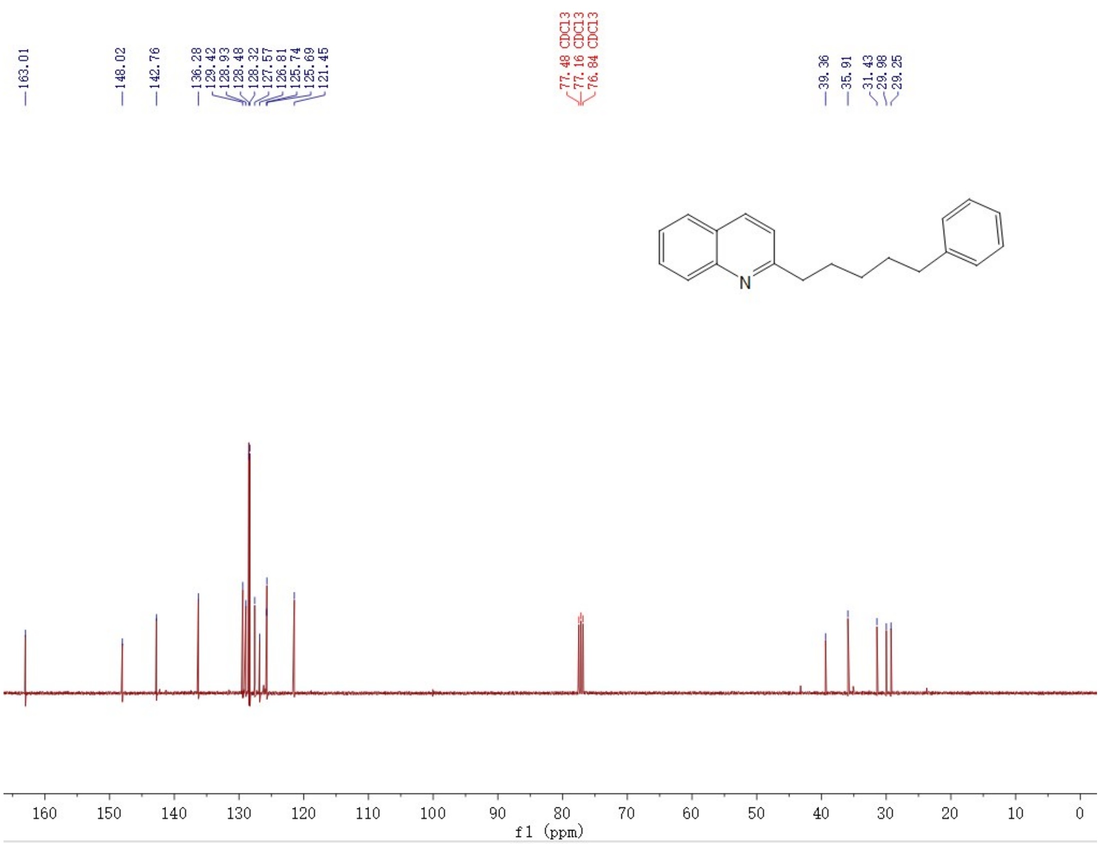
2-heptylquinoline (3dl), ^{13}C NMR (101 MHz, $CDCl_3$)



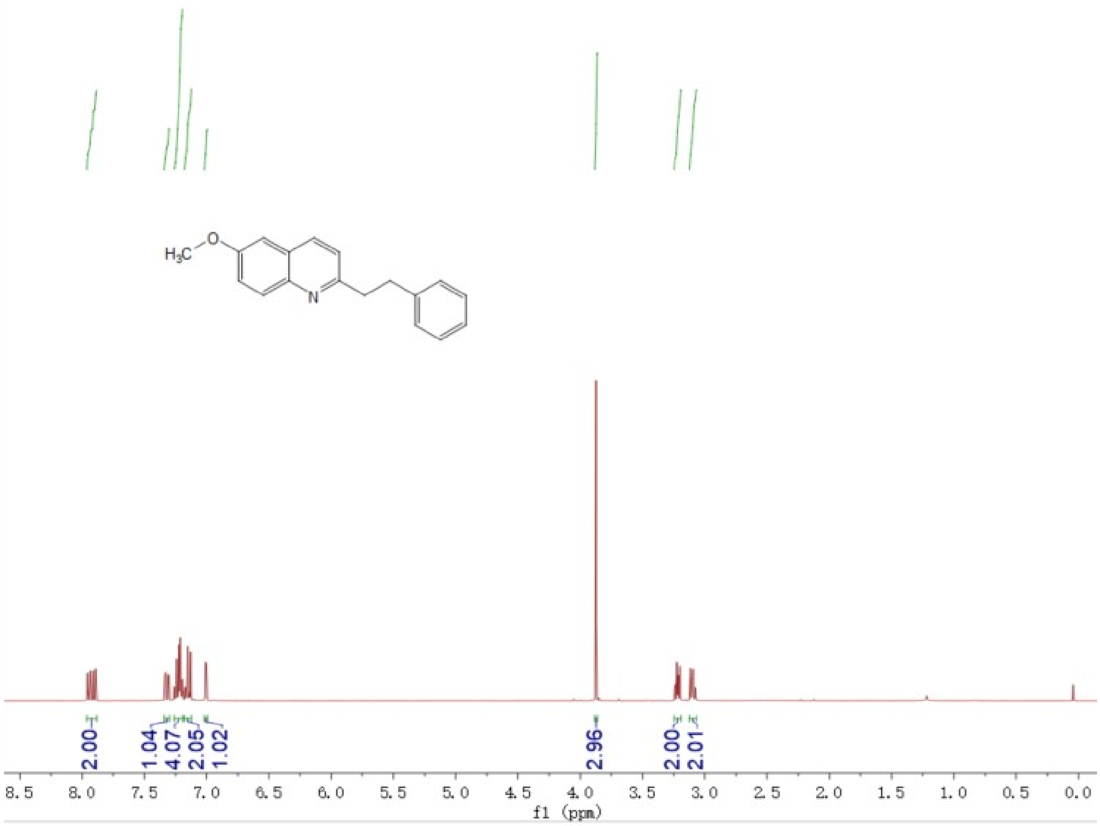
2-(5-phenylpentyl)quinoline (3dm), ^{1}H NMR (400 MHz, $CDCl_3$)



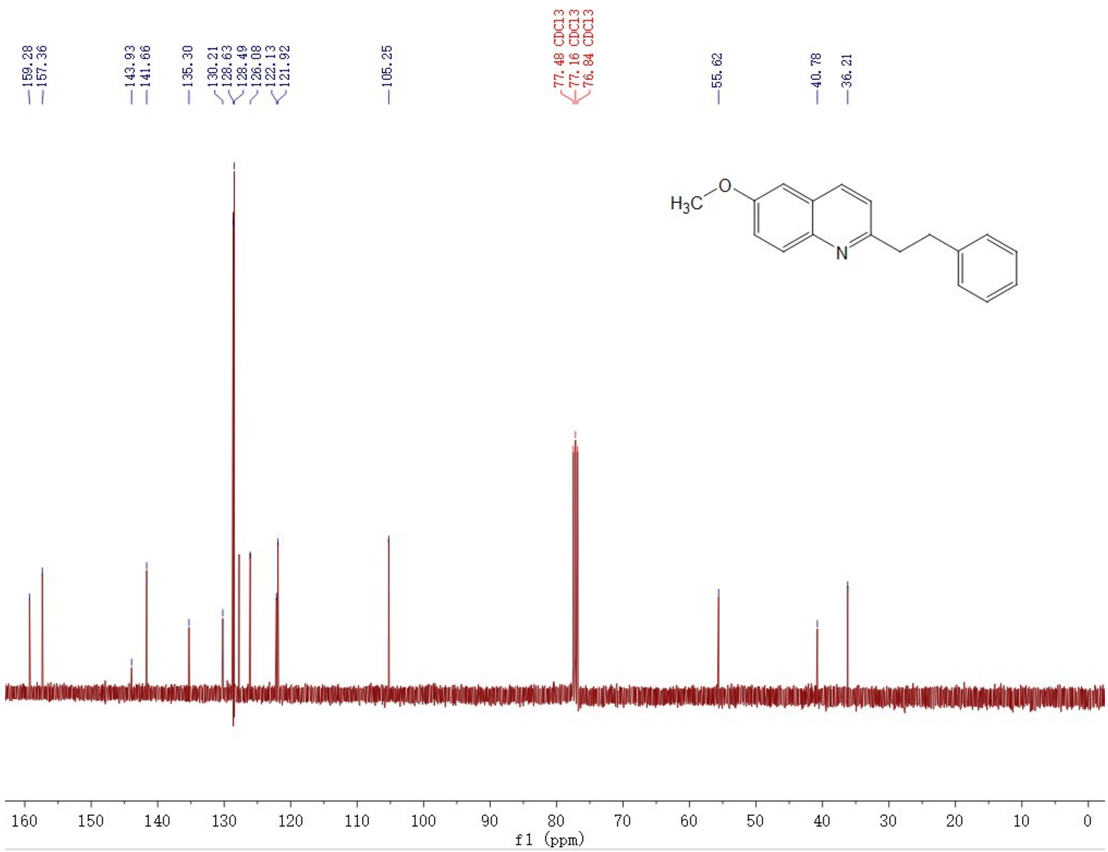
2-(5-phenylpentyl)quinoline (3dm), ^{13}C NMR (101 MHz, $CDCl_3$)



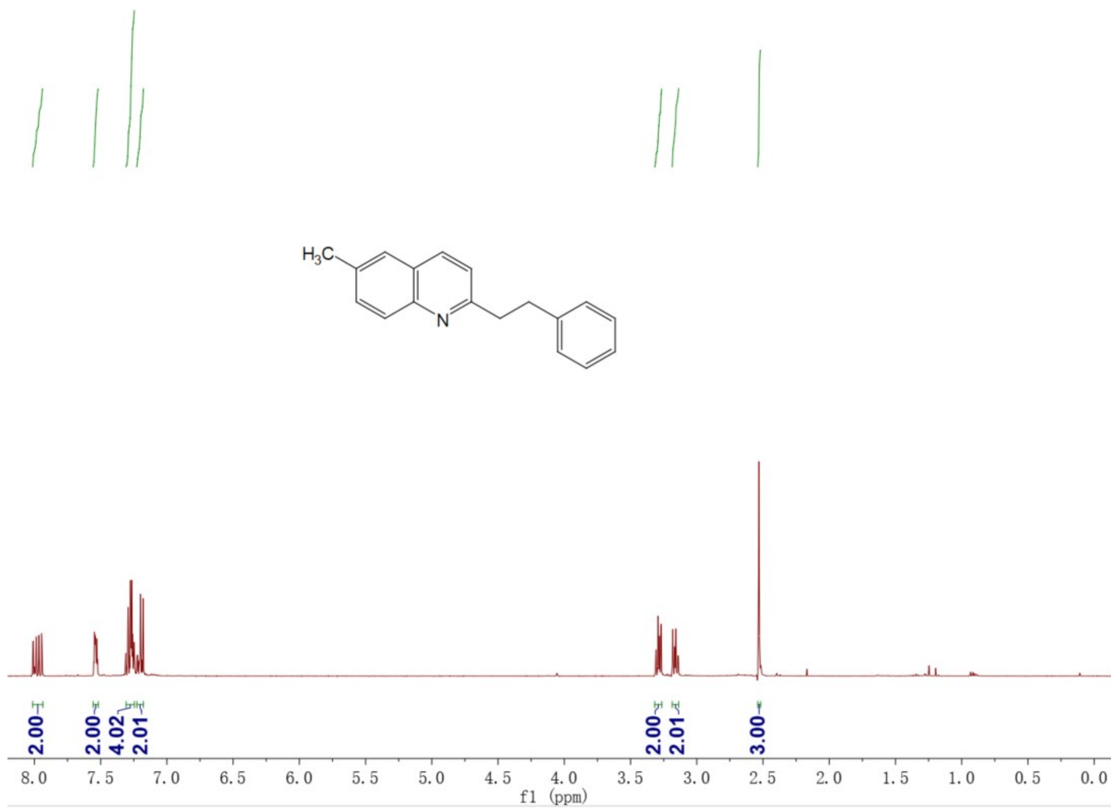
6-methoxy-2-phenethylquinoline (3ea), ^{1}H NMR (400 MHz, CDCl$_3$)



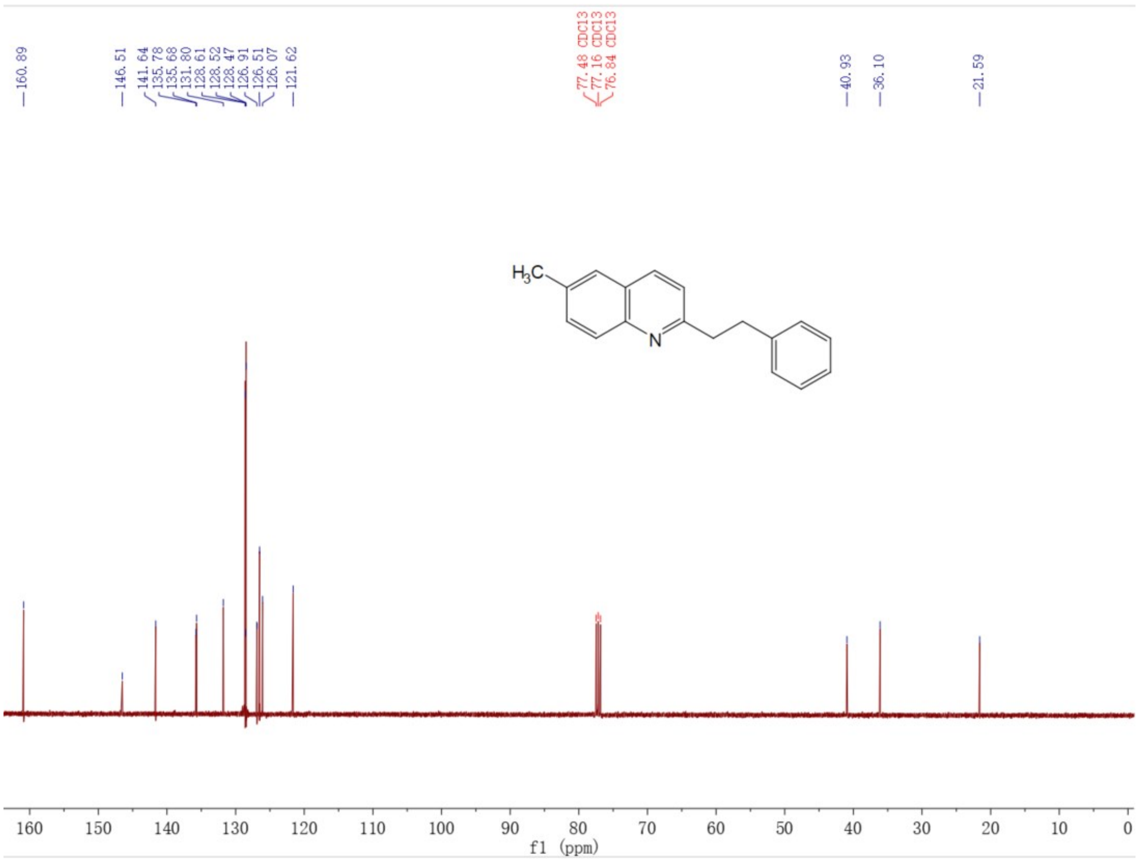
6-methoxy-2-phenethylquinoline (3ea), ^{13}C NMR (101 MHz, CDCl$_3$)



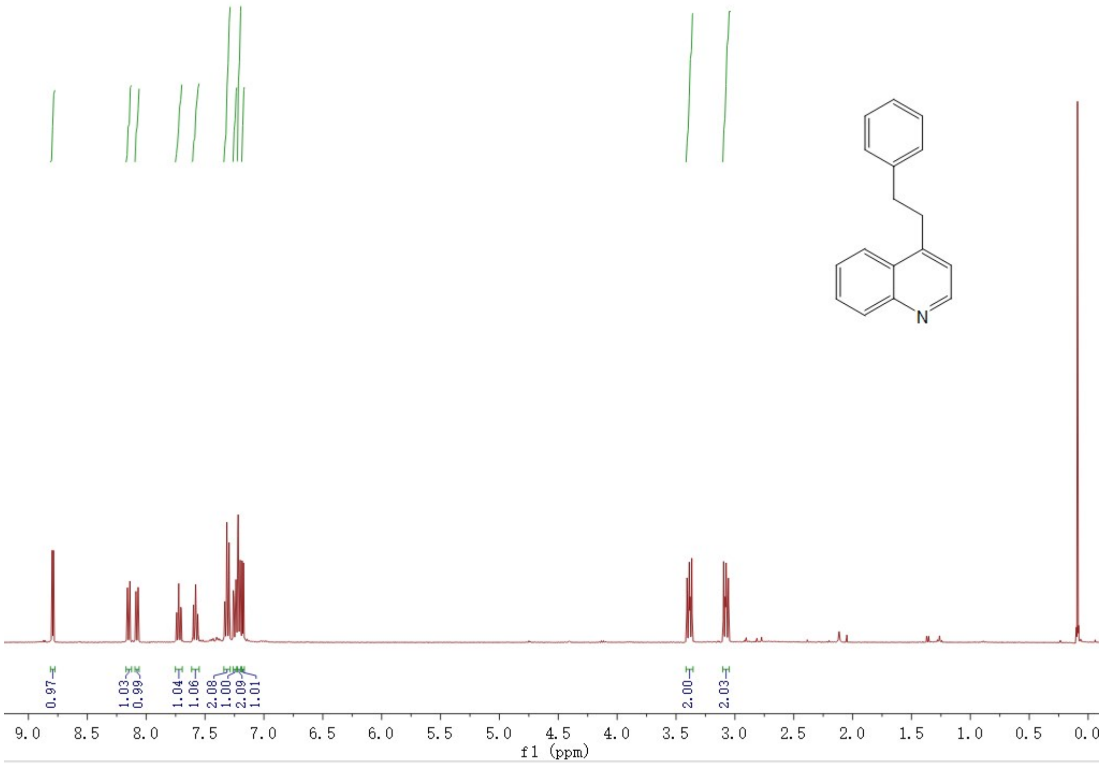
6-methyl-2-phenethylquinoline (3fa), ^{1}H NMR (400 MHz, $CDCl_3$)



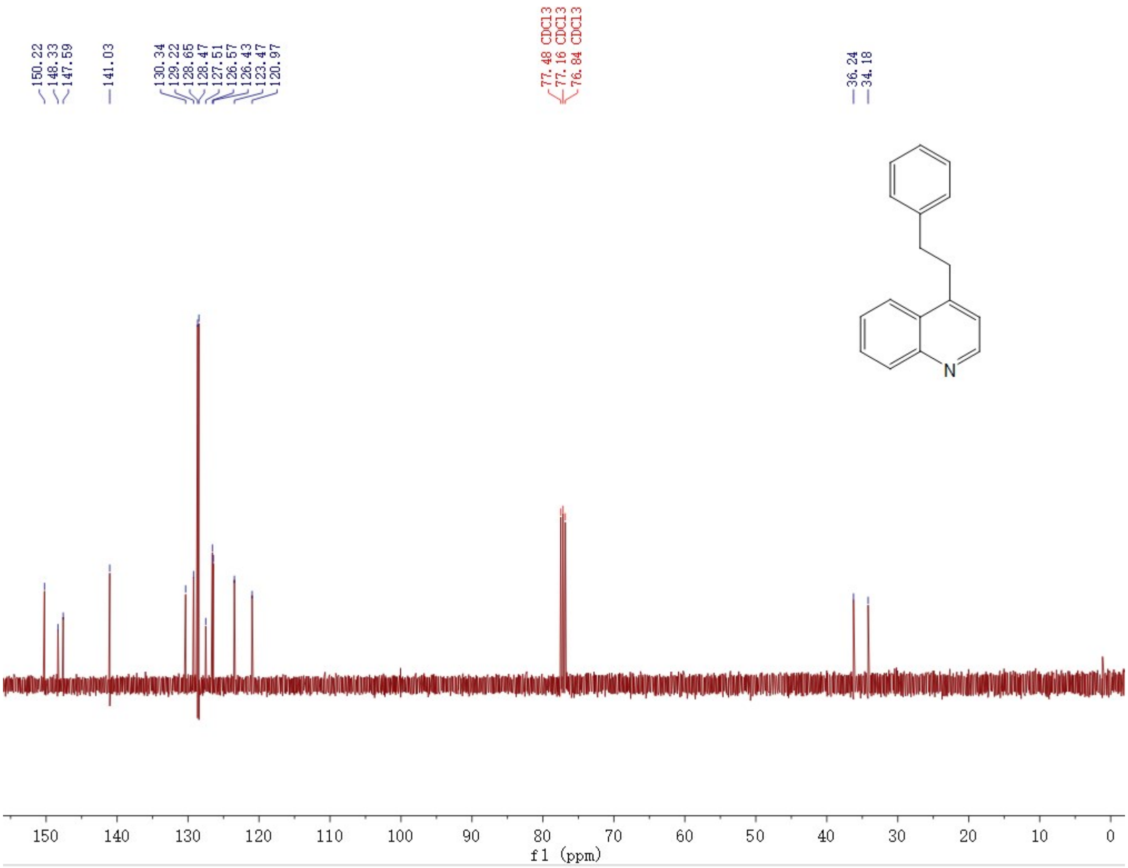
6-methyl-2-phenethylquinoline (3fa), ^{13}C NMR (101 MHz, $CDCl_3$)



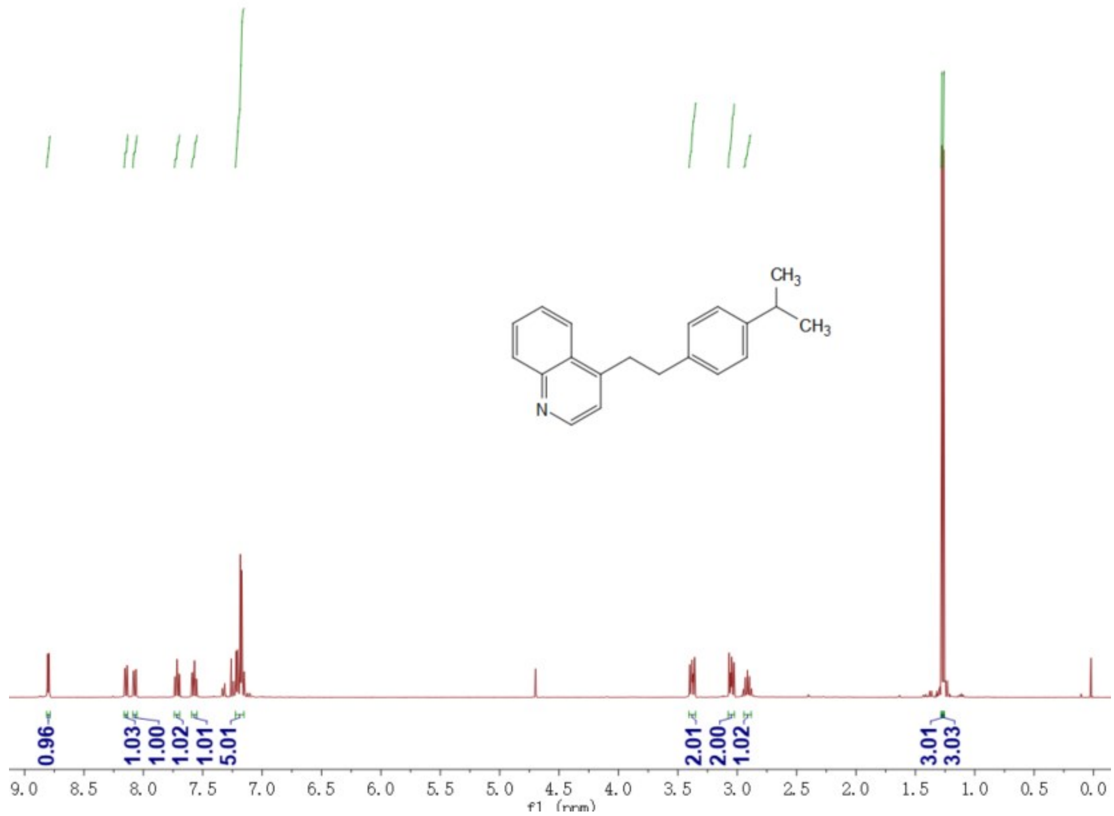
4-phenethylquinoline (3ga), ^{1}H NMR (400 MHz, CDCl$_3$)



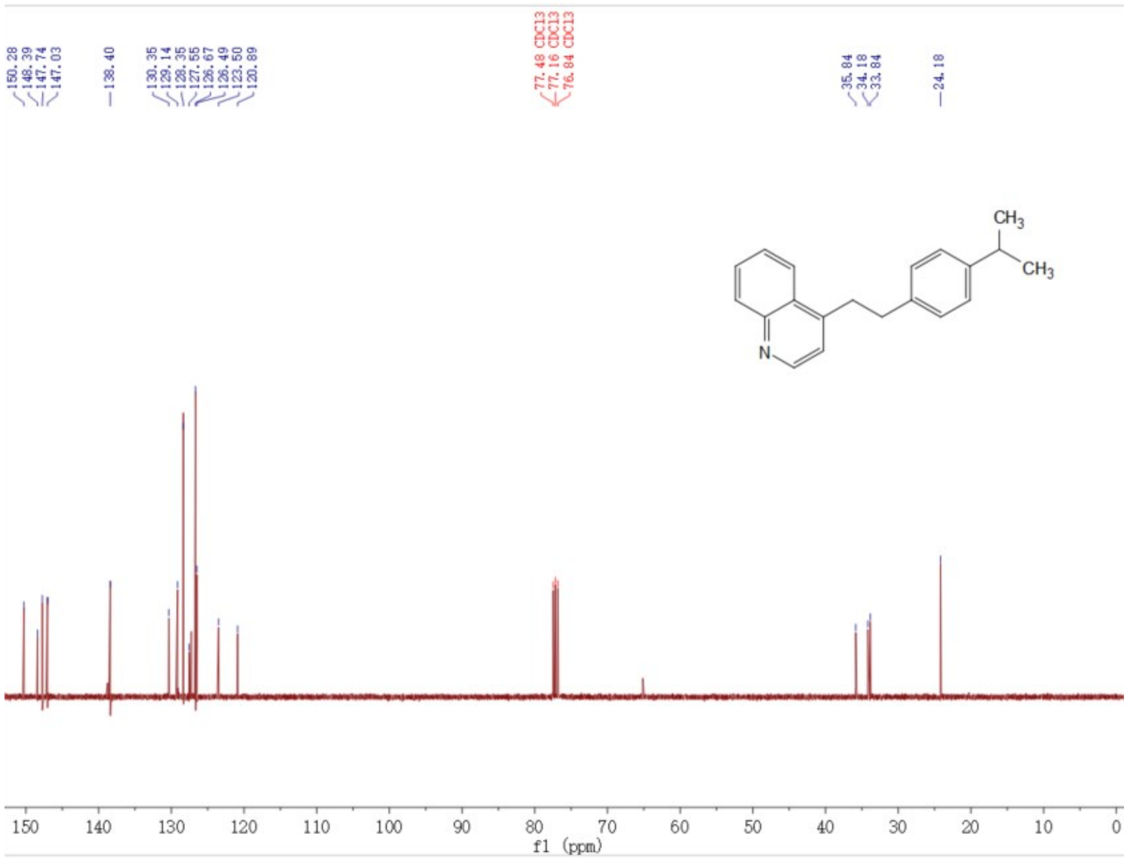
4-phenethylquinoline (3ga), ^{13}C NMR (101 MHz, CDCl$_3$)



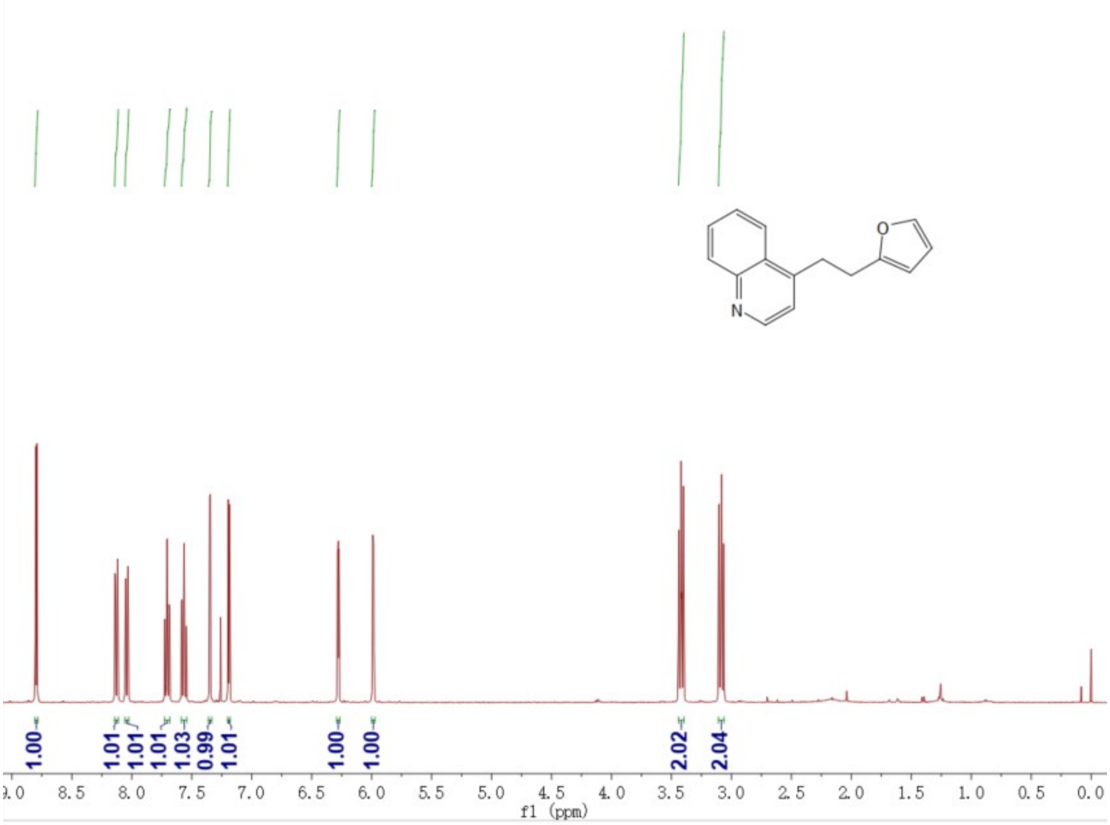
4-(4-isopropylphenethyl)quinoline (3gc), ^{1}H NMR (400 MHz, CDCl$_3$)



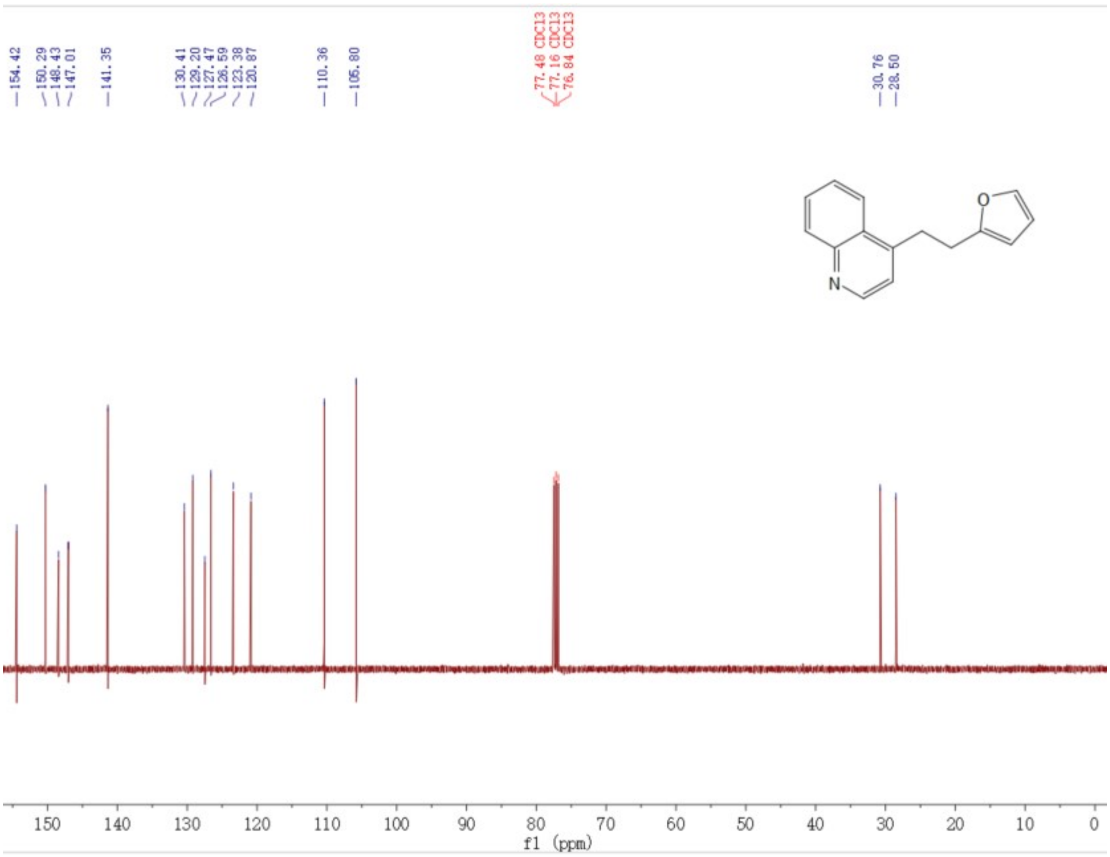
4-(4-isopropylphenethyl)quinoline (3gc), ^{13}C NMR (101 MHz, CDCl$_3$)



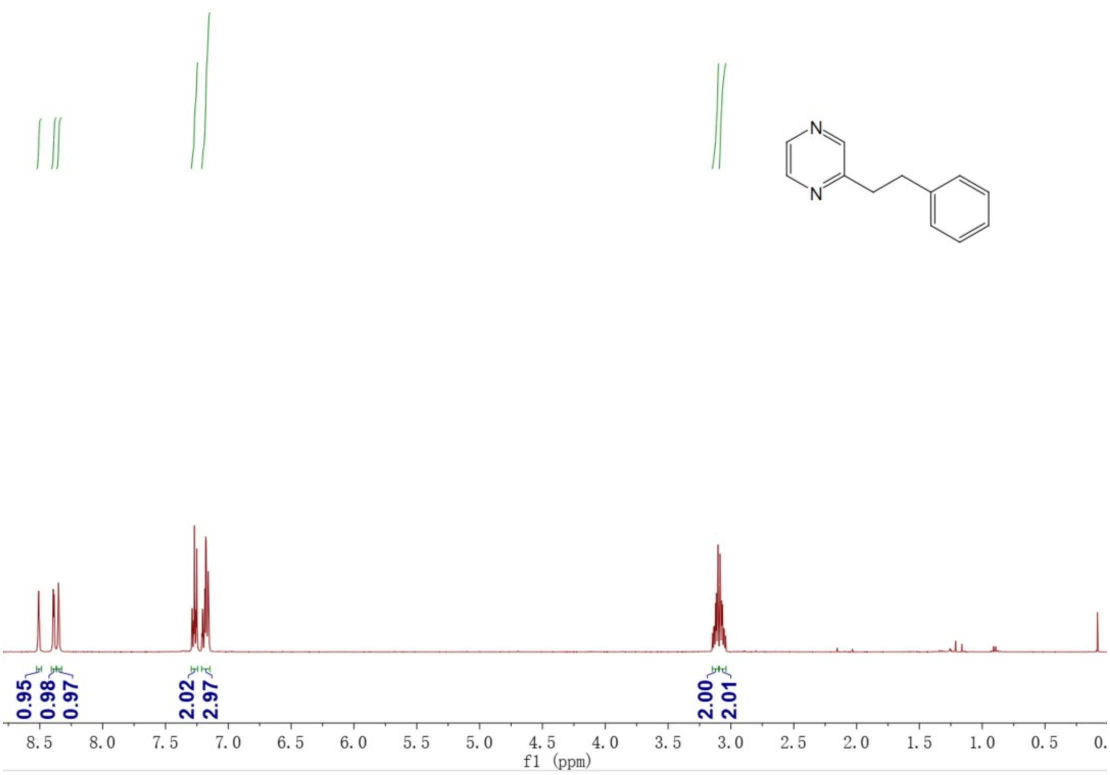
4-(2-(furan-2-yl)ethyl)quinoline (3gh), ^{1}H NMR (400 MHz, $CDCl_3$)



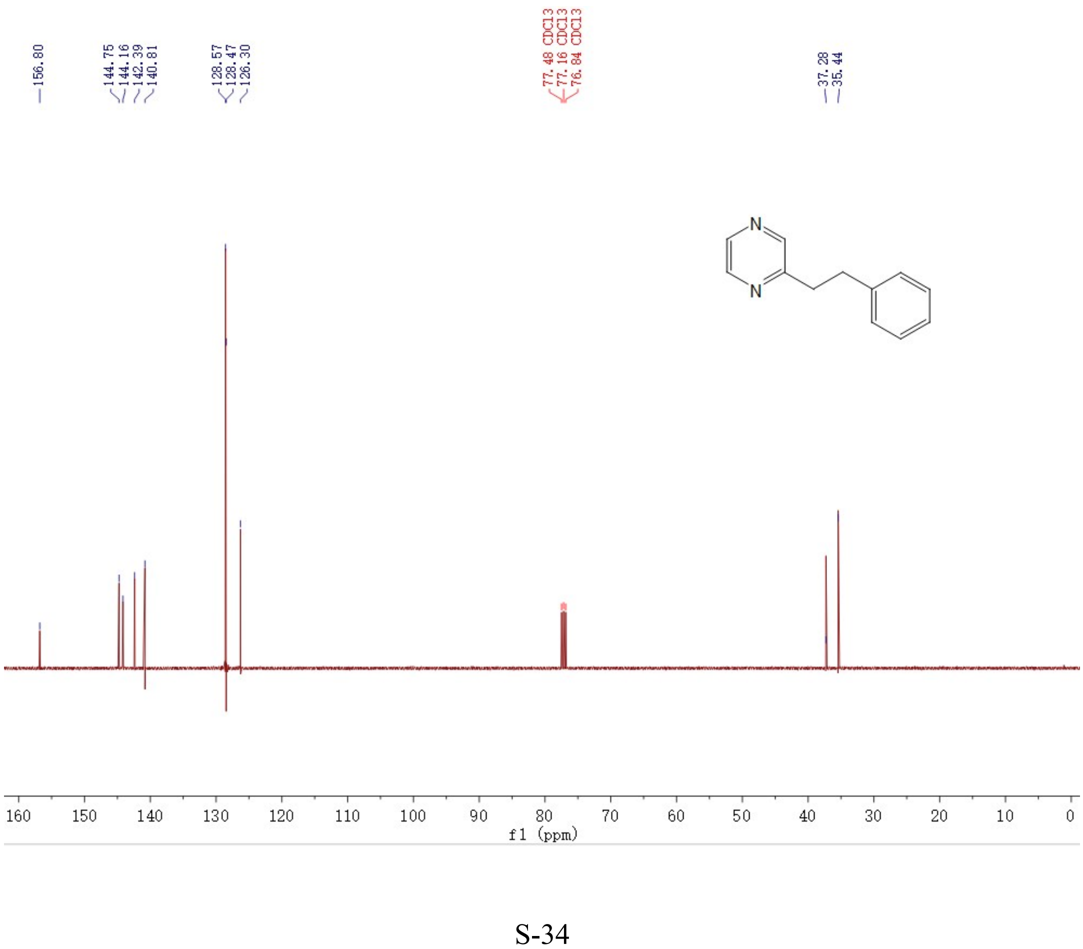
4-(2-(furan-2-yl)ethyl)quinoline (3gh), ^{13}C NMR (101 MHz, $CDCl_3$)



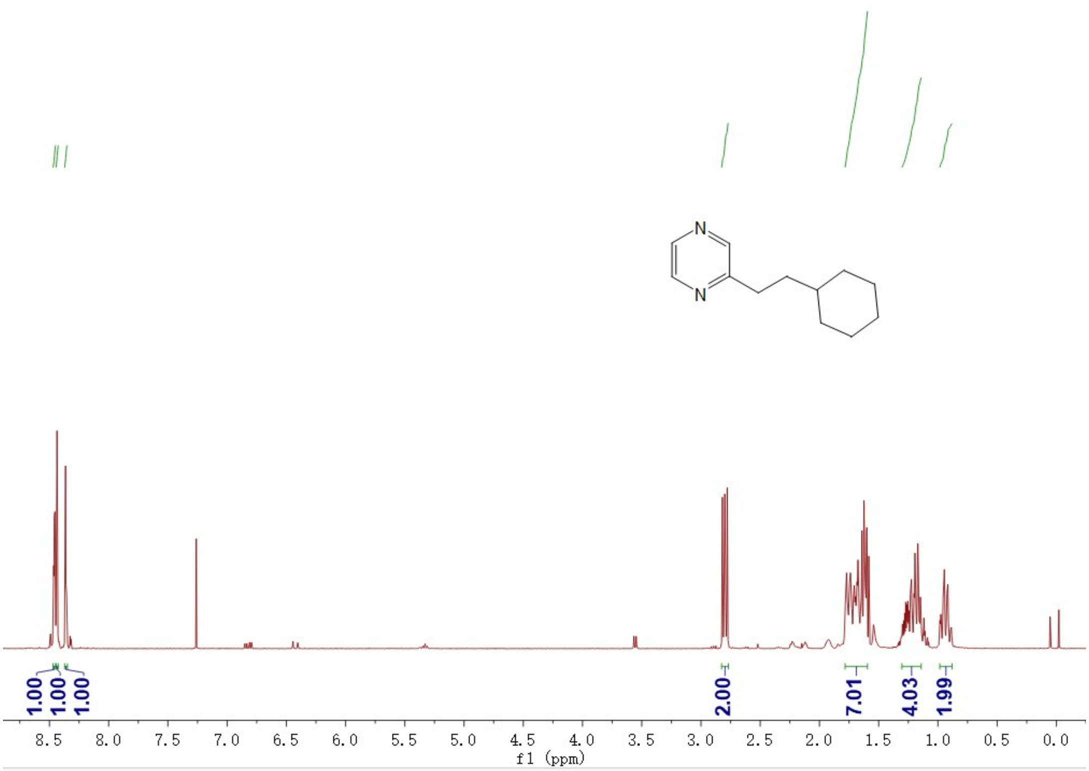
2-phenethylpyrazine (3ha), .[1]H NMR (400 MHz, CDCl$_3$)



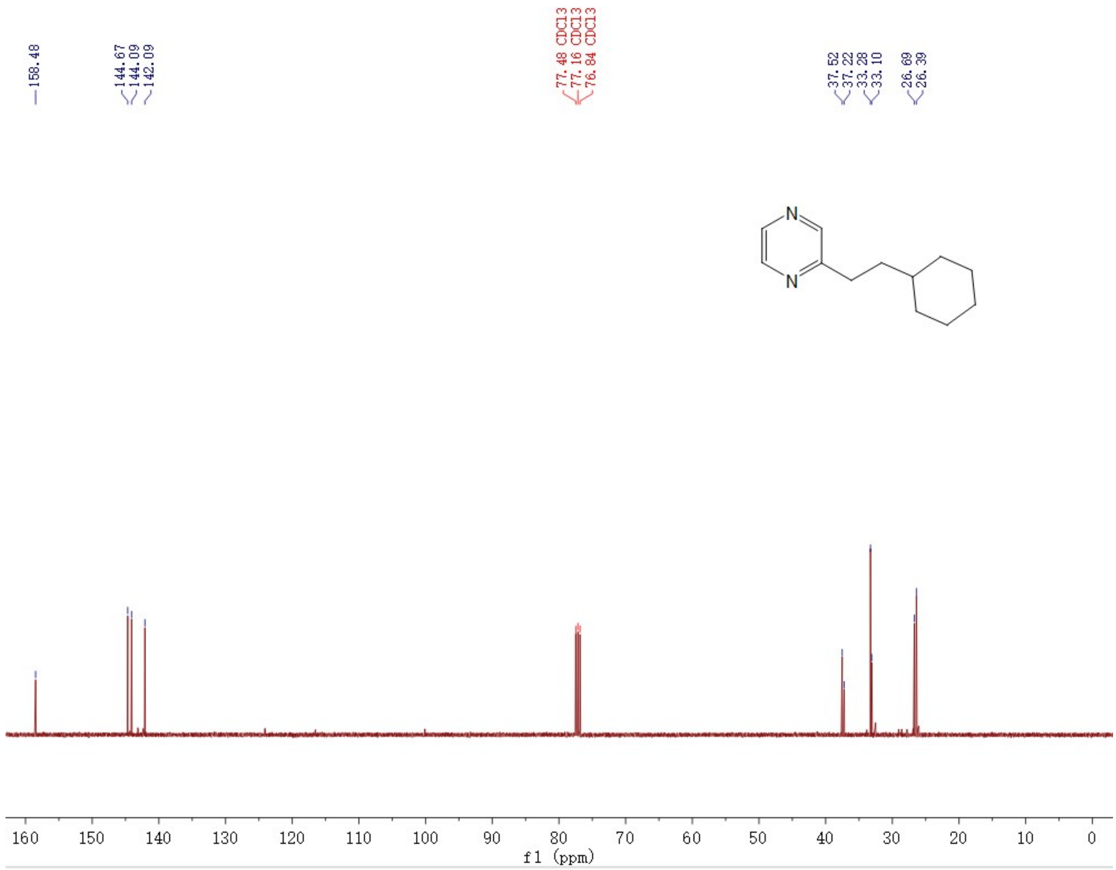
2-phenethylpyrazine (3ha), ^{13}C NMR (101 MHz, CDCl$_3$)



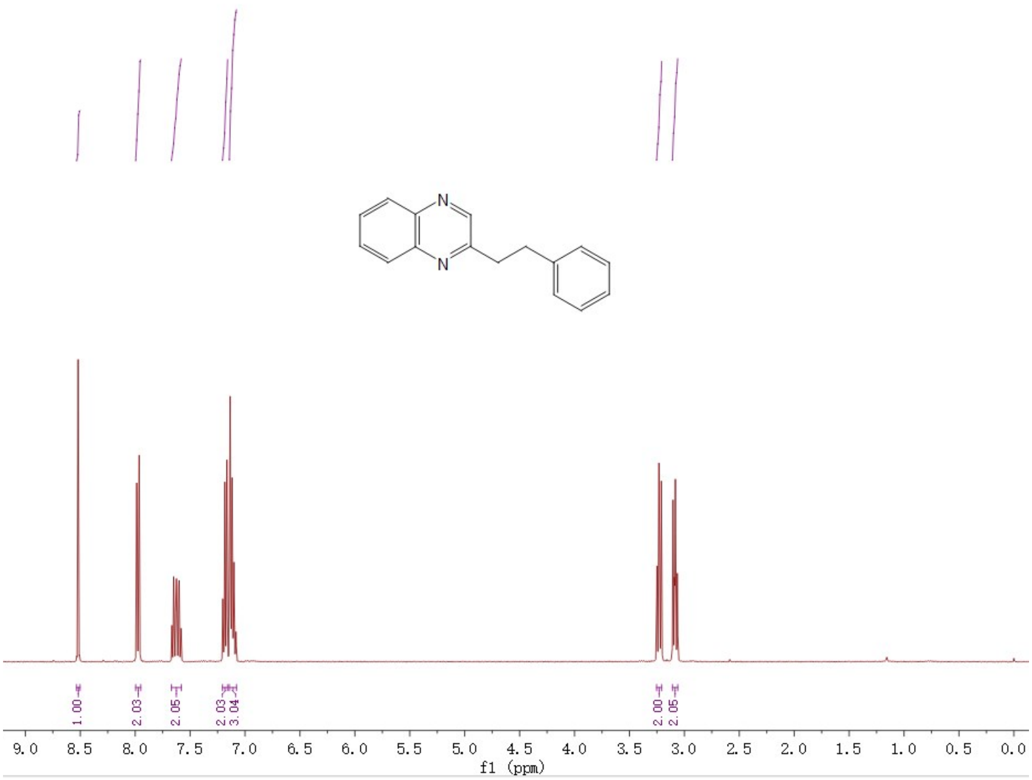
2-(2-cyclohexylethyl)pyrazine (3hj), ^{1}H NMR (400 MHz, CDCl$_3$



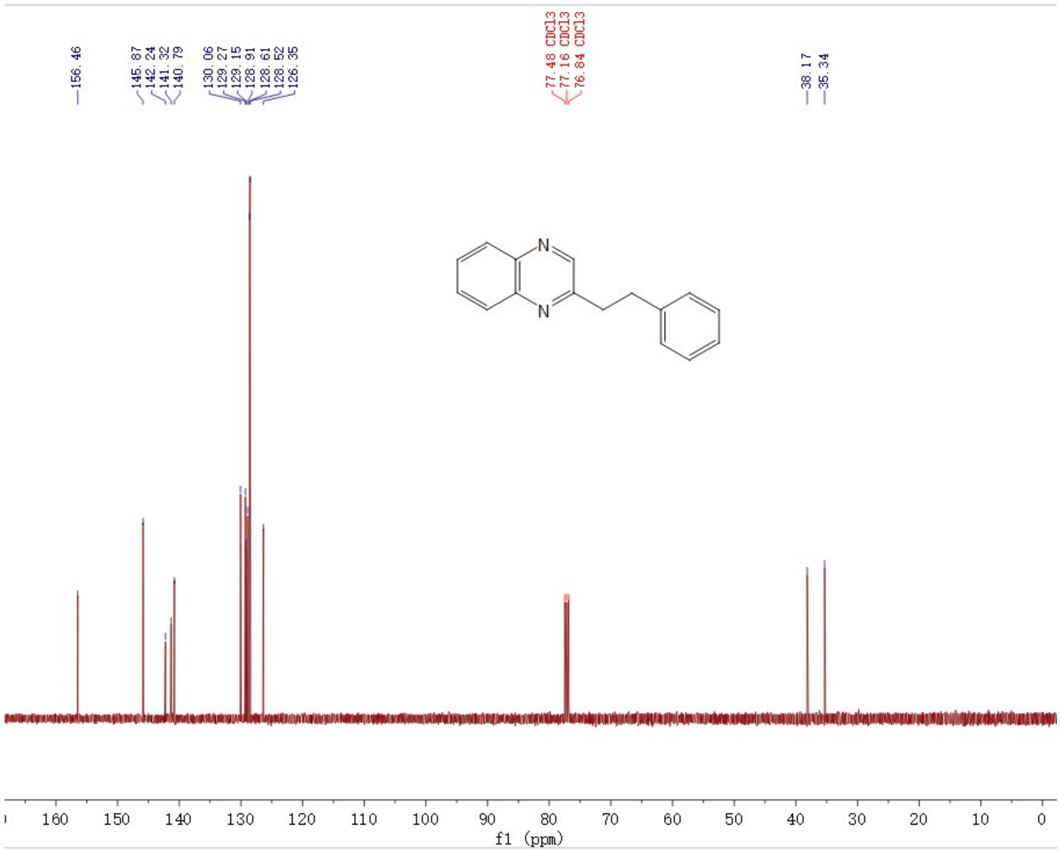
2-(2-cyclohexylethyl)pyrazine (3hj), ^{13}C NMR (101 MHz, CDCl$_3$)



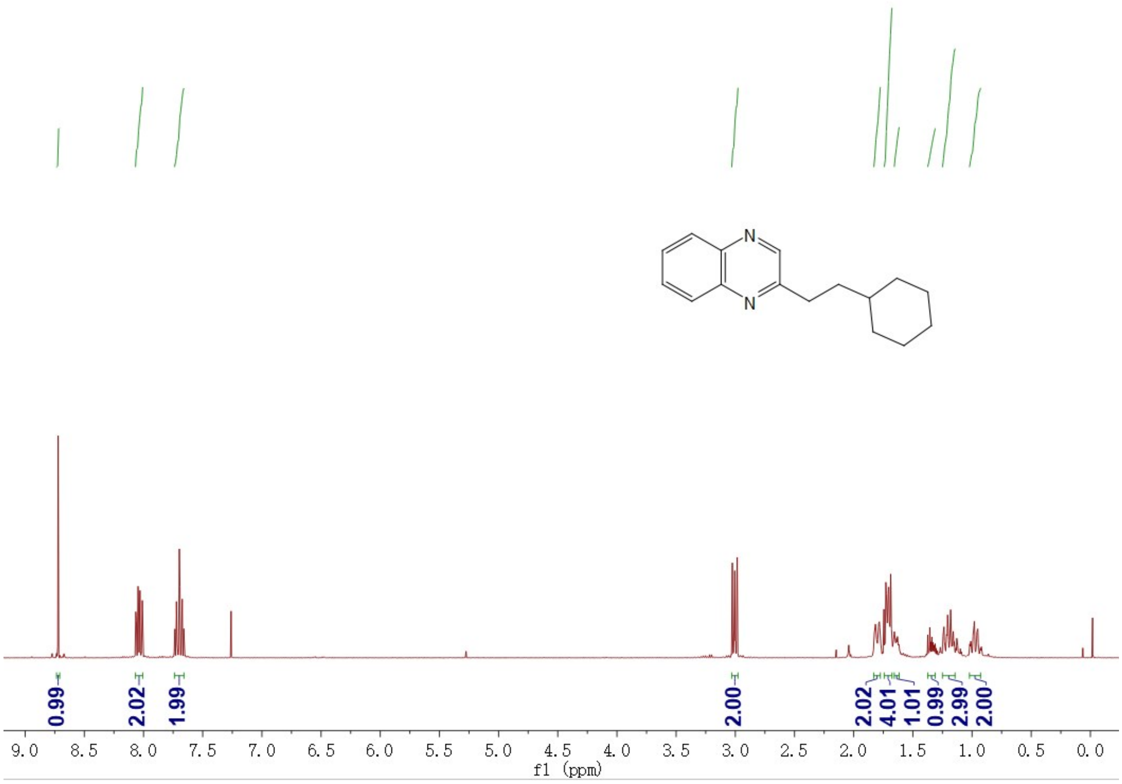
2-phenethylquinoxaline (3ia), ^{1}H NMR (400 MHz, CDCl$_3$)



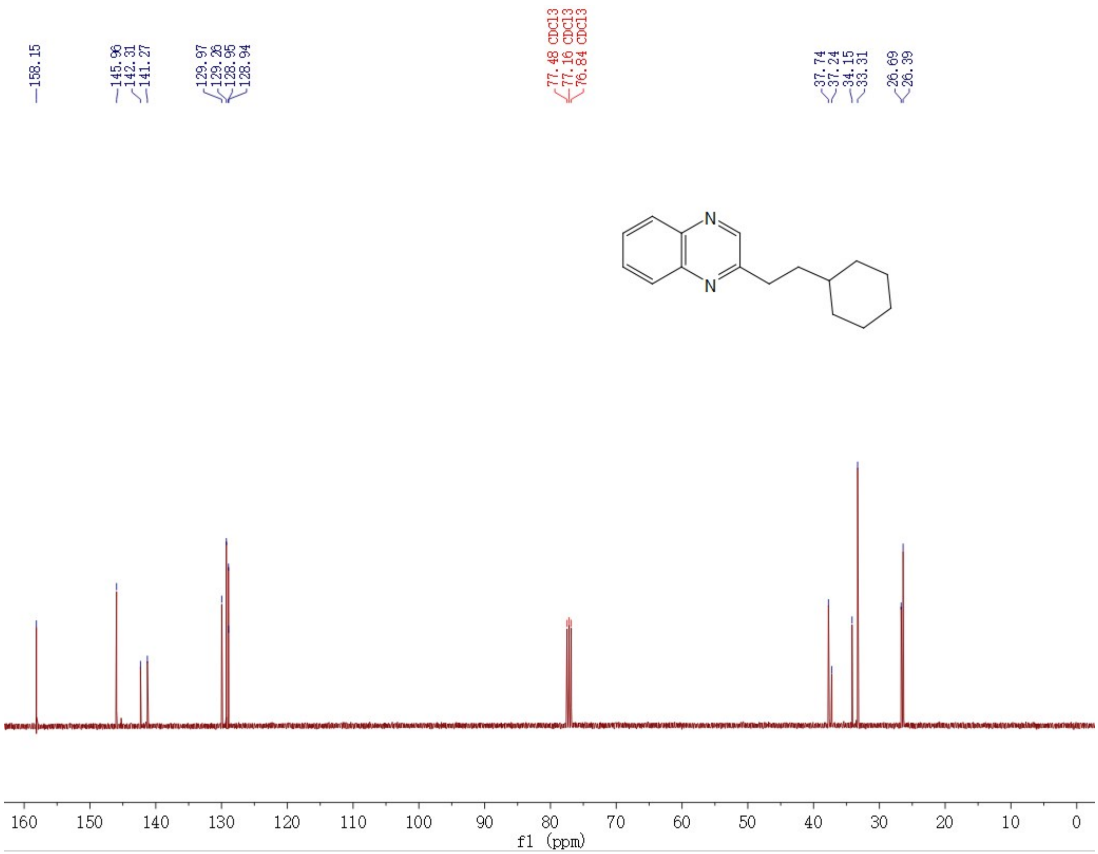
2-phenethylquinoxaline (3ia), ^{13}C NMR (101 MHz, CDCl$_3$)



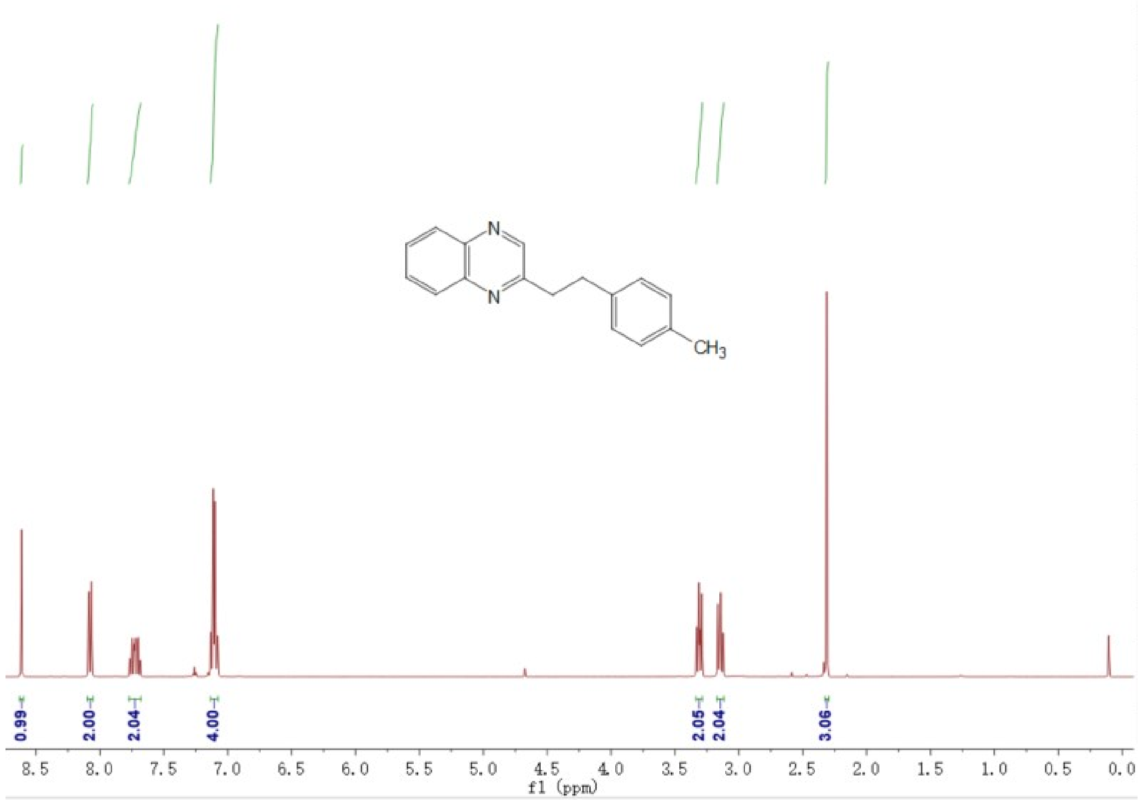
2-(2-cyclohexylethyl)quinoxaline (3ij), ^{1}H NMR (400 MHz, $CDCl_3$)



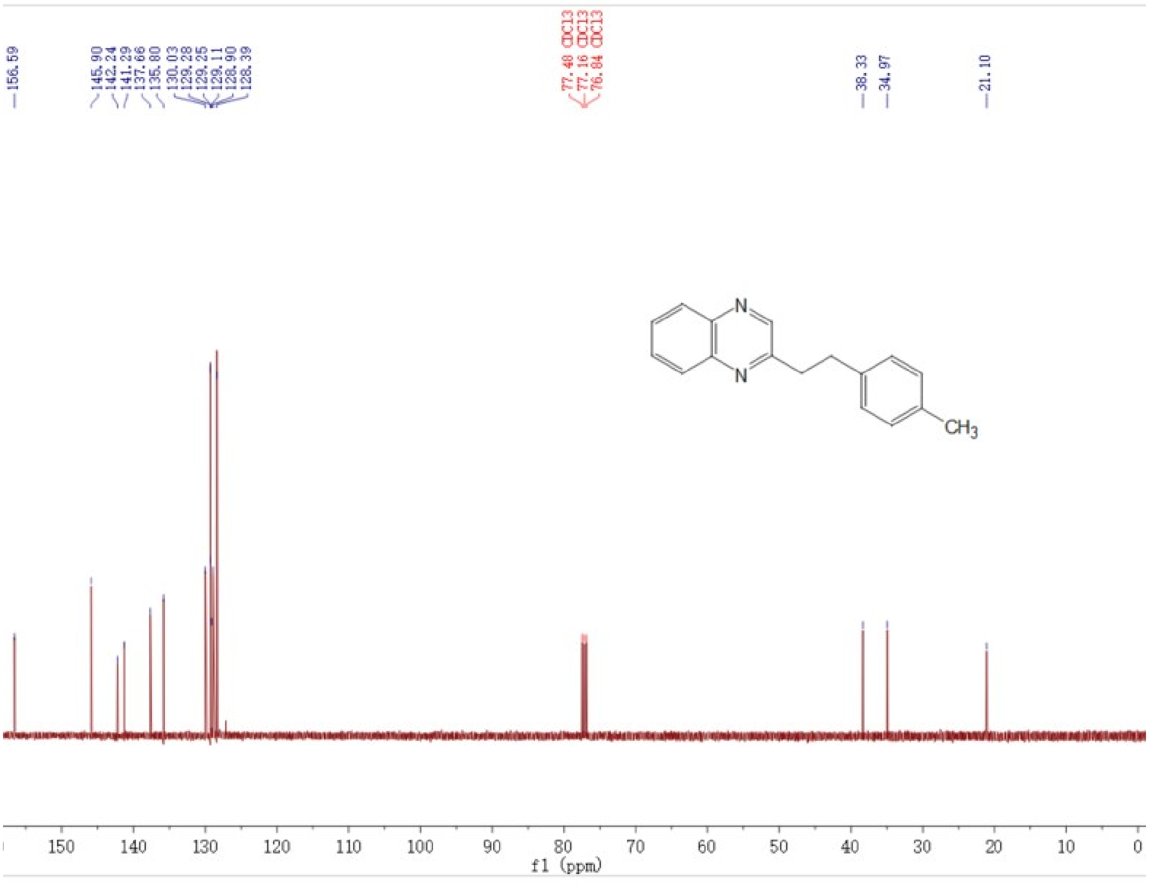
2-(2-cyclohexylethyl)quinoxaline (3ij), ^{13}C NMR (101 MHz, $CDCl_3$)



2-(4-methylphenethyl)quinoxaline (3in), ^{1}H NMR (400 MHz, $CDCl_3$)



2-(4-methylphenethyl)quinoxaline (3in), ^{13}C NMR (101 MHz, $CDCl_3$)



5. Computational details

Calculations were carried out with the Gaussian 16 program[10] at the DFT level of theory using the M062X functional.[11] All the different atoms (C, N, H, O) have been described with a 6-311+G(d,p) triple-ζ basis set.[12] Geometry optimisations were carried out without any symmetry restrictions. The nature of all stationary points were fully characterized via a subsequent analytical frequency calculation either as *minima* or as first order transition states (one imaginary frequency). IRC calculations 8 were used to confirm the *minima* linked by each transition state.[13] To model solvation effect (dimethylformamide) conductor-like polarizable continuum model (C-PCM) is used.[14]

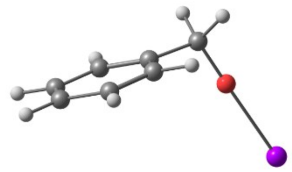
We used the default SCF option in Gaussian16 (Tight) and also the default grid (Ultrafine)

Cartesian coordinates for the optimized structure (PCM)

Energies in a.u.

$PhCH_2OK$ (2a)

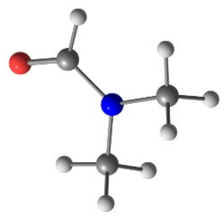
C	3.001012000000	-0.946879000000	-0.193659000000
C	2.381991000000	-0.895907000000	1.053782000000
C	1.274544000000	-0.073625000000	1.249322000000
C	0.764739000000	0.709309000000	0.210674000000
C	1.396847000000	0.648742000000	-1.033573000000
C	2.504800000000	-0.170450000000	-1.239036000000
H	3.865415000000	-1.582233000000	-0.348466000000
H	2.766297000000	-1.492678000000	1.873697000000
H	0.796185000000	-0.033512000000	2.223882000000
H	1.013968000000	1.255231000000	-1.849531000000
H	2.984884000000	-0.200305000000	-2.211006000000
C	-0.493688000000	1.546053000000	0.406923000000
H	-0.466537000000	1.920778000000	1.451701000000
H	-0.379224000000	2.446270000000	-0.232669000000
O	-1.639236000000	0.841244000000	0.127539000000
K	-3.670422000000	-0.353459000000	-0.352875000000



Sum of electronic and thermal Free Energies= -946.022037

DMF

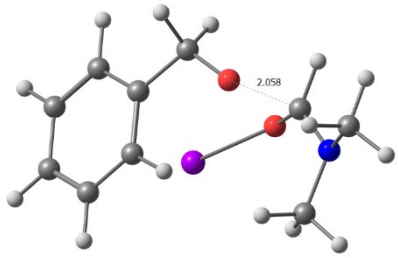
N	0.333999000000	-0.023270000000	-0.000135000000
C	1.581006000000	-0.767204000000	0.000018000000
H	1.372159000000	-1.836226000000	-0.000293000000
H	2.167285000000	-0.519775000000	-0.888028000000
H	2.166853000000	-0.520196000000	0.888472000000
C	0.434519000000	1.425598000000	0.000092000000
H	0.975541000000	1.761900000000	-0.887641000000
H	-0.565980000000	1.850485000000	-0.000567000000
H	0.974294000000	1.761777000000	0.888642000000
C	-0.858518000000	-0.641360000000	0.000007000000
H	-0.767055000000	-1.737987000000	-0.000265000000
O	-1.950391000000	-0.087412000000	-0.000011000000



Sum of electronic and thermal Free Energies= -248.406870

TS1 (5’a)

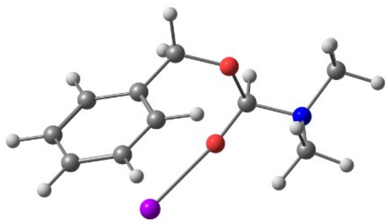
C	-0.160203000000	-1.812724000000	-0.769707000000
H	0.069402000000	-2.892879000000	-0.875649000000
H	-0.176596000000	-1.426234000000	-1.812919000000
C	1.071665000000	-1.185013000000	-0.118090000000
C	0.983096000000	-0.607087000000	1.147923000000
C	2.306483000000	-1.165706000000	-0.775865000000
C	2.098593000000	-0.018298000000	1.745416000000
H	0.014683000000	-0.611060000000	1.633653000000
C	3.422150000000	-0.573199000000	-0.189096000000
H	2.388931000000	-1.608592000000	-1.764966000000
C	3.321508000000	0.006958000000	1.076974000000
H	2.012402000000	0.430347000000	2.729039000000
H	4.368558000000	-0.557767000000	-0.717859000000
H	4.186893000000	0.471534000000	1.534546000000
O	-1.065238000000	0.938201000000	-0.998397000000
N	-3.019243000000	0.440116000000	0.100743000000
K	1.249447000000	1.871669000000	-0.747279000000
O	-1.332123000000	-1.590536000000	-0.110148000000
C	-2.049766000000	0.190786000000	-0.849574000000
H	-2.430436000000	-0.408948000000	-1.685771000000
C	-4.005710000000	-0.603440000000	0.305864000000
H	-3.618816000000	-1.387191000000	0.965459000000
H	-4.909042000000	-0.171394000000	0.741914000000
H	-4.263484000000	-1.056252000000	-0.652385000000
C	-2.590804000000	1.098623000000	1.320124000000
H	-2.099843000000	0.389174000000	1.999082000000
H	-1.890714000000	1.896015000000	1.077970000000
H	-3.459908000000	1.523996000000	1.825550000000



Sum of electronic and thermal Free Energies= -1194.403337

Adduct 1 (5’a)

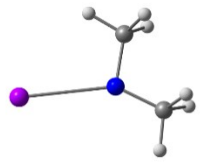
C	-0.241313000000	-1.789525000000	-0.617413000000
H	-0.225284000000	-2.860960000000	-0.383922000000
H	-0.265020000000	-1.695119000000	-1.711509000000
C	1.043028000000	-1.174693000000	-0.097197000000
C	1.107624000000	-0.672156000000	1.204420000000
C	2.187479000000	-1.126520000000	-0.894569000000
C	2.290489000000	-0.125531000000	1.696011000000
H	0.211512000000	-0.689565000000	1.813838000000
C	3.373161000000	-0.576694000000	-0.407450000000
H	2.147557000000	-1.505802000000	-1.911040000000
C	3.427971000000	-0.071164000000	0.889666000000
H	2.324786000000	0.266631000000	2.706098000000
H	4.249877000000	-0.535364000000	-1.043427000000
H	4.346037000000	0.361813000000	1.268442000000
O	-0.960549000000	0.820359000000	-1.025819000000
N	-3.018348000000	0.447868000000	0.025641000000
K	1.172838000000	1.945549000000	-0.601835000000
O	-1.396136000000	-1.253245000000	-0.038985000000
C	-1.902262000000	-0.054377000000	-0.781028000000
H	-2.365469000000	-0.502124000000	-1.689032000000
C	-4.069866000000	-0.534685000000	0.225241000000
H	-3.775587000000	-1.335690000000	0.919090000000
H	-4.961120000000	-0.043434000000	0.625428000000
H	-4.332830000000	-0.991680000000	-0.732133000000
C	-2.587071000000	1.019515000000	1.291061000000
H	-2.237865000000	0.251912000000	1.999020000000
H	-1.772958000000	1.720943000000	1.108994000000
H	-3.421074000000	1.556007000000	1.751500000000



Sum of electronic and thermal Free Energies= -1194.410634

Me$_2$NK

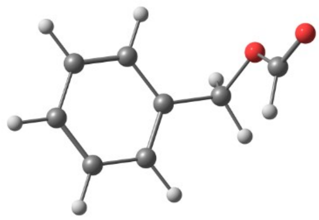
N	0.771741000000	-0.145572000000	0.000000000000
C	2.119974000000	-0.638518000000	0.000000000000
H	2.145089000000	-1.735383000000	-0.000001000000
H	2.718421000000	-0.307671000000	-0.881614000000
H	2.718421000000	-0.307672000000	0.881614000000
C	0.835995000000	1.291187000000	0.000000000000
H	1.367782000000	1.719149000000	-0.882166000000
H	-0.166827000000	1.744073000000	0.000001000000
H	1.367782000000	1.719148000000	0.882167000000
K	-1.748144000000	-0.709754000000	-0.000002000000



Sum of electronic and thermal Free Energies= -734.425078

Formamide (5a)

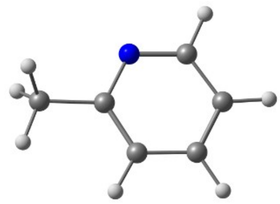
C	0.978450000000	0.699132000000	1.140340000000
H	1.216031000000	1.746470000000	0.943479000000
H	0.993274000000	0.536063000000	2.216500000000
C	-0.350957000000	0.320181000000	0.541482000000
C	-1.132421000000	1.271603000000	-0.109866000000
C	-0.811140000000	-0.995031000000	0.642067000000
C	-2.366329000000	0.916963000000	-0.652040000000
H	-0.775983000000	2.292692000000	-0.196131000000
C	-2.037445000000	-1.351433000000	0.095011000000
H	-0.202557000000	-1.737788000000	1.146947000000
C	-2.818644000000	-0.394026000000	-0.551465000000
H	-2.967995000000	1.663494000000	-1.156571000000
H	-2.387863000000	-2.373566000000	0.175337000000
H	-3.775799000000	-0.672346000000	-0.976212000000
O	3.279500000000	-0.575807000000	-1.142876000000
O	2.043952000000	-0.140186000000	0.640669000000
C	2.436079000000	0.088982000000	-0.611671000000
H	1.927716000000	0.934708000000	-1.098833000000



Sum of electronic and thermal Free Energies= -459.946962

Me-Pyridine (1a)

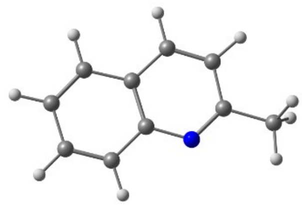
C	-0.875336000000	0.003563000000	-0.000049000000
C	-0.161678000000	1.203433000000	-0.000055000000
C	1.226946000000	1.168547000000	-0.000008000000
C	1.865635000000	-0.065013000000	0.000036000000
C	1.074616000000	-1.208625000000	0.000022000000
H	-0.693413000000	2.147054000000	-0.000102000000
H	1.799384000000	2.088751000000	-0.000014000000
H	2.944852000000	-0.146200000000	0.000065000000
H	1.535983000000	-2.191574000000	0.000041000000
C	-2.378485000000	-0.016816000000	0.000030000000
H	-2.746007000000	-0.548622000000	-0.880022000000
H	-2.745918000000	-0.546391000000	0.881480000000
H	-2.790990000000	0.991708000000	-0.001170000000
N	-0.259154000000	-1.186466000000	-0.000019000000



Sum of electronic and thermal Free Energies= -287.466958

Me-Quinoline (1d)

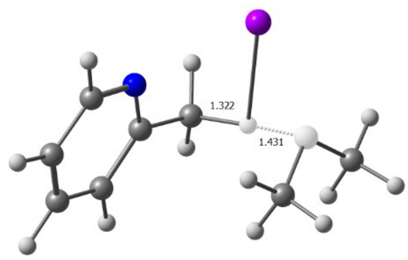
C	-4.178331000000	-0.758831000000	-0.351581000000
C	-2.806906000000	-0.721868000000	-0.351752000000
C	-2.123031000000	0.519835000000	-0.351820000000
C	-2.878779000000	1.719261000000	-0.351708000000
C	-4.294189000000	1.653799000000	-0.351533000000
C	-4.931650000000	0.439373000000	-0.351470000000
H	-4.693518000000	-1.712150000000	-0.351530000000
H	-2.215892000000	-1.630274000000	-0.351839000000
C	-2.159782000000	2.943475000000	-0.351782000000
H	-4.860898000000	2.578699000000	-0.351449000000
H	-6.013875000000	0.391715000000	-0.351336000000
C	-0.797056000000	2.915730000000	-0.351953000000
C	-0.118613000000	1.659809000000	-0.352055000000
H	-2.703538000000	3.882364000000	-0.351700000000
H	-0.215169000000	3.829776000000	-0.352014000000
C	1.384328000000	1.643061000000	-0.352245000000
H	1.770837000000	2.162589000000	-1.232420000000
H	1.771062000000	2.162617000000	0.527815000000
H	1.749844000000	0.617999000000	-0.352276000000
N	-0.755115000000	0.512418000000	-0.351990000000



Sum of electronic and thermal Free Energies= -441.044205

TS2 (1a→1'a)

C	0.247954000000	-1.954027000000	0.007306000000
C	1.090886000000	-0.905815000000	0.444942000000
C	0.645105000000	0.398706000000	0.417063000000
C	-0.646695000000	0.671102000000	-0.048306000000
C	-1.414682000000	-0.405274000000	-0.459788000000
H	2.086146000000	-1.145279000000	0.801544000000
H	1.287719000000	1.203648000000	0.756941000000
H	-1.040461000000	1.678132000000	-0.086321000000
H	-2.423952000000	-0.243091000000	-0.829400000000
N	-0.998425000000	-1.677557000000	-0.443808000000
K	-1.660242000000	-3.602279000000	-2.367906000000
N	0.971246000000	-3.661810000000	-2.797888000000
C	1.522824000000	-2.351878000000	-3.068504000000
H	2.304808000000	-2.059884000000	-2.333978000000
H	1.993862000000	-2.278872000000	-4.063685000000
H	0.742132000000	-1.582139000000	-3.017308000000
C	2.027869000000	-4.642044000000	-2.900266000000
H	2.492010000000	-4.672266000000	-3.900962000000
H	2.858301000000	-4.453495000000	-2.185203000000
H	1.645807000000	-5.647080000000	-2.689718000000
C	0.704066000000	-3.338782000000	-0.079776000000
H	1.628918000000	-3.519335000000	0.468215000000
H	0.842281000000	-3.558540000000	-1.375981000000
H	-0.069643000000	-4.046756000000	0.228905000000

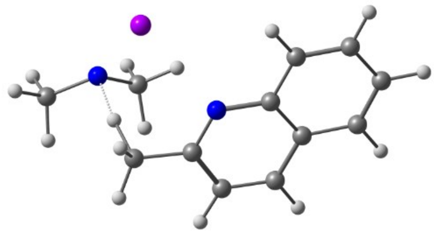


Sum of electronic and thermal Free Energies= -1021.875312

Quinoline series (1d→1'd)

C	-0.313211000000	-2.103469000000	0.098138000000
C	0.480674000000	-0.983324000000	0.530356000000
C	-0.050816000000	0.265637000000	0.553841000000
C	-1.402357000000	0.462640000000	0.141547000000
C	-2.124164000000	-0.686680000000	-0.271541000000
H	1.505208000000	-1.162037000000	0.835379000000
H	0.533427000000	1.119231000000	0.882892000000

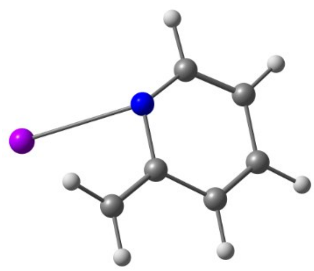
N	-1.574363000000	-1.937931000000	-0.293355000000
K	-2.024266000000	-3.756749000000	-2.394659000000
N	0.606811000000	-3.570746000000	-2.762031000000
C	1.002619000000	-2.188785000000	-2.916779000000
H	1.709108000000	-1.856027000000	-2.124078000000
H	1.506399000000	-1.988414000000	-3.878047000000
H	0.132500000000	-1.521694000000	-2.856749000000
C	1.777749000000	-4.406147000000	-2.897523000000
H	2.273048000000	-4.298372000000	-3.878150000000
H	2.557616000000	-4.178900000000	-2.137816000000
H	1.515543000000	-5.463462000000	-2.781307000000
C	0.287613000000	-3.425756000000	-0.026275000000
H	1.227428000000	-3.527125000000	0.515064000000
H	0.456594000000	-3.569790000000	-1.301092000000
H	-0.406182000000	-4.226653000000	0.238511000000
C	-2.029041000000	1.728252000000	0.133775000000
H	-1.459015000000	2.594186000000	0.454874000000
C	-3.471598000000	-0.522847000000	-0.681288000000
H	-4.027121000000	-1.402980000000	-0.986069000000
C	-3.336286000000	1.860921000000	-0.273341000000
H	-3.812674000000	2.833710000000	-0.278698000000
C	-4.059858000000	0.720153000000	-0.682921000000
H	-5.091133000000	0.826681000000	-0.999430000000



Sum of electronic and thermal Free Energies= -1175.454532

Pyridinium (1’a)

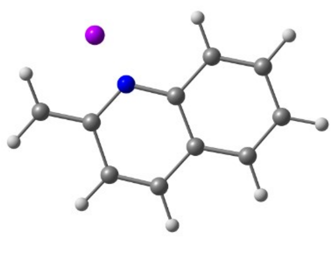
C	-0.215323000000	0.881648000000	0.334723000000
C	-1.409665000000	1.162956000000	-0.438711000000
C	-2.357821000000	0.200650000000	-0.633073000000
C	-2.178941000000	-1.095982000000	-0.089338000000
C	-1.006282000000	-1.311539000000	0.612813000000
H	-1.538120000000	2.159919000000	-0.846961000000
H	-3.250751000000	0.432102000000	-1.206235000000
H	-2.908175000000	-1.883673000000	-0.220098000000
H	-0.811439000000	-2.297656000000	1.033133000000
N	-0.046780000000	-0.405746000000	0.829496000000
C	0.761201000000	1.837022000000	0.554845000000
H	0.636157000000	2.845516000000	0.182223000000
H	1.577134000000	1.643646000000	1.242693000000
K	2.371771000000	-0.532008000000	-0.423094000000



Sum of electronic and thermal Free Energies= -886.840362

Quinoline series (1’d)

C	-4.395215000000	-0.464804000000	-0.936237000000
C	-3.145596000000	-0.212573000000	-1.465857000000
C	-2.243391000000	0.690526000000	-0.839456000000
C	-2.693014000000	1.326653000000	0.356146000000
C	-3.966350000000	1.052536000000	0.875022000000
C	-4.823210000000	0.164834000000	0.245899000000
H	-5.056095000000	-1.161736000000	-1.441055000000
H	-2.820322000000	-0.705482000000	-2.376179000000
C	-1.779984000000	2.257304000000	0.971349000000
H	-4.273108000000	1.556029000000	1.787698000000
H	-5.804910000000	-0.041046000000	0.654277000000
C	-0.570472000000	2.480679000000	0.421397000000
C	-0.151016000000	1.777670000000	-0.793730000000
H	-2.085476000000	2.771996000000	1.877950000000
H	0.127242000000	3.178101000000	0.873011000000

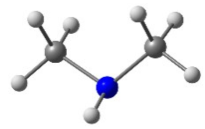


C	1.093378000000	2.021797000000	-1.329550000000
H	1.462010000000	1.441318000000	-2.168323000000
H	1.771449000000	2.716297000000	-0.851454000000
N	-1.027790000000	0.908825000000	-1.398053000000
K	-0.821203000000	2.263358000000	-3.726065000000

Sum of electronic and thermal Free Energies= -1040.426537

$HNMe_2$

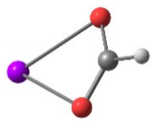
N	-0.028311000000	0.594675000000	0.000000000000
C	-0.028311000000	-0.224948000000	1.206590000000
H	0.038325000000	0.412313000000	2.089240000000
H	-0.966671000000	-0.782658000000	1.261356000000
H	0.797350000000	-0.951433000000	1.234655000000
C	-0.028311000000	-0.224948000000	-1.206590000000
H	-0.966671000000	-0.782658000000	-1.261356000000
H	0.038325000000	0.412313000000	-2.089240000000
H	0.797350000000	-0.951433000000	-1.234655000000
H	0.799899000000	1.180204000000	0.000000000000



Sum of electronic and thermal Free Energies= -135.065717

HCOOK

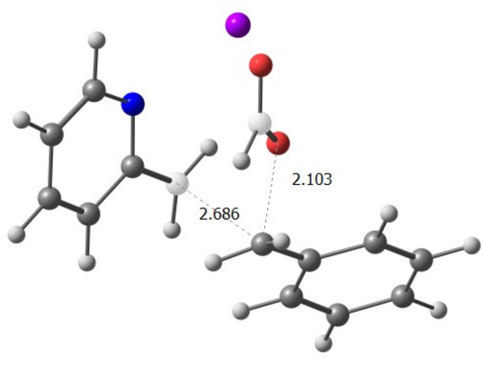
O	-0.983735000000	1.118425000000	0.000034000000
C	-1.547954000000	0.000000000000	-0.000056000000
H	-2.659647000000	-0.000001000000	-0.000076000000
K	1.457217000000	0.000000000000	-0.000007000000
O	-0.983735000000	-1.118425000000	0.000034000000



Sum of electronic and thermal Free Energies= -789.189159

TS3 (3’aa)

C	-1.514410000000	-1.180225000000	-0.724794000000
C	-1.919614000000	-2.409092000000	-0.101563000000
C	-3.132754000000	-2.495310000000	0.535474000000
C	-3.988599000000	-1.379317000000	0.558250000000
C	-3.549721000000	-0.236522000000	-0.098659000000
H	-1.250470000000	-3.262294000000	-0.139917000000
H	-3.429764000000	-3.422824000000	1.014234000000
H	-4.953936000000	-1.404393000000	1.045322000000
H	-4.189154000000	0.644327000000	-0.123067000000
N	-2.380145000000	-0.111662000000	-0.722478000000
C	-0.233476000000	-1.031599000000	-1.257424000000
H	0.389648000000	-1.904811000000	-1.391931000000
H	0.065193000000	-0.120622000000	-1.756957000000
K	-1.337894000000	2.375155000000	-1.327652000000
C	1.030788000000	-0.691701000000	1.087755000000
H	0.504400000000	-1.614809000000	0.896315000000
H	0.864033000000	-0.271032000000	2.069569000000
C	2.350336000000	-0.502949000000	0.529381000000
C	2.937432000000	-1.469820000000	-0.305806000000
C	3.099227000000	0.631286000000	0.884360000000
C	4.237673000000	-1.310005000000	-0.758694000000
H	2.374082000000	-2.354608000000	-0.577699000000
C	4.394229000000	0.797539000000	0.413190000000

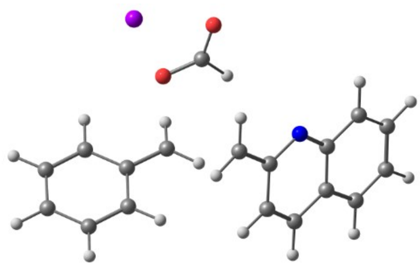


H	2.642243000000	1.379864000000	1.521220000000
C	4.966495000000	-0.171881000000	-0.408520000000
H	4.686426000000	-2.068383000000	-1.388873000000
H	4.961174000000	1.678892000000	0.688179000000
H	5.978341000000	-0.043982000000	-0.774455000000
O	0.092775000000	1.142092000000	0.663980000000
C	-0.878220000000	1.391021000000	1.442101000000
H	-1.053956000000	0.658863000000	2.256197000000
O	-1.630722000000	2.371778000000	1.357808000000

Sum of electronic and thermal Free Energies= -1346.712451

Quinoline series (3'da)

C	1.394262000000	-0.151882000000	1.280463000000
C	1.709130000000	-1.571820000000	1.177462000000
C	2.858720000000	-1.987344000000	0.595219000000
C	3.783036000000	-1.023346000000	0.081543000000
C	3.418326000000	0.351942000000	0.221986000000
H	1.006958000000	-2.289670000000	1.589270000000
H	3.095908000000	-3.044255000000	0.517275000000
N	2.271643000000	0.771462000000	0.794314000000
C	0.175002000000	0.237195000000	1.810650000000
H	-0.499026000000	-0.492524000000	2.240495000000
H	-0.071529000000	1.286348000000	1.905339000000
C	-1.098001000000	-0.789559000000	-0.890955000000
H	-0.214190000000	-0.914925000000	-0.284559000000
H	-1.011104000000	-0.257380000000	-1.826264000000
C	-2.284183000000	-1.485680000000	-0.591777000000
C	-2.354672000000	-2.337168000000	0.535506000000
C	-3.406313000000	-1.373557000000	-1.444981000000
C	-3.501694000000	-3.064190000000	0.786585000000
H	-1.496593000000	-2.414344000000	1.193100000000
C	-4.552388000000	-2.100473000000	-1.184120000000
H	-3.351589000000	-0.708513000000	-2.299251000000
C	-4.599551000000	-2.944086000000	-0.070902000000
H	-3.554186000000	-3.722052000000	1.644762000000
H	-5.412038000000	-2.017989000000	-1.837057000000
H	-5.500084000000	-3.511695000000	0.132025000000
O	-1.873354000000	1.483779000000	-0.604666000000
C	-0.868896000000	2.234608000000	-0.468368000000
H	0.121248000000	1.785527000000	-0.681073000000
O	-0.898703000000	3.428137000000	-0.105045000000
C	4.998212000000	-1.380086000000	-0.532319000000
H	5.243248000000	-2.434363000000	-0.622577000000
C	5.863441000000	-0.418373000000	-1.010748000000
H	6.796942000000	-0.700116000000	-1.482024000000
C	5.516522000000	0.944154000000	-0.877332000000
H	6.193133000000	1.705270000000	-1.250885000000
C	4.335904000000	1.321016000000	-0.282264000000
H	4.071288000000	2.367917000000	-0.181638000000
K	-3.550767000000	3.363110000000	0.344561000000

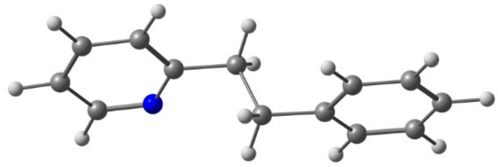


Sum of electronic and thermal Free Energies= -1500.294658

Final Product (3a*a*)

C	-1.906416000000	0.042578000000	-0.369585000000
C	-2.667262000000	1.212464000000	-0.319012000000
C	-4.018699000000	1.128749000000	-0.011241000000
C	-4.571328000000	-0.121706000000	0.238582000000
C	-3.737284000000	-1.231847000000	0.167115000000
H	-2.199379000000	2.168540000000	-0.521871000000
H	-4.629802000000	2.022723000000	0.030858000000
H	-5.619559000000	-0.240363000000	0.480526000000

H	-4.133448000000	-2.225487000000	0.353087000000
N	-2.437401000000	-1.162611000000	-0.127084000000
C	-0.428447000000	0.084372000000	-0.652318000000
H	-0.169422000000	1.012160000000	-1.168389000000
H	-0.165843000000	-0.751863000000	-1.305284000000
C	0.387669000000	-0.019135000000	0.650748000000
H	0.125904000000	0.819507000000	1.302195000000
H	0.104282000000	-0.939693000000	1.167771000000
C	1.869681000000	-0.014482000000	0.374623000000
C	2.587346000000	1.183068000000	0.345283000000
C	2.543832000000	-1.205091000000	0.092949000000
C	3.946956000000	1.192504000000	0.044763000000
H	2.075669000000	2.115262000000	0.563959000000
C	3.902884000000	-1.200916000000	-0.207912000000
H	1.997362000000	-2.143054000000	0.113885000000
C	4.608958000000	-0.000571000000	-0.232997000000
H	4.489696000000	2.130677000000	0.030723000000
H	4.411431000000	-2.134463000000	-0.419558000000
H	5.667585000000	0.004406000000	-0.464301000000



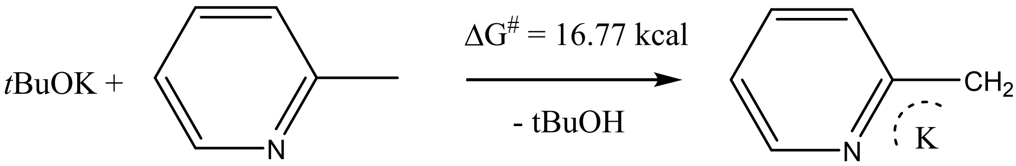
Sum of electronic and thermal Free Energies= -557.684921

Quinoline series (3da)

C	0.619483000000	-0.403597000000	0.478085000000
C	1.129798000000	-1.711171000000	0.230115000000
C	2.458313000000	-1.872809000000	-0.035030000000
C	3.303720000000	-0.734003000000	-0.060403000000
C	2.708486000000	0.527879000000	0.195914000000
H	0.454406000000	-2.558193000000	0.260333000000
H	2.879364000000	-2.854722000000	-0.223680000000
N	1.375464000000	0.669655000000	0.459711000000
C	-0.855107000000	-0.219852000000	0.718743000000
H	-1.242597000000	-1.045888000000	1.321883000000
H	-1.013651000000	0.710164000000	1.267868000000
C	-1.626519000000	-0.165332000000	-0.615235000000
H	-1.450698000000	-1.091363000000	-1.170296000000
H	-1.230753000000	0.657993000000	-1.216038000000
C	-3.104771000000	0.024267000000	-0.387327000000
C	-3.940136000000	-1.076192000000	-0.182189000000
C	-3.658208000000	1.304906000000	-0.327633000000
C	-5.297413000000	-0.902608000000	0.073495000000
H	-3.522075000000	-2.077204000000	-0.227231000000
C	-5.015227000000	1.483590000000	-0.072361000000
H	-3.019450000000	2.168218000000	-0.486412000000
C	-5.839199000000	0.379278000000	0.129061000000
H	-5.932511000000	-1.767629000000	0.226025000000
H	-5.429509000000	2.484478000000	-0.034133000000
H	-6.896096000000	0.516203000000	0.325022000000
C	4.694219000000	-0.809806000000	-0.325537000000
H	5.137240000000	-1.780724000000	-0.519652000000
C	5.460235000000	0.327168000000	-0.335471000000
H	6.522537000000	0.267082000000	-0.538809000000
C	4.867149000000	1.587347000000	-0.079626000000
H	5.484192000000	2.478030000000	-0.090246000000
C	3.524457000000	1.687818000000	0.180269000000
H	3.055666000000	2.644678000000	0.378159000000

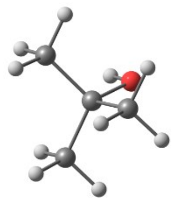
Sum of electronic and thermal Free Energies= -711.261387

Reaction using *t*BuOH



***t*BuOH**

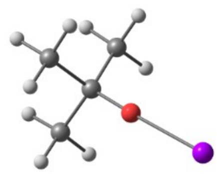
C	-6.283638000000	0.470007000000	-0.033862000000
O	-5.833097000000	1.203312000000	1.116351000000
C	-5.697985000000	-0.926120000000	0.123785000000
H	-6.057153000000	-1.384170000000	1.047944000000
H	-5.992244000000	-1.558153000000	-0.716366000000
H	-4.607499000000	-0.876115000000	0.158175000000
C	-7.809923000000	0.421265000000	-0.039899000000
H	-8.175521000000	-0.036485000000	0.881832000000
H	-8.226445000000	1.429743000000	-0.117583000000
H	-8.173495000000	-0.162337000000	-0.888724000000
C	-5.757853000000	1.139628000000	-1.301572000000
H	-4.666931000000	1.186309000000	-1.278440000000
H	-6.065589000000	0.581021000000	-2.188441000000
H	-6.148644000000	2.157629000000	-1.388546000000
H	-6.180426000000	2.099625000000	1.057672000000



Sum of electronic and thermal Free Energies= -233.529920

***t*BuOK**

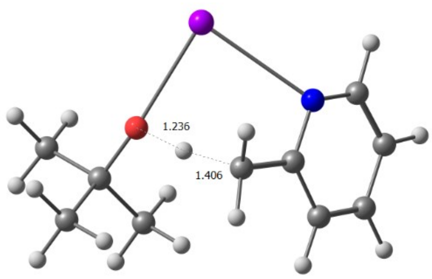
C	-6.379488000000	0.612242000000	-0.120248000000
O	-6.130343000000	1.577387000000	0.830030000000
K	-5.788721000000	3.265257000000	2.506431000000
C	-5.696355000000	-0.720224000000	0.254378000000
H	-6.075623000000	-1.071300000000	1.219064000000
H	-5.869928000000	-1.504428000000	-0.490640000000
H	-4.617052000000	-0.564830000000	0.348272000000
C	-7.894908000000	0.350880000000	-0.254026000000
H	-8.297842000000	0.028851000000	0.711102000000
H	-8.402985000000	1.275771000000	-0.544073000000
H	-8.124535000000	-0.418388000000	-0.999421000000
C	-5.846553000000	1.046579000000	-1.502230000000
H	-4.767331000000	1.219690000000	-1.443220000000
H	-6.034341000000	0.296313000000	-2.278112000000
H	-6.326670000000	1.982571000000	-1.804230000000



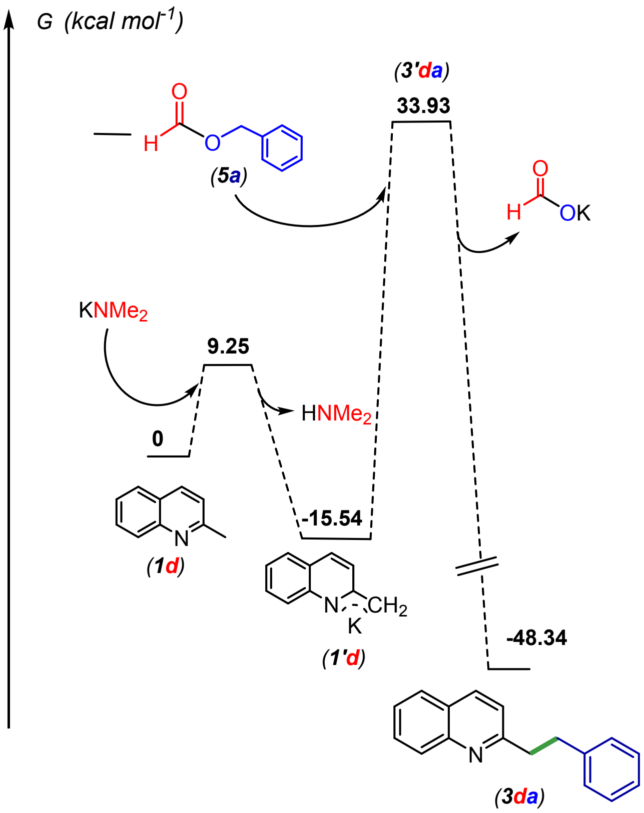
Sum of electronic and thermal Free Energies= -832.922787

TS_deprotonation step

C	-0.034645000000	-2.253844000000	-0.082874000000
C	1.044449000000	-1.583223000000	0.545856000000
C	1.140851000000	-0.209025000000	0.481835000000
C	0.163125000000	0.517101000000	-0.207295000000
C	-0.860361000000	-0.204146000000	-0.800697000000
H	1.783363000000	-2.165851000000	1.084036000000
H	1.963796000000	0.303308000000	0.968715000000
H	0.194693000000	1.596085000000	-0.279707000000
H	-1.641769000000	0.314931000000	-1.350264000000
N	-0.969773000000	-1.536366000000	-0.756248000000
K	-1.686959000000	-3.175993000000	-2.904792000000
C	1.944584000000	-4.592914000000	-2.754549000000
C	-0.124389000000	-3.702005000000	-0.127049000000
H	0.499172000000	-4.198537000000	0.617356000000
H	0.327486000000	-4.050663000000	-1.411939000000
H	-1.155136000000	-4.062151000000	-0.078154000000
O	0.586797000000	-4.269858000000	-2.600084000000
C	2.822864000000	-3.505565000000	-2.115758000000
H	2.605902000000	-2.536213000000	-2.574278000000
H	2.612097000000	-3.429741000000	-1.045660000000
H	3.887078000000	-3.722871000000	-2.247087000000
C	2.260231000000	-4.686615000000	-4.249499000000
H	3.310348000000	-4.942716000000	-4.420382000000
H	1.635817000000	-5.453447000000	-4.716097000000
H	2.052688000000	-3.729525000000	-4.735814000000
C	2.242661000000	-5.942208000000	-2.083395000000
H	1.629408000000	-6.726380000000	-2.535870000000
H	3.295595000000	-6.220753000000	-2.187685000000
H	2.001740000000	-5.888607000000	-1.018014000000



Sum of electronic and thermal Free Energies= -1120.363023



6. References

1. Y. Obora, S. Ogawa and N. Yamamoto, *J. Org. Chem.* **2012**, *77*, 9429-9433.
2. Y. Wang, X. Li, F. Leng, H. Zhu, J. Li, D. Zou, Y, Wu and Y. Wu, *Adv. Synth. Catal*. **2014**, *356*, 3307-3313.
3. M. Lautens, A. Roy, K. Fukuoka, K. Fagnou and B. M. Matute, *J. Am. Chem. Soc.* **2001**, *123*, 5358-5359.
4. M. Onoda and K. Fujita, *Org. Lett*. **2020**, *18*, 7295-7299.
5. Y. Ito, K. Kobayashi and T. Saegusa, *Journal of Organometallic Chemistry*, **1986**, *303*, 301-308.
6. L. M. Kabadwal, S. Bera and D. Banerjee, *Chem. Commun*., **2020**, *56*, 4777-4780.
7. A. Mishra, A. D. Dwivedi, S. Shee and S. Kundu, *Chem. Commun*., **2020**, *56*, 249-252.
8. K. D. Kim and J. H. Lee, *Org. Lett.* **2018**, *20*, 7712-7716.
9. J. C. Lewis, R. G. Bergman, J. A. Ellman, *J. Am. Chem. Soc*. **2007**, *129*, 5332-5333.
10. Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, *Inc., Wallingford CT*, **2016**.
11. Y. Zhao, D. G. Truhlar, Theor. *Chem. Acc*., **2008**, *120*, 215-241.
12. a) R. Krishnan, J. S. Binkley, R. Seeger, J. A. Pople, *J. Chem. Phys*., **1980**, *72*, 4244-4245; b) T. Clark, J. Chandrasekhar, G. W. Spitznagel, P. V. R. Schleyer, *J. Comp. Chem*., **1983**, *4*, 294-301.
13. a) K. Fukui, *Acc. Chem. Res*., **1981**, *14*, 363-368; b) H. P. Hratchian and H. B. Schlegel, *in Theory and Applications of Computational Chemistry: The First 40 Years*, Eds. C. E. Dykstra, G. Frenking, K. S. Kim, and G. Scuseria, **2005**, *Elsevier: Amsterdam*, 195-249.
14. J. Tomasi, B. Mennucci, R. Cammi, *Chem. Rev*., **2005**, *105*, 2999-3094.