Supporting Information

A Convenient Reagent for the Conversion of Aldoximes into Nitriles and Isonitriles

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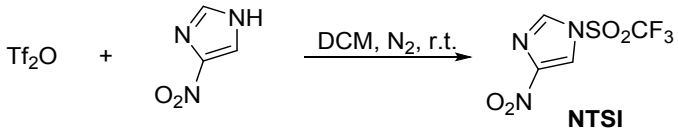
I. General information:

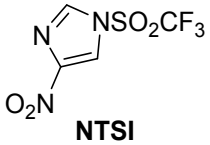
^{1}H, ^{13}C and ^{19}F NMR spectra were detected on a 400 MHz NMR spectrometer. Data for ^{1}H NMR, ^{13}C NMR and ^{19}F NMR were recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, coupling constant(s) in Hz). Mass spectra were obtained on GC-MS (EI). High resolution mass data were recorded on a high resolution mass spectrometer in the EI or ESI mode. The mass analyzer types for HRMS-EI and HRMS-ESI are time-of-flight and Fourier transform mass spectrometer, respectively.

II. The procedure for the preparation of NTSI:



NTSI

The mixture of nitro-imidazole (22.6 g, 200 mmol), dichloromethane (200 mL)，and trifluoromethanesulfonic anhydride (28.2 g, 100 mmol) was stirred at room temperature for overnight under a N_2 atmosphere. After the reaction was finished as monitored by ^{19}F NMR spectroscopy, the solid was filtered through a short pad of Celite, and the solid was washed with dichloromethane. The combined organic phase was concentrated under vacuum to remove the solvent and the product was obtained as a pale yellow solid (19.6 g, 80 mmol, 80%). NTSI is sensitive to moisture but stable under dry atmosphere.

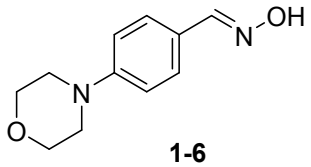


NTSI

4-Nitro-1-((trifluoromethyl)sulfonyl)-1H-imidazole (**NTSI**): Pale yellow solid, m.p. 55-56 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, J = 1.4 Hz, 1H), 8.01 (d, J = 1.4 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -74.9 (s, 3F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.4, 136.6, 118.6 (q, J = 323.0 Hz), 118.0. HRMS (EI): Calculated for $C_4H_2F_3N_3SO_4$ [M^+]: 244.9718; Found: 244.9728. IR (KBr): 3152, 1560, 1526, 1443, 1354, 1229, 1131, 1056, 995, 971, 852, 823, 747, 645, 598, 531 cm^{-1}.

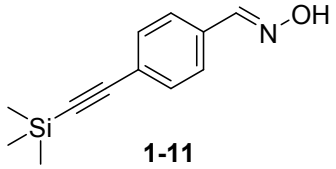
III. The procedure for the preparation of aldoximes:

All aldoximes were synthesized according to the literature [1-3]. The new compounds **1-6** and **1-11** were prepared according to Ref. [1], and **1-14** was prepared according to Ref. [3]. Their characterization data are shown as follows:



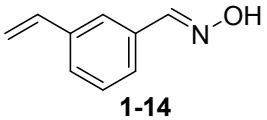
1-6

(E)-4-Morpholinobenzaldehyde oxime (**1-6**): White solid, m.p. 188-190 °C, 73%. ^{1}H NMR (400 MHz, d_6-acetone) δ 9.95 (s, 1H), 8.03 (s, 1H), 7.49 (d, J = 8.8 Hz, 2H), 6.95 (d, J = 8.8 Hz, 2H), 3.77 (t, J = 4.8 Hz, 4H), 3.18 (t, J = 4.8 Hz, 4H). ^{13}C NMR (100 MHz, d_6-acetone) δ 153.1, 149.1, 128.5, 125.0, 115.6, 67.2, 49.2. HRMS (ESI): Calculated for $C_{11}H_{15}N_2O_2$ $[M+H]^+$: 207.1128; Found: 207.1127. IR (KBr): 3317, 2821, 1609, 1445, 1266, 1110, 953, 933, 813, 532 cm^{-1}.



1-11

(E)-4-((Trimethylsilyl)ethynyl)benzaldehyde oxime (**1-11**): White solid, m.p. 110-112 °C, 47%. ^{1}H NMR (400 MHz, d_6-acetone) δ 10.57 (s, 1H), 8.16 (s, 1H), 7.63 (d, J = 8.0 Hz, 2H), 7.48 (d, J = 8.0 Hz, 2H), 0.23 (s, 9H). ^{13}C NMR (100 MHz, d_6-acetone) δ 148.7, 134.5, 132.9, 127.5, 124.7, 105.6, 96.0, -0.1. HRMS (ESI): Calculated for $C_{12}H_{16}ONSi$ $[M+H]^+$: 218.0996; Found: 218.0994. IR (KBr): 3290, 2957, 2156, 1512, 1301, 1248, 977, 844, 761, 654, 547, 458 cm^{-1}.

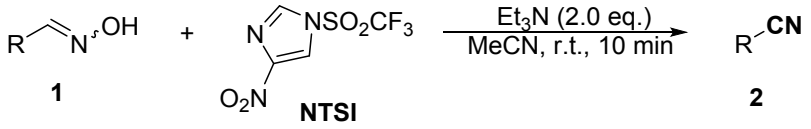


1-14

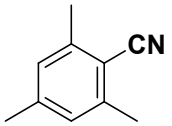
(E)-3-Vinylbenzaldehyde oxime (**1-14**): White solid, m.p. 49-51 °C, 63%. ^{1}H NMR (400 MHz, d_6-acetone) δ 10.44 (s, 1H), 8.19 (s, 1H), 7.71 (s, 1H), 7.55 (d, J = 7.6 Hz, 1H), 7.46 (d, J = 8.0 Hz, 1H), 7.35 (t, J = 7.6 Hz, 1H), 6.75 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1H), 5.83 (dd, J_1 = 17.6 Hz, J_2 = 0.8 Hz, 1H), 5.26 (dd, J_1 = 11.0 Hz, J_2

= 0.8 Hz, 1H). ^{13}C NMR (100 MHz, d_6-acetone) δ 149.2, 138.9, 137.3, 134.6, 129.7, 127.8, 126.8, 125.3, 114.9. HRMS (ESI): Calculated for $C_9H_{10}NO$ $[M+H]^+$: 148.0757; Found: 148.0756. IR (KBr): 3373, 1727, 1631, 1484, 1442, 1308, 1167, 947, 800, 709, 669 cm^{-1}.

IV. The general procedure for the conversion of aldoximes into nitriles:

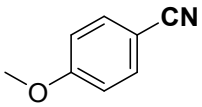


Into a sealed tube was added aldoxime **1** (0.5 mmol), NTSI (147 mg, 0.6 mmol), dry CH_3CN (2 mL) and Et_3N (101 mg, 1.0 mmol) under a N_2 atmosphere. The tube was sealed and the mixture was stirred at room temperature for 10 min. The desired product was isolated by flash column chromatography.



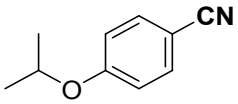
2-1

2,4,6-Trimethylbenzonitrile (**2-1**)[4]: White solid, 82%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.93 (s, 2H), 2.47 (s, 6H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 141.9, 128.1, 117.6, 110.2, 21.5, 20.6. MS (EI): Calculated for $C_{10}H_{11}N$ $[M^+]$: 145.1; Found: 145.1.



2-2

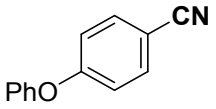
4-Methoxybenzonitrile (**2-2**)[4]: White solid, 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 8.8 Hz, 2H), 6.95 (d, J = 8.8 Hz, 2H), 3.86 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7, 133.8, 119.1, 114.6, 103.8, 55.4. MS (EI): Calculated for C_8H_7NO $[M^+]$: 133.1; Found: 133.0.



2-3

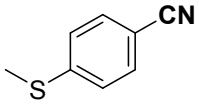
4-Isopropoxybenzonitrile (**2-3**)[5]: Pale yellow oil, 92%. ^{1}H NMR (400 MHz,

$CDCl_3$) δ 7.56 (d, *J* = 9.2 Hz, 2H), 6.91 (d, *J* = 8.8 Hz, 2H), 4.62 (sep, *J* = 6.0 Hz, 1H), 1.36 (d, *J* = 6.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.2, 133.8, 119.2, 115.9, 103.2, 70.3, 21.6. MS (EI): Calculated for $C_{10}H_{11}NO$ [M^+]: 161.1; Found: 161.1.



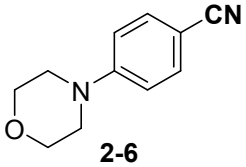
2-4

4-Phenoxybenzonitrile (**2-4**)[6]: Colorless oil, 92%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.8 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.05 (d, *J* = 7.6 Hz, 2H), 6.99 (d, *J* = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 154.6, 133.9, 130.1, 125.0, 120.2, 118.6, 117.7, 105.6. MS (EI): Calculated for $C_{13}H_9NO$ [M^+]: 195.1; Found: 195.0.



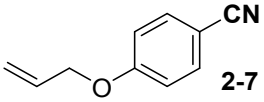
2-5

4-(Methylthio)benzonitrile (**2-5**)[7]: White solid, 93%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.9, 131.9, 125.2, 118.8, 107.3, 14.4. MS (EI): Calculated for C_8H_7NS [M^+]: 149.0; Found: 149.0.



2-6

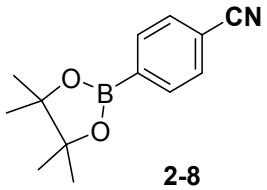
4-Morpholinobenzonitrile (**2-6**)[8]: White solid, 62%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 3.86-3.84 (m, 4H), 3.29-3.27 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 133.3, 119.7, 113.9, 100.6, 66.2, 47.1. MS (EI): Calculated for $C_{11}H_{12}N_2O$ [M^+]: 188.1; Found: 188.0.



2-7

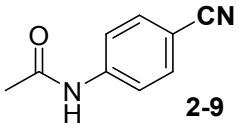
4-(Allyloxy)benzonitrile (**2-7**)[6]: White solid, 96%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.4 Hz, 2H), 6.96 (d, *J* = 8.4 Hz, 2H), 6.08-5.98 (m, 1H), 5.42 (d, *J* = 17.2 Hz, 1H), 5.33 (d, *J* = 10.4 Hz, 1H), 4.59 (d, *J* = 5.2 Hz, 2H). ^{13}C NMR (100 MHz,

$CDCl_3$) δ 161.6, 133.7, 131.9, 119.0, 118.2, 115.3, 103.8, 68.8. MS (EI): Calculated for $C_{10}H_9NO$ [M^+]: 159.1; Found: 159.1.



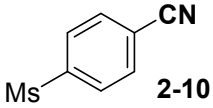
2-8

4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)benzonitrile (**2-8**)[8]: White solid, 35%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.0 Hz, 2H), 7.64 (d, *J* = 8.0 Hz, 2H), 1.36 (s, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.0, 131.1, 118.8, 114.5, 84.4, 24.8.



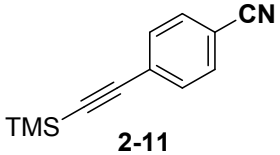
2-9

***N*-(4-Cyanophenyl)acetamide** (**2-9**)[9]: White solid, 84%. ^{1}H NMR (400 MHz, d_6-DMSO) δ 10.37 (s, 1H), 7.75 (s, 4H), 2.09 (s, 3H). ^{13}C NMR (100 MHz, d_6-DMSO) δ 169.2, 143.5, 133.2, 119.1, 118.9, 104.7, 24.2. MS (EI): Calculated for $C_9H_8N_2O$ [M^+]: 160.1; Found: 160.1.



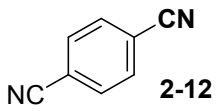
2-10

4-(Methylsulfonyl)benzonitrile (**2-10**)[10]: White solid, 77%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.2 Hz, 2H), 7.92 (d, *J* = 8.0 Hz, 2H), 3.12 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 133.1, 128.1, 117.4, 117.0, 44.1. MS (EI): Calculated for $C_8H_7NO_2S$ [M^+]: 181.0; Found: 181.0.



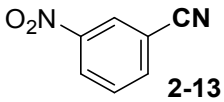
2-11

4-((Trimethylsilyl)ethynyl)benzonitrile (**2-11**)[11]: White solid, 97%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.52 (d, *J* = 8.0 Hz, 2H), 0.27 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.3, 131.8, 127.8, 118.2, 111.6, 102.8, 99.4, -0.4. MS (EI): Calculated for $C_{12}H_{13}NSi$ [M^+]: 199.1; Found: 199.1.



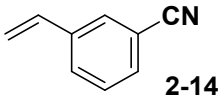
2-12

Terephthalonitrile (**2-12**)[8]: White solid, 69%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.7, 117.0, 116.7. MS (EI): Calculated for $C_8H_4N_2$ [M^+]: 128.0; Found: 128.0.



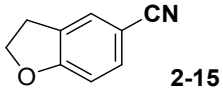
2-13

3-Nitrobenzonitrile (**2-13**)[6]: White solid, 97%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 8.52 (d, J = 8.2 Hz, 1H), 8.07 (d, J = 7.8 Hz, 1H), 7.81 (t, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.0, 137.6, 130.6, 127.4, 127.0, 116.4, 113.9. MS (EI): Calculated for $C_7H_4N_2O_2$ [M^+]: 148.0; Found: 148.1.



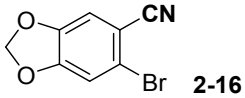
2-14

3-Vinylbenzonitrile (**2-14**)[9]: Colorless oil, 62%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (s, 1H), 7.62 (d, J = 8.0 Hz, 1H), 7.53 (d, J = 8.0 Hz, 1H), 7.43 (t, J = 8.0 Hz, 1H), 6.69 (dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1H), 5.82 (d, J = 17.6 Hz, 1H), 5.39 (d, J = 10.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 134.7, 131.0, 130.3, 129.6, 129.3, 118.7, 116.5, 112.7. MS (EI): Calculated for C_9H_7N [M^+]: 129.1; Found: 129.1.



2-15

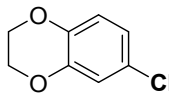
2,3-Dihydrobenzofuran-5-carbonitrile (**2-15**)[12]: White solid, 81%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.41 (m, 2H), 6.81 (d, J = 8.4 Hz, 1H), 4.66 (t, J = 8.9 Hz, 2H), 3.25 (t, J = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 133.3, 128.7, 128.5, 119.4, 110.0, 103.2, 72.0, 28.8. MS (EI): Calculated for C_9H_7NO [M^+]: 145.1; Found: 145.0.



2-16

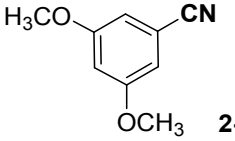
6-Bromobenzo[d][1,3]dioxole-5-carbonitrile (**2-16**)[13]: White solid, 93%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07 (s, 1H), 7.01 (s, 1H), 6.13 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 147.3, 118.7, 117.2, 113.2, 112.3, 107.6, 103.0. MS (EI):

Calculated for $C_8H_4NO_2Br$ [M^+]: 224.9; Found: 224.9.



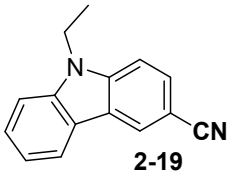
2-17

2,3-Dihydrobenzo[b][1,4]dioxine-6-carbonitrile (**2-17**)[8]: White solid, 97%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13-7.11 (m, 2H), 6.91 (d, *J* = 9.2 Hz, 1H), 4.33-4.26 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 143.7, 125.8, 121.1, 118.8, 118.1, 104.3, 64.5, 64.0. MS (EI): Calculated for $C_9H_7NO_2$ [M^+]: 161.0; Found: 161.0.



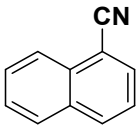
2-18

3,5-Dimethoxybenzonitrile (**2-18**)[14]: White solid, 94%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.75 (d, *J* = 2.2 Hz, 2H), 6.65 (t, *J* = 2.2 Hz, 1H), 3.80 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 118.6, 113.2, 109.7, 105.4, 55.5. MS (EI): Calculated for $C_9H_9NO_2$ [M^+]: 163.1; Found: 163.0.



2-19

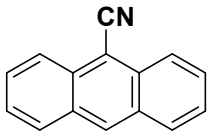
9-Ethyl-9H-carbazole-3-carbonitrile (**2-19**)[15]: White solid, 80%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.95 (d, *J* = 7.6 Hz, 1H), 7.59-7.56 (m, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.36 (d, *J* = 8.4 Hz, 1H), 7.29-7.21 (m, 2H), 4.22 (q, *J* = 7.2 Hz, 2H), 1.34 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.2, 140.1, 128.5, 126.9, 124.8, 122.7, 121.6, 120.47, 120.45, 120.0, 108.9, 108.8, 101.0, 37.5, 13.5. MS (EI): Calculated for $C_{15}H_{12}N_2$ [M^+]: 220.1; Found: 220.0.



2-20

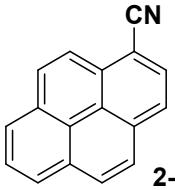
1-Naphthonitrile (**2-20**)[4]: Pale yellow oil, 94%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.4 Hz, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.89-7.85 (m, 2H), 7.67-7.62 (m, 1H), 7.60-7.56 (m, 1H), 7.49-7.45 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.2, 132.8, 132.5, 132.3, 128.6, 128.5, 127.5, 125.0, 124.8, 117.7, 110.1. MS (EI):

Calculated for $C_{11}H_7N$ [M^+]: 153.1; Found: 153.1.



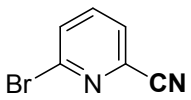
2-21

Anthracene-9-carbonitrile (**2-21**)[14]: Yellow solid, 82%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.26 (d, *J* = 8.8 Hz, 2H), 7.92 (d, *J* = 8.4 Hz, 2H), 7.60 (t, *J* = 7.2 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.0, 132.5, 130.3, 128.8, 128.7, 126.2, 125.0, 117.1, 105.1. MS (EI): Calculated for $C_{15}H_9N$ [M^+]: 203.1; Found: 203.1.



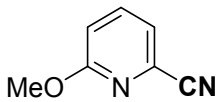
2-22

Pyrene-1-carbonitrile (**2-22**)[16]: Yellow solid, 82%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.6 Hz, 1H), 8.01-7.98 (m, 2H), 7.92-7.88 (m, 3H), 7.85 (d, *J* = 8.8 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.5, 132.2, 130.3, 130.0, 129.9, 129.8, 128.9, 126.64, 126.58, 126.5, 126.3, 123.8, 123.23, 123.16, 122.8, 118.6, 105.0. MS (EI): Calculated for $C_{17}H_9N$ [M^+]: 227.1; Found: 227.2.



2-23

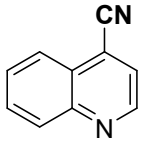
6-Bromopicolinonitrile (**2-23**)[17]: White solid, 86%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82-7.77 (m, 2H), 7.75-7.23 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.8, 139.2, 133.5, 132.1, 127.5, 115.8. MS (EI): Calculated for $C_6H_3N_2Br$ [M]: 181.9; Found: 181.9.



2-24

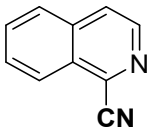
6-Methoxypicolinonitrile (**2-24**)[18]: White solid, 79%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (t, *J* = 7.8 Hz, 1H), 7.31 (d, *J* = 7.2 Hz, 1H), 6.98 (d, *J* = 8.4 Hz, 1H), 3.96 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2, 138.9, 130.2, 122.1, 117.2, 116.0,

53.9. MS (EI): Calculated for $C_7H_6N_2O$ [M^+]: 134.0; Found: 134.1.



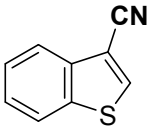
2-25

Quinoline-4-carbonitrile (**2-25**)[19]: White solid, 88%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.04 (d, *J* = 4.4 Hz, 1H), 8.21-8.16 (m, 2H), 7.88-7.84 (m, 1H), 7.77-7.32 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.3, 147.9, 131.0, 130.2, 129.0, 125.5, 124.74, 124.68, 118.5, 115.3. MS (EI): Calculated for $C_{10}H_6N_2$ [M^+]: 154.1; Found: 154.0.



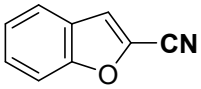
2-26

Isoquinoline-1-carbonitrile (**2-26**)[19]: White solid, 96%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 5.6 Hz, 1H), 8.26 (d, *J* = 8.2 Hz, 1H), 7.95 (d, *J* = 8.2 Hz, 1H), 7.91 (d, *J* = 5.6 Hz, 1H), 7.83 (t, *J* = 7.9 Hz, 1H), 7.78 (t, *J* = 7.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.0, 135.6, 134.4, 131.6, 129.7, 129.0, 127.2, 124.9, 124.3, 115.6. MS (EI): Calculated for $C_{10}H_6N_2$ [M^+]: 154.1; Found: 154.0.



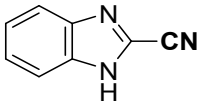
2-27

Benzo[b]thiophene-3-carbonitrile (**2-27**)[18]: White solid, 93%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.52-7.43 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.3, 137.4, 137.0, 126.0, 125.8, 122.7, 122.3, 114.2, 106.9. MS (EI): Calculated for C_9H_5NS [M^+]: 159.0; Found: 159.0.



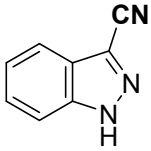
2-28

Benzofuran-2-carbonitrile (**2-28**)[18]: Pale yellow solid, 80%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.0 Hz, 1H), 7.54-7.48 (m, 2H), 7.44 (s, 1H), 7.37-7.33 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.5, 128.4, 127.1, 125.4, 124.5, 122.5, 118.4, 111.9, 111.7. MS (EI): Calculated for C_9H_5NO [M^+]: 143.0; Found: 143.0.



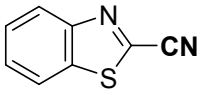
2-29

1H-Benzo[d]imidazole-2-carbonitrile (**2-29**)[20]: White solid, 73%. ^{1}H NMR (400 MHz, d_6-DMSO) δ 14.20 (br, 1H), 7.76 (s, 2H), 7.45-7.43 (m, 2H). MS (EI): Calculated for $C_8H_5N_3$ [M^+]: 143.0; Found: 143.1.



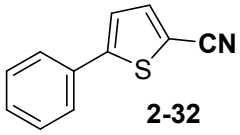
2-30

1H-Indazole-3-carbonitrile (**2-30**)[21]: White solid, 48%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.23 (s, 1H), 7.87 (d, J = 8.2 Hz, 1H), 7.80 (d, J = 8.2 Hz, 1H), 7.56 (t, J = 7.8 Hz, 1H), 7.40 (t, J = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.0, 128.7, 124.3, 124.0, 119.6, 119.4, 113.6, 111.0. MS (EI): Calculated for $C_8H_5N_3$ [M^+]: 143.0; Found: 143.1.



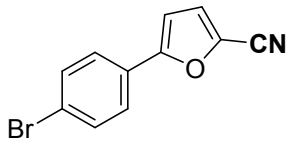
2-31

Benzo[d]thiazole-2-carbonitrile (**2-31**)[22]: White solid, 79%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23-8.19 (m, 1H), 8.01-7.97 (m, 1H), 7.68-7.61 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 136.4, 135.2, 128.6, 127.8, 125.1, 121.7, 112.9. MS (EI): Calculated for $C_8H_4N_2S$ [M^+]: 160.0; Found: 160.0.



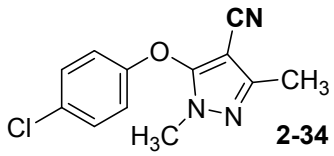
2-32

5-Phenylthiophene-2-carbonitrile (**2-32**)[23]: Yellow solid, 82%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58-7.55 (m, 3H), 7.44-7.36 (m, 3H), 7.25 (d, J = 4.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 138.3, 132.1, 129.3, 129.2, 126.3, 123.1, 114.3, 108.0. MS (EI): Calculated for $C_{11}H_7NS$ [M^+]: 185.0; Found: 185.1.



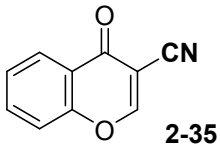
2-33

5-(4-Bromophenyl)furan-2-carbonitrile (**2-33**)[24]: White solid, 82%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (s, 4H), 7.15 (d, J = 2.8 Hz, 1H), 6.71 (d, J = 2.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 132.0, 127.4, 126.1, 125.2, 123.9, 123.6, 111.6, 106.4. MS (EI): Calculated for $C_{11}H_6NBrO$ [M^+]: 247.0; Found: 247.0.



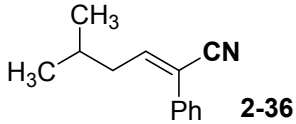
2-34

5-(4-Chlorophenoxy)-1,3-dimethyl-1H-pyrazole-4-carbonitrile (**2-34**): White solid, m.p.: 73-75 ºC, 86%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, J = 8.8 Hz, 2H), 7.06 (d, J = 8.8 Hz, 2H), 3.69 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 152.7, 150.4, 130.8, 130.0, 118.9, 111.6, 78.2, 34.4, 13.0. HRMS (EI): Calculated for $C_{12}H_{10}ClN_3O$ [M^+]: 247.0512; Found: 247.0506. IR (KBr): 2951, 2227, 1556, 1417, 1245, 1195, 1090, 1012, 831, 635, 496 cm^{-1}.



2-35

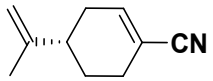
4-Oxo-4H-chromene-3-carbonitrile (**2-35**)[25]: White solid, 83%. ^{1}H NMR (400 MHz, CD_3CN) δ 8.64 (s, 1H), 8.11 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.86-7.82 (m, 1H), 7.60 (d, J = 8.4 Hz, 1H), 7.56-7.53 (m, 1H). ^{13}C NMR (100 MHz, CD_3CN) δ 173.9, 165.0, 156.8, 136.5, 128.0, 126.3, 124.1, 119.7, 113.8, 102.8. MS (EI): Calculated for $C_{10}H_5NO_2$ [M^+]: 171.0; Found: 171.1.



2-36

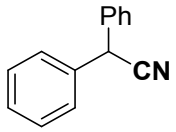
(E)-5-Methyl-2-phenylhex-2-enenitrile (**2-36**)[26]: Colorless oil, 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.34 (m, 5H), 6.66 (t, J = 7.6 Hz, 1H), 2.23 (t, J = 6.8 Hz, 2H), 1.82-1.72 (m, 1H), 0.91 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 132.4, 128.7, 128.61, 128.60, 119.6, 115.7, 38.3, 28.4, 22.2. MS (EI):

Calculated for $C_{13}H_{15}N$ [M^+]: 185.1; Found: 185.1.



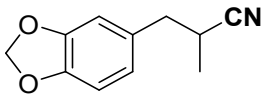
2-37

(S)-4-(Prop-1-en-2-yl)cyclohex-1-ene-1-carbonitrile (**2-37**)[27]: Colorless oil, 64%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66-7.64 (m, 1H), 4.80-4.78 (m, 1H), 4.71 (s, 1H), 2.37-2.28 (m, 3H), 2.22-2.04 (m, 2H), 1.92-1.86 (m, 1H), 1.74 (s, 3H), 1.57-1.47 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 144.5, 119.4, 111.9, 109.7, 39.0, 30.8, 26.8, 26.1, 20.5. MS (EI): Calculated for $C_{10}H_{13}N$ [M^+]: 147.1; Found: 147.0.



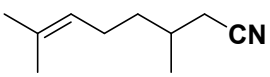
2-38

2,2-Diphenylacetonitrile (**2-38**)[28]: White solid, 78%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.25 (m, 10H), 5.09 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.8, 129.0, 128.1, 127.5, 119.6, 42.4. MS (EI): Calculated for $C_{14}H_{11}N$ [M^+]: 193.1; Found: 193.1.



2-39

3-(Benzo[d][1,3]dioxol-5-yl)-2-methylpropanenitrile (**2-39**)[7]: Colorless oil, 75%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.76 (d, J = 8.0 Hz, 1H), 6.71-6.67 (m, 2H), 5.93 (s, 2H), 2.85-2.71 (m, 3H), 1.31 (d, J = 6.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 146.6, 130.4, 122.4, 122.1, 109.2, 108.3, 100.9, 39.6, 27.6, 17.4. MS (EI): Calculated for $C_{11}H_{11}NO_2$ [M^+]: 189.1; Found: 189.0.

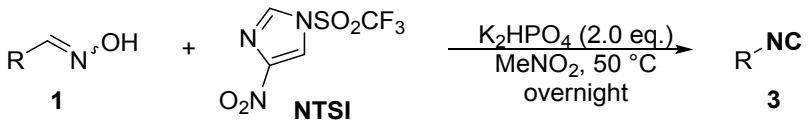


2-40

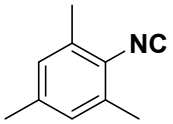
3,7-Dimethyloct-6-enenitrile (**2-40**)[23]: Colorless oil, 75%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.07 (tt, J_1 = 6.8 Hz, J_2 = 1.3 Hz 1H), 2.33 (dd, J_1 = 16.4 Hz, J_2 = 5.6 Hz, 1H), 2.24 (dd, J_1 = 16.4 Hz, J_2 = 6.8 Hz, 1H), 2.06-1.96 (m, 2H), 1.92-1.81 (m, 1H), 1.69 (s, 3H), 1.61 (s, 3H), 1.53-1.30 (m, 2H), 1.08 (d, J = 6.8 Hz, 3H). ^{13}C NMR (100

MHz, $CDCl_3$) δ 132.2, 123.4, 118.8, 35.8, 29.9, 25.6, 25.2, 24.4, 19.3, 17.6. MS (EI): Calculated for $C_{10}H_{17}N$ [M^+]: 151.1; Found: 151.2.

V. The general procedure for the conversion of aldoximes into isonitriles

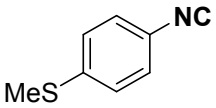


Into a sealed tube were sequentially added aldoxime **1** (0.5 mmol), NTSI (147 mg, 0.6 mmol)，K_2HPO_4 (174, mg, 1.0 mmol) and dry $MeNO_2$ (2.0 mL) under a N_2 atmosphere. The tube was sealed and the mixture was stirred at 50 ^oC for overnight. The product was isolated by flash column chromatography.



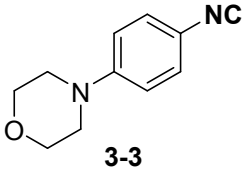
3-1

2-Isocyano-1,3,5-trimethylbenzene (**3-1**)[29]: White solid, 51%. ^1H NMR (400 MHz, $CDCl_3$) δ 6.89 (s, 2H), 2.37 (s, 6H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6 (t, J = 5.4 Hz), 138.7, 134.5, 128.4, 124.0 (t, J = 12.7 Hz), 21.1, 18.7. MS (EI): Calculated for $C_{10}H_{11}N$ [M^+]: 145.1; Found: 145.1.



3-2

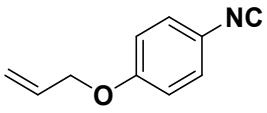
(4-Isocyanophenyl)(methyl)sulfane (**3-2**)[30]: Green oil, 71%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, J = 8.6 Hz, 2H), 7.19 (d, J = 8.6 Hz, 2H), 2.48 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0, 141.1, 126.4, 126.1, 122.9 (t, J = 13.8 Hz), 15.1. MS (EI): Calculated for C_8H_7NS [M^+]: 149.0; Found: 149.0.



3-3

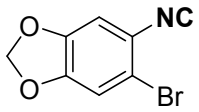
4-(4-Isocyanophenyl)morpholine (**3-3**)[31]: Brown oil, 57%. ^1H NMR (400 MHz, $CDCl_3$) δ 7.28-7.24 (m, 2H), 6.84-6.80 (m, 2H), 3.85 (t, J = 4.8 Hz, 4H), 3.19 (t, J =

4.8 Hz, 4 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1, 151.2, 127.3, 117.8 (t, J =13.1 Hz), 114.9, 66.5, 48.1. MS (EI): Calculated for $C_{11}H_{12}N_2O$ [M^+]: 188.0; Found: 188.0.



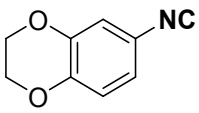
3-4

1-(Allyloxy)-4-isocyanobenzene (**3-4**)[32]: Colorless oil, 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, J = 8.8 Hz, 2H), 6.88 (d, J = 8.8 Hz, 2H), 6.07-5.97 (m, 1H), 5.41 (dd, J_1 = 17.2 Hz, J_2 = 0.9 Hz, 1H), 5.31 (dd, J_1 = 10.5 Hz, J_2 = 0.8 Hz, 1H), 4.54 (d, J = 5.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6 (t, J = 5.4 Hz), 158.8, 132.3, 127.6, 119.5 (t, J = 13.1 Hz), 118.1, 115.3, 69.0. MS (EI): Calculated for $C_{10}H_9NO$ [M^+]: 159.1; Found: 159.0.



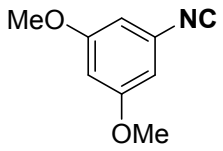
3-5

5-Bromo-6-isocyanobenzo[d][1,3]dioxole (**3-5**): Pale pink solid, m.p. 86-88 °C, 48%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.03 (s, 1H), 6.88 (s, 1H), 6.07 (s, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 149.0, 147.4, 120.5 (t, J = 12.5 Hz), 112.3, 112.1, 107.8, 102.8. HRMS (EI): Calculated for $C_8H_4NO_2Br$ [M^+]: 224.9425; Found: 224.9431. IR (KBr) 3052, 2127, 1606, 1504, 1410, 1358, 1259, 1174, 1124, 1037, 928, 869, 769, 667, 574, 446 cm^{-1}.



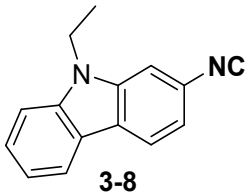
3-6

6-Isocyano-2,3-dihydrobenzo[b][1,4]dioxine (**3-6**): White solid, m.p. 85-86 °C, 73%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.90-6.81 (m, 3H), 4.27 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1, 144.5, 143.4, 119.6, 119.5 (t, J = 12.8 Hz) 117.7, 115.5, 64.2, 64.1. HRMS (EI): Calculated for $C_9H_7NO_2$ [M^+]: 161.0477; Found: 161.0479. IR (KBr) 3075, 2129, 1593, 1504, 1457, 1293, 1244, 1205, 1117, 1063, 1043, 912, 871, 807, 756, 716, 602, 502, 456 cm^{-1}.



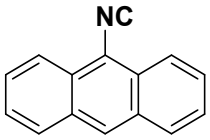
3-7

1-Isocyano-3,5-dimethoxybenzene (**3-7**): White solid, m.p. 70-72 °C, 42%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.51 (d, *J* = 2.0 Hz, 2H), 6.48-6.47 (t, *J* = 2.0 Hz, 1H), 3.78 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.5, 160.9, 127.6 (t, *J* = 13.2 Hz), 104.7, 102.0, 55.6. HRMS (EI): Calculated for $C_9H_9NO_2$ [M^+]: 163.0633; Found: 163.0635. IR (KBr) 3004, 2135, 1598, 1465, 1350, 1214, 1195, 1163, 1133, 1066, 938, 843, 821, 756, 668, 530 cm^{-1}.



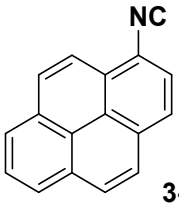
3-8

9-Ethyl-2-isocyano-9H-carbazole (**3-8**): Pale yellow oil, 71%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96-7.95 (m, 2H), 7.50-7.46 (m, 1H), 7.37-7.34 (m, 2H), 7.25-7.20 (m, 2H), 4.23 (q, *J* = 7.2 Hz, 2H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.6, 140.4, 139.0, 126.7, 123.5, 122.6, 121.8, 120.5, 119.6, 118.4, 117.7 (t, *J* = 13.3 Hz), 108.8, 108.6, 37.5, 13.6. HRMS (EI): Calculated for $C_{15}H_{12}N_2$ [M^+]: 220.1000; Found: 220.1003. IR (KBr) 3054, 2976, 2119, 1597, 1479, 1384, 1332, 1291, 1234, 1150, 880, 803, 746, 726, 602, 554, 423 cm^{-1}.



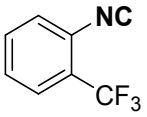
3-9

9-Isocyanoanthracene (**3-9**): Yellow solid, 71%, m.p. 151-153 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 8.15 (d, *J* = 8.3 Hz, 2H), 7.83 (d, *J* = 8.0 Hz, 2H), 7.53 (t, *J* = 7.7 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 130.5, 128.4, 128.3, 127.8, 126.5, 126.0, 122.7, 118.1 (t, *J* = 13.2 Hz). HRMS (EI): Calculated for $C_{15}H_9N$ [M^+]: 203.0735; Found: 203.0738. IR (KBr) 2110, 1341, 1265, 951, 888, 841, 777, 728, 601, 548, 410 cm^{-1}.



3-10

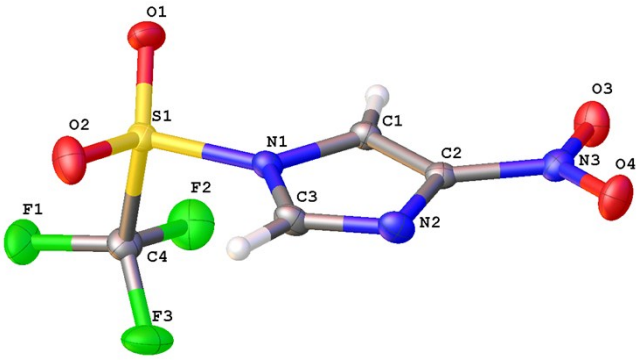
1-Isocyanopyrene (3-10)[33]: White solid, 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10-8.03 (m, 3H), 7.96-7.92 (m, 3H), 7.82-7.94 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 131.2, 130.6, 130.3, 129.3, 128.7, 126.6, 126.4, 126.3, 126.2, 126.0, 124.2, 123.9, 123.5, 123.2, 121.2, 119.4 (t, *J* = 13.5 Hz). MS (EI): Calculated for $C_{17}H_9N$ [M^+]: 227.1; Found: 227.1.

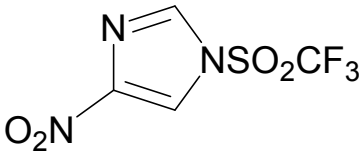


3-11

1-Isocyano-2-(trifluoromethyl)benzene (3-11)[34]: Yellow oil, 15% NMR yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.56 - 7.52 (m, 2H). ^{19}F NMR (376Hz, CDCl3) δ -62.9 (s, 3F). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 132.9, 129.4, 128.8, 126.9 (q, *J* = 32.0 Hz), 126.7 (q, *J* = 4.8 Hz), 124.0-123.6 (m, *C*-(N≡C)), 122.2 (q, *J* = 272.0 Hz). MS (EI): Calculated for $C_8H_4F_3N$ [M^+]: 171.0; Found: 171.0.

VI. The X-ray structure of NTSI





NTSI

Bond precision: C-C = 0.0030 A Wavelength = 1.34139

Cell: a=12.0715(9) Å b=5.7257(4) Å c=12.5111(10) Å

alpha=90° beta=101.199(4)° gamma=90°

Temperature: 170 K

	Caculated	Reported
Volume	848.27(11)	848.27(11)
Space group	P 21/c	P 1 21/c 1
Hall group	-p 2ybc	-p 2ybc
Moiety formula	$C_4H_2F_3N_3O_4S$	$C_4H_2F_3N_3O_4S$
Sum formula	$C_4H_2F_3N_3O_4S$	$C_4H_2F_3N_3O_4S$
Mr	245.15	245.15
Dx, g cm^{-3}	1.920	1.920
Z	4	4
Mu (mm^{-1})	2.631	2.610
F000	488.0	488.0
F000’	490.91	
h, k, lmax	14, 6, 15	14, 6, 15
Nref	1602	1595
Tmin, Tmax	0.829, 0.855	0.423, 0.751
Tmin’	0.812	

Correction method = # Reported T Limits: Tmin = 0.423 Tmax = 0.751

AbsCorr = MULTI-SCAN

Data completeness = 0.996 Theta(max) = 54.921

R (reflections) = 0.0589(1513) wR2 (reflections) = 0.1481(1595)

S = 1.131 Npar= 136

VII. References:

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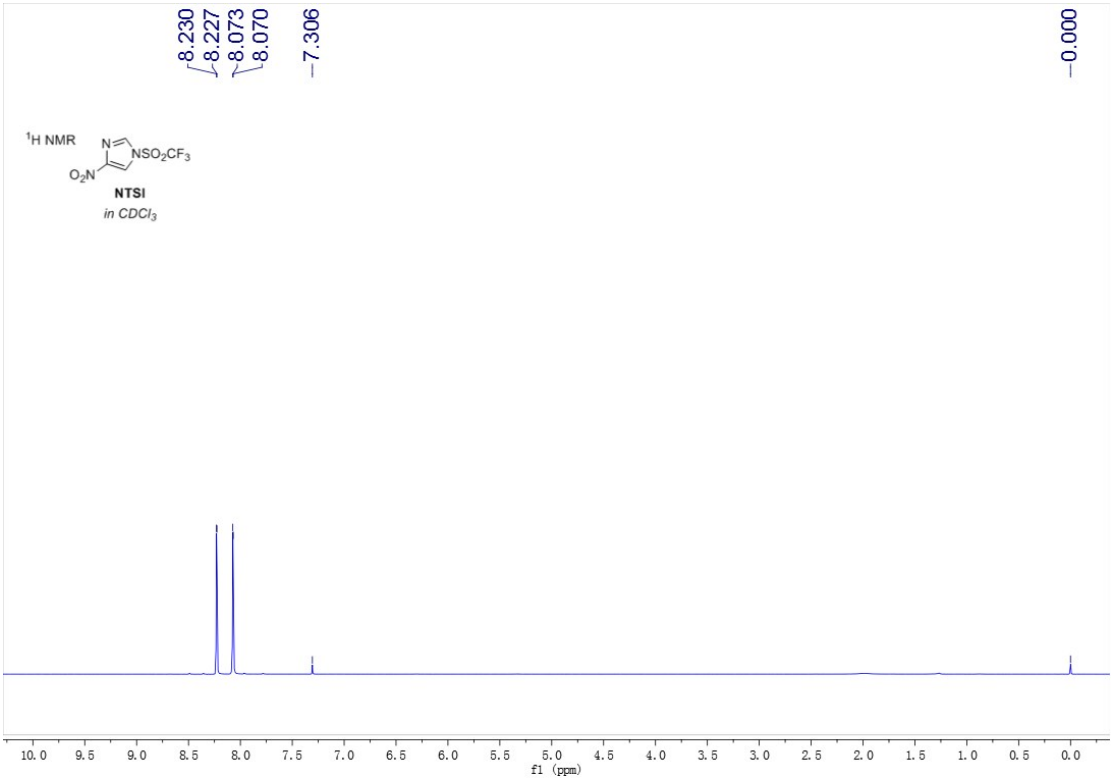
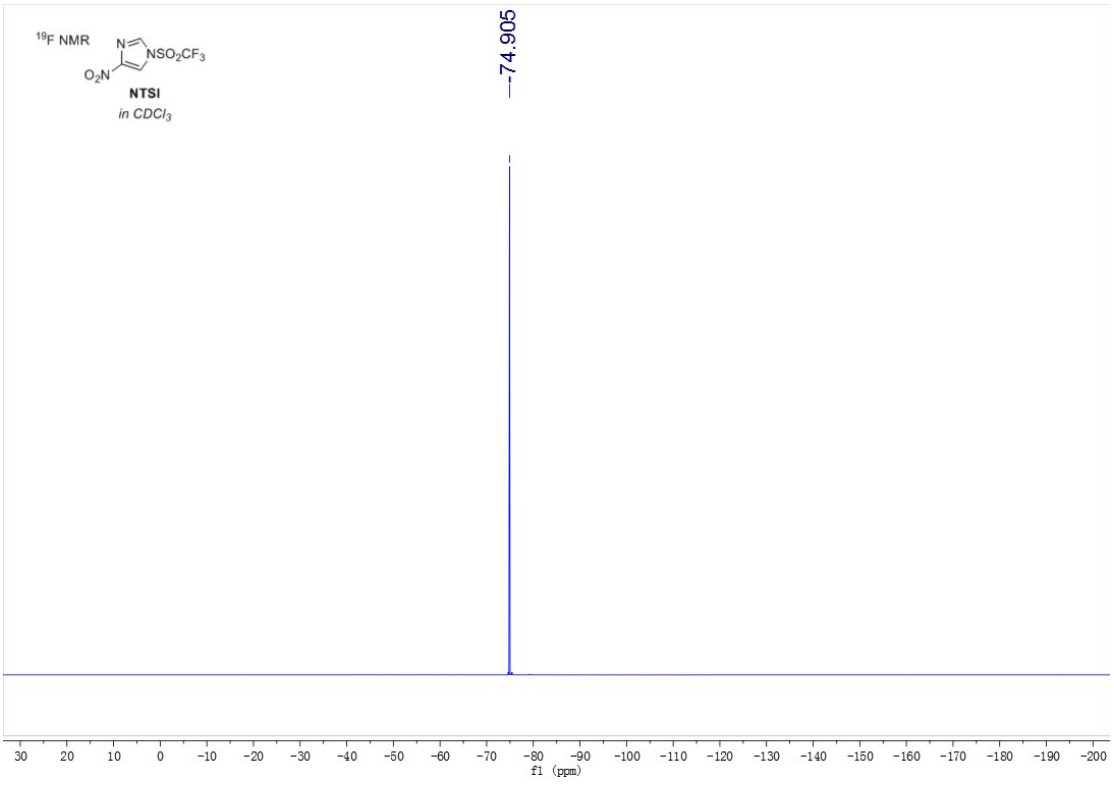
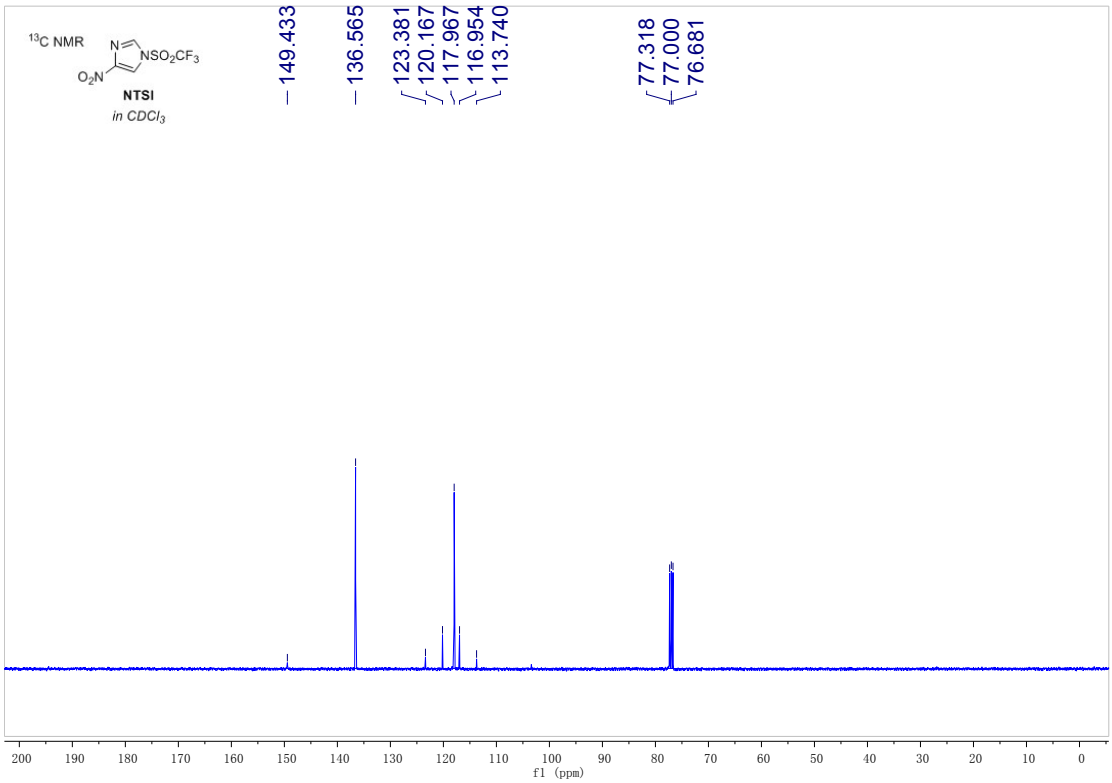
VIII. Copies of NMR spectra of the products



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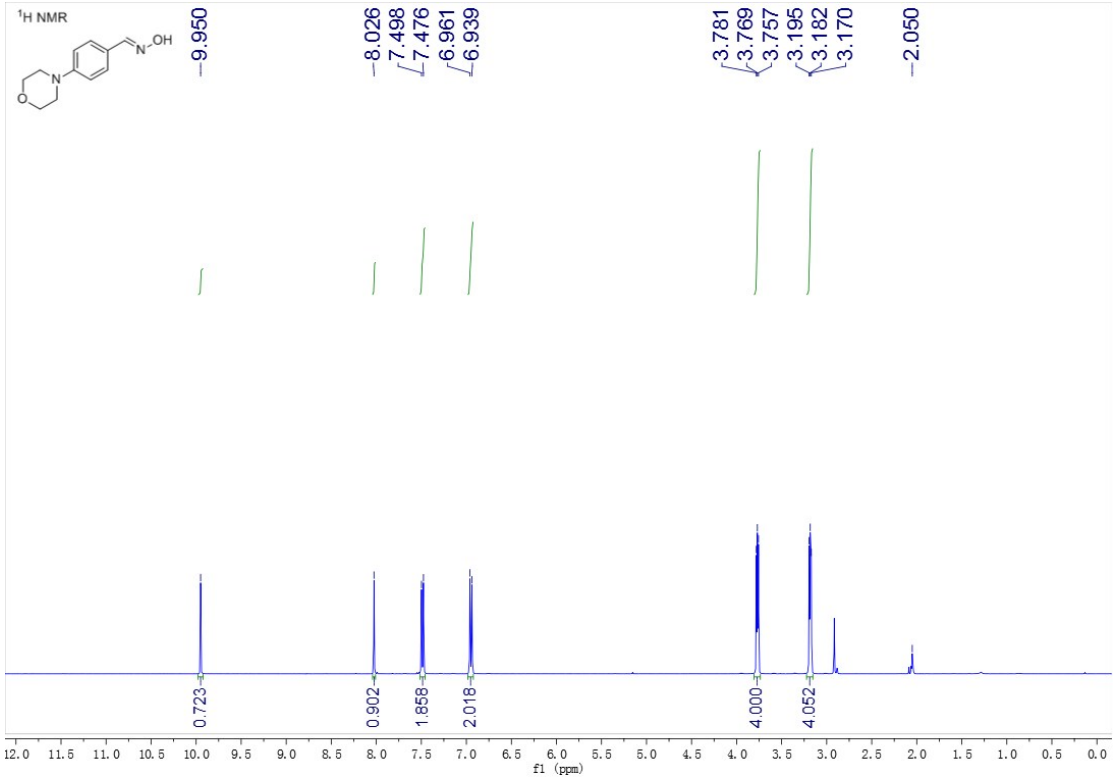
77.000
76.681
f1 (ppm)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7.476
6.961
6.939
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3.170
2.050
0.723
0.902
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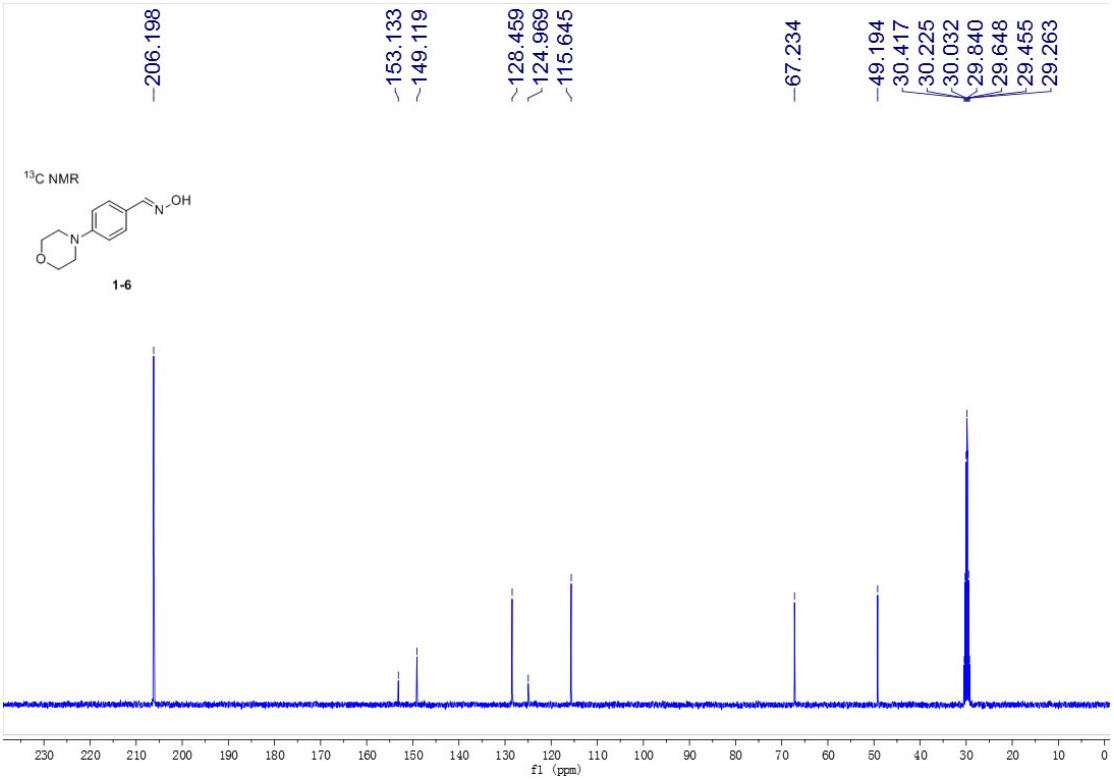
2.018
4.000
4.052
f1 (ppm)


206.198
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149.119
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49.194
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30.225
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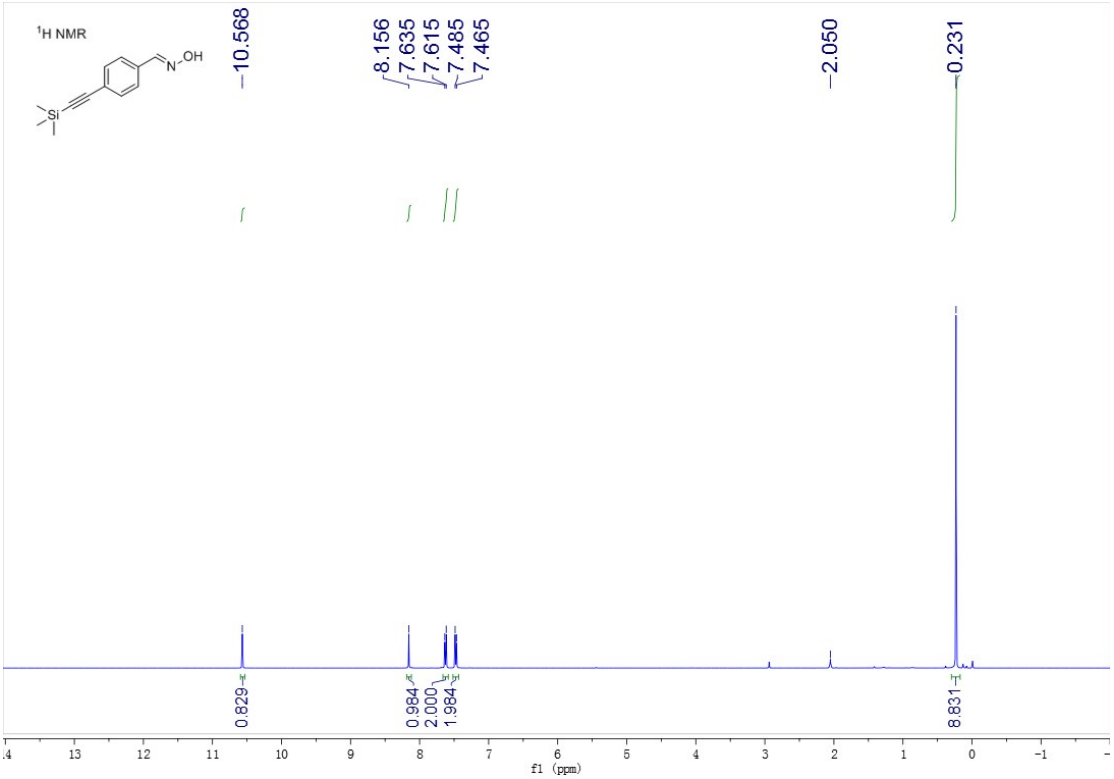
29.840
29.648
29.455
29.263
13C NMR
OH
N
O
1-6
f1 (ppm)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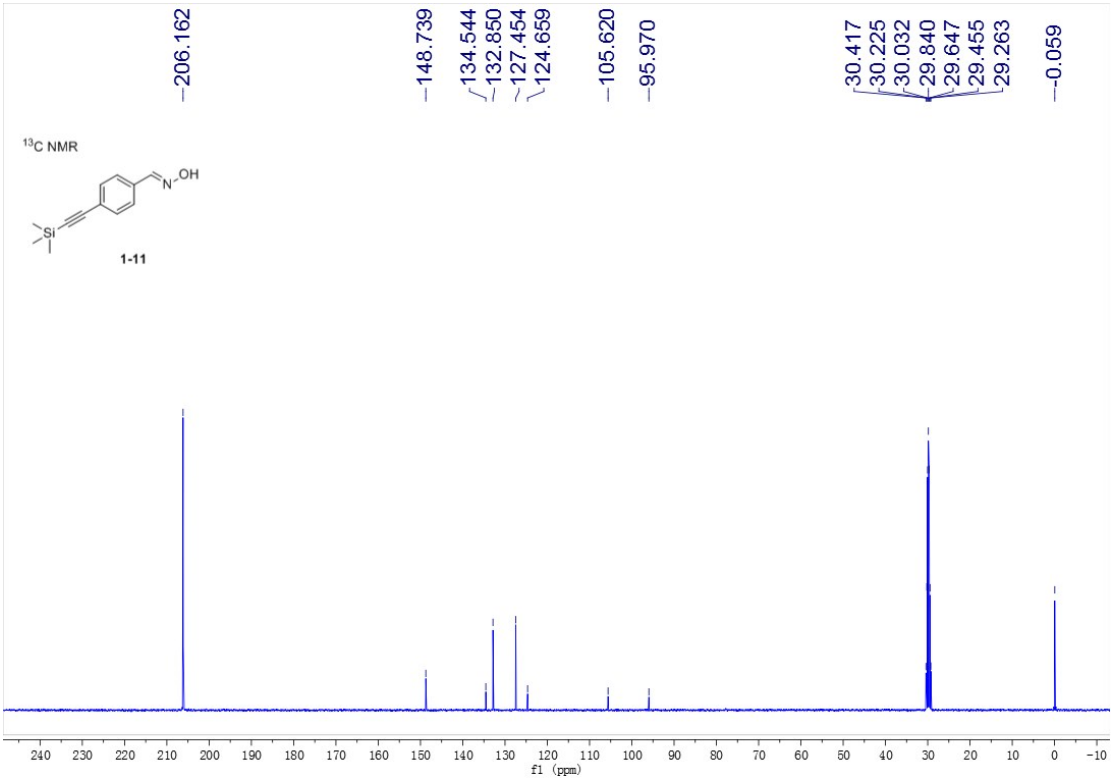
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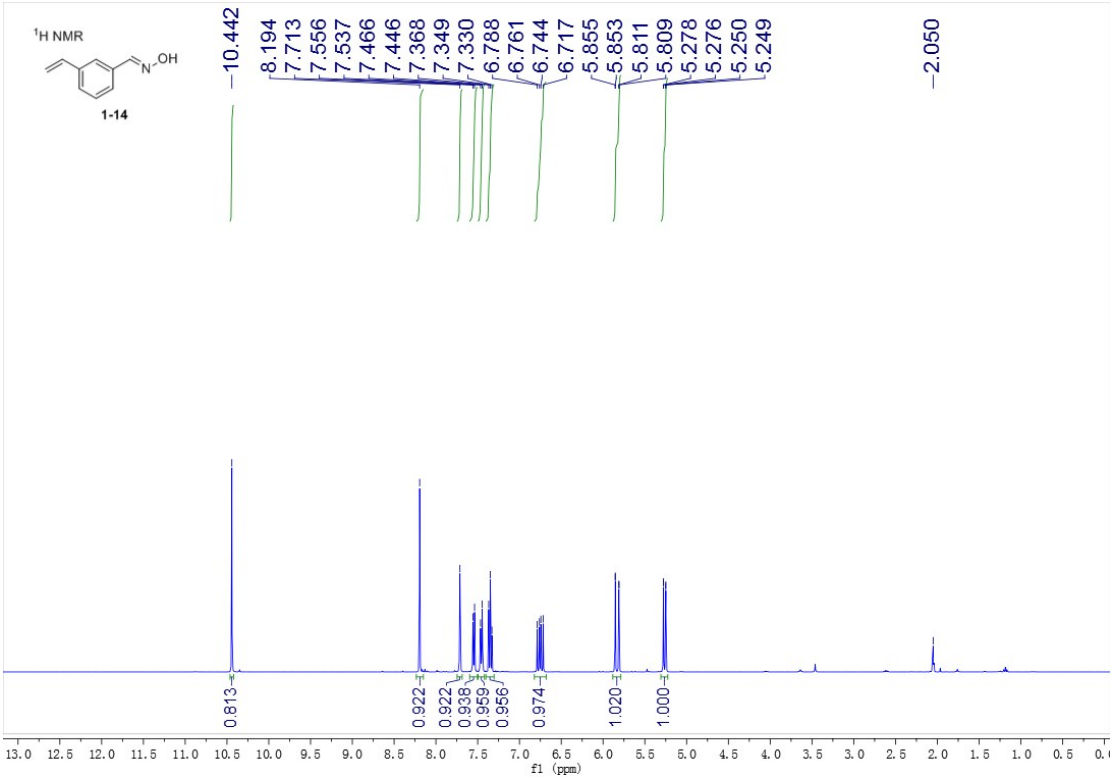
OH
N
Si
1-11
f1 (ppm)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N
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5.809
5.278
5.276
5.250
5.249
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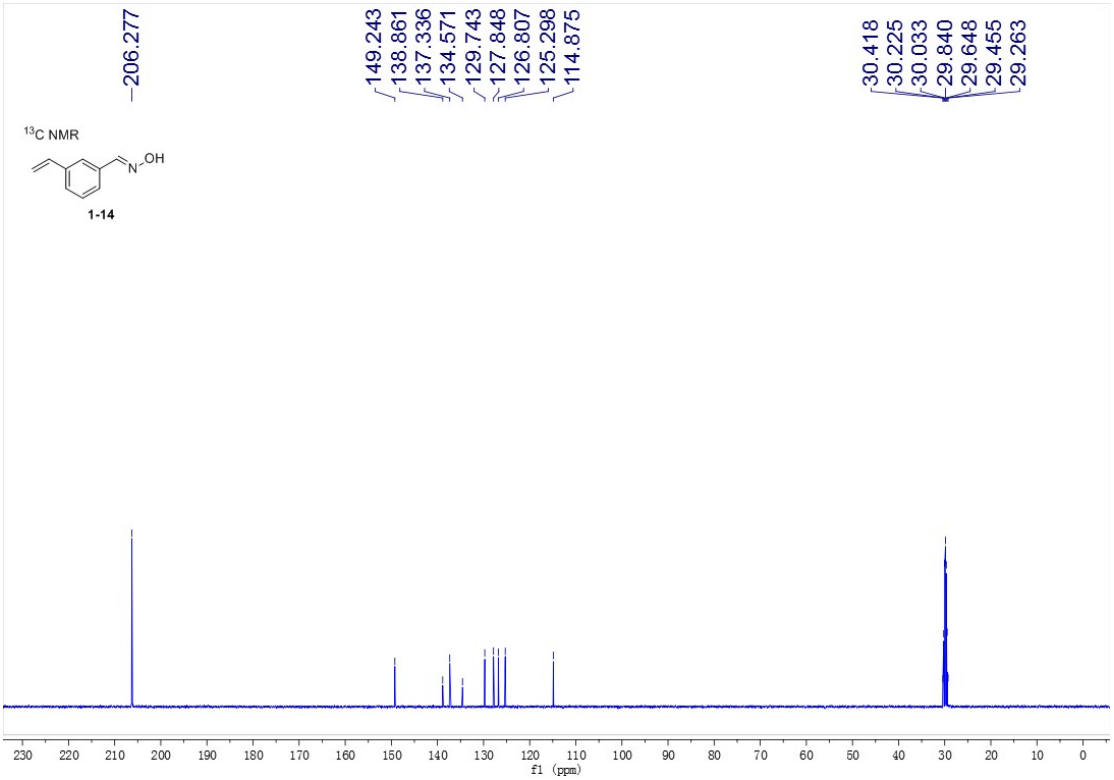
f1 (ppm)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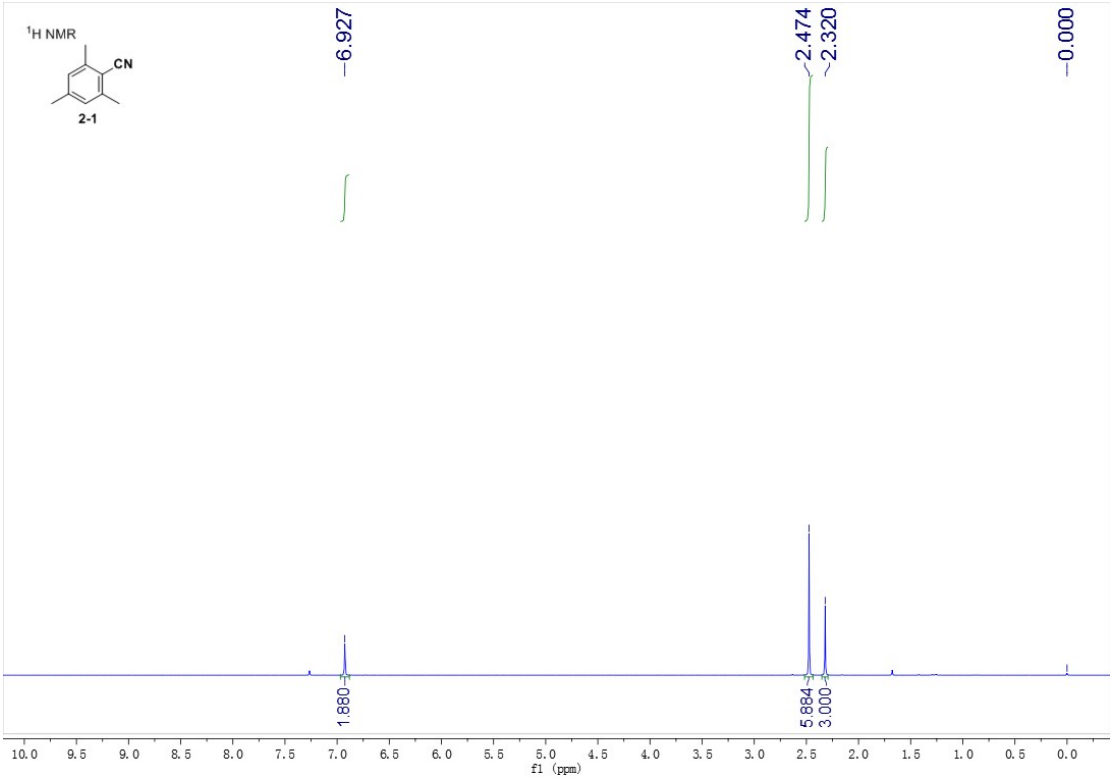
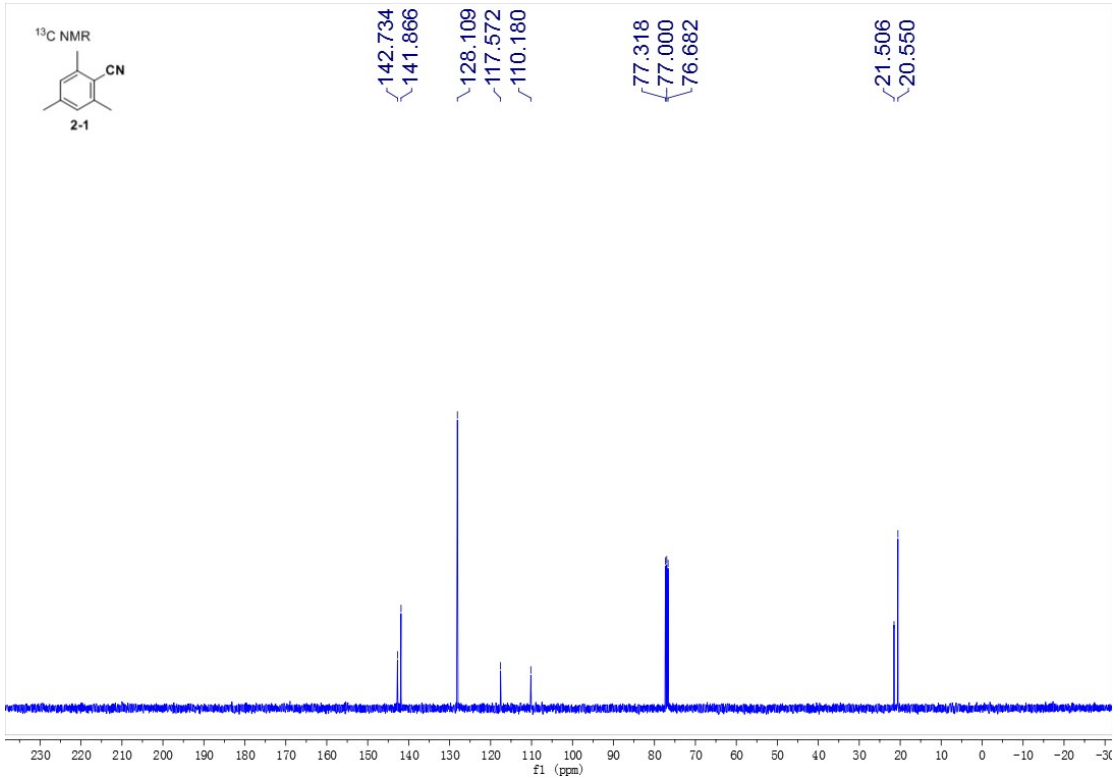
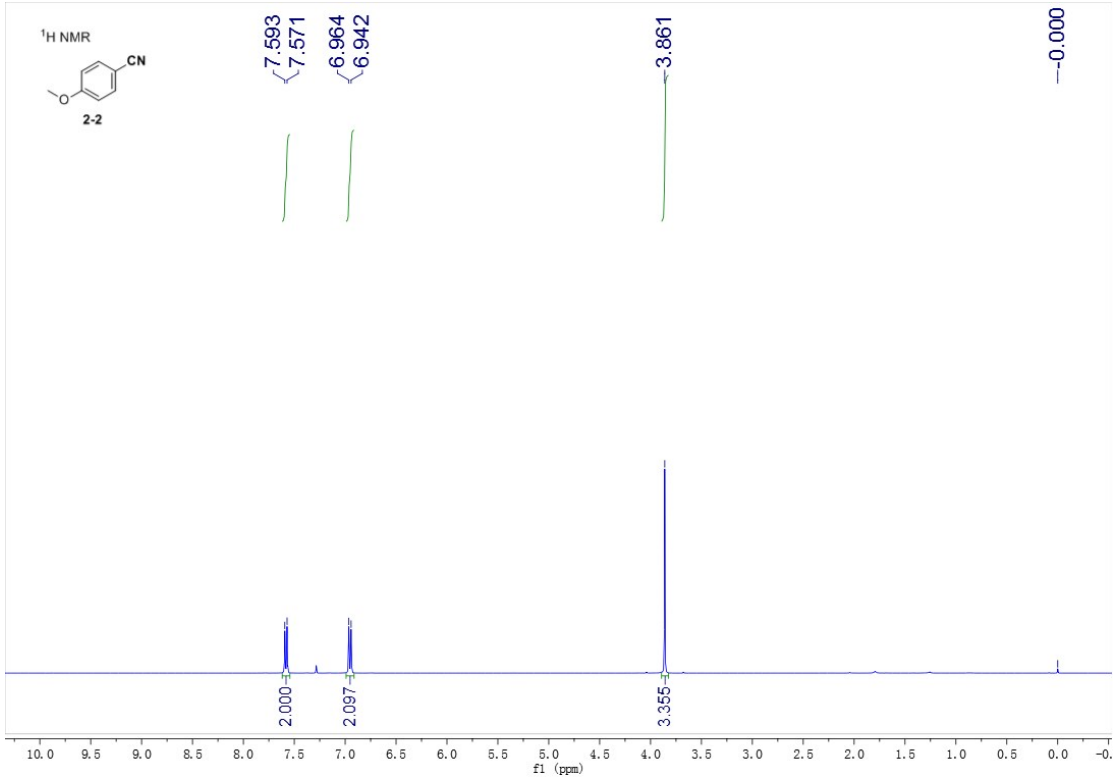
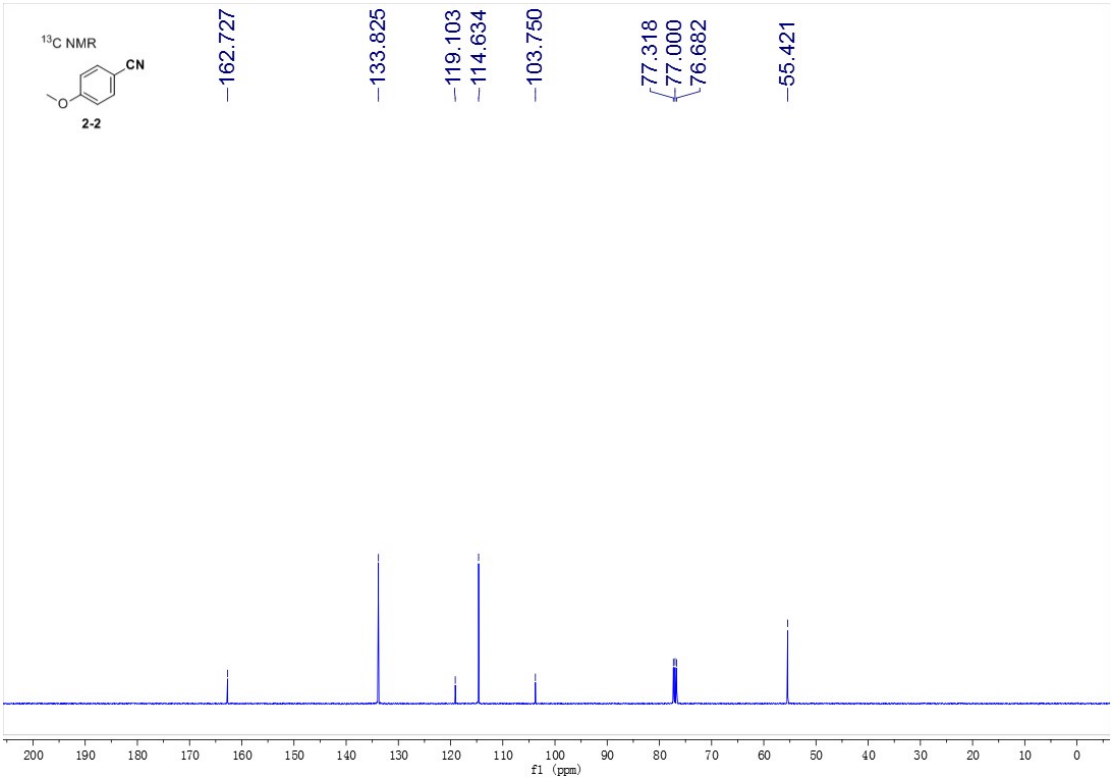
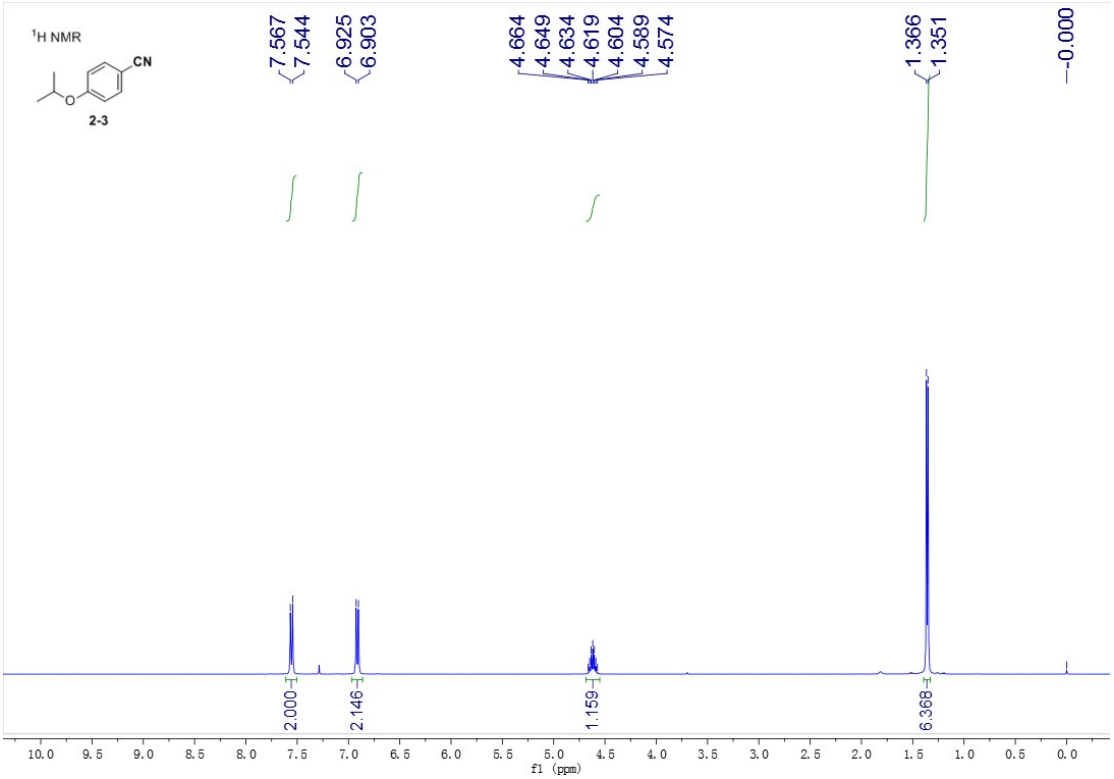
30.225
30.033
29.840
29.648
29.455
29.263
13C NMR
OH
N
1-14
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

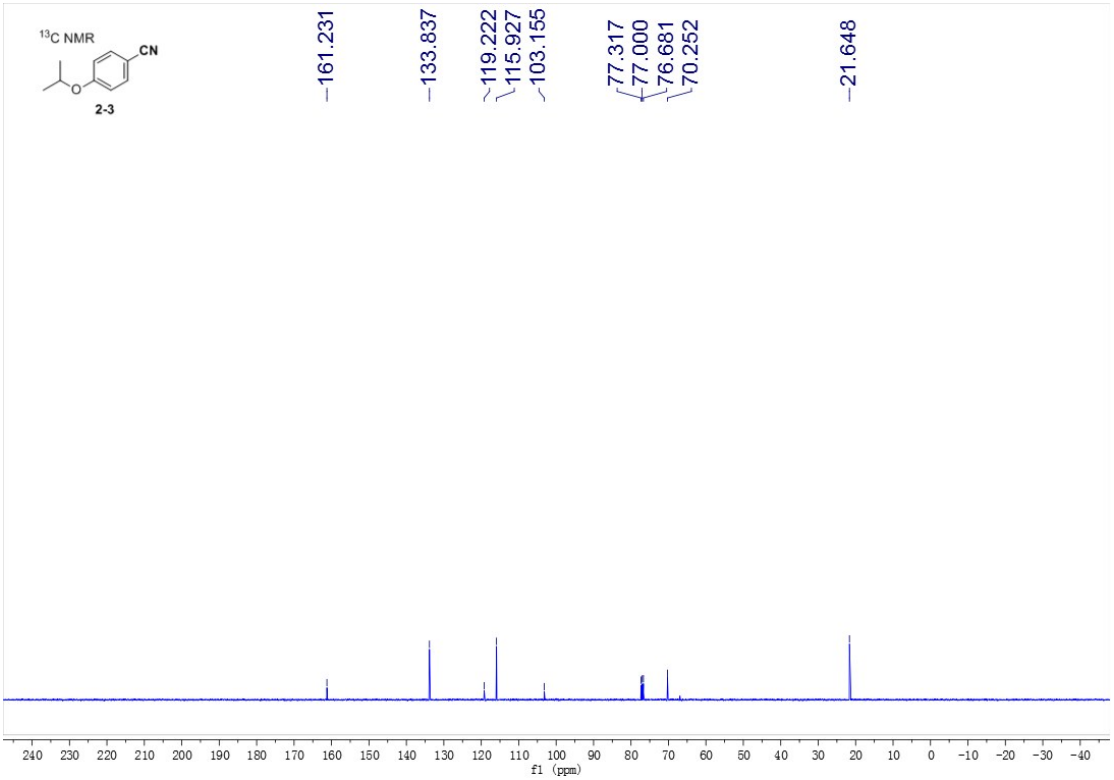

1H NMR
CN
2-1
6.927
2.474
2.320
0.000
1.880
5.884
3.000
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

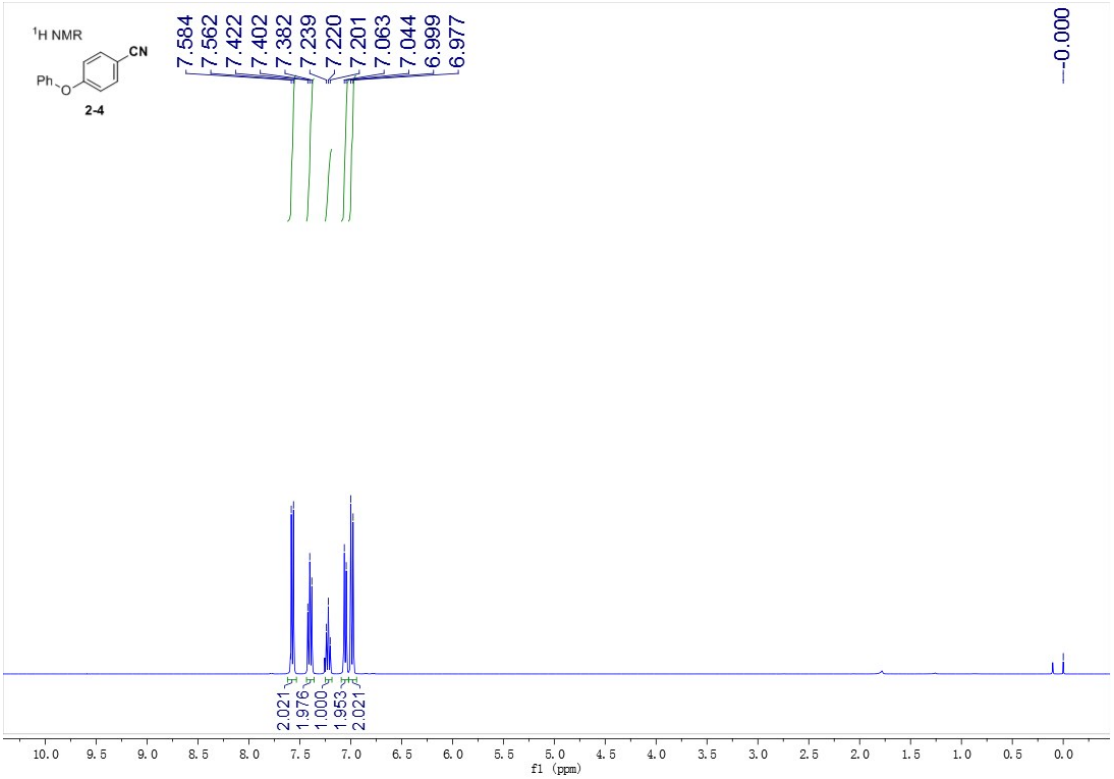

13C NMR
CN
2-1
142.734
141.866
128.109
117.572
110.180
77.318
77.000
76.682
21.506
20.550
f1 (ppm)

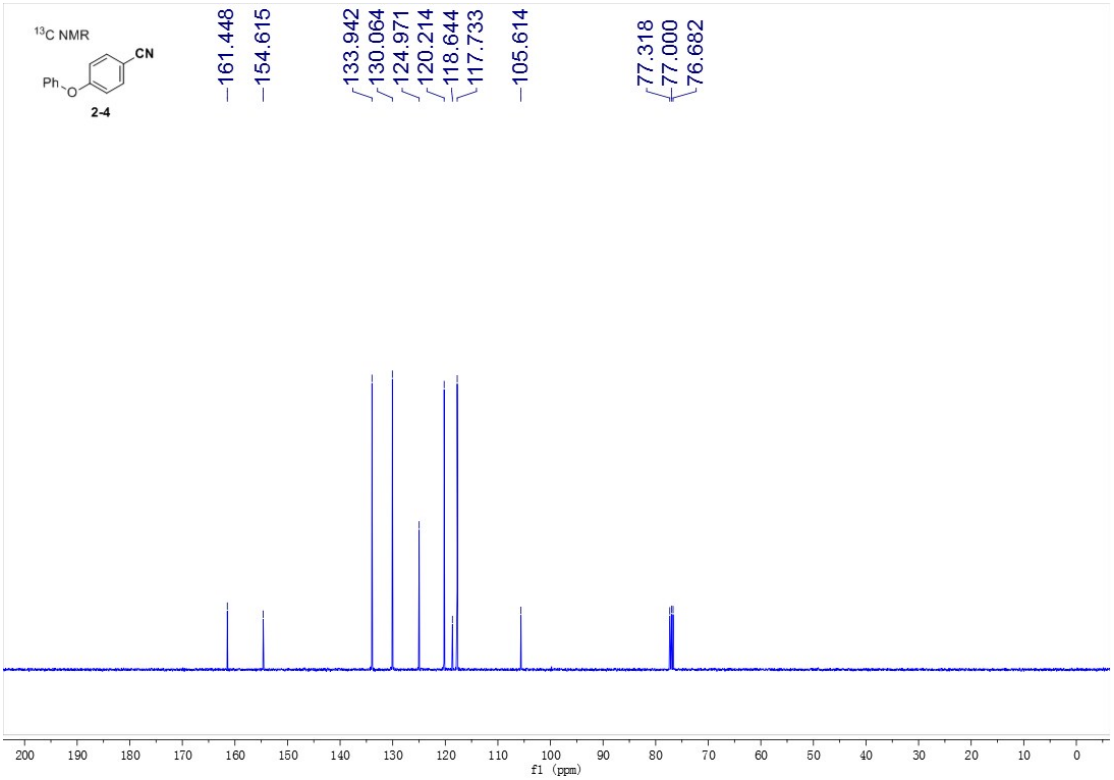

1H NMR
CN
O
2-2
7.593
7.571
6.964
6.942
3.861
0.000
2.000
2.097
3.355
f1 (ppm)

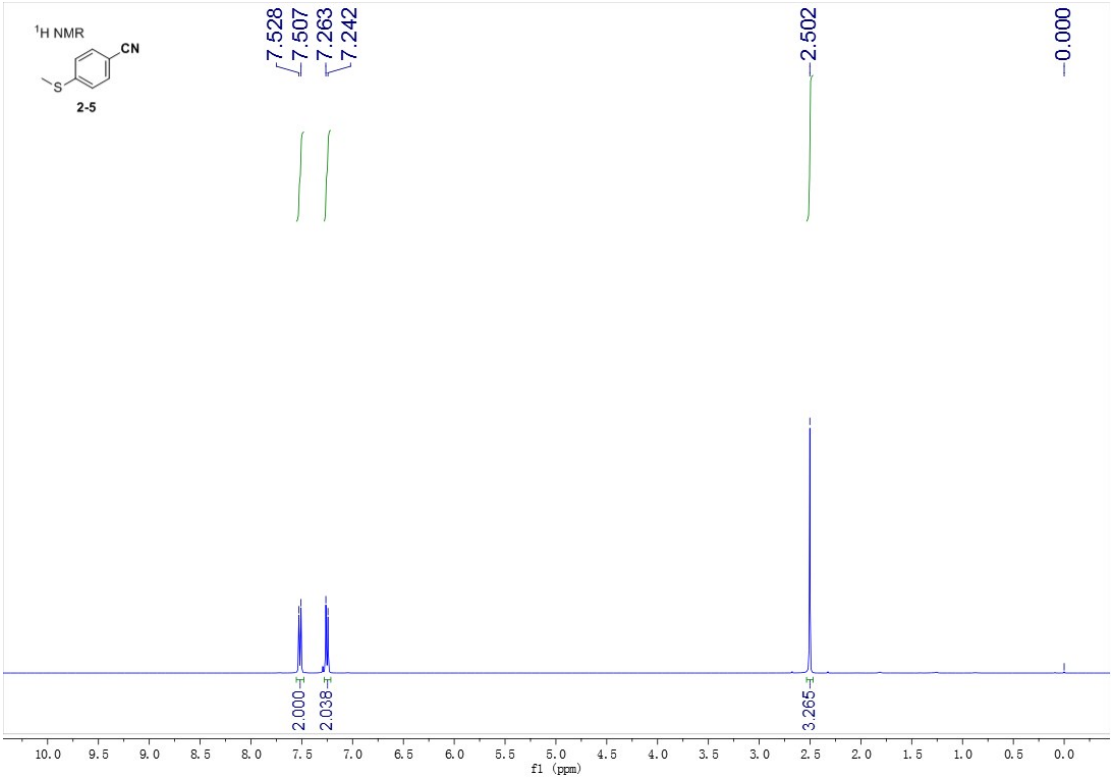

13C NMR
CN
O
2-2
162.727
133.825
119.103
114.634
103.750
77.318
77.000
76.682
55.421
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

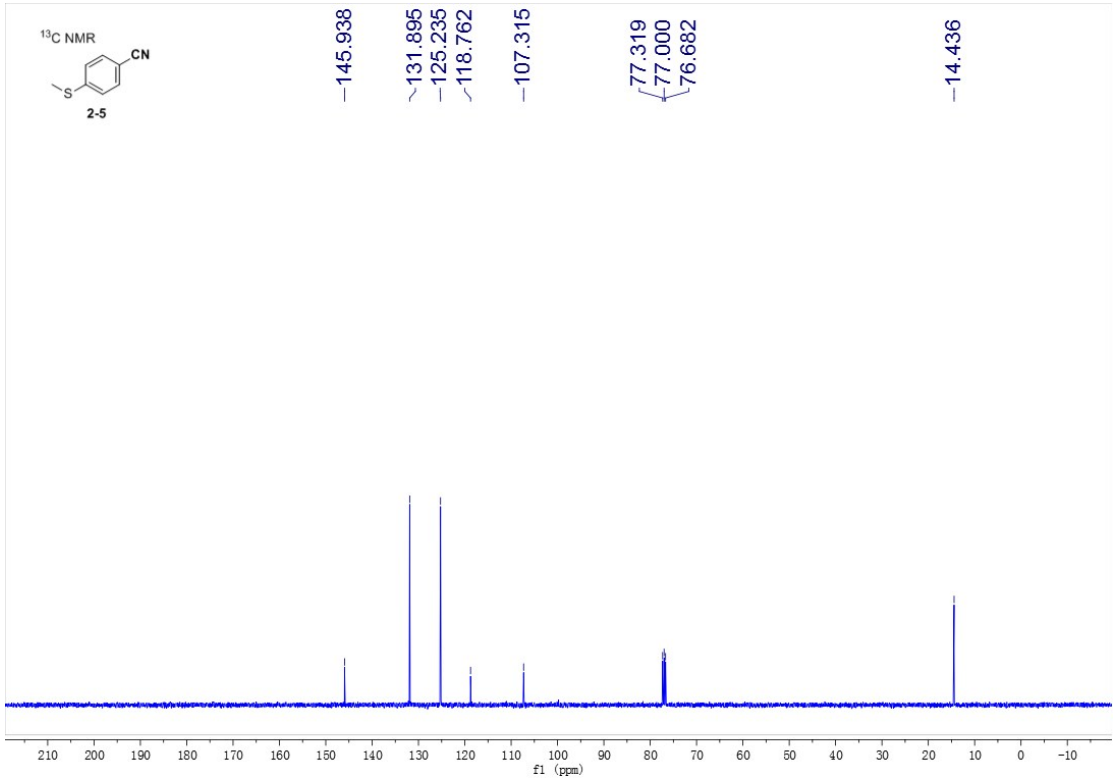

1H NMR
CN
O
2-3
7.567
7.544
6.925
6.903
4.664
4.649
4.634
4.619
4.604
4.589
4.574
1.366
1.351
0.000
2.000
2.146
1.159
6.368
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

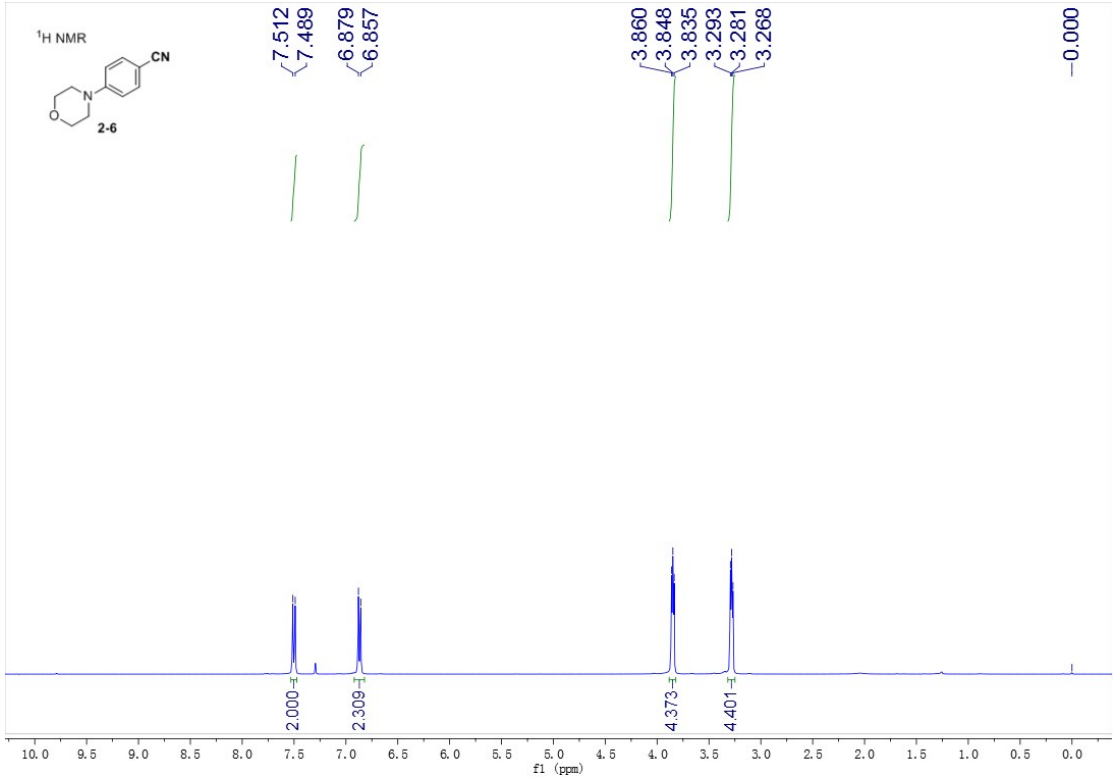

13C NMR
CN
O
2-3
161.231
133.837
119.222
115.927
103.155
77.317
77.000
76.681
70.252
21.648
f1 (ppm)

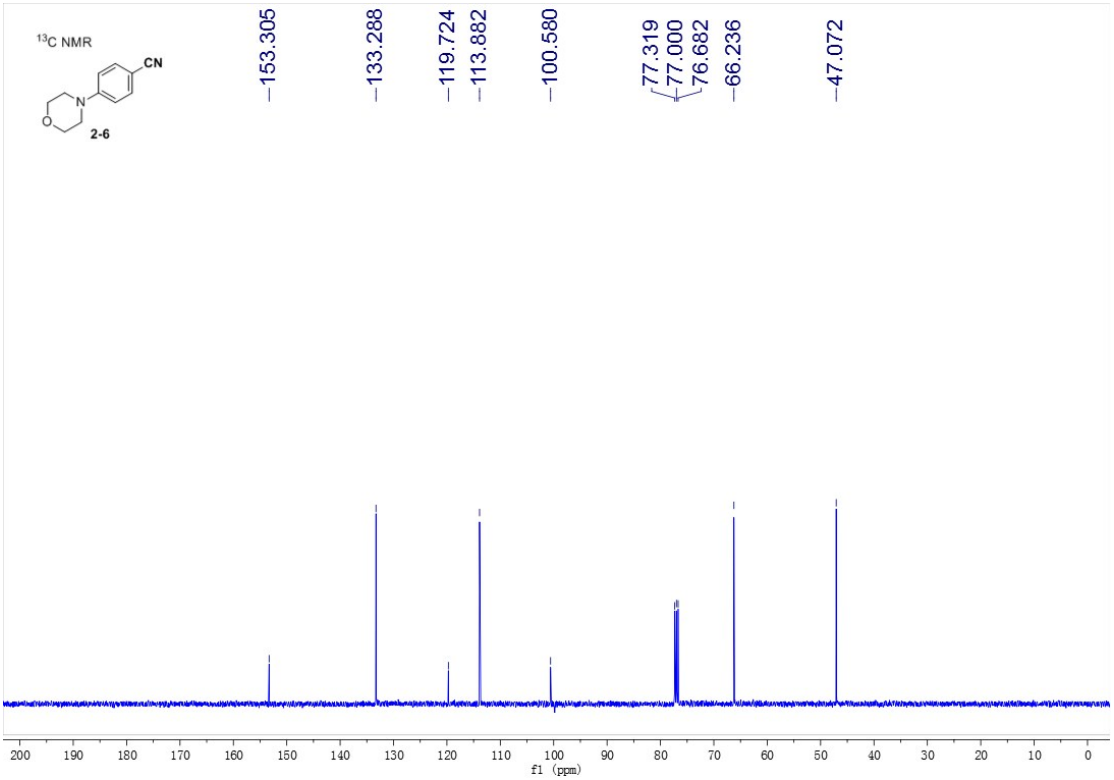

1H NMR
CN
Ph
O
2-4
7.584
7.562
7.422
7.402
7.382
7.239
7.220
7.201
7.063
7.044
6.999
6.977
0.000
2.021
1.976
1.000
1.953
2.021
f1 (ppm)

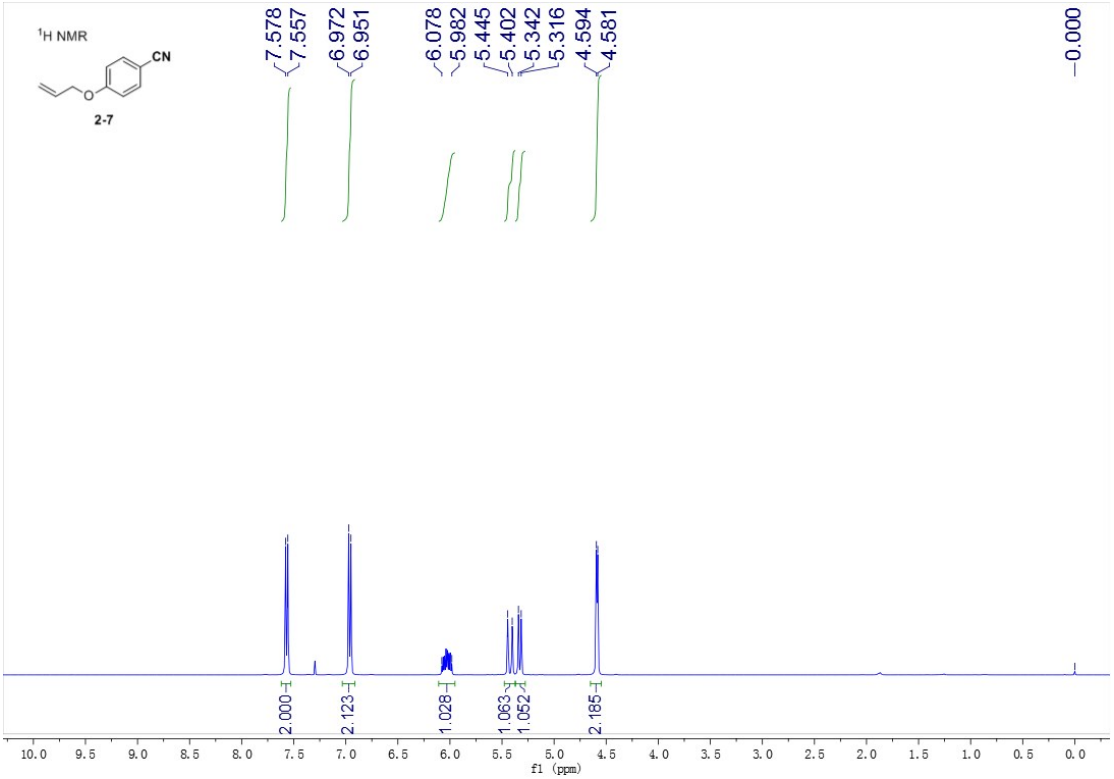

13C NMR
CN
Ph
O
2-4
161.448
154.615
133.942
130.064
124.971
120.214
118.644
117.733
105.614
77.318
77.000
76.682
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

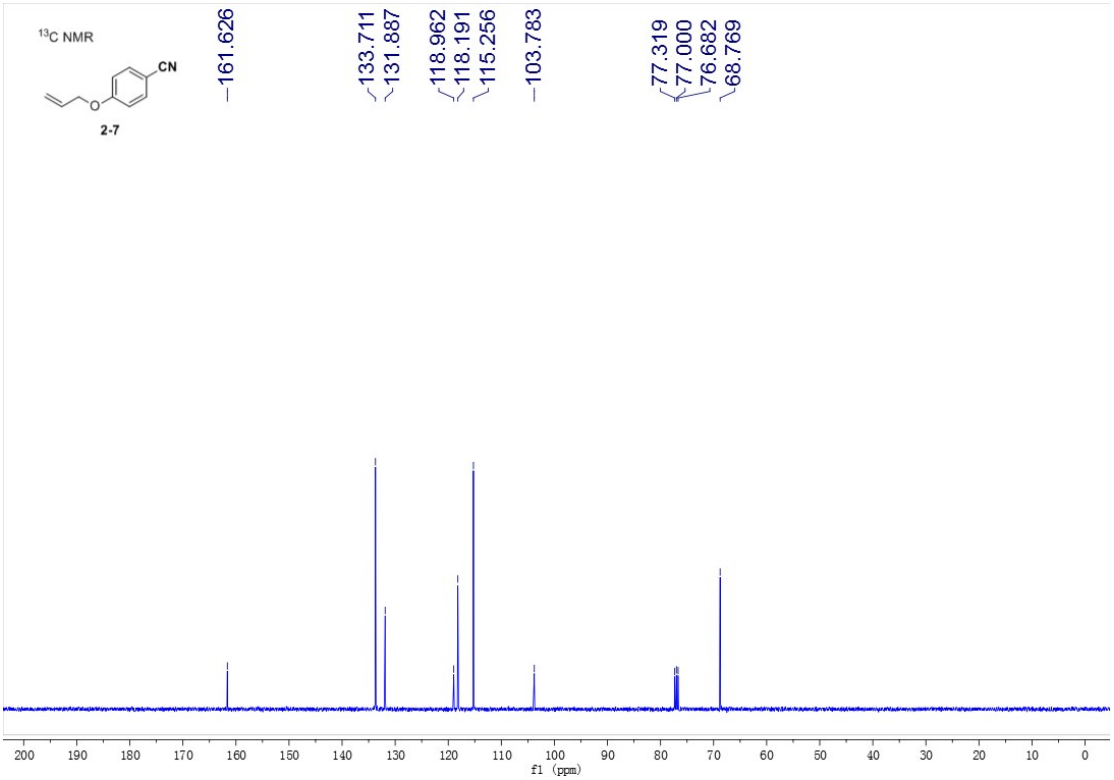

1H NMR
CN
S
2-5
7.528
7.507
7.263
7.242
2.502
0.000
2.000
2.038
3.265
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

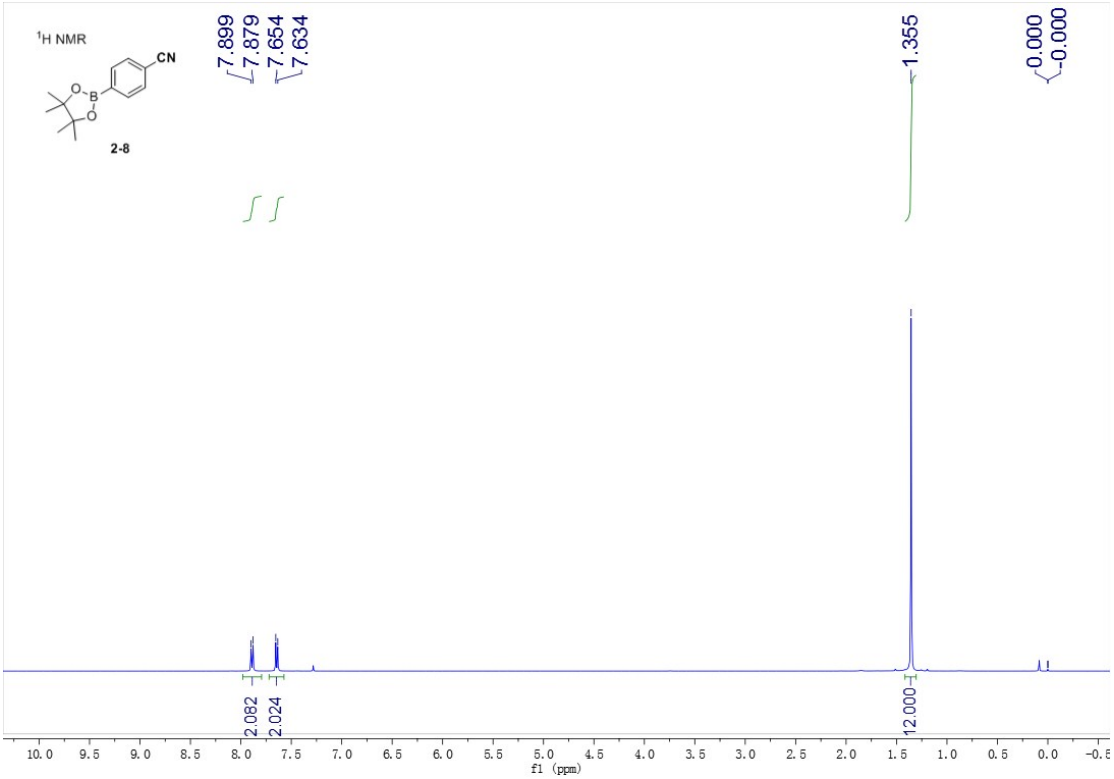

13C NMR
CN
S
2-5
145.938
131.885
125.235
118.762
107.315
77.319
77.000
76.682
14.436
f1 (ppm)

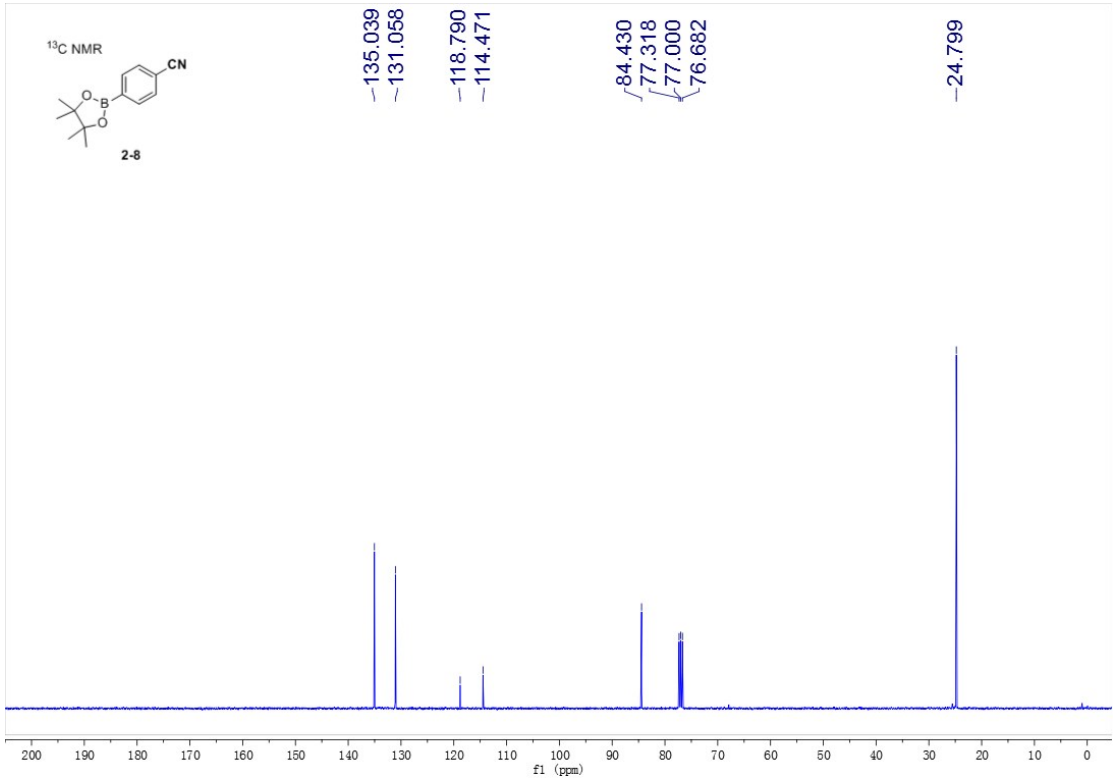

1H NMR
CN
N
O
2-6
7.512
7.489
6.879
6.857
3.860
3.848
3.835
3.293
3.281
3.268
0.000
2.000
2.309
4.373
4.401
f1 (ppm)

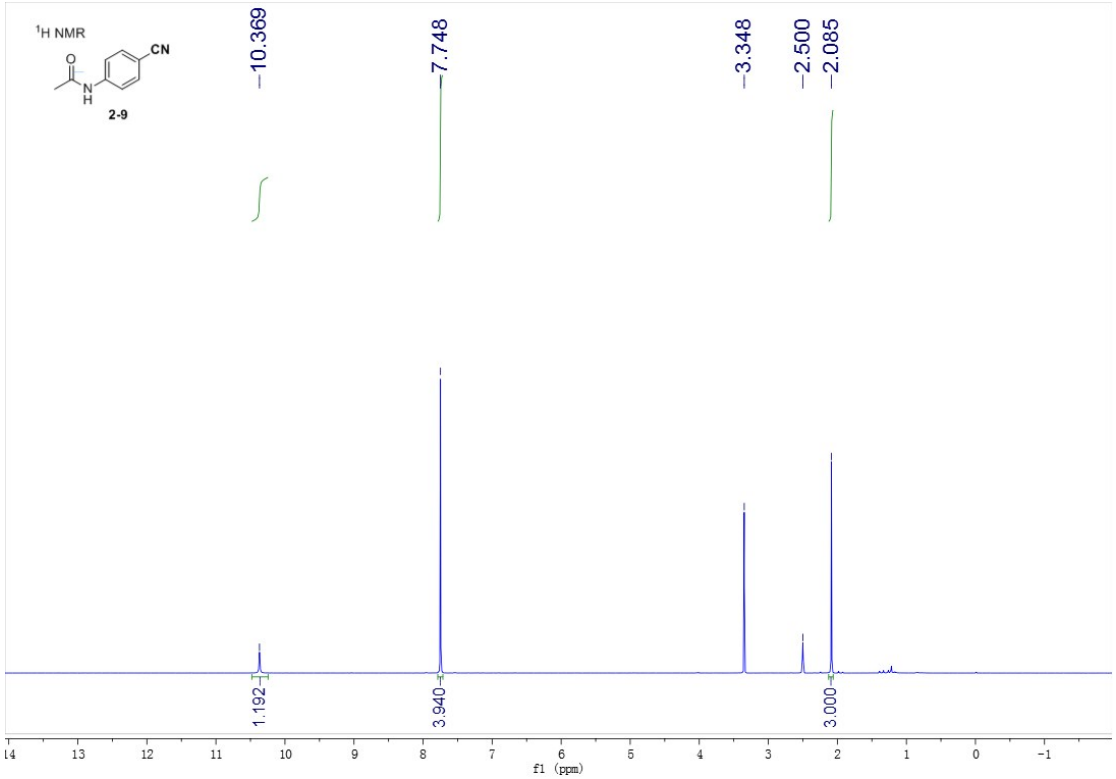

13C NMR
CN
N
O
2-6
153.305
133.288
119.724
113.882
100.580
77.319
77.000
76.682
66.236
47.072
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

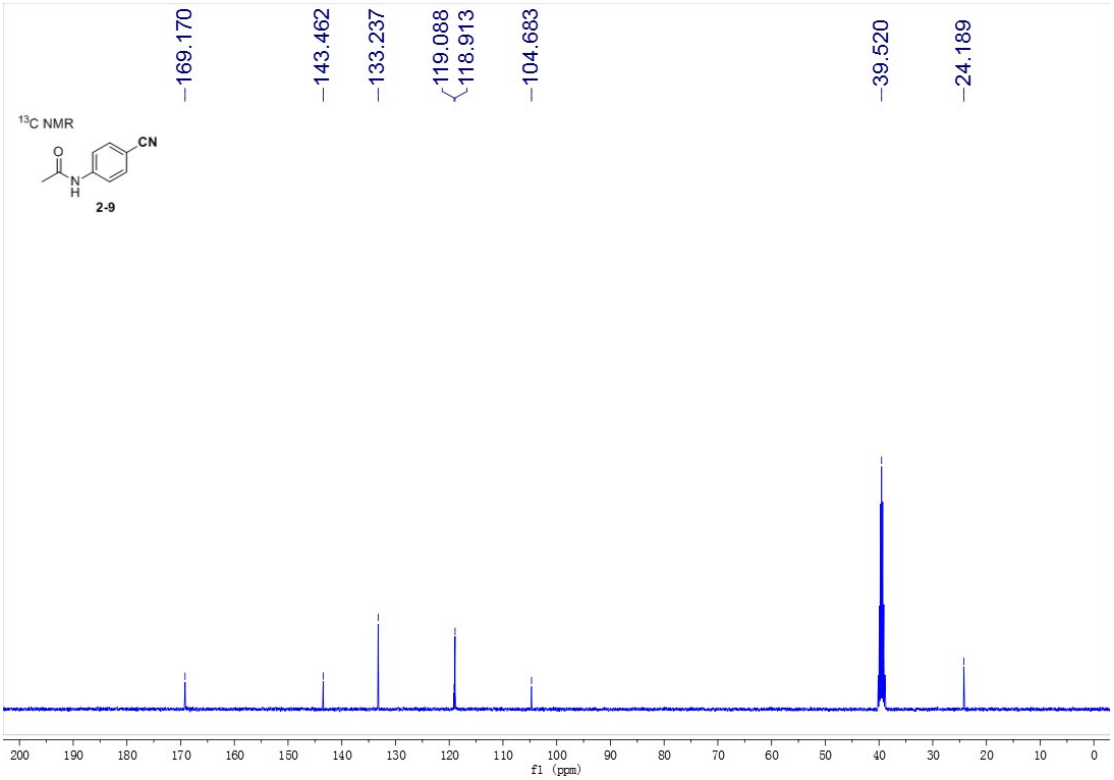

1H NMR
CN
O
2-7
7.578
7.557
6.972
6.951
6.078
5.982
5.445
5.402
5.342
5.316
4.594
4.581
0.000
2.000
2.123
1.028
1.063
1.052
2.185
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

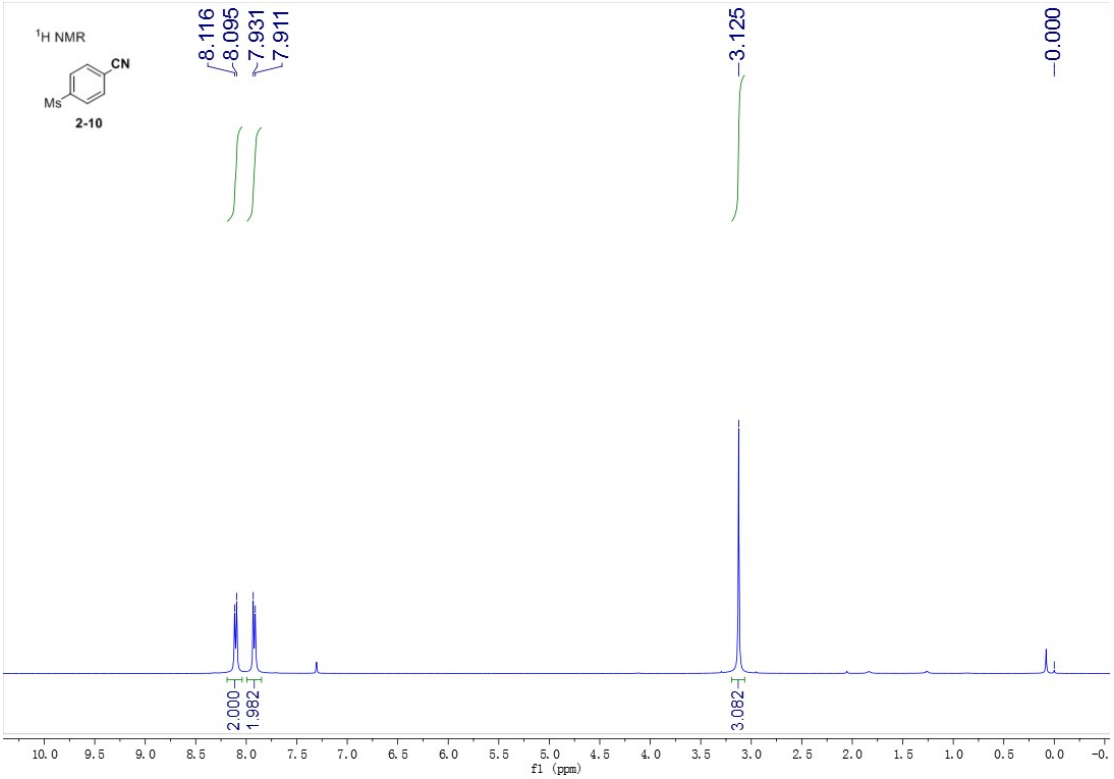

13C NMR
CN
2-7
161.626
133.711
131.887
118.962
118.191
115.256
103.783
77.319
77.000
76.682
68.769
f1 (ppm)

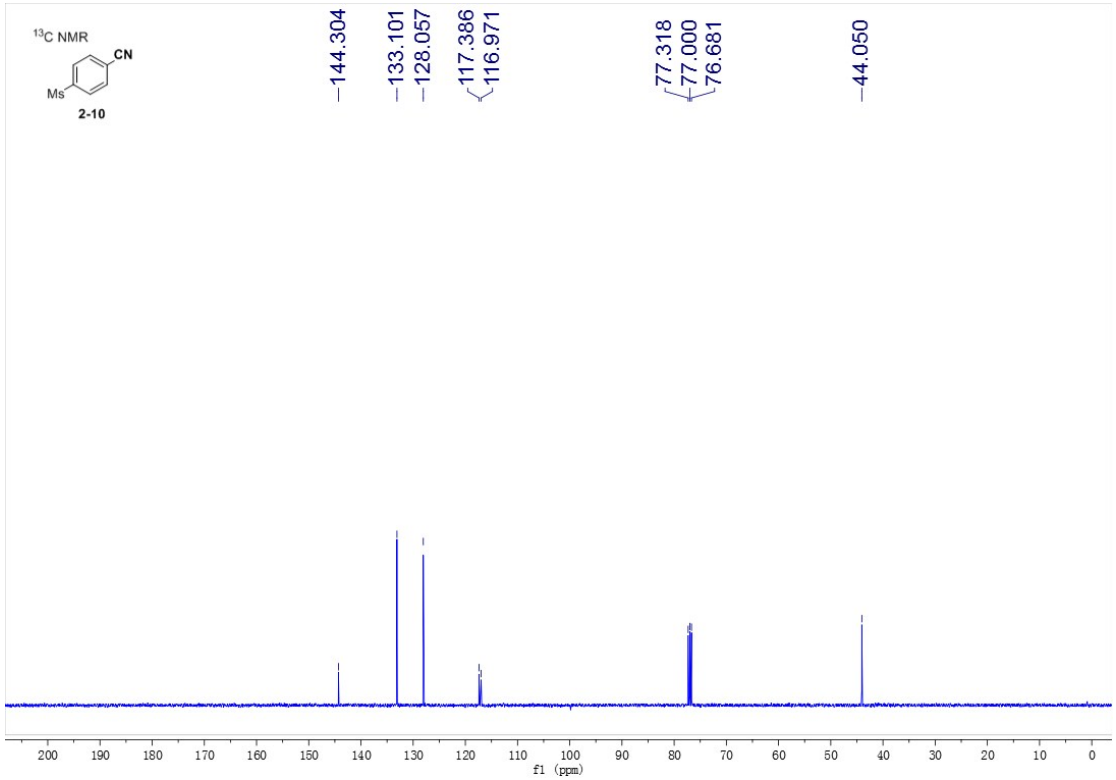

1H NMR
CN
2-8
7.899
7.879
7.654
7.634
1.355
0.000
-0.000
2.082
2.024
12.000
f1 (ppm)

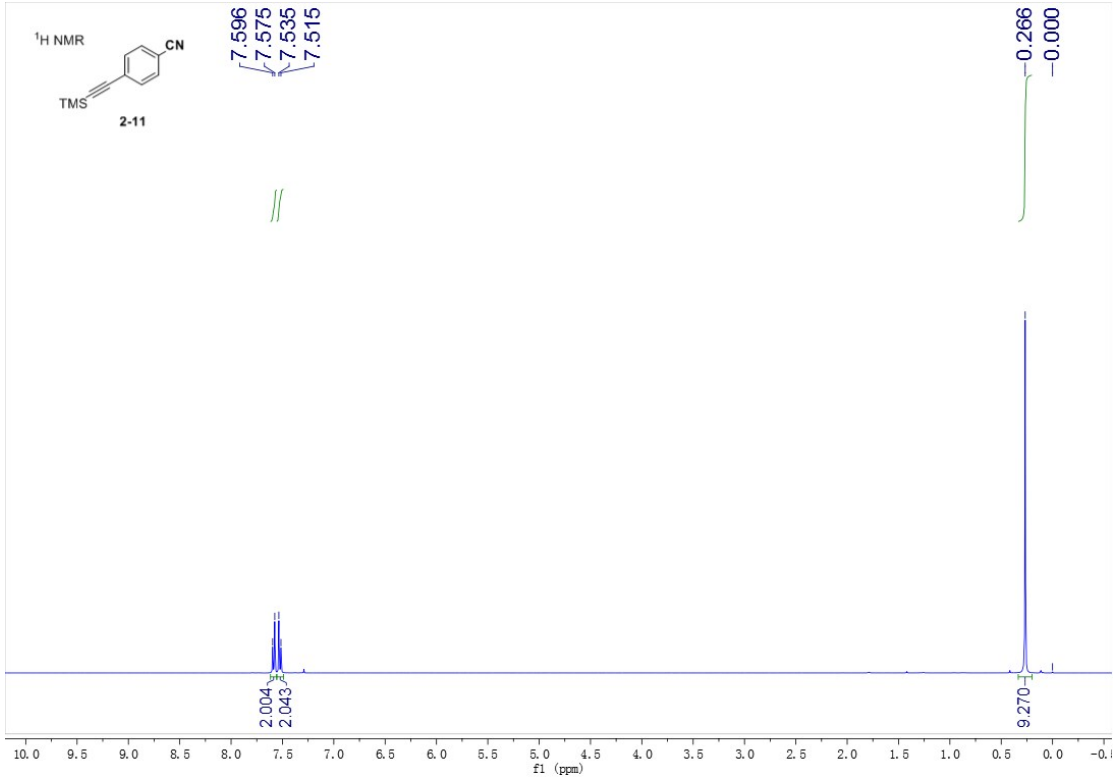

^{13}C NMR
CN
2-8
135.039
131.058
118.790
114.471
84.430
77.318
77.000
76.682
24.799
f1 (ppm)

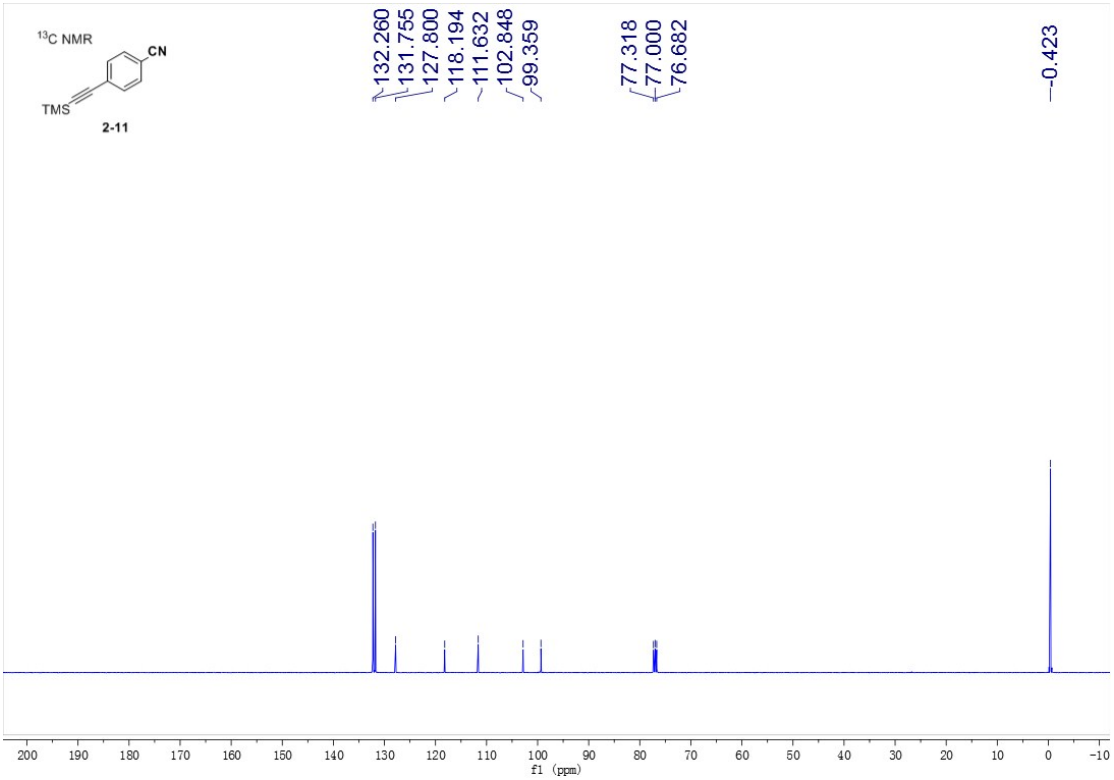

^{1}H NMR
CN
2-9
10.369
7.748
3.348
2.500
2.085
1.192
3.940
3.000
f1 (ppm)

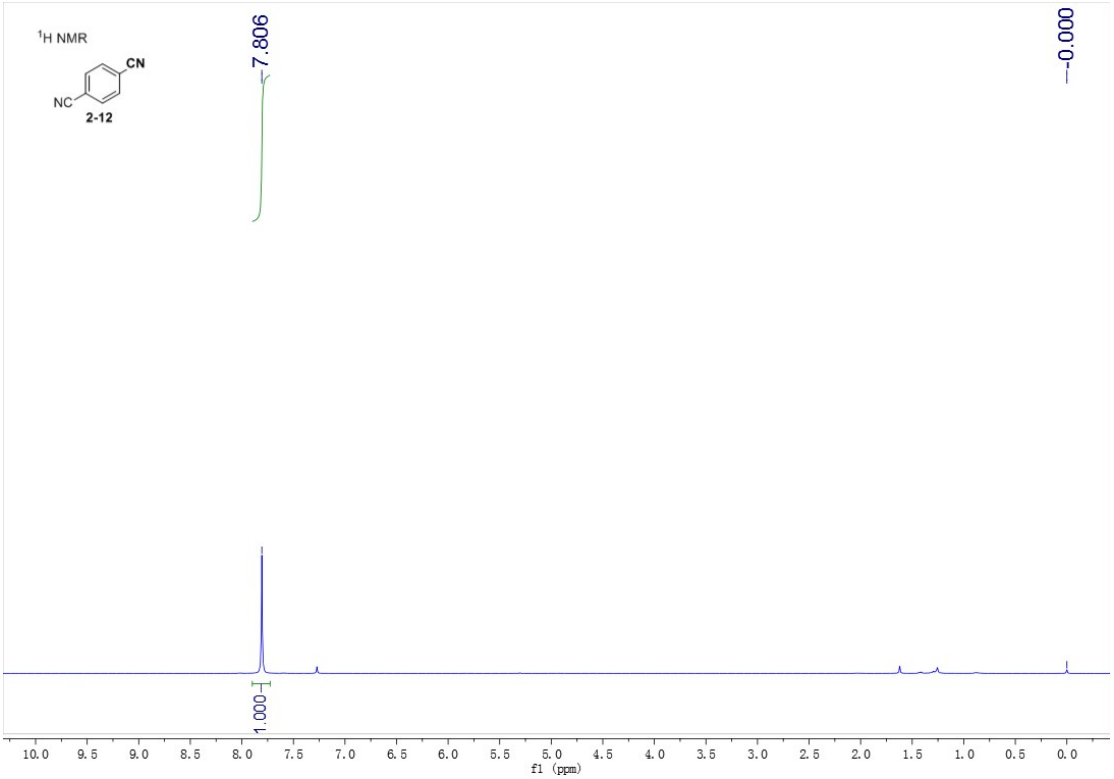

169.170
143.462
133.237
119.088
118.913
104.683
39.520
24.189
13C NMR
CN
O
N
H
2-9
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

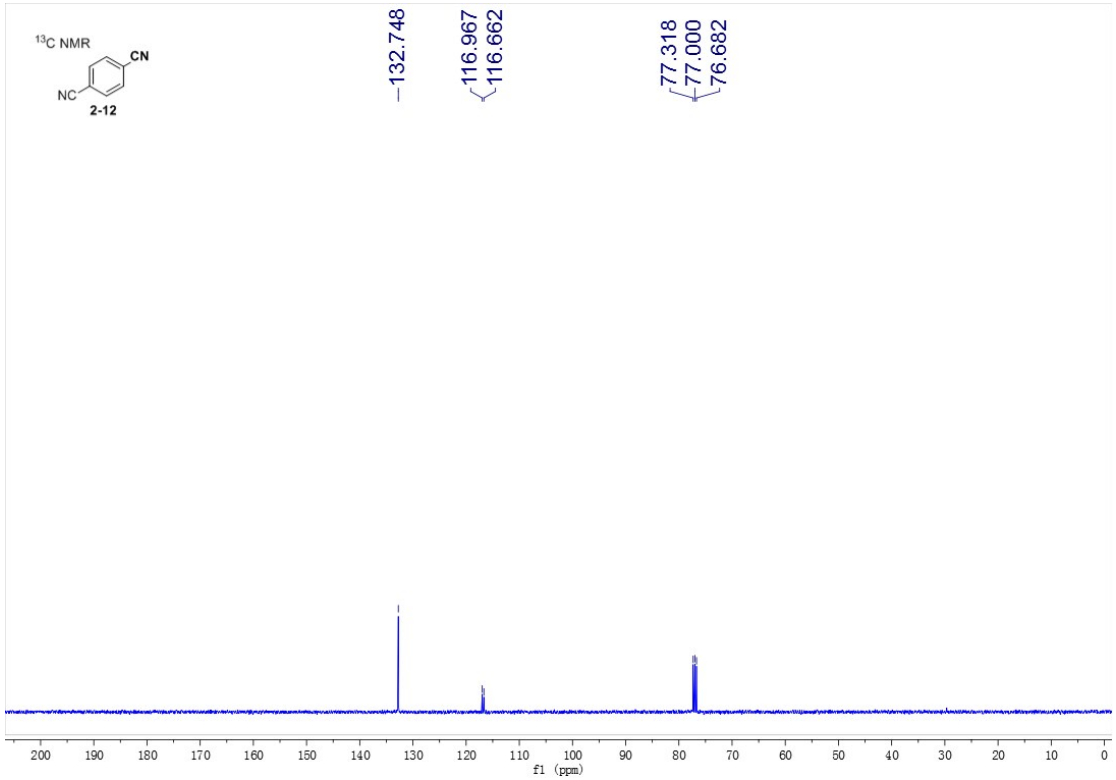

1H NMR
CN
Ms
2-10
8.116
8.095
7.931
7.911
3.125
0.000
2.000
1.982
3.082
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

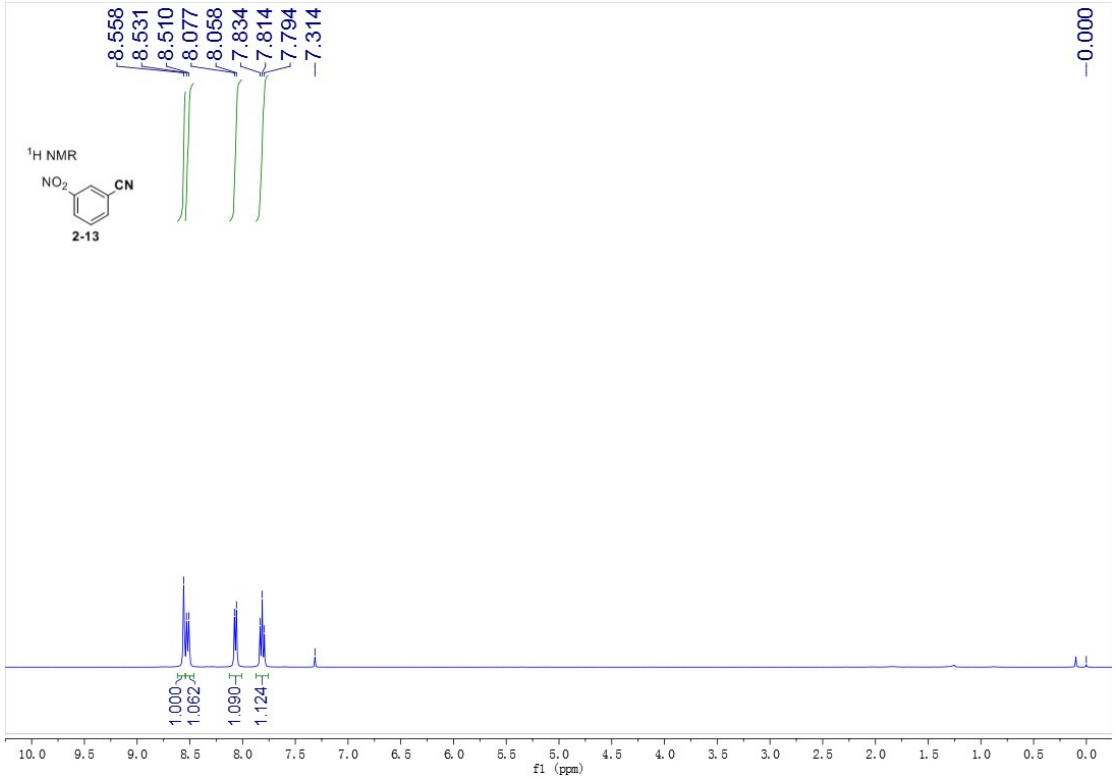

13C NMR
CN
Ms
2-10
144.304
133.101
128.057
117.386
116.971
77.318
77.000
76.681
44.050
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

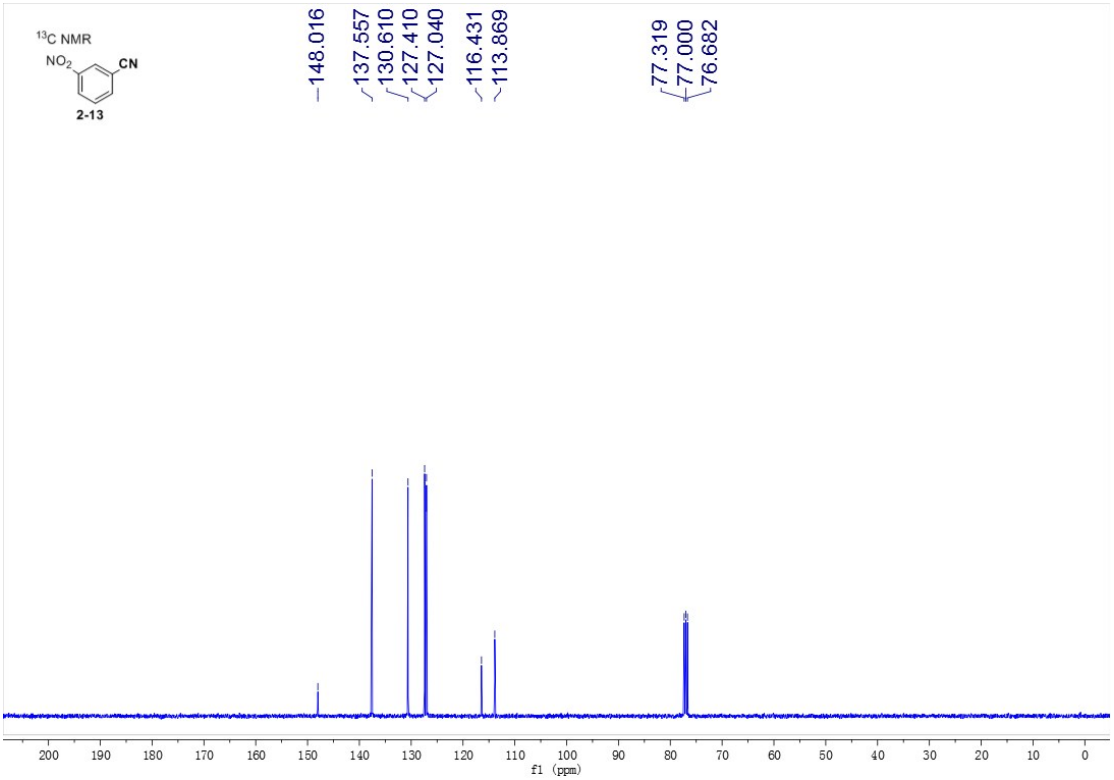

1H NMR
CN
TMS
2-11
7.596
7.575
7.535
7.515
0.266
0.000
2.004
2.043
9.270
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

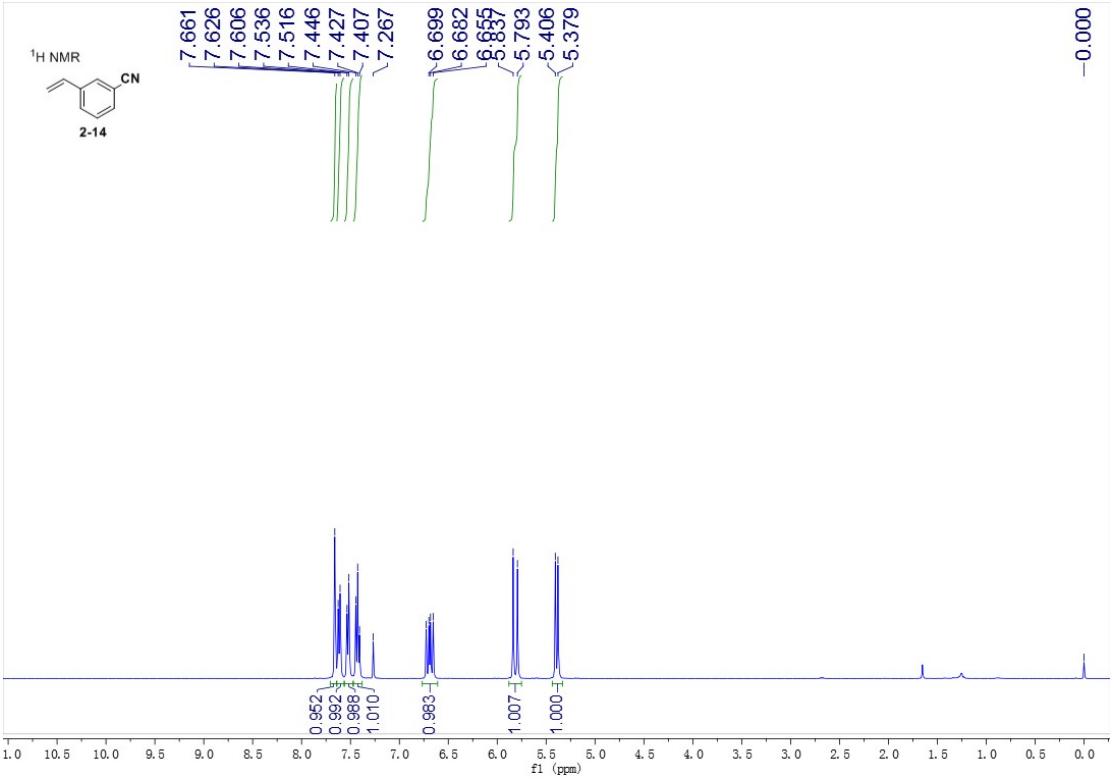

13C NMR
CN
TMS
2-11
132.260
131.755
127.800
118.194
111.632
102.848
99.359
77.318
77.000
76.682
-0.423
f1 (ppm)

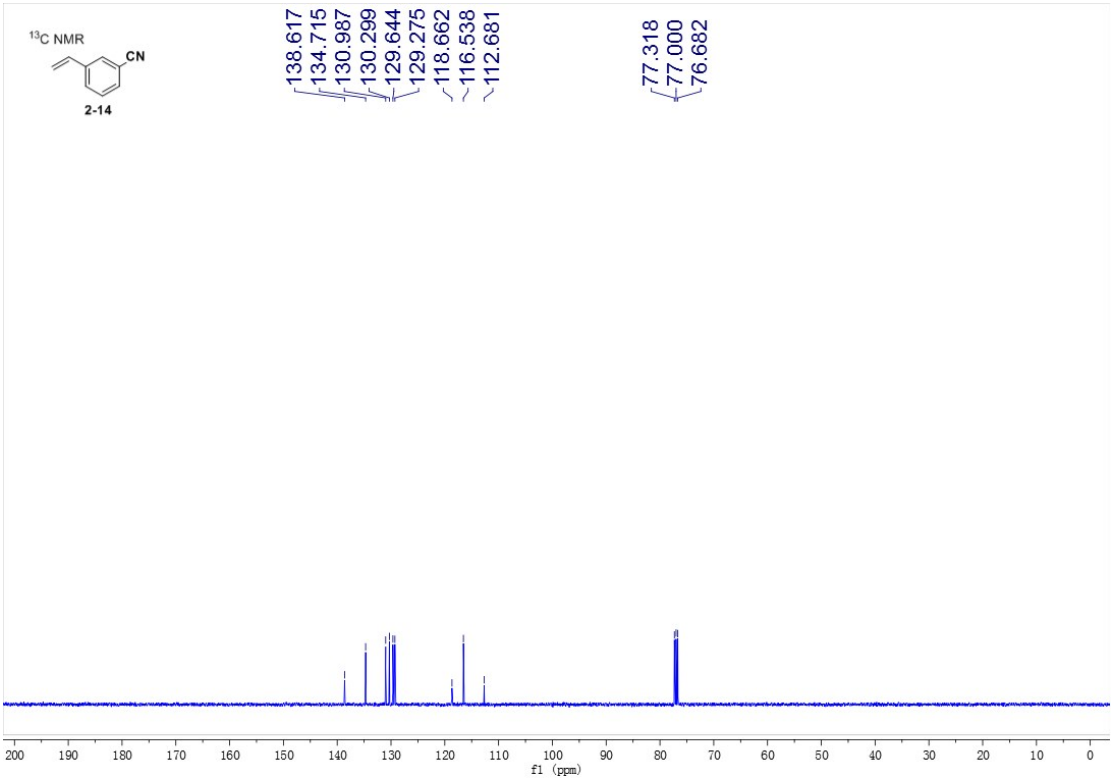

1H NMR
CN
NC
2-12
7.806
-0.000
1.000
f1 (ppm)

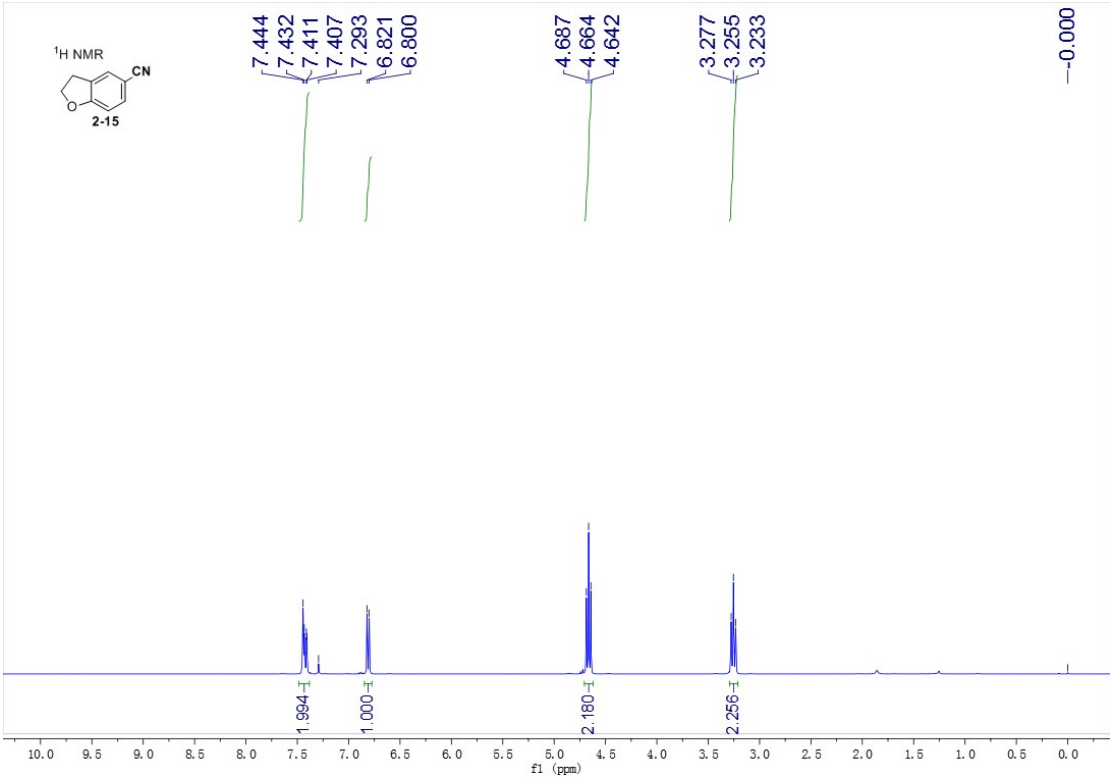

13C NMR
CN
NC
2-12
132.748
116.967
116.662
77.318
77.000
76.682
f1 (ppm)

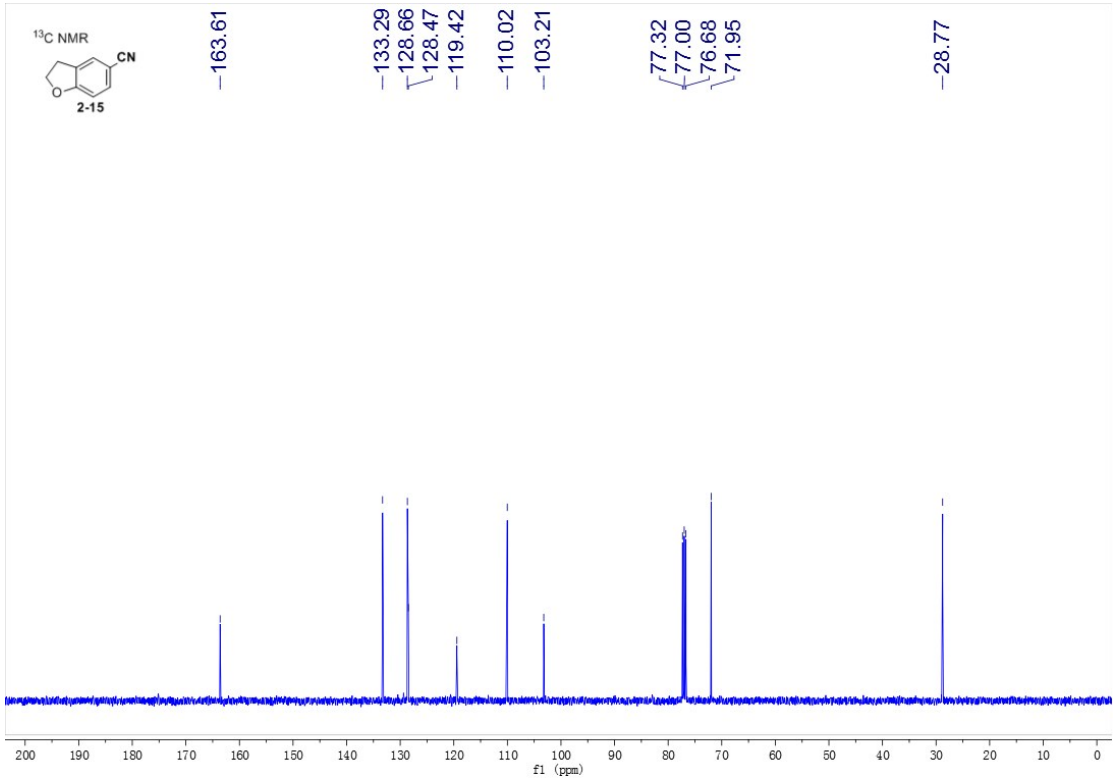

8.558
8.531
8.510
8.077
8.058
7.834
7.814
7.794
7.314
0.000
1H NMR
NO2
CN
2-13
1.000
1.062
1.090
1.124
f1 (ppm)

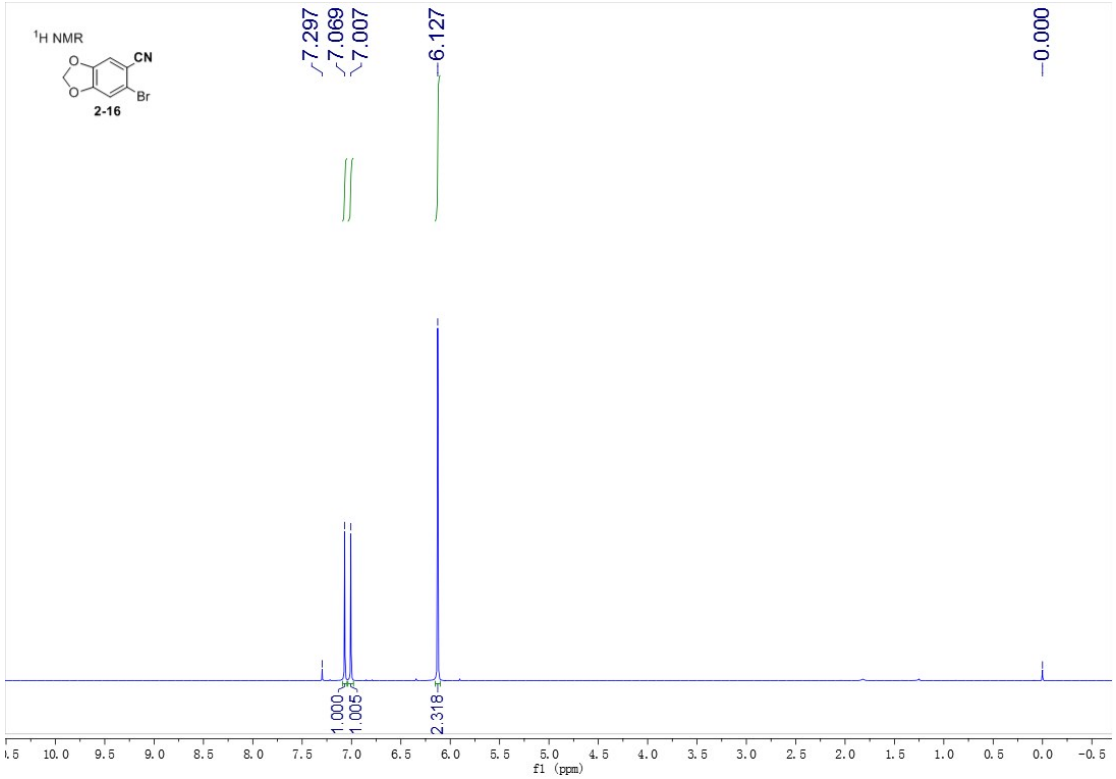

13C NMR
NO2
CN
2-13
148.016
137.557
130.610
127.410
127.040
116.431
113.869
77.319
77.000
76.682
f1 (ppm)

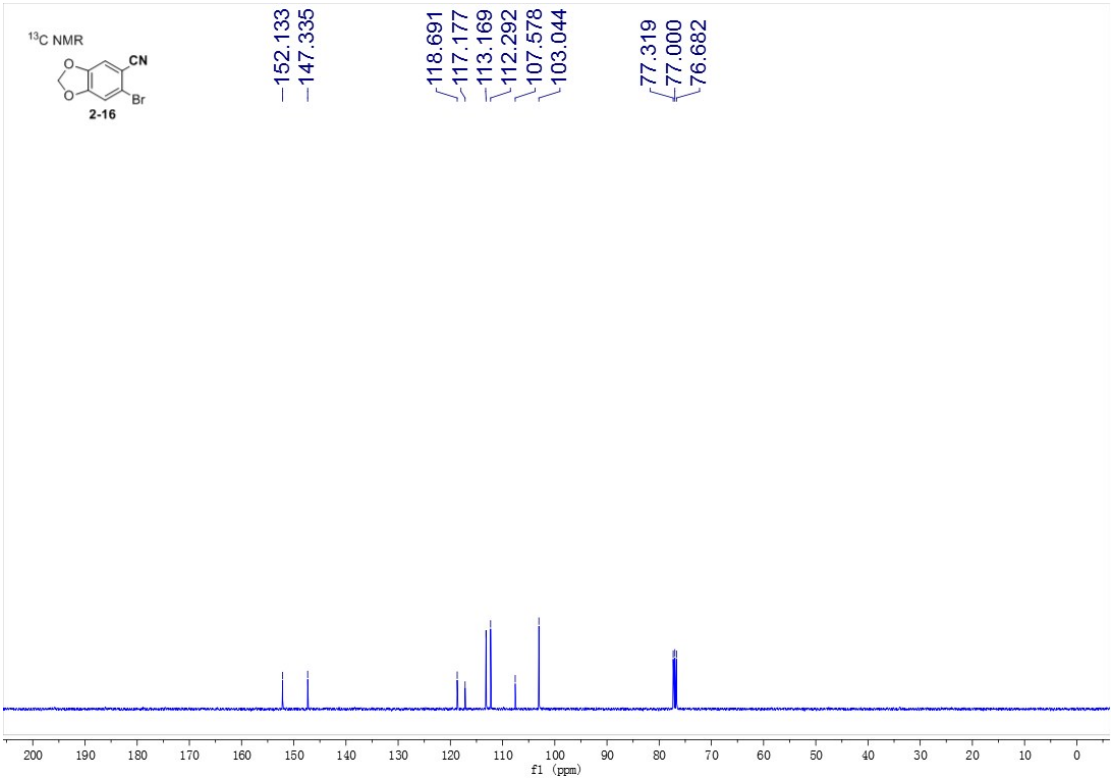

1H NMR
CN
2-14
7.661
7.626
7.606
7.536
7.516
7.446
7.427
7.407
7.267
6.699
6.682
6.655
5.837
5.793
5.406
5.379
0.000
0.952
0.992
0.988
1.010
0.983
1.007
1.000
f1 (ppm)

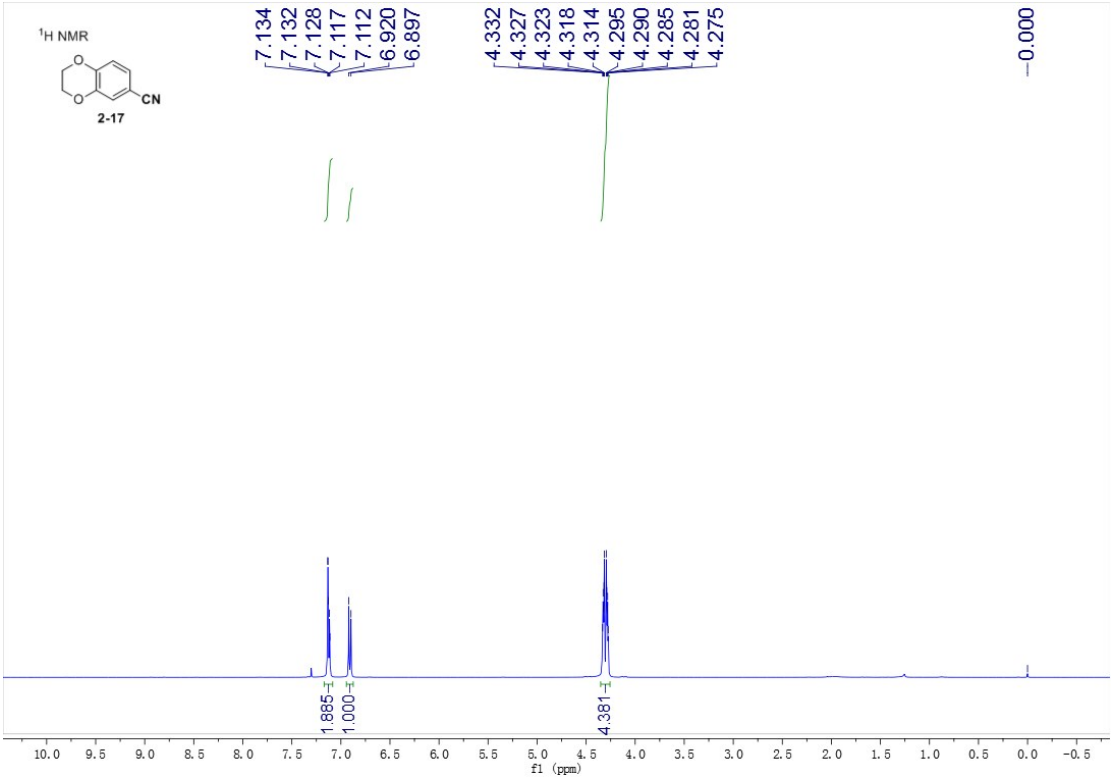

13C NMR
CN
2-14
138.617
134.715
130.987
130.299
129.644
129.275
118.662
116.538
112.681
77.318
77.000
76.682
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

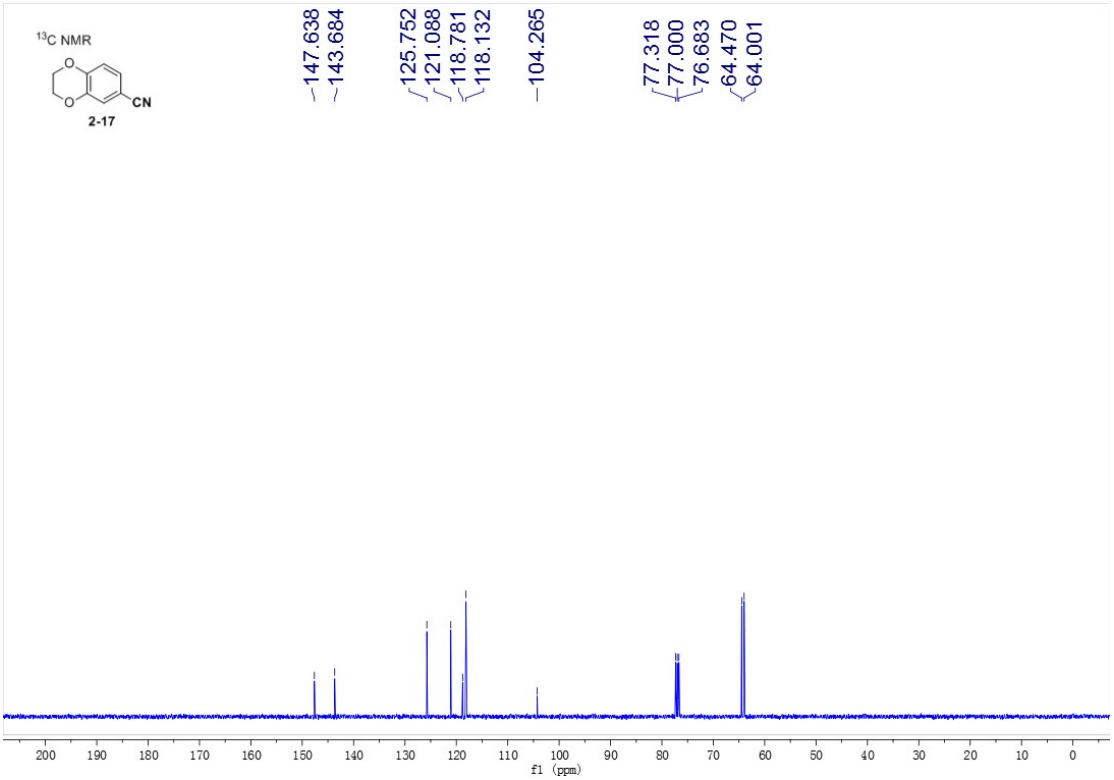

1H NMR
CN
O
2-15
7.444
7.432
7.411
7.407
7.293
6.821
6.800
4.687
4.664
4.642
3.277
3.255
3.233
-0.000
1.994
1.000
2.180
2.256
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

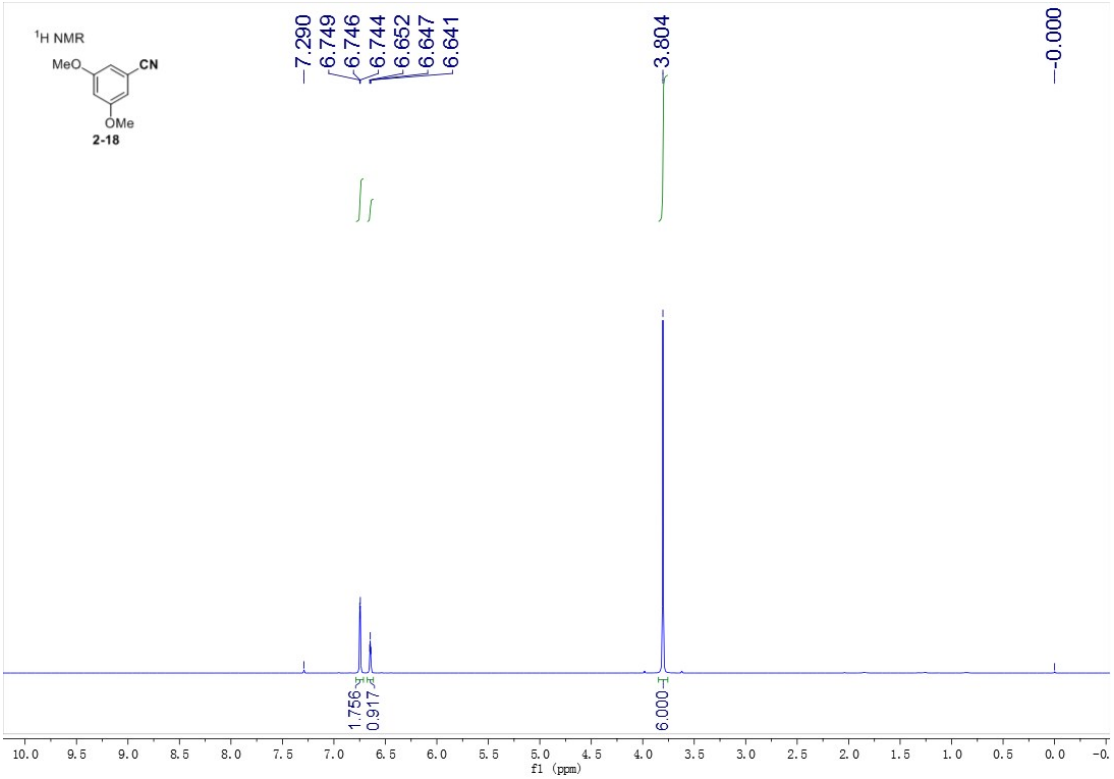

^{13}C NMR
CN
2-15
163.61
133.29
128.66
128.47
119.42
110.02
103.21
77.32
77.00
76.68
71.95
28.77
f1 (ppm)

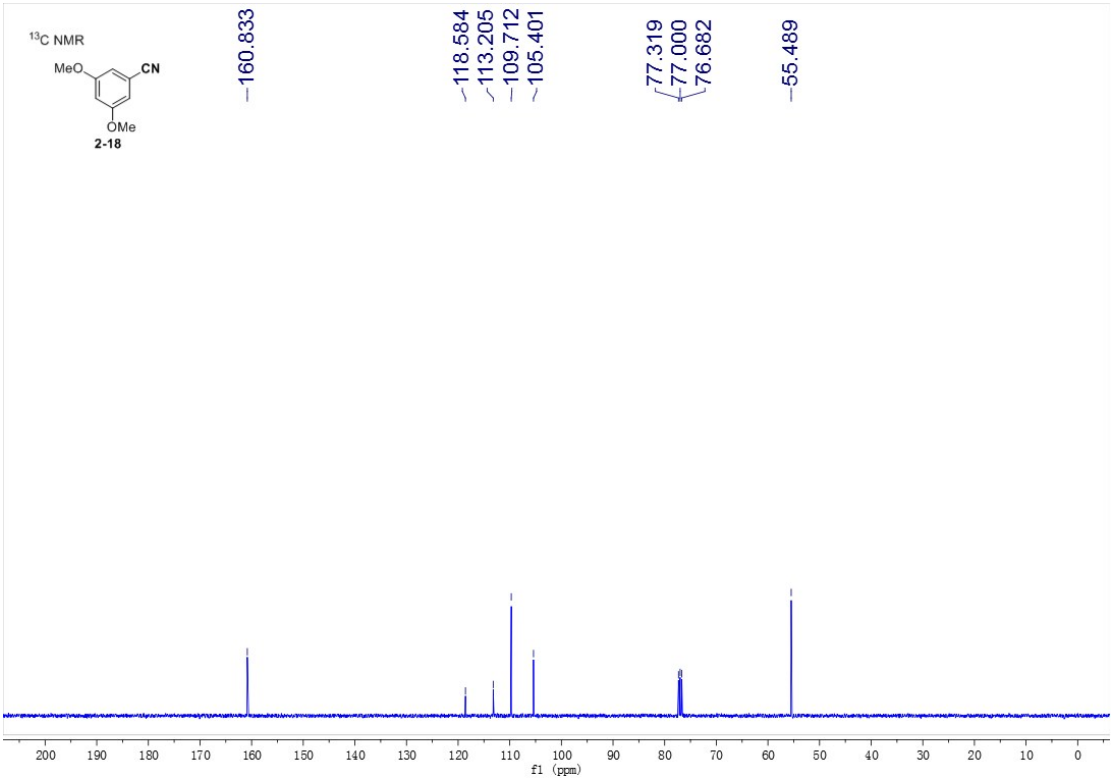

^{1}H NMR
CN
Br
2-16
7.297
7.069
7.007
6.127
0.000
1.000
1.005
2.318
f1 (ppm)

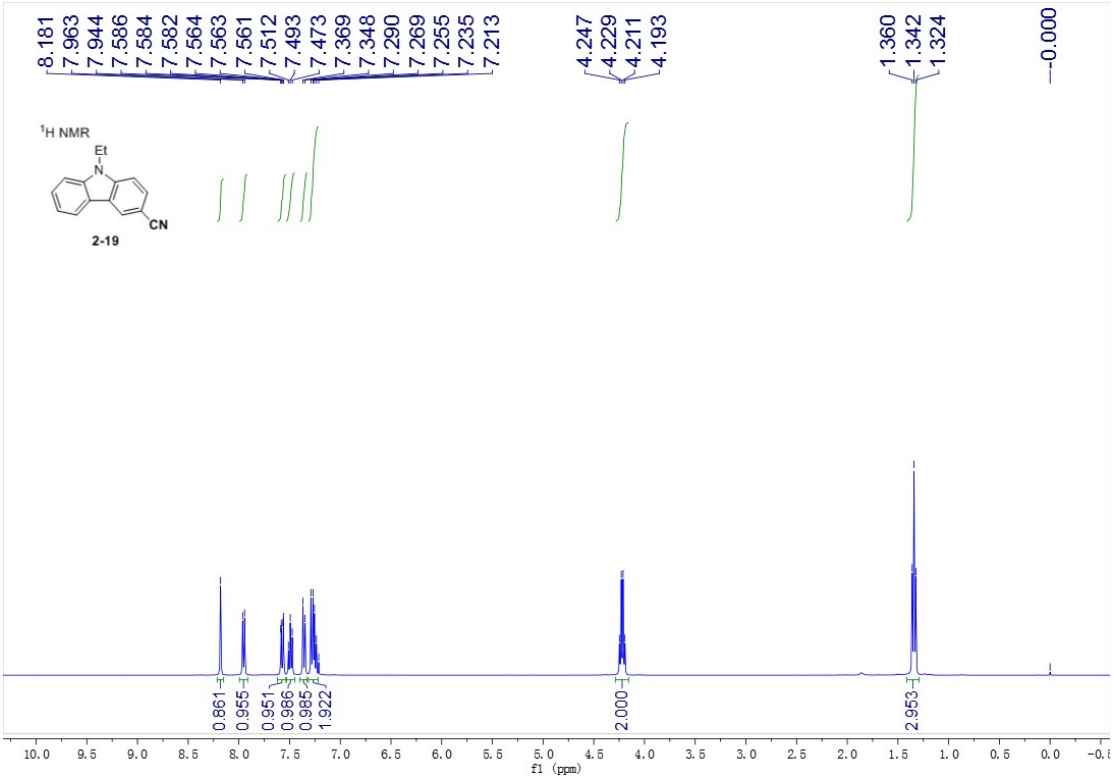

13C NMR
CN
Br
2-16
152.133
147.335
118.691
117.177
113.169
112.292
107.578
103.044
77.319
77.000
76.682
f1 (ppm)

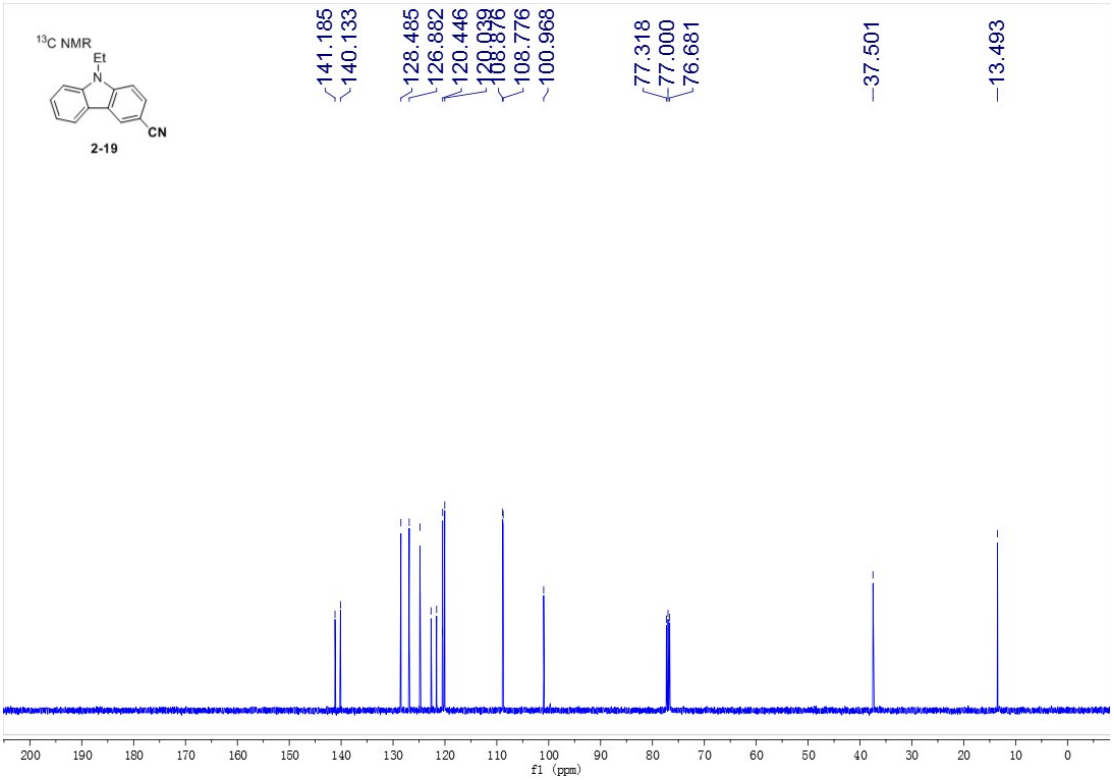

1H NMR
CN
2-17
7.134
7.132
7.128
7.117
7.112
6.920
6.897
4.332
4.327
4.323
4.318
4.314
4.295
4.290
4.285
4.281
4.275
0.000
1.885
1.000
4.381
f1 (ppm)

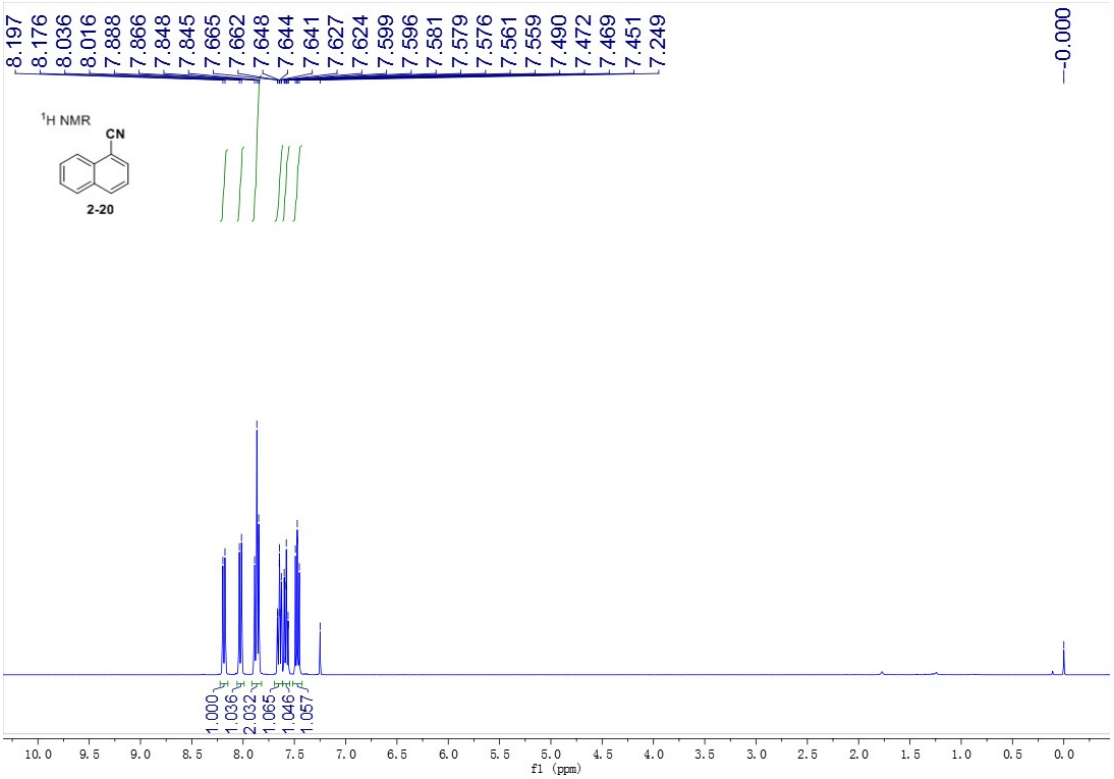

13C NMR
CN
2-17
147.638
143.684
125.752
121.088
118.781
118.132
104.265
77.318
77.000
76.683
64.470
64.001
f1 (ppm)

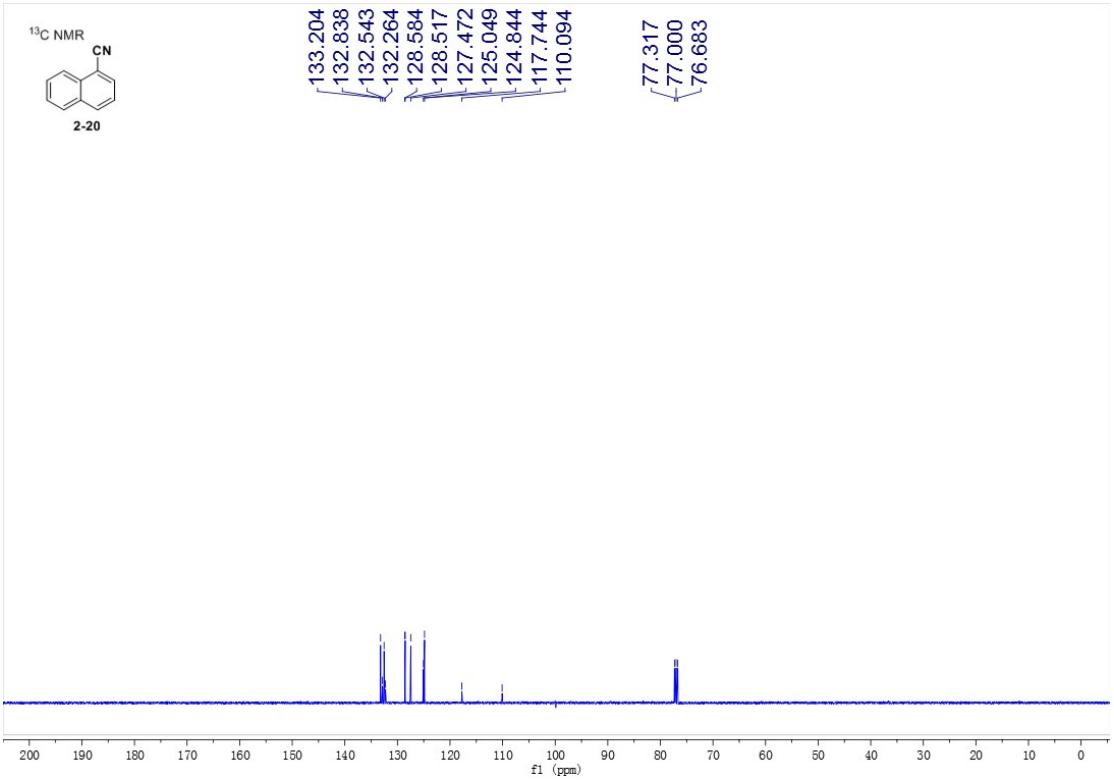

1H NMR
MeO
CN
OMe
2-18
7.290
6.749
6.746
6.744
6.652
6.647
6.641
3.804
0.000
1.756
0.917
6.000
f1 (ppm)

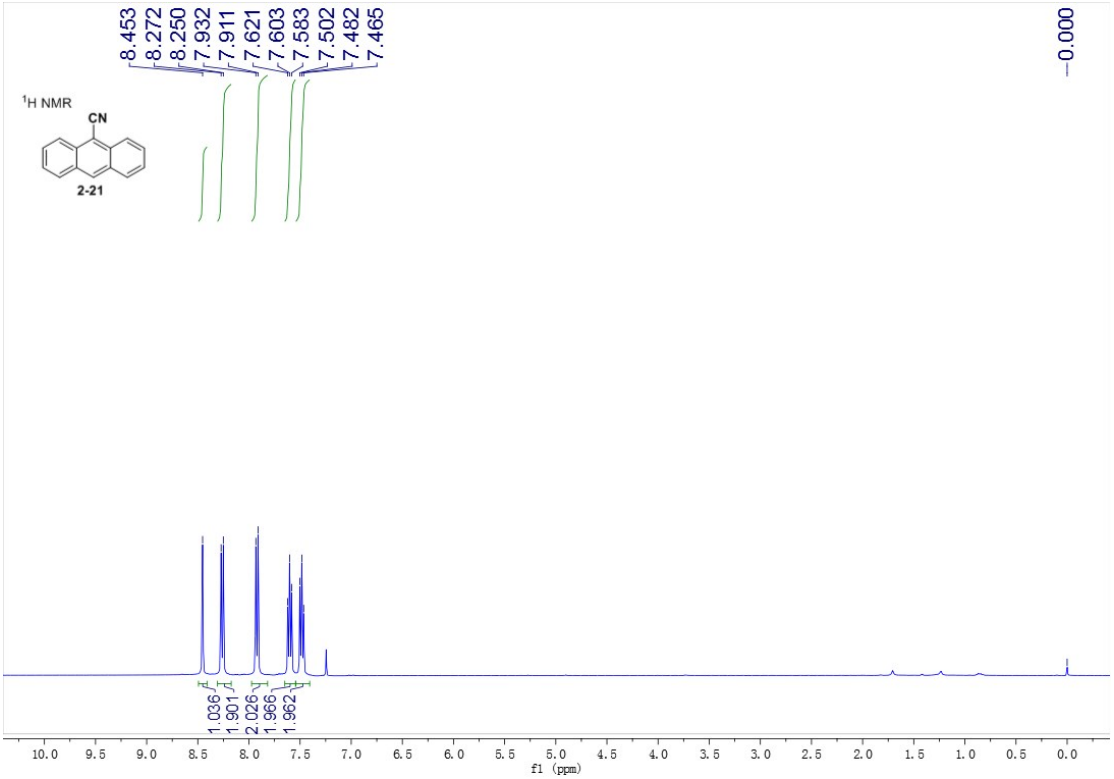

13C NMR
MeO
CN
OMe
2-18
160.833
118.584
113.205
109.712
105.401
77.319
77.000
76.682
55.489
f1 (ppm)

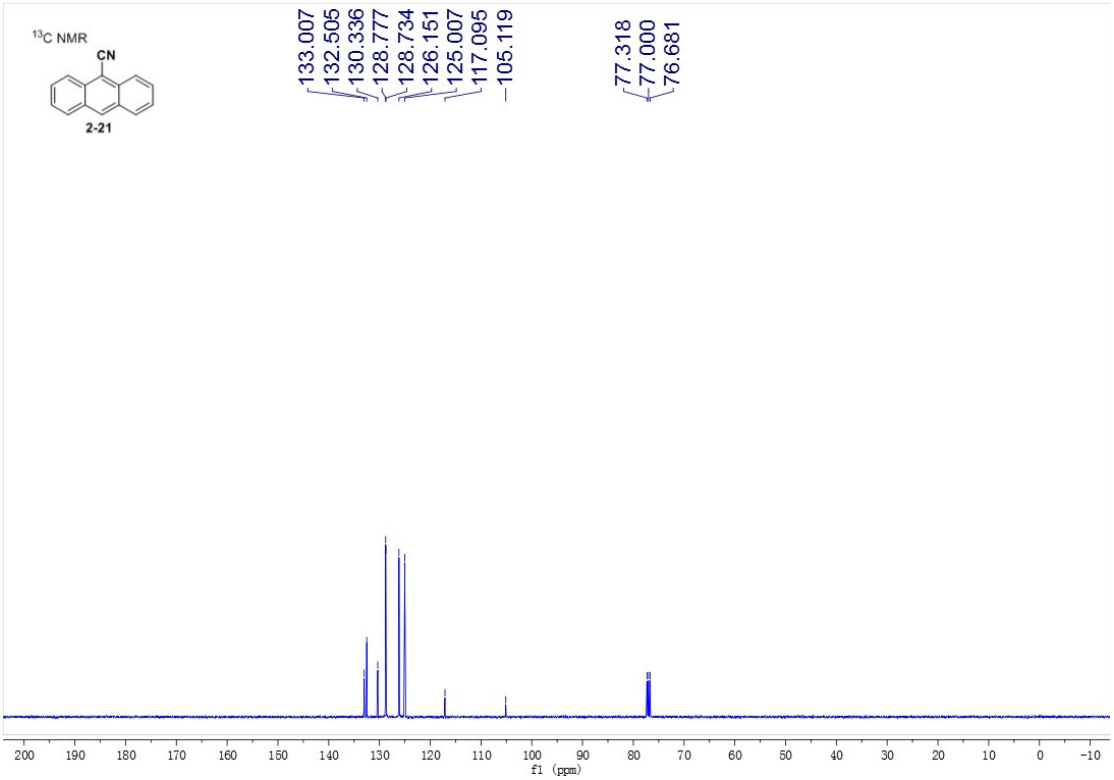

8.181
7.963
7.944
7.586
7.584
7.582
7.564
7.563
7.561
7.512
7.493
7.473
7.369
7.348
7.290
7.269
7.255
7.235
7.213
4.247
4.229
4.211
4.193
1.360
1.342
1.324
0.000
1H NMR
Et
N
CN
2-19
0.861
0.955
0.951
0.986
0.985
1.922
2.000
2.953
f1 (ppm)

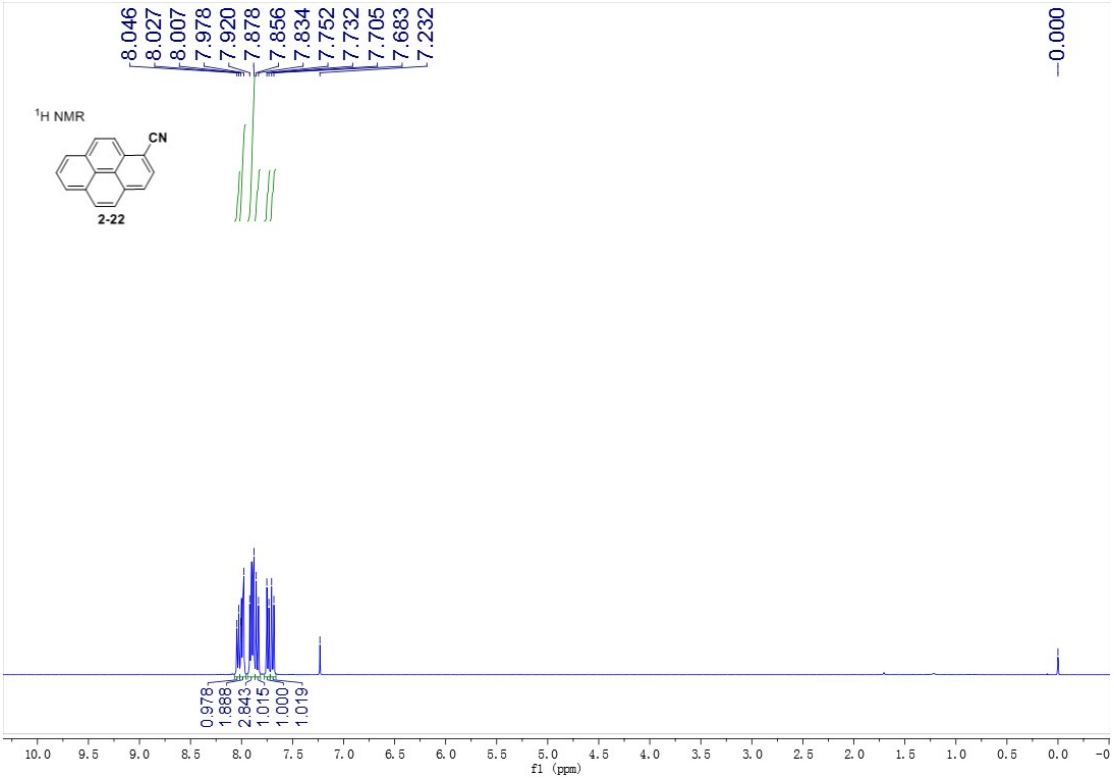

13C NMR
Et
N
CN
2-19
141.185
140.133
128.485
126.882
120.446
120.039
108.876
108.776
100.968
77.318
77.000
76.681
37.501
13.493
f1 (ppm)

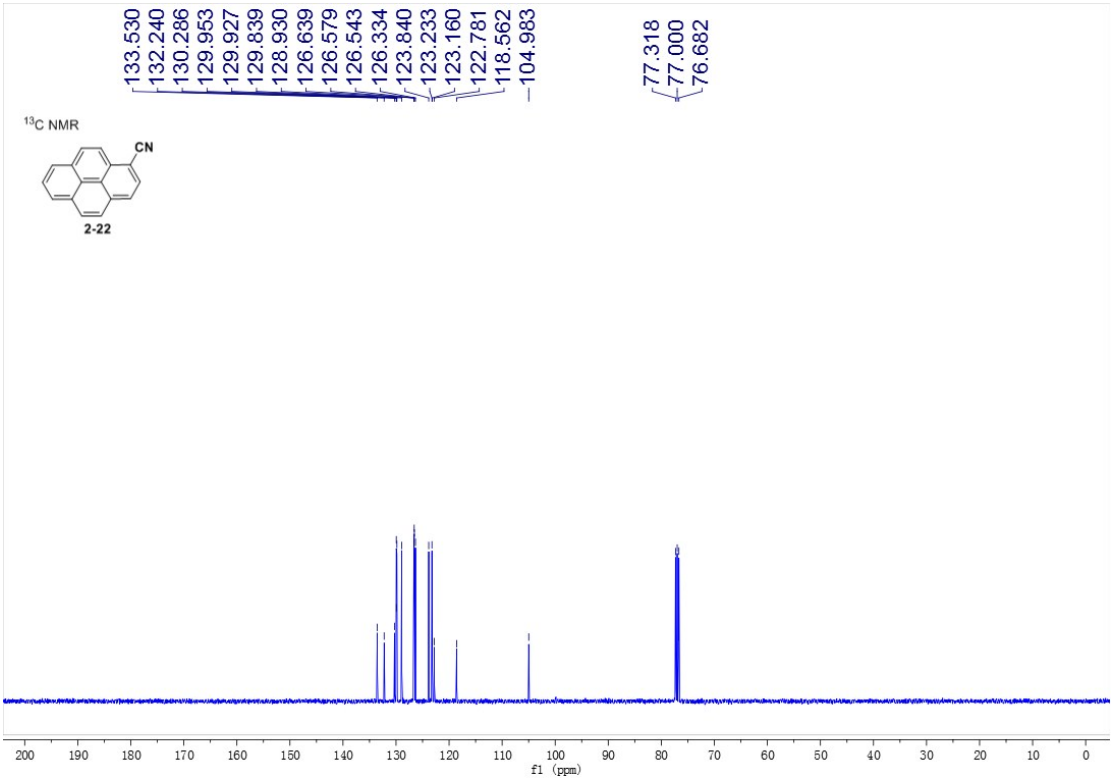

8.197
8.176
8.036
8.016
7.888
7.866
7.848
7.845
7.665
7.662
7.648
7.644
7.641
7.627
7.624
7.599
7.596
7.581
7.579
7.576
7.561
7.559
7.490
7.472
7.469
7.451
7.249
0.000
1H NMR
CN
2-20
1.000
1.036
2.032
1.065
1.046
1.057
f1 (ppm)

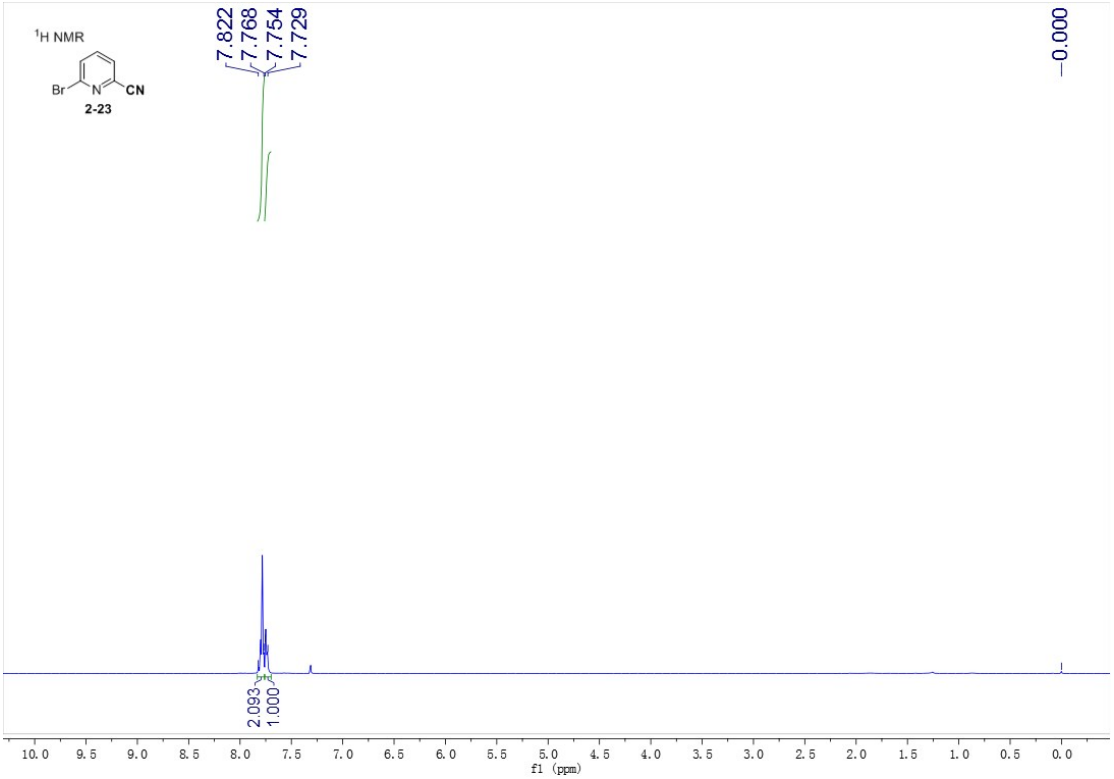

13C NMR
CN
2-20
133.204
132.838
132.543
132.264
128.584
128.517
127.472
125.049
124.844
117.744
110.094
77.317
77.000
76.683
f1 (ppm)

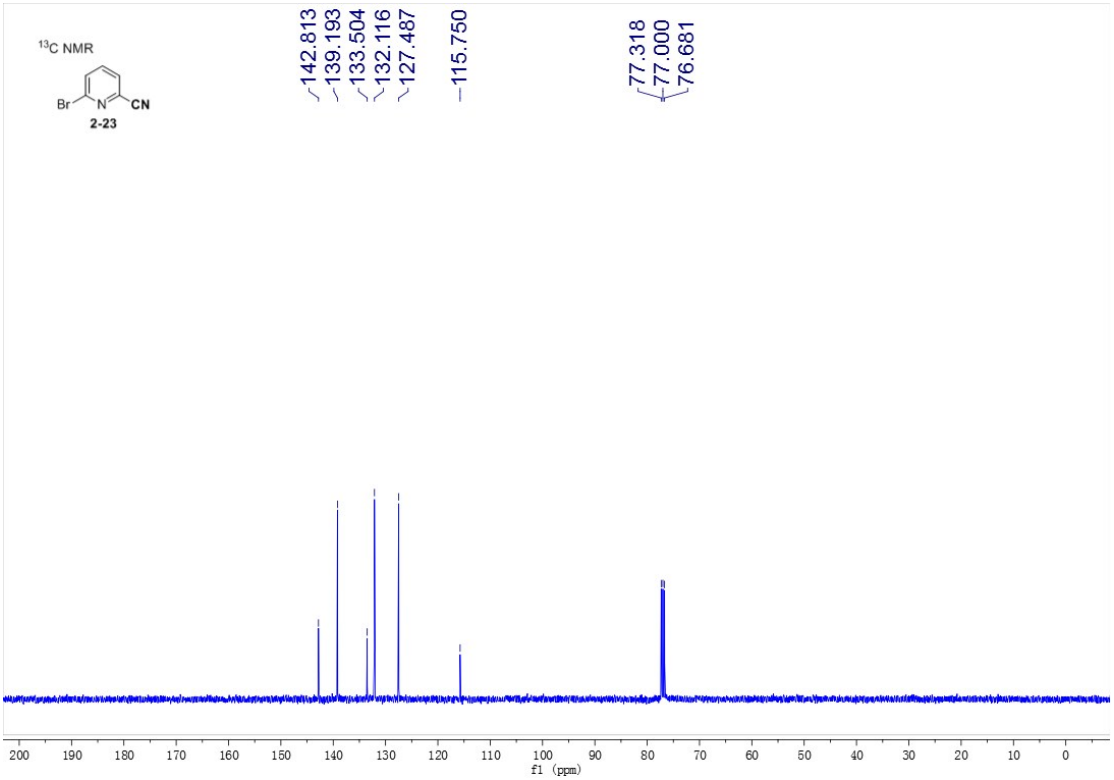

1H NMR
CN
2-21
8.453
8.272
8.250
7.932
7.911
7.621
7.603
7.583
7.502
7.482
7.465
0.000
1.036
1.901
2.026
1.966
1.962
f1 (ppm)

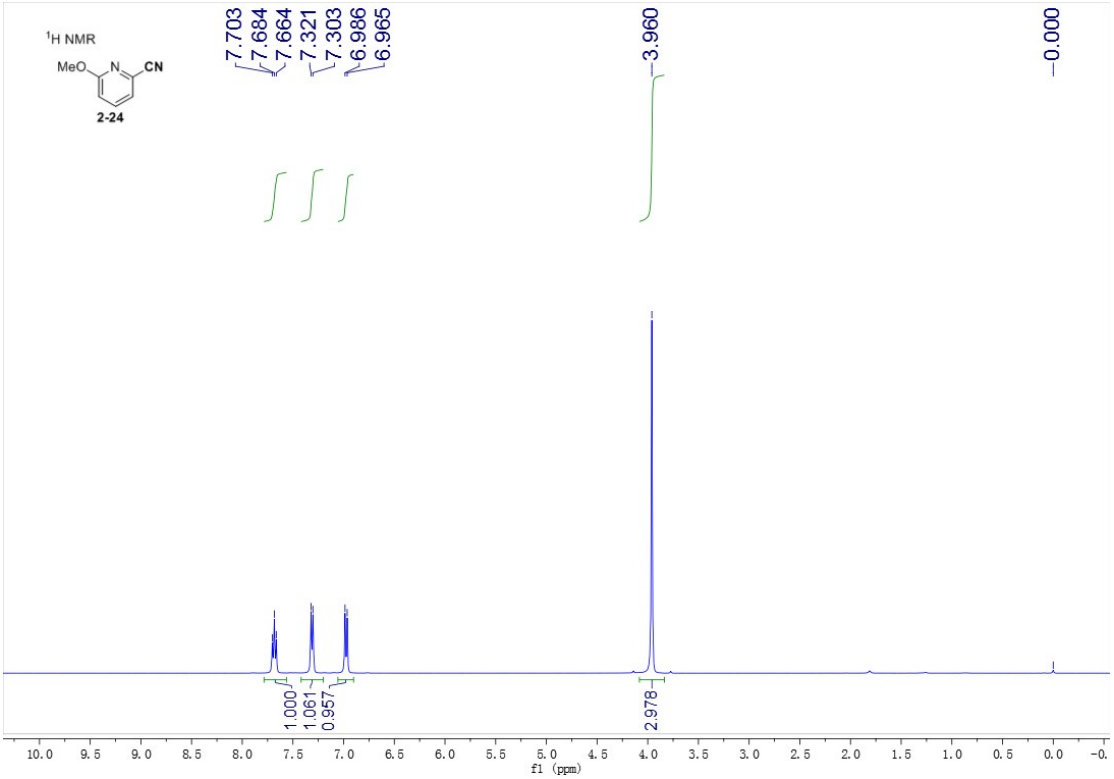

13C NMR
CN
2-21
133.007
132.505
130.336
128.777
128.734
126.151
125.007
117.095
105.119
77.318
77.000
76.681
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

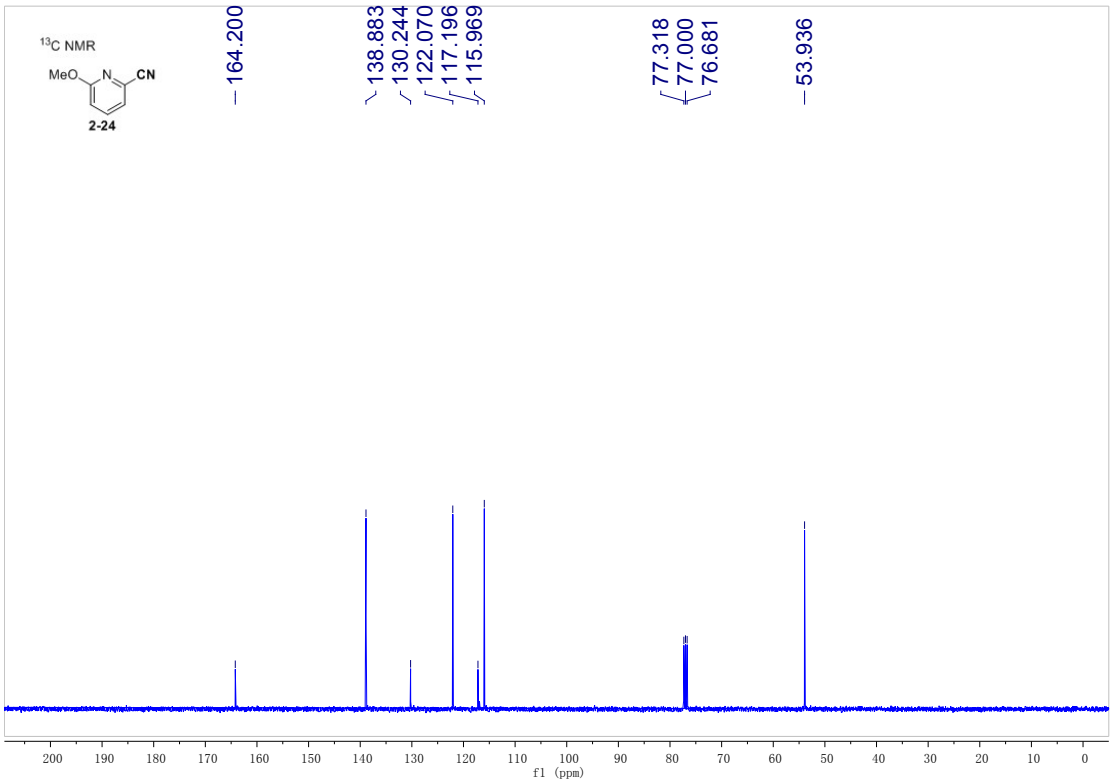

8.046
8.027
8.007
7.978
7.920
7.878
7.856
7.834
7.752
7.732
7.705
7.683
7.232
0.000
1H NMR
CN
2-22
0.978
1.888
2.843
1.015
1.000
1.019
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

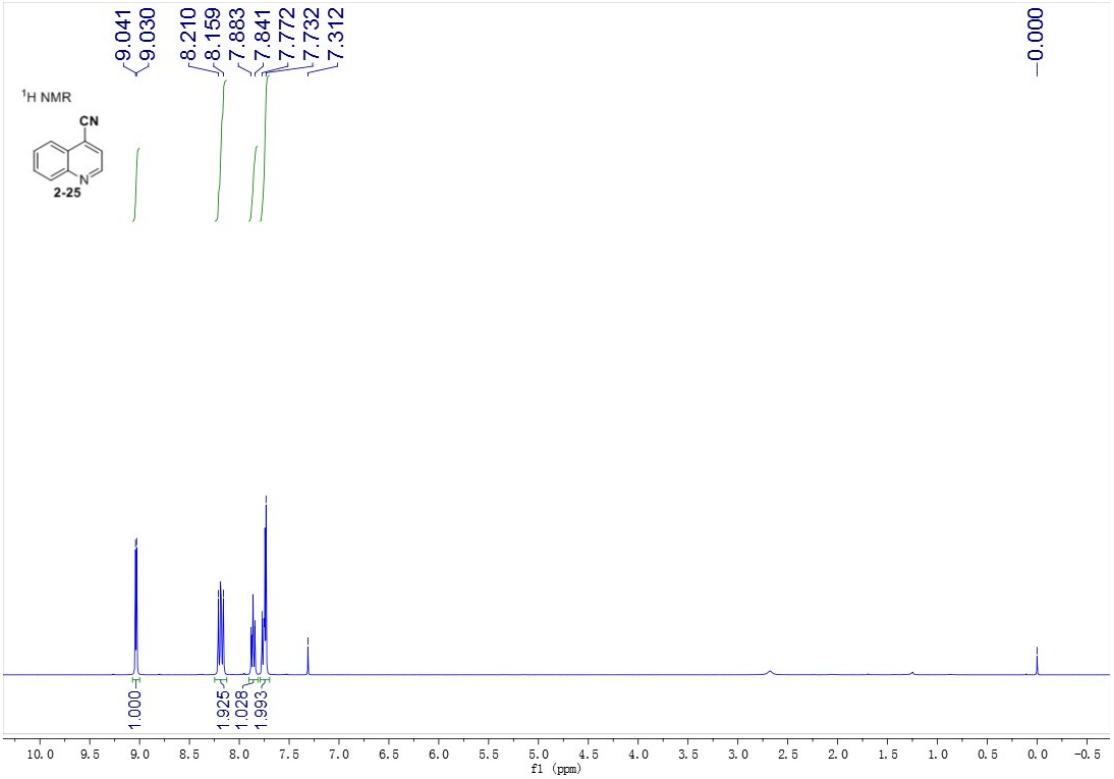

133.530
132.240
130.286
129.953
129.927
129.839
128.930
126.639
126.579
126.543
126.334
123.840
123.233
123.160
122.781
118.562
104.983
77.318
77.000
76.682
13C NMR
CN
2-22
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

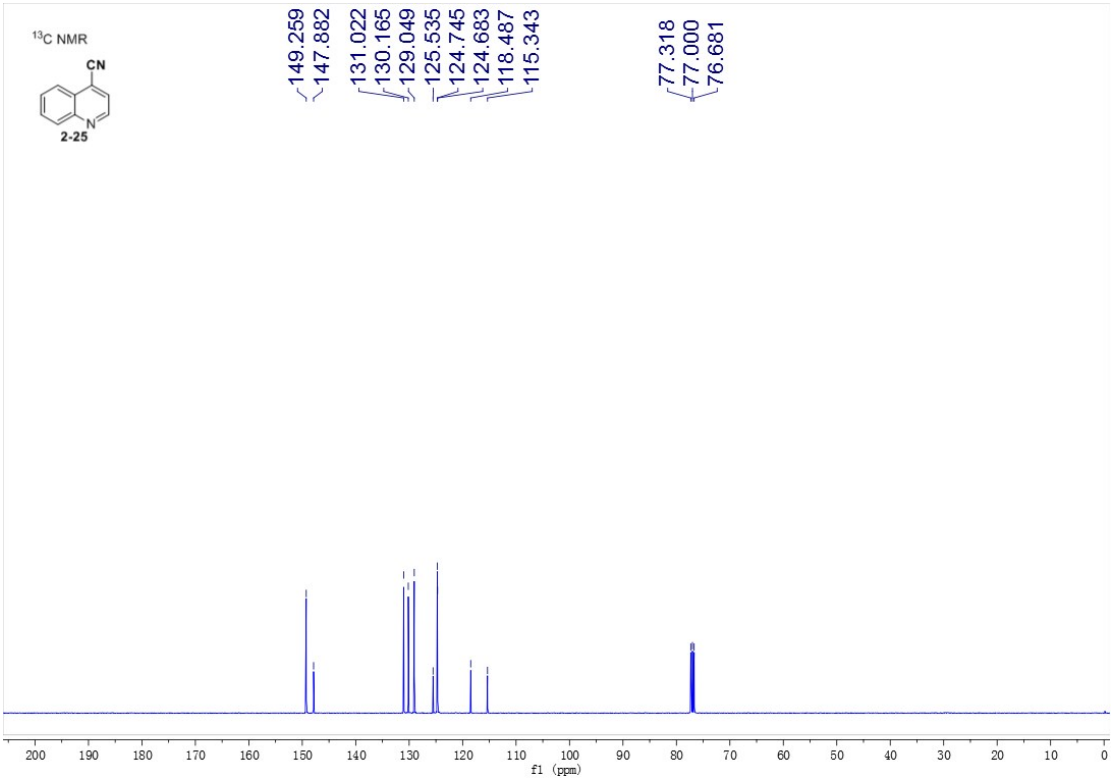

1H NMR
Br
N
CN
2-23
7.822
7.768
7.754
7.729
0.000
2.093
1.000
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

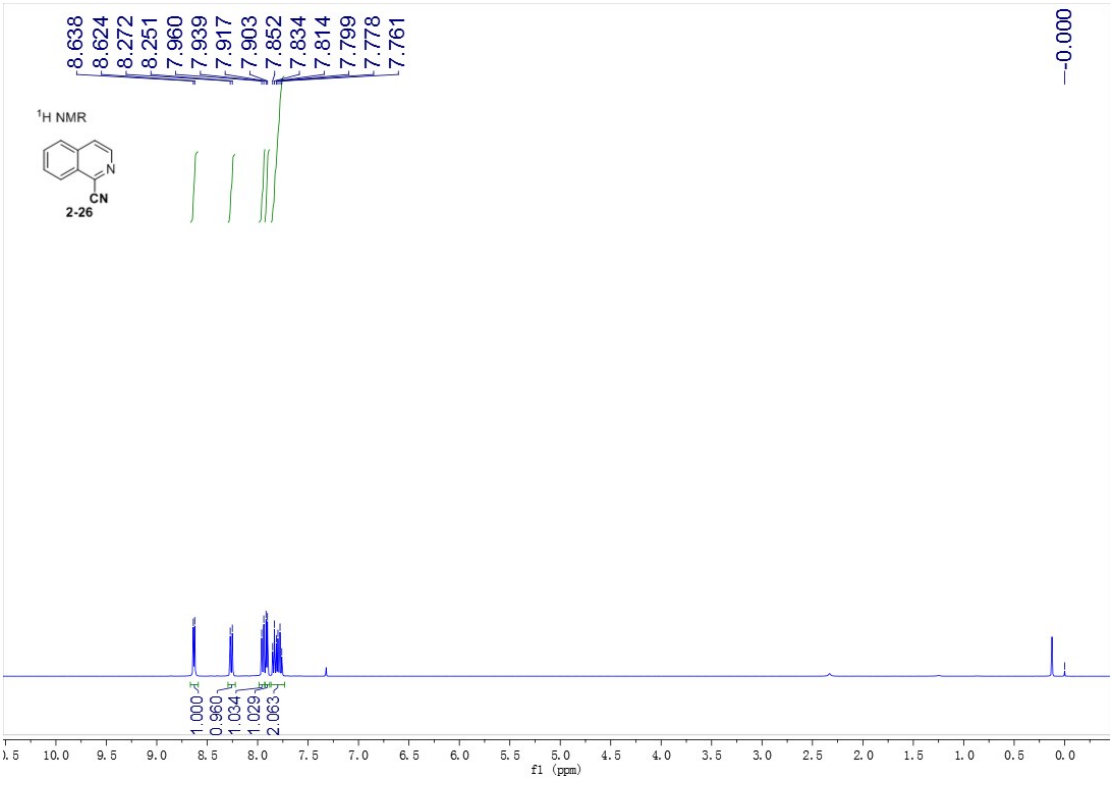

13C NMR
Br
N
CN
2-23
142.813
139.193
133.504
132.116
127.487
115.750
77.318
77.000
76.681
f1 (ppm)

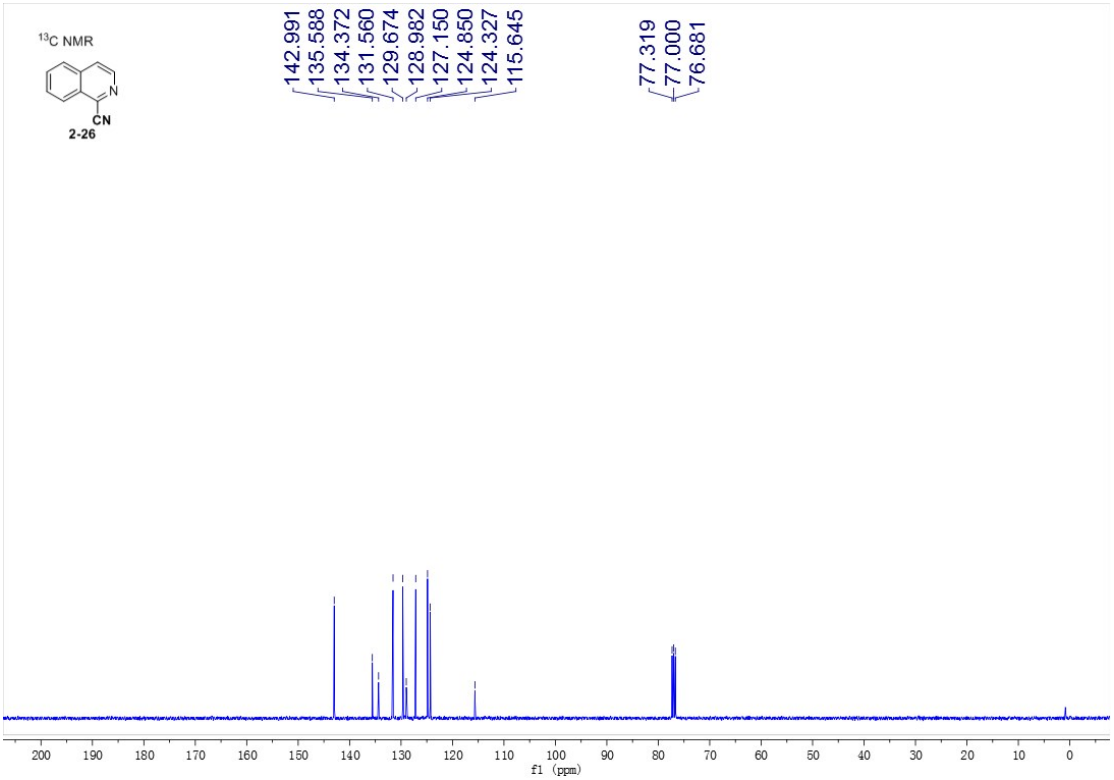

1H NMR
MeO
N
CN
2-24
7.703
7.684
7.664
7.321
7.303
6.986
6.965
3.960
0.000
1.000
1.061
0.957
2.978
f1 (ppm)

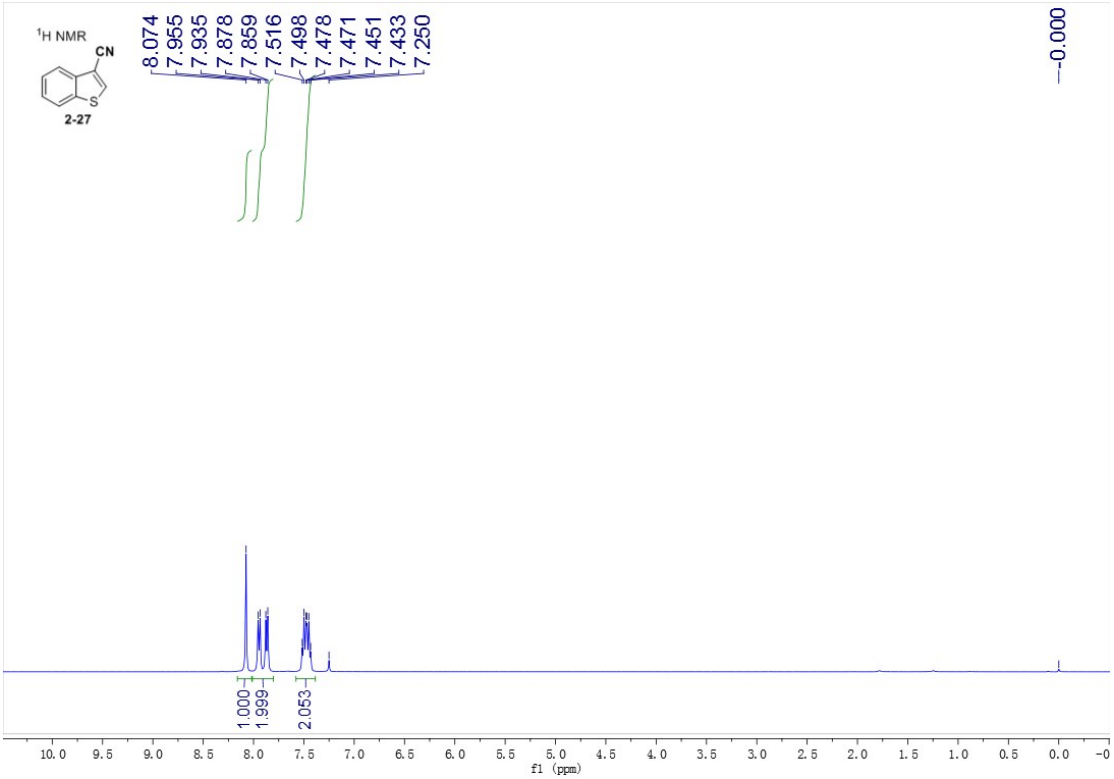

13C NMR
MeO
N
CN
2-24
164.200
138.883
130.244
122.070
117.196
115.969
77.318
77.000
76.681
53.936
f1 (ppm)

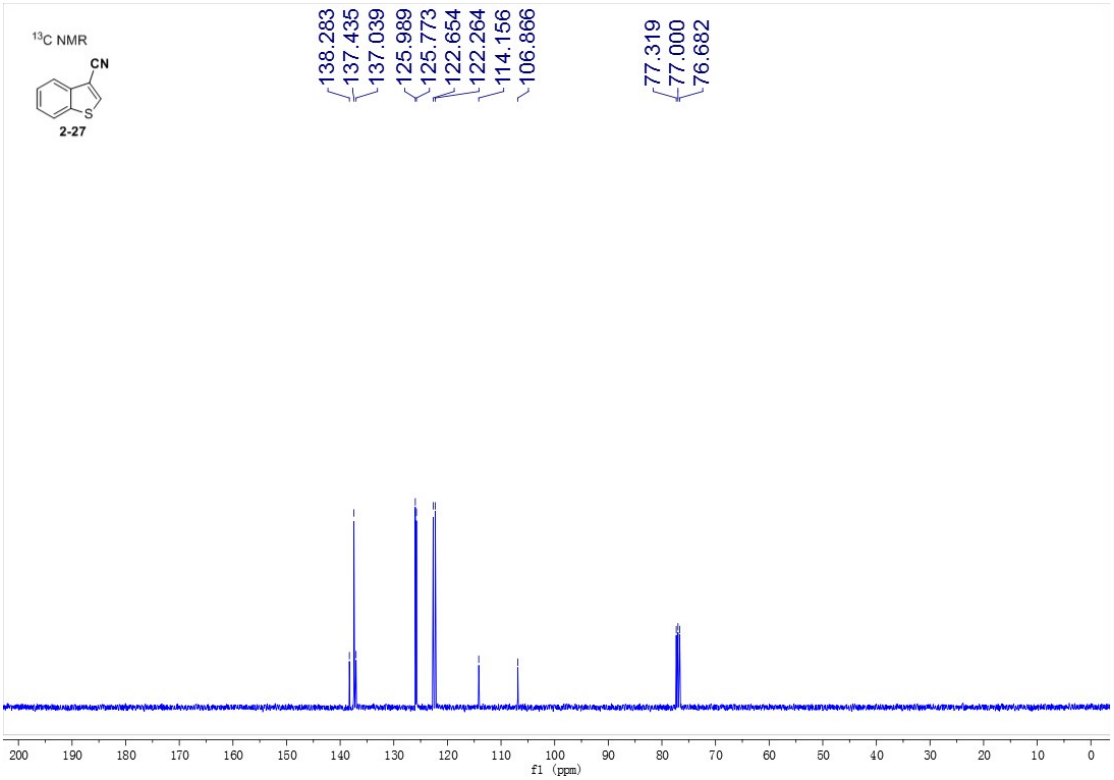

1H NMR
CN
N
2-25
9.041
9.030
8.210
8.159
7.883
7.841
7.772
7.732
7.312
0.000
1.000
1.925
1.028
1.993
f1 (ppm)

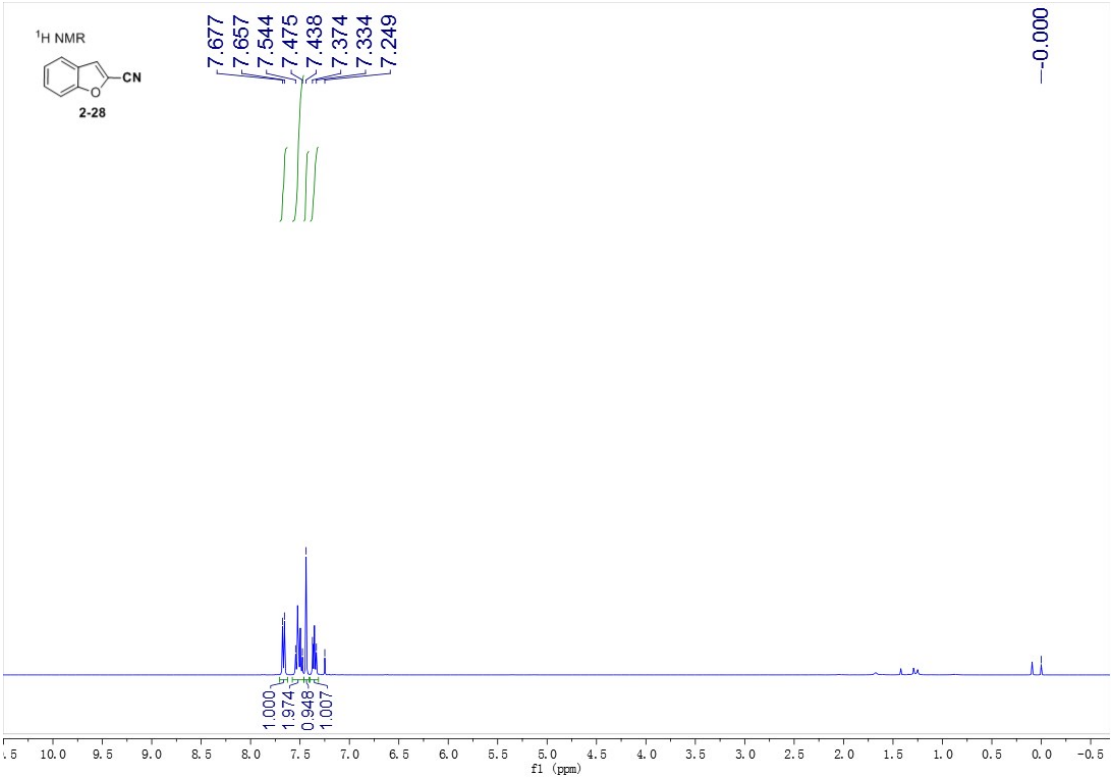

13C NMR
CN
N
2-25
149.259
147.882
131.022
130.165
129.049
125.535
124.745
124.683
118.487
115.343
77.318
77.000
76.681
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

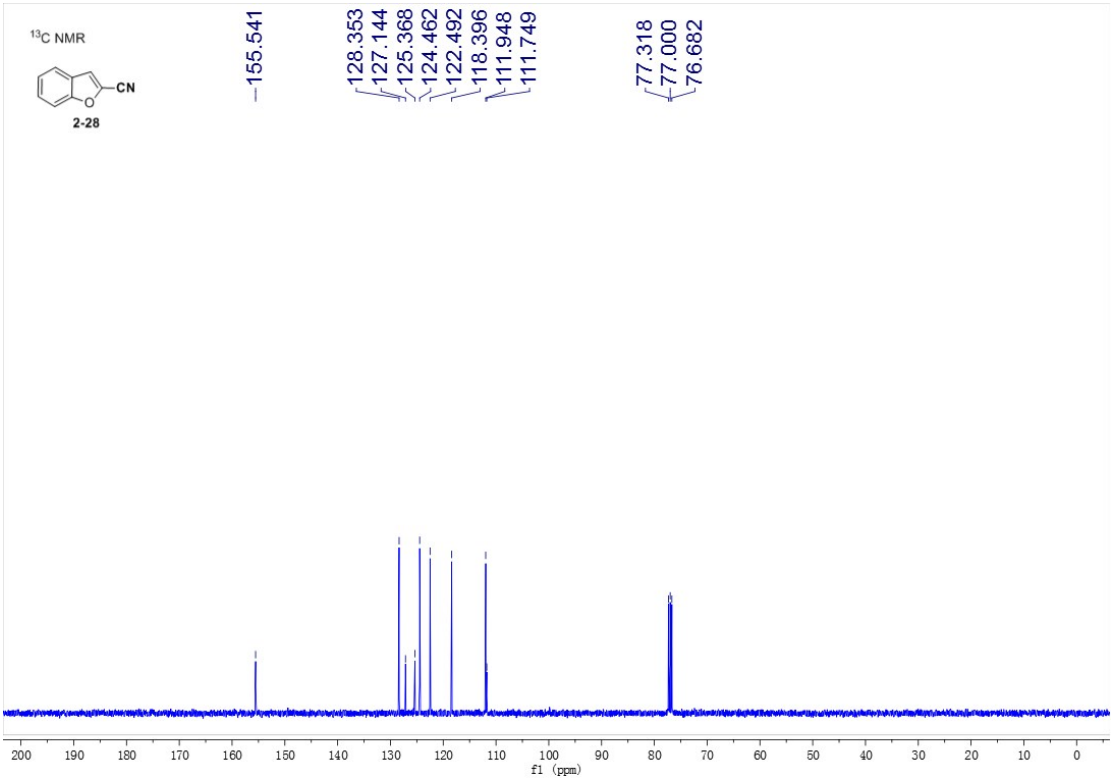

8.638
8.624
8.272
8.251
7.960
7.939
7.917
7.903
7.852
7.834
7.814
7.799
7.778
7.761
0.000
1H NMR
N
CN
2-26
1.000
0.960
1.034
1.029
2.063
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

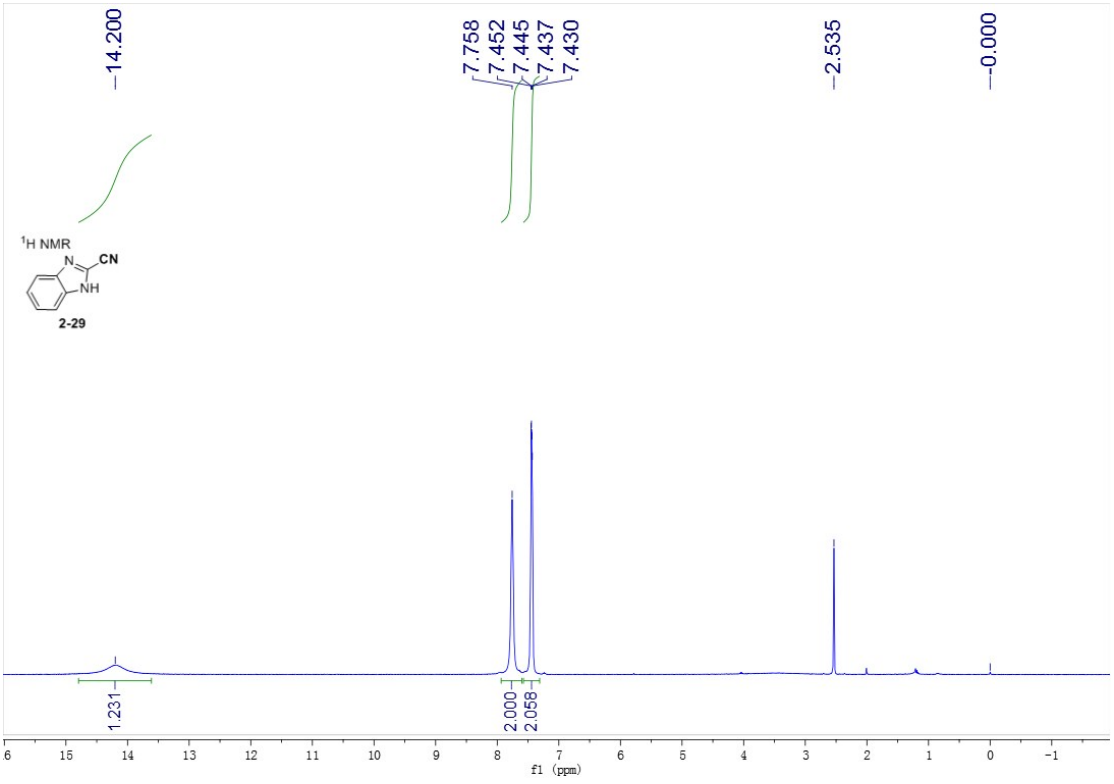

13C NMR
CN
2-26
142.991
135.588
134.372
131.560
129.674
128.982
127.150
124.850
124.327
115.645
77.319
77.000
76.681
f1 (ppm)

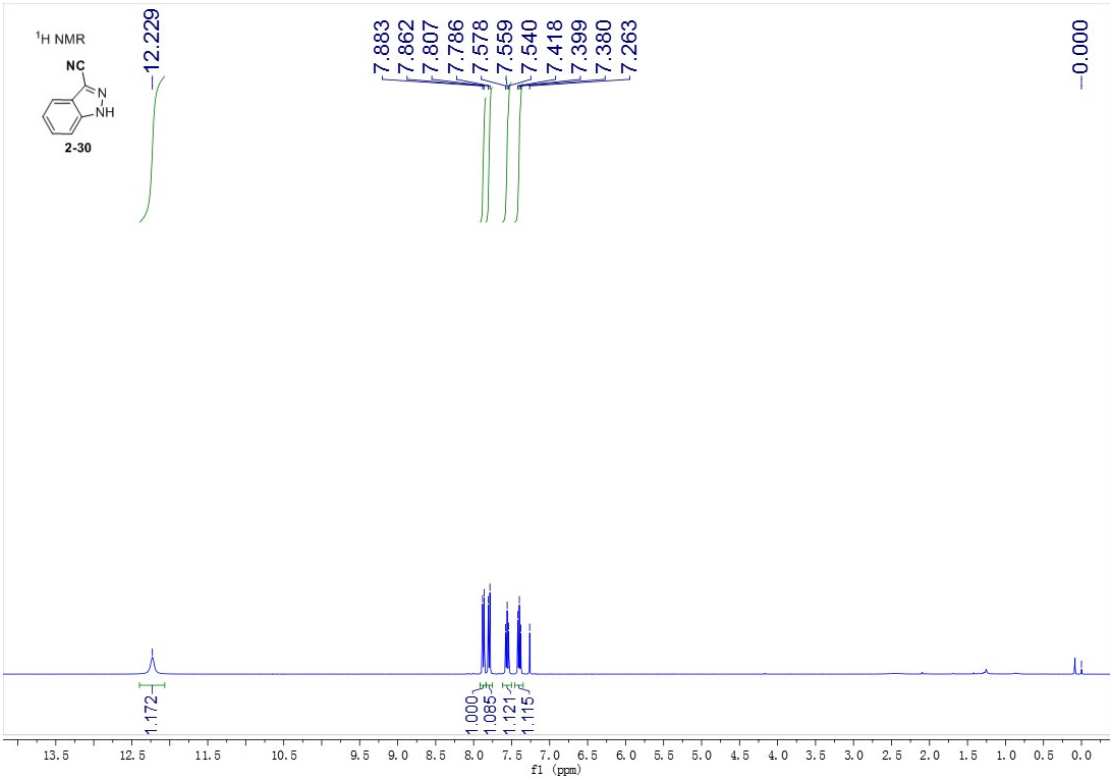

1H NMR
CN
S
2-27
8.074
7.955
7.935
7.878
7.859
7.516
7.498
7.478
7.471
7.451
7.433
7.250
-0.000
1.000
1.999
2.053
f1 (ppm)

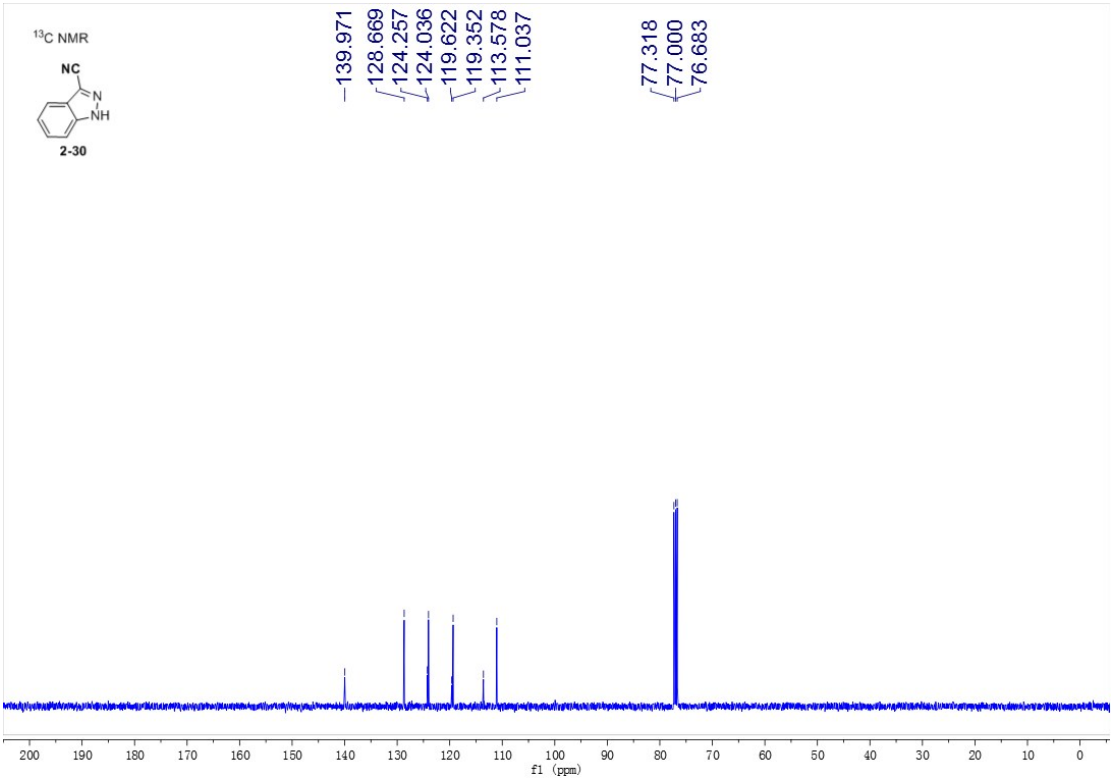

13C NMR
CN
S
2-27
138.283
137.435
137.039
125.989
125.773
122.654
122.264
114.156
106.866
77.319
77.000
76.682
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

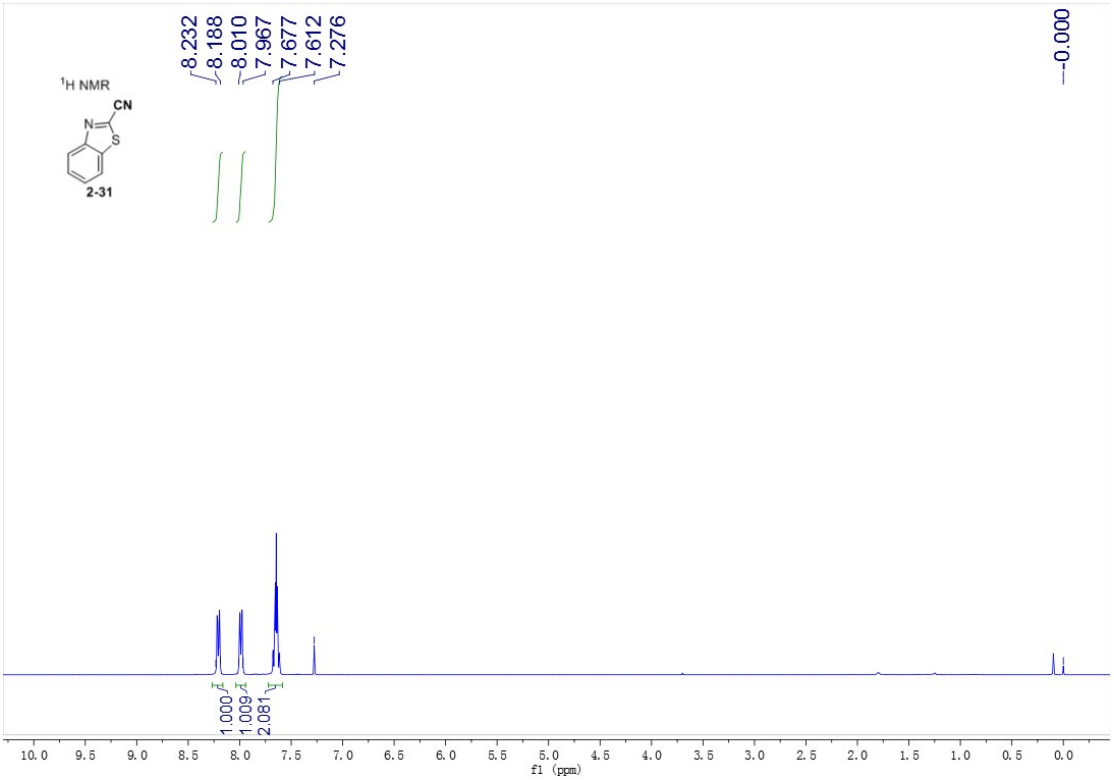

1H NMR
CN
O
2-28
7.677
7.657
7.544
7.475
7.438
7.374
7.334
7.249
-0.000
1.000
1.974
0.948
1.007
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

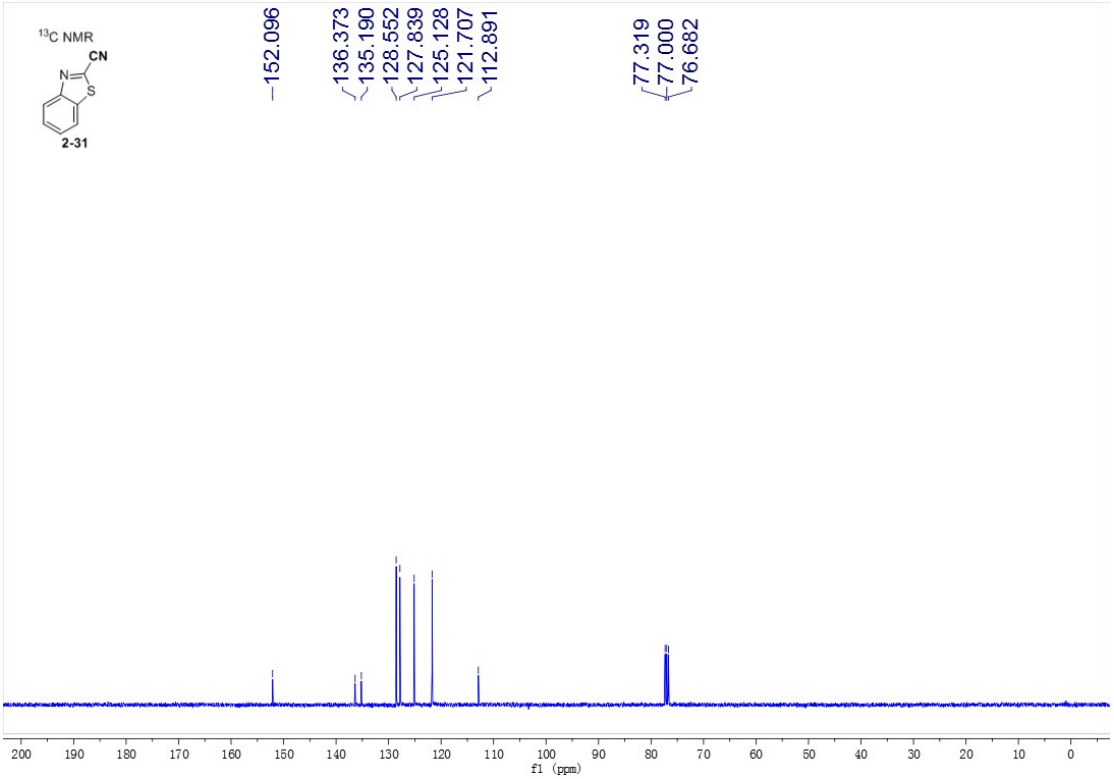

13C NMR
CN
2-28
155.541
128.353
127.144
125.368
124.462
122.492
118.396
111.948
111.749
77.318
77.000
76.682
f1 (ppm)

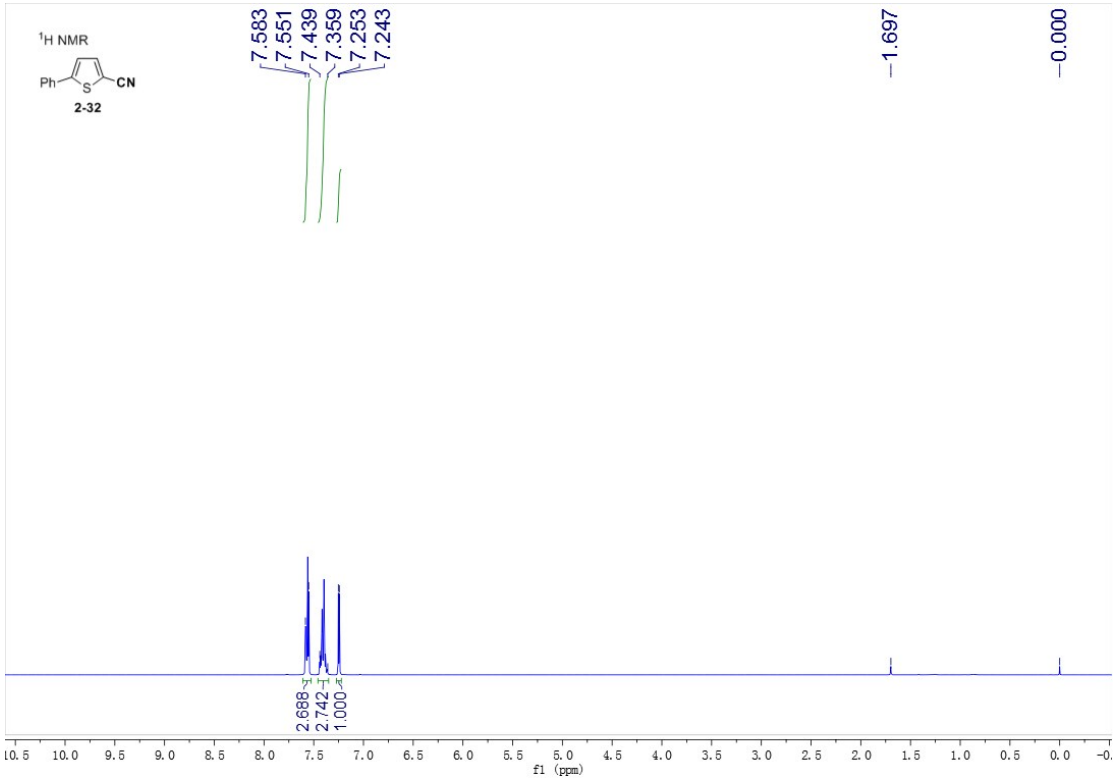

14.200
7.758
7.452
7.445
7.437
7.430
2.535
0.000
1H NMR
CN
NH
2-29
1.231
2.000
2.058
f1 (ppm)

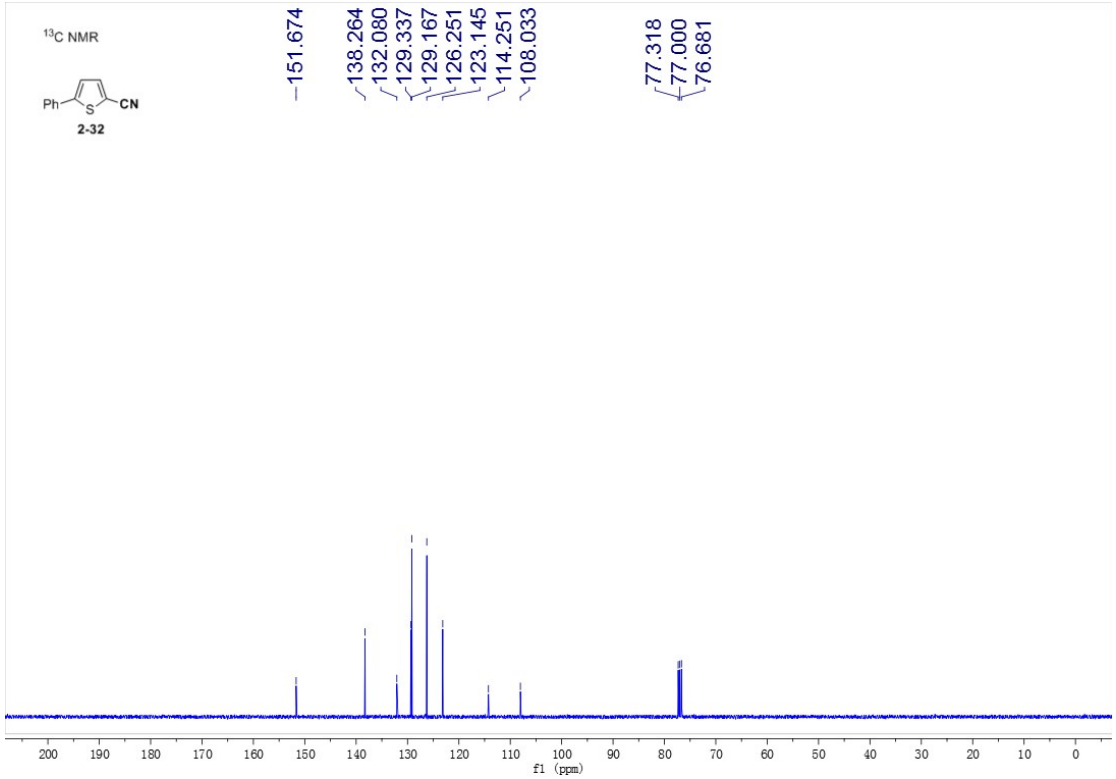

1H NMR
NC
N
NH
2-30
12.229
7.883
7.862
7.807
7.786
7.578
7.559
7.540
7.418
7.399
7.380
7.263
0.000
1.172
1.000
1.085
1.121
1.115
f1 (ppm)

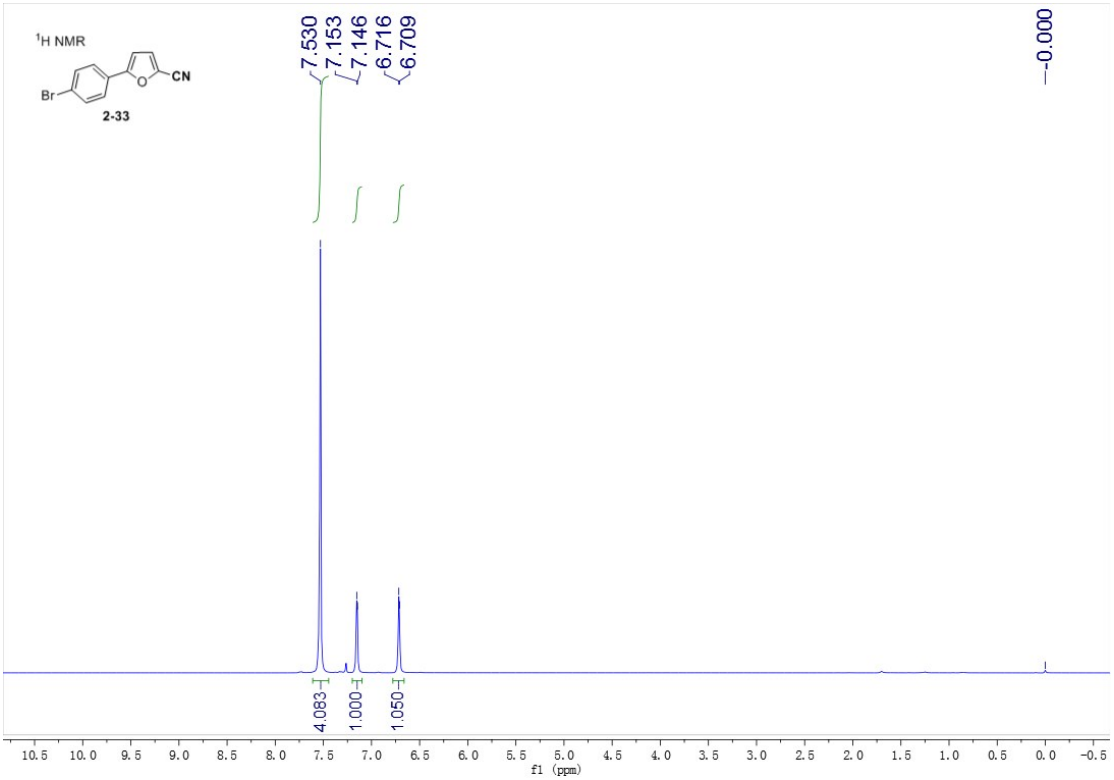

13C NMR
NC
N
NH
2-30
139.971
128.669
124.257
124.036
119.622
119.352
113.578
111.037
77.318
77.000
76.683
f1 (ppm)

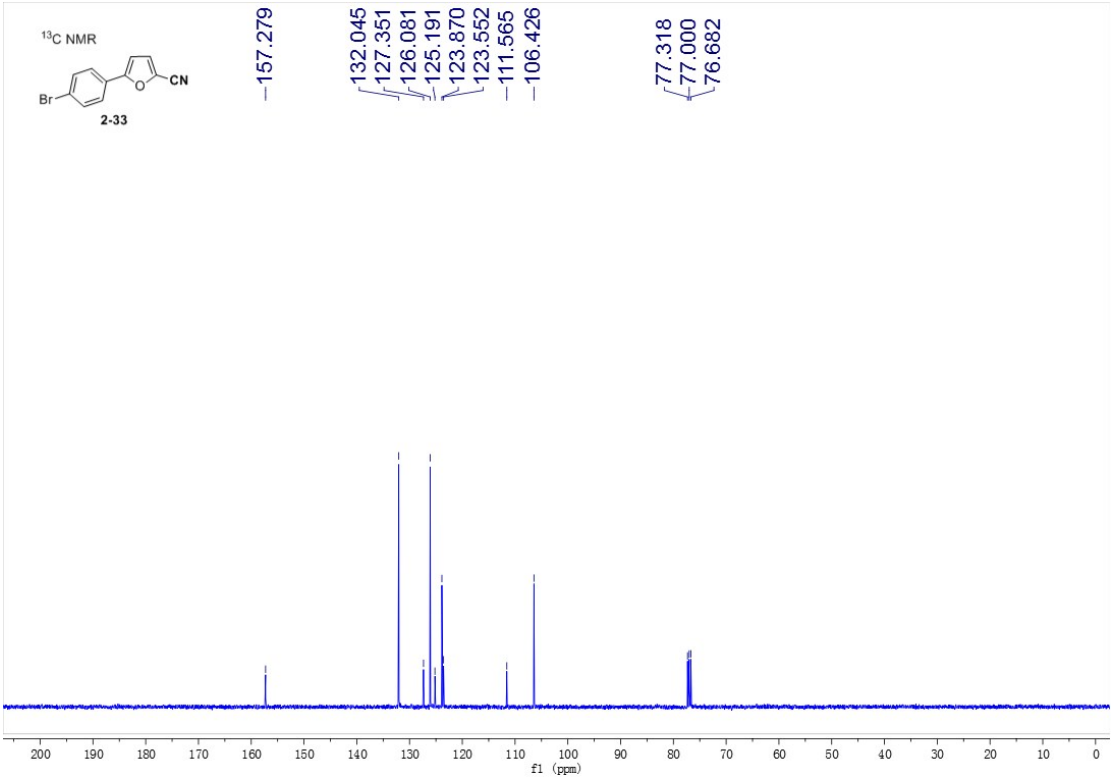

^{1}H NMR
CN
N
S
2-31
8.232
8.188
8.010
7.967
7.677
7.612
7.276
0.000
1.000
1.009
2.081
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

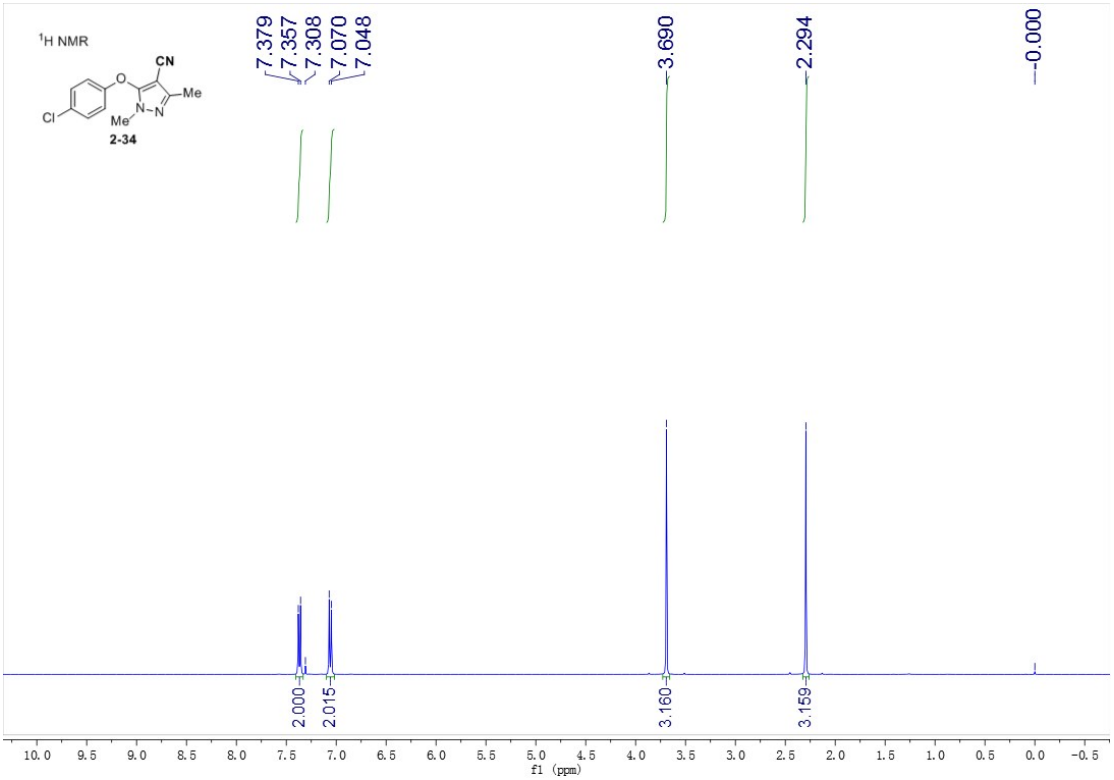

^{13}C NMR
CN
N
S
2-31
152.096
136.373
135.190
128.552
127.839
125.128
121.707
112.891
77.319
77.000
76.682
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

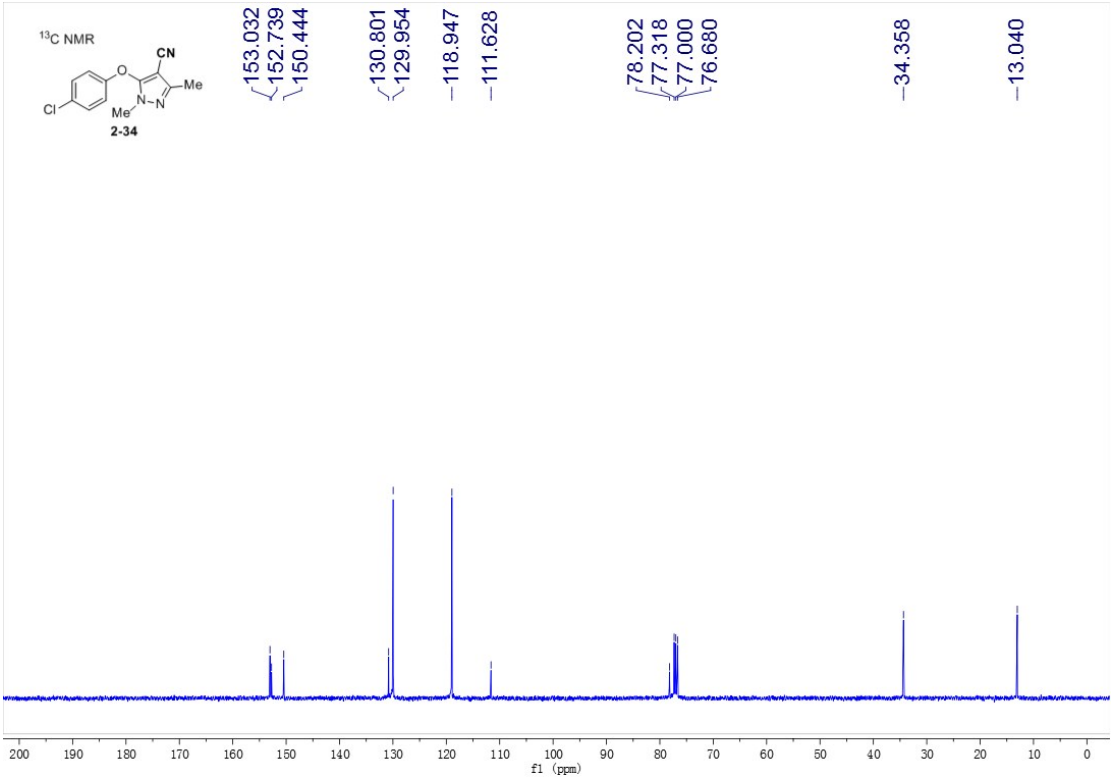

1H NMR
Ph
S
CN
2-32
7.583
7.551
7.439
7.359
7.253
7.243
1.697
0.000
2.688
2.742
1.000
f1 (ppm)

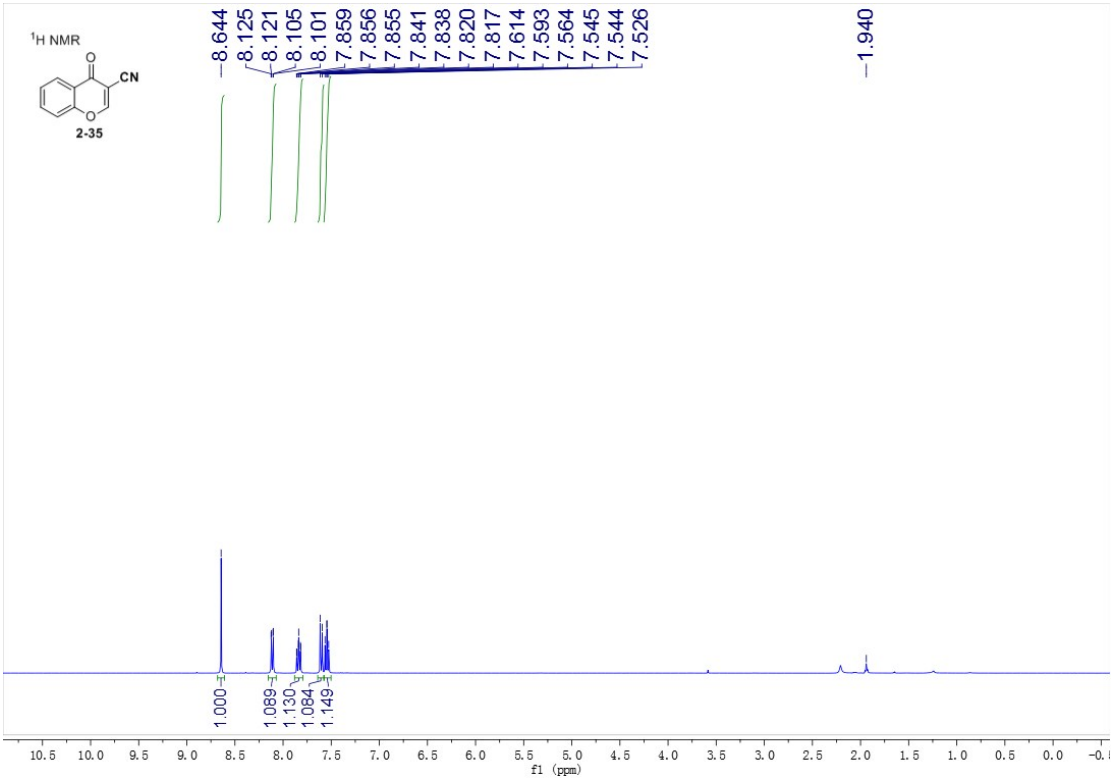

13C NMR
Ph
S
CN
2-32
151.674
138.264
132.080
129.337
129.167
126.251
123.145
114.251
108.033
77.318
77.000
76.681
f1 (ppm)

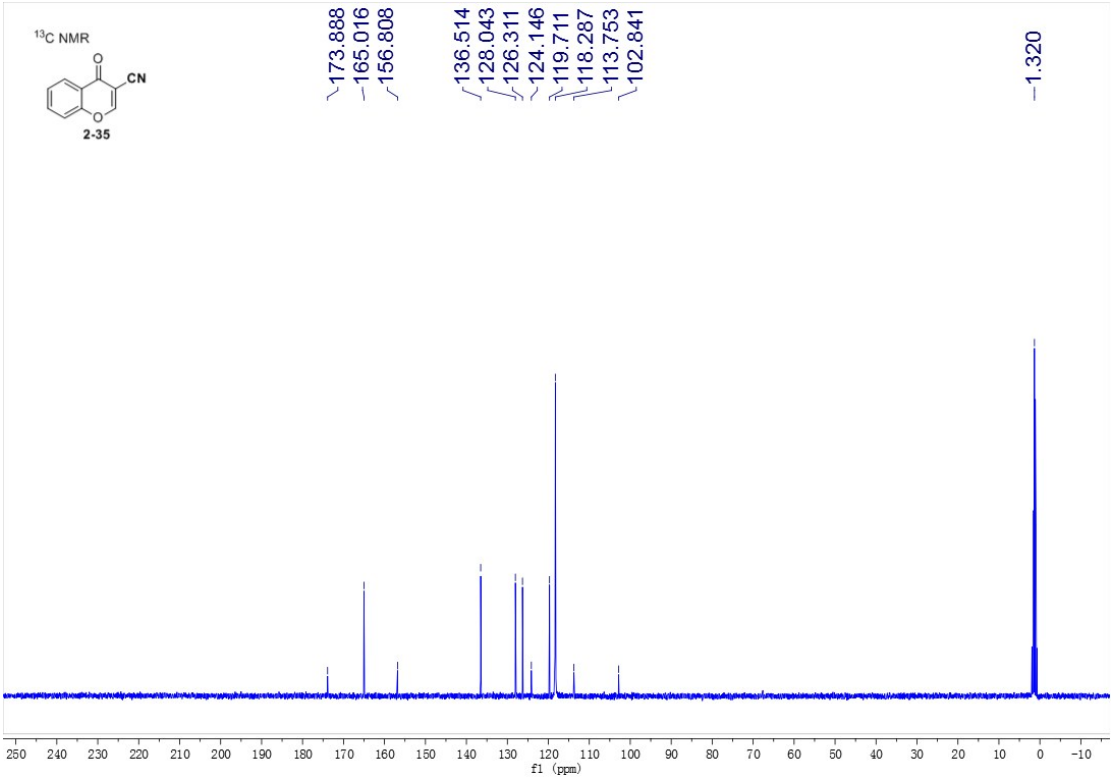

^{1}H NMR
Br
CN
2-33
7.530
7.153
7.146
6.716
6.709
0.000
4.083
1.000
1.050
f1 (ppm)

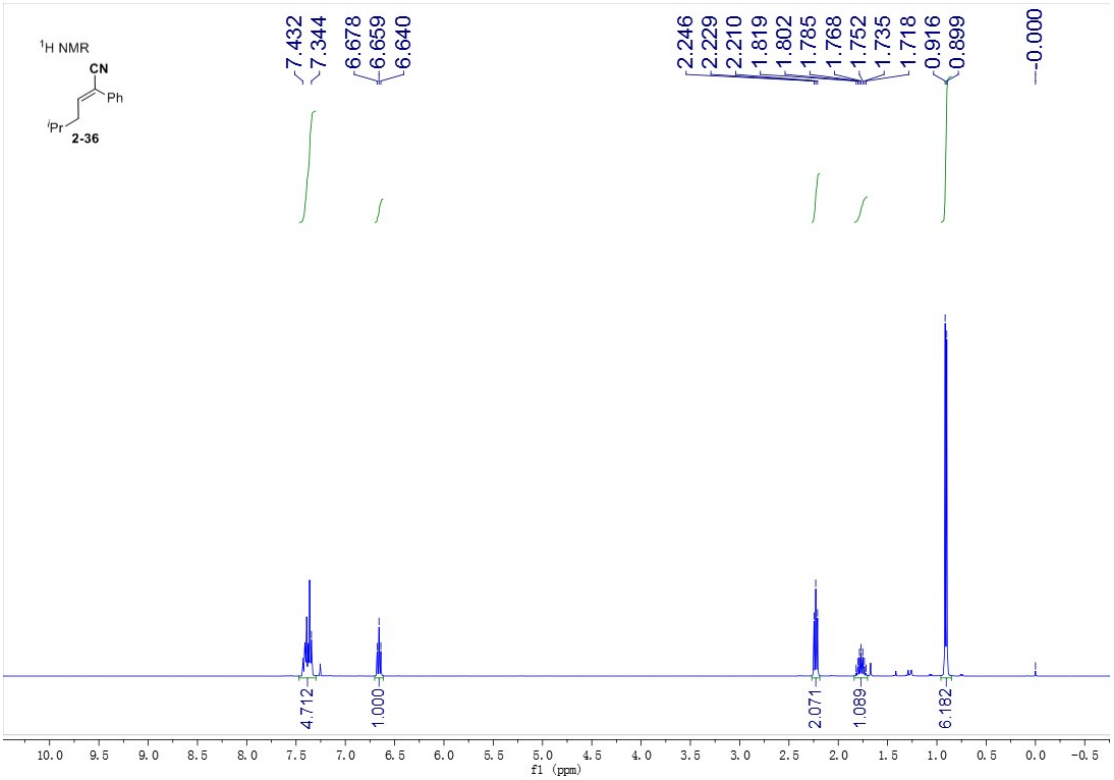

^{13}C NMR
Br
CN
2-33
157.279
132.045
127.351
126.081
125.191
123.870
123.552
111.565
106.426
77.318
77.000
76.682
f1 (ppm)

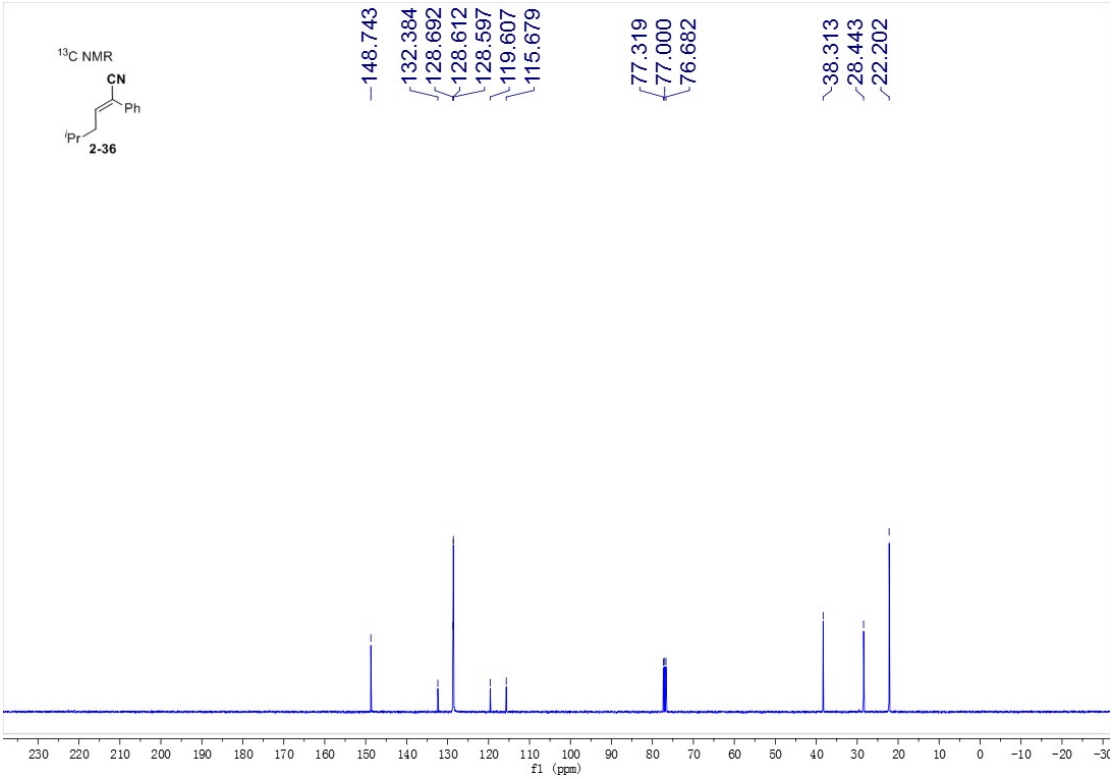

1H NMR
2-34
7.379
7.357
7.308
7.070
7.048
3.690
2.294
0.000
2.000
2.015
3.160
3.159
f1 (ppm)

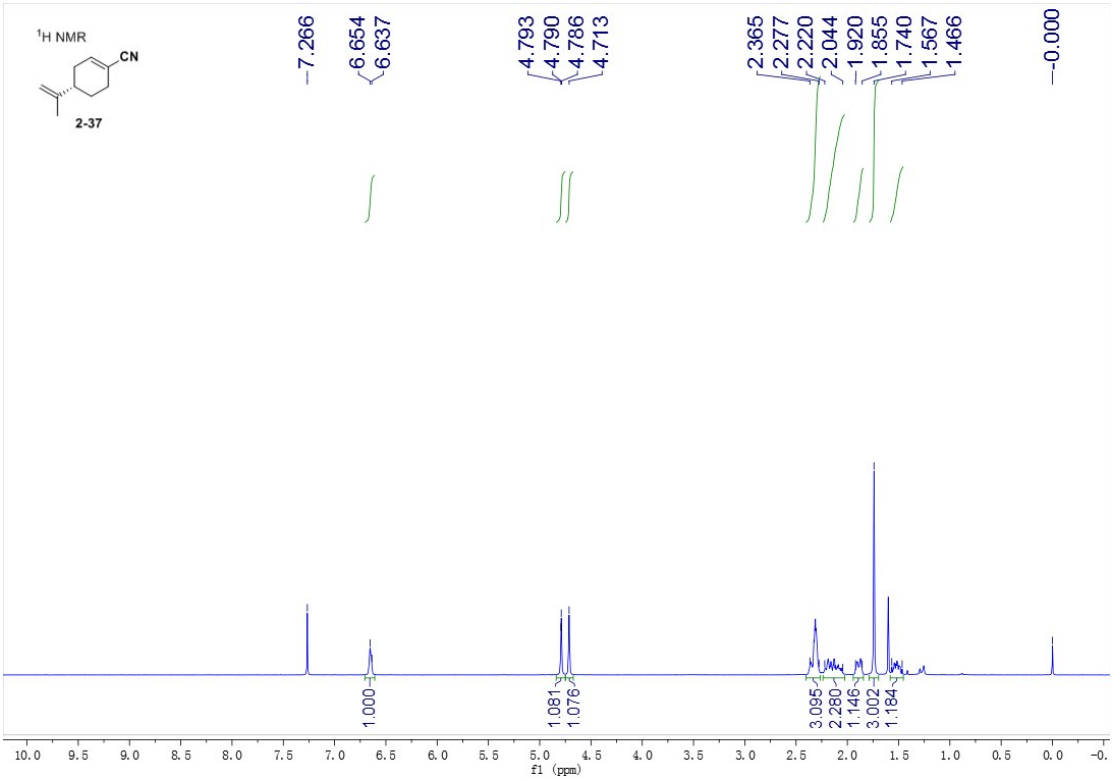

13C NMR
2-34
153.032
152.739
150.444
130.801
129.954
118.947
111.628
78.202
77.318
77.000
76.680
34.358
13.040
f1 (ppm)

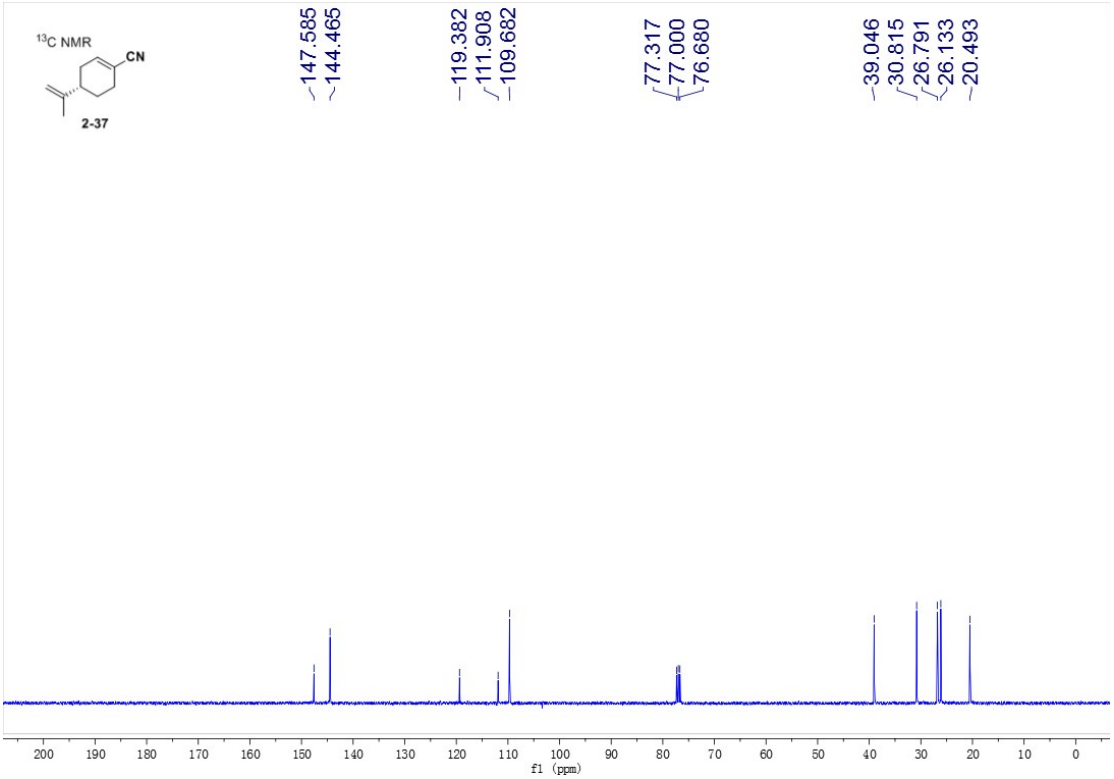

^{1}H NMR
2-35
8.644
8.125
8.121
8.105
8.101
7.859
7.856
7.855
7.841
7.838
7.820
7.817
7.614
7.593
7.564
7.545
7.544
7.526
1.940
1.000
1.089
1.130
1.084
1.149
f1 (ppm)

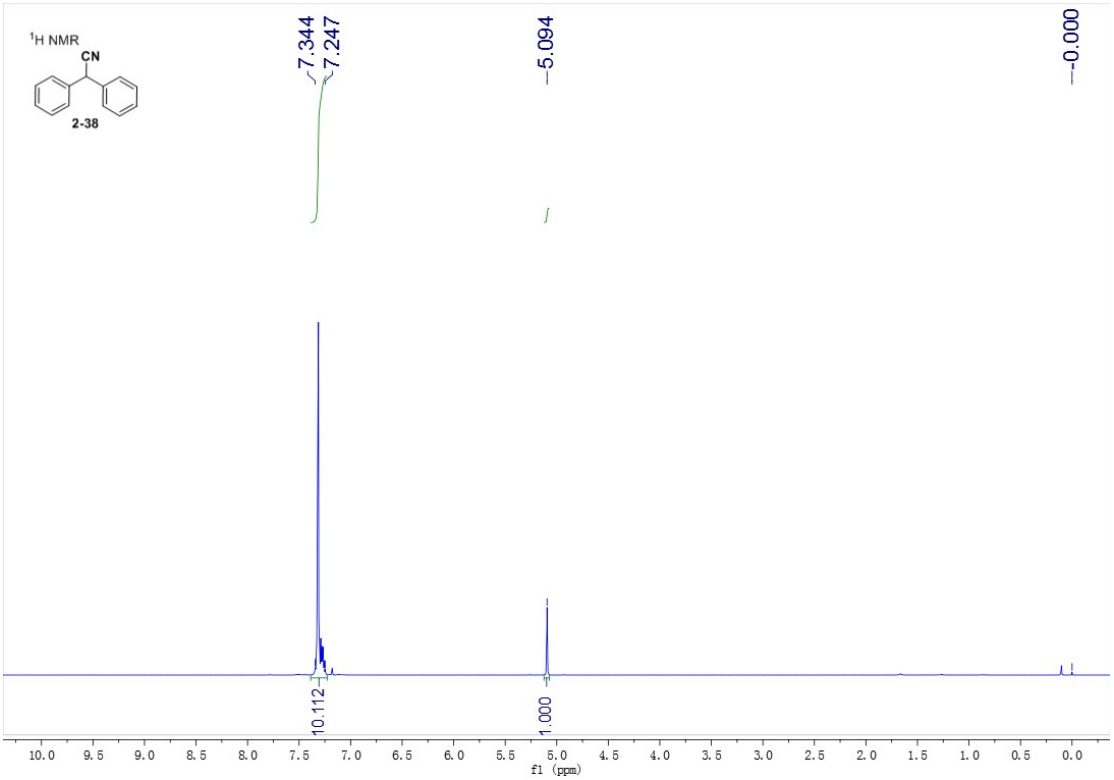

^{13}C NMR
2-35
173.888
165.016
156.808
136.514
128.043
126.311
124.146
119.711
118.287
113.753
102.841
1.320
f1 (ppm)

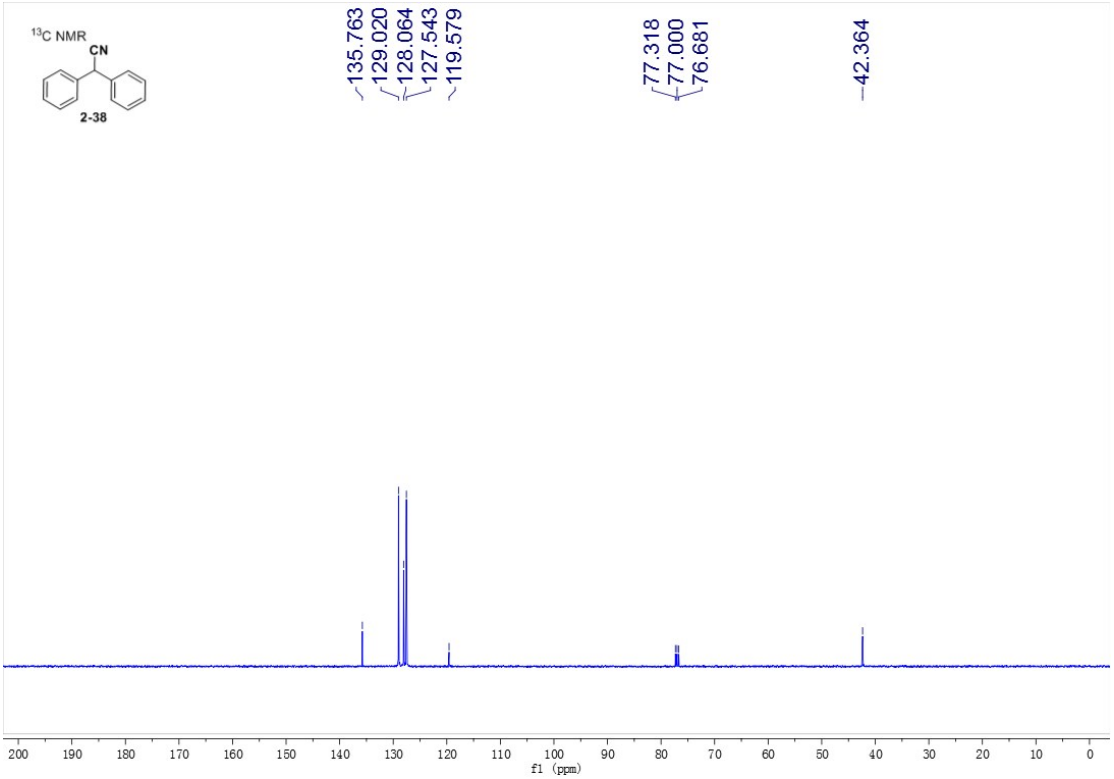

^{1}H NMR
CN
Ph
^{i}Pr
2-36
7.432
7.344
6.678
6.659
6.640
2.246
2.229
2.210
1.819
1.802
1.785
1.768
1.752
1.735
1.718
0.916
0.899
0.000
4.712
1.000
2.071
1.089
6.182
f1 (ppm)

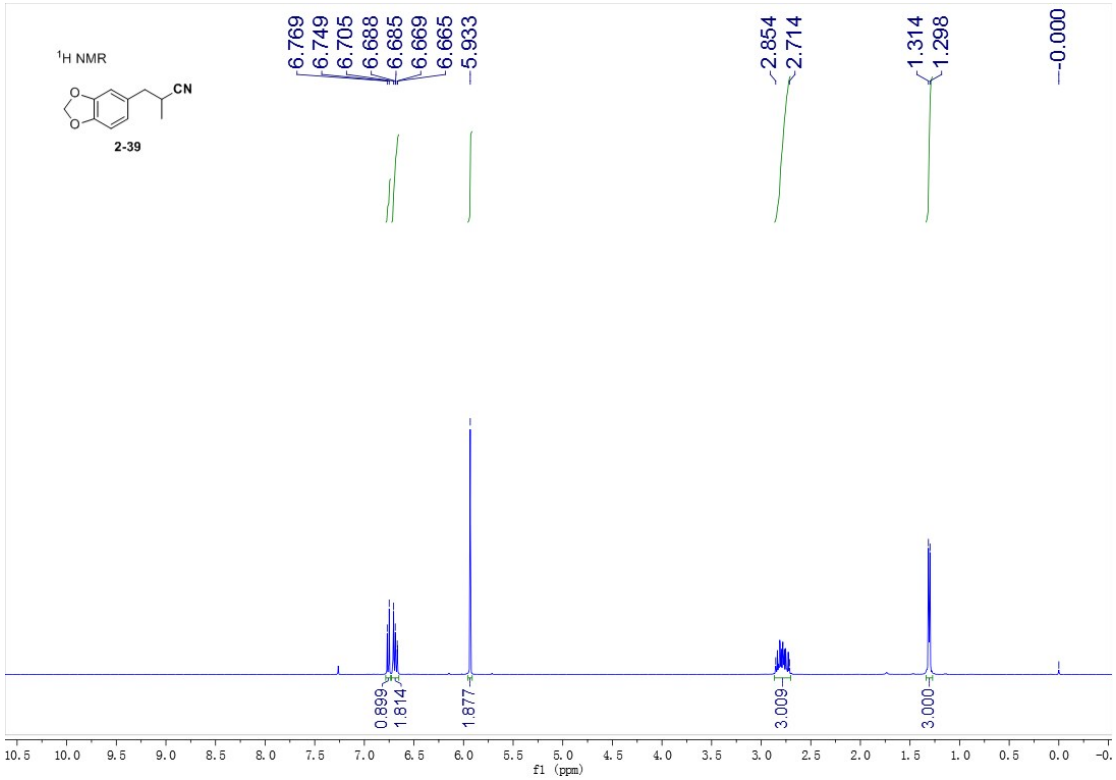

^{13}C NMR
CN
Ph
^{i}Pr
2-36
148.743
132.384
128.692
128.612
128.597
119.607
115.679
77.319
77.000
76.682
38.313
28.443
22.202
f1 (ppm)

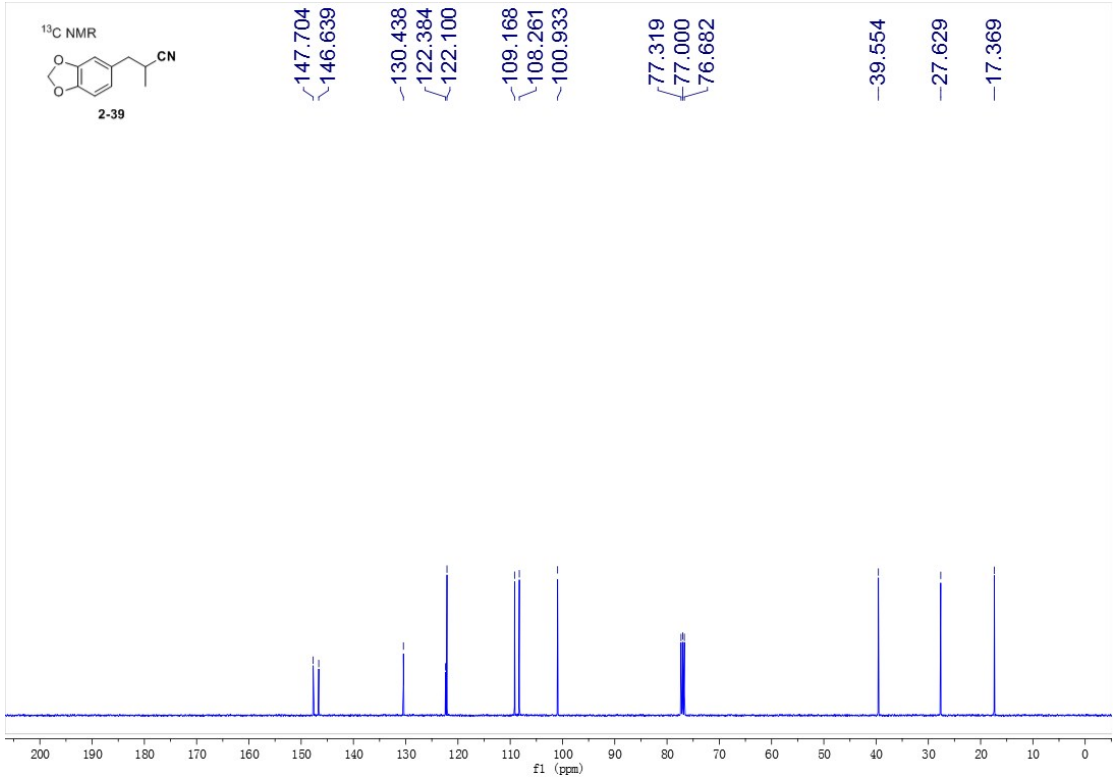

1H NMR
CN
2-37
7.266
6.654
6.637
4.793
4.790
4.786
4.713
2.365
2.277
2.220
2.044
1.920
1.855
1.740
1.567
1.466
0.000
1.000
1.081
1.076
3.095
2.280
1.146
3.002
1.184
f1 (ppm)

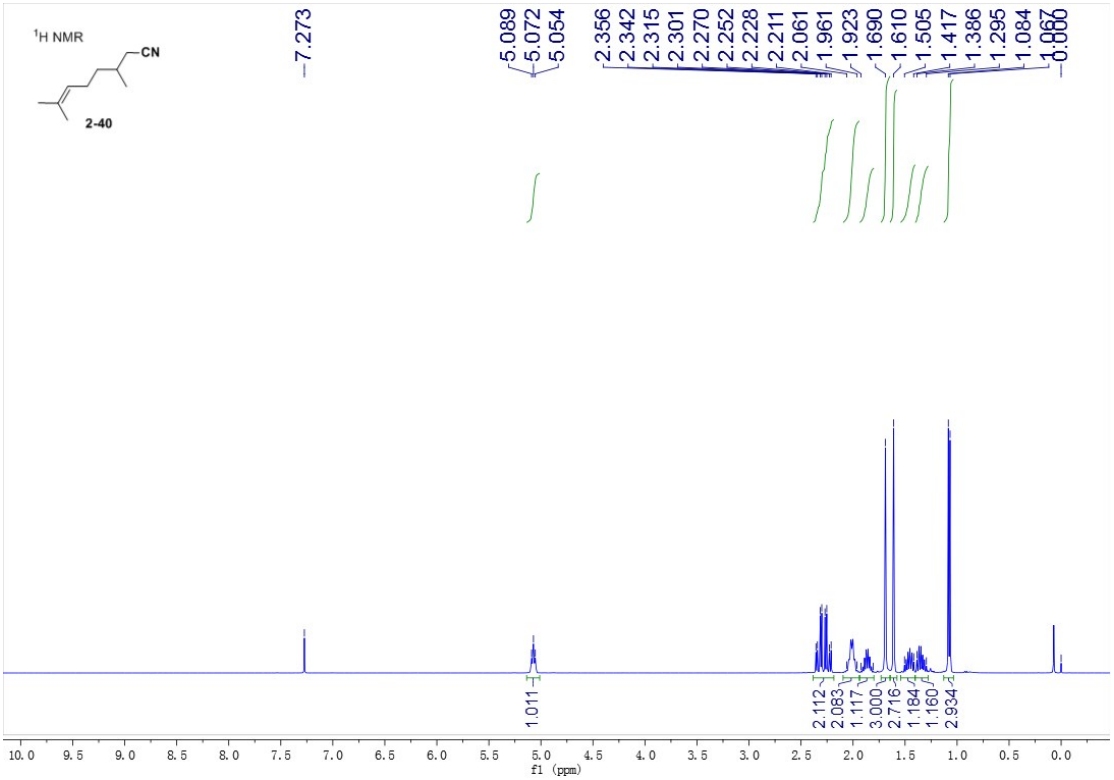

13C NMR
CN
2-37
147.585
144.465
119.382
111.908
109.682
77.317
77.000
76.680
39.046
30.815
26.791
26.133
20.493
f1 (ppm)

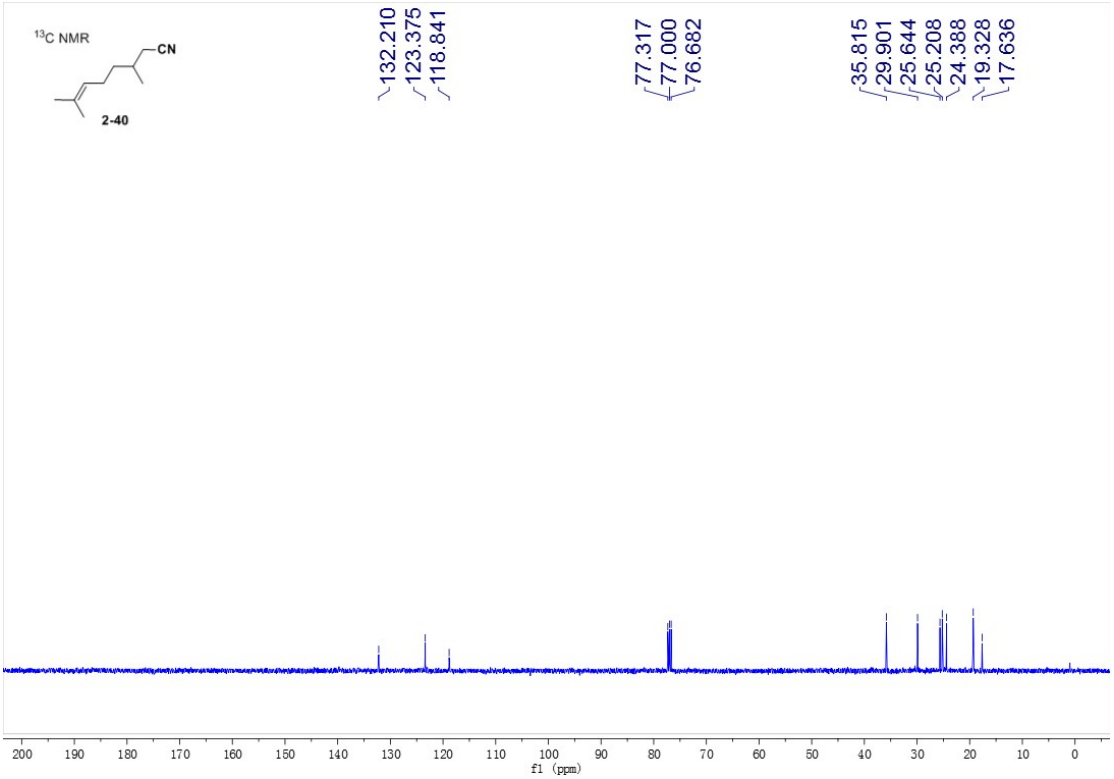

1H NMR
CN
2-38
7.344
7.247
5.094
0.000
10.112
1.000
f1 (ppm)

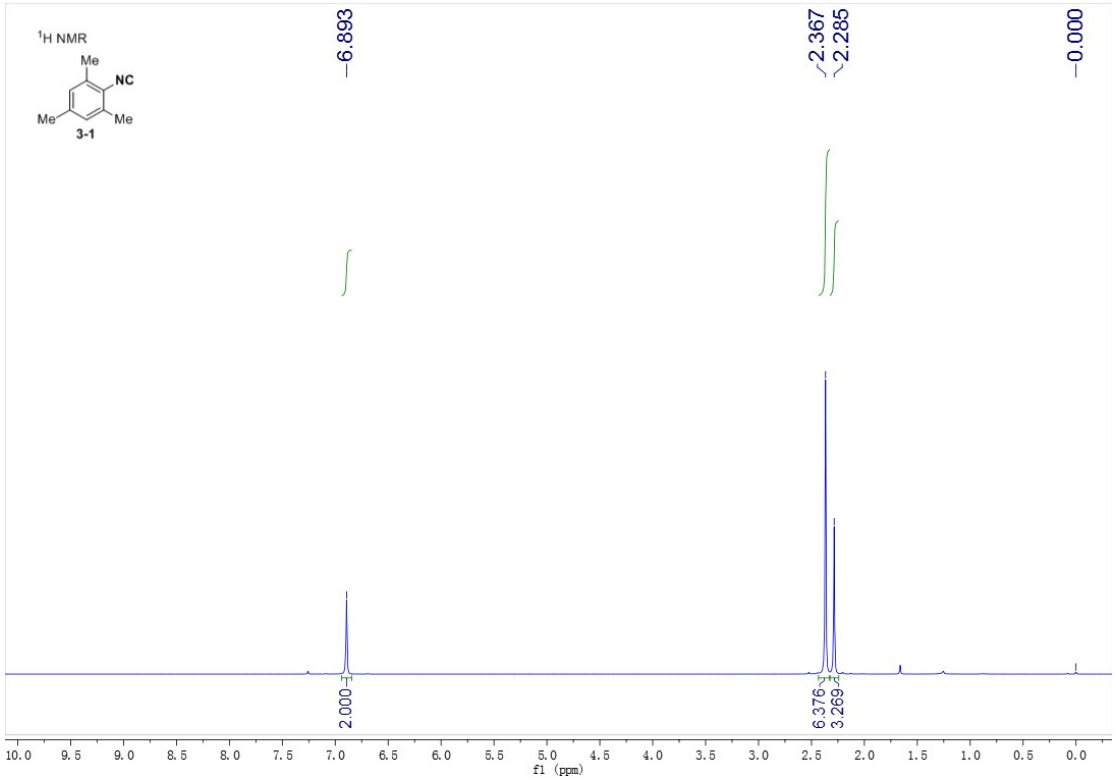

13C NMR
CN
2-38
135.763
129.020
128.064
127.543
119.579
77.318
77.000
76.681
42.364
f1 (ppm)

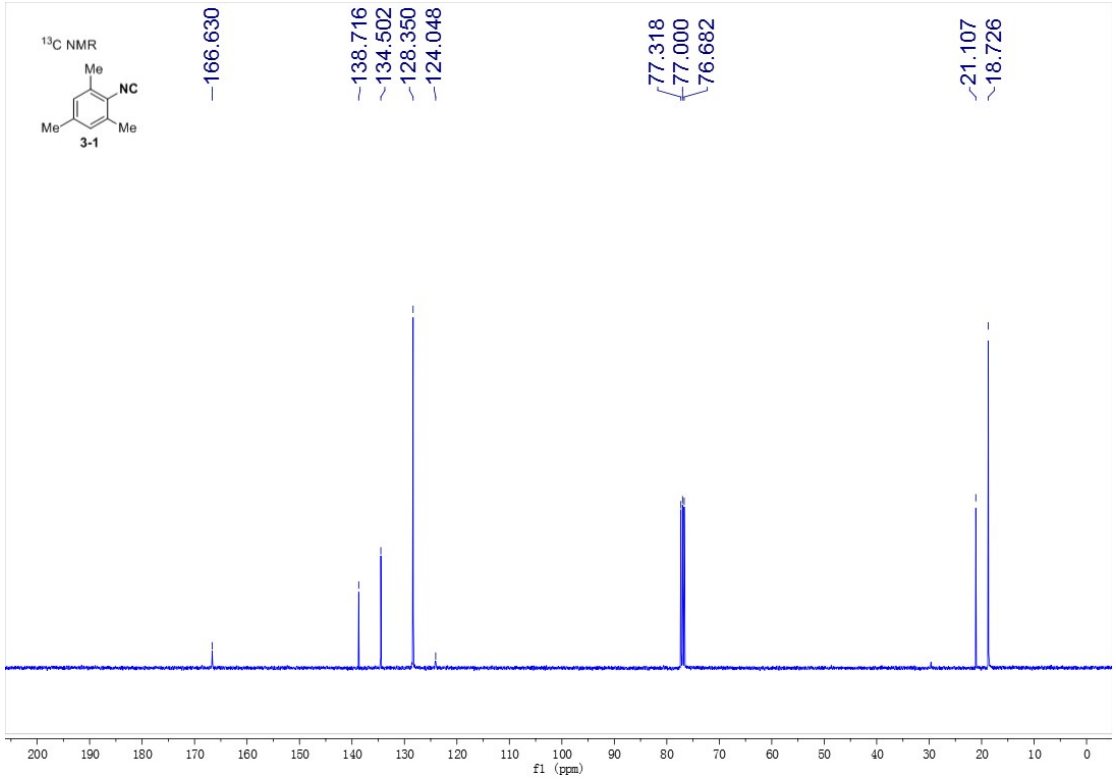

^{1}H NMR
CN
2-39
6.769
6.749
6.705
6.688
6.685
6.669
6.665
5.933
2.854
2.714
1.314
1.298
0.000
0.899
1.814
1.877
3.009
3.000
f1 (ppm)

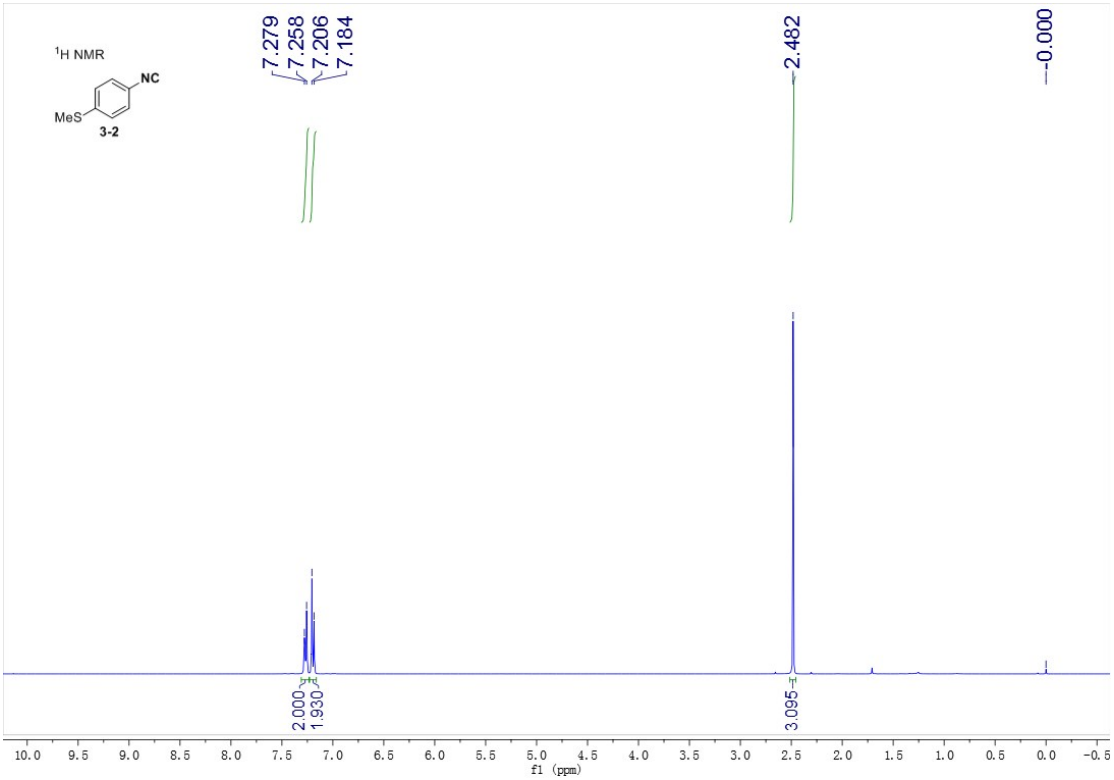

^{13}C NMR
CN
2-39
147.704
146.639
130.438
122.384
122.100
109.168
108.261
100.933
77.319
77.000
76.682
39.554
27.629
17.369
f1 (ppm)

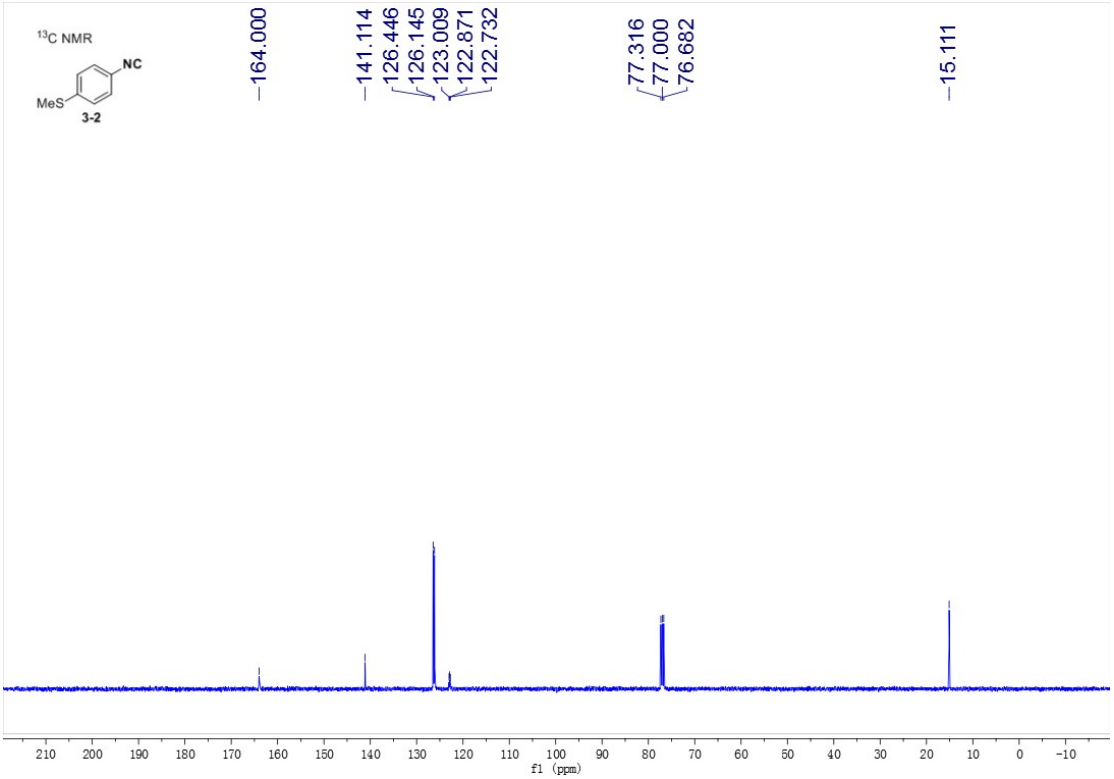

^{1}H NMR
CN
2-40
7.273
5.089
5.072
5.054
2.356
2.342
2.315
2.301
2.270
2.252
2.228
2.211
2.061
1.961
1.923
1.690
1.610
1.505
1.417
1.386
1.295
1.084
1.067
0.000
1.011
2.112
2.083
1.117
3.000
2.716
1.184
1.160
2.934
f1 (ppm)

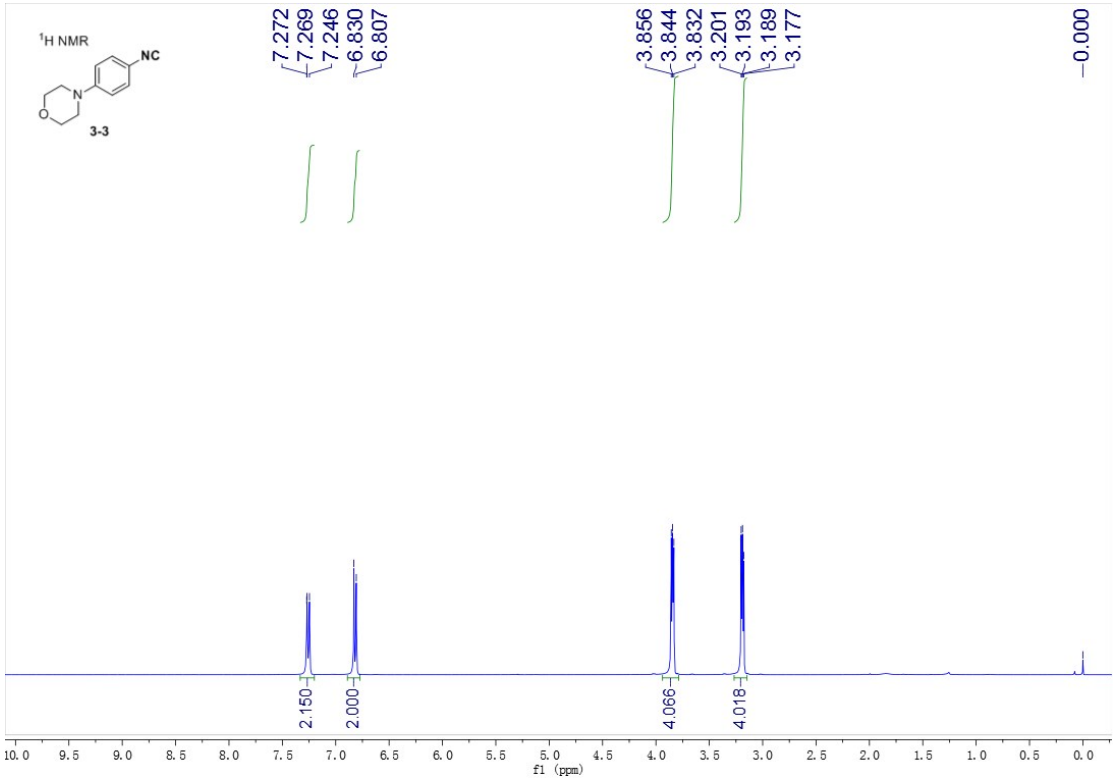

^{13}C NMR
CN
2-40
132.210
123.375
118.841
77.317
77.000
76.682
35.815
29.901
25.644
25.208
24.388
19.328
17.636
f1 (ppm)

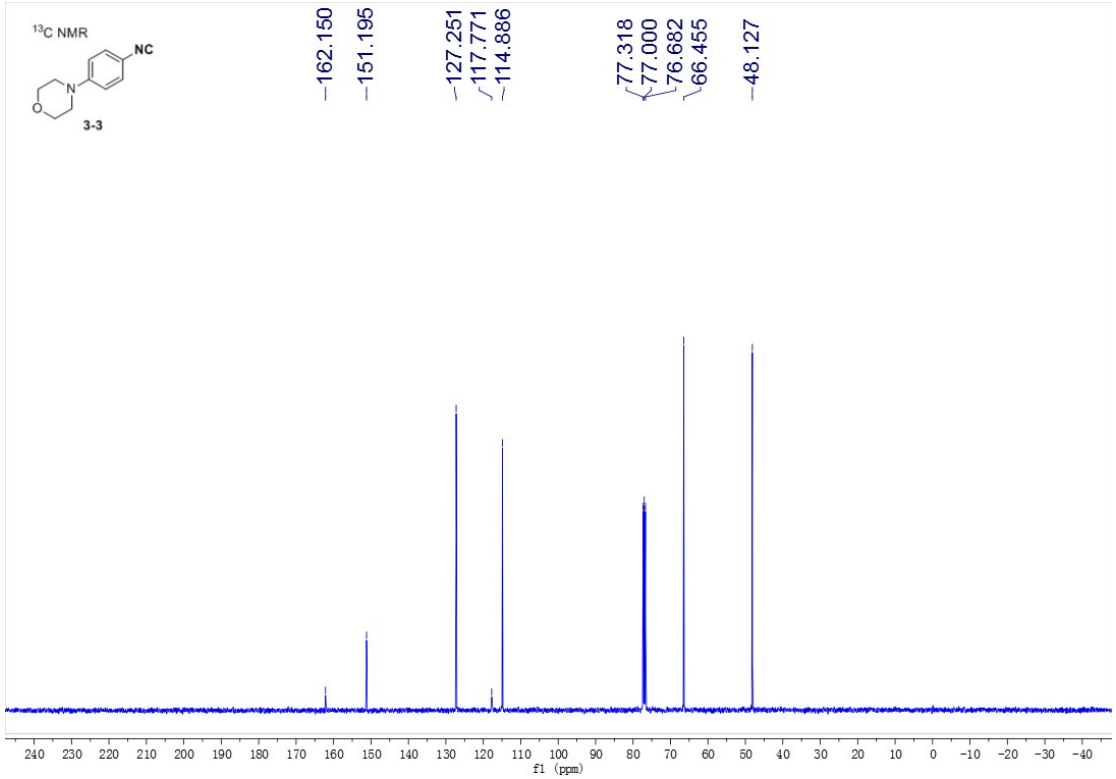

1H NMR
Me
NC
Me
Me
3-1
6.893
2.367
2.285
0.000
2.000
6.376
3.269
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

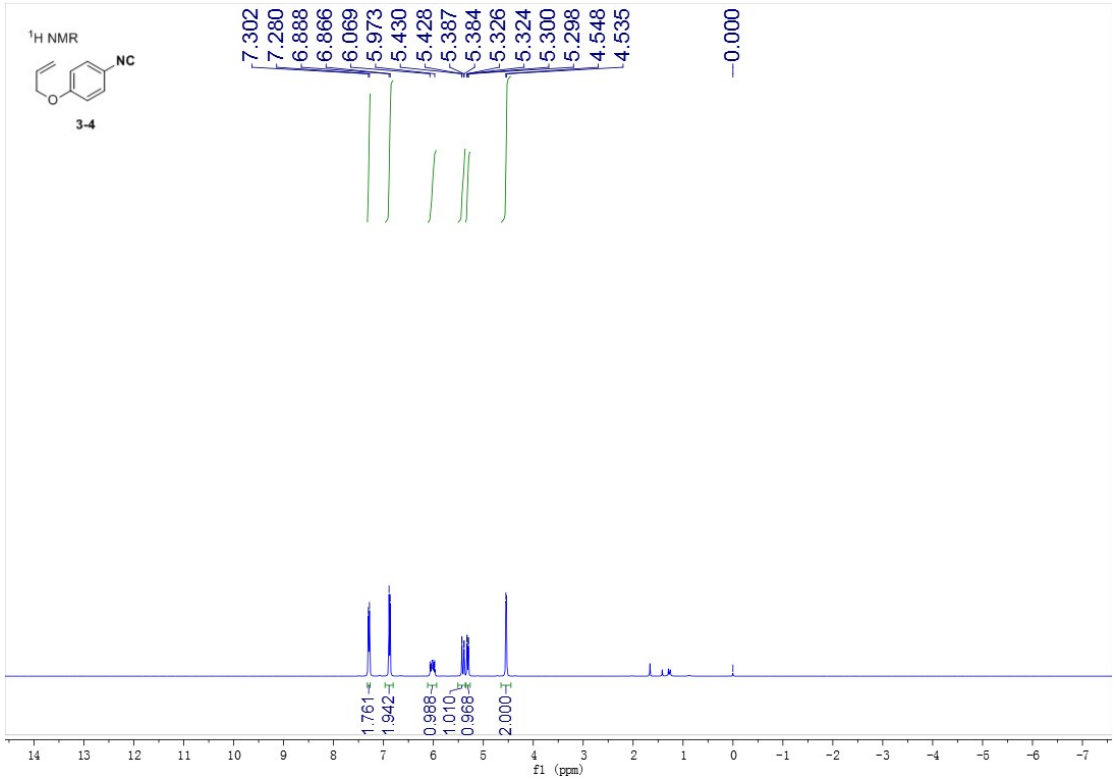

13C NMR
Me
NC
Me
Me
3-1
166.630
138.716
134.502
128.350
124.048
77.318
77.000
76.682
21.107
18.726
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

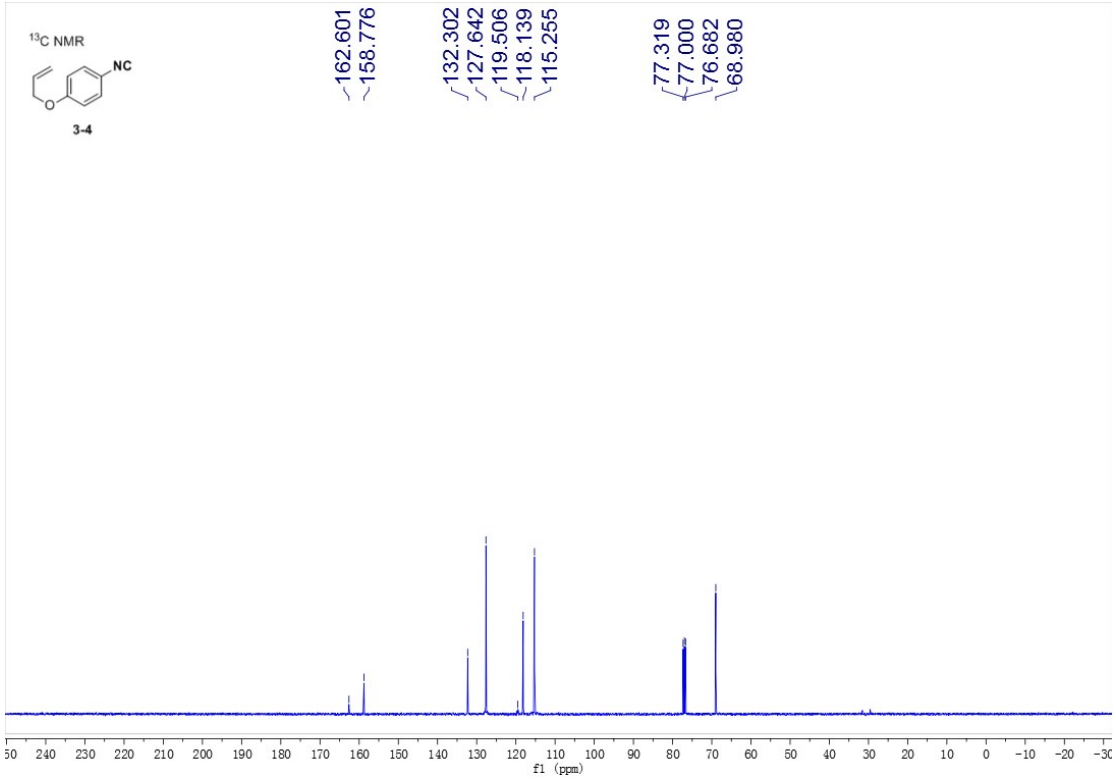

^{1}H NMR
NC
MeS
3-2
7.279
7.258
7.206
7.184
2.482
0.000
2.000
1.930
3.095
f1 (ppm)

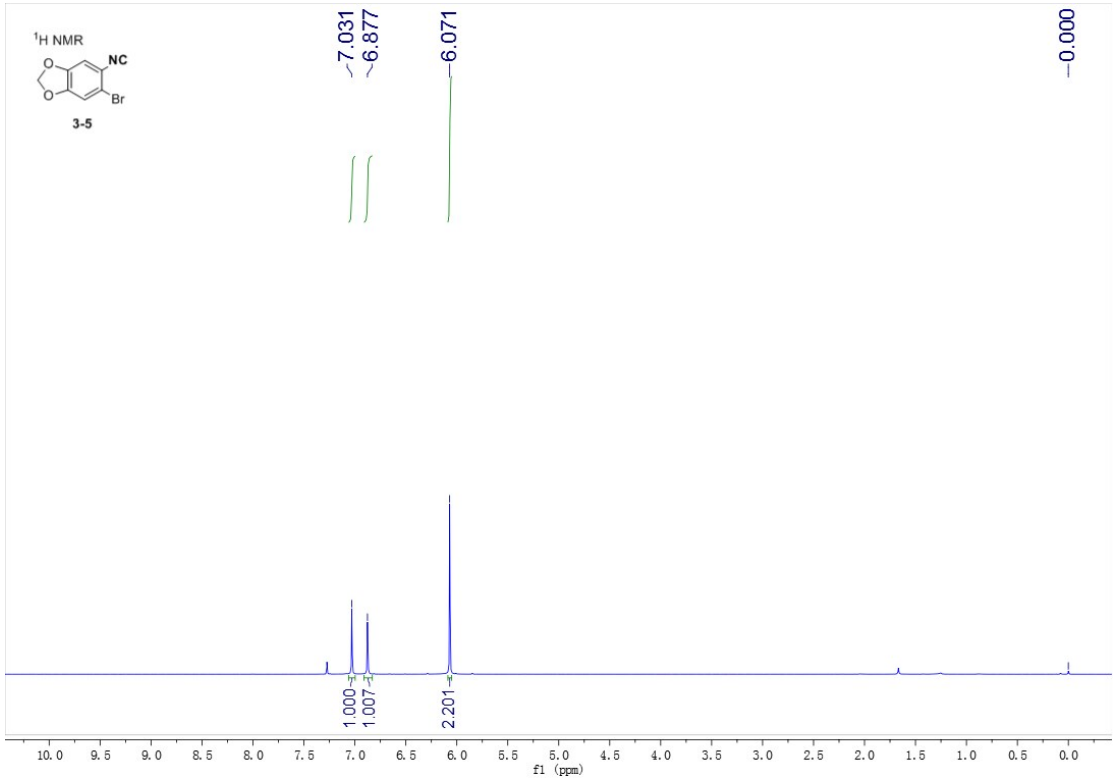

^{13}C NMR
NC
MeS
3-2
164.000
141.114
126.446
126.145
123.009
122.871
122.732
77.316
77.000
76.682
15.111
f1 (ppm)

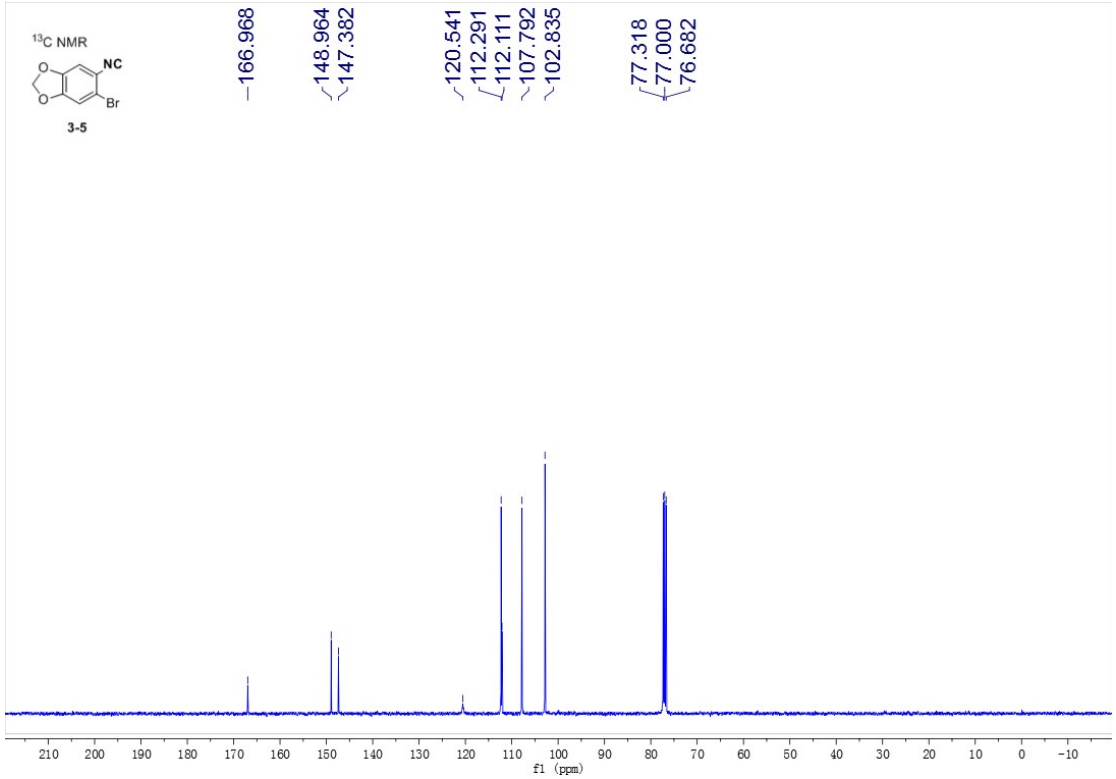

1H NMR
NC
3-3
7.272
7.269
7.246
6.830
6.807
3.856
3.844
3.832
3.201
3.193
3.189
3.177
0.000
2.150
2.000
4.066
4.018
f1 (ppm)

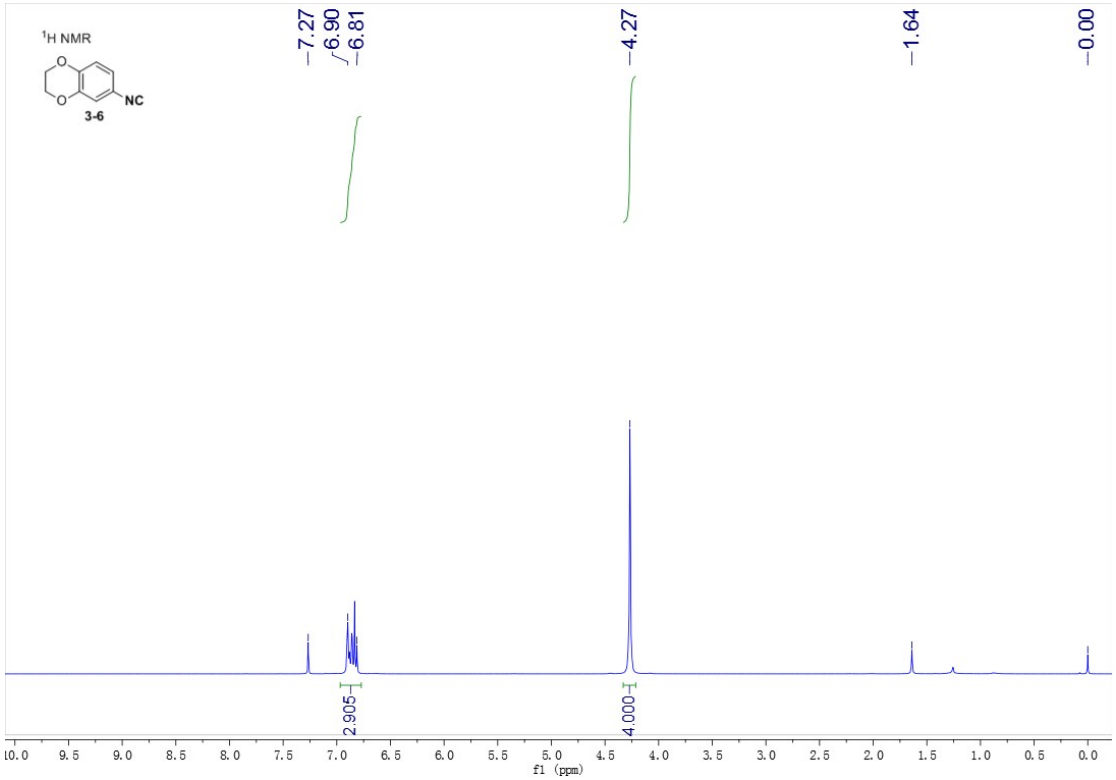

13C NMR
NC
3-3
162.150
151.195
127.251
117.771
114.886
77.318
77.000
76.682
66.455
48.127
f1 (ppm)


1H NMR
NC
O
3-4
7.302
7.280
6.888
6.866
6.069
5.973
5.430
5.428
5.387
5.384
5.326
5.324
5.300
5.298
4.548
4.535
0.000
1.761
1.942
0.988
1.010
0.968
2.000
f1 (ppm)


13C NMR
NC
O
3-4
162.601
158.776
132.302
127.642
119.506
118.139
115.255
77.319
77.000
76.682
68.980
f1 (ppm)


1H NMR
NC
Br
3-5
7.031
6.877
6.071
0.000
1.000
1.007
2.201
f1 (ppm)


13C NMR
NC
Br
3-5
166.968
148.964
147.382
120.541
112.291
112.111
107.792
102.835
77.318
77.000
76.682
f1 (ppm)


1H NMR
NC
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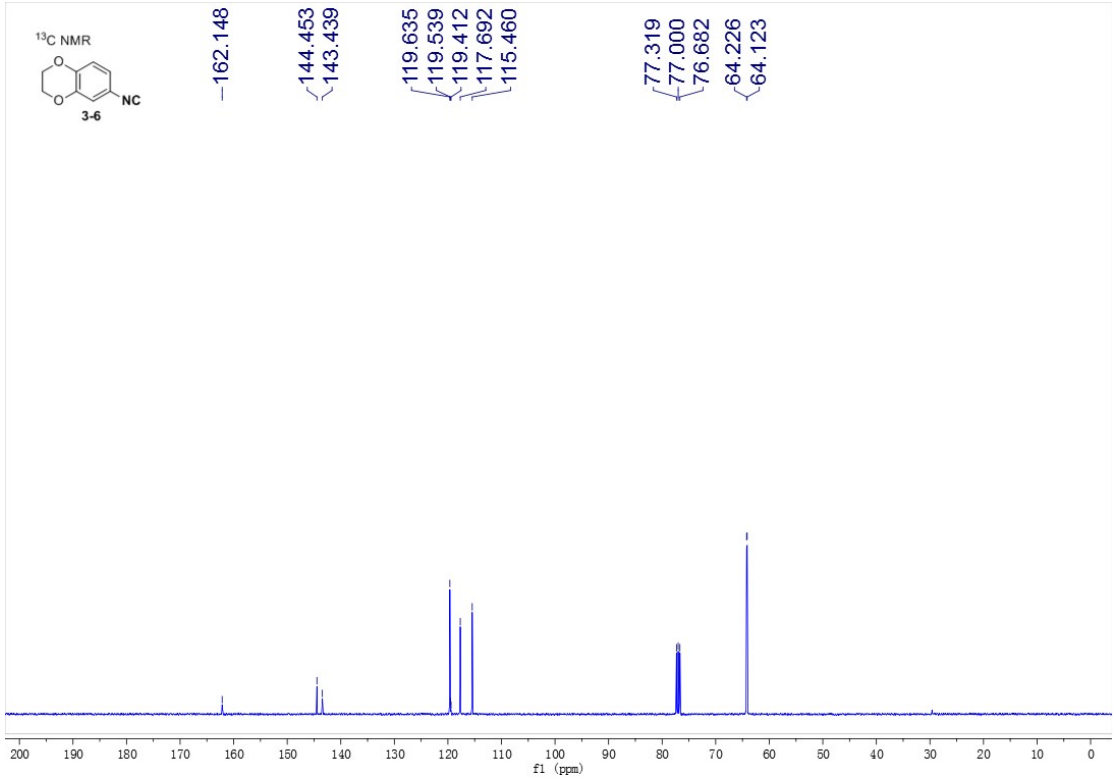
6.90
6.81
4.27
1.64
0.00
2.905
4.000
f1 (ppm)


13C NMR
NC
3-6
162.148
144.453
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117.692
115.460
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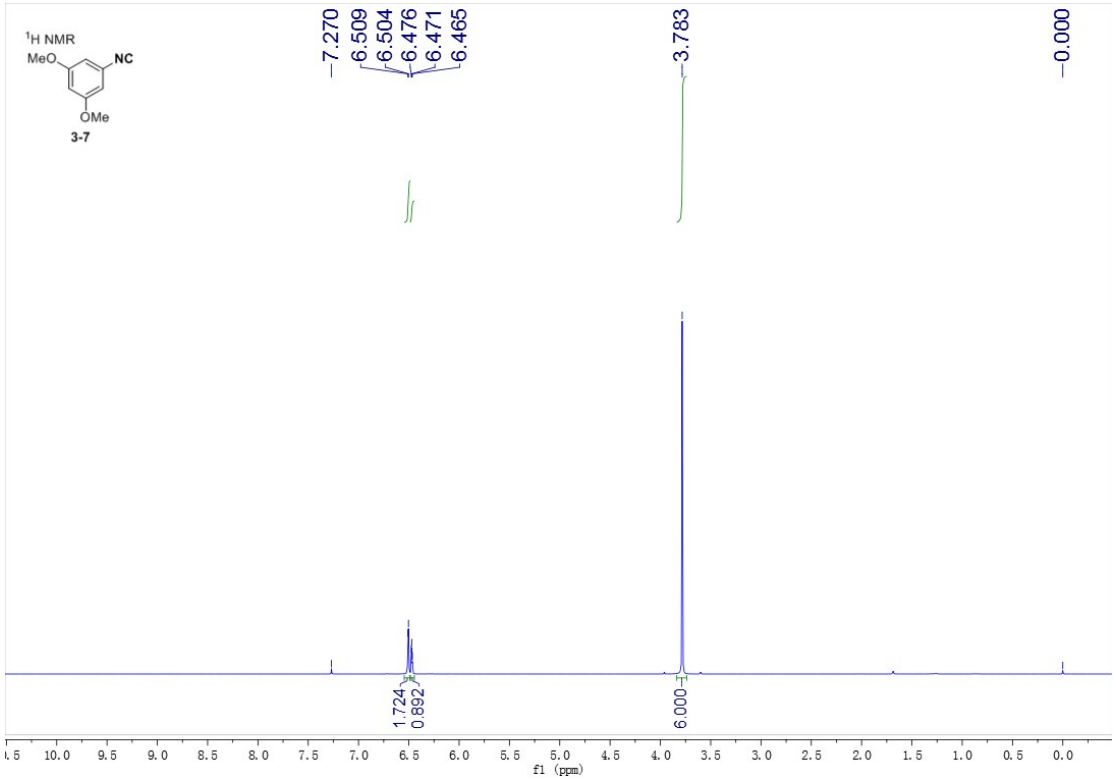
77.000
76.682
64.226
64.123
f1 (ppm)


1H NMR
MeO
NC
OMe
3-7
7.270
6.509
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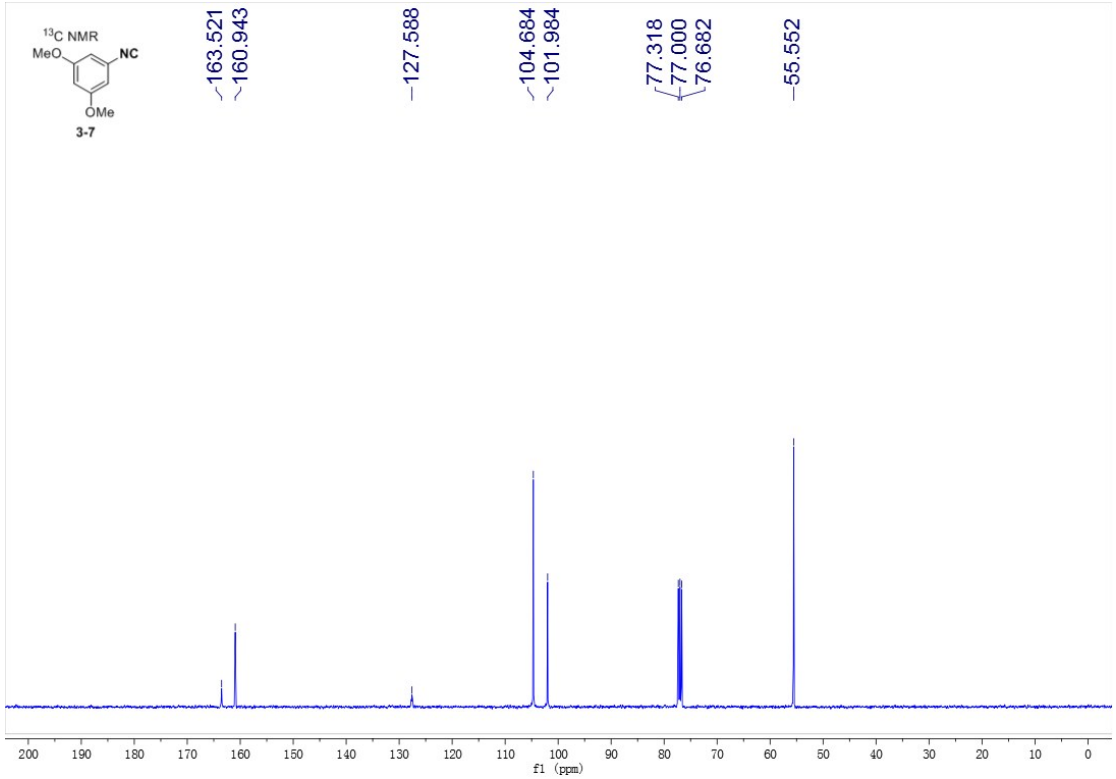
6.476
6.471
6.465
3.783
0.000
1.724
0.892
6.000
f1 (ppm)


13C NMR
MeO
NC
OMe
3-7
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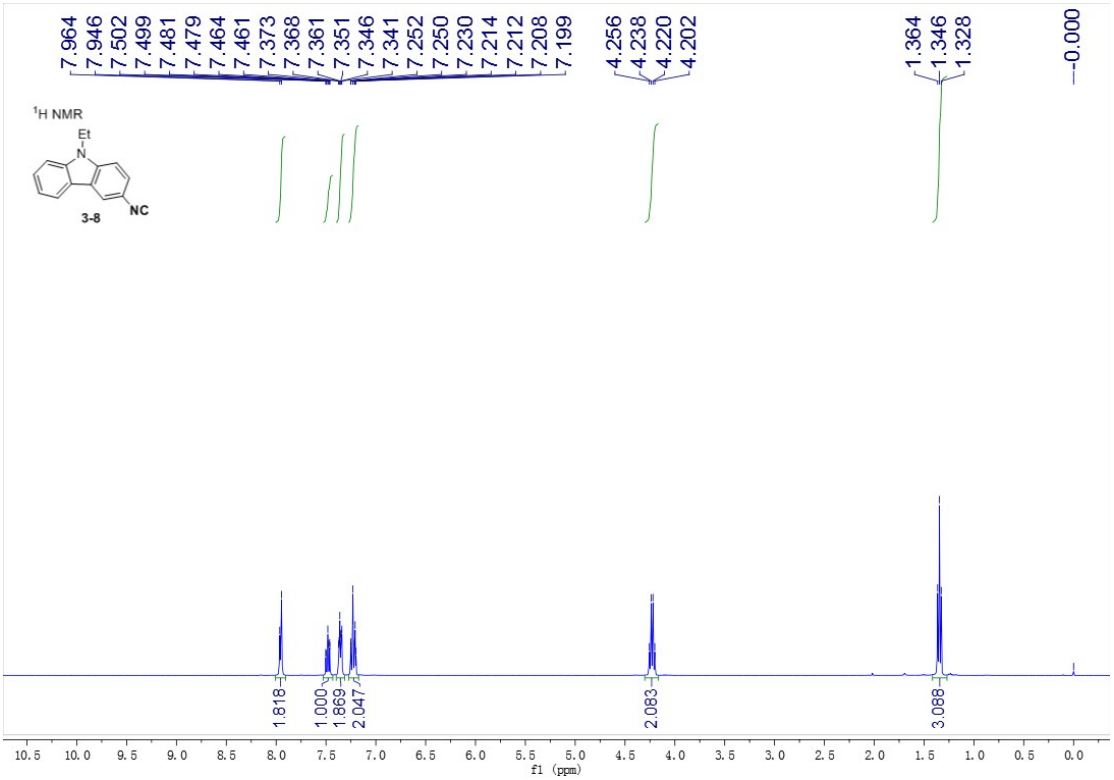
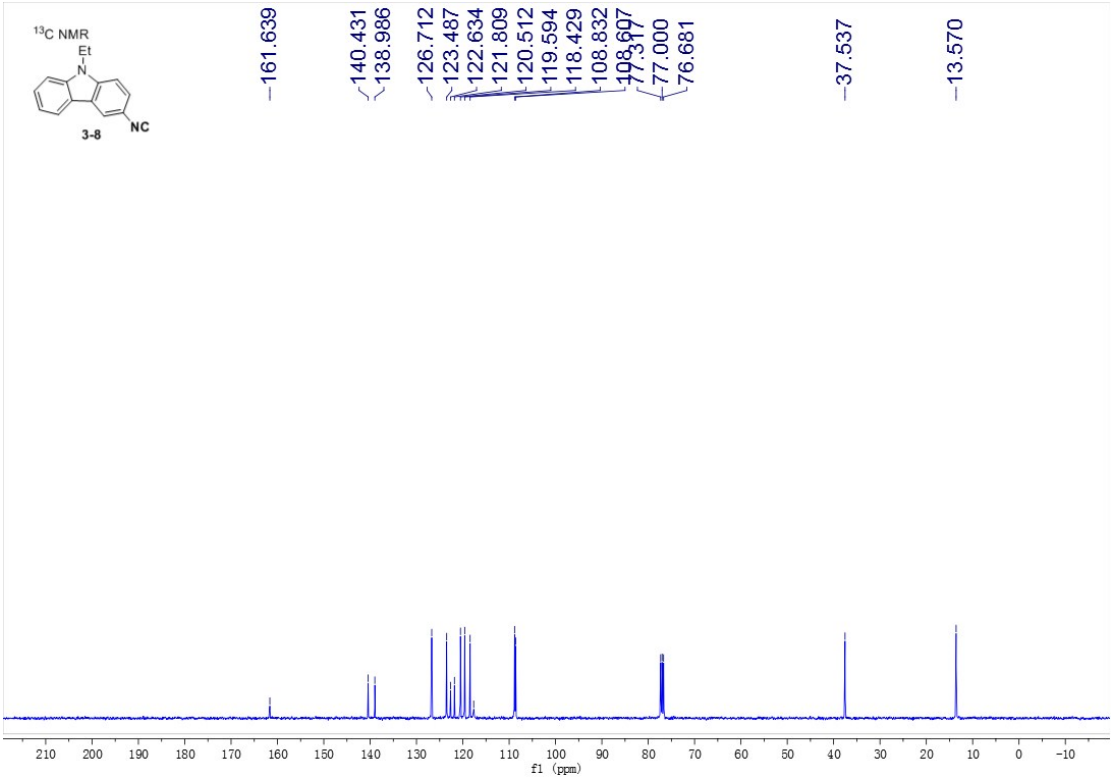
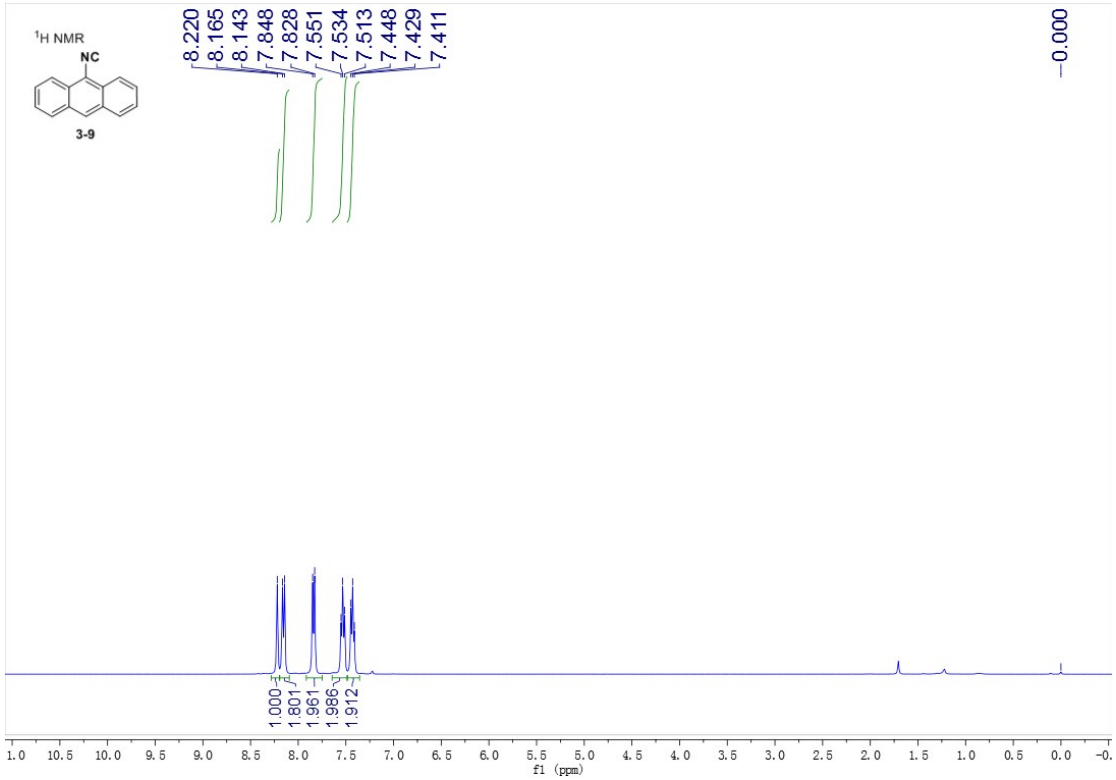
160.943
127.588
104.684
101.984
77.318
77.000
76.682
55.552
f1 (ppm)


7.964
7.946
7.502
7.499
7.481
7.479
7.464
7.461
7.373
7.368
7.361
7.351
7.346
7.341
7.252
7.250
7.230
7.214
7.212
7.208
7.199
4.256
4.238
4.220
4.202
1.364
1.346
1.328
0.000
1H NMR
Et
N
NC
3-8
1.818
1.000
1.869
2.047
2.083
3.088
f1 (ppm)


161.639
140.431
138.986
126.712
123.487
122.634
121.809
120.512
119.594
118.429
108.832
108.607
77.317
77.000
76.681
37.537
13.570
13C NMR
Et
N
NC
3-8
f1 (ppm)


1H NMR
NC
3-9
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8.165
8.143
7.848
7.828
7.551
7.534
7.513
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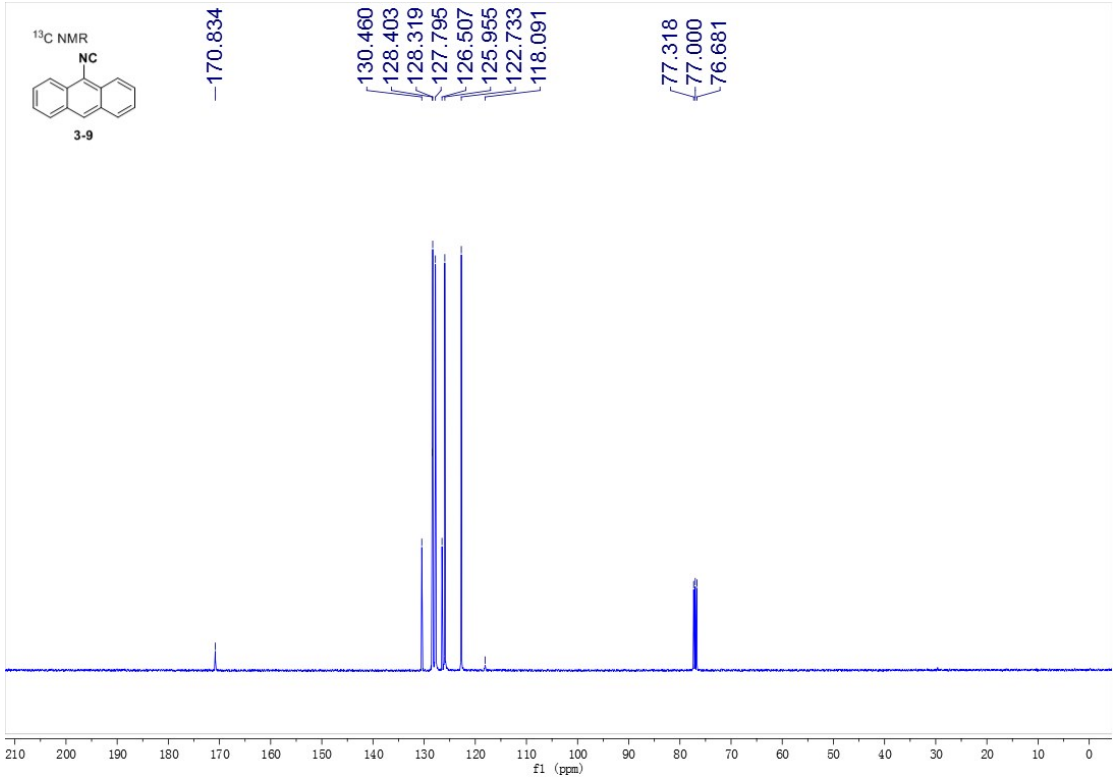
7.429
7.411
0.000
1.000
1.801
1.961
1.986
1.912
f1 (ppm)


13C NMR
NC
3-9
170.834
130.460
128.403
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127.795
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122.733
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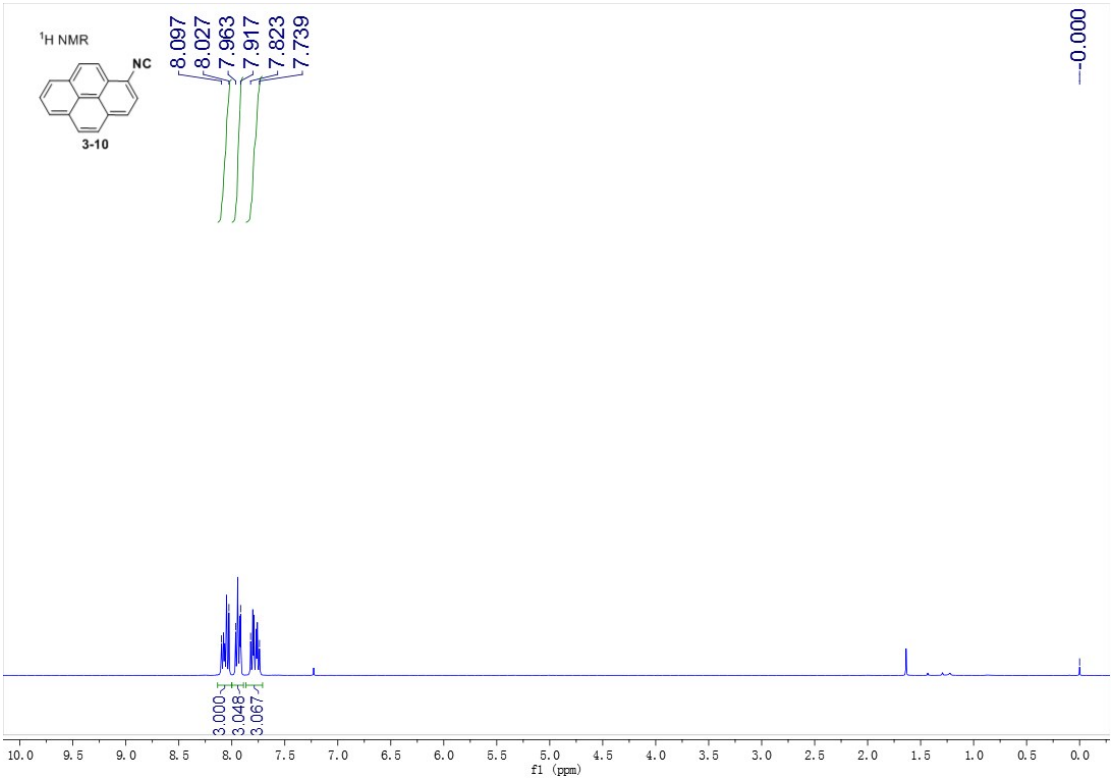
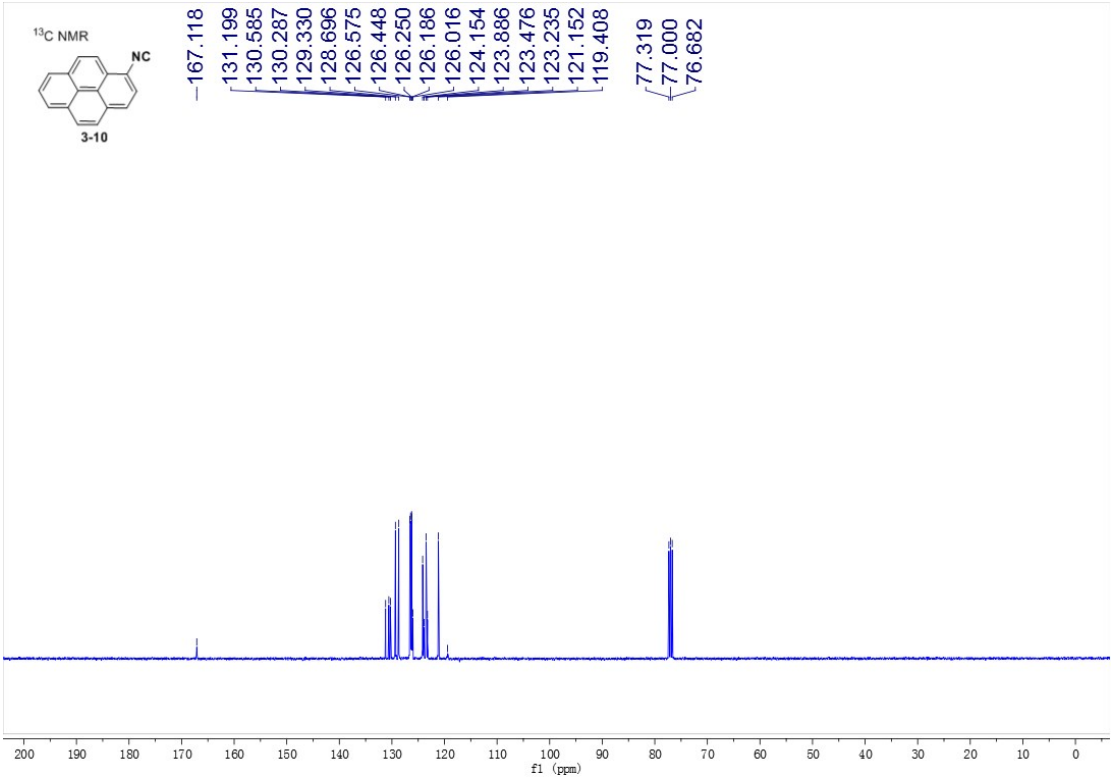
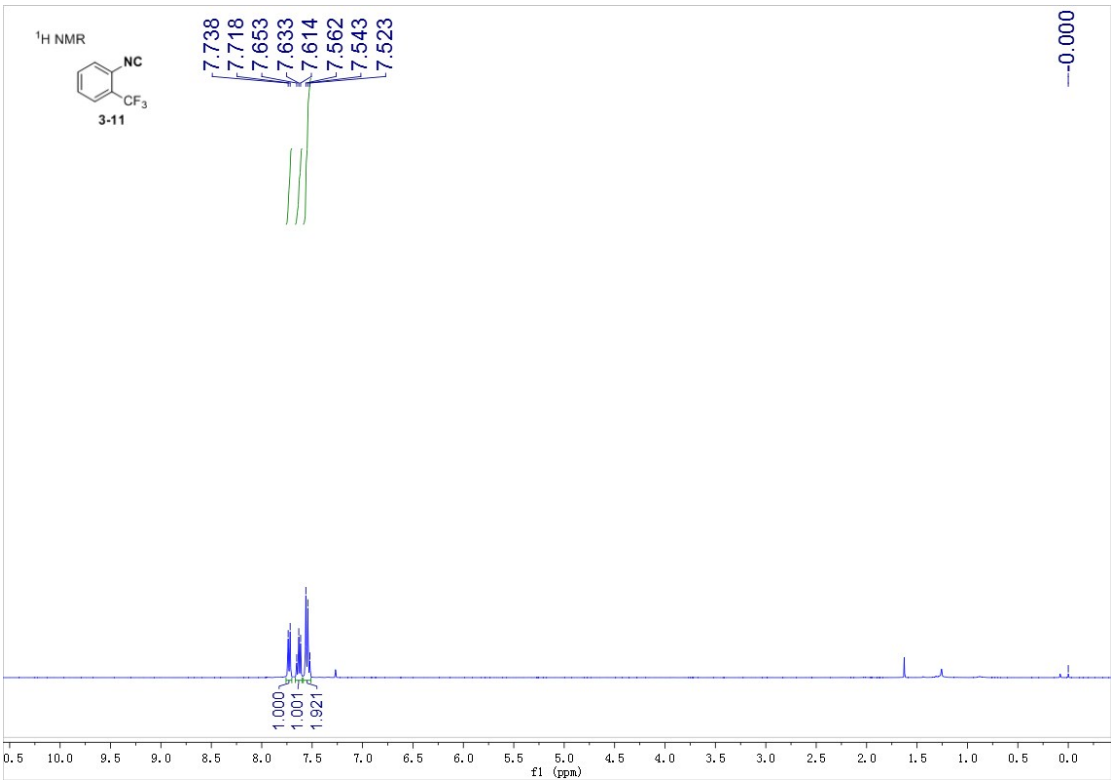
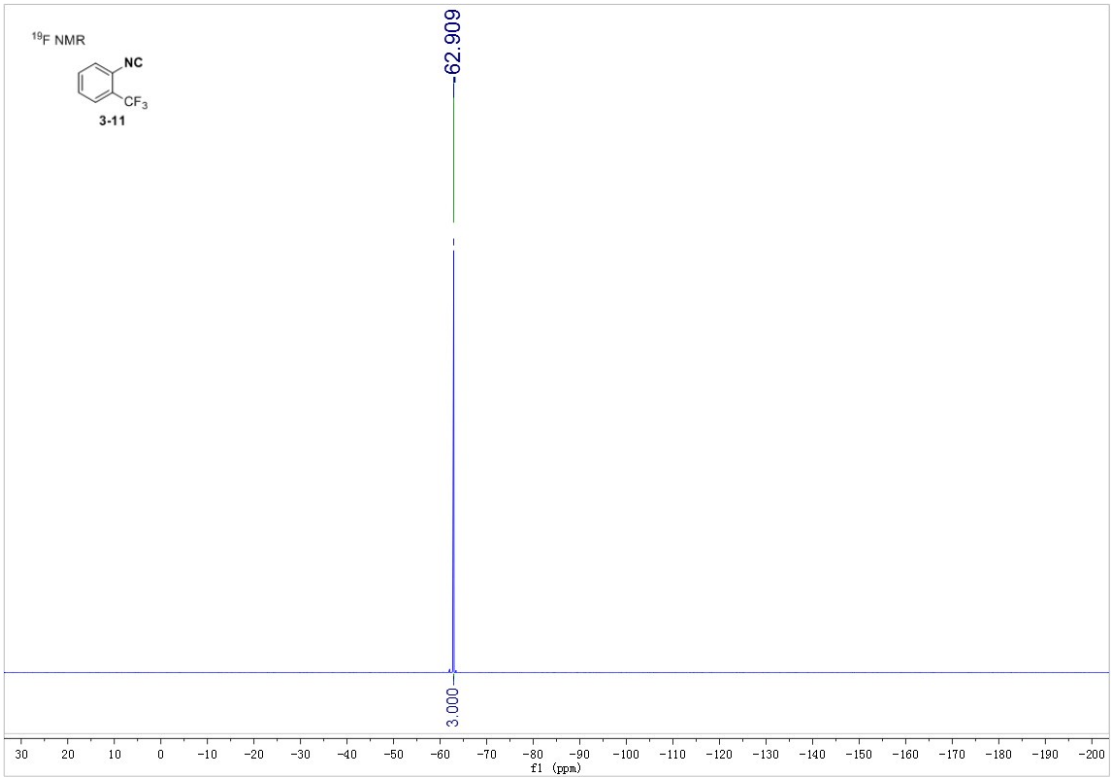
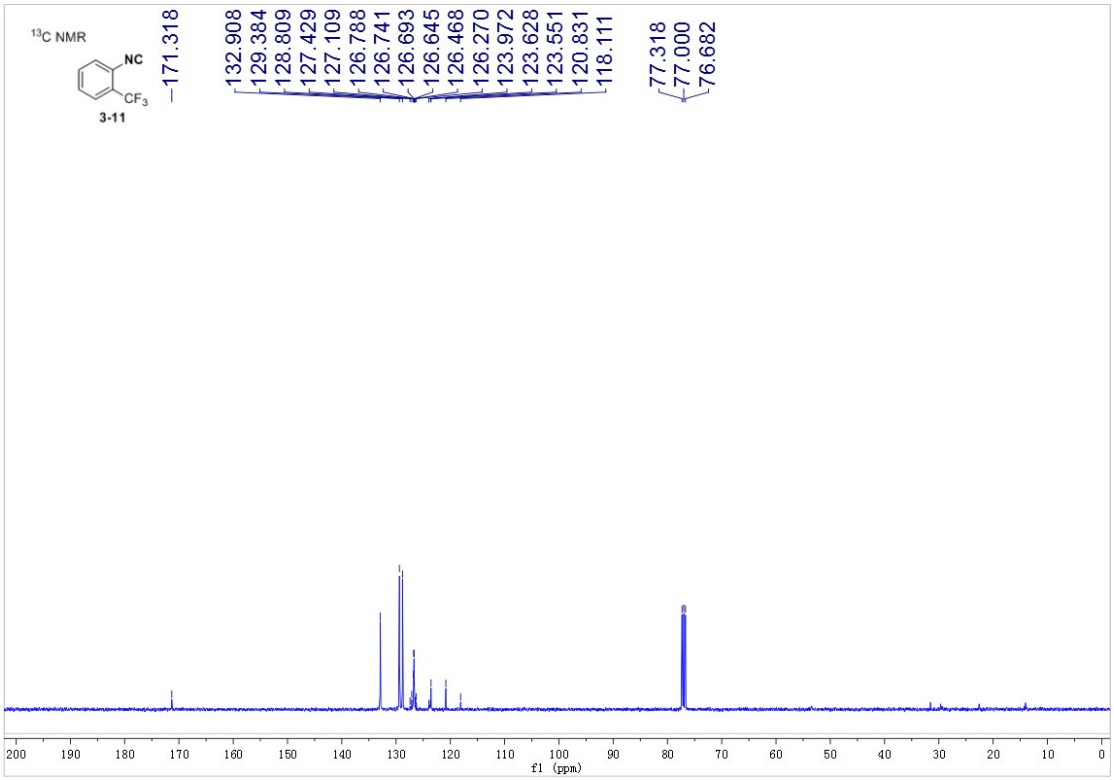
77.318
77.000
76.681
f1 (ppm)


1H NMR
NC
3-10
8.097
8.027
7.963
7.917
7.823
7.739
0.000
3.000
3.048
3.067
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


13C NMR
NC
3-10
167.118
131.199
130.585
130.287
129.330
128.696
126.575
126.448
126.250
126.186
126.016
124.154
123.886
123.476
123.235
121.152
119.408
77.319
77.000
76.682
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


1H NMR
NC
CF3
3-11
7.738
7.718
7.653
7.633
7.614
7.562
7.543
7.523
0.000
1.000
1.001
1.921
f1 (ppm)


19F NMR
NC
CF3
3-11
-62.909
3.000
f1 (ppm)


13C NMR
NC
CF3
3-11
171.318
132.908
129.384
128.809
127.429
127.109
126.788
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126.693
126.645
126.468
126.270
123.972
123.628
123.551
120.831
118.111
77.318
77.000
76.682
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)