Supporting Information

for

N^1-Selective alkenylation of 1-sulfonyl-1,2,3-trizoles with alkyne via gold catalysis

Chenyang Sun, Xiao Yuan, Yan Li, Xiaoxiao Li*and Zhigang Zhao*

College of Chemistry and Environmental Protection Engineering, Southwest University for Nationalities, Chengdu 610041, PR China

lixiaoxiao.2005@163.com ; zzg63129@163.com

Table of Contents

1. General information

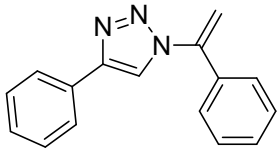
All reactions were performed using Schlenk tubes, septa, and syringes without protection of nitrogen. THF、toluene and DCM、DCE were freshly distilled over sodium/benzophenone and calcium hydride, respectively. Commercial reagents were used as supplied or were purified by standard techniques where necessary. Column chromatography was performed using Qingdao Haiyang Chemical Co., Ltd silica gel (200–300 mesh) with the appropriate solvent system, as determined by TLC analysis (Qingdao Haiyang Chemical Co., Ltd, silica gel F254) using UV light and $KMnO_4$ stain to visualize the reaction components. Melting points were determined using a WRS-1B digital melting point instrument. IR spectra were recorded on a Nicoletisso FTIR spectrometer using KBr disks. Unless otherwise noted, nuclear magnetic resonance spectra were recorded at room temperature on an Agilent 400 MHz spectrometer using $CDCl_3$ as the solvent and TMS as the internal reference. Chemical shifts for ^{13}C NMR spectra were recorded in parts per million relative to tetramethylsilane using the central peak of deuterochloroform (77.0 ppm) as the internal standard. HRMS was performed using a Bruker Daltonics Bio TOF mass spectrometer.

1-Sulfonyl-1,2,3-trizoles **1a-1j** were prepared according to the published methods.[1] Alkyne were obtained commercially and used without further purification.

General procedure for N^1-Selective gold-catalyzed alkenylation of 4-phenyl-1-sulfonyl-1,2,3-trizole 1a with phenylacetylene 2a.

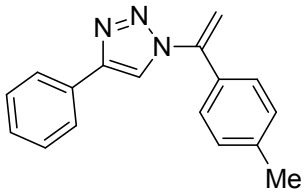
To a Schlenk tube charged with nitrogen was added IPrAuCl/AgOTf (5 mol%) in dry DCE (3 mL). After three minutes, 4-phenyl-1-sulfonyl-1,2,3-trizole **1a** (0.1 mmol), phenylacetylene **2a** (0.5 mmol) and H_2O (0.2 mmol) were added to the reaction. Then the reaction mixture was stirred at 80 ℃ for 12 h until complete consumption of starting material as monitored by TLC. Concentration of the reaction mixture in vacuo followed by purification through flash chromatography on silica gel column (hexane/EtOAc = 30/1) afforded **3a** (22.8 mg, 92% yield) as yellow oily liquid.

2. Spectral Data



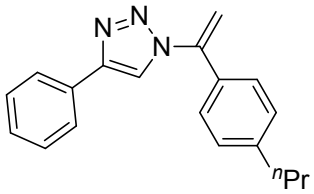
4-phenyl-1-(1-phenylvinyl)-1*H*-1,2,3-triazole (**3a**)

Yellow oily liquid; yield, 92% (22.8 mg); IR (neat) 3038, 2934, 1496, 1459, 756 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.6 Hz, 2H), 7.79 (s, 1H), 7.43 – 7.21 (m, 8H), 5.85 (s, 1H), 5.54 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.48, 142.86, 134.51, 130.09, 129.83, 128.80, 128.79, 128.27, 127.26, 125.71, 119.78, 109.37; HRMS (ESI) calcd for $C_{16}H_{14}N_3^+$ $[M+H]^+$ 248.1182; found, 248.1182.



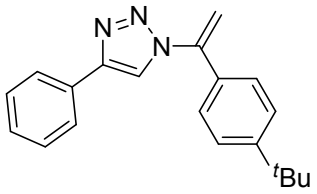
4-phenyl-1-(1-(*p*-tolyl)vinyl)-1*H*-1,2,3-triazole (**3b**)

Yellow oily liquid; yield, 88% (23.0 mg); IR (neat) 3038, 2937, 1499, 1457, 756 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.2 Hz, 2H), 7.80 (s, 1H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.24 (q, *J* = 8.0 Hz, 4H), 5.80 (s, 1H), 5.50 (s, 1H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.39, 142.85, 140.04, 131.69, 130.12, 129.47, 128.78, 128.25, 127.18, 125.71, 119.80, 108.58, 21.24; HRMS (ESI) calcd for $C_{17}H_{16}N_3^+$ $[M+H]^+$ 262.1339; found, 262.1339.



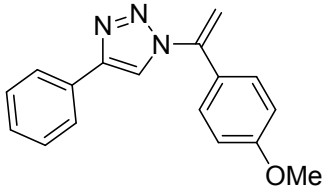
4-phenyl-1-(1-(4-propylphenyl)vinyl)-1*H*-1,2,3-triazole (**3c**)

Yellow oily liquid; yield, 86% (24.9 mg); IR (neat) 3038, 2937, 1496, 1460, 762 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.1 Hz, 2H), 7.81 (s, 1H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.28 (d, *J* = 8.2 Hz, 2H), 7.22 (d, *J* = 8.2 Hz, 2H), 5.80 (s, 1H), 5.51 (s, 1H), 2.65 – 2.60 (m, 2H), 1.71 – 1.62 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.42, 144.82, 142.92, 131.92, 130.18, 128.88, 128.78, 128.24, 127.16, 125.74, 119.84, 108.64, 37.72, 24.32, 13.77. HRMS (ESI) calcd for $C_{19}H_{20}N_3^+$ $[M+H]^+$ 290.1652; found, 290.1652.



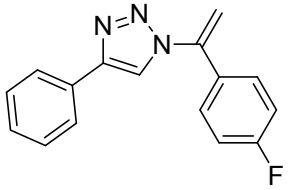
1-(1-(4-(*tert*-butyl)phenyl)vinyl)-4-phenyl-1*H*-1,2,3-triazole (**3d**)

Yellow oily liquid; yield, 88% (26.7 mg); IR (neat) 3041, 2937, 1502, 1457, 756 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.6 Hz, 2H), 7.81 (s, 1H), 7.45 – 7.40 (m, 4H), 7.35 – 7.30 (m, 3H), 5.82 (s, 1H), 5.52 (s, 1H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.22, 147.48, 142.86, 131.68, 130.24, 128.81, 128.26, 127.04, 125.79, 125.78, 119.86, 108.69, 34.78, 31.18; HRMS (ESI) calcd for $C_{20}H_{22}N_3^+$ $[M+H]^+$ 304.1808; found, 304.1807.



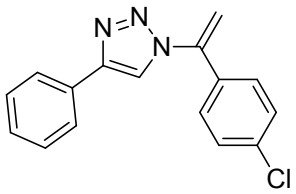
1-(1-(4-methoxyphenyl)vinyl)-4-phenyl-1*H*-1,2,3-triazole (**3e**)

Yellow oily liquid; yield, 78% (21.6 mg); IR (neat) 3035, 2931, 1499, 1457, 759 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.85 (d, *J* = 7.2 Hz, 2H), 7.46 – 7.36 (m, 5H), 6.94 (d, *J* = 8.8 Hz, 2H), 5.87 (s, 1H), 5.33 (s, 1H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.40, 148.56, 145.75, 132.32, 129.92, 129.63, 128.88, 128.80, 127.20, 126.18, 113.71, 110.00, 105.98, 55.34; HRMS (ESI) calcd for $C_{17}H_{16}N_3O^+$ $[M+H]^+$ 278.1288; found, 278.1288.



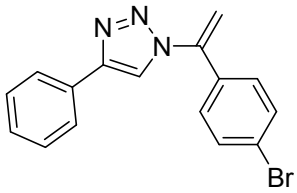
1-(1-(4-fluorophenyl)vinyl)-4-phenyl-1*H*-1,2,3-triazole (**3f**)

Yellow oily liquid; yield, 63% (16.7 mg); IR (neat) 3035, 2937, 1499, 1457, 758 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.3 Hz, 2H), 7.81 (s, 1H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.39 – 7.33 (m, 3H), 7.12 (t, *J* = 8.6 Hz, 2H), 5.82 (s, 1H), 5.52 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.55 (d, *J* = 249.2 Hz), 147.63, 142.02, 129.94 (d, *J* = 4.8 Hz), 129.32 (d, *J* = 8.4 Hz), 128.86, 128.42, 127.94, 125.78, 119.69, 115.95 (d, *J* = 21.8 Hz), 109.28; HRMS (ESI) calcd for $C_{16}H_{13}FN_3^+$ $[M+H]^+$ 266.1088; found, 266.1089.



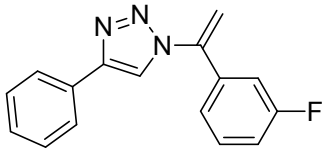
1-(1-(4-chlorophenyl)vinyl)-4-phenyl-1*H*-1,2,3-triazole (**3g**)

White solid; M p, 109.7 – 111.6 ℃; yield, 75% (21.1 mg); IR (neat) 3038, 2934, 1496, 1454, 762 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.7 Hz, 2H), 7.81 (s, 1H), 7.45 – 7.39 (m, 4H), 7.37 – 7.31 (m, 3H), 5.84 (s, 1H), 5.56 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.73, 142.01, 135.97, 133.01, 129.98, 129.10, 128.87, 128.63, 128.43, 125.78, 119.66, 109.78; HRMS (ESI) calcd for $C_{16}H_{13}ClN_3^+$ $[M+H]^+$ 282.0793; found, 282.0793.



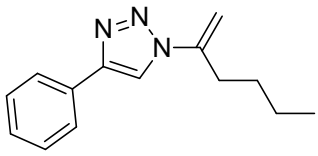
1-(1-(4-bromophenyl)vinyl)-4-phenyl-1*H*-1,2,3-triazole (**3h**)

Yellow oily liquid; yield, 81% (26.3 mg); IR (neat) 3038, 2935, 1496, 1460, 762 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.1 Hz, 2H), 7.81 (s, 1H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.44 (t, *J* = 7.4 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 1H), 7.25 (d, *J* = 6.4 Hz, 2H), 5.86 (s, 1H), 5.57 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.77, 142.09, 133.49, 132.09, 129.98, 128.88, 128.45, 125.79, 124.24, 119.64, 109.99, 109.84; HRMS (ESI) calcd for $C_{16}H_{13}BrN_3^+$ $[M+H]^+$ 326.0287; found, 326.0287.



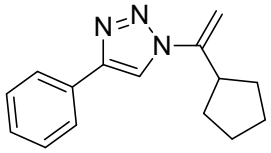
1-(1-(3-fluorophenyl)vinyl)-4-phenyl-1*H*-1,2,3-triazole (**3i**)

Yellow oily liquid; yield, 25% (6.7 mg); IR (neat) 3035, 2934, 1501, 758, 702 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.3 Hz, 2H), 7.82 (s, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.40 – 7.34 (m, 2H), 7.19 – 7.07 (m, 3H), 5.88 (s, 1H), 5.61 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.76 (d, *J* = 274.3 Hz), 147.65, 141.80, 130.53 (d, *J* = 8.3 Hz), 128.88, 128.45, 125.82, 123.02 (d, *J* = 3.1 Hz), 119.72, 116.92 (d, *J* = 21.1 Hz), 114.44 (d, *J* = 23.1 Hz), 110.48; HRMS (ESI) calcd for $C_{16}H_{13}FN_3^+$ $[M+H]^+$ 266.1088; found, 266.1088.



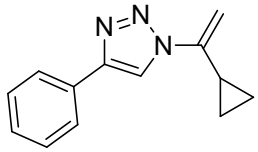
1-(hex-1-en-2-yl)-4-phenyl-1*H*-1,2,3-triazole (**3j**)

White solid; M p, 78.8 – 79.9 ℃; yield, 64% (24.9 mg); IR (neat) 3038, 2934, 1499, 1459, 702 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.97 (s, 1H), 7.87 (d, *J* = 7.4 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 1H), 5.47 (s, 1H), 5.01 (s, 1H), 2.79 (t, *J* = 7.6 Hz, 2H), 1.62 – 1.54 (m, 2H), 1.47 – 1.38 (m, 2H), 0.94 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.48, 143.87, 130.24, 128.85, 128.31, 125.79, 117.28, 109.99, 104.00, 32.58, 29.16, 22.12, 13.79; HRMS (ESI) calcd for $C_{14}H_{18}N_3^+$ $[M+H]^+$ 228.1495; found, 228.1498.



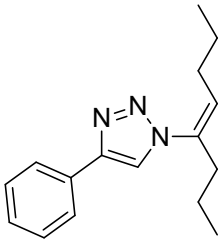
1-(1-cyclopentylvinyl)-4-phenyl-1*H*-1,2,3-triazole (**3k**)

White solid; M p, 56.9 – 57.8 ℃; yield, 80% (19.2 mg); IR (neat) 3041, 2934, 1608, 1499, 756 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.97 (s, 1H), 7.87 (d, *J* = 7.2 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 1H), 5.44 (s, 1H), 5.07 (s, 1H), 3.38 – 3.28 (m, 1H), 2.06 – 2.02 (m, 2H), 1.80 – 1.73 (m, 2H), 1.72 – 1.63 (m, 2H), 1.61 – 1.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.63, 147.20, 130.31, 128.78, 128.17, 125.69, 117.85, 103.04, 42.45, 31.18, 24.72; HRMS (ESI) calcd for $C_{15}H_{18}N_3^+$ $[M+H]^+$ 240.1495; found, 240.1493.



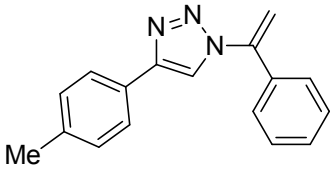
1-(1-cyclopropylvinyl)-4-phenyl-1*H*-1,2,3-triazole (**3l**)

Yellow oily liquid; yield, 64% (13.5 mg); IR (neat) 3041, 2934, 1605, 1501, 1457, 761 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.81 (d, *J* = 6.8 Hz, 2H), 7.38 (t, *J* = 7.2 Hz, 2H), 7.28 (t, *J* = 7.3 Hz, 1H), 5.67 (s, 1H), 4.89 (s, 1H), 1.86 – 1.79 (m, 1H), 0.95 – 0.90 (m, 2H), 0.73 – 0.70 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 130.32, 128.82, 128.22, 125.72, 117.32, 109.97, 102.91, 13.39, 6.44; HRMS (ESI) calcd for $C_{13}H_{14}N_3^+$ $[M+H]^+$ 212.1182; found, 212.1182.



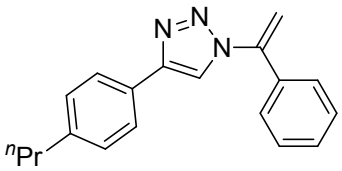
(*Z*)-1-(oct-4-en-4-yl)-4-phenyl-1*H*-1,2,3-triazole (**3m**)[2]

Yellow oily liquid; yield, 58% (14.7 mg); IR (neat) 3061, 2974, 2381, 1429, 768 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.7 Hz, 2H), 7.68 (s, 1H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.27 (t, *J* = 7.3 Hz, 1H), 5.54 (t, *J* = 7.4 Hz, 1H), 2.46 (t, *J* = 7.3 Hz, 2H), 1.89 (q, *J* = 7.2 Hz, 2H), 1.38 – 1.30 (m, 4H), 0.87 – 0.83 (m, 3H), 0.83 – 0.79 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.85, 136.00, 130.46, 128.82, 128.12, 127.31, 125.66, 120.21, 109.97, 38.10, 29.16, 22.49, 20.12, 13.68, 13.26.



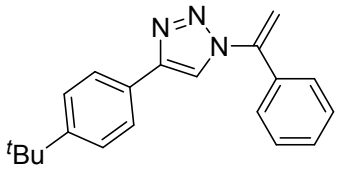
1-(1-phenylvinyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (**4b**)

Yellow oily liquid; yield, 67% (17.5 mg); IR (neat) 3041, 2934, 1501, 1457, 759 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 3.3 Hz, 2H), 7.72 (s, 1H), 7.47 – 7.34 (m, 5H), 7.22 (d, *J* = 7.6 Hz, 2H), 5.84 (s, 1H), 5.53 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.60, 142.94, 138.15, 134.60, 129.81, 129.48, 128.79, 127.30, 125.65, 119.43, 109.26, 21.24; HRMS (ESI) calcd for $C_{17}H_{16}N_3^+$ $[M+H]^+$ 262.1339; found, 262.1339.



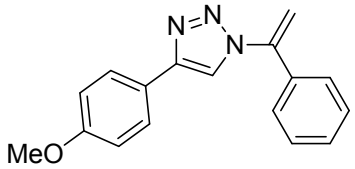
1-(1-phenylvinyl)-4-(4-propylphenyl)-1*H*-1,2,3-triazole (**4c**)

Yellow oily liquid; yield, 84% (24.4 mg); IR (neat) 3035, 2934, 1496, 1457, 703 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.77 (m, 2H), 7.76 (s, 1H), 7.44 – 7.42 (m, 3H), 7.39 – 7.37 (m, =2H), 7.26 – 7.24 (m, 2H), 5.88 (s, 1H), 5.56 (s, 1H), 2.61 (t, *J* = 7.5 Hz, 2H), 1.71 – 1.61 (m, 2H), 0.95 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.25, 142.94, 134.53, 129.92, 129.00, 128.88, 127.84, 127.36, 125.78, 119.60, 110.00, 109.55, 37.81, 24.44, 13.76; HRMS (ESI) calcd for $C_{19}H_{20}N_3^+$ $[M+H]^+$ 290.1652; found, 290.1652.



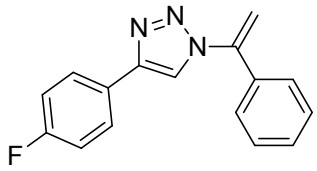
4-(4-(*tert*-butyl)phenyl)-1-(1-phenylvinyl)-1*H*-1,2,3-triazole (**4d**)

Yellow oily liquid; yield, 75% (23.1 mg); IR (neat) 3038, 2937, 1499, 1454, 758, 700 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.77 (m, 3H), 7.51 – 7.31 (m, 7H), 5.85 (s, 1H), 5.54 (s, 1H), 1.34 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.43, 147.53, 142.93, 134.63, 129.82, 128.80, 127.30, 125.73, 125.50, 119.50, 109.29, 34.63, 31.23; HRMS (ESI) calcd for $C_{20}H_{22}N_3^+$ $[M+H]^+$ 304.1808; found, 304.1807.



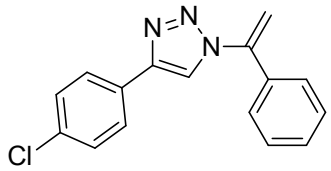
4-(4-methoxyphenyl)-1-(1-phenylvinyl)-1*H*-1,2,3-triazole (**4e**)

Yellow oily liquid; yield, 47% (13.3 mg); IR (neat) 3038, 2932, 1628, 1499, 756 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 8.8 Hz, 2H), 7.72 (s, 1H), 7.49 – 7.40 (m, 3H), 7.39 – 7.37 (m, 2H), 6.96 (d, J = 7.8 Hz, 2H), 5.86 (s, 1H), 5.55 (s, 1H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.82, 142.98, 134.58, 129.91, 128.87, 127.38, 127.20, 122.58, 119.06, 114.30, 110.01, 109.45, 55.33; HRMS (ESI) calcd for $C_{17}H_{16}N_3O^+$ $[M+H]^+$ 278.1288; found, 278.1287.



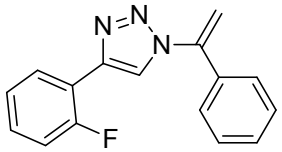
4-(4-fluorophenyl)-1-(1-phenylvinyl)-1*H*-1,2,3-triazole (**4f**)

Yellow oily liquid; yield, 64% (17.1 mg); IR (neat) 3035, 2934, 1499, 1457, 761 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.78 (m, 2H), 7.76 (s, 1H), 7.48 – 7.39 (m, 3H), 7.38 – 7.36 (m, 2H), 7.11 (t, J = 8.6 Hz, 2H), 5.85 (s, 1H), 5.55 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.69 (d, J = 246.1 Hz), 146.67, 142.88, 134.49, 129.89, 128.84, 127.50 (d, J = 8.2 Hz), 127.29, 126.38 (d, J = 3.3 Hz), 119.55, 115.81 (d, J = 21.6 Hz), 109.44; HRMS (ESI) calcd for $C_{16}H_{13}FN_3^+$ $[M+H]^+$ 266.1088; found, 266.1088.



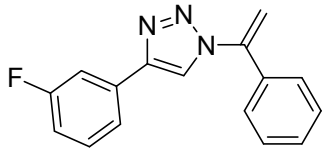
4-(4-chlorophenyl)-1-(1-phenylvinyl)-1*H*-1,2,3-triazole (**4g**)

Yellow oily liquid; yield, 70% (20.0 mg); IR (neat) 3041,2937,1496,1460,705 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.78 (m, 2H), 7.77 (s, 1H), 7.48 – 7.32 (m, 7H), 5.86 (s, 1H), 5.56 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.47, 142.86, 134.44, 134.09, 129.95, 129.04, 128.88, 127.80, 127.31, 127.02, 119.87, 109.57; HRMS (ESI) calcd for $C_{16}H_{13}ClN_3^+$ $[M+H]^+$ 282.0793; found, 282.0792.



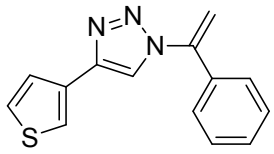
4-(2-fluorophenyl)-1-(1-phenylvinyl)-1*H*-1,2,3-triazole (**4h**)

Yellow oily liquid; yield, 62% (16.5 mg); IR (neat) 3035, 2931, 1496, 1457, 758 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.37 (td, *J* = 7.6, 1.8 Hz, 1H), 7.99 (d, *J* = 3.6 Hz, 1H), 7.44 – 7.40 (m, 3H), 7.39 – 7.36 (m, 2H), 7.34 – 7.27 (m, 2H), 7.15 – 7.11 (m, 1H), 5.86 (s, 1H), 5.59 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.17 (d, *J* = 246.8 Hz), 142.97, 134.47, 129.89, 129.50 (d, *J* = 8.5 Hz), 128.83, 127.92 (d, *J* = 3.5 Hz), 127.24, 124.62 (d, *J* = 3.3 Hz), 122.92 (d, *J* = 12.8 Hz), 115.65 (d, *J* = 21.5 Hz), 109.64; HRMS (ESI) calcd for $C_{16}H_{13}FN_3^+$ $[M+H]^+$ 266.1088; found, 266.1084.



4-(3-fluorophenyl)-1-(1-phenylvinyl)-1*H*-1,2,3-triazole (**4i**)

Yellow oily liquid; yield, 58% (15.5 mg); IR (neat) 3035, 2931, 1496, 1457, 758 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.59 (t, *J* = 10.2 Hz, 2H), 7.45 – 7.41 (m, 3H), 7.38 (s, 3H), 7.03 (t, *J* = 8.4 Hz, 1H), 5.87 (s, 1H), 5.57 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.12 (d, *J* = 244.5 Hz), 142.85, 134.46, 132.32 (d, *J* = 8.5 Hz), 130.43 (d, *J* = 8.5 Hz), 129.97, 128.90, 127.32, 121.37 (d, *J* = 3.0 Hz), 120.17, 115.14 (d, *J* = 21.1 Hz), 112.73 (d, *J* = 22.9 Hz), 109.98, 109.60; HRMS (ESI) calcd for $C_{16}H_{13}FN_3^+$ $[M+H]^+$ 266.1088; found, 266.1088.



1-(1-phenylvinyl)-4-(thiophen-3-yl)-1*H*-1,2,3-triazole (**4j**)

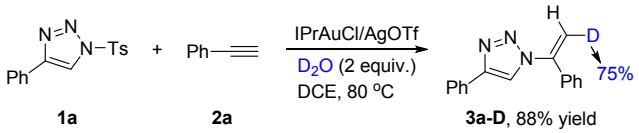
Yellow oily liquid; yield, 84% (21.3 mg); IR (neat) 3038, 2934, 1501, 1460, 759 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.70 (s, 1H), 7.46 – 7.41 (m, 4H), 7.39 – 7.36 (m, 3H), 5.85 (s, 1H), 5.55 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.74, 142.87, 134.56, 131.37, 129.87, 128.83, 127.30, 126.39, 125.74, 121.42, 119.57, 109.42; HRMS (ESI) calcd for $C_{14}H_{12}N_3S^+$ $[M+H]^+$ 254.0746; found, 254.0747.

3. References

1. E. J. Yoo, M. Ahlquist, S. H. Kim, I. Bae, V. V. Fokin, K. B. Sharpless, S. Chang, *Angew. Chem. Int. Ed.,* 2007, **46**, 1730.

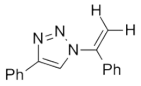
2. H. F. Duan, W. M. Yan, S. Sengupta and X. D. Shi, *Bioorg. Med. Chem. Lett.*, 2009, **19**, 3899.

4. Deuterium-Labeling Experiment Result

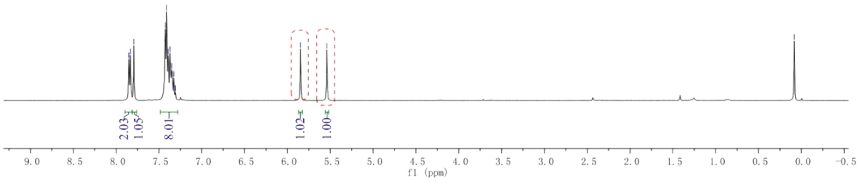


1a **2a** **3a-D**, 88% yield

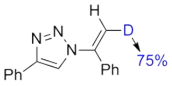
H^1 NMR of **3a**



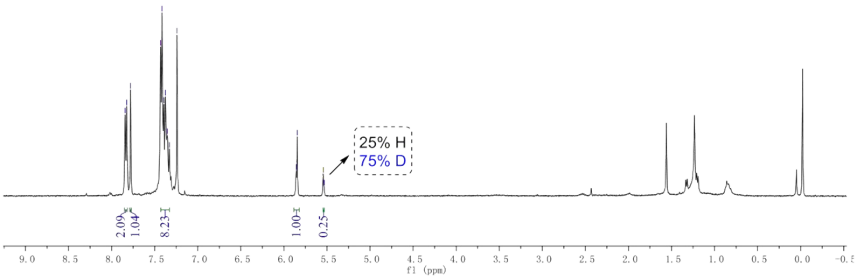
3a



H^1 NMR of **3a-D**

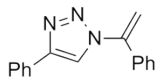


3a-D

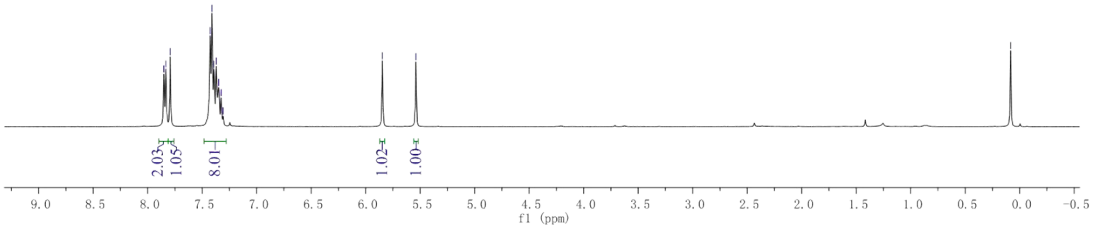


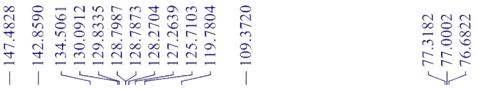
The incorporation of deuterium at the f1 = 5.53 ppm of **3a** is (1-0.25)/1*100% = 75%.

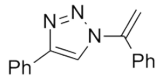
5. ^{1}H and ^{13}C NMR Spectra



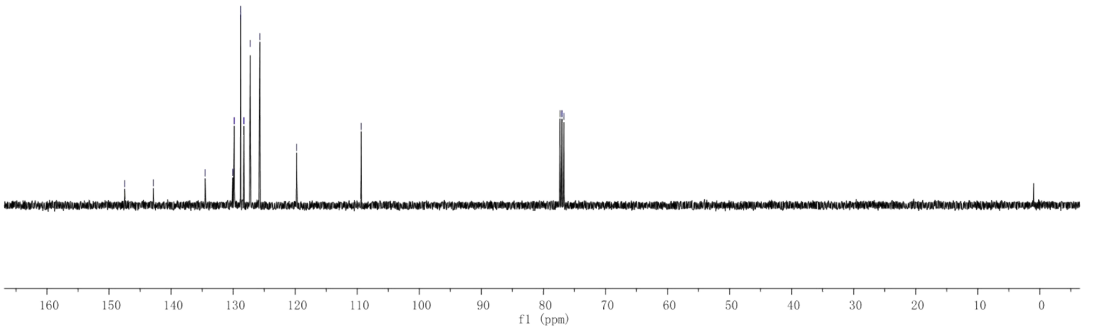
3a

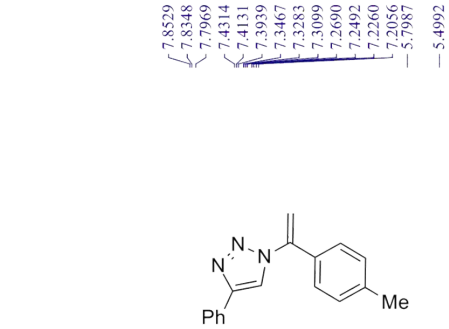




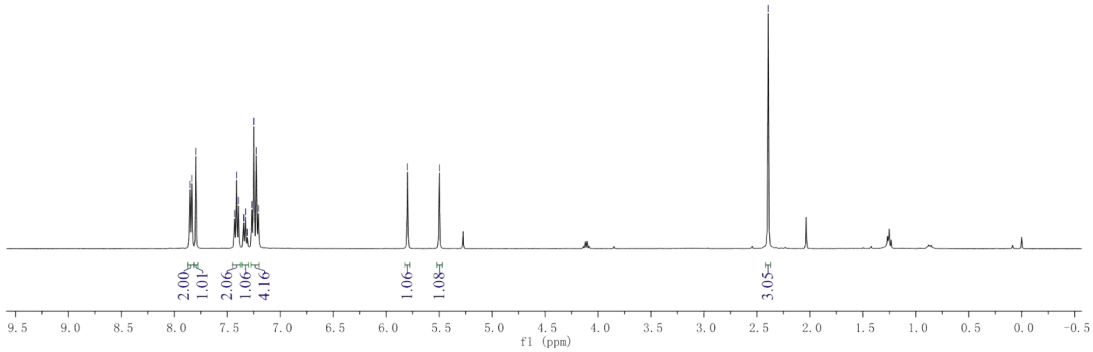


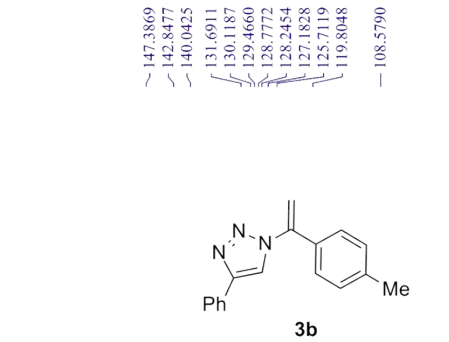
3a



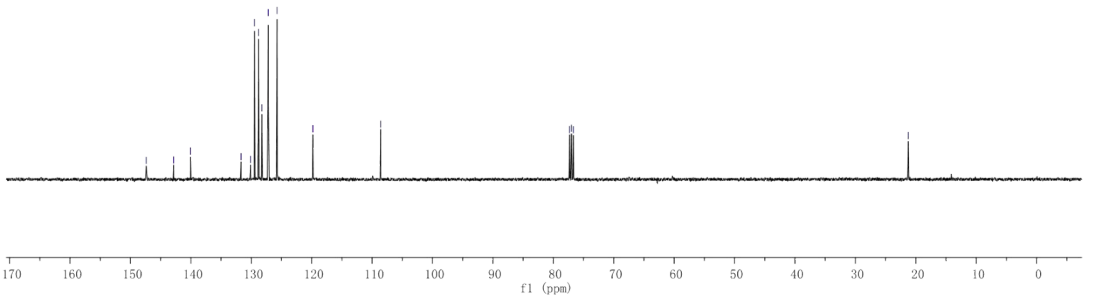

7.8529
7.8348
7.7969
7.4314
7.4131
7.3939
7.3467
7.3283
7.3099
7.2690
7.2492
7.2260
7.2056
5.7987
5.4992
2.3929
N
N
N
Ph
Me

3b

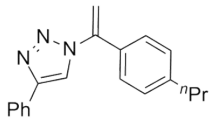

2.00
1.01
2.06
1.06
4.16
1.06
1.08
3.05
f1 (ppm)


147.3869
142.8477
140.0425
131.6911
130.1187
129.4660
128.7772
128.2454
127.1828
125.7119
119.8048
108.5790
77.3176
76.9998
76.6818
21.2446
N
N
N
Ph
Me

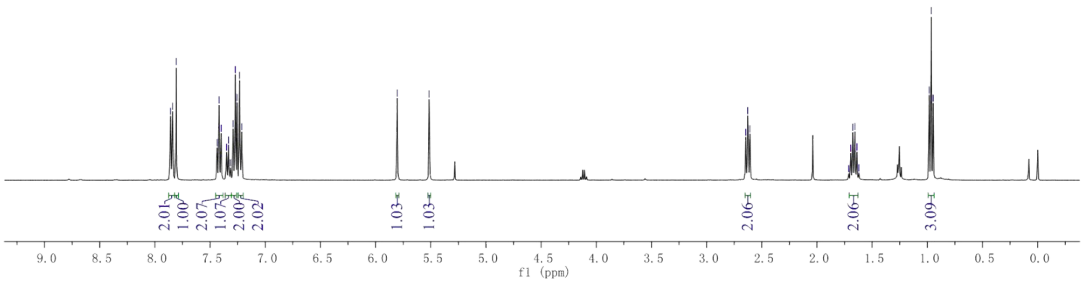
3b


f1 (ppm)

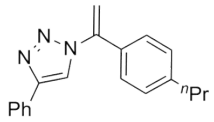

7.8585
7.8407
7.8069
7.4367
7.4186
7.3993
7.3509
7.3325
7.2916
7.2710
7.2554
7.2330
5.5145
2.6460
2.6274
2.6077
1.7128
1.6943
1.6756
1.6566
1.6379
1.6195
0.9835
0.9652
0.9468


N
N
N
Ph
nPr

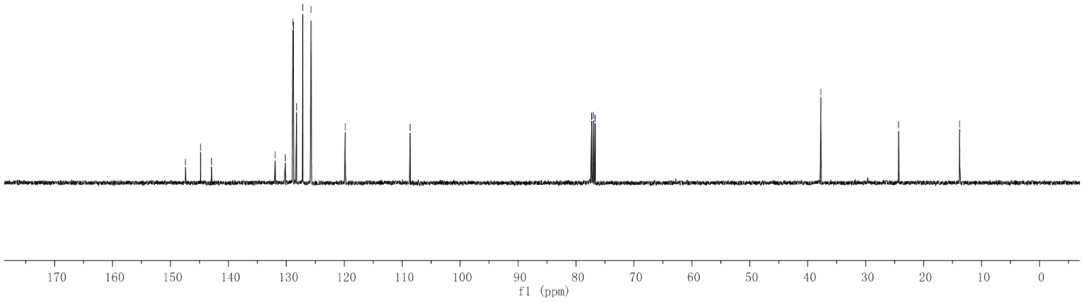
3c

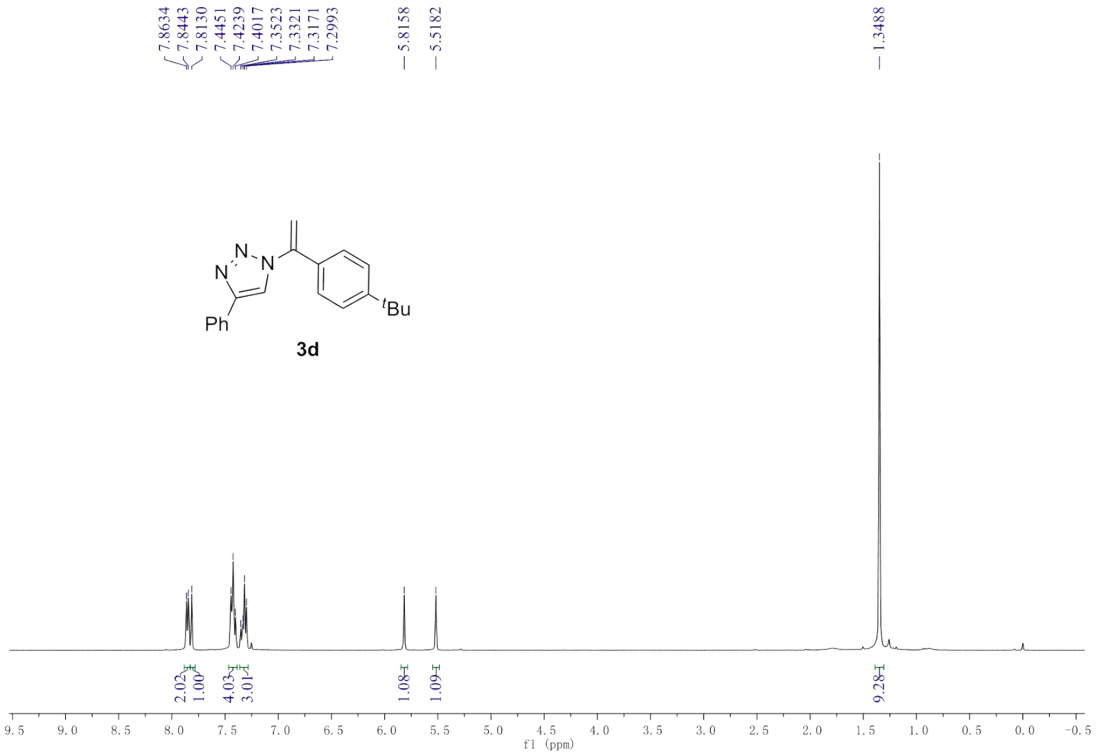

2.01
1.00
2.07
1.07
2.00
2.02
1.03
1.03
2.06
2.06
3.09
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


147.4215
144.8192
142.9162
131.9241
130.1850
128.8845
128.7848
128.2415
127.1620
125.7363
119.8426
108.6399
77.3190
77.0002
76.6825
37.7239
24.3198
13.7708

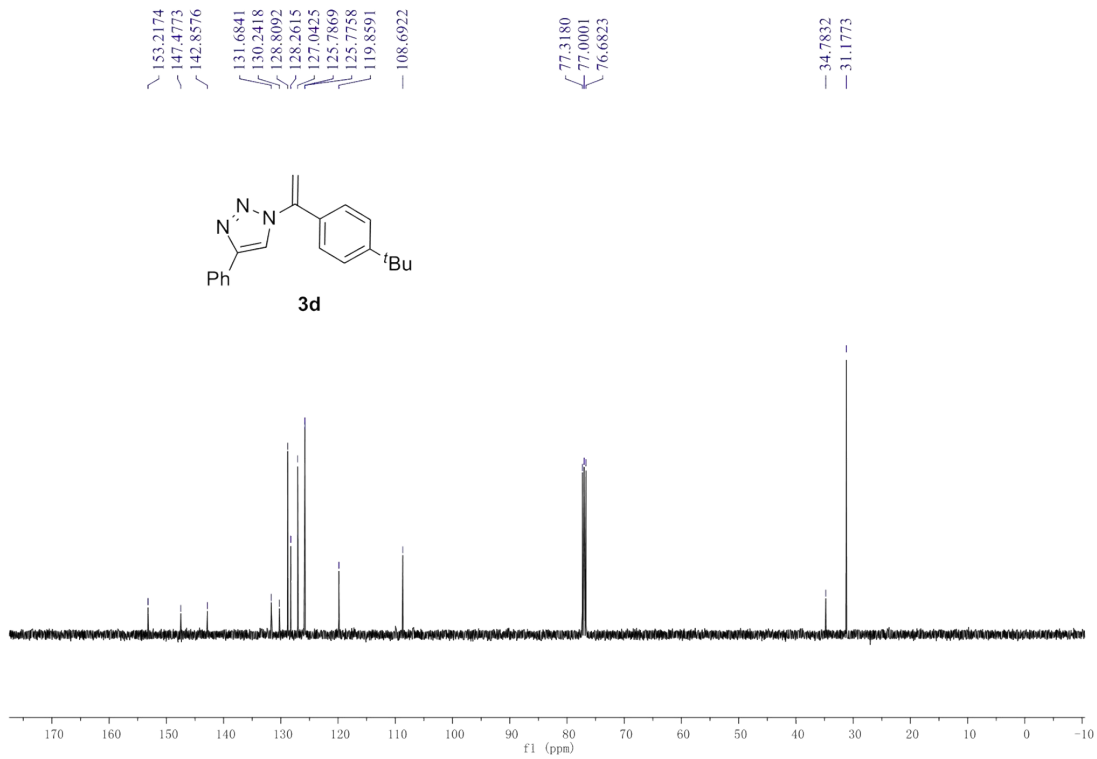

N
N
N
Ph
nPr

3c

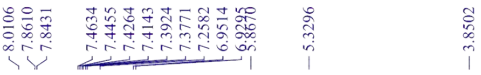

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

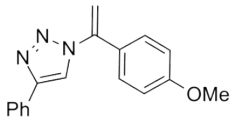

7.8634
7.8443
7.8130
7.4451
7.4239
7.4017
7.3523
7.3321
7.3171
7.2993
5.8158
5.5182
1.3488
N
N
N
Ph
tBu
2.02
1.00
4.03
3.01
1.08
1.09
9.28
f1 (ppm)

3d

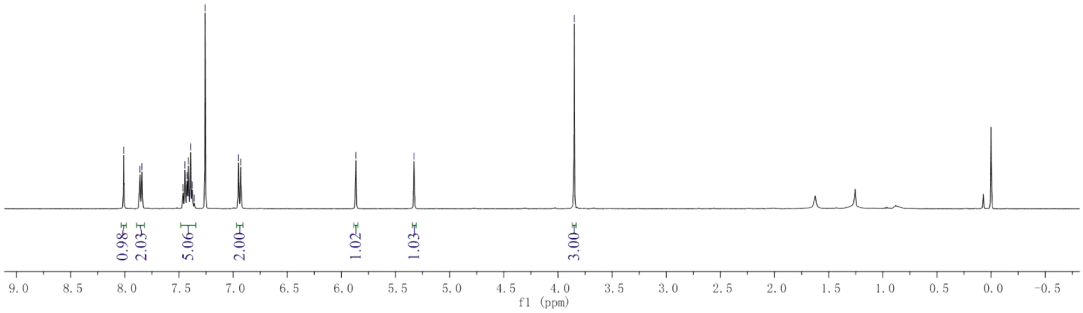

153.2174
147.4773
142.8576
131.6841
130.2418
128.8092
128.2615
127.0425
125.7869
125.7758
119.8591
108.6922
77.3180
77.0001
76.6823
34.7832
31.1773
N
N
N
Ph
tBu
f1 (ppm)

3d

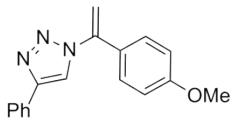

8.0106
7.8610
7.8431
7.4634
7.4455
7.4264
7.4143
7.3924
7.3771
7.2582
6.9514
6.9295
5.8670
5.3296
3.8502


N
N
N
Ph
OMe

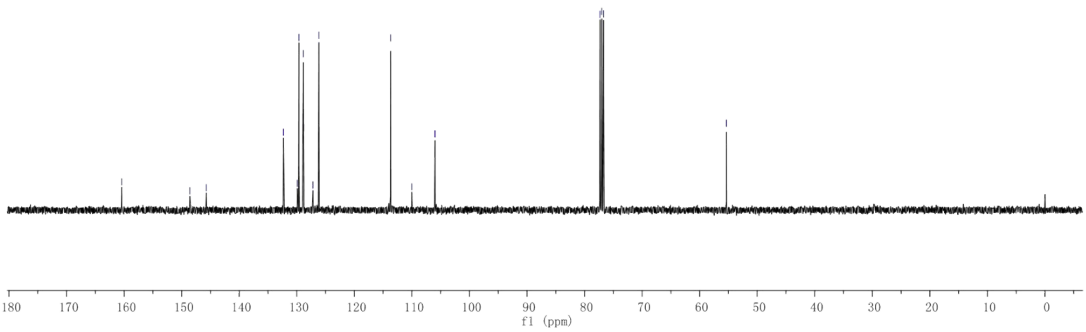
3e


0.98
2.03
5.06
2.00
1.02
1.03
3.00
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)

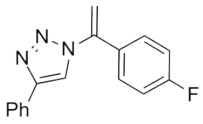

160.3958
148.5636
145.7457
132.3186
129.9204
129.6323
128.8759
128.8025
127.1978
126.1808
113.7052
110.0016
105.9776
77.3176
77.0000
76.6825
55.3396


N
N
N
Ph
OMe

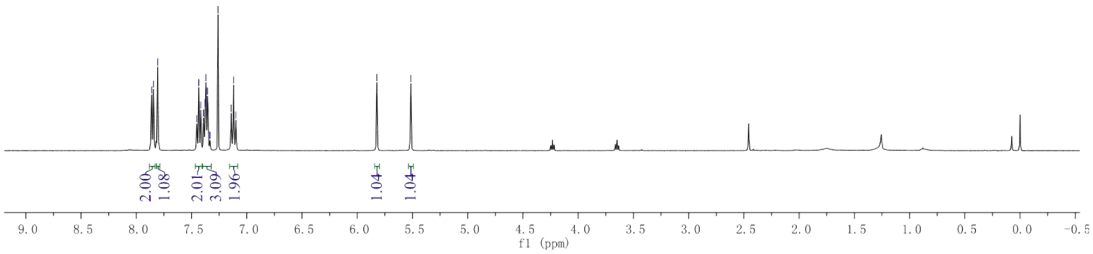
3e


180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

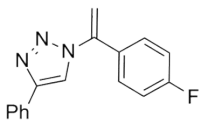

7.8623
7.8440
7.8067
7.4345
7.4152
7.3905
7.3770
7.3694
7.3553
7.2603
7.1411
7.1198
5.5153


N
N
N
Ph
F

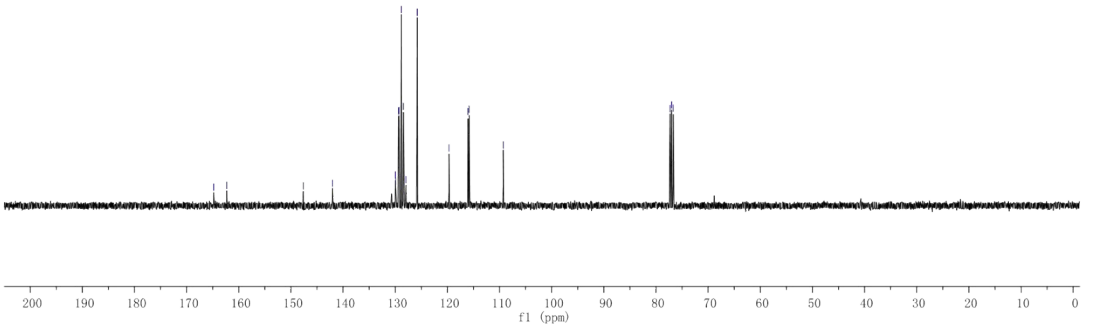
3f


2.00
1.08
2.01
3.09
1.96
1.04
1.04
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)

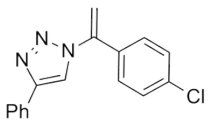

164.7973
162.3053
147.6278
142.0224
129.9609
129.9130
129.3648
129.2807
128.8559
128.4190
127.9388
125.7759
119.6924
116.0543
115.8362
109.2816
77.3183
77.0005
76.6826


N
N
N
Ph
F

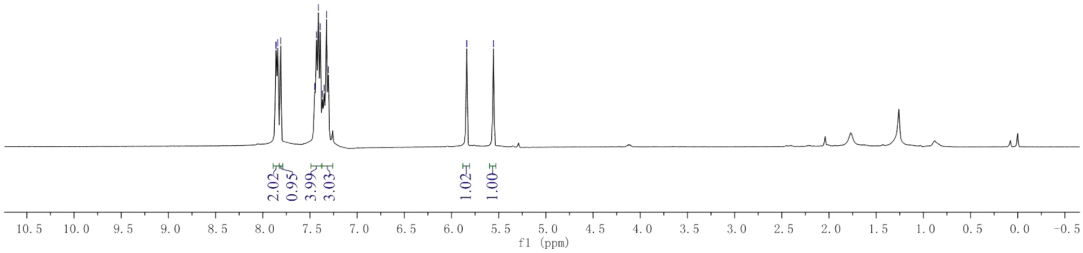
3f


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

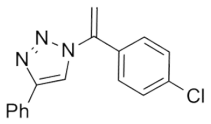

7.8598
7.8406
7.8101
7.4486
7.4307
7.4108
7.3891
7.3674
7.3489
7.3244
7.3038
5.8384
5.5552


N
N
N
Ph
Cl

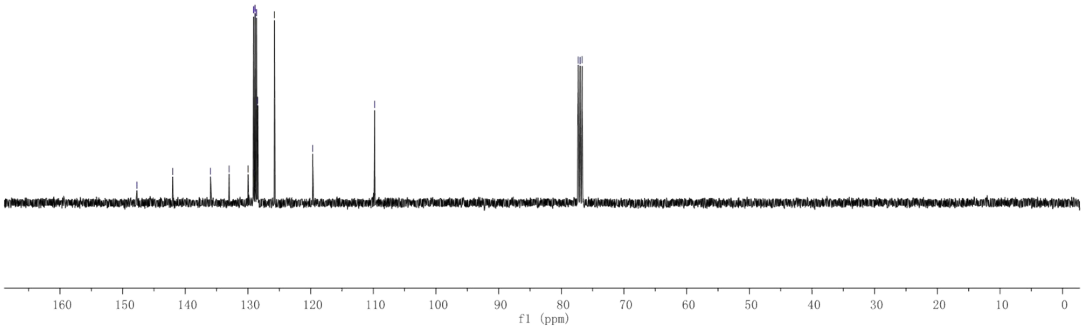
3g


2.02
0.95
3.99
3.03
1.02
1.00
10.5 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)

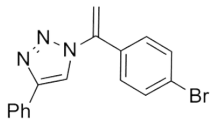

147.7257
142.0124
129.9797
129.1039
128.8661
128.6267
128.4298
125.7775
119.8614
109.7828
77.3177
77.0001
76.6821


N
N
N
Ph
Cl

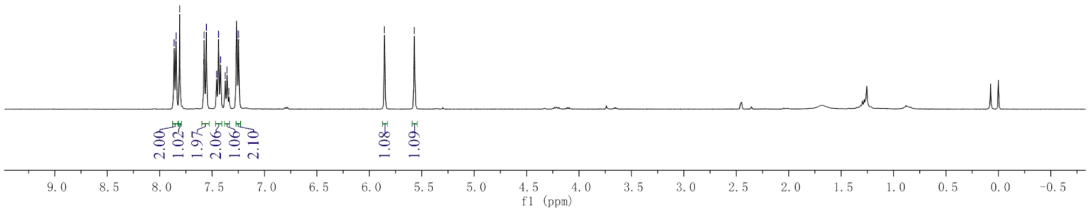
3g

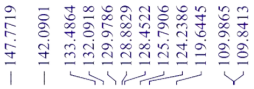

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

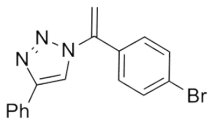

7.8617
7.8439
7.8092
7.5763
7.5549
7.4566
7.4386
7.4194
7.3750
7.3568
7.3382
7.2625
7.2465
5.8562
5.5715


N
N
N
Ph
Br

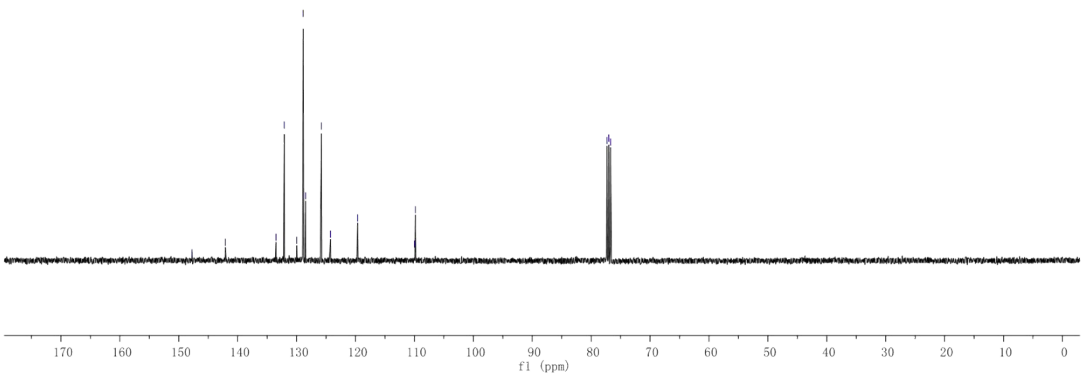
3h

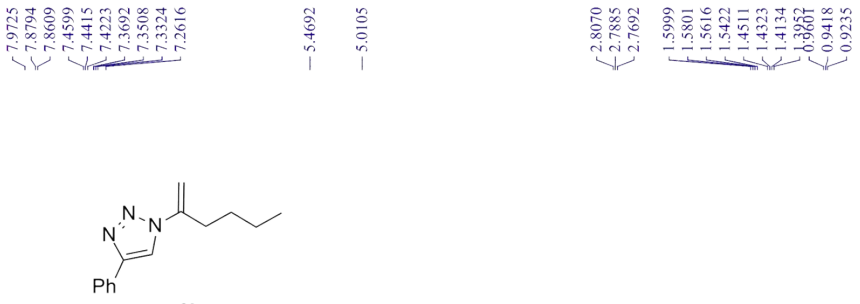

2.00
1.02
1.97
2.06
1.06
2.10
1.08
1.09
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


147.7719
142.0901
133.4864
132.0918
129.9786
128.8829
128.4522
125.7906
124.2386
119.6445
109.9865
109.8413
77.3182
77.0004
76.6826


N
N
N
Ph
Br

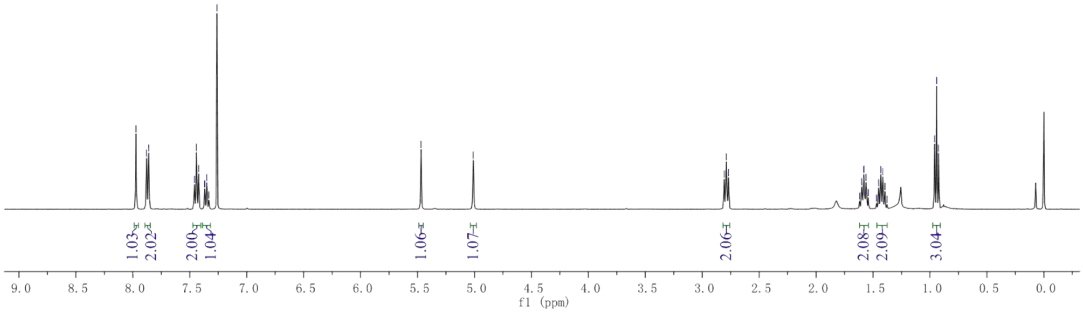
3h

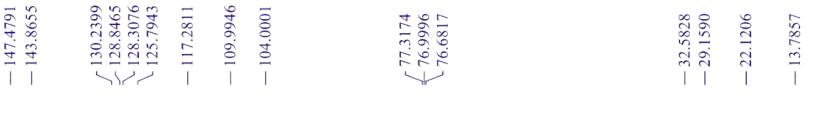

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

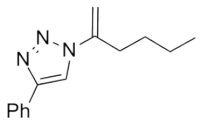

7.9725
7.8794
7.8609
7.4599
7.4415
7.4223
7.3692
7.3508
7.3324
7.2616
5.4692
5.0105
2.8070
2.7885
2.7692
1.5999
1.5801
1.5616
1.5422
1.4511
1.4323
1.4134
1.3952
0.9601
0.9418
0.9235

N
N
N
Ph

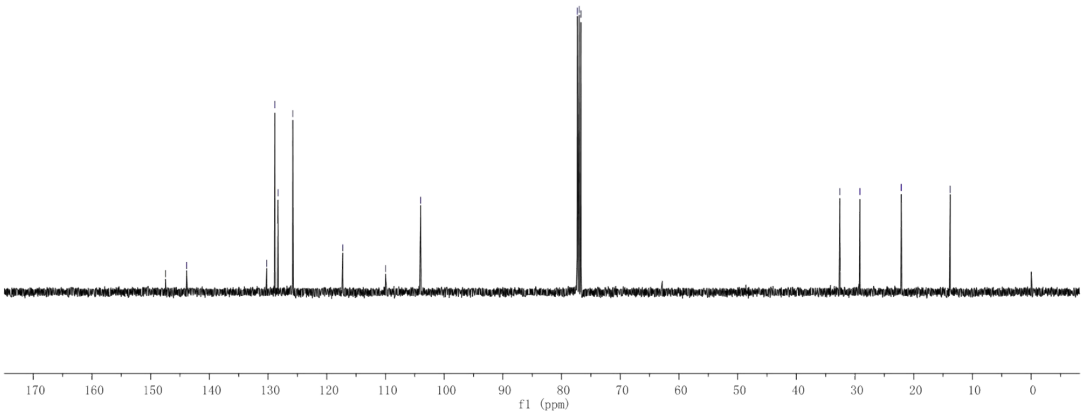
3j


1.03
2.02
2.00
1.04
1.06
1.07
2.06
2.08
2.09
3.04
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)


147.4791
143.8655
130.2399
128.8465
128.3076
125.7943
117.2811
109.9946
104.0001
77.3174
76.9996
76.6817
32.5828
29.1590
22.1206
13.7857

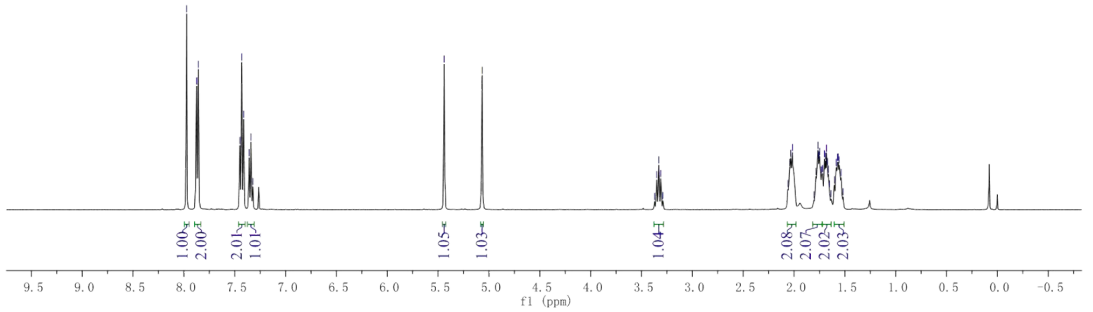

N
N
N
Ph

3j


170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.9733
7.8764
7.8583
7.4494
7.4310
7.4117
7.3578
7.3396
7.3209
5.4403
5.0670
3.3713
3.3504
3.3304
3.3099
3.2899
2.0421
2.0331
2.0159
1.7843
1.7640
1.7536
1.7476
1.7304
1.7202
1.7006
1.6887
1.6808
1.6700
1.6615
1.6033
1.5853
1.5714
1.5662
1.5559
1.5365
N
N
N
Ph

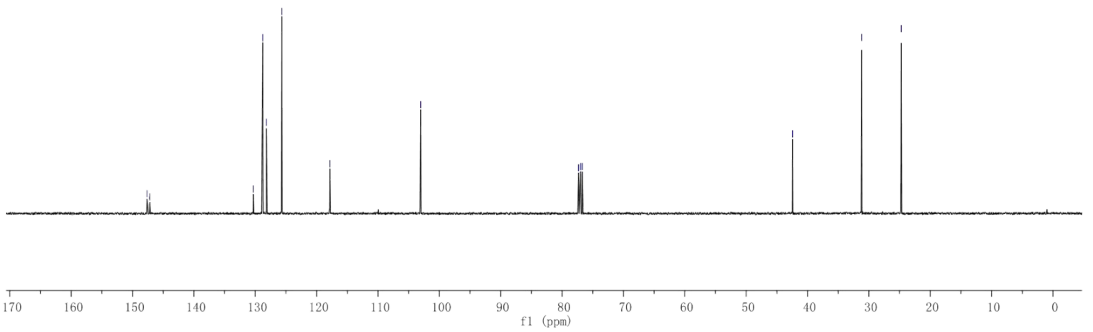
3k

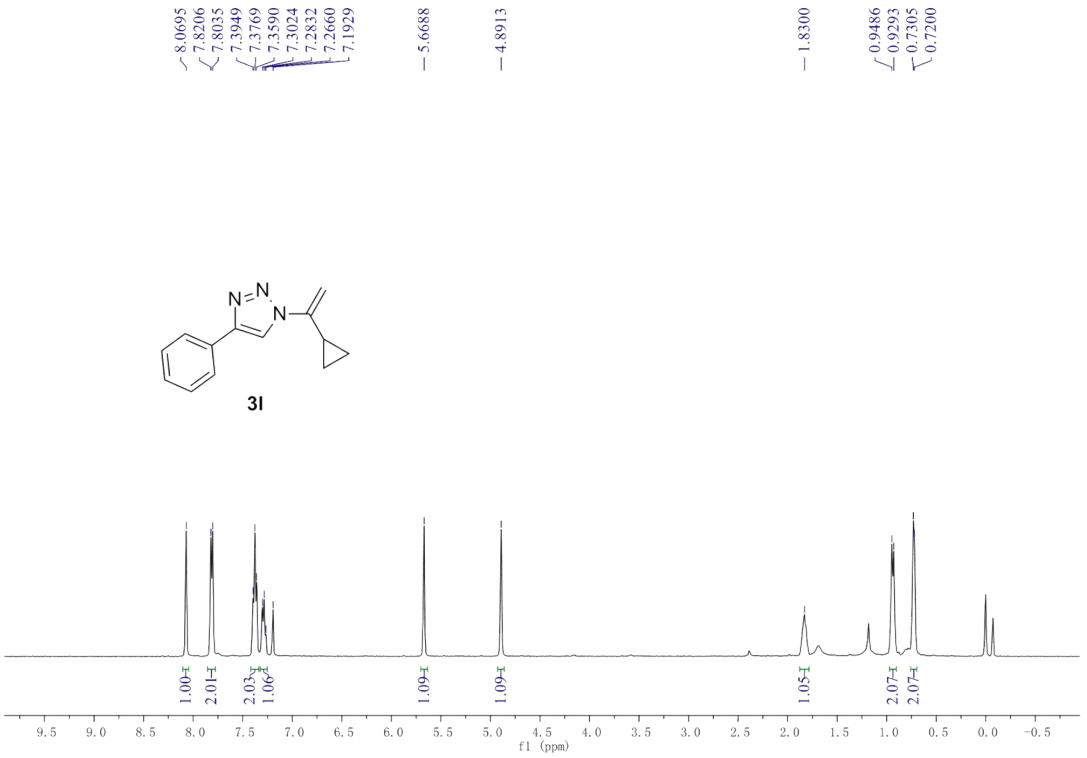

1.00
2.00
2.01
1.01
1.05
1.03
1.04
2.08
2.07
2.02
2.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

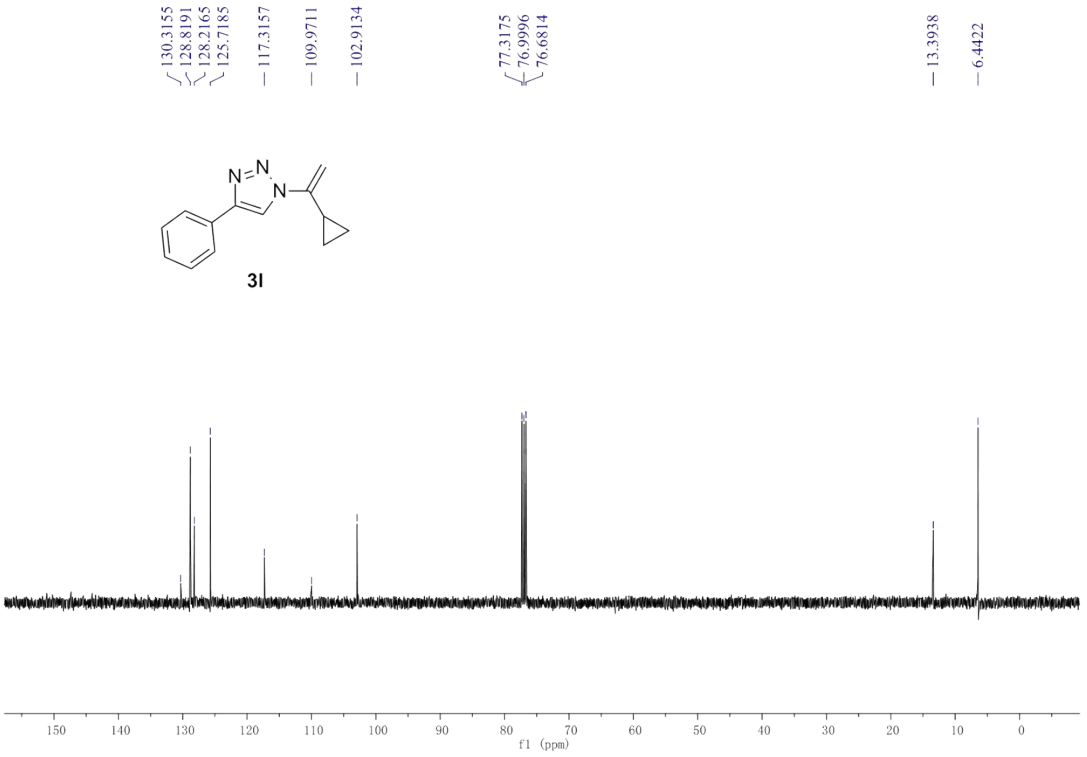

147.6284
147.2016
130.3061
128.7767
128.1724
125.6850
117.8481
103.0419
77.3183
77.0001
76.6824
42.4494
31.1817
24.7214

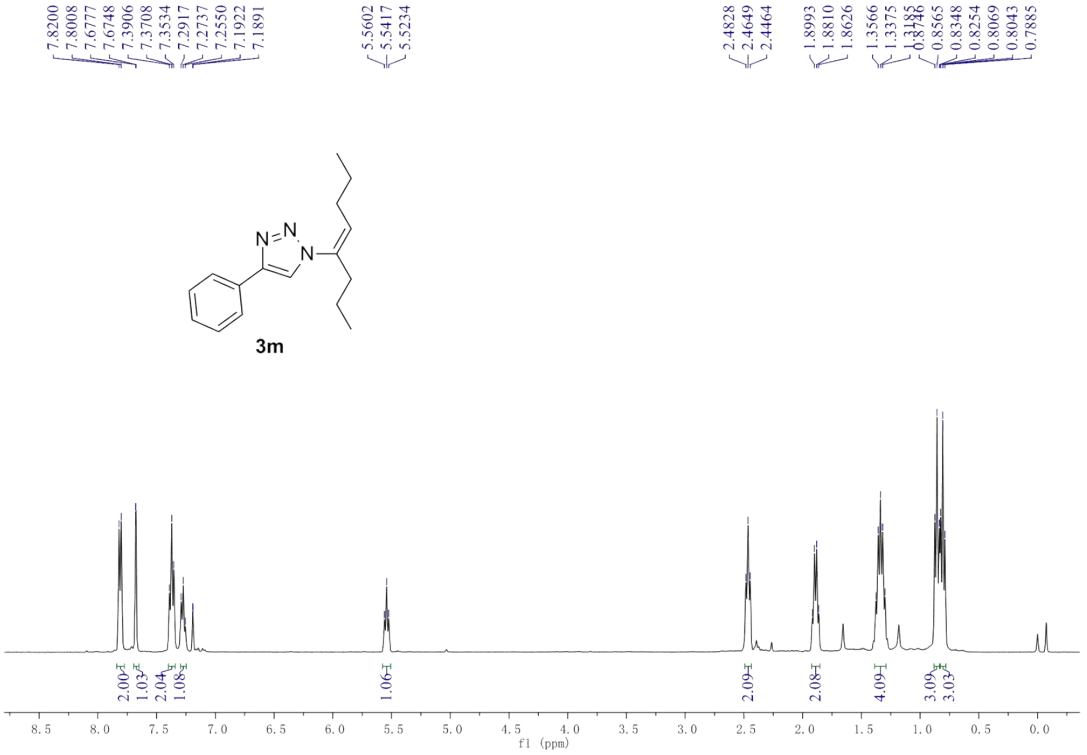
N
N
N
Ph

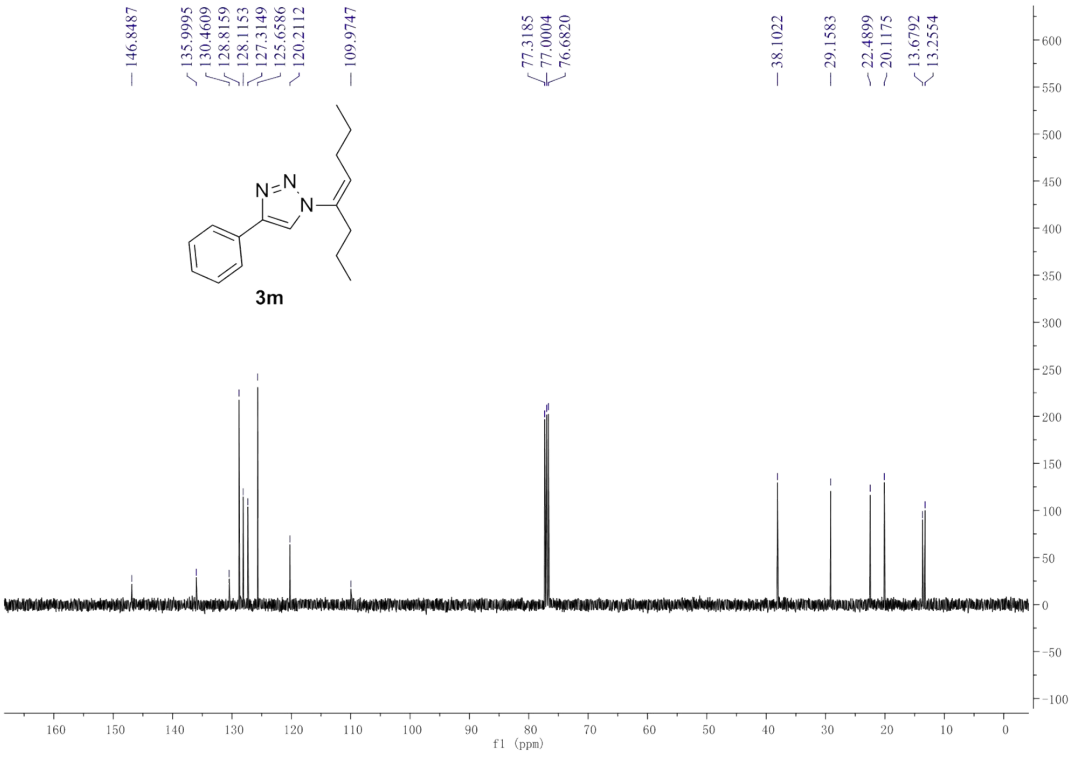
3k

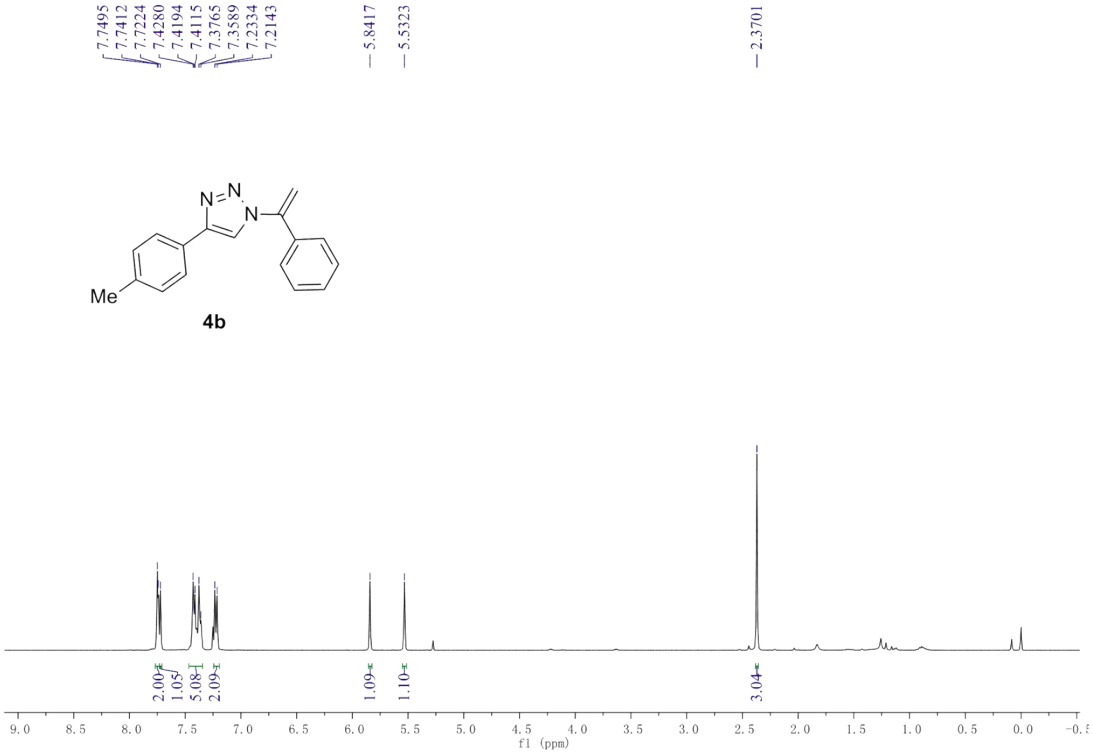

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

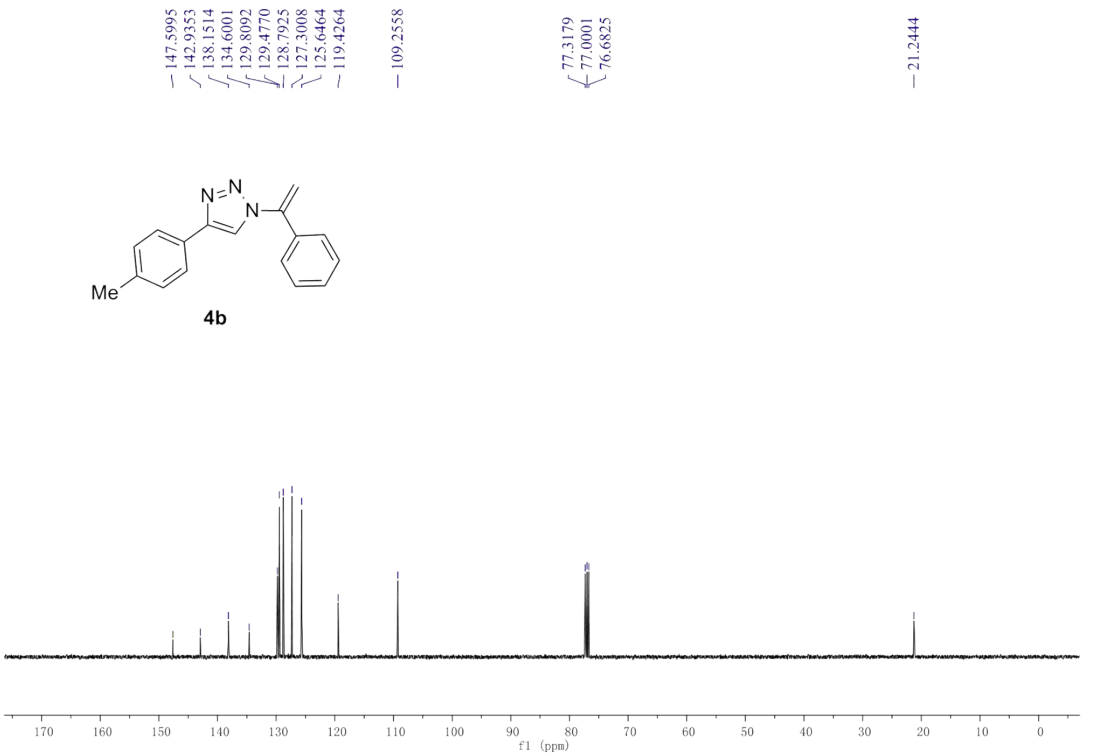

8.0695
7.8206
7.8035
7.3949
7.3769
7.3590
7.3024
7.2832
7.2660
7.1929
5.6688
4.8913
1.8300
0.9486
0.9293
0.7305
0.7200
3l
1.00
2.01
2.03
1.06
1.09
1.09
1.05
2.07
2.07
f1 (ppm)

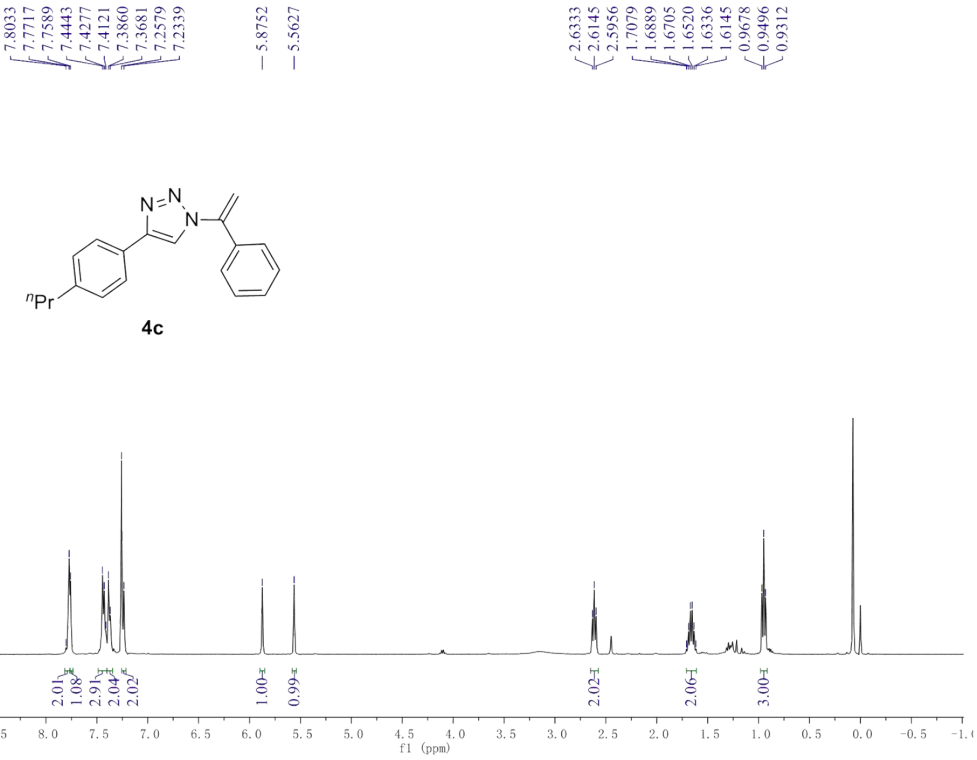

130.3155
128.8191
128.2165
125.7185
117.3157
109.9711
102.9134
77.3175
76.9996
76.6814
13.3938
6.4422
3l
f1 (ppm)

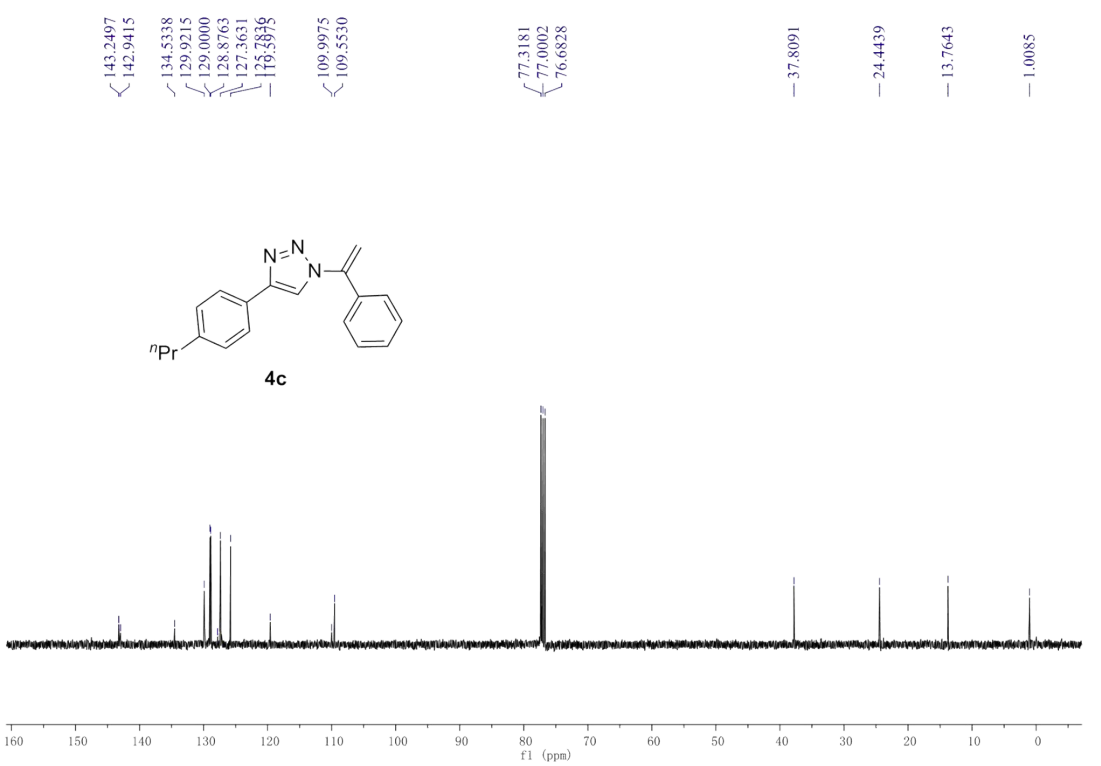

7.8200
7.8008
7.6777
7.6748
7.3906
7.3708
7.3534
7.2917
7.2737
7.2550
7.1922
7.1891
5.5602
5.5417
5.5234
2.4828
2.4649
2.4464
1.8993
1.8810
1.8626
1.3566
1.3375
1.3185
0.8746
0.8565
0.8348
0.8254
0.8069
0.8043
0.7885
3m
2.00
1.03
2.04
1.08
1.06
2.09
2.08
4.09
3.09
3.03
f1 (ppm)

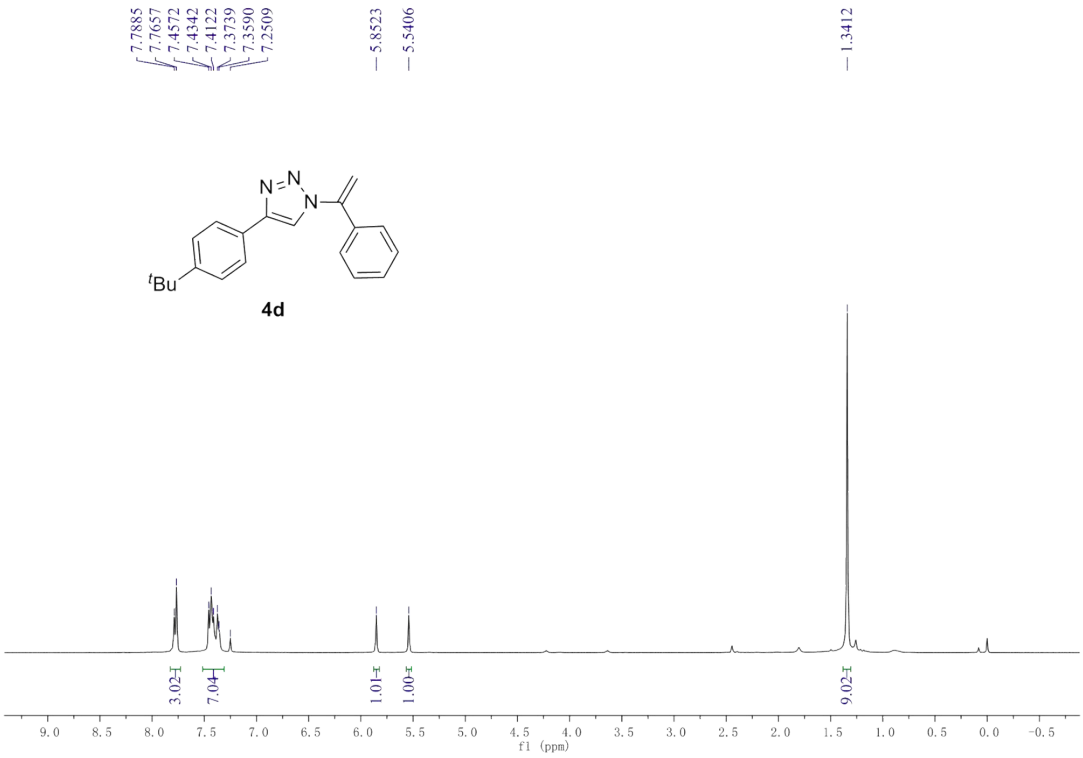

146.8487
135.9995
130.4609
128.8159
128.1153
127.3149
125.6586
120.2112
109.9747
77.3185
77.0004
76.6820
38.1022
29.1583
22.4899
20.1175
13.6792
13.2554
3m
f1 (ppm)

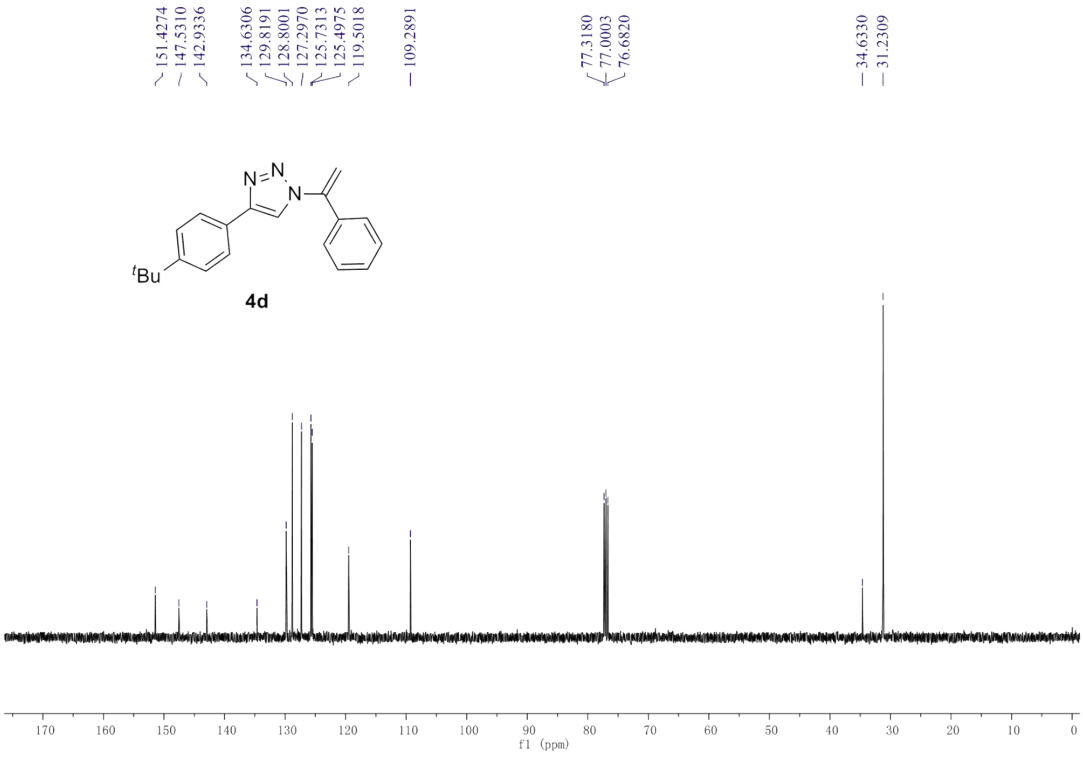

7.7495
7.7412
7.7224
7.4280
7.4194
7.4115
7.3765
7.3589
7.2334
7.2143
5.8417
5.5323
2.3701
Me
4b
2.00
1.05
5.08
2.09
1.09
1.10
3.04
f1 (ppm)

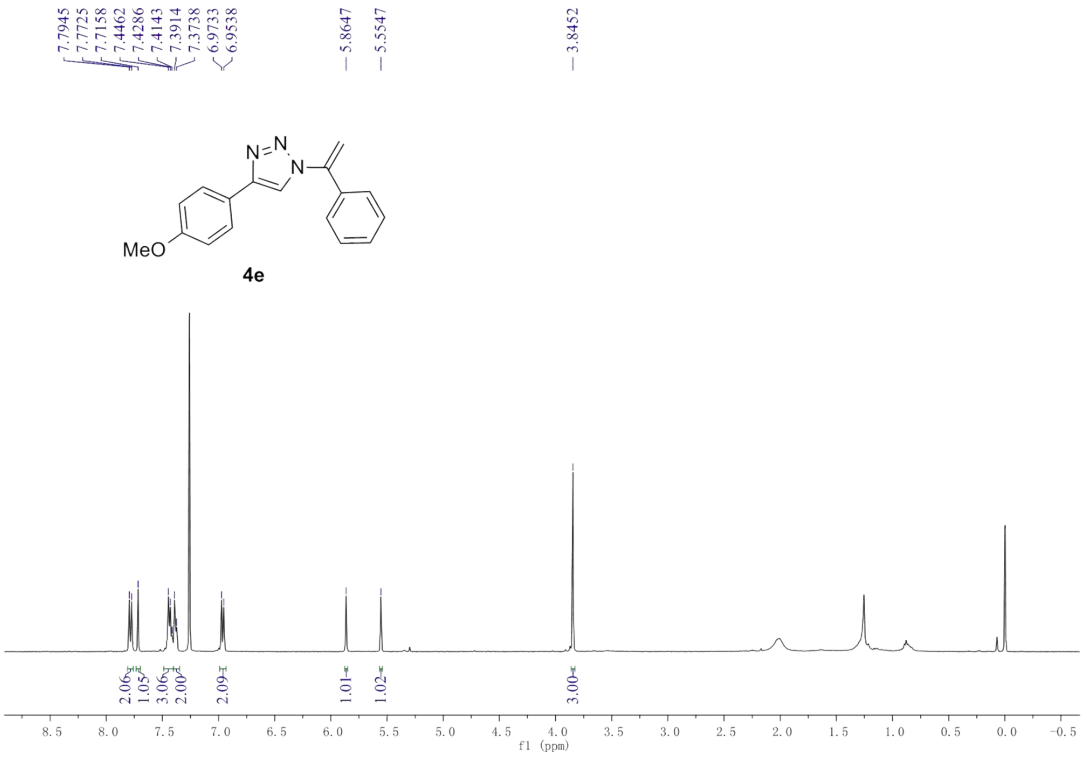

147.5995
142.9353
138.1514
134.6001
129.8092
129.4770
128.7925
127.3008
125.6464
119.4264
109.2558
77.3179
77.0001
76.6825
21.2444
Me
4b
f1 (ppm)

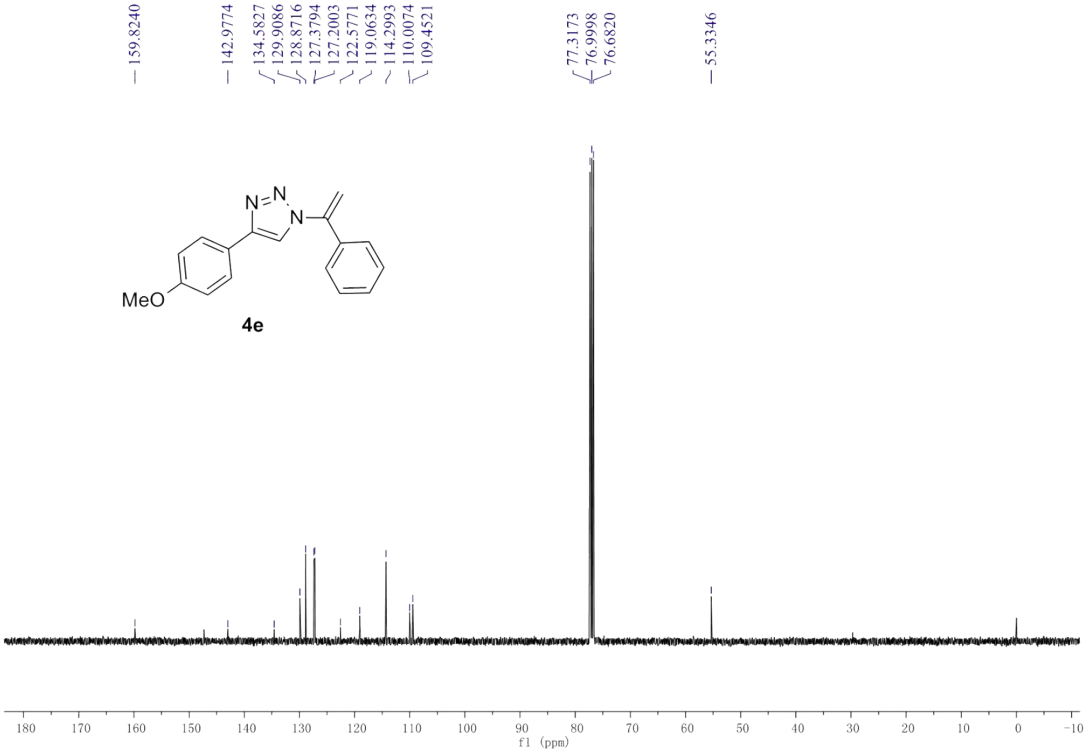

7.8033
7.7717
7.7589
7.4443
7.4277
7.4121
7.3860
7.3681
7.2579
7.2339
5.8752
5.5627
2.6333
2.6145
2.5956
1.7079
1.6889
1.6705
1.6520
1.6336
1.6145
0.9678
0.9496
0.9312
nPr
4c
2.01
1.08
2.91
2.04
2.02
1.00
0.99
2.02
2.06
3.00
f1 (ppm)


143.2497
142.9415
134.5338
129.9215
129.0000
128.8763
127.3631
109.9975
109.5530
77.3181
77.0002
76.6828
37.8091
24.4439
13.7643
1.0085
nPr
4c
f1 (ppm)

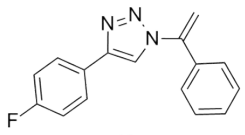

7.7885
7.7657
7.4572
7.4342
7.4122
7.3739
7.3590
7.2509
5.8523
5.5406
1.3412
tBu
4d
3.02
7.04
1.01
1.00
9.02
f1 (ppm)


151.4274
147.5310
142.9336
134.6306
129.8191
128.8001
127.2970
125.7313
125.4975
119.5018
109.2891
77.3180
77.0003
76.6820
34.6330
31.2309
tBu
4d
f1 (ppm)

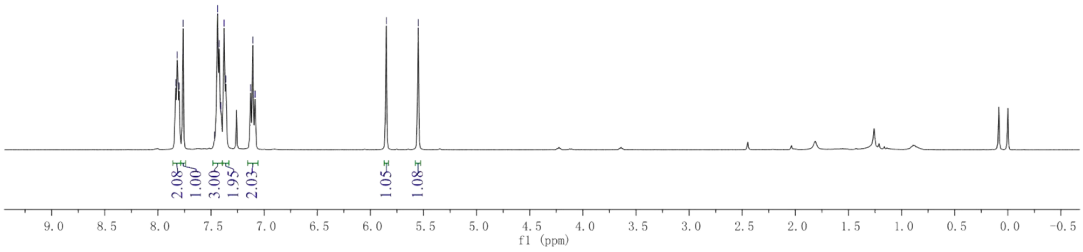

7.7945
7.7725
7.7158
7.4462
7.4286
7.4143
7.3914
7.3738
6.9733
6.9538
5.8647
5.5547
3.8452
MeO
4e
2.06
1.05
3.06
2.00
2.09
1.01
1.02
3.00
f1 (ppm)

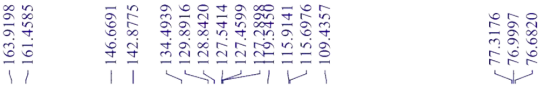

159.8240
142.9774
134.5827
129.9086
128.8716
127.3794
127.2003
122.5771
119.0634
114.2993
110.0074
109.4521
77.3173
76.9998
76.6820
55.3346
MeO
4e
f1 (ppm)

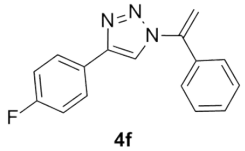

7.8321
7.8184
7.7993
7.7630
7.4679
7.4378
7.4220
7.4080
7.3775
7.3605
7.1279
7.1063
7.0847
5.8499
5.5492


N
N
N
F

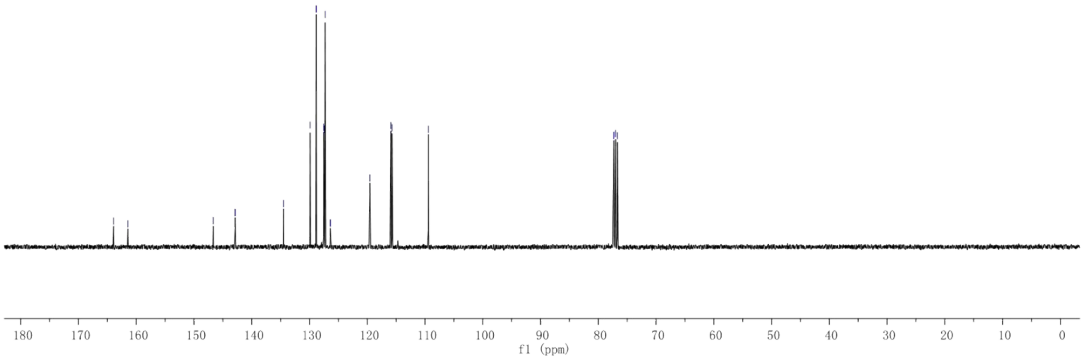
4f


2.08
1.00
3.00
1.95
2.03
1.05
1.08
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)

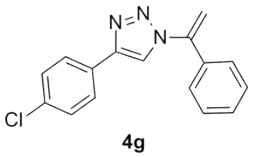

163.9198
161.4585
146.6691
142.8775
134.4939
129.8916
128.8420
127.5414
127.4599
127.2898
119.5450
115.9141
115.6976
109.4357
77.3176
76.9997
76.6820


N
N
N
F

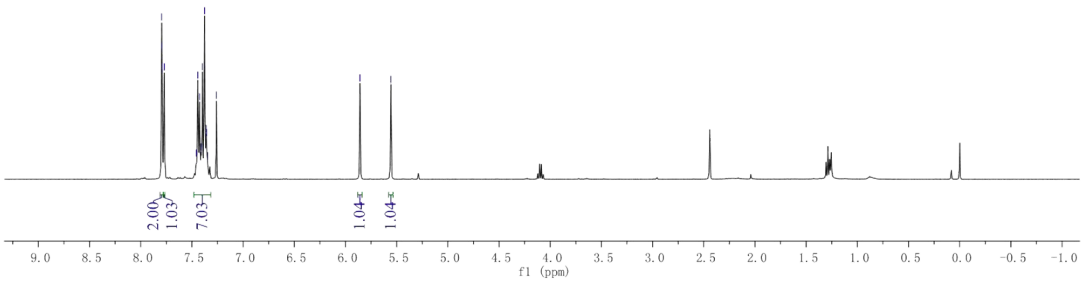
4f


180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

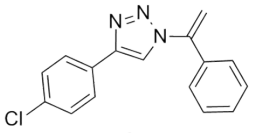

7.7958
7.7925
7.7704
7.4563
7.4432
7.4252
7.4110
7.3977
7.3764
7.3600
7.3555
7.3464
7.2606
5.8586
5.5572


N
N
N
Cl

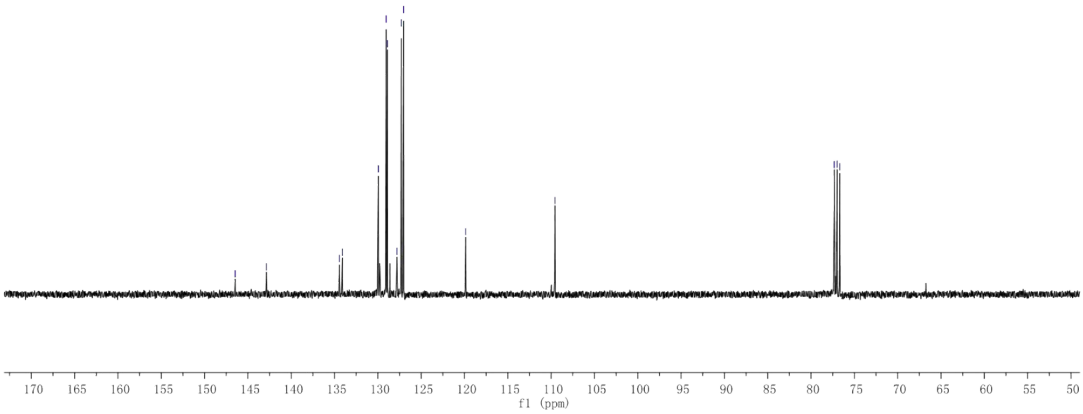
4g


2.00
1.03
7.03
1.04
1.04
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 -1.0
f1 (ppm)

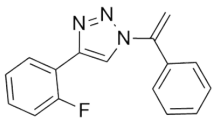

146.4696
142.8613
134.4415
134.0933
129.9453
129.0403
128.8816
127.7981
127.3101
127.0222
119.8701
109.5659
77.3179
77.0003
76.6824


N
N
N
Cl

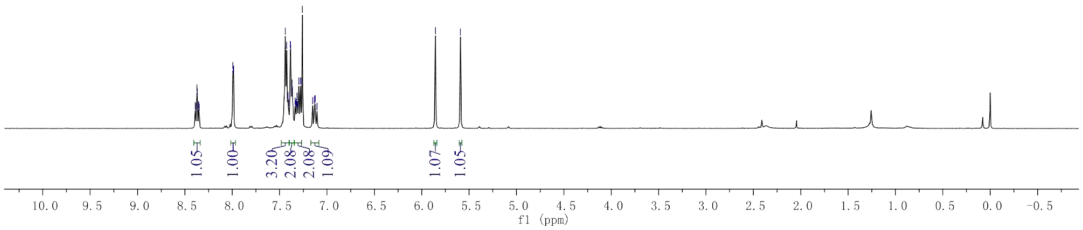
4g


170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50
f1 (ppm)

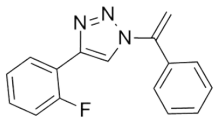

8.3920
8.3879
8.3731
8.3689
8.3546
8.3499
7.9942
7.9853
7.4410
7.4251
7.3871
7.3836
7.3683
7.3637
7.2983
7.2791
5.5912


N
N
N
F

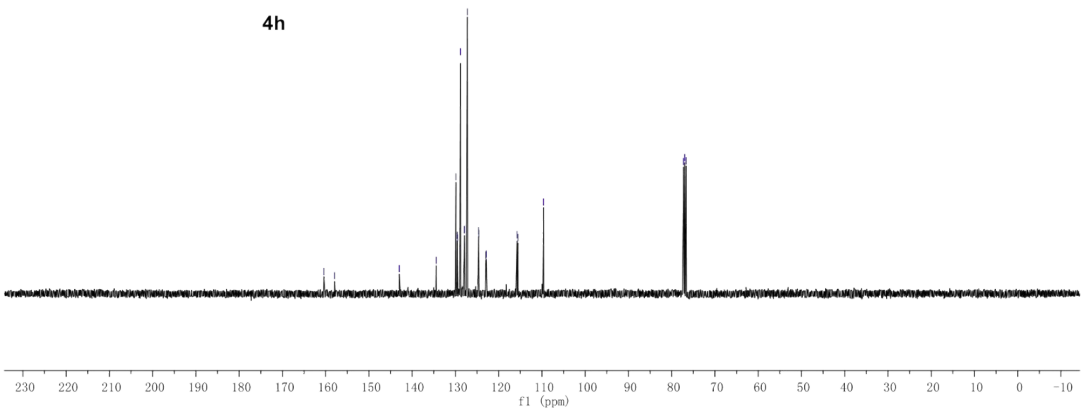
4h

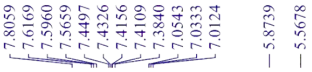

1.05
1.00
3.20
2.08
2.08
1.09
1.07
1.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

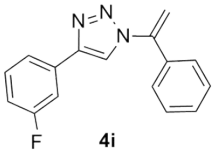

160.4058
157.9381
142.9733
134.4654
129.8880
129.5413
129.4567
128.8343
127.9354
127.9009
127.2396
124.6384
124.6052
122.9838
122.8554
115.7547
115.5400
109.6372
77.3176
76.9997
76.6815


N
N
N
F

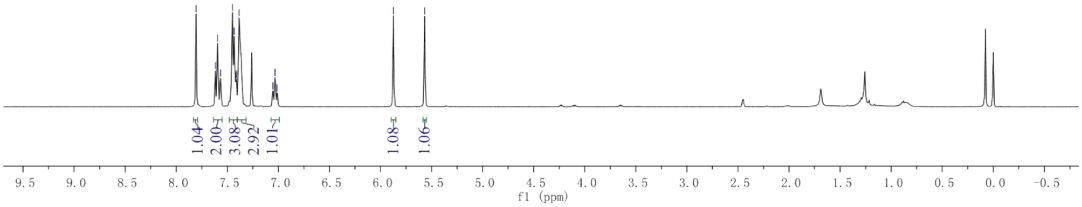
4h

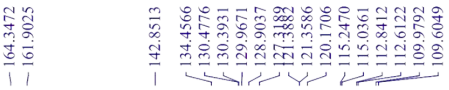

230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

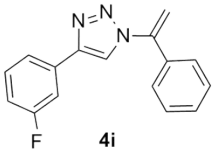

7.8059
7.6169
7.5960
7.5659
7.4497
7.4326
7.4156
7.4109
7.3840
7.0543
7.0333
7.0124
5.8739
5.5678


N
N
N
F

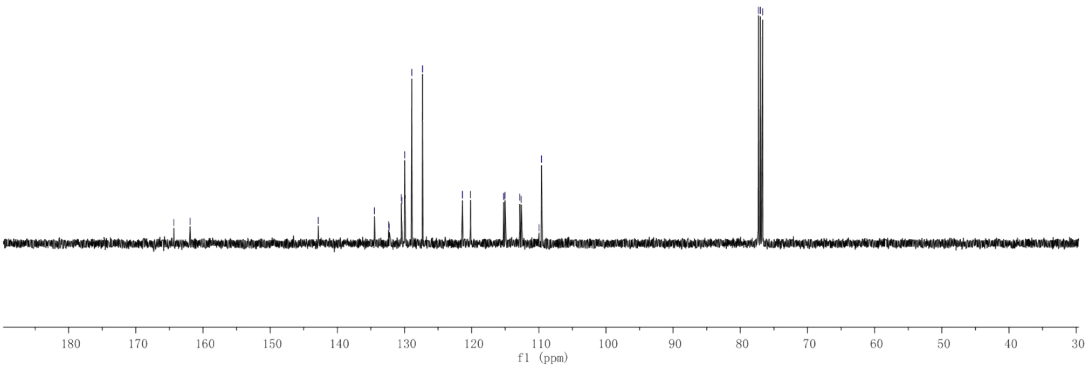
4i


1.04
2.00
3.08
2.92
1.01
1.08
1.06
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)

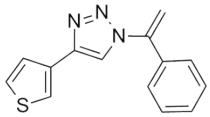

164.3472
161.9025
142.8513
134.4566
130.4776
130.3931
129.9671
128.9037
127.3189
127.3082
121.3586
120.1706
115.2470
115.0361
112.8412
112.6122
109.9792
109.6049
77.3179
77.0005
76.6825


N
N
N
F

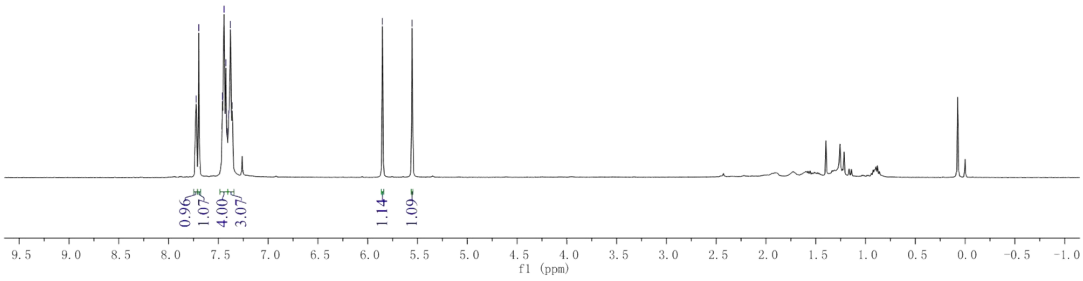
4i

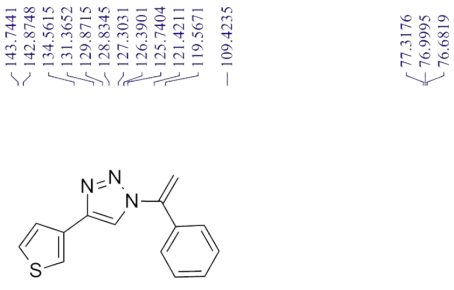

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30
f1 (ppm)


7.7237
7.6968
7.4597
7.4437
7.4250
7.4116
7.3937
7.3789
7.3620
5.8521
5.5540

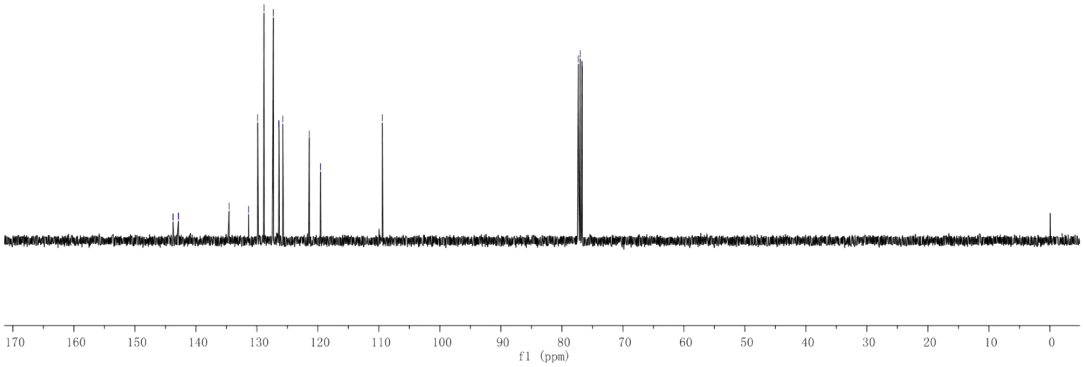


4j


0.96
1.07
4.00
3.07
1.14
1.09
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 -1.0
f1 (ppm)


143.7441
142.8748
134.5615
131.3652
129.8715
128.8345
127.3031
126.3901
125.7404
121.4211
119.5671
109.4235
77.3176
76.9995
76.6819

4j


170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)