Supporting information

Pd-Catalyzed regio- and stereoselective allylic substitution of vinylethylene carbonates with 1,2,4-triazoles

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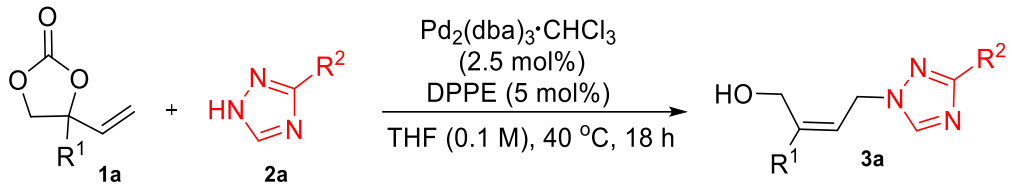
General experimental details

Analytical thin-layer chromatography (TLC) was carried out using 0.2-mm commercial silica gel plates (Yantai Jiangyou Silica Gel Development Co., Ltd., silica gel HSGF 254). Preparative column chromatography employing silica gel (Qingdao Shenghai Fine Silica Gel Chemical Co., Ltd., 200-300 mesh) was performed according to the method of Still. High-resolution mass spectra (HRMS) were performed at Instrumental Analysis Center of Shanghai Jiao Tong University using ESI method. Proton nuclear magnetic resonance (^{1}H NMR) spectra were recorded with a Bruker AVANCE III HD 500 (500 MHz) spectrometer. Chemical shifts are reported in delta (δ) units, parts per million (ppm) downfield from trimethylsilane or deuterated water and ppm relative to the center of the singlet at 7.26 ppm for deuteriochloroform, or ppm relative to the center of the quintet at 3.34 ppm for deuteriomethanol. Coupling constants are reported in Hertz (Hz). Carbon-13 nuclear magnetic resonance (^{13}C NMR) spectra were recorded with a Bruker AVANCE III HD 500 (125 MHz) spectrometer. Chemical shifts are reported in delta (δ) units, ppm relative to the center of the triplet at 77.0 ppm for deuteriochloroform and ppm relative to the center of the septet at 49.54 ppm for deuteriomethanol. ^{13}C NMR spectra were routinely run with broadband decoupling. All of the palladium sources and phosphine ligands were purchased from Sinocompound Co. and used as received.

General procedure for the synthesis of substituted 1,2,4-triazoles (2p-2r)

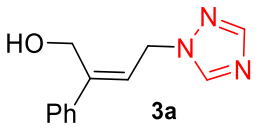
1,2,4-Triazoles **2p-2r** were synthesized according to reported procedure, all characterization data are in accordance with literature.[1]

General procedure for Pd-catalyzed allylic amination of vinylethylene carbonates 1a with 1,2,4-triazoles 2a



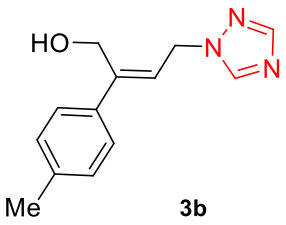
To an oven dried screw-cap reaction tube equipped with a magnetic stir bar, $Pd_2(dba)_3{\cdot}CHCl_3$ (5.2 mg, 0.005 mmol, 2.5 mol%), DPPE (3.98 mg, 0.02 mmol, 5 mol%), Ph-VEC **1a** (38.0 mg, 0.2 mmol) and 1,2,4-Triazole **2a** (20.7 mg, 0.3 mmol) were added. The reaction tube was sealed with rubber-septum, then evacuated and backfilled with nitrogen (this process was repeated a total of three times). Anhydrous THF (2 mL) was added via syringe. The resulting mixture was stirred at 40 ºC for 18 h. The reaction mixture was cooled to room temperature and the solvent was removed by rotary evaporation under vacuum. The crude product was purified by flash column chromatography on silica gel to afford the corresponding product **3a**.

(*Z*)-2-phenyl-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



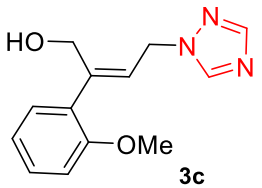
Yield: 96% (41.3 mg); light yellow solid; (*Z*:*E* = >20:1); Purification: petroleum ether/EtOAc = 1:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.92 (s, 1H), 7.48–7.46 (m, 2H), 7.36–7.28 (m, 3H), 5.99 (t, *J* = 7.8 Hz, 1H), 5.04 (d, *J* = 7.8 Hz, 2H), 4.67 (s, 2H), 4.31 (bs, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.9, 146.1, 142.9, 140.0, 128.5, 128.1, 126.3, 122.2, 59.8, 46.8; HRMS (ESI-MS): Calcd. for $C_{12}H_{13}N_3O$ (M+Na): 238.0956, Found: 238.0961.

(*Z*)-2-(*p*-tolyl)-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



Yield: 93% (42.6 mg); light yellow oil; (*Z*:*E* = >20:1); Purification: petroleum ether/EtOAc = 2:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.92 (s, 1H), 7.36 (d, *J* = 10.2 Hz, 2H), 7.14 (d, *J* = 9.8 Hz, 2H), 5.97 (t, *J* = 9.6 Hz, 1H), 5.02 (d, *J* = 9.8 Hz, 2H), 4.65 (s, 2H), 3.92 (bs, 1H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.0, 146.0, 143.0, 138.0, 137.0, 129.2, 126.2, 121.4, 59.8, 46.8, 21.0; HRMS (ESI-MS): Calcd. for $C_{13}H_{15}N_3O$ (M+Na): 252.1113, Found: 252.1108.

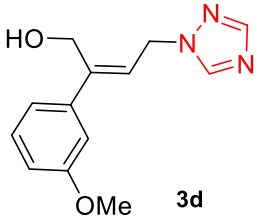
(*Z*)-2-(2-methoxyphenyl)-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



3c

Yield: 83% (40.7 mg); light yellow oil; (*Z*:*E* = >20:1); Purification: petroleum ether/EtOAc = 1:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (s, 1H), 7.95 (s, 1H), 7.31–7.27 (m, 1H), 7.14 (dd, *J* = 9.2, 2.2 Hz, 1H), 6.96–6.89 (m, 2H), 5.85 (t, *J* = 9.2 Hz, 1H), 5.09 (d, *J* = 9.2 Hz, 2H), 4.49 (s, 2H), 3.86 (s, 3H), 3.00 (bs, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.2, 151.9, 145.2, 143.0, 130.3, 130.0, 129.3, 125.4, 121.0, 110.6, 60.9, 55.5, 47.0; HRMS (ESI-MS): Calcd. for $C_{13}H_{15}N_3O_2$ (M+Na): 268.1062, Found: 268.1055.

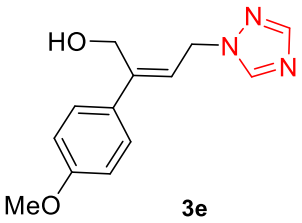
(*Z*)-2-(3-methoxyphenyl)-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



3d

Yield: 90% (44.1 mg); yellow oil; (*Z*:*E* = >20:1); Purification: petroleum ether/EtOAc = 3:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.93 (s, 1H), 7.28–7.23 (m, 1H), 7.05–7.00 (m, 2H), 6.84 (dd, *J* = 10.4, 3.1 Hz, 1H), 5.99 (t, *J* = 9.6 Hz, 1H), 5.04 (d, *J* = 9.6 Hz, 2H), 4.64 (s, 2H), 3.79 (s, 3H), 4.47 (bs, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.6, 152.0, 145.9, 143.0, 141.5, 129.5, 122.5, 118.8, 113.4, 112.2, 59.9, 55.2, 46.8; HRMS (ESI-MS): Calcd. for $C_{13}H_{15}N_3O_2$ (M+Na): 268.1062, Found: 268.1059.

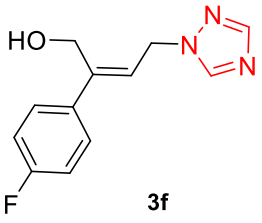
(*Z*)-2-(4-methoxyphenyl)-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



3e

Yield: 93% (45.6 mg); light yellow solid; (*Z*:*E* = >20:1); Purification: petroleum ether/EtOAc = 1:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.92 (s, 1H), 7.41 (d, *J* = 8.8 Hz, 2H), 7.86 (d, *J* = 8.8 Hz, 2H), 5.93 (t, *J* = 7.8 Hz, 1H), 5.01 (d, *J* = 7.8 Hz, 2H), 4.64 (s, 2H), 4.32 (bs, 1H), 3.79 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.5, 151.9, 145.4, 142.8, 132.2, 127.5, 120.5, 113.8, 59.7, 55.2, 46.8; HRMS (ESI-MS): Calcd. for $C_{13}H_{15}N_3O_2$ (M+H): 246.1243, Found: 246.1272.

(*Z*)-2-(4-fluorophenyl)-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol

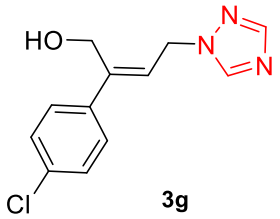


3f

Yield: 95% (44.6 mg); light yellow oil; (*Z*:*E* = 20:1); Purification: petroleum ether/EtOAc = 2:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.95 (s, 1H), 7.48–7.44 (m, 2H), 7.02 (dd, *J* = 8.7, 8.6 Hz, 2H), 5.93 (t, *J* = 7.9 Hz, 1H), 5.03 (d, *J* = 7.9 Hz, 2H), 4.65 (s, 2H), 4.08 (bs, 1H); ^{13}C NMR (125 MHz, $CDCl_3$)

δ 163.7, 161.7, 152.2, 145.6, 143.0, 136.3, 136.2, 128.2, 128.1, 122.1, 115.5, 115.4, 59.9, 46.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.72; HRMS (ESI-MS): Calcd. for $C_{12}H_{12}FN_3O$ (M+H): 234.1043, Found: 234.1046.

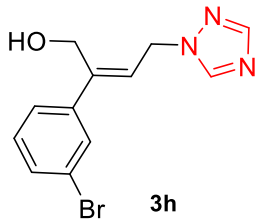
(*Z*)-2-(4-chlorophenyl)-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



3g

Yield: 95% (44.8 mg); light yellow oil; (*Z*:*E* = 17:1); Purification: petroleum ether/EtOAc = 1:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.95 (s, 1H), 7.41 (d, *J* = 10.6 Hz, 2H), 7.30 (d, *J* = 10.8 Hz, 2H), 5.99 (t, *J* = 9.8 Hz, 1H), 5.04 (d, *J* = 9.8 Hz, 2H), 4.64 (s, 2H), 3.36 (bs, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.1, 145.3, 143.02 , 138.5, 134.0, 128.6, 127.7, 122.6, 59.7, 46.6; HRMS (ESI-MS): Calcd. for $C_{12}H_{12}ClN_3O$ (M+H): 250.0747, Found: 250.0733.

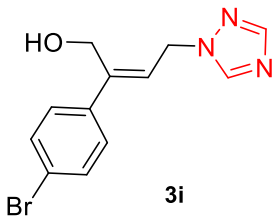
(*Z*)-2-(3-bromophenyl)-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



3h

Yield: 97% (56.8 mg); light yellow oil; (*Z*:*E* = 13:1); Purification: petroleum ether/EtOAc = 1:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.96 (s, 1H), 7.62 (dd, *J* = 4.6, 2.4 Hz, 1H), 7.44–7.39 (m, 2H), 7.20 (d, *J* = 9.9, 9.8 Hz, 1H), 6.00 (t, *J* = 9.8 Hz, 1H), 5.05 (d, *J* = 9.8 Hz, 2H), 4.64 (s, 2H), 3.57 (bs, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.1, 145.2, 143.0, 142.3, 131.0, 130.0, 129.4, 125.0, 123.3, 122.6, 59.7, 46.6; HRMS (ESI-MS): Calcd. for $C_{12}H_{12}BrN_3O$ (M+H): 294.0242, Found: 294.0237.

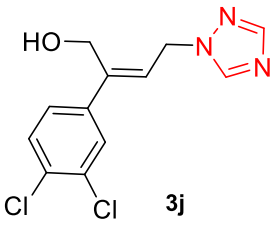
(*Z*)-2-(4-bromophenyl)-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



3i

Yield: 94% (55.1 mg); light yellow solid; 108-110 ℃; (*Z*:*E* = >20:1); Purification: petroleum ether/EtOAc = 1:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.95 (s, 1H), 7.46 (d, *J* = 8.6 Hz, 2H), 7.35 (d, *J* = 8.6 Hz, 2H), 6.00 (t, *J* = 7.9 Hz, 1H), 5.03 (d, *J* = 7.8 Hz, 2H), 4.64 (s, 2H), 4.24 (bs, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.1, 145.4, 143.0, 139.0, 131.6, 1278.0, 122.6, 122.2, 59.6, 46.6; HRMS (ESI-MS): Calcd. for $C_{12}H_{12}BrN_3O$ (M+H): 294.0242, Found: 294.0256.

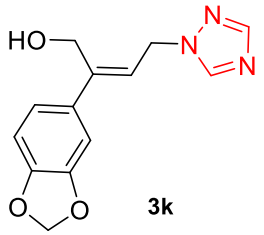
(*Z*)-2-(3,4-dichlorophenyl)-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



3j

Yield: 90% (50.9 mg); yellow oil; (*Z*:*E* = 10:1); Purification: petroleum ether/EtOAc = 1:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.96 (s, 1H), 7.58 (d, *J* = 2.6 Hz, 1H), 7.41–7.37 (m, 1H), 7.33–7.30 (m, 1H), 6.02 (t, *J* = 9.8 Hz, 1H), 5.05 (d, *J* = 9.8 Hz, 2H), 4.62 (s, 2H), 3.54 (bs, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.2, 144.4, 143.0, 140.1, 132.6, 132.1, 130.4, 128.3, 125.7, 123.5, 59.5, 46.5; HRMS (ESI-MS): Calcd. for $C_{12}H_{11}Cl_2N_3O$ (M+H): 284.0357, Found: 284.0352.

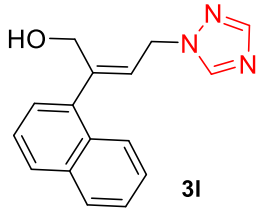
(*Z*)-2-(benzo[*d*][1,3]dioxol-4-yl)-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



3k

Yield: 89% (46.1 mg); yellow oil; (*Z*:*E* = 20:1); Purification: petroleum ether/EtOAc = 2:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.94 (s, 1H), 6.98–6.95 (m, 2H), 6.77 (d, *J* = 10.7 Hz, 1H), 5.94 (s, 2H), 5.91 (t, *J* = 9.8 Hz, 1H), 5.01 (d, *J* = 9.8 Hz, 2H), 4.61 (s, 2H), 4.28 (bs, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.9, 147.8, 147.5, 145.8, 142.9, 134.2, 121.1, 120.1, 108.2, 106.8, 101.1, 59.8, 46.8; HRMS (ESI-MS): Calcd. for $C_{13}H_{13}N_3O_3$ (M+Na): 282.0855, Found: 282.0854.

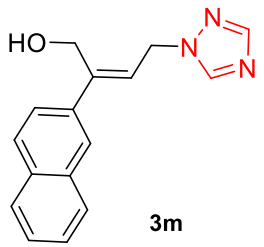
(*Z*)-2-(naphthalen-1-yl)-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



3l

Yield: 79% (41.9 mg); light yellow oil; (*Z*:*E* = 20:1); Purification: petroleum ether/EtOAc = 2:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.97 (s, 1H), 7.89–7.83 (m, 2H), 7.78 (d, *J* = 8.2 Hz, 1H), 7.49–7.44 (m, 2H), 7.42–7.39 (m, 1H), 7.30 (dd, *J* = 7.0, 1.4 Hz, 1H), 5.85 (t, *J* = 7.8 Hz, 1H), 5.15 (d, *J* = 7.8 Hz, 2H), 4.65 (s, 2H), 3.98 (bs, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.0, 146.5, 142.9, 138.8, 133.6, 131.0, 128.4, 128.1, 126.3, 125.9, 125.9, 125.2, 125.1, 125.0, 62.2, 46.6; HRMS (ESI-MS): Calcd. for $C_{16}H_{15}N_3O$ (M+H): 266.1293, Found: 266.1287.

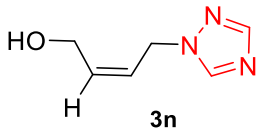
(*Z*)-2-(naphthalen-2-yl)-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



3m

Yield: 94% (49.8 mg); light brown solid; (*Z*:*E* = 20:1); Purification: petroleum ether/EtOAc = 1:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.94 (s, 1H), 7.93 (s, 1H), 7.81–7.76 (m, 3H), 7.55 (dd, *J* = 10.7, 2.3 Hz, 1H), 7.48–7.43 (m, 2H), 6.09 (t, *J* = 9.7 Hz, 1H), 5.02 (d, *J* = 9.8 Hz, 2H), 4.74 (s, 2H), 4.30 (bs, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.9, 146.0, 142.9, 137.2, 133.2, 132.9, 128.1, 128.1, 127.5, 126.3, 126.2, 125.5, 124.2, 122.6, 59.8, 46.8; HRMS (ESI-MS): Calcd. for $C_{16}H_{15}N_3O$ (M+Na): 288.1113, Found: 288.1108.

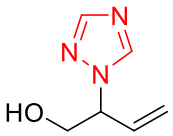
(*Z*)-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



3n

Yield: 53% (14.7 mg); light yellow oil; (*Z*:*E* = 5:1, l:b = 1.3:1); Purification: petroleum ether/EtOAc = 1:1; ^{1}H NMR (500 MHz, $CDCl_3$) for *Z* isomer: δ 8.13 (s, 1H), 7.94 (s, 1H), 6.03–5.97 (m, 1H), 5.77–5.70 (m, 1H), 4.92 (d, *J* = 9.1 Hz, 2H), 4.33 (d, *J* = 7.0 Hz, 2H), 3.18 (bs, 1H); ^{1}H NMR (500 MHz, $CDCl_3$) for *E* isomer: δ 8.11(s, 1H), 7.94 (s, 1H), 5.93–5.91 (m, 2H), 4.80 (d, *J* = 5.3 Hz, 2H), 4.19 (d, *J* = 1.7 Hz, 2H), 2.56 (bs, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) for *Z* isomer: δ 151.7, 142.6, 135.0, 123.8, 58.0, 46.2; ^{13}C NMR (125 MHz, $CDCl_3$) for *E* isomer: δ 151.6, 142.7, 135.4, 123.0, 61.8, 51.0; HRMS (ESI-MS): Calcd. for $C_6H_9N_3O$ (M+H): 140.0824, Found: 140.0809.

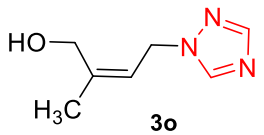
2-(1*H*-1,2,4-triazol-1-yl)but-3-en-1-ol



3n'

Yield: 40% (11.2 mg); light yellow oil; Purification: petroleum ether/EtOAc = 5:1; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.13 (s, 1H), 7.92 (s, 1H), 6.07 (ddd, *J* = 17.4, 10.5, 7.1 Hz, 1H), 5.42 (d, *J* = 10.5 Hz, 1H), 5.30 (d, *J* = 17.2 Hz, 1H), 4.91 (tdd, *J* = 6.9, 3.0, 1.2 Hz, 1H), 4.14–3.94 (m, 2H), 3.83 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 151.6, 143.1, 132.0, 120.4, 64.5, 64.0; HRMS (ESI-MS): Calcd. for $C_6H_9N_3O$ (M+H): 140.0824, Found: 140.0818.

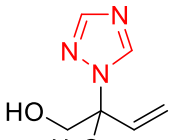
(*Z*)-2-methyl-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



3o

Yield: 32% (9.8 mg); light yellow oil; (*Z*:*E* = 17:1, l:b = 1:3); Purification: petroleum ether/EtOAc = 2:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.94 (s, 1H), 5.54 (t, *J* = 7.8 Hz, 1H), 4.87 (d, *J* = 7.8 Hz, 2H), 4.26 (s, 2H), 3.70 (bs, 1H), 1.88 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.9, 143.8, 142.7, 119.2, 61.4, 46.3, 22.0; HRMS (ESI-MS): Calcd. for $C_7H_{11}N_3O$ (M+H): 154.0980, Found: 154.0975.

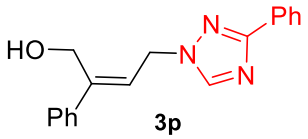
2-methyl-2-(1*H*-1,2,4-triazol-1-yl)but-3-en-1-ol



3o'

Yield: 51% (15.7 mg); light yellow oil; Purification: petroleum ether/EtOAc = 5:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (s, 1H), 8.01–7.64 (m, 1H), 6.14 (dd, *J* = 17.5, 10.8 Hz, 1H), 5.39 (d, *J* = 10.8 Hz, 1H), 5.20 (d, *J* = 17.5 Hz, 1H), 4.13 (bs, 1H), 3.99 (d, *J* = 11.8 Hz, 1H), 3.85 (d, *J* = 11.3 Hz, 1H), 1.69 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.1, 142.2, 137.6, 117.4, 68.4, 65.6, 21.7; HRMS (ESI-MS): Calcd. for $C_7H_{11}N_3O$ (M+H): 154.0980, Found: 154.0975.

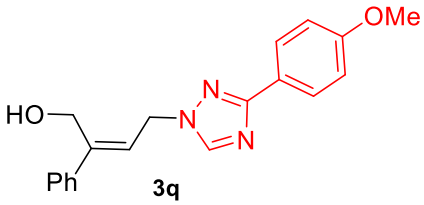
(*Z*)-2-phenyl-4-(3-phenyl-1*H*-1,2,4-triazol-1-yl)but-2-en-1-ol



3p

Yield: 96% (55.9 mg); light yellow oil; (*Z*:*E* = >20:1); Purification: petroleum ether/EtOAc = 1:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (s, 1H), 8.05–7.03 (m, 2H), 7.51–7.49 (m, 2H), 7.44–7.37 (m, 3H), 7.36–7.28 (m, 3H), 6.05 (t, *J* = 8.0 Hz, 1H), 5.03 (d, *J* = 8.1 Hz, 2H), 4.72 (s, 2H), 4.47 (bs, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.0, 146.8, 143.8, 140.2, 130.3, 129.5, 128.7, 128.5, 128.2, 126.3, 126.3, 122.2, 60.0, 46.8; HRMS (ESI-MS): Calcd. for $C_{18}H_{17}N_3O$ (M+H): 292.1450, Found: 292.1445.

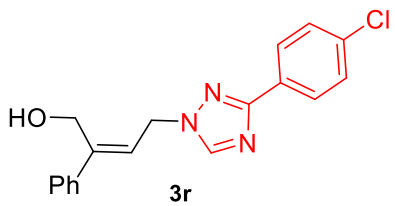
(*E*)-4-(3-(4-methoxyphenyl)-1*H*-1,2,4-triazol-1-yl)-2-phenylbut-2-en-1-ol



3q

Yield: 96% (61.7 mg); light yellow oil; (*Z*:*E* = 5:1); Purification: petroleum ether/EtOAc = 2:1; ^{1}H NMR (500 MHz, $CDCl_3$) for *Z* isomer: δ 8.09 (s, 1H), 7.98–7.94 (m, 2H), 7.51–7.49 (m, 2H), 7.36–7.28 (m, 3H), 6.95–7.92 (m, 2H), 6.05 (t, *J* = 8.0 Hz, 1H), 5.01 (d, *J* = 8.0 Hz, 2H), 4.70 (d, *J* = 4.6 Hz, 2H), 4.56 (dd, *J* = 6.0, 6.0 Hz, 1H), 3.83 (s, 3H); ^{1}H NMR (500 MHz, $CDCl_3$) for *E* isomer: δ 7.94 (s, 1H), 7.60–7.58 (m, 2H), 7.51–7.49 (m, 2H), 7.36–7.28 (m, 3H), 7.04–7.03 (m, 2H), 6.02 (t, *J* = 7.8 Hz, 1H), 5.05 (d, *J* = 7.9 Hz, 2H), 4.65 (d, *J* = 5.0 Hz, 2H), 4.27 (dd, *J* = 6.6, 4.3 Hz, 1H), 3.87 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) for *Z* isomer: δ 162.9, 160.6, 146.8, 143.6, 140.3, 128.5, 128.4, 128.1, 127.7, 126.3, 122.2, 114.0, 59.9, 55.3, 46.7; ^{13}C NMR (125 MHz, $CDCl_3$) for *E* isomer: δ 161.2, 154.7, 150.9, 146.3, 140.4, 130.3, 128.0, 126.4, 123.0, 122.8, 119.8, 114.4, 60.0, 55.4, 46.4; HRMS (ESI-MS): Calcd. for $C_{19}H_{19}N_3O_2$ (M+H): 322.1256, Found: 322.1245.

(*Z*)-4-(3-(4-chlorophenyl)-1*H*-1,2,4-triazol-1-yl)-2-phenylbut-2-en-1-ol

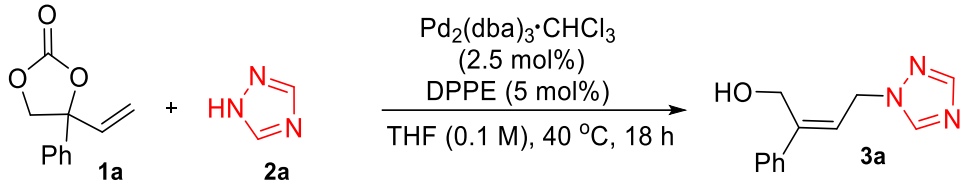


3r

Yield: 96% (59.9 mg); light yellow oil; (*Z*:*E* = 20:1); Purification: petroleum ether/EtOAc = 1:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.97 (d, *J* = 8.6 Hz, 2H), 7.51–7.49 (m, 2H), 7.39 (d, *J* = 8.6 Hz, 2H), 7.37–7.29 (m, 3H), 6.06 (t, *J* = 8.0 Hz, 1H), 5.05 (d, *J* = 8.0 Hz, 2H), 4.72 (s, 2H), 4.20 (dd, *J* = 6.3, 6.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ ^{13}C NMR (126 MHz, Chloroform-*d*) δ 162.1, 146.9, 143.9,

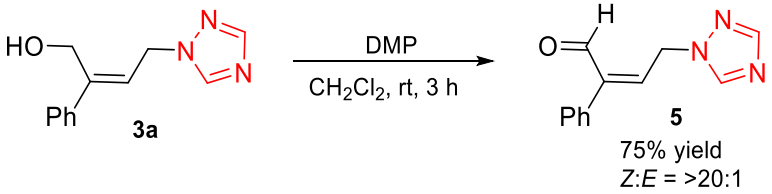
140.0, 135.4, 128.9, 128.9, 128.6, 128.2, 127.6, 126.3, 122.2, 60.0, 46.9; HRMS (ESI-MS): Calcd. for $C_{18}H_{16}ClN_3O$ (M+H): 326.1060, Found: 326.1064.

Procedure for gram scale reaction of 3a

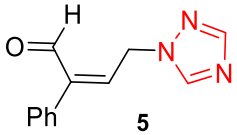


To an oven dried screw-cap reaction tube equipped with a magnetic stir bar, $Pd_2(dba)_3{\cdot}CHCl_3$ (0.156 g, 0.15 mmol, 2.5 mol%), DPPE (0.119 g, 0.30 mmol, 5 mol%), Ph-VEC **1a** (1.140 g, 6.0 mmol) and 1,2,4-triazole **2a** (0.621 g, 9.0 mmol) were added. The reaction flask was sealed with rubber-septum, then evacuated and backfilled with nitrogen (this process was repeated a total of three times). Anhydrous THF (30 mL) was added via syringe. The resulting mixture was stirred at 40 ºC for 18 h. The reaction mixture was cooled to room temperature and the solvent was removed by rotary evaporation under vacuum. The crude product was purified by flash column chromatography on silica gel to afford the corresponding product **3a** as light yellow soild in 91% (1.174 g) and *Z*:*E* = >20:1.

Procedure for Dess-Martin oxidation of 3a

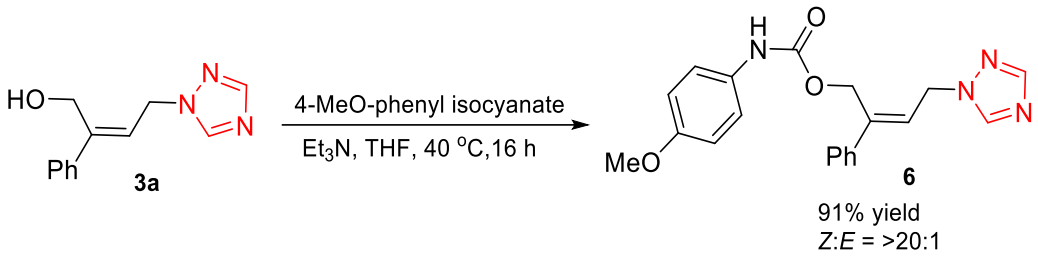


(*Z*)-2-phenyl-4-(1*H*-1,2,4-triazol-1-yl)but-2-enal

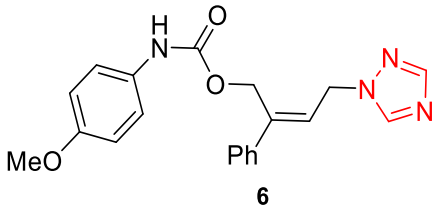


A screw-capped vial was charged with the **3a** (43.0 mg, 0.2 mmol), DMP (93.3 mg, 0.220 mmol, 1.10 equiv.), CH_2Cl_2 (5 mL). The reaction mixture was stirred for 3 hours at room temperature. The mixture reaction washed twice with a saturated solution (5 mL) of $NaHCO_3/Na_2S_2O_3$ (1:1). And then the liquid was extracted with CH_2Cl_2 three times. After drying over Na_2SO_4 for 30 minutes, the combined organic phase was concentrated by evaporated under reduced pressure, and then the residue was purified by chromatography on silica gel to afford **5** as yellow oil in 75% yield (34.4 mg).[2] (*Z*:*E* = >20:1); Purification: petroleum ether/EtOAc = 3:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.70 (s, 1H), 8.05 (s, 1H), 7.00 (s, 1H), 7.49–7.42 (m, 3H), 7.24–7.22 (m, 2H), 6.83 (t, *J* = 6.5 Hz, 1H), 5.08 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.1, 152.5, 145.6, 144.0, 143.0, 130.8, 129.1, 129.0, 128.7, 47.8; HRMS (ESI-MS): Calcd. for $C_{12}H_{11}N_3O$ (M+H): 294.0980, Found: 294.0977.

Procedure for carbamate synthesis from 3a

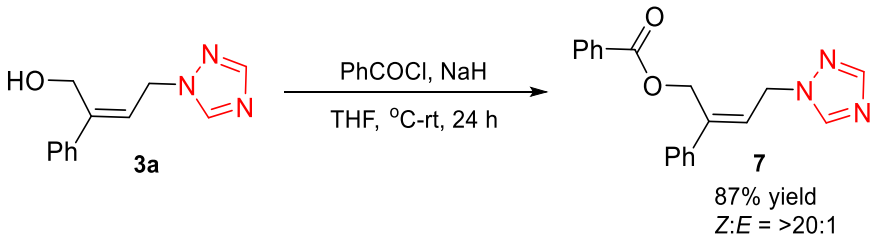


(*Z*)-2-phenyl-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-yl(4-methoxyphenyl)carbamate

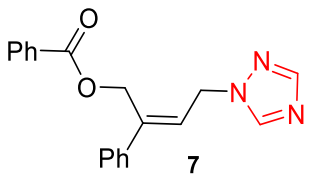


A screw-capped vial was charged with the **3a** (43.0 mg, 0.2 mmol), 4-MeO-phenyl isocyanate (35.8 mg, 0.240 mmol, 1.2 equiv.), Et_3N (36.2 uL, 0.260 mmol, 1.3 equiv.) and THF (2.0 mL). The reaction mixture was stirred for 16 hours under N_2 at 40 ºC. After filtration, the mixture was extracted with EtOAc, dried over anhydrous Na_2SO_4, and the solvent was removed in vacuum. The crude product was purified by flash column chromatography on silica gel to get the desired product **6** as light yellow oil in 91% yield (66.3 mg). (*Z*:*E* = >20:1); Purification: petroleum ether/EtOAc = 1:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.70 (s, 1H), 8.18 (s, 1H), 7.95 (s, 1H), 7.44–7.42 (m, 2H), 7.36–7.31 (m, 3H), 7.27–7.21 (m, 2H), 7.07 (bs, 1H), 6.85–6.81 (m, 2H), 6.12 (t, *J* = 7.0 Hz, 1H), 5.18 (s, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.0, 153.6, 151.9, 143.0, 139.3, 138.8, 130.6, 128.6, 128.3, 126.4, 125.8, 120.7, 114.2, 61.0, 55.4, 47.4; HRMS (ESI-MS): Calcd. for $C_{20}H_{20}N_4O_3$ (M+H): 365.1614, Found: 365.1604.

Procedure for ester synthesis from 3a



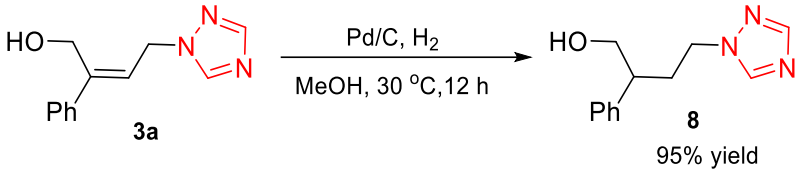
(*Z*)-2-phenyl-4-(1*H*-1,2,4-triazol-1-yl)but-2-en-1-yl benzoate



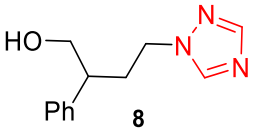
A screw-capped vial was charged with the **3a** (43.0 mg, 0.2 mmol), benzoyl chloride (30.2 uL, 0.260 mmol, 1.3 equiv.), NaH (10.4 mg, 0.433 mmol, 1.3 equiv.) and THF (2.0 mL). The reaction mixture was initially stirred at 0 ºC for 30 minutes and then stirred under N_2 atmosphere at room temperature for 24

hours. After filtration, the mixture was extracted with EtOAc, dried over anhydrous Na_2SO_4, and the solvent was removed in vacuum. The crude product was purified by flash column chromatography on silica gel to get the target product **7** as colorless oil in 87% yield (55.5 mg). (*Z*:*E* = >20:1); Purification: petroleum ether/EtOAc = 7:3; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.97 (s, 1H), 7.96–7.94 (m, 2H), 7.57–7.54 (m, 1H), 7.50–7.48 (m, 2H), 7.43–7.40 (m, 2H), 7.39–7.32 (m, 3H), 6.20 (t, *J* = 7.0 Hz, 1H), 5.38 (s, 2H), 7.05 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.3, 152.2, 143.0, 139.0, 139.0, 133.3, 129.6, 129.6, 128.6, 128.5, 128.4, 126.4, 126.2, 61.3, 47.6; HRMS (ESI-MS): Calcd. for $C_{19}H_{17}N_3O_2$ (M+H): 320.1399, Found: 320.1405.

Procedure for Hydrogenation of 3a



2-phenyl-4-(1*H*-1,2,4-triazol-1-yl)butan-1-ol



A screw-capped vial was charged with the **3a** (43.0 mg, 0.2 mmol), the Pd/C (10%) catalyst (2.1 mg, 10 mol%) and MeOH (2.0 mL). The reaction mixture was stirred for 12 hours under H_2 at room temperature. After filtration, the mixture was extracted with EtOAc, dried over anhydrous Na_2SO_4, and the solvent was removed in vacuum. The crude product was purified by flash column chromatography on silica gel to afford **8** as colorless oil in 95% yield (41.2 mg).[3] Purification: petroleum ether/EtOAc = 1:2; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.83 (s, 1H), 7.36–7.33 (m, 2H), 7.29–7.25 (m, 1H), 7.19–7.17 (m, 2H), 4.11–3.98 (m, 2H), 3.77–3.69 (m, 2H), 2.72–2.66 (m, 1H), 2.55 (bs, 1H), 2.49–2.42 (m, 1H), 2.19–2.11 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.8, 142.9, 140.4, 128.9, 127.9, 127.2, 67.0, 47.5, 45.6, 31.7; HRMS (ESI-MS): Calcd. for $C_{12}H_{15}N_3O$ (M+H): 218.1293, Found: 218.1302.

X-rays crystallography of 3i (CCDC 1975292)

A single crystal of **3i** was obtained from THF/n-Hexane solvent at room temperature. Diffraction data were collected on Bruker SMART Apex-III CMOS-Based X-ray diffractometer with Cu-Kα. Radiation (λ = 1.54178). The empirical absorption correction was applied by using the SADABS program. The structure was solved using direct method, and refined by full matrix least-squares on F2 (G.M Sheldrick, SHELXTL2014, program of crystal structure refinement, University of Göttingen, Germany).

Table 1. Crystal data and structure refinement for 3i

Identification code	**3i**
Empirical formula	$C_{12}H_{12}BrN_3O$
Formula weight	294.16
Temperature	296(2) K
Wavelength	1.54178 A
Crystal system, space group	Monoclinic, P2(1)/n

Unit cell dimensions	a = 4.7996(13) A alpha = 90 deg. b = 9.8909(15) A beta = 92.99(2) deg. c = 26.029(4) A gamma = 90 deg.
Volume	1234.0(4) A^3
Z, Calculated density	4, 1.583 Mg/m^3
Absorption coefficient	4.444 mm^-1
F(000)	592
Crystal size	0.180 x 0.160 x 0.150 mm
Theta range for data collection	3.400 to 68.419 deg.
Limiting indices	-5<=h<=5, -11<=k<=11, -30<=l<=31
Reflections collected / unique	14924 / 2262 [R(int) = 0.0443]
Completeness to theta = 67.679	99.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2262 / 0 / 156
Goodness-of-fit on F^2	1.025
Final R indices [I>2sigma(I)]	R1 = 0.0462, wR2 = 0.1139
R indices (all data)	R1 = 0.0652, wR2 = 0.1306
Extinction coefficient	n/a
Largest diff. peak and hole	0.369 and -0.577 e.A^-3

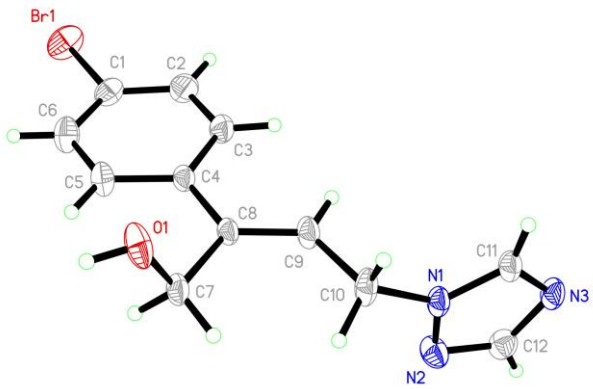
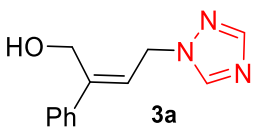


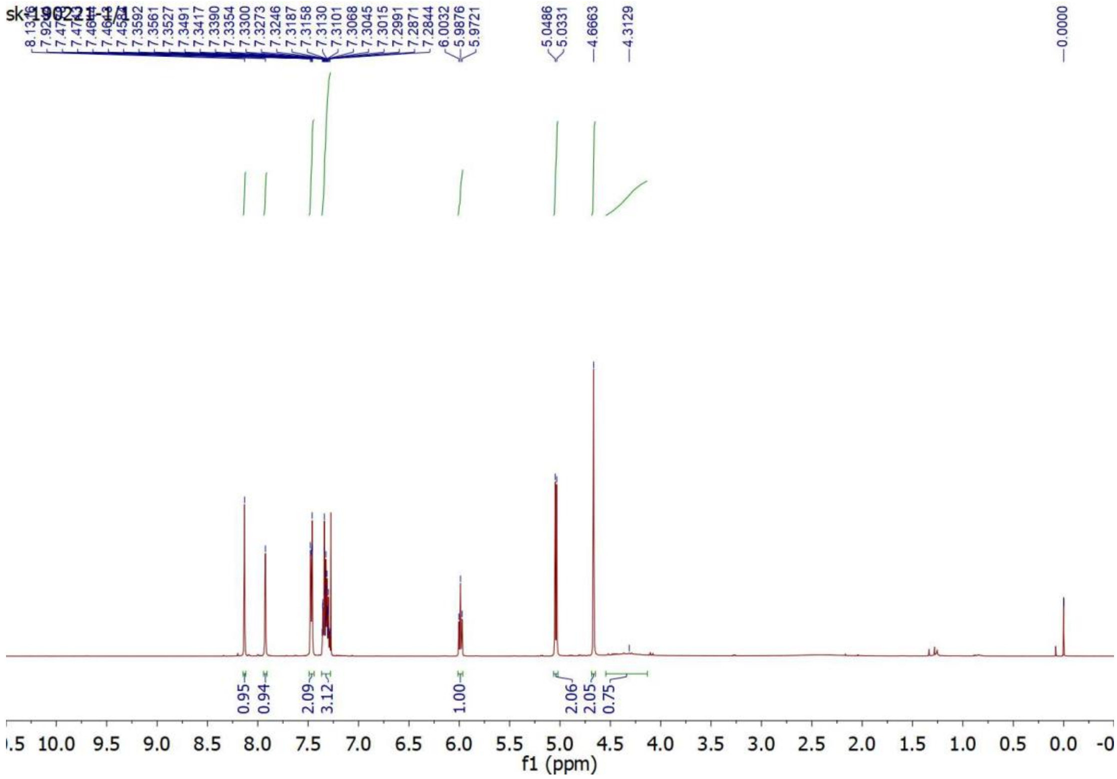
Figure S1: Molecular structure of **3i**

References:

(1) X. Sun, Z. Hong, M. Liu, S. Guo, D. Yang, Y. Wang, T. Lan, L. Gao, H. Qi, P. Gong and Y. Liu, *Bioorg. Med. Chem.*, 2017, **25**, 2800.
(2) L. Wavrin and J. Viala, *Synthesis*, 2002, **2002**, 0326.
(3) T. Ikawa, H. Sajiki and K. Hirota, *Tetrahedron*, 2005, **61**, 2217.



3a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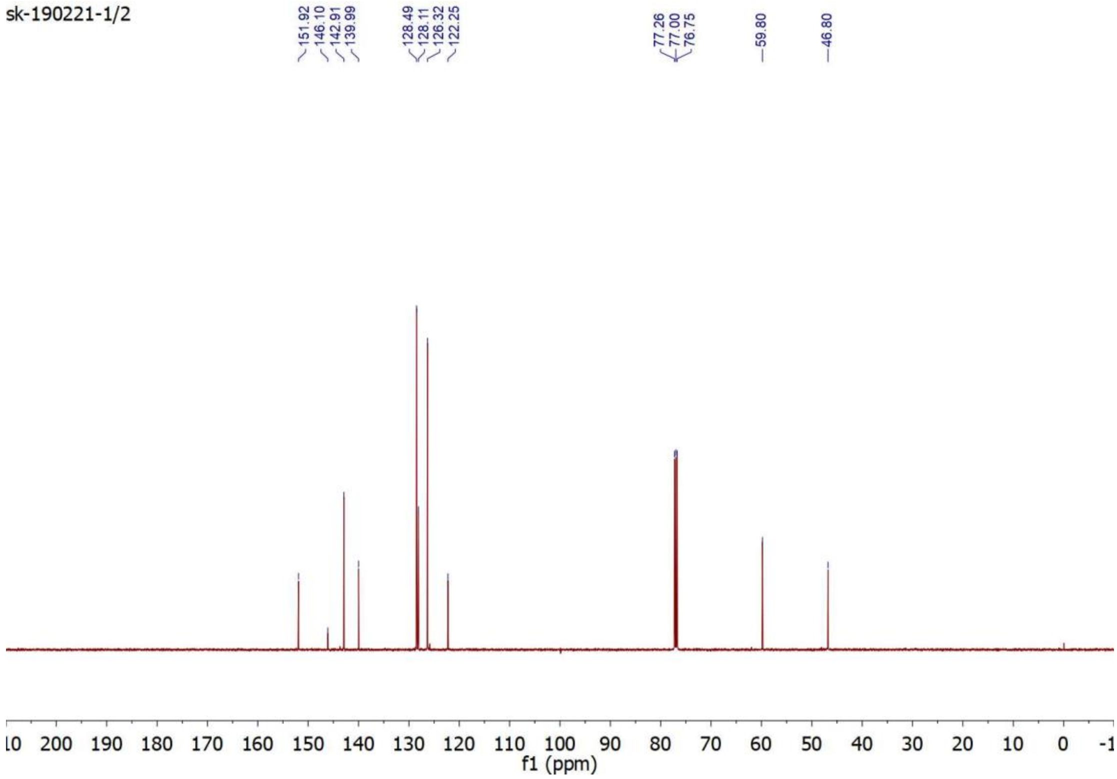
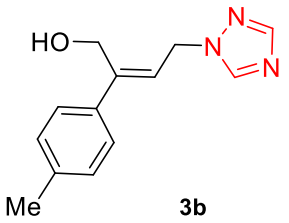
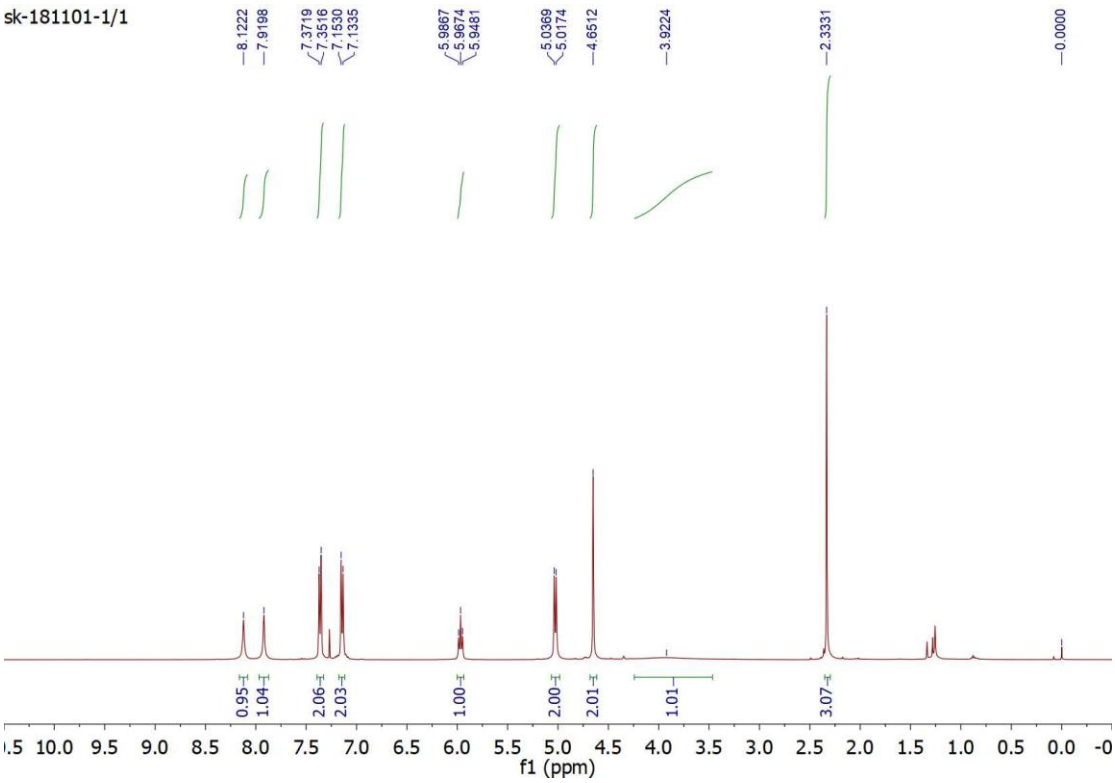
f1 (ppm)


sk-190221-1/2
f1 (ppm)


HO
N
N
N
Me

3b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5.0174
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3.9224
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1.04
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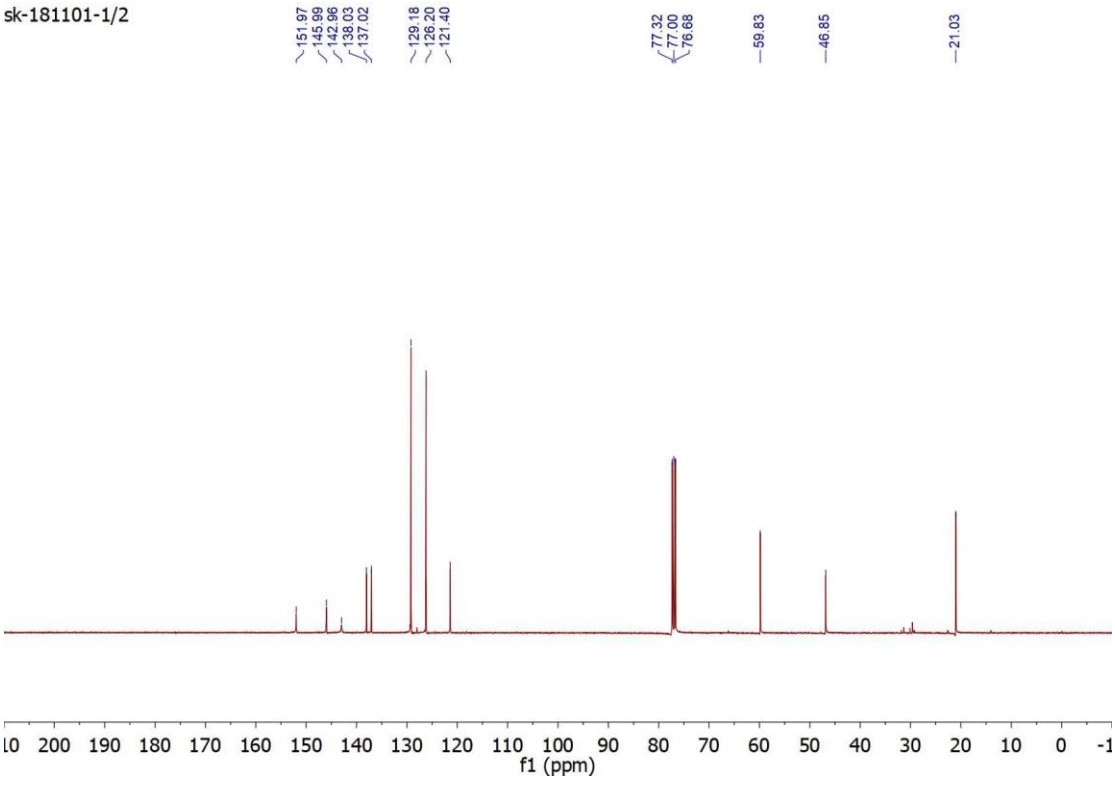
2.03
1.00
2.00
2.01
1.01
3.07
f1 (ppm)


sk-181101-1/2
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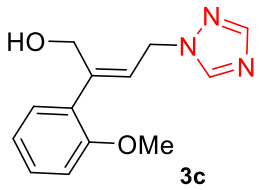
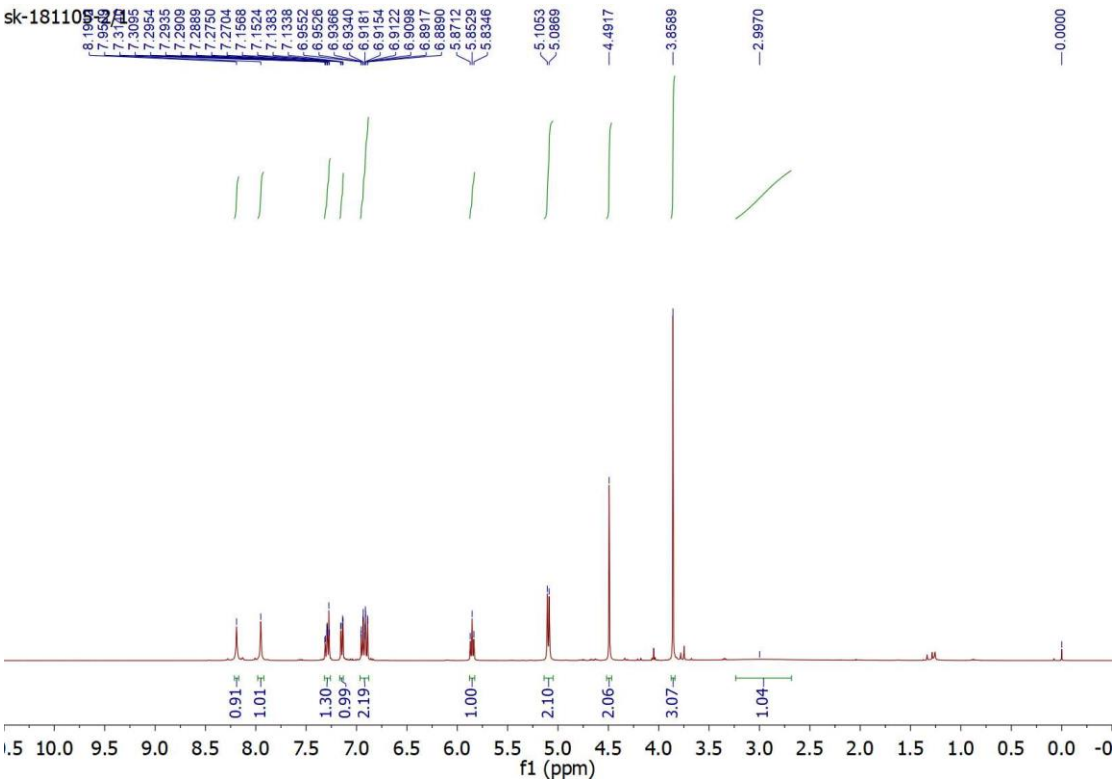
145.99
142.96
138.03
137.02
129.18
126.20
121.40
77.32
77.00
76.68
59.83
46.85
21.03
f1 (ppm)


HO
N
N
N
OMe

3c


sk-181105
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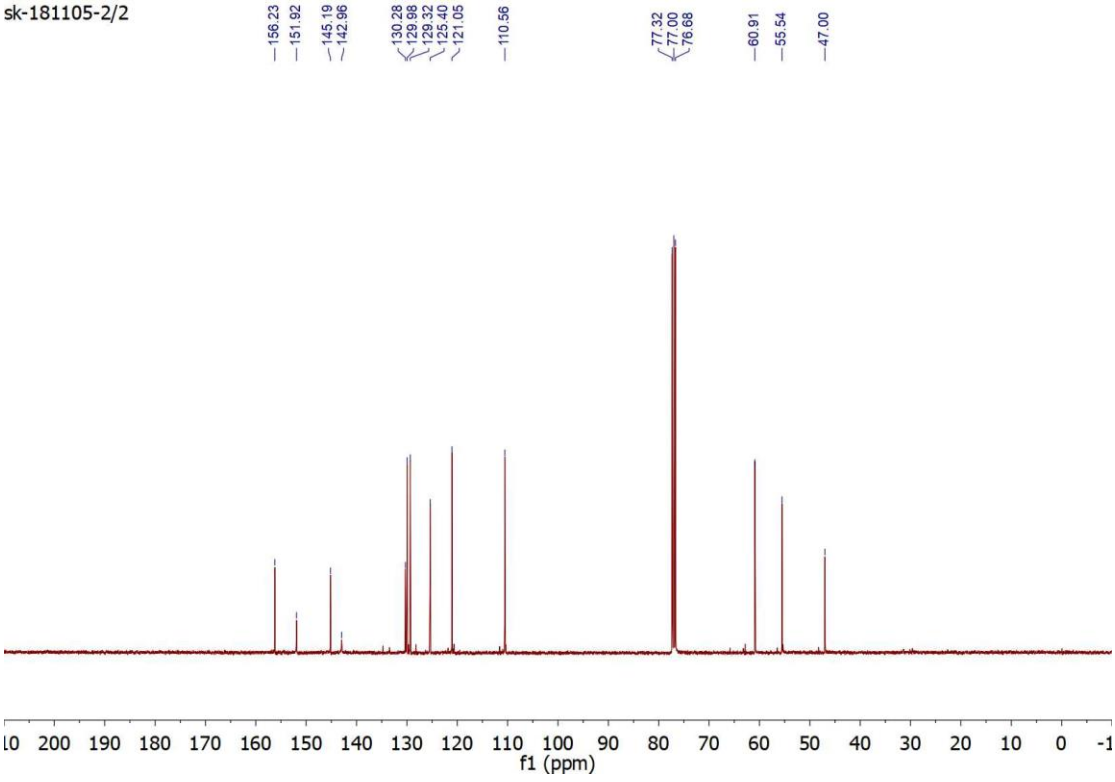
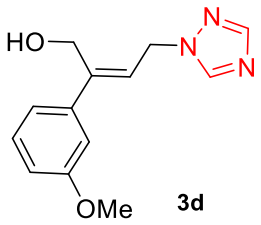
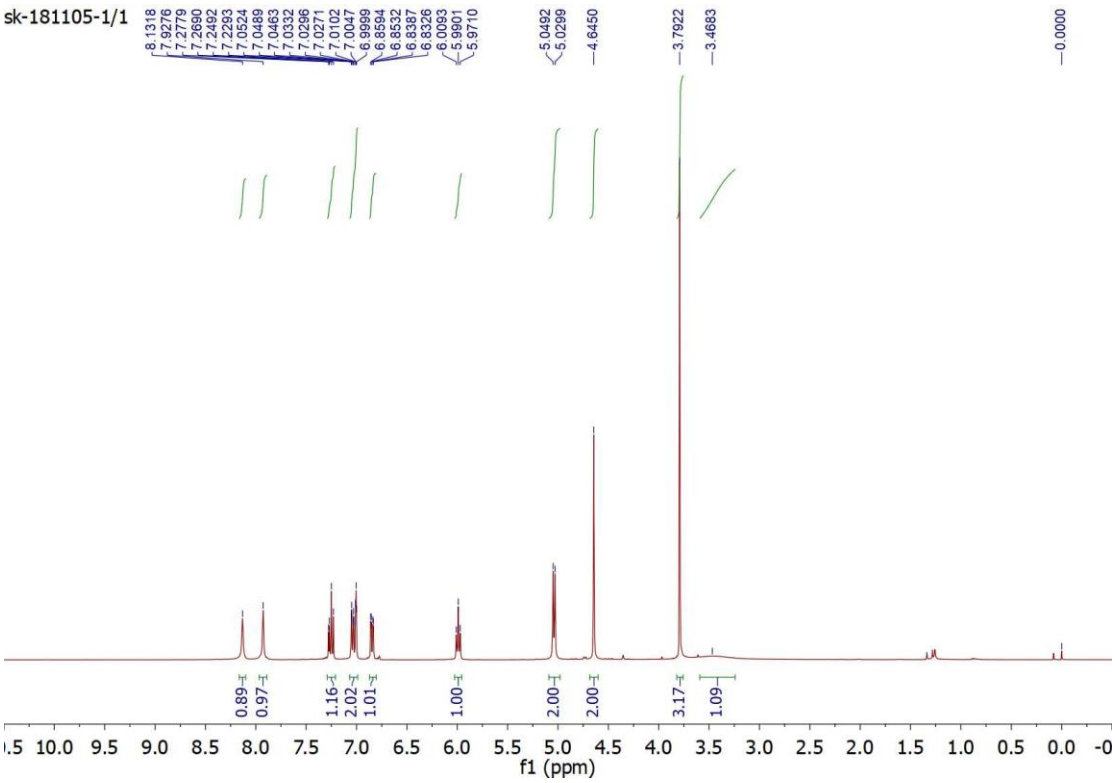
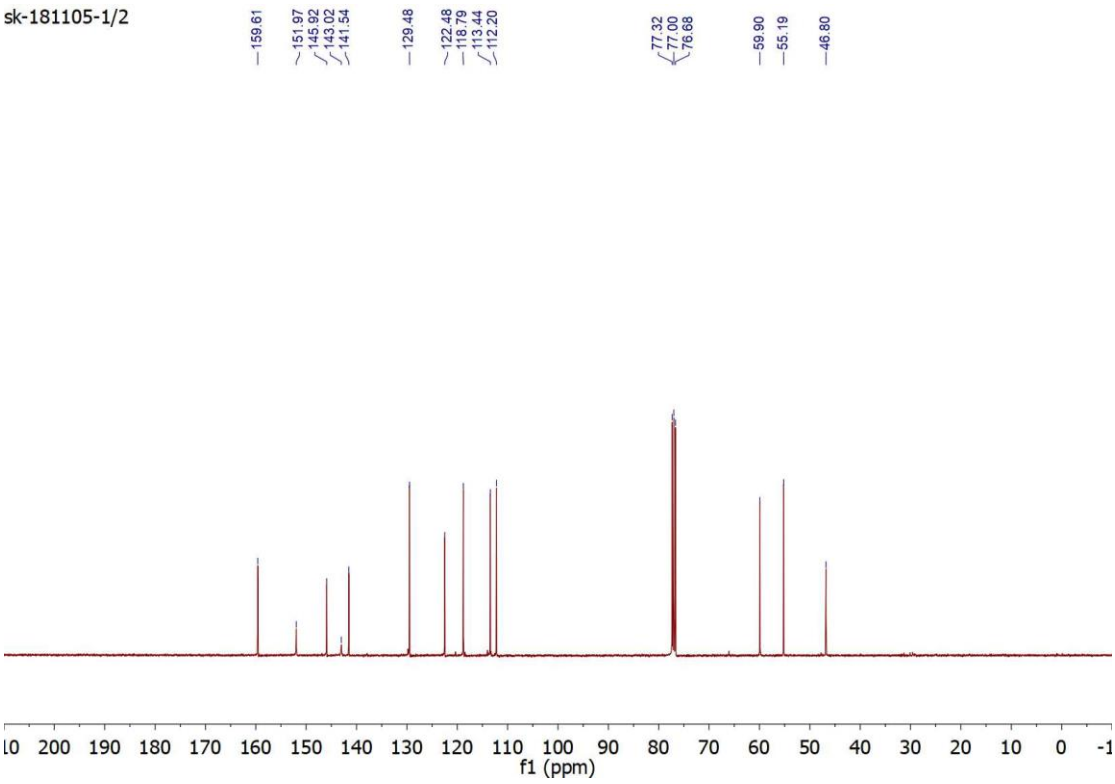
7.9543
7.3112
7.3095
7.2954
7.2935
7.2909
7.2889
7.2750
7.2704
7.1568
7.1524
7.1383
7.1338
6.9552
6.9526
6.9366
6.9340
6.9181
6.9154
6.9122
6.9098
6.8917
6.8890
5.8712
5.8529
5.8346
5.1053
5.0869
4.4917
3.8589
2.9970
0.0000
0.91
1.01
1.30
0.99
2.19
1.00
2.10
2.06
3.07
1.04
f1 (ppm)

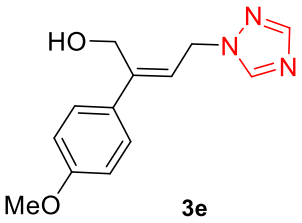

sk-181105-2/2
156.23
151.92
145.19
142.96
130.28
129.98
129.32
125.40
121.05
110.56
77.32
77.00
76.68
60.91
55.54
47.00
f1 (ppm)


HO
N
N
N
OMe

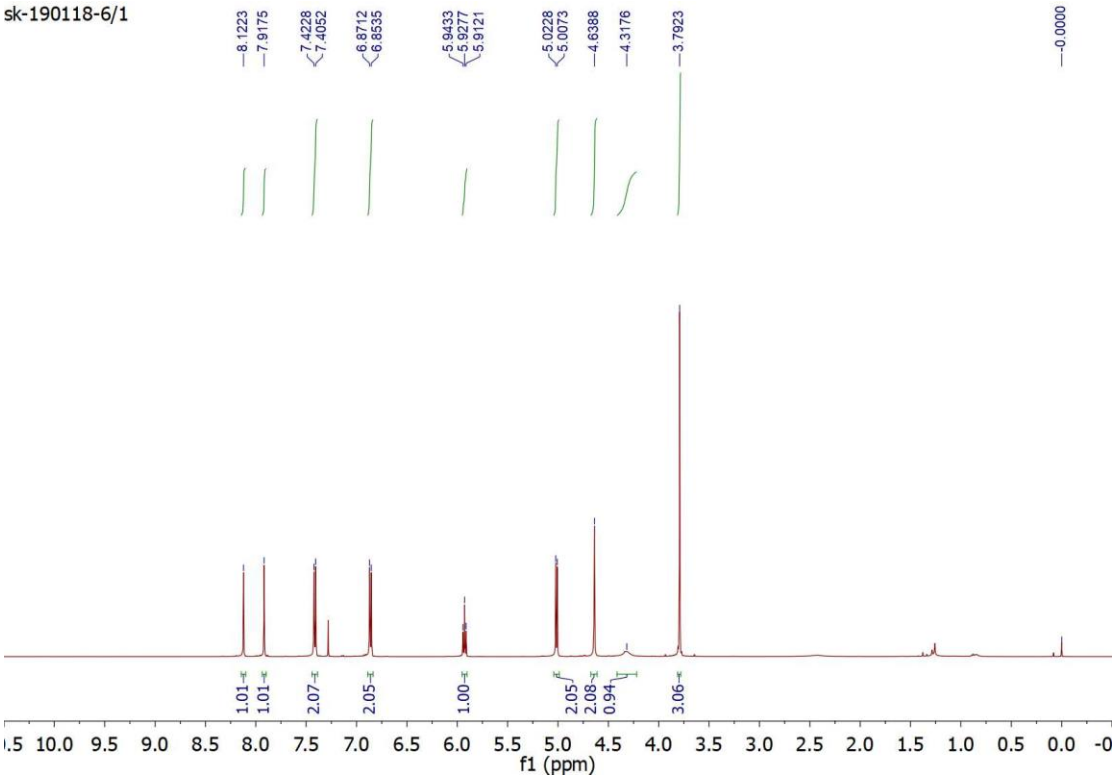
3d

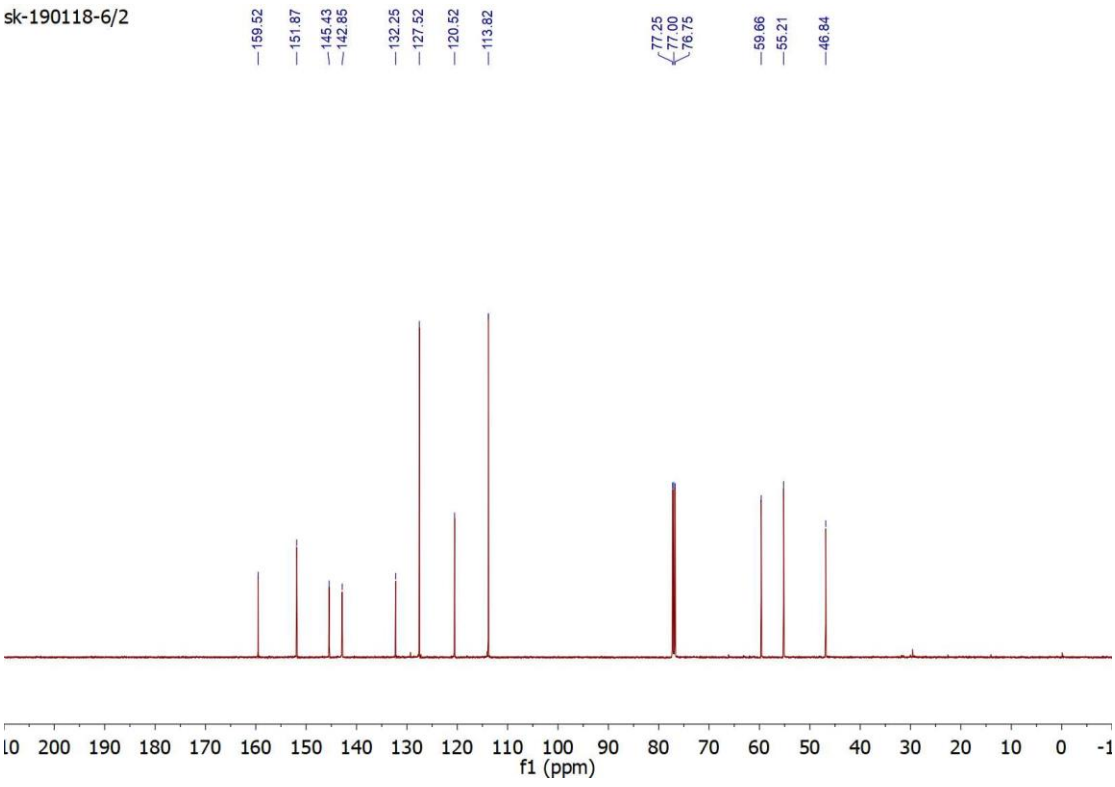

sk-181105-1/1
8.1318
7.9276
7.2779
7.2690
7.2492
7.2293
7.0524
7.0489
7.0463
7.0332
7.0296
7.0271
7.0102
7.0047
6.9999
6.8994
6.8532
6.8387
6.8326
6.0093
5.9901
5.9710
5.0492
5.0299
4.6450
3.7922
3.4683
0.0000
0.89
0.97
1.16
2.02
1.01
1.00
2.00
2.00
3.17
1.09
f1 (ppm)

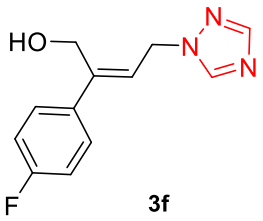

sk-181105-1/2
159.61
151.97
145.92
143.02
141.54
129.48
122.48
118.79
113.44
112.20
77.32
77.00
76.68
59.90
55.19
46.80
f1 (ppm)


HO
N
N
N
MeO

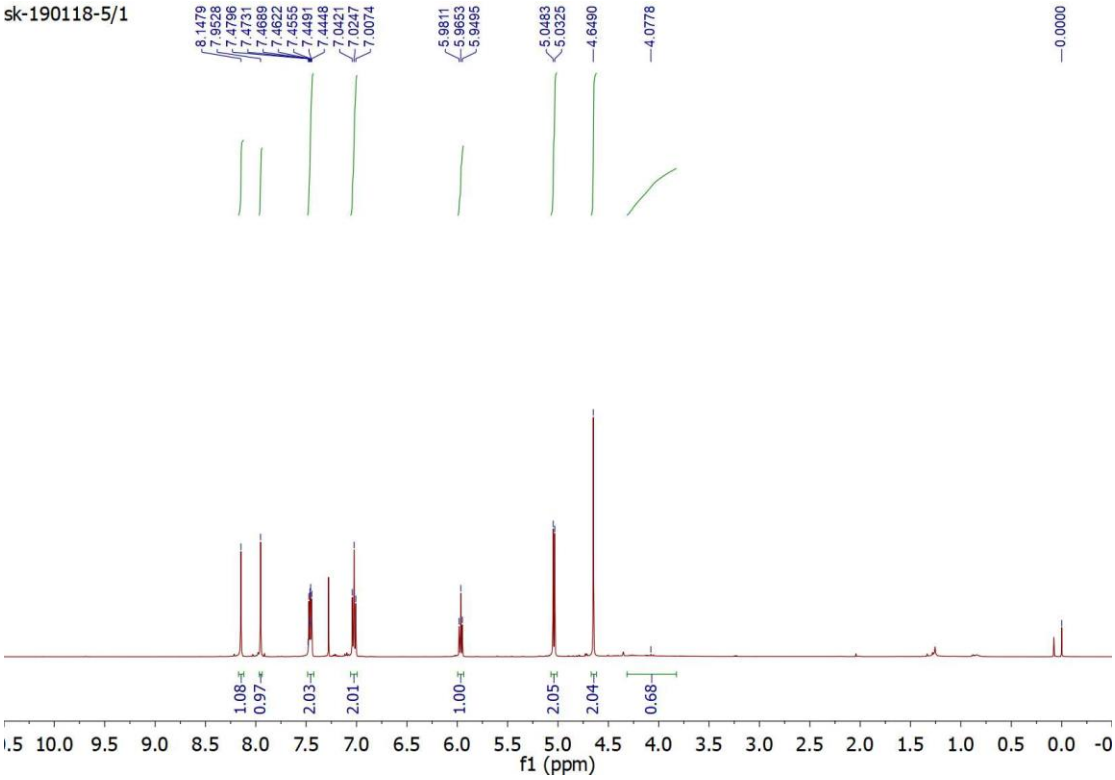
3e

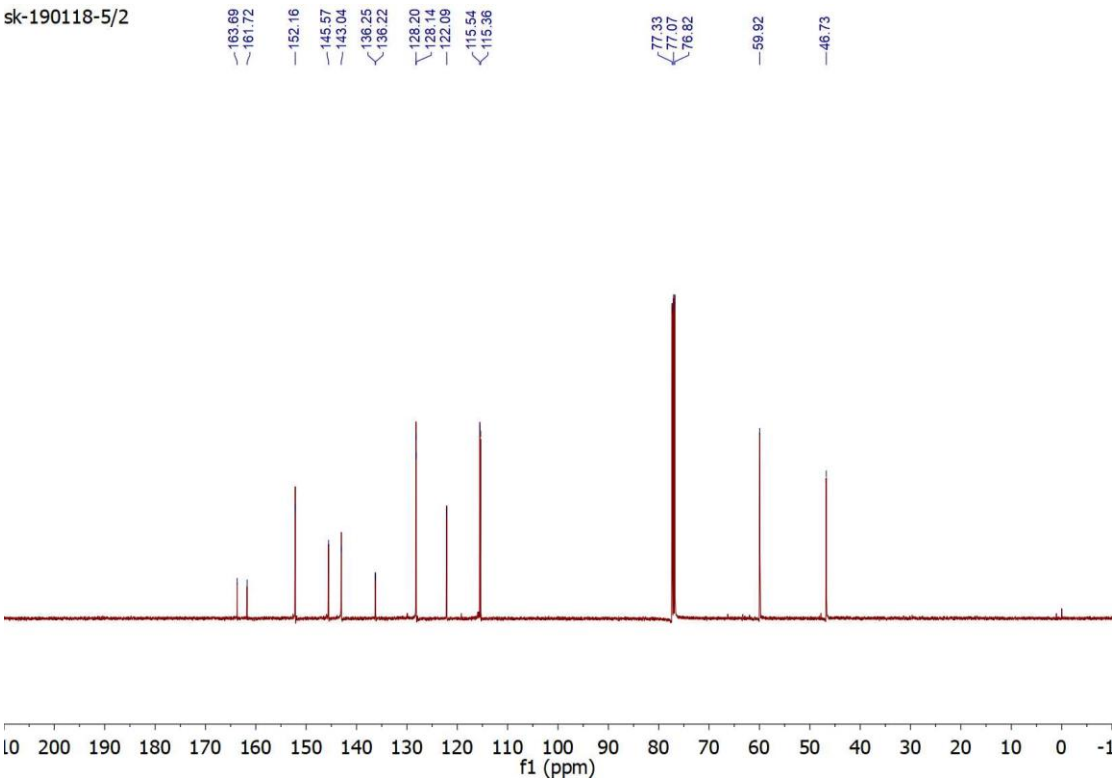

sk-190118-6/1
8.1223
7.9175
7.4228
7.4052
6.8712
6.8535
5.9433
5.9277
5.9121
5.0228
5.0073
4.6388
4.3176
3.7923
0.0000
1.01
1.01
2.07
2.05
1.00
2.05
2.08
0.94
3.06
f1 (ppm)

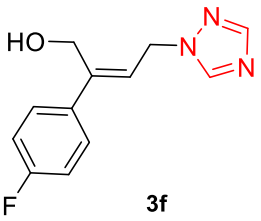

sk-190118-6/2
159.52
151.87
145.43
142.85
132.25
127.52
120.52
113.82
77.25
77.00
76.75
59.66
55.21
46.84
f1 (ppm)


HO
N
N
N
F

3f

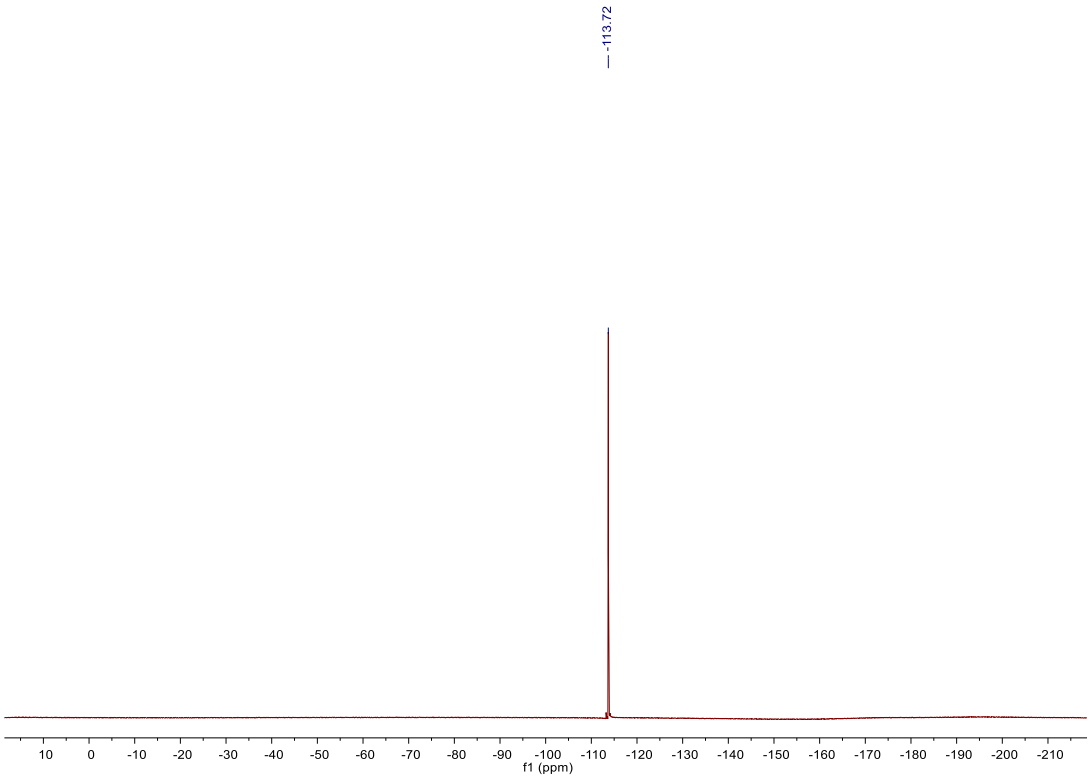

sk-190118-5/1
8.1479
7.9528
7.4796
7.4731
7.4689
7.4622
7.4555
7.4491
7.4448
7.0421
7.0247
7.0074
5.9811
5.9653
5.9495
5.0483
5.0325
4.6490
4.0778
0.0000
1.08
0.97
2.03
2.01
1.00
2.05
2.04
0.68
f1 (ppm)

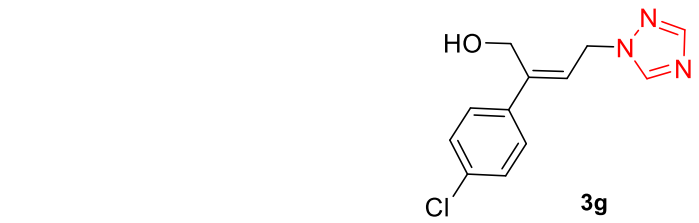

sk-190118-5/2
163.69
161.72
152.16
145.57
143.04
136.25
136.22
128.20
128.14
122.09
115.54
115.36
77.33
77.07
76.82
59.92
46.73
f1 (ppm)



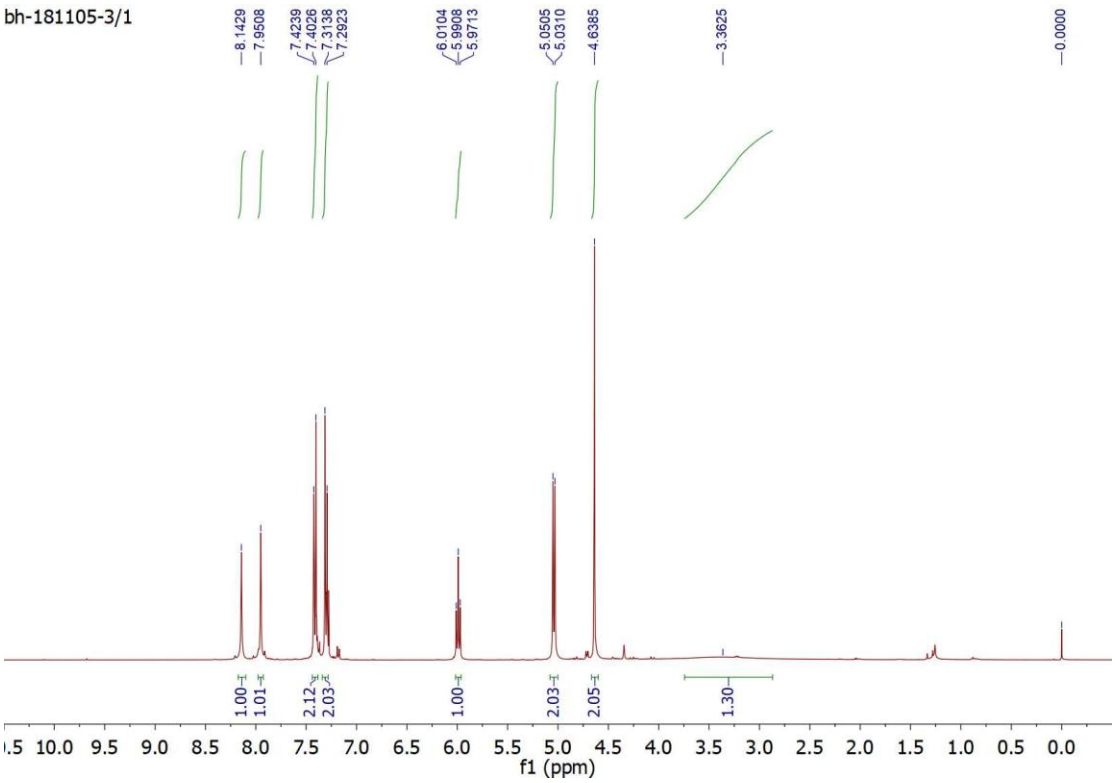
3f

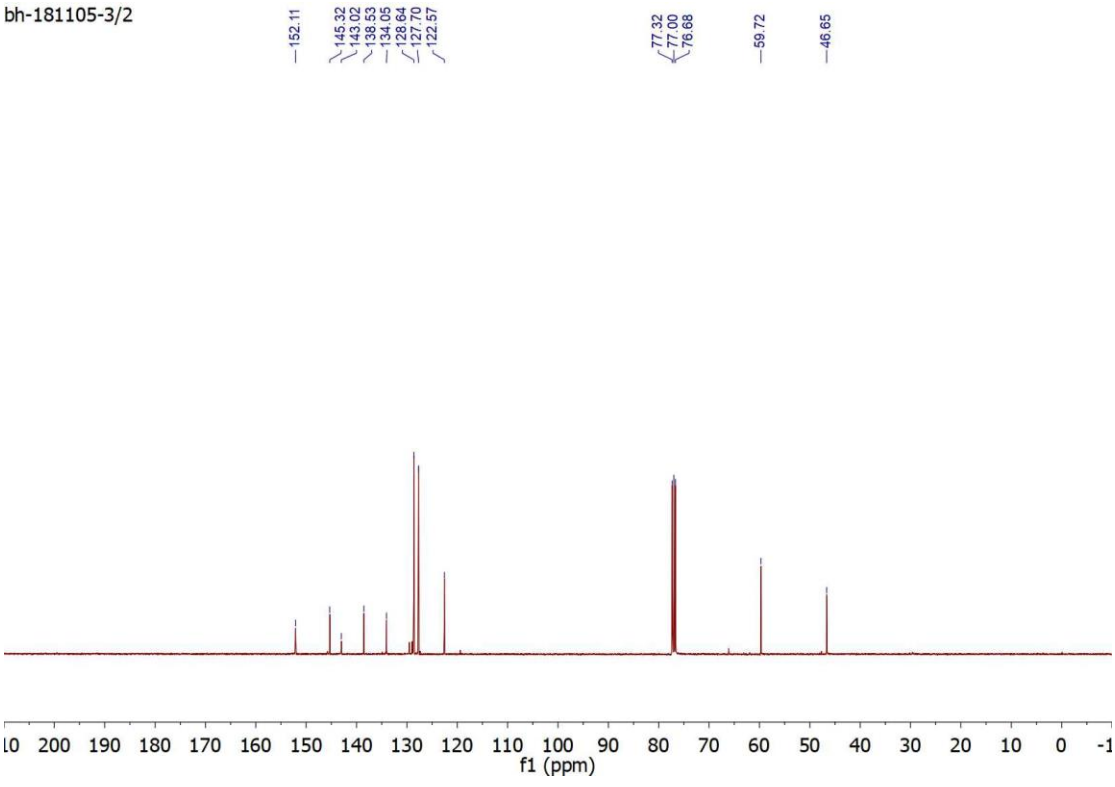
^{19}F NMR spectrum for **3f**

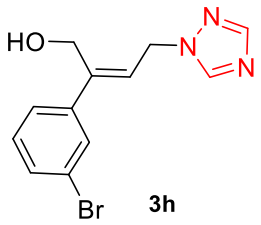



HO
N
N
N
Cl

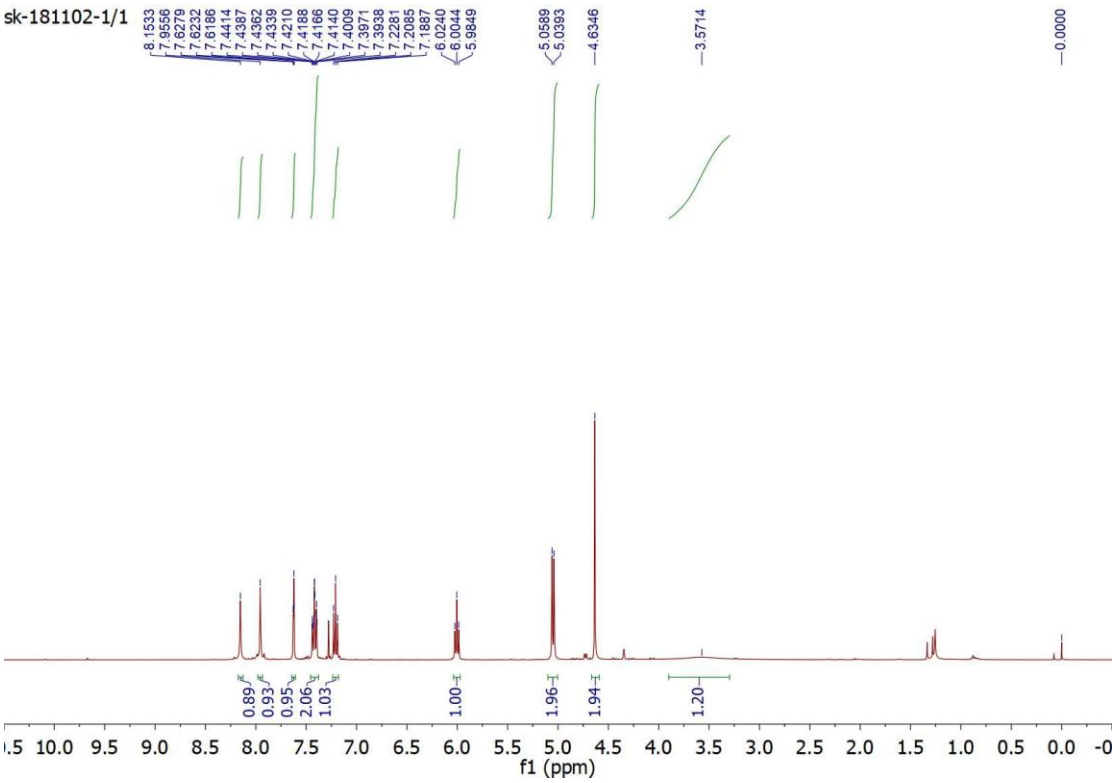
3g

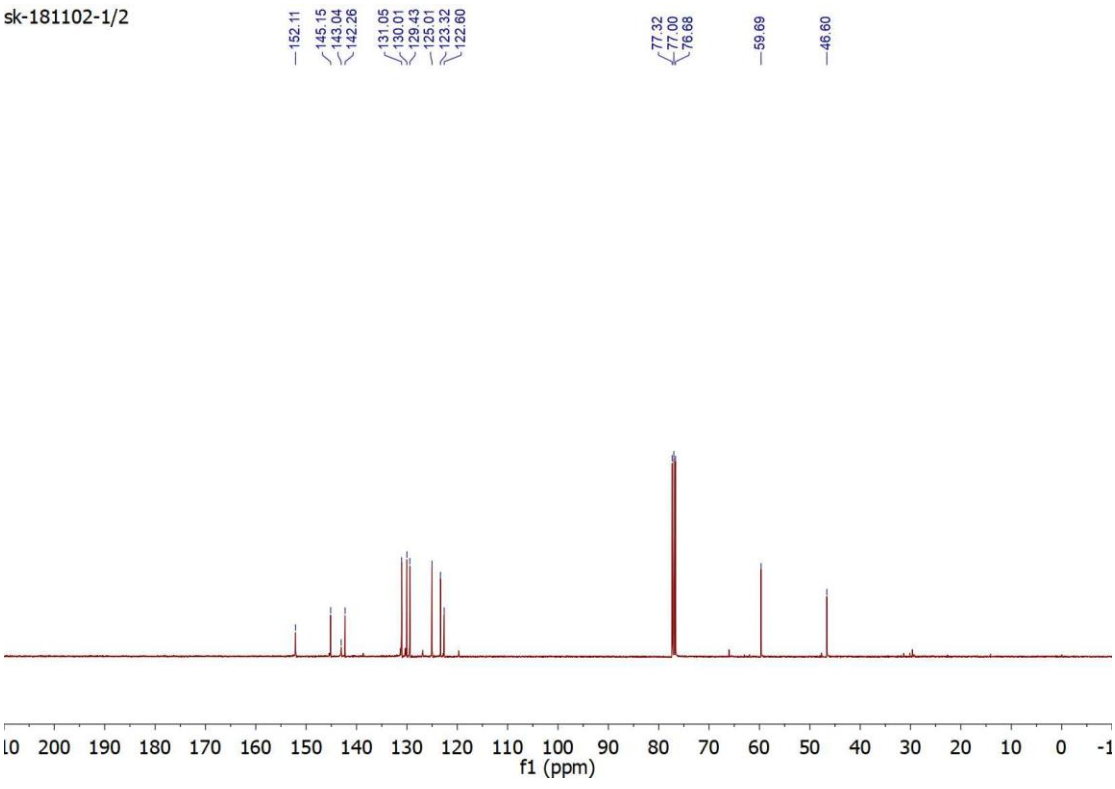

bh-181105-3/1
8.1429
7.9508
7.4239
7.4026
7.3138
7.2923
6.0104
5.9908
5.9713
5.0505
5.0310
4.6385
3.3625
0.0000
1.00
1.01
2.12
2.03
1.00
2.03
2.05
1.30
f1 (ppm)

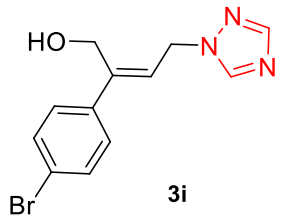

bh-181105-3/2
152.11
145.32
143.02
138.53
134.05
128.64
127.70
122.57
77.32
77.00
76.68
59.72
46.65
f1 (ppm)


HO
N
N
N
Br

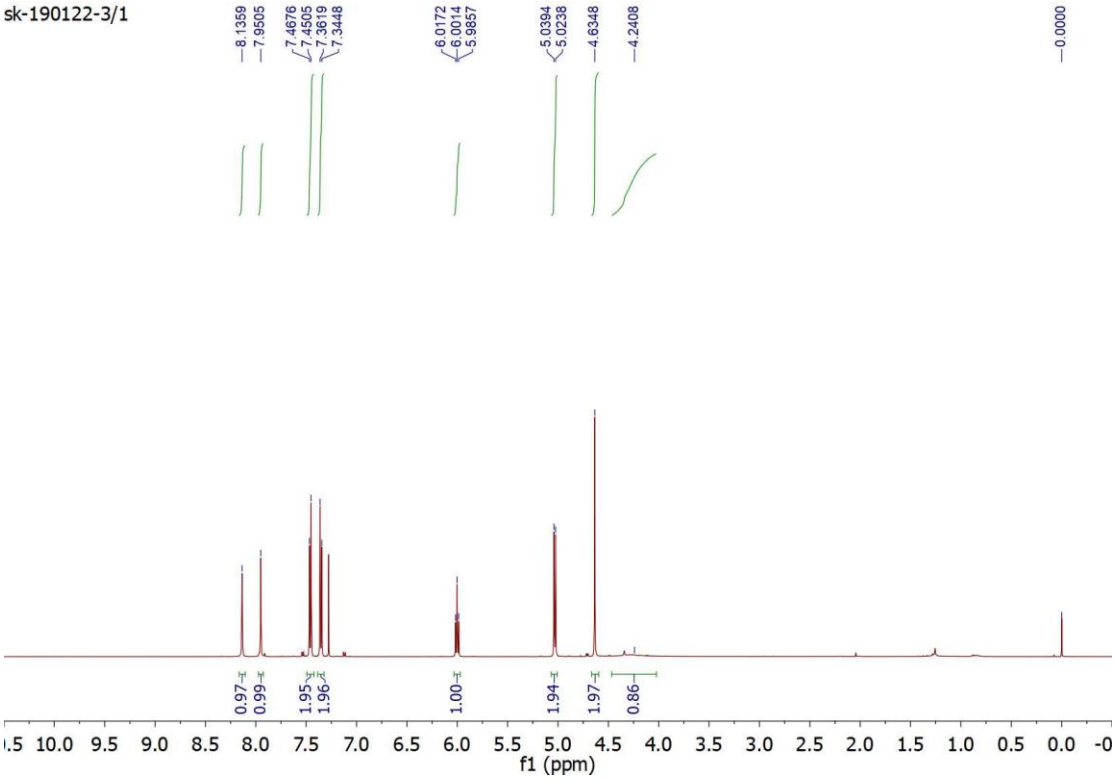
3h

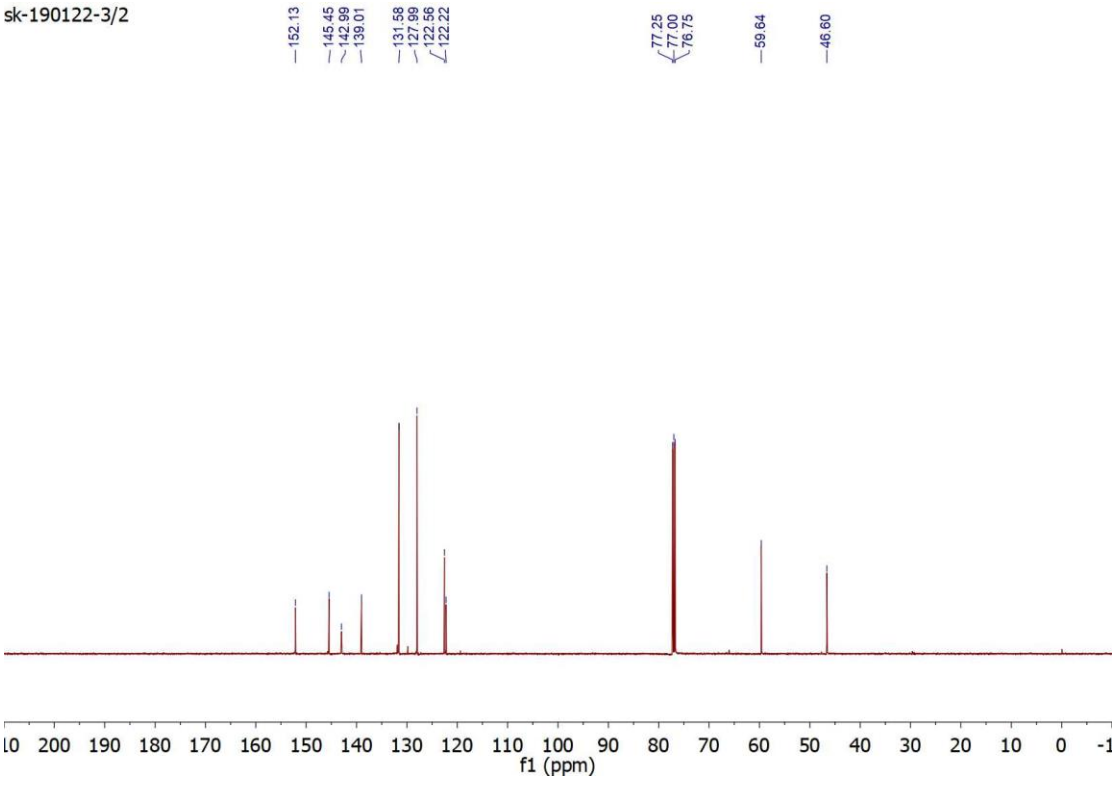

sk-181102-1/1
8.1533
7.9556
7.6279
7.6232
7.6186
7.4414
7.4387
7.4362
7.4339
7.4210
7.4188
7.4166
7.4140
7.4009
7.3971
7.3938
7.2281
7.2085
7.1887
6.0240
6.0044
5.9849
5.0589
5.0393
4.6346
3.5714
0.0000
0.89
0.93
0.95
2.06
1.03
1.00
1.96
1.94
1.20
f1 (ppm)

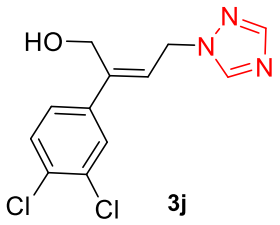

sk-181102-1/2
152.11
145.15
143.04
142.26
131.05
130.01
129.43
125.01
123.32
122.60
77.32
77.00
76.68
59.69
46.60
f1 (ppm)


HO
N
N
N
Br

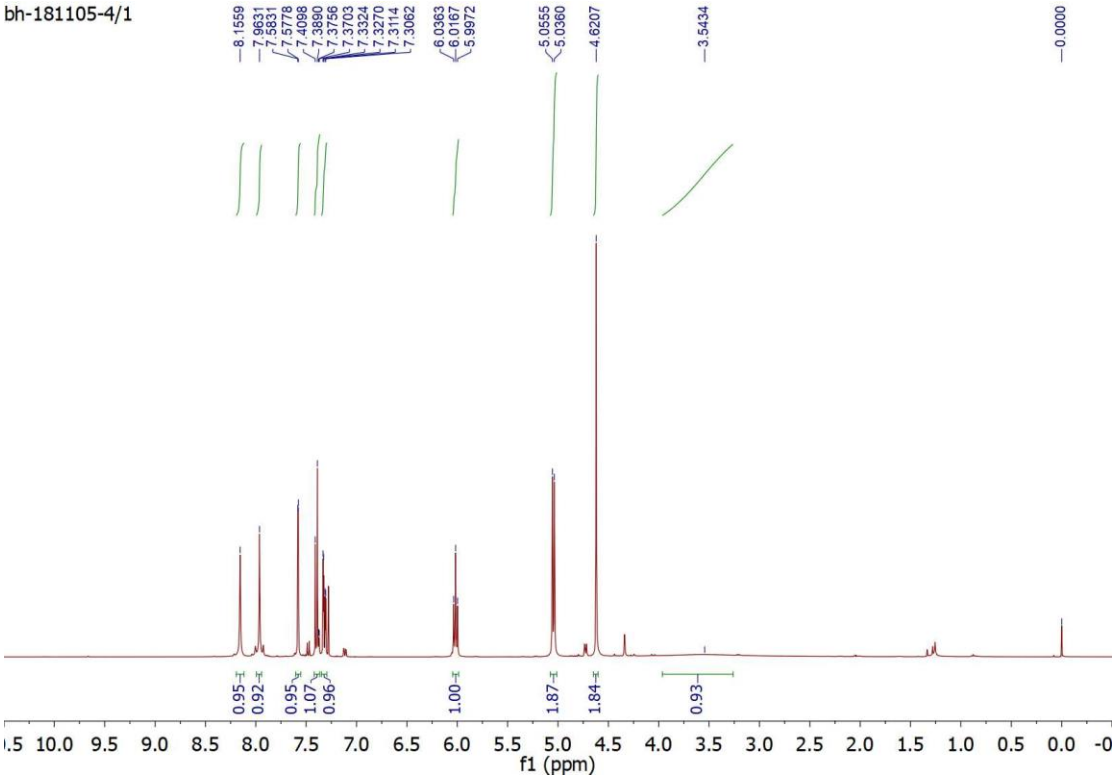
3i

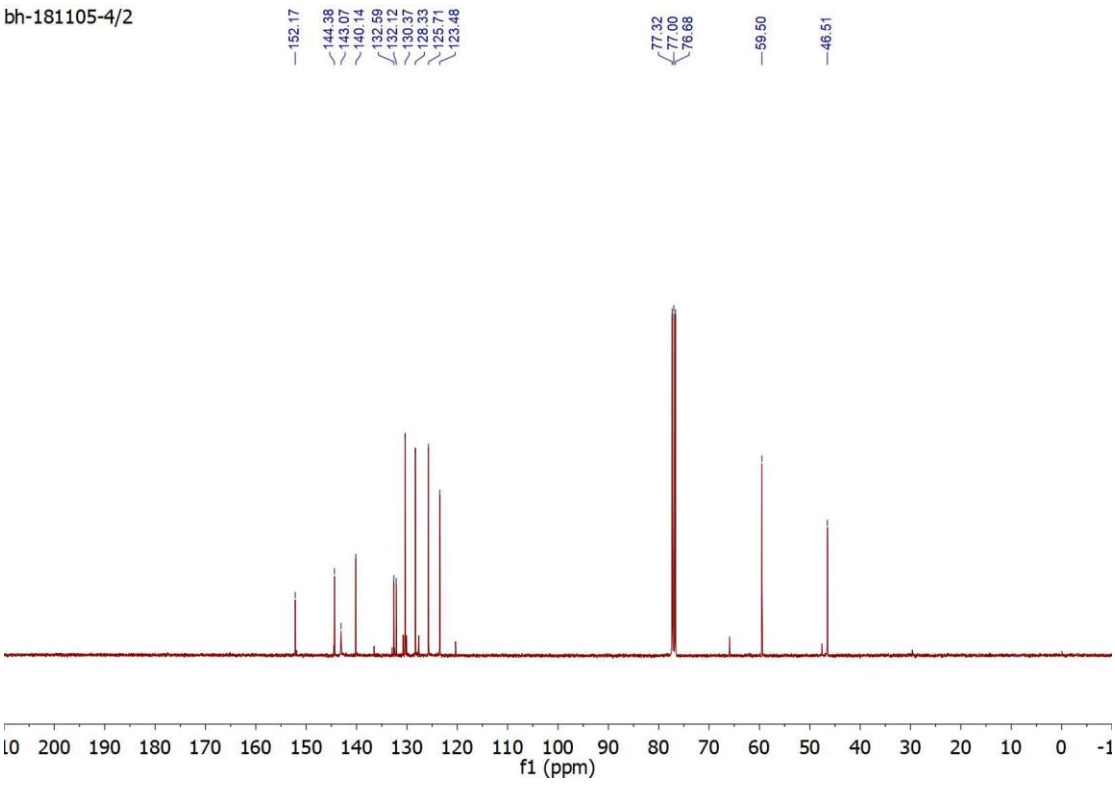

sk-190122-3/1
8.1359
7.9505
7.4676
7.4505
7.3619
7.3448
6.0172
6.0014
5.9857
5.0394
5.0238
4.6348
4.2408
0.0000
0.97
0.99
1.95
1.96
1.00
1.94
1.97
0.86
f1 (ppm)

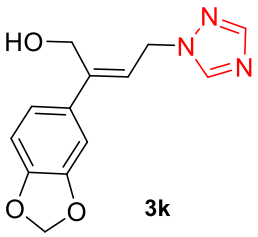

sk-190122-3/2
152.13
145.45
142.99
139.01
131.58
127.99
122.56
122.22
77.25
77.00
76.75
59.64
46.60
f1 (ppm)


HO
N
N
N
Cl
Cl

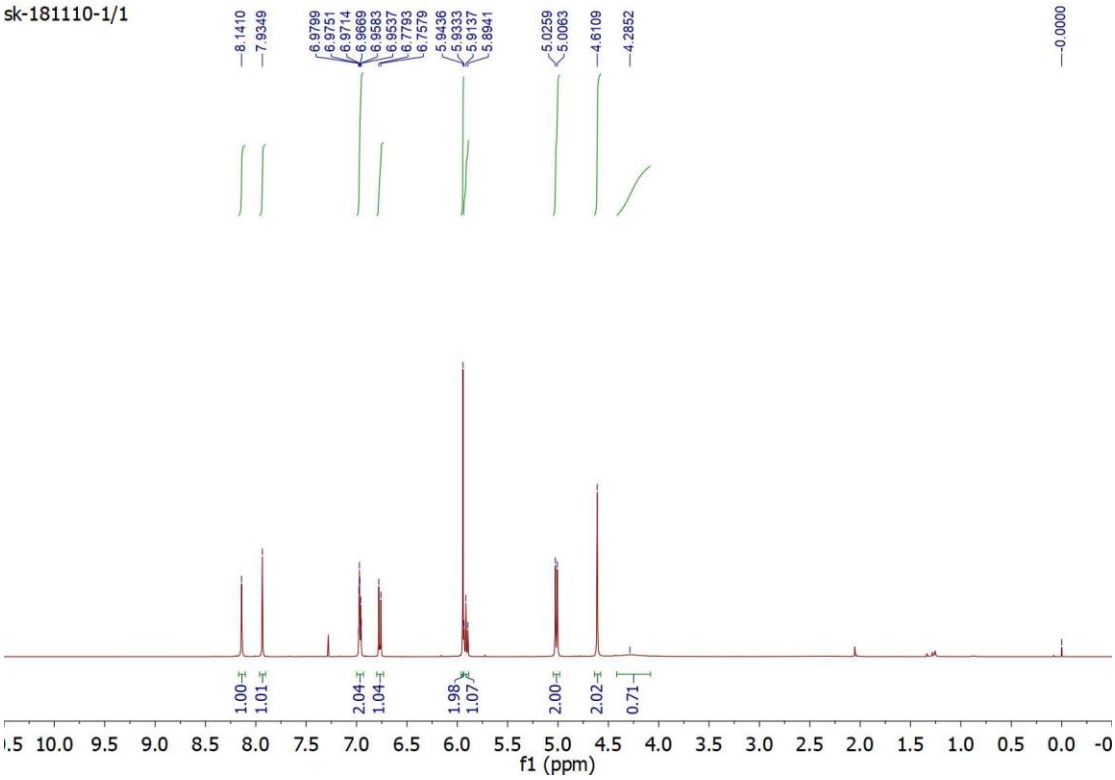
3j

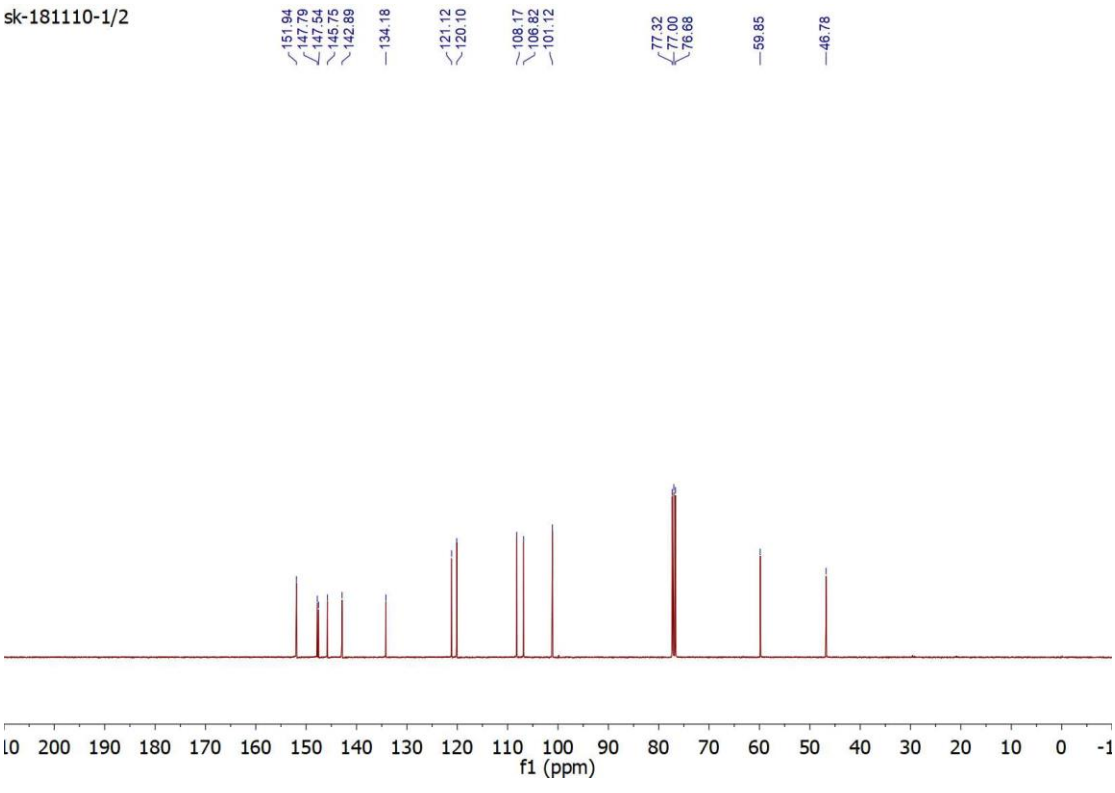

bh-181105-4/1
8.1559
7.9631
7.5831
7.5778
7.4098
7.3890
7.3756
7.3703
7.3324
7.3270
7.3114
7.3062
6.0363
6.0167
5.9972
5.0555
5.0360
4.6207
3.5434
0.0000
0.95
0.92
0.95
1.07
0.96
1.00
1.87
1.84
0.93
f1 (ppm)

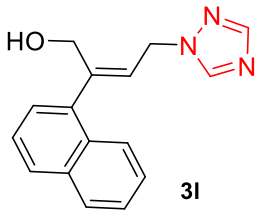

bh-181105-4/2
152.17
144.38
143.07
140.14
132.59
132.12
130.37
128.33
125.71
123.48
77.32
77.00
76.68
59.50
46.51
f1 (ppm)


HO
N
N
N
O
O

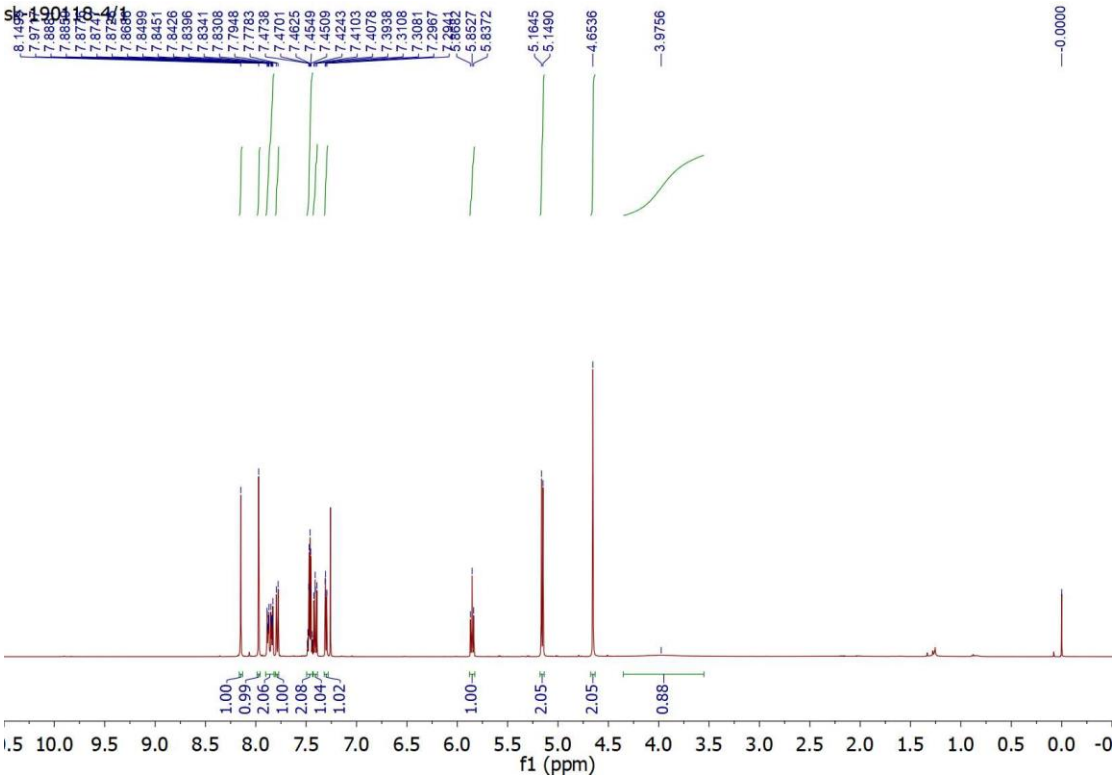
3k

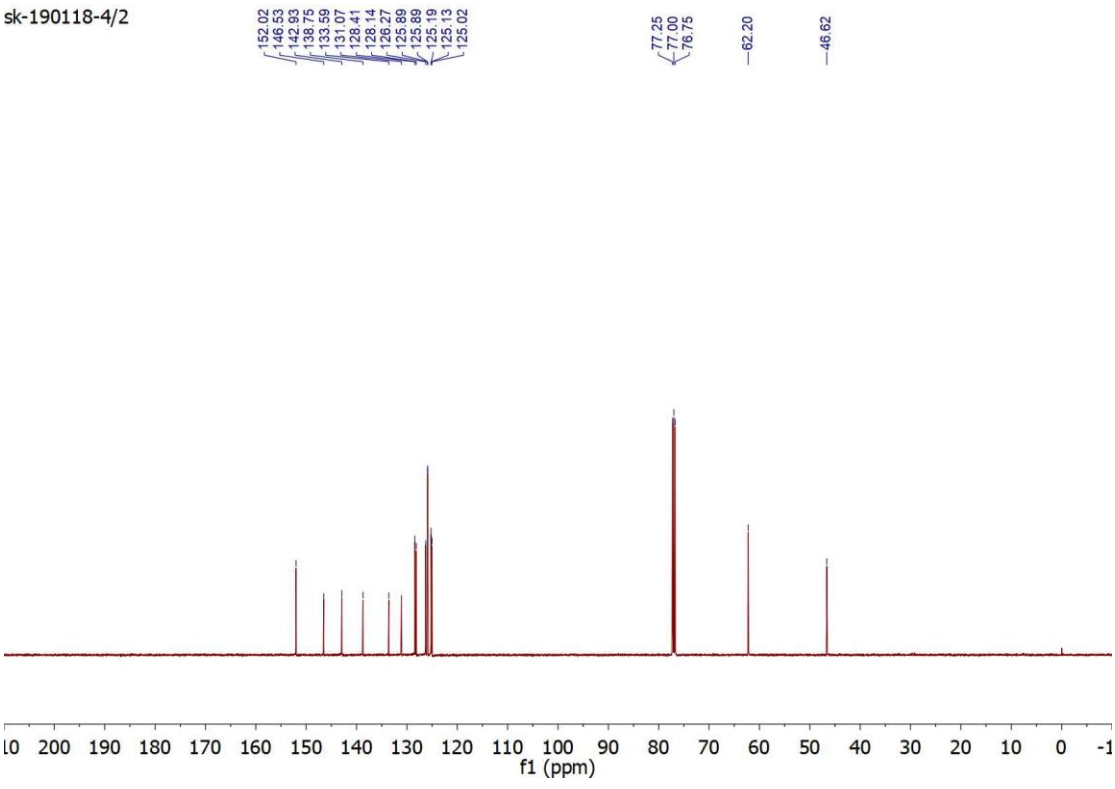

sk-181110-1/1
8.1410
7.9349
6.9799
6.9751
6.9714
6.9669
6.9583
6.9537
6.7793
6.7579
5.9436
5.9333
5.9137
5.8941
5.0259
5.0063
4.6109
4.2852
0.0000
1.00
1.01
2.04
1.04
1.98
1.07
2.00
2.02
0.71
f1 (ppm)


sk-181110-1/2
151.94
147.79
147.54
145.75
142.89
134.18
121.12
120.10
108.17
106.82
101.12
77.32
77.00
76.68
59.85
46.78
f1 (ppm)


HO
N
N
N

3l


sk-190118-4/1
5.1645
5.1490
4.6536
3.9756
0.0000
1.00
0.99
2.06
1.00
2.08
1.04
1.02
1.00
2.05
2.05
0.88
f1 (ppm)


sk-190118-4/2
152.02
146.53
142.93
138.75
133.59
131.07
128.41
128.14
126.27
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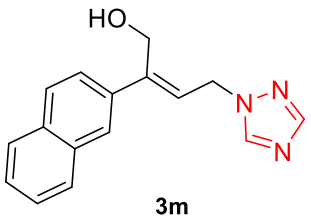
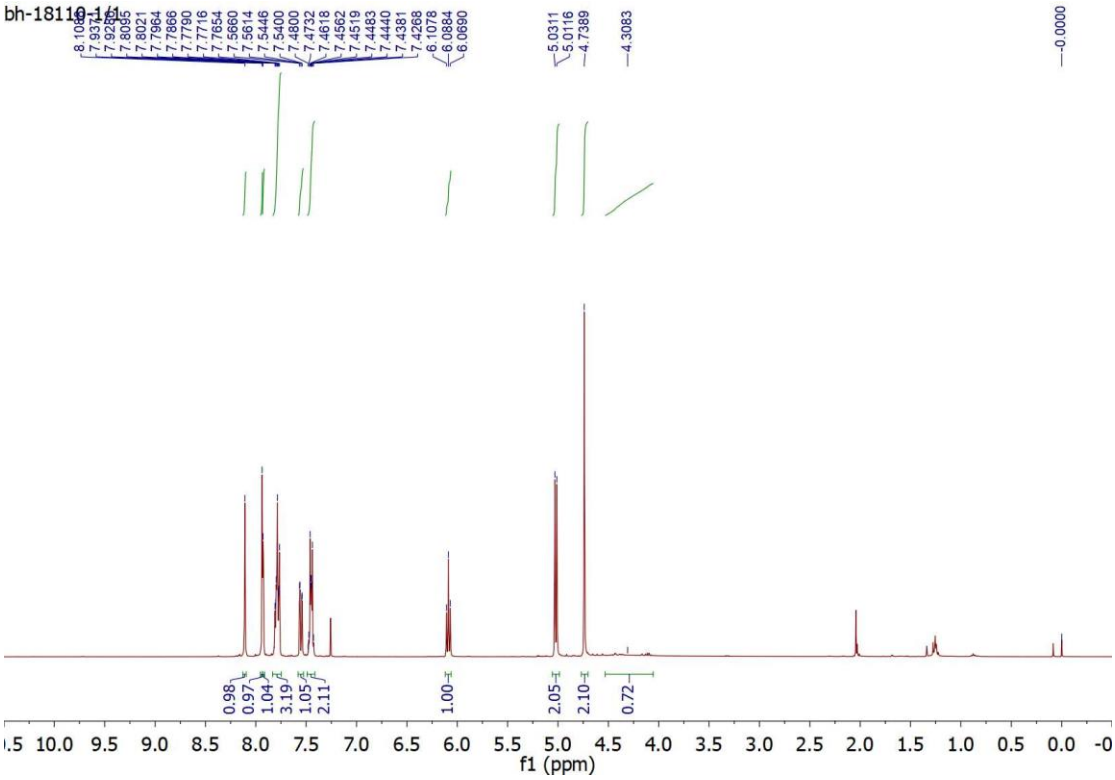
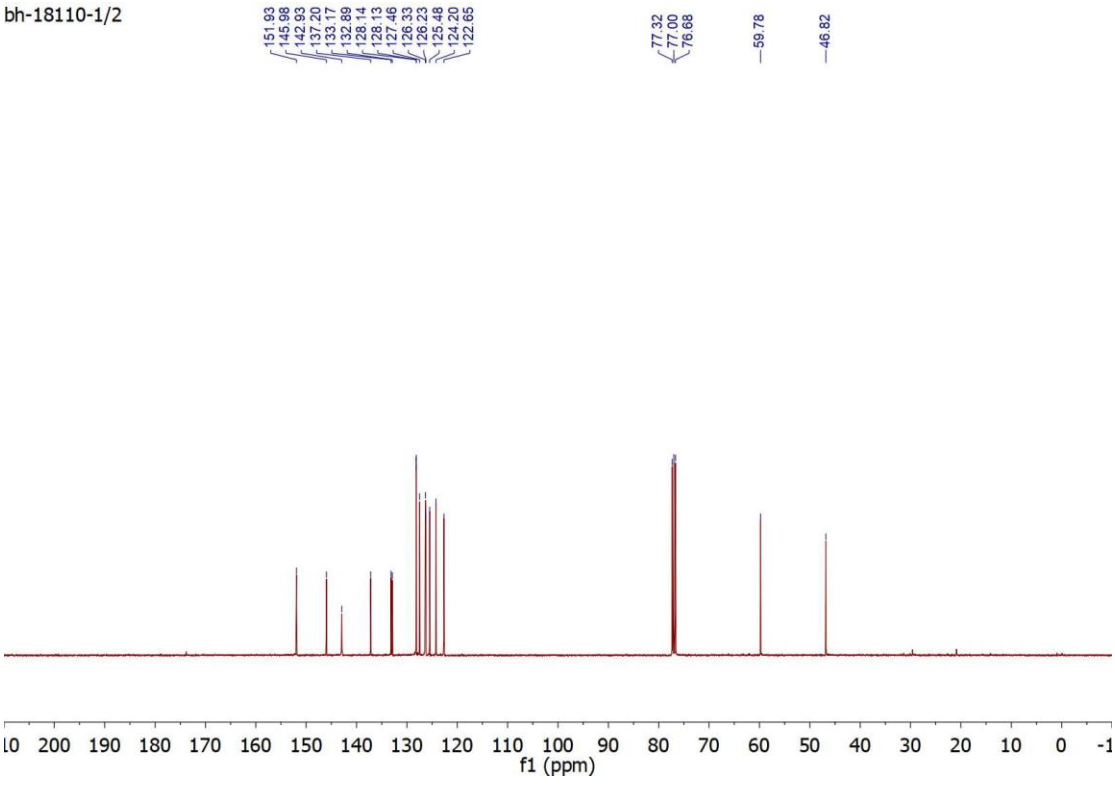
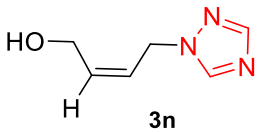
77.00
76.75
62.20
46.62
f1 (ppm)


HO
N
N
N

3m

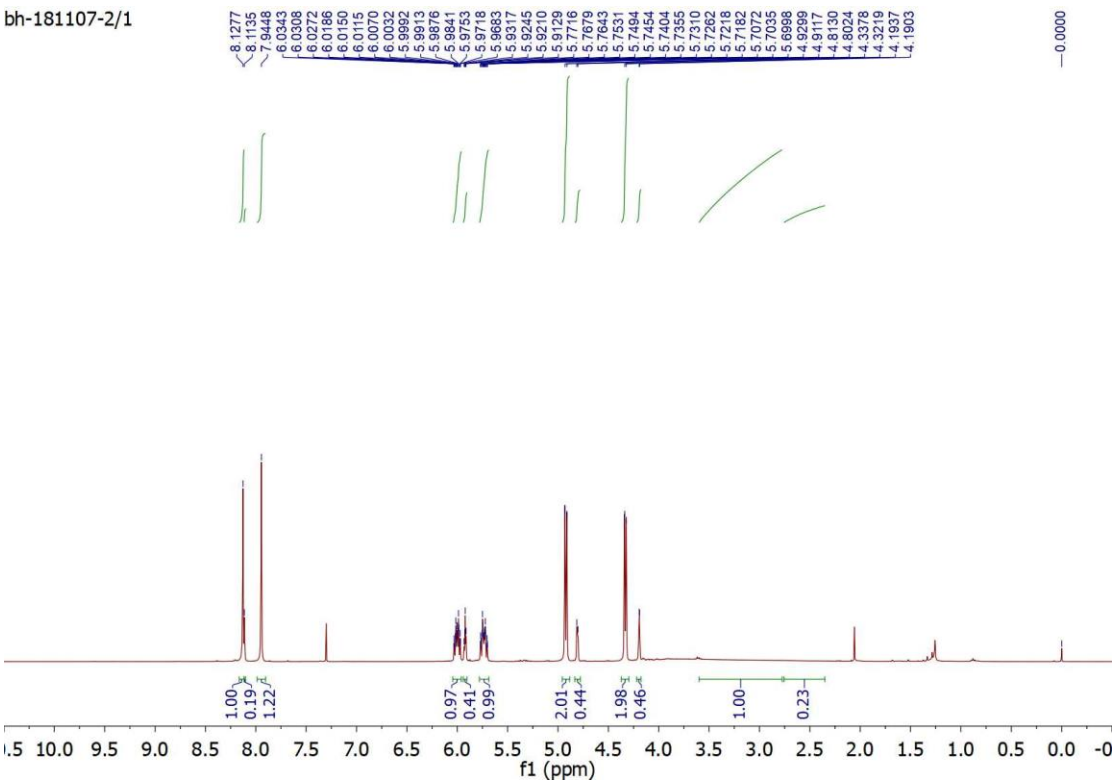

bh-18110-1/1
8.1087
7.9377
7.9285
7.8095
7.8021
7.7964
7.7866
7.7790
7.7716
7.7654
7.5660
7.5614
7.5446
7.5400
7.4800
7.4732
7.4618
7.4562
7.4519
7.4483
7.4440
7.4381
7.4268
6.1078
6.0884
6.0690
5.0311
5.0116
4.7389
4.3083
0.0000
0.98
0.97
1.04
3.19
1.05
2.11
1.00
2.05
2.10
0.72
f1 (ppm)


bh-18110-1/2
151.93
145.98
142.93
137.20
133.17
132.89
128.14
128.13
127.46
126.33
126.23
125.48
124.20
122.65
77.32
77.00
76.68
59.78
46.82
f1 (ppm)

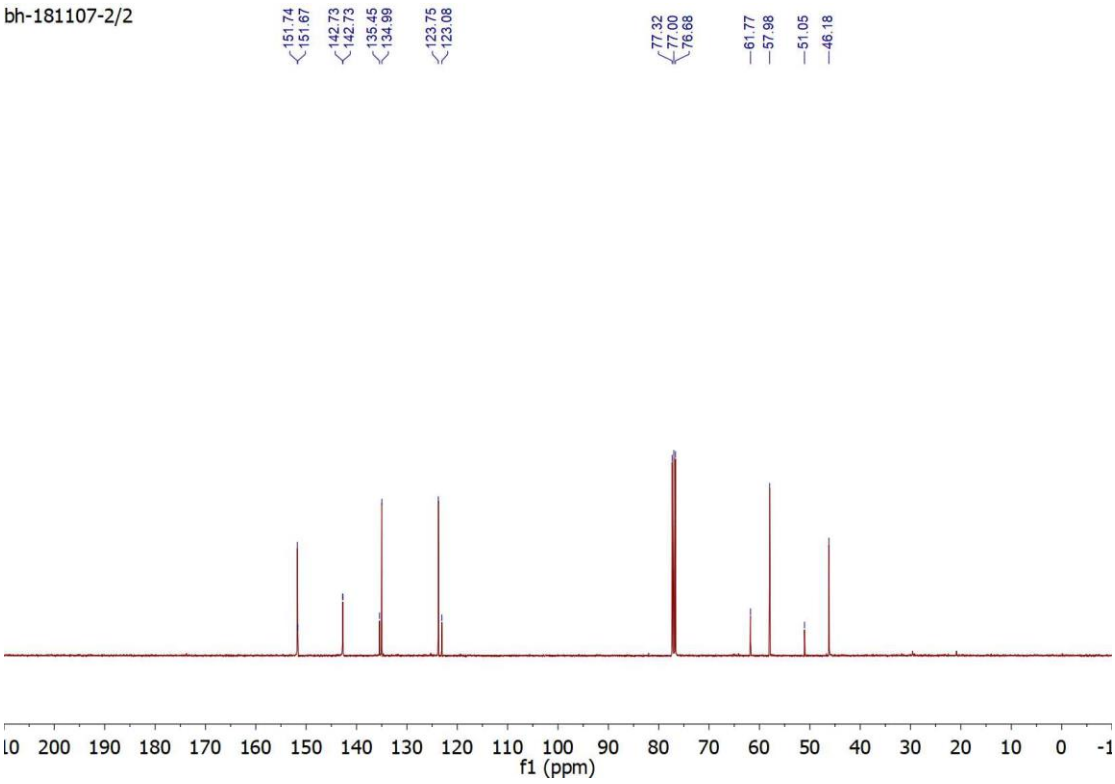


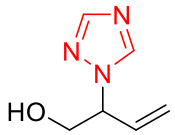
3n

bh-181107-2/1

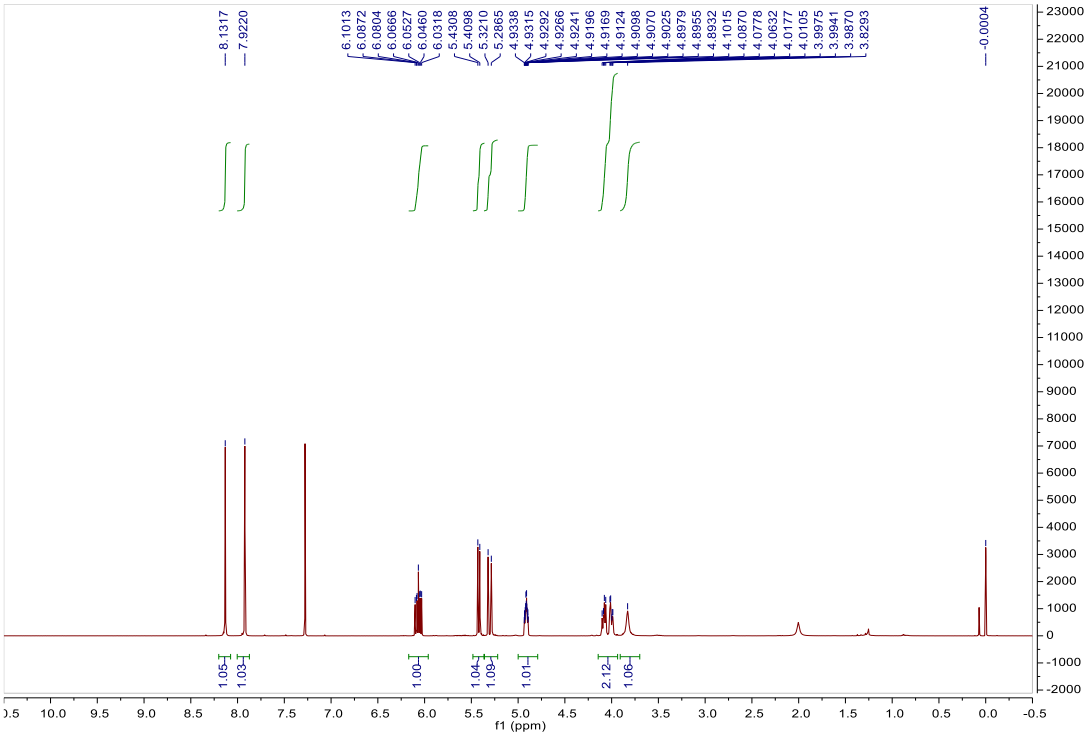


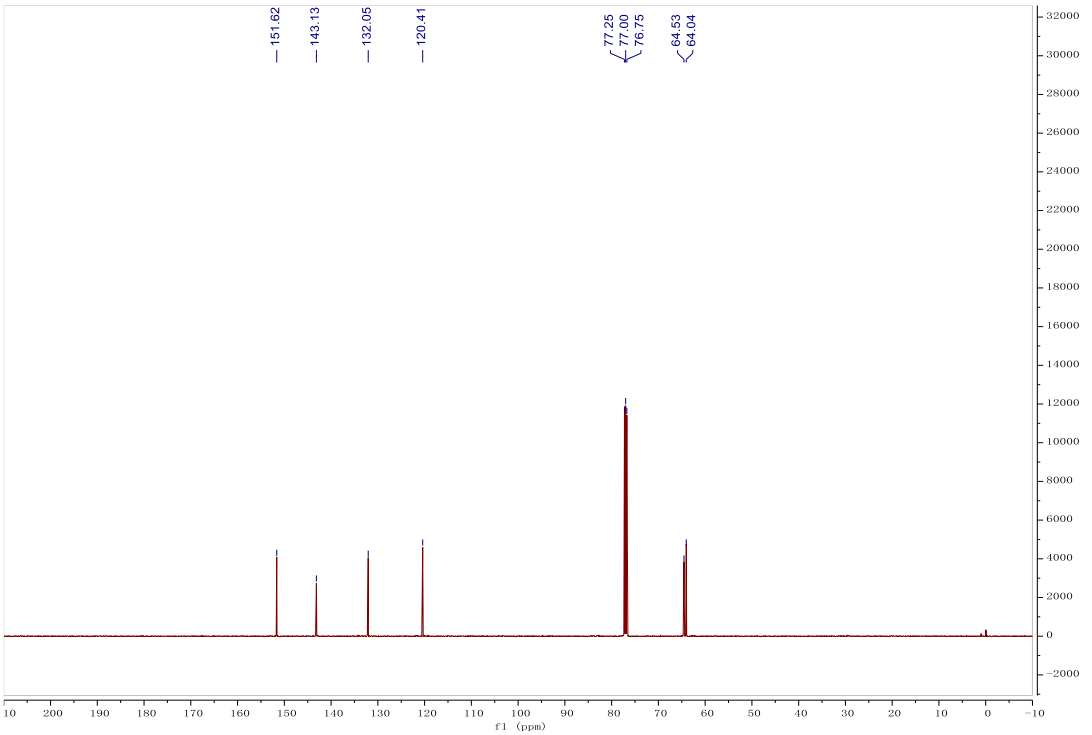
bh-181107-2/2

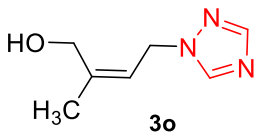



N
N
N
HO

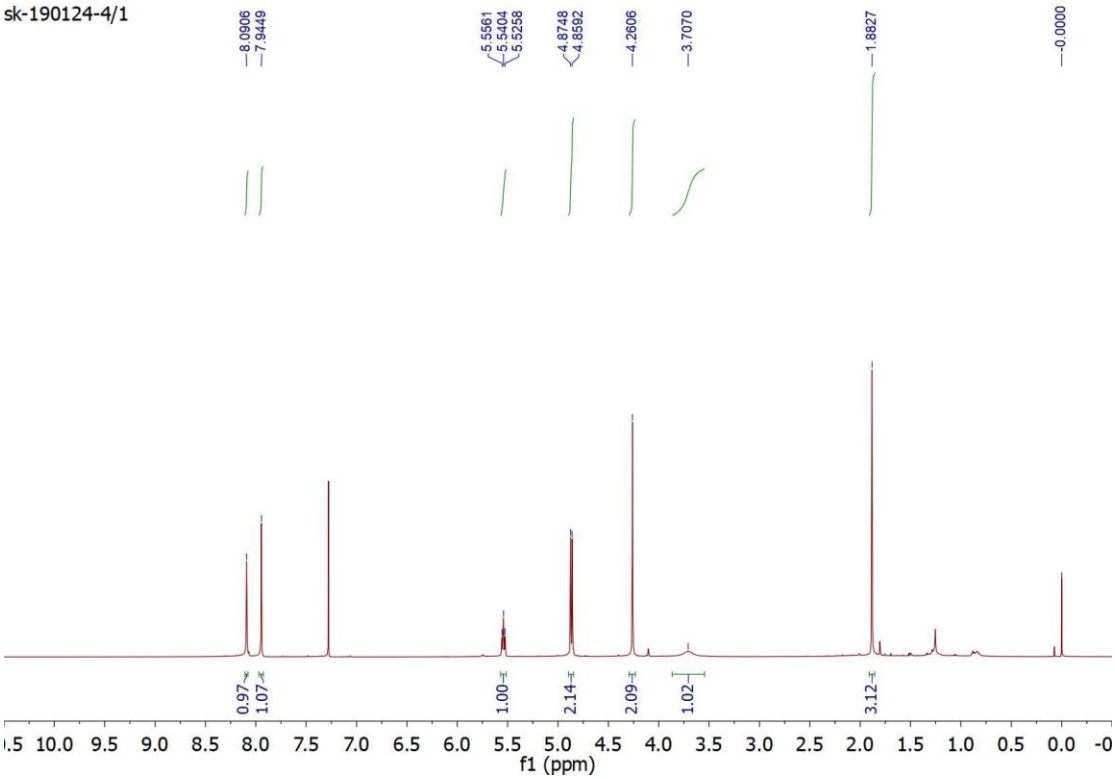
3n'

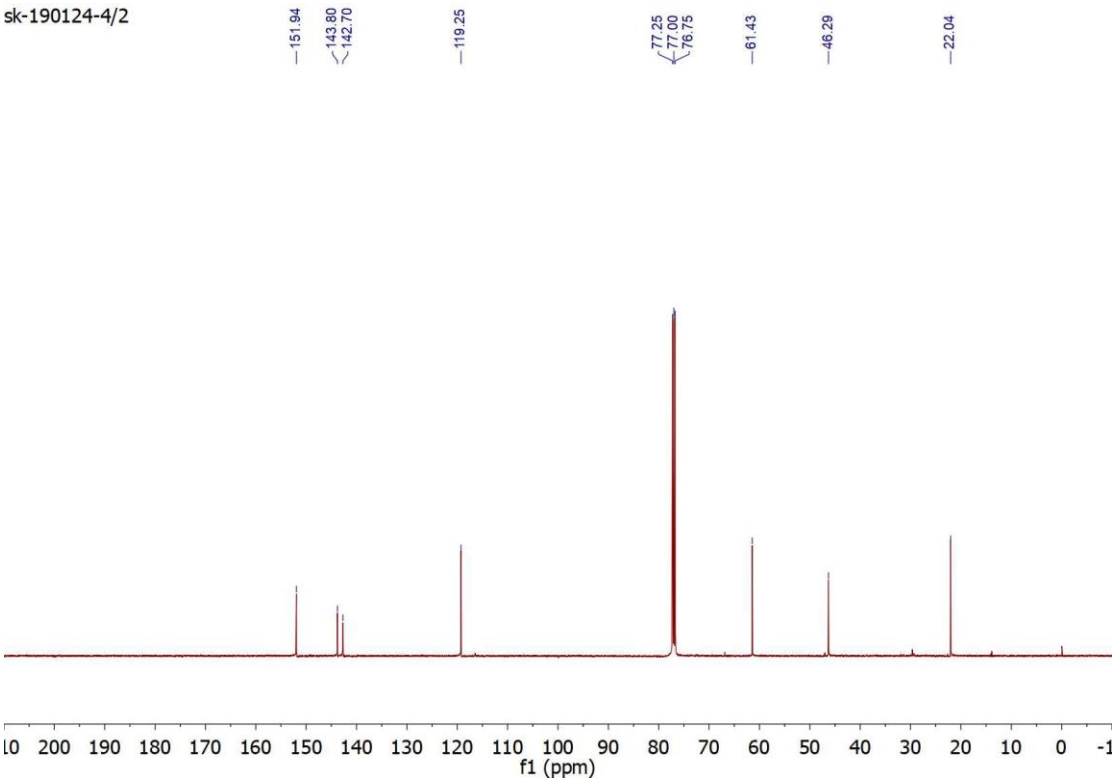

8.1317
7.9220
6.1013
6.0872
6.0804
6.0666
6.0527
6.0460
6.0318
5.4308
5.4098
5.3210
5.2865
4.9338
4.9315
4.9292
4.9266
4.9241
4.9196
4.9169
4.9124
4.9098
4.9070
4.9025
4.8979
4.8955
4.8932
4.1015
4.0670
4.0778
4.0632
4.0177
4.0105
3.9975
3.9941
3.9870
3.8293
-0.0004
1.05
1.03
1.00
1.04
1.09
1.01
2.12
1.06
f1 (ppm)

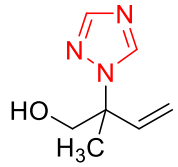

151.62
143.13
132.05
120.41
77.25
77.00
76.75
64.53
64.04
f1 (ppm)


HO
N
N
N
H_3C

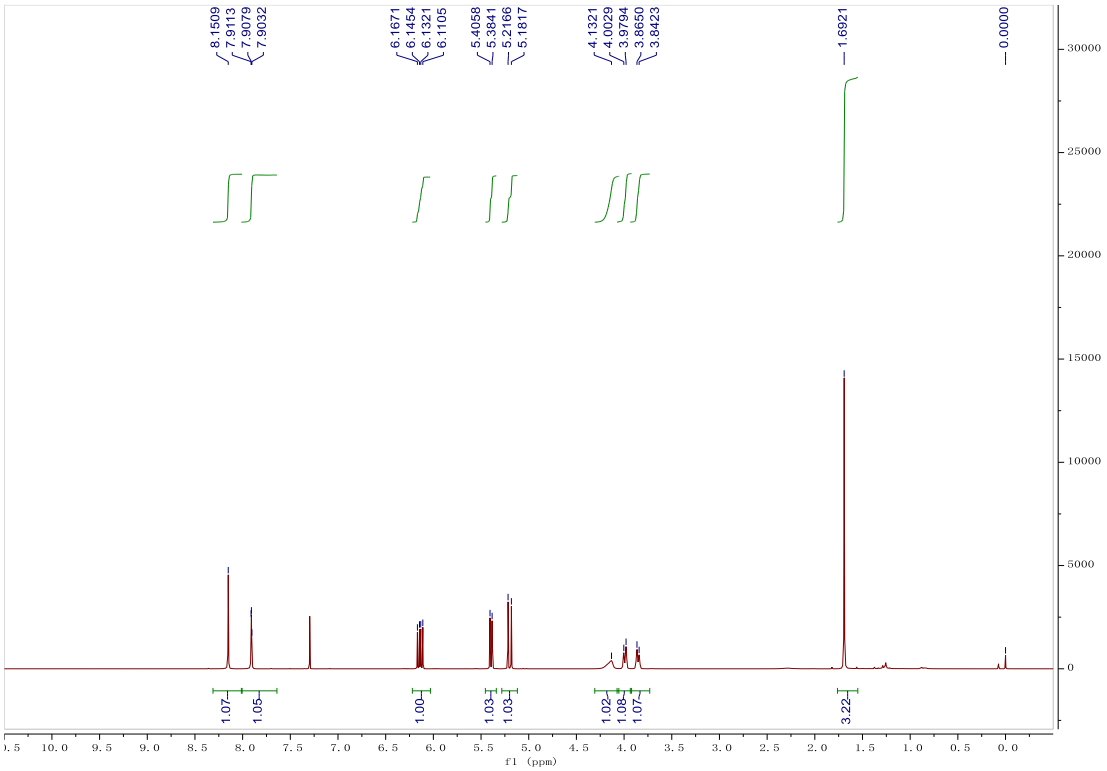
3o

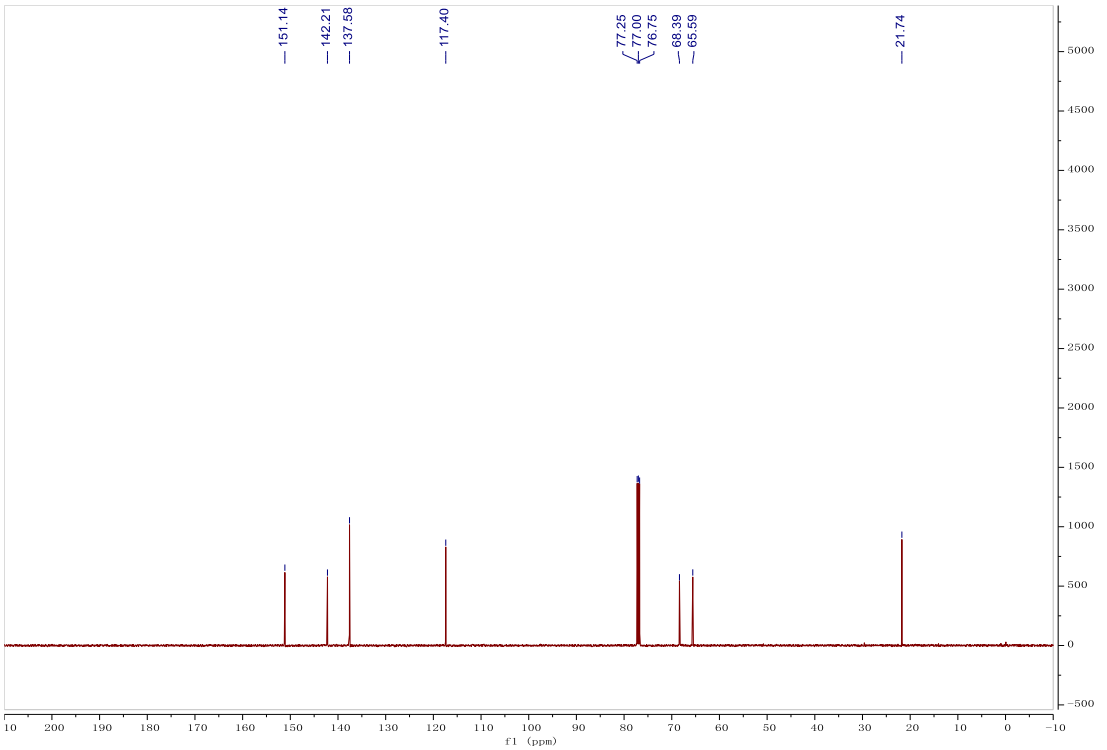

sk-190124-4/1
8.0906
7.9449
5.5561
5.5404
5.5258
4.8748
4.8592
4.2606
3.7070
1.8827
0.0000
0.97
1.07
1.00
2.14
2.09
1.02
3.12
f1 (ppm)

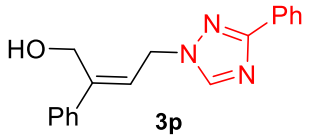

sk-190124-4/2
151.94
143.80
142.70
119.25
77.25
77.00
76.75
61.43
46.29
22.04
f1 (ppm)


N
N
N
HO
H3C

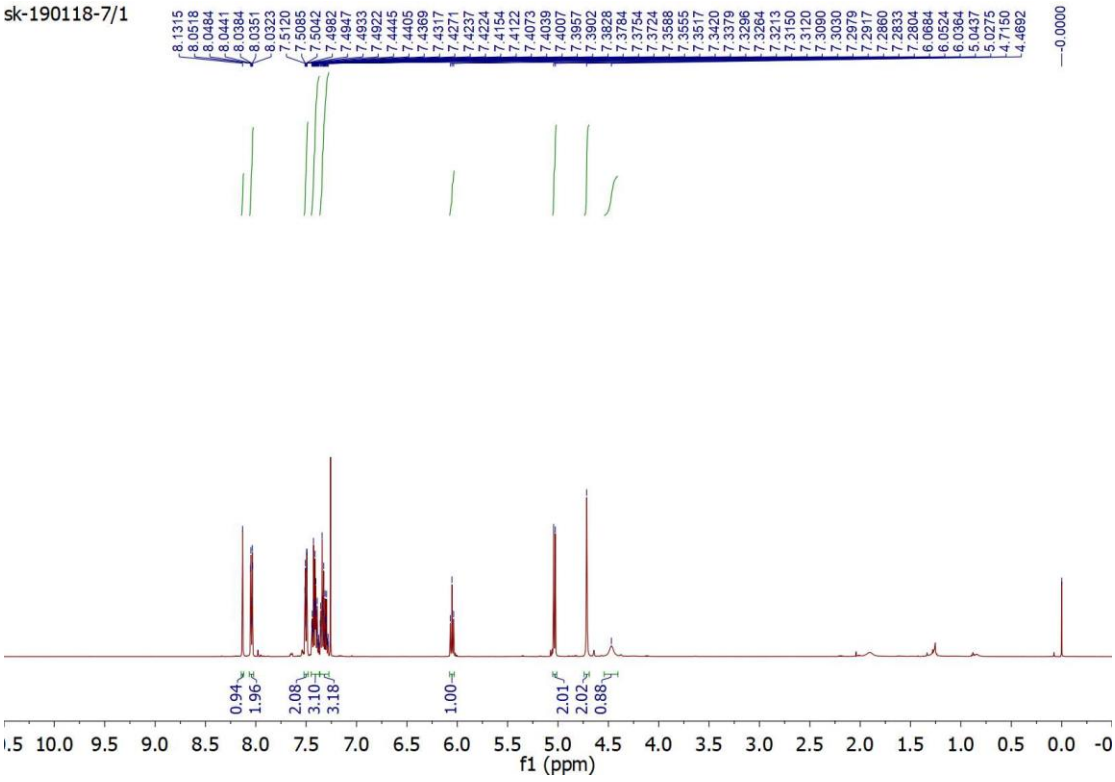
3o'

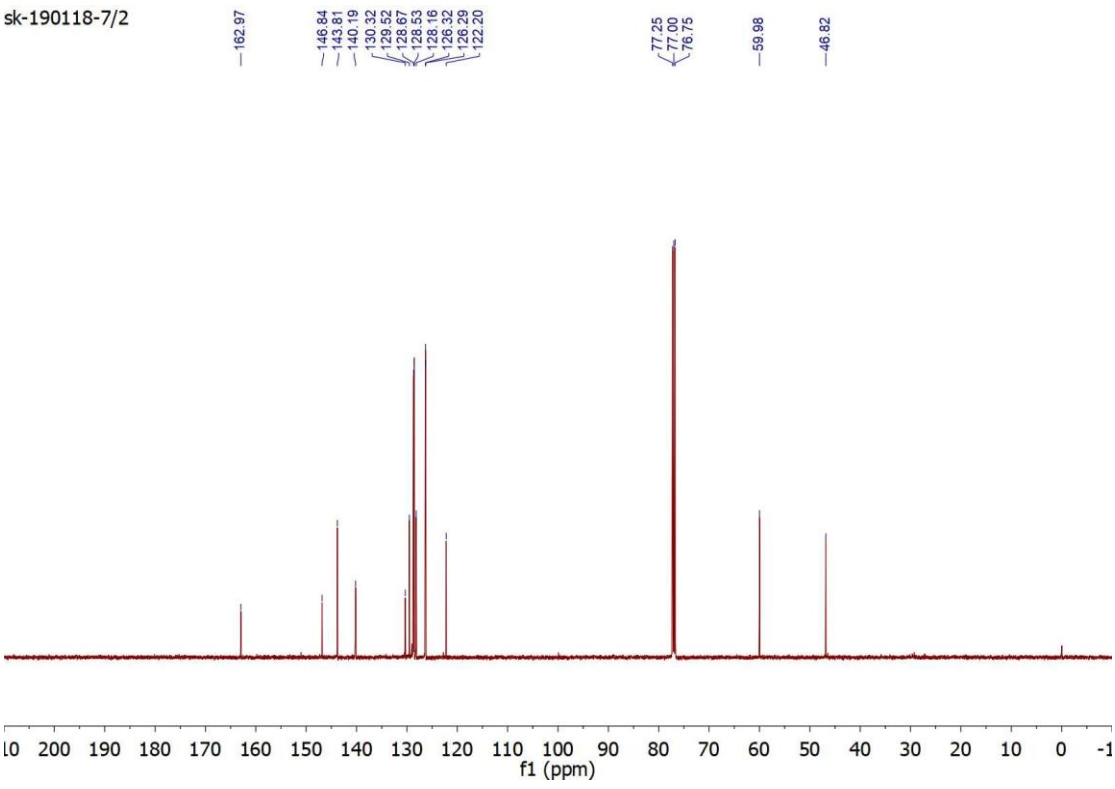

8.1509
7.9113
7.9079
7.9032
6.1671
6.1454
6.1321
6.1105
5.4058
5.3841
5.2166
5.1817
4.1321
4.0029
3.9794
3.8650
3.8423
1.6921
0.0000
1.07
1.05
1.00
1.03
1.03
1.02
1.08
1.07
3.22
f1 (ppm)

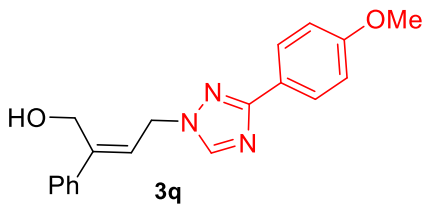

151.14
142.21
137.58
117.40
77.25
77.00
76.75
68.39
65.59
21.74
f1 (ppm)



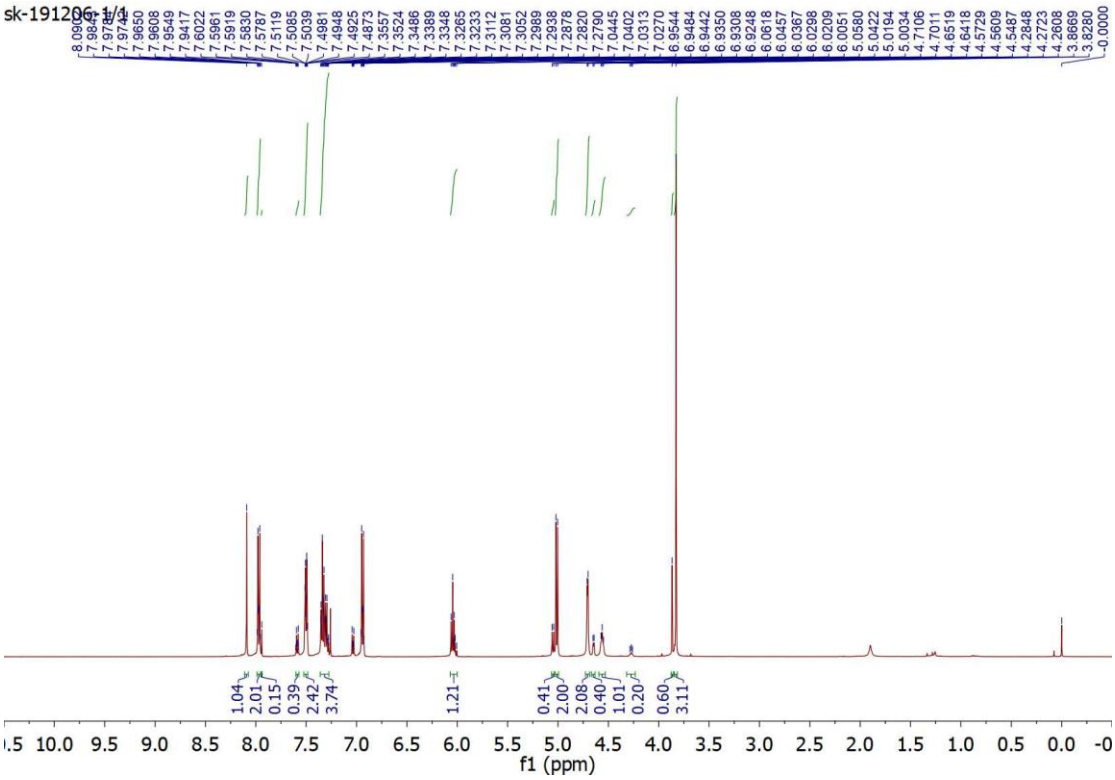
3p

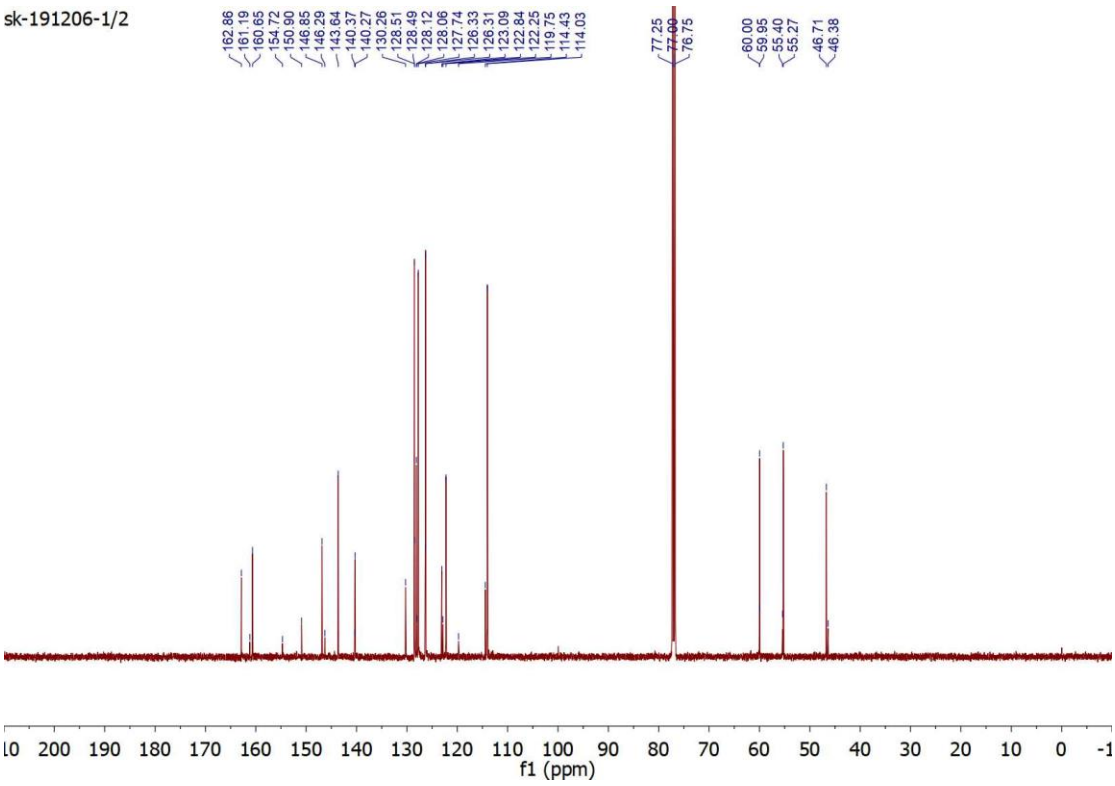


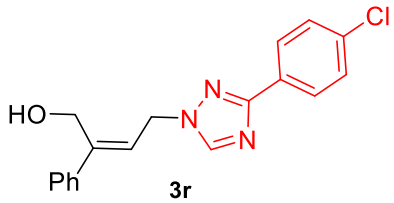



OMe
HO
N
N
N
Ph

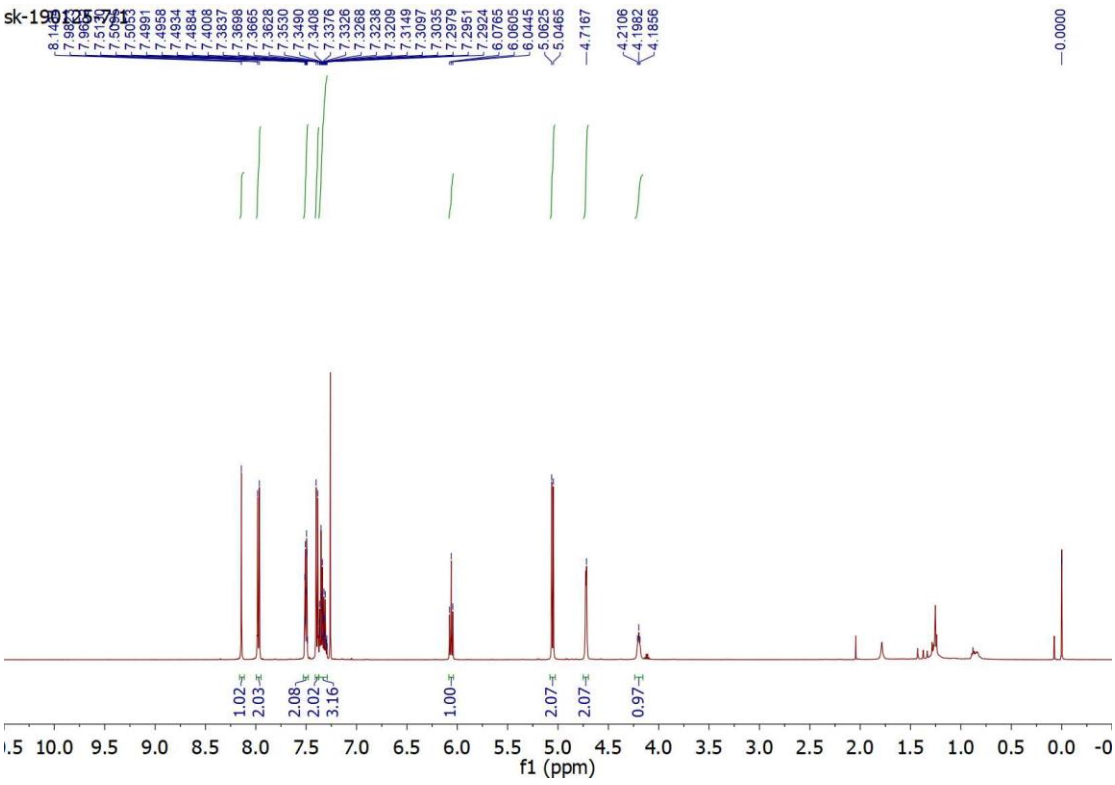
3q

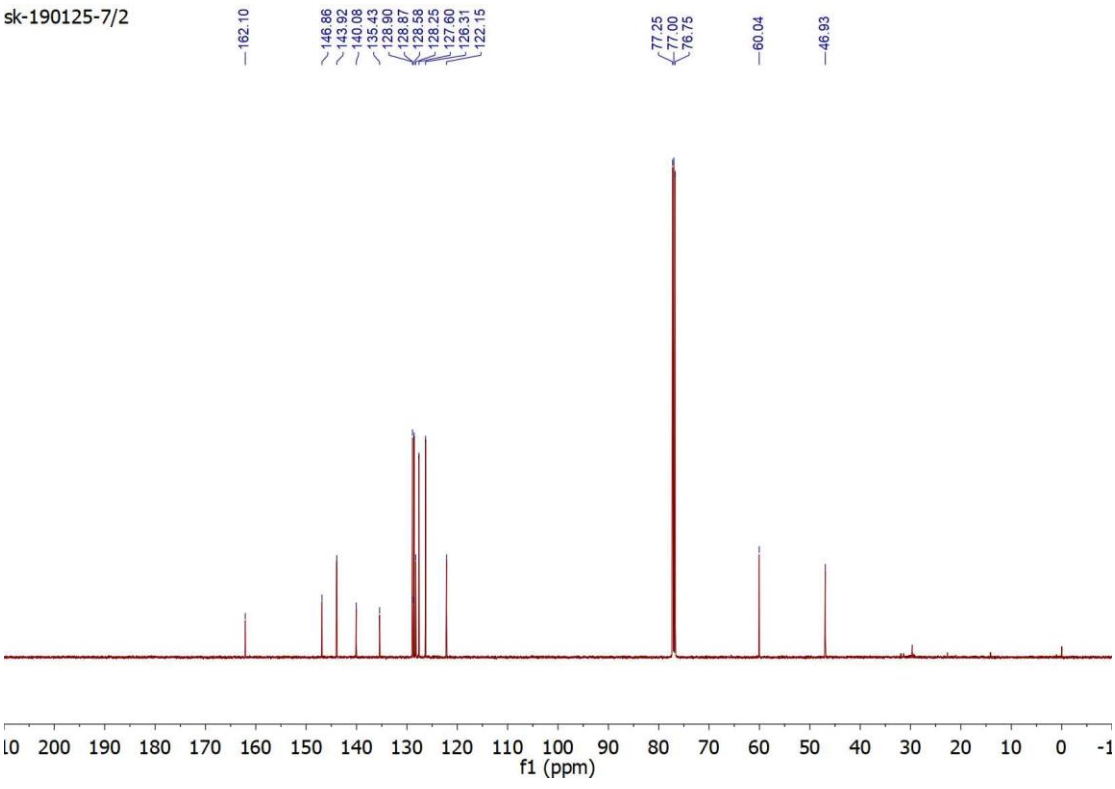

sk-191206-1/1
1.04
2.01
0.15
0.39
2.42
3.74
1.21
0.41
2.00
2.08
0.40
1.01
0.20
0.60
3.11
f1 (ppm)

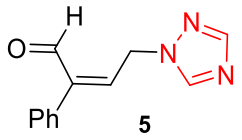

sk-191206-1/2
f1 (ppm)


Cl
HO
N
N
N
Ph

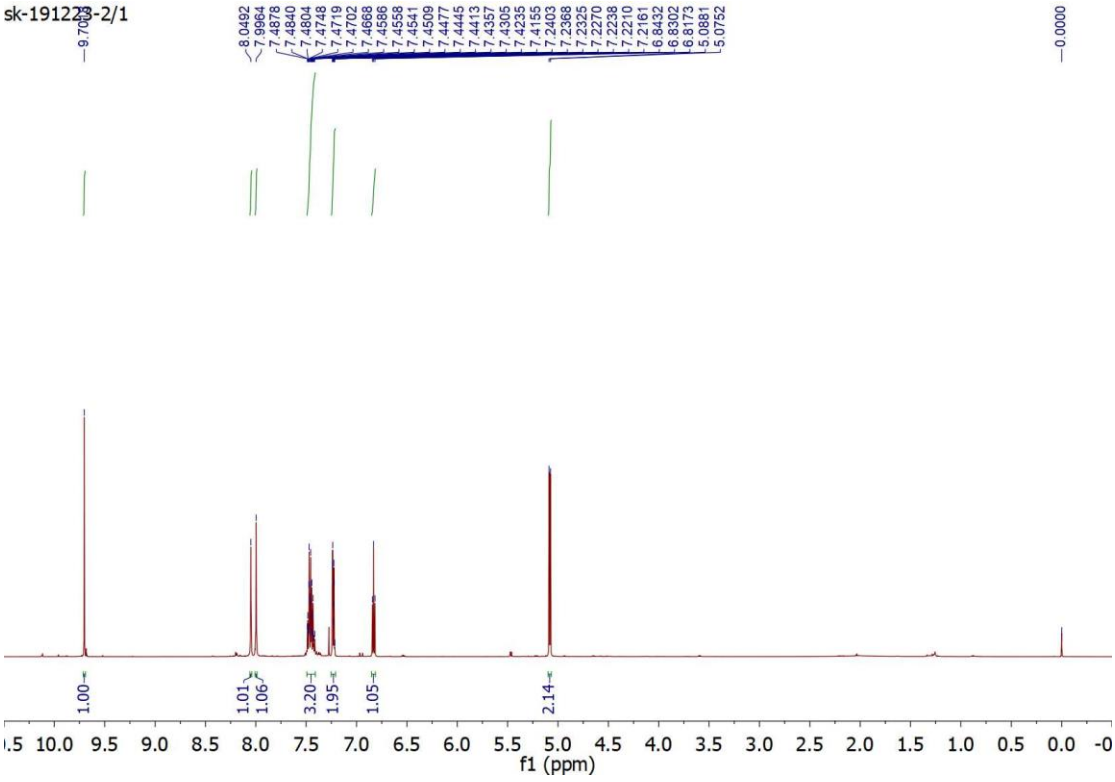
3r

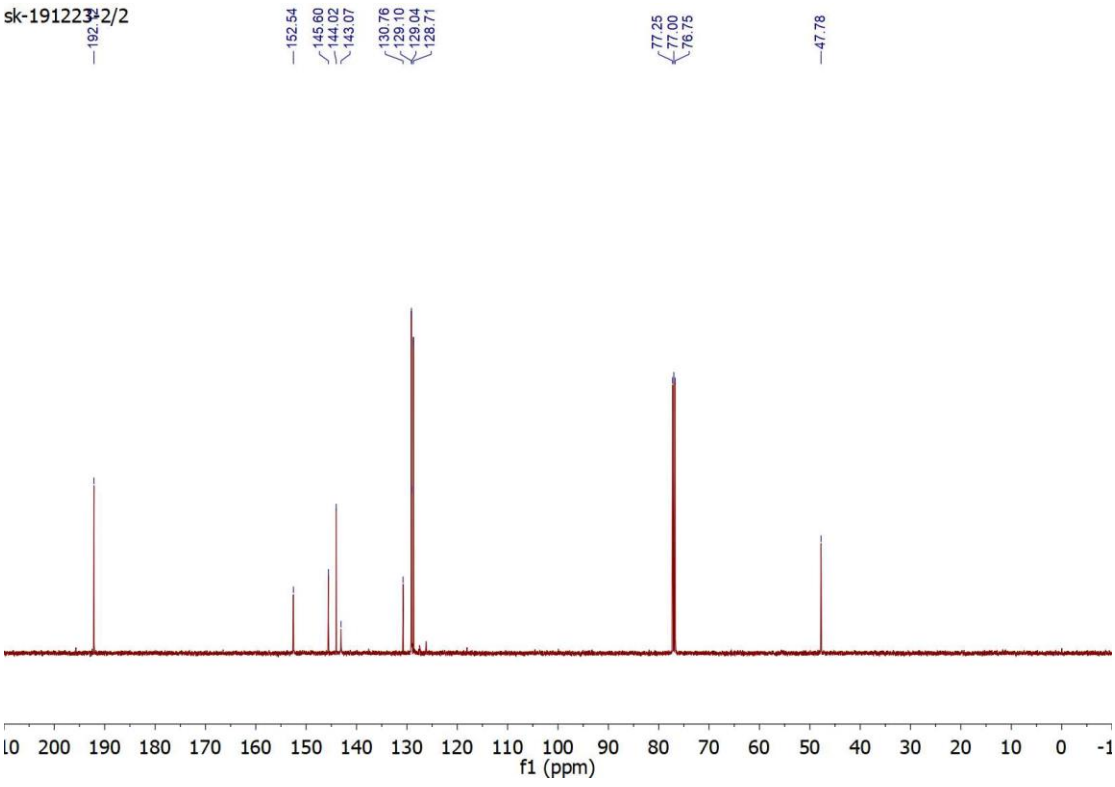

sk-190125-7/1
1.02
2.03
2.08
2.02
3.16
1.00
2.07
2.07
0.97
f1 (ppm)

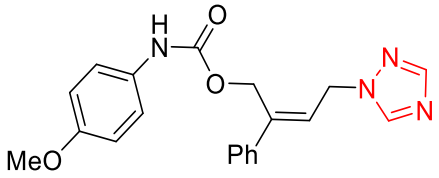

sk-190125-7/2
f1 (ppm)


H
O
N
N
N
Ph

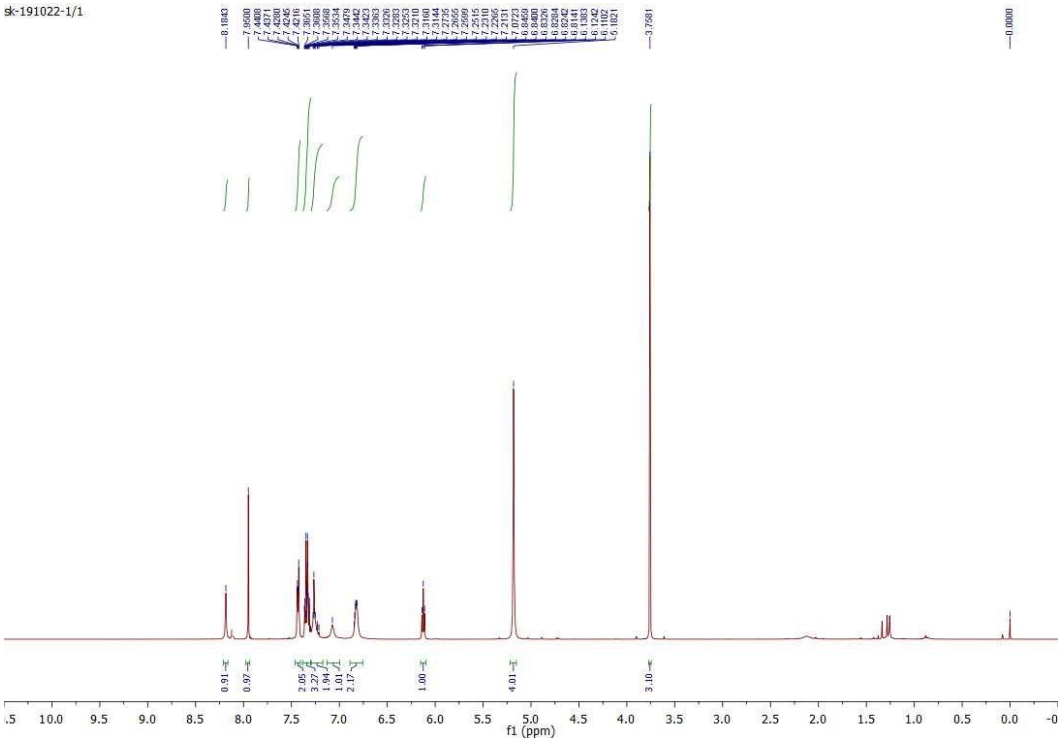
5

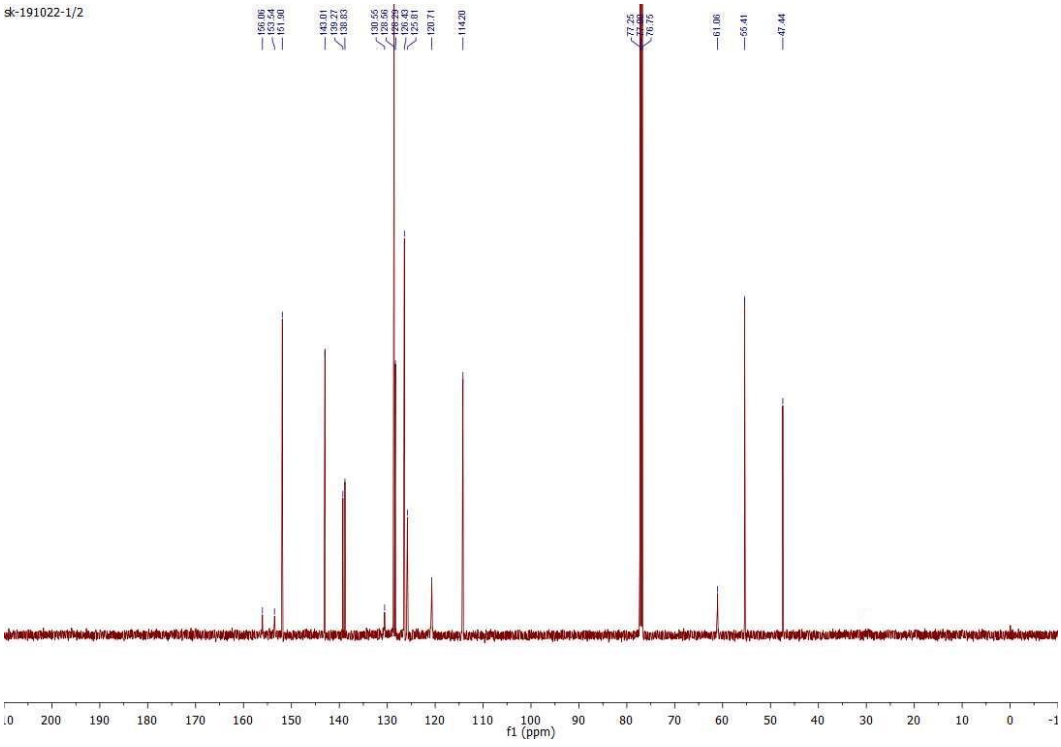

sk-191223-2/1
9.7023
8.0492
7.9964
7.4878
7.4840
7.4804
7.4748
7.4719
7.4702
7.4668
7.4586
7.4558
7.4541
7.4509
7.4477
7.4445
7.4413
7.4357
7.4305
7.4235
7.4155
7.2403
7.2368
7.2325
7.2270
7.2238
7.2210
7.2161
6.8432
6.8302
6.8173
5.0881
5.0752
0.0000
1.00
1.01
1.06
3.20
1.95
1.05
2.14
f1 (ppm)

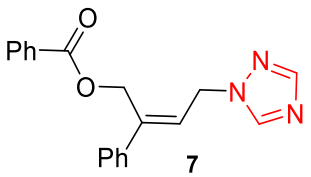

sk-191223-2/2
192.42
152.54
145.60
144.02
143.07
130.76
129.10
129.04
128.71
77.25
77.00
76.75
47.78
f1 (ppm)



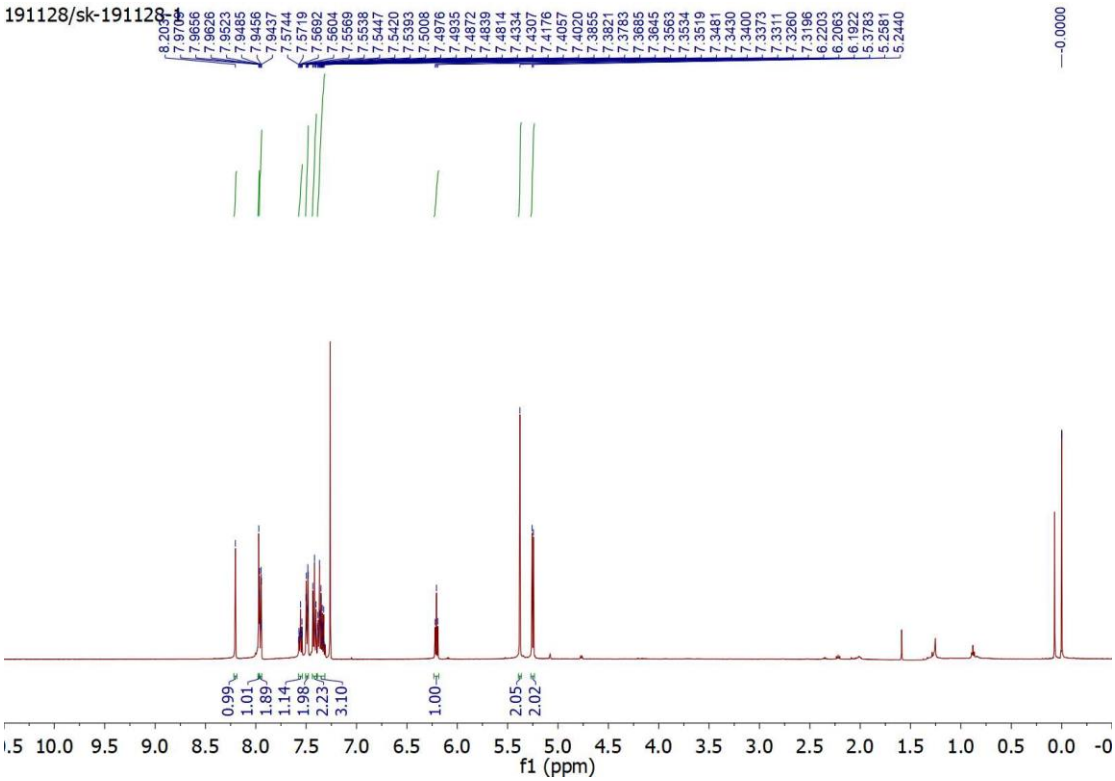
6

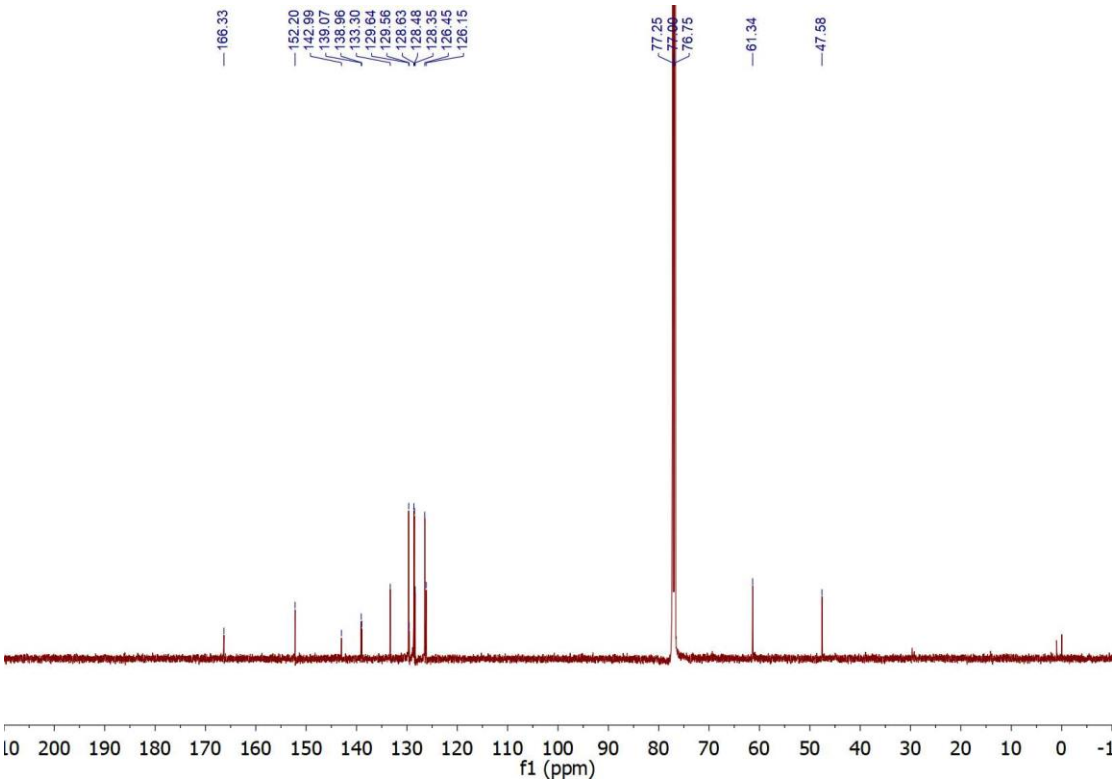


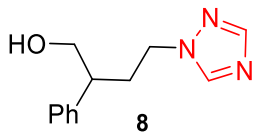



Ph
O
O
N
N
N
Ph

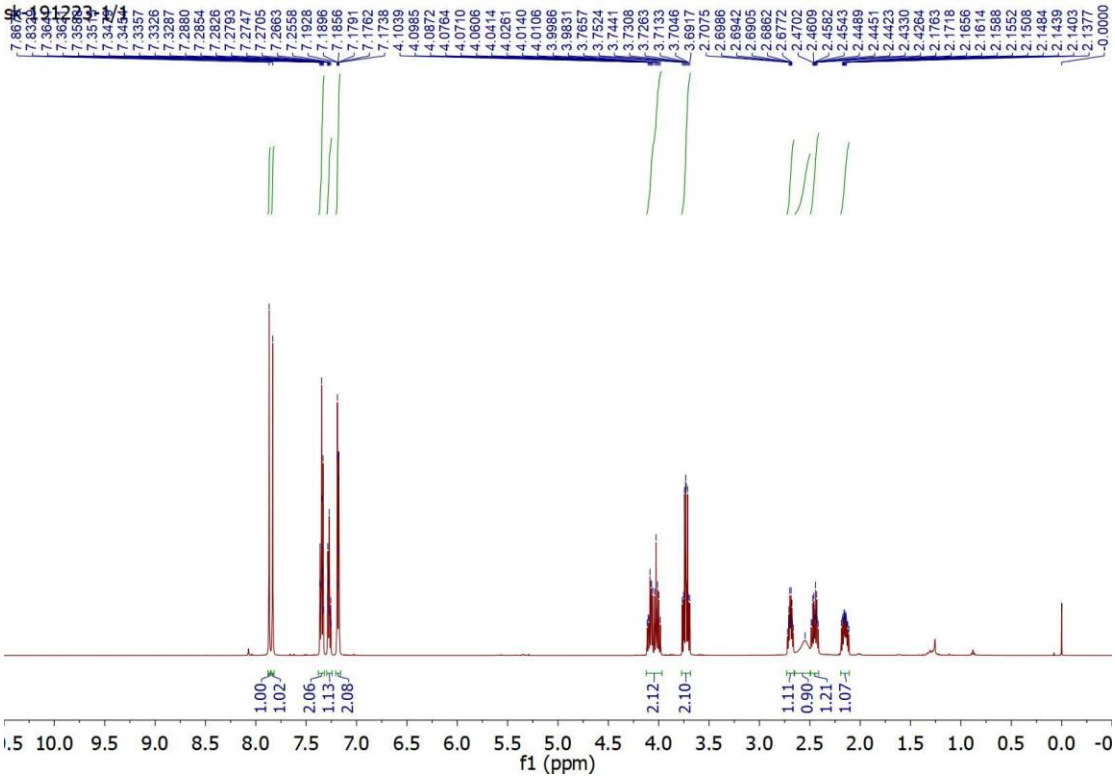
7

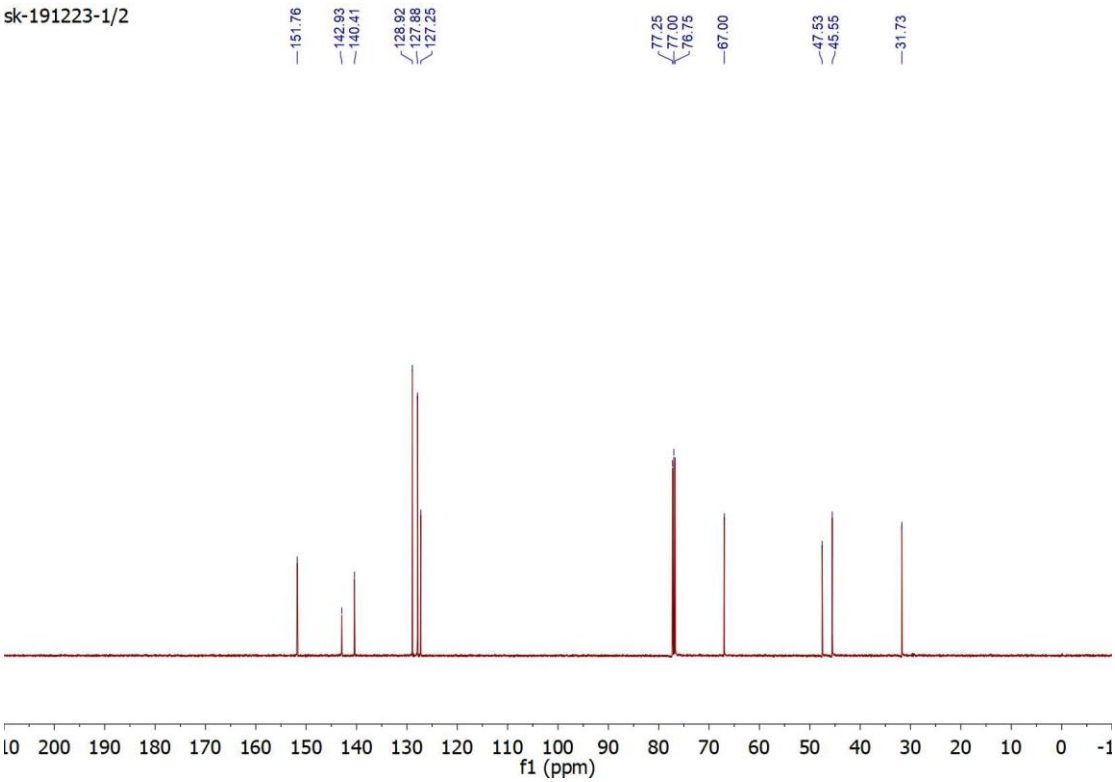

191128/sk-191128-1
0.99
1.01
1.89
1.14
1.98
2.23
3.10
1.00
2.05
2.02
f1 (ppm)


166.33
152.20
142.99
139.07
138.96
133.30
129.64
129.56
128.63
128.48
128.35
126.45
126.15
77.25
77.00
76.75
61.34
47.58
f1 (ppm)


HO
N
N
N
Ph

8


sk-191223-1/1
1.00
1.02
2.06
1.13
2.08
2.12
2.10
1.11
0.90
1.21
1.07
f1 (ppm)


sk-191223-1/2
151.76
142.93
140.41
128.92
127.88
127.25
77.25
77.00
76.75
67.00
47.53
45.55
31.73
f1 (ppm)