Supplementary Information

Selective assembly of N1- and N2-alkylated 1,2,3-triazoles via copper-catalyzed decarboxylative cycloaddition of alkynyl carboxylic acids with ethers and azidotrimethylsilane

Pengli Bao,[a] Na Meng,[a] Yufen Lv,*[a] Huilan Yue,*[b] Jiang-Sheng Li,[c] Wei Wei[a,b*]

[a]*School of Chemistry and Chemical Engineering, Qufu Normal University, Qufu 273165, Shandong, China. E-mail: weiweiqfnu@163.com; yufenlv06@163.com*

[b]*Qinghai Provincial Key Laboratory of Tibetan Medicine Research and Key Laboratory of Tibetan Medicine Research, Northwest Institute of Plateau Biology, Chinese Academy of Sciences, Qinghai 810008, China. E-mail: hlyue@nwipb.cas.cn*

[c]*School of Chemistry and food Engineering, Changsha University of Science and Technology, Changsha, 410114, P. R. China*

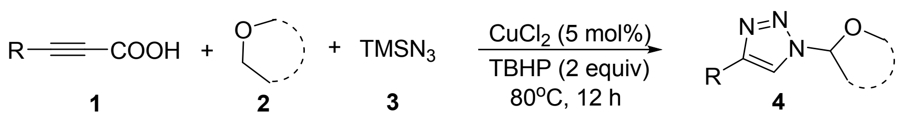
Contents

1. General information

All commercially available reagent grade chemicals were purchased from Aldrich, Acros, Alfa Aesar and Energy Chemical Company and used as received without further purification unless otherwise stated. All solvents were dried according to standard procedures. ^{1}H NMR and ^{13}C NMR were recorded in $CDCl_3$ on a Bruker Avance III 400 spectrometer with TMS as internal standard (500 MHz ^{1}H, 125 MHz ^{13}C) at room temperature, the chemical shifts (δ) were expressed in ppm and J values were given in Hz. The following abbreviations are used to indicate the multiplicity: singlet (s), doublet (d), triplet (t), quartet (q), doublet of doublets (dd), doublet of triplets (dt), and multiplet (m). All first order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted were designated as multiplet (m). Mass analyses and HRMS were obtained on a Finnigan-LCQDECA mass spectrometer and a Bruker Daltonics Bio-TOF-Q mass spectrometer by the ESI method, respectively. Column chromatography was performed on silica gel (200-300 mesh).

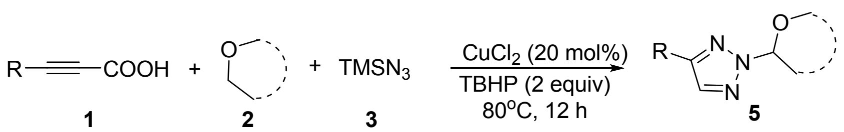
2 General procedure for the selective synthesis of N1-and N2-alkylated 1,2,3-triazoles from alkynyl carboxylic acid, ether and $TMSN_3$.

2.1 General procedure for the synthesis of N1-alkylated 1,2,3-triazoles.



In a tube (15 mL), $CuCl_2$ (5 mol%, 1.4 mg), alkynyl carboxylic acid **1** (0.2 mmol), ether **2** (2 mL), $TMSN_3$ **3** (0.3 mmol, 42 μL), and TBHP (0.4 mmol, 56 μL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 12 h. After completion of the reaction, the solution was concentrated in vacuum, the crude mixtures were purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired N1-alkylated 1,2,3-triazole **4**.

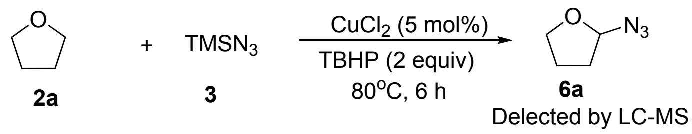
2.2 General procedure for the synthesis of N2-alkylated 1,2,3-triazoles.



In a tube (15 mL), $CuCl_2$ (20 mol%, 5.4 mg), alkynyl carboxylic acid **1** (0.2 mmol), ether **2** (2 mL), $TMSN_3$ **3** (0.3 mmol, 42 μL), and TBHP (0.4 mmol, 56 μL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 ^{o}C for 12 h. After completion of the reaction, the solution was concentrated in vacuum, the crude mixtures were purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired N2-alkylated 1,2,3-triazole **5**.

3. Preliminary mechanistic studies

3.1 The Reaction of THF ether with $TMSN_3$ under the standard conditions.



In a tube (15 mL), $CuCl_2$ (1.4 mg), TBHP (0.4mmol, 56 μL) , $TMSN_3$ **3** (0.3 mmol, 42 μL), and THF (2 mL) were added. The reaction vessel was allowed to stir at 80 ^{o}C for 6 h. After completion of the reaction, the solution was concentrated in vacuum, the alkylated azide **6a** was detected by LC-MS (Figure S3).

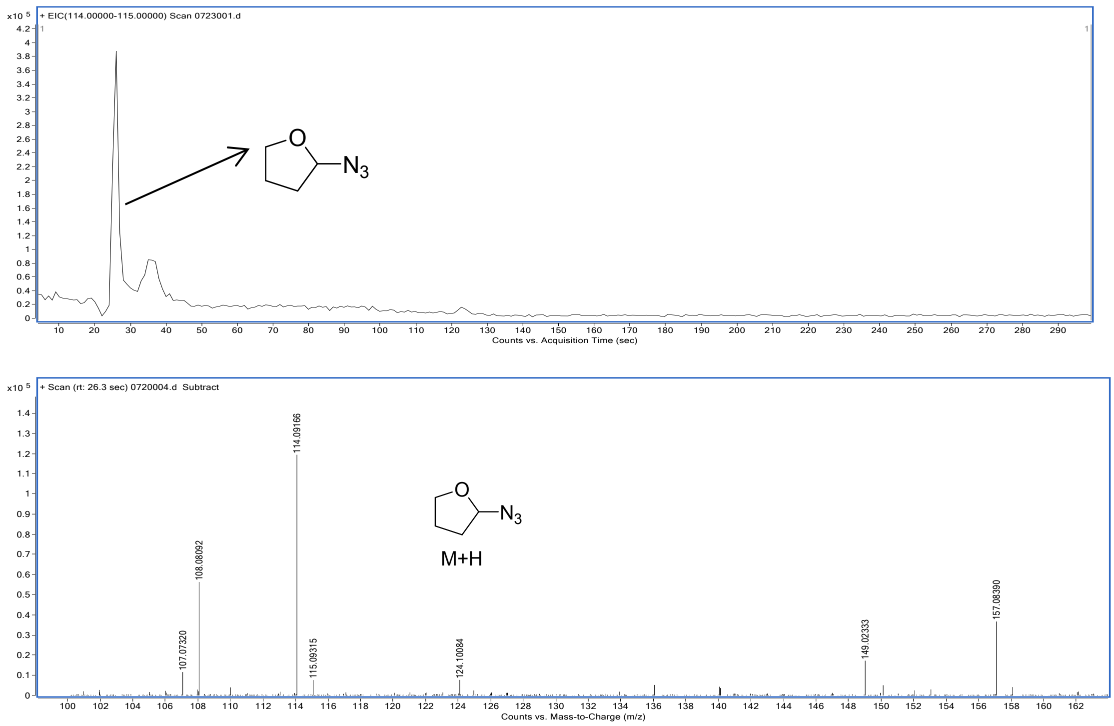
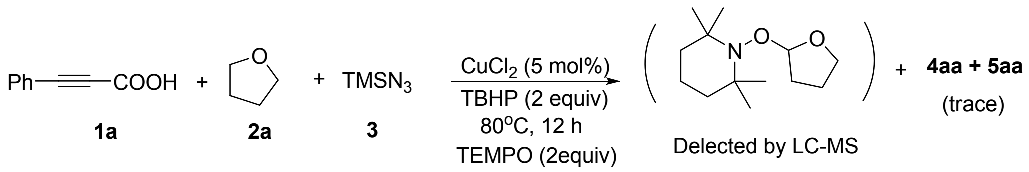
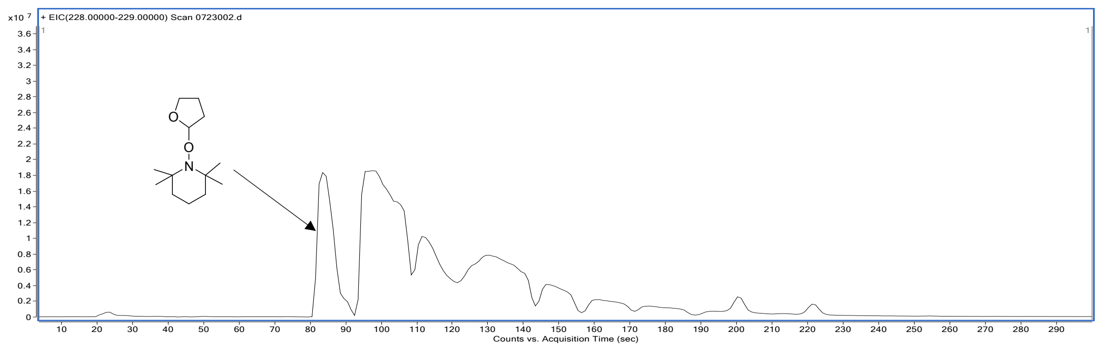


Figure S3. LC-MS spectra of oxyalkylated azide **6a**.

3.2 The addition of TEMPO in the model reaction system.



In a tube (15 mL), $CuCl_2$ (5 mol%, 1.4 mg), TEMPO (0.4mmol, 62.8mg), phenylpropynic acid **1a** (0.2 mmol, 29.2 mg), THF **2a** (2 ml), $TMSN_3$ **3** (0.3 mmol, 42 μL), and TBHP (0.4 mmol, 56 μL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 12 h. The reaction was extremely restrained and TEMPO-trapped complex (TEMPO-THF) was detected by LC-MS analysis (Figure S4).



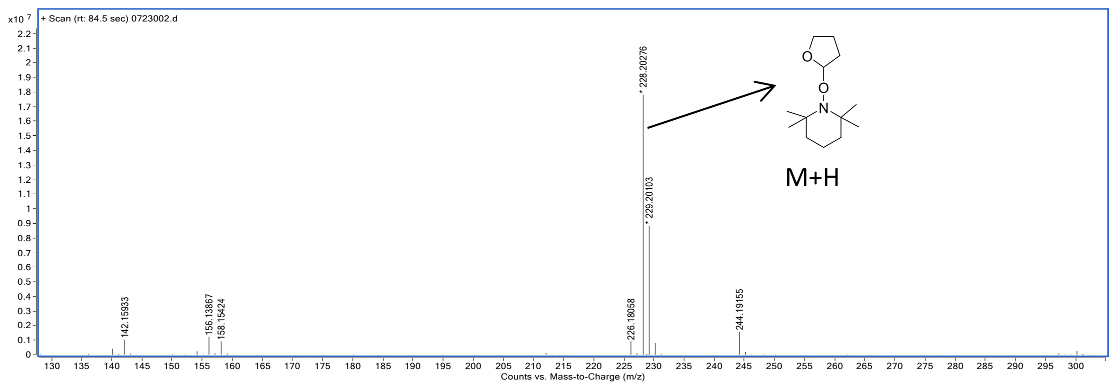
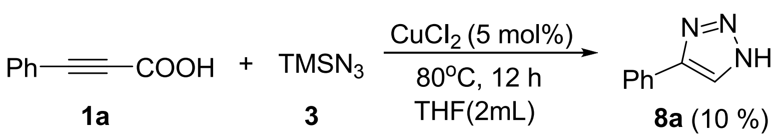


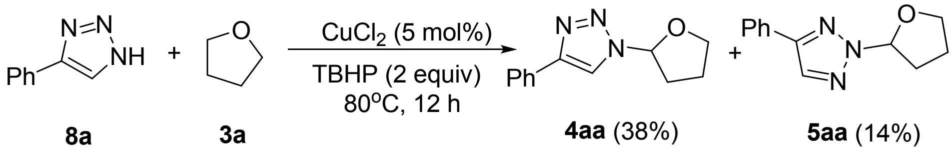
Figure S4. LC-MS spectra of TEMPO-THF.

3.3The model reaction was carried out in the absence of TBHP.



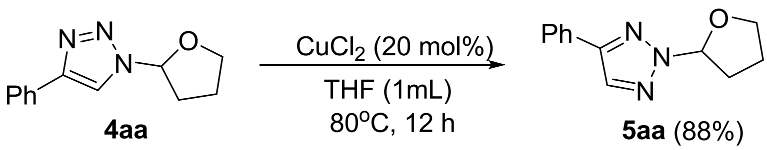
In a tube (15 mL), $CuCl_2$ (20 mol%, 5.4 mg), 3-phenylpropiolic acid **1a** (0.2 mmol, 29.2 mg), $TMSN_3$ **3** (0.3 mmol, 42 μL), and THF (2 mL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 12 h. After completion of the reaction, the solution was concentrated in vacuum. The residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **8a** in 10% yield.

3.4 The reactions of 4-phenyl-1H-1,2,3-triazole with THF under the standard conditions.



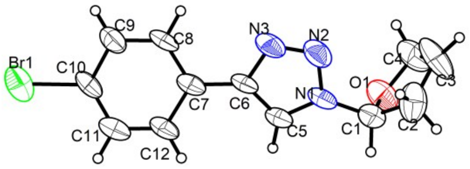
In a tube (15 mL), $CuCl_2$ (5 mol%, 1.4 mg), 4-phenyl-1H-1,2,3-triazole **10a** (0.2 mmol, 29mg), THF **3a** (2 ml), and TBHP (0.4mmol, 56 μL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 12 h. After completion of the reaction, the solution was concentrated in vacuum. The residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **4aa** in 38% yield (10.3 mg), and product **5aa** in 14 % yield (4.5 mg).

3.5 The transformation of product 4aa to product 5aa under the standard conditions.



In a tube (15 mL), 4-phenyl-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole **4aa** (0.1 mmol, 21.5 mg), $CuCl_2$ (20 mol%, 2.7 mg), and THF (1 mL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 12 h. After completion of the reaction, the solution was concentrated in vacuum. The residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the product **5aa** in 88% yield (18.9 mg) and product **4aa** was remained in 10% yield.

4. Crystallographic data of product 4ja.



CCDC-1949074

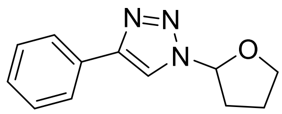
Table S1. Crystallographic data and structure refinement for complex **4ja**.

Identification code	Complex
formula	$C_{12}H_{12}BrN_3O$
MW	293.65
cryst	White block
Cryst size(mm)	0.40 x 0.30 x 0.20 mm
λ (Å)	0.71073
temp(K)	298(2) K
cryst syst	Triclinic
space group	P-1
a (Å)	10.2294(8)
b (Å)	10.6907(8)
c (Å)	11.7250(9)
α (°)	98.227(2)
β (°)	103.378(3)
γ (°)	91.2920(10)
vol(Å^3)	1232.54(16)
Z	4
Density(cale)(Mg m^{-3})	1.582
Abs coeff (mm^{-1})	3.322
F(000)	590
θrange (deg)	2.89 to 25.02
Index ranges	-12<=h<=11,-10<=k<=12, -13<=l<=10
Reflns collected	5903
Indep reflns	4092 [R(int) = 0.0486
Date/restraints/params	4092 / 0 / 308
Final R indices	R1 = 0.0935
[1＞2σ(1)]	wR2 = 0.1995
R indices (all date)	R1 = 0.1778, wR2 = 0.2262
GOF	1.060
Largest diff.peak and hole(e Å^{-3})	0.864 and -1.118

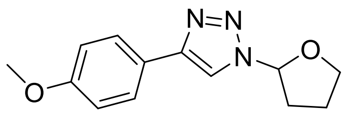
Table S2. Selected Bond Lengths (Å) and Angles (deg) for complex **4ja**.

Bond/angle	Complex
Br(1)-C(10)	1.904(8)
N(1)-C(5)	1.317(10)
N(1)-N(2)	1.365(9)
N(1)-C(1)	1.489(11)
N(2)-N(3)	1.301(9)
N(3)-C(6)	1.364(9)
O(1)-C(4)	1.392(10)
O(1)-C(1)	1.403(10)
C(5)-N(1)-N(2)	110.9(7)
C(5)-N(1)-C(1)	128.2(7)
N(2)-N(1)-C(1)	120.3(7)
N(3)-N(2)-N(1)	160.4(6)
N(2)-N(3)-C(6)	110.2(6)
O(1)-C(1)-N(1)	108.6(8)
N(1)-C(1)-C(2)	113.6(7)
N(1)-C(1)-H(1)	108.8
N(1)-C(5)-C(6)	106.0(7)
N(1)-C(5)-H(5)	127.0
N(3)-C(6)-C(5)	106.5(7)

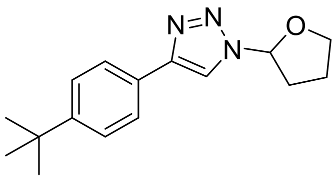
5.Characterization data of products 4aa-5af



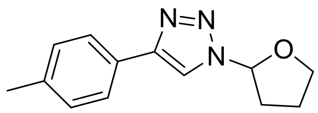
4-phenyl-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4aa** was obtained in 92% yield (38.7 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.70 (s, 1H), 7.94 – 7.87 (m, 2H), 7.46 (t, J = 4.7 Hz, 2H), 7.35 (t, J = 4.3 Hz, 1H), 6.39 – 6.27 (m, 1H), 4.11 – 4.07 (m, 1H), 3.99 – 3.95 (m, 1H), 2.51 – 2.44 (m, 2H), 2.25 – 2.15 (m, 1H), 2.10 – 2.01 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 146.8, 130.9, 129.1, 128.2, 125.5, 120.0, 89.1, 69.2, 31.9, 24.0. HRMS calc. for $C_{12}H_{13}N_3NaO$ $(M+Na)^+$, 238.0956; found, 238.0959.



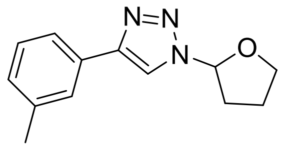
4-(4-methoxyphenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4ba** was obtained in 80% yield (39.2 mg) according to the general procedure (0.2 mmol). White solid, mp = 51.4 °C – 51.8 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.21 (s, 1H), 7.78 (d, J = 8.6 Hz, 2H), 7.01 (d, J = 8.6 Hz, 2H), 6.31 – 6.29 (m, 1H), 4.03 – 4.00 (m, 1H), 3.99 – 3.93 (m, 1H), 3.72 (s, 3H), 2.53 – 2.40 (m, 2H), 2.24 – 2.15 (m, 1H), 2.09 – 2.00 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 160.0, 147.6, 131.8, 127.6, 122.9, 114.9, 92.1, 69.3, 55.7, 40.3, 40.2, 40.0, 39.8, 39.7, 31.3, 24.7. HRMS calc. for $C_{13}H_{15}N_3NaO_2$ $(M+Na)^+$, 268.1062; found, 268.1071.



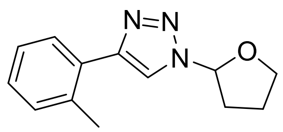
4-(4-tert-butylphenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4ca** was obtained in 70% yield (37.9 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.63 (s, 1H), 7.79 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 8.4 Hz, 2H), 6.36 – 6.34 (m, 1H), 4.10 – 4.04 (m, 1H), 3.98 – 3.94 (m, 1H), 2.50 – 2.40 (m, 2H), 2.22 – 2.16 (m, 1H), 2.08 – 2.03 (m, 1H), 1.30 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 150.9, 147.0, 128.4, 126.1, 125.5, 119.9, 89.2, 69.4, 40.3, 40.2, 40.0, 39.8, 39.7, 34.8, 32.1, 31.6, 24.3. HRMS calc. for $C_{16}H_{21}N_3NaO$ $(M+Na)^+$, 294.1582; found, 294.1581.



1–**(tetrahydrofuran-2-yl)-4-p-tolyl-1H-1,2,3-triazole**, Compound **4da** was obtained in 76% yield (34.8 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.62 (s, 1H), 7.76 (d, J = 8.1 Hz, 2H), 7.24 (d, J = 7.9 Hz, 2H), 6.35 – 6.33 (m, 1H), 4.08 – 4.04 (m, 1H), 3.97 – 3.92 (m, 1H), 2.47 – 2.38 (m, 2H), 2.32 (s, 3H), 2.22 – 2.13 (m, 1H), 2.07 – 2.00 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 147.0, 137.7, 129.8, 128.4, 125.6, 119.8, 89.2, 69.4, 32.1, 24.3, 21.3. HRMS calc. for $C_{13}H_{15}N_3NaO$ $(M+Na)^+$, 252.1113; found, 252.1115.

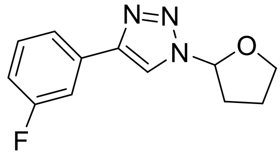


1-(tetrahydrofuran-2-yl)-4-m-tolyl-1H-1,2,3-triazole, Compound **4ea** was obtained in 70% yield (32.1 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.67 (s, 1H), 7.72 – 7.67 (m, 2H), 7.33 (t, J = 7.6 Hz, 1H), 7.15 (d, J = 7.5 Hz, 1H), 6.38 – 6.36 (m, 1H), 4.11 – 4.07 (m, 1H), 3.99 – 3.94 (m, 1H), 2.51 – 2.44 (m, 2H), 2.36 (s, 3H), 2.22 – 2.16 (m, 1H), 2.08 – 2.00 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 147.1, 138.5, 131.1, 129.2, 129.0, 126.3, 122.9, 120.1, 89.3, 69.4, 32.1, 24.3, 21.5. HRMS calc. for $C_{13}H_{15}N_3NaO$ $(M+Na)^+$, 252.1113; found, 252.1109.

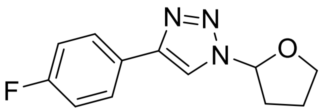


1-(tetrahydrofuran-2-yl)-4-o-tolyl-1H-1,2,3-triazole, Compound **4fa** was obtained in 75% yield (34.4 mg) according to the general procedure (0.2 mmol). White solid, mp = 52.2 °C – 52.3 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.47 (s, 1H), 7.73 – 7.71 (m, 1H), 7.32 – 7.26 (m, 3H), 6.40 – 6.39 (m, 1H), 4.11 –4.08 (m, 1H), 4.02 – 3.96 (m, 1H), 2.61

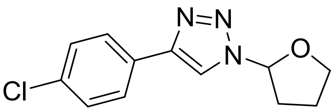
– 2.48 (m, 2H), 2.45 (s, 3H), 2.26 – 2.18 (m, 1H), 2.10 – 2.01 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 146.3, 135.5, 131.3, 130.4, 128.9, 128.3, 126.5, 122.2, 89.1, 69.4, 32.0, 24.4, 21.5. HRMS calc. for $C_{13}H_{15}N_3NaO$ $(M+Na)^+$, 252.1113; found, 252.1117.



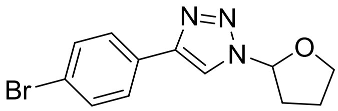
4-(3-fluorophenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4ga** was obtained in 75% yield (35.0 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.77 (s, 1H), 7.75 (d, J = 7.8 Hz, 1H), 7.71 – 7.68 (m, 1H), 7.51 – 7.47 (m, 1H), 7.19 – 7.15 (m, 1H), 6.38 (t, J = 4.7 Hz, 1H), 4.11 – 4.08 (m, 1H), 3.99 – 3.95 (m, 1H), 2.50 – 2.43 (m, 2H), 2.21 – 2.15 (m, 1H), 2.09 – 2.03 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.38 (d, J = 242.5 Hz), 147.23 (q, J = 2.5 Hz), 134.84 (d, J = 8.8 Hz), 132.80 (d, J = 8.8 Hz), 123.02 (d, J = 2.5 Hz), 122.27, 116.40 (d, J = 21.3 Hz), 113.62 (d, J = 22.5 Hz), 90.75, 70.83, 33.48, 25.49; ^{19}F NMR (470 MHz, DMSO-d_6) δ -112.82. HRMS calc. for $C_{12}H_{12}FN_3NaO$ $(M+Na)^+$, 256.0862; found, 256.0863.



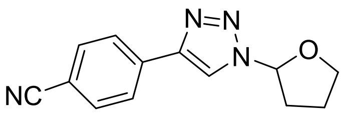
4-(4-fluorophenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4ha** was obtained in 66% yield (30.8 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.70 (s, 1H), 7.95 – 7.92 (m, 2H), 7.32 – 7.28 (m, 2H), 6.37 (t, J = 4.7 Hz, 1H), 4.11 – 4.07 (m, 1H), 4.00 – 3.95 (m, 1H), 2.52 – 2.43 (m, 2H), 2.23 – 2.17 (m, 1H), 2.10 – 2.04 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 167.04 (d, J = 242.5 Hz), 150.88, 132.46 (q, J = 22.5 Hz), 132.45, 124.90 (d, J = 25.0 Hz), 121.01 (d, J = 22.5 Hz), 94.08, 74.20, 36.85, 28.97. ^{19}F NMR (470 MHz, DMSO-d_6) δ -114.08. HRMS calc. for $C_{12}H_{12}FN_3NaO$ $(M+Na)^+$, 256.0862; found, 256.0859.



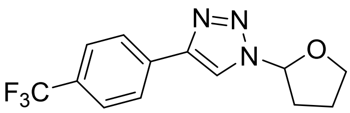
4-(4-chlorophenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4ia** was obtained in 80% yield (39.8 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.75 (s, 1H), 7.93 – 7.91 (m, 2H), 7.53 – 7.51 (m, 2H), 6.37 (t, J = 4.7 Hz, 1H), 4.11 – 4.07 (m, 1H), 3.99 – 3.95 (m, 1H), 2.50 – 2.44 (m, 2H), 2.22 – 2.16 (m, 1H), 2.08 – 2.03 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 145.9, 132.8, 130.1, 129.4, 127.4, 120.6, 89.4, 69.5, 32.1, 24.2. HRMS calc. for $C_{12}H_{13}ClN_3O$ $(M+H)^+$, 250.0747; found, 250.0756.



4-(4-bromophenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4ja** was obtained in 82% yield (48.1 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.75 (s, 1H), 7.84 (d, J = 6.3, 2H), 7.64 (d, J = 4.7, 2H), 6.38 – 6.36 (m, 1H), 4.10 – 4.06 (m, 1H), 3.99 – 3.94 (m, 1H), 2.50 – 2.43 (m, 2H), 2.20 – 2.15 (m, 1H), 2.09 – 2.03 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 145.9, 132.3, 130.4, 127.7, 121.4, 120.6, 89.4, 69.5, 32.1, 24.2. HRMS calc. for $C_{12}H_{13}BrN_3O$ $(M+H)^+$, 294.0242; found, 294.0243.

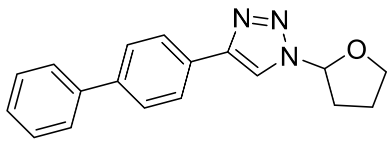


4-(1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazol-4-yl)benzonitrile, Compound **4ka** was obtained in 68% yield (32.6 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.89 (s, 1H), 8.09 – 8.07 (m, 2H), 7.92 – 7.91 (m, 2H), 6.39 (t, J = 4.6 Hz, 1H), 4.10 – 4.07 (m, 1H), 4.00 – 3.95 (m, 1H), 2.50 – 2.44 (m, 2H), 2.20 – 2.14 (m, 1H), 2.09 – 2.03 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 145.4, 135.6, 133.4, 126.3, 122.0, 119.3, 110.6, 89.5, 69.6, 32.2, 24.1. HRMS calc. for $C_{13}H_{12}N_4NaO$ $(M+Na)^+$, 263.0903; found, 263.0901.

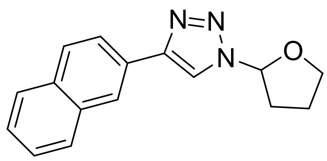


1-(tetrahydrofuran-2-yl)-4-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazole, Compound **4la** was obtained in 65% yield (36.8 mg) according to the general procedure (0.2 mmol). Yellow solid, mp = 55.4 ^{o}C – 55.7 ^{o}C. ^{1}H NMR (500 MHz, DMSO-d_6) δ

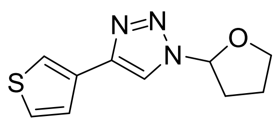
8.83 (s, 1H), 8.06 (d, J = 8.1 Hz, 2H), 7.76 (d, J = 8.3 Hz, 2H), 6.36 – 6.34 (m, 1H), 4.07 – 4.03 (m, 1H), 3.95 – 3.90 (m, 1H), 2.45 – 2.37 (m, 2H), 2.17 – 2.11 (m, 1H), 2.13 – 1.98 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 145.60, 135.11, 128.48 (q, J = 32.5 Hz), 126.33 (q, J = 3.8 Hz), 126.20, 123.64, 121.56, 89.48, 69.54, 31.16, 24.17. ^{19}F NMR (470 MHz, DMSO-d_6) δ -60.98. HRMS calc. for $C_{13}H_{12}F_3N_3NaO$ (M+Na)$^+$, 306.0830; found, 306.0833.



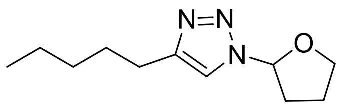
4-(biphenyl-4-yl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4ma** was obtained in 57% yield (33.2 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.76 (s, 1H), 7.98 (d, J = 7.9 Hz, 2H), 7.78 – 7.72 (m, 4H), 7.49 (t, J = 7.5 Hz, 2H), 7.38 (t, J = 7.3 Hz, 1H), 6.50 – 6.22 (m, 1H), 4.13 – 4.08 (m, 1H), 3.98 (q, J = 7.5 Hz, 1H), 2.50 – 2.46 (m, 2H), 2.24 – 2.18 (m, 1H), 2.09 – 2.04 (m, 1H).; ^{13}C NMR (125 MHz, DMSO-d_6) δ 146.6, 140.1, 140.0, 130.3, 129.5, 128.0, 127.6, 127.0, 126.3, 120.4, 89.3, 69.5, 32.1, 24.3. HRMS calc. for $C_{19}H_{17}N_3O$ (M+H)$^+$, 292.1450; found, 292.1451.



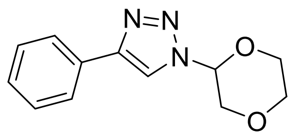
4-**(naphthalen-2-yl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole**, Compound **4na** was obtained in 61% yield (32.3 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.79 – 8.75 (m, 1H), 8.42 (s, 1H), 8.05 – 8.01 (m, 1H), 8.00 – 7.93 (m, 2H), 7.90 (d, J = 7.2 Hz, 1H), 7.53 – 7.48 (m, 2H), 6.58 – 6.21 (m, 1H), 4.12 – 4.07 (m, 1H), 3.98 – 3.94 (m, 1H), 2.51 – 2.44 (m, 2H), 2.26 – 2.13 (m, 1H), 2.10 – 1.98 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 147.1, 133.6, 133.1, 129.0, 128.4, 128.2, 127.1, 126.7, 124.1, 124.1, 120.6, 89.4, 69.5, 32.1, 24.3. HRMS calc. for $C_{16}H_{15}N_3NaO$ (M+Na)$^+$, 288.1113; found, 288.1122.



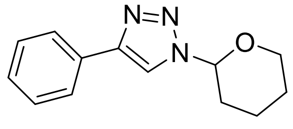
1-(tetrahydrofuran-2-yl)-4-(thiophen-3-yl)-1H-1,2,3-triazole, Compound **4oa** was obtained in 75% yield (36.6 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-*d₆*) δ 8.55 (s, 1H), 7.87 – 7.86 (m, 1H), 7.66 – 7.64 (m, 1H), 7.56 – 7.54 (m, 1H), 6.47 – 6.18 (m, 1H), 4.09 – 4.05 (m, 1H), 3.99 – 3.94 (m, 1H), 2.48 – 2.41 (m, 2H), 2.20 – 2.13 (m, 1H), 2.09 – 2.03 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 143.5, 132.5, 127.6, 126.3, 121.4, 120.0, 89.2, 69.4, 32.1, 24.2. HRMS calc. for $C_{10}H_{11}N_3NaOS$ $(M+Na)^+$, 244.0521; found, 244.0527.



4-pentyl-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4pa** was obtained in 60 % yield (25.0 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-*d6*): δ 7.94 (s, 1H), 6.25 (t, J = 4.8 Hz, 1H), 4.01 – 3.97 (m, 1H), 3.93 – 3.89 (m, 1H), 2.59 (t, J = 7.6 Hz, 2H), 2.40 – 2.37 (m, 2H), 2.20 – 2.09 (m, 1H), 2.05 – 1.97 (m, 1H), 1.62 – 1.56 (m, 2H), 1.35 – 1.25 (m, 4H), 0.87 (t, J = 6.8 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-*d6*): δ 147.6, 120.7, 88.8, 69.2, 31.9, 31.3, 29.1, 25.4, 24.4, 22.3, 14.4. HRMS calc. for $C_{11}H_{19}N_3NaO$ $(M+Na)^+$, 232.1426; found, 232.1431.

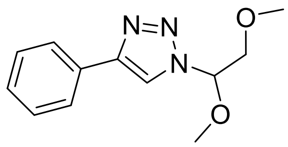


1-(1,4-dioxan-2-yl)-4-phenyl-1H-1,2,3-triazole, Compound **4ab** was obtained in 40% yield (18.5 mg) according to the general procedure (0.2 mmol). Yellow oil.^{1}H NMR (500 MHz, DMSO-d_6) δ 8.81 (s, 1H), 7.92 – 7.90 (m, 2H), 7.47 (t, J = 7.6 Hz, 2H), 7.38 – 7.35 (m, 1H), 6.01 – 5.99 (m, 1H), 4.17 – 4.09 (m, 2H), 3.87 – 3.85 (m, 2H), 3.83 – 3.79 (m, 1H), 3.75 – 3.70 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 151.6, 135.6, 134.2, 133.3, 130.6, 125.9, 86.6, 72.2, 70.6, 69.3. HRMS calc. for $C_{12}H_{13}N_3NaO_2$ $(M+Na)^+$, 254.0905; found, 254.0914.

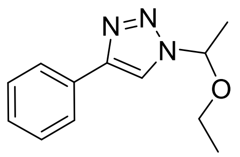


4-phenyl-1-(tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazole, Compound **4ac** was obtained in 60 % yield (27.5 mg) according to the general procedure (0.2 mmol).

Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.76 (s, 1H), 7.90 – 7.78 (m, 2H), 7.44 (t, J = 7.7 Hz, 2H), 7.33 (t, J = 7.4 Hz, 1H), 5.82 – 5.79 (m, 1H), 3.94 (d, J = 12.2 Hz, 1H), 3.74 – 3.69 (m, 1H), 2.19 – 2.10 (m, 1H), 2.08 – 2.01 (m, 1H), 1.99 – 1.92 (m, 1H), 1.78 – 1.68 (m, 1H), 1.61 – 1.55 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 146.9, 131.1, 129.4, 128.4, 125.7, 120.4, 86.0, 67.4, 30.3, 24.9, 21.9. HRMS calc. for $C_{13}H_{15}N_3NaO$ (M+H)$^+$, 252.1113; found, 252.1110.

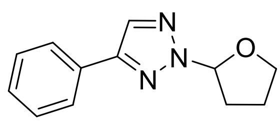


1-(1,2-dimethoxyethyl)-4-phenyl-1H-1,2,3-triazole, Compound **4ad** was obtained in 40% yield (18.6 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.79 (s, 1H), 7.90 – 7.89 (m, 2H), 7.47 (t, J = 7.6 Hz, 2H), 7.36 (d, J = 7.3 Hz, 1H), 5.87 (t, J = 5.9 Hz, 1H), 3.87 (d, J = 6.0 Hz, 2H), 3.33 (s, 1H), 3.29 (s, 3H), 2.50 (d, J = 1.5 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 147.3, 131.0, 129.4, 128.5, 125.7, 120.1, 88.8, 72.2, 59.0, 56.6. HRMS calc. for $C_{12}H_{15}N_3NaO_2$ (M+Na)$^+$, 256.1062; found, 256.1067.

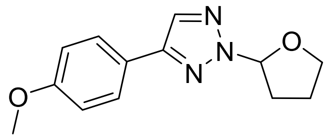


1-(1-ethoxyethyl)-4-phenyl-1H-1,2,3-triazole, Compound **4ae** was obtained in 71% yield (30.6 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.81 (s, 1H), 7.90 (d, J = 7.2 Hz, 2H), 7.46 (t, J = 7.5 Hz, 2H), 7.35 (d, J = 7.2 Hz, 1H), 5.94 (q, J = 6.0 Hz, 1H), 3.55-3.50 (m, 1H), 3.30-3.27 (m, 1H), 1.71 (d, J = 6.1 Hz, 3H), 1.08 (d, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 147.3, 131.1, 129.4, 128.5, 125.7, 119.2, 86.2, 64.2, 21.8, 15.1. HRMS calc. for $C_{12}H_{16}N_3O_2$ (M+H)$^+$, 218.1293; found, 218.1297.

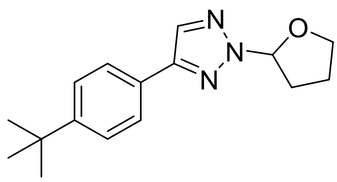
Characterization data of products 5aa-5af:



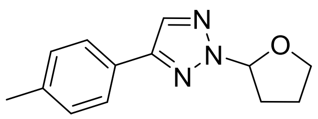
4-phenyl-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5aa** was obtained in 85% yield (36.6 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.85 – 7.76 (m, 2H), 7.42 (t, J = 7.5 Hz, 2H), 7.38 – 7.30 (m, 1H), 6.35 – 6.32 (m, 1H), 4.21 – 4.17 (m, 1H), 4.03 – 4.09 (m, 1H), 2.74 – 2.67 (m, 1H), 2.50 – 2.38 (m, 2H), 2.14 – 2.06 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.1, 131.4, 130.4, 128.8, 128.5, 126.1, 92.4, 69.6, 31.4, 24.5. HRMS calc. for $C_{12}H_{13}N_3NaO$ $(M+Na)^+$, 238.0956; found, 238.0955.



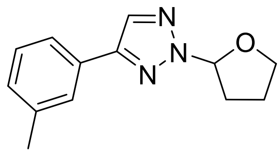
4-(4-methoxyphenyl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5ba** was obtained in 80% yield (39.2 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.73 – 7.72 (m, 2H), 6.96 – 6.95 (m, 2H), 6.33 – 6.31 (m, 1H), 4.21 – 4.17 (m, 1H), 4.08 – 4.03 (m, 1H), 3.85 (s, 3H), 2.71 – 2.67 (m, 1H), 2.44 – 2.37 (m, 2H), 2.12 – 2.04 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.5, 147.6, 130.6, 127.0, 122.7, 113.9, 91.9, 61.9, 54.9, 30.9, 24.2. HRMS calc. for $C_{13}H_{15}N_3NaO_2$ $(M+Na)^+$, 268.1062; found, 268.1071.



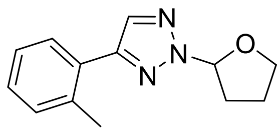
4-(4-tert-butylphenyl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5ca** was obtained in 71% yield (38.5 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.84 (s, 1H), 7.73 (d, J = 8.3 Hz, 2H), 7.46 (d, J = 8.3 Hz, 2H), 6.33 – 6.32 (m, 1H), 4.22 – 4.17 (m, 1H), 4.08 – 4.03 (m, 1H), 2.72 – 2.65 (m, 1H), 2.49 – 2.38 (m, 2H), 2.13 – 2.06 (m, 1H), 1.34 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 151.9, 147.3, 131.5, 127.7, 125.0, 124.9, 91.5, 68.7, 33.9, 30.6, 30.5, 23.7. HRMS calc. for $C_{16}H_{21}N_3NaO$ $(M+Na)^+$, 294.1582; found, 294.1579.



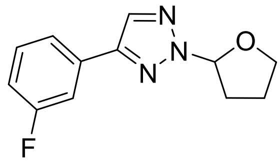
2-(tetrahydrofuran-2-yl)-4-p-tolyl-2H-1,2,3-triazole, Compound **5da** was obtained in 80% yield (36.6 mg) according to the general procedure (0.2 mmol). Yellow oil.^{1}H NMR (500 MHz, $CDCl_3$) *δ* 7.83 (s, 1H), 7.68 (d, *J* = 8.1 Hz, 2H), 7.24 (d, *J* = 7.9 Hz, 2H), 6.34 – 6.33 (m, 1H), 4.21 – 4.16 (m, 1H), 4.07 – 4.03 (m, 1H), 2.73 – 2.65 (m, 1H), 2.52 – 2.39 (m, 2H), 2.38 (s, 3H), 2.13 – 2.04 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): *δ* 138.4, 131.3, 129.5, 127.5, 126.0, 92.3, 69.6, 31.4, 24.5, 21.3. HRMS calc. for $C_{13}H_{15}N_3NaO$ $(M+Na)^+$, 252.1113, found, 252.1117.



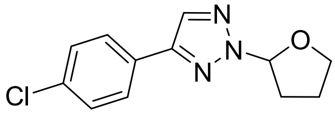
2-(tetrahydrofuran-2-yl)-4-m-tolyl-2H-1,2,3-triazole, Compound **5ea** was obtained in 76% yield (34.8 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$): *δ* 7.85 (s, 1H), 7.63 (s, 1H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.17 (d, *J* = 7.4 Hz, 1H), 6.34 – 6.32 (m, 1H), 4.22 – 4.18 (m, 1H), 4.08 – 4.04 (m, 1H), 2.74 – 2.67 (m, 1H), 2.55 – 2.41 (m, 2H), 2.40 (s, 3H), 2.14 – 2.06 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) *δ* 148.2, 138.5, 131.5, 130.2, 129.3, 128.7, 126.7, 123.2, 92.3, 69.6, 31.4, 24.5, 21.4. HRMS calc. for $C_{13}H_{15}N_3NaO$ $(M+Na)^+$, 252.1113, found, 252.1115.



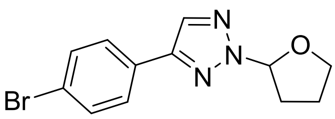
2-(tetrahydrofuran-2-yl)-4-o-tolyl-2H-1,2,3-triazole, Compound **5fa** was obtained in 75% yield (34.4 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$): *δ* 7.76 (s, 1H), 7.58 (d, *J* = 6.3 Hz, 1H), 7.28 – 7.26 (m, 2H), 6.37 – 6.35 (m, 1H), 4.22 – 4.18 (m, 1H), 4.08 – 4.04 (m, 1H), 2.71 – 2.67 (m, 1H), 2.48 (s, 3H), 2.47 – 2.38 (m, 2H), 2.15 – 2.05 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 148.0, 136.2, 133.7, 131.0, 129.8, 129.1, 128.4, 126.0, 92.3, 69.6, 31.4, 24.5, 21.3. HRMS calc. for $C_{13}H_{15}N_3NaO$ $(M+Na)^+$, 252.1113, found, 252.1111.



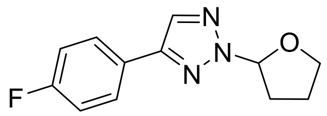
4-(3-fluorophenyl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5ga** was obtained in 75% yield (35.0 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.86 (s, 1H), 7.56 (d, J = 7.8 Hz, 2H), 7.53 – 7.50 (m, 1H), 7.41 – 7.36 (m, 1H), 7.06 – 7.03 (m, 1H), 6.34 – 6.32 (m, 1H), 4.22 – 4.18 (m, 1H), 4.09 – 4.05 (m, 1H), 2.71 – 2.66 (m, 1H), 2.49 – 2.39 (m, 2H), 2.13 – 2.09 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 163.11 (d, J = 245.0 Hz), 146.97, 132.47 (d, J = 8.7 Hz), 131.50, 130.39 (d, J = 8.7 Hz), 121.61 (d, J = 2.5 Hz), 115.31 (d, J = 21.2 Hz), 112.92 (d, J = 22.5 Hz), 92.43, 69.62, 31.37, 24.41. ^{19}F NMR (470 MHz, $CDCl_3$) δ -112.66. HRMS calc. for $C_{12}H_{12}FN_3NaO$ (M+Na)$^+$, 256.0862; found, 256.0865.



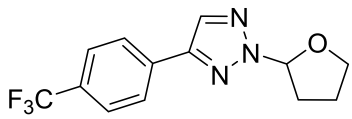
4-(4-chlorophenyl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5ha** was obtained in 70% yield (34.9 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.71 – 7.66 (m, 2H), 7.37 – 7.32 (m, 2H), 6.29 – 6.27 (m, 1H), 4.17 – 4.13 (m, 1H), 4.04 – 3.99 (m, 1H), 2.68 – 2.59 (m, 1H), 2.45 – 2.31 (m, 2H), 2.11 – 1.99 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 147.6, 134.9, 131.9, 129.4, 127.8, 90.3, 70.2, 32.9, 25.0. HRMS calc. for $C_{12}H_{13}ClN_3O$ (M+H)$^+$, 250.0747; found, 250.0752.



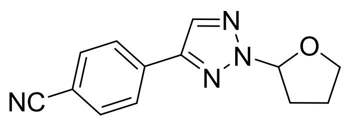
4-(4-bromophenyl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5ia** was obtained in 71% yield (41.6 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.85 (s, 1H), 7.67 (d, J = 8.3 Hz, 2H), 7.55 (d, J = 8.4 Hz, 2H), 6.33 – 6.32 (m, 1H), 4.21 – 4.17 (m, 1H), 4.08 – 4.03 (m, 1H), 2.72 – 2.66 (m, 1H), 2.48 – 2.40 (m, 2H), 2.15 – 2.04 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 147.1, 132.0, 131.4, 129.3, 127.6, 122.5, 92.4, 69.6, 31.4, 24.5. HRMS calc. for $C_{12}H_{13}BrN_3O$ (M+H)$^+$, 294.0242; found, 294.0239.



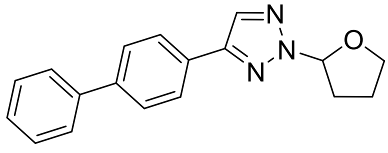
4-(4-fluorophenyl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5ja** was obtained in 79% yield (36.8 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (s, 1H), 7.79 – 7.74 (m, 2H), 7.11 (t, J = 8.7 Hz, 2H), 6.33 – 6.31 (m, 1H), 4.22 – 4.17 (m, 1H), 4.08 – 4.04 (m, 1H), 2.71 – 2.66 (m, 1H), 2.48 – 2.39 (m, 2H), 2.14 – 2.07 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 162.9 (d, J = 246.3 Hz), 147.25, 131.17, 127.81 (d, J = 7.5 Hz), 126.58 (d, J = 3.8 Hz), 115.86 (d, J = 21.3 Hz), 92.37, 69.61, 31.37, 24.5. ^{19}F NMR (470 MHz, $CDCl_3$) δ -113.02. HRMS calc. for $C_{12}H_{12}FN_3NaO$ $(M+Na)^+$, 256.0862; found, 256.0861.



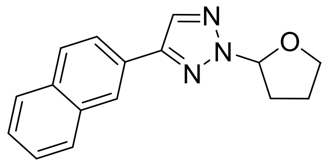
2-(tetrahydrofuran-2-yl)-4-(4-(trifluoromethyl)phenyl)-2H-1,2,3-triazole, Compound **5ka** was obtained in 70% yield (39.6 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.92 (s, 1H), 7.91(d, J = 8.7 Hz, 2H), 7.68 (d, J = 8.2 Hz, 2H), 6.36 – 6.34 (m, 1H), 4.23 – 4.18 (m, 1H), 4.11 – 4.06 (m, 1H), 2.71 – 2.67 (m, 1H), 2.49 – 2.40 (m, 2H), 2.16 – 2.10 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 146.71, 133.81, 131.78, 130.35 (q, J = 32.50 Hz), 126.21, 125.84 (q, J = 3.75 Hz), 124.07 (q, J = 270 Hz), 92.59, 69.72, 31.45, 24.45. ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.66. HRMS calc. for $C_{13}H_{12}F_3N_3NaO$ $(M+Na)^+$, 306.0830; found, 306.0833.



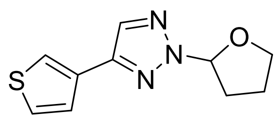
4-(2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazol-4-yl)benzonitrile, Compound **5la** was obtained in 70% yield (33.6 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.69 – 7.65 (m, 3H), 7.72 – 7.70 (m, 2H), 6.11 – 6.09 (m, 1H), 3.99 – 3.94 (m, 1H), 3.86 – 3.81 (m, 1H), 2.45 – 2.41 (m, 1H), 2.24 – 2.16 (m, 2H), 1.91 – 1.86 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 146.4, 134.9, 132.9, 132.1, 126.6, 118.8, 112.1, 92.9, 69.9, 31.6, 24.6. HRMS calc. for $C_{13}H_{12}N_4NaO$ $(M+Na)^+$, 263.0909; found, 263.0914.



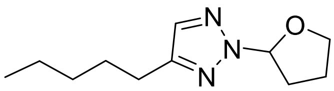
4-(biphenyl-4-yl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5ma** was obtained in 56% yield (32.6 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl3) δ 7.83 – 7.79 (m, 3H), 7.67 – 7.51 (m, 4H), 7.38 (t, J = 7.6 Hz, 2H), 7.29 (t, J = 7.4 Hz, 1H), 6.29 – 6.27 (m, 1H), 4.20 – 4.08 (m, 1H), 4.02 – 3.98 (m, 1H), 2.74 – 2.56 (m, 1H), 2.51 – 2.28 (m, 2H), 2.17 – 1.93 (m, 1H).; ^{13}C NMR (126 MHz, CDCl3) δ 152.0, 146.8, 140.3, 139.5, 130.5, 128.3, 127.8, 126.5, 126.0, 125.4, 91.4, 68.6, 30.4, 23.5. HRMS calc. for $C_{19}H_{17}N_3O$ $(M+H)^+$, 292.1450; found, 292.1453.



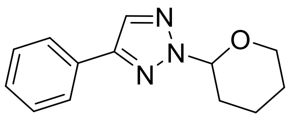
4-**(naphthalen-2-yl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole**, Compound **5na** was obtained in 60% yield (31.8 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl3) δ 8.25 (s, 1H), 7.99 (s, 1H), 7.93 (d, J = 8.6 Hz, 1H), 7.91 – 7.85 (m, 2H), 7.84 – 7.80 (m, 1H), 7.57 – 7.40 (m, 2H), 6.37 – 6.36 (m, 1H), 4.24 – 4.20 (m, 1H), 4.09 – 4.04 (m, 1H), 2.87 – 2.59 (m, 1H), 2.54 – 2.34 (m, 2H), 2.17 – 1.97 (m, 1H); ^{13}C NMR (126 MHz, CDCl3) δ 148.1, 133.5, 133.4, 131.7, 128.6, 128.2, 127.8, 127.8, 126.5, 126.3, 124.9, 124.0, 92.5, 69.7, 31.4, 24.6. HRMS calc.for $C_{16}H_{15}N_3NaO$ $(M+Na)^+$, 288.1113; found, 288.1120.



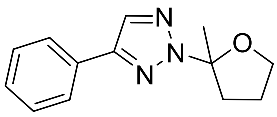
2-(tetrahydrofuran-2-yl)-4-(thiophen-3-yl)-2H-1,2,3-triazole, Compound **5oa** was obtained in 73% yield (32.3 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, $CDCl_3$): δ 7.76 (s, 1H), 7.63 – 7.62 (m, 1H), 7.47 – 7.45 (m, 1H), 7.39 – 7.37 (m, 1H), 6.32 – 6.30 (m, 1H), 4.24 – 4.14 (m, 1H), 4.09 – 4.01 (m, 1H), 2.75 – 2.63 (m, 1H), 2.49 – 2.36 (m, 2H), 2.14 – 2.04 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.3, 131.7, 131.6, 126.4, 126.0, 121.8, 92.3, 69.6, 31.3, 24.5. HRMS calc. for $C_{10}H_{11}N_3NaO$ $(M+Na)^+$, 244.0521; found, 244.0529.



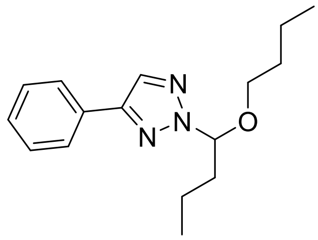
4-pentyl-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5pa** was obtained in 70 % yield (29.1 mg) according to the general procedure (0.2 mmol). Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.39 (s, 1H), 6.24-6.22 (m, 1H), 4.14 – 4.10 (m, 1H), 4.04 – 3.99 (m, 1H), 2.67-2.61 (m, 3H), 2.41 – 2.33 (m, 2H), 1.67 – 1.64 (m, 3H), 1.42 – 1.34 (m, 3H), 0.89 (t, J = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 149.2, 133.2, 91.8, 69.3, 31.5, 31.1, 28.9, 25.5, 24.6, 22.4, 14.0. HRMS calc. for $C_{11}H_{19}N_3NaO$ $(M+Na)^+$, 232.1426; found, 232.1433.



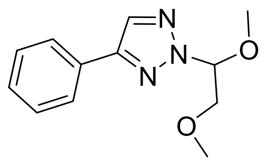
5-**phenyl-2-(tetrahydro-2H-pyran-2-yl)-2H-1,2,3-triazole**, Compound **5ab** was obtained in 66% yield (30.2 mg) according to the general procedure (0.2 mmol). Yellow solid, mp = 69.7 °C – 70.3 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.0 (s, 1H), 7.84 (d, J = 7.3 Hz, 2H), 7.42 (t, J = 7.6 Hz, 2H), 7.33 (t, J = 7.4 Hz, 1H), 5.77 – 5.74 (m, 1H), 4.09 – 3.94 (m, 1H), 3.83 – 3.68 (m, 1H), 2.29 – 2.11 (m, 2H), 2.10 – 1.97 (m, 1H), 1.90 – 1.55 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 147.7, 130.6, 128.8, 128.2, 125.8, 117.9, 86.4, 67.4, 30.8, 24.8, 21.6. HRMS calc. for $C_{13}H_{15}N_3NaO$ $(M+Na)^+$, 252.1113; found, 252.1117.



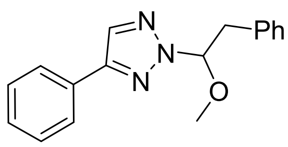
2-**(2-methyltetrahydrofuran-2-yl)-4-phenyl-2H-1,2,3-triazole**, Compound **5ac** was obtained in 40% yield (18.3 mg) according to the general procedure (0.2 mmol). Yellow oil.^{1}H NMR (500 MHz, $CDCl_3$): δ 7.86 (s, 1H), 7.81 (t, J = 7.2 Hz, 2H), 7.42 (t, J = 7.4 Hz, 2H), 7.36 – 7.32 (m, 1H), 4.15 – 4.11 (m, 1H), 4.07 – 3.98 (m, 1H), 3.14 – 3.11 (m, 1H), 2.26 – 2.10 (m, 3H), 1.99 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 147.7, 130.9, 130.6, 128.8, 128.4, 126.0, 100.3, 69.6, 37.5, 26.0, 24.8. HRMS calc. for $C_{13}H_{15}N_3NaO$ $(M+Na)^+$, 252.1113; found, 252.1112.



2-(1-butoxybutyl)-4-phenyl-2H-1,2,3-triazole, Compound **5ad** was obtained in 41% yield (22.4 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, $CDCl_3$): δ 7.83 – 7.82 (m, 1H), 7.80 – 7.79 (m, 2H), 7.38 – 7.35 (m, 2H), 7.30 – 7.26 (m, 2H),5.68 – 5.64 (m, 1H), 3.43 – 3.39 (m, 1H), 3.30 – 3.25 (m, 1H), 2.02 – 1.96 (m, 1H), 1.88 – 1.83 (m, 1H), 1.48 – 1.44 (m, 2H), 1.29 – 1.22 (m, 3H), 0.91 – 0.87 (m, 3H), 0.82 – 0.79 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 148.3, 128.9, 128.5, 128.3, 125.7, 116.1, 90.3, 69.2, 38.1, 31.3, 19.2, 18.0, 13.7, 13.5. HRMS calc. for $C_{16}H_{23}F_3N_3NaO$ $(M+Na)^+$, 296.1739; found, 296.1743.



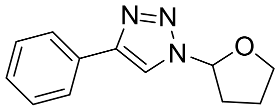
2-(1,2-dimethoxyethyl)-4-phenyl-2H-1,2,3-triazole，Compound **5ae** was obtained in 40% yield (18.6 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, $CDCl_3$): δ 8.02 (s, 1H), 7.88 – 7.87 (m, 2H), 7.46 – 7.42 (m, 2H), 7.35 (t, J = 7.4 Hz, 1H), 5.81 (t, J = 4.6 Hz, 1H), 3.87 – 3.81 (m, 2H), 3.43 (s, 3H), 3.37 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 148.3, 130.4, 128.9, 128.3, 125.8, 117.7, 89.4, 73.2, 59.7, 57.1. HRMS calc. for $C_{12}H_{15}N_3NaO$ $(M+Na)^+$, 256.1062; found, 256.1064.

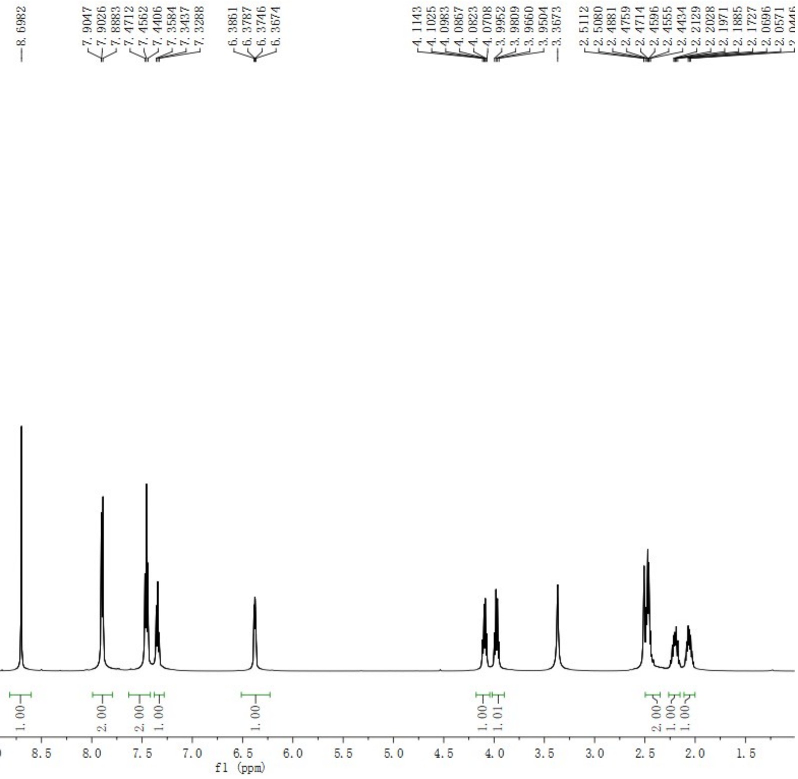


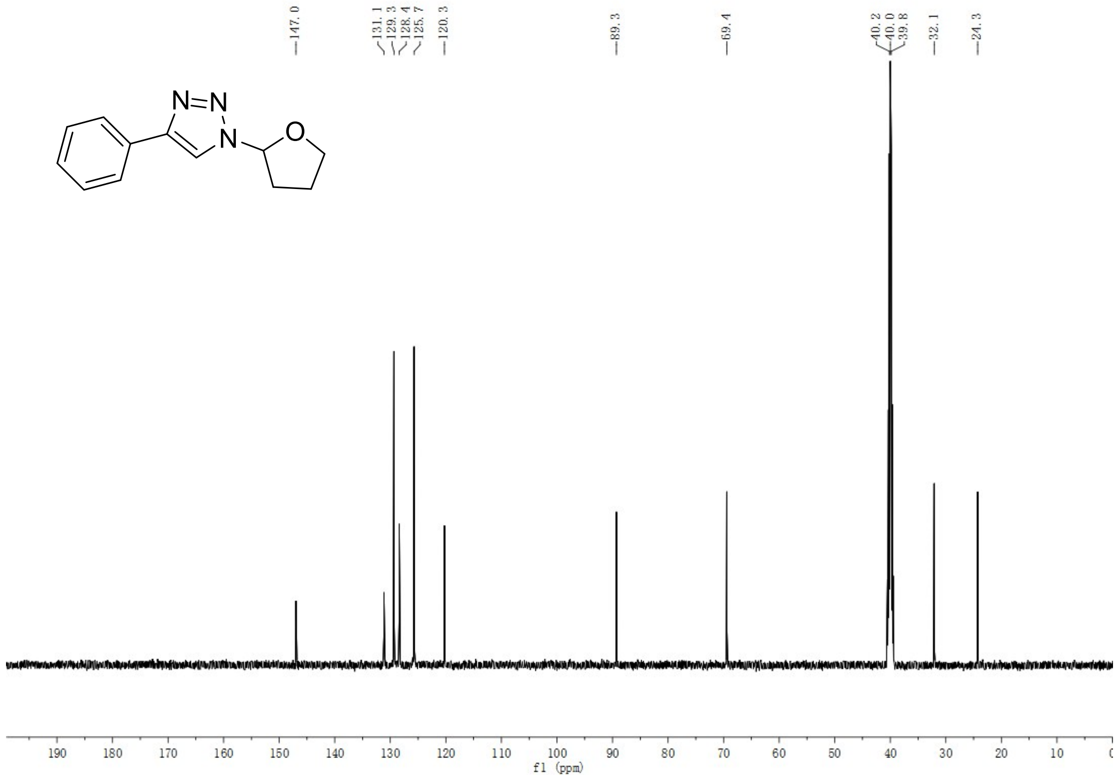
2-(1-methoxy-2-phenylethyl)-4-phenyl-2H-1,2,3-triazole, Compound **5af** was obtained in 68% yield (37.9 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, $CDCl_3$): δ 7.83 (d, J = 7.4 Hz, 2H), 7.81 (s, 1H), 7.42 (t, J = 7.6 Hz, 2H), 7.34 (t, J = 7.4 Hz, 1H), 7.31 – 7.25 (m, 3H), 7.17 – 7.15 (m, 2H), 5.85 –

5.82 (m, 1H), 3.38 – 3.34 (m, 1H), 3.30 – 3.28 (m, 3H), 3.26 (d, J = 5.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 148.2, 134.7, 130.5, 129.5, 128.9, 128.6, 128.3, 127.3, 125.8, 116.8, 92.1, 57.0, 42.4. HRMS calc. for $C_{17}H_{17}N_3NaO$ $(M+Na)^+$, 302.1296; found, 302.1299.

6. Copies of NMR Spectra for 4aa-5af



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128.4
125.7
120.3
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69.4
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32.1
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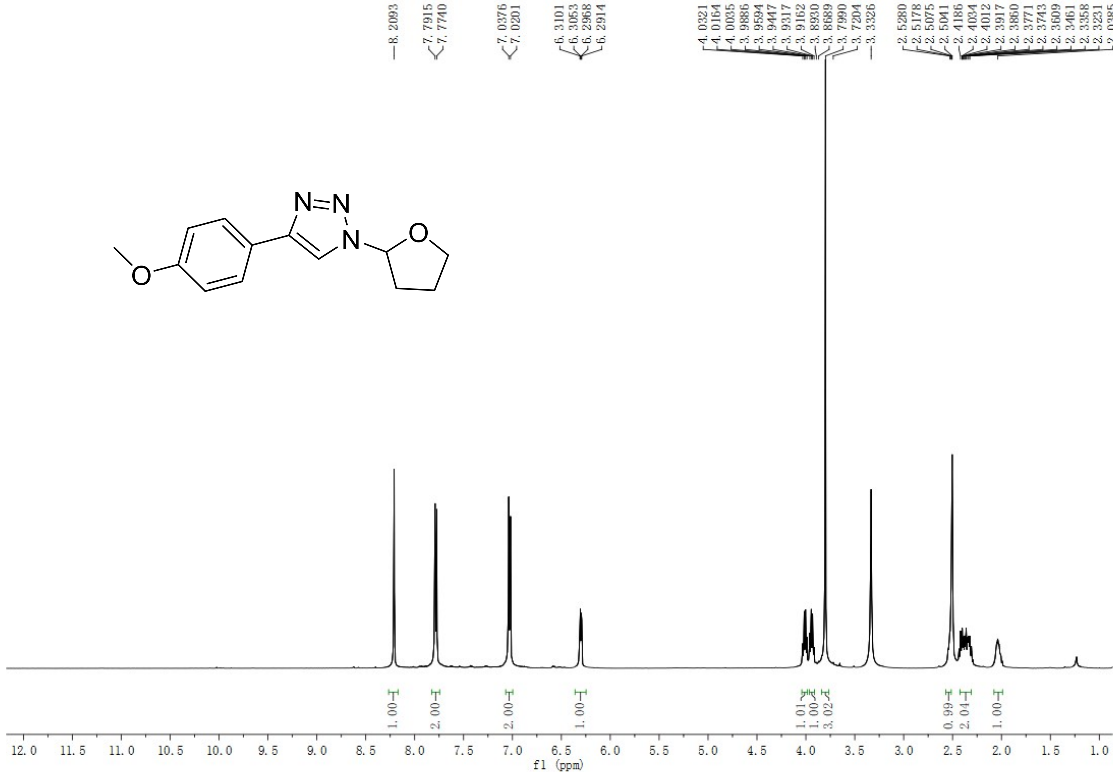
f1 (ppm)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2.00
2.00
1.00
1.01
1.00
3.02
0.99
2.04
1.00
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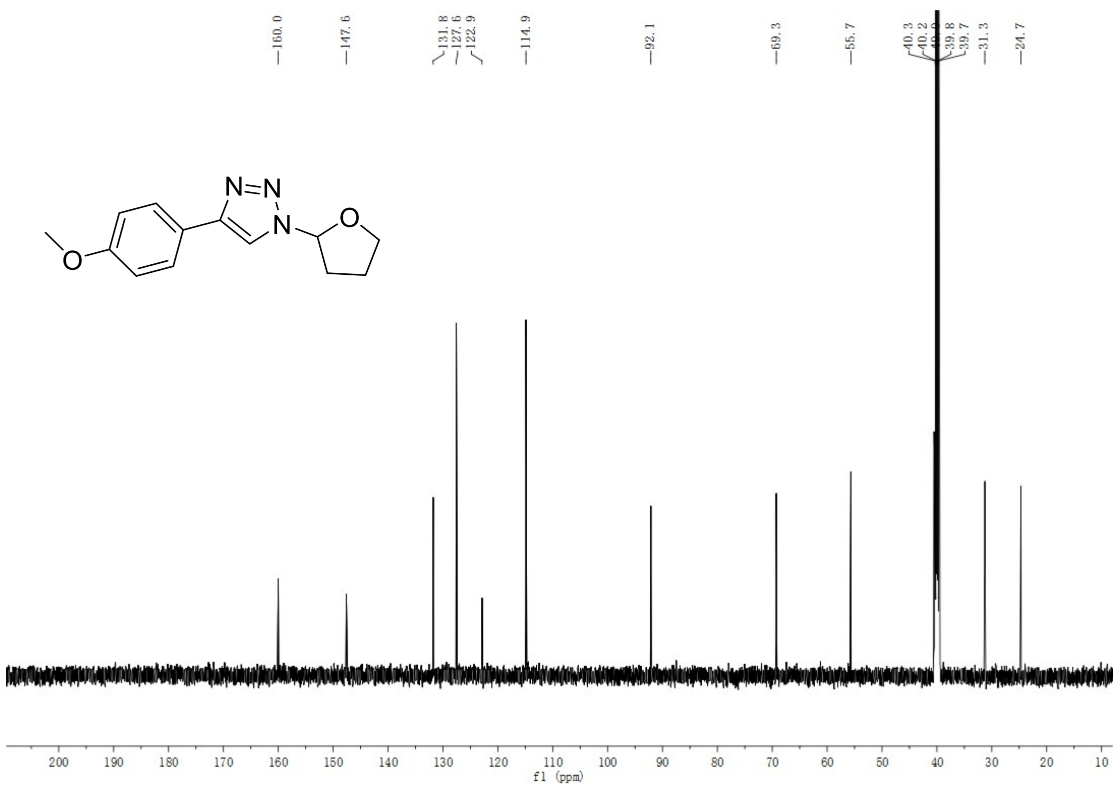
f1 (ppm)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114.9
92.1
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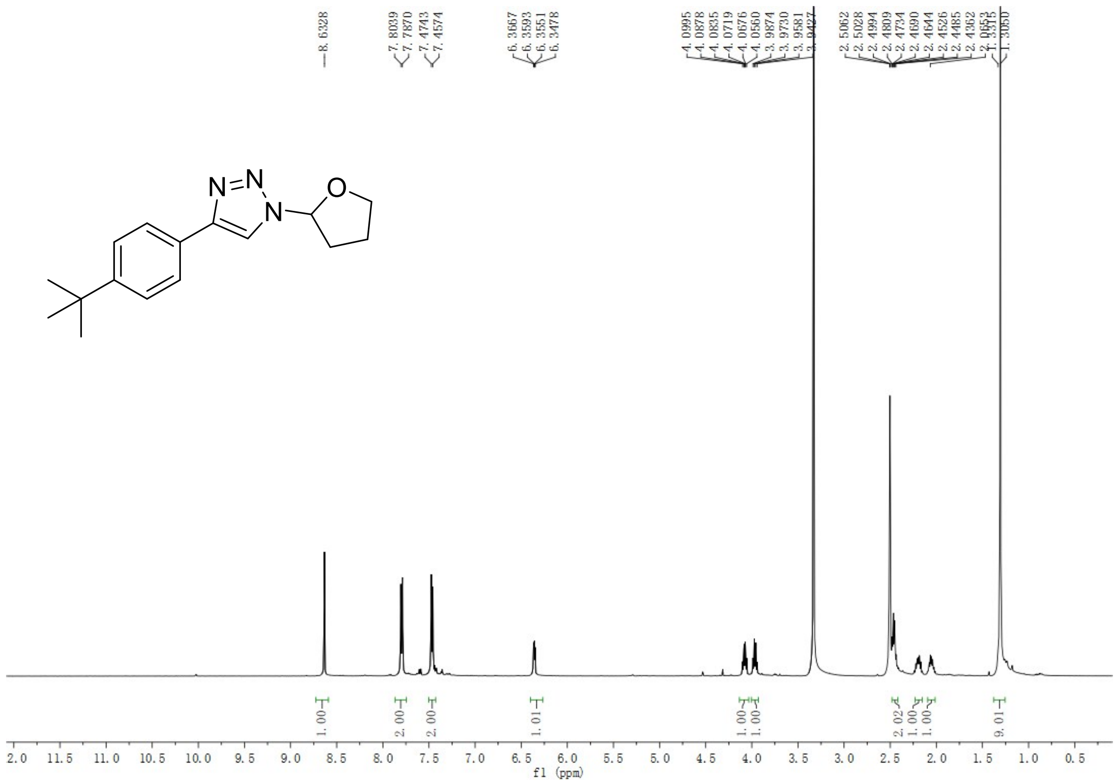
f1 (ppm)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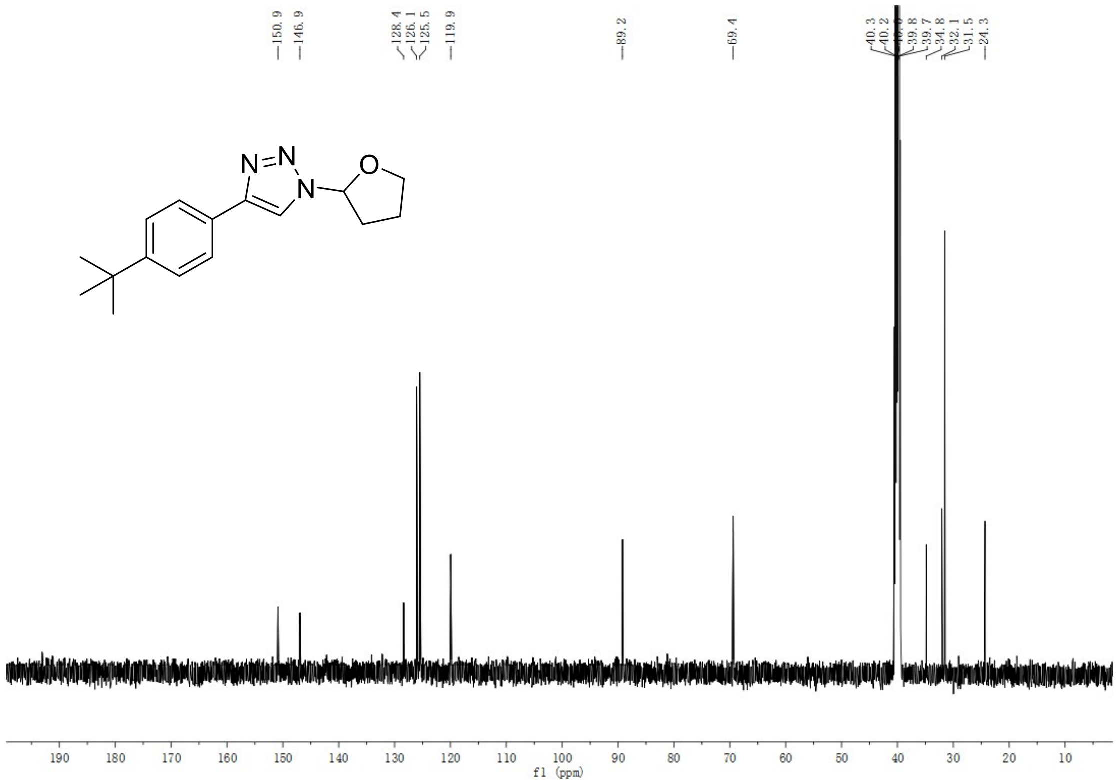
9.01
f1 (ppm)



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128.4
126.1
125.5
119.9
89.2
69.4
40.3
40.2
39.8
39.7
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31.5
24.3
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N
N
O
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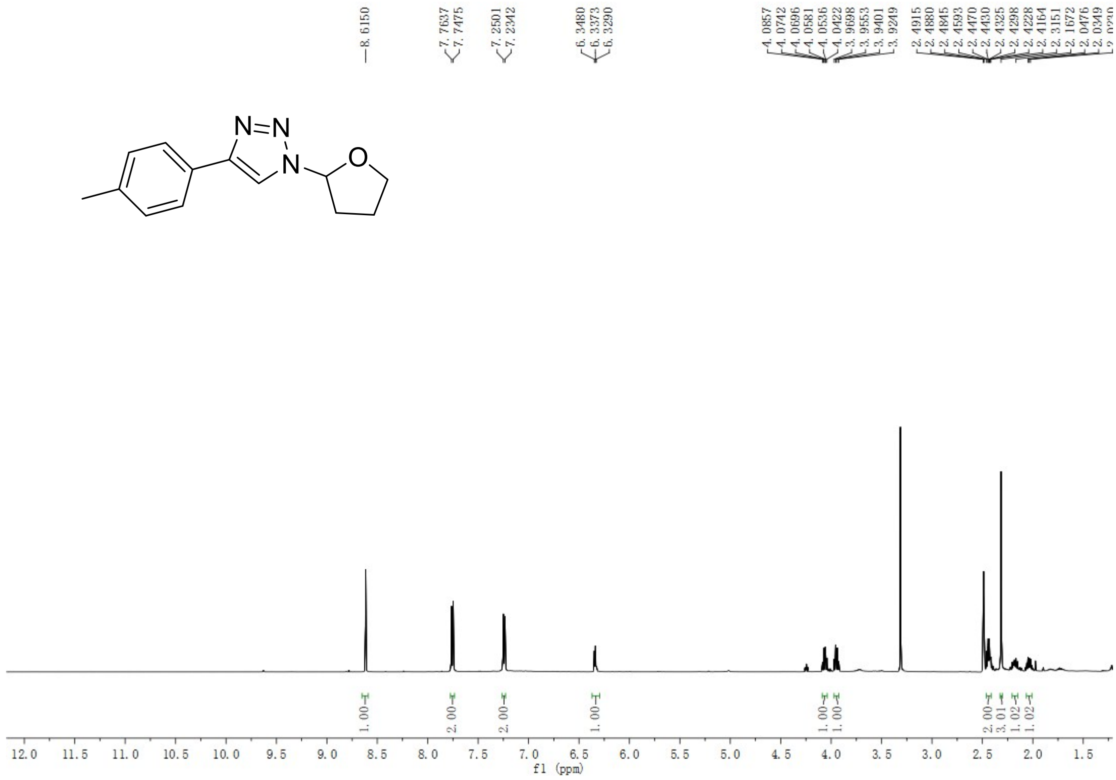
f1 (ppm)



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1.00
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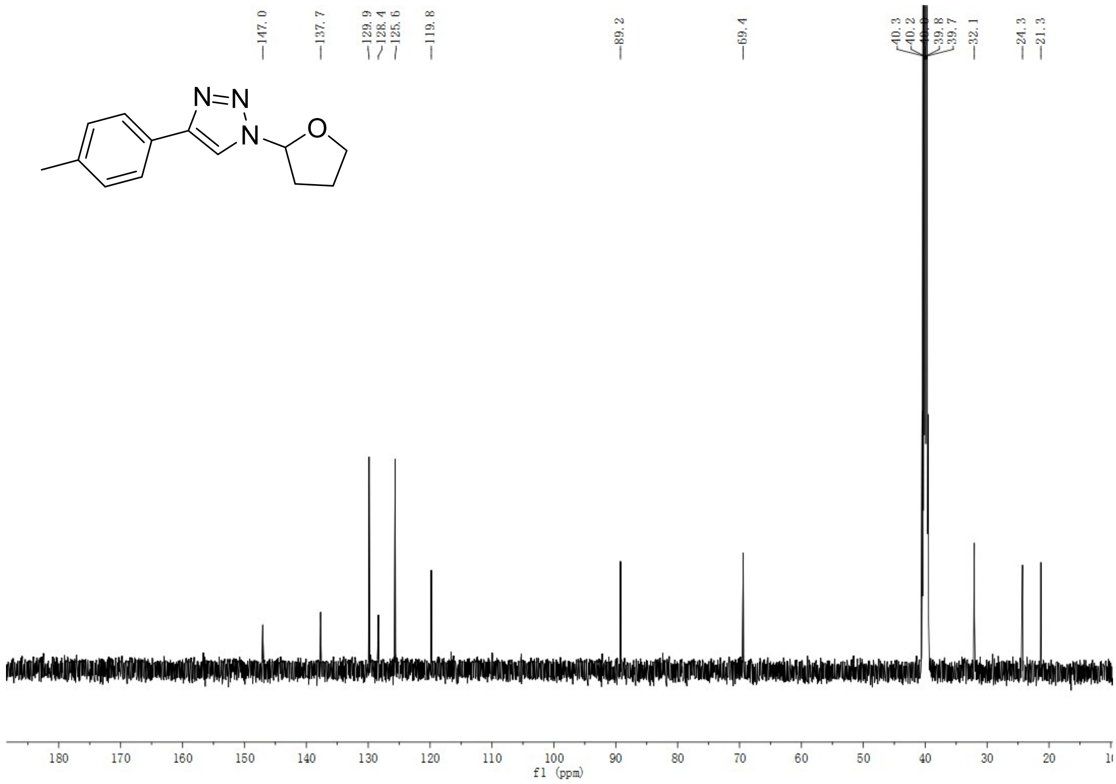
1.00
2.00
3.01
1.02
1.02
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)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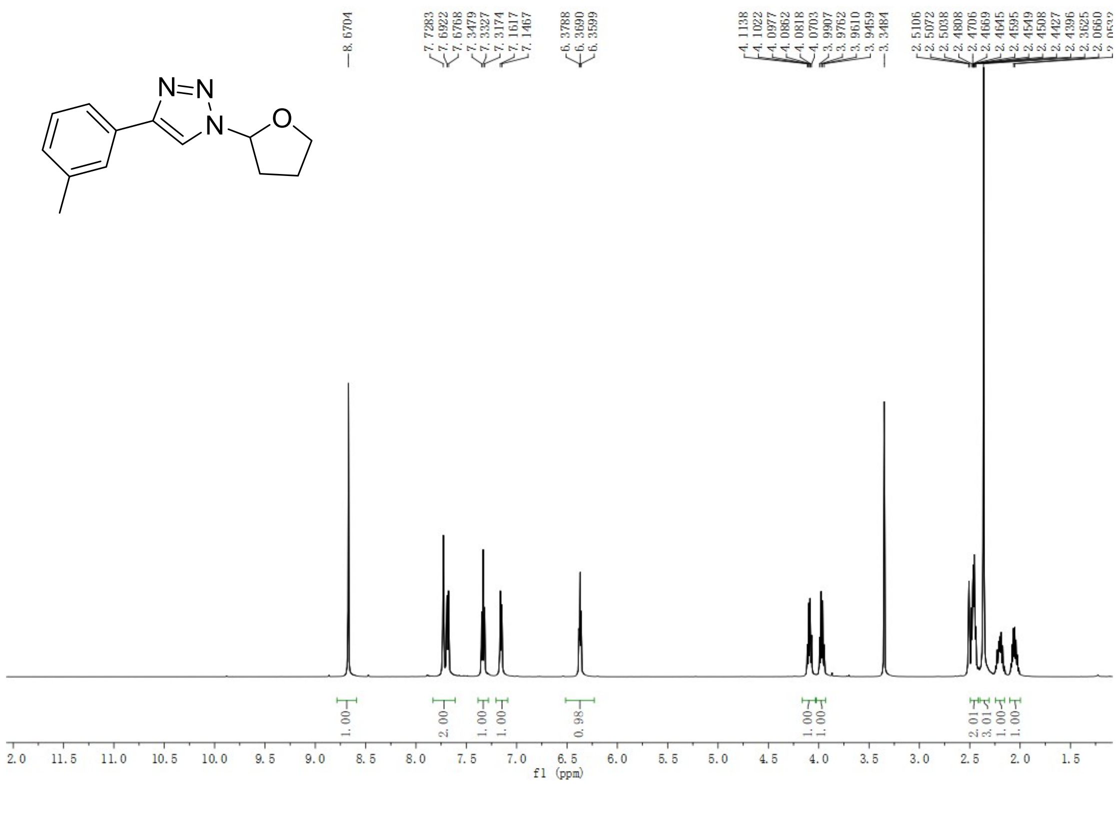
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3.3484
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2.0660
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N
O
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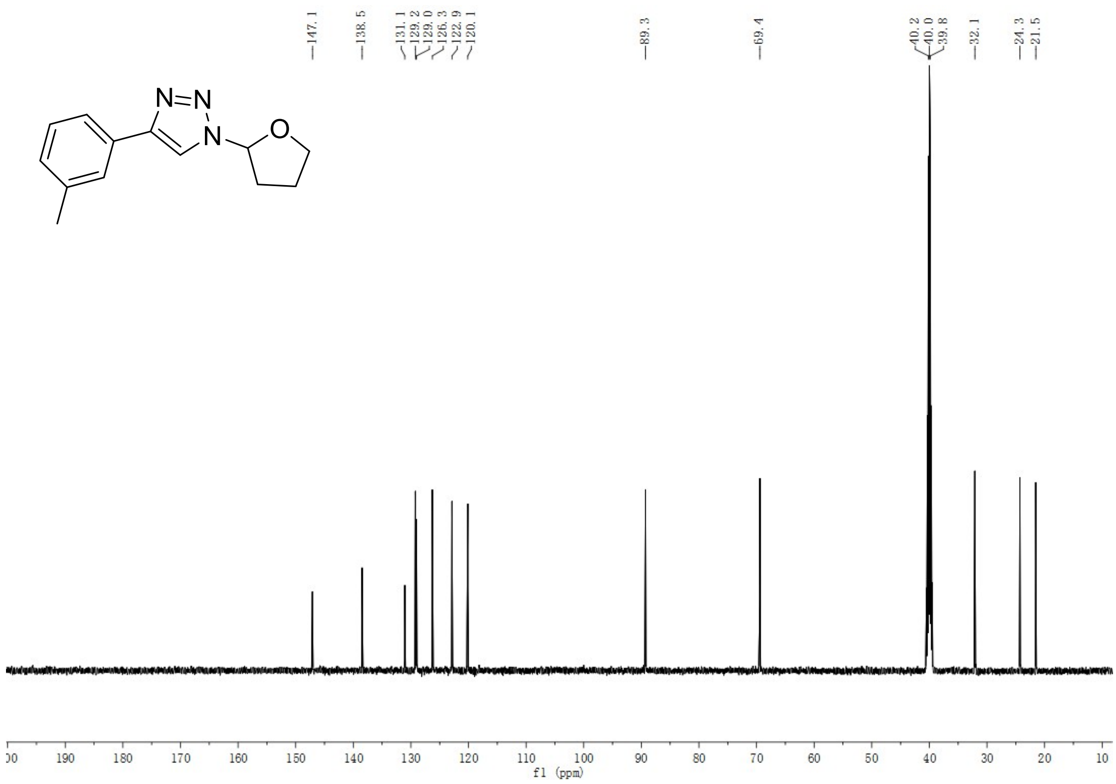
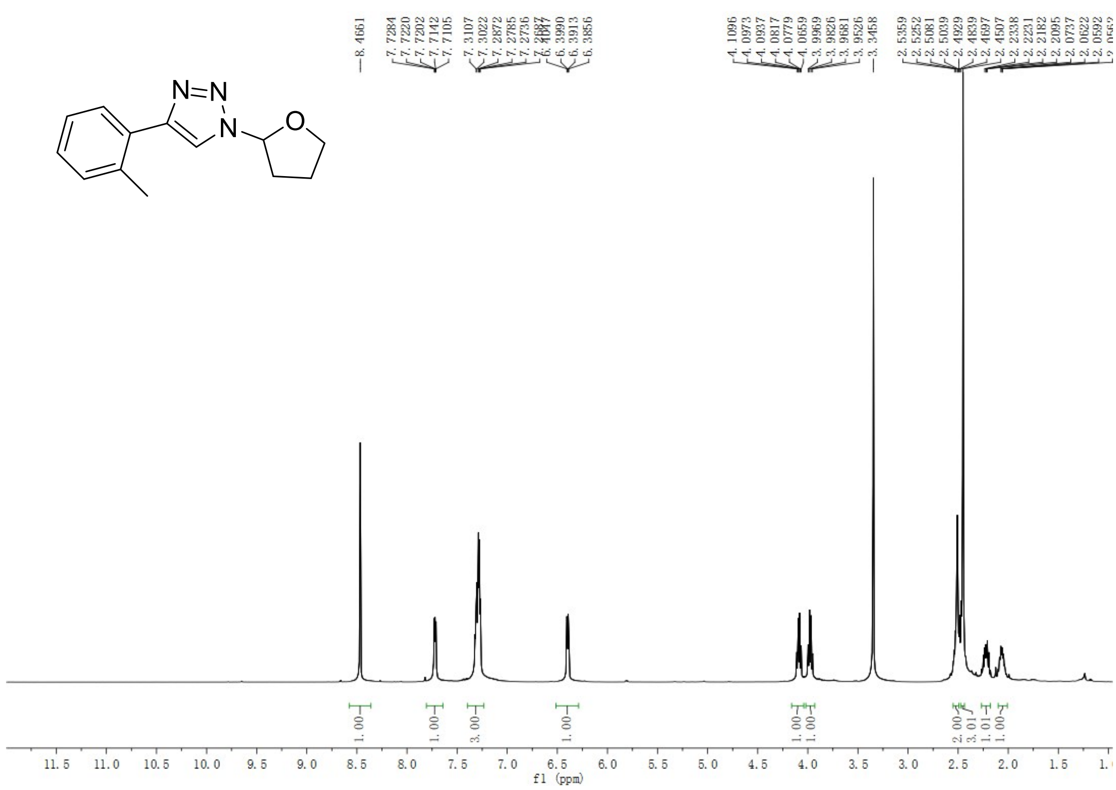
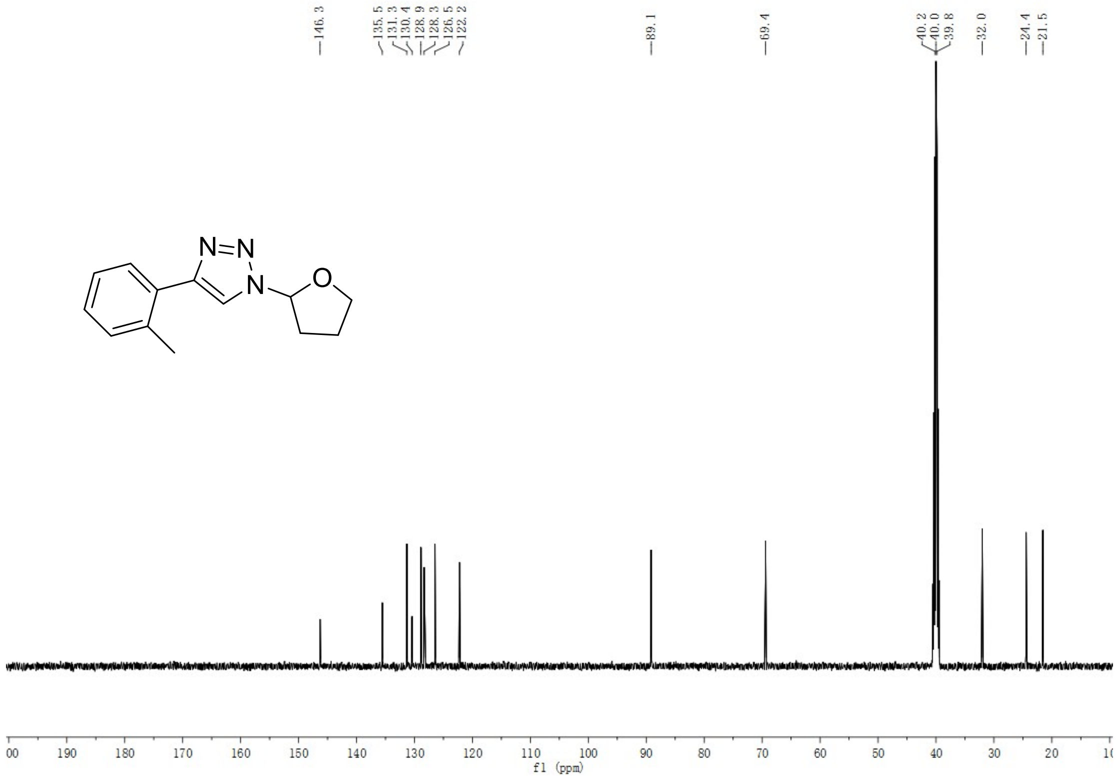
2.00
1.00
1.00
0.98
1.00
1.00
2.01
3.01
1.00
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)



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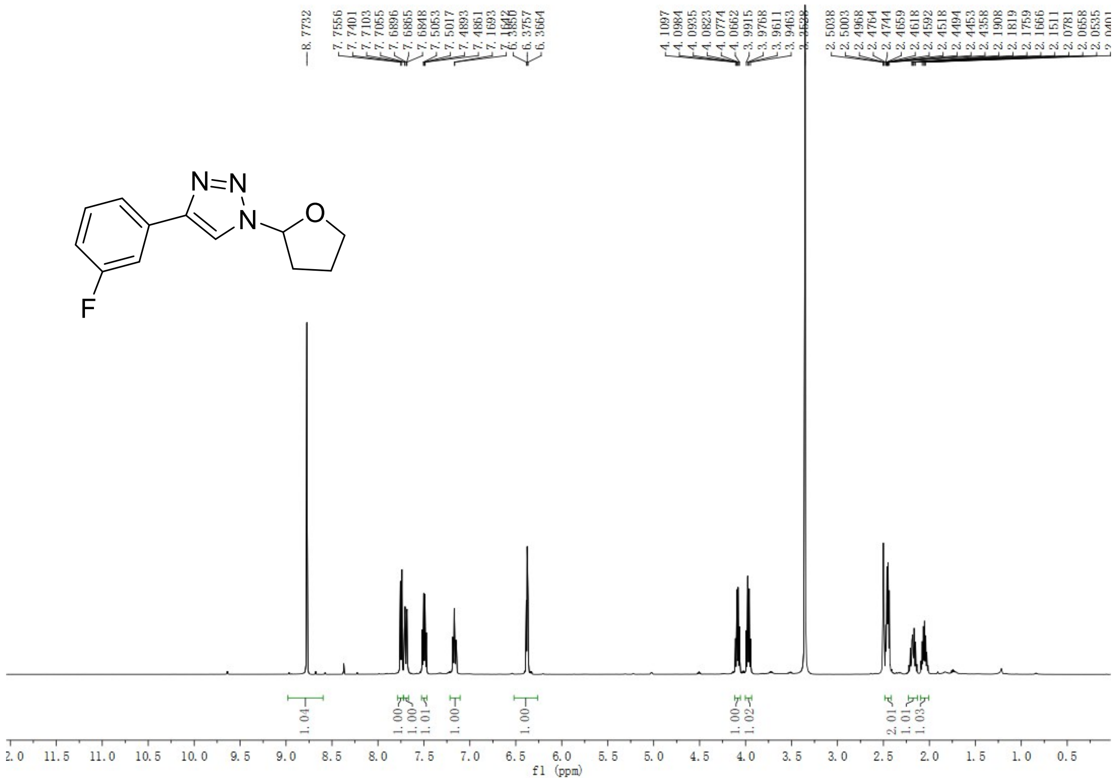
N
O
f1 (ppm)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7.4893
7.4861
7.1693
6.3757
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4.0774
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2.4764
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2.4618
2.4592
2.4518
2.4494
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2.4358
2.1908
2.1819
2.1759
2.1666
2.1511
2.0781
2.0658
2.0535
N=N
N
O
F
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1.01
1.00
1.00
1.00
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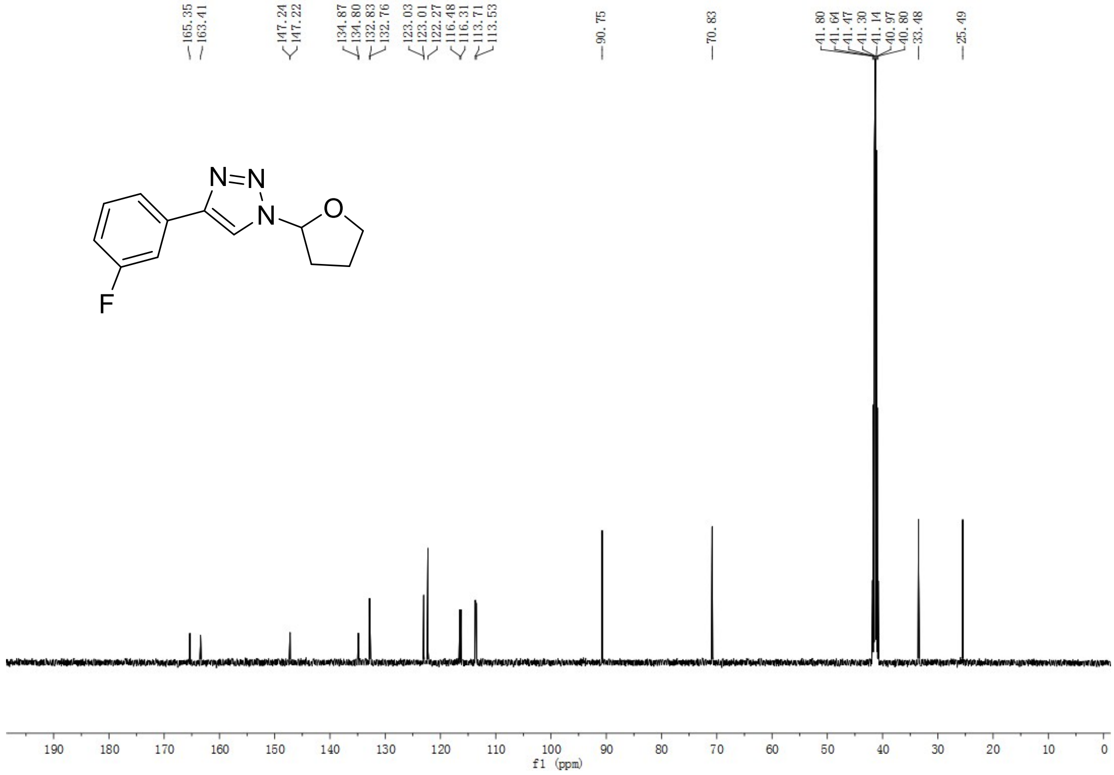
2.01
1.01
1.03
f1 (ppm)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132.76
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123.01
122.27
116.48
116.31
113.71
113.53
90.75
70.83
41.80
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41.47
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41.14
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40.80
33.48
25.49
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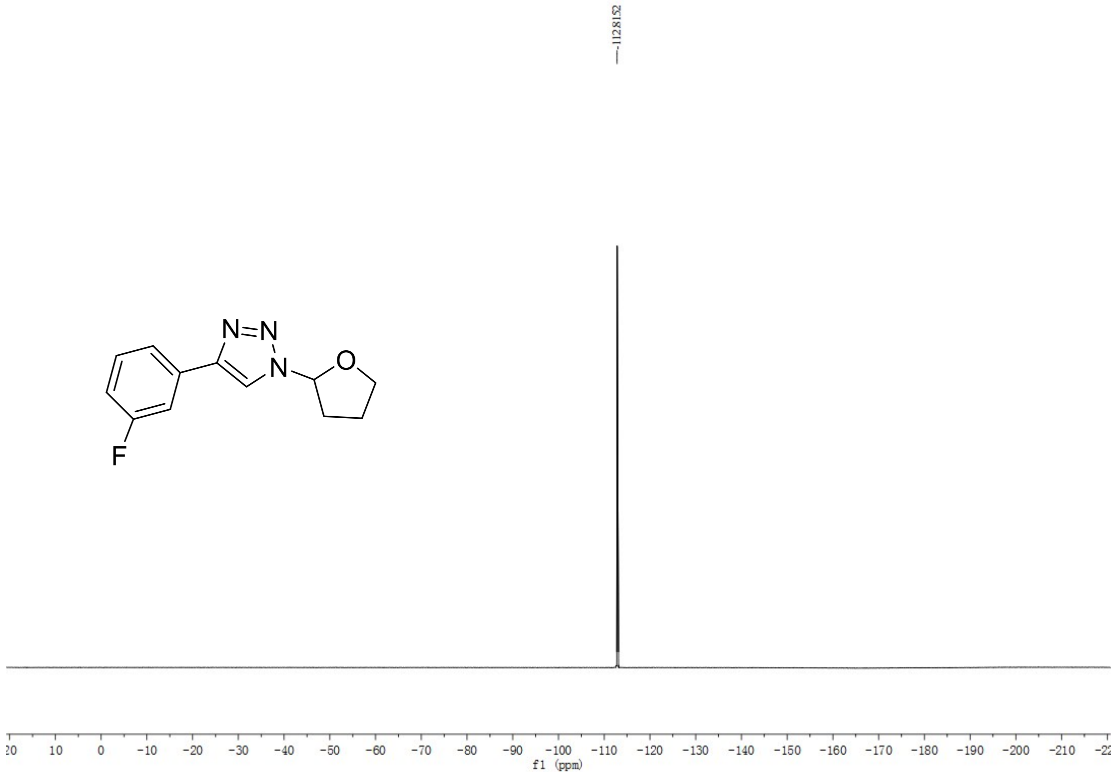
N
O
F
f1 (ppm)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O
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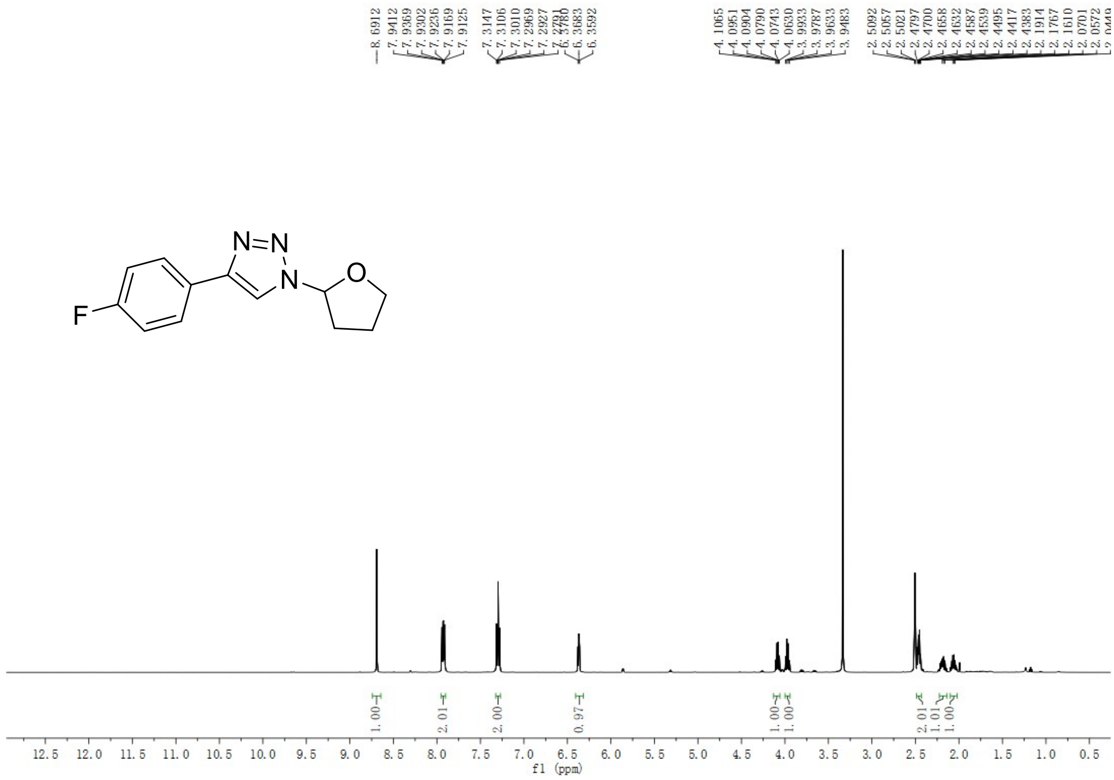
f1 (ppm)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7.2969
7.2927
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6.3780
6.3683
6.3592
4.1065
4.0951
4.0904
4.0790
4.0743
4.0630
3.9933
3.9787
3.9633
3.9483
2.5092
2.5057
2.5021
2.4797
2.4700
2.4658
2.4632
2.4587
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2.1914
2.1767
2.1610
2.0701
2.0572
N=N
N
O
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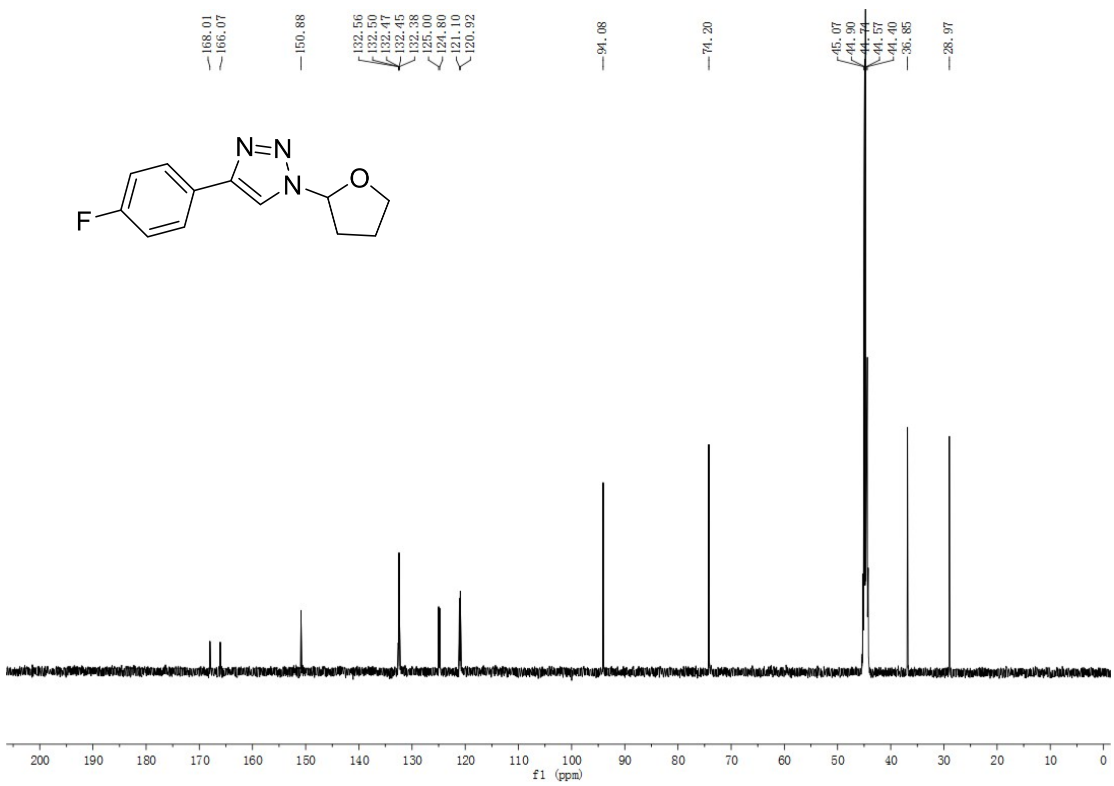
2.01
2.00
0.97
1.00
1.00
2.01
1.01
1.00
f1 (ppm)



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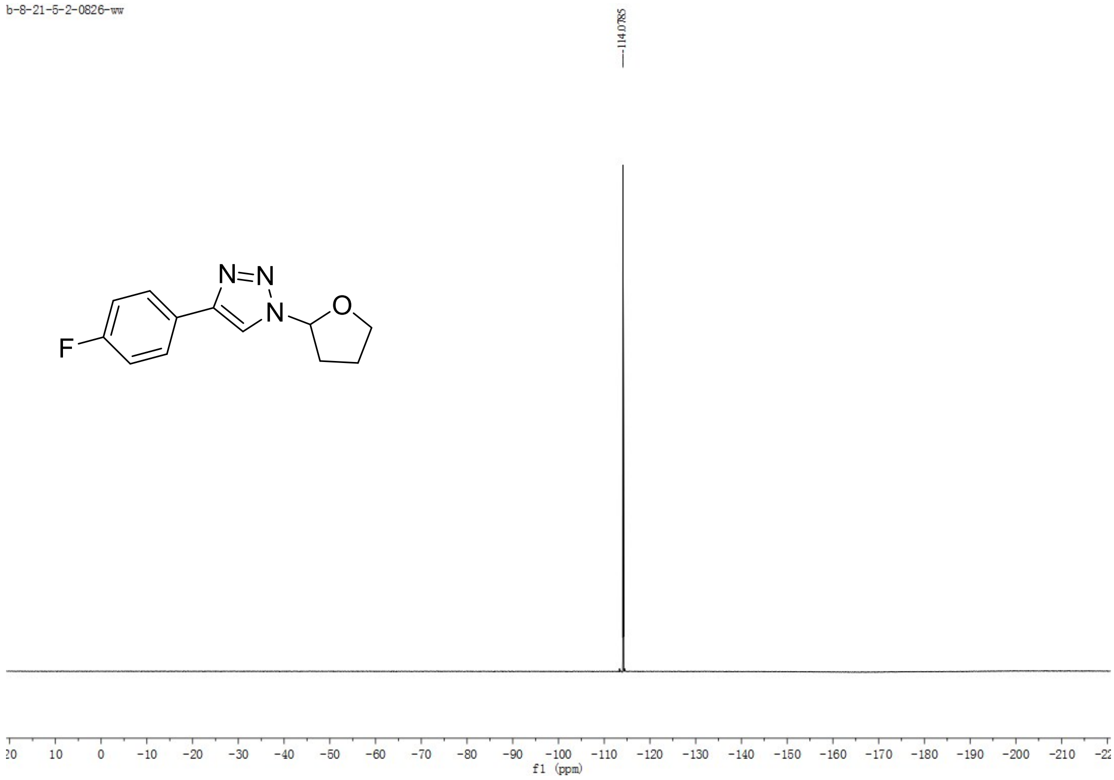

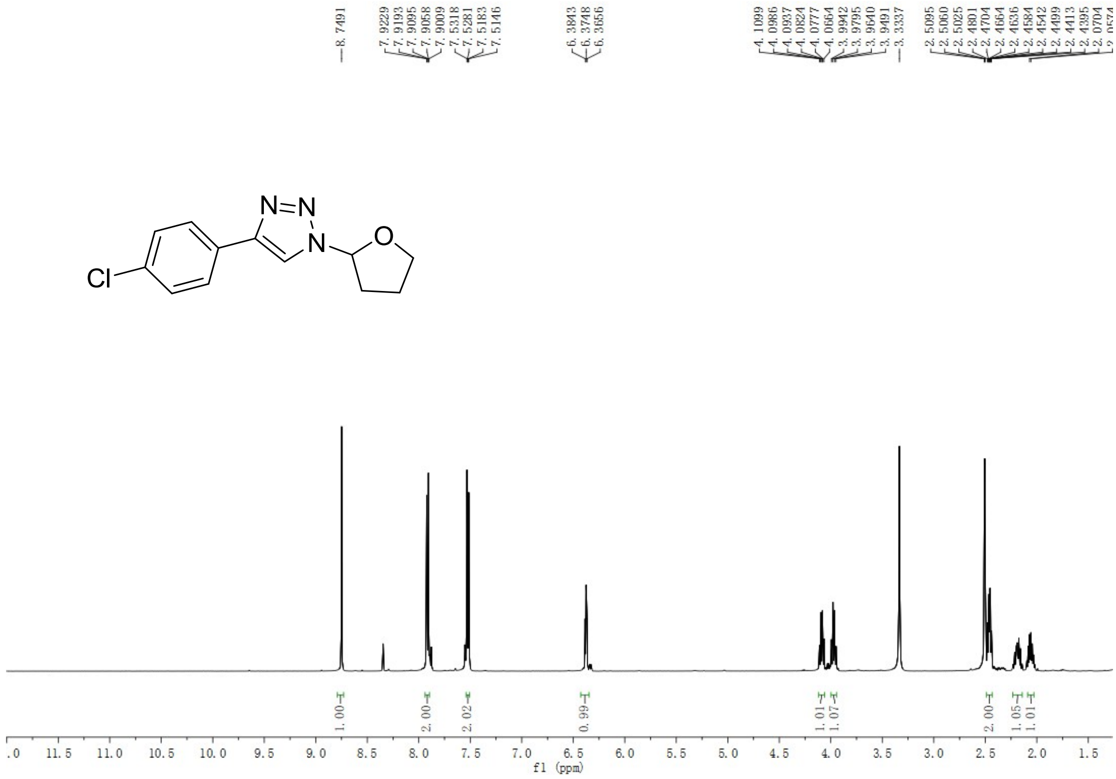
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7.5183
7.5146
6.3843
6.3748
6.3656
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4.0986
4.0937
4.0824
4.0777
3.9640
3.9491
3.3337
2.5095
2.5060
2.5025
2.4801
2.4704
2.4636
2.4584
2.4542
2.4499
2.4413
2.4395
2.0704
N=N
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Cl
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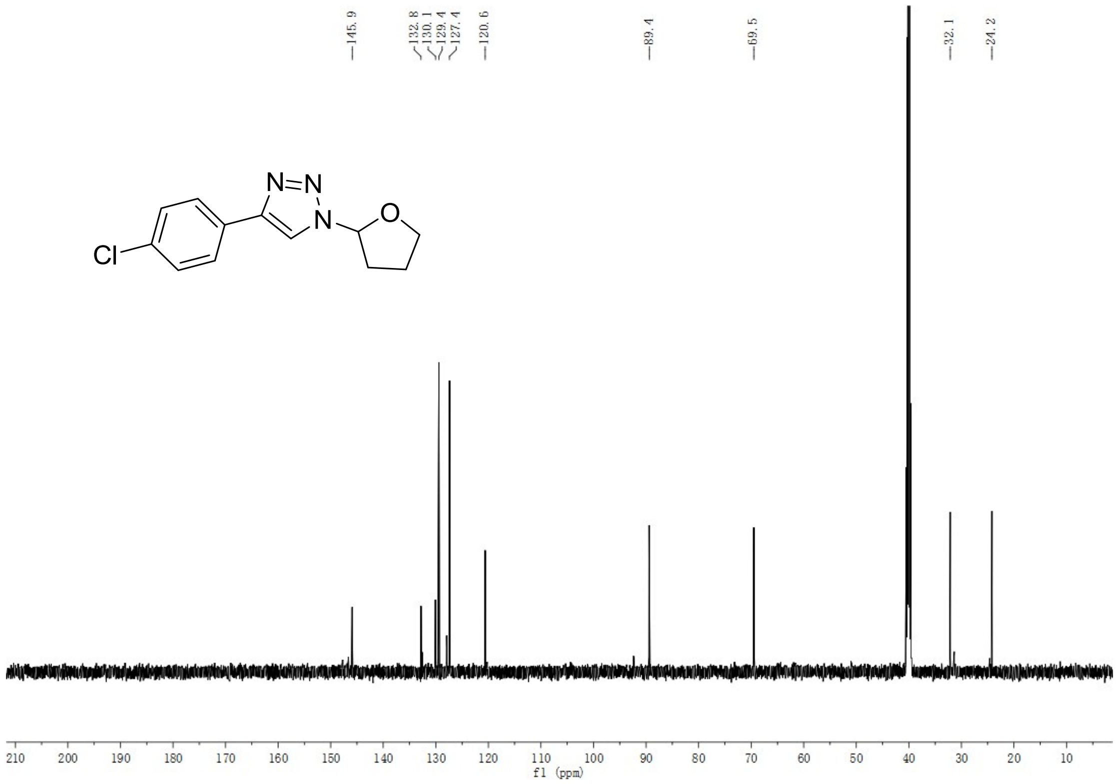
2.00
2.02
0.99
1.01
1.07
2.00
1.05
1.01
f1 (ppm)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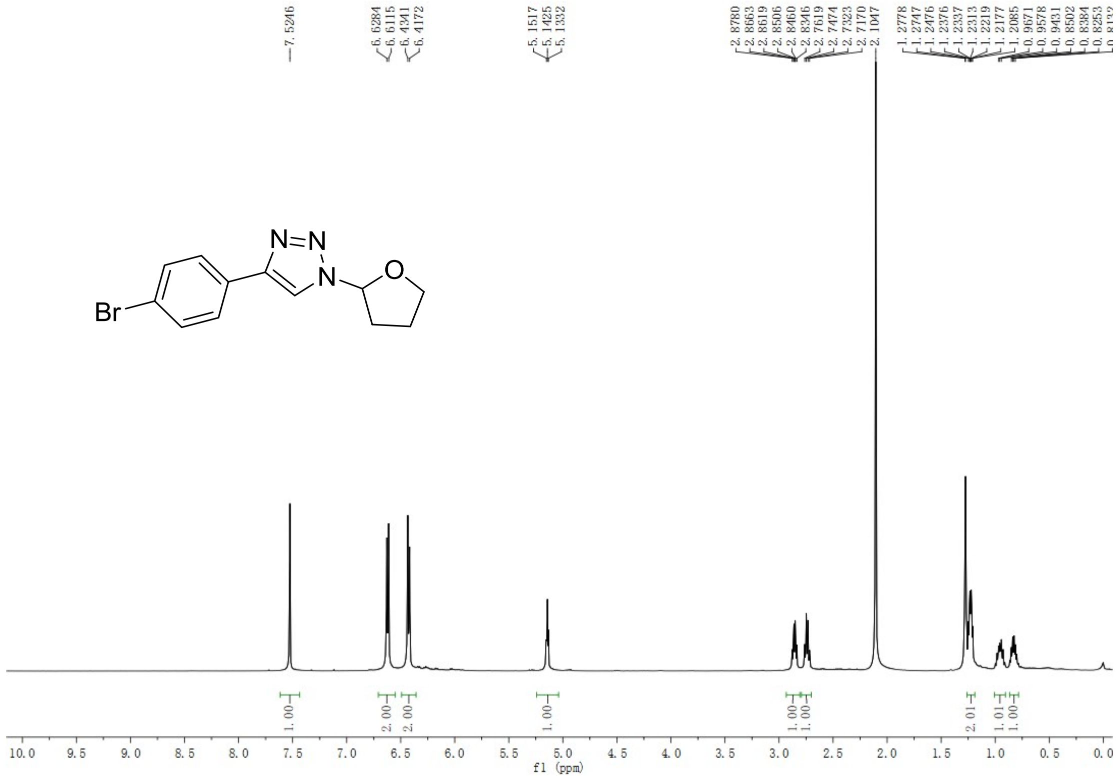
132.8
130.1
129.4
127.4
120.6
89.4
69.5
32.1
24.2
N=N
N
O
Cl
f1 (ppm)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2.8506
2.8460
2.8346
2.7619
2.7474
2.7323
2.7170
2.1047
1.2778
1.2747
1.2476
1.2376
1.2337
1.2313
1.2219
1.2177
1.2085
0.9671
0.9578
0.9431
0.8502
0.8384
0.8253
Br
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N
O
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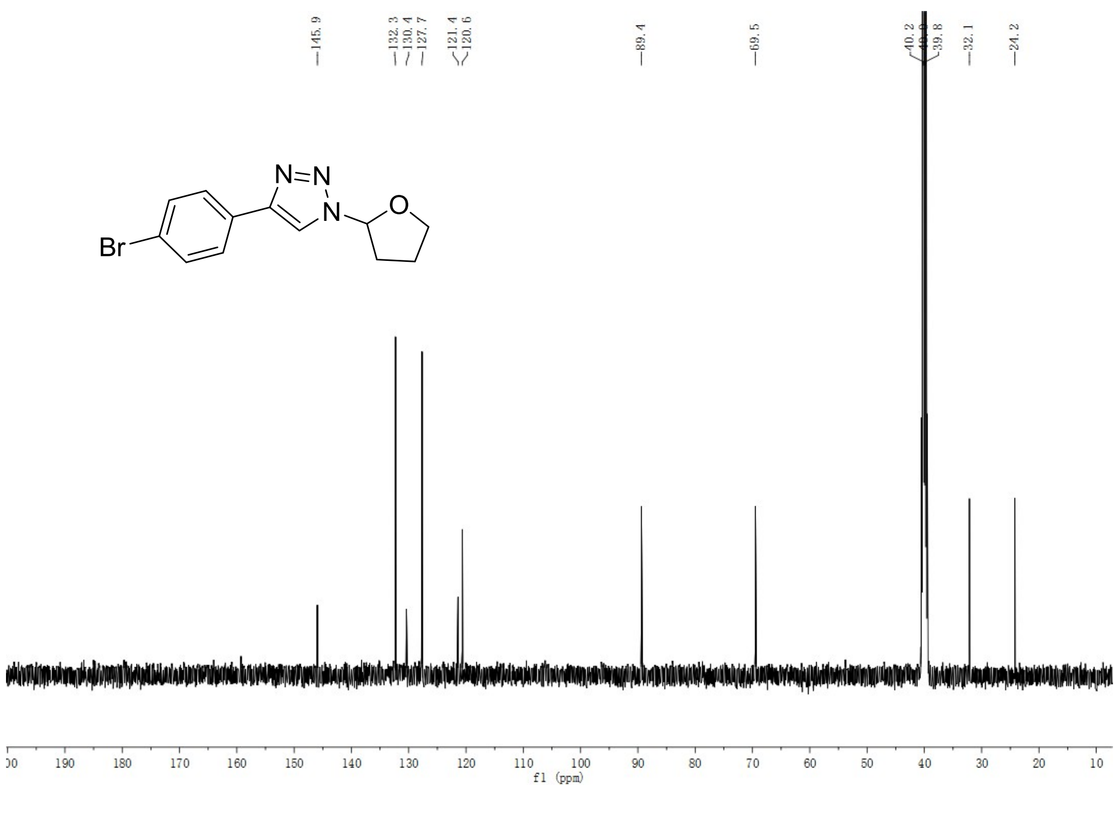
2.00
2.00
1.00
1.00
1.00
2.01
1.01
1.00
f1 (ppm)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132.3
130.4
127.7
121.4
120.6
89.4
69.5
40.2
39.8
32.1
24.2
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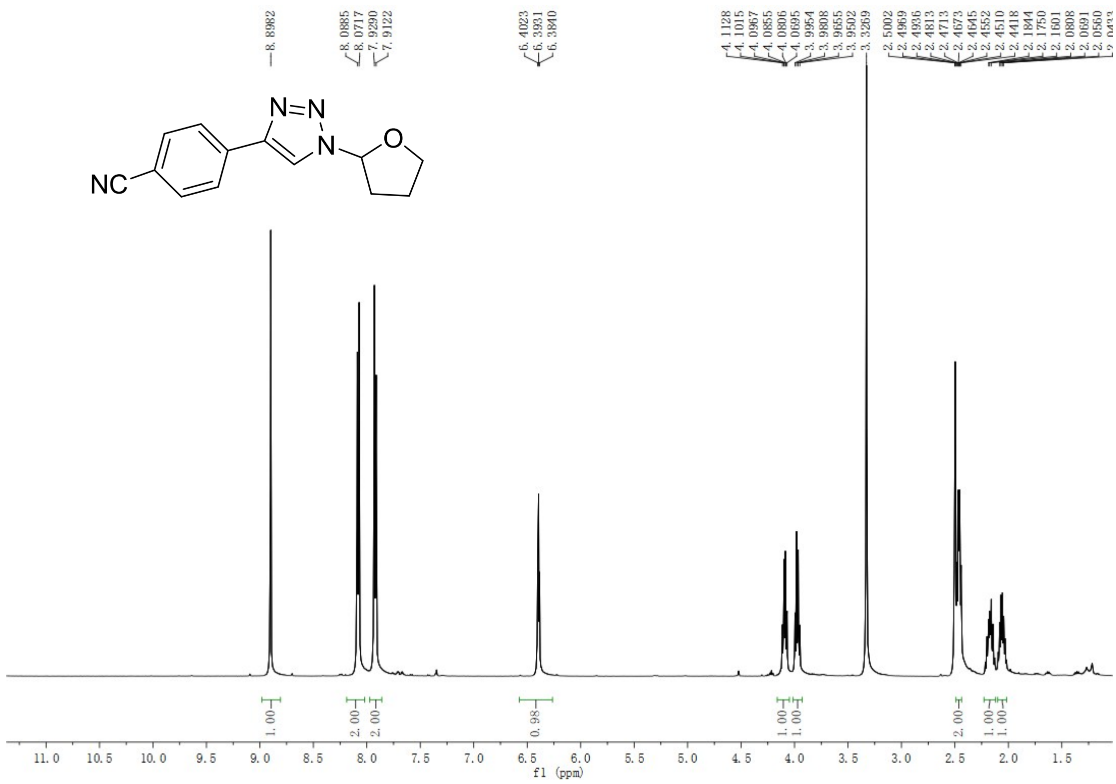
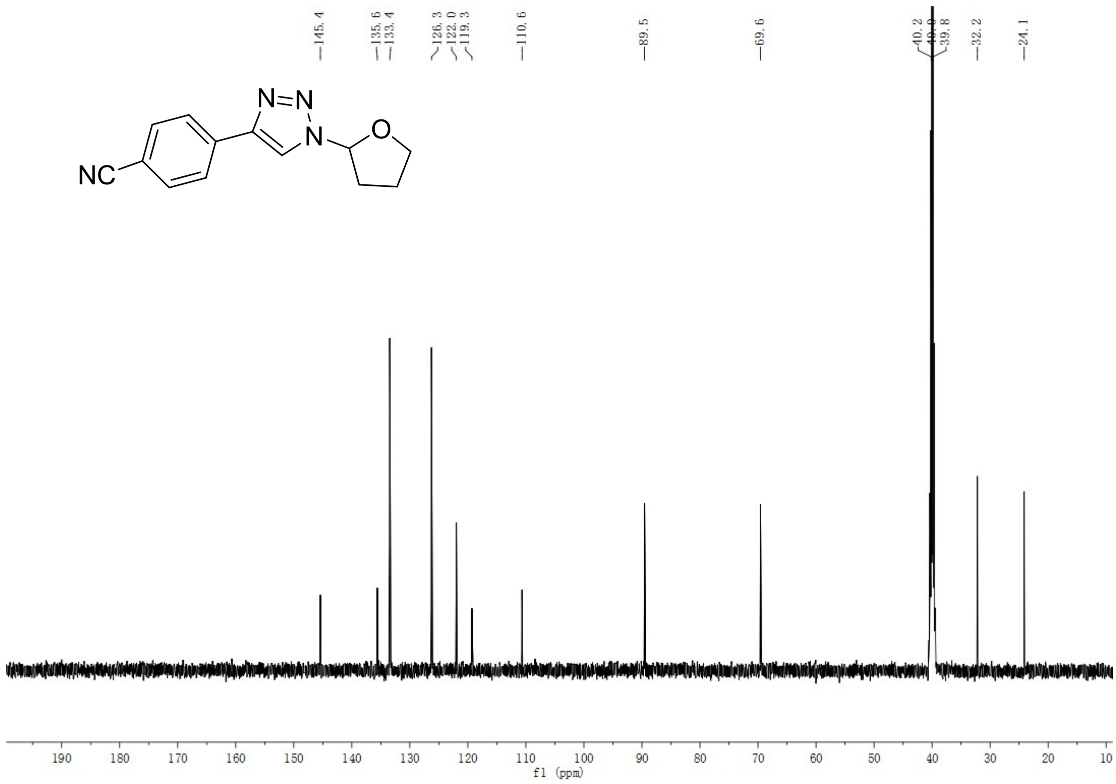
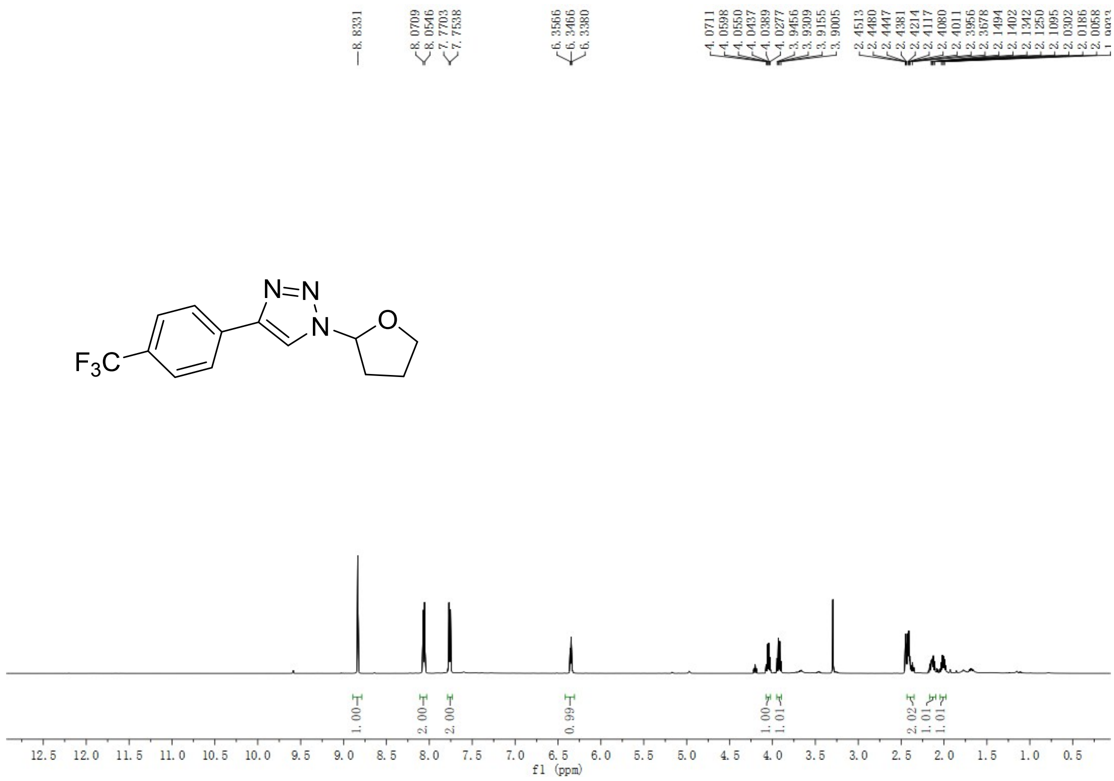
N
O
f1 (ppm)



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3.9005
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2.4447
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2.3578
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2.1402
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2.1250
2.1095
2.0392
2.0186
2.0058
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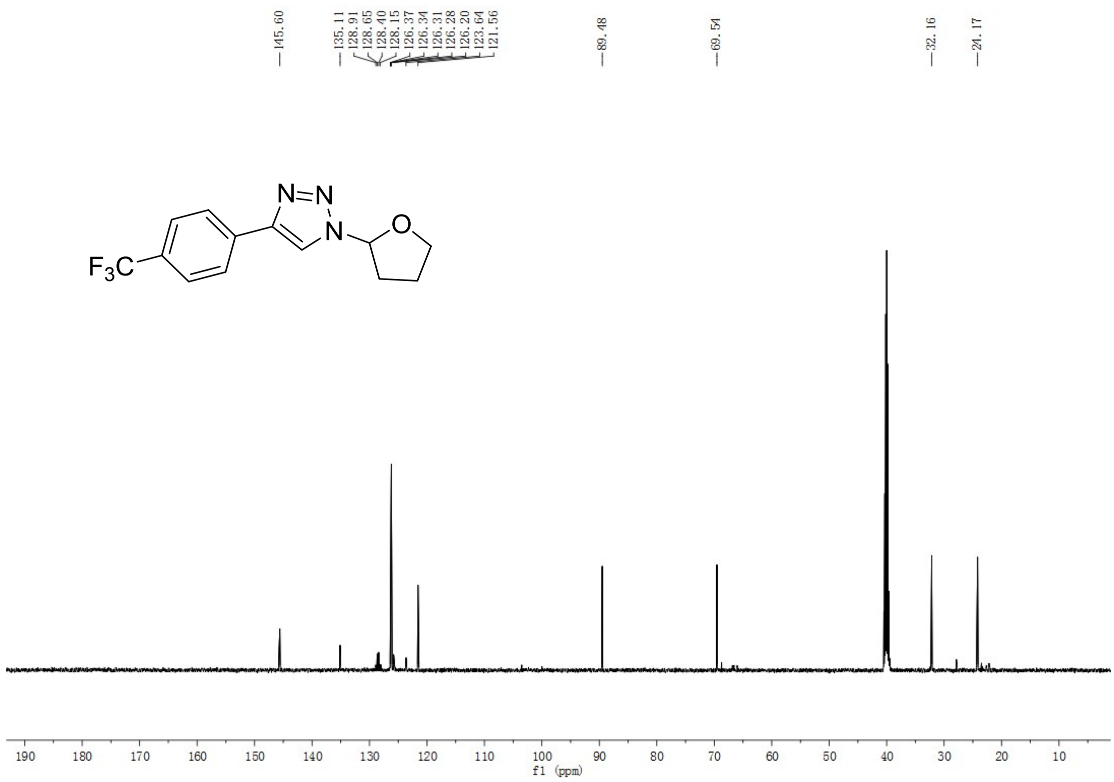
N
O
F3C
1.00
2.00
2.00
0.99
1.00
1.01
2.02
1.01
1.01
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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128.15
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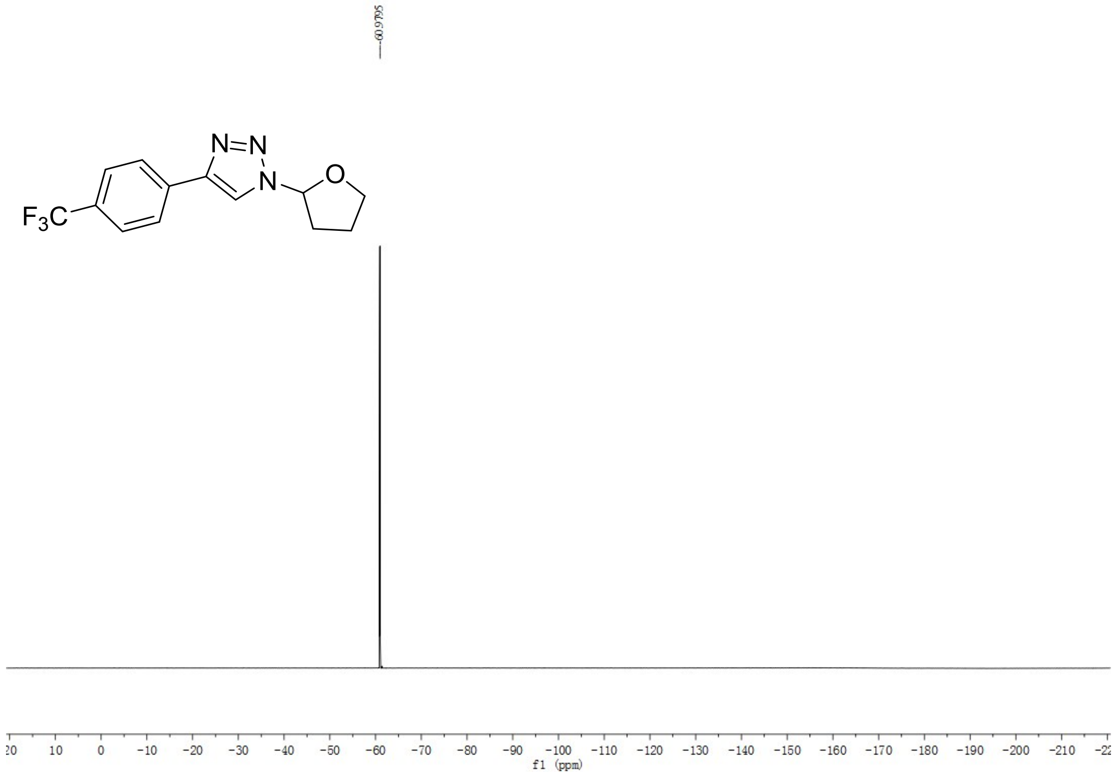
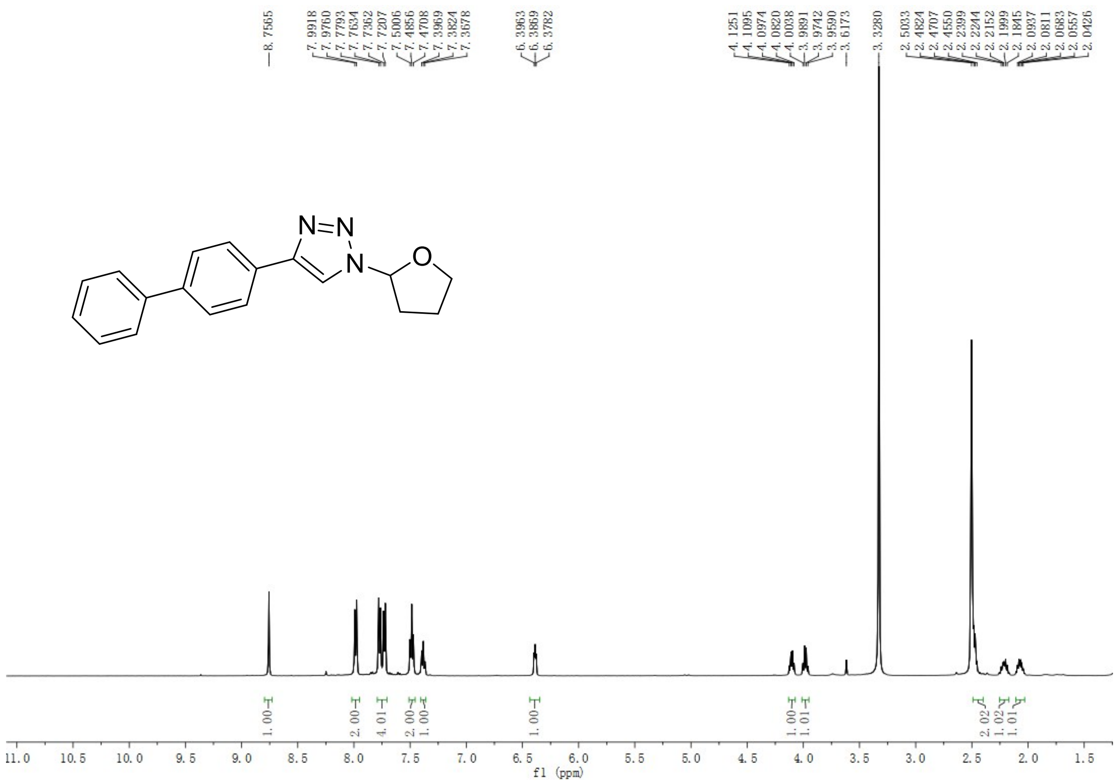
126.34
126.31
126.28
126.20
123.64
121.56
89.48
69.54
32.16
24.17
N=N
N
O
F3C
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)



-60.9795
F3C
N=N
N
O
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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6.3782
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2.0937
2.0811
2.0683
2.0557
2.0426
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N
O
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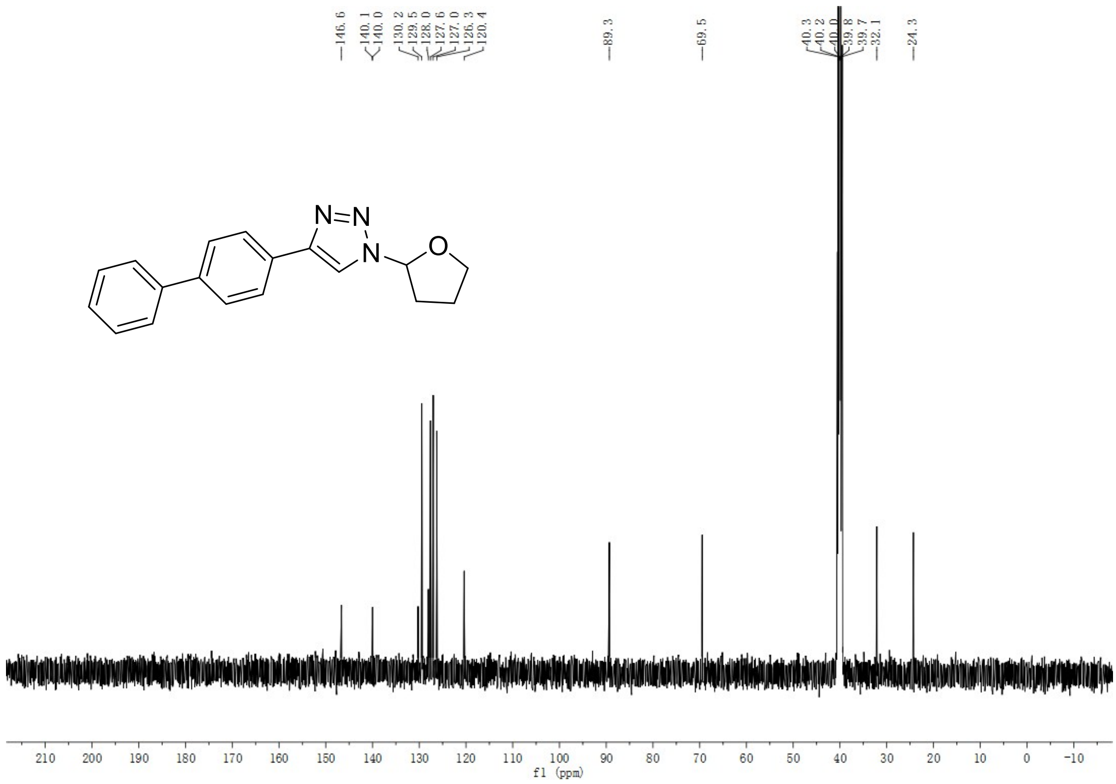
2.00
4.01
2.00
1.00
1.00
1.00
1.01
2.02
1.02
1.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)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127.0
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120.4
89.3
69.5
40.3
40.2
40.0
39.8
39.7
32.1
24.3
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N
O
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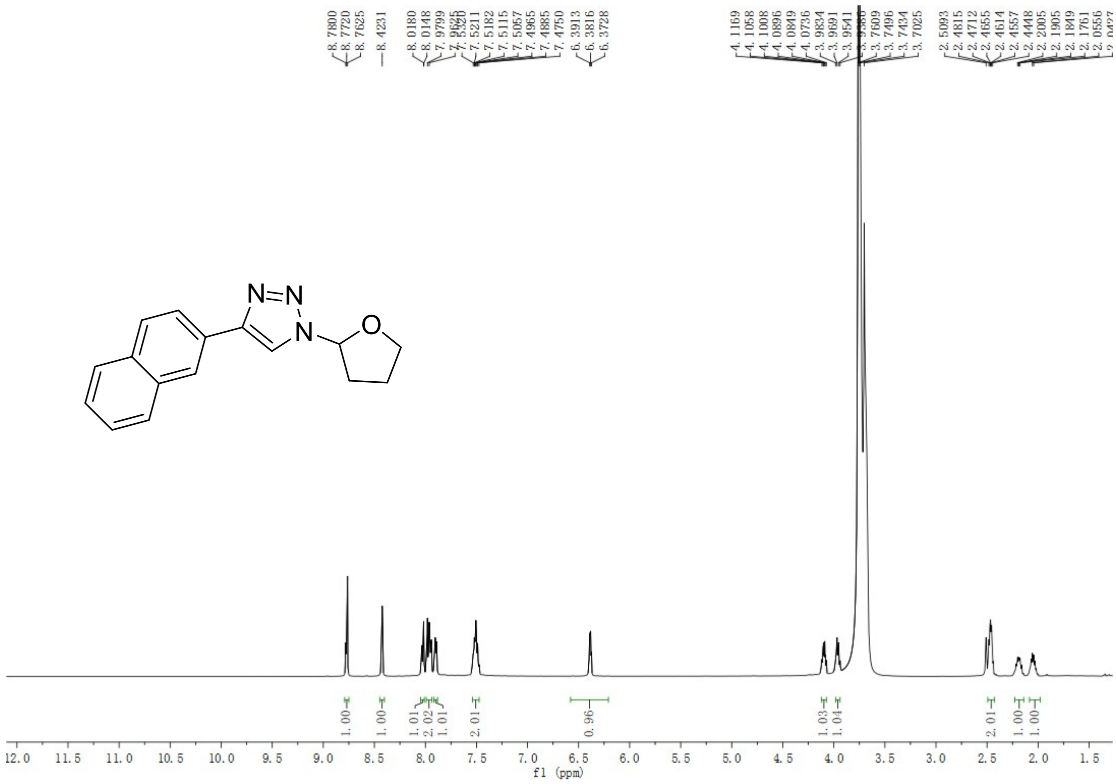
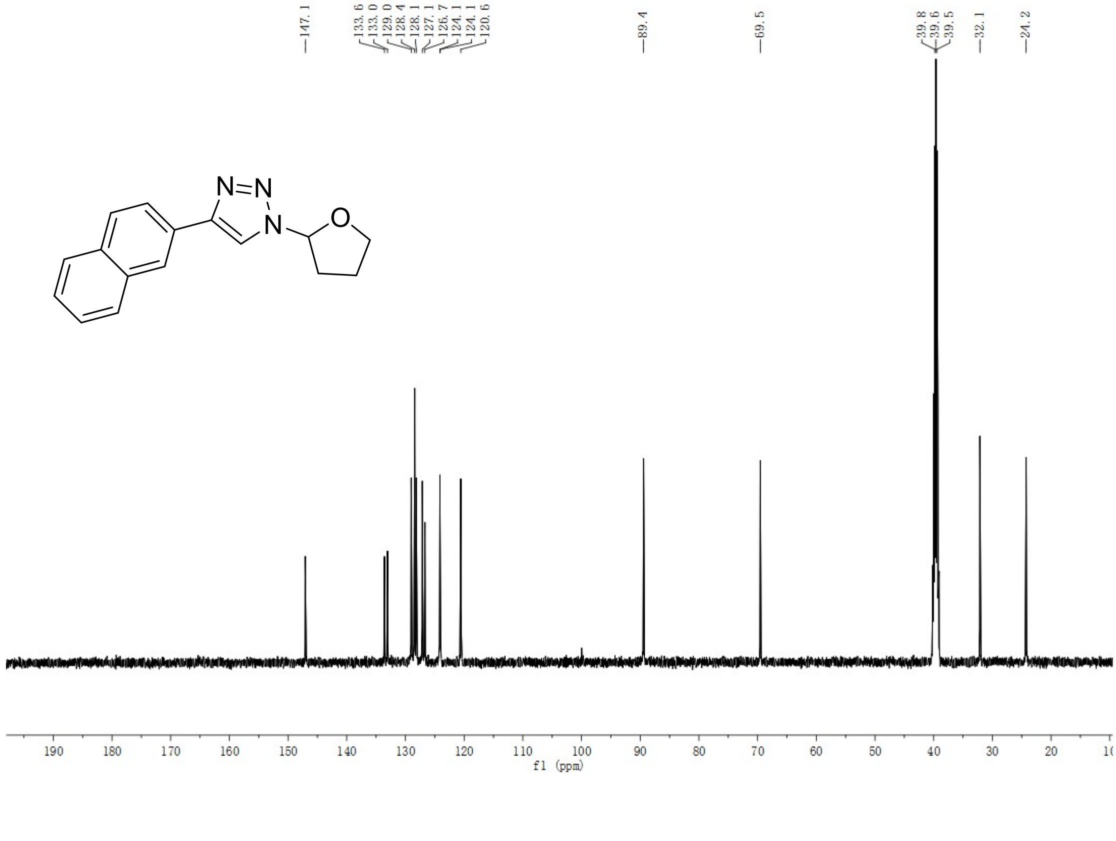
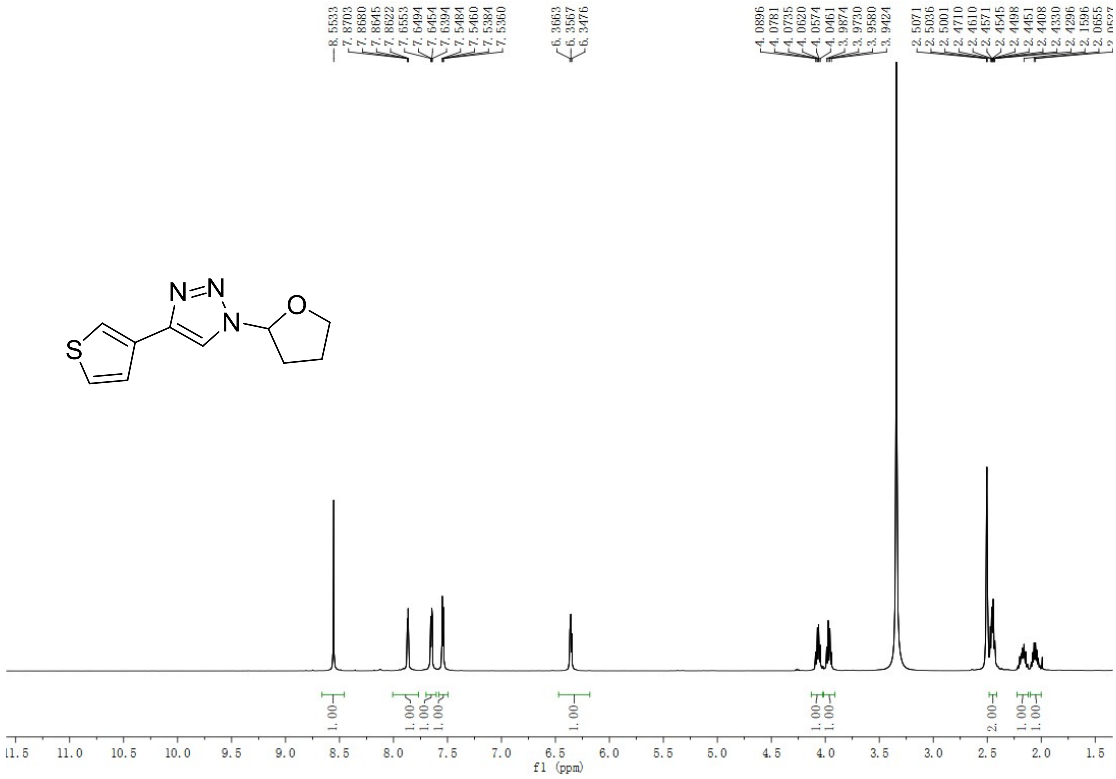
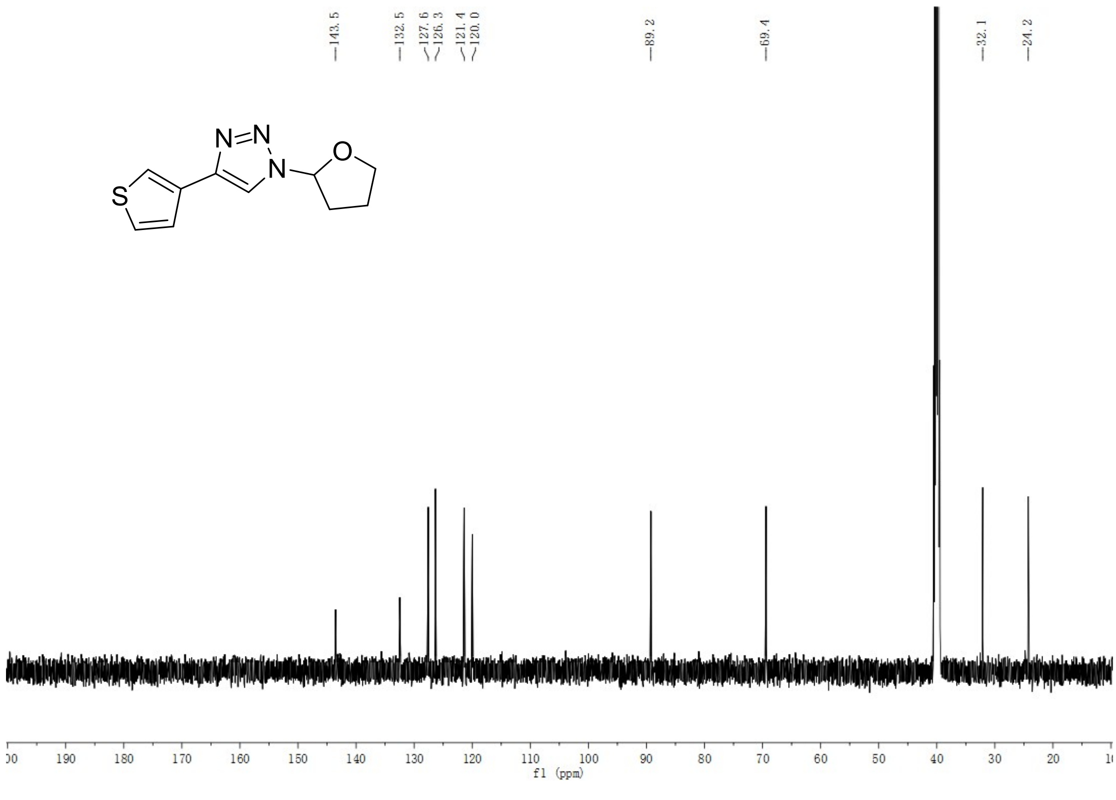
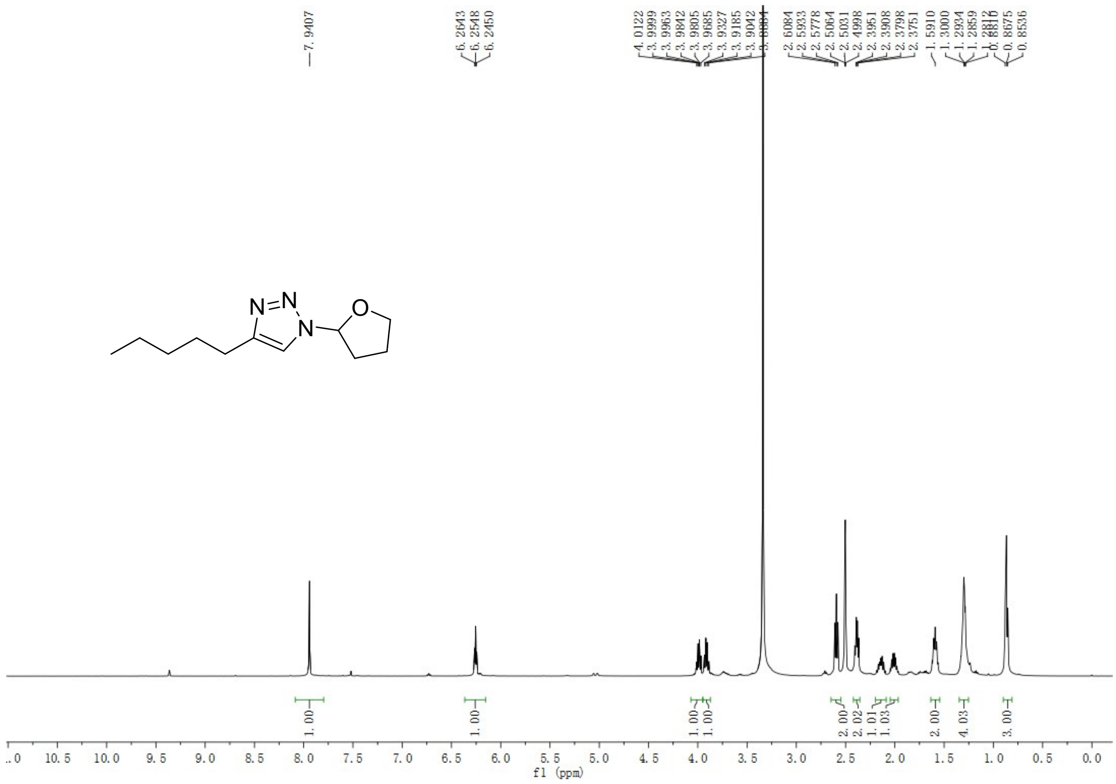
f1 (ppm)







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1.5910
1.3000
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1.2859
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1.00
1.00
1.00
2.00
2.02
1.01
1.03
2.00
4.03
3.00
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10.0
9.5
9.0
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8.0
7.5
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6.5
6.0
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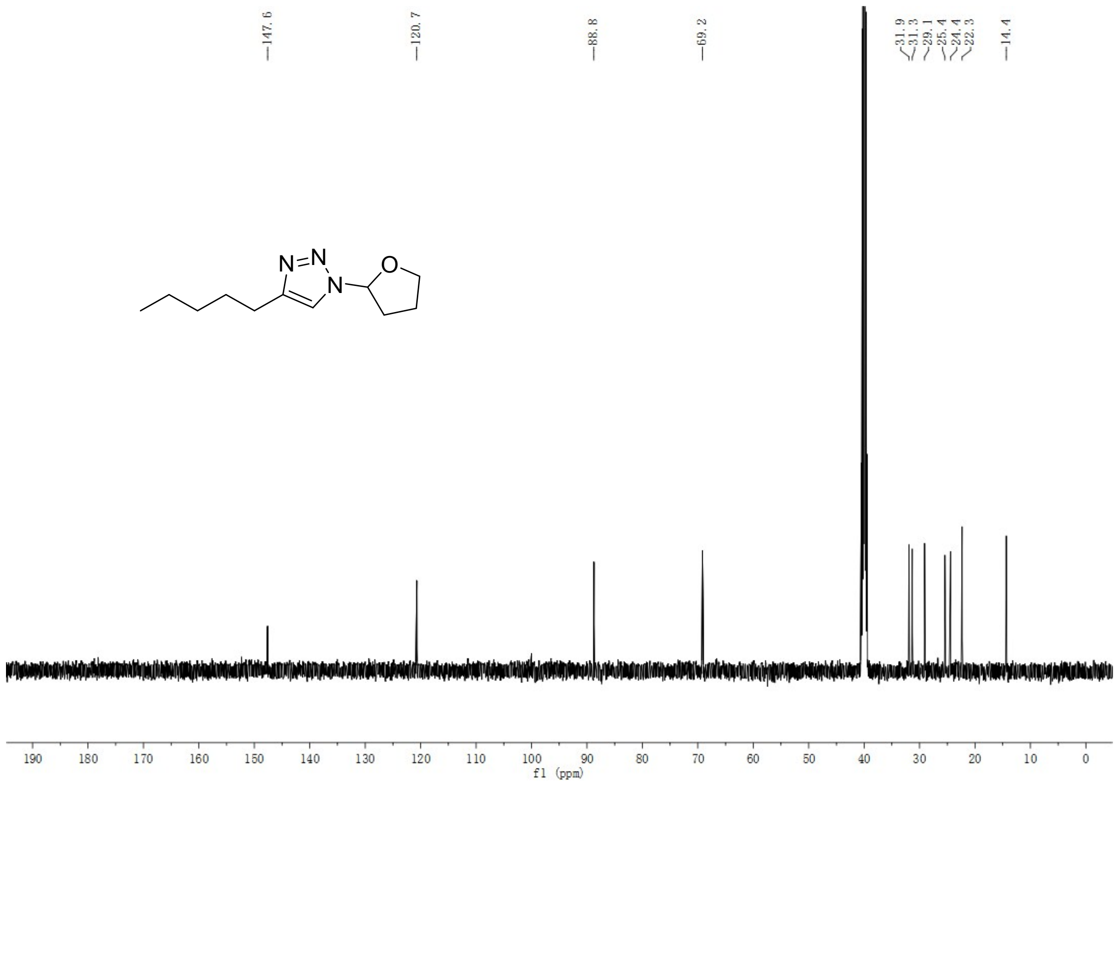
f1 (ppm)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22.3
14.4
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180
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110
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70
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50
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20
10
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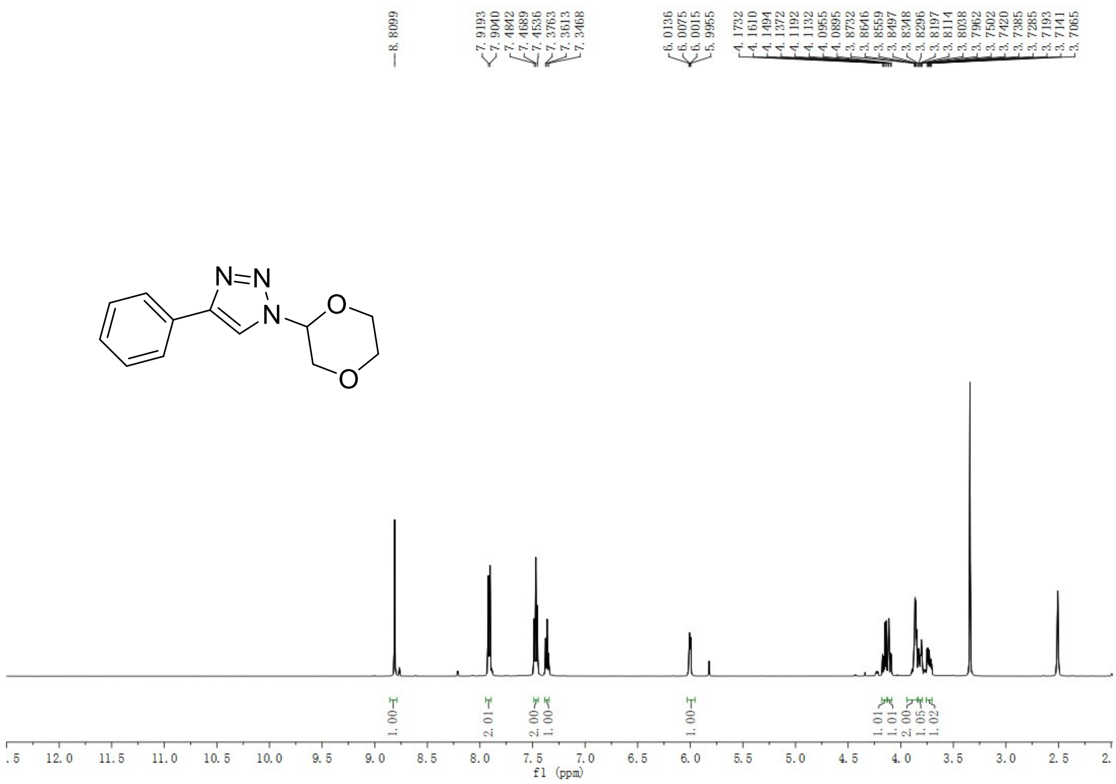
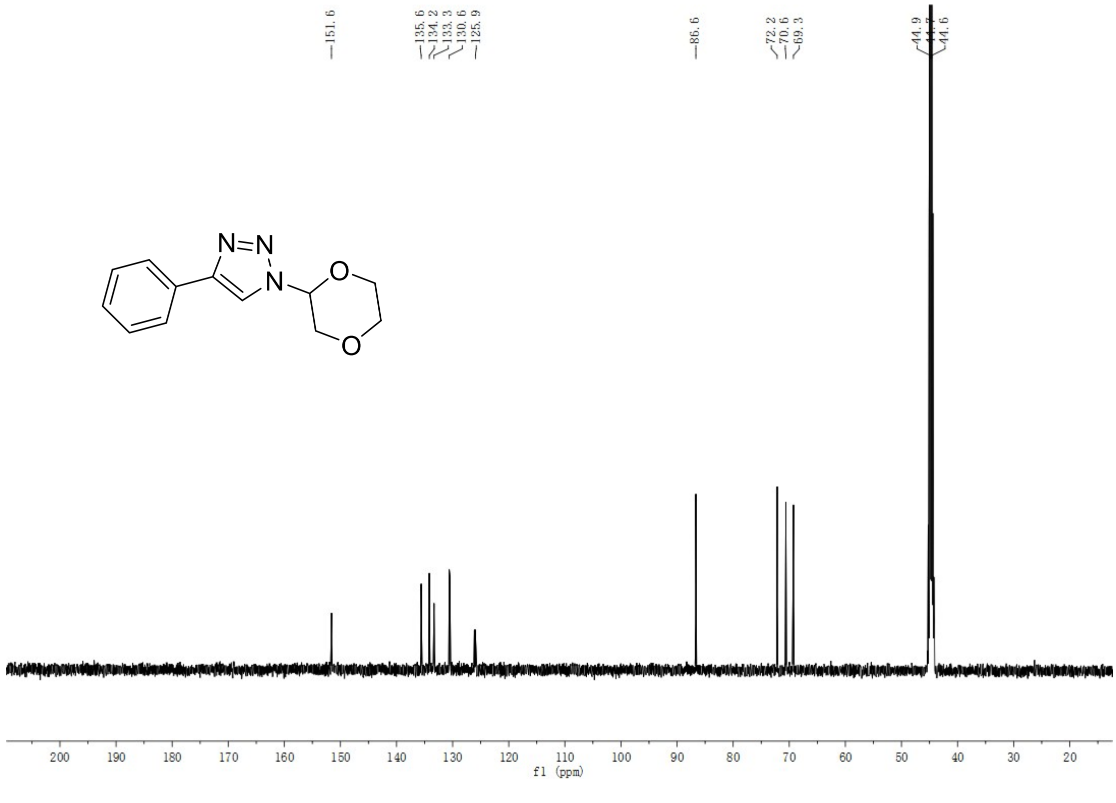
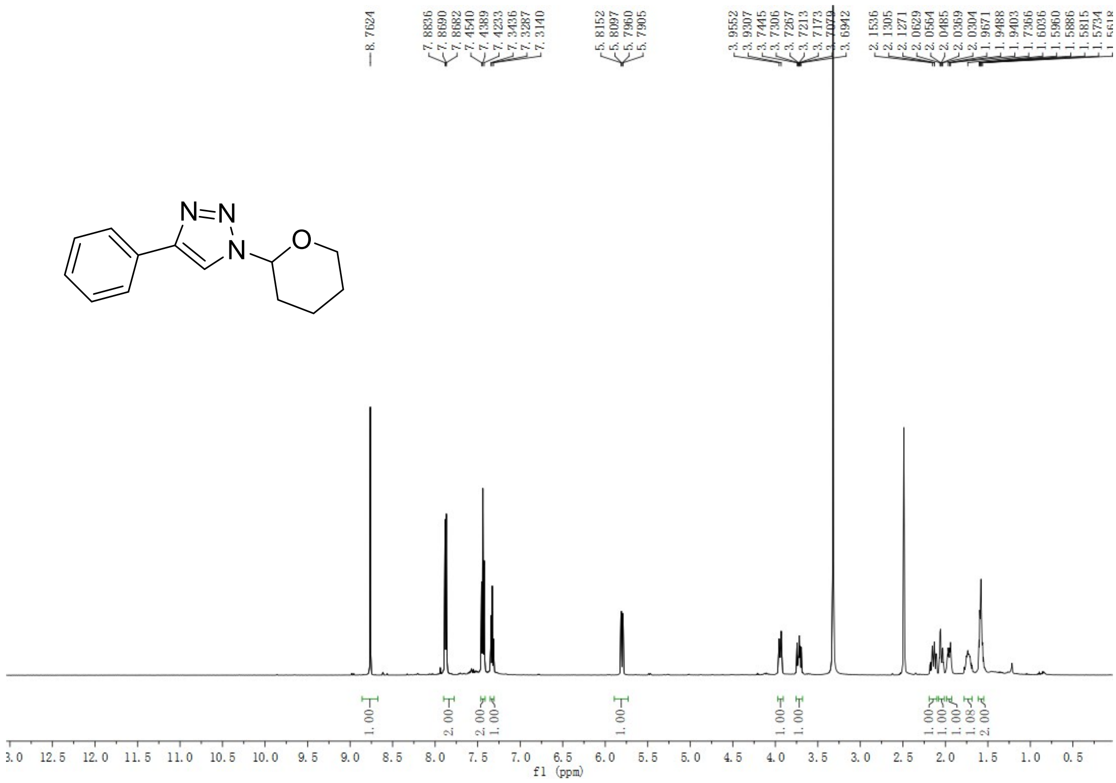
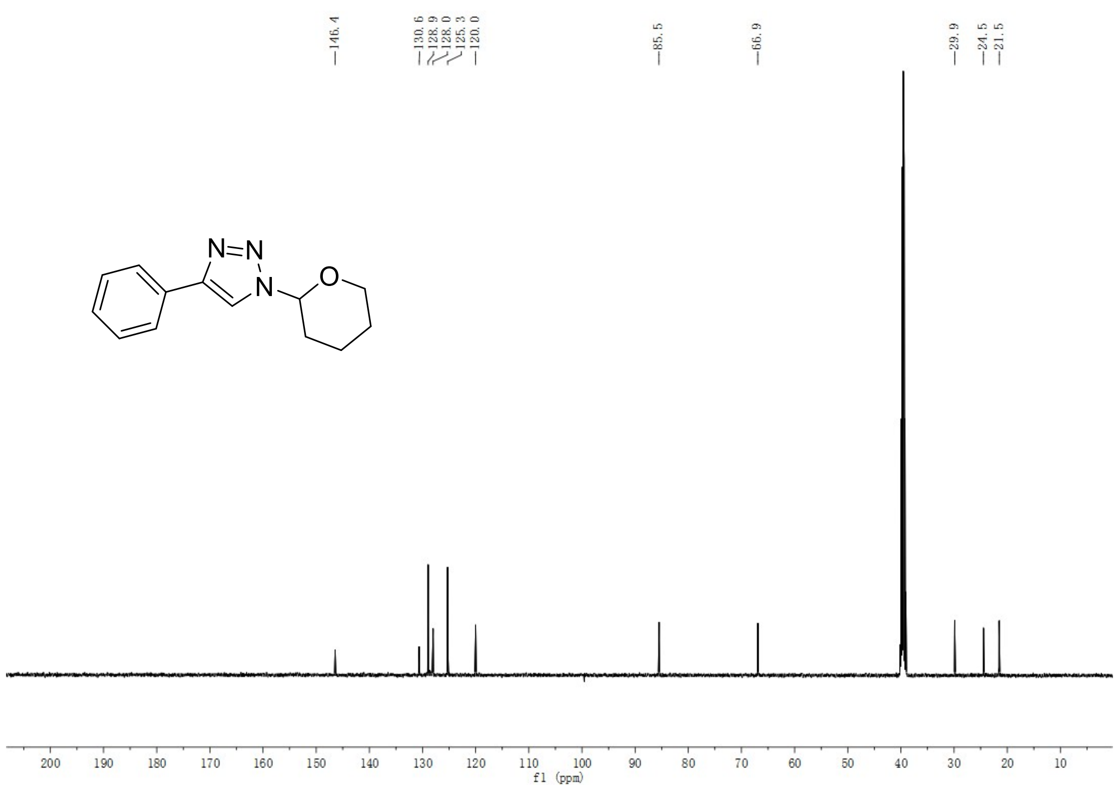
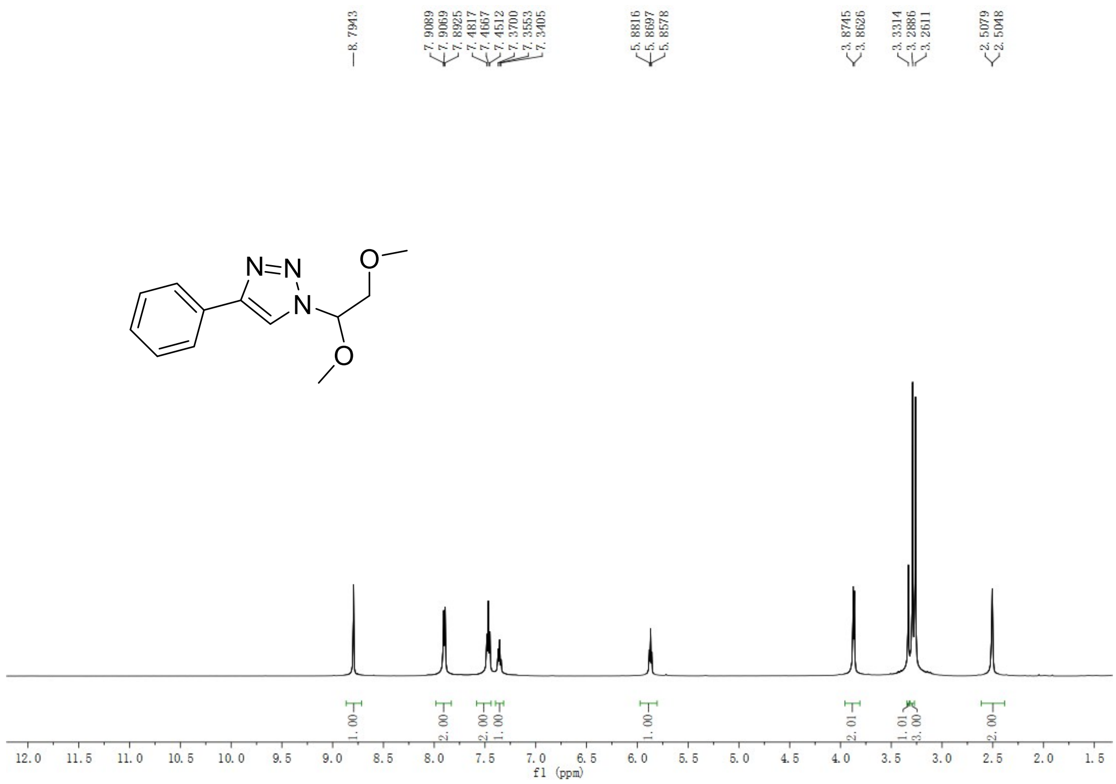
f1 (ppm)

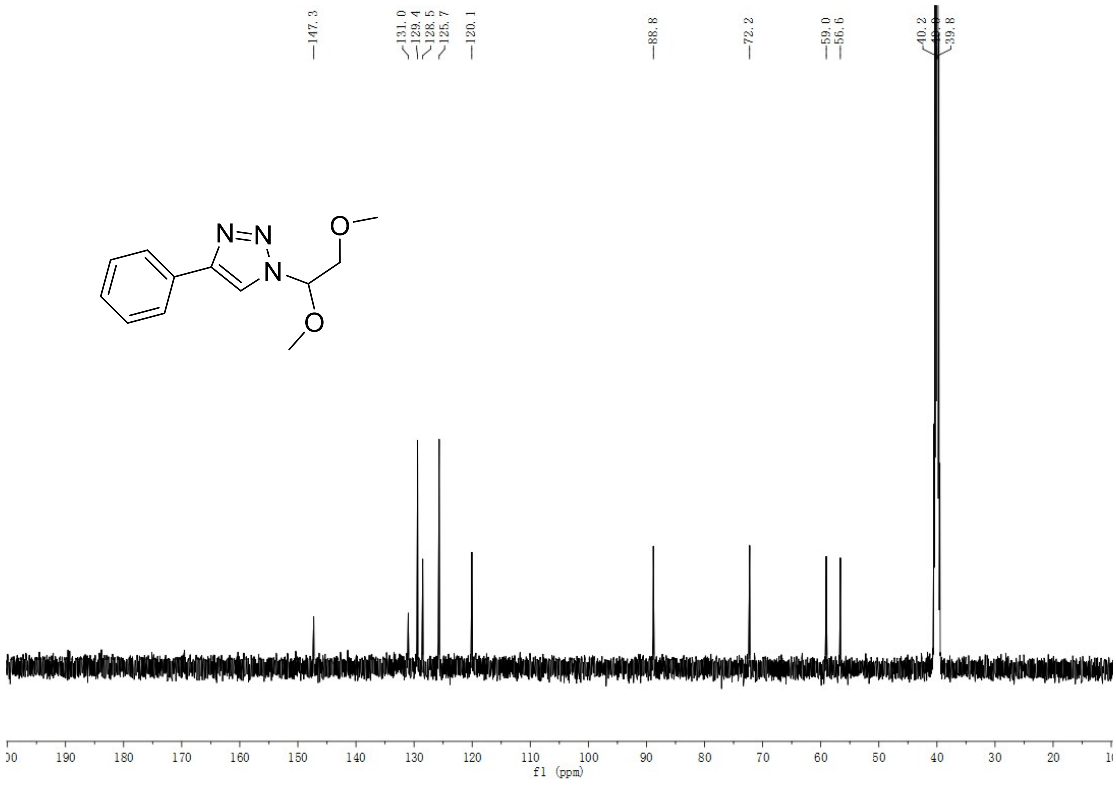


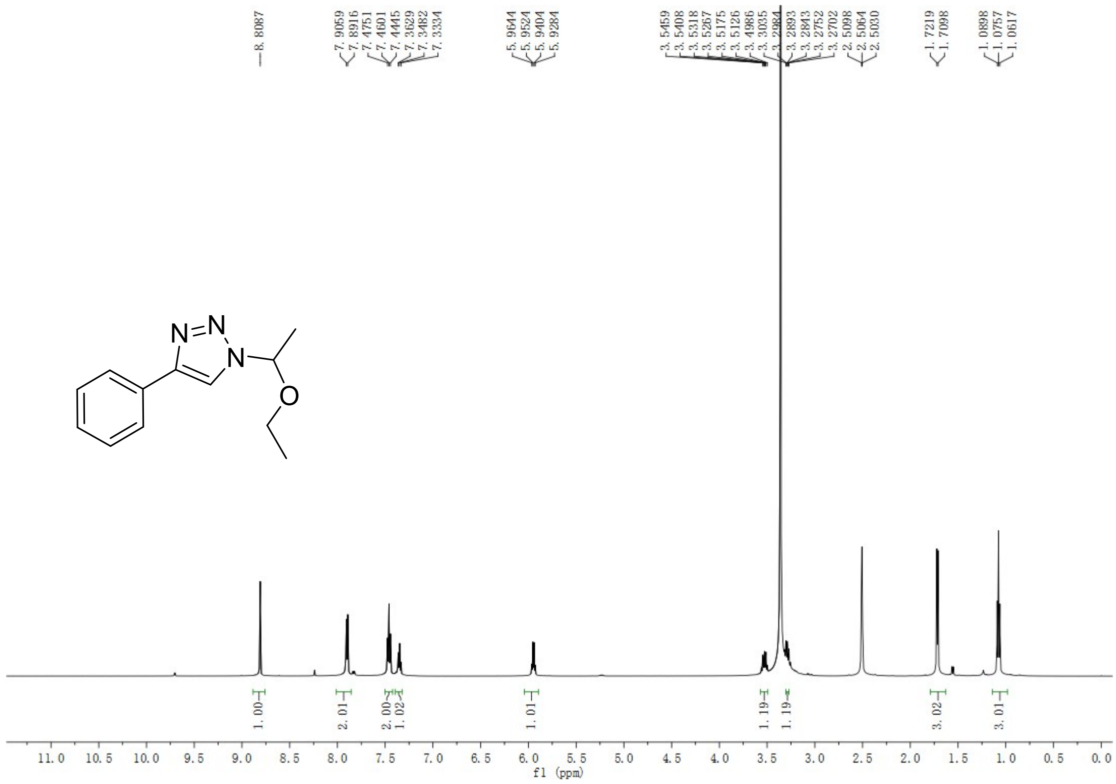








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3.2752
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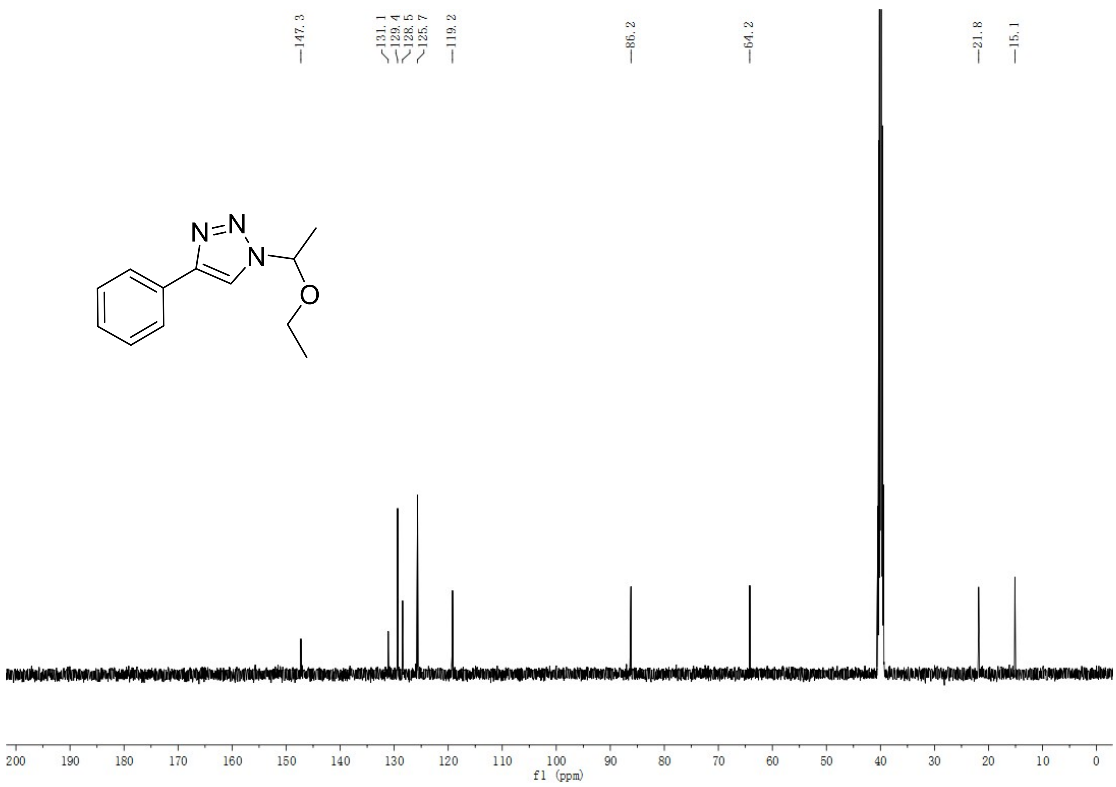
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64.2
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15.1
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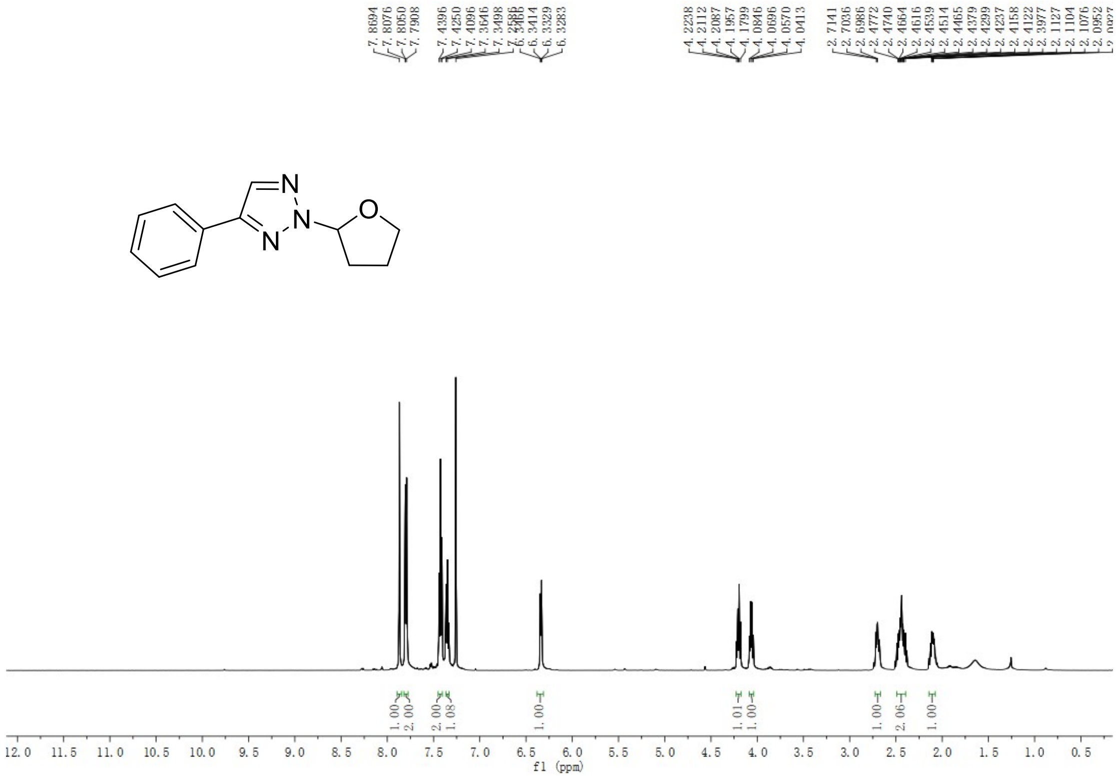
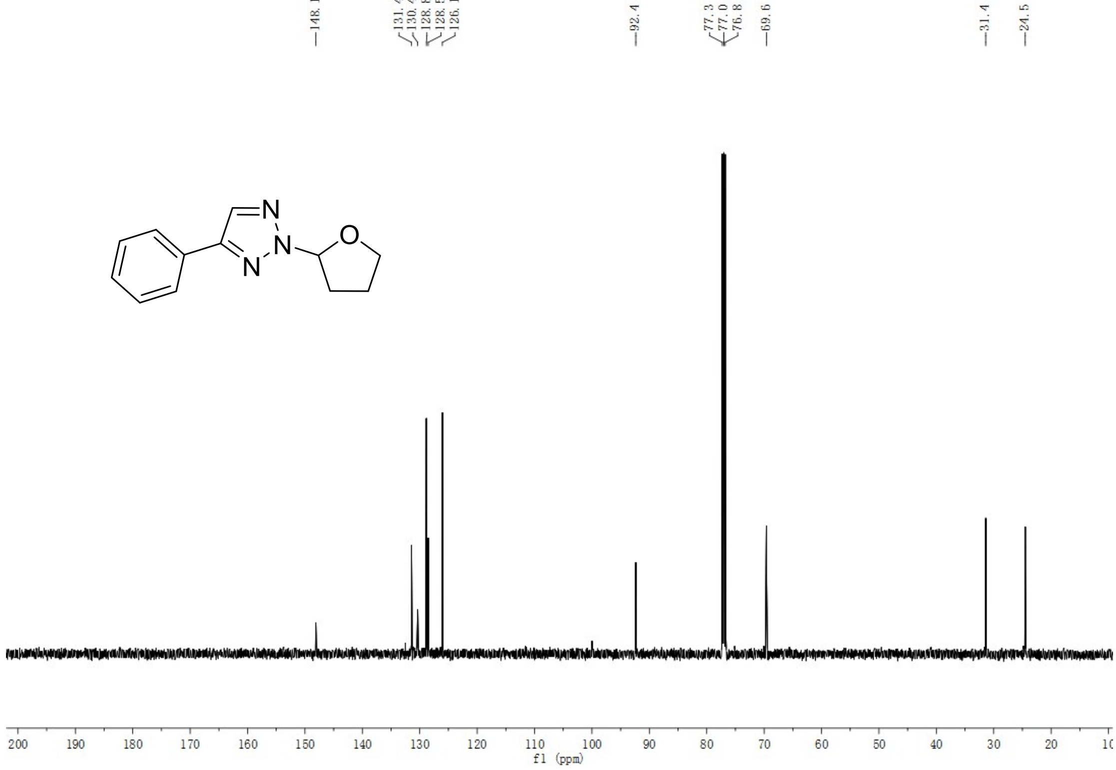
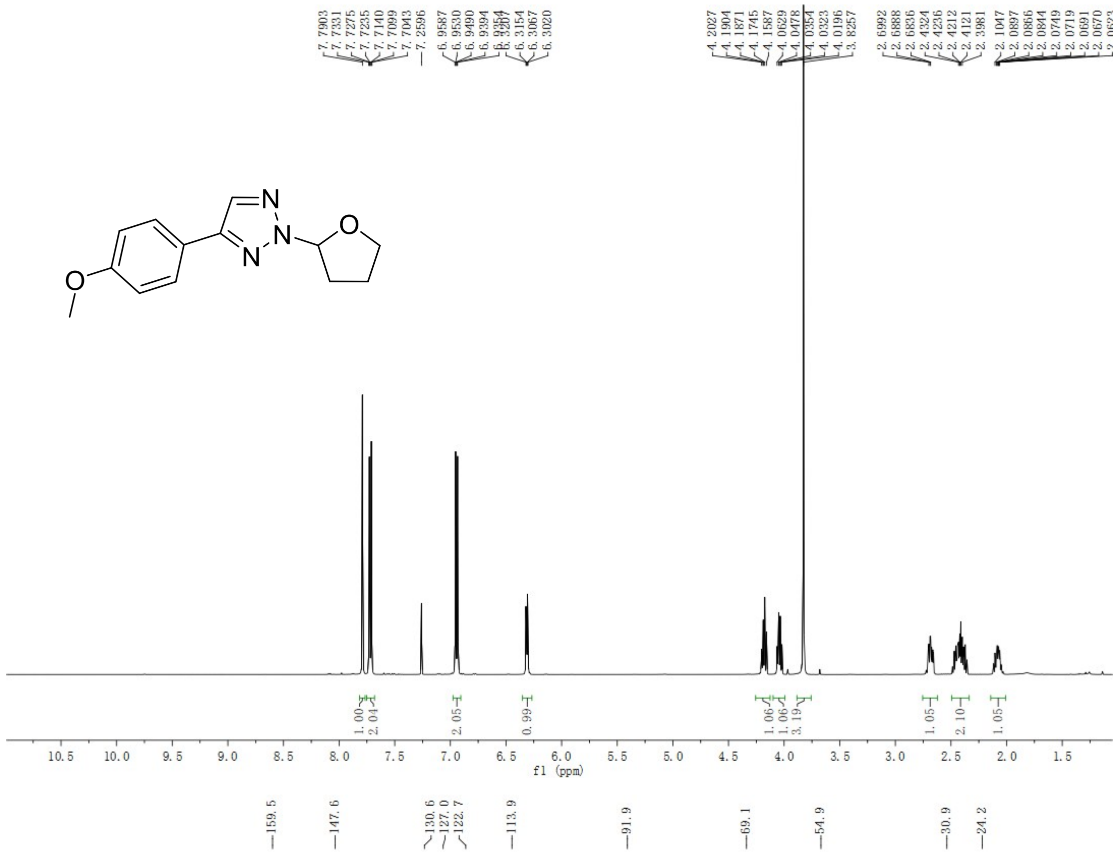
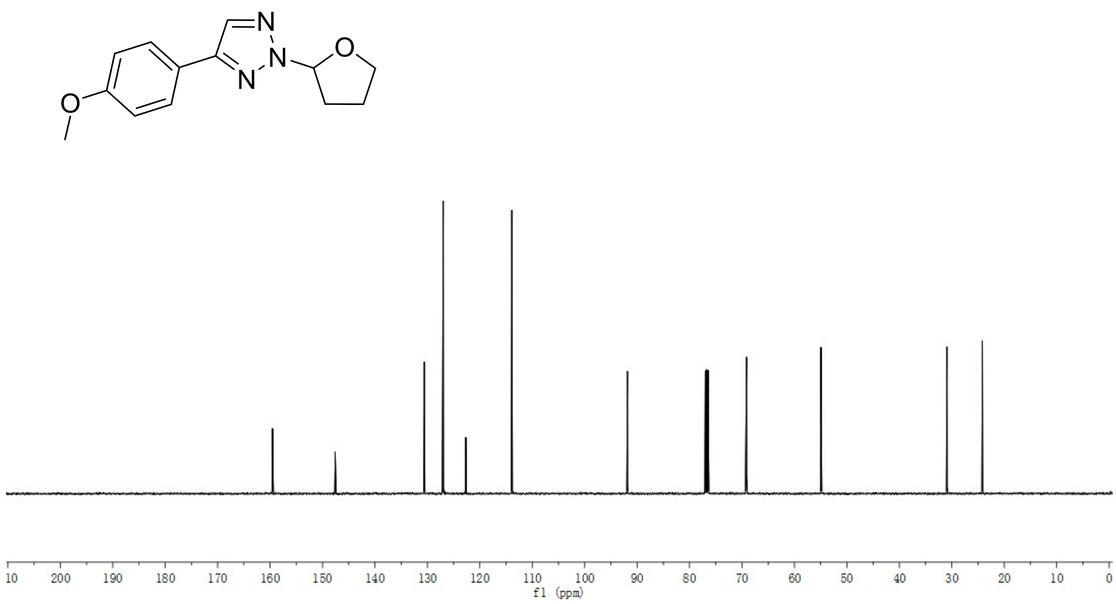
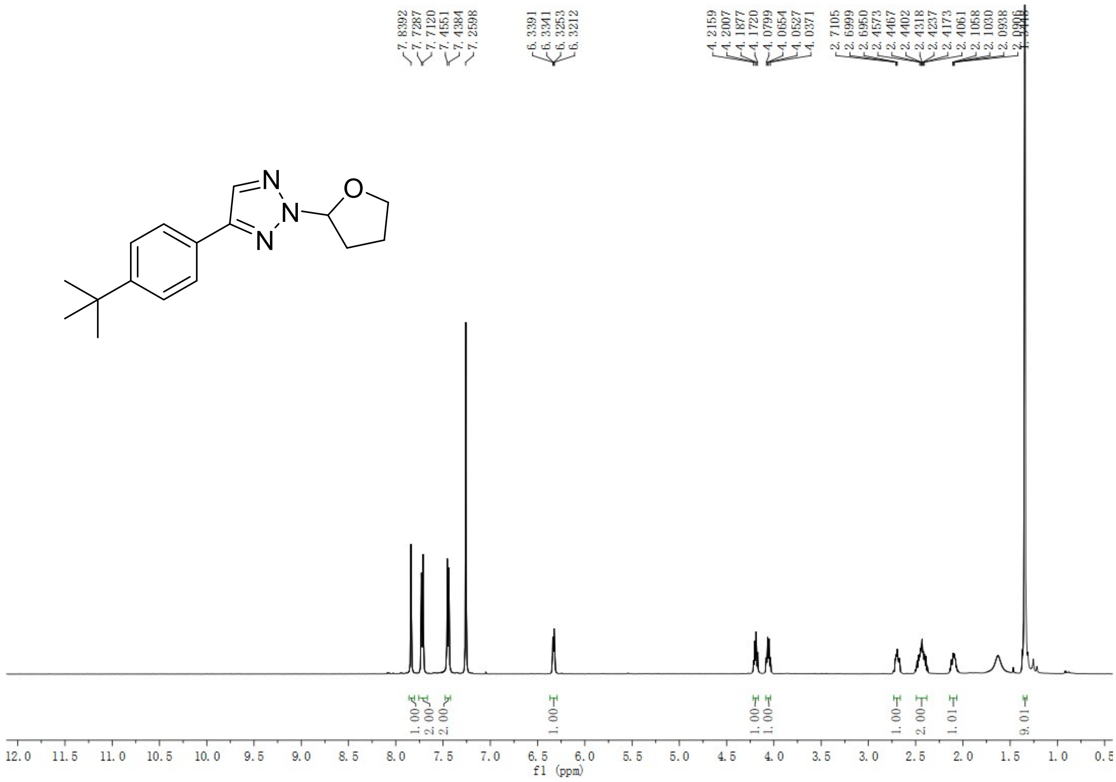
N
O
f1 (ppm)

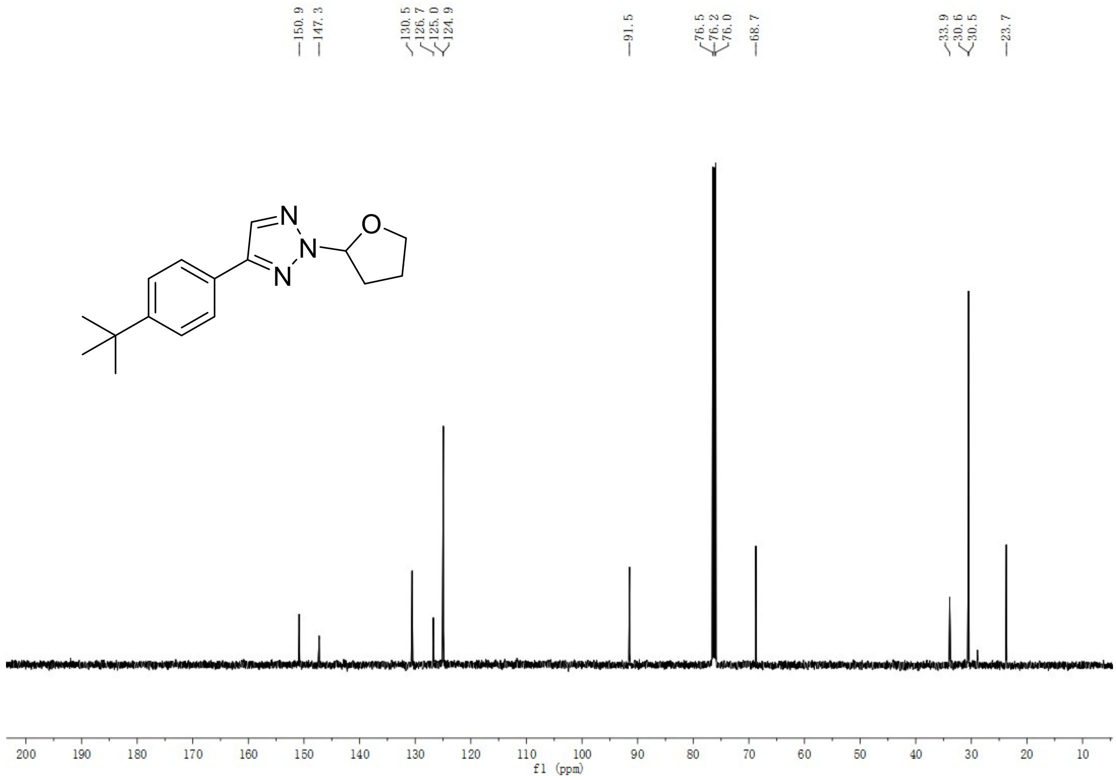


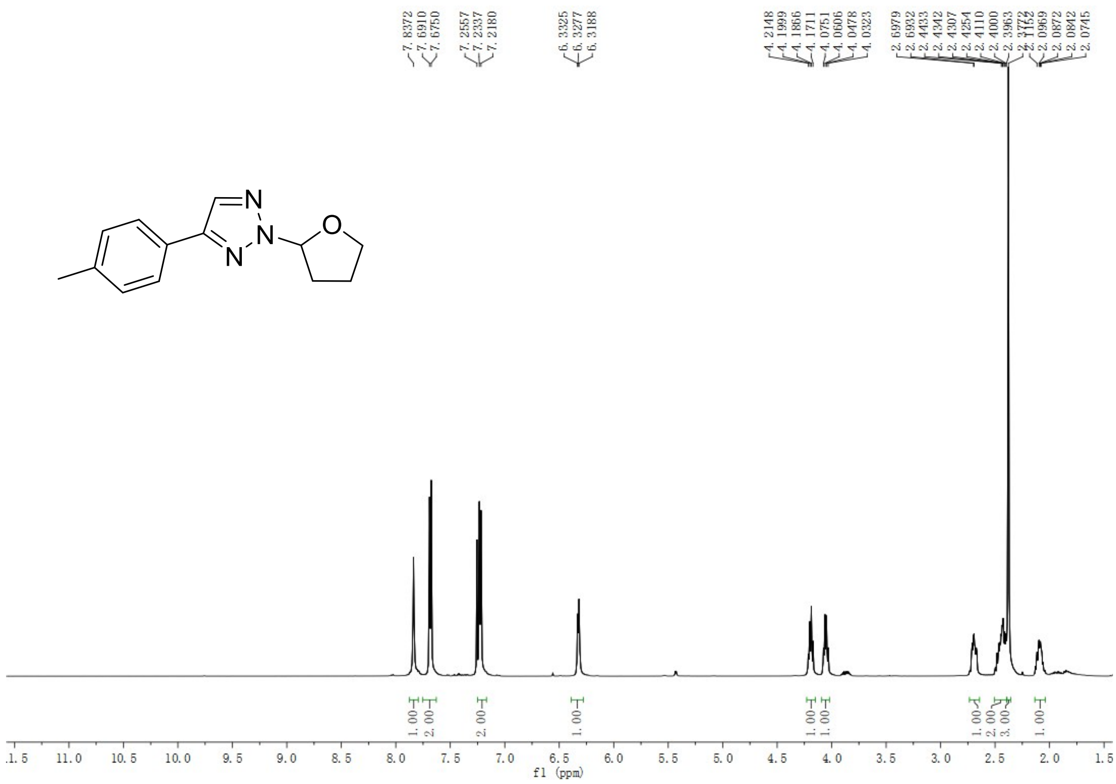








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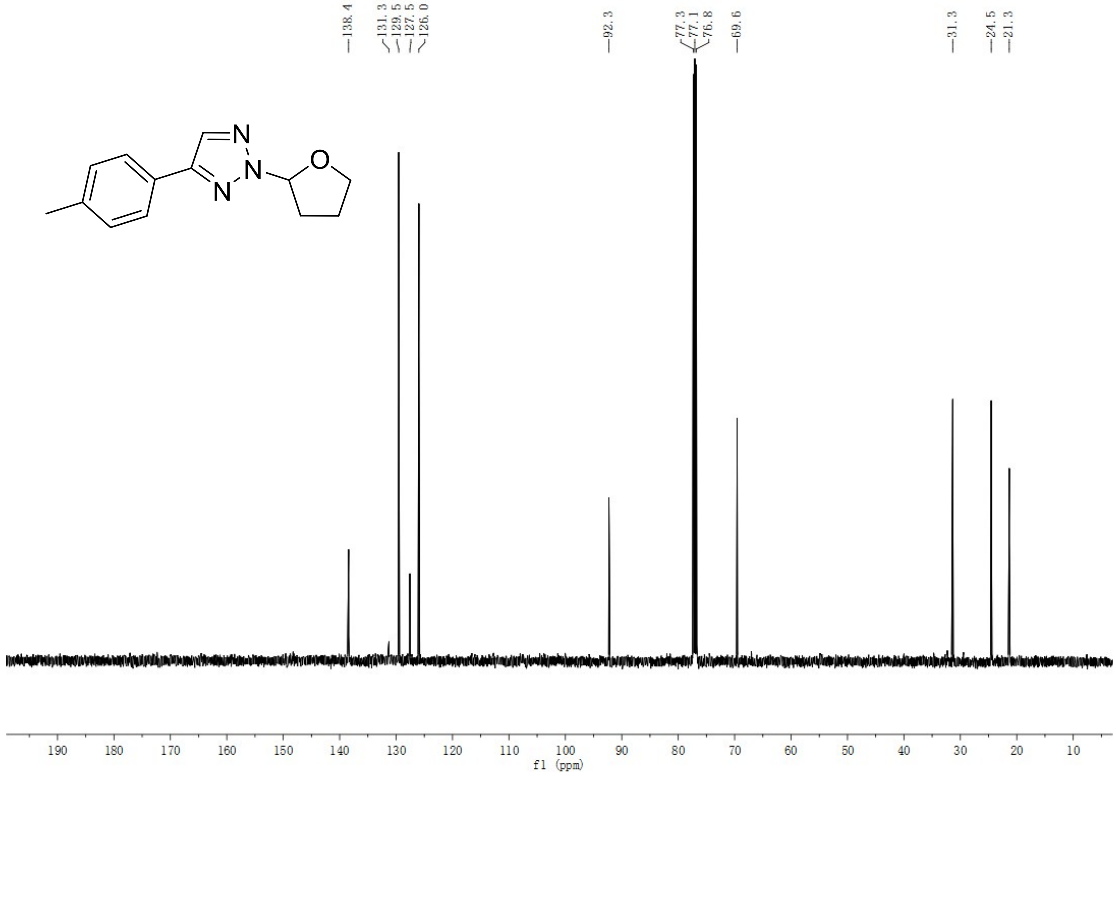
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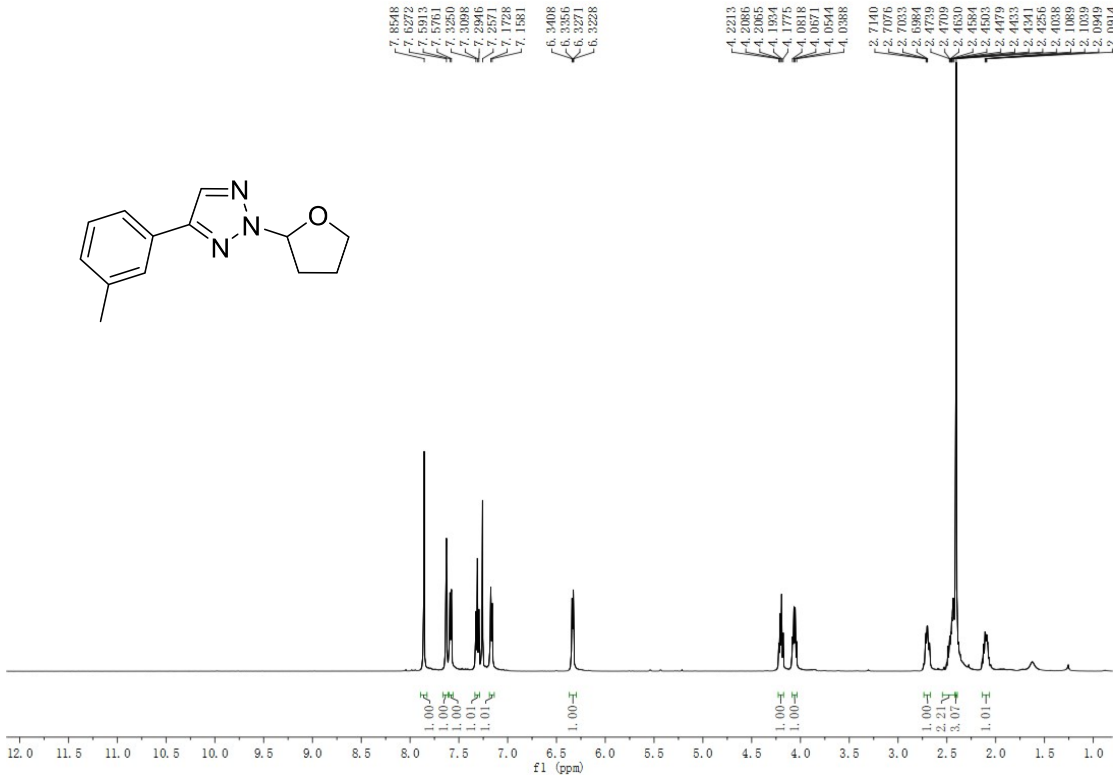
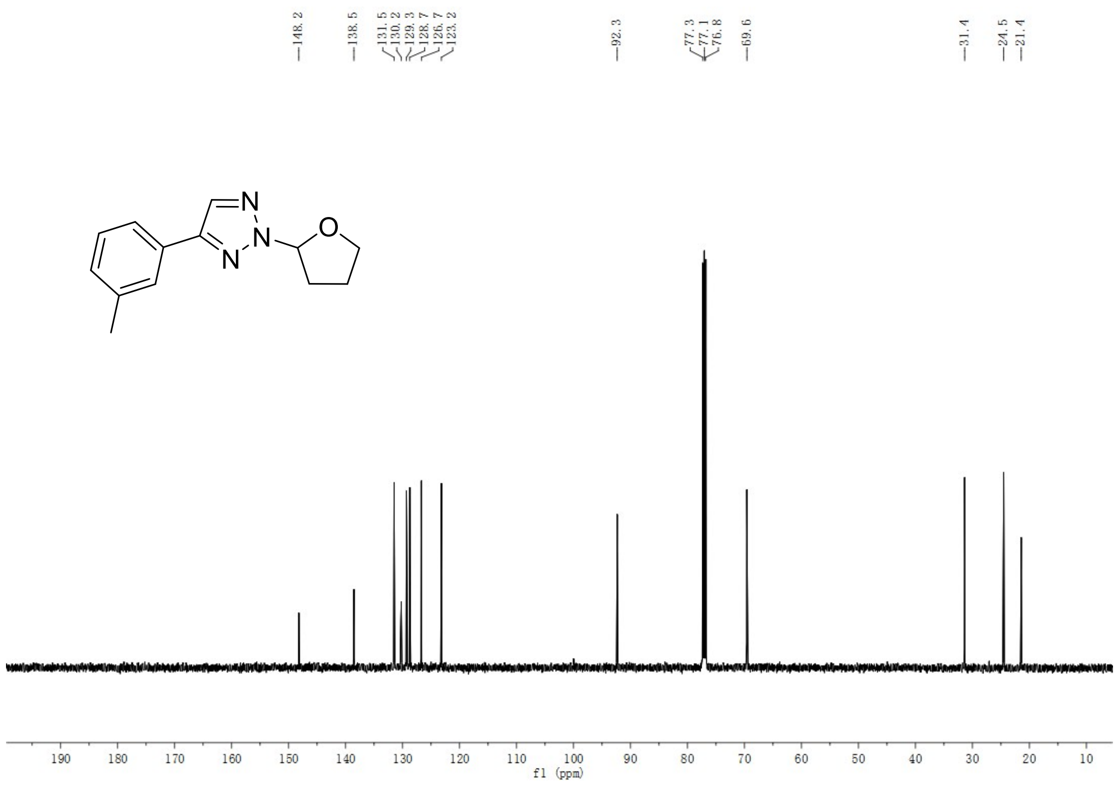
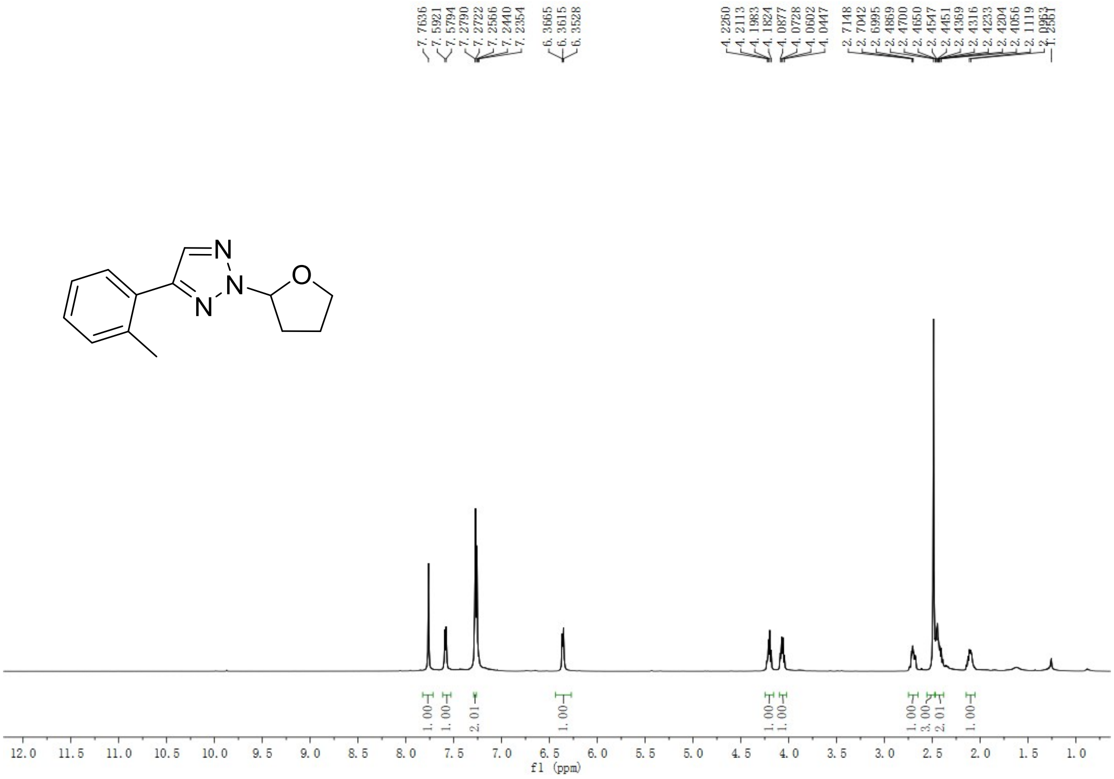
f1 (ppm)



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2.0963
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N
N
O
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1.00
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1.00
1.00
1.00
1.00
3.00
2.01
1.00
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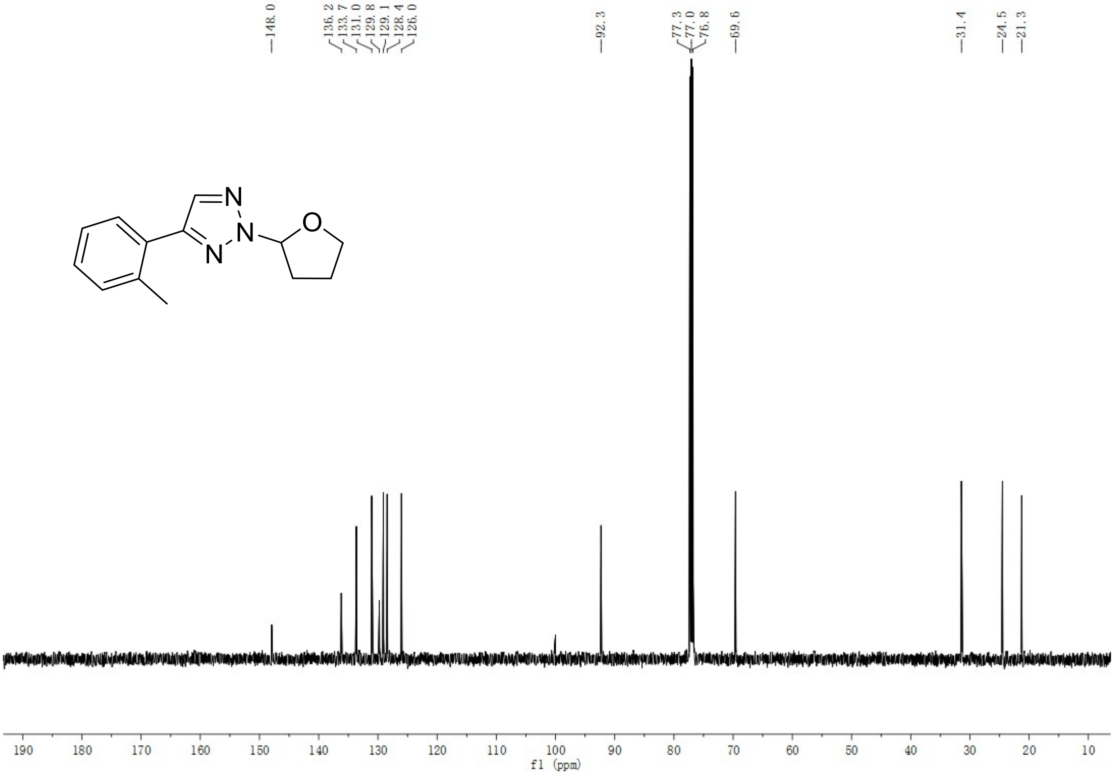
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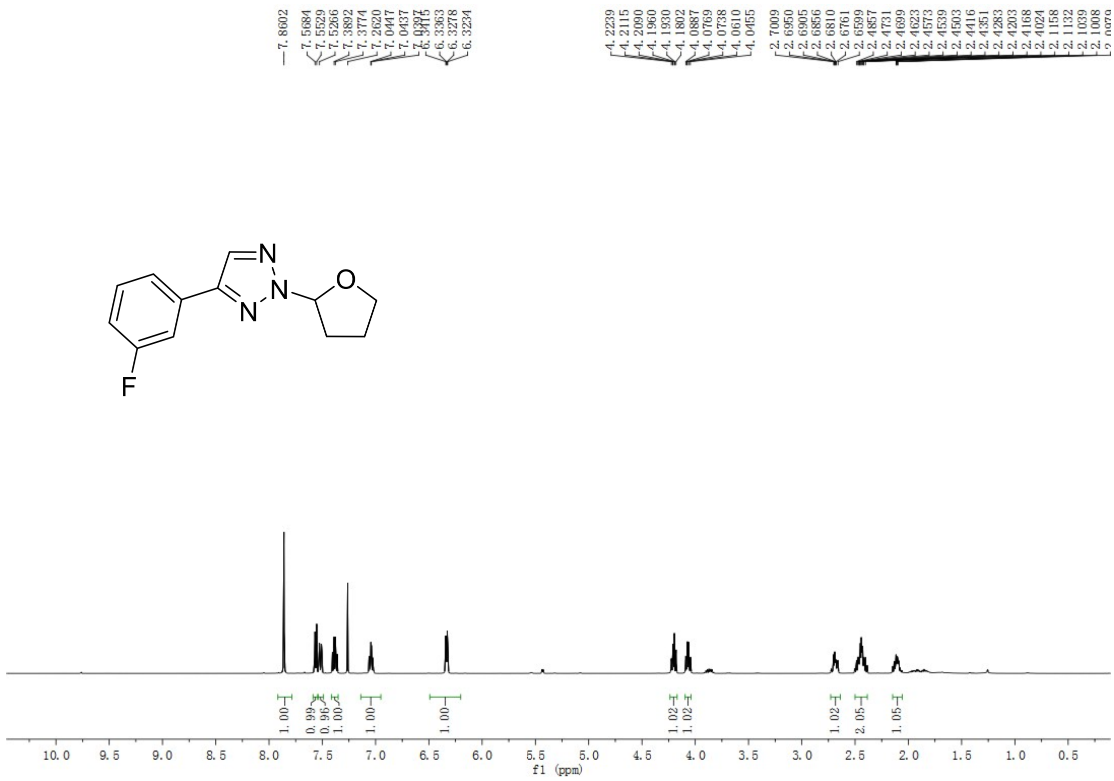
f1 (ppm)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6.3234
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4.1930
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4.0610
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2.4539
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2.1039
2.1008
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N
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1.02
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1.05
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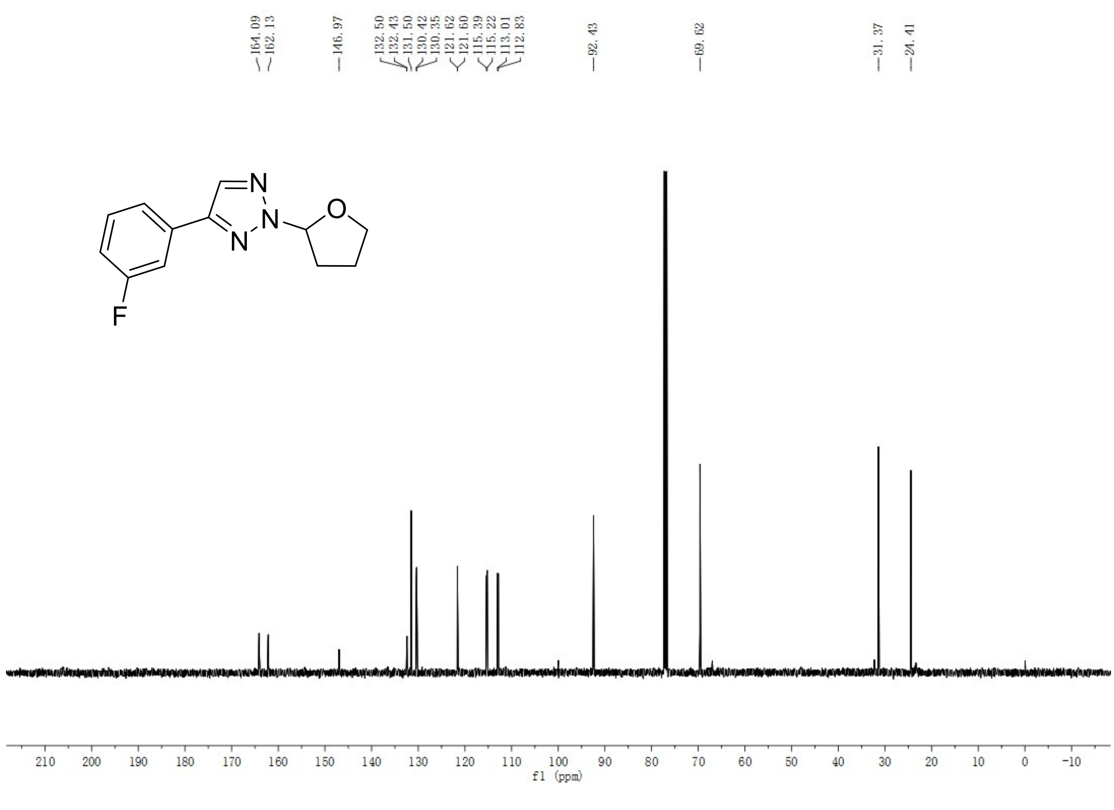
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121.60
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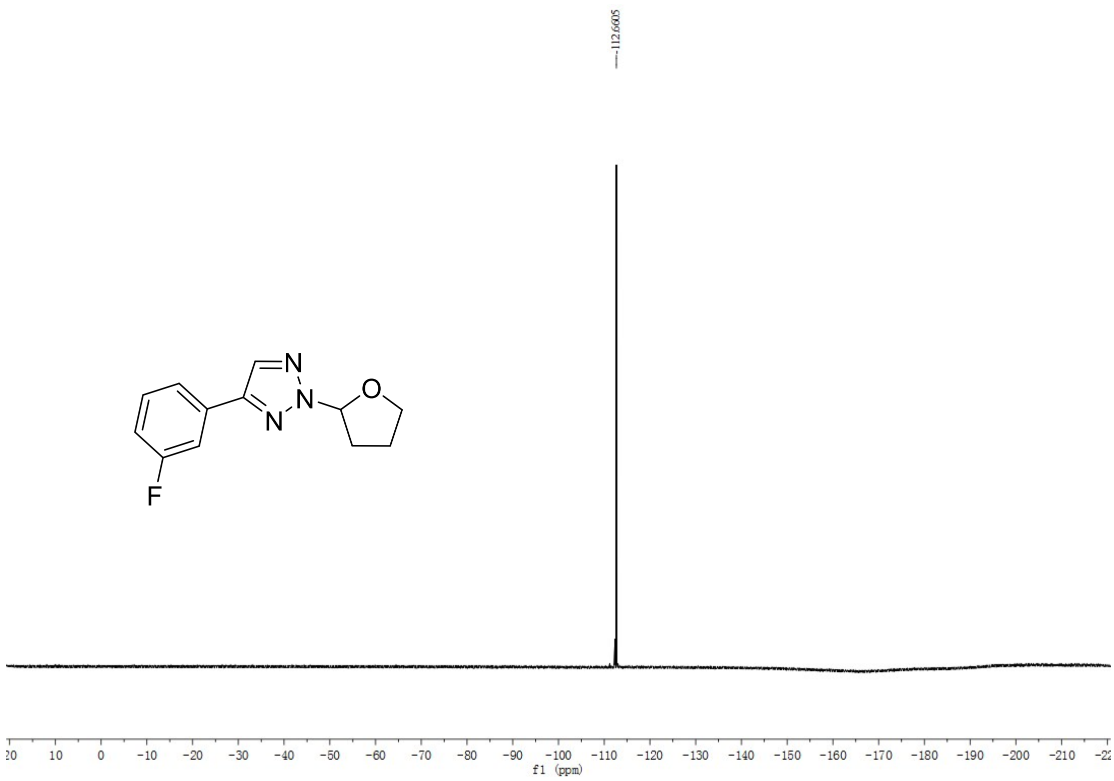
N
N
O
F
f1 (ppm)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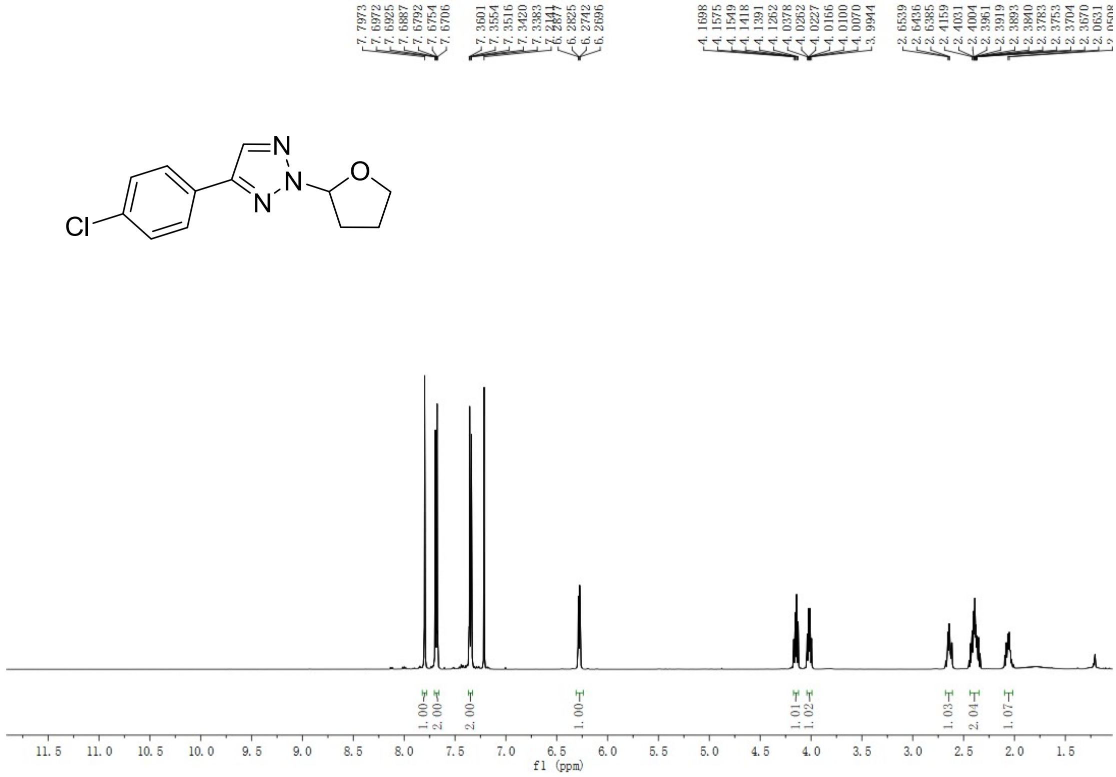
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6.2742
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4.1575
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4.0100
4.0070
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2.4031
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2.3753
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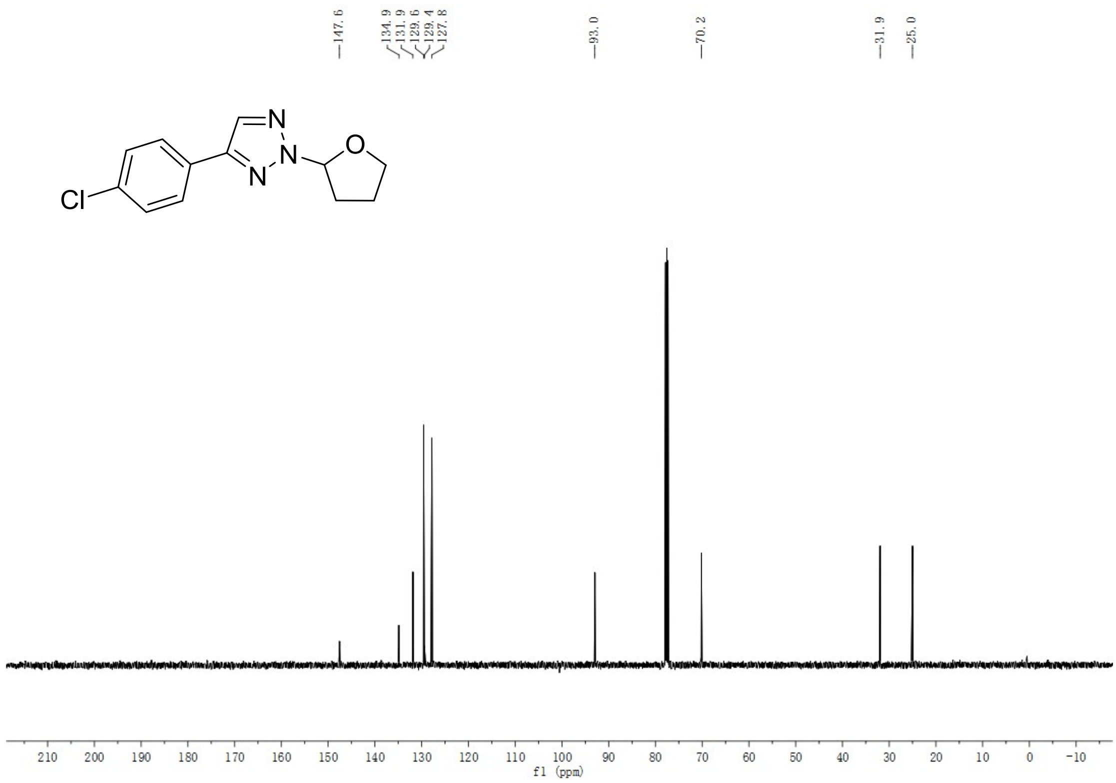
2.0631
f1 (ppm)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127.8
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70.2
31.9
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Cl
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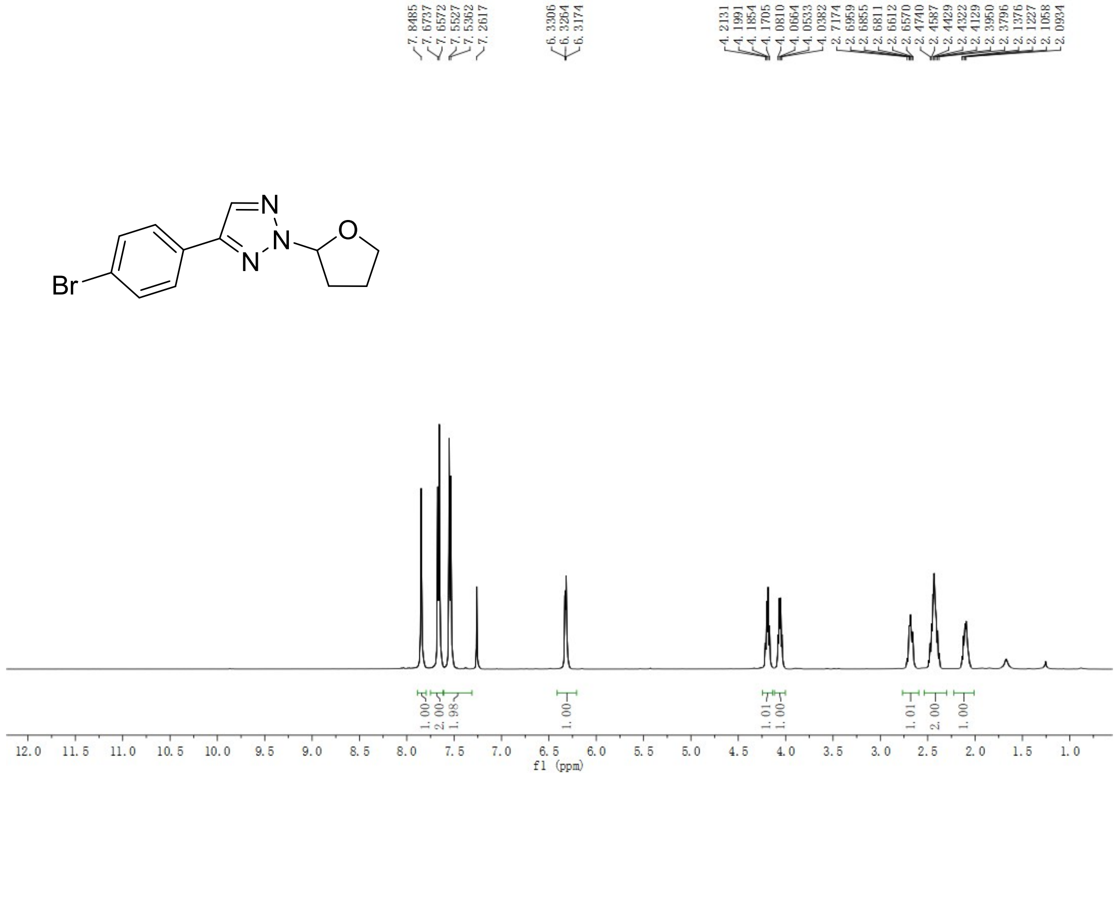
N
N
O
f1 (ppm)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2.6612
2.6570
2.4740
2.4587
2.4429
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2.3950
2.3796
2.1376
2.1227
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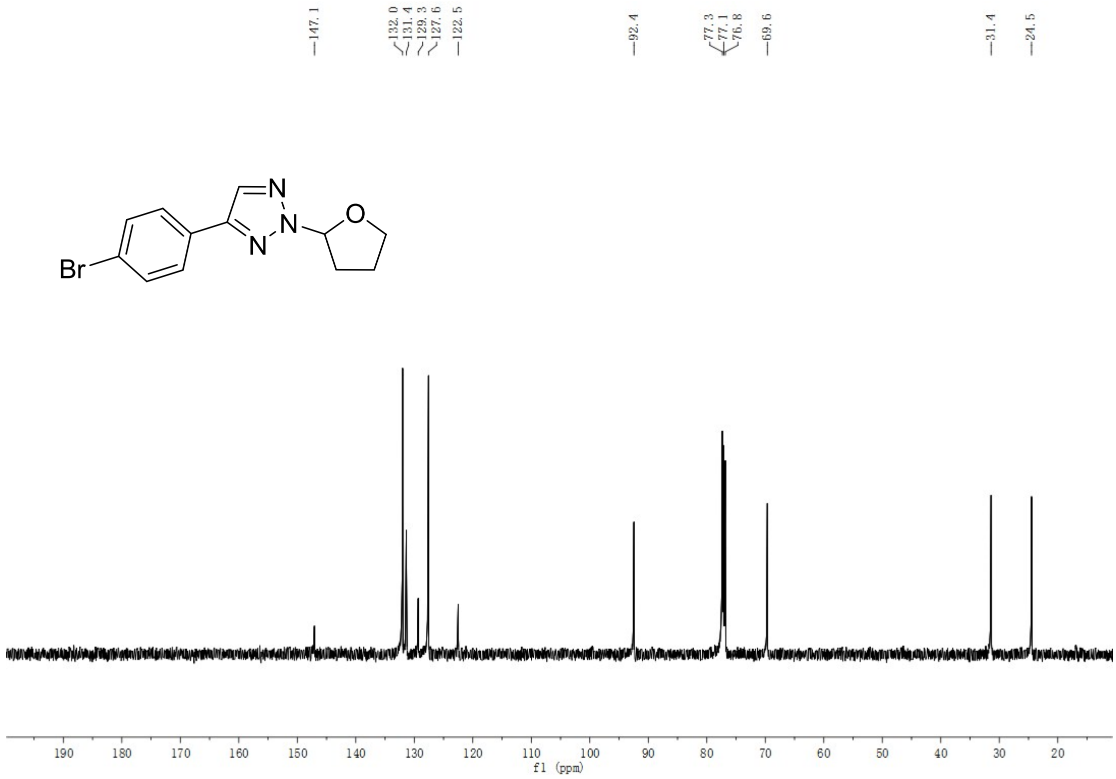
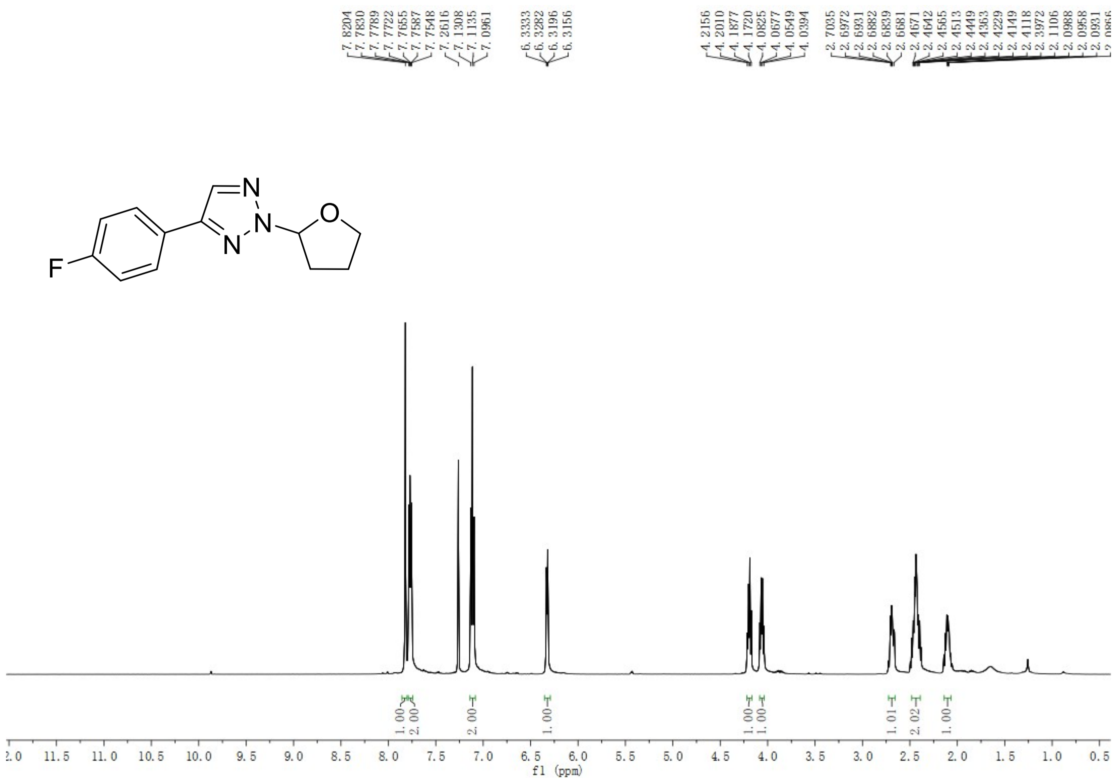
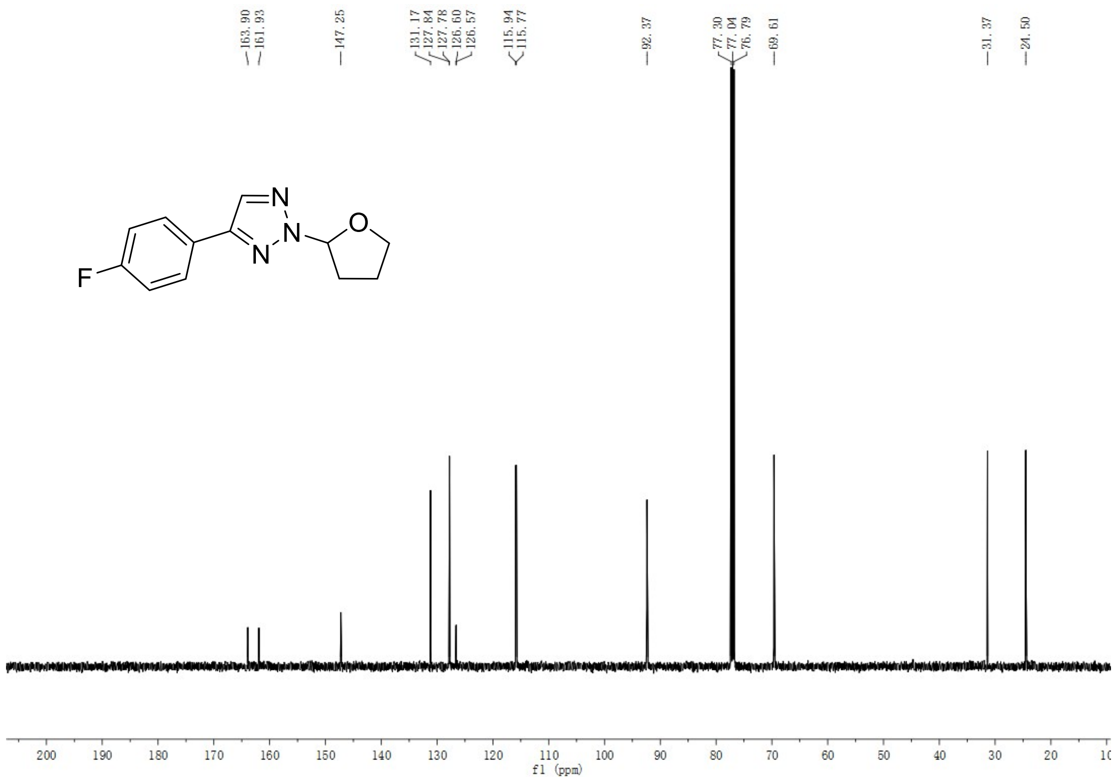
1.00
f1 (ppm)



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92.37
77.30
77.04
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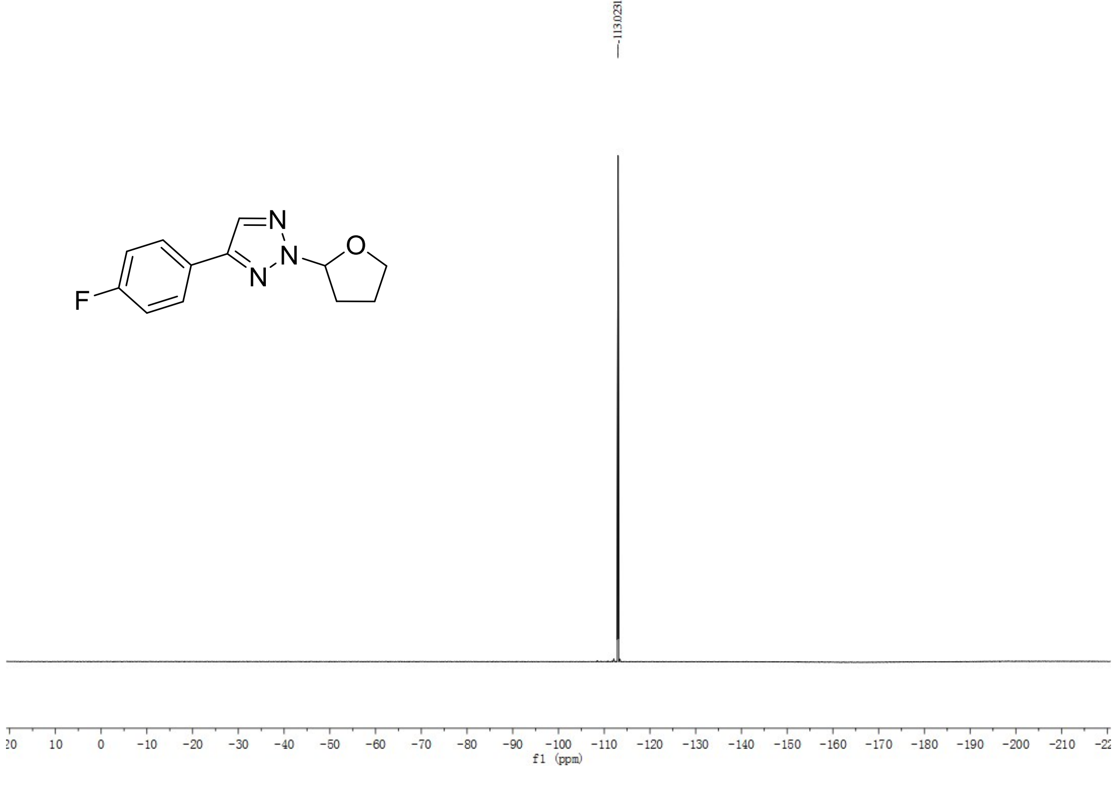
69.61
31.37
24.50
f1 (ppm)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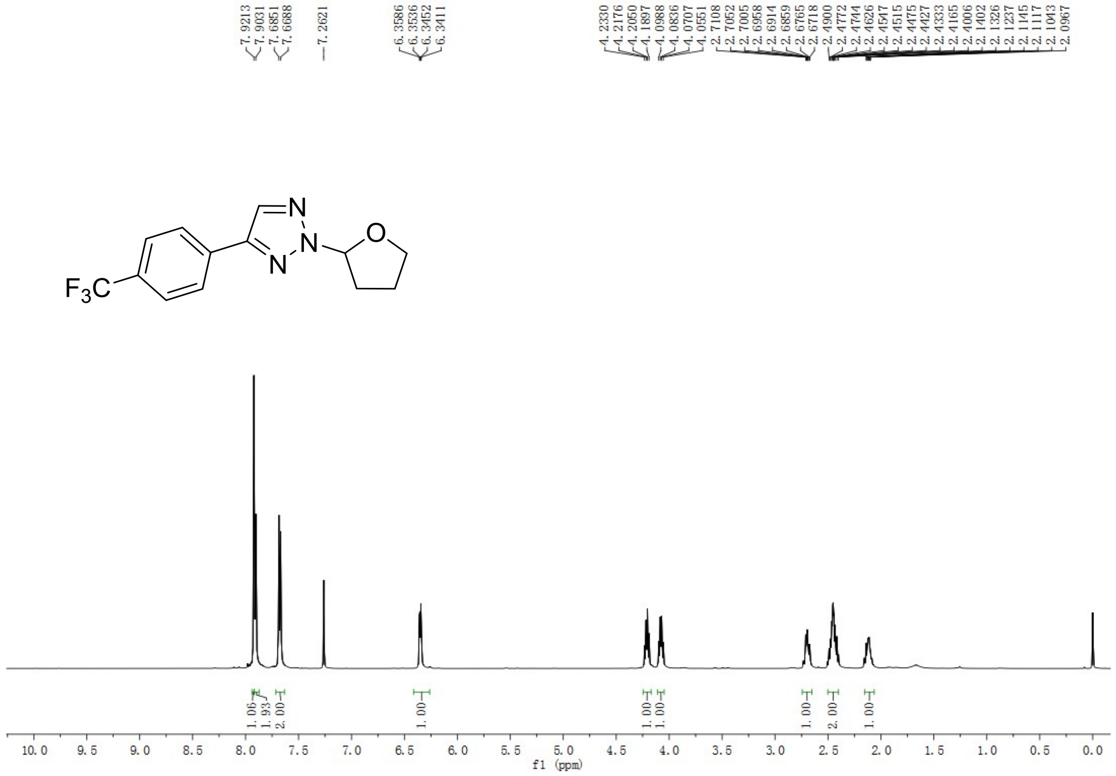

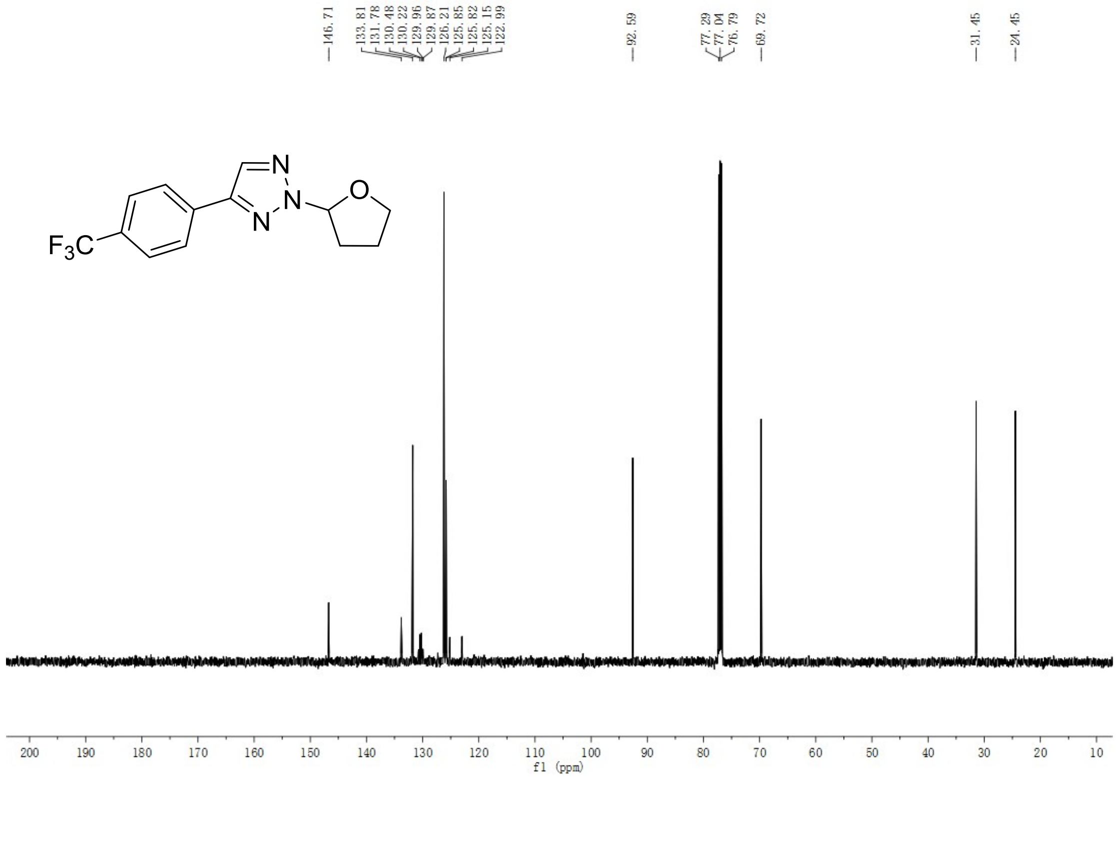

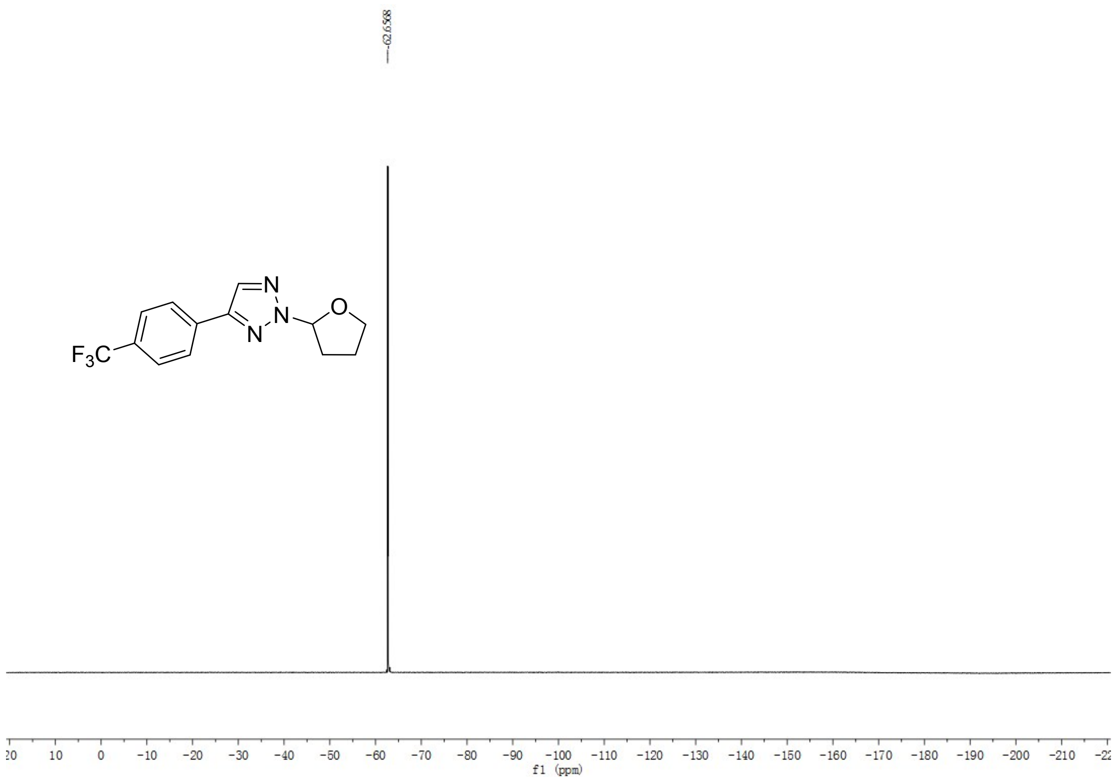

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−180
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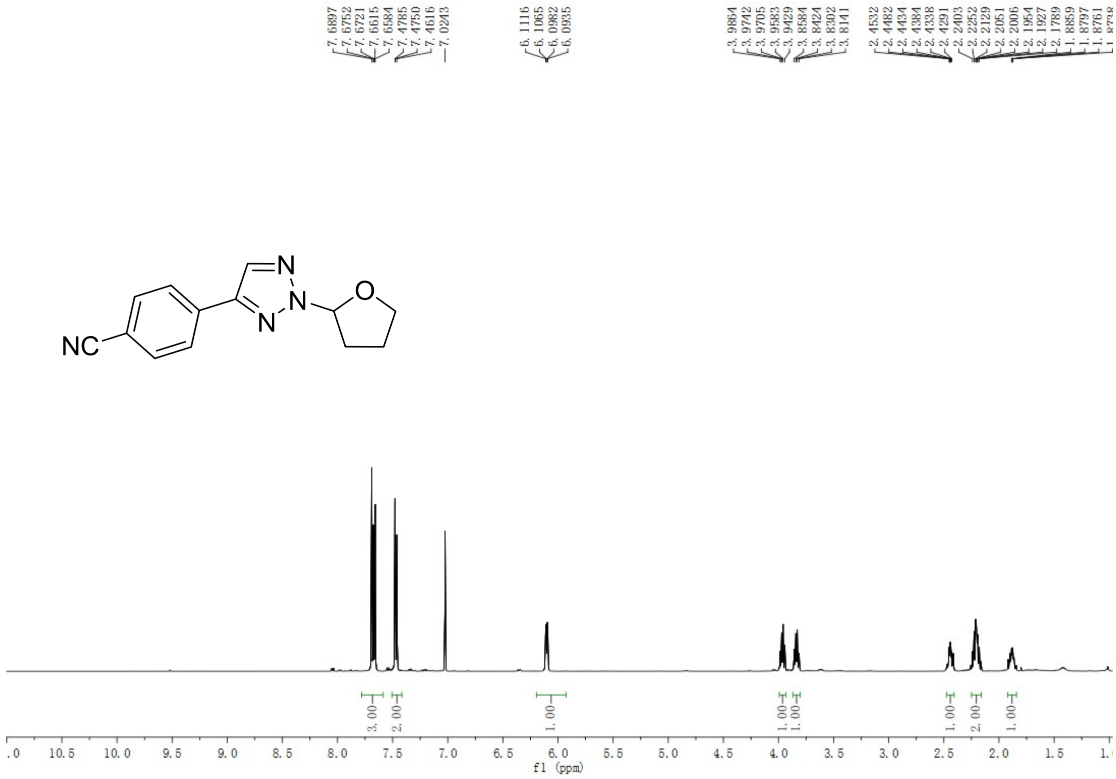
−210
f1 (ppm)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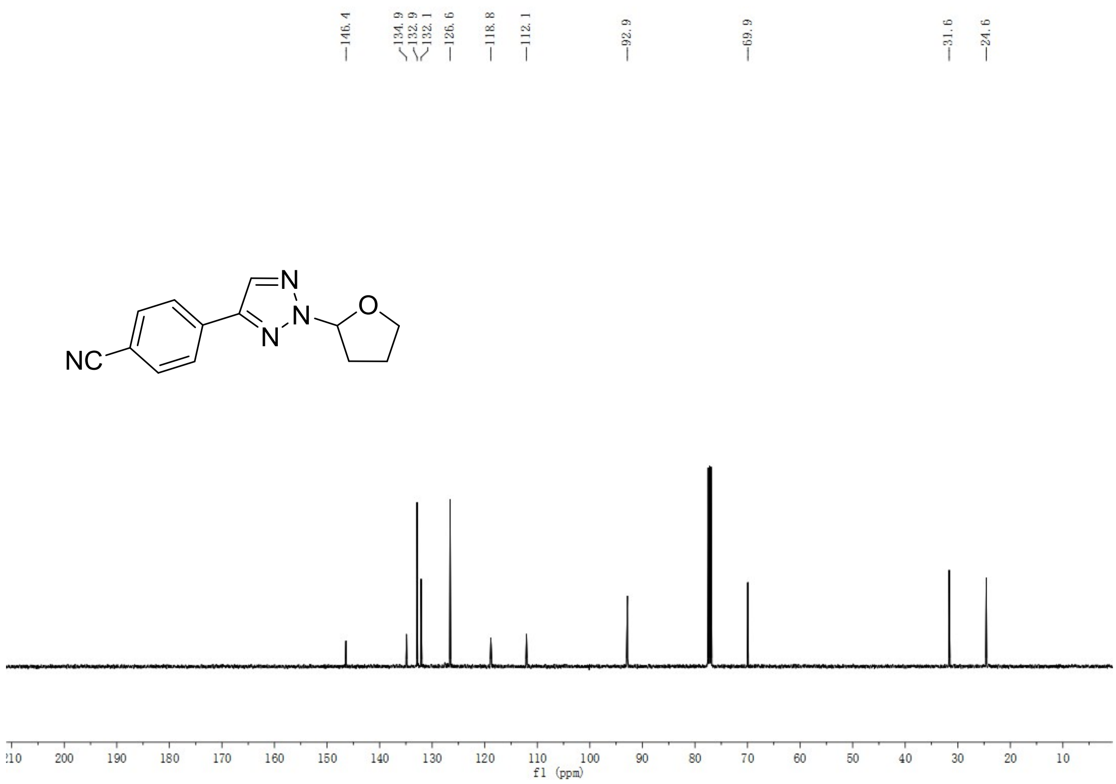
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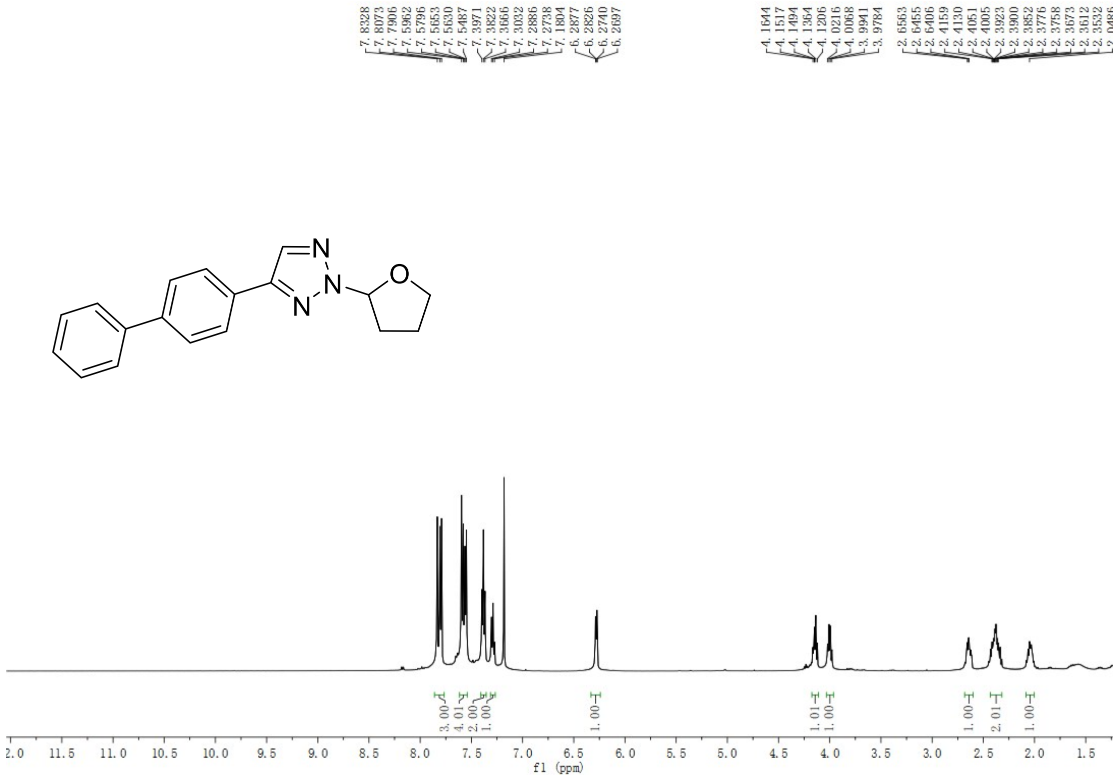
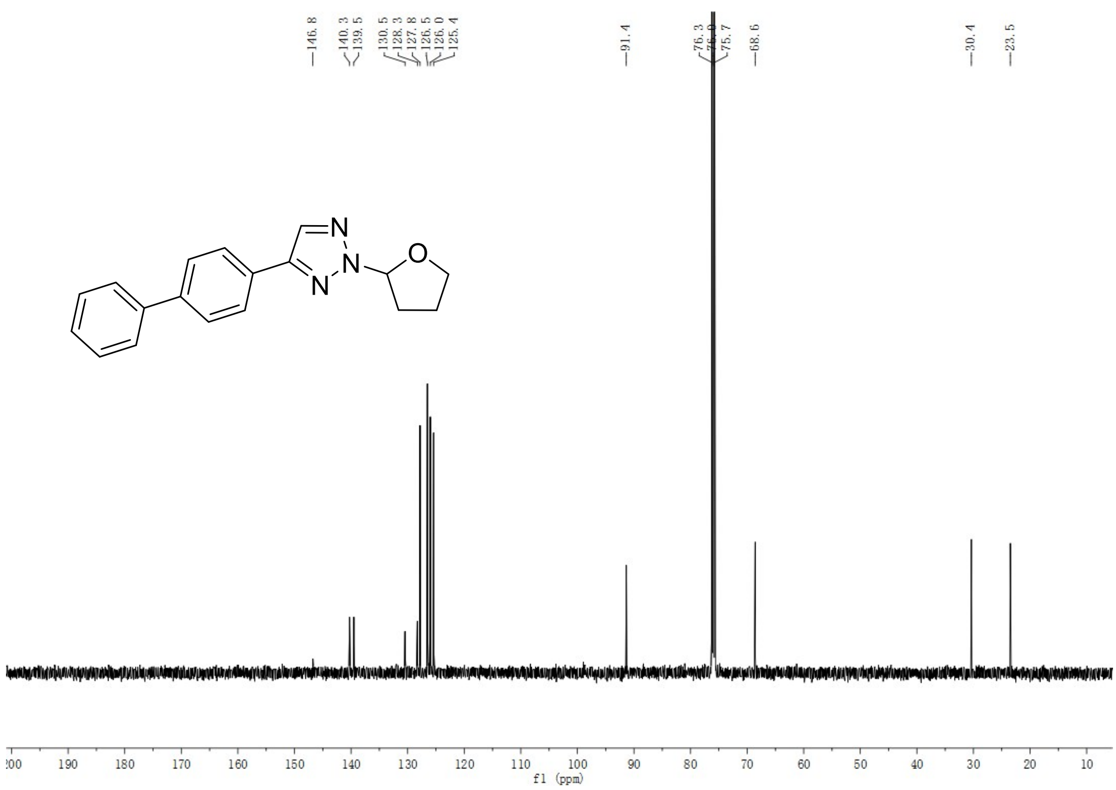
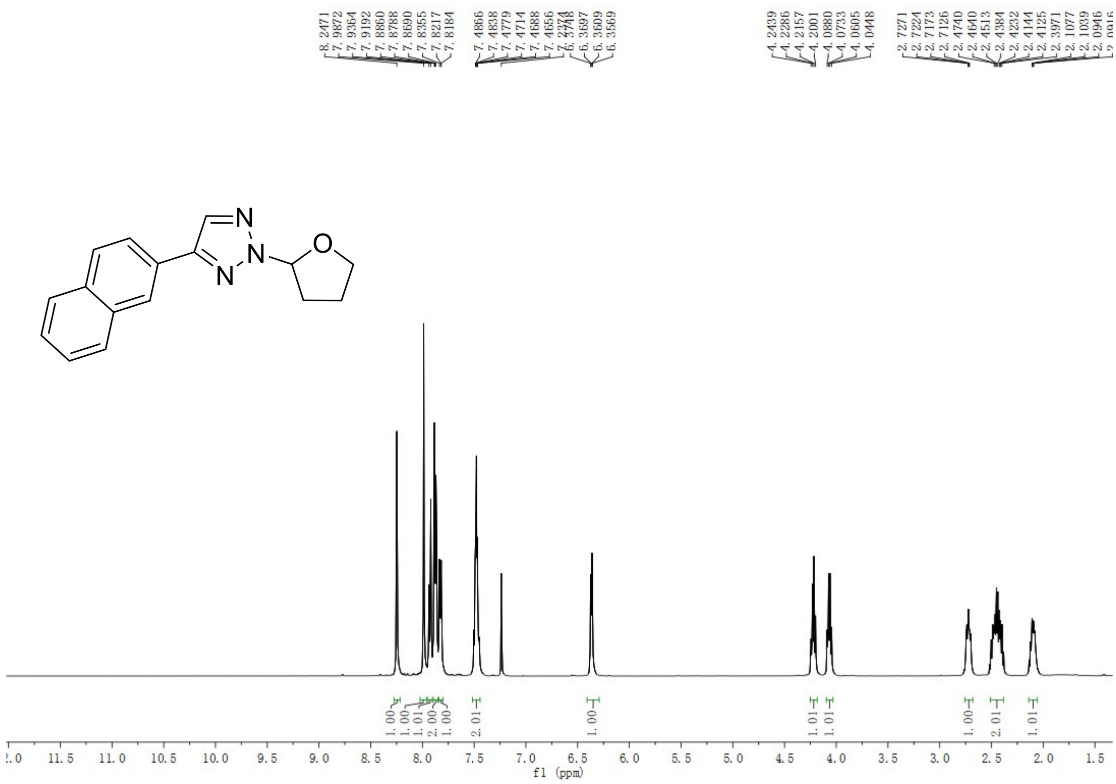
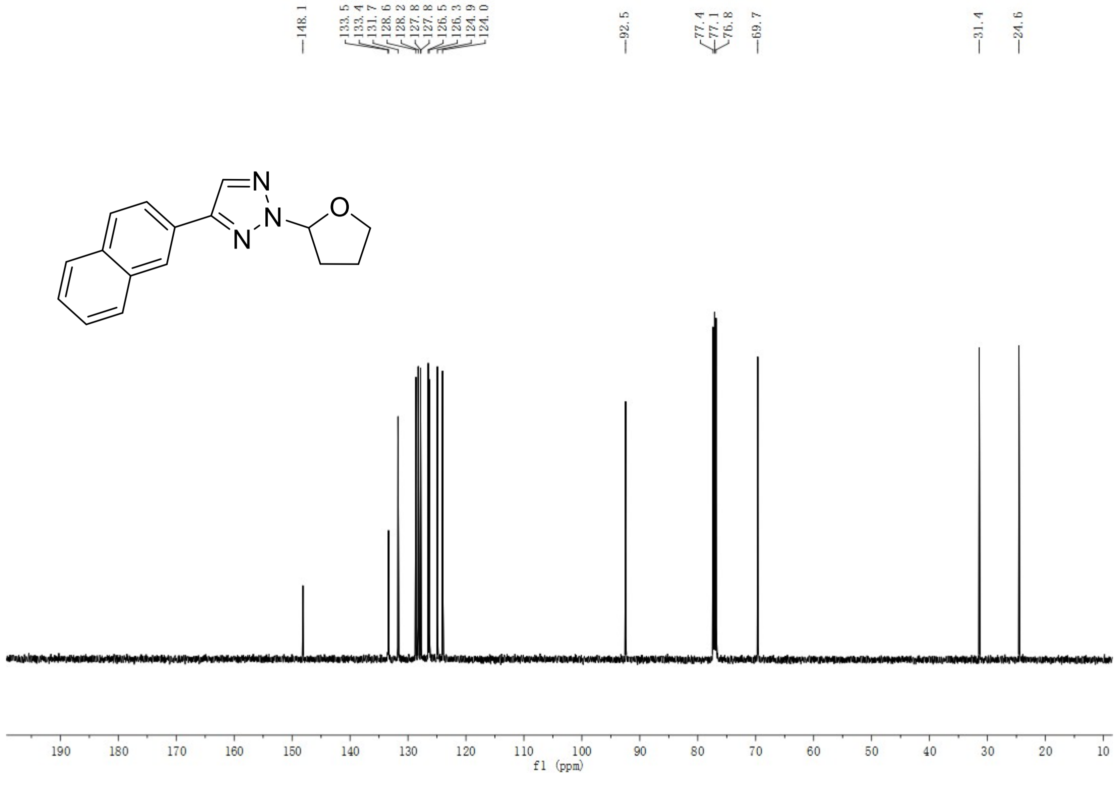
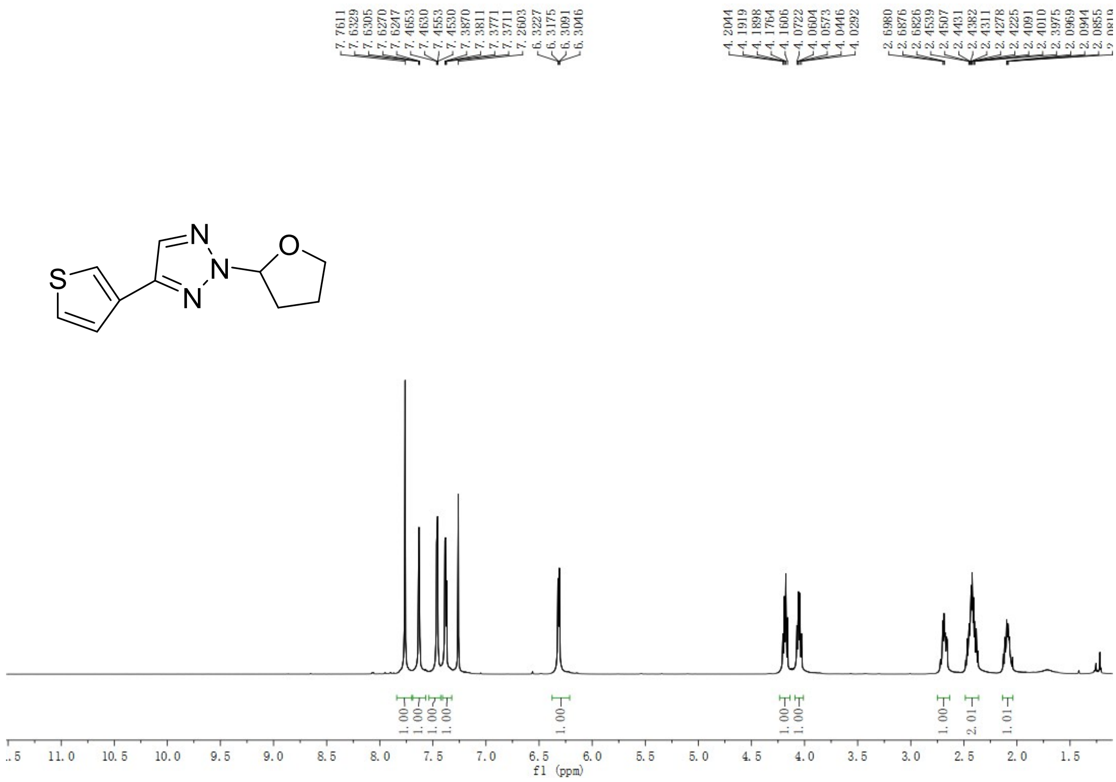
N
O
f1 (ppm)







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6.3046
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4.0722
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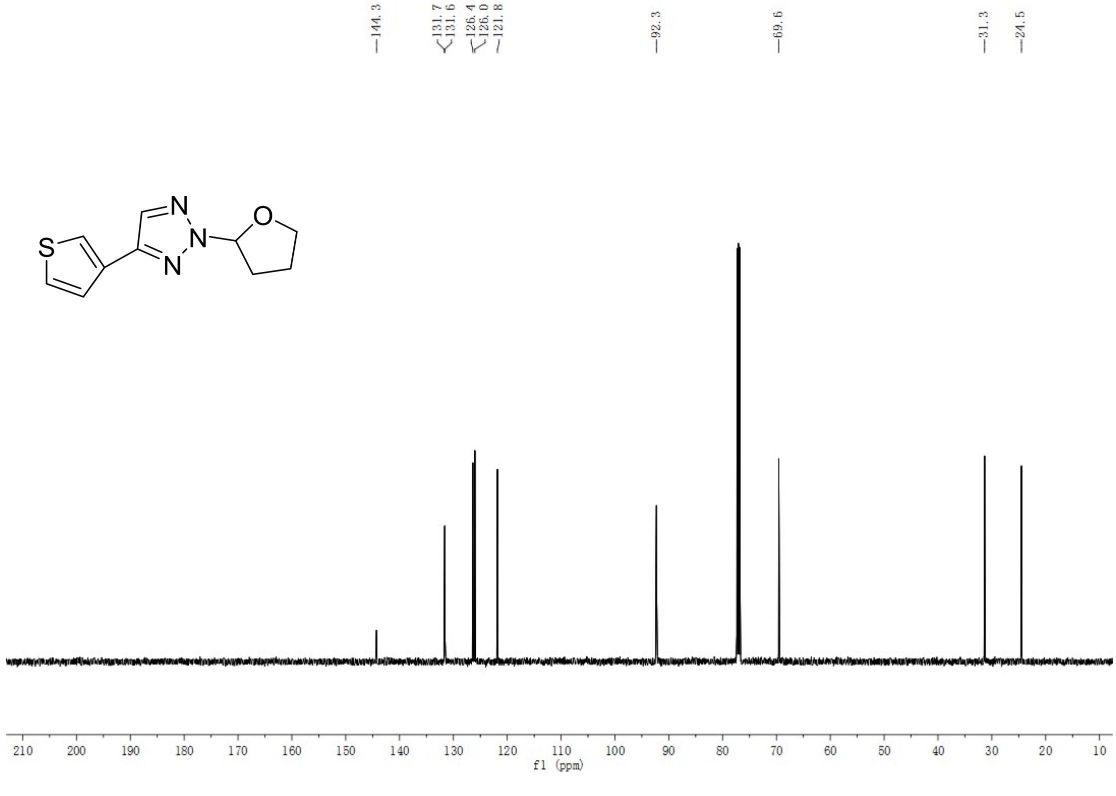
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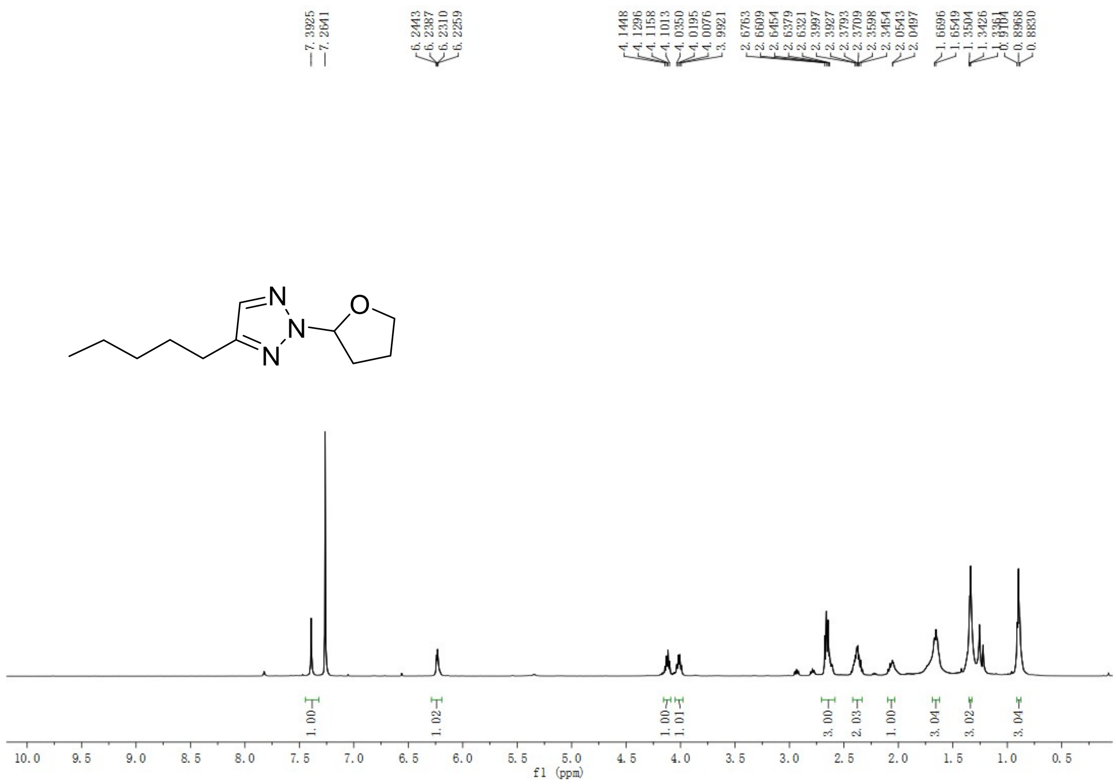
O
f1 (ppm)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1.00
1.01
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2.03
1.00
3.04
3.02
3.04
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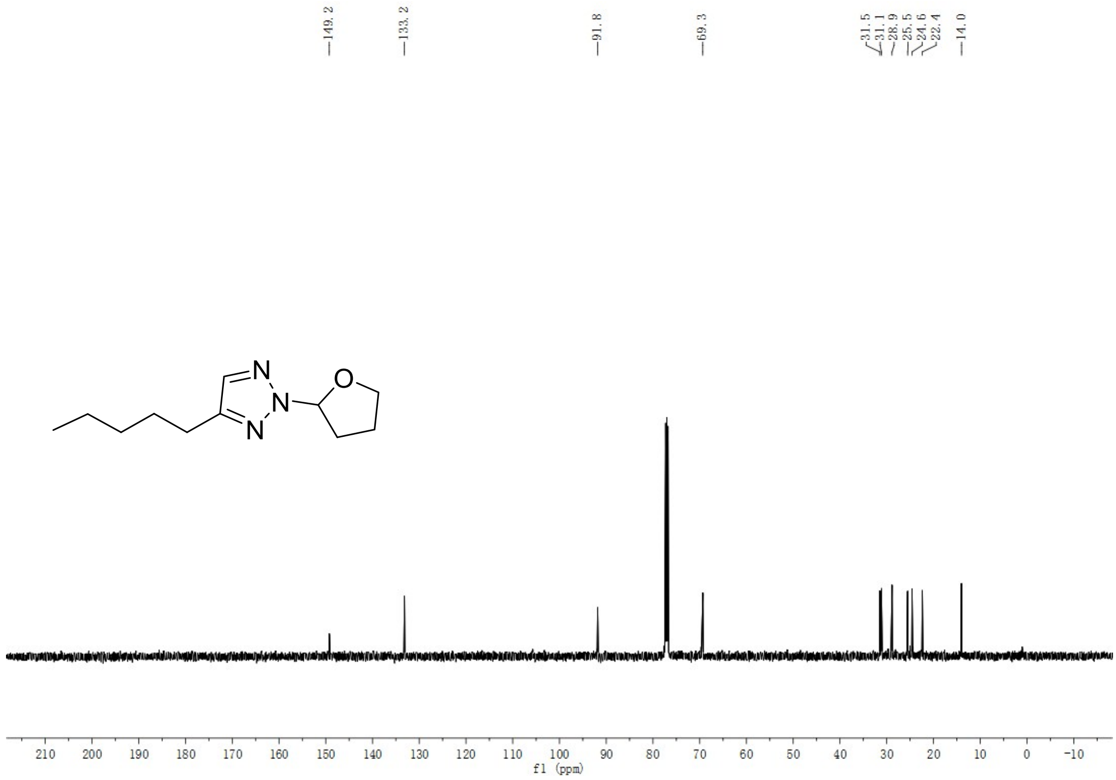
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N
O
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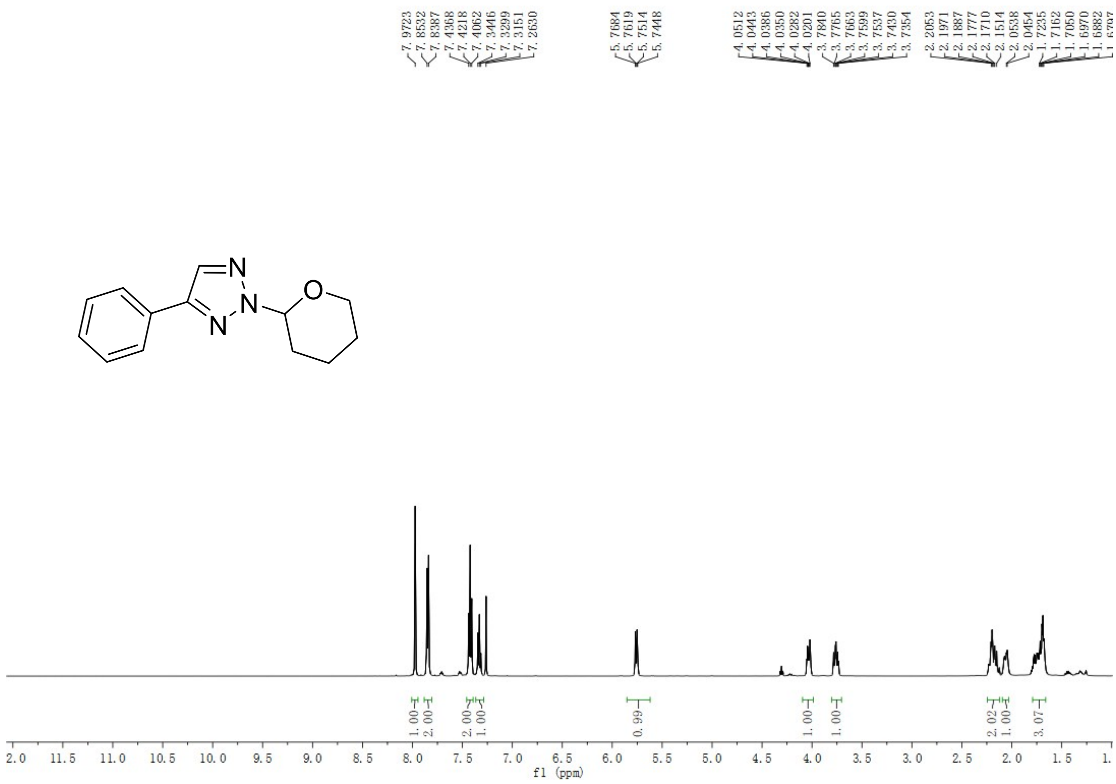
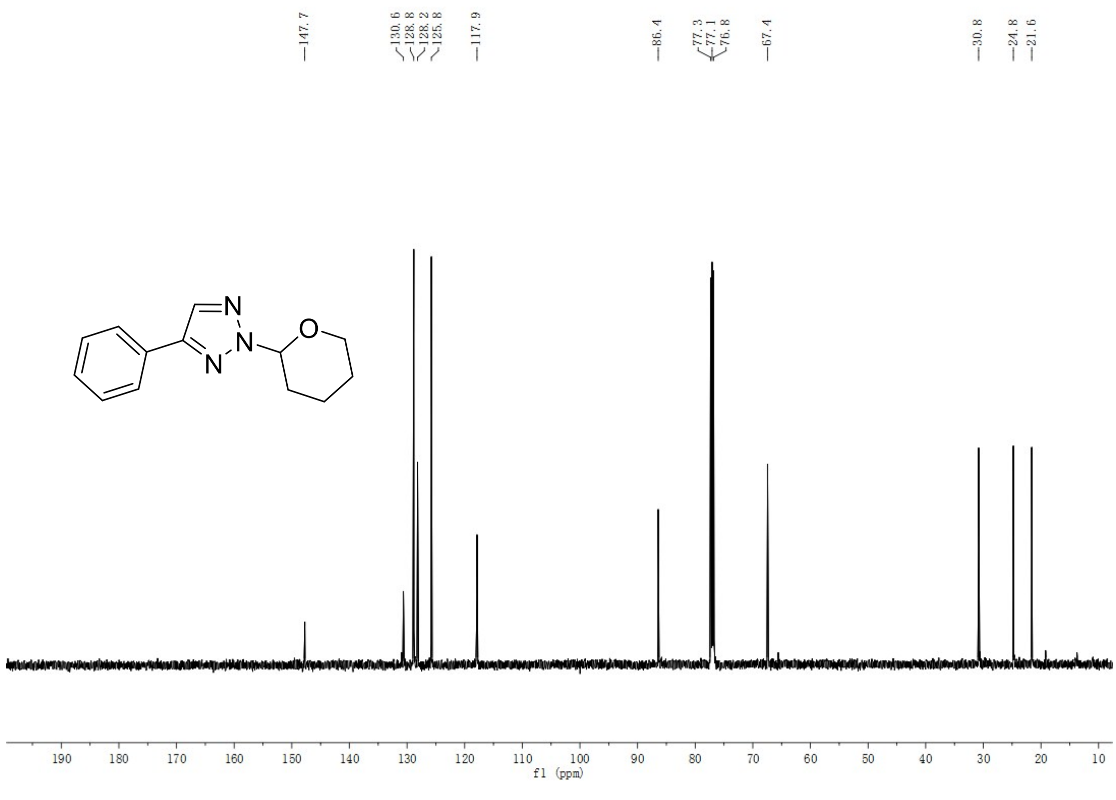
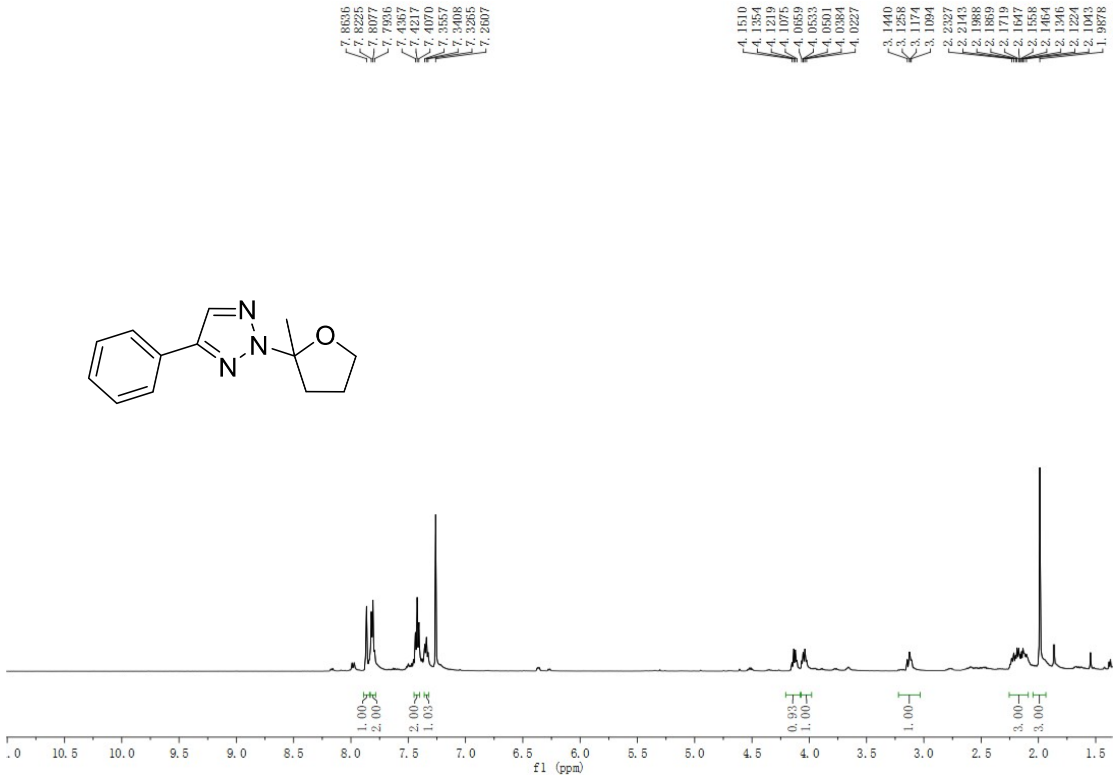
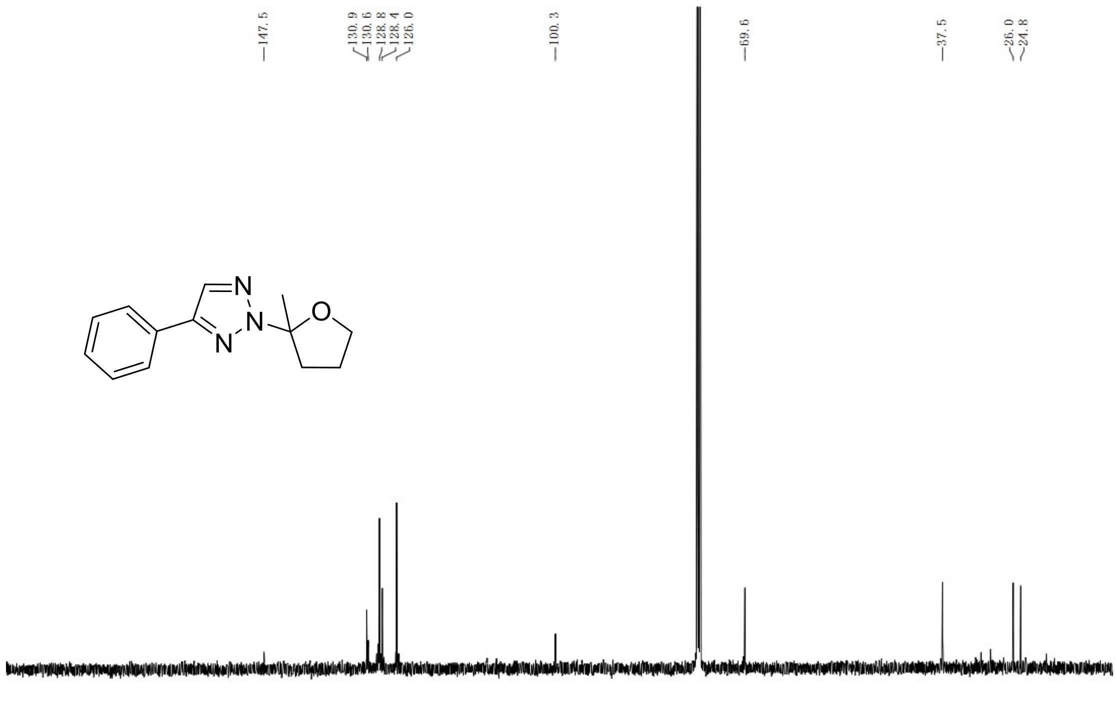
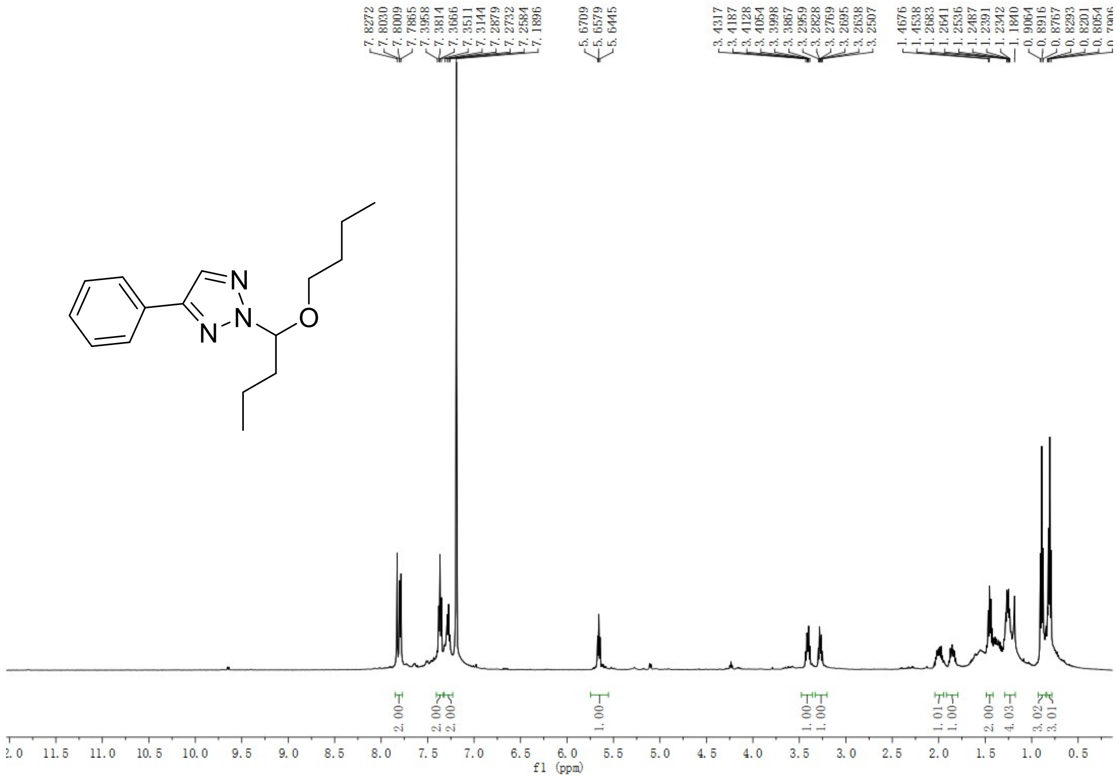
f1 (ppm)

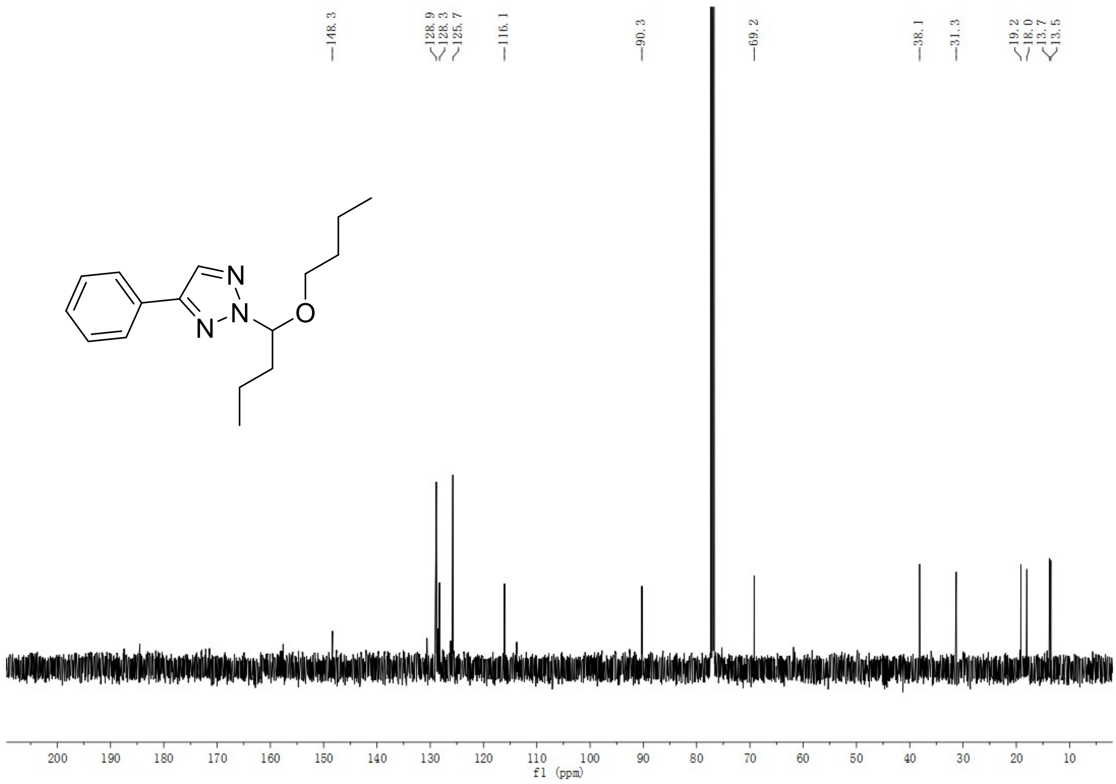


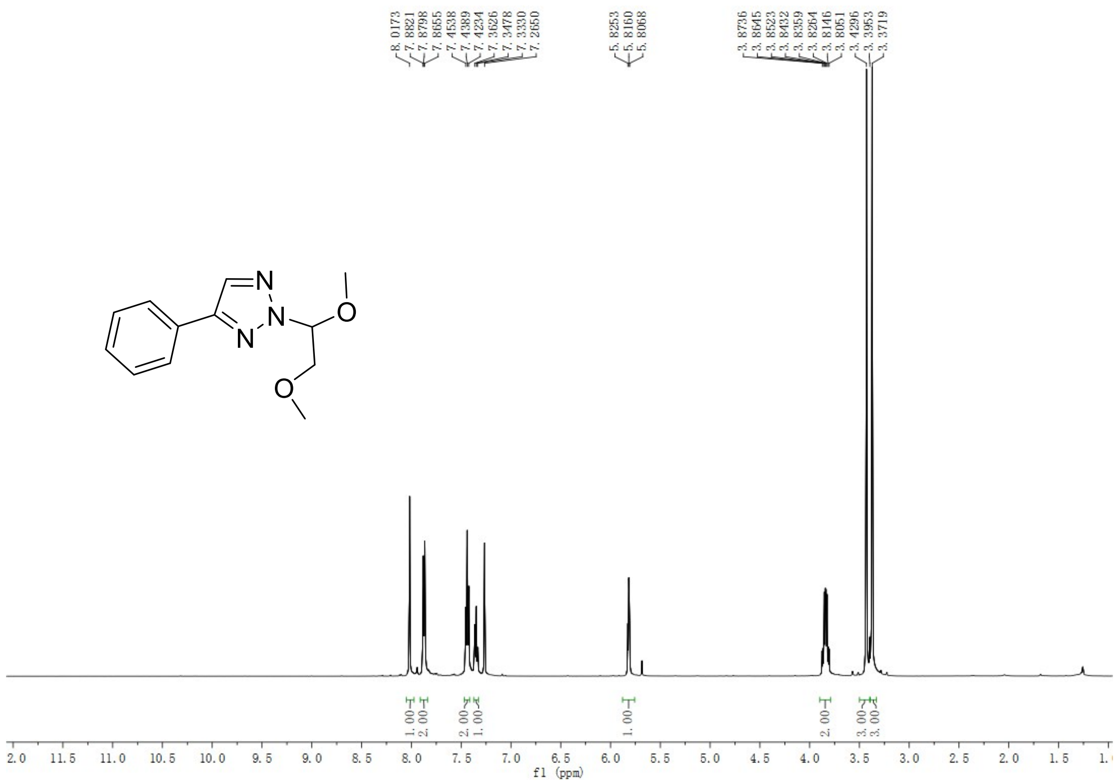








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2.00
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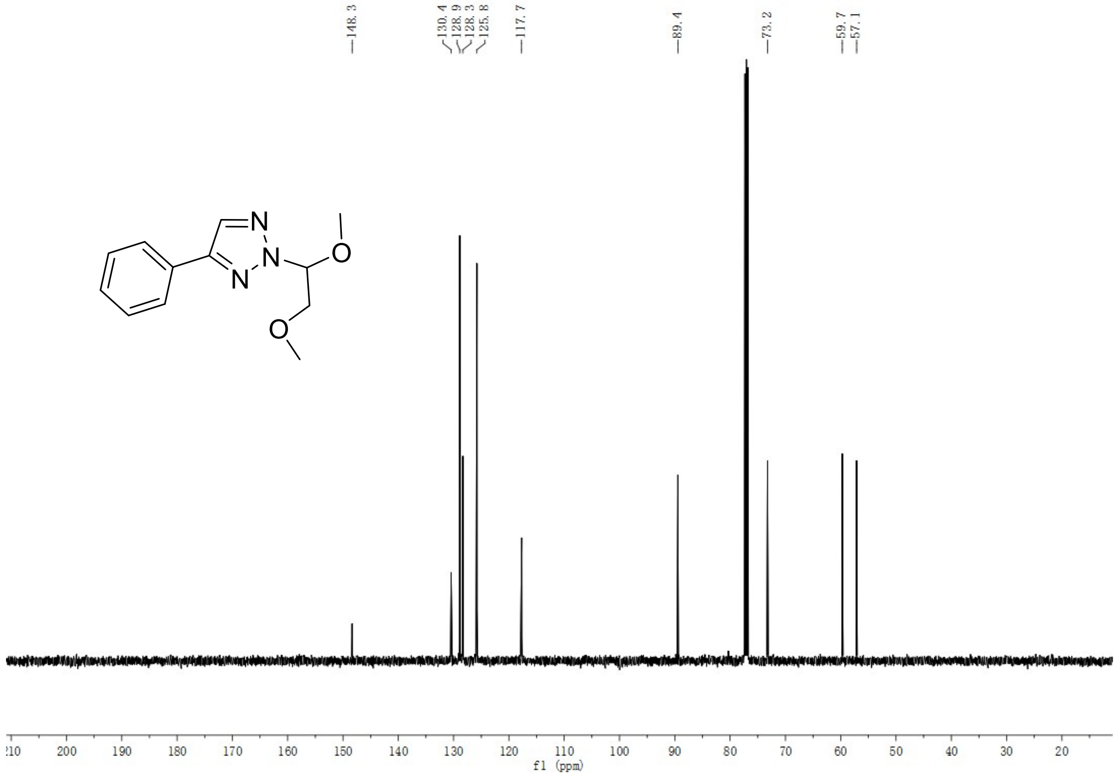
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O
O
f1 (ppm)