

Supplementary Information

Copper-Catalyzed Three Component Reaction of Alkynes, TMSN₃ and Ethers: Regiocontrollable Synthesis of N¹- and N²-Oxyalkylated 1,2,3-Triazoles

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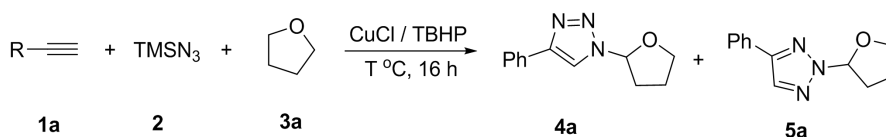
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1. General information

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. ^1H NMR and ^{13}C NMR were recorded in CDCl_3 on a Bruker Avance III 400 spectrometer with TMS as internal standard (500 MHz ^1H , 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. The screening of Reaction Temperature.

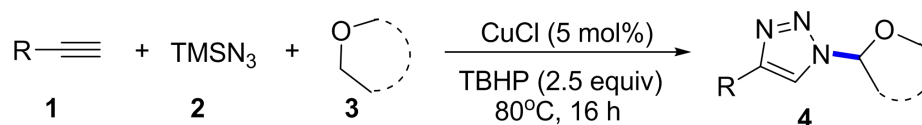


entry	Cat.	T/ °C	Yield (4a) ^b	Yield (5a) ^b
1	CuCl (5%)	25	0	0
2	CuCl (5%)	60	trace	trace
3	CuCl (5%)	70	60%	trace
4	CuCl (5%)	80	85%	trace
5	CuCl (5%)	90	70%	trace
6	CuCl (20%)	60	trace	trace
7	CuCl (20%)	70	25%	60%
8	CuCl (20%)	80	<5%	86%
9	CuCl (20%)	90	6%	80%

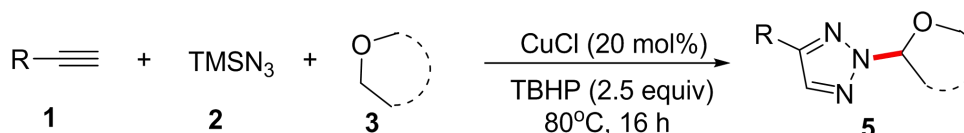
Reaction conditions: ^a Phenylacetylene **1a** (0.2 mmol, 22 μL), TMSN₃ **2** (0.4 mmol, 56 μL), TBHP (0.5 mmol, 70

μL), THF **3a** (2 mL) 16 h. ^b Isolated yield based on **1a**.

3. General procedure for copper catalyzed selective synthesis of N¹- and N²-oxyalkylated 1,2,3-triazoles.

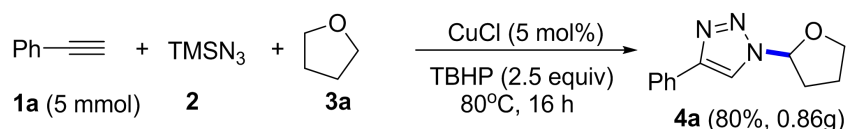


In a tube (15 mL), CuCl (5 mol%, 1 mg), alkyne **1** (0.2 mmol), TMSN₃ **2** (0.4 mmol, 56 μL), ether **3** (2 mL), and TBHP (0.5 mmol, 70 μL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 16 h. After completion of the reaction, the solution was concentrated 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-oxyalkylated 1,2,3-triazole **4**.



In a tube (15 mL), CuCl (20 mol%, 4 mg), alkynes **1** (0.2 mmol), TMSN₃ **2** (0.4 mmol, 56 μL), ether (2 mL), and TBHP (0.5 mmol, 70 μL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 16 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-oxyalkylated 1,2,3-triazole **5**.

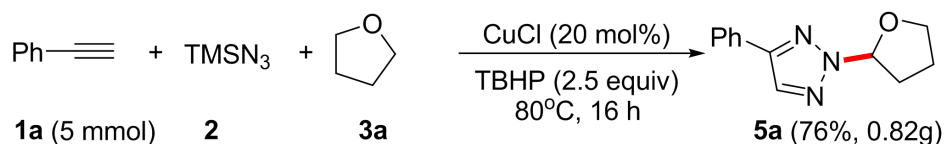
The experimental procedure for the synthesis of N¹-oxyalkylated 1,2,3-triazole (**5 mmol**)



In a tube (35 mL), CuCl (5 mol%, 25 mg), phenylacetylene **1a** (5 mmol), TMSN₃ **2** (10 mmol, 1400 μL), THF **3a** (20 mL), and TBHP (12.5 mmol, 1750 μL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 16 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-oxyalkylated 1,2,3-triazole **4a** in 80% yield (0.86 g).

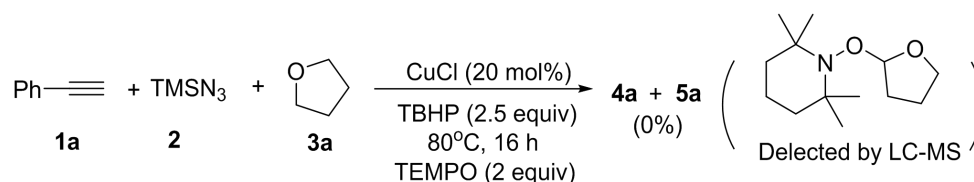
The experimental procedure for the synthesis of N²-oxyalkylated 1,2,3-triazole (**5a** mmol)



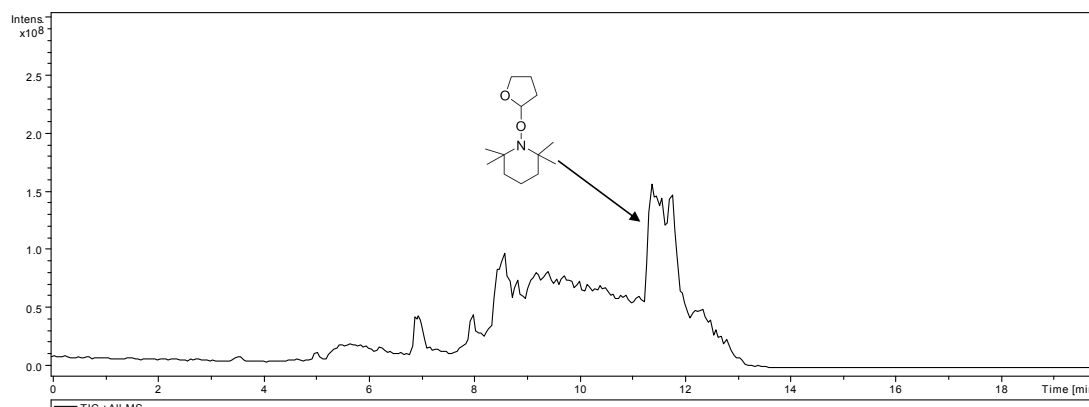
In a tube (35 mL), CuCl (20 mol%, 100 mg), phenylacetylene **1a** (5 mmol), TMSN₃ **2** (10 mmol, 1400 μL), THF **3a** (20 mL), and TBHP (12.5 mmol, 1750 μL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 16 h. After completion of the reaction, the solution 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-oxyalkylated 1,2,3-triazole **5a** in 76% yield (0.82 g).

4. Preliminary mechanistic studies

4.1 The addition of TEMPO in the model reaction system.



In a tube (15 mL), CuCl (20 mol%, 4 mg), TEMPO (0.4 mmol, 62.8 mg), phenylacetylene **1a** (0.2 mmol, 22 μL), TMSN₃ **2** (0.4 mmol, 56 μL), THF **3a** (2 mL), and TBHP (0.5 mmol, 70 μL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 16 h. The reaction was completely inhibited and TEMPO-trapped complex (TEMPO-THF) was detected by LC-MS analysis.



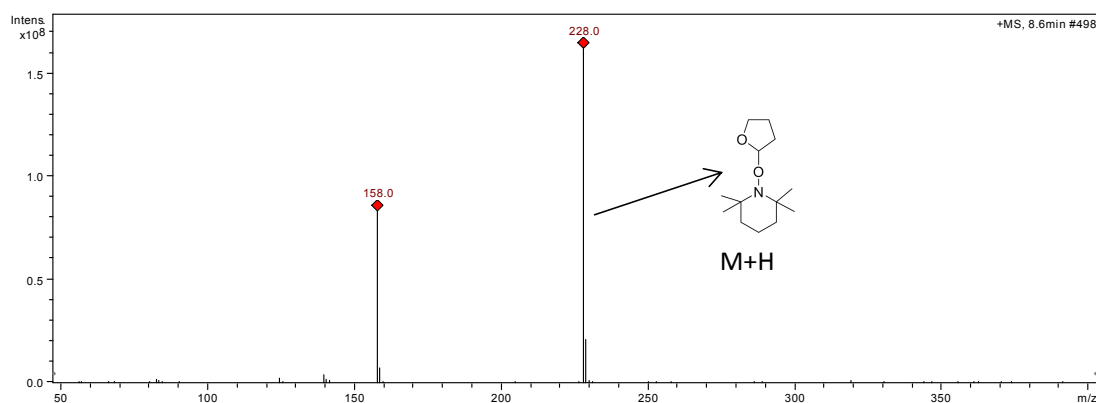
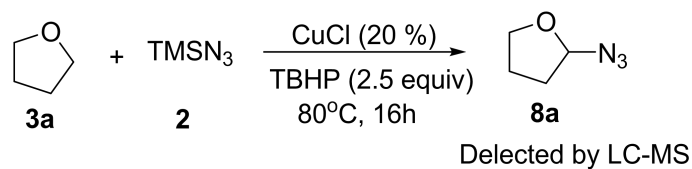
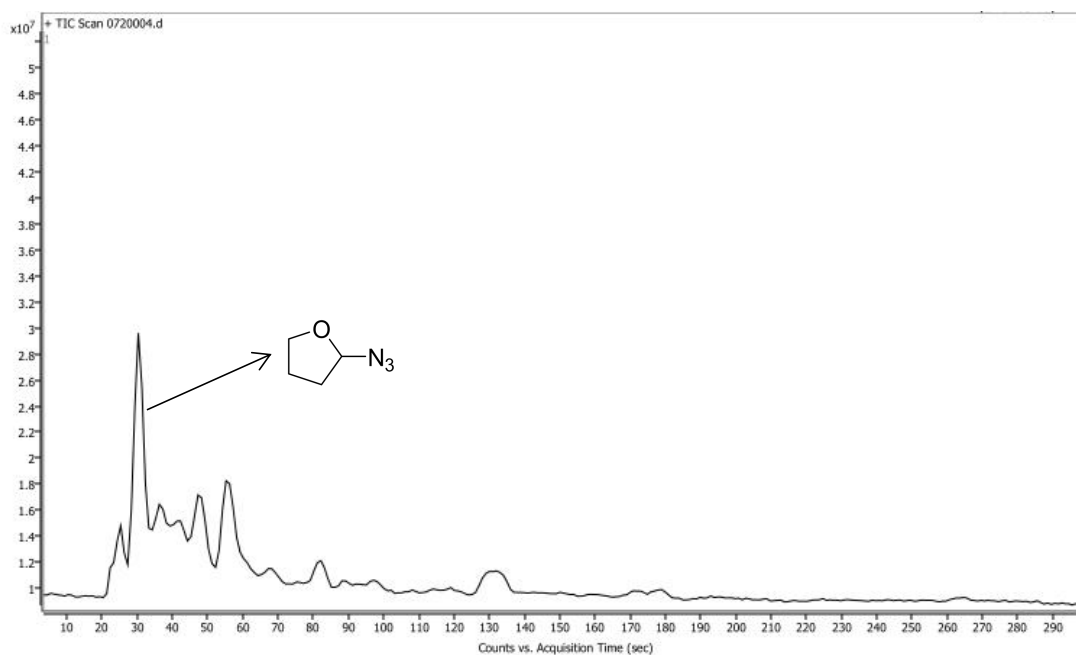


Figure S1. LC-MS spectra of TEMPO-THF.

4.2 The Reaction of THF with TMSN_3 under the standard conditions.



In a tube (15 mL), CuCl (20 mol%, 4 mg), TBHP (0.5mmol, 70 μL), TMSN_3 **2** (0.4 mmol, 56 μL), and THF **3a** (2 mL) were added. The reaction vessel was allowed to stir at 80 $^\circ\text{C}$ for 16 h. After completion of the reaction, the solution was concentrated in vacuum, the oxyalkylated azide **8a** was detected by LC-MS (Figure S4).



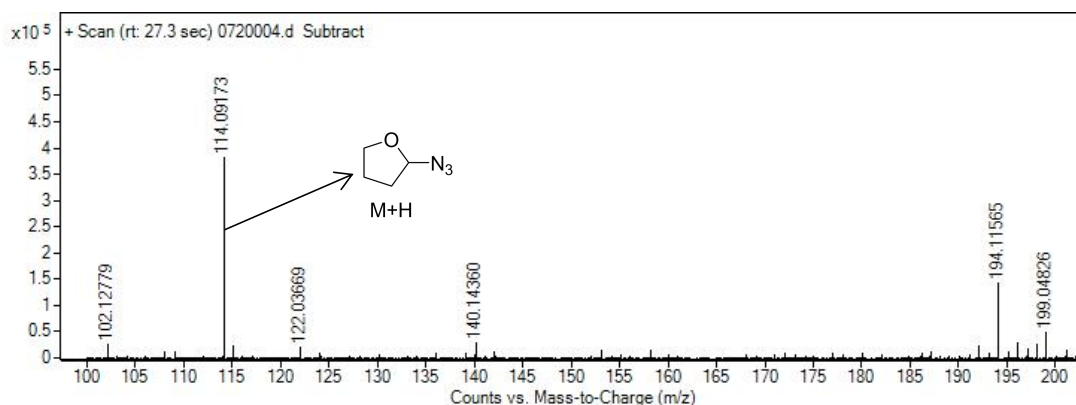
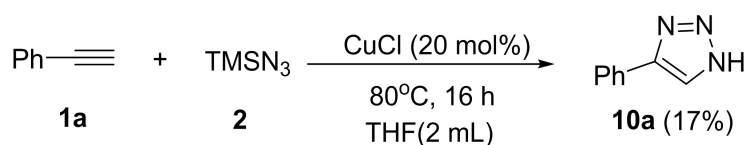


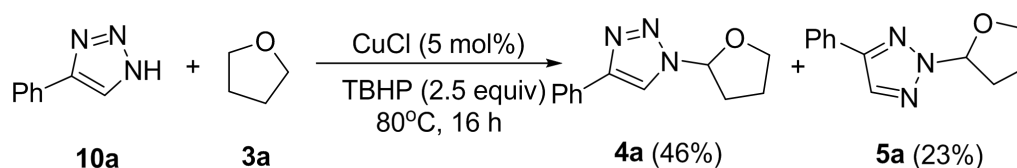
Figure S2. LC-MS spectra of oxyalkylated azide **8a**.

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



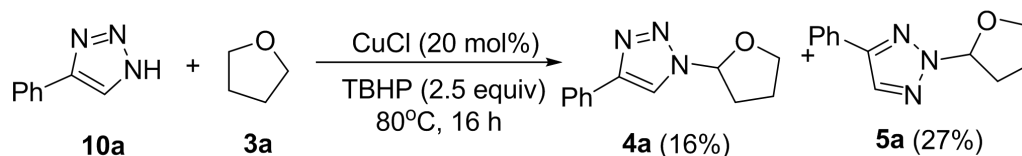
In a tube (15 mL), CuCl (20 mol%, 4 mg), phenylacetylene **1a** (0.2 mmol, 22 μL), TMSN₃ **2** (0.4 mmol, 56 μL), and THF (2 mL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 16 h. After completion of the reaction, the solution was concentrated in vacuum. The residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **10a** in 17% yield.

4.4 The reactions of 4-phenyl-1H-1,2,3-triazole **10a** with THF under CuCl (5 mol%) catalyzed conditions.



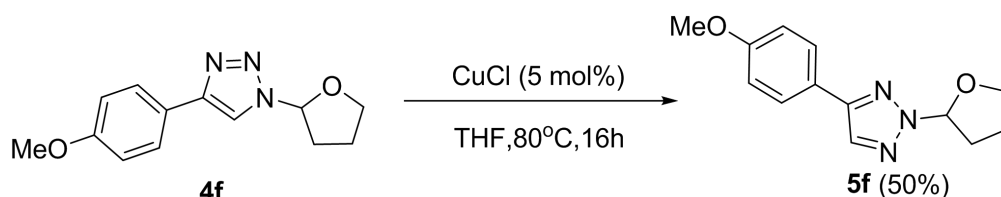
In a tube (15 mL), CuCl (5 mol%, 1 mg), 4-phenyl-1H-1,2,3-triazole **10a** (0.2 mmol, 29mg), THF **3a** (2 ml), and TBHP (0.5mmol, 70 μL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 16 h. After completion of the reaction, the solution was concentrated 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 **4a** in 46% yield (19.8 mg), and product **5a** in 23 % yield (10.0 mg).

4.5 The reactions of 4-phenyl-1H-1,2,3-triazole **10a** with THF under CuCl (20 mol%) catalyzed conditions.



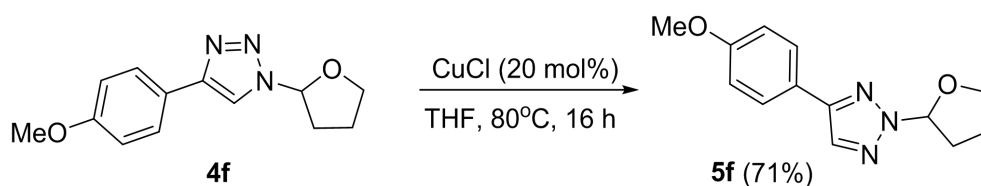
In a tube (15 mL), CuCl (20 mol%, 4 mg), 4-phenyl-1H-1,2,3-triazole **10a** (0.2 mmol, 29mg), THF **3a** (2 ml), and TBHP (0.5mmol, 70 μ L) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 16 h. After completion of the reaction, the solution was concentrated 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 **4a** in 16% yield (6.9 mg), and product **5a** in 27 % yield (11.4 mg).

4.6 The transformation of product **4f** to product **5f** under CuCl (5 mol%) catalyzed conditions.



In a tube (15 mL), 4-(4-methoxyphenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole **4f** (0.1 mmol, 24.5 mg), CuCl (5 mol%, 0.5 mg), and THF (1 mL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 16 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 **5f** in 50% yield (12.3 mg) and product **4f** was remained in 46% yield.

4.7 The transformation of product **4f** to product **5f** under CuCl (20 mol%) catalyzed conditions.



In a tube (15 mL), 4-(4-methoxyphenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole **4f** (0.1 mmol, 24.5 mg), CuCl (20 mol%, 2 mg), and THF (1 mL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 80 °C for 16 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 **5f** in 71% yield (17.4 mg) and product **4f** was remained in 24% yield.

4.8 Characterization data of products **4f** and **5f**.

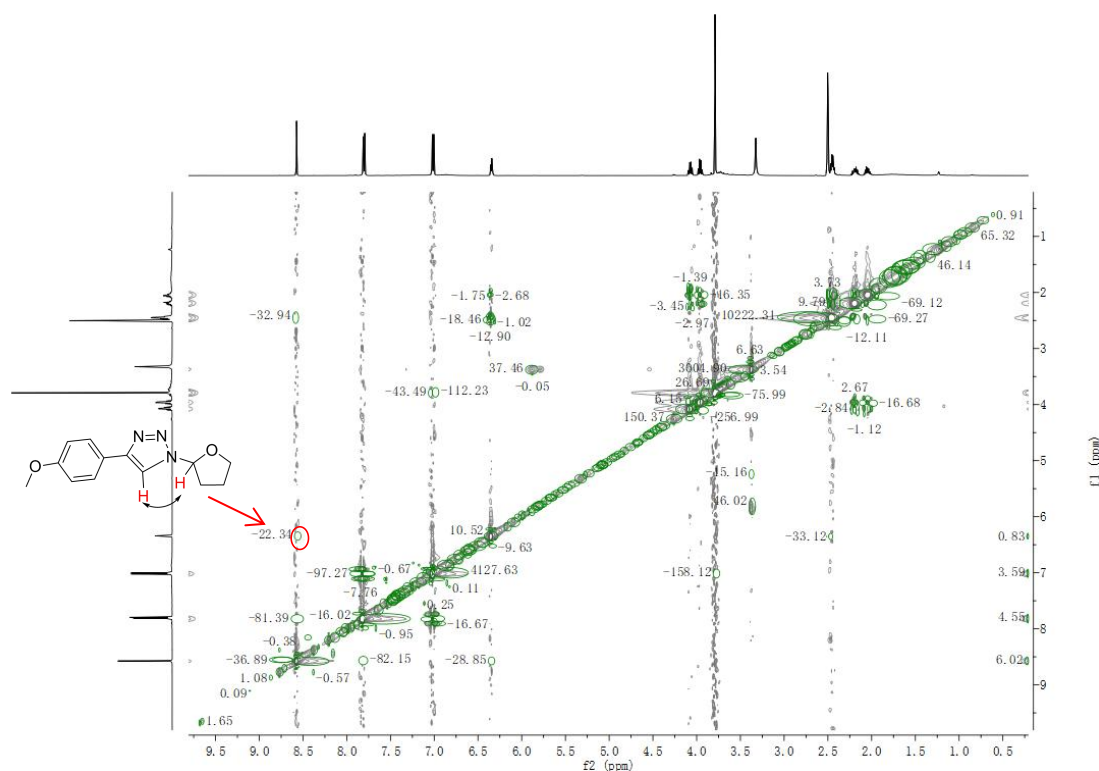
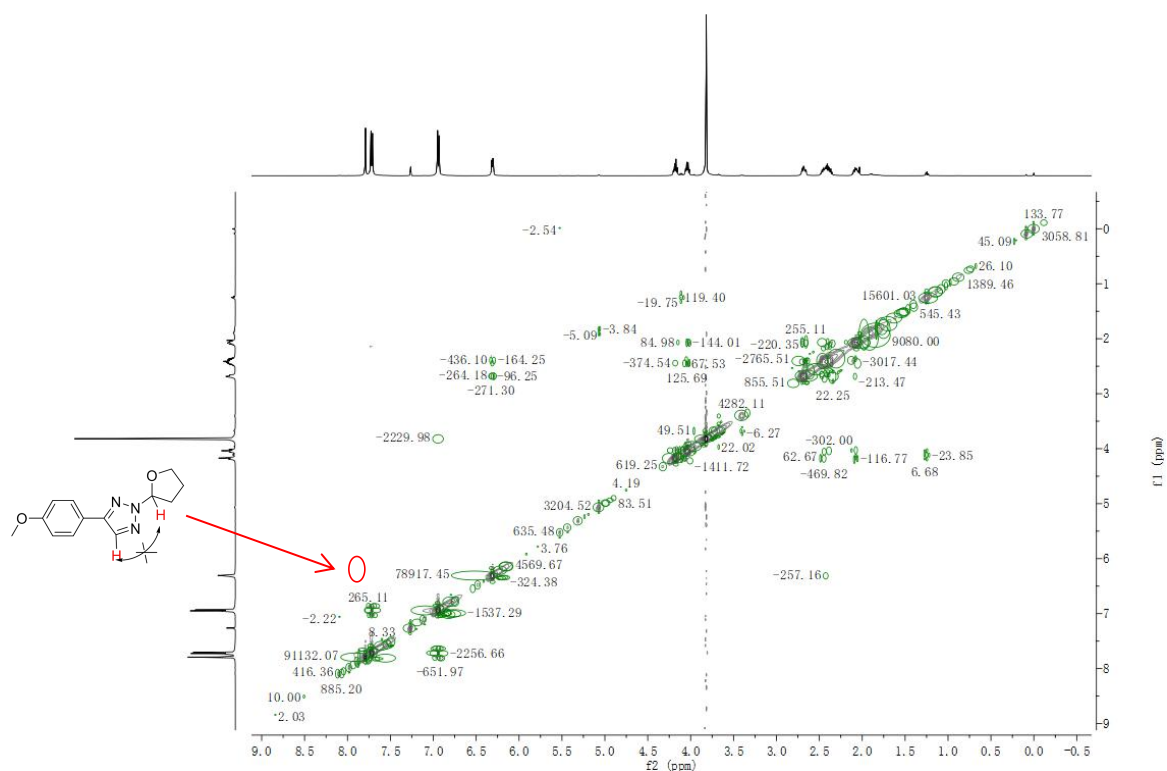
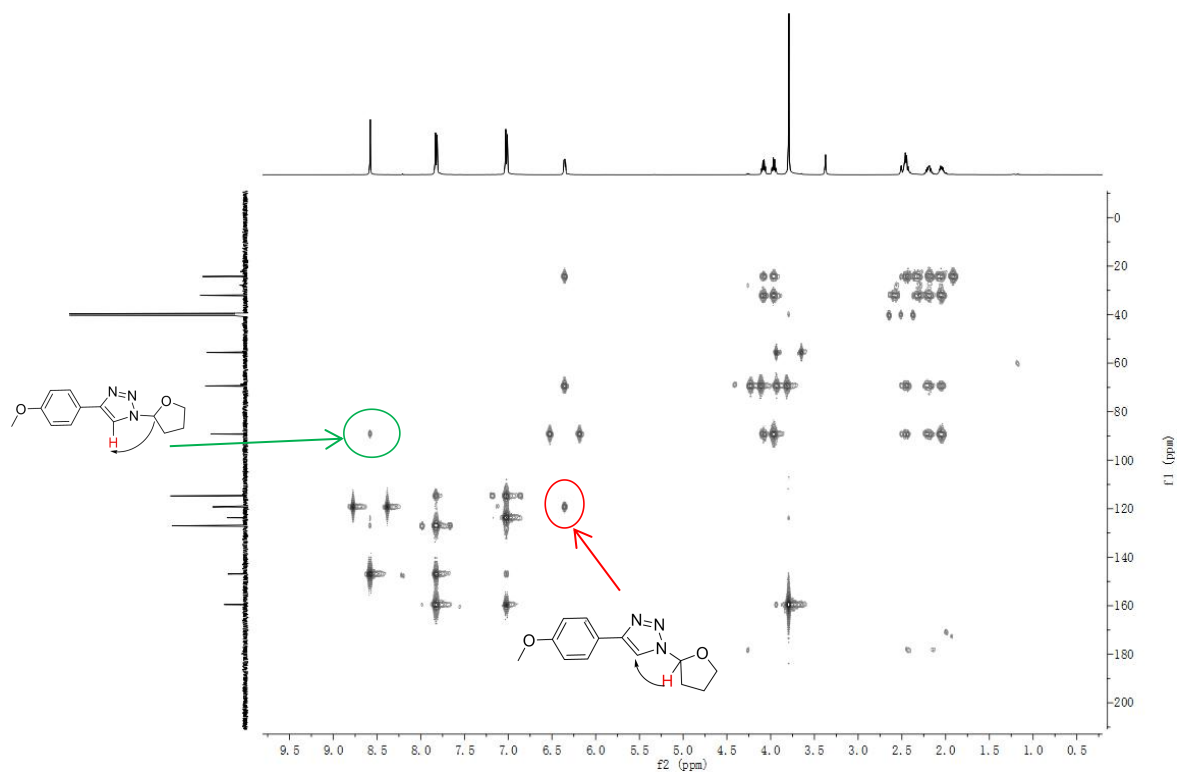


Figure S3. 1H-1H NOESY spectrum of product **4f**.



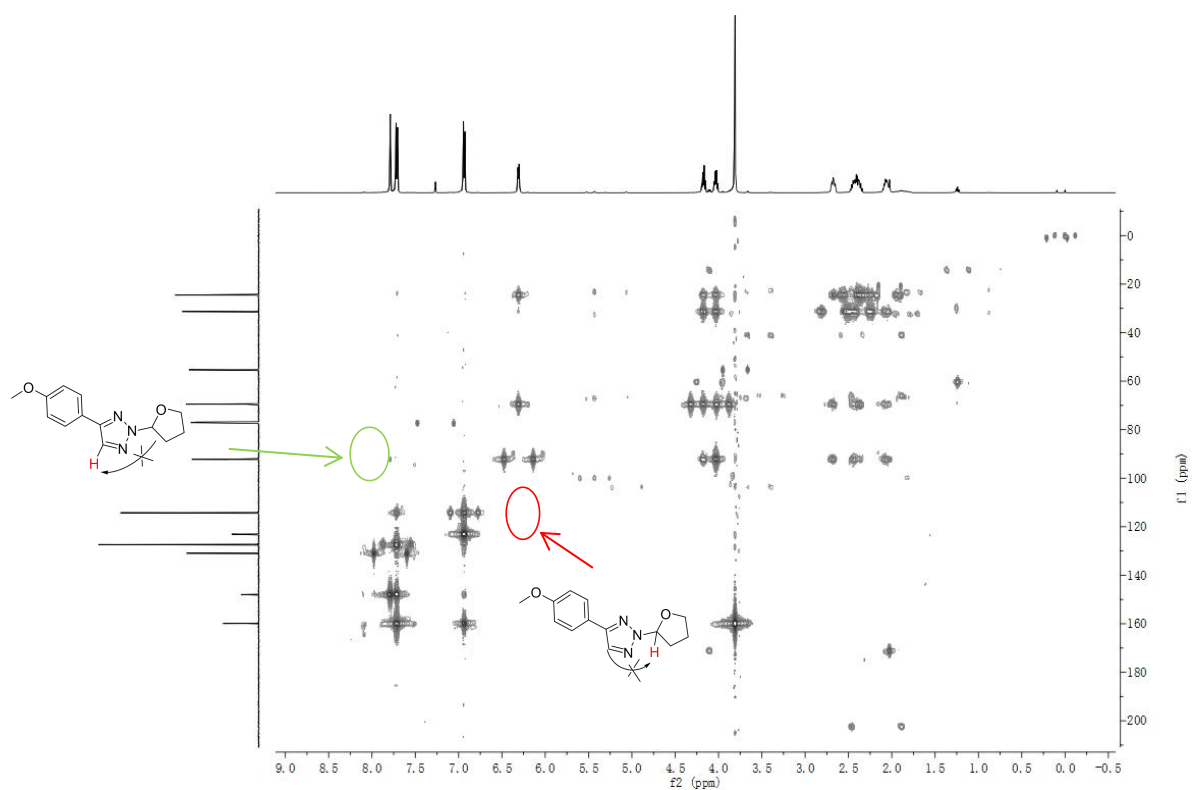
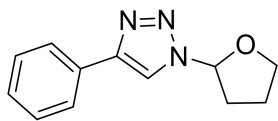
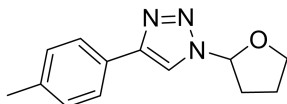


Figure S6. HMBC spectrum of product **5f**.

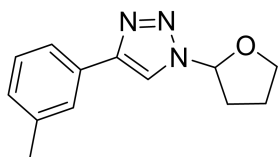
5 Characterization data of products 4a-4u and 5a-5u.



4-phenyl-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4a** was obtained in 85 % yield (36.6 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 8.70 (s, 1H), 7.93 – 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, $\text{DMSO}-d_6$): δ 147.0, 131.1, 129.3, 128.4, 125.7, 120.3, 89.3, 69.4, 32.1, 24.3; HRMS calc. for $\text{C}_{12}\text{H}_{13}\text{N}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 238.0956; found, 238.0955.

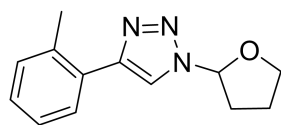


1-(tetrahydrofuran-2-yl)-4-p-tolyl-1H-1,2,3-triazole, Compound **4b** was obtained in 66 % yield (30.2 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 8.63 (s, 1H), 7.76 (d, J = 8.1 Hz, 2H), 7.25 (d, J = 7.9 Hz, 2H), 6.36 – 6.34 (m, 1H), 4.10 – 4.05 (m, 1H), 3.98 – 3.93 (m, 1H), 2.51 – 2.36 (m, 2H), 2.33 (s, 3H), 2.22 – 2.13 (m, 1H), 2.07 – 2.00 (m, 1H); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): δ 147.0, 137.7, 129.9, 128.4, 125.6, 119.8, 89.2, 69.4, 32.1, 24.3, 21.3; HRMS calc. for $\text{C}_{13}\text{H}_{15}\text{N}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 252.1113; found, 252.1109.

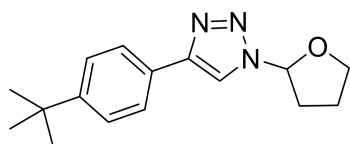


1-(tetrahydrofuran-2-yl)-4-m-tolyl-1H-1,2,3-triazole, Compound **4c** was obtained in 75 % yield (34.4 mg) according to the general procedure (0.2 mmol). Yellow oil ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 8.67 (s, 1H), 7.78 – 7.67 (m, 2H), 7.33 (t, J = 7.6 Hz, 1H), 7.15 (d, J = 7.5 Hz, 1H), 6.45 – 6.29 (m, 1H), 4.11 – 4.07 (m, 1H), 3.99 – 3.984 (m, 1H), 2.51 – 2.44 (m, 2H), 2.36 (s, 3H), 2.24 – 2.16 (m, 1H), 2.09 – 2.00 (m, 1H); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): δ 147.1, 138.5, 131.1, 129.2, 129.0, 126.3, 122.9,

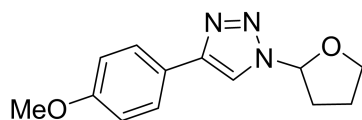
120.1, 89.3, 69.4, 32.1, 24.3, 21.5; HRMS calc. for $C_{13}H_{15}N_3NaO$ ($M+Na$)⁺, 252.1113; found, 252.1104.



1-(tetrahydrofuran-2-yl)-4-o-tolyl-1H-1,2,3-triazole, Compound **4d** was obtained in 70 % yield (32.1 mg) according to the general procedure (0.2 mmol). White solid, mp = 52.3°C – 52.5°C. ¹H NMR (500 MHz, DMSO-*d*₆): δ 8.47 (s, 1H), 7.74 – 7.72 (m, 1H), 7.32 – 7.27 (m, 3H), 6.41 – 6.39 (m, 1H), 4.11 – 4.07 (m, 1H), 4.00 – 3.95 (m, 1H), 2.61 – 2.48 (m, 2H), 2.45 (s, 3H), 2.26 – 2.18 (m, 1H), 2.10 – 2.01 (m, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 146.3, 135.6, 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, 252.1105.

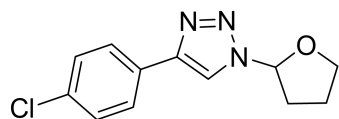


4-(4-tert-butylphenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4e** was obtained in 76 % yield (41.2 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, DMSO-*d*₆): δ 8.64 (s, 1H), 7.81 (d, *J* = 8.4 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 2H), 6.38 – 6.36 (m, 1H), 4.11 – 4.06 (m, 1H), 3.99 – 3.94 (m, 1H), 2.49 – 2.35 (m, 2H), 2.20 (m, 1H), 2.10 – 2.01 (m, 1H), 1.30 (s, 9H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 150.9, 147.0, 128.4, 126.0, 125.5, 119.9, 89.2, 69.4, 34.8, 32.1, 31.5, 24.3; HRMS calc. for $C_{16}H_{21}N_3NaO$ ($M+Na$)⁺, 294.1582; found, 294.1573.

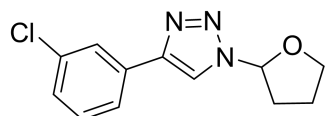


4-(4-methoxyphenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4f** was obtained in 66 % yield (32.3 g) according to the general procedure (0.2 mmol). White solid, mp = 51.3°C – 51.8°C. ¹H NMR (500 MHz, DMSO-*d*₆): δ 8.57 (s, 1H), 7.80 (d, *J* = 8.6 Hz, 2H), 7.01 (d, *J* = 8.6 Hz, 2H), 6.42 – 6.28 (m, 1H), 4.11 – 4.03 (m, 1H), 3.98 – 3.93 (m, 1H), 3.79 (s, 3H), 2.48 – 2.42 (m, 2H), 2.24 – 2.15 (m, 1H), 2.09 – 2.02 (m, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 159.5, 146.9, 127.1, 123.7, 119.3,

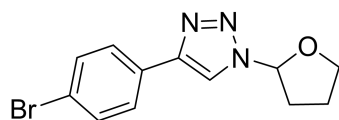
114.7, 89.2, 69.4, 55.6, 32.1, 24.3; HRMS calc. for $C_{13}H_{15}N_3NaO_2$ ($M+Na$)⁺, 268.1062; found, 268.1071.



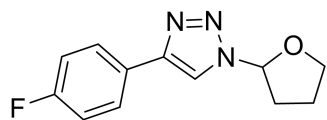
4-(4-chlorophenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4g** was obtained in 71 % yield (35.4 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, DMSO-*d*₆): δ 8.75 (s, 1H), 7.94 – 7.90 (m, 2H), 7.54 – 7.51 (m, 2H), 6.37 (t, *J* = 4.7 Hz, 1H), 4.11 – 4.07 (m, 1H), 3.99 – 3.95 (m, 1H), 2.49 – 2.43 (m, 2H), 2.23 – 2.14 (m, 1H), 2.09 – 2.03 (m, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 145.9, 132.8, 130.0, 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.



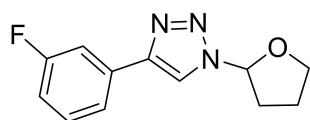
4-(3-chlorophenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4h** was obtained in 65 % yield (32.4 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, DMSO-*d*₆): δ 8.81 (s, 1H), 7.95 (t, *J* = 1.7 Hz, 1H), 7.88 (d, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 7.9 Hz, 1H), 7.44 – 7.37 (m, 1H), 6.39 – 6.37 (m, 1H), 4.12 – 4.08 (m, 1H), 4.00 – 3.95 (m, 1H), 2.52 – 2.43 (m, 2H), 2.24 – 2.14 (m, 1H), 2.09 – 2.03 (m, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 145.6, 134.2, 133.2, 131.3, 128.2, 125.3, 124.2, 121.0, 89.4, 69.5, 32.2, 24.2; HRMS calc. for $C_{12}H_{13}ClN_3O$ ($M+H$)⁺, 250.0747; found, 250.0745.



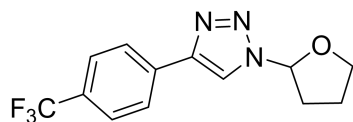
4-(4-bromophenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4i** was obtained in 69 % yield (40.4 mg) according to the general procedure (0.2 mmol). Yellow Solid, mp = 52.1°C – 52.5°C. ¹H NMR (500 MHz, DMSO-*d*₆): δ 8.75 (s, 1H), 7.85 (d, *J* = 6.3, 2H), 7.65 (d, *J* = 4.7, 2H), 6.39 – 6.37 (m, 1H), 4.11 – 4.07 (m, 1H), 3.99 – 3.95 (m, 1H), 2.49 – 2.42 (m, 2H), 2.23 – 2.14 (m, 1H), 2.09 – 2.01 (m, 1H); ¹³C 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, 294.0234.



4-(4-fluorophenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4j** was obtained in 60 % yield (28.0 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 8.69 (s, 1H), 7.95 – 7.90 (m, 2H), 7.32 – 7.27 (m, 2H), 6.37 (t, J = 4.7 Hz, 1H), 4.11 – 4.06 (m, 1H), 3.99 – 3.95 (m, 1H), 2.49 – 2.43 (m, 2H), 2.23 – 2.14 (m, 1H), 2.06 (m, 1H); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): δ 162.29 (d, J = 242.5 Hz), 146.12, 127.73 (d, J = 8.75 Hz), 127.72, 120.16, 116.27 (d, J = 22.5 Hz), 89.32, 69.45, 32.10, 24.22; HRMS calc. for $\text{C}_{12}\text{H}_{12}\text{FN}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 256.0862; found, 256.0859.

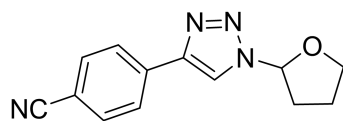


5-(3-fluorophenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4k** was obtained in 68 % yield (31.7 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 8.79 (s, 1H), 7.76 (d, J = 7.8 Hz, 1H), 7.72 – 7.69 (m, 1H), 7.53 – 7.49 (m, 1H), 7.20 – 7.16 (m, 1H), 6.39 (t, J = 4.7 Hz, 1H), 4.12 – 4.08 (m, 1H), 4.00 – 3.96 (m, 1H), 2.52 – 2.45 (m, 2H), 2.22 – 2.16 (m, 1H), 2.10 – 2.04 (m, 1H); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): δ 163.06 (d, J = 242.5 Hz), 145.90 (d, J = 2.5 Hz), 133.49 (d, J = 8.7 Hz), 131.47 (d, J = 8.5 Hz), 121.69 (d, J = 2.5 Hz), 120.94, 115.07 (d, J = 20.9 Hz), 112.29 (d, J = 22.8 Hz), 89.42, 69.50, 32.15, 24.16; HRMS calc. for $\text{C}_{12}\text{H}_{12}\text{FN}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 256.0862; found, 256.0858.

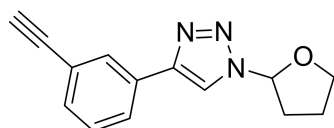


1-(tetrahydrofuran-2-yl)-4-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazole, Compound **4l** was obtained in 69 % yield (39.1 mg) according to the general procedure (0.2 mmol). Yellow solid, mp = 55.6°C – 55.8°C. ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 8.89 (s, 1H), 8.12 (d, J = 8.1 Hz, 2H), 7.83 (d, J = 8.3 Hz, 2H), 6.42 – 6.39 (m, 1H), 4.13 – 4.09 (m, 1H), 4.00 – 3.96 (m, 1H), 2.51 – 2.43 (m, 2H), 2.22 – 2.15 (m, 1H), 2.11 – 2.05 (m, 1H); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): δ 145.60, 135.11,

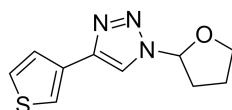
128.53 (q, $J = 32.5$ Hz), 126.35 (q, $J = 3.8$ Hz), 126.22, 123.65, 121.57, 89.49, 69.55, 32.17, 24.18; HRMS calc. for $C_{13}H_{12}F_3N_3NaO$ ($M+Na$)⁺, 306.0830; found, 306.0828.



4-(1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazol-4-yl)benzonitrile, Compound **4m** was obtained in 57 % yield (27.4 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, DMSO-*d*₆): δ 8.91 (s, 1H), 8.11 – 8.06 (m, 2H), 7.95 – 7.84 (m, 2H), 6.40 (t, $J = 4.6$ Hz, 1H), 4.12 – 4.08 (m, 1H), 4.00 – 3.96 (m, 1H), 2.49 – 2.45 (m, 2H), 2.23 – 2.14 (m, 1H), 2.11 – 2.03 (m, 1H); ¹³C 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 $C_{13}H_{12}N_4NaO$ ($M+Na$)⁺, 263.0909; found, 263.0901.

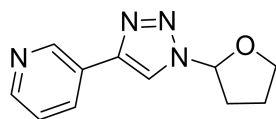


4-(3-ethynylphenyl)-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4n** was obtained in 60 % yield (28.7 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, DMSO-*d*₆): δ 8.80 (s, 1H), 8.00 (s, 1H), 7.97 – 7.92 (m, 1H), 7.46 (m, 2H), 6.41 – 6.33 (m, 1H), 4.26 (s, 1H), 4.12 – 4.08 (m, 1H), 3.99 – 3.95 (m, 1H), 2.51 – 2.44 (m, 2H), 2.24 – 2.15 (m, 1H), 2.10 – 2.02 (m, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 146.0, 131.6, 131.5, 129.8, 128.7, 126.1, 122.8, 120.7, 89.4, 83.7, 81.6, 69.5, 32.2, 24.2. HRMS calc. for $C_{14}H_{14}N_3O$ ($M+H$)⁺, 240.1137; found, 240.1133.

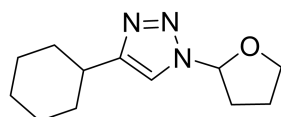


1-(tetrahydrofuran-2-yl)-4-(thiophen-3-yl)-1H-1,2,3-triazole, Compound **4o** was obtained in 72 % yield (31.8 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, DMSO-*d*₆): δ 8.54 (s, 1H), 7.86 – 7.84 (m, 1H), 7.63 – 7.62 (m, 1H), 7.54 – 7.53 (m, 1H), 6.36 – 6.32 (m, 1H), 4.07 – 4.03 (m, 1H), 3.97 – 3.92 (m, 1H), 2.49 – 2.41 (m, 2H), 2.18 – 2.12 (m, 1H), 2.06 – 2.00 (m, 1H); ¹³C

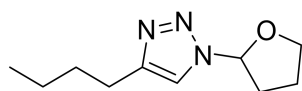
NMR (125 MHz, DMSO-*d*₆): δ 143.5, 132.5, 127.6, 126.3, 121.4, 120.0, 89.3, 69.4, 32.1, 24.2; HRMS calc. for C₁₀H₁₂N₃OS (M+H)⁺, 222.0701; found, 222.0697.



3-(1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazol-4-yl)pyridine, Compound **4p** was obtained in 67 % yield (28.9 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, DMSO-*d*₆): δ 8.69 (s, 1H), 8.61 (s, 1H), 8.05 (d, *J* = 7.6 Hz, 1H), 7.92 – 7.89 (m, 1H), 7.43 – 7.27 (m, 1H), 6.43 – 6.41 (m, 1H), 4.13 – 4.08 (m, 1H), 3.99 – 3.95 (m, 1H), 2.51 – 2.41 (m, 2H), 2.25 – 2.16 (m, 1H), 2.09 – 2.00 (m, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 150.3, 150.0, 147.8, 137.7, 123.5, 122.1, 120.0, 89.4, 69.5, 32.1, 24.4; HRMS calc. for C₁₁H₁₂N₄NaO (M+Na)⁺, 239.0909; found, 239.0905.

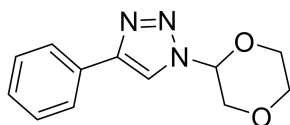


4-cyclohexyl-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4q** was obtained in 60 % yield (26.5 mg) according to the general procedure (0.2 mmol). Yellow oil ¹H NMR (500 MHz, DMSO-*d*₆): δ 7.93 (s, 1H), 6.25 (t, *J* = 4.9 Hz, 1H), 4.02 – 3.98 (m, 1H), 3.93 – 3.89 (m, 1H), 2.67 – 2.63 (m, 1H), 2.44 – 2.33 (m, 2H), 2.22 – 2.09 (m, 1H), 2.05 – 2.00 (m, 1H), 1.99 – 1.91 (m, 2H), 1.75 – 1.66 (m, 3H), 1.43 – 1.30 (m, 4H), 1.24 – 1.21 (m, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆): δ 152.8, 119.5, 88.7, 69.2, 35.1, 33.0, 33.0, 31.9, 26.1, 24.5. HRMS calc. for C₁₂H₁₉N₃NaO (M+Na)⁺, 244.1426; found, 244.1423.

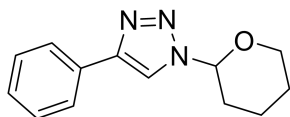


4-butyl-1-(tetrahydrofuran-2-yl)-1H-1,2,3-triazole, Compound **4r** was obtained in 65 % yield (25.3 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, DMSO-*d*₆): δ 7.94 (s, 1H), 6.25 (t, *J* = 4.8 Hz, 1H), 4.02 – 3.96 (m, 1H), 3.93 – 3.89 (m, 1H), 2.60 (t, *J* = 7.6 Hz, 2H), 2.40 – 2.37 (m, 2H), 2.17 – 2.11 (m, 1H), 2.03 – 1.99 (m, 1H), 1.61 – 1.54 (m, 2H), 1.34 – 1.30 (m, 2H), 0.89 (t, *J* = 7.4 Hz,

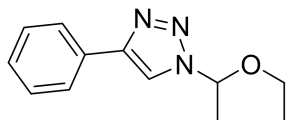
3H); ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$): δ 147.6, 120.7, 88.8, 69.2, 31.9, 31.5, 25.1, 24.4, 22.2, 14.2. HRMS calc. for $\text{C}_{10}\text{H}_{17}\text{N}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 218.1269; found, 218.1266.



1-(1,4-dioxan-2-yl)-4-phenyl-1H-1,2,3-triazole, Compound **4s** was obtained in 55 % yield (25.4 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, $\text{DMSO-}d_6$): δ 8.81 (s, 1H), 7.91 (d, $J = 7.7$ Hz, 2H), 7.47 (t, $J = 7.6$ Hz, 2H), 7.36 (t, $J = 7.4$ Hz, 1H), 6.01 – 5.99 (m, 1H), 4.17 – 4.14 (m, 1H), 4.12 – 4.09 (m, 1H), 3.87 – 3.80 (m, 2H), 3.84 – 3.79 (m, 1H), 3.76 – 3.70 (m, 1H); ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$): δ 146.8, 130.9, 129.4, 128.6, 125.8, 121.3, 81.9, 67.4, 65.9, 64.5. HRMS calc. for $\text{C}_{12}\text{H}_{13}\text{N}_3\text{NaO}_2$ ($\text{M}+\text{Na}$) $^+$, 254.0905; found, 254.0914.



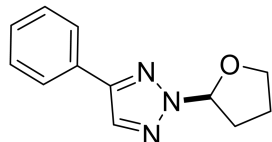
4-phenyl-1-(tetrahydro-2H-pyran-2-yl)-1H-1,2,3-triazole, Compound **4t** was obtained in 60% yield (27.5 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 8.78 (s, 1H), 7.90 – 7.88 (m, 2H), 7.45 (t, $J = 7.7$ Hz, 2H), 7.34 (t, $J = 7.4$ Hz, 1H), 5.83 – 5.80 (m, 1H), 3.96 (d, $J = 12.2$ Hz, 1H), 3.76 – 3.70 (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, $\text{DMSO-}d_6$): δ 145.9, 130.1, 128.5, 127.5, 124.8, 119.5, 85.0, 66.4, 29.4, 24.0, 21.0. HRMS calc. for $\text{C}_{13}\text{H}_{15}\text{N}_3\text{NaO}$ ($\text{M}+\text{H}$) $^+$, 252.1113; found, 252.1109.



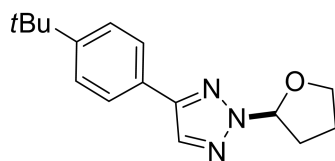
1-(1-ethoxyethyl)-4-phenyl-1H-1,2,3-triazole, Compound **4u** was obtained in 35 % yield (15.2 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, $\text{DMSO-}d_6$): δ 8.80 (s, 1H), 7.90 – 7.89 (m, 2H), 7.45 (t, $J = 7.7$ Hz, 2H), 7.34 (t, $J = 7.4$ Hz, 1H), 5.94 (q, $J = 6.0$ Hz, 1H), 3.54 – 3.50 (m, 1H), 3.30 – 3.26 (m, 1H), 1.72 (t, $J = 9.8$ Hz, 3H), 1.07 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (125 MHz,

DMSO-d₆): δ 146.8, 130.6, 128.9, 128.0, 125.2, 125.1, 86.7, 63.7, 21.3, 14.6. HRMS calc. for C₁₂H₁₅N₃NaO (M+Na)⁺, 240.1113; found, 240.1108.

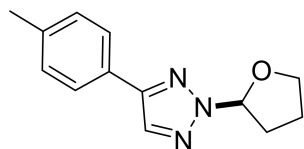
Characterization data of products 5a-5u:



4-phenyl-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole,^[1] Compound **5a** was obtained in 86% yield (37.0 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, CDCl₃): δ 7.87 (s, 1H), 7.80 – 7.79 (m, 2H), 7.42 (t, J = 7.5 Hz, 2H), 7.36 – 7.33 (m, 1H), 6.34 – 6.33 (m, 1H), 4.22 – 4.18 (m, 1H), 4.08 – 4.04 (m, 1H), 2.72 – 2.67 (m, 1H), 2.49 – 2.38 (m, 2H), 2.14 – 2.08 (m, 1H); ¹³C NMR (125 MHz, CDCl₃): δ 148.1, 131.4, 130.4, 128.8, 128.5, 126.1, 92.4, 69.6, 31.4, 24.5. HRMS calc. for C₁₂H₁₃N₃NaO (M+Na)⁺, 238.0956; found, 238.0953.

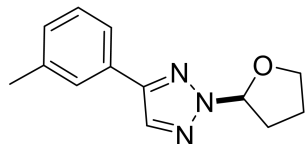


4-(4-tert-butylphenyl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5b** was obtained in 80% yield (43.4 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, CDCl₃): δ 7.84 (s, 1H), 7.72 (d, J = 8.3 Hz, 2H), 7.45 (d, J = 8.3 Hz, 2H), 6.34 – 6.32 (m, 1H), 4.21 – 4.17 (m, 1H), 4.08 – 4.03 (m, 1H), 2.71 – 2.66 (m, 1H), 2.48 – 2.37 (m, 2H), 2.13 – 2.06 (m, 1H), 1.34 (s, 9H); ¹³C NMR (125 MHz, CDCl₃): δ 151.7, 149.1, 131.4, 127.6, 125.8, 125.8, 92.3, 69.6, 34.7, 31.4, 31.3, 24.5. HRMS calc. for C₁₆H₂₁N₃NaO (M+Na)⁺, 294.1582; found, 294.1574.

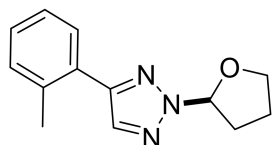


2-(tetrahydrofuran-2-yl)-4-p-tolyl-2H-1,2,3-triazole, Compound **5c** was obtained in 64% yield (29.3 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, CDCl₃): δ 7.83 (s, 1H), 7.68 (d, J = 8.1 Hz, 2H), 7.23 (d, J = 7.9 Hz, 2H), 6.33 – 6.31 (m, 1H), 4.21 – 4.17 (m, 1H), 4.07 – 4.03 (m, 1H), 2.71 – 2.66 (m,

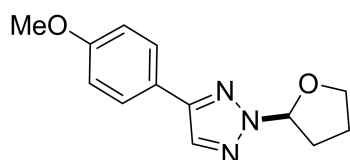
1H), 2.48 – 2.39 (m, 2H), 2.38 (s, 3H), 2.13 – 2.06 (m, 1H); ¹³C NMR (125 MHz, CDCl₃): δ 148.2, 138.4, 131.3, 129.5, 127.5, 126.0, 92.3, 69.6, 31.4, 24.5, 21.3. HRMS calc. for C₁₃H₁₅N₃NaO (M+Na)⁺, 252.1113, found, 252.1106.



2-(tetrahydrofuran-2-yl)-4-m-tolyl-2H-1,2,3-triazole, Compound **5d** was obtained in 67% yield (30.7 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, CDCl₃): δ 7.86 (s, 1H), 7.63 (s, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.16 (d, *J* = 7.5 Hz, 1H), 6.34 – 6.32 (m, 1H), 4.22 – 4.18 (m, 1H), 4.08 – 4.03 (m, 1H), 2.72 – 2.67 (m, 1H), 2.49 – 2.41 (m, 2H), 2.40 (s, 3H), 2.14 – 2.07 (m, 1H); ¹³C NMR (125 MHz, CDCl₃): 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 C₁₃H₁₅N₃NaO (M+Na)⁺, 252.1113; found, 252.1105.

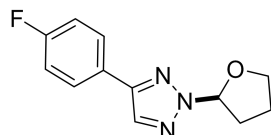


2-(tetrahydrofuran-2-yl)-4-o-tolyl-2H-1,2,3-triazole, Compound **5e** was obtained in 67% yield (30.7 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, CDCl₃): δ 7.81 (s, 1H), 7.59 (d, *J* = 6.2 Hz, 1H), 7.28 – 7.26 (m, 3H), 6.36 (d, *J* = 4.9 Hz, 1H), 4.24 – 4.20 (m, 1H), 4.10 – 4.06 (m, 1H), 2.72 – 2.68 (m, 1H), 2.49 (s, 3H), 2.46 – 2.41 (m, 2H), 2.13 – 2.10 (m, 1H); ¹³C NMR (125 MHz, CDCl₃): δ 147.9, 136.1, 133.6, 131.0, 129.7, 129.0, 128.4, 126.0, 92.3, 69.5, 31.4, 24.5, 21.2. HRMS calc. for C₁₃H₁₅N₃NaO (M+Na)⁺, 252.1113; found, 252.1111.

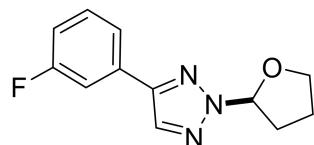


4-(4-methoxyphenyl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5f** was obtained in 80% yield (39.2 mg) according to the general procedure (0.2 mmol). Yellow oil. ¹H NMR (500 MHz, CDCl₃): δ 7.79 (s, 1H), 7.73 – 7.70 (m, 2H), 6.96 – 6.93 (m, 2H), 6.32 – 6.30 (m, 1H), 4.20 – 4.16 (m, 1H), 4.06 – 4.01 (m, 1H), 3.83 (s,

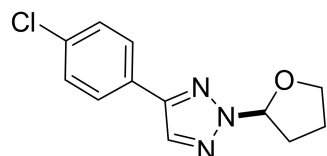
3H), 2.71 – 2.66 (m, 1H), 2.44 – 2.37 (m, 2H), 2.10 – 2.06 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 160.1, 148.1, 131.1, 127.5, 123.2, 114.4, 92.4, 69.7, 55.5, 31.5, 24.7. HRMS calc. for $\text{C}_{13}\text{H}_{15}\text{N}_3\text{NaO}_2$ ($\text{M}+\text{Na}$) $^+$, 268.1062; found, 268.1071.



4-(4-fluorophenyl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5g** was obtained in 74% yield (34.5 g) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 7.81 (s, 1H), 7.77 – 7.74 (m, 2H), 7.10 (t, $J = 8.7$ Hz, 2H), 6.32 – 6.30 (m, 1H), 4.20 – 4.16 (m, 1H), 4.07 – 4.03 (m, 1H), 2.70 – 2.65 (m, 1H), 2.43 – 2.39 (m, 2H), 2.13 – 2.06 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 163.12 (d, $J = 243.7$ Hz), 132.47 (d, $J = 7.5$ Hz), 131.55, 130.39 (d, $J = 7.5$ Hz), 121.67 (d, $J = 2.5$ Hz), 114.12(q, $J = 23.3$ Hz), 92.44, 69.62, 31.38, 24.42. HRMS calc. for $\text{C}_{12}\text{H}_{12}\text{FN}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 256.0862; found, 256.0859.

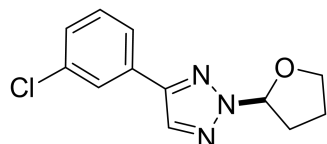


4-(3-fluorophenyl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5h** was obtained in 75 % yield (35.0 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 7.86 (s, 1H), 7.57 – 7.51 (m, 2H), 7.39 – 7.26 (m, 1H), 7.06 – 7.02 (m, 1H), 6.34 – 6.32 (m, 1H), 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 163.16 (d, $J = 243.7$ Hz), 147.01, 132.51 (d, $J = 8.7$ Hz), 131.55, 130.43 (d, $J = 7.5$ Hz), 121.66 (d, $J = 2.5$ Hz), 115.36 (d, $J = 21.3$ Hz), 112.97 (d, $J = 22.5$ Hz), 92.48, 69.67, 31.42, 24.46. HRMS calc. for $\text{C}_{12}\text{H}_{12}\text{FN}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 256.0862; found, 256.0858.

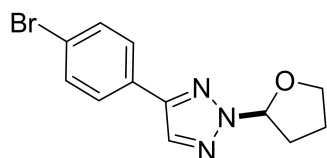


4-(4-chlorophenyl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5i** was obtained in 71% yield (35.4 mg) according to the general procedure (0.2 mmol).

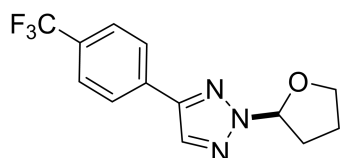
Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 7.84 (s, 1H), 7.74 – 7.71 (m, 2H), 7.41 – 7.38 (m, 2H), 6.33 – 6.32 (m, 1H), 4.22 – 4.17 (m, 1H), 4.08 – 4.04 (m, 1H), 2.72 – 2.66 (m, 1H), 2.48 – 2.40 (m, 2H), 2.14 – 2.07 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 147.1, 134.3, 131.4, 129.1, 128.9, 127.3, 92.4, 69.7, 31.4, 24.5. HRMS calc. for $\text{C}_{12}\text{H}_{12}\text{ClN}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 272.0567; found, 272.0569.



4-(3-chlorophenyl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5j** was obtained in 70% yield (34.9 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 7.86 (s, 1H), 7.81 (t, J = 1.6 Hz, 1H), 7.68 – 7.66 (m, 1H), 7.37 – 7.31 (m, 2H), 6.34 – 6.32 (m, 1H), 4.22 – 4.18 (m, 1H), 4.09 – 4.05 (m, 1H), 2.71 – 2.66 (m, 1H), 2.47 – 2.40 (m, 2H), 2.13 – 2.09 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 146.8, 134.8, 132.1, 131.5, 130.1, 128.5, 126.1, 124.1, 92.50, 69.7, 31.4, 24.5. HRMS calc. for $\text{C}_{12}\text{H}_{12}\text{ClN}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 272.0567; found, 272.0564.



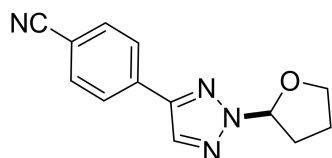
4-(4-bromophenyl)-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5k** was obtained in 66% yield (38.7 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 7.85 (s, 1H), 7.67 (d, J = 8.3 Hz, 2H), 7.55 (d, J = 8.4 Hz, 2H), 6.33 – 6.31 (m, 1H), 4.21 – 4.17 (m, 1H), 4.08 – 4.04 (m, 1H), 2.70 – 2.66 (m, 1H), 2.48 – 2.40 (m, 2H), 2.12 – 2.08 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 147.1, 132.0, 131.4, 129.3, 127.6, 122.5, 92.5, 69.7, 31.4, 24.5. HRMS calc. for $\text{C}_{12}\text{H}_{13}\text{BrN}_3\text{O}$ ($\text{M}+\text{H}$) $^+$, 294.0242; found, 294.0244.



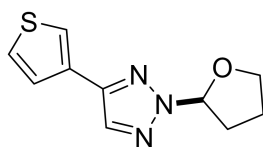
2-(tetrahydrofuran-2-yl)-4-(4-(trifluoromethyl)phenyl)-2H-1,2,3-triazole,

Compound **5l** was obtained in 78% yield (44.1 mg) according to the general

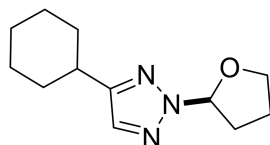
procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 7.92 (s, 1H), 7.91 (d, $J = 8.2$ Hz, 3H), 7.68 (d, $J = 8.2$ Hz, 2H), 6.36 – 6.34 (m, 1H), 4.23 – 4.19 (m, 1H), 4.10 – 4.06 (m, 1H), 2.71 – 2.67 (m, 1H), 2.49 – 2.40 (m, 2H), 2.16 – 2.10 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 146.71, 133.81, 131.78, 130.35 (q, $J = 32.5$ Hz), 126.21, 125.84 (q, $J = 3.7$ Hz), 124.07 (d, $J = 270$ Hz), 92.59, 69.73, 31.45, 24.45. HRMS calc. for $\text{C}_{13}\text{H}_{12}\text{F}_3\text{N}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 306.0830; found, 306.0828.



4-(2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazol-4-yl)benzonitrile, Compound **5m** was obtained in 76% yield (36.5 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 7.93 (s, 1H), 7.91 (d, $J = 8.4$ Hz, 2H), 7.71 (d, $J = 8.4$ Hz, 2H), 6.36 – 6.34 (m, 1H), 4.23 – 4.19 (m, 1H), 4.10 – 4.06 (m, 1H), 2.70 – 2.66 (m, 1H), 2.49 – 2.41 (m, 2H), 2.16 – 2.11 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 146.2, 134.7, 132.7, 132.0, 126.4, 118.7, 111.9, 92.7, 69.8, 31.5, 24.4. HRMS calc. for $\text{C}_{13}\text{H}_{12}\text{N}_4\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 263.0909; found, 263.0906.

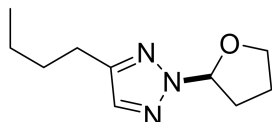


2-(tetrahydrofuran-2-yl)-4-(thiophen-3-yl)-2H-1,2,3-triazole, Compound **5n** was obtained in 77% yield (34.0 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 7.76 (s, 1H), 7.63 – 7.62 (m, 1H), 7.46 – 7.45 (m, 1H), 7.38 – 7.37 (m, 1H), 6.32 – 6.30 (m, 1H), 4.20 – 4.16 (m, 1H), 4.07 – 4.03 (m, 1H), 2.72 – 2.66 (m, 1H), 2.48 – 2.36 (m, 2H), 2.12 – 2.05 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 143.9, 131.7, 131.6, 126.4, 126.0, 121.8, 92.3, 69.6, 31.3, 24.5. HRMS calc. for $\text{C}_{10}\text{H}_{11}\text{N}_3\text{ONaS}$ ($\text{M}+\text{Na}$) $^+$, 244.0521; found, 244.0517.

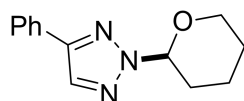


4-cyclohexyl-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5o** was obtained in 66% yield (29.2 mg) according to the general procedure (0.2 mmol).

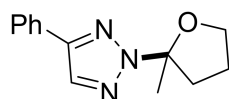
Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 7.52 (s, 1H), 6.52 (s, 1H), 6.18 (d, $J = 6.4$ Hz, 1H), 4.10 – 4.08 (m, 1H), 4.06 – 4.02 (m, 1H), 2.81 – 2.66 (m, 1H), 2.44 – 2.38 (m, 3H), 2.29 – 1.93 (m, 5H), 1.72 (m, 5H); ^{13}C NMR (125 MHz, CDCl_3): δ 149.4, 127.3, 125.0, 116.9, 89.4, 69.5, 32.1, 26.4, 25.3, 23.9, 22.5, 22.2. HRMS calc. for $\text{C}_{12}\text{H}_{19}\text{N}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 244.1426; found, 244.1425.



4-butyl-2-(tetrahydrofuran-2-yl)-2H-1,2,3-triazole, Compound **5p** was obtained in 78% yield (30.4 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 7.39 (s, 1H), 6.24 – 6.23 (m, 1H), 4.14 – 4.10 (m, 1H), 4.03 – 4.00 (m, 1H), 2.70 – 2.65 (m, 2H), 2.43 – 2.32 (m, 2H), 2.10 – 2.01 (m, 1H), 1.64 (m, 2H), 1.38 (m, 2H), 1.33 – 1.22 (m, 1H), 0.93 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (125 MHz, CDCl_3): δ 149.2, 133.2, 91.8, 69.4, 31.3, 31.1, 25.3, 24.6, 22.4, 13.8; HRMS calc. for $\text{C}_{10}\text{H}_{17}\text{N}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 218.1269; found, 218.1267.

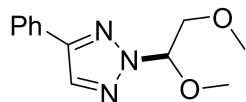


4-phenyl-2-(tetrahydro-2H-pyran-2-yl)-2H-1,2,3-triazole^[1], Compound **5q** was obtained in 78% yield (35.7 mg) according to the general procedure (0.2 mmol). Yellow solid, mp = 69.7 °C – 70.3°C. ^1H NMR (500 MHz, CDCl_3): δ 7.97 (s, 1H), 7.85 (d, $J = 7.8$ Hz, 2H), 7.42 (t, $J = 7.6$ Hz, 2H), 7.33 (t, $J = 7.4$ Hz, 1H), 5.76 – 5.74 (m, 1H), 4.05 – 4.02 (m, 1H), 3.80 – 3.71 (m, 1H), 2.24 – 2.12 (m, 2H), 2.09 – 2.02 (m, 1H), 1.81 – 1.67 (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 $\text{C}_{13}\text{H}_{15}\text{N}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 252.1113; found, 252.1109.

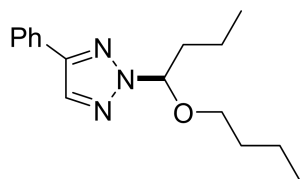


2-(5-methyltetrahydrofuran-2-yl)-4-phenyl-2H-1,2,3-triazole, Compound **5r** was obtained in 40% yield (18.3 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 7.79 (s, 1H), 7.74 (d, $J = 7.4$ Hz, 2H), 7.35 (t, $J = 7.5$ Hz, 2H), 7.27 (t, $J = 7.4$ Hz, 1H), 4.08 – 4.04 (m, 1H), 4.00 – 3.95 (m, 1H),

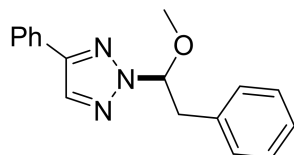
3.07 – 3.03 (m, 1H), 2.17 – 2.04 (m, 3H), 1.99 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 147.7, 131.0, 130.8, 128.9, 128.5, 126.2, 100.4, 69.7, 37.7, 26.2, 25.0. HRMS calc. for $\text{C}_{13}\text{H}_{15}\text{N}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 252.1113; found, 252.1110.



2-(1,2-dimethoxyethyl)-4-phenyl-2H-1,2,3-triazole, Compound **5s** was obtained in 57% yield (26.6 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 8.02 (s, 1H), 7.88 – 7.86 (m, 2H), 7.45 – 7.42 (m, 2H), 7.36 – 7.34 (m, 1H), 5.82 (t, J = 4.6 Hz, 1H), 3.86 – 3.84 (m, 1H), 3.83 – 3.80 (m, 1H), 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 $\text{C}_{12}\text{H}_{15}\text{N}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 256.1062; found, 256.1059.



2-(1-butoxybutyl)-4-phenyl-2H-1,2,3-triazole, Compound **5t** was obtained in 30% yield (16.4 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 7.83 (s, 1H), 7.80 – 7.79 (m, 2H), 7.38 – 7.35 (m, 2H), 7.29 – 7.27 (m, 2H), 5.66 (t, J = 6.6 Hz, 1H), 3.42 – 3.38 (m, 1H), 3.28 – 3.26 (m, 1H), 2.01 – 1.96 (m, 1H), 1.88 – 1.83 (m, 1H), 1.47 – 1.43 (m, 2H), 1.28 – 1.23 (m, 3H), 0.92 – 0.87 (m, 3H), 0.81 – 0.79 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 148.3, 130.7, 128.9, 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 $\text{C}_{16}\text{H}_{23}\text{F}_3\text{N}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 296.1739; found, 296.1737.



2-(1-methoxy-2-phenylethyl)-4-phenyl-2H-1,2,3-triazole, Compound **5u** was obtained in 51% yield (28.5 mg) according to the general procedure (0.2 mmol). Yellow oil. ^1H NMR (500 MHz, CDCl_3): δ 7.84 – 7.81 (m, 3H), 7.43 (t, J = 7.7 Hz, 2H), 7.34 (t, J = 7.4 Hz, 1H), 7.30 – 7.25 (m, 4H), 7.17 (d, J = 6.6 Hz, 2H), 5.86 –

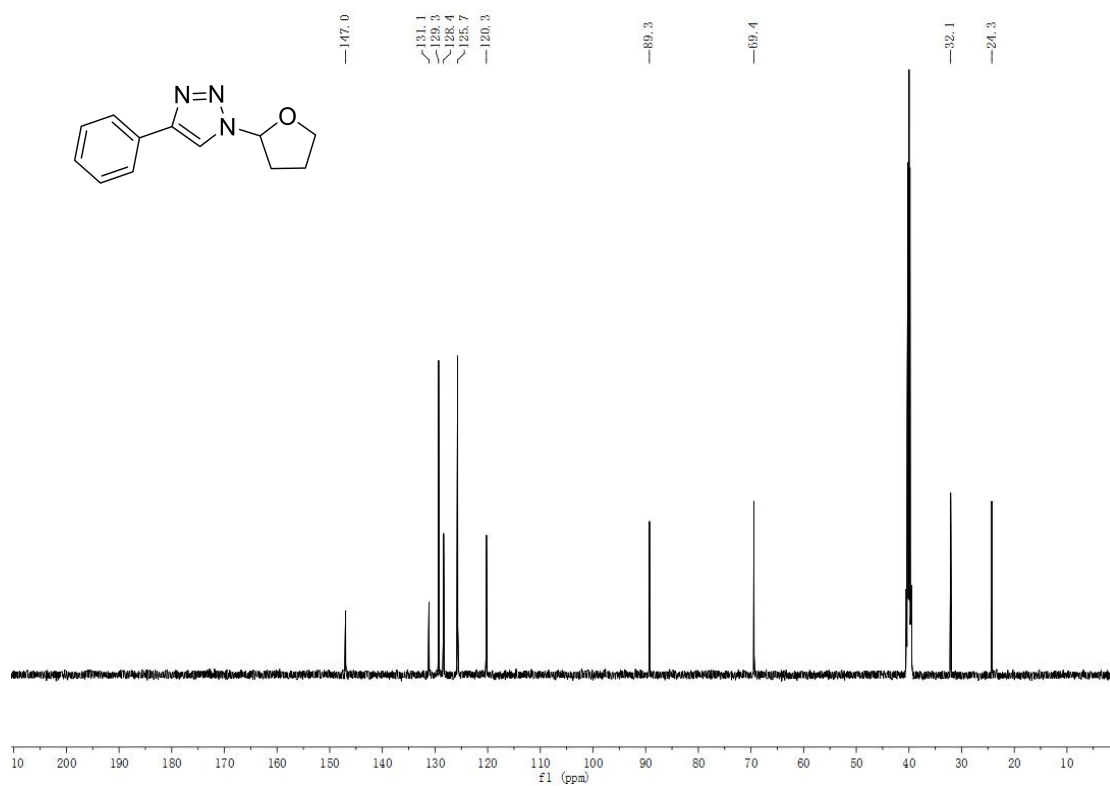
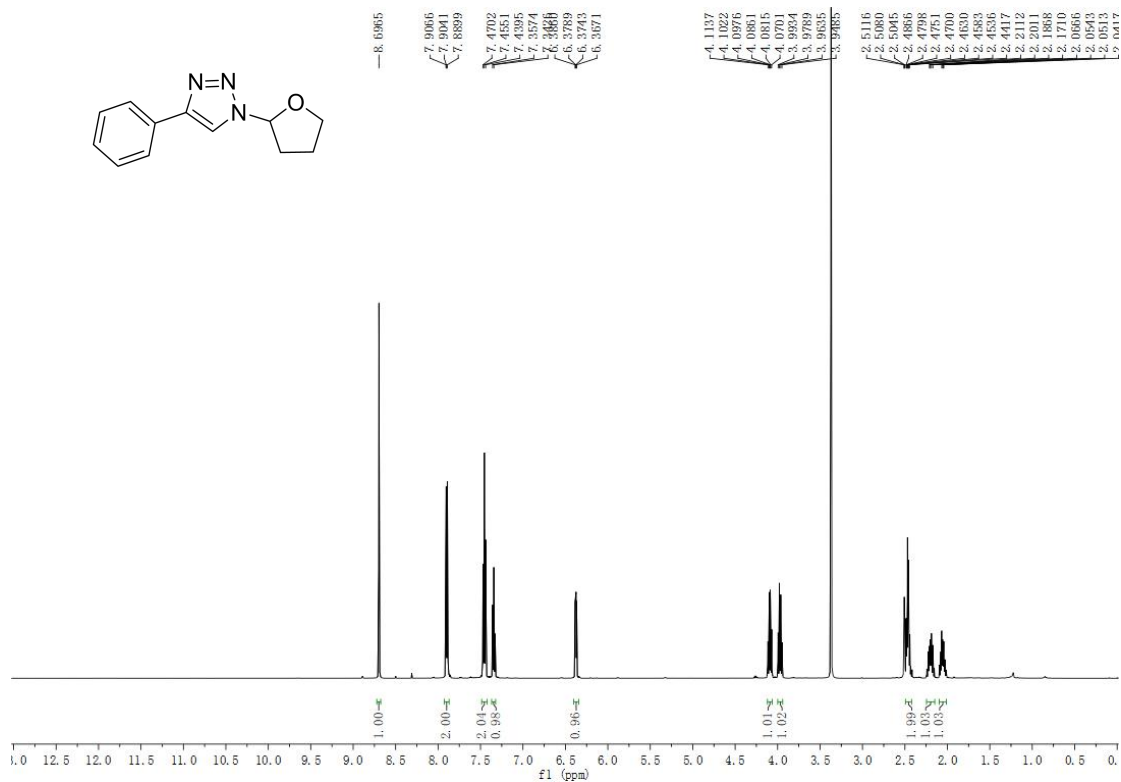
5.83 (m, 1H), 3.38 – 3.34 (m, 1H), 3.29 (s, 3H), 3.28 – 3.27 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 148.2, 134.7, 130.5, 129.5, 128.9, 128.6, 128.3, 127.3, 125.8, 116.8, 92.1, 57.0, 42.4. HRMS calc. for $\text{C}_{17}\text{H}_{17}\text{N}_3\text{NaO}$ ($\text{M}+\text{Na}$) $^+$, 302.1269; found, 302.1273.

References:

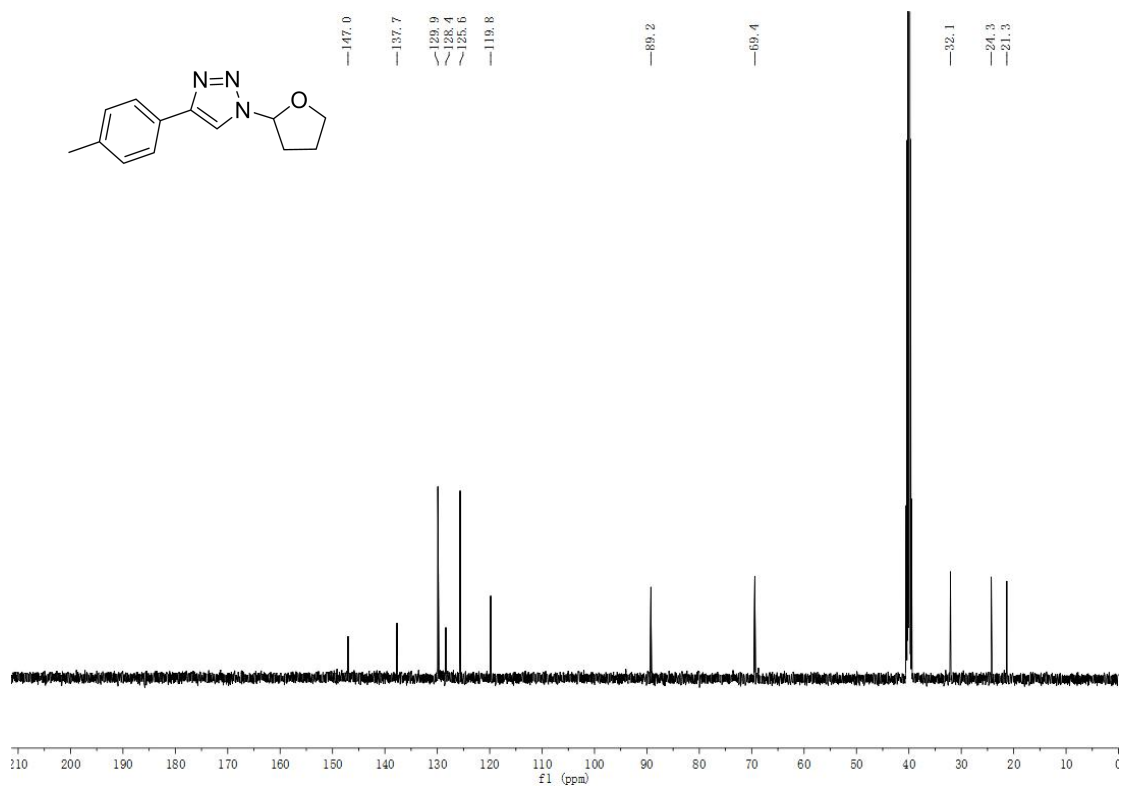
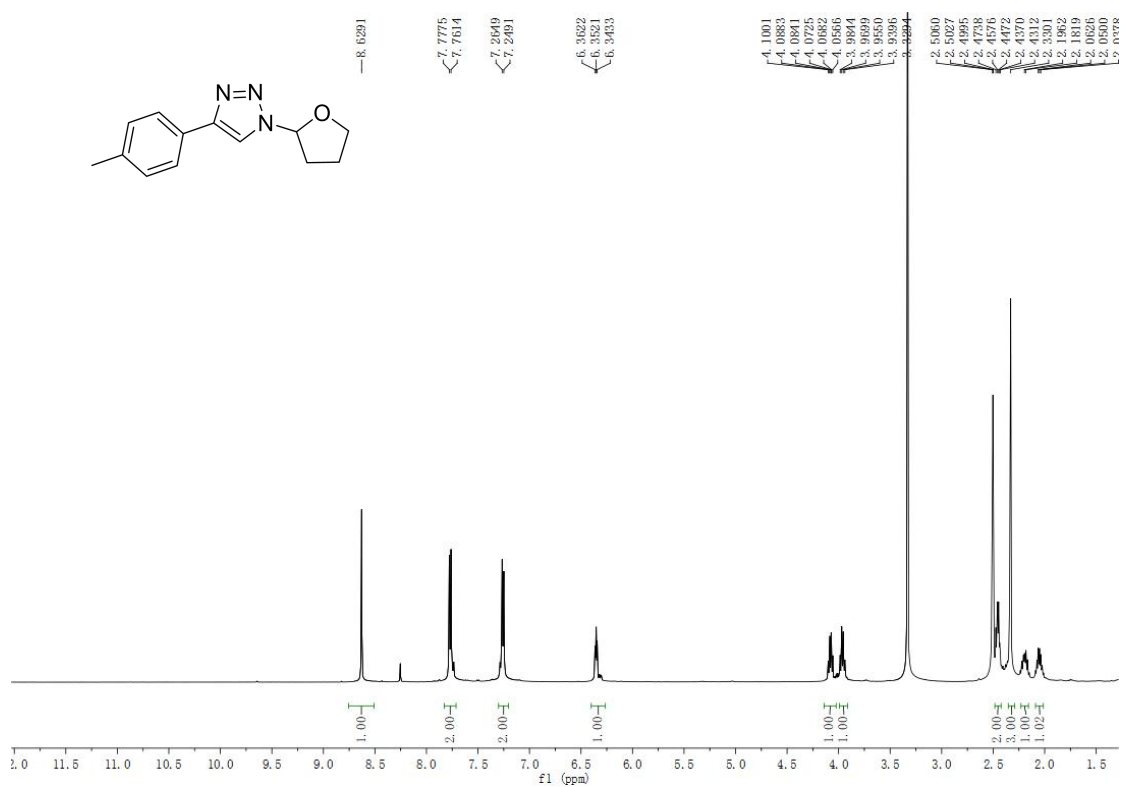
- [1] (a) Luo, G.; Sun, C.; Li, Y.; Li, X.; Zhao, Z. *RSC Adv.* **2018**, 8, 27610-27615. (b) Ma, T.; Sun, C. Y.; Yuan, X.; Li, X. X.; Zhao, Z. G. *RSC Adv.*, **2017**, 7, 1062-1066.

6. Copies of NMR Spectra for 4a-5u

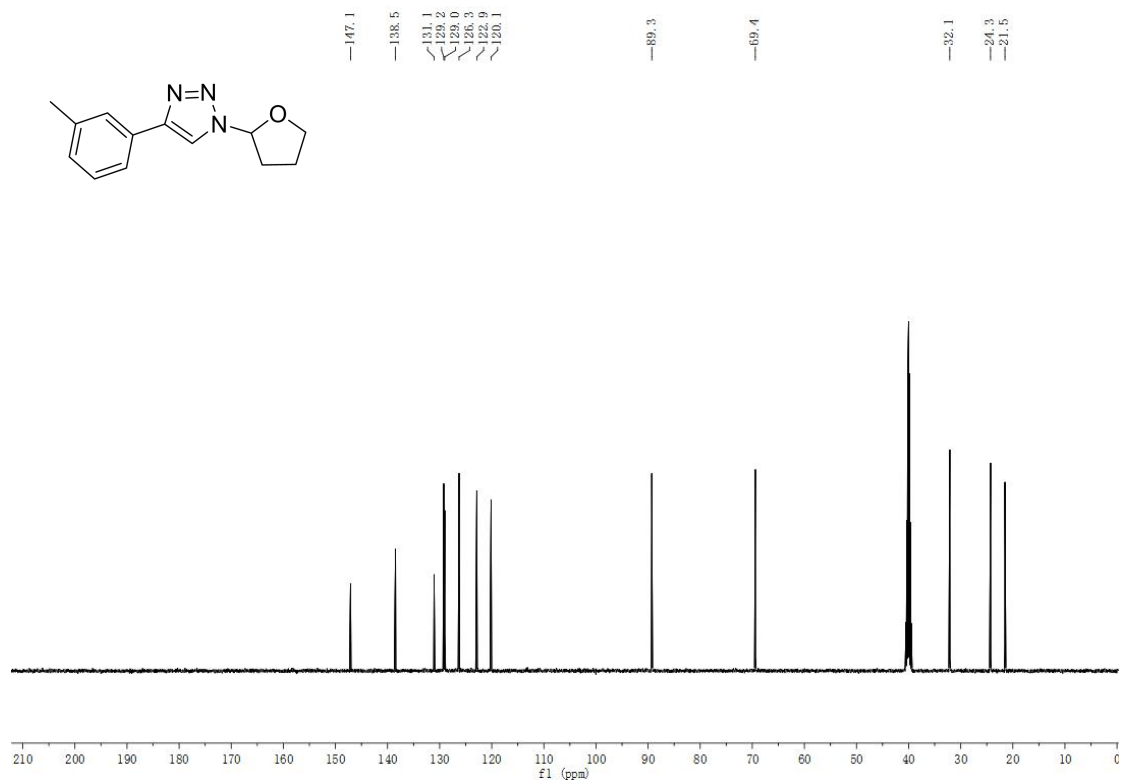
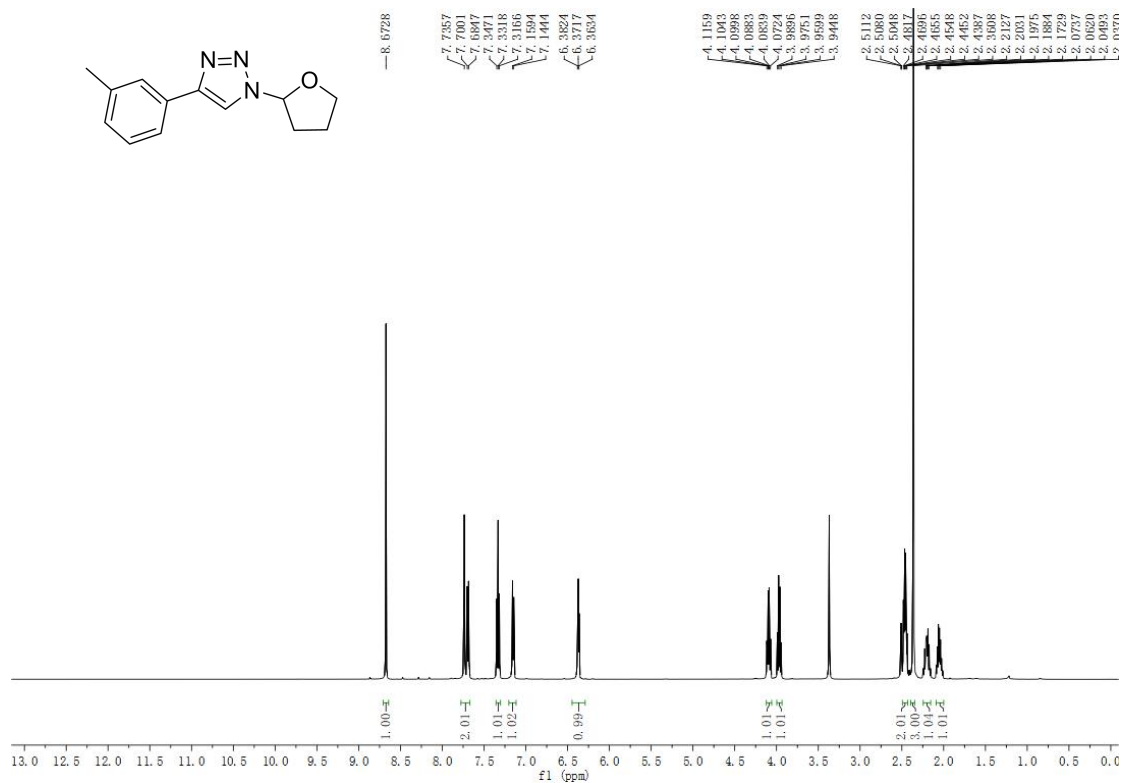
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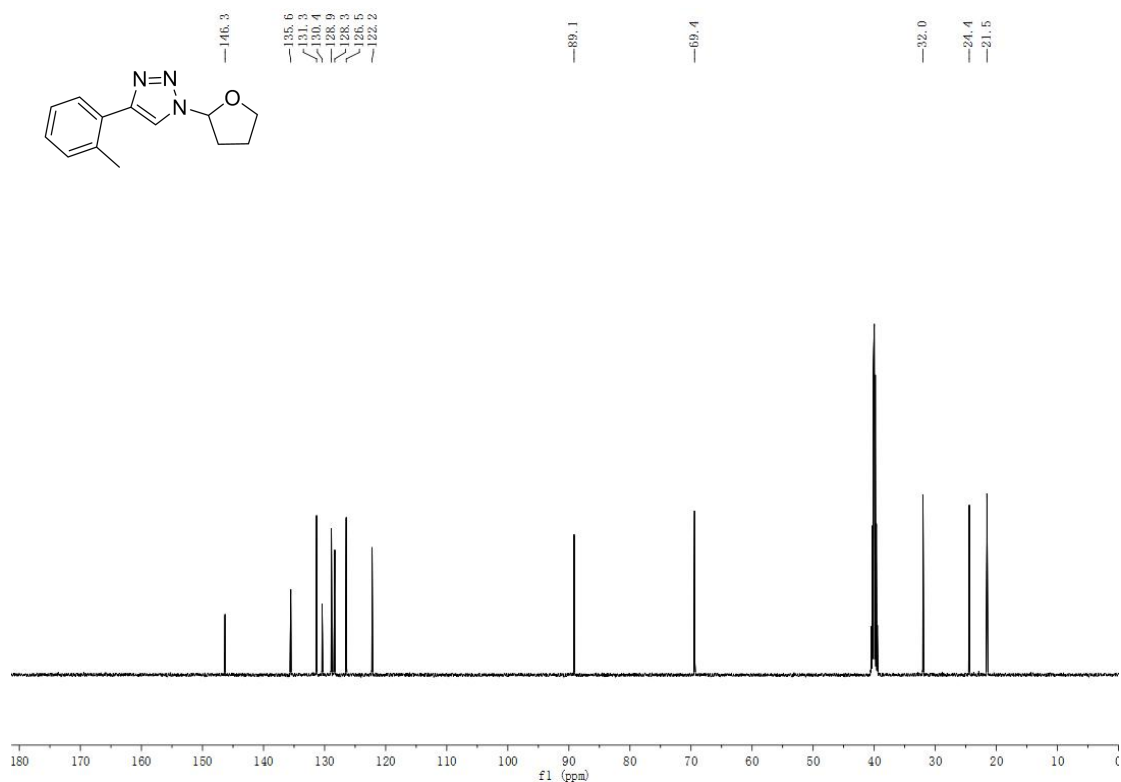
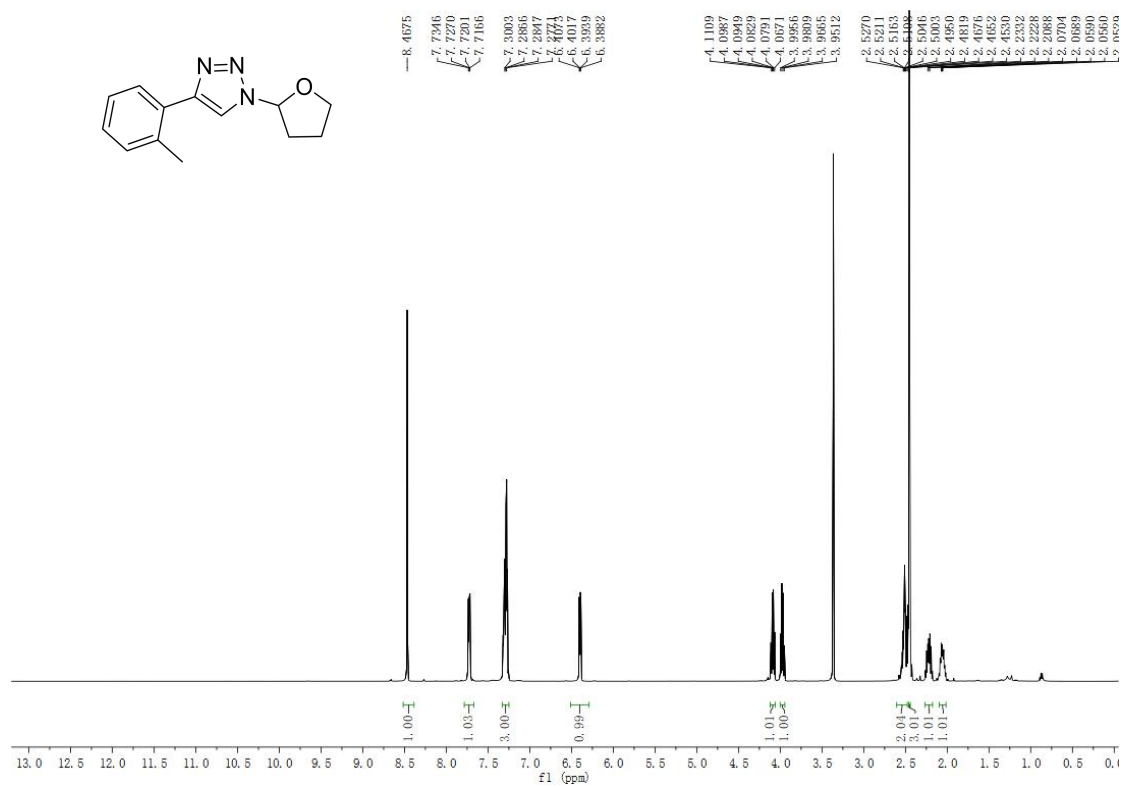
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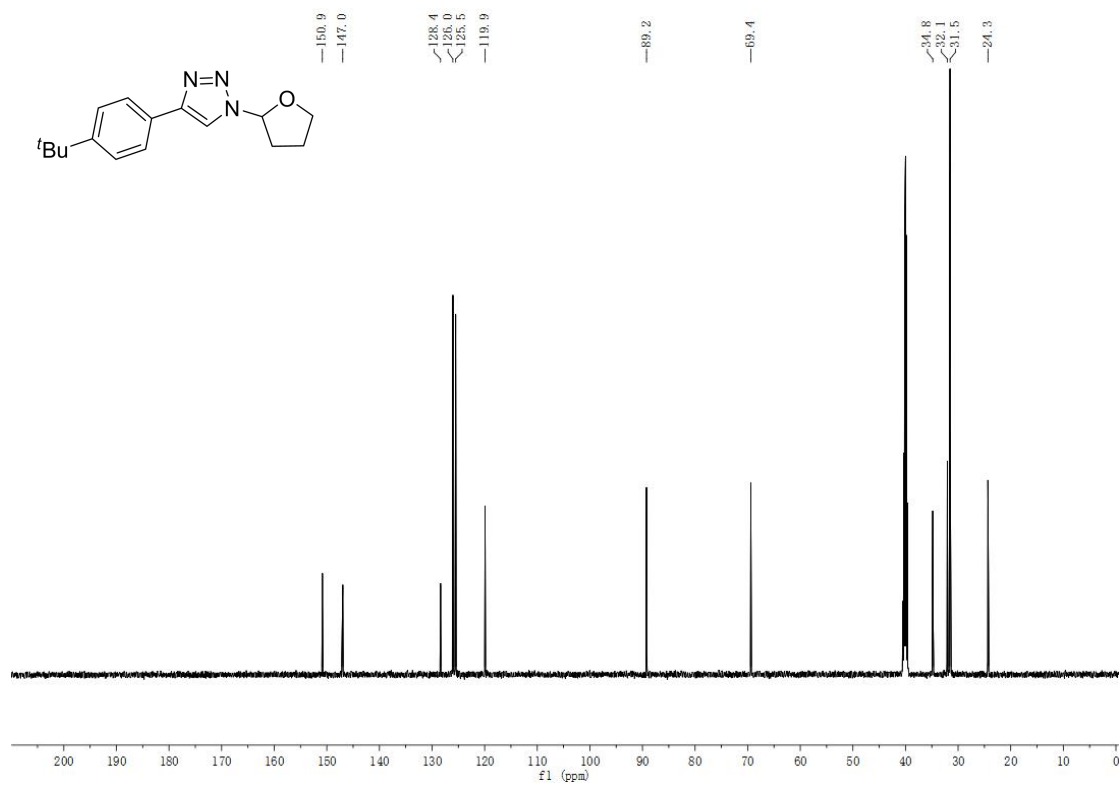
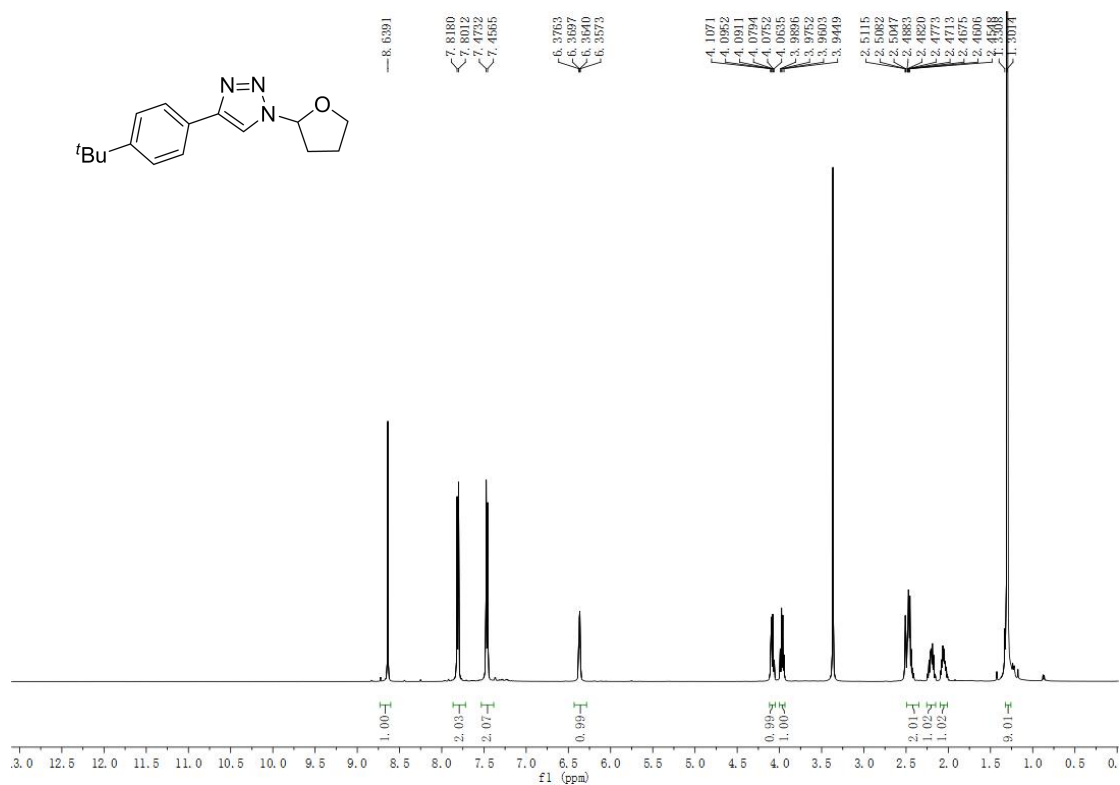
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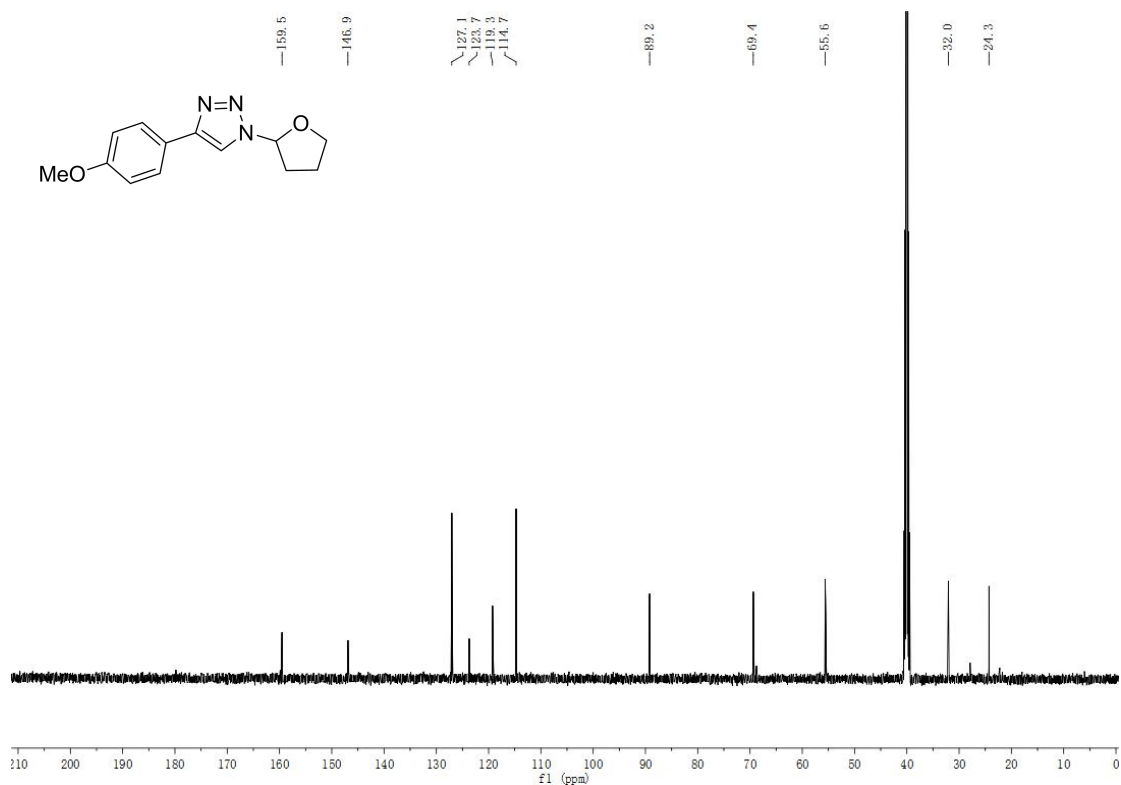
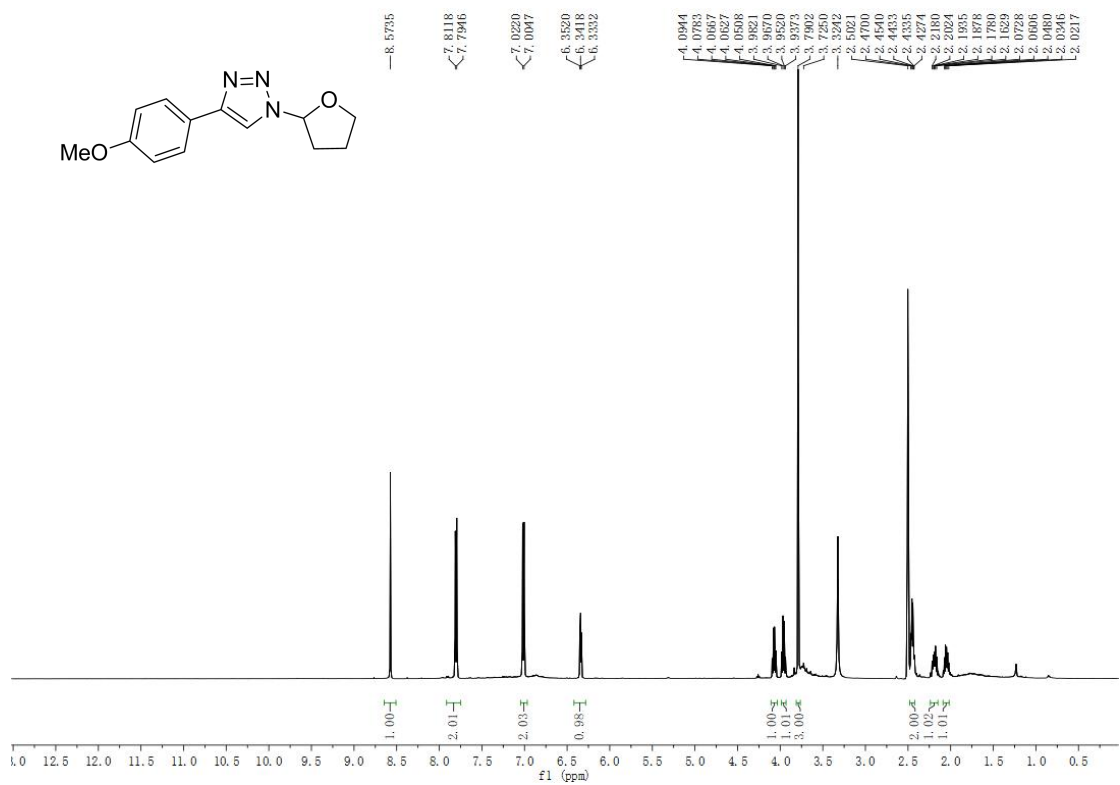
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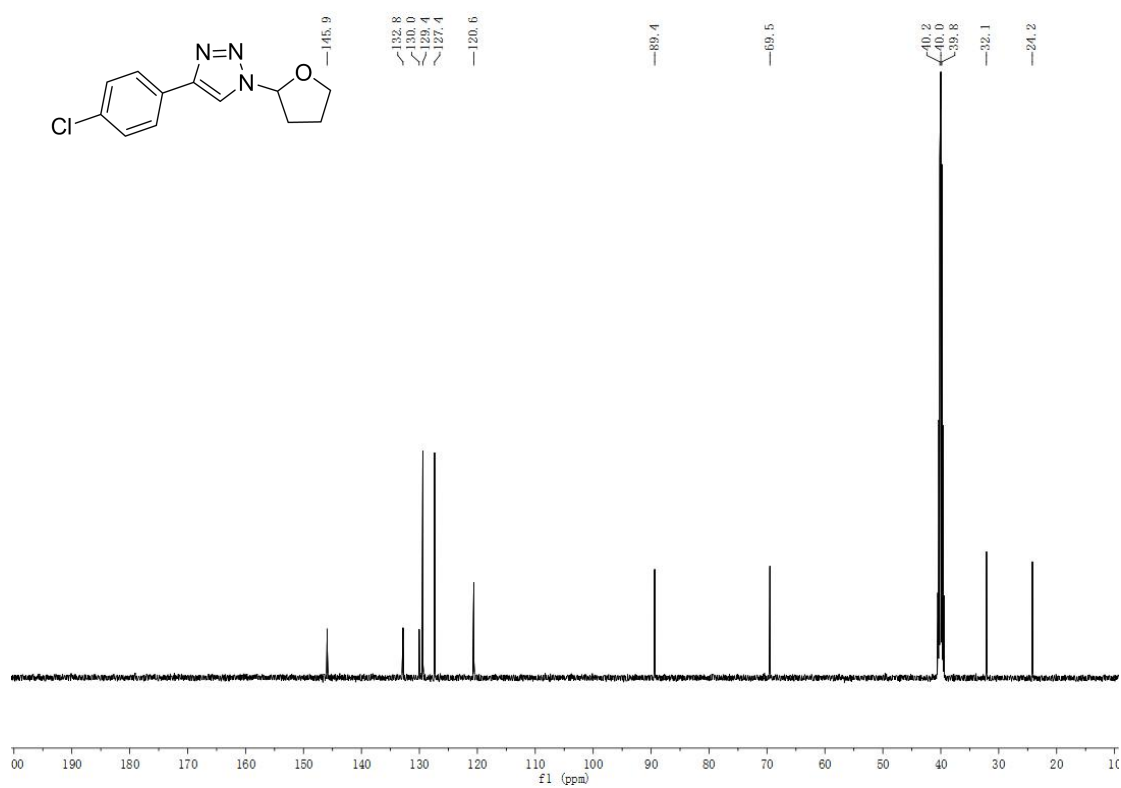
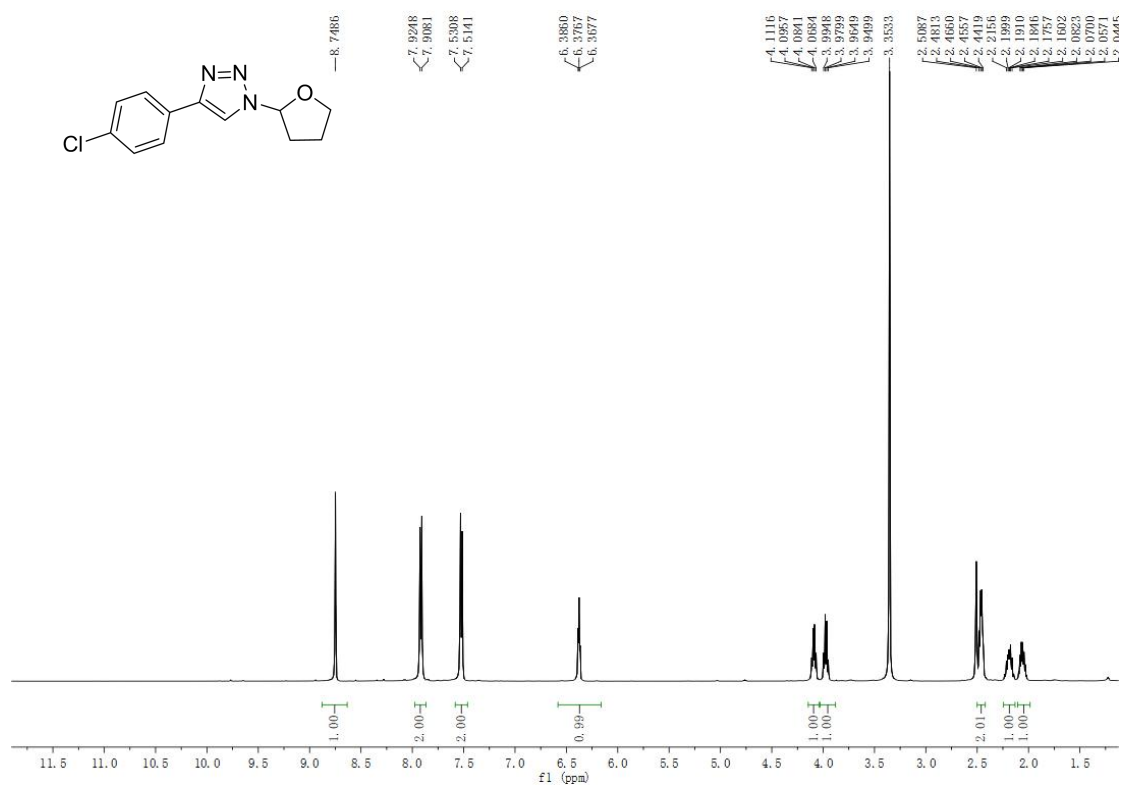
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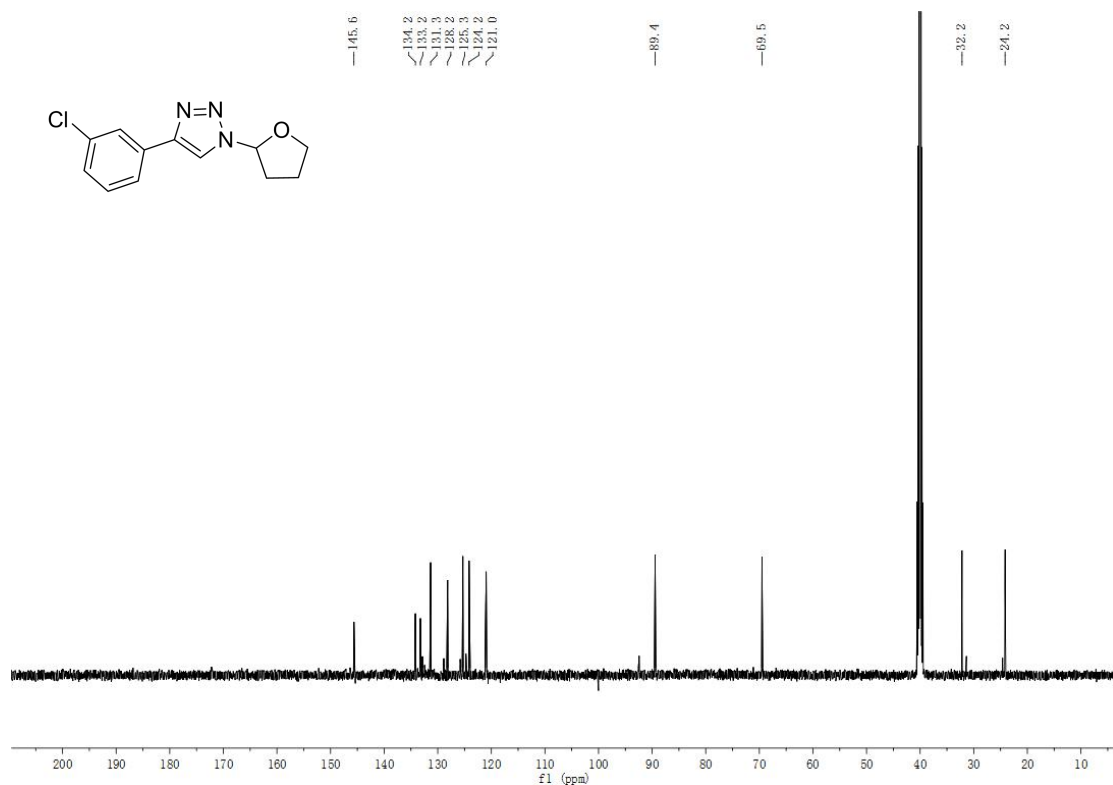
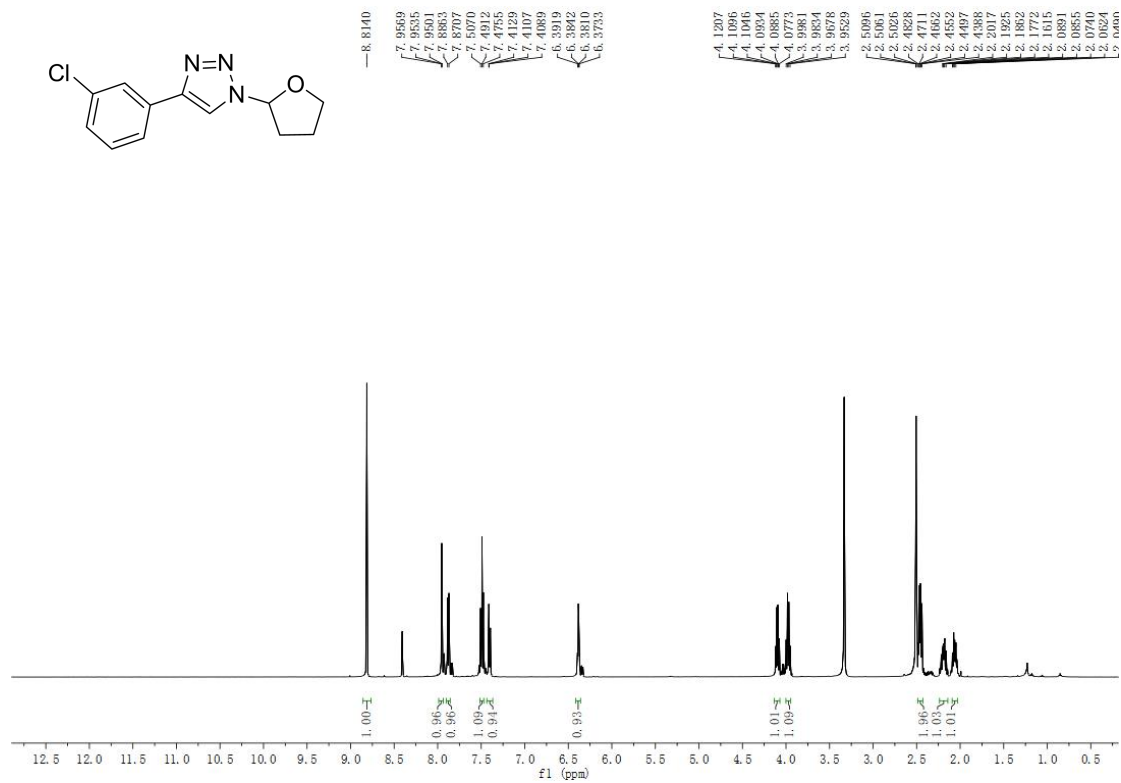
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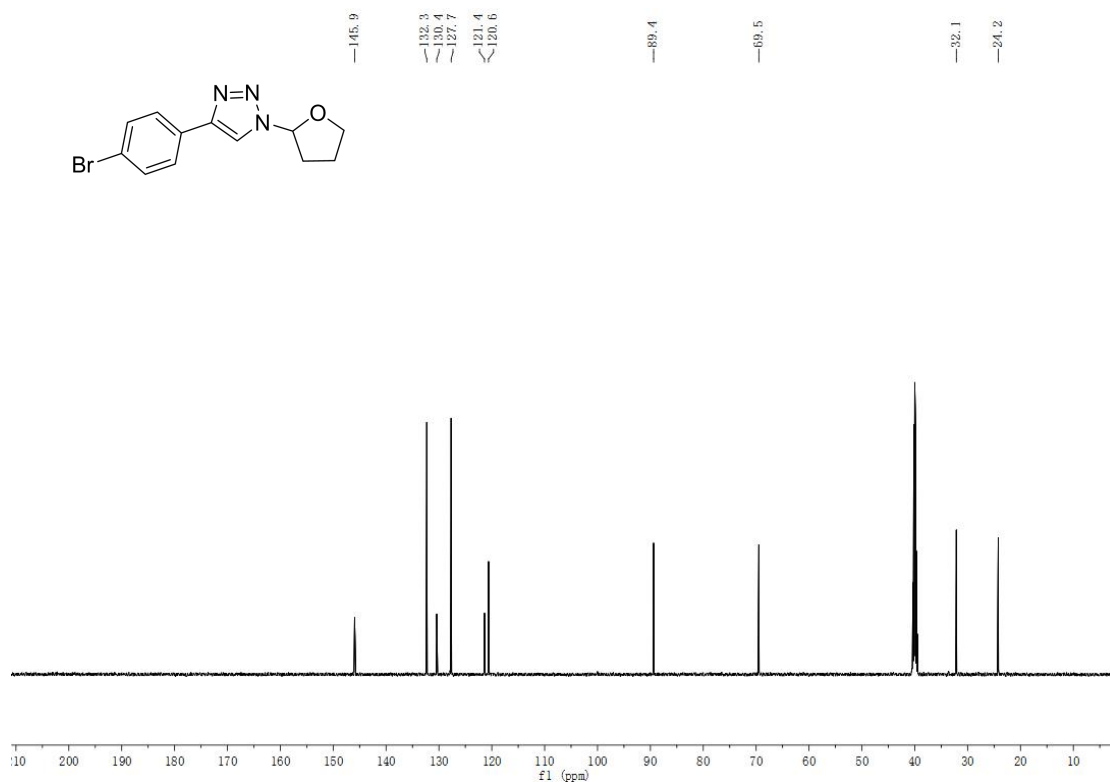
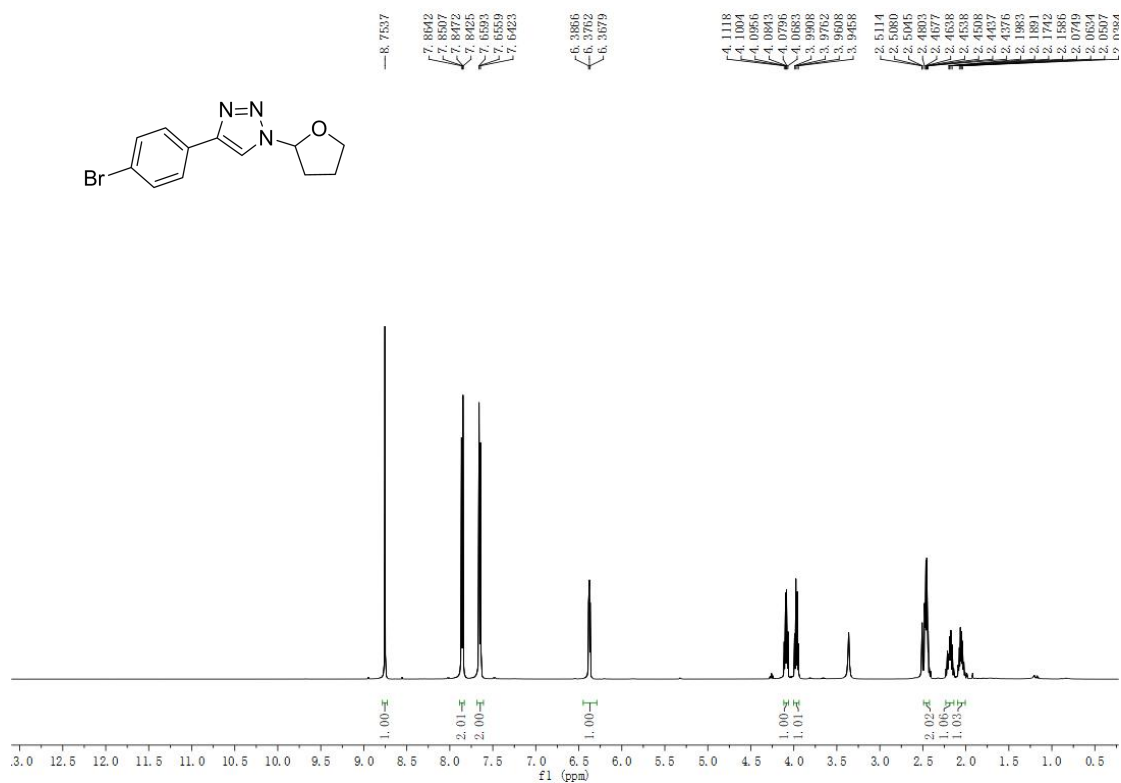
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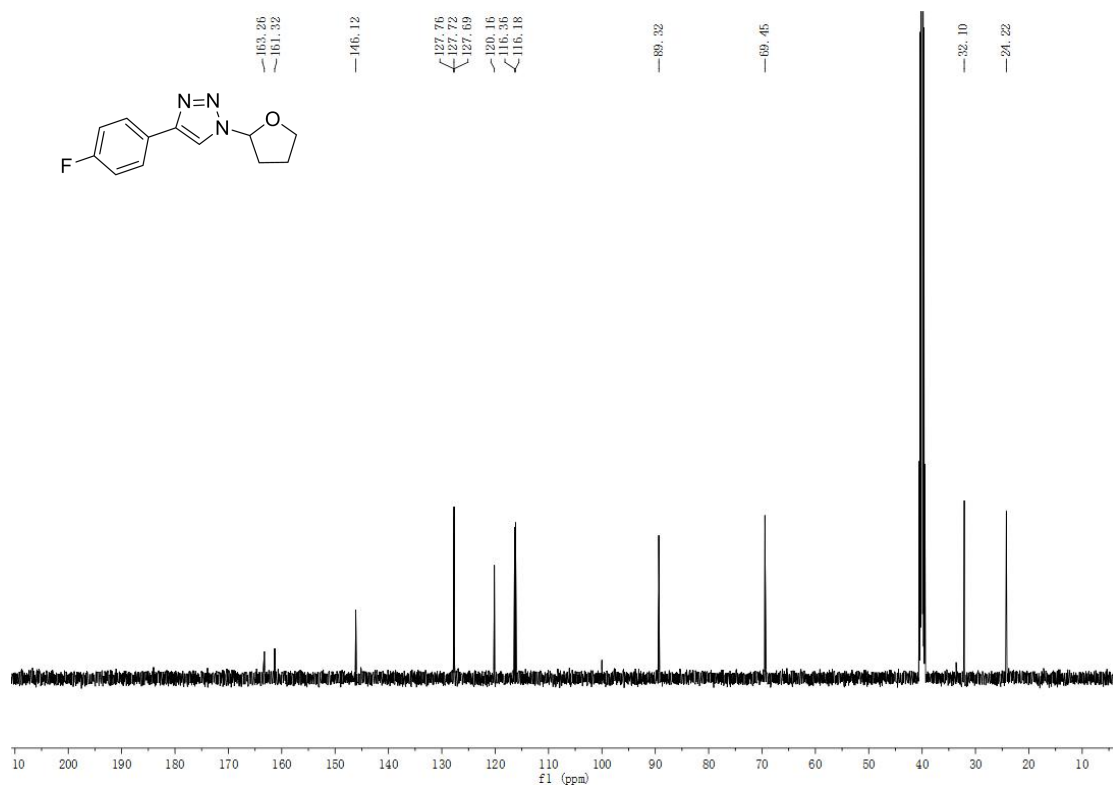
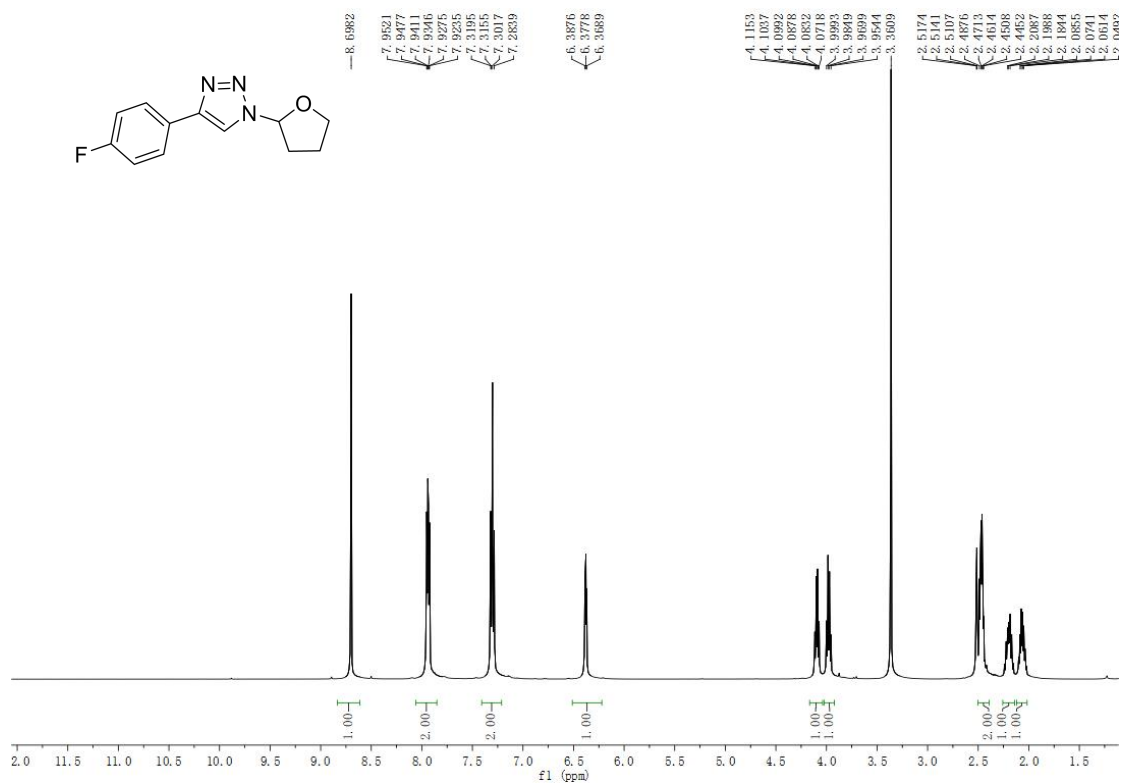
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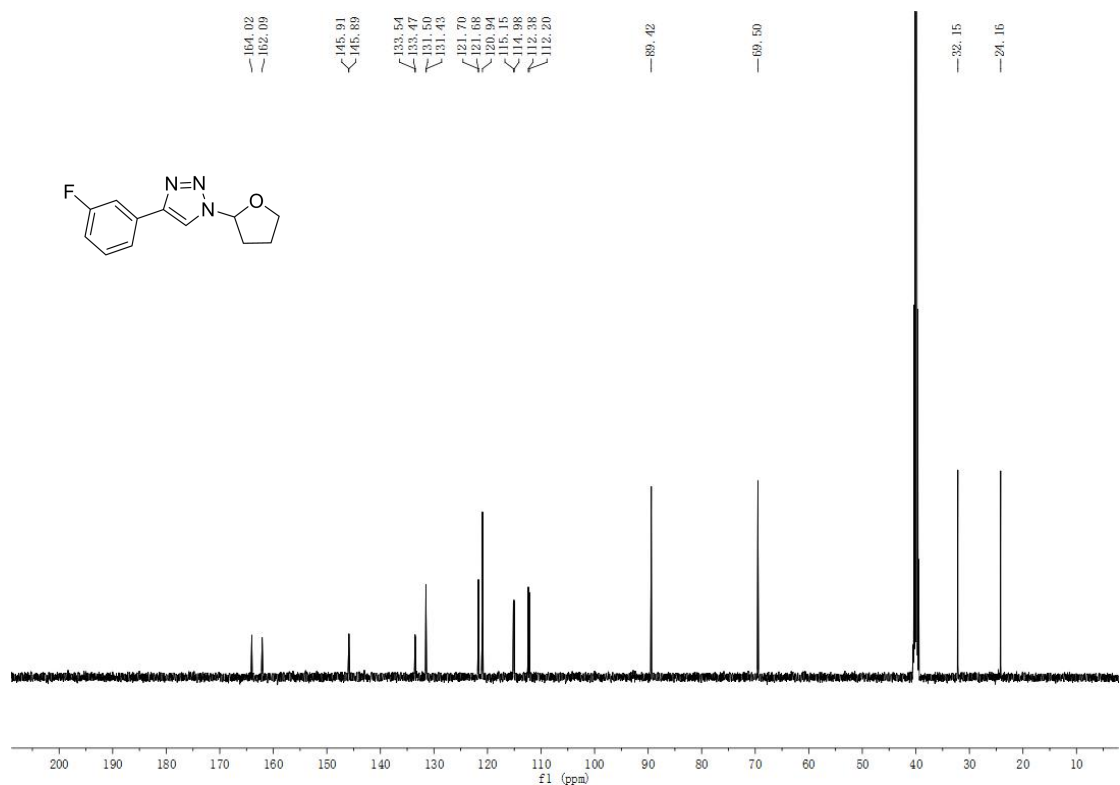
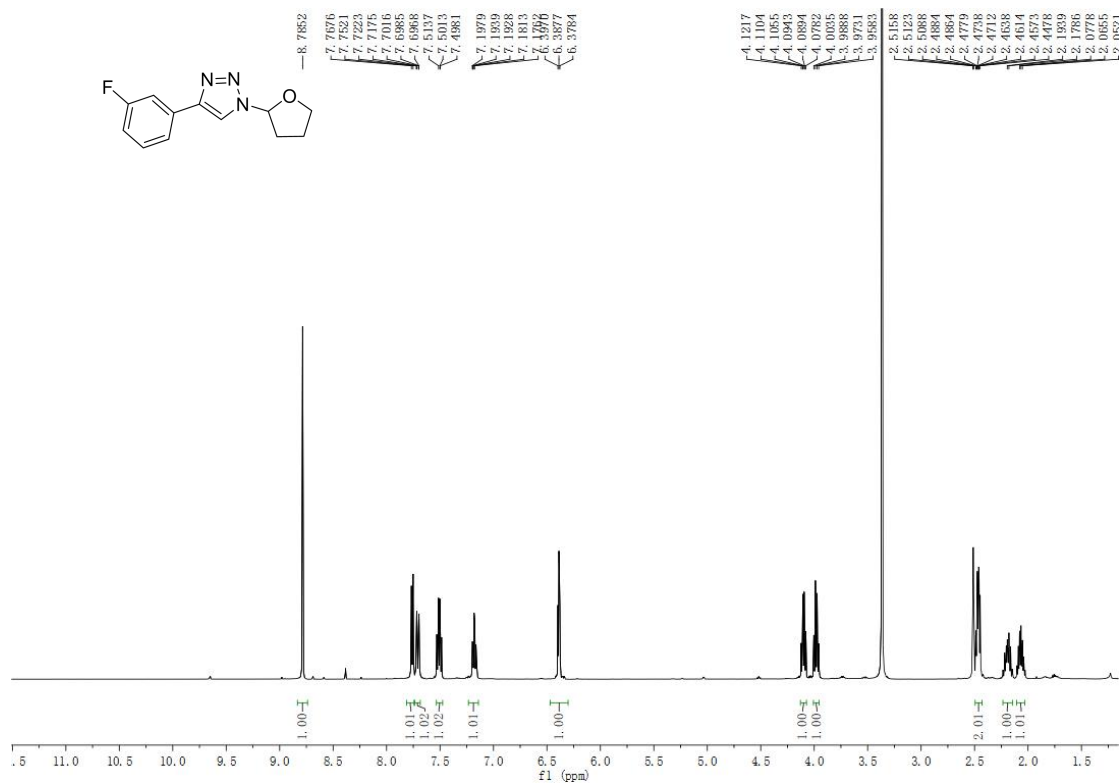
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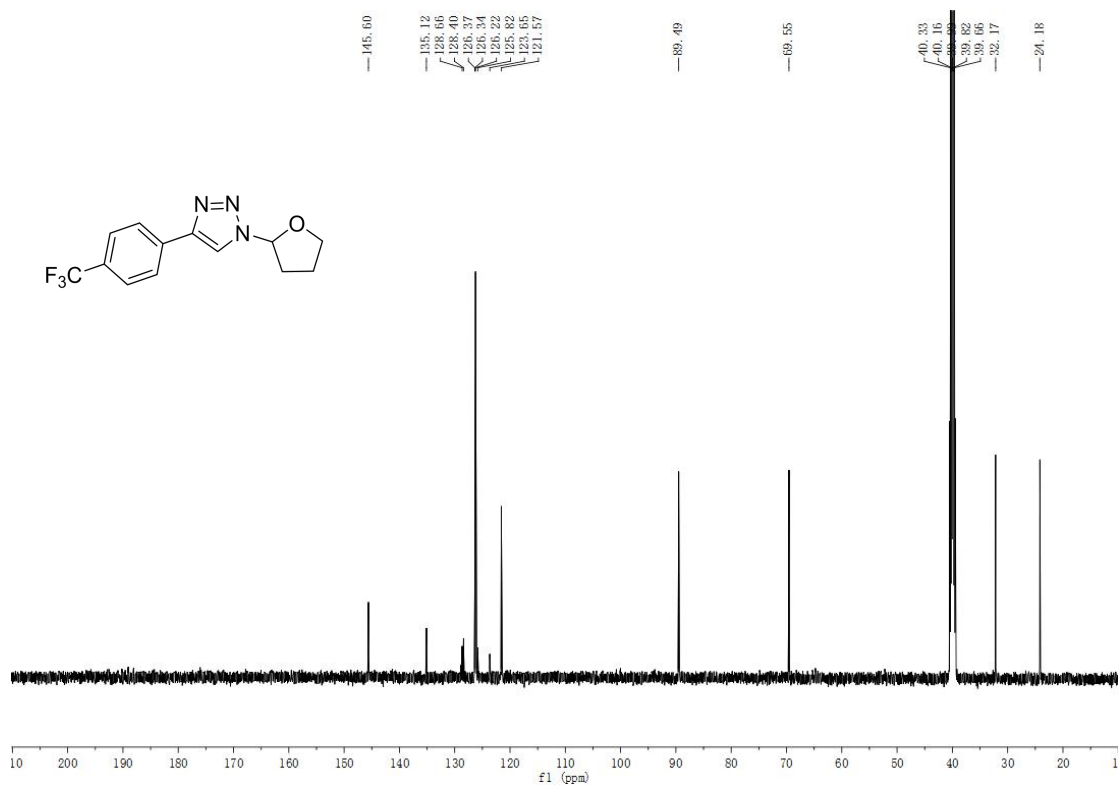
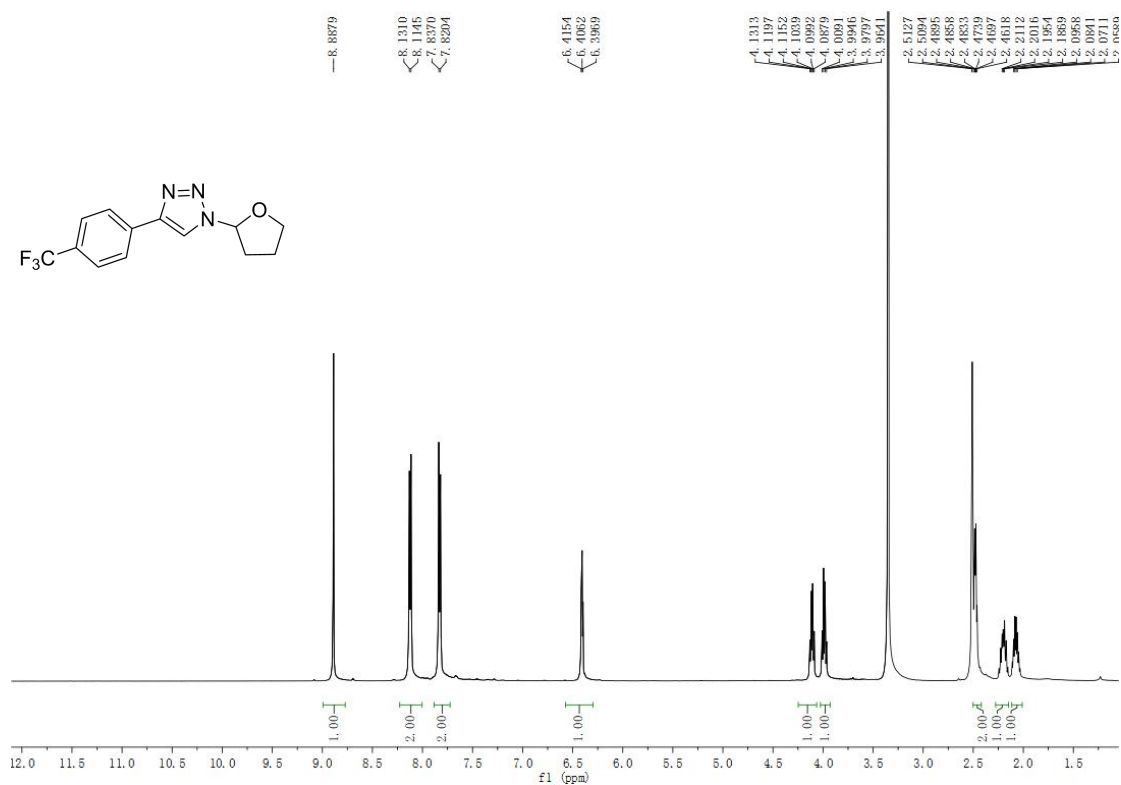
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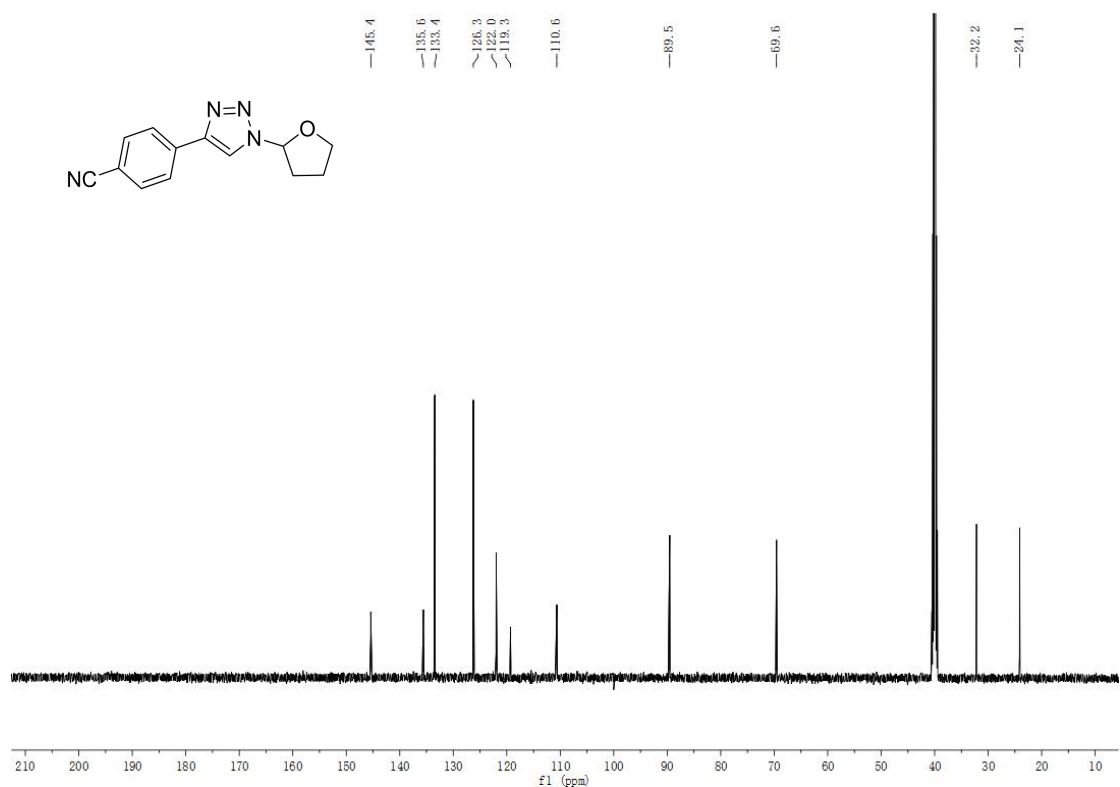
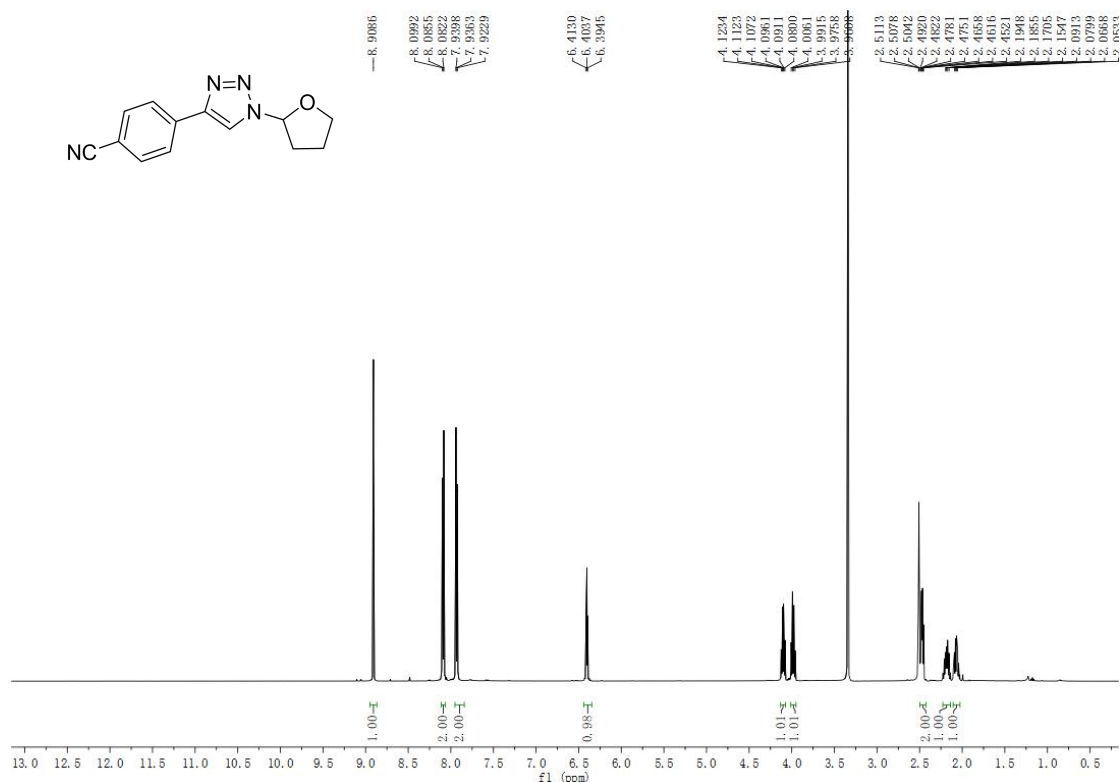
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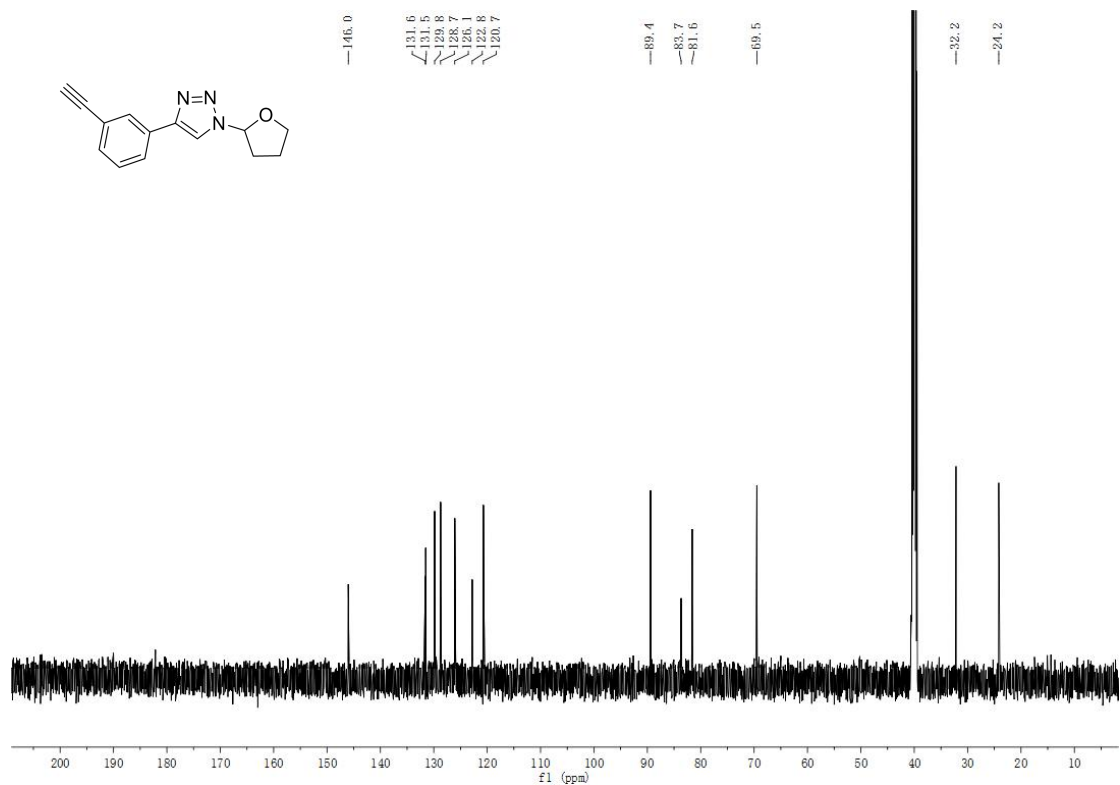
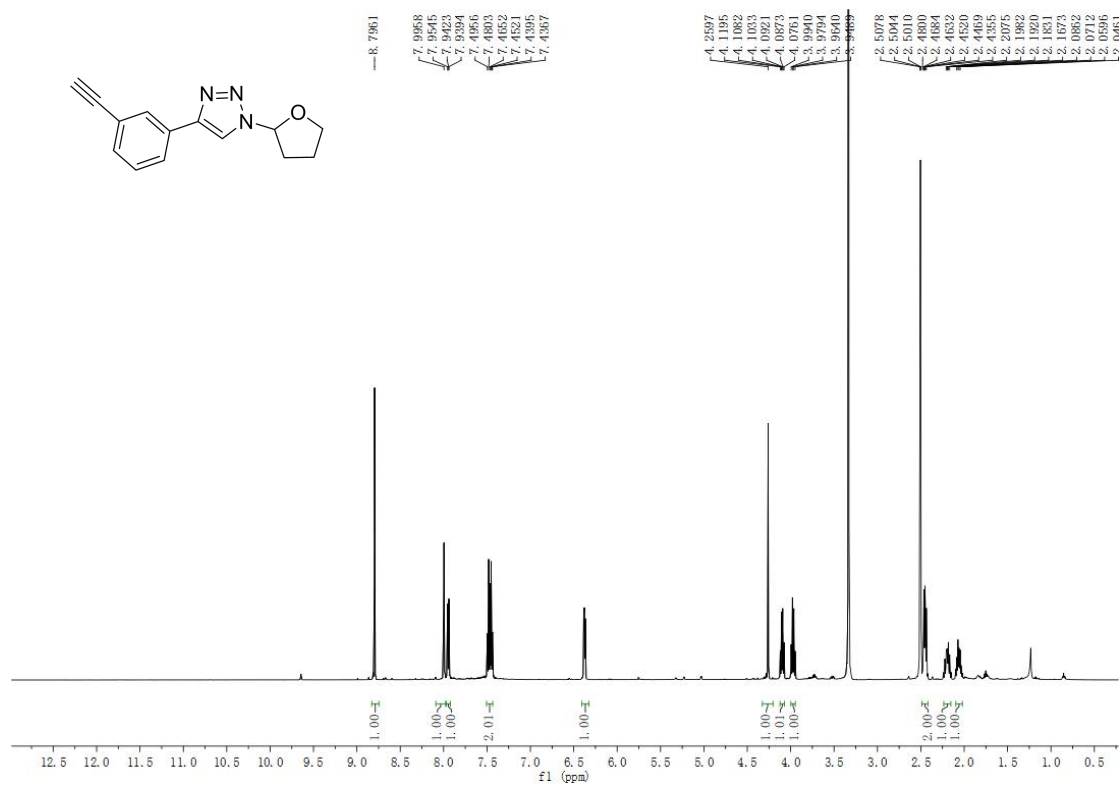
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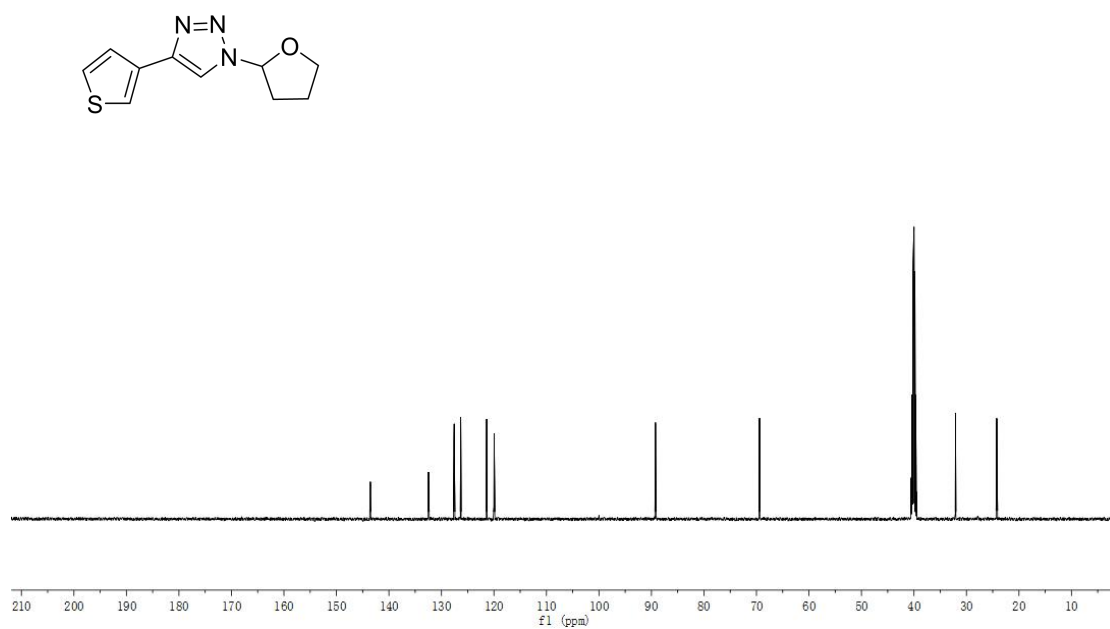
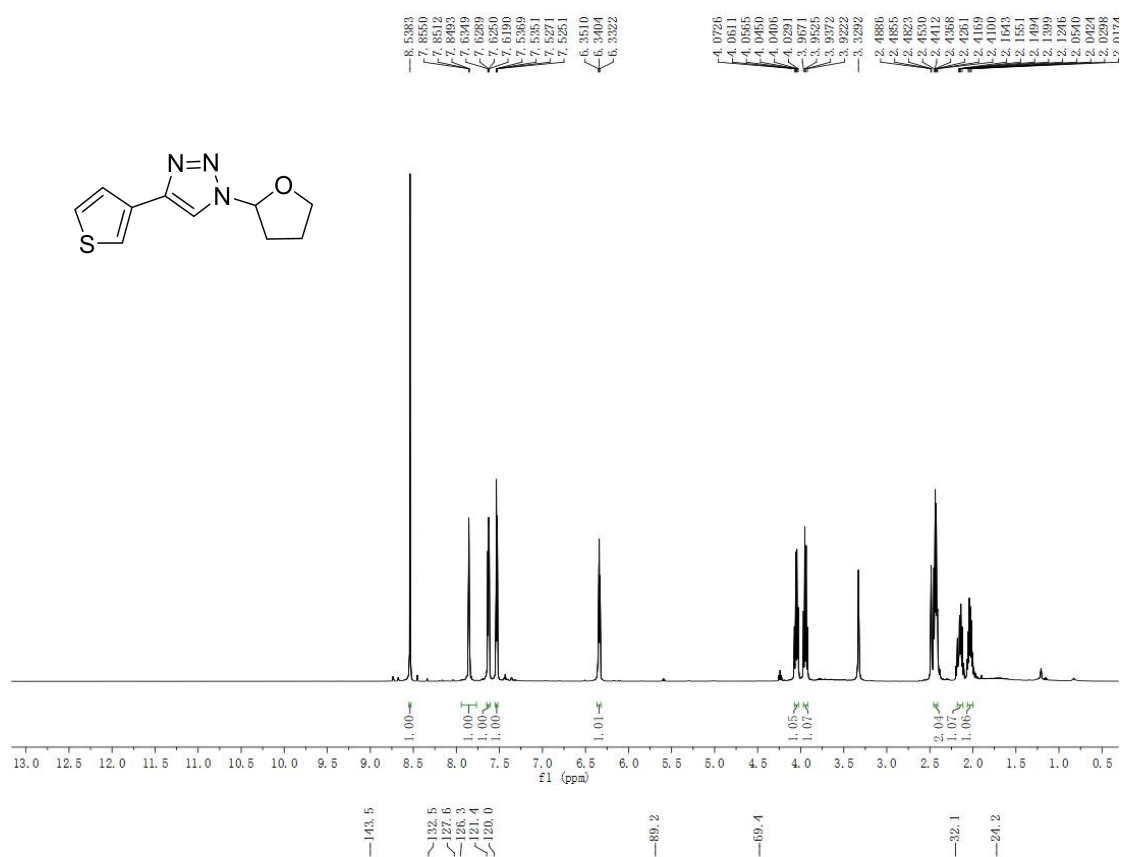
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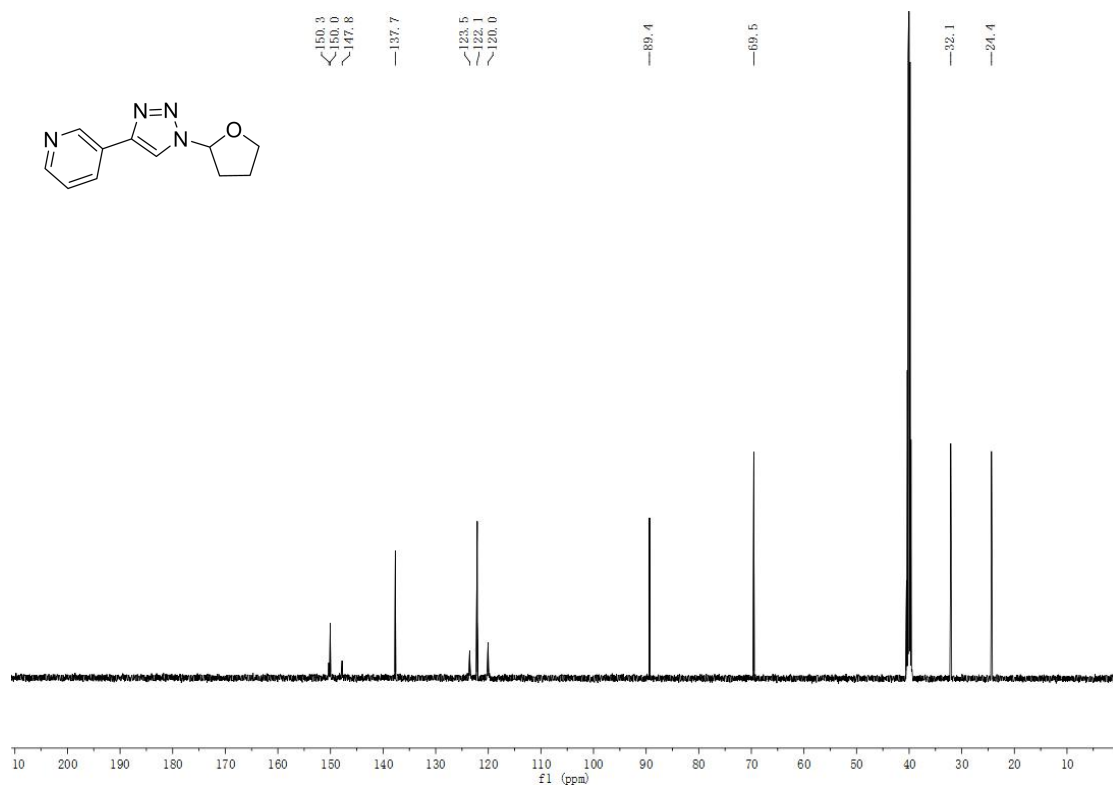
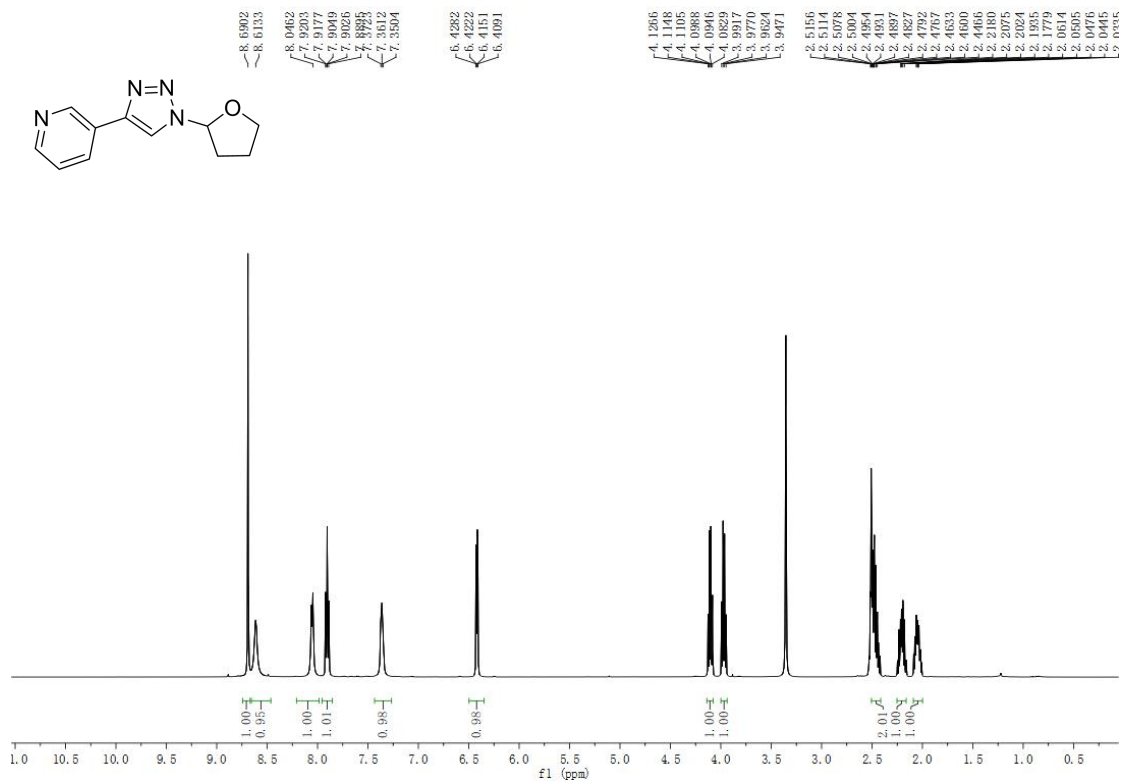
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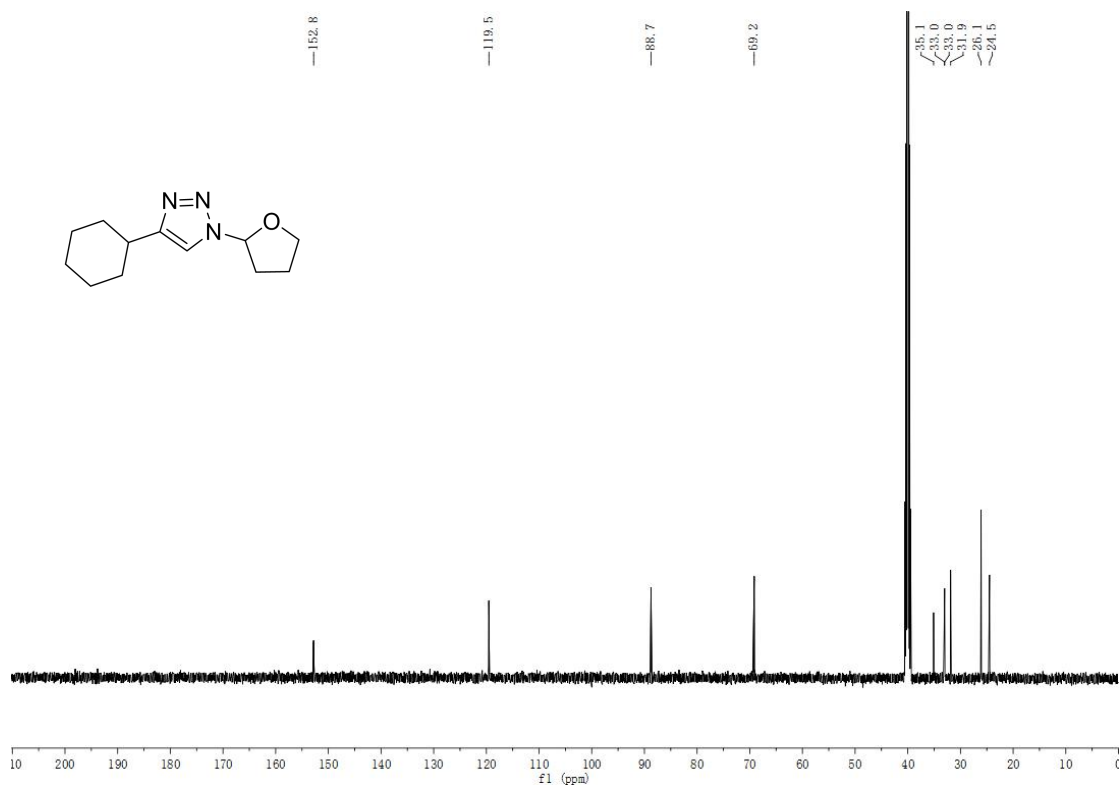
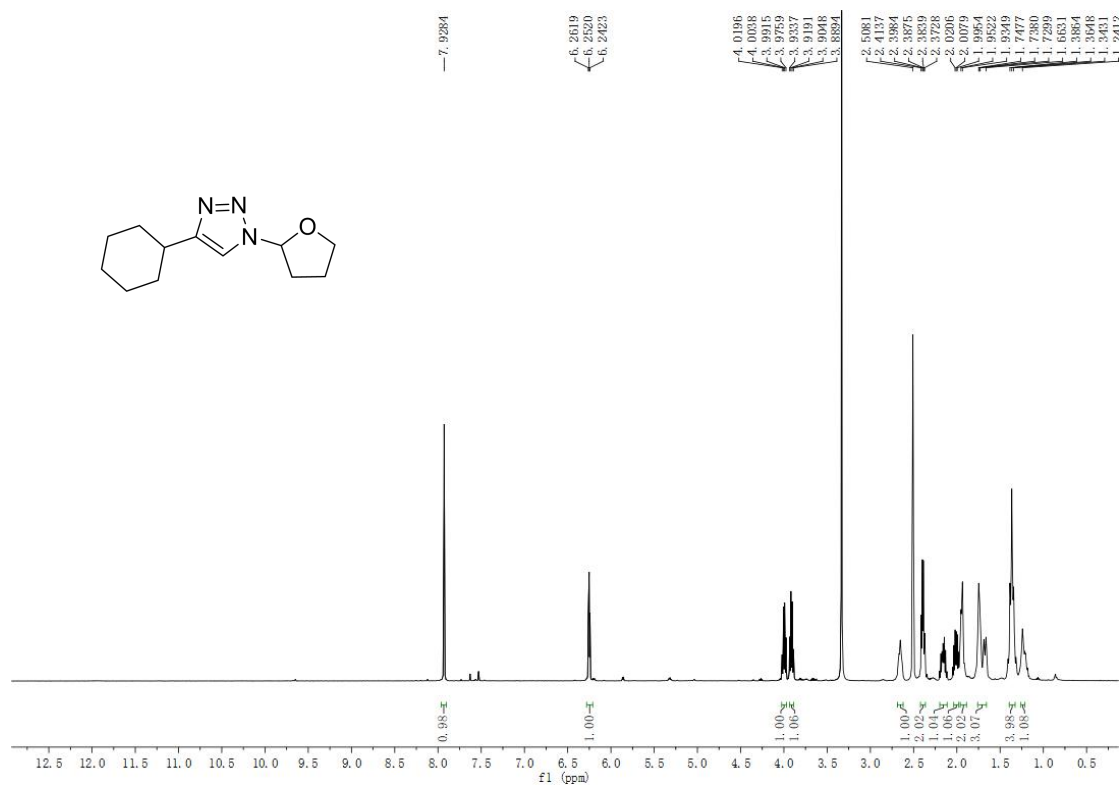
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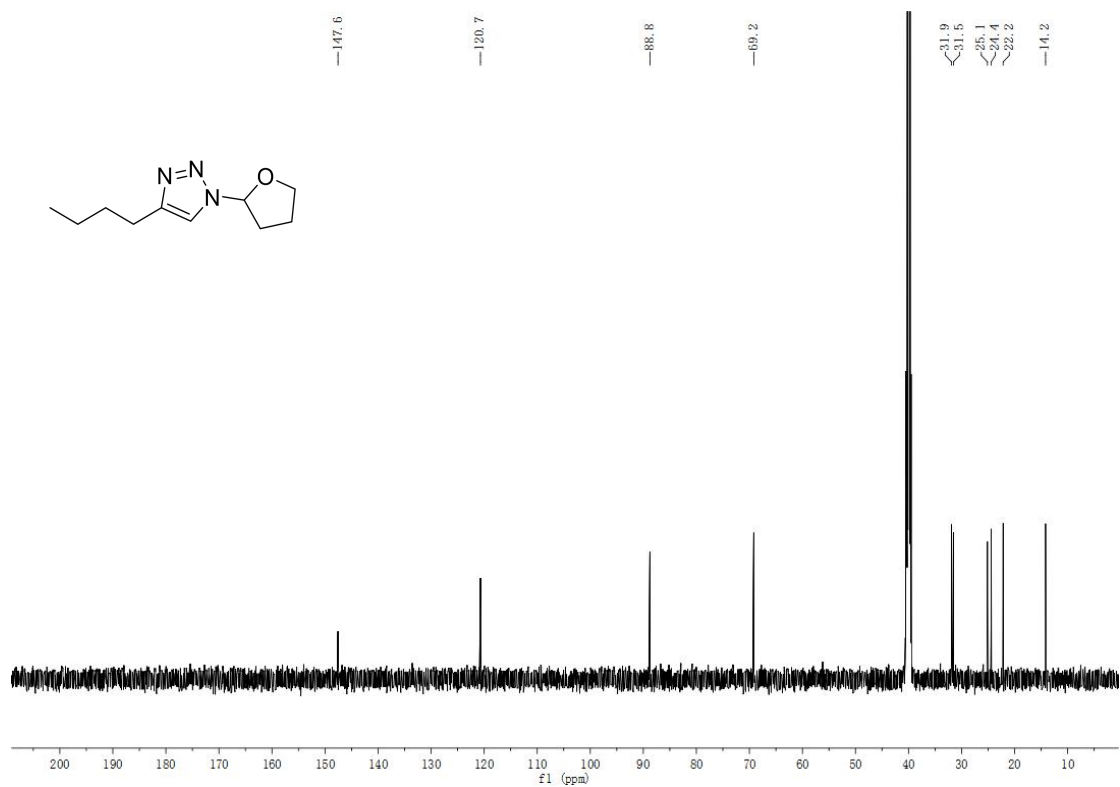
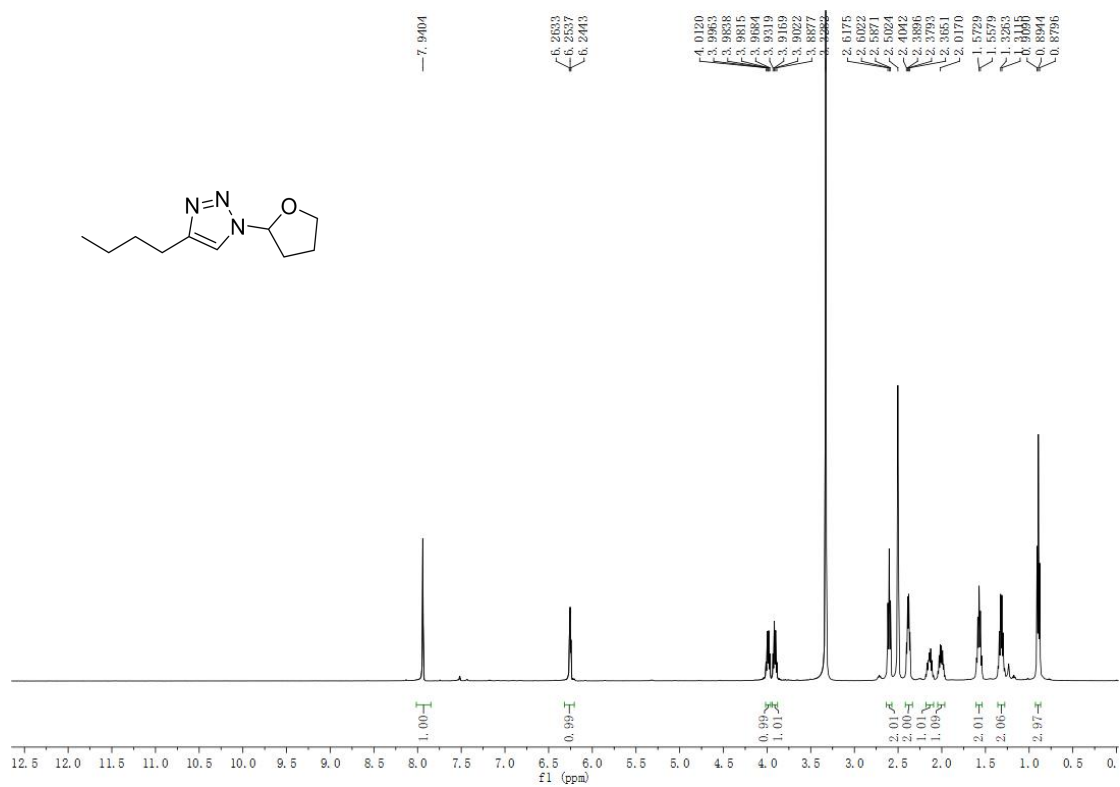
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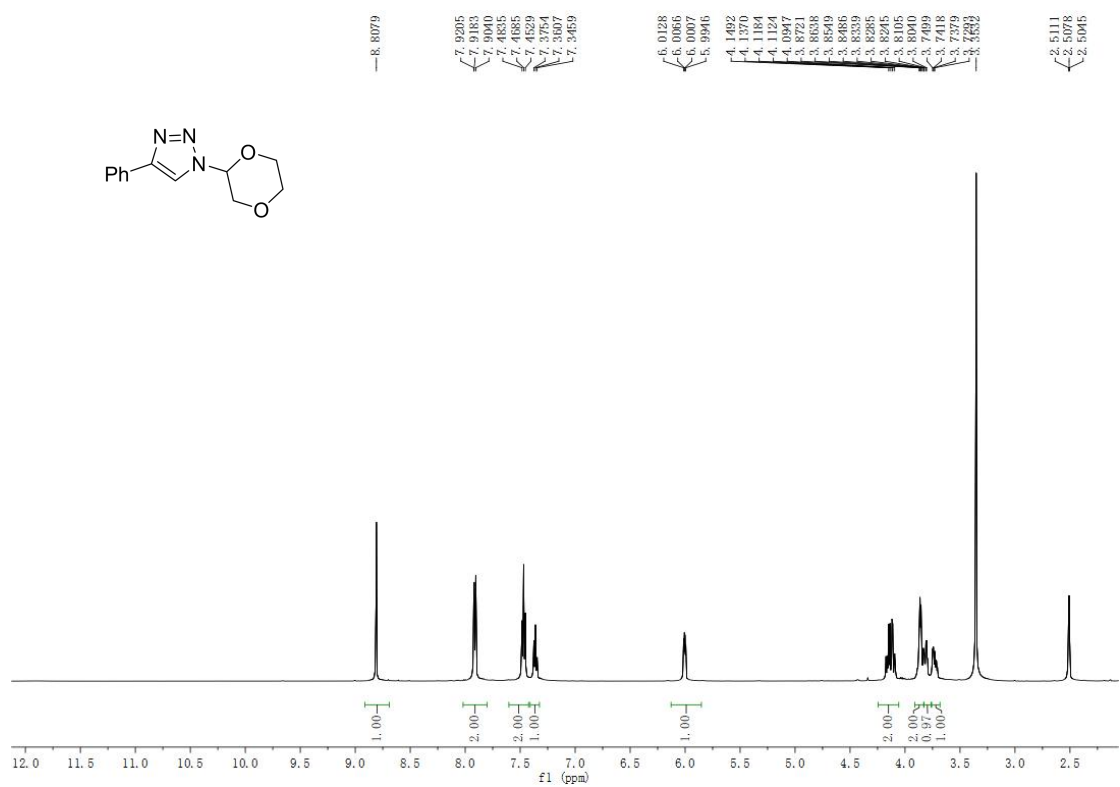
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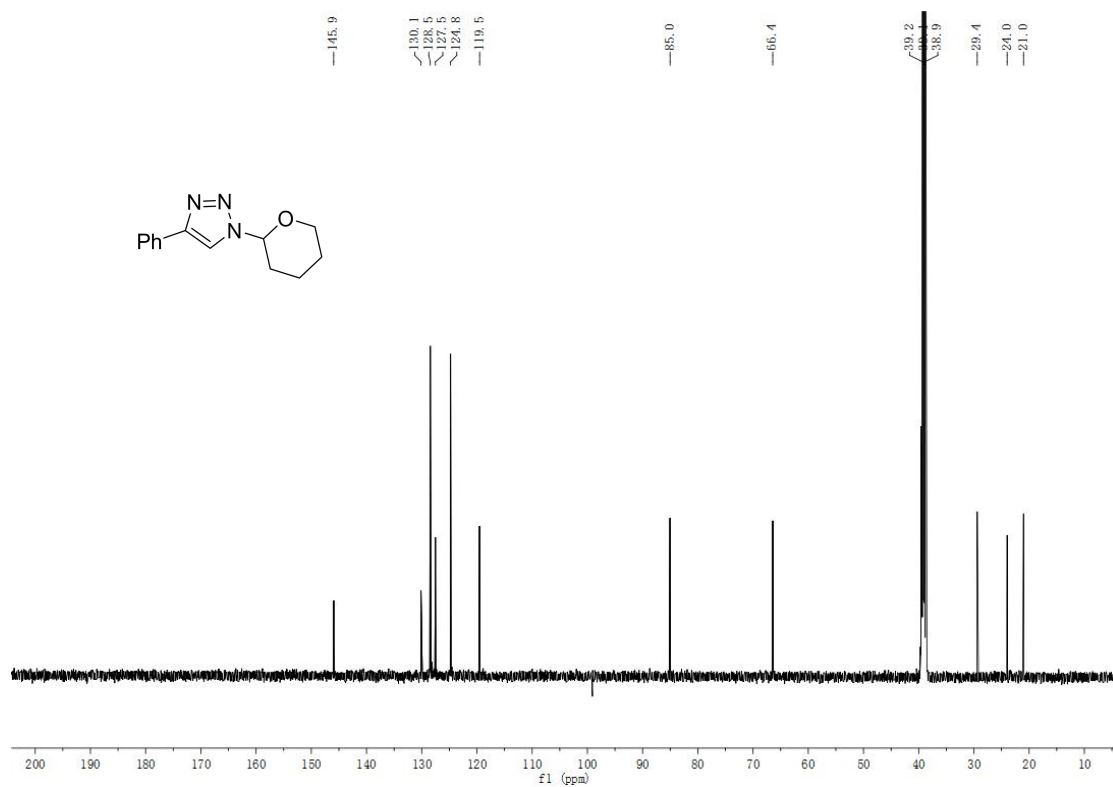
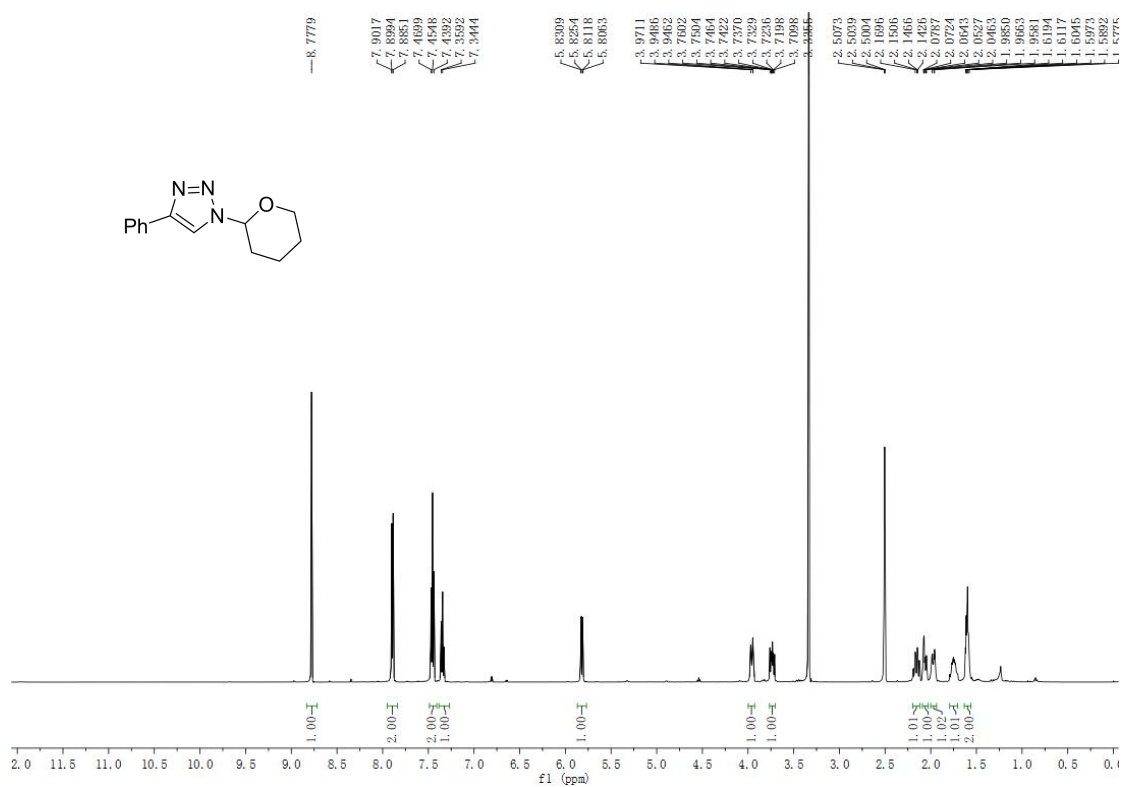
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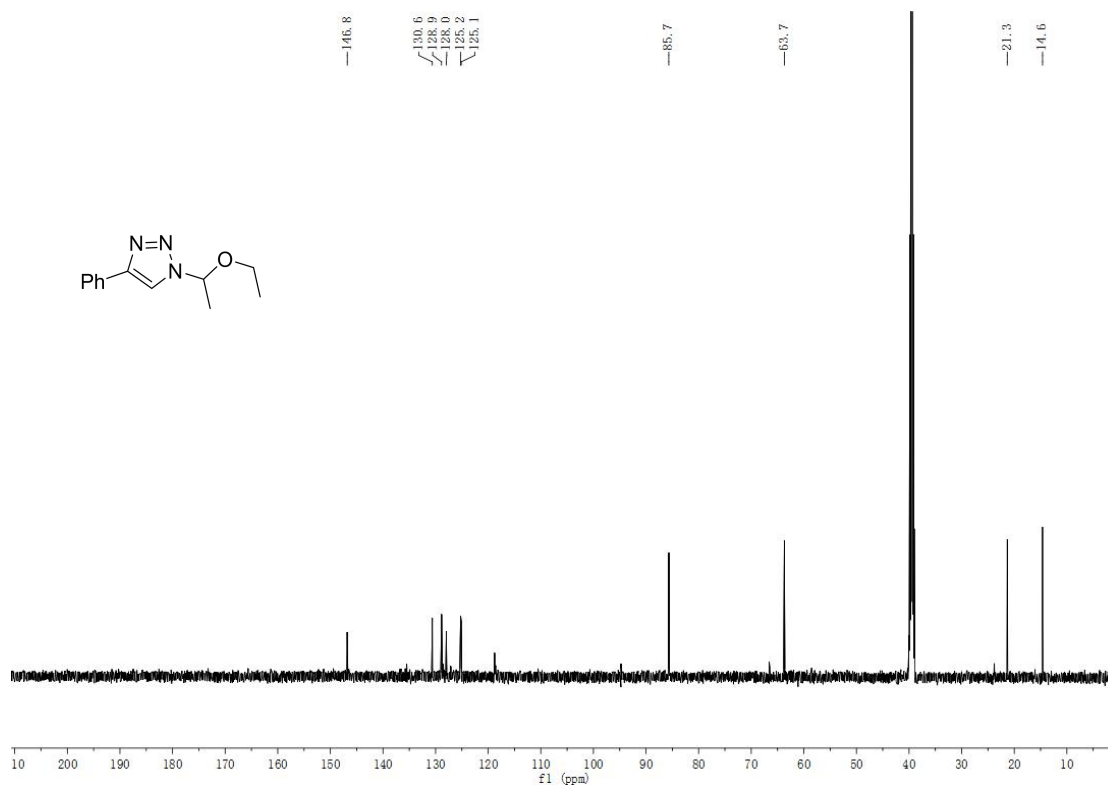
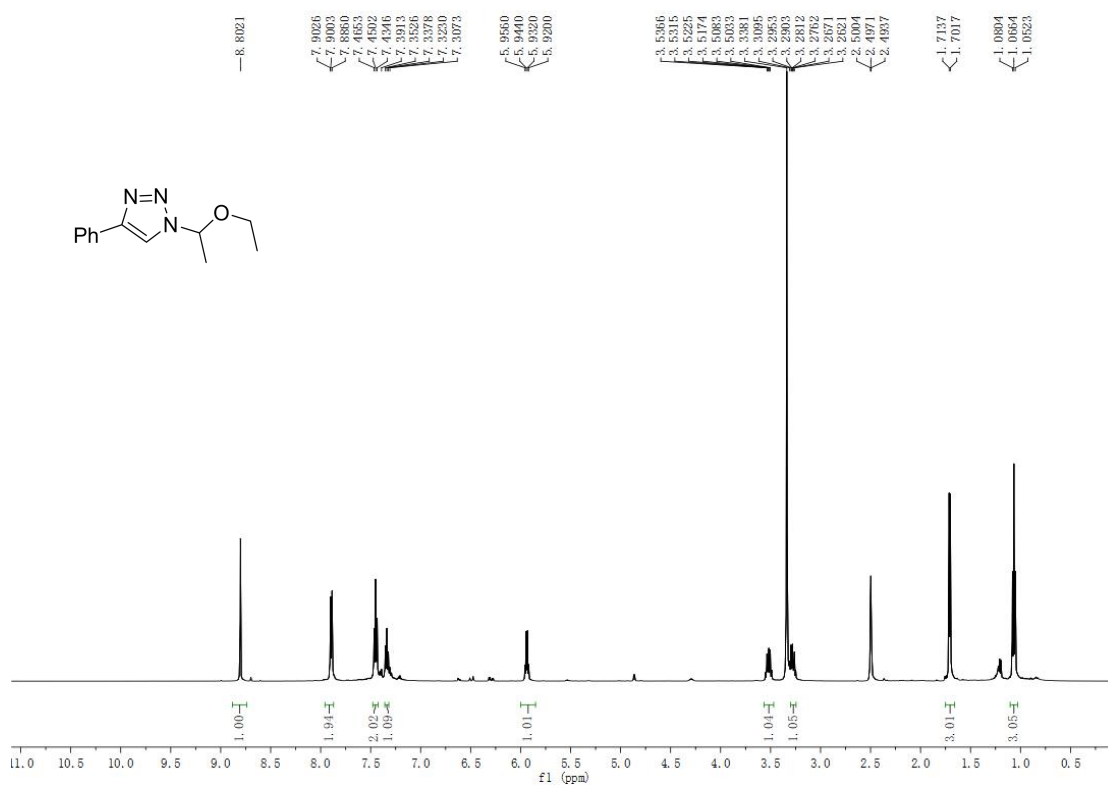
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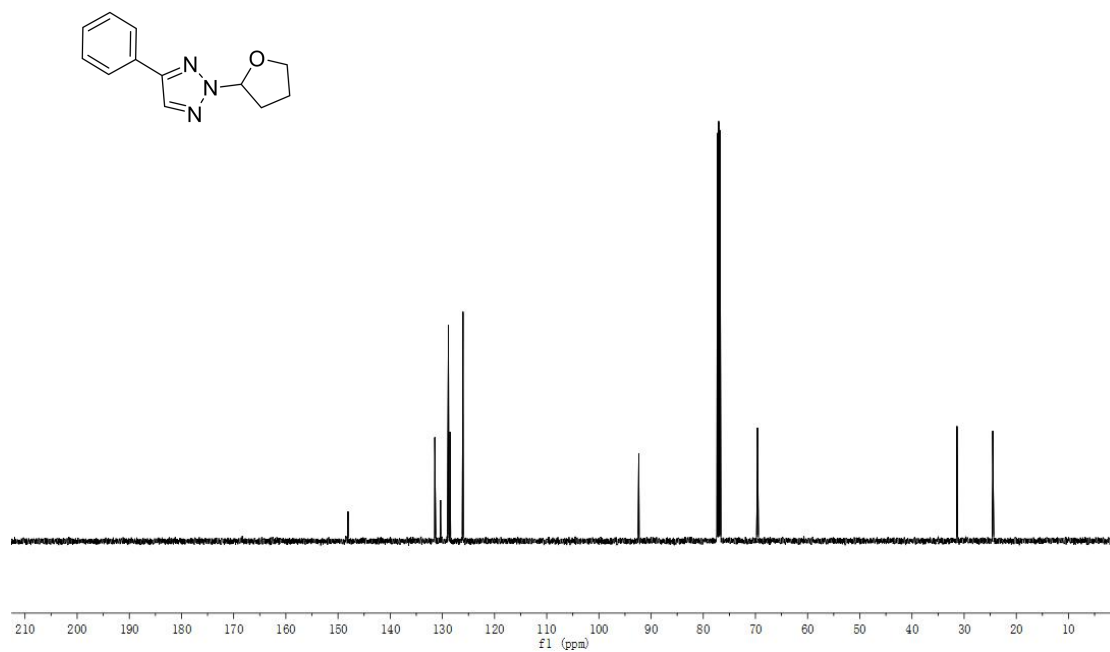
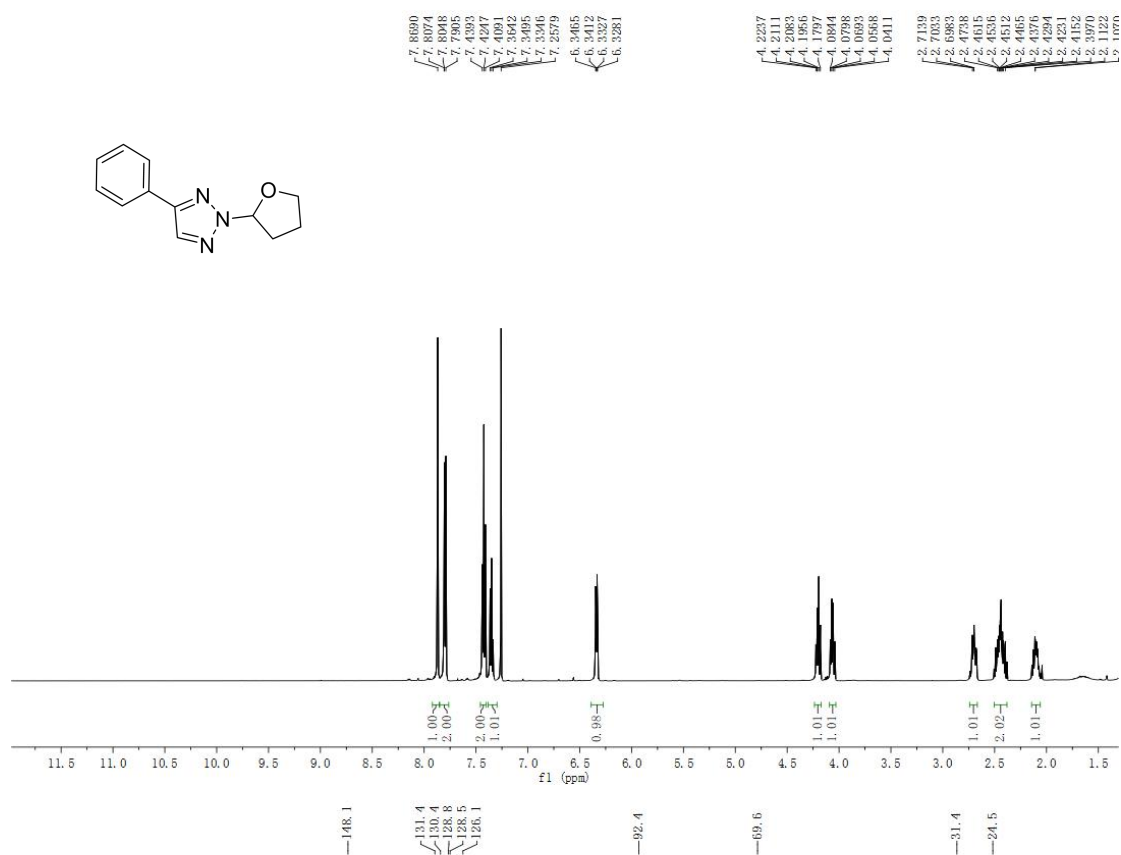
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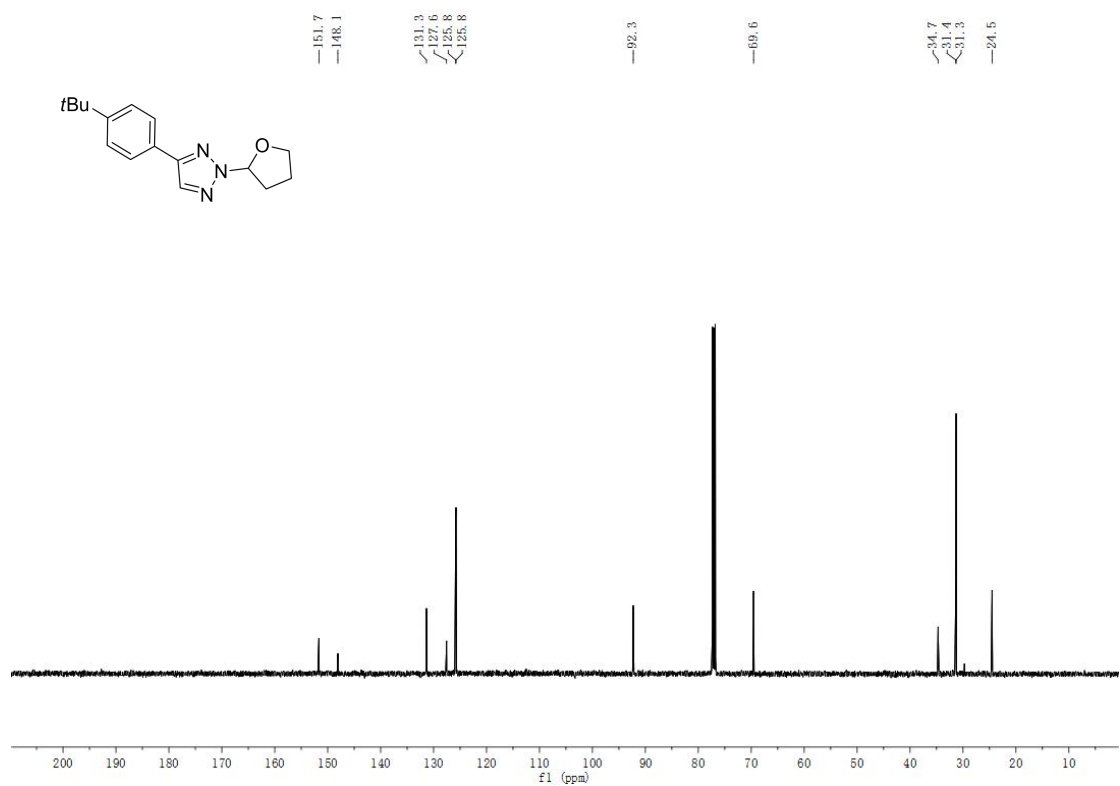
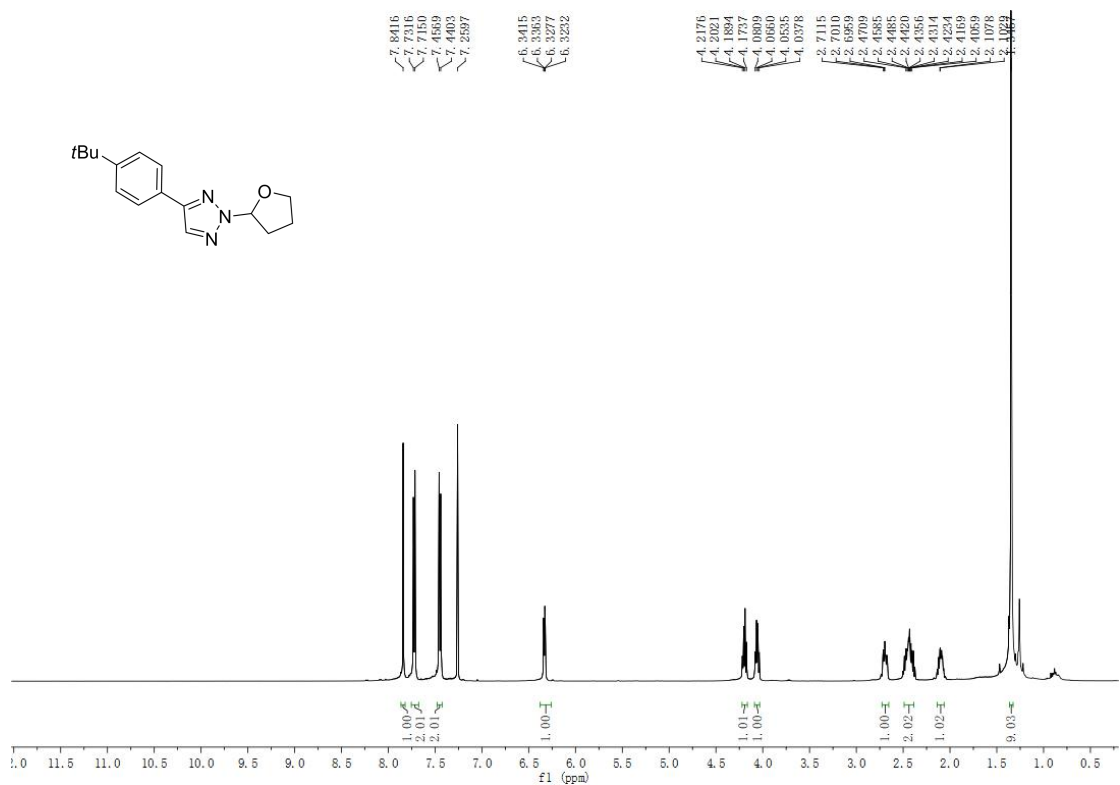
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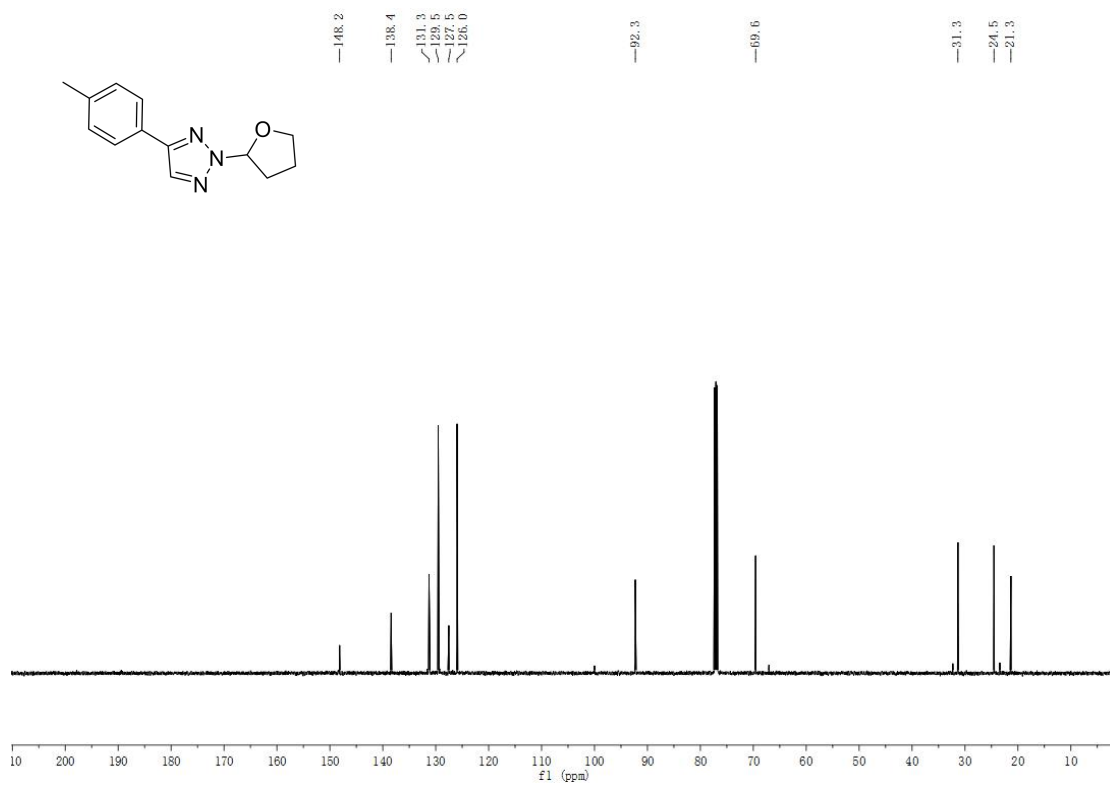
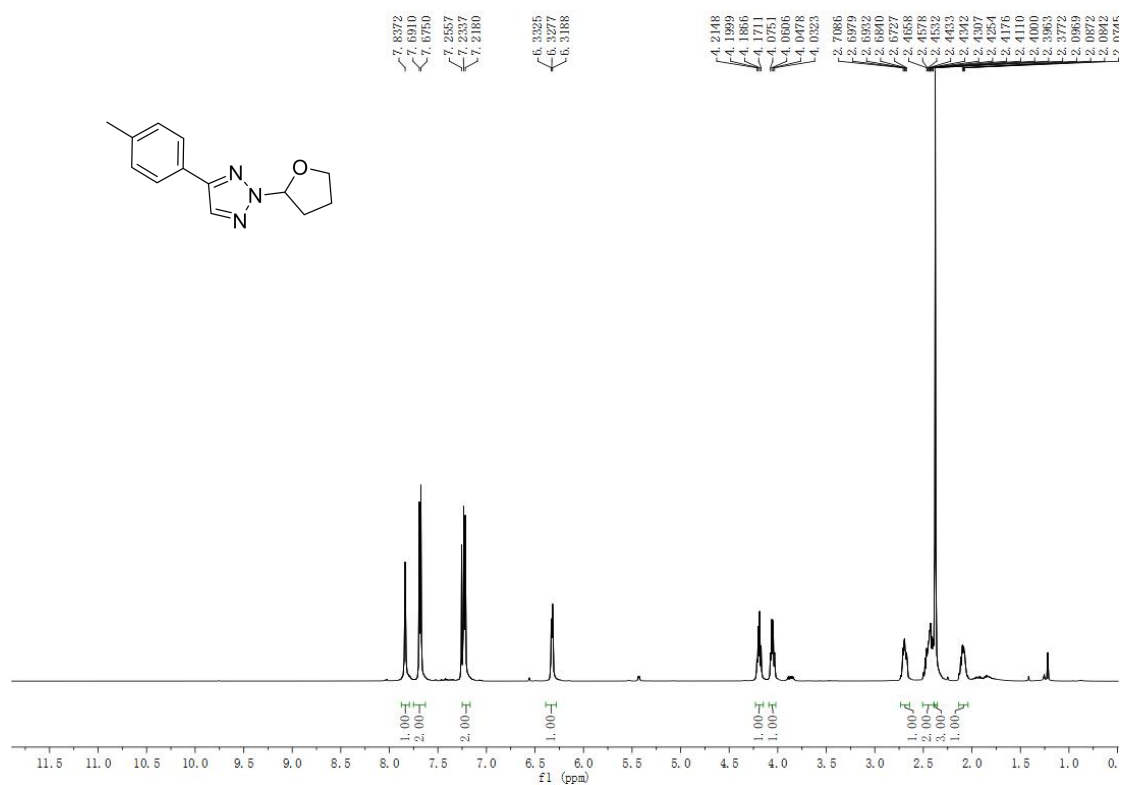
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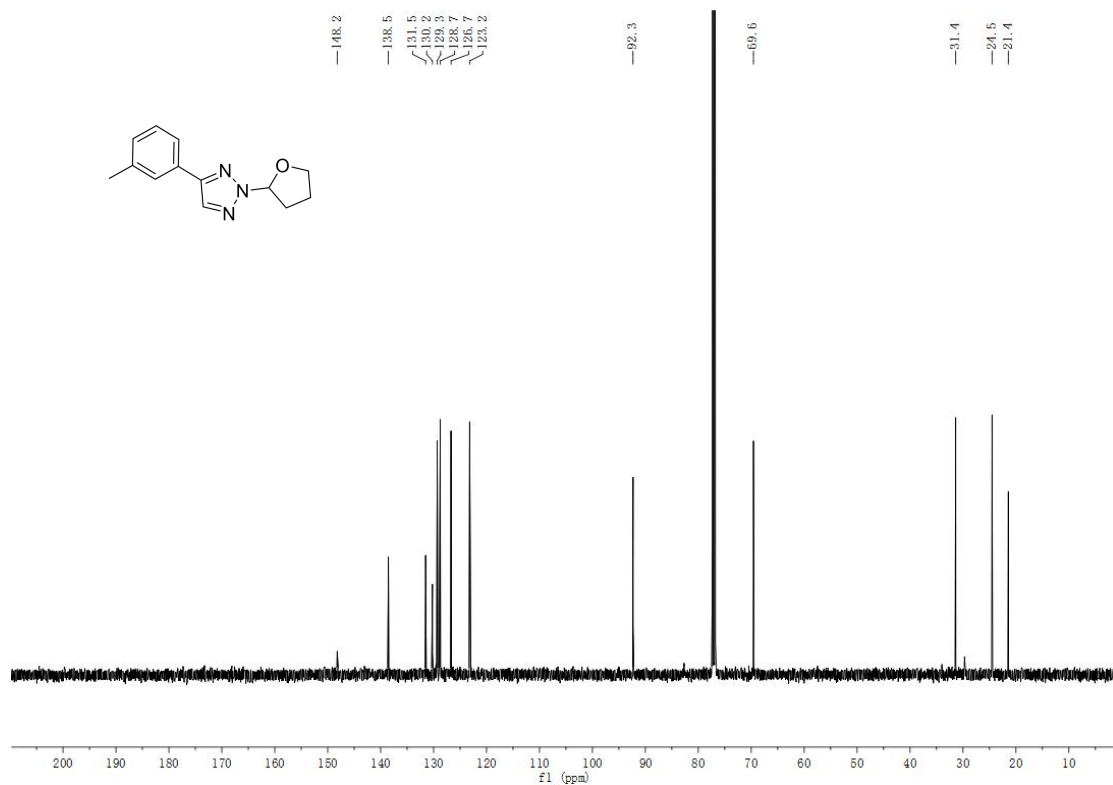
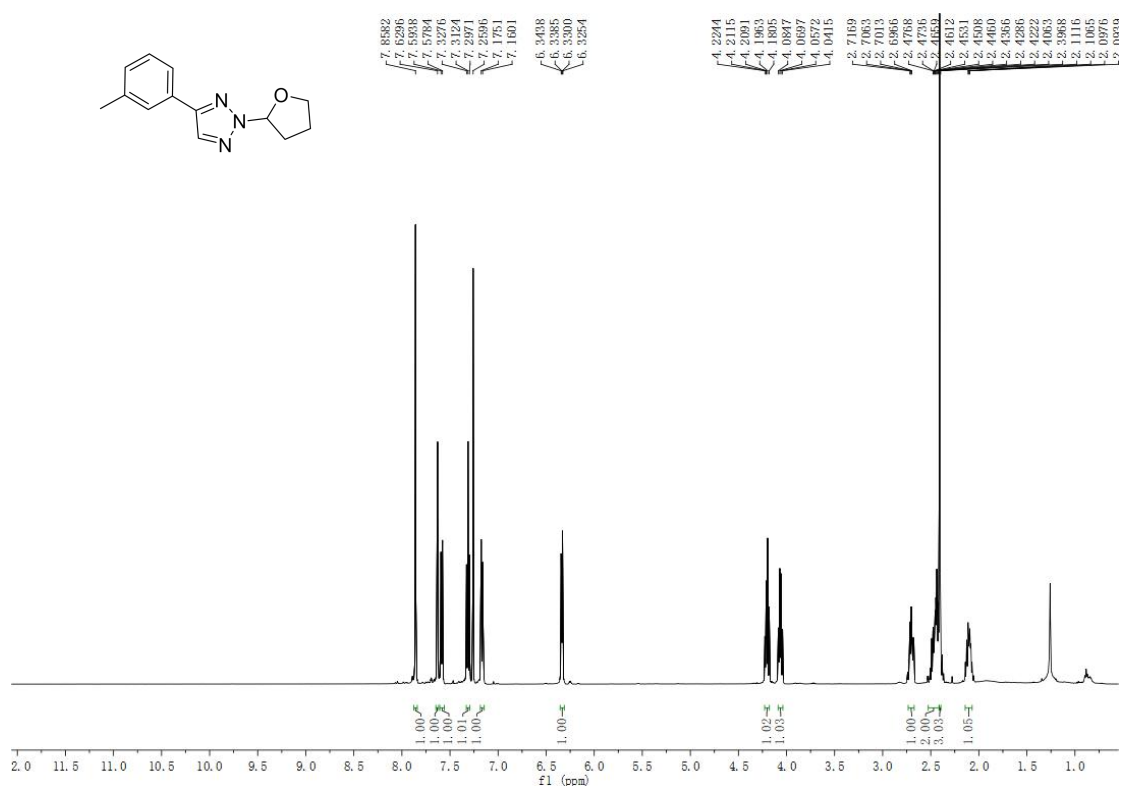
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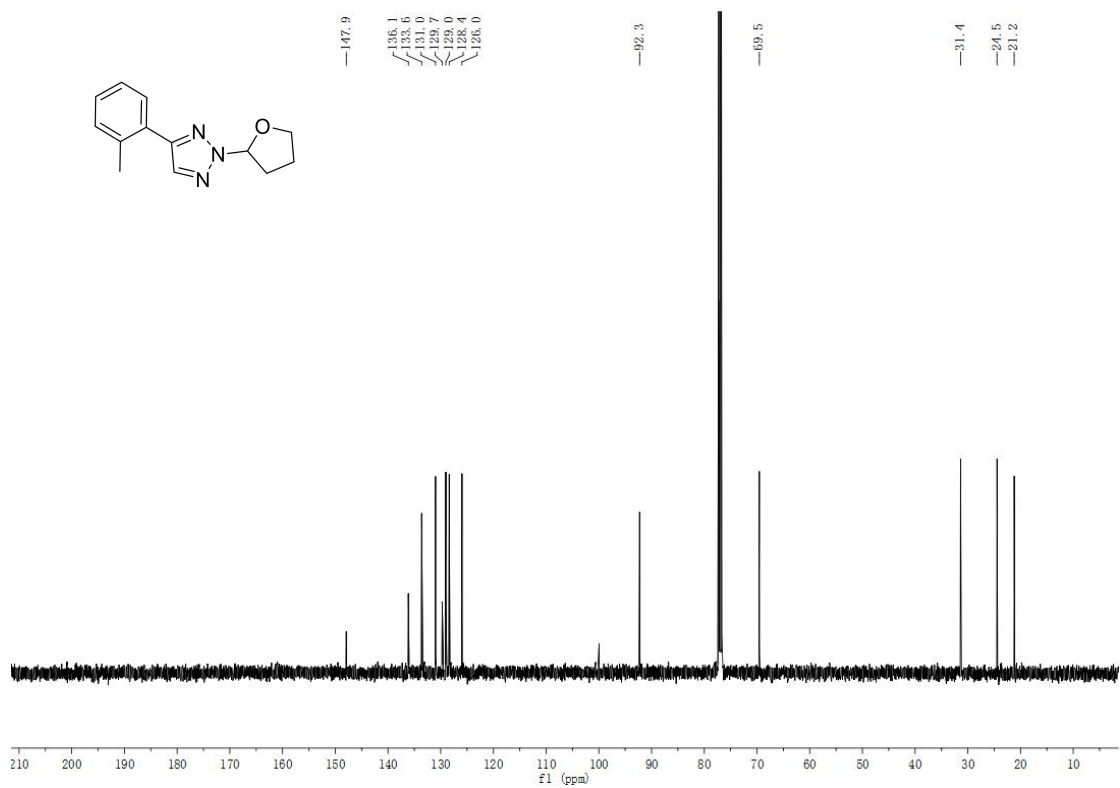
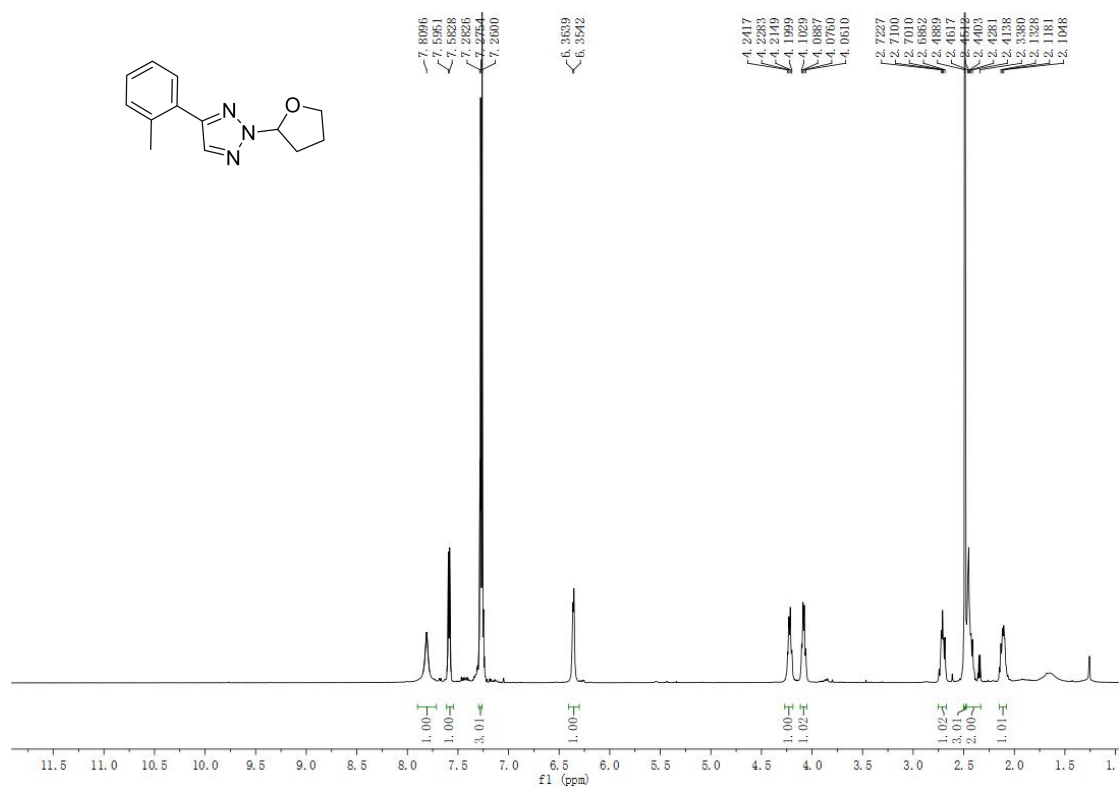
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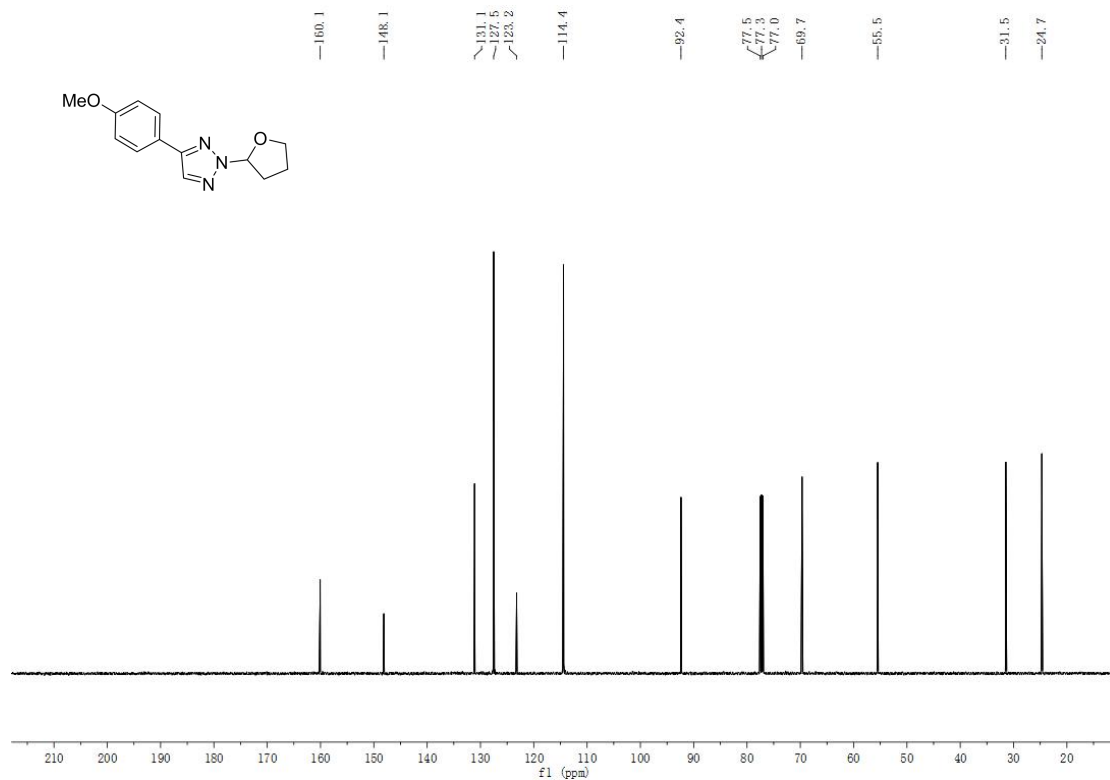
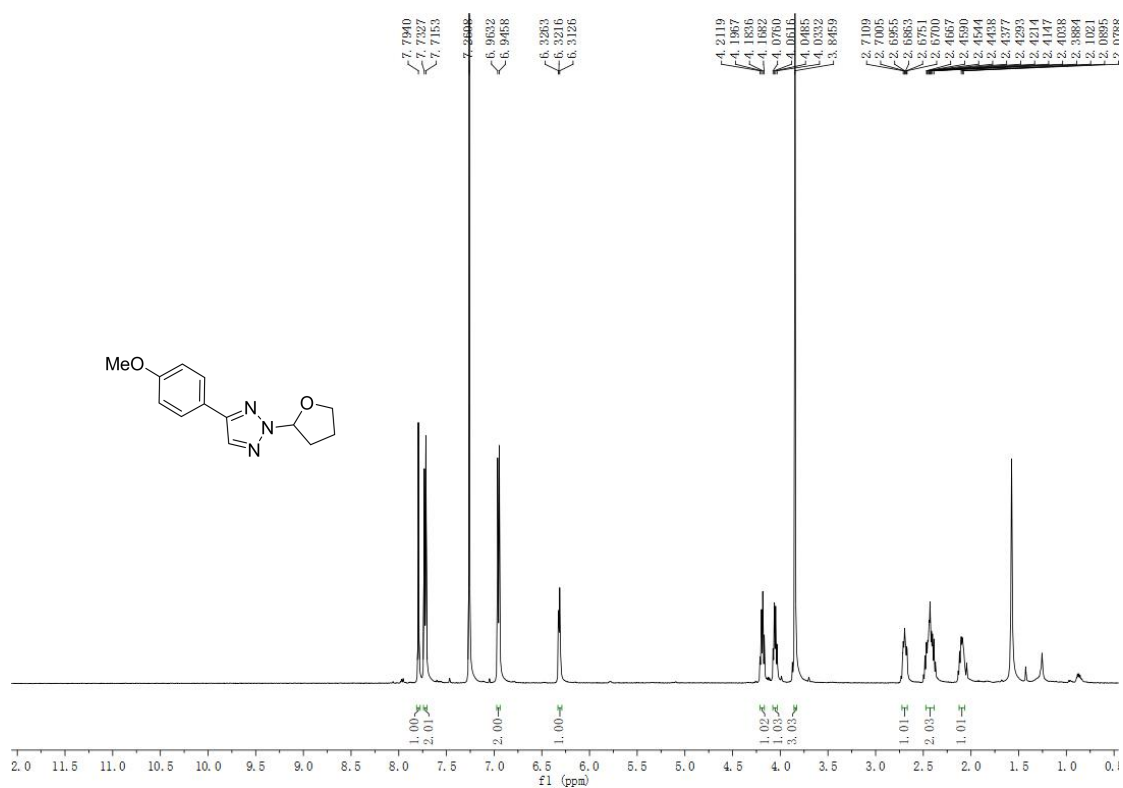
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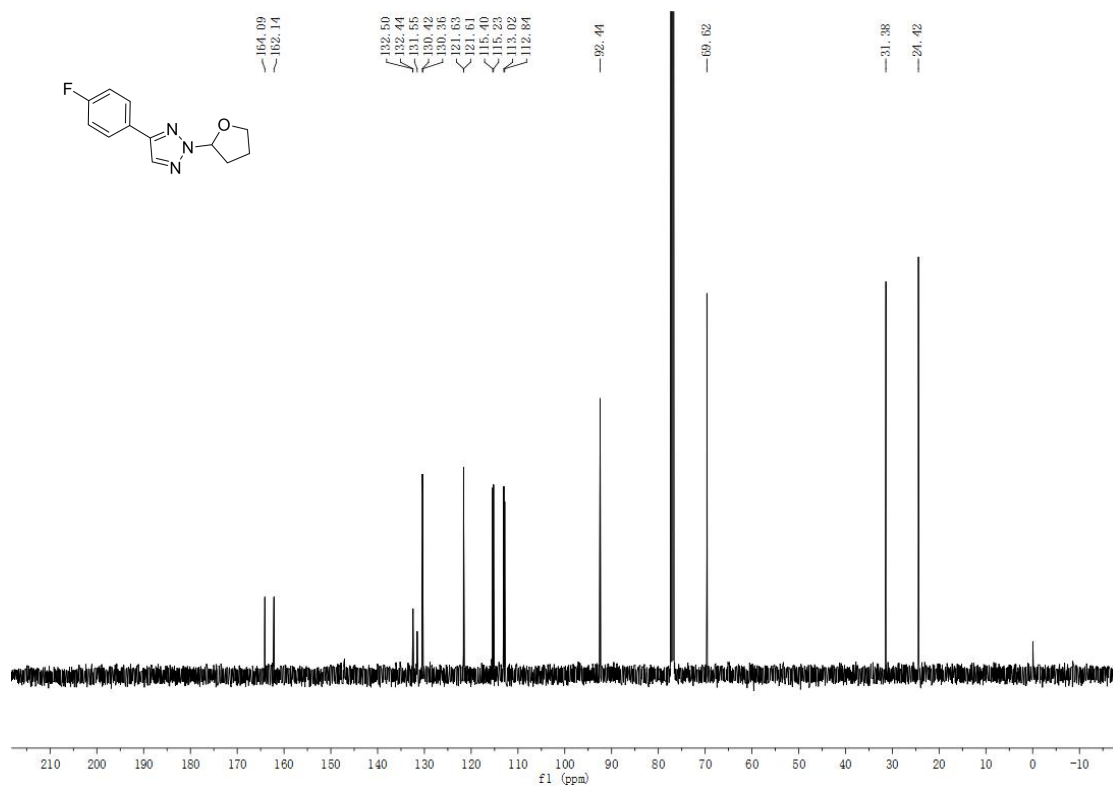
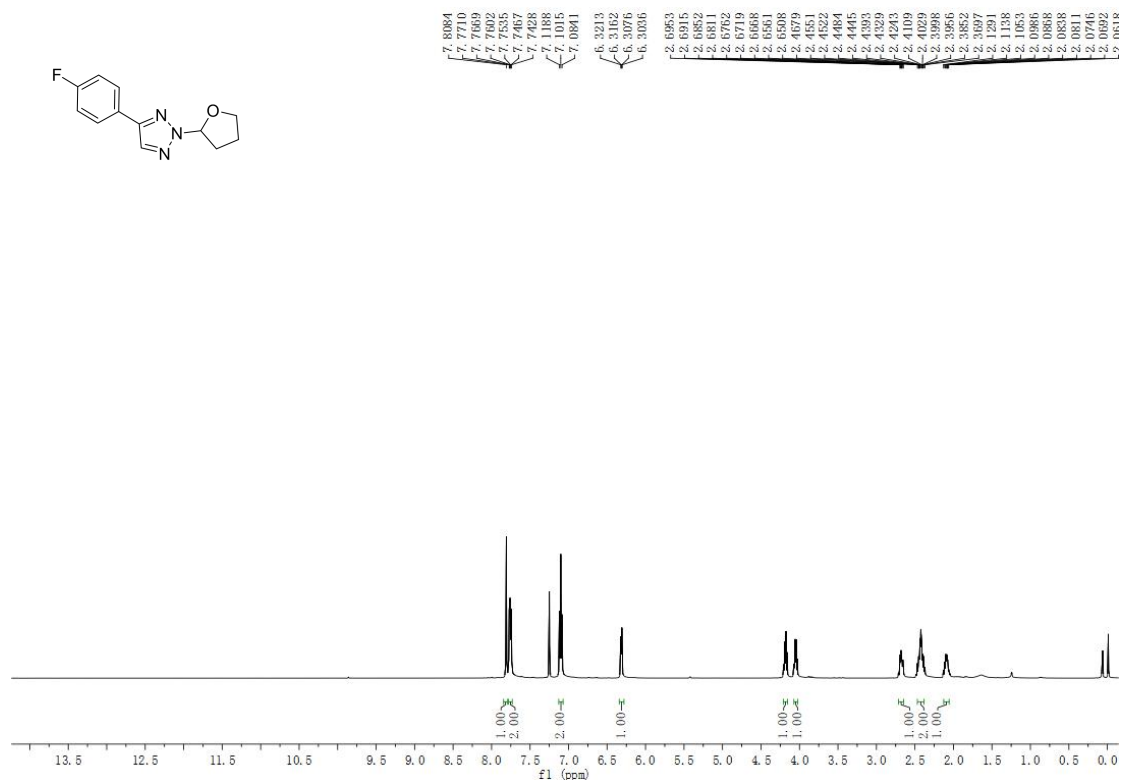
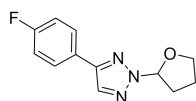
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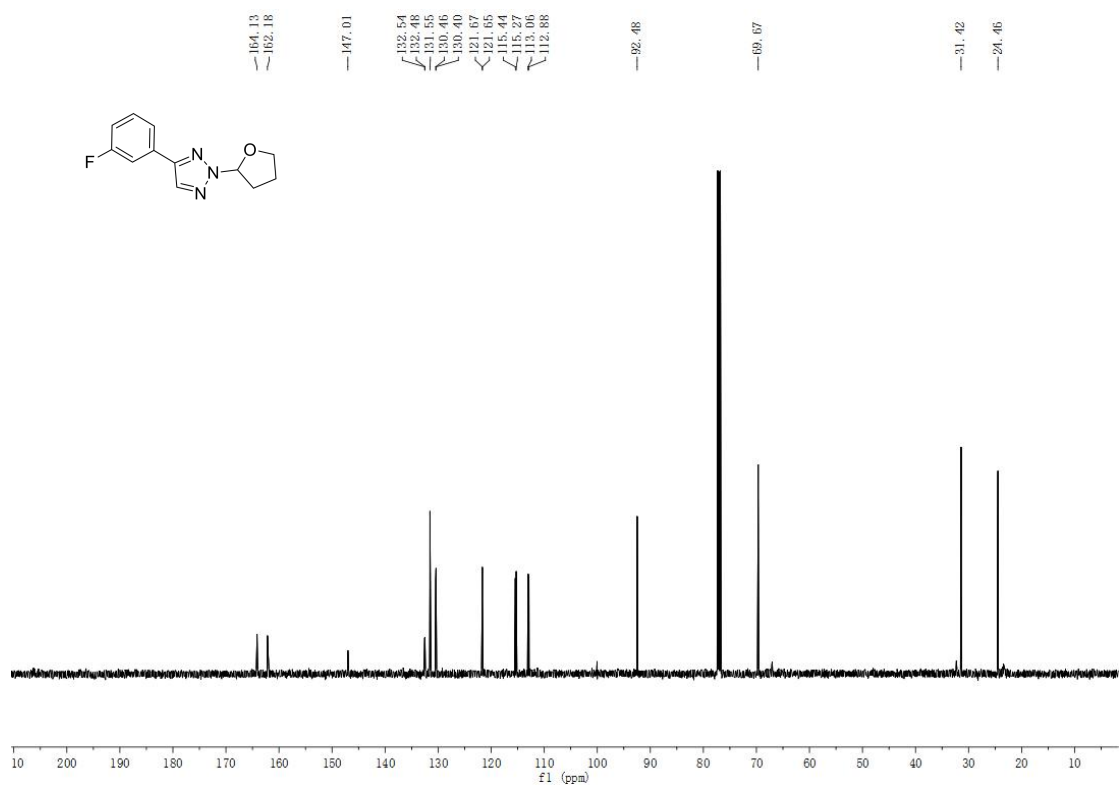
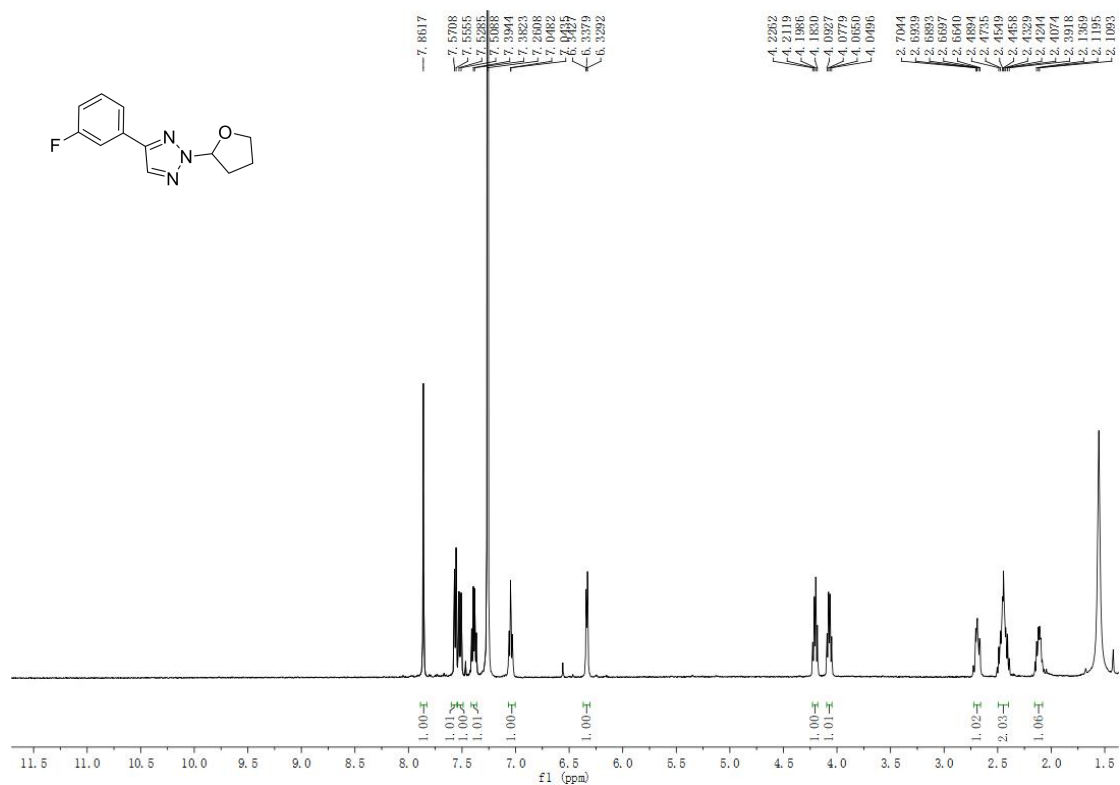
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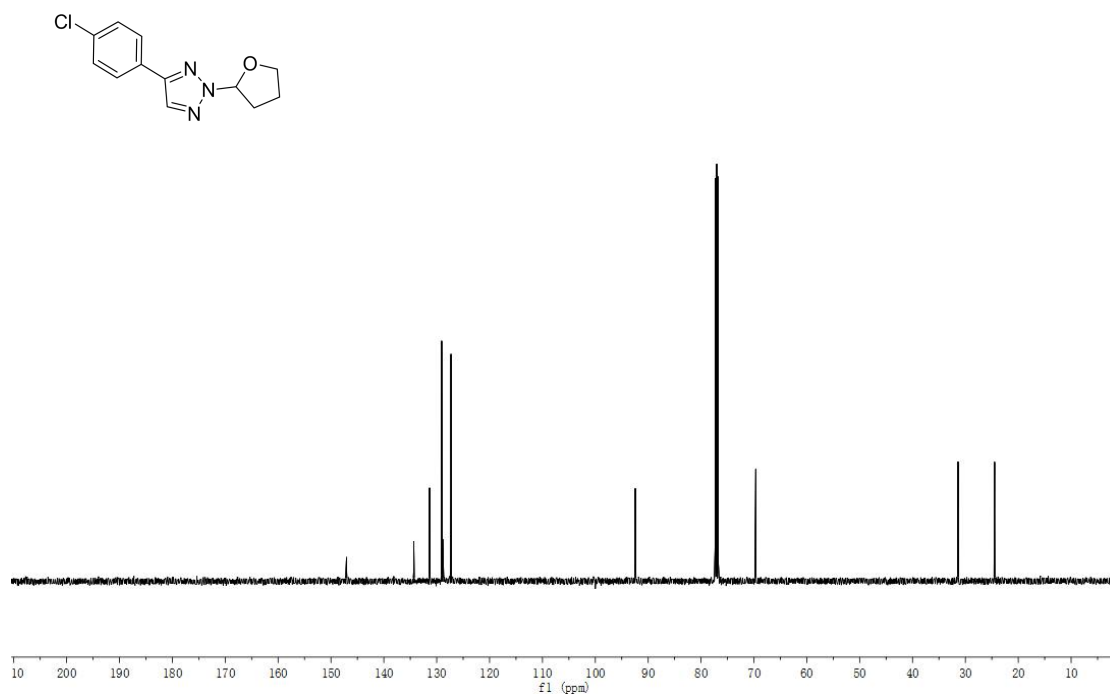
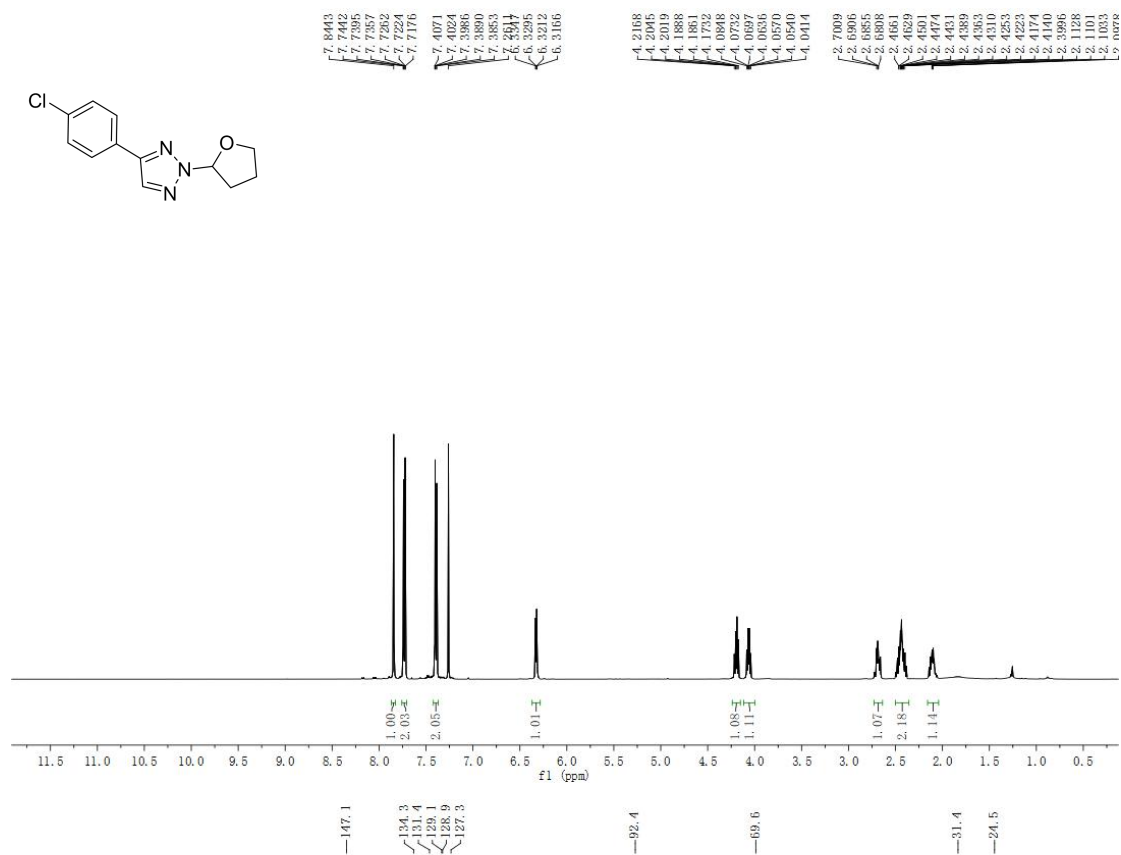
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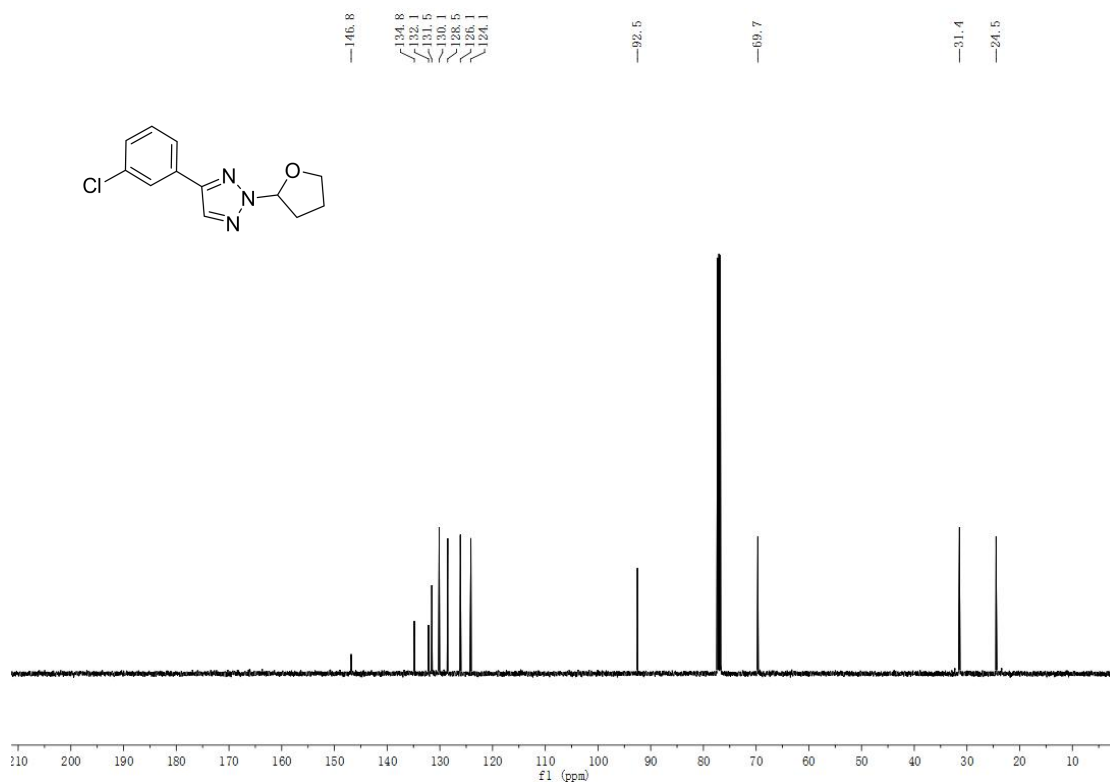
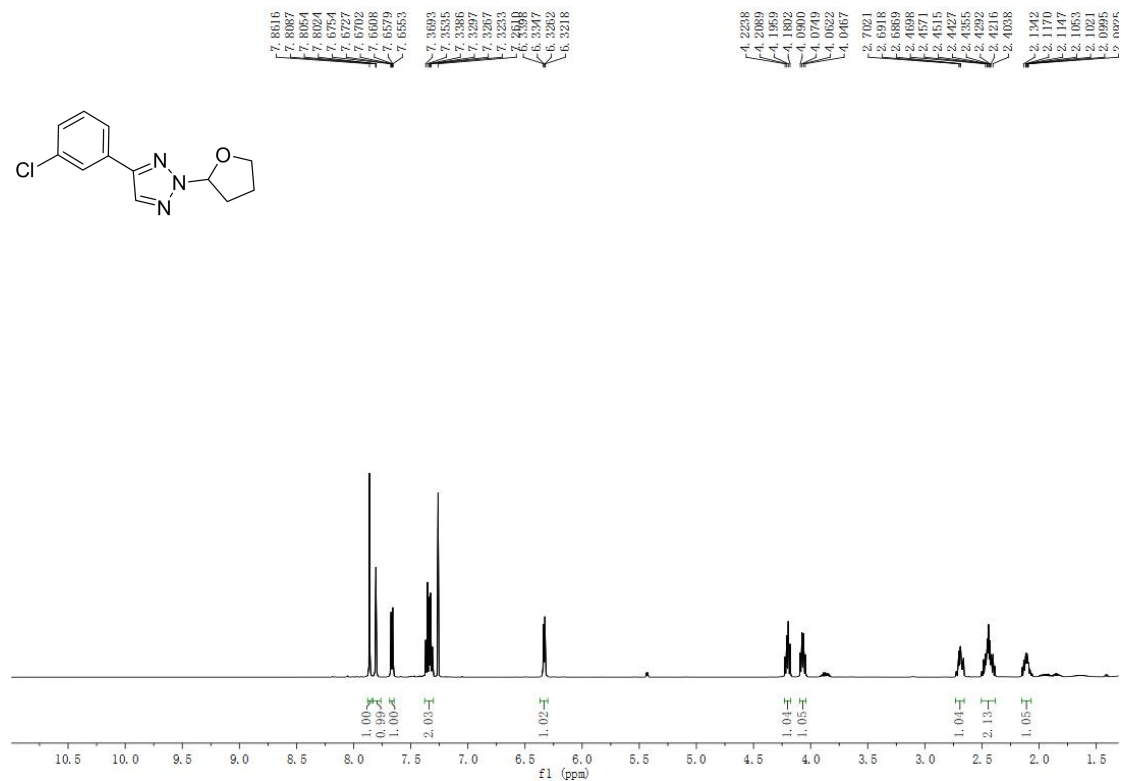
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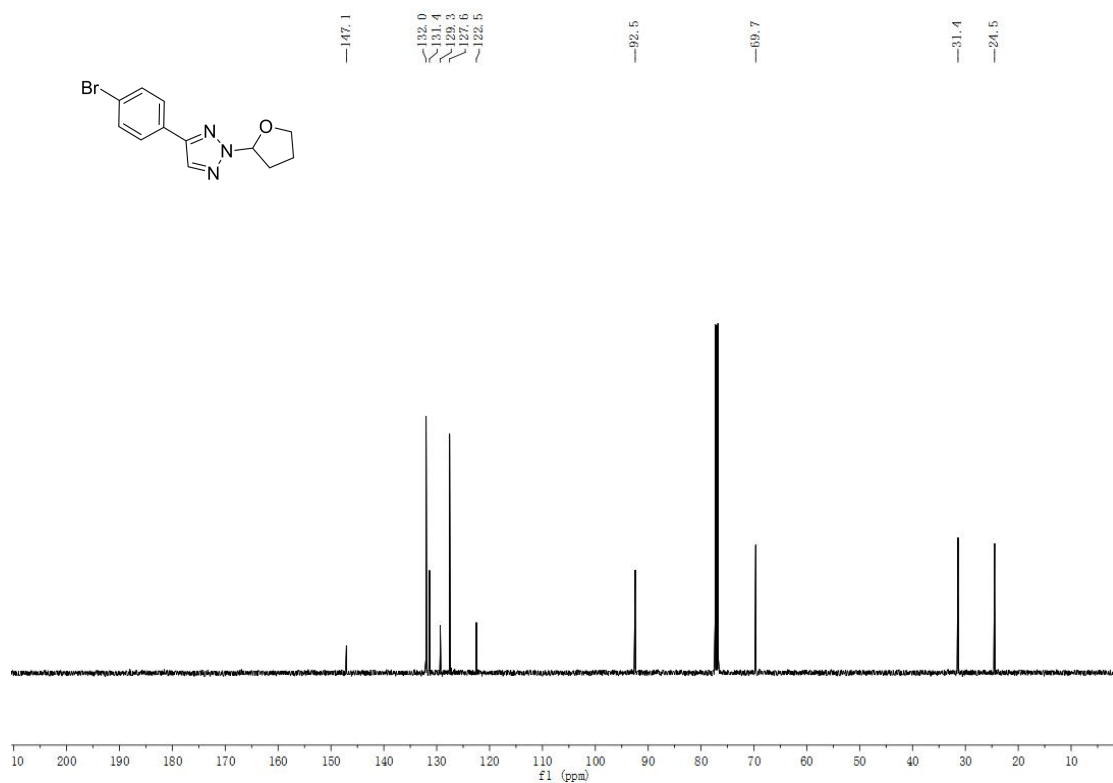
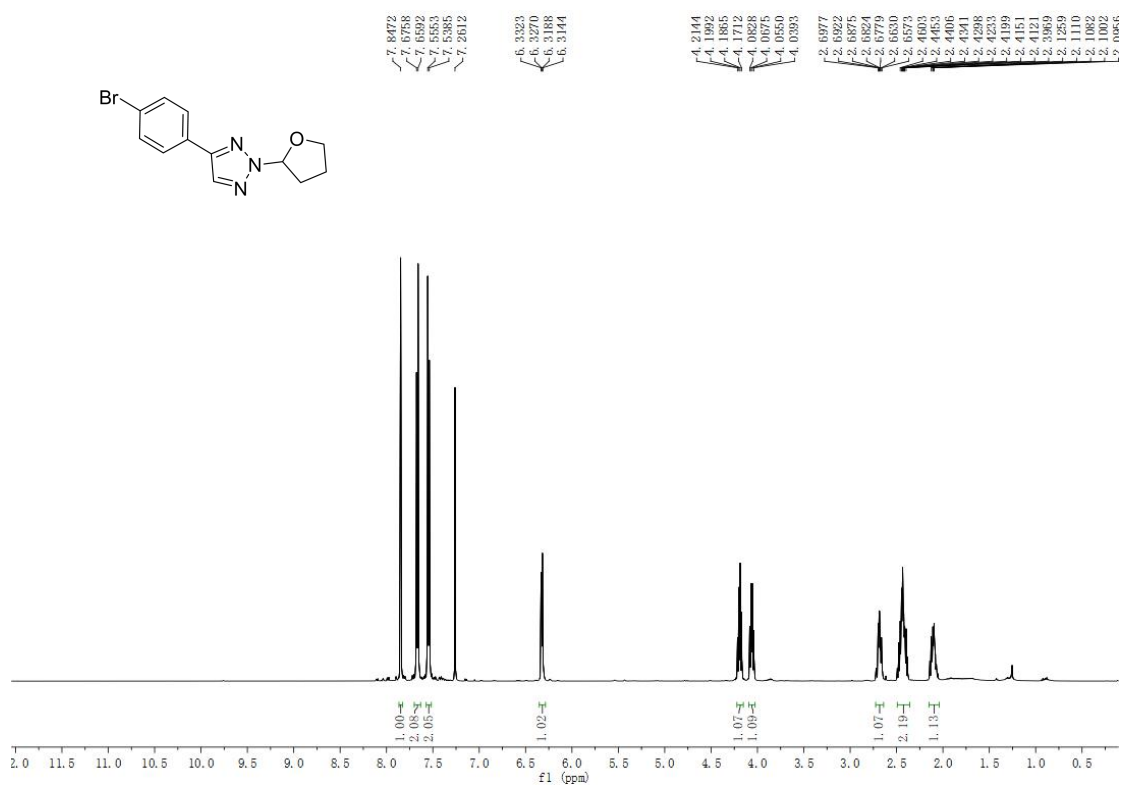
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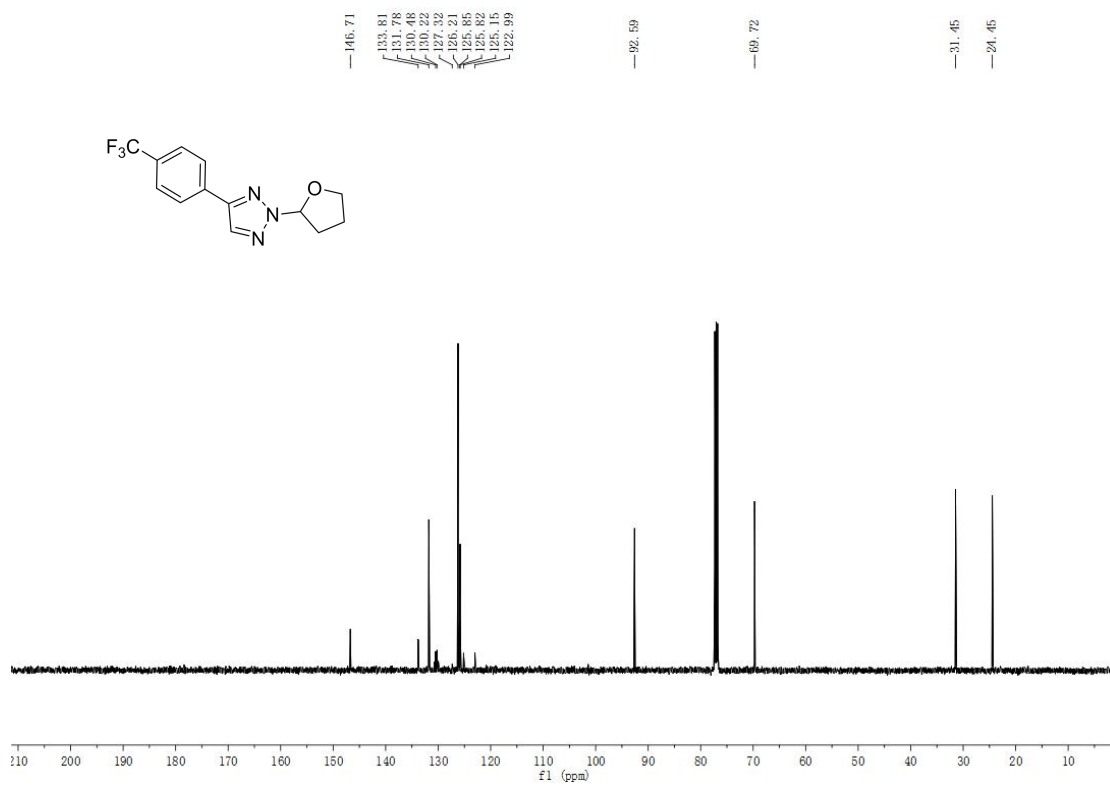
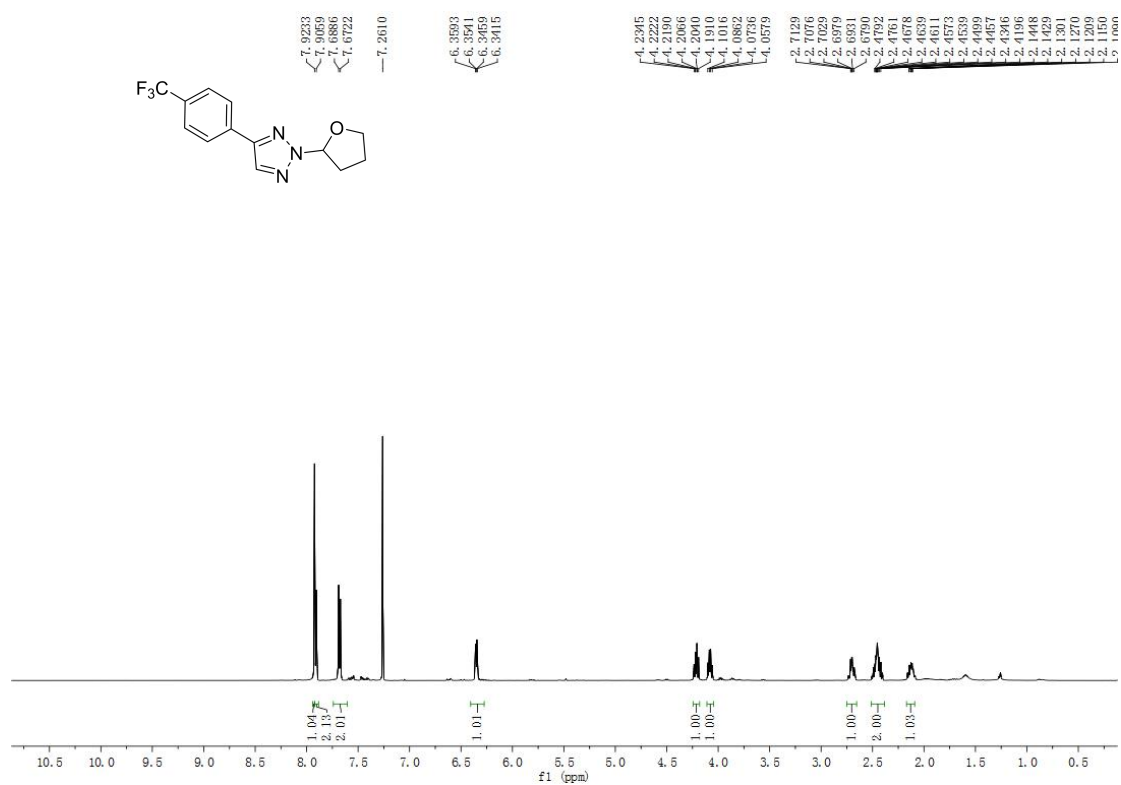
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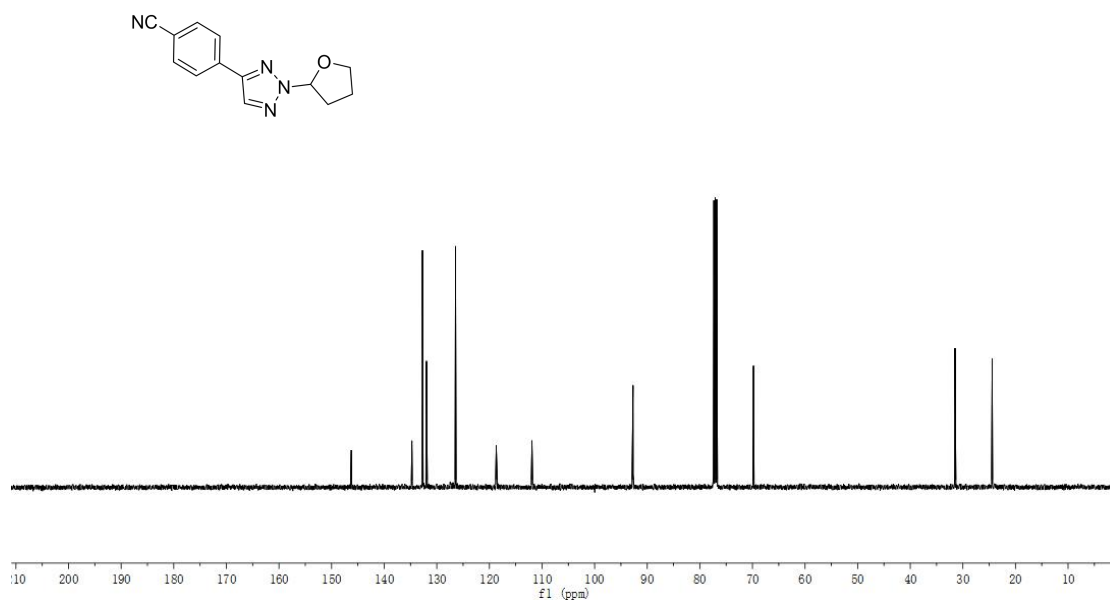
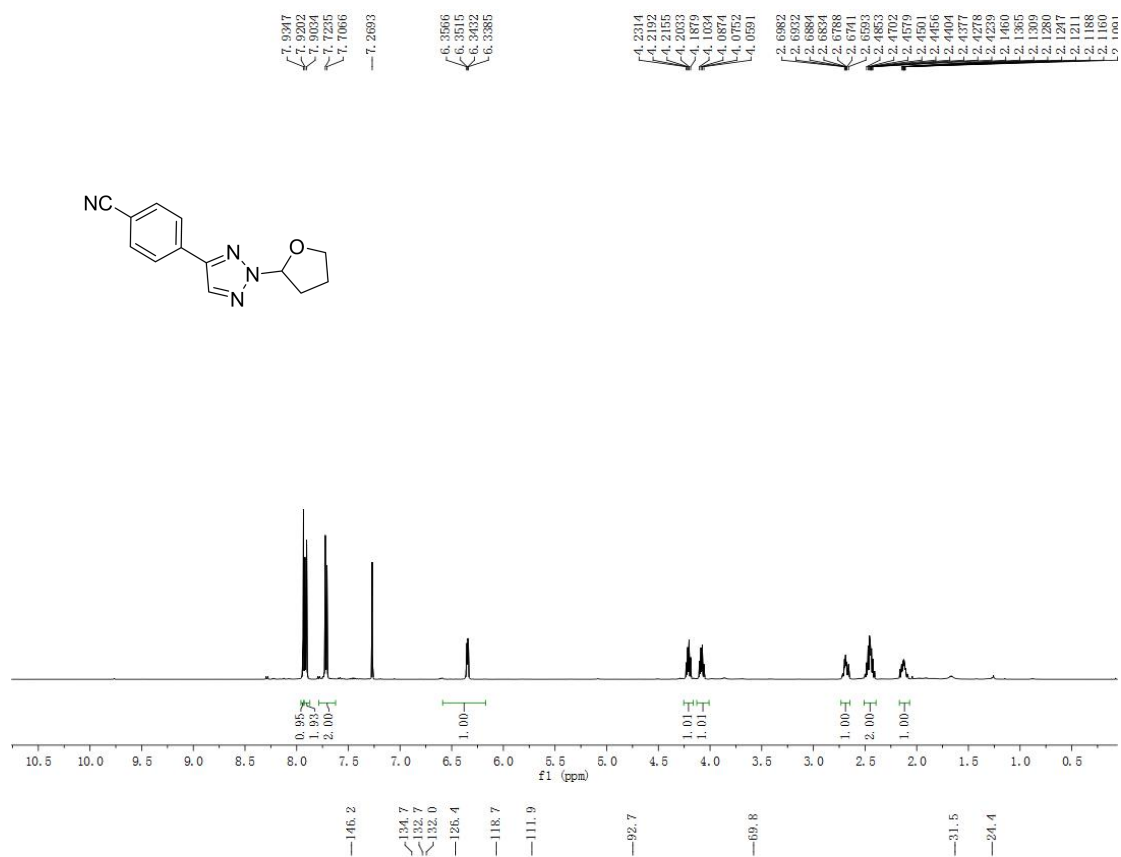
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51

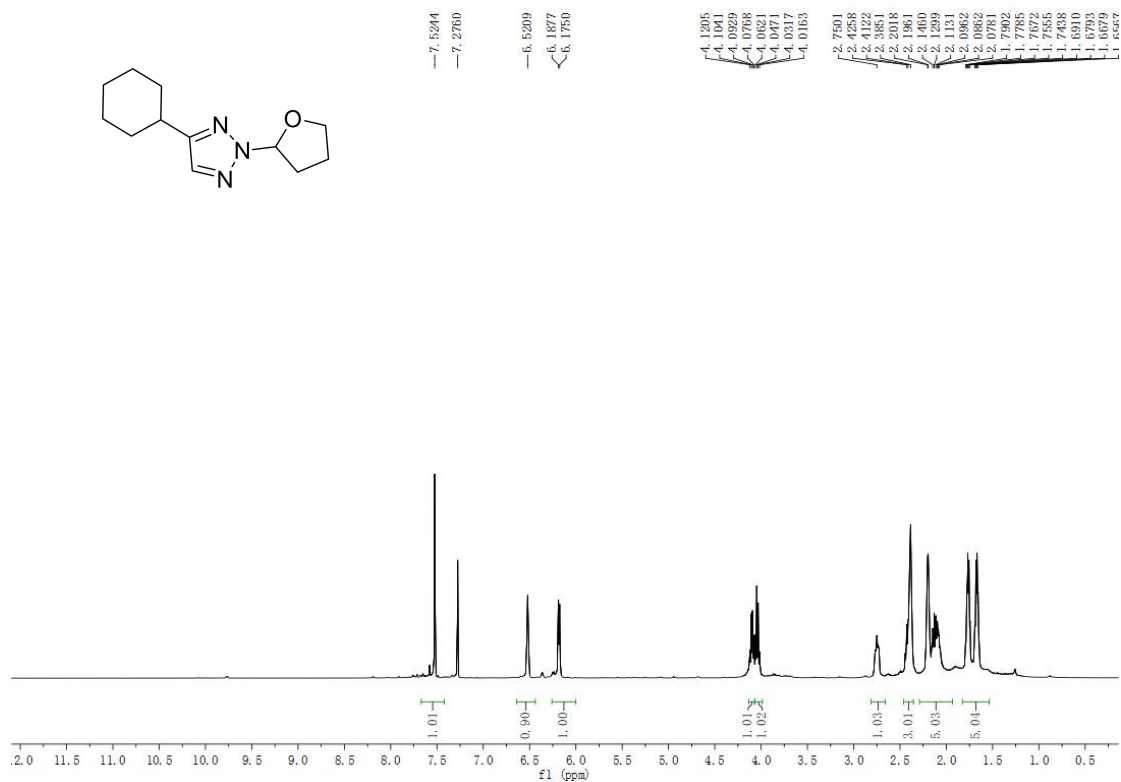


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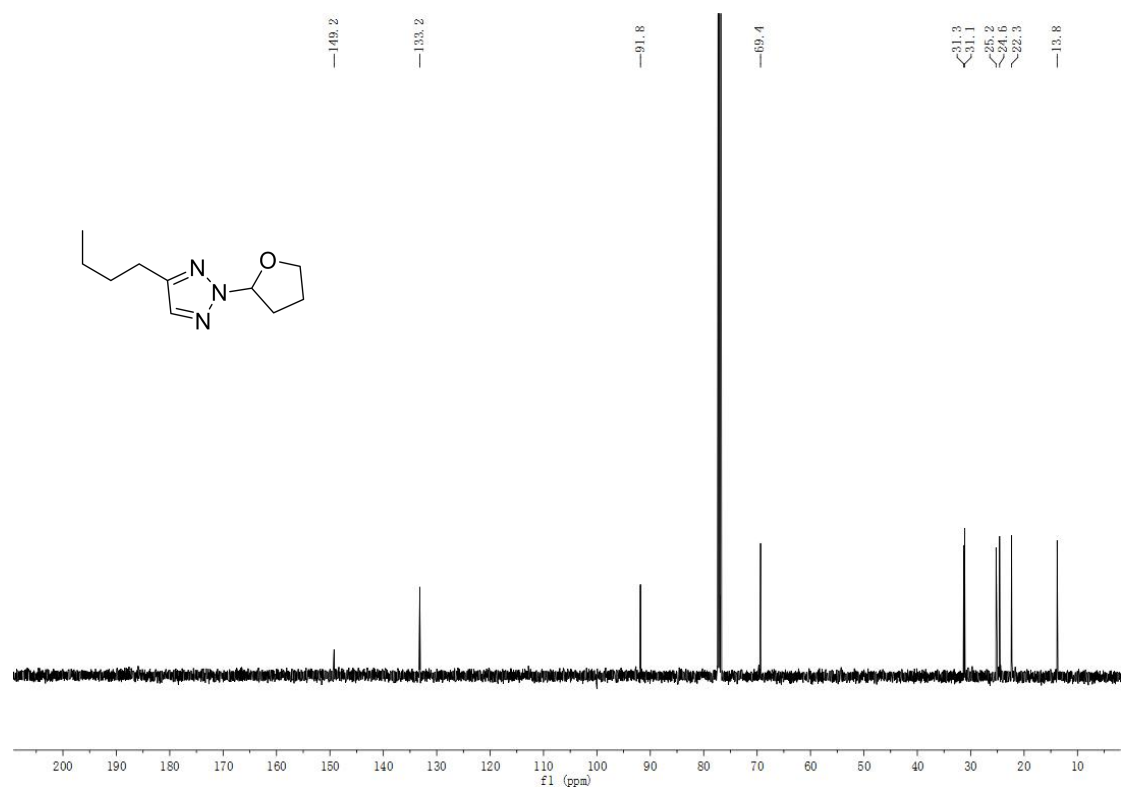
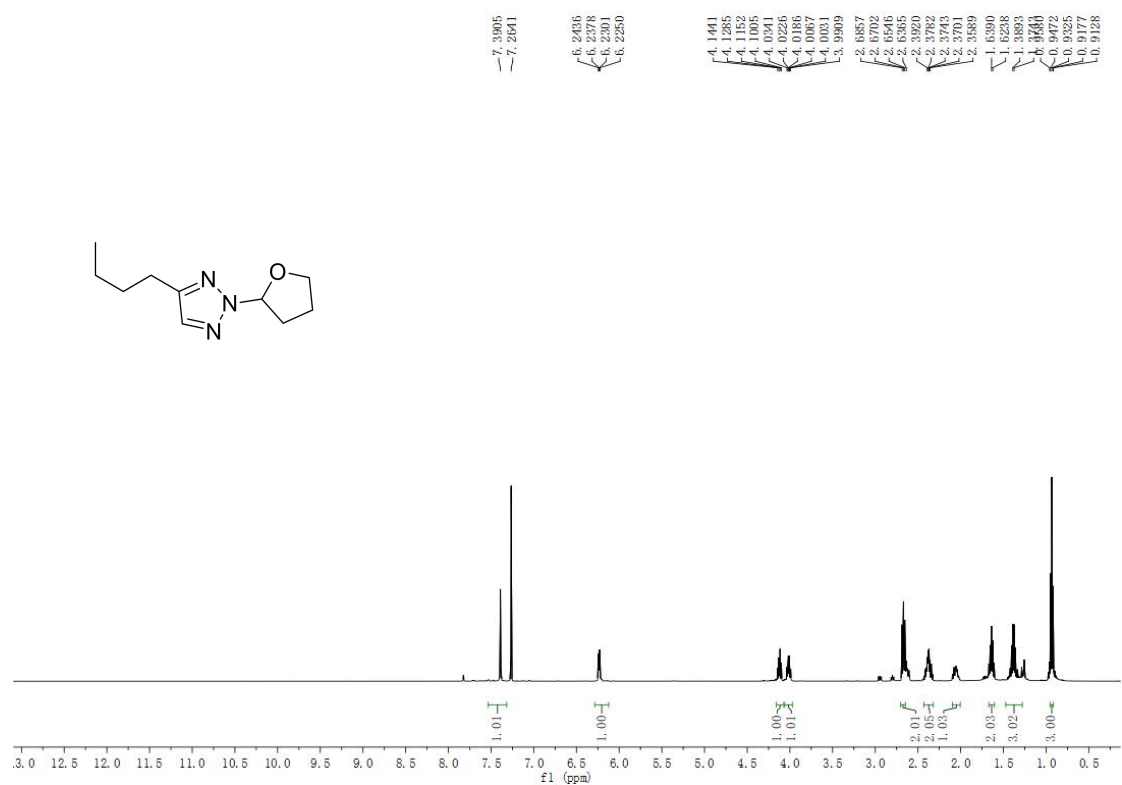


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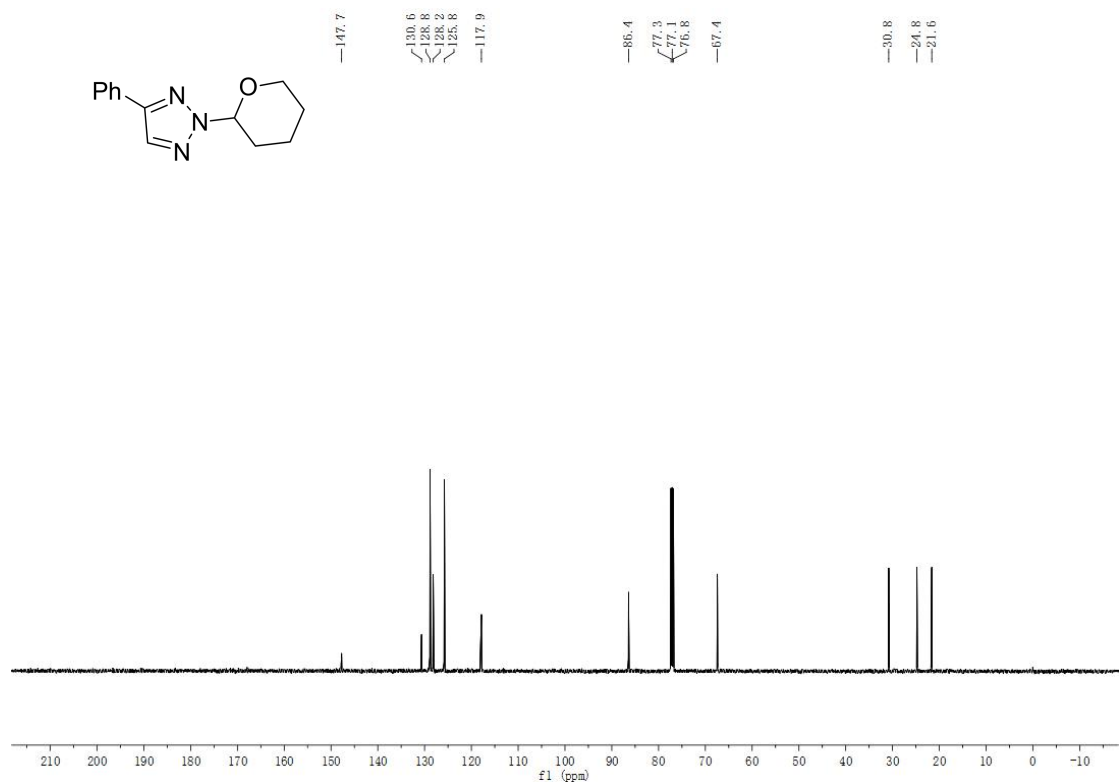
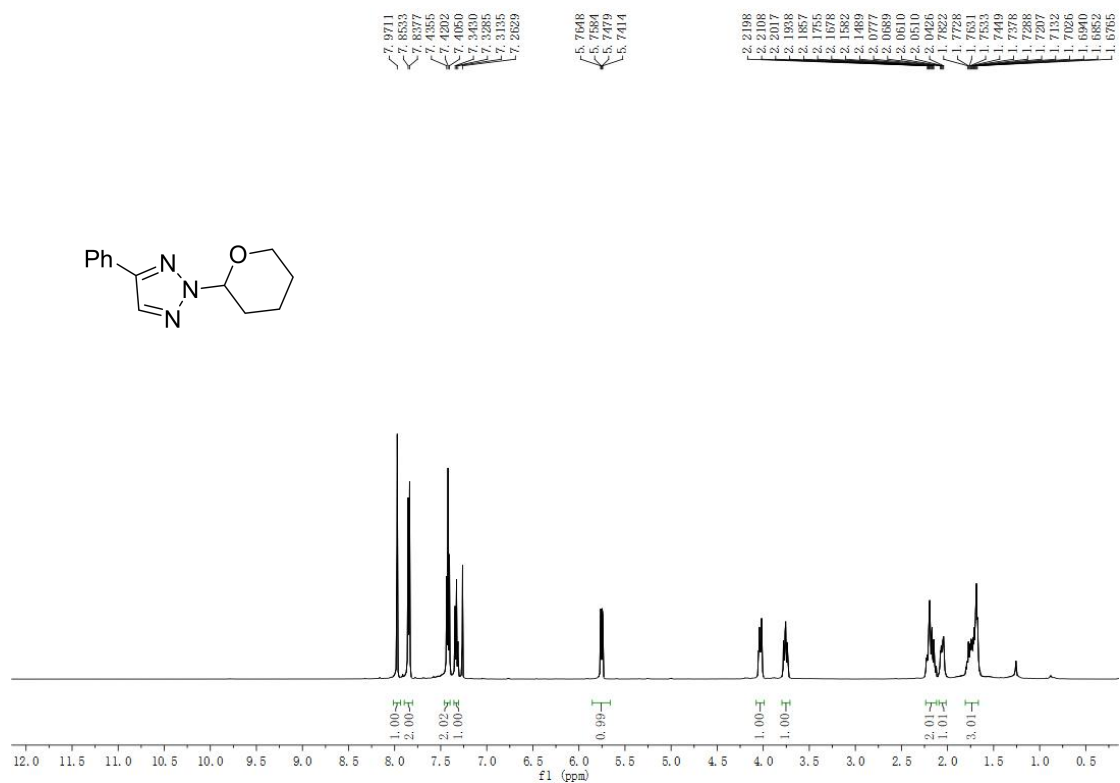
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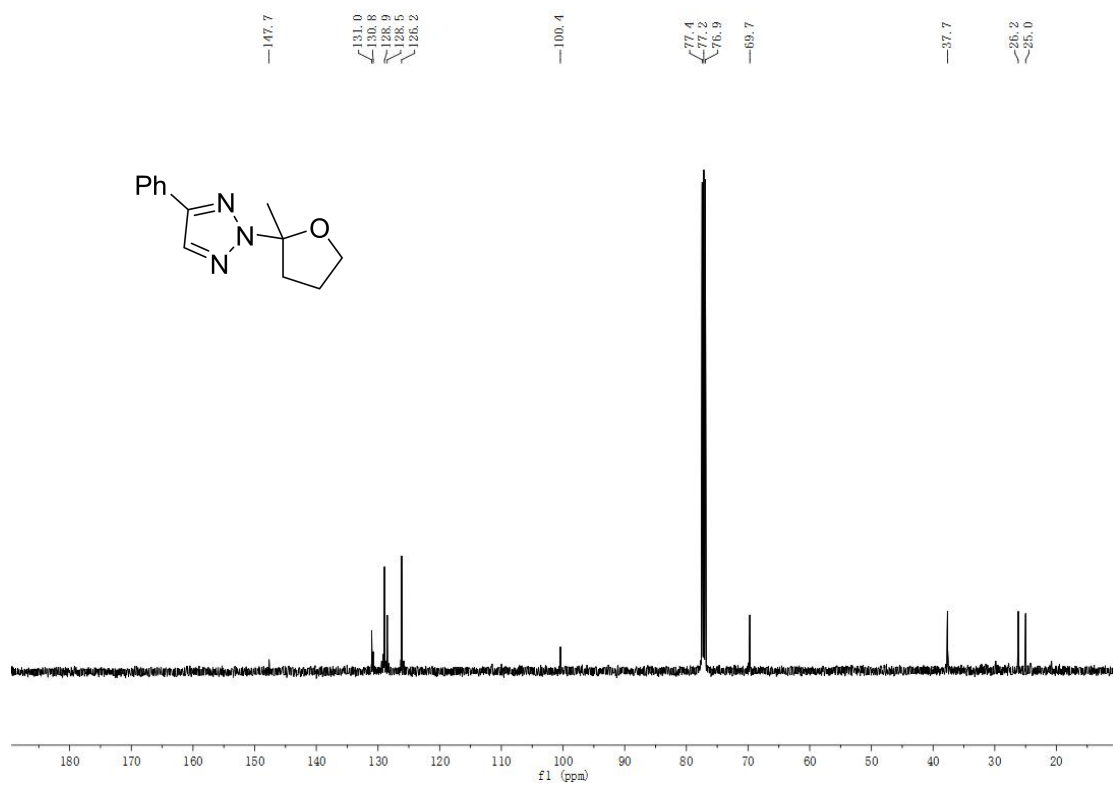
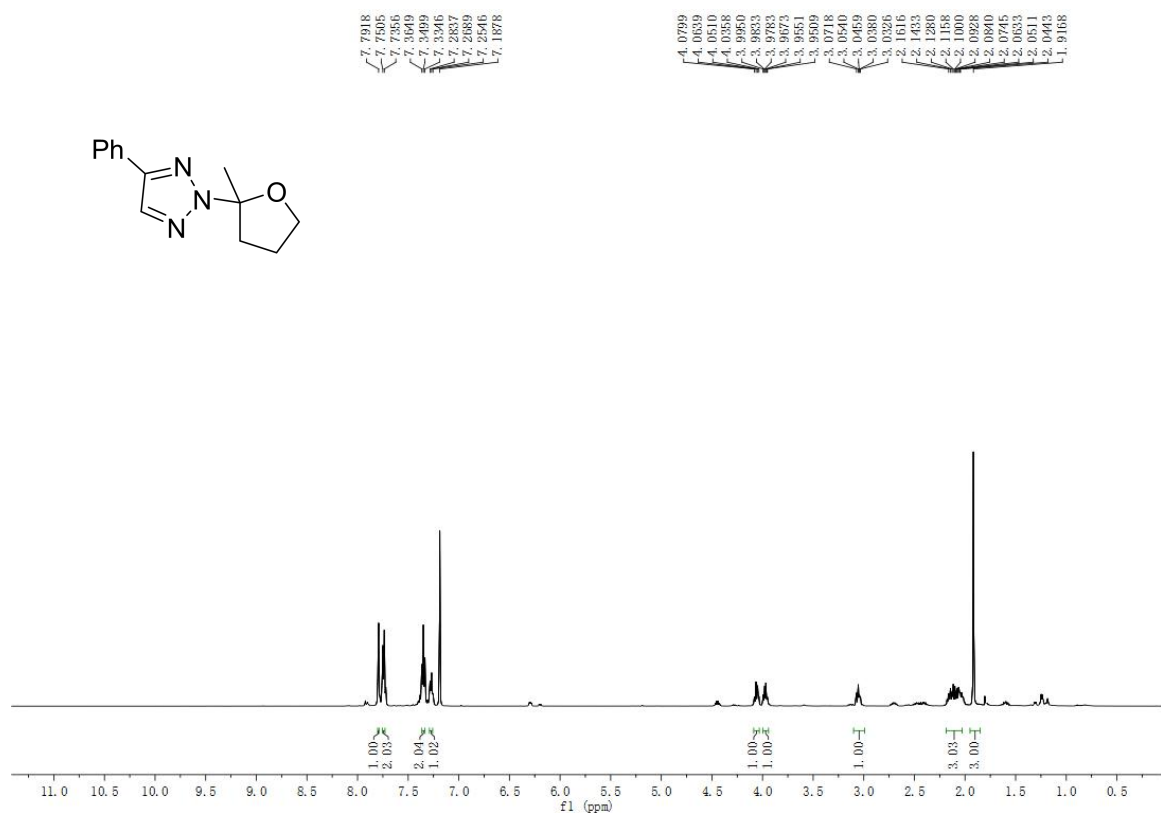
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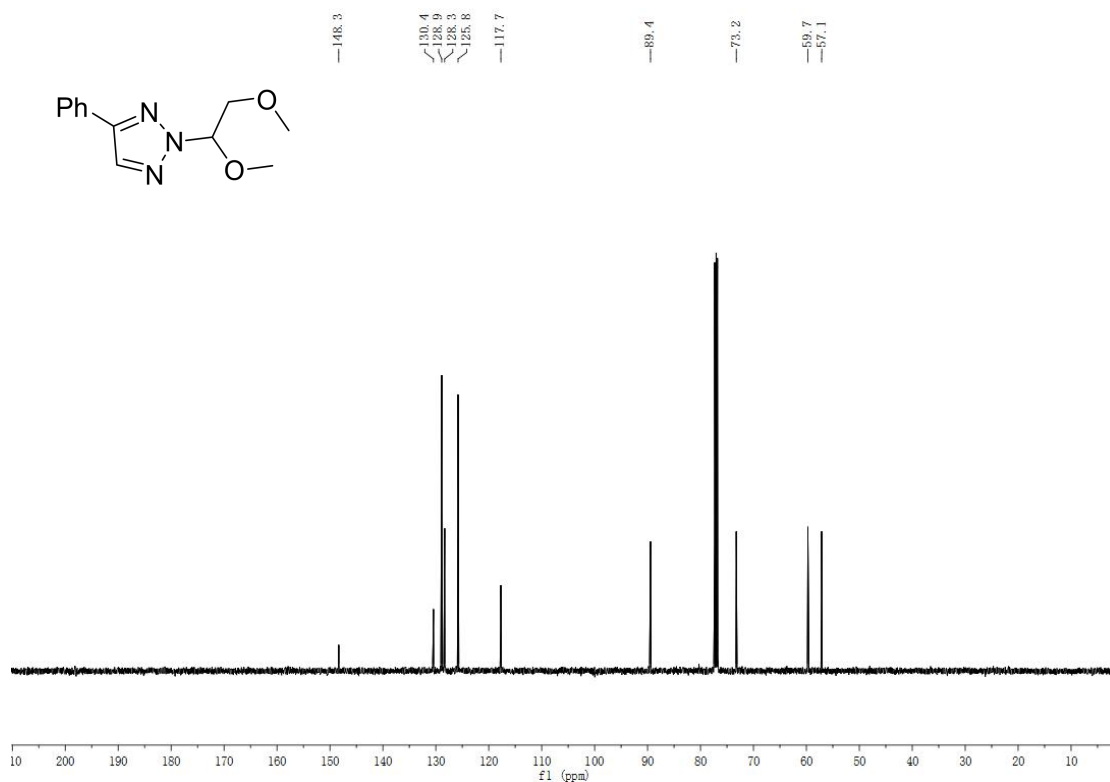
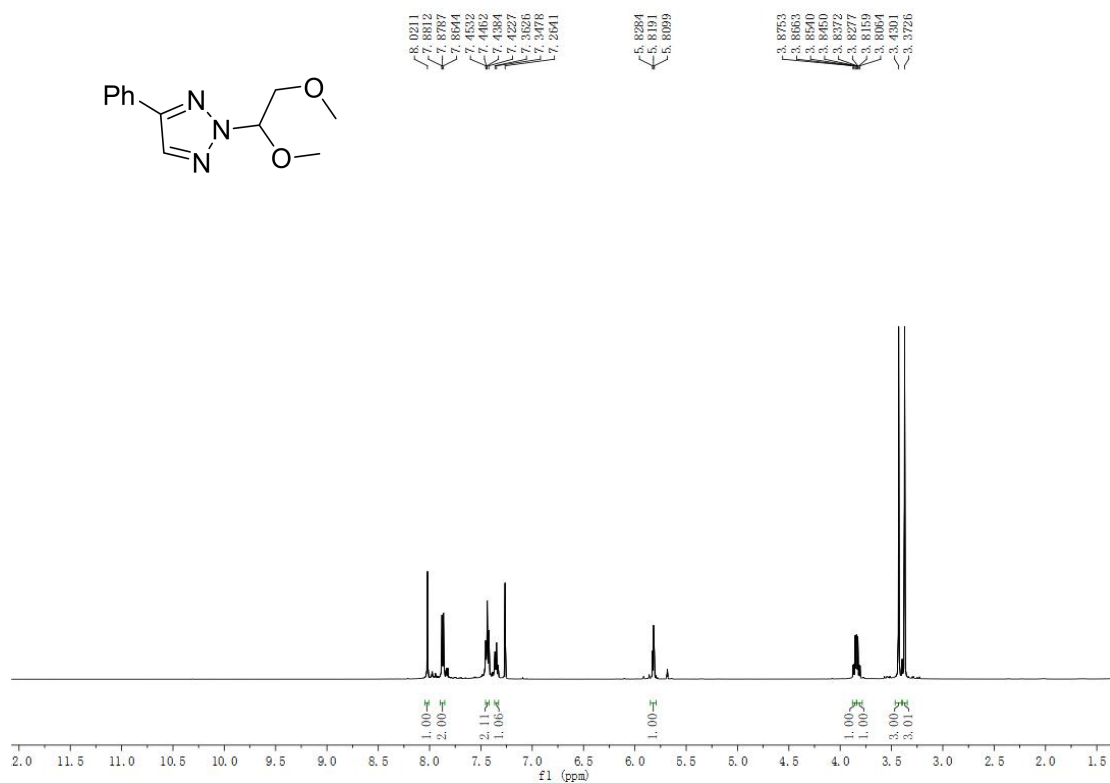
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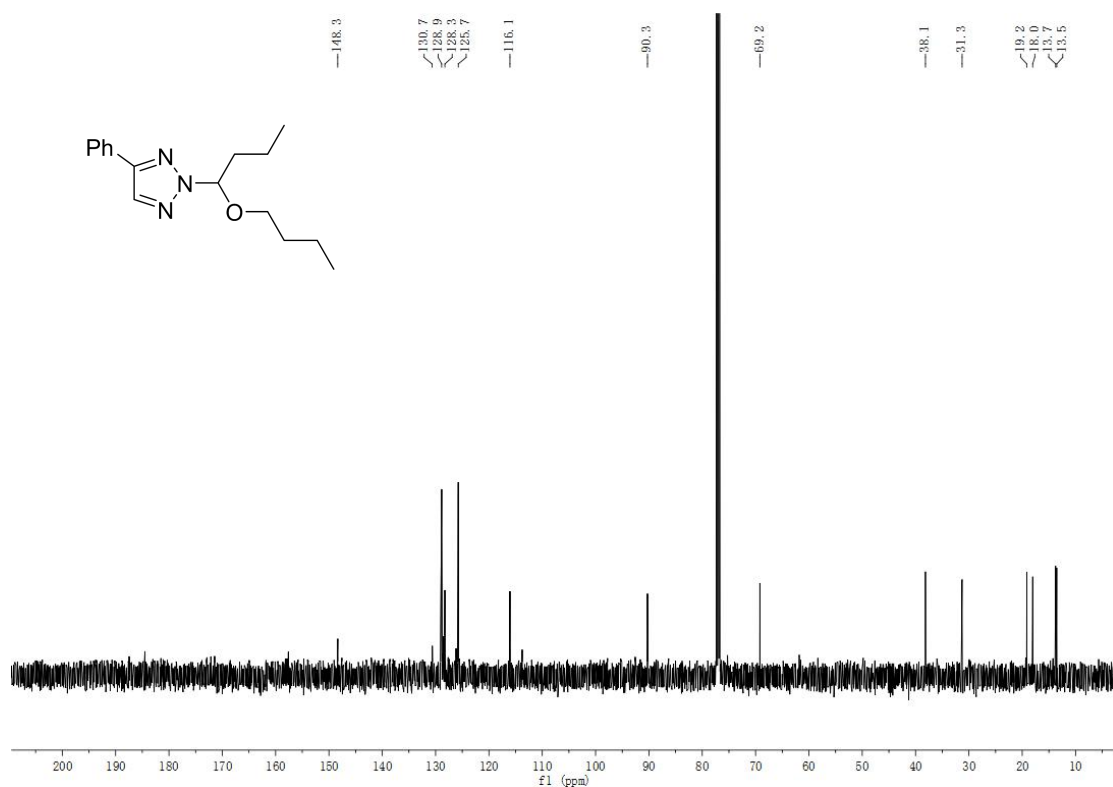
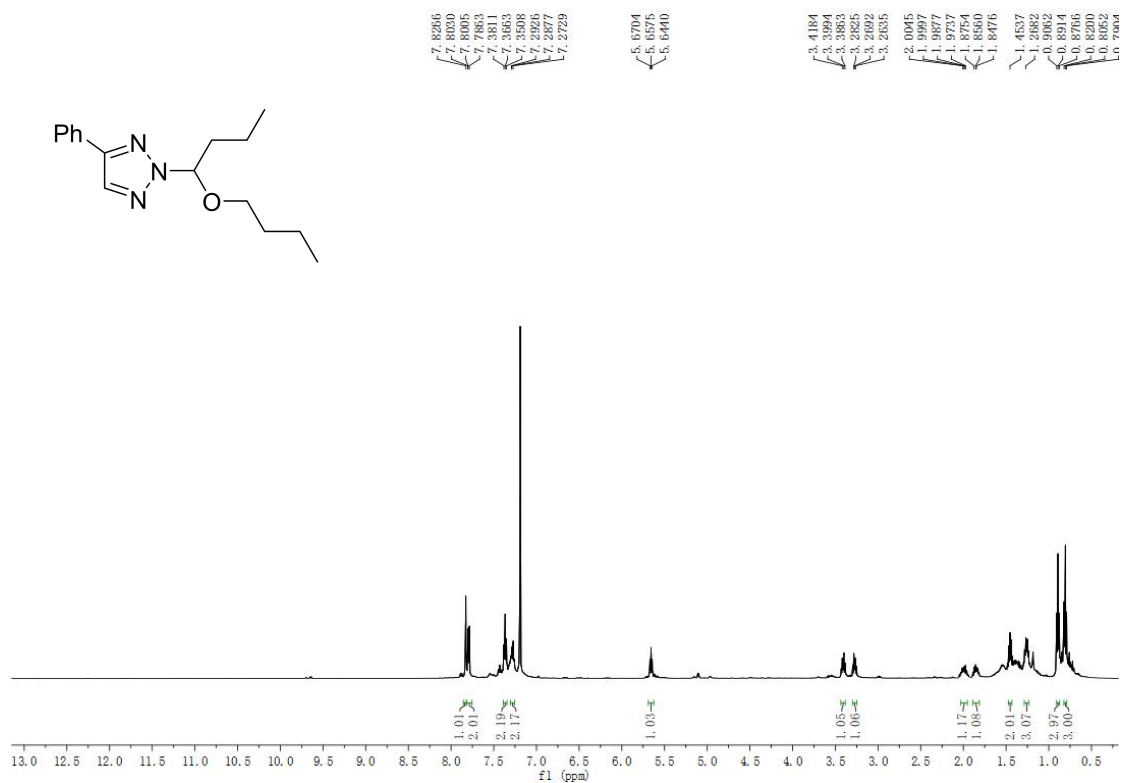
5r



5s



5t



5u

