Supporting Information

Regioselective N^1- and N^2-Heterocycloalkylation of N^1-Sulfonyl-1,2,3-Triazoles

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General Information

All solvents were dried or distilled prior to use according to the standard methods unless otherwise noted. THF was distilled over Na/benzophenone and toluene was distilled over Na. Reagents were purchased from commercial sources at the highest commercial quality. TsN_3 was 75% w/w in ethyl acetate solution. All products could be purified by column chromatography using petroleum ether (PE) and ethyl acetate (EA) as eluent. Glassware was dried in an oven before use. All new compounds were characterized by NMR spectroscopy, IR spectroscopy, high-resolution mass spectroscopy (HRMS).

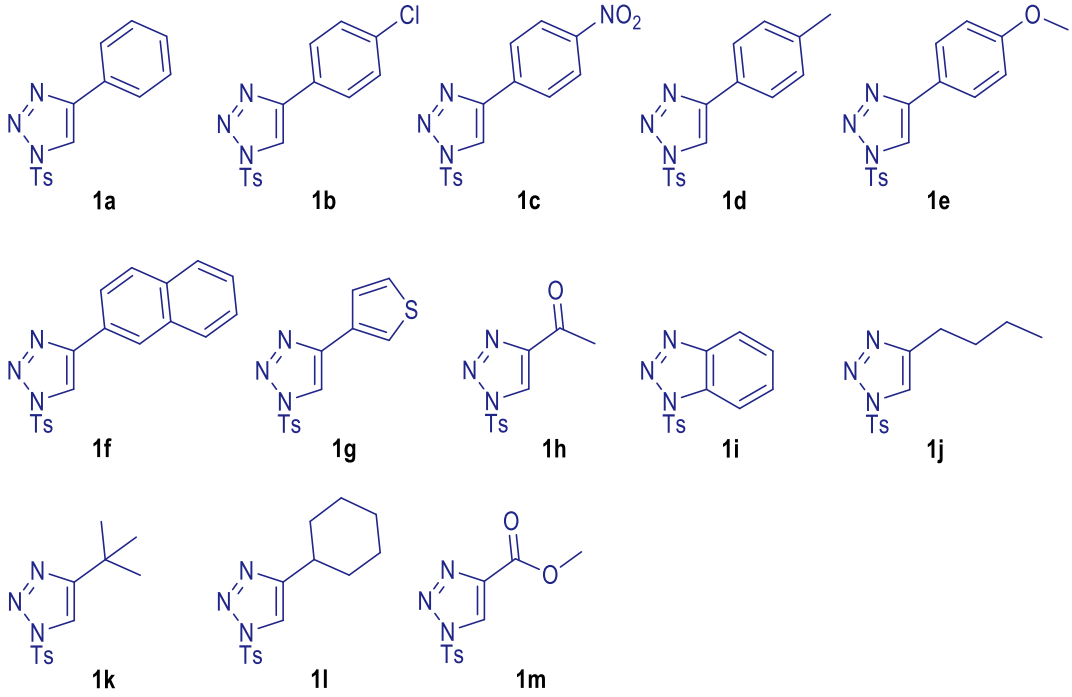
^1H and ^{13}C NMR spectra were recorded on Bruker 500 spectrometer (^1H at 500 MHz and ^{13}C at 125 MHz). Chemical shifts for ^1H NMR spectra are reported as δ in units of parts per million (ppm) downfield from $SiMe_4$ (δ 0.00) and relative to the signal of $SiMe_4$ (δ 0.00 singlet). ^1H NMR splitting patterns are designated as singlet (s), doublet (d), triplet (t), quartet (q), multiplets (m), doublet of doublet (dd), triplet of doublet (td). Coupling constants are reported as a *J* value in Hz. ^{13}C NMR spectra are reported as δ in units of parts per million (ppm) downfield from $SiMe_4$ (δ 0.00) and relative to the signal of chloroform-*d* (δ 77.00 triplet).^{13}C NMR spectra were recorded on the same spectrometer with complete proton decoupling.

Infrared (IR) spectra were measured on Thermofisher Nicolet iN10 FM-IR spectrometer using KBr plates. High resolution mass spectral analysis (HRMS) was performed a Bruker Daltonics APEX II 47e FT-ICR mass spectrometer by using electrospray ionization (ESI) techniques or performed on Bruker solariX 7.0T. Single crystal X-ray diffraction measurements were performed on an Agilent SuperNova-CCD X-ray diffractometer.

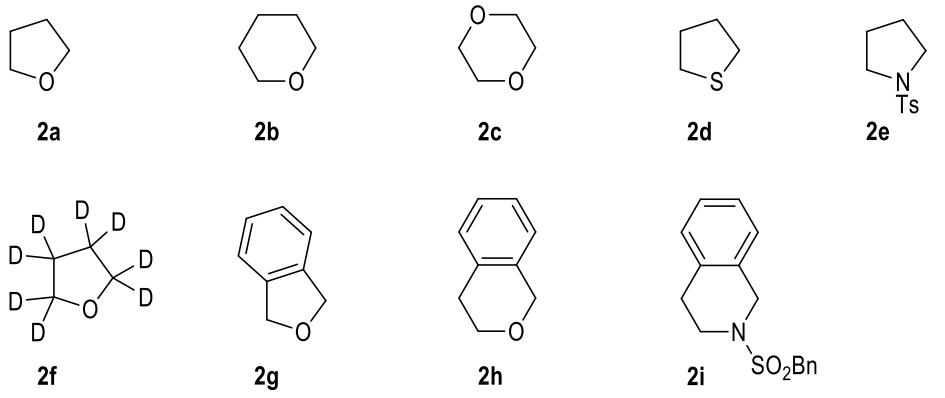
Column chromatographic was performed on 200–300 mesh silica gel and reactions were monitored by thin layer chromatography (TLC) using silica gel GF254 plates. Visualisation was by ultraviolet fluorescene (λ = 254 nm) and staining with phosphomolybdic acid.

Preparation of substrates

N[1]-sulfonyl-1,2,3-triazoles **1a**,[1] **1b**,[2] **1c**,[3] **1d**,[4] **1e**,[5] **1f**,[6] **1g**,[2] **1h**,[7] **1i**,[8] **1j**,[9] **1k**,[10] **1l**,[11] **1m**[12] were synthesized according to literatures.

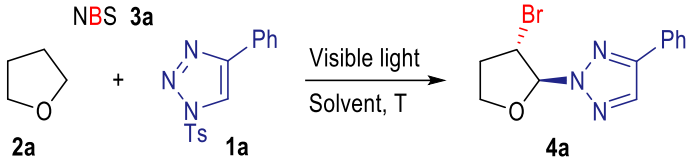


Saturated heterocycles **2a–2i** are commercially available.



Conditions optimization

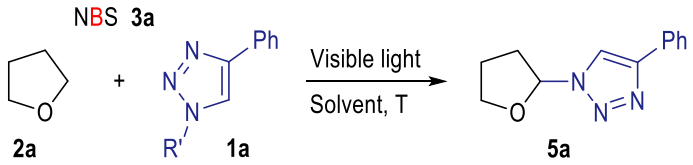
The reaction condition optimization for *N*^{2}-heteroalkylations 1,2,3-triazoles[a,b]



entry	R'	NBS **3a**	solvent	conditions	yield **4a** (%)
1	Ts	1.5 equiv.	THF	90 °C, 3.0 h, Ar	9
2	Ts	1.5 equiv.	THF	90 °C, 12.0 h, Ar	20
3	Ts	1.5 equiv.	PhCl	90 °C, 12.0 h, Ar	42
4	Ts	1.5 equiv.	PhCl	90 °C, 12.0 h, air	56
5	Ts	1.5 equiv.	PhCl	80 °C, 12.0 h, air	34
6	Ts	1.5 equiv.	PhCl	100 °C, 3.0 h, air	55
7	Ts	1.5 equiv.	$PhCF_3$	90 °C, 12.0 h, air	58
8	Ts	1.5 equiv.	PhBr	90 °C, 12.0 h, air	61
9	Ts	1.5 equiv.	PhF	90 °C, 12.0 h, air	68
10	Ts	2.0 equiv.	PhF	90 °C, 12.0 h, air	76
11	Ts	**3.0 equiv.**	**PhF**	**90 °C, 12.0 h, air**	**85**
12	Ms	3.0 equiv.	PhF	90 °C, 12.0 h, air	79

[a]Unless noted, all reactions were carried out on a 0.20 mmol scale (**1a**/**2a** = 1.0/1.2) in 2.0 mL solvent. [b]Isolated yields.

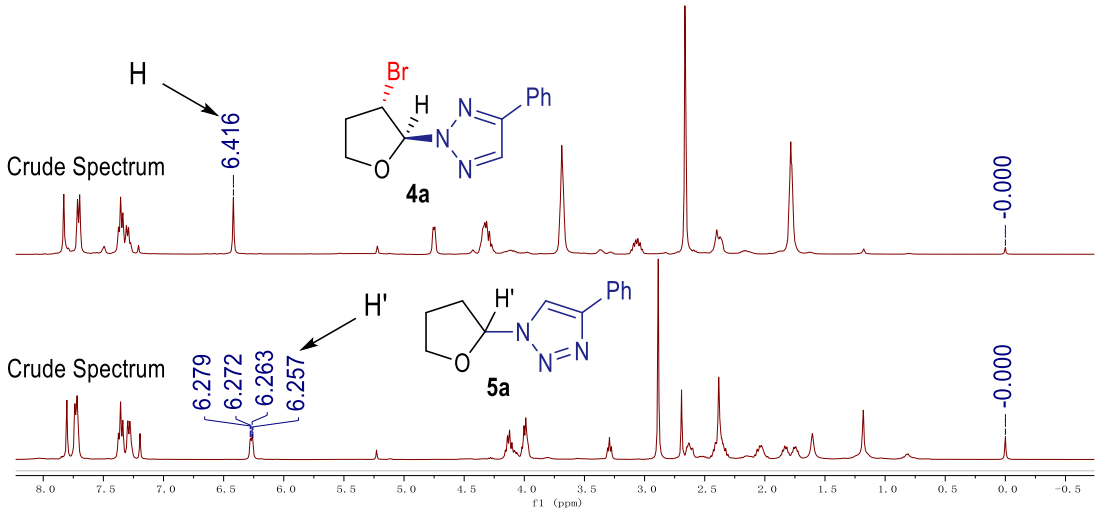
The reaction condition optimization for *N*[1]-heteroalkylations 1,2,3-triazoles[a,b]



entry	R'	NBS **3a**	solvent	conditions	yield **5a** (%)
1	Ts	0.2 equiv.	DCM	r.t., 3.0 h, Ar	13
2	Ts	0.2 equiv.	DCM	r.t., 3.0 h, air	8
3	Ts	0.4 equiv.	DCM	r.t., 3.0 h, Ar	20
4	Ts	0.6 equiv.	DCM	r.t., 3.0 h, Ar	31
5	Ts	1.2 equiv.	DCM	r.t., 3.0 h, Ar	40
6	Ts	1.5 equiv.	DCM	r.t., 3.0 h, Ar	52
7	Ts	1.5 equiv.	Chloroform	r.t., 3.0 h, Ar	trace
8	Ts	1.5 equiv.	1,2–DCE	r.t., 3.0 h, Ar	trace
9	Ts	1.5 equiv.	Mesitylene	r.t., 3.0 h, Ar	trace
10	Ts	1.5 equiv.	THF	r.t., 3.0 h, Ar	70
11	Ts	1.5 equiv.	Acetone	r.t., 3.0 h, Ar	20
12	Ts	1.5 equiv.	MeCN	r.t., 3.0 h, Ar	trace
13	Ts	1.5 equiv.	MeOH	r.t., 3.0 h, Ar	trace
14	Ts	1.5 equiv.	DMSO	r.t., 3.0 h, Ar	trace
15	Ts	1.5 equiv.	Cyclohexane	r.t., 3.0 h, Ar	89
16	**Ts**	**1.5 equiv.**	**Hexane**	**r.t., 3.0 h, Ar**	**94**
17	Ms	1.5 equiv.	Hexane	r.t., 3.0 h, Ar	90

[a]Unless noted, all reactions were carried out on a 0.20 mmol scale (**1a**/**2a** = 1.0/1.2) in 2.0 mL solvent. [b]Isolated yields.

Crude ^{1}H NMR Spectra of Compounds 4a and 5a in $CDCl_3$



The corresponding reactions were performed under optimal conditions, products of direct N^2-alkylation (**4a'**), N^3-alkylation, and α-N^1-1,2,3-triazole-β-bromination (**5a'**) were not observed.

X-ray structure

The single crystal was obtained by slow evaporation of a saturated solution in ethyl acetate in a lossely capped vial. Structure information was deposited at the Cambridge Crystallographic Data Center (CCDC).

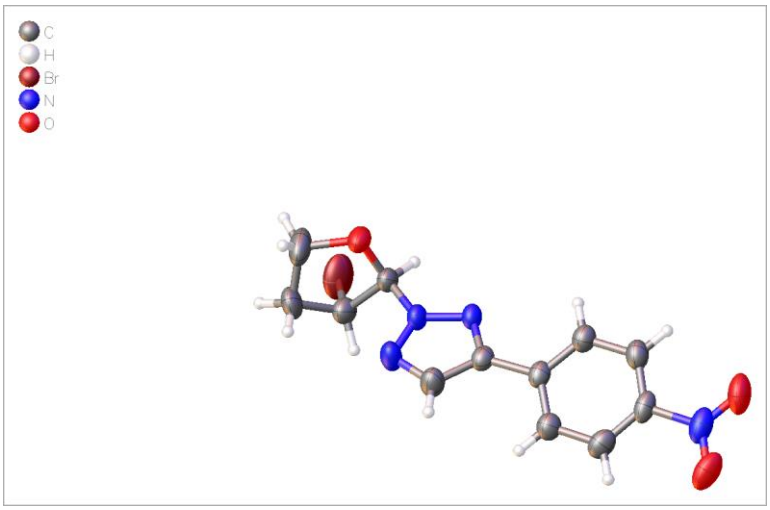
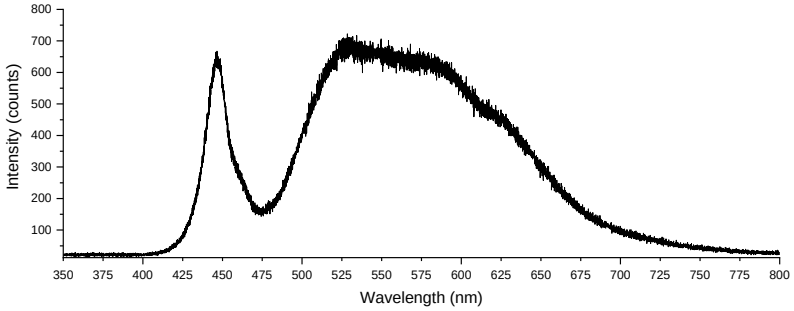


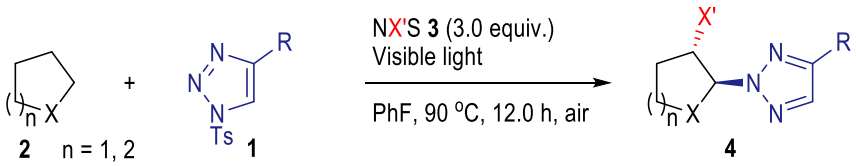
Fig. X-ray crystallographic sturcture of **4c** (CCDC 1974384).

General Procedure A: Syntheses of products 4

A common ring-shaped white light LED lamp (5W) was used as the light source emitter of visible light in our reaction. For further confirmation of wavelength, we measured the wavelength of this LED lamp by a spectrometer (HORIBA Jobin Yvon S.A.S) coupled with a CCD (Charge-Coupled Device). As below figure shown, the result indicate that the wavelength of the current white light LED lamp is between 400 nm and 780 nm.



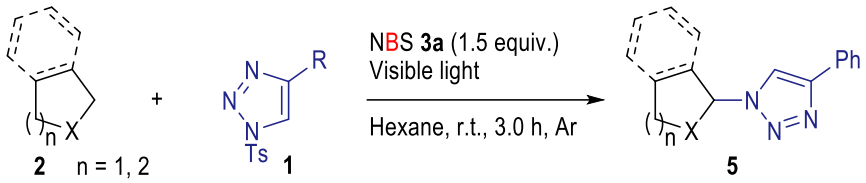
Details of experiment procedure:



N[1]-tosyl-1,2,3-triazoles **1** (0.20 mmol), saturated heterocycles **2** (0.24 mmol), *N*-halogenated succinimide NX'S **3** (0.60 mmol) and PhF (2.0 mL) were added to an oven-dried 10.0 mL reaction tube. The reaction tube is placed in the center directly below the white light LED lamp which is placed 10 cm above reactor (as right photo shown). The reaction mixture was stirred at 90 ºC for 12.0 hours. After triazole was completely consumed by TLC analysis, the reaction mixture was cooled to room temperature, and directly purified by flash chromatography (PE/EA = 50:1) to afford the products **4**.

General Procedure B: Syntheses of products 5

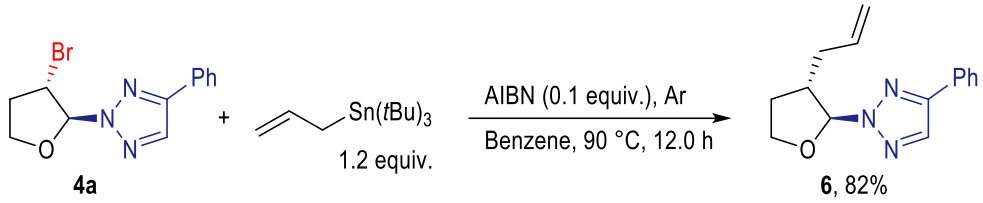
The condition of photocatalytic was the same as General Procedure A. The wavelength of the current white light LED lamp is between 400 nm and 780 nm.



N^1-tosyl-1,2,3-triazoles **1** (0.20 mmol), saturated heterocycles **2** (0.24 mmol), NBS **3a** (53.4 mg, 0.30 mmol) and hexane (2.0 mL) were added to an oven-dried 10.0 mL flask under argon atmosphere. The flask is placed in the center directly below the white light LED lamp which is placed 10 cm above reactor. The reaction mixture was stirred at room temperature for 3.0 hours. After triazole was completely consumed by TLC analysis, the reaction mixture was directly purified by flash chromatography (PE/EA = 30:1) to afford the products **5**.

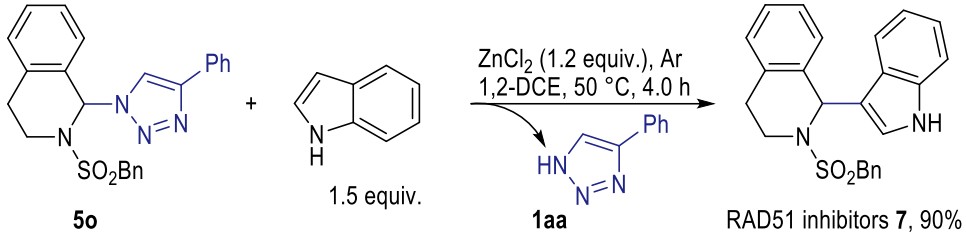
Synthetic transformations and applications

Transformation of product 4a *via* Keck reaction[13]



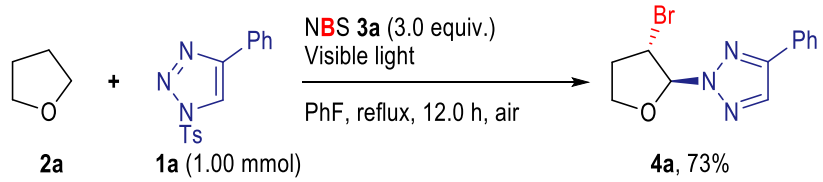
Product **4a** (58.6 mg, 0.20 mmol), allyltributyltin (79.5 mg, 0.24 mmol), AIBN (3.3 mg, 0.02 mmol) and benzene (2.0 mL) were added to an oven-dried 10.0 mL sealed tube under argon atmosphere. The reaction was stirred at 90 ºC for 12.0 hours. After triazole was completely consumed by TLC analysis, the reaction was cooled to room temperature, then the reaction mixture was directly purified by flash chromatography (PE/EA = 80:1) to afford **6** (41.8 mg) in 82% yield.

Synthesis of bioactive compound RAD51 inhibitor



Product **5o** (86.0 mg, 0.20 mmol), indole (35.1 mg, 0.30 mmol), Zinc chloride (32.7 mg, 0.24 mmol) and 1,2-DCE (2.0 mL) were added to an oven-dried 10.0 mL sealed tube under argon atmosphere. The reaction was stirred at 50 ºC for 4.0 hours. After triazole was completely consumed by TLC analysis, the reaction was cooled to room temperature, then the reaction mixture was directly purified by flash chromatography (PE/EA = 5:1) to afford the RAD51 inhibitor **7** (72.4 mg) in 90% yield.

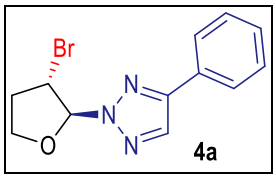
Up-scale reaction for product 4a



N[1]-tosyl-4-phenyl-1,2,3-triazole **1a** (1.00 mmol), THF **2a** (1.20 mmol), NBS **3a** (0.60 mmol) and PhF (10.0 mL) were added to an oven-dried 50.0 mL sealed flask. The reaction was placed under white LED light source, stirred and refluxed for 12.0 hours. After triazole was completely consumed by TLC analysis, the reaction was cooled to room temperature, the reaction mixture was directly purified by flash chromatography (PE/EA = 50:1) to afford the products **4a** (213.9 mg) in 73% yield.

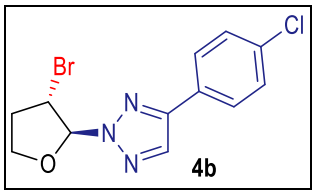
Characterization data for compounds

trans-2-(3-bromotetrahydrofuran-2-yl)-4-phenyl-1,2,3-triazole (**4a**)



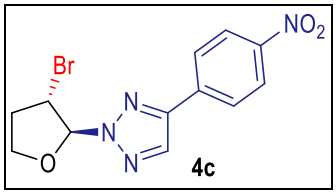
Compound **4a** was obtained from triazole **1a**, THF **2a** and NBS **3a** *via* the General Procedure A as a colorless oil (49.8 mg) in 85% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.80 (s, 1H), 7.69 (d, *J* = 7.0 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 6.41 (s, 1H), 4.74 – 4.73 (m, 1H), 4.35 – 4.27 (m, 2H), 3.09 – 3.02 (m, 1H), 2.38 – 2.35 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 148.6, 131.9, 129.8, 128.9, 128.7, 126.0, 98.2, 69.3, 48.6, 35.3; **IR (cm^{-1})**: *v* 3441, 2978, 1609, 1477, 1296, 1086, 1055, 979, 769, 693; **HRMS**: m/z (ESI) calcd for $C_{12}H_{13}BrN_3O$ $(M+H)^+$ 294.0237, found 294.0239.

trans-2-(3-bromotetrahydrofuran-2-yl)-4-(4-chlorophenyl)-1,2,3-triazole (**4b**)



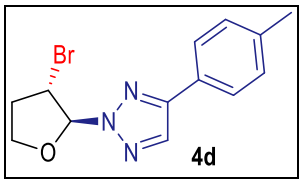
Compound **4b** was obtained from triazole **1b**, THF **2a** and NBS **3a** *via* the General Procedure A as a colorless oil (45.8 mg) in 70% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.79 (s, 1H), 7.63 (d, *J* = 7.0 Hz, 2H), 7.32 (d, *J* = 7.0 Hz, 2H), 6.40 (s, 1H), 4.74 – 4.73 (m, 1H), 4.35 – 4.28 (m, 2H), 3.08 – 3.01 (m, 1H), 2.41 – 2.36 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 147.6, 134.6, 131.9, 129.1, 128.3, 127.3, 98.3, 69.3, 48.4, 35.3; **IR (cm^{-1})**: *v* 3448, 2926, 1479, 1378, 1306, 1085, 1051, 980, 833, 818; **HRMS**: m/z (ESI) calcd for $C_{12}H_{19}BrClN_3O$ $(M+H)^+$ 326.9847, found 326.9843.

trans-2-(3-bromotetrahydrofuran-2-yl)-4-(4-nitrophenyl)-1,2,3-triazole (**4c**)



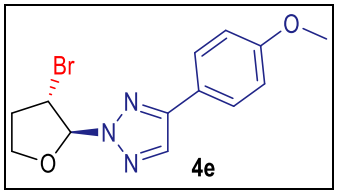
Compound **4c** was obtained from triazole **1c**, THF **2a** and NBS **3a** *via* the General Procedure A as a colorless soild (54.1 mg) in 80% yield. **m.p.**: 82 °C. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.20 (d, *J* = 8.0 Hz, 2H), 7.93 (s, 1H), 7.88 (d, *J* = 7.5 Hz, 2H), 6.43 (s, 1H), 4.75 – 4.74 (m, 1H), 4.36 – 4.30 (m, 2H), 3.08 – 3.01 (m, 1H), 2.43 – 2.37 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 147.7, 146.3, 136.0, 132.7, 126.6, 124.2, 98.5, 69.5, 48.2, 35.2; **IR (cm^{-1})**: *v* 3448, 2902, 1603, 1518, 1342, 1297, 1085, 1055, 981, 855; **HRMS**: m/z (ESI) calcd for $C_{12}H_{12}BrN_4O_3$ $(M+H)^+$ 339.0087, found 339.0089.

trans-2-(3-bromotetrahydrofuran-2-yl)-4-(*p*-tolyl)-1,2,3-triazole (**4d**)



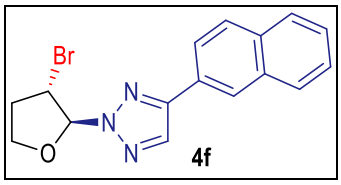
Compound **4d** was obtained from triazole **1d**, THF **2a** and NBS **3a** *via* the General Procedure A as a colorless oil (36.8 mg) in 60% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.78 (s, 1H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 7.5 Hz, 2H), 6.40 (s, 1H), 4.75 – 4.74 (m, 1H), 4.35 – 4.27 (m, 2H), 3.10 – 3.02 (m, 1H), 2.40 – 2.34 (m, 1H), 2.30 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 148.7, 138.7, 131.8, 129.5, 127.0, 125.9, 98.2, 69.3, 48.6, 35.3, 21.3; **IR (cm^{-1})**: *v* 3438, 2924, 2360, 1735, 1620, 1296, 1083, 1055, 981, 821; **HRMS**: m/z (ESI) calcd for $C_{13}H_{15}BrN_3O$ $(M+H)^+$ 308.0393, found 308.0399.

trans-2-(3-bromotetrahydrofuran-2-yl)-4-(4-methoxyphenyl)-1,2,3-triazole (**4e**)



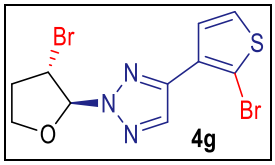
Compound **4e** was obtained from triazole **1e**, THF **2a** and NBS **3a** *via* the General Procedure A as a colorless oil (40.1 mg) in 62% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.74 (s, 1H), 7.63 (d, *J* = 8.5 Hz, 2H), 6.88 (d, *J* = 8.5 Hz, 2H), 6.40 (s, 1H), 4.75 – 4.74 (m, 1H), 4.35 – 4.27 (m, 2H), 3.77 (s, 3H), 3.10 – 3.03 (m, 1H), 2.40 – 2.36 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 160.1, 148.5, 131.5, 127.4, 122.5, 114.3, 98.1, 69.2, 55.3, 48.6, 35.4; **IR (cm^{-1})**: *v* 3448, 2959, 1614, 1469, 1252, 1176, 1092, 1035, 992, 836; **HRMS**: m/z (ESI) calcd for $C_{13}H_{15}BrN_3O$ $(M+H)^+$ 324.0342, found 324.0349.

trans-2-(3-bromotetrahydrofuran-2-yl)-4-(naphthalen-2-yl)-1,2,3-triazole (**4f**)



Compound **4f** was obtained from triazole **1f**, THF **2a** and NBS **3a** *via* the General Procedure A as a colorless oil (48.7 mg) in 71% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.12 (s, 1H), 7.89 (s, 1H), 7.80 – 7.76 (m, 3H), 7.73 (d, *J* = 6.5 Hz, 1H), 7.41 – 7.36 (m, 2H), 6.43 (s, 1H), 4.75 – 4.74 (m, 1H), 4.35 – 4.26 (m, 2H), 3.08 – 3.01 (m, 1H), 2.37 – 2.33 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 148.6, 133.4, 133.3, 132.1, 128.6, 128.1, 127.7, 127.1, 126.5, 126.4, 125.0, 123.8, 98.2, 69.3, 48.6, 35.3; **IR (cm^{-1})**: *v* 3454, 3051, 2970, 2905, 1434, 1298, 1086, 1052, 828, 752; **HRMS**: m/z (ESI) calcd for $C_{16}H_{15}BrN_3O$ $(M+H)^+$ 344.0393, found 344.0398.

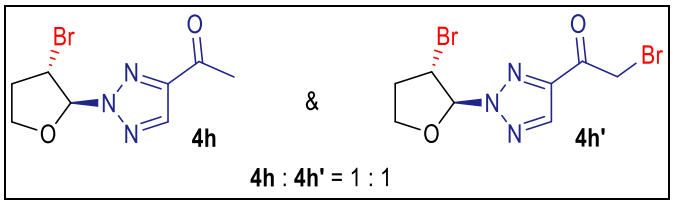
trans-2-(3-bromotetrahydrofuran-2-yl)-4-(2-bromothiophen-3-yl)-1,2,3-triazole (**4g**)



Compound **4g** was obtained from triazole **1g**, THF **2a** and NBS **3a** *via* the General Procedure A as a colorless oil (56.5 mg) in 75% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.15 (s, 1H), 7.28 (d, *J* = 5.0 Hz, 1H), 7.24 (d, *J* = 5.0 Hz, 1H), 6.42 (s, 1H), 4.73 (s, 1H), 4.35 – 4.31 (m, 2H), 3.10 – 3.03 (m, 1H), 2.41 – 2.36 (m, 1H); **^{13}C NMR (125**

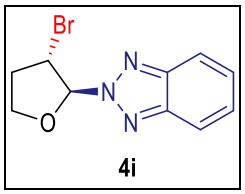
MHz, $CDCl_3$) δ 143.2, 133.0, 130.6, 127.9, 126.7, 110.2, 98.2, 69.4, 48.5, 35.3; **IR (cm^{-1})**: *v* 3445, 2916, 1476, 1298, 1088, 1055, 979, 765; **HRMS**: m/z (ESI) calcd for $C_{10}H_{10}Br_2N_3OS$ $(M+H)^+$ 377.8906, found 377.8902.

trans-1-(2-(3-bromotetrahydrofuran-2-yl)-1,2,3-triazol-4-yl)ethan-1-one and *trans*-2-bromo-1-(2-(3-bromotetrahydrofuran-2-yl)-1,2,3-triazol-4-yl)ethan-1-one (**4h** and **4h'**)



The 1:1 mixture of **4h** and **4h'** was obtained from triazole **1h**, THF **2a** and NBS **3a** *via* the General Procedure A as a colorless oil (35.8 mg) in 60% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.09 (s, 1H), 8.00 (s, 1H), 6.43 (s, 1H), 6.42 (s, 1H), 4.70 (s, 2H), 4.44 (s, 2H), 4.36 – 4.32 (m, 4H), 3.03 – 2.98 (m, 2H), 2.54 (s, 3H), 2.44 – 2.38 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 184.8 (191.9), 144.8 (147.6), 135.5 (136.4), 98.8 (99.0), 69.7 (69.8), 48.0 (48.1), 35.0 (35.1), 27.3 (31.3); **IR (cm^{-1})**: *v* 3448, 3133, 2982, 2903, 1697, 1296, 1094, 1056, 991, 805; **HRMS**: m/z (ESI) calcd for $C_8H_{11}BrN_3O_2$ $(M+H)^+$ 260.0029, found 260.0036; $C_8H_{10}Br_2N_3O_2$ $(M+H)^+$ 337.9134, found 337.9140.

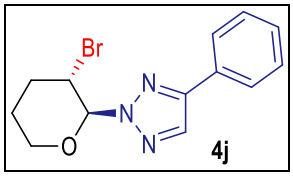
trans-2-(3-bromotetrahydrofuran-2-yl)-benzo[*d*][1,2,3]triazole (**4i**)



Compound **4i** was obtained from triazole **1i**, THF **2a** and NBS **3a** *via* the General Procedure A as a colorless oil (22.4 mg) in 42% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.80 (dd, *J* = 7.0, 3.0 Hz, 2H), 7.34 (dd, *J* = 6.5, 3.0 Hz, 2H), 6.68 (s, 1H), 4.80 (d, *J* = 5.0Hz, 1H), 4.49 – 4.45 (m, 1H), 4.43 – 4.38 (m, 1H), 3.14 – 3.07 (m, 1H), 2.45 – 2.40 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 144.4, 127.1, 118.5, 99.8, 70.0, 48.9,

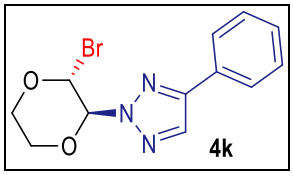
35.1; **IR (cm^{-1})**: *v* 3426, 2928, 1624, 1385, 1265, 1119, 856, 747; **HRMS**: m/z (ESI) calcd for $C_{10}H_{11}BrN_3O$ $(M+H)^+$ 268.0080, found 268.0089.

trans-2-(3-bromotetrahydro-pyran-2-yl)-4-phenyl-1,2,3-triazole (**4j**)



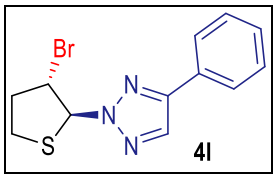
Compound **4j** was obtained from triazole **1a**, tetrahydropyran **2b** and NBS **3a** *via* the General Procedure A as a colorless oil (35.6 mg) in 58% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.88 (s, 1H), 7.75 (d, *J* = 7.5 Hz, 2H), 7.35 (t, *J* = 7.0 Hz, 2H), 7.28 (t, *J* = 7.0 Hz, 1H), 5.66 – 5.63 (m, 1H), 4.72 – 4.67 (m, 1H), 4.13 – 4.09 (m, 1H), 3.75 – 3.69 (m, 1H), 2.63 – 2.59 (m, 1H), 2.14 – 2.06 (m, 1H), 1.94 – 1.86 (m, 1H), 1.72 – 1.68 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 148.7, 132.1, 129.8, 128.8, 128.8, 126.2, 92.7, 68.1, 46.9, 34.5, 26.7; **IR (cm^{-1})**: *v* 3456, 2953, 1455, 1396, 1300, 1069, 1039, 944, 779, 731; **HRMS**: m/z (ESI) calcd for $C_{13}H_{15}BrN_3O$ $(M+H)^+$ 308.0393, found 308.0401.

trans-2-(3-bromo-1,4-dioxan-2-yl)-4-phenyl-1,2,3-triazole (**4k**)



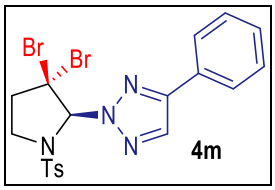
Compound **4k** was obtained from triazole **1a**, 1,4-dioxane **2c** and NBS **3a** *via* the General Procedure A as a colorless oil (30.9 mg) in 50% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.92 (s, 1H), 7.75 (d, *J* = 7.0 Hz, 2H), 7.38 (dd, *J* = 7.5, 7.0 Hz, 2H), 7.31 (t, *J* = 7.5 Hz, 1H), 6.85 (s, 1H), 6.05 (s, 1H), 4.38 (td, *J* = 12.0, 3.0 Hz, 1H), 4.18 (dd, *J* = 12.0, 2.5 Hz, 1H), 3.80 (d, *J* = 11.0 Hz, 2H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 148.8, 132.3, 129.6, 129.0, 128.9, 126.2, 87.4, 82.8, 61.5, 61.0; **IR (cm^{-1})**: *v* 3435, 2925, 1627, 1457, 1385, 1124, 1102, 977, 942, 769; **HRMS**: m/z (ESI) calcd for $C_{12}H_{13}BrN_3O_2$ $(M+H)^+$ 310.0186, found 310.0194.

trans-2-(3-bromotetrahydrothiophen-2-yl)-4-phenyl-1,2,3-triazole (**4l**)



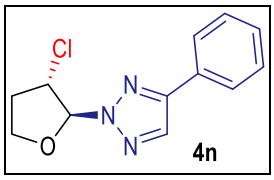
Compound **4l** was obtained from triazole **1a**, tetrahydrothiophene **2d** and NBS **3a** *via* the General Procedure A as a colorless oil (32.8 mg) in 53% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.81 (s, 1H), 7.70 (d, *J* = 7.0 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 1H), 6.33 (d, *J* = 2.5 Hz, 1H), 4.92 (dd, *J* = 7.5, 4.5 Hz, 1H), 3.31 – 3.23 (m, 2H), 3.03 – 2.96 (m, 1H), 2.53 – 2.48 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 148.6, 132.0, 129.8, 128.9, 128.8, 126.0, 78.0, 53.4, 38.9, 31.2; **IR (cm^{-1})**: *v* 3449, 1536, 1475, 1293, 1205, 1092, 992, 978, 808, 769; **HRMS**: m/z (ESI) calcd for $C_{12}H_{13}BrN_3S$ $(M+H)^+$ 310.0008, found 310.0013.

2-(3,3-dibromo-1-tosylpyrrolidin-2-yl)-4-phenyl-1,2,3-triazole (**4m**)



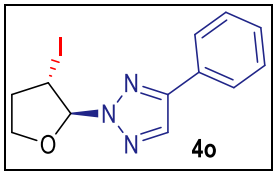
Compound **4m** was obtained from triazole **1a**, *N*-tosylpyrrolidine **2e** and NBS **3a** *via* the General Procedure A as a colorless oil (62.9 mg) in 60% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.73 (d, *J* = 7.0 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 7.0 Hz, 4H), 7.08 (d, *J* = 8.0 Hz, 2H), 6.50 (s, 1H), 3.77 – 3.74 (m, 2H), 3.45 – 3.38 (m, 1H), 2.90 – 2.86 (m, 1H), 2.20(s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 146.2, 144.4, 134.3, 130.0, 129.6, 129.2, 128.5, 128.3, 127.4, 127.1, 86.0, 58.6, 46.8, 44.9, 21,4; **IR (cm^{-1})**: *v* 3448, 2924, 1597, 1454, 1360, 1167, 1127, 1040, 1007, 770; **HRMS**: m/z (ESI) calcd for $C_{19}H_{19}Br_2N_4O_2S$ $(M+H)^+$ 524.9590, found 524.9585.

trans-2-(3-chlorotetrahydrofuran-2-yl)-4-phenyl-1,2,3-triazole (**4n**)



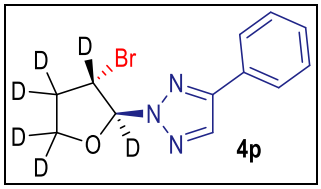
Compound **4n** was obtained from triazole **1a**, THF **2a** and NCS **3b** *via* the General Procedure A as a colorless oil (30.4 mg) in 61% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.82 (s, 1H), 7.71 (d, *J* = 8.0 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 1H), 6.30 (s, 1H), 4.80 – 4.79 (m, 1H), 4.37 – 4.28 (m, 2H), 3.03 – 2.96 (m, 1H), 2.33 – 2.29 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 148.7, 132.0, 129.8, 128.9, 128.8, 126,1, 97.8, 69.2, 60.1, 34.8; **IR (cm^{-1})**: *v* 3448, 2924, 1630, 1477, 1384, 1297, 1088, 1062, 980, 770; **HRMS**: m/z (ESI) calcd for $C_{12}H_{13}ClN_3O$ $(M+H)^+$ 250.0742, found 250.0747.

trans-2-(3-iodotetrahydrofuran-2-yl)-4-phenyl-1,2,3-triazole (**4o**)



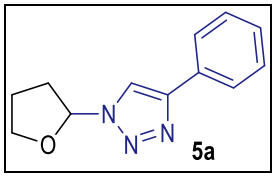
Compound **4o** was obtained from triazole **1a**, THF **2a** and NIS **3c** *via* the General Procedure A as a colorless oil (35.5 mg) in 52% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.82 (s, 1H), 7.71 (d, *J* = 7.0 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 1H), 6.50 (s, 1H), 4.74 – 4.72 (m, 1H), 4.34 – 4.23 (m, 2H), 3.03 – 2.95 (m, 1H), 2.41 – 2.34 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 148.6, 131.9, 129.9, 128.9, 128.8, 126.1, 100.1, 69.5, 37.2, 21.1; **IR (cm^{-1})**: *v* 3448, 2970, 1637, 1477, 1294, 1084, 1047, 979, 802, 769; **HRMS**: m/z (ESI) calcd for $C_{12}H_{13}IN_3O$ $(M+H)^+$ 342.0098, found 342.0108.

trans-2-(3-bromotetrahydrofuran-2-yl-2,3,4,4,5,5-d_6)-4-phenyl-1,2,3-triazole (**4p**)



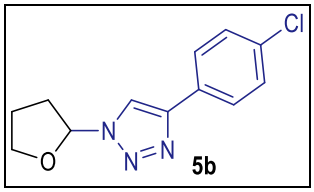
Compound **4p** was obtained from triazole **1a**, THF-d_8 **2f** and NBS **3a** *via* the General Procedure A as a colorless oil (44.7 mg) in 78% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.81 (s, 1H), 7.70 (d, *J* = 8.5 Hz, 2H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.28 (t, *J* = 7.5 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 148.7, 132.0, 129.9, 128.9, 128.9, 126.1, 98.3, 69.4, 48.6, 35.4; **IR (cm^{-1})**: *v* 3128, 3076, 3036, 2239, 1459, 1298, 1078, 1043, 978, 771; **HRMS**: m/z (ESI) calcd for $C_{12}H_7D_6BrN_3O$ $(M+H)^+$ 300.0613, found 300.0620.

4-phenyl-1-(tetrahydrofuran-2-yl)-1,2,3-triazole (**5a**)[14]



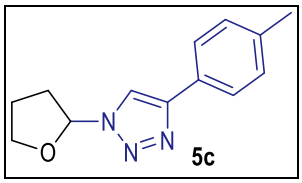
Compound **5a** was obtained from triazole **1a**, THF **2a** and NBS **3a** *via* the General Procedure B as a colorless oil (40.4 mg) in 94% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.79 (s, 1H), 7.72 (d, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.27 (t, *J* = 7.5 Hz, 1H), 6.26 – 6.25 (m, 1H), 4.14 – 4.10 (m, 1H), 4.00 – 3.96 (m, 1H), 2.65 – 2.59 (m, 1H), 2.42 – 2.29 (m, 2H), 2.05 – 1.97 (m, 1H).

4-(4-chlorophenyl)-1-(tetrahydrofuran-2-yl)-1,2,3-triazole (**5b**)[15]



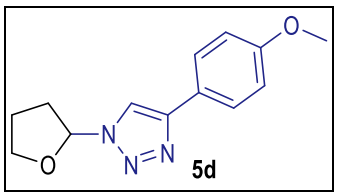
Compound **5b** was obtained from triazole **1b**, THF **2a** and NBS **3a** *via* the General Procedure B as a colorless oil (34.4 mg) in 69% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.77 (s, 1H), 7.65 (d, *J* = 8.5 Hz, 2H), 7.31 (d, *J* = 8.5 Hz, 2H), 6.25 (dd, *J* = 6.5, 2.0 Hz, 1H), 4.14 – 4.09 (m, 1H), 4.05 – 3.96 (m, 1H), 2.64 – 2.58 (m, 1H), 2.38 – 2.33 (m, 2H), 2.06 – 1.99 (m, 1H).

1-(tetrahydrofuran-2-yl)-4-(p-tolyl)-1,2,3-triazole (**5c**)[15]



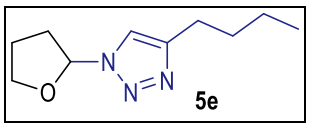
Compound **5c** was obtained from triazole **1d**, THF **2a** and NBS **3a** *via* the General Procedure B as a colorless oil (39.4 mg) in 86% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.75 (s, 1H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 7.5 Hz, 2H), 6.24 (dd, *J* = 7.0, 2.5 Hz, 1H), 4.11 – 4.08 (m, 1H), 3.99 – 3.94 (m, 1H), 2.63 – 2.58 (m, 1H), 2.41 – 2.29 (m, 5H), 2.04 – 1.95 (m, 1H).

4-(4-methoxyphenyl)-1-(tetrahydrofuran-2-yl)-1,2,3-triazole (**5d**)[16]



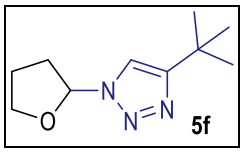
Compound **5d** was obtained from triazole **1e**, THF **2a** and NBS **3a** *via* the General Procedure B as a colorless oil (44.6 mg) in 91% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.72 (s, 1H), 7.64 (d, *J* = 9.0 Hz, 2H), 6.87 (d, *J* = 9.0 Hz, 2H), 6.24 (dd, *J* = 7.0, 2.5 Hz, 1H), 4.13 – 4.08 (m, 1H), 3.99 – 3.95 (m, 1H), 3.75 (s, 3H), 2.65 – 2.58 (m, 1H), 2.41 – 2.29 (m, 2H), 2.05 – 1.96 (m, 1H).

4-butyl-1-(tetrahydrofuran-2-yl)-1,2,3-triazole (**5e**)[17]



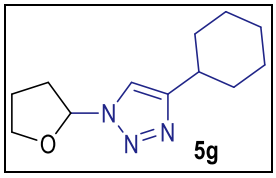
Compound **5e** was obtained from triazole **1j**, THF **2a** and NBS **3a** *via* the General Procedure B as a colorless oil (35.1 mg) in 90% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.32 (s, 1H), 6.17 (dd, *J* = 6.5, 2.5 Hz, 1H), 4.07 – 4.03 (m, 1H), 3.97 – 3.92 (m, 1H), 2.60 (t, *J* = 7.5 Hz, 2H), 2.57 – 2.54 (m, 1H), 2.33 – 2.28 (m, 2H), 2.03 – 1.96 (m, 1H), 1.60 – 1.54 (m, 2H), 1.35 – 1.27 (m, 2H), 0.86 (t, *J* = 7.5 Hz, 3H).

4-(*tert*-butyl)-1-(tetrahydrofuran-2-yl)-1,2,3-triazole (**5f**)



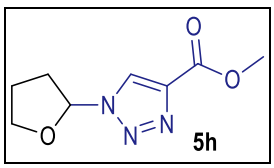
Compound **5f** was obtained from triazole **1k**, THF **2a** and NBS **3a** *via* the General Procedure B as a colorless oil (31.2 mg) in 80% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.35 (s, 1H), 6.17 – 6.16 (m, 1H), 4.05 (q, *J* = 7.0 Hz, 1H), 3.93 (q, *J* = 7.0 Hz, 1H), 2.59 – 2.54 (m, 1H), 2.35 – 2.25 (m, 2H), 2.03 – 1.95 (m, 1H), 1.25 (s, 9H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 157.8, 131.0, 91.8, 69.3, 31.1, 30.8, 30.3, 24.5; **IR (cm^{-1})**: *v* 2965, 2932, 2906, 2872, 1513, 1462, 1297, 1229, 1072, 1015, 813, 729; **HRMS**: m/z (ESI) calcd for $C_{10}H_{18}N_3O$ $(M+H)^+$ 196.1444, found 196.1450.

4-cyclohexyl-1-(tetrahydrofuran-2-yl)-1,2,3-triazole (**5g**)[17]



Compound **5g** was obtained from triazole **1l**, THF **2a** and NBS **3a** *via* the General Procedure B as a colorless oil (40.3 mg) in 91% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.32 (s, 1H), 6.17 – 6.16 (m, 1H), 4.07 – 4.02 (m, 1H), 3.96 – 3.91 (m, 1H), 2.66 – 2.62 (m, 1H), 2.57 – 2.53 (m, 1H), 2.36 – 2.25 (m, 2H), 2.02 – 1.92 (m, 3H), 1.73 (d, *J* = 12 Hz, 2H), 1.64 (d, *J* = 12.5 Hz, 1H), 1.39 – 1.27 (m, 4H), 1.22 – 1.17 (m, 1H).

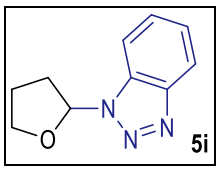
methyl 1-(tetrahydrofuran-2-yl)-1,2,3-triazole-4-carboxylate (**5h**)



Compound **5h** was obtained from triazole **1m**, THF **2a** and NBS **3a** *via* the General Procedure B as a colorless oil (32.4 mg) in 83% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.00 (s, 1H), 6.29 (dd, *J* = 6.5, 2.5 Hz, 1H), 4.16 – 4.12 (m, 1H), 4.02 – 3.98 (m, 1H), 3.88 (s, 3H), 2.58 – 2.52 (m, 1H), 2.39 – 2.33 (m, 2H), 2.06 – 1.98 (m, 1H); **^{13}C NMR**

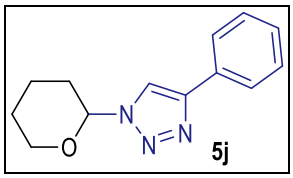
(125 MHz, $CDCl_3$) δ 161.0, 139.7, 137.1, 93.3, 69.9, 52.2, 31.7, 24.2; **IR (cm^{-1})**: *v* 3141, 2958, 2897, 1733, 1513, 1439, 1299, 1227, 955, 890; **HRMS** m/z (ESI) calcd for $C_8H_{11}N_3NaO_3$ $(M+Na)^+$ 220.0693, found 220.0691.

1-(tetrahydrofuran-2-yl)-benzo[*d*][1,2,3]triazole (**5i**)[18]



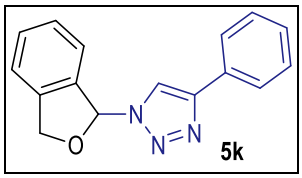
Compound **5i** was obtained from triazole **1i**, THF **2a** and NBS **3a** *via* the General Procedure B as a colorless oil (32.5 mg) in 86% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.00 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.5 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.31 (t, *J* = 7.5 Hz, 1H), 6.44 (dd, *J* = 6.5, 2.5 Hz, 1H), 4.05 – 4.01 (m, 1H), 3.99 – 3.94 (m, 1H), 3.12 – 3.07 (m, 1H), 2.49 – 2.42 (m, 1H), 2.37 – 2.29 (m, 1H), 2.15 – 2.10 (m, 1H).

4-phenyl-1-(tetrahydro-2*H*-pyran-2-yl)-1,2,3-triazole (**5j**)[17]



Compound **5j** was obtained from triazole **1a**, tetrahydropyran **2b** and NBS **3a** *via* the General Procedure B as a colorless oil (28.4 mg) in 62% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.92 (s, 1H), 7.83 – 7.81 (m, 2H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.35 (t, *J* = 7.5 Hz, 1H), 5.75 (dd, *J* = 9.0, 3.0 Hz, 1H), 4.11 – 4.06 (m, 1H), 3.79 – 3.74 (m, 1H), 2.52 – 2.44 (m, 1H), 2.19 – 2.09 (m, 2H), 1.81 – 1.73 (m, 2H), 1.70 – 1.64 (m, 1H).

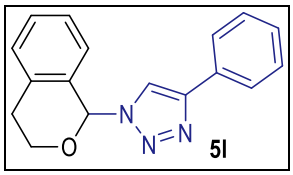
1-(1,3-dihydroisobenzofuran-1-yl)-4-phenyl-1,2,3-triazole (**5k**)



Compound **5k** was obtained from triazole **1a**, 1,3-dihydrobenzofuran **2g** and NBS **3a** *via* the General Procedure B as a colorless oil (41.6 mg) in 79% yield. **^{1}H NMR (500**

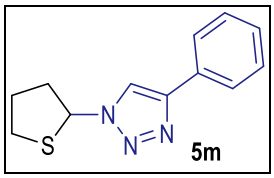
MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.69 (d, *J* = 7.5 Hz, 2H), 7.39 – 7.36 (m, 2H), 7.32 (t, *J* = 7.0 Hz, 3H), 7.29 – 7.23 (m, 3H), 5.44 (d, *J* = 12.5 Hz, 1H), 5.16 (d, *J* = 12.5 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 148.4, 139.9, 135.4, 132.3, 130.1, 129.7, 128.8, 128.6, 128.0, 126.1, 122.8, 121.3, 95.5, 74.0; **IR (cm^{-1})**: *v* 3055, 2990, 2949, 2887, 1629, 1542, 1464, 1436, 1342, 1275, 1073, 900, 750, 697; **HRMS** m/z (ESI) calcd for $C_{16}H_{13}N_3NaO$ $(M+Na)^+$ 286.0951, found 286.0950.

1-(isochroman-1-yl)-4-phenyl-1,2,3-triazole (**5l**)[19]



Compound **5l** was obtained from triazole **1a**, isochromane **2h** and NBS **3a** *via* the General Procedure B as a colorless oil (37.7 mg) in 68% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.82 (s, 1H), 7.72 (d, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.27 – 7.22 (m, 2H), 7.18 (d, *J* = 7.5 Hz, 1H), 7.12 (t, *J* = 7.5 Hz, 1H), 6.98 (s, 1H), 6.94 (d, *J* = 8.0 Hz, 1H), 4.30 – 4.25 (m, 1H), 4.01 – 3.98 (m, 1H), 3.10 – 3.03 (m, 1H), 2.87 (d, *J* = 16.0 Hz, 1H).

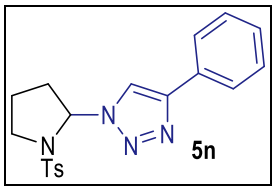
4-phenyl-1-(tetrahydrothiophen-2-yl)-1,2,3-triazole (**5m**)



Compound **5m** was obtained from triazole **1a**, tetrahydrothiophene **2d** and NBS **3a** *via* the General Procedure B as a colorless oil (37.0 mg) in 80% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.78 (s, 1H), 7.72 – 7.70 (m, 2H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 1H), 6.24 (dd, *J* = 6.5, 2.5 Hz, 1H), 3.24 – 3.20 (m,1H), 2.97 – 2.92 (m, 1H), 2.72 – 2.69 (m, 1H), 2.59 – 2.51 (m, 1H), 2.33 – 2.27 (m, 1H), 2.26 – 2.19 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 147.9, 131.3, 130.3, 128.8, 128.5, 126.0, 71.6, 37.5, 33.7, 29.6; **IR (cm^{-1})**: *v* 3052, 2919, 2849, 1620, 1474, 1458, 1365, 1089, 978, 768,

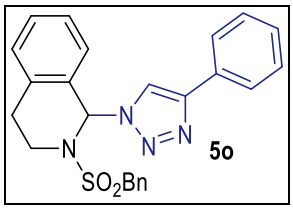
692, 556; **HRMS** m/z (ESI) calcd for $C_{12}H_{13}N_3NaS$ $(M+Na)^+$ 254.0722, found 254.0721.

4-phenyl-1-(1-tosylpyrrolidin-2-yl)-1,2,3-triazole (**5n**)



Compound **5n** was obtained from triazole **1a**, *N*-tosylpyrrolidine **2e** and NBS **3a** *via* the General Procedure B as a colorless oil (44.2 mg) in 60% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.59 (s, 1H), 7.52 (d, *J* = 7.0 Hz, 2H), 7.36 – 7.31 (m, 4H), 7.27 (t, *J* = 7.5 Hz, 1H), 6.98 (d, *J* = 8.0 Hz, 2H), 6.38 (d, *J* = 7.0 Hz, 1H), 3.70 – 3.62 (m, 2H), 2.52 – 2.43 (m, 1H), 2.37 – 2.29 (m, 1H), 2.22 – 2.14 (m, 1H), 2.07 (s, 3H), 2.12 – 2.02 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 147.7, 143.3, 135.5, 130.6, 129.9, 129.2, 128.7, 128.4, 126.8, 125.8, 77.0, 48.2, 35.6, 23.2, 21.2; **IR (cm^{-1})**: *v* 3500, 2925, 1645, 1456, 1261, 1091, 768; **HRMS** m/z (ESI) calcd for $C_{19}H_{20}N_4NaO_2S$ $(M+Na)^+$ 391.1199, found 391.1197.

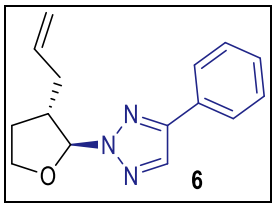
2-(benzylsulfonyl)-1-(4-phenyl-1,2,3-triazol-1-yl)-1,2,3,4-tetrahydroisoquinoline (**5o**)



Compound **5o** was obtained from triazole **1a**, *N*-protected tetrahydroisoquinoline **2i** and NBS **3a** *via* the General Procedure B as a colorless oil (71.4 mg) in 83% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.97 (s, 1H), 7.84 (d, *J* = 8.0 Hz, 2H), 7.54 (s, 1H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.34 – 7.27 (m, 2H), 7.21 – 7.17 (m, 4H), 7.08 (d, *J* = 7.5 Hz, 1H), 6.95 (d, *J* = 7.5 Hz, 2H), 4.15 (d, *J* = 14.0 Hz, 1H), 4.06 (d, *J* = 14.0 Hz, 1H), 3.56 – 3.46 (m, 2H), 3.07 – 3.00 (m, 1H), 2.78 (d, J = 16.5 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 148.5, 134.3, 130.6, 129.9, 129.7, 129.2, 129.0, 128.9, 128.7, 128.7, 128.7, 128.5, 128.1, 127.8, 126.8, 126.3, 126.1, 71.8, 59.5, 40.8, 29.2;

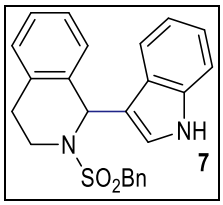
IR (cm^{-1}): *v* 2965, 2851, 1508, 1347, 1065, 926, 817; **HRMS** m/z (ESI) calcd for $C_{24}H_{22}N_4NaO_2S$ $(M+Na)^+$ 453.1356, found 453.1363.

trans-2-(3-allyltetrahydrofuran-2-yl)-4-phenyl-1,2,3-triazole (**6**)



Compound **6** was obtained as a colorless oil (41.8 mg) in 82% yield. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.81 (s, 1H), 7.73 (d, *J* = 7.0 Hz, 2H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.27 (t, *J* = 7.5 Hz, 1H), 5.93 (d, *J* = 7.0 Hz, 1H), 5.75 – 5.67 (m, 1H), 5.05 (d, *J* = 17.0 Hz, 1H), 5.00 (d, *J* = 10.0 Hz, 1H), 4.15 (d, *J* = 7.5 Hz, 1H), 4.09 – 4.05 (m, 1H), 3.08 – 3.01 (m, 1H), 2.50 – 2.44 (m, 1H), 2.35 – 2.29 (m, 1H), 2.25 – 2.19 (m, 1H), 1.81 – 1.76 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 148.2, 135.3, 131.5, 130.3, 128.8, 128.5, 126.0, 117.3, 96.6, 69.3, 44.0, 37.1, 30.7; **IR(cm^{-1})**: *v* 3450, 3059, 1688, 1597, 1345, 1161, 1023, 756, 698, 517; **HRMS**: m/z: $(M+H)^+$ calculated for $C_{15}H_{18}N_3O^+$, 256.1444, found 256.1452.

2-(benzylsulfonyl)-1-(1H-indol-3-yl)-1,2,3,4-tetrahydroisoquinoline (**7**)[20]



Compound **7** was obtained as a colorless oil (72.4 mg) in 90% yield. **^{1}H NMR (500 MHz, CDCl3)** δ 8.12 (s, 1H), 7.70 (d, *J* = 7.5 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.17 – 7.13 (m, 3H), 7.10 – 6.98 (m, 5H), 6.94 (d, *J* = 8.0 Hz, 1H), 6.80 – 6.80 (m, 1H), 6.76 (d, *J* = 8.0 Hz, 2H), 6.39 (s, 1H), 3.93 (d, *J* = 13.5 Hz, 1H), 3.81 (d, *J* = 13.5 Hz, 1H), 3.43 – 3.39 (m, 1H), 3.12 – 3.06 (m, 1H), 2.96 – 2.87 (m, 1H), 2.66 – 2.62 (m, 1H).

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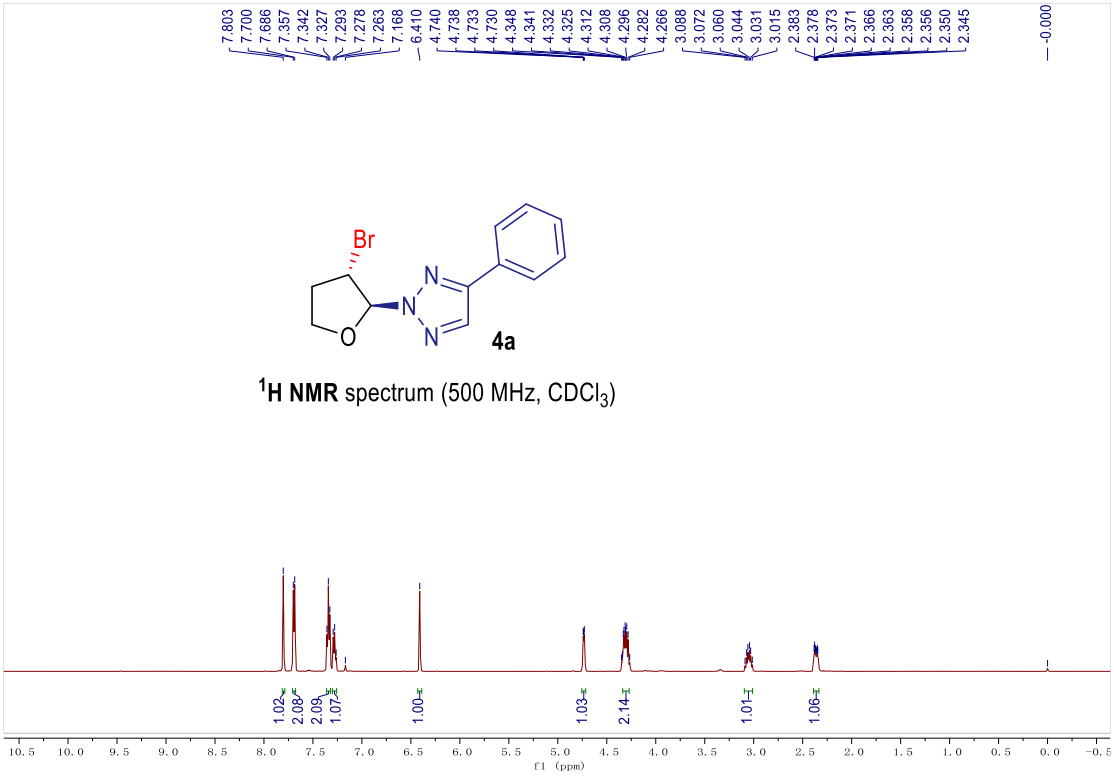
Copies of NMR spectra

4a



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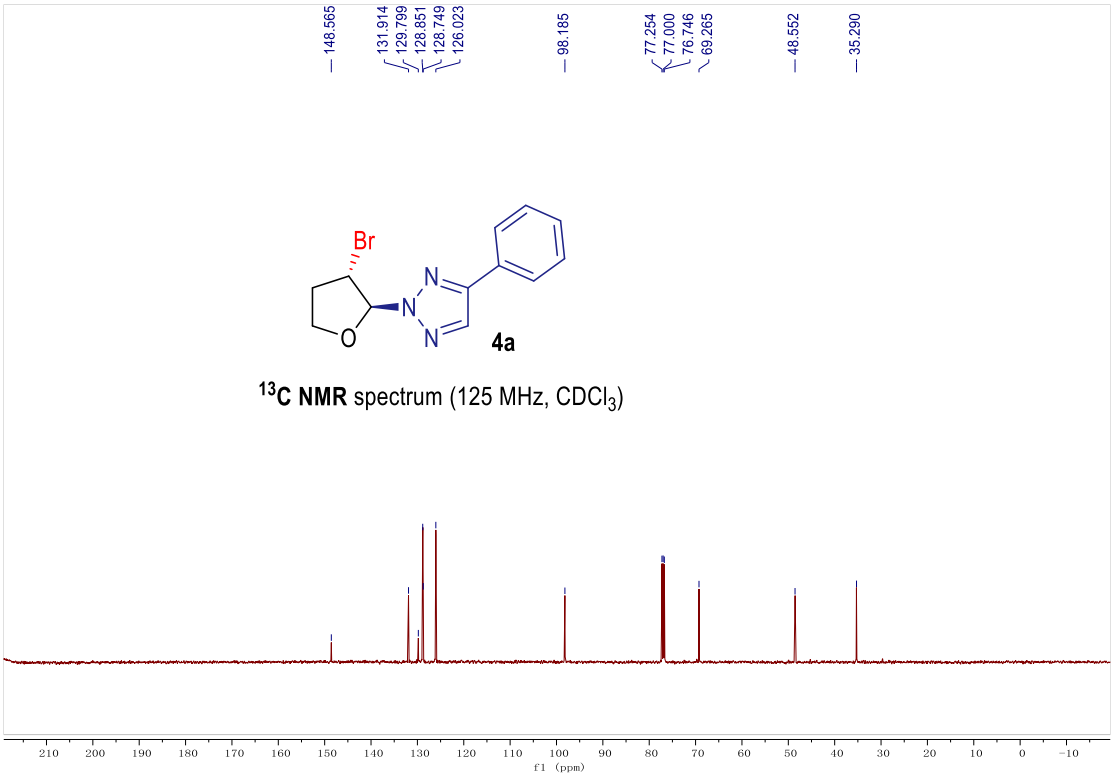

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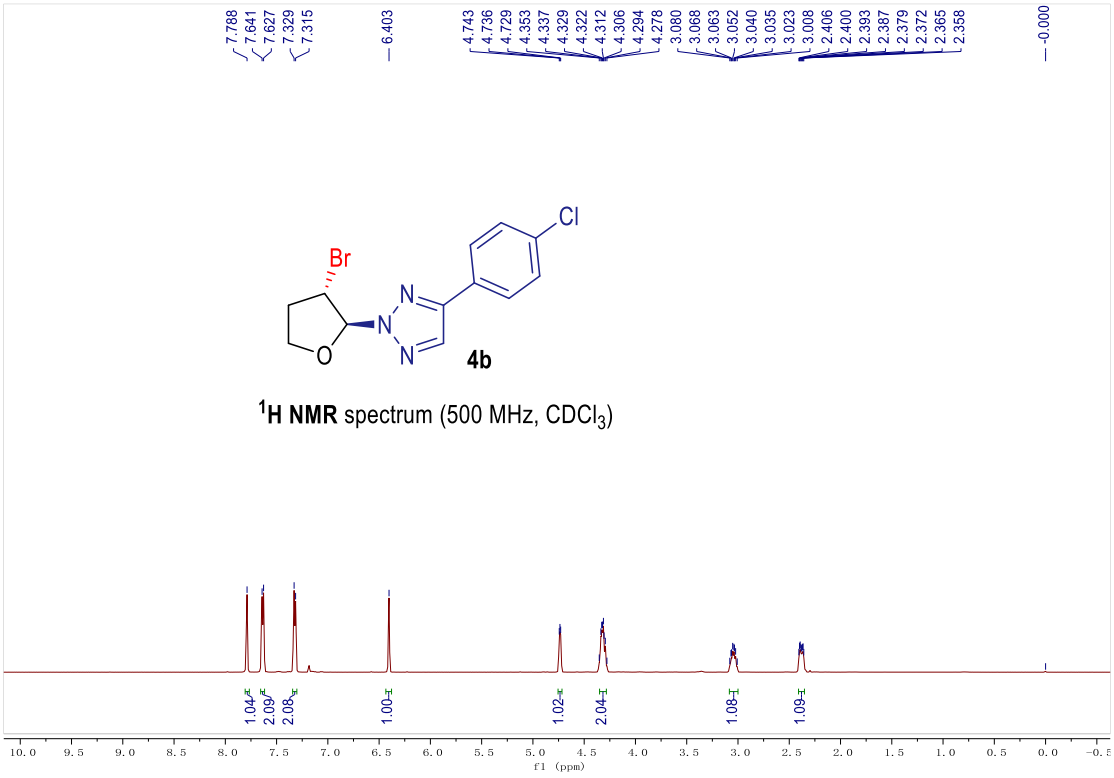
4b



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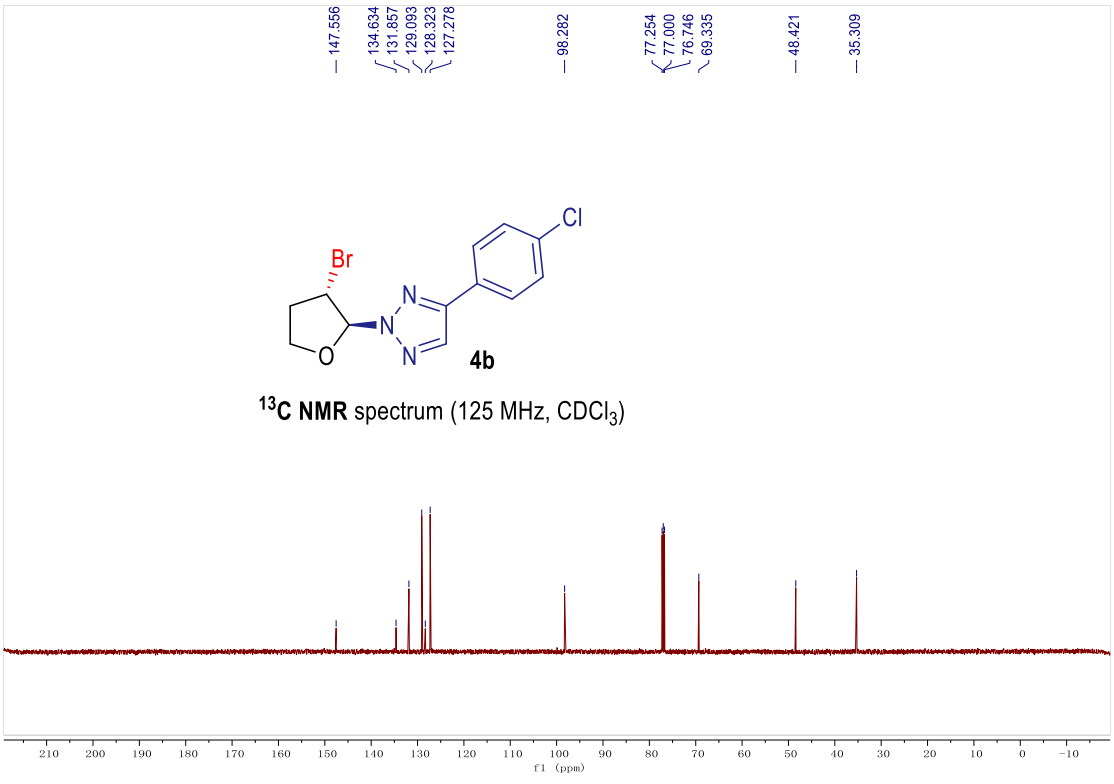
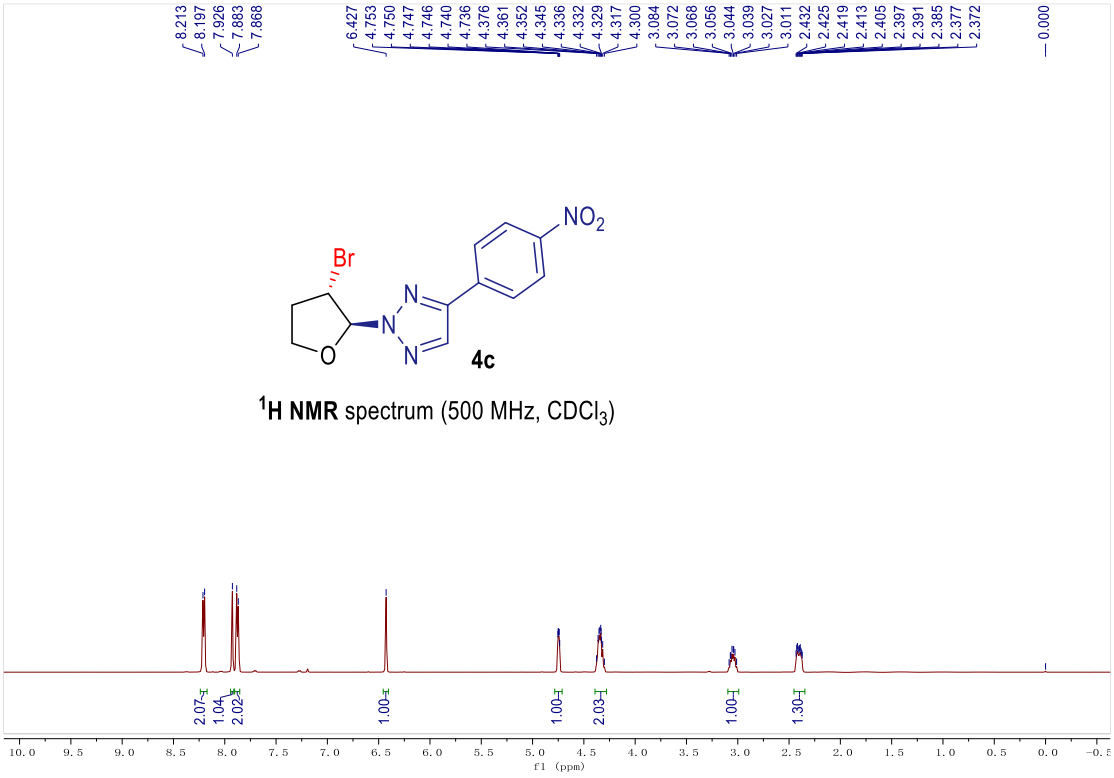


^{13}C NMR spectrum (125 MHz, $CDCl_3$)

4c



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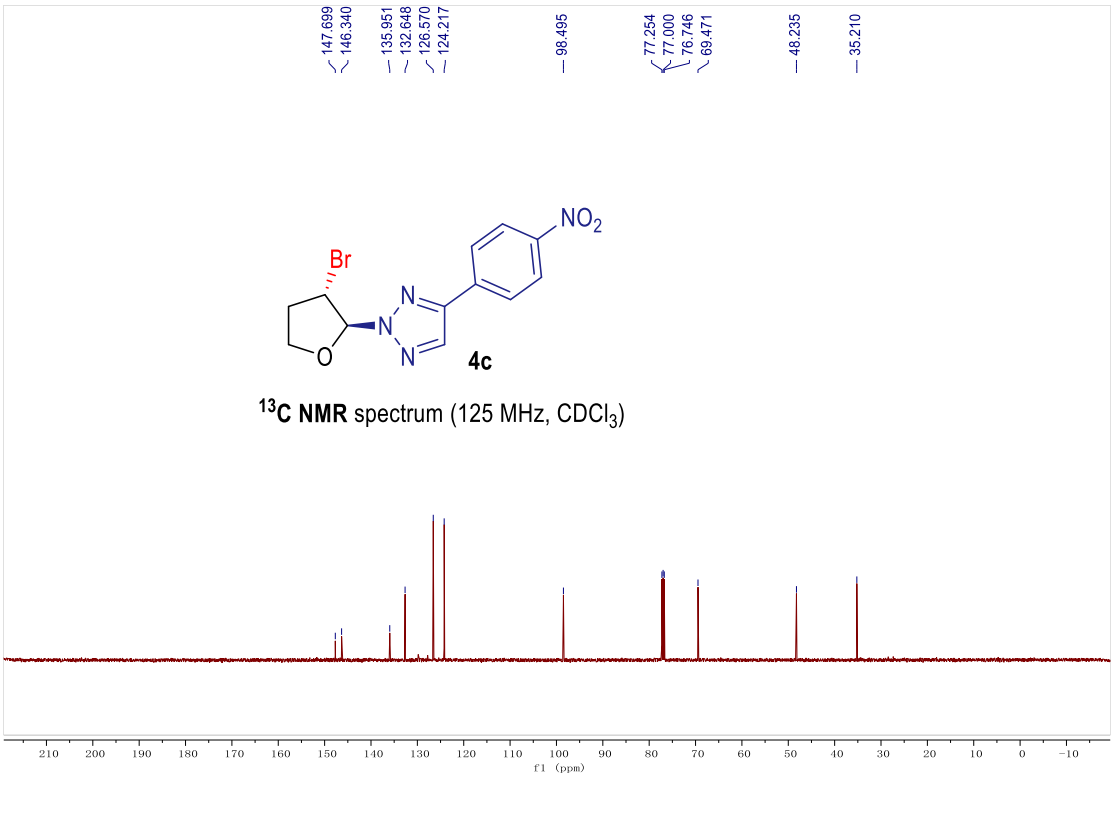

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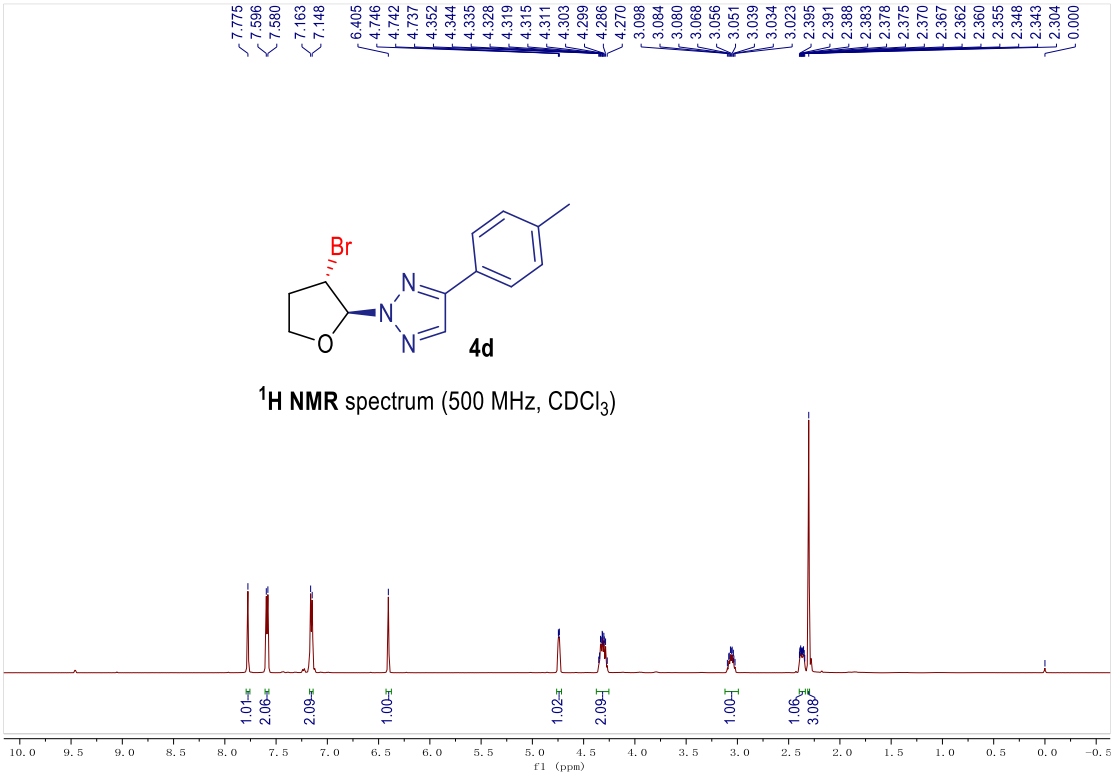
4d



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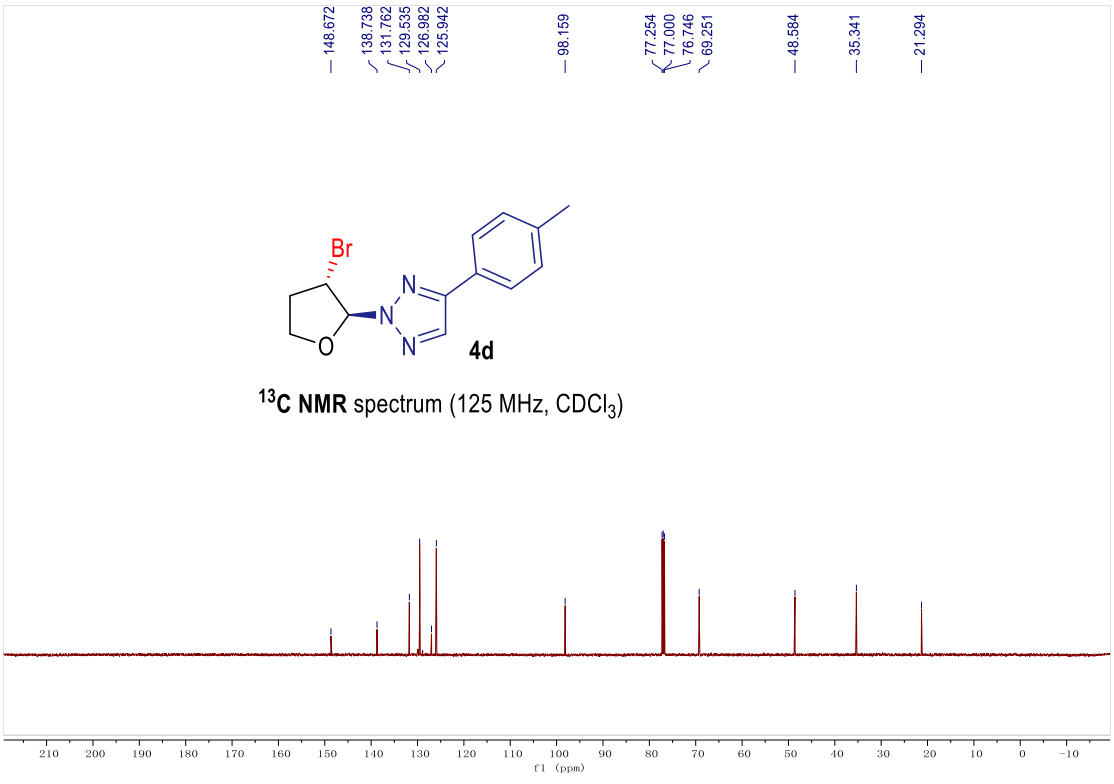
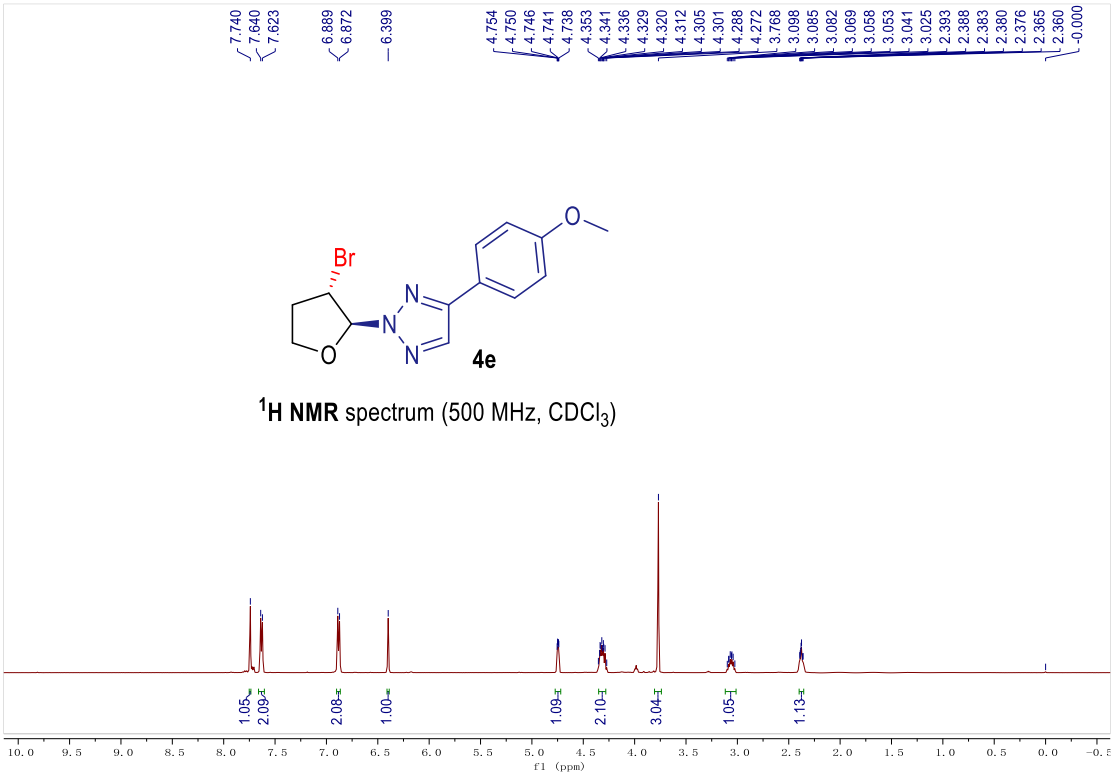


^{13}**C NMR** spectrum (125 MHz, $CDCl_3$)

4e



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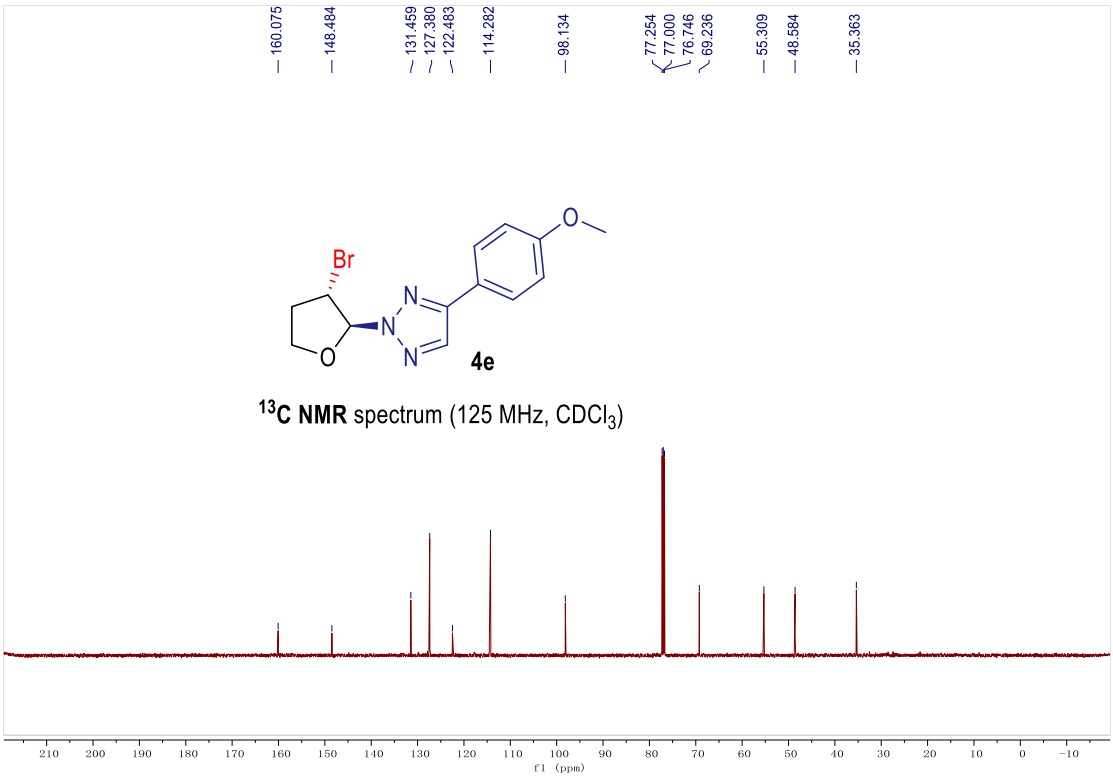
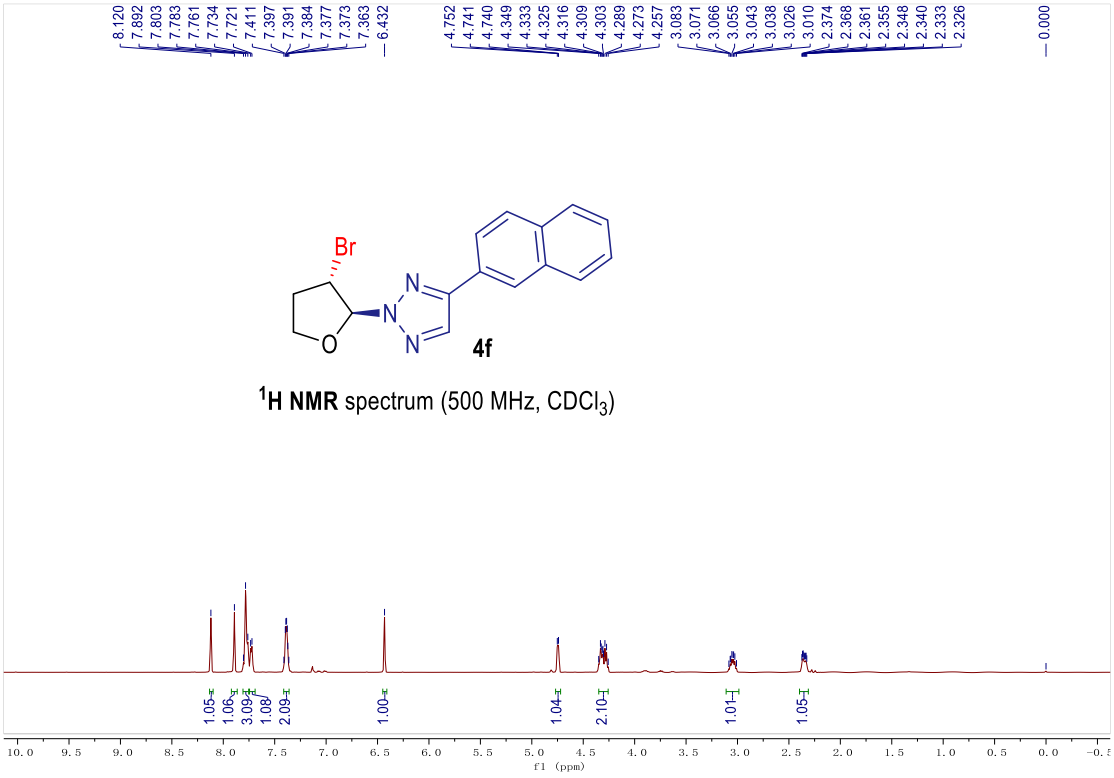
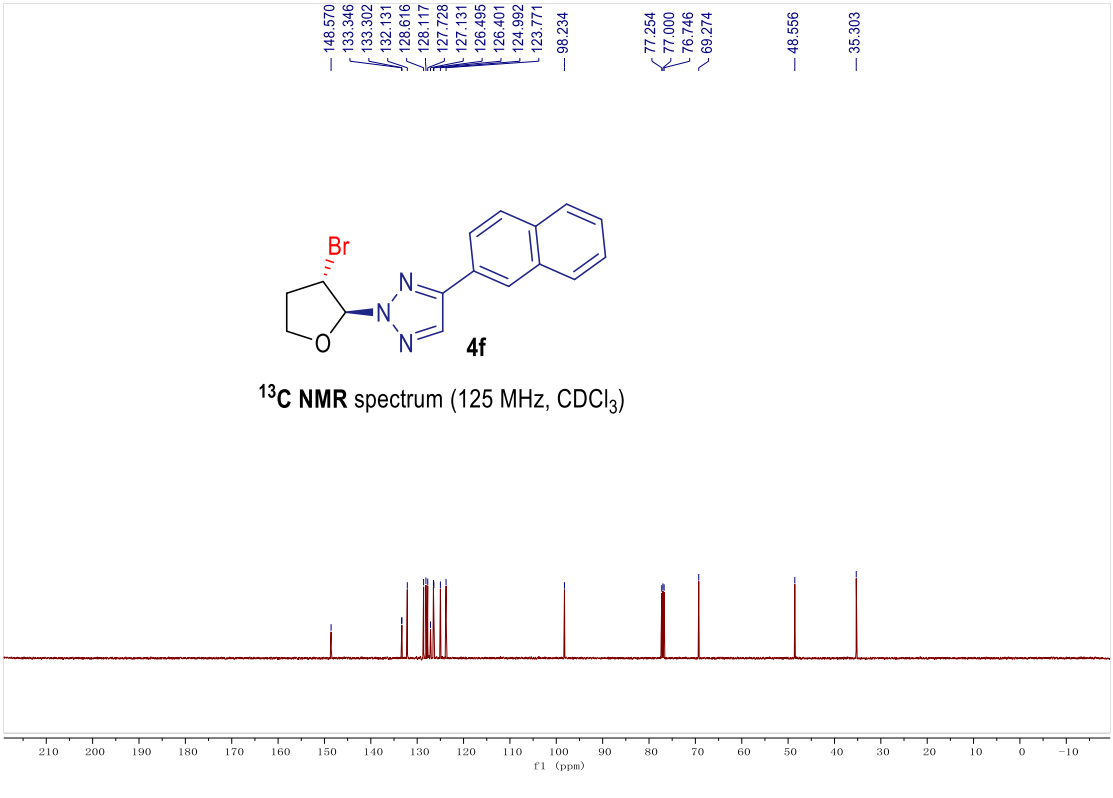


^{13}**C NMR** spectrum (125 MHz, $CDCl_3$)

4f

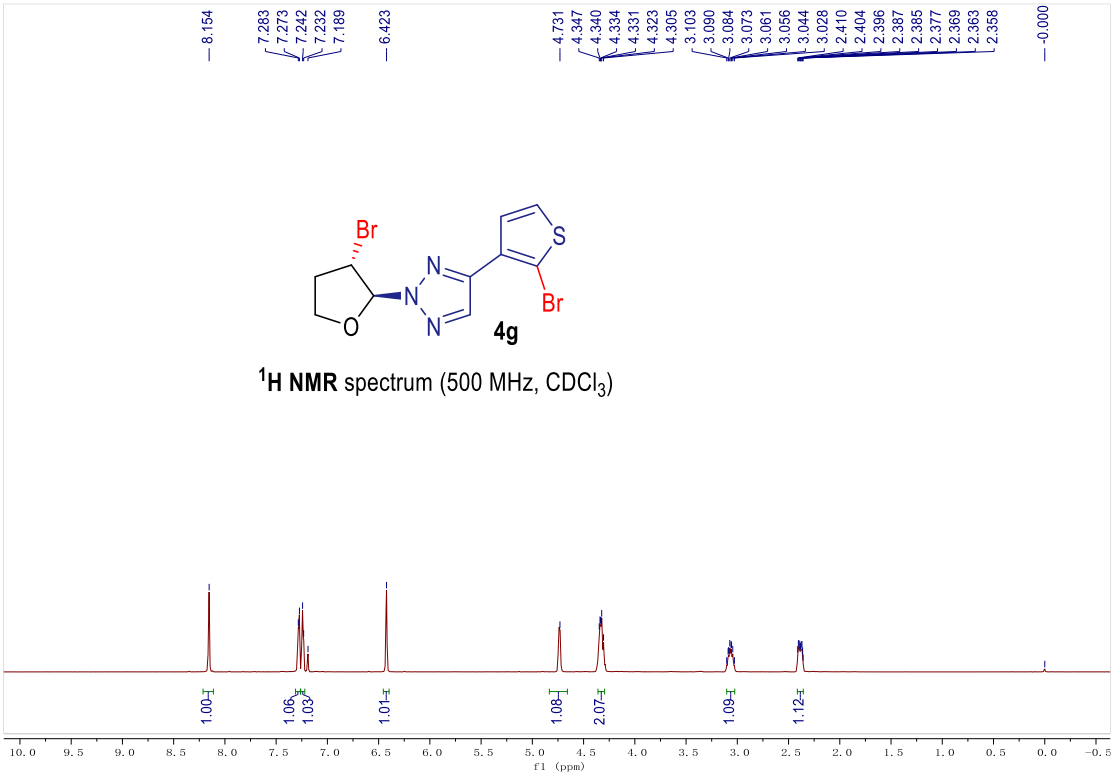


^{1}**H NMR** spectrum (500 MHz, $CDCl_3$)

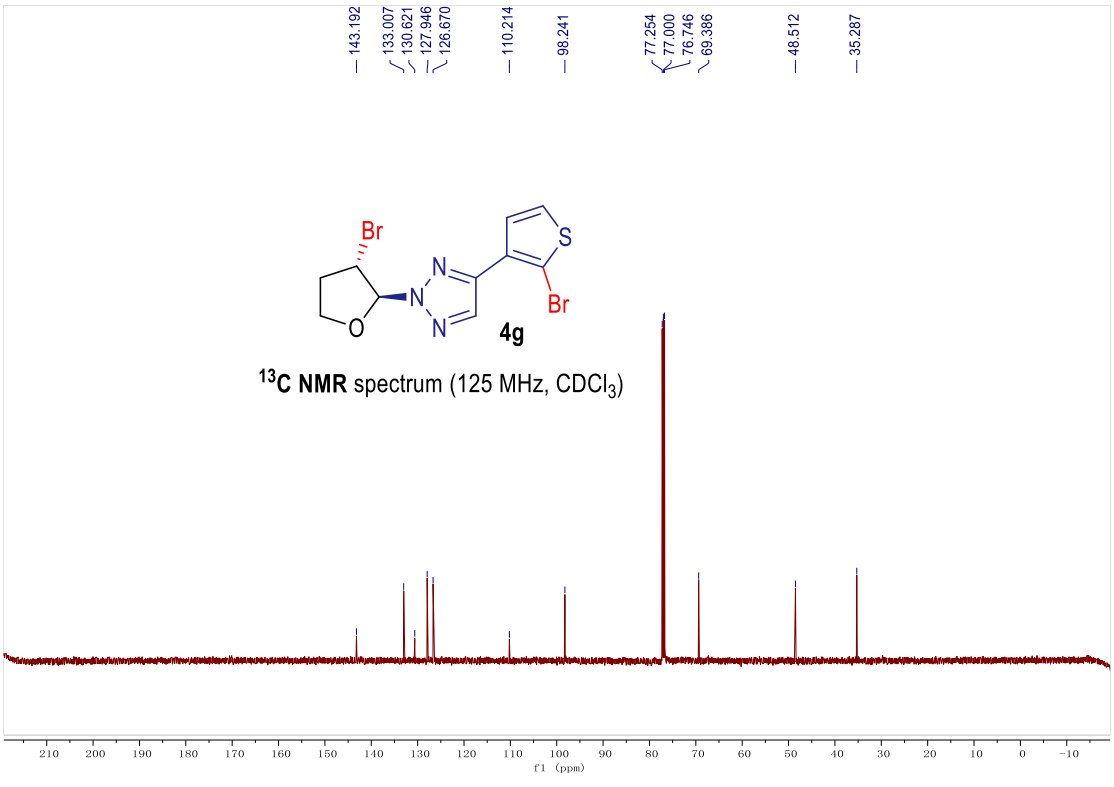


^{13}**C NMR** spectrum (125 MHz, $CDCl_3$)

4g

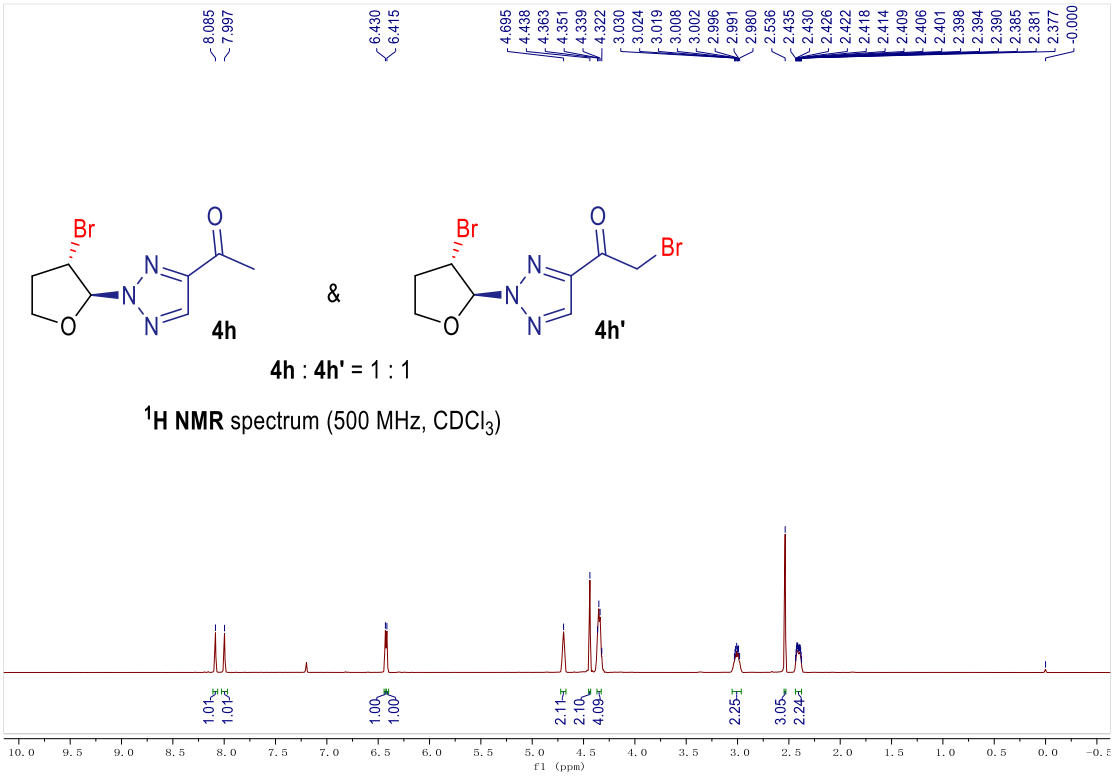


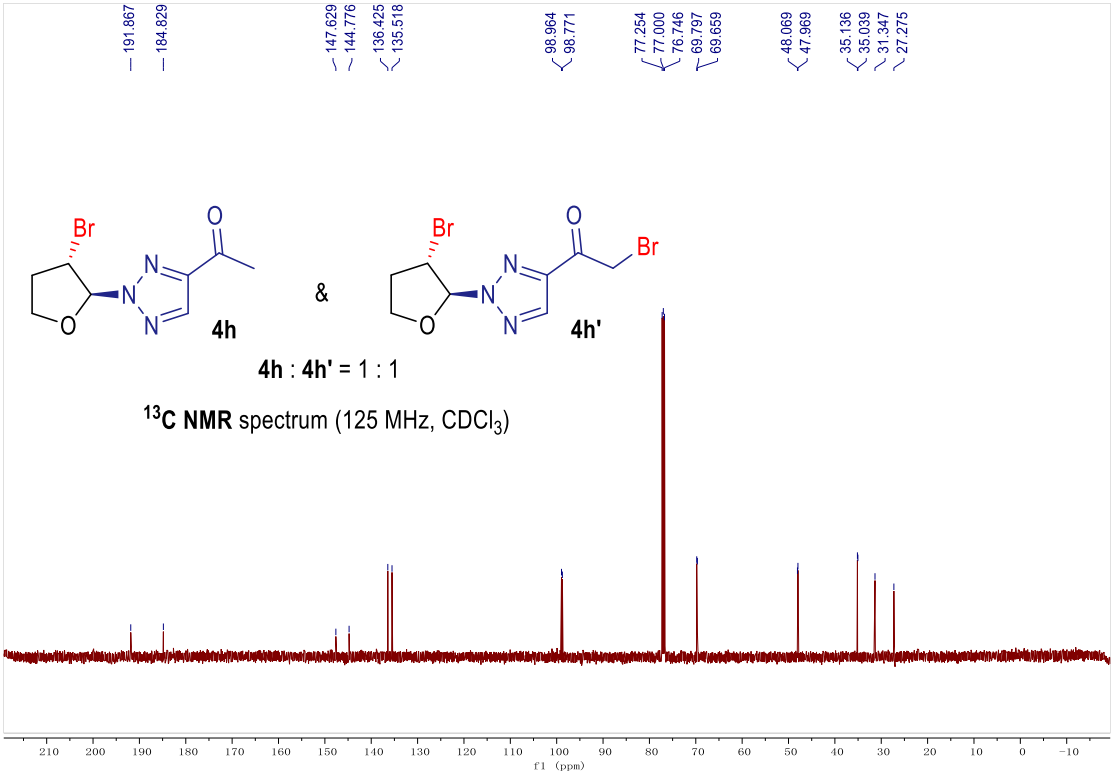
^{1}H NMR spectrum (500 MHz, $CDCl_3$)



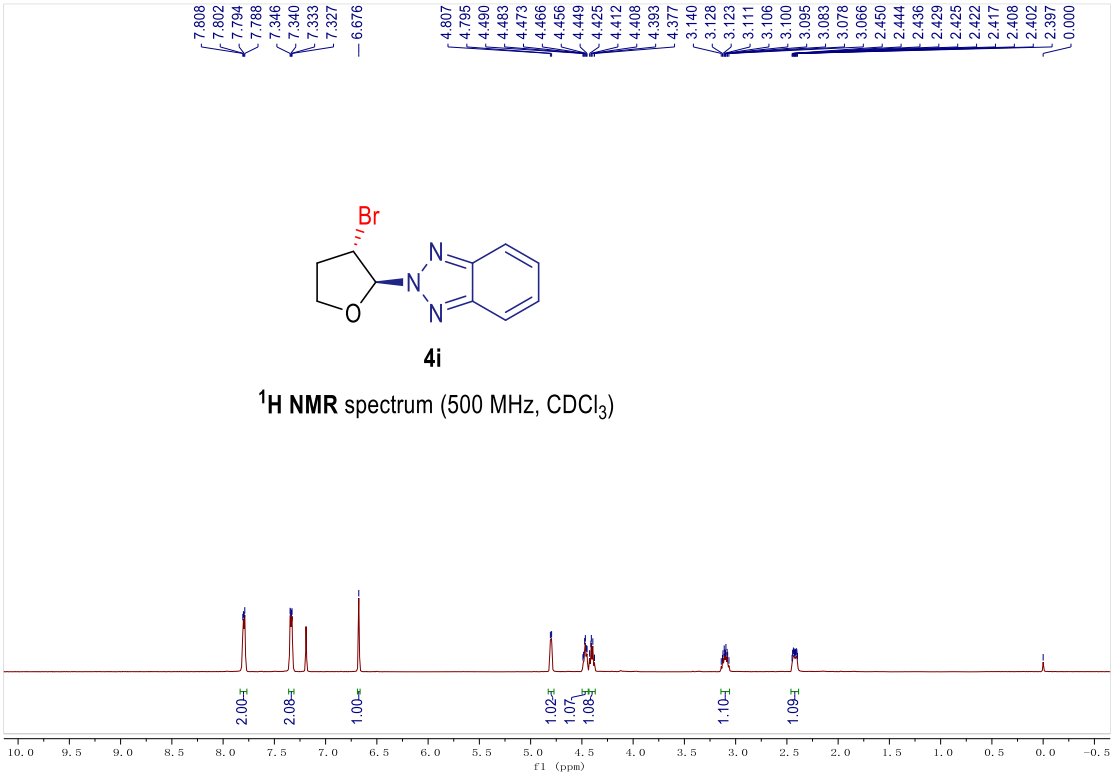
^{13}C NMR spectrum (125 MHz, $CDCl_3$)

4h : **4h'** = 1 : 1


8.085
7.997
6.430
6.415
4.695
4.438
4.363
4.351
4.339
4.322
3.030
3.024
3.019
3.008
3.002
2.996
2.991
2.980
2.536
2.435
2.430
2.426
2.422
2.418
2.414
2.409
2.406
2.401
2.398
2.394
2.390
2.385
2.381
2.377
-0.000
Br
O
N
N
N
O
4h
&
Br
O
Br
N
N
N
O
4h'
4h : 4h' = 1 : 1
1H NMR spectrum (500 MHz, CDCl3)
1.01
1.01
1.00
1.00
2.11
2.10
4.09
2.25
3.05
2.24
f1 (ppm)

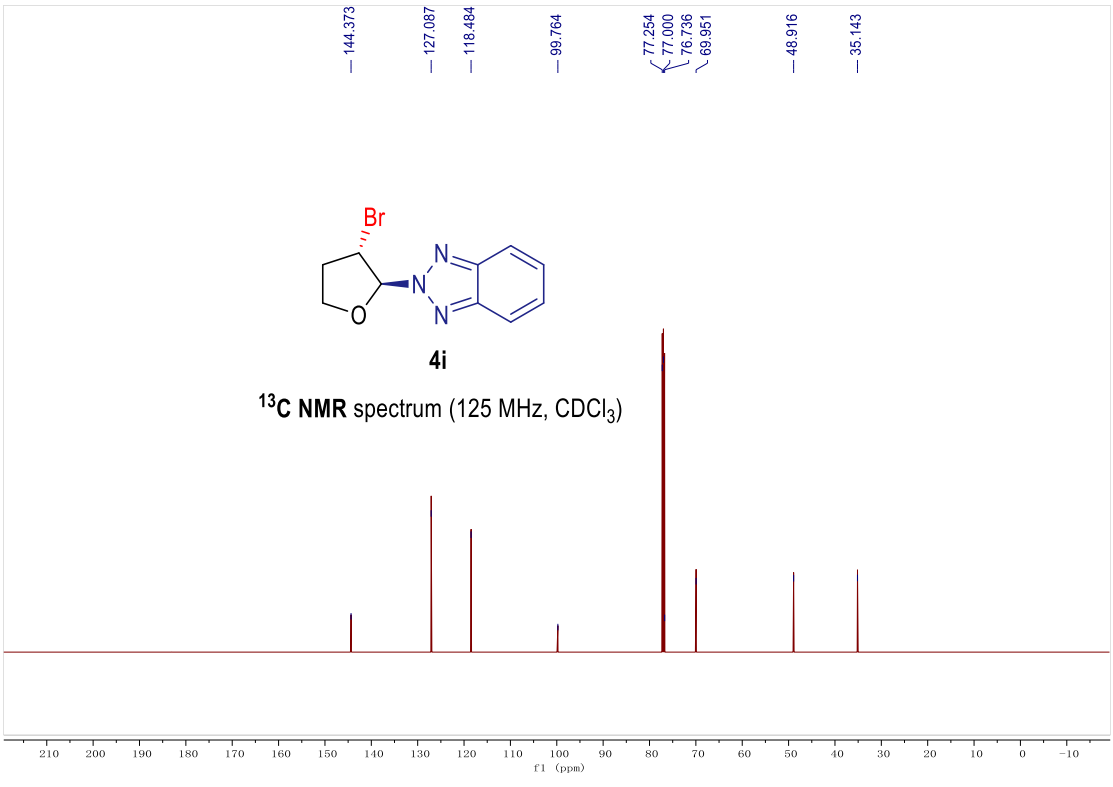

191.867
184.829
147.629
144.776
136.425
135.518
98.964
98.771
77.254
77.000
76.746
69.797
69.659
48.069
47.969
35.136
35.039
31.347
27.275
Br
O
N
N
N
O
4h
&
Br
O
Br
N
N
N
O
4h'
4h : 4h' = 1 : 1
13C NMR spectrum (125 MHz, CDCl3)
f1 (ppm)

4i



4i

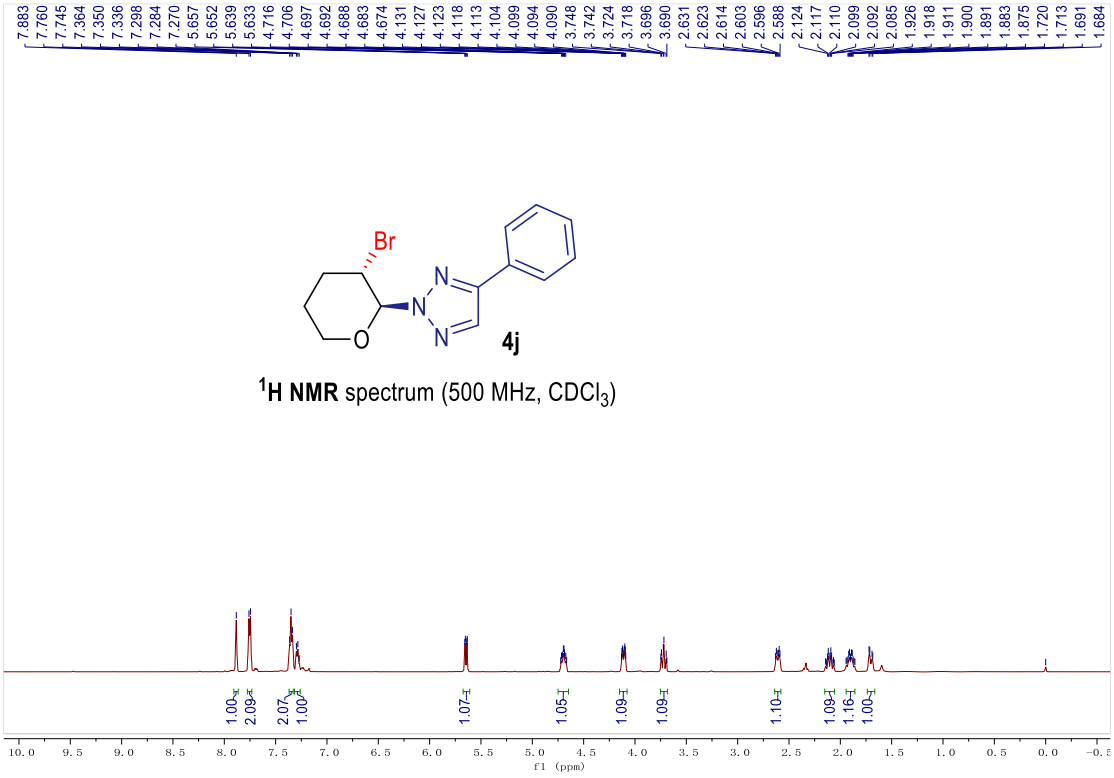
^{1}H NMR spectrum (500 MHz, $CDCl_3$)



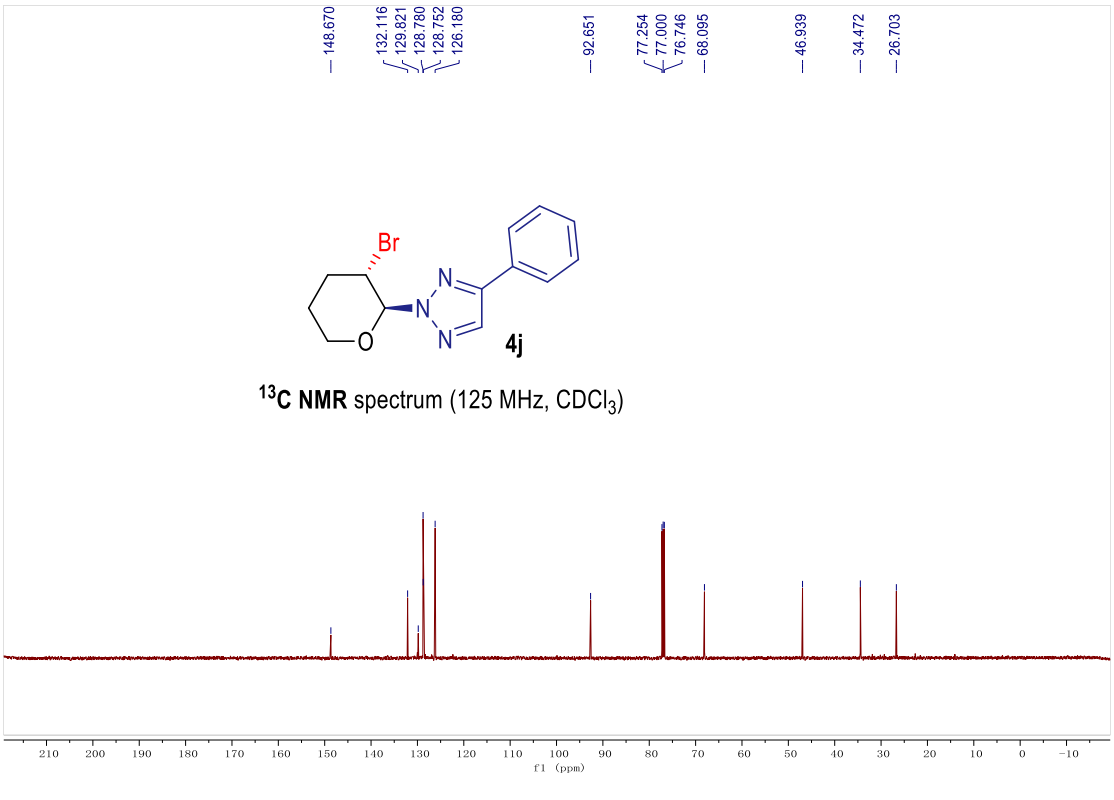
4i

^{13}C NMR spectrum (125 MHz, $CDCl_3$)

4j

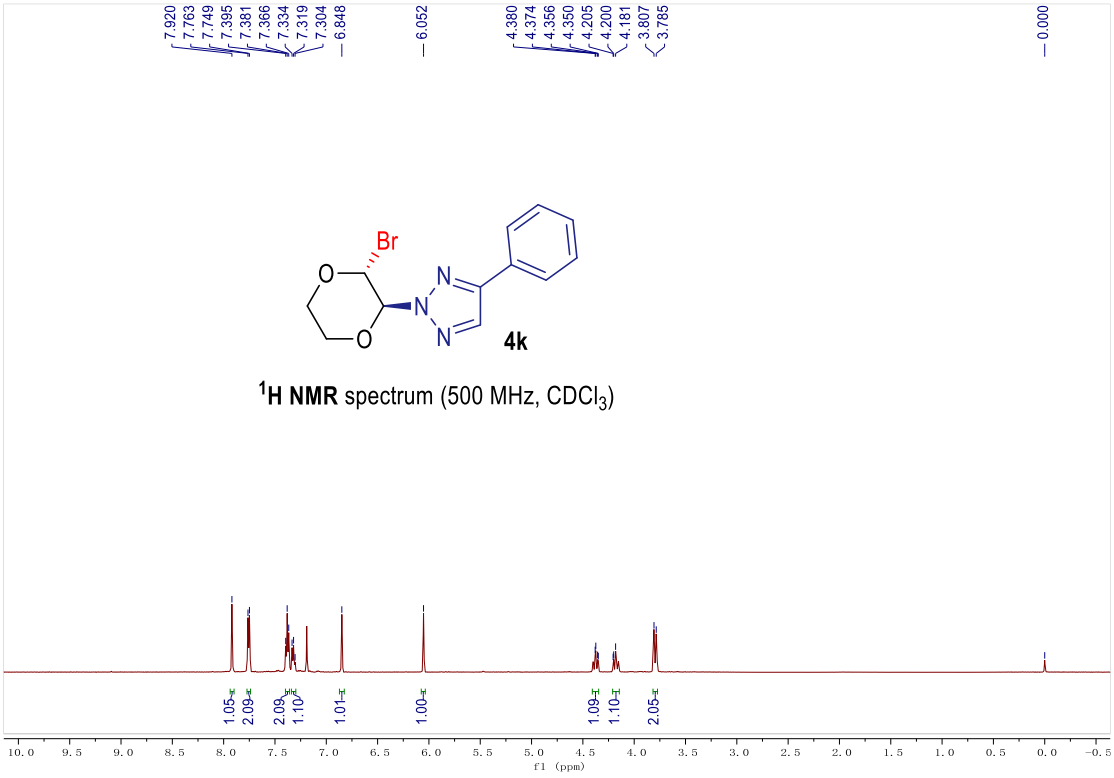


^{1}H NMR spectrum (500 MHz, $CDCl_3$)

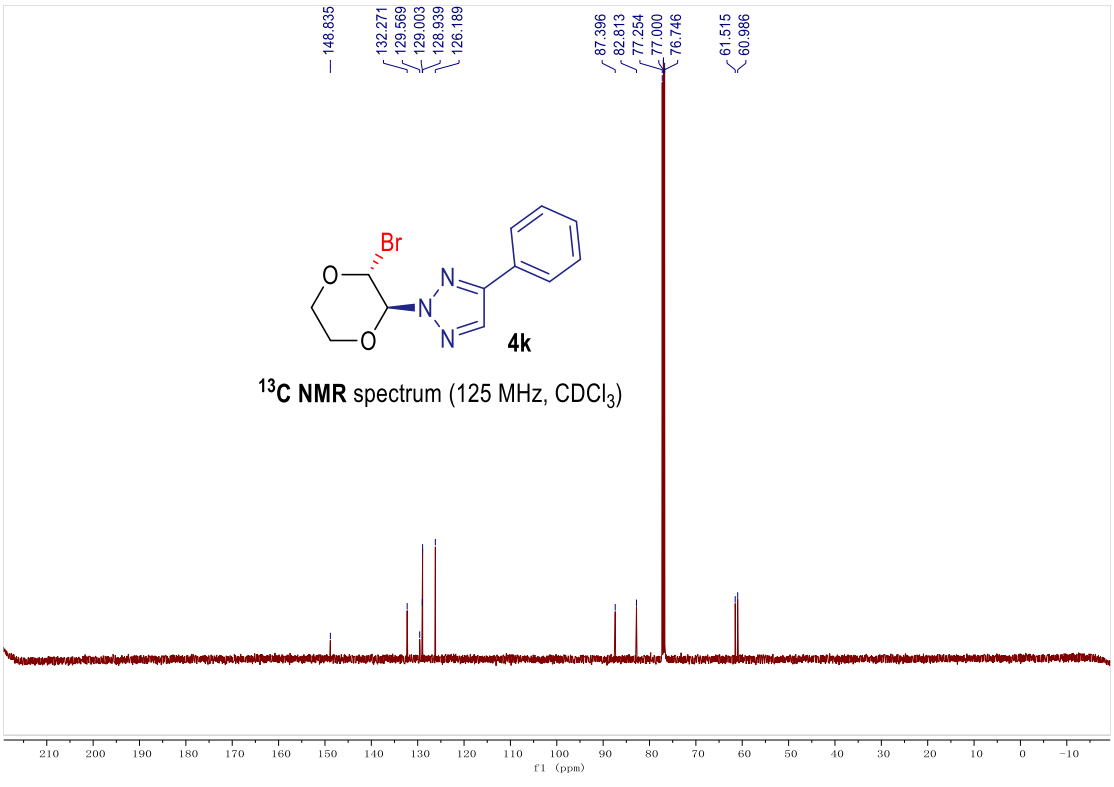


^{13}C NMR spectrum (125 MHz, $CDCl_3$)

4k

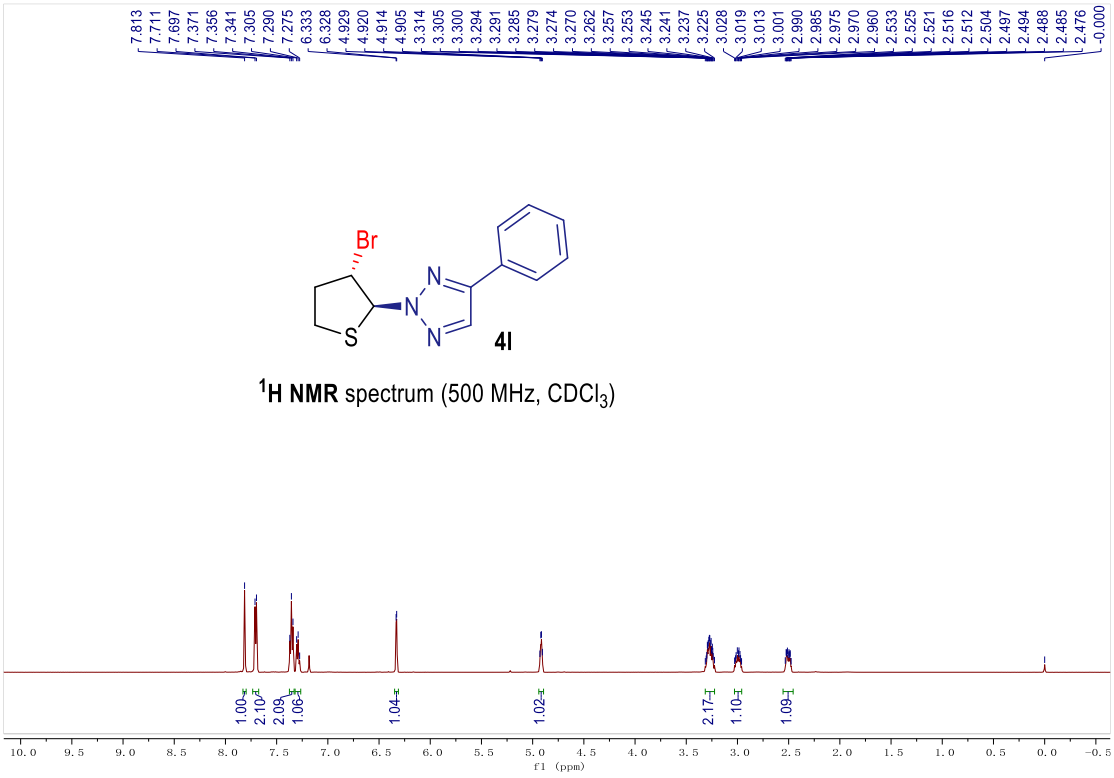


^{1}**H NMR** spectrum (500 MHz, $CDCl_3$)

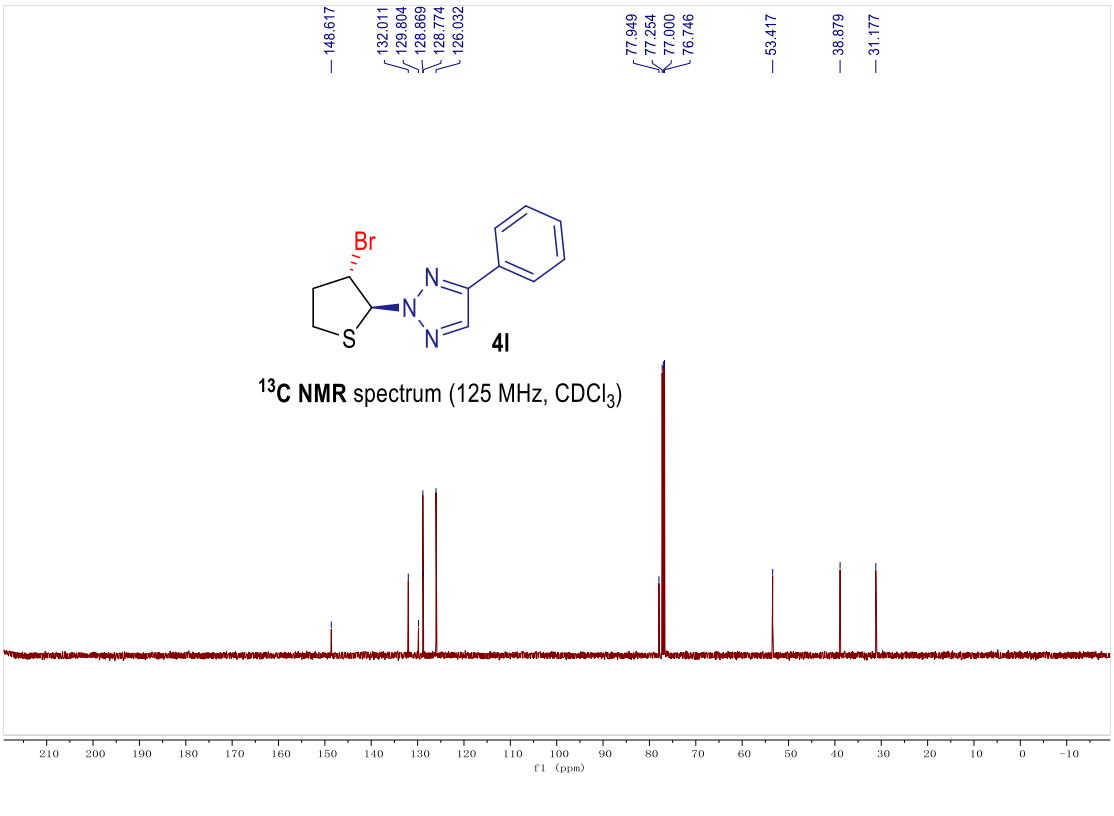


^{13}**C NMR** spectrum (125 MHz, $CDCl_3$)

4l

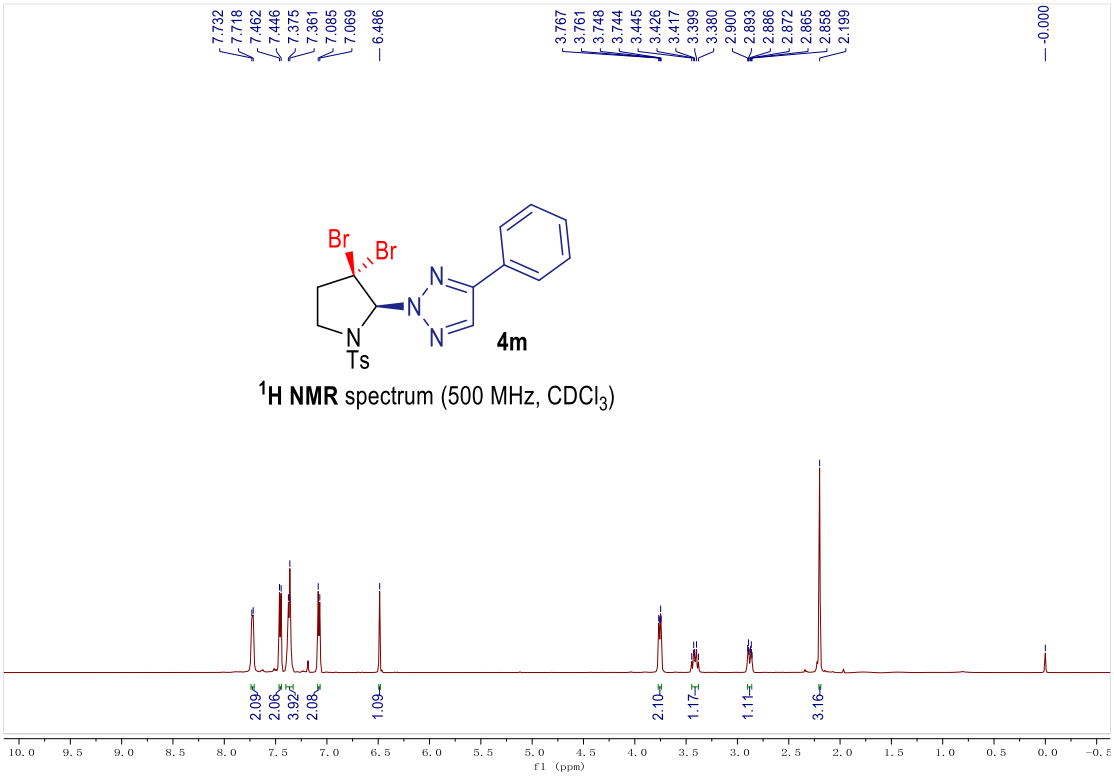


^{1}**H NMR** spectrum (500 MHz, $CDCl_3$)

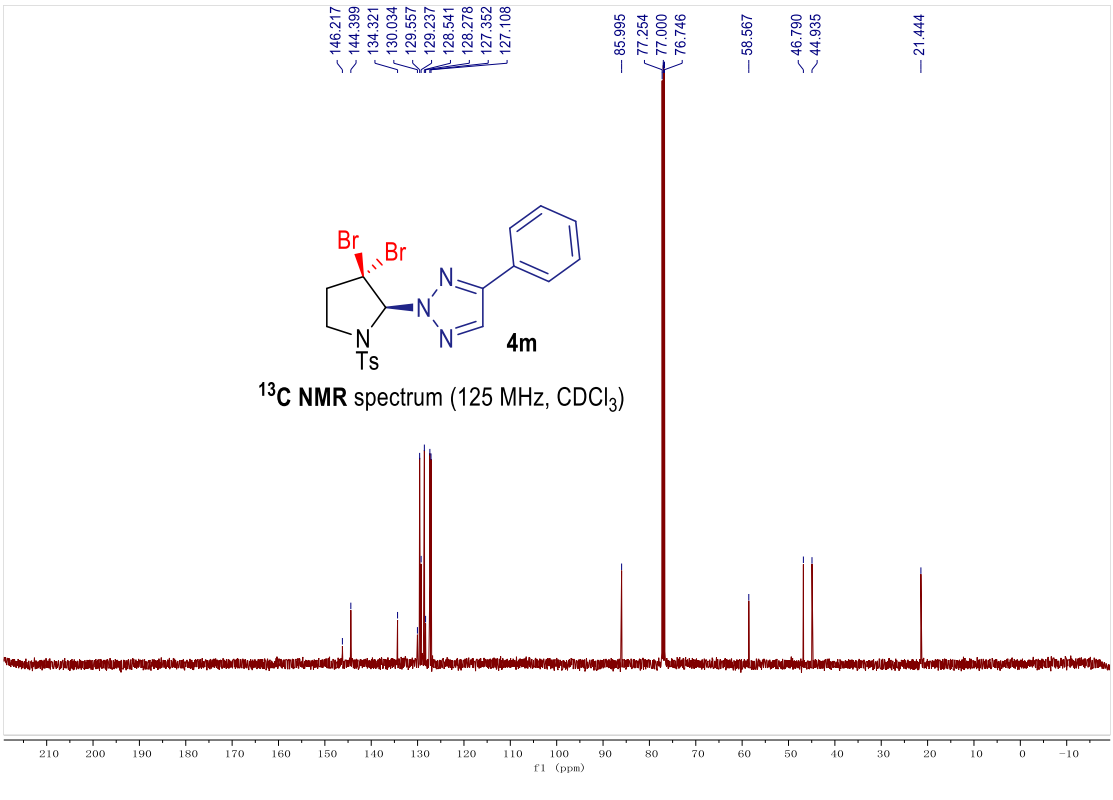


^{13}**C NMR** spectrum (125 MHz, $CDCl_3$)

4m

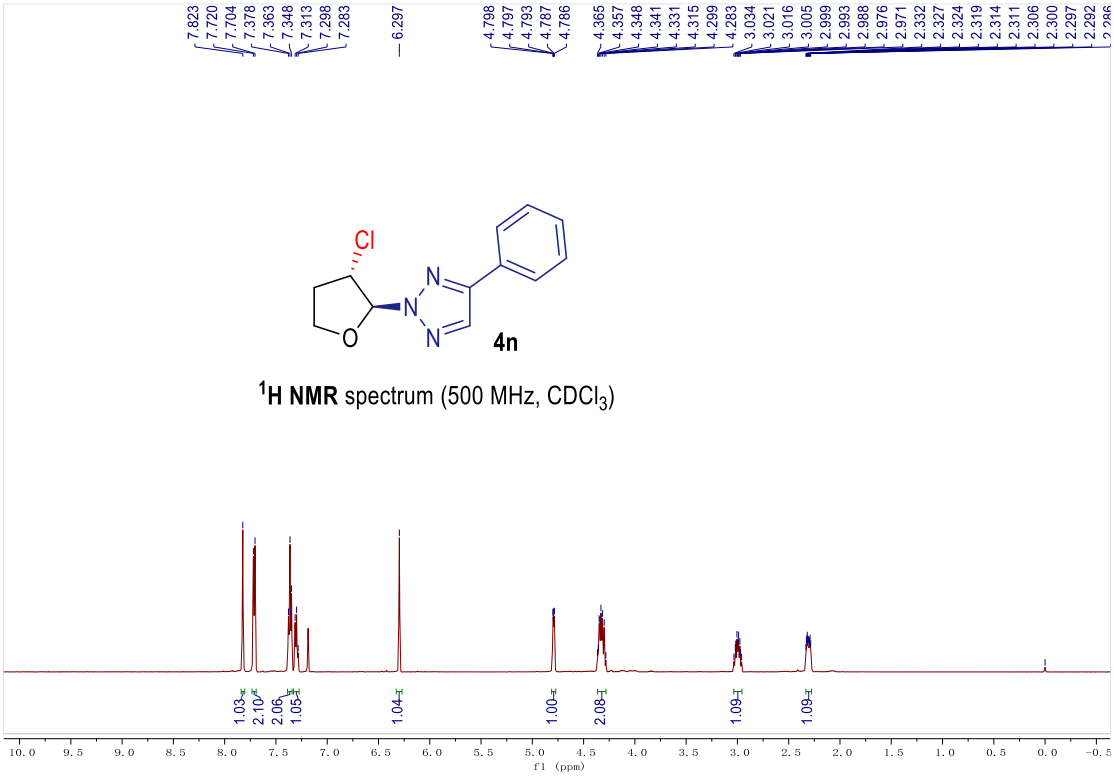


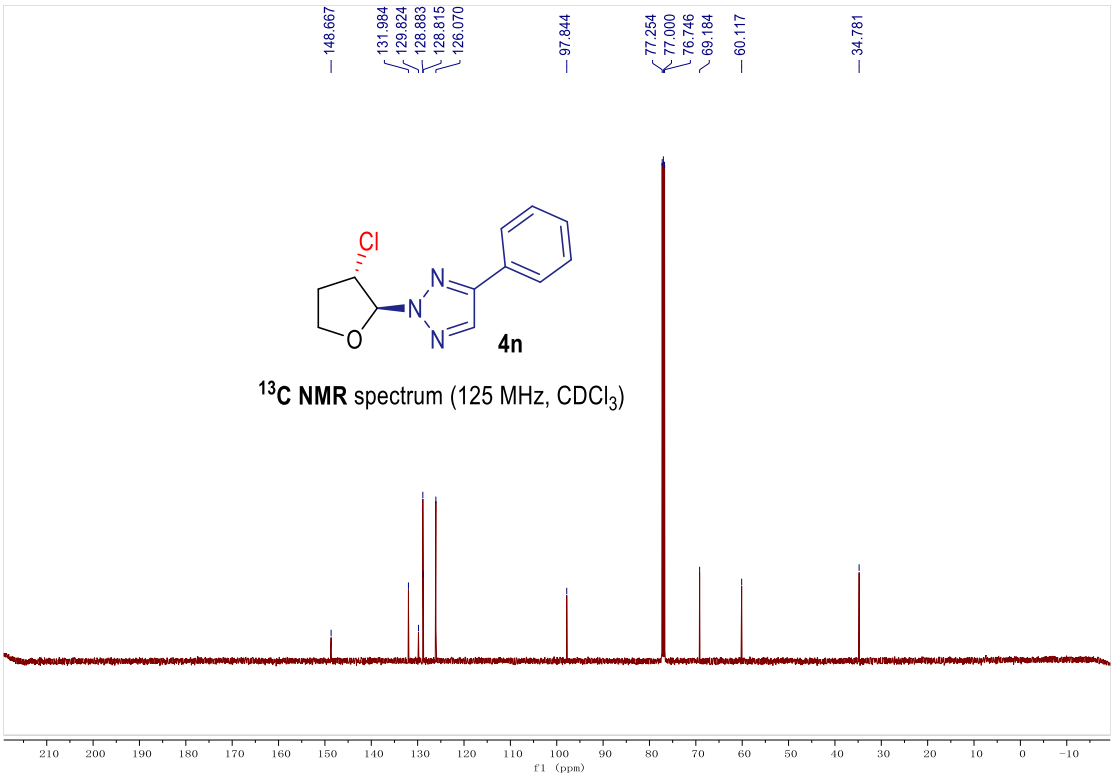
^{1}H NMR spectrum (500 MHz, $CDCl_3$)



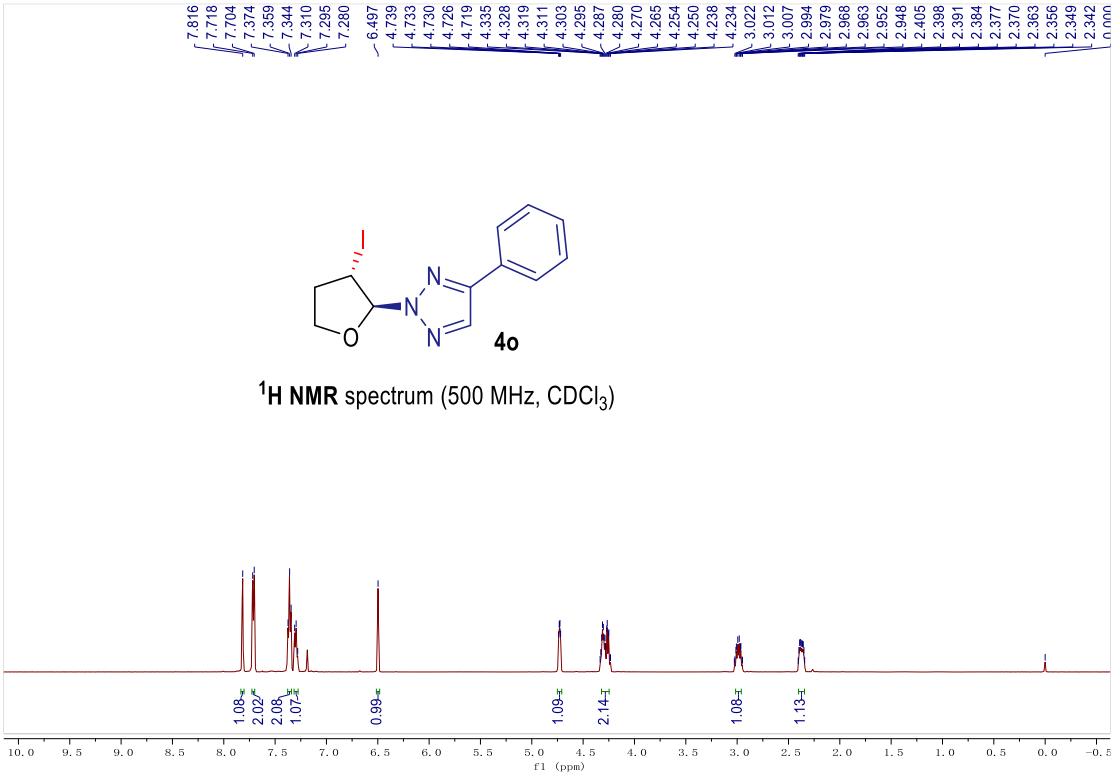
^{13}C NMR spectrum (125 MHz, $CDCl_3$)

4n

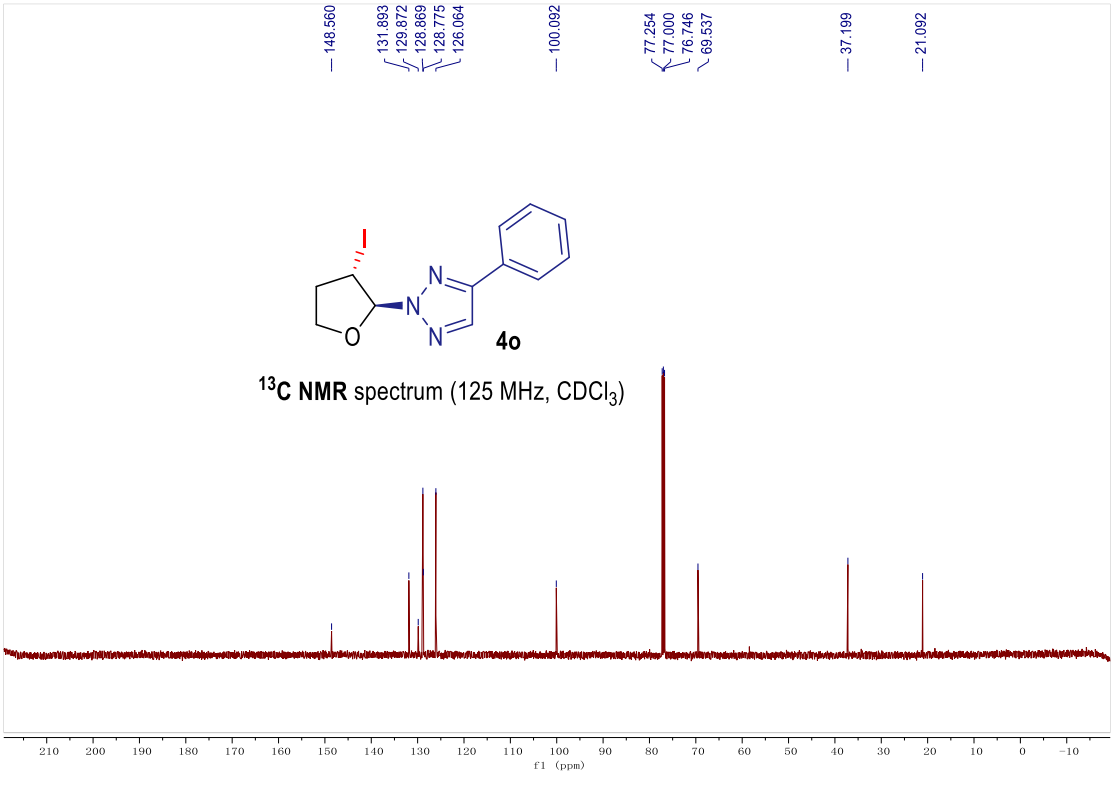

7.823
7.720
7.704
7.378
7.363
7.348
7.313
7.298
7.283
6.297
4.798
4.797
4.793
4.787
4.786
4.365
4.357
4.348
4.341
4.331
4.315
4.299
4.283
3.034
3.021
3.016
3.005
2.999
2.993
2.988
2.976
2.971
2.332
2.327
2.324
2.319
2.314
2.311
2.306
2.300
2.297
2.292
Cl
N
N
N
O
4n
1H NMR spectrum (500 MHz, CDCl3)
1.03
2.10
2.06
1.05
1.04
1.00
2.08
1.09
1.09
f1 (ppm)


148.667
131.984
129.824
128.883
128.815
126.070
97.844
77.254
77.000
76.746
69.184
60.117
34.781
Cl
N
N
N
O
4n
13C NMR spectrum (125 MHz, CDCl3)
f1 (ppm)

4o

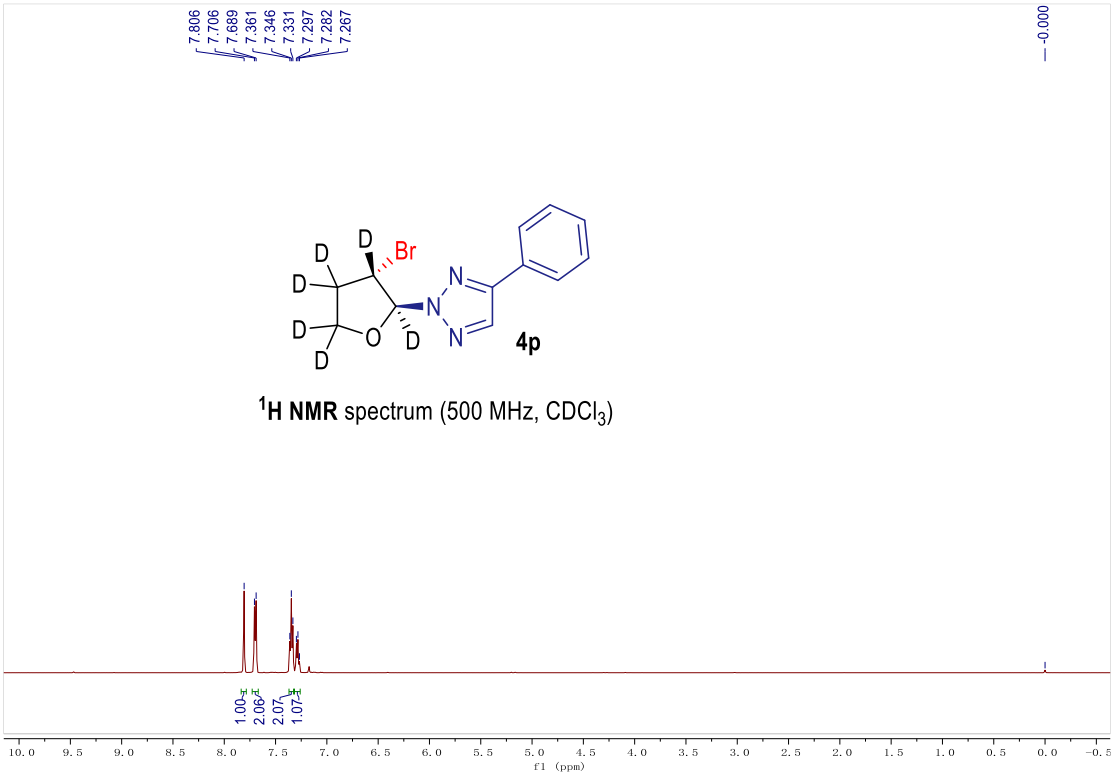


^{1}**H NMR** spectrum (500 MHz, $CDCl_3$)

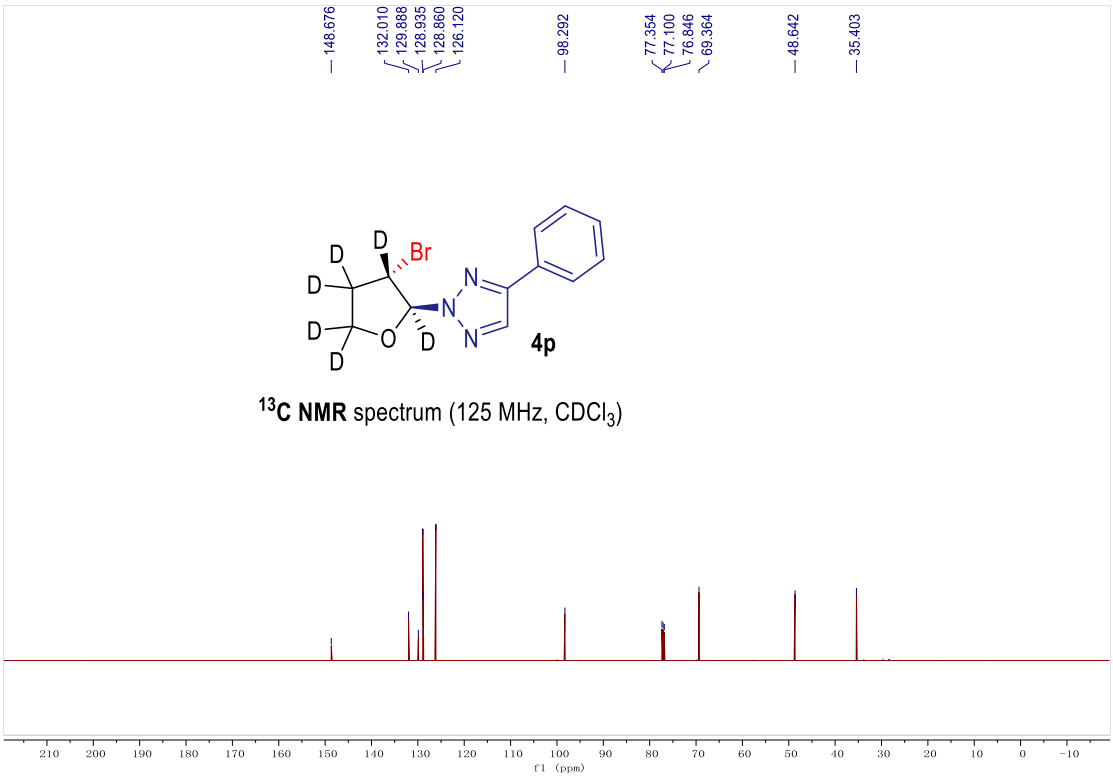


^{13}**C NMR** spectrum (125 MHz, $CDCl_3$)

4p

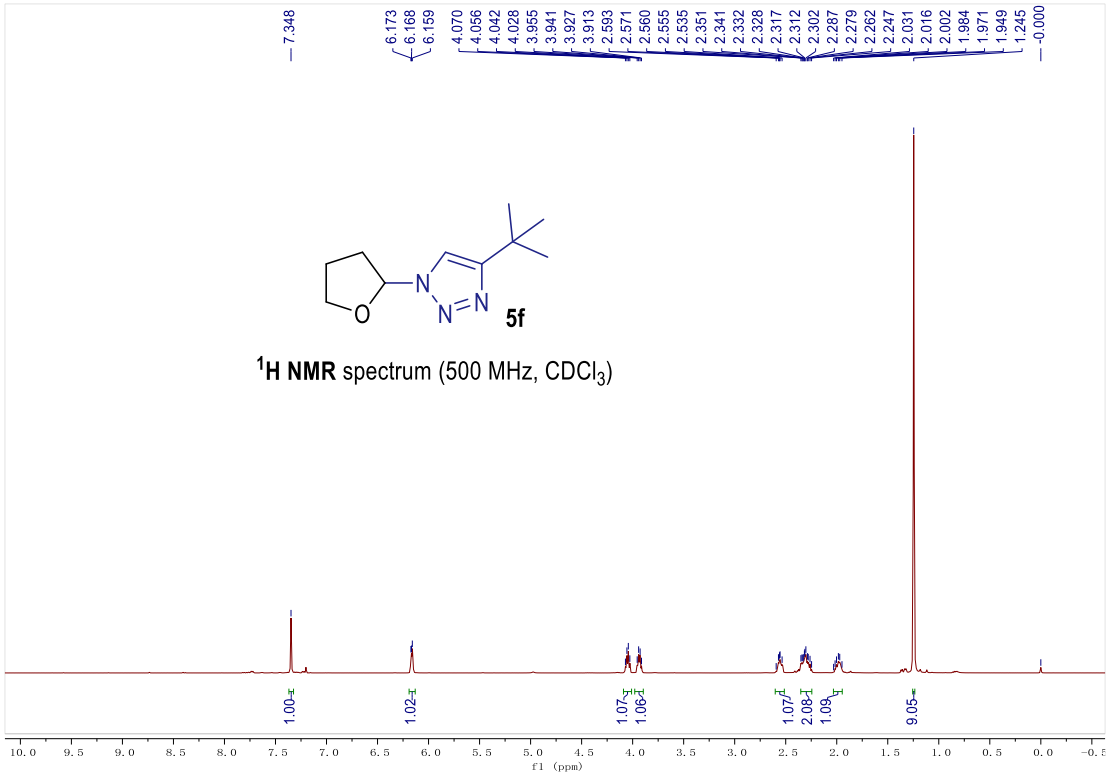


^{1}**H NMR** spectrum (500 MHz, $CDCl_3$)



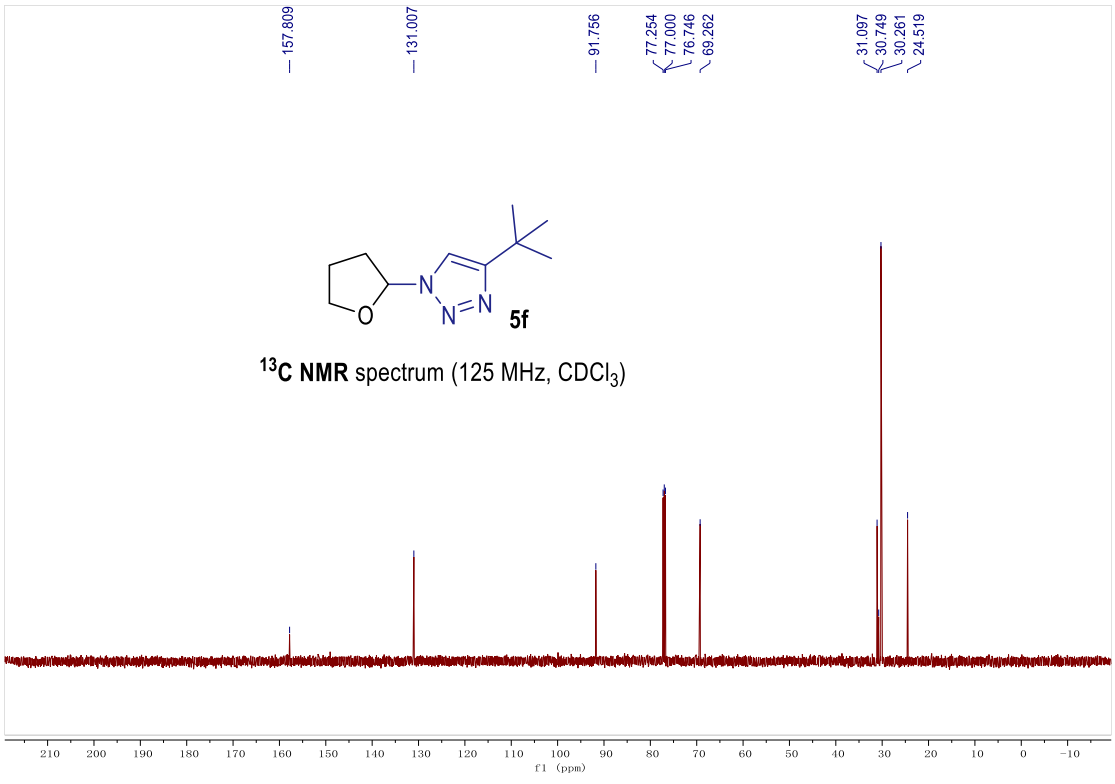
^{13}**C NMR** spectrum (125 MHz, $CDCl_3$)

5f



5f

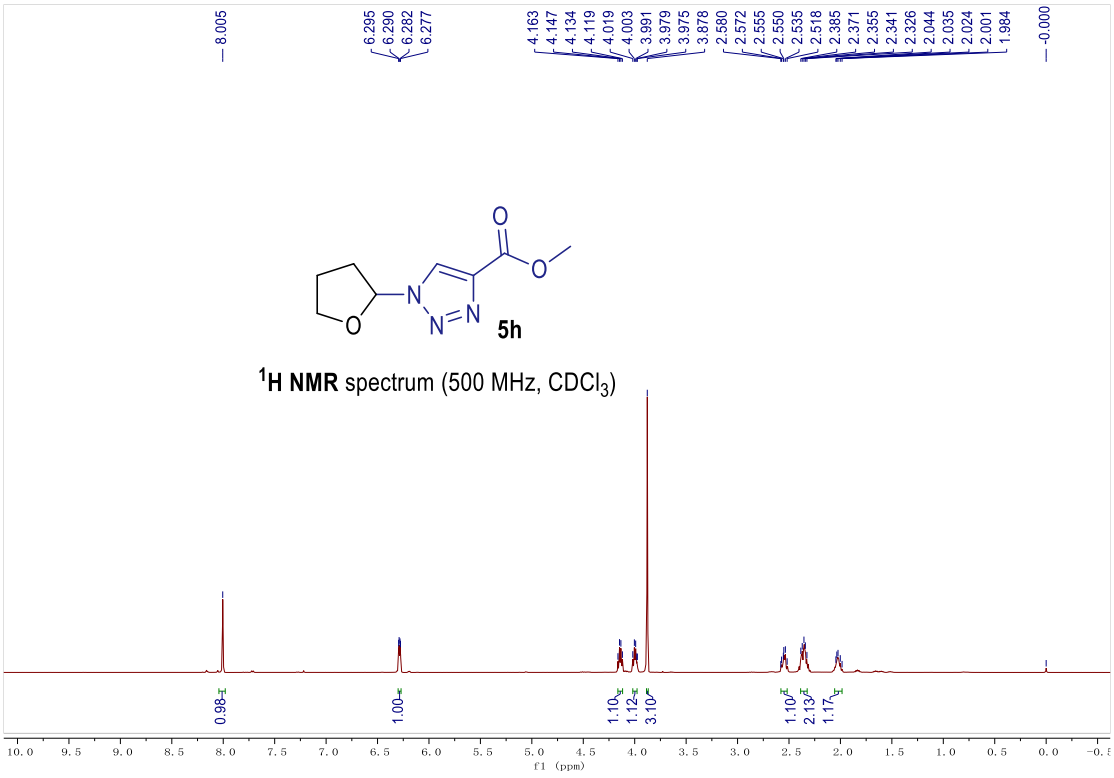
^{1}**H NMR** spectrum (500 MHz, $CDCl_3$)



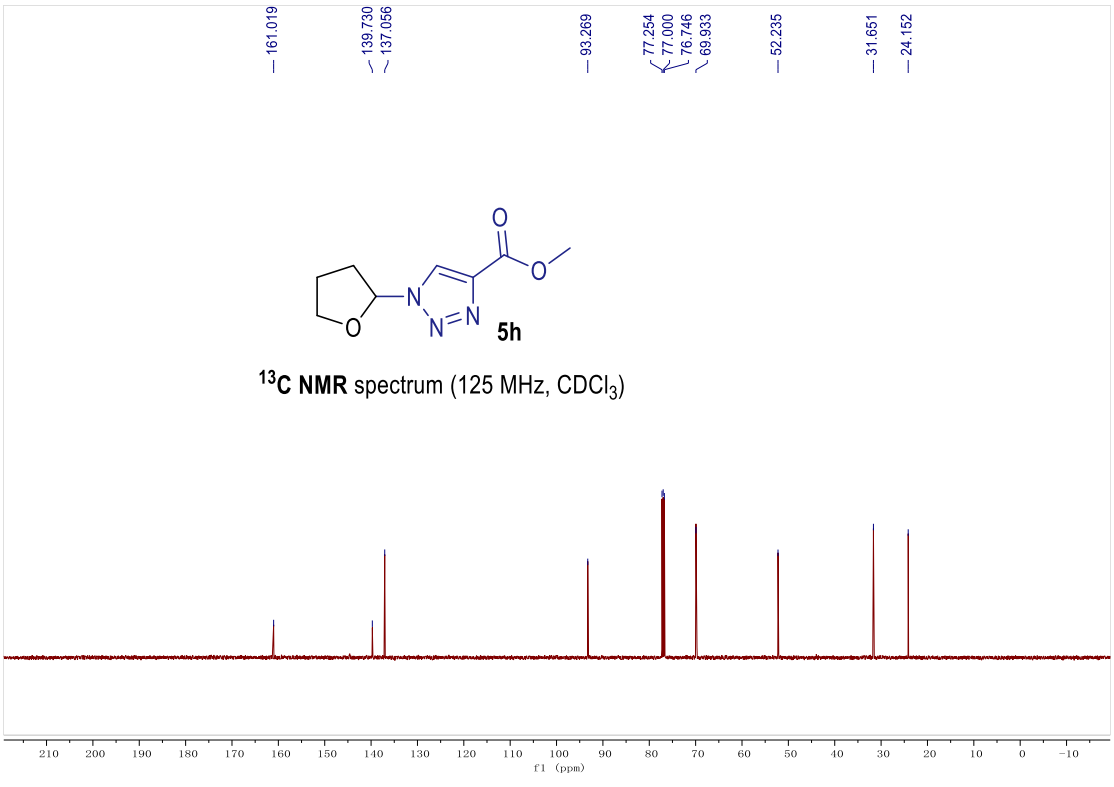
5f

^{13}**C NMR** spectrum (125 MHz, $CDCl_3$)

5h

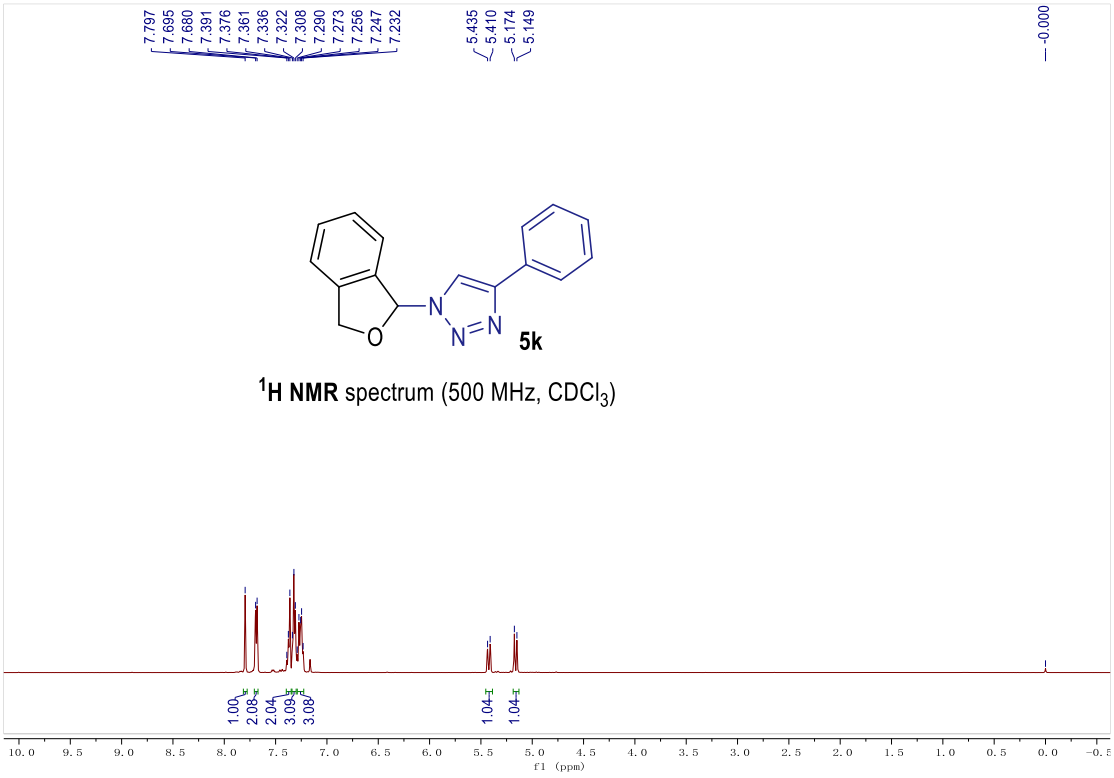


^{1}H NMR spectrum (500 MHz, $CDCl_3$)

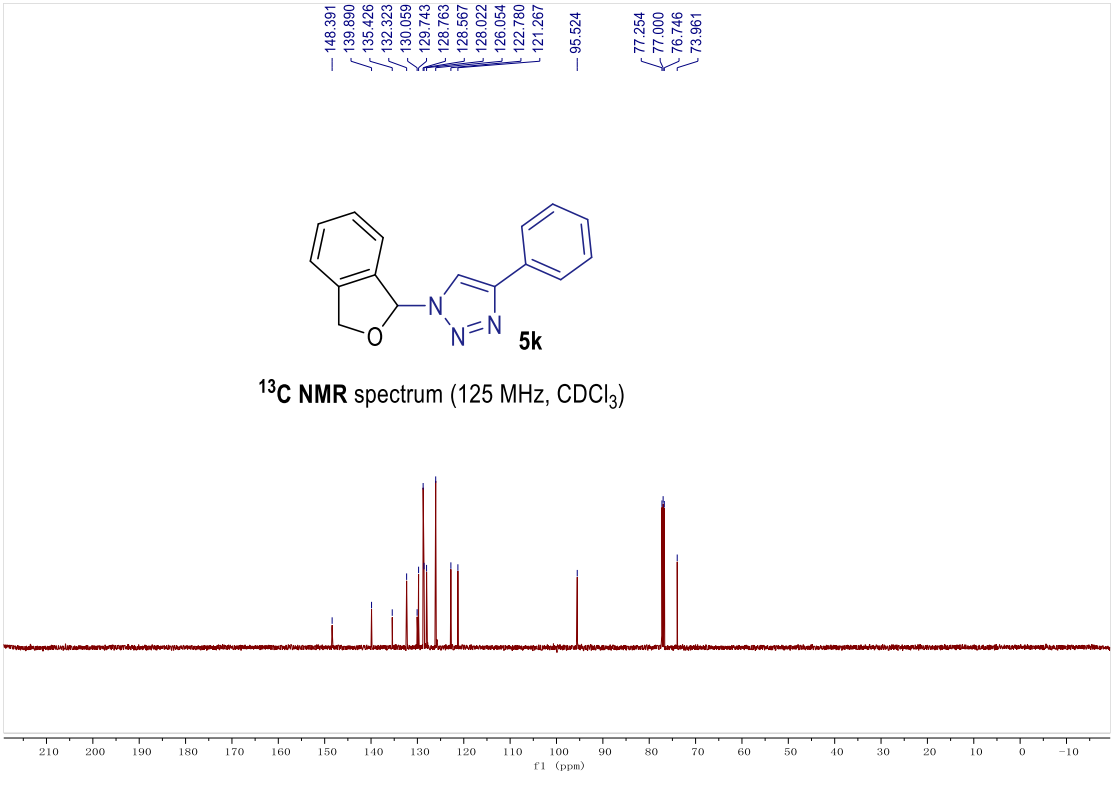


^{13}C NMR spectrum (125 MHz, $CDCl_3$)

5k

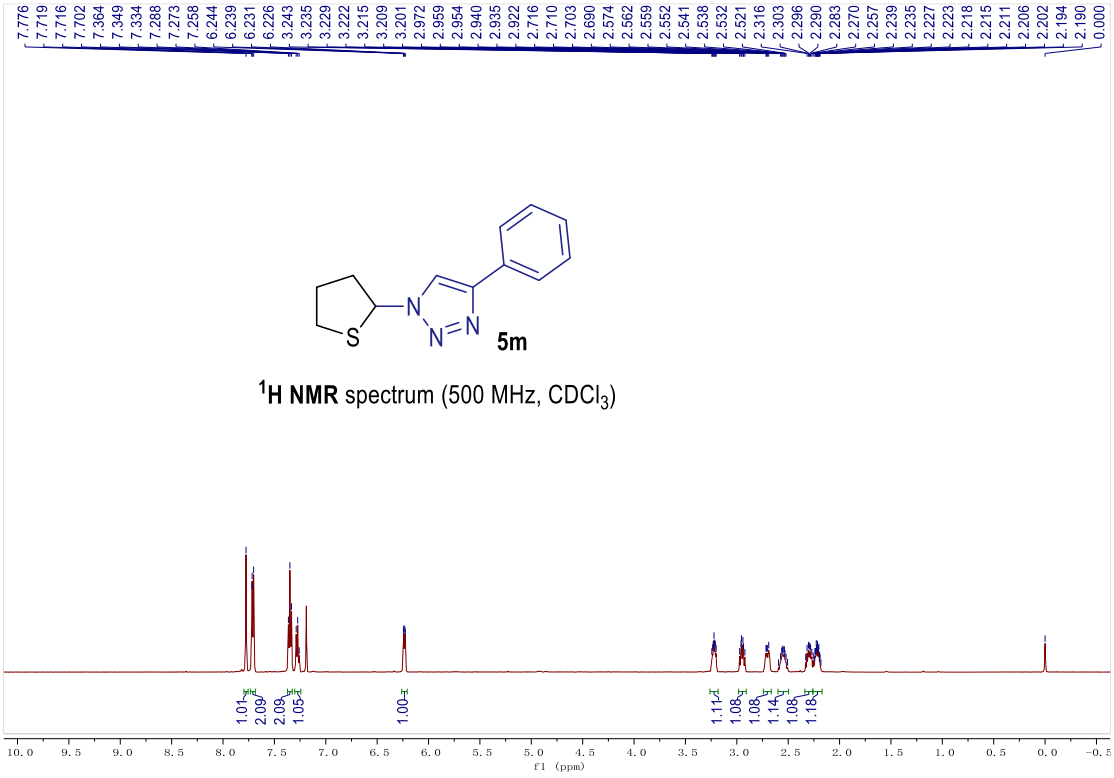


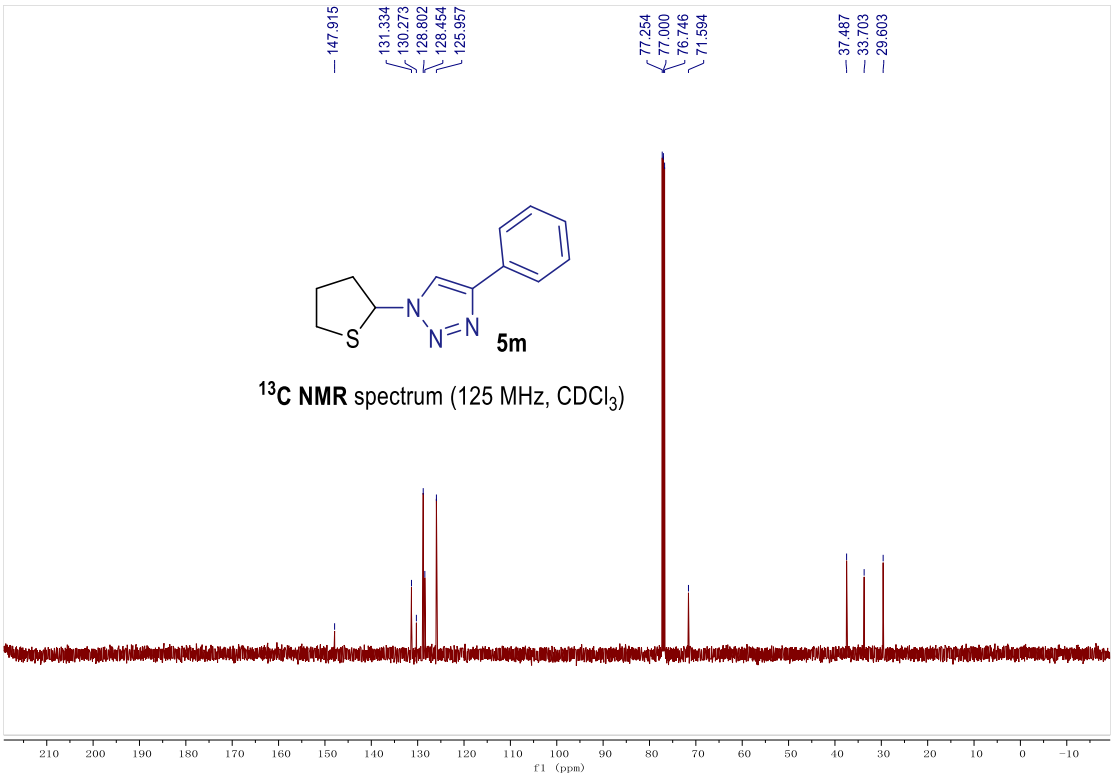
^{1}**H NMR** spectrum (500 MHz, $CDCl_3$)



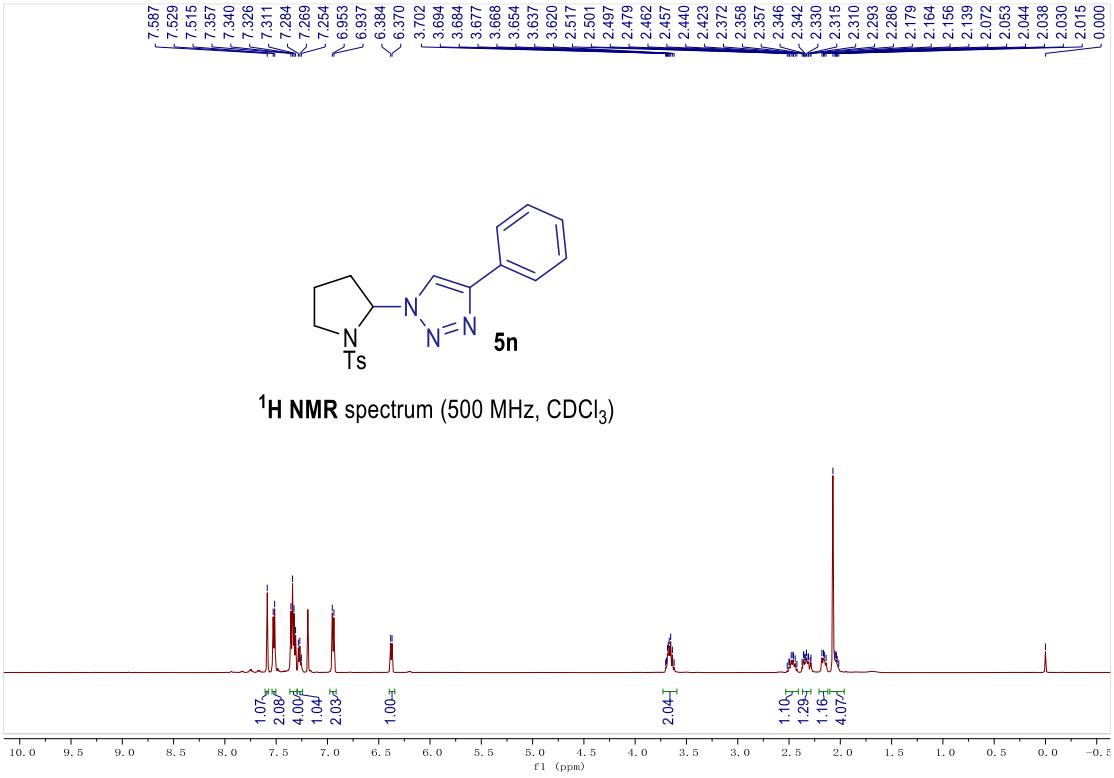
^{13}**C NMR** spectrum (125 MHz, $CDCl_3$)

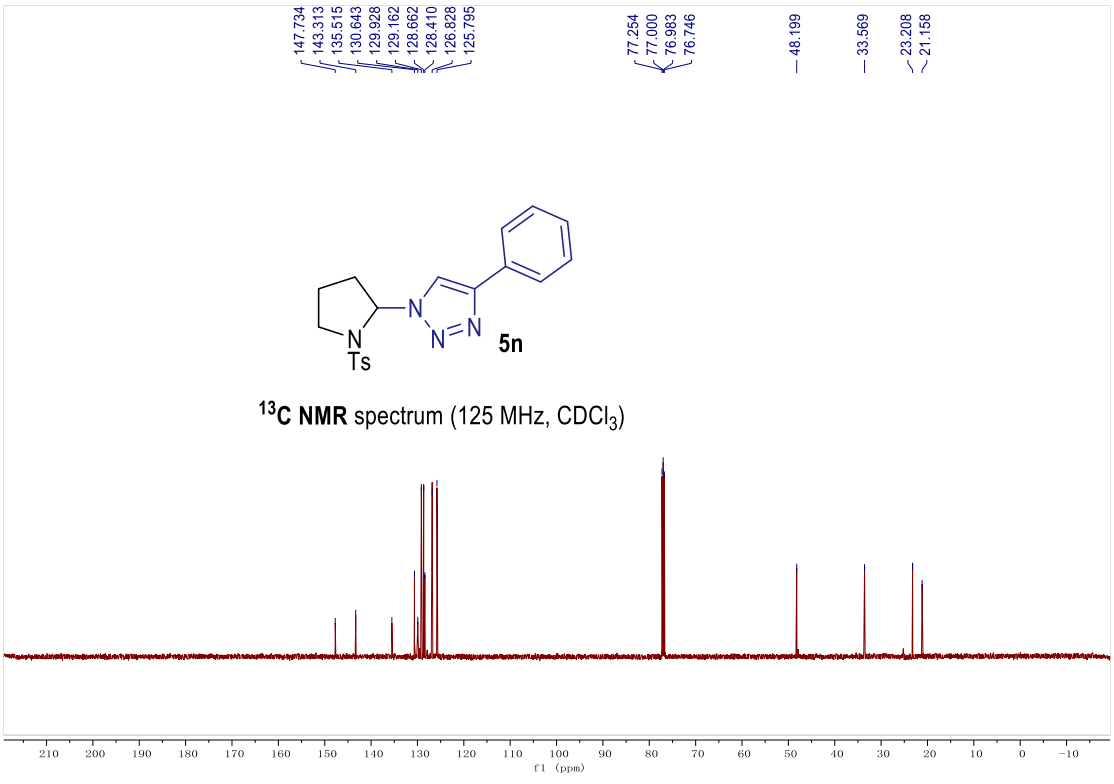
5m


7.776
7.719
7.716
7.702
7.364
7.349
7.334
7.288
7.273
7.258
6.244
6.239
6.231
6.226
3.243
3.235
3.229
3.222
3.215
3.209
3.201
2.972
2.959
2.954
2.940
2.935
2.922
2.716
2.710
2.703
2.690
2.574
2.562
2.559
2.552
2.541
2.538
2.532
2.521
2.316
2.303
2.296
2.290
2.283
2.270
2.257
2.239
2.235
2.227
2.223
2.218
2.215
2.211
2.206
2.202
2.194
2.190
0.000
5m
1H NMR spectrum (500 MHz, CDCl3)
1.01
2.09
2.09
1.05
1.00
1.11
1.08
1.08
1.14
1.08
1.18
f1 (ppm)

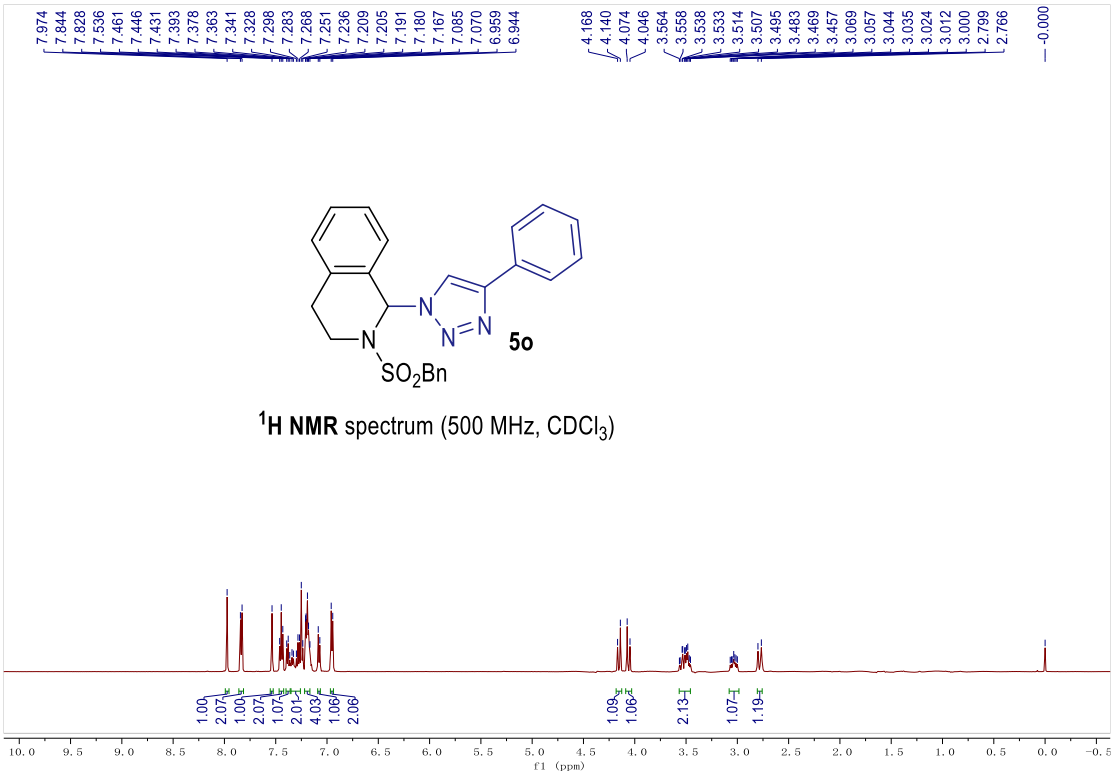

147.915
131.334
130.273
128.802
128.454
125.957
77.254
77.000
76.746
71.594
37.487
33.703
29.603
5m
13C NMR spectrum (125 MHz, CDCl3)
f1 (ppm)

5n

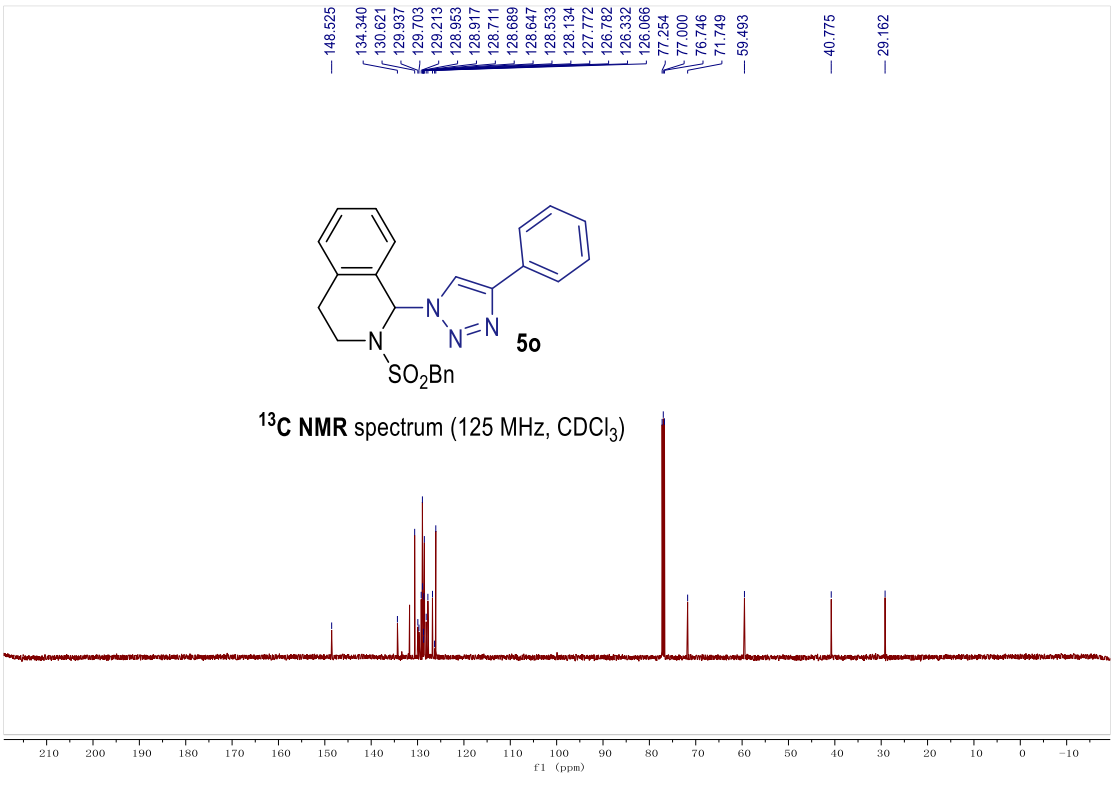

7.587
7.529
7.515
7.357
7.340
7.326
7.311
7.284
7.269
7.254
6.953
6.937
6.384
6.370
3.702
3.694
3.684
3.677
3.668
3.654
3.637
3.620
2.517
2.501
2.497
2.479
2.462
2.457
2.440
2.423
2.372
2.358
2.357
2.346
2.342
2.330
2.315
2.310
2.293
2.286
2.179
2.164
2.156
2.139
2.072
2.053
2.044
2.038
2.030
2.015
0.000
N
N
N
Ts
5n
1H NMR spectrum (500 MHz, CDCl3)
1.07
2.08
4.00
1.04
2.03
1.00
2.04
1.10
1.29
1.16
4.07
f1 (ppm)


147.734
143.313
135.515
130.643
129.928
129.162
128.662
128.410
126.828
125.795
77.254
77.000
76.983
76.746
48.199
33.569
23.208
21.158
N
N
N
Ts
5n
13C NMR spectrum (125 MHz, CDCl3)
f1 (ppm)

5o

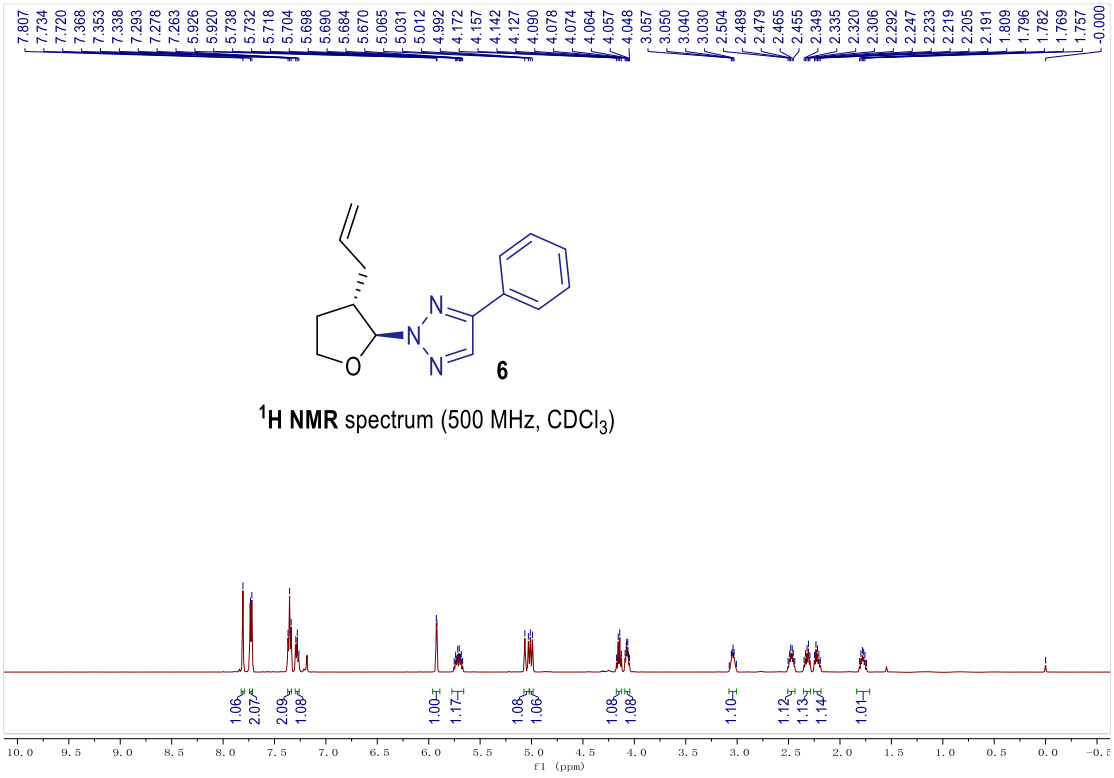


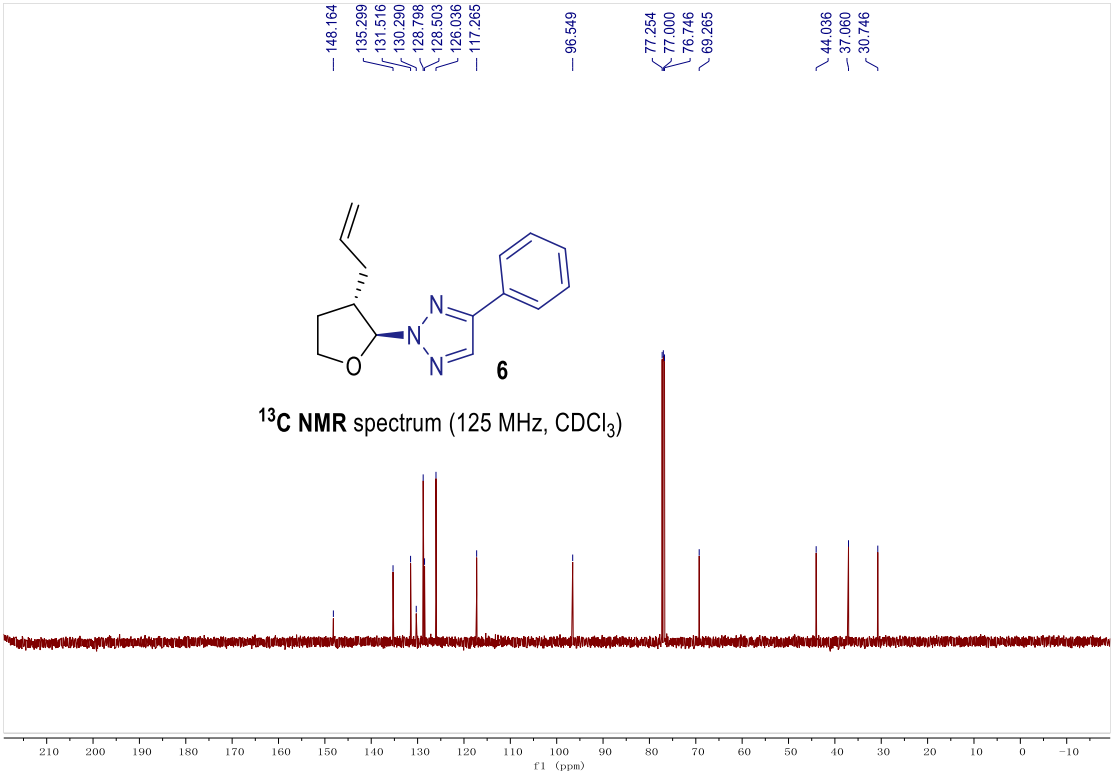
^{1}H NMR spectrum (500 MHz, $CDCl_3$)



^{13}C NMR spectrum (125 MHz, $CDCl_3$)

6


7.807
7.734
7.720
7.368
7.353
7.338
7.293
7.278
7.263
5.926
5.920
5.738
5.732
5.718
5.704
5.698
5.690
5.684
5.670
5.065
5.031
5.012
4.992
4.172
4.157
4.142
4.127
4.090
4.078
4.074
4.064
4.057
4.048
3.057
3.050
3.040
3.030
2.504
2.489
2.479
2.465
2.455
2.349
2.335
2.320
2.306
2.292
2.247
2.233
2.219
2.205
2.191
1.809
1.796
1.782
1.769
1.757
-0.000
N
N
N
O
6
1H NMR spectrum (500 MHz, CDCl3)
1.06
2.07
2.09
1.08
1.00
1.17
1.08
1.06
1.08
1.08
1.10
1.12
1.13
1.14
1.01
f1 (ppm)


148.164
135.299
131.516
130.290
128.798
128.503
126.036
117.265
96.549
77.254
77.000
76.746
69.265
44.036
37.060
30.746
N
N
N
O
6
13C NMR spectrum (125 MHz, CDCl3)
f1 (ppm)