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Iodide ion Enabled High Regioselective α-C(sp^3)–H Triazolization of Ethers with *N*-Sulfonyl-1,2,3-triazoles

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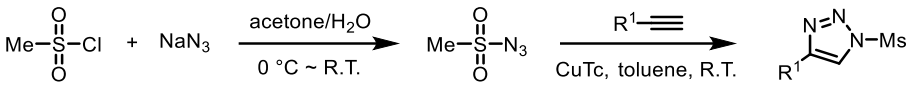
1.General Experimental Details

All reactions and manipulations were carried out under an air atmosphere. All commercial anhydrous solvents and materials were commercialized. All ^{1}H NMR, ^{19}F NMR and ^{13}C NMR spectra were recorded using a Brucker 400 MHz spectrometer in $CDCl_3$. Tetramethylsilane (TMS) served as an internal standard ($\delta = 0$) for ^{1}H NMR, and $CDCl_3$ was used as internal standard ($\delta = 77.0$) for ^{13}C NMR. Chemical shifts are reported in parts per million as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad). Column chromatography was performed on silica gel (300-400 mesh). High-resolution mass spectrometry (HRMS) was performed on IonSpec FT-ICR or Waters Micromass Q-TOF micro Synapt High-Definition Mass Spectrometer. The X-ray diffraction analysis was performed using a Bruker Smart-1000 X-ray diffractometer.

2. General Procedure

2.1 General procedure A: the preparation of Sulfonyl-1,2,3-triazoles[1]



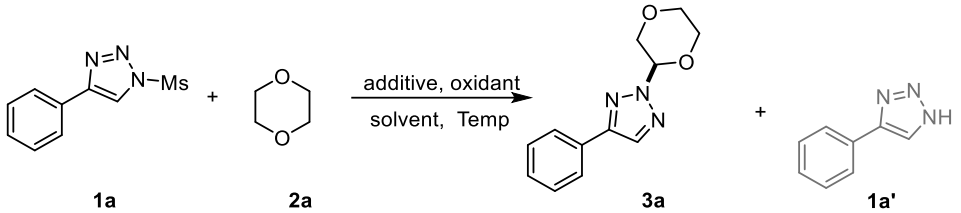
Sulfonyl chloride (20 mmol) was dissolved in 50 mL of acetone, then sodium azide (1.95g, 30 mmol) dissolved in water was slowly added dropwise at 0°C. The reaction was stirred at 0°C for 1 h and then stirred at room temperature for 2 h. After the reaction was complete, the solution was concentrated. Upon complete consumption of the starting materials, the reaction mixture was quenched with saturated aqueous solution of NH_4Cl (20 mL), extracted with EA (3 × 30 mL), washed by brine. The combined extracts were dried with Na_2SO_4 and concentrated and used directly in the next reaction step.

The substituted acetylene (10 mmol) was dissolved in 50 mL of toluene, then CuTc (Copper(I) thiophene-2-carboxylate) (19mg, 0.1 mmol) was added and stirred for 5 minutes. The sulfonyl azide (9 mmol) was added slowly dropwise at 0°C and the mixture stirred overnight. After the reaction is complete, the residue was purified by

flash column chromatography using a mixture of petroleum ether and ethyl acetate (10:1~4:1) as eluent to give the desired products. ***Attention!*** *Sulfonyl azides are potentially explosive materials and must be handled with caution!*

2.2 Optimization of amination of C(sp^3)−H reaction conditions

Table S1. Optimization of amination of C(sp^3)−H reaction conditions



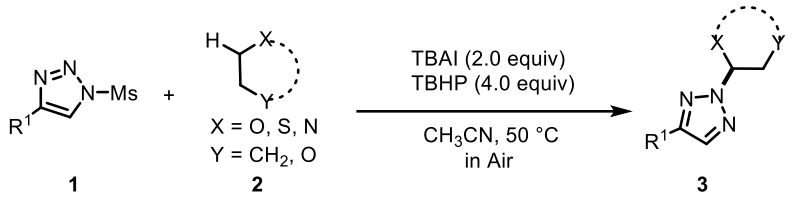
1a **2a** **3a** **1a'**

entry	additive (equiv.)	oxidant (equiv.)	solvent	*T*/°C	yield of **3a** [b]	byproduct
1	$Cu(OAc)_2$ [a]	TBHP (4)	1,4-dioxiane	50	trace	**1a'** (100%)
2	$Cu(OAc)_2$ [b]	TBHP (4)	1,4-dioxiane	50	trace	**1a'** (100%)
3	CuI [c]	TBHP (4)	1,4-dioxiane	50	trace	**1a'** (100%)
4	CuCl (2)	TBHP (4)	1,4-dioxiane	50	trace	**1a'** (100%)
5	$FeCl_3$ (2)	TBHP (4)	1,4-dioxiane	50	trace	**1a'** (100%)
6	KI (2)	TBHP (4)	1,4-dioxiane	50	trace	**1a'** (100%)
7	I_2 (1)	TBHP (4)	1,4-dioxiane	50	trace	**1a'** (100%)
8	TBAI (1.5)	H_2O_2 (1)	1,4-dioxiane	50	trace	**1a'** (100%)
9	TBAF (2)	TBHP (4)	1,4-dioxiane	50	trace	**1a'** (100%)
10	TBAB (2)	TBHP (4)	1,4-dioxiane	50	trace	**1a'** (100%)
11	I_2 (1)	$[Bu_4N]^+[OH]^-$ (2)	1,4-dioxiane	50	trace	**1a'** (100%)
12	TBAI (2)	TBHP (4)	1,4-dioxiane	50	83%	-
13	TBAI (1.5)	TBHP (4)	1,4-dioxiane	50	<40%	**1a'** (60%)
14	TBAI (1.2)	TBHP (4)	1,4-dioxiane	50	<20%	**1a**(40%) + **1a'** (40%)
15	TBAI (1.0)	TBHP (4)	1,4-dioxiane	50	<10%	**1a**(45%) +**7**(45%)
16	TBAI (0.8)	TBHP (4)	1,4-dioxiane	50	<10%	**1a**(30%) + **1a'** (67%)
17	TBAI (0.4)	TBHP (4)	1,4-dioxiane	50	trace	**1a**(85%) + **1a'**13%)
18	TBAI (0.2)	TBHP (4)	1,4-dioxiane	50	trace	**1a**(89%) + **1a'** (10%)
19	TBAI (0.1)	TBHP (4)	1,4-dioxiane	50	trace	**1a**(91%)+ **1a'** (8%)
20	-	TBHP (4)	1,4-dioxiane	50	trace	**6** (100%)
21	TBAI (2)	-	1,4-dioxiane	50	trace	**1a'** (100%)
22	TBAI (2)	TBHP (4)	1,4-dioxiane	70	68%	**1a'** (15%)
23	TBAI (2)	TBHP (4)	1,4-dioxiane	90	61%	**1a'** (10%)
24	TBAI (2)	TBHP (4)	1,4-dioxiane	r.t.	trace	**1a'** (100%)
25	TBAI (2)	TBHP (4)	PEG400	50	trace	**1a'** (100%)
26	TBAI (2)	TBHP (4)	H_2O	50	22%	**1a'** (75%)
27	TBAI (2)	TBHP (4)	DCE	50	42%	-
28	**TBAI (2)**	**TBHP (4)**	**CH_3CN**	**50**	**76%**	-

29	TBAI (2) [d]	TBAI (2)	TBHP (4)	CH_3CN	50	71%
30[e]	TBN (0.2)	DDQ (0.2)	CH_3CN	rt	trace	**1a**(95%)+ **1a'** (5%)
31[e]	RB (0.2)	-	CH_3CN	rt	trace	**1a**(98%)+ **1a'** (2%)
32	$AgNO_3$ (0.2)	$NH_4S_2O_8$(0.2)	CH_3CN	50	trace	**1a**(65%)+ **1a'** (35%)

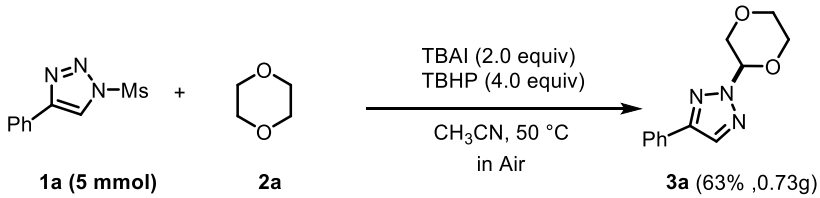
Reaction conditions: Unless otherwise noted, all reactions were conducted on a 0.2 mmol scale of **1a**, **1a**:**2a** = 1:2; **1a** (0.2 mmol, 1 equiv.), **2a** (0.4 mmol, 2 equiv.), solvent (2 mL), additive (x equiv.), oxidant (0.8 mmol, 4 equiv.), T/°C, 2-12h. Isolated yield. In air. [a] $Cu(OAc)_2$ (0.04 mmol), TBAI (0.04 mmol). [b] $Cu(OAc)_2$ (0.04 mmol), TBAI (0.2 mmol). [c] CuI (0.04 mmol). [d] Under N_2. [e] Blue led, rt.

2.3 General procedures B: C(sp^3)−H Amination of Ethers



In a 4 mL sealed vial equipped with a stir bar, *N*-sulfonyl-1,2,3-triazoles **1** (0.2 mmol) and 2 mL acetonitrile were added. Then ethers **2** (1 mmol) and TBAI (147mg, 0.4 mmol) and TBHP (72mg, 0.8 mmol) were added to the mixture. Then, the reaction was allowed to stir at 50 °C for 2-8h. After the completion of the reaction and the evaporation of the solvent under the reduced pressure, the mixture was purified by column chromatography using petroleum ether/ethyl acetate mixture (4:1) as eluent to afford product in high yield and purity.

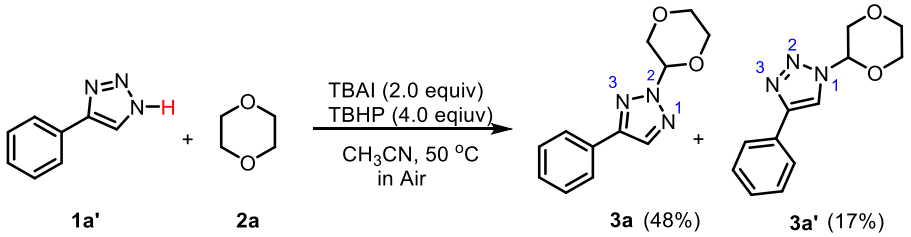
2.4 The experimental procedure for the synthesis of 3a (5 mmol)



In a tube (35 mL), 1-(methylsulfonyl)-4-phenyl-1*H*-1,2,3-triazole **1a** (1.17g, 5 mmol), 1,4-dioxane **2a** (5 mL), TBAI (3.69g, 10 mmol) and TBHP (2800 μL, 20 mmol) were added to 20 mL acetonitrile. Then, the tube was sealed and the reaction was allowed to stir at 50°C for 8h. 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 (10:1~4:1) as eluent to give the desired product **3a** in 63% yield (0.73 g).

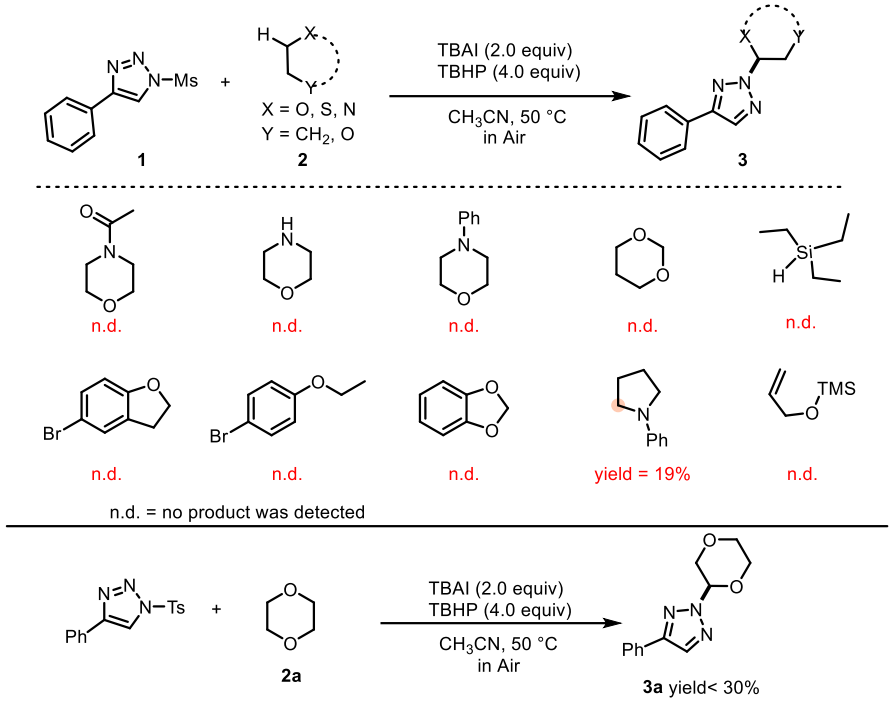
2.5 Perform reactions by using 4-phenyl-1*H*-1,2,3-triazole



Scheme S1. Perform reactions by using 4-phenyl-1*H*-1,2,3-triazole

In a 4 mL sealed vial equipped with a stir bar, 4-phenyl-1*H*-1,2,3-triazole **1a'** (0.2 mmol) and 2 mL acetonitrile were added. Then the 1,4-dioxane **2a** (1 mmol,) and TBAI (147mg, 0.4 mmol) and TBHP (78mg, 0.8 mmol) were added to the mixture. Then, reaction was allowed to stir at 50°C for 8 h. After the completion of the reaction, the mixture was purified by column chromatography using petroleum ether/ethyl acetate mixture (4:1) as eluent to afford the desired N^2-product **3a** in 48% yield and N^1-product **3a'** in 17 % yield.

3. Attempts for other ethers with *N*-sulfonyl-1,2,3-triazoles



Scheme S2. Attempts for other ethers with *N*-sulfonyl-1,2,3-triazoles

4. Single crystal X-ray structures

4.1 Single crystal X-ray structures of 3g (CCDC Number: 2234198)

The method for the crystal growth of **3g** is as follows: In a 10 mL vial, **3g** (10 mg) was dissolved in 1.5 mL DCM, then 5mL hexane was added carefully, making a clear stratification of solution. The vial was placed at room temperature about three days.

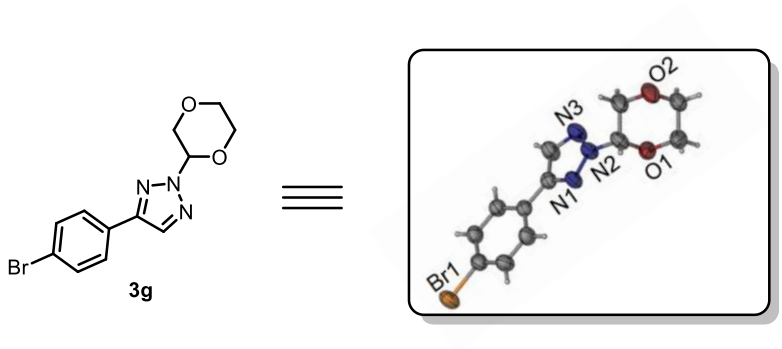


Fig. S1. ORTEP diagram for the compound **3g**. Thermal ellipsoids are shown at the 50% probability level.

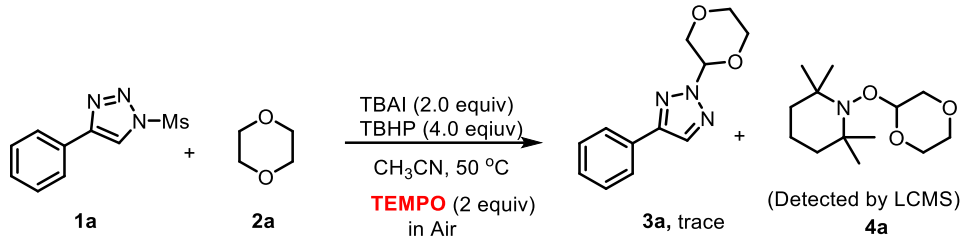
* Crystal data and structure refinement for exp_2860.

Identification code	exp_2860
Empirical formula	$C_{12}H_{12}BrN_3O_2$
Formula weight	310.16
Temperature/K	297.52(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.8086(2)
b/Å	9.1808(2)
c/Å	9.3863(2)
α/°	90
β/°	97.2030(10)
γ/°	90
Volume/Å^3	1266.04(4)

Z	4
ρ_{calc}g/cm^3	1.627
μ/mm^{-1}	4.428
F(000)	624.0
Crystal size/mm^3	0.38 × 0.26 × 0.22
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.016 to 134.146
Index ranges	-17 ⩽ h ⩽ 17, -10 ⩽ k ⩽ 10, -11 ⩽ l ⩽ 11
Reflections collected	26271
Independent reflections	2253 [R_{int} = 0.0498, R_{sigma} = 0.0190]
Data/restraints/parameters	2253/0/163
Goodness-of-fit on F^2	1.100
Final R indexes [I>=2σ (I)]	R_1 = 0.0384, wR_2 = 0.1080
Final R indexes [all data]	R_1 = 0.0415, wR_2 = 0.1105
Largest diff. peak/hole / e Å^{-3}	0.44/-0.52

5.Preliminary mechanistic studies

5.1 The addition of TEMPO in the model reaction system



In a tube (4 mL), TEMPO (0.4mmol, 62.8mg), *N*-sulfonyl-1,2,3-triazoles **1a** (0.2 mmol), 1,4-dioxane **2a** (1 mmol), TBAI (147mg, 0.4 mmol), and TBHP (78mg, 0.8 mmol) were dissolved into 2 mL CH_3CN. Then, the tube was sealed and the reaction was allowed to stir at 50 °C for 8 h. The reaction was completely inhibited and TEMPO-trapped complex (TEMPO-1,4-dioxane) **4a** was detected by LC-MS analysis.

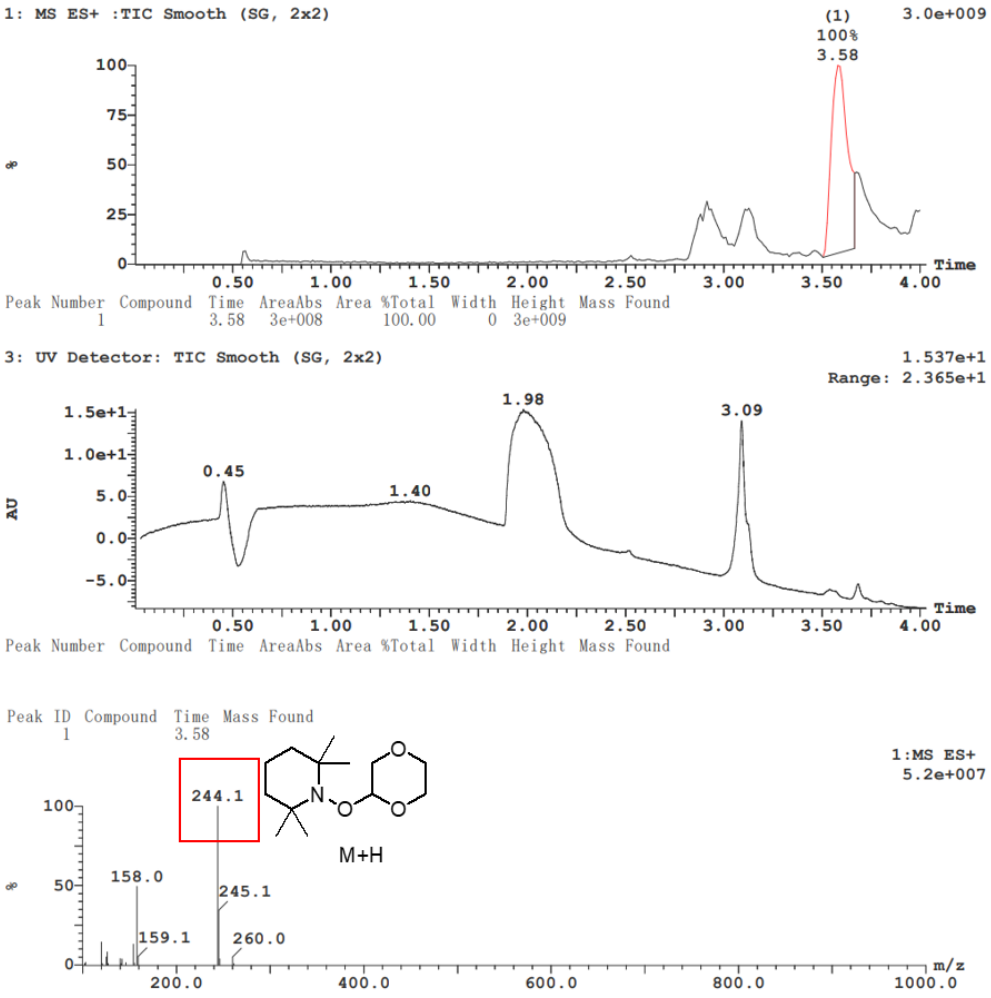
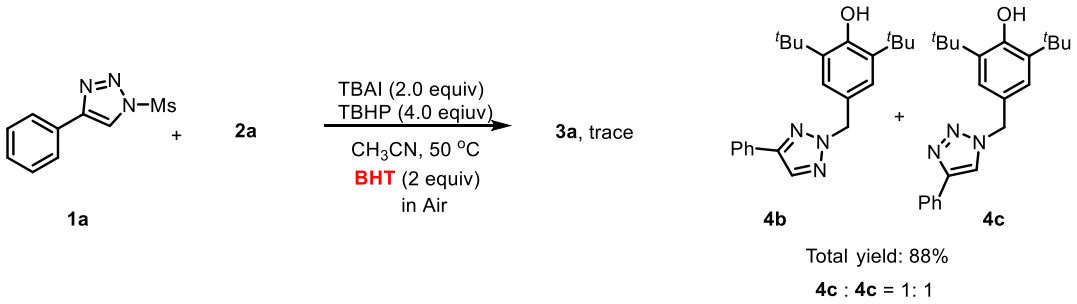
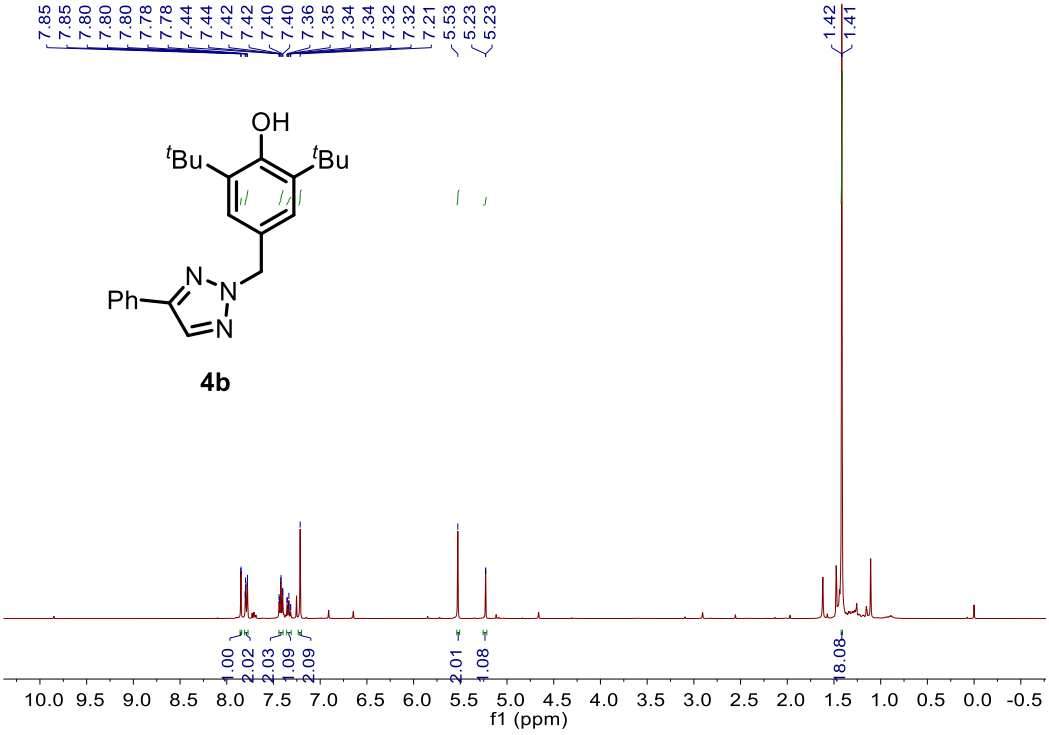
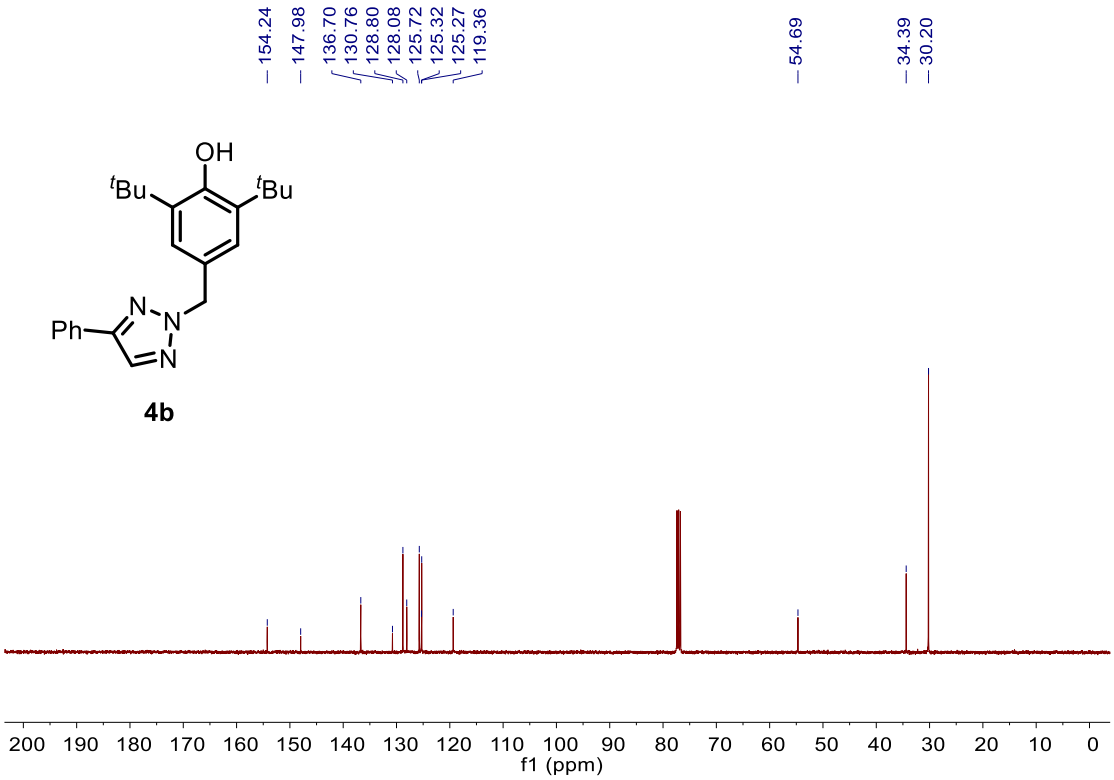


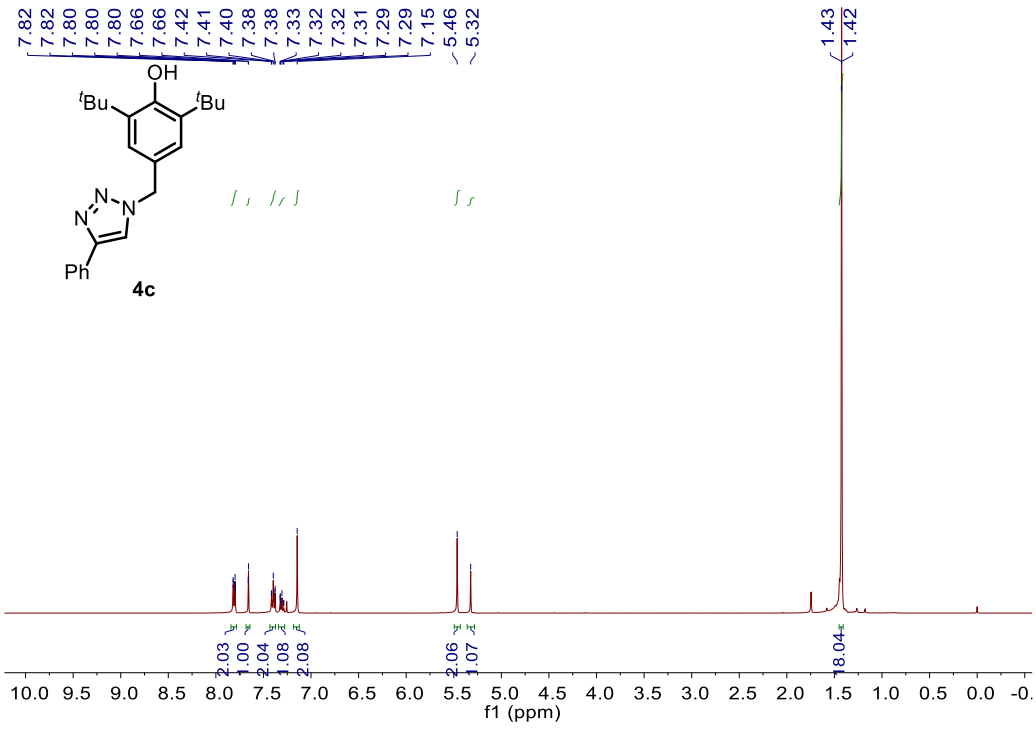
Fig. S2. LCMS spectra of TEMPO-1,4-dioxane under standard condition

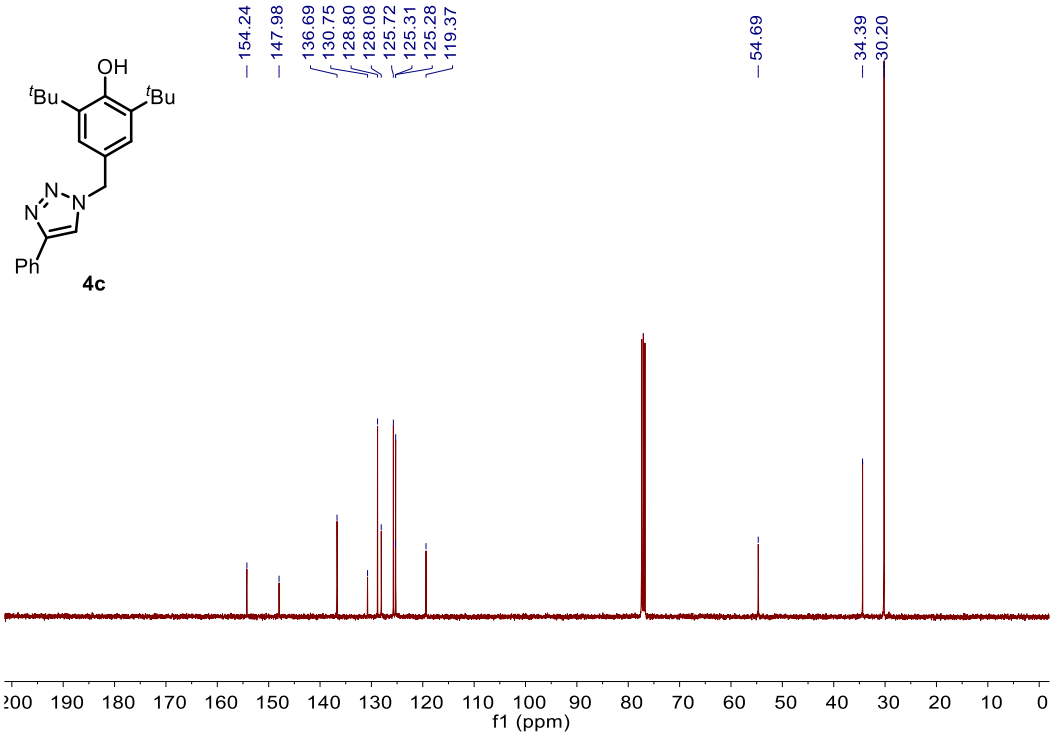


The same reactions were repeated in the presence of BHT (88 mg, 0.4 mmol) under otherwise identical conditions which revealed that the yields of the desired product **3a** and **3a** were <1% by using NMR detected, while the scavenger was observed to form phenyl triazole-substituted BHT in 88% isolated yield.

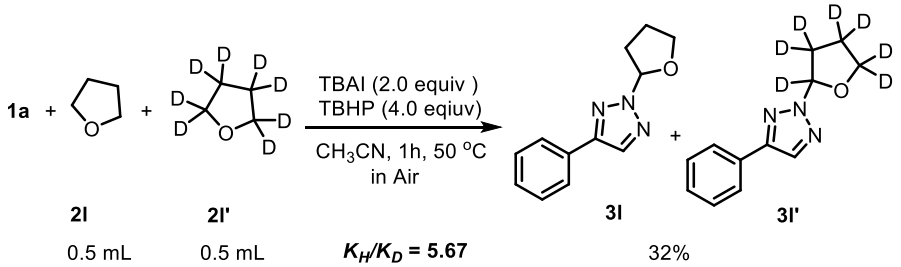



154.24
147.98
136.70
130.76
128.80
128.08
125.72
125.32
125.27
119.36
54.69
34.39
30.20
OH
tBu
tBu
N
N
N
Ph
4b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

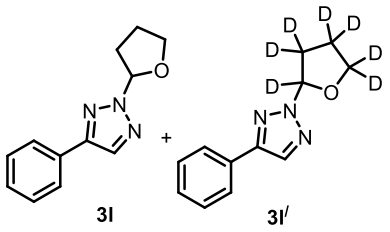

7.82
7.82
7.80
7.80
7.80
7.66
7.66
7.42
7.41
7.40
7.38
7.38
7.33
7.32
7.32
7.31
7.29
7.29
7.15
5.46
5.32
1.43
1.42
OH
tBu
tBu
N
N
N
Ph
4c
2.03
1.00
2.04
1.08
2.08
2.06
1.07
18.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

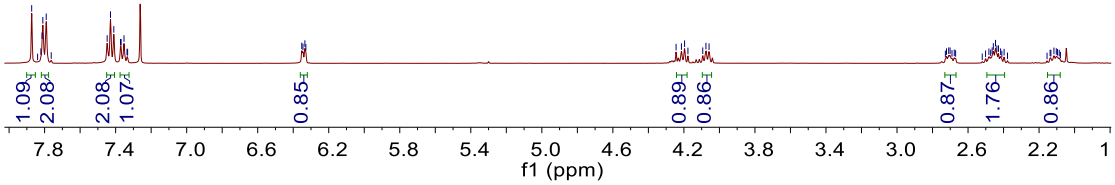


5.2 Intermolecular Kinetic Isotopic Effect (KIE)

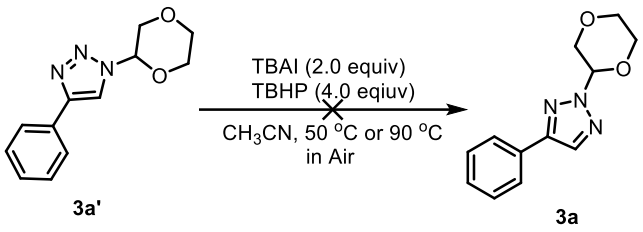


In a tube (4 mL), *N*-sulfonyl-1,2,3-triazoles **1a** (0.2 mmol, 46.6 mg), THF **2l** (0.5 mL), d_8-THF **2l'** (0.5 mL), TBAI (147mg, 0.4 mmol), and TBHP (78mg, 0.8 mmol) were dissolved into 2mL CH_3CN. Then, the tube was sealed and the reaction was allowed to stir at 50°C for 1 h. When the reaction was finished, the pure product was obtained by flash column chromatography on silica gel with a total yield of 32% and detected by ^{1}H NMR to determine the exact KIE value. From the following ^{1}H NMR spectrum, we can calculate the KIE value to be k_H/k_D = 0.85/0.15 = 5.67.



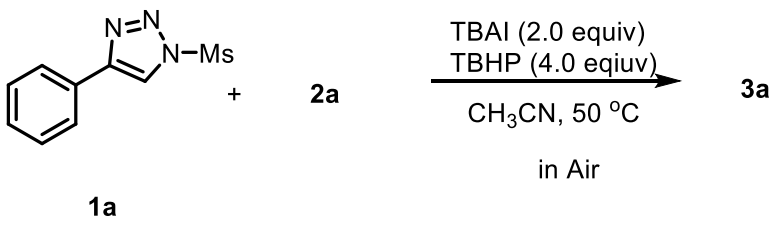


5.3 The transformation of product 3a' to product 3a under standard condition



3a' were prepared according to previously reported synthetic procedures.[2] And then in a 4 mL sealed vial equipped with a stir bar, **3a'** (46.4 mg, 0.2 mmol) and 2 mL acetonitrile were added. Then the 1,4-dioxane **2a** (1 mmol) and TBAI (147mg, 0.4 mmol) and TBHP (78mg, 0.8 mmol) were added to the mixture. Then, the reaction was allowed to stir at 50°C or 90°C for 8 h under standard conditions. But **3a** was not detected in the reaction system.

5.4 Negative-ion ESI mass spectrum of the reaction mixture



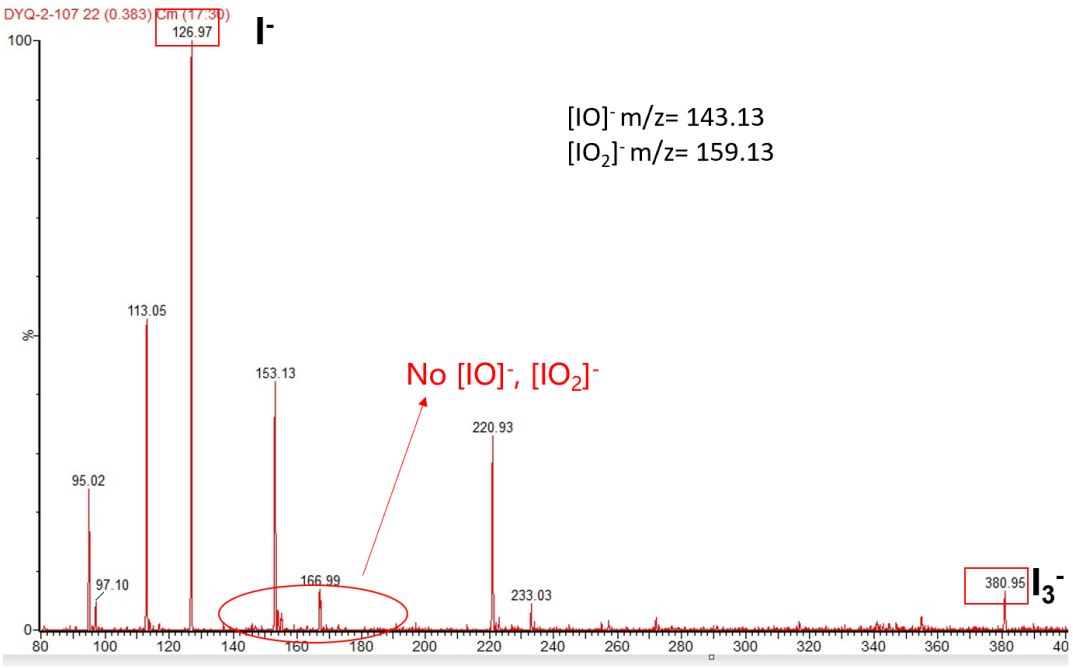
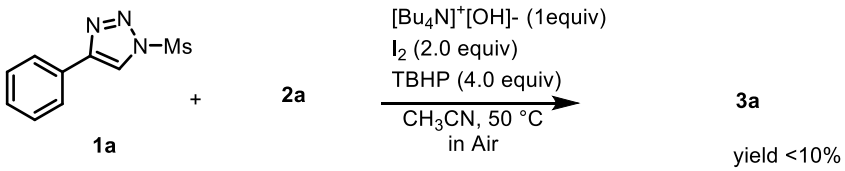


Fig. S3. Negative-ion ESI mass spectrum of the reaction mixture.

5.5 Clarify how to form the desired carbon-centered radicals



In a tube (4 mL), *N*-sulfonyl-1,2,3-triazoles **1a** (0.2 mmol, 46.6 mg), **2a** (0.5 mL) or **4a** (0.4 mmol), $[Bu_4N]^+[OH]^-$ (0.2 mmol), TBHP (0.8 mmol) and I_2 (0.4 mmol) were dissolved into 2mL CH_3CN. Then, the tube was sealed and the reaction was allowed to stir at 50 °C for 8 h. **3a** was observed in micro yields.

6. DFT calculation

Computational Methods: All the DFT calculations were carried out in the Gaussian16 software package. The geometrical structures of reactants, transition states and products were directly optimized with using the functional B3LYP-D3(BJ) combined with a basis set def2-SVP. Single-point energies were calculated with a larger basis set def2-TZVP, denoted as the B3LYP-D3(BJ)/def2-TZVP method. The solvent effect of 1,4-Dioxane is described by using the SMD model. The frequency analysis was performed at the same computational level as single point calculation to identify the minima or transition states. The calculated Gibbs free energy is in kcal/mol at the temperature of 298.15 K.

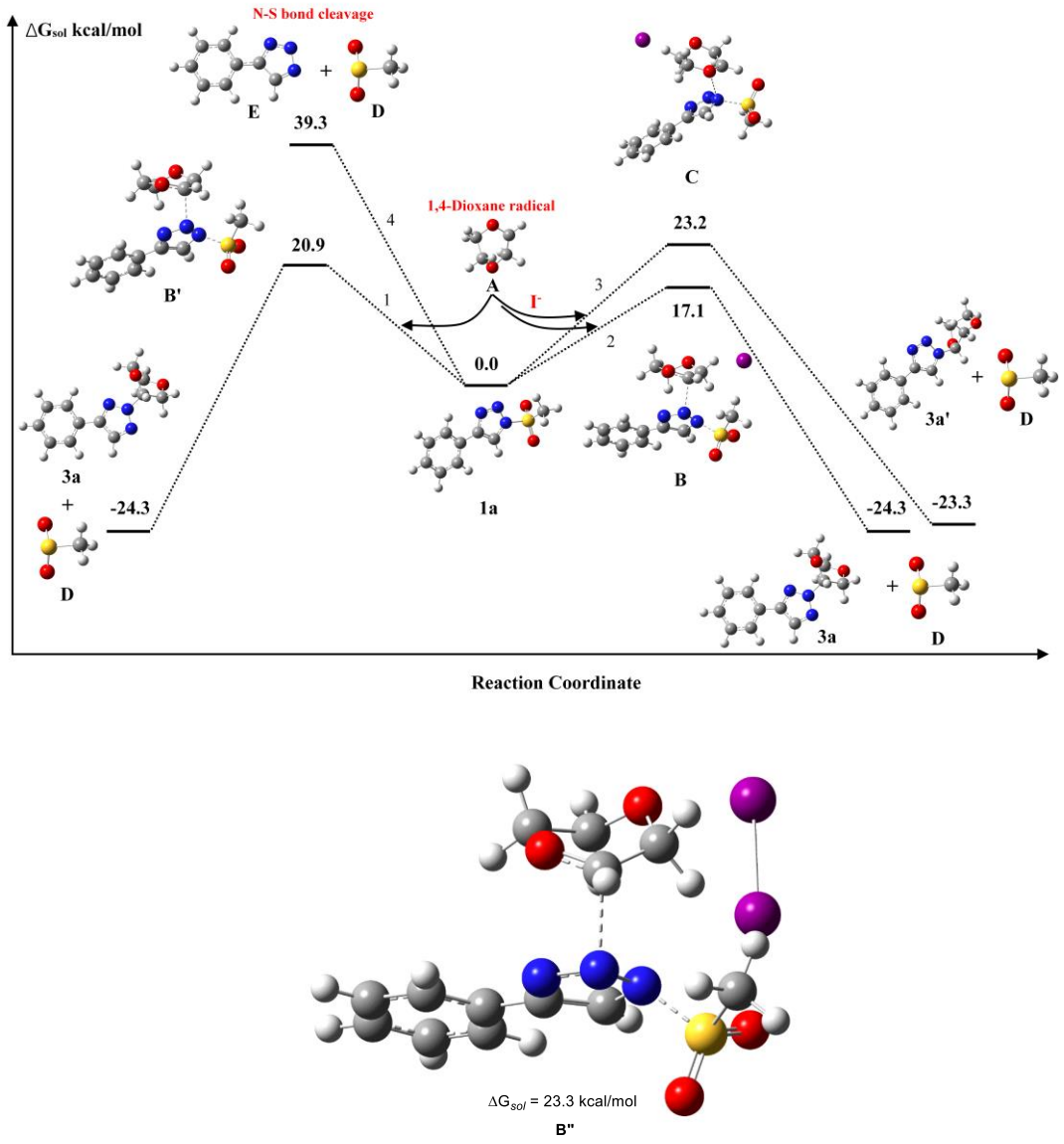


Fig. S4. Calculated free energy profile for *N*-Sulfonyl-1,2,3-triazole **1a** with possible reaction pathways

Coordinates of Optimized Structures

1a

C	-0.75648900	-0.27957700	0.03183200
C	0.29541500	0.62105300	0.01460800
N	1.40185200	-0.17594200	0.05390200
H	0.36858900	1.70273000	-0.02299600
C	-2.20562500	-0.04923100	0.00582100
C	-2.73560600	1.25153600	-0.03498600
C	-3.08734000	-1.14352700	0.02189000
C	-4.11527000	1.45383200	-0.06009300
H	-2.06621800	2.11485400	-0.04593400
C	-4.46647700	-0.93718800	-0.00310000
H	-2.67138100	-2.15130400	0.05489000
C	-4.98630800	0.36006400	-0.04440700
H	-4.51284200	2.47096800	-0.09120700
H	-5.14140300	-1.79633500	0.01030900
H	-6.06697900	0.51921200	-0.06357800
N	-0.21899800	-1.54653300	0.07450600
N	1.06829900	-1.48446400	0.09404500
S	3.08187500	0.32968600	0.11768000
O	3.65529300	-0.18214700	1.34796500
O	3.02859000	1.75283500	-0.18962000
C	3.72390100	-0.60114500	-1.26629300
H	4.80568900	-0.41074600	-1.27804100
H	3.50487000	-1.65993600	-1.07981400
H	3.24333100	-0.23624300	-2.18204800

3a

C	-0.88682500	0.73064100	-0.16327700
C	-0.39723100	2.04828400	0.01665800
N	0.91690400	2.04820500	-0.20630700
H	-0.92098100	2.96307900	0.28296700
C	-2.24823500	0.19512400	-0.03781600
C	-3.30313300	1.00646600	0.41327900
C	-2.51889900	-1.14441900	-0.36923500
C	-4.59529600	0.49259300	0.52953400
H	-3.11350600	2.04814500	0.68063000
C	-3.81052000	-1.65552900	-0.25072600
H	-1.70127900	-1.77354000	-0.72421300
C	-4.85460400	-0.84026700	0.19859400
H	-5.40404700	1.13694900	0.88241400
H	-4.00572800	-2.69816400	-0.51323500
H	-5.86636400	-1.24224200	0.28995700
N	0.16139600	-0.03858600	-0.49877600

N	1.19115200	0.78798300	-0.50126000
C	2.76730500	-1.15766500	1.27894000
C	2.53646700	-1.87488000	-0.04571900
C	2.57450500	0.37134600	-0.86758500
C	3.58276900	0.78352900	0.22894400
H	3.03929900	-1.88581500	2.05722500
H	3.32459800	-2.62664900	-0.20794200
H	3.20331100	1.68799700	0.73815300
H	1.55240500	-2.37106100	-0.05665100
H	1.85136600	-0.63578100	1.61517200
H	4.53736200	1.03517500	-0.25743000
H	2.80670400	0.91265600	-1.79701400
O	3.84857700	-0.26077900	1.14077500
O	2.61803300	-0.97238400	-1.15767200

3a'

C	-1.18967300	0.10931400	0.12608100
C	-0.22575500	-0.88594200	0.18818000
N	0.95217100	-0.21592000	0.28452300
H	-0.27632500	-1.97008300	0.17011800
C	-2.65125200	0.01845100	0.02991300
C	-3.30524400	-1.22417200	-0.02621100
C	-3.42287600	1.19288100	-0.00890200
C	-4.69547600	-1.29175200	-0.11860800
H	-2.72426600	-2.14906000	0.00159900
C	-4.81257100	1.12191700	-0.10144500
H	-2.91062100	2.15488600	0.03486100
C	-5.45536200	-0.11872000	-0.15658900
H	-5.18861100	-2.26585600	-0.16162700
H	-5.39968700	2.04308900	-0.13069200
H	-6.54420300	-0.17197400	-0.22901000
N	-0.53433600	1.31260200	0.17474800
N	0.73993800	1.11545100	0.26409300
C	2.30779600	-0.76359900	0.25131700
C	3.22862600	0.00968700	1.21801700
H	3.10268900	-0.37324400	2.24041900
C	3.62930600	0.36073000	-1.33899200
C	4.87212100	0.33293100	-0.43922900
H	3.90999800	0.29389700	-2.39915100
H	5.29426200	1.35399900	-0.34912600
O	4.56438000	-0.20122900	0.84070500
O	2.82217500	-0.77349300	-1.05179600
H	3.04487600	1.28698400	-1.20119200
H	5.64662100	-0.32201100	-0.86699900

H	2.95301200	1.07855100	1.21953400
H	2.21755500	-1.81669600	0.55525200

B'

C	2.55276200	-0.49724400	-0.23166900
C	1.84490400	-1.36753600	0.57486900
N	0.53624100	-1.27346100	0.12872300
H	2.11140400	-1.99718800	1.41678700
C	3.96712900	-0.11095700	-0.18340500
C	4.84124500	-0.62833900	0.78860100
C	4.47150900	0.80748800	-1.12227800
C	6.18007500	-0.23762300	0.82291700
H	4.46750400	-1.34108100	1.52697000
C	5.81106100	1.19528300	-1.08640000
H	3.78710600	1.19935600	-1.87607600
C	6.67250000	0.67665000	-0.11426100
H	6.84415100	-0.64957700	1.58736300
H	6.18690100	1.90898100	-1.82449800
H	7.72150200	0.98247400	-0.08636800
N	1.70151300	0.06171000	-1.14618400
N	0.48114500	-0.40228000	-0.95107000
S	-0.46221400	-2.73521700	0.08139100
O	-0.49529000	-3.17709300	1.47662800
O	0.06406500	-3.63209300	-0.94939200
C	-2.01900200	-2.05900300	-0.44478900
H	-2.69745900	-2.91926300	-0.51452800
H	-2.41793000	-1.32068100	0.26698200
H	-1.86663700	-1.59796800	-1.42687100
C	1.10060200	2.33846300	1.24778600
C	0.96022700	2.99600900	-0.11345700
C	-0.75516100	1.36284000	-0.40765100
C	-0.97028500	1.26573200	1.07204300
H	1.68942300	2.99069600	1.91221600
H	0.63695700	4.04425900	0.01116900
H	-0.78931900	0.21975300	1.40208400
H	1.90985400	2.97492100	-0.67070600
H	1.63322100	1.37466500	1.16282600
H	-2.03608400	1.47901300	1.27177400
H	-1.57812800	1.04691700	-1.05206900
O	-0.17347300	2.17165200	1.81985700
O	-0.02687400	2.35273100	-0.92484200
I	-4.53079500	0.57536300	-0.12870600

B

C	0.93152700	-0.65110400	-0.18649900
C	-0.05246300	-1.19284900	0.61892900
N	-1.24619500	-0.68516400	0.11605800
H	-0.03454600	-1.83786000	1.49091700
C	2.39240900	-0.75949700	-0.08808400
C	3.00430100	-1.47253900	0.95683000
C	3.20435200	-0.13168600	-1.04906900
C	4.39411300	-1.55360200	1.04061900
H	2.38981200	-1.96599400	1.71295900
C	4.59419800	-0.21569600	-0.96288800
H	2.72307000	0.41159100	-1.86352200
C	5.19485200	-0.92504100	0.08152200
H	4.85546200	-2.11112100	1.85917500
H	5.21364900	0.27388300	-1.71831300
H	6.28342700	-0.98995200	0.14787900
N	0.34574300	0.11701400	-1.15534700
N	-0.96441600	0.09763200	-1.00177200
S	-2.64116300	-1.75848000	0.00985500
O	-2.89612500	-2.15314900	1.39172300
O	-2.42531500	-2.75319000	-1.03377100
C	-3.88251600	-0.59965400	-0.55397000
H	-4.79400000	-1.19819800	-0.68302600
H	-4.02617400	0.17353000	0.20932400
H	-3.54186600	-0.18791000	-1.51134100
C	0.36525300	2.56839800	1.15477000
C	0.60428800	3.10304900	-0.24596900
C	-1.53186100	2.11267700	-0.66679500
C	-1.91163500	2.21654500	0.79031900
H	1.06312200	3.04294300	1.85979800
H	0.69458600	4.20101500	-0.22375600
H	-2.08936100	1.19765200	1.19851900
H	1.51180500	2.67238600	-0.69462100
H	0.52819400	1.47721800	1.19987300
H	-2.85764100	2.77843000	0.88557800
H	-2.33433400	2.05811600	-1.40462800
O	-0.94826600	2.90131700	1.55801900
O	-0.49447300	2.80996700	-1.12513900

C

C	-1.64917600	1.52921600	-0.27686200
C	-1.87903000	0.52179300	0.65957800
N	-2.33168600	-0.53867300	-0.06761800
H	-1.71516100	0.45244300	1.72973200
N	-2.01398200	1.04841800	-1.50259400

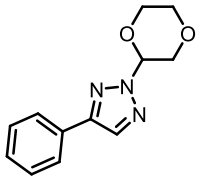
N	-2.44523200	-0.18096100	-1.37306000
C	-1.10820600	2.87946800	-0.10268000
C	-0.94925500	3.72493800	-1.21628500
C	-0.73459100	3.35993300	1.16514300
C	-0.43680100	5.01200400	-1.06178500
H	-1.23112200	3.34352000	-2.19863400
C	-0.22012700	4.64778200	1.31594100
H	-0.84004900	2.71599600	2.04094400
C	-0.06973500	5.48160600	0.20396300
H	-0.31485200	5.65360100	-1.93858300
H	0.07296900	4.99964300	2.30836900
H	0.33974300	6.48799600	0.32191400
S	-3.95338300	-1.57801300	0.54183700
O	-3.78254600	-2.95644400	0.04943200
O	-4.11509100	-1.31826400	1.98156600
C	-5.30697700	-0.80256200	-0.37741000
H	-5.04056400	-0.86235800	-1.43894900
H	-6.22025300	-1.36619500	-0.14110100
H	-5.37668300	0.23930000	-0.04122700
C	1.14408000	-1.09472300	-1.06411400
C	1.24682500	-1.16614000	0.44071700
C	-0.76162800	-2.47258300	0.28972500
C	-0.51484400	-2.73160100	-1.15862800
H	2.14512600	-0.84526600	-1.44458000
H	2.11730200	-1.76790800	0.74670100
H	-1.29515600	-2.19083800	-1.74111200
H	1.33973000	-0.17949500	0.90821500
H	0.41573600	-0.32864200	-1.39003200
H	-0.65881000	-3.80932900	-1.35258100
H	-1.56077300	-2.98452300	0.82768700
O	0.77495800	-2.37324200	-1.57182400
O	0.04934600	-1.78289900	1.02933000
I	4.76673000	-0.61319300	0.18726200

B”

C	-2.81126100	-0.17425100	-0.29533400
C	-1.66322300	-0.64124700	-0.90634600
N	-1.09830700	-1.52946900	0.01023900
H	-1.17052600	-0.40205800	-1.84246600
C	-3.75903200	0.85414600	-0.74153000
C	-3.63432200	1.46579800	-2.00037300
C	-4.80632500	1.25078800	0.10855200
C	-4.53405300	2.45400700	-2.39886300
H	-2.83001400	1.16596100	-2.67558900

C	-5.70562400	2.23822400	-0.29447500
H	-4.89885500	0.76771000	1.08231700
C	-5.57293500	2.84414700	-1.54749400
H	-4.42556700	2.92104700	-3.38052500
H	-6.51690900	2.53659500	0.37390800
H	-6.27776300	3.61757300	-1.86154200
N	-2.95444900	-0.78618300	0.91830000
N	-1.94840800	-1.60814300	1.12553300
S	-0.52717600	-3.06807600	-0.62432000
O	0.57507900	-2.69873000	-1.52833000
O	-1.63536100	-3.86518100	-1.13225600
C	0.12035100	-3.83392900	0.85393300
H	0.42736600	-4.83987400	0.53879800
H	0.97735600	-3.25368300	1.21408700
H	-0.69563400	-3.87750700	1.58547100
C	-0.25611300	1.46051500	1.72954400
C	-1.47767800	1.52050800	2.62750500
C	-1.02996800	-0.81448800	2.89000200
C	0.42406800	-0.60814000	2.55322700
H	0.11901800	2.47404100	1.52898000
H	-1.29324200	2.19016700	3.48218000
H	0.67562900	-1.16760200	1.63143300
H	-2.37262700	1.86299200	2.08619700
H	-0.48986500	0.99061600	0.75855600
H	1.05028800	-1.01270700	3.36761900
H	-1.31720100	-1.70227800	3.45600900
O	0.76390900	0.74862300	2.40146900
O	-1.78811000	0.23064000	3.19075800
I	2.19289300	-0.45806200	-0.90868500
I	3.55039200	1.79514700	-0.12259900

7. ^{1}H NMR, ^{19}F NMR and ^{13}C NMR data of compounds



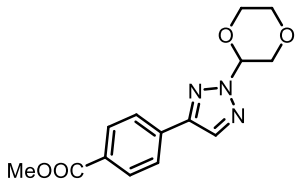
3a

2-(1,4-dioxan-2-yl)-4-phenyl-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3a**. Yield: 83%. 37.6 mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 (s, 1H), 7.91 – 7.74 (m, 2H), 7.50 – 7.38 (m, 3H), 5.88 (dd, J = 7.6, 2.8 Hz, 1H), 4.41 (dd, J = 11.7, 7.6 Hz, 1H), 4.16 (dd, J = 11.8, 2.8 Hz, 1H), 4.12 – 4.03 (m, 1H), 3.99 (dd, J = 11.8, 5.1 Hz, 1H), 3.87 (dd, J = 5.4, 3.7 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.8, 132.2, 130.0, 128.9, 128.9, 126.2, 85.2, 67.7, 65.9, 65.7.

HRMS calc. for $C_{12}H_{13}N_3NaO_2$ $(M+Na)^+$, 254.0900; found, 254.0904.



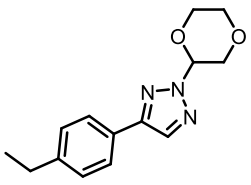
3b

methyl 4-(2-(1,4-dioxan-2-yl)-2*H*-1,2,3-triazol-4-yl) benzoate was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3b**. Yield:72%. 41.6mg. White solid, mp = 62.3 °C – 62.5 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.11 (d, J = 8.0 Hz, 2H), 8.02 (s, 1H), 7.90 (d, J = 8.0 Hz, 2H), 5.87 (dd, J = 7.4, 2.8 Hz, 1H), 4.39 (dd, J = 11.7, 7.5 Hz, 1H), 4.19 – 4.10 (m, 1H), 4.09 –3.97 (m, 2H), 3.94 (s, 3H), 3.88 – 3.84 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7, 147.7, 134.0, 132.6, 130.3, 130.2, 126.0, 85.3, 67.6, 65.9, 65.6, 52.2.

HRMS calc. for $C_{14}H_{15}N_3NaO_4$ $(M+Na)^+$, 312.0955; found, 312.0957.



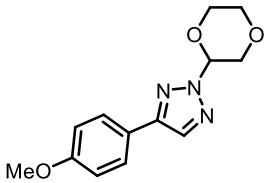
3c

2-(1,4-dioxan-2-yl)-4-(thiophen-2-yl)-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3c**. Yield:76%. 39.3mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (s, 1H), 7.73 (d, *J* = 7.5 Hz, 2H), 7.27 (d, *J* = 7.5 Hz, 2H), 5.95 – 5.77 (dt, *J* = 7.3, 1.7 Hz, 1H), 4.38 (dd, *J* = 11.6, 7.8 Hz, 1H), 4.20 – 4.09 (m, 1H), 4.07 – 4.01 (m, 1H), 3.97 (dt, *J* = 11.8, 5.7 Hz, 1H), 3.88 – 3.78 (m, 2H), 2.68 (q, *J* = 7.6 Hz, 2H), 1.26 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.9, 145.2, 132.1, 128.4, 127.2, 126.2, 85.1, 67.7, 65.9, 65.7, 28.7, 15.5.

HRMS calc. for $C_{14}H_{17}N_3NaO_2$ $(M+Na)^+$, 282.1213; found, 282.1221.



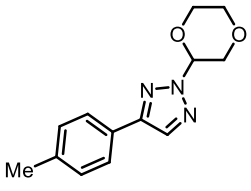
3d

methyl 4-(2-(1,4-dioxan-2-yl)-2*H*-1,2,3-triazol-4-yl) benzoate was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3d.** Yield:75%. 39.1mg. White solid, mp = 57.6 °C – 57.9 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (s, 1H), 7.75 (d, *J* = 7.7 Hz, 2H), 6.96 (d, *J* = 7.8 Hz, 2H), 5.84 (dt, *J* = 7.9, 2.2 Hz, 1H), 4.37 (dd, *J* = 11.6, 7.8 Hz, 1H), 4.13 (d, *J* = 11.7 Hz, 1H), 4.08 – 3.91 (m, 2H), 3.85 (m, 5H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1, 148.6, 131.7, 127.5, 122.5, 114.3, 85.1, 67.7, 65.9, 65.8, 55.4.

HRMS calc. for $C_{13}H_{15}N_3NaO_3$ $(M+Na)^+$, 284.1006; found, 284.1002.

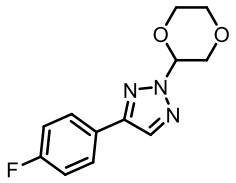


3e

2-(1,4-dioxan-2-yl)-4-(p-tolyl)-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3e**. Yield: 83 %. 40.6mg. Yellow oil. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.92 (s, 1H), 7.71 (dd, *J* = 8.0, 1.5 Hz, 2H), 7.26 (d, *J* = 4.2 Hz, 2H), 5.85 (dt, *J* = 7.7, 1.9 Hz, 1H), 4.38 (ddd, *J* = 11.7, 7.7, 1.4 Hz, 1H), 4.18 – 4.10 (m, 1H), 4.08 – 3.93 (m, 2H), 3.84 (dd, *J* = 5.5, 3.0 Hz, 2H), 2.39 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.9, 138.8, 132.1, 129.6, 126.9, 126.1, 85.1, 67.7, 65.9, 65.8, 21.4.

HRMS calc. for $C_{13}H_{15}N_3NaO_2$ $(M+Na)^+$, 268.1056; found, 268.1061.



3f

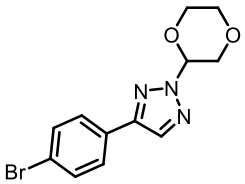
2-(1,4-dioxan-2-yl)-4-(4-fluorophenyl)-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3f**. Yield: 77%. 46.0mg. White solid, mp = 64.1 °C – 64.6 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (s, 1H), 7.94 (d, *J* = 8.3 Hz, 2H), 7.70 (q, *J* = 10.6, 8.8 Hz, 2H), 5.88 (dd, *J* = 7.5, 2.8 Hz, 1H), 4.39 (dd, *J* = 11.8, 7.4 Hz, 1H), 4.14 (dd, *J* = 11.8, 2.8 Hz, 1H), 4.10 – 4.03 (m, 1H), 3.98 (dt, *J* = 11.9, 7.2, 4.6 Hz, 1H), 3.90 – 3.82 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.4, 132.5, 129.3, 128.9, 128.2, 126.4, 125.87 (dd, *J* = 6.9, 2.6 Hz), 85.3, 67.6, 65.9, 65.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.69.

HRMS calc. for $C_{12}H_{12}FN_3NaO_2$ $(M+Na)^+$, 272.0806; found, 272.0807.



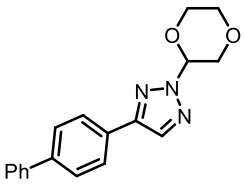
3g

4-(4-bromophenyl)-2-(1,4-dioxan-2-yl)-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3g**. Yield: 75%. 46.3mg. White solid, mp = 55.3 °C – 56.6 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 (s, 1H), 7.69 (d, *J* = 7.9 Hz, 2H), 7.56 (d, *J* = 7.7 Hz, 2H), 5.85 (dt, *J* = 7.1, 2.0 Hz, 1H), 4.37 (dd, *J* = 11.6, 7.6 Hz, 1H), 4.13 (dt, *J* = 11.8, 2.0 Hz, 1H), 4.08 – 4.01 (m, 1H), 3.97 (dt, *J* = 11.8, 5.3 Hz, 1H), 3.88 – 3.79 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.8, 132.1, 132.1, 128.8, 127.7, 122.9, 85.2, 67.6, 65.9, 65.7.

HRMS calc. for $C_{12}H_{12}BrN_3NaO_2$ $(M+Na)^+$, 332.0005; found, 332.0007.



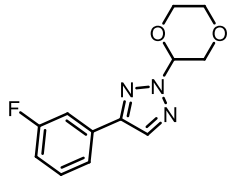
3h

4-([1,1'-biphenyl]-4-yl)-2-(1,4-dioxan-2-yl)-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3h**. Yield: 82%. 50.3mg. White solid, mp = 62.3 °C – 62.5 °C.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 1.3 Hz, 1H), 7.89 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.70 – 7.65 (m, 2H), 7.66 – 7.60 (m, 2H), 7.49 – 7.41 (m, 2H), 7.40 – 7.32 (m, 1H), 5.87 (dd, *J* = 8.3, 2.8 Hz, 1H), 4.40 (m, *J* = 11.8, 7.6, 1.3 Hz, 1H), 4.15 (dd, *J* = 11.9, 2.9 Hz, 1H), 4.10 – 4.03 (m, 1H), 3.98 (dt, *J* = 11.8, 5.8 Hz, 1H), 3.85 (dd, *J* = 5.7, 3.2 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.5, 141.6, 140.4, 132.3, 128.9, 128.7, 127.6, 127.6, 127.1, 126.6, 85.2, 67.7, 65.9, 65.8.

HRMS calc. for $C_{18}H_{17}N_3NaO_2$ $(M+Na)^+$, 330.1213; found, 330.1215.



3i

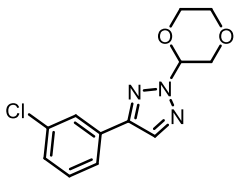
2-(1,4-dioxan-2-yl)-4-(3-fluorophenyl)-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3i**. Yield:72%. 35.8mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95 (s, 1H), 7.56 (dd, *J* = 17.5, 8.7 Hz, 2H), 7.40 (q, *J* = 7.6 Hz, 1H), 7.07 (t, *J* = 7.4 Hz, 1H), 5.86 (dd, *J* = 7.4, 2.3 Hz, 1H), 4.38 (dd, *J* = 11.5, 7.6 Hz, 1H), 4.13 (dd, *J* = 11.7, 2.4 Hz, 1H), 4.05 (dt, *J* = 12.2, 3.0 Hz, 1H), 3.98 (dt, *J* = 11.7, 5.1 Hz, 1H), 3.88 – 3.82 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.15 (d, *J* = 246.1 Hz), 147.71 (d, *J* = 2.9 Hz), 132.3, 131.93 (d, *J* = 8.4 Hz), 130.52 (d, *J* = 8.4 Hz), 121.82 (d, *J* = 3.0 Hz), 115.74 (d, *J* = 21.1 Hz), 113.16 (d, *J* = 23.1 Hz), 85.2, 67.6, 65.9, 65.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -112.42.

HRMS calc. for $C_{12}H_{12}FN_3NaO_2$ $(M+Na)^+$, 272.0806; found, 272.0811.



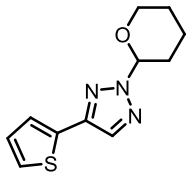
3j

4-(3-chlorophenyl)-2-(1,4-dioxan-2-yl)-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3j**. Yield:75%. 39.7mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95 (s, 1H), 7.83 (d, *J* = 2.0 Hz, 1H), 7.69 (dd, *J* = 6.9, 1.7 Hz, 1H), 7.36 (d, *J* = 7.4 Hz, 2H), 5.86 (dd, *J* = 7.6, 2.8 Hz, 1H), 4.38 (dd, *J* = 11.7, 7.5 Hz, 1H), 4.13 (dd, *J* = 11.8, 2.9 Hz, 1H), 4.08 – 4.02 (m, 1H), 4.01 – 3.94 (m, 1H), 3.89 – 3.81 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.5, 134.9, 132.3, 131.6, 130.2, 128.9, 126.3, 124.3, 85.2, 67.6, 65.9, 65.7.

HRMS calc. for $C_{12}H_{12}ClN_3NaO_2$ $(M+Na)^+$, 288.0510; found, 288.0514.



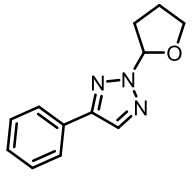
3k

2-(tetrahydro-2*H*-pyran-2-yl)-4-(thiophen-2-yl)-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3k**. Yield: 71%. 33.6mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 (s, 1H), 7.40 (d, *J* = 3.4 Hz, 1H), 7.32 (d, *J* = 5.0 Hz, 1H), 7.07 (t, *J* = 4.2 Hz, 1H), 5.96 – 5.55 (m, 1H), 4.06 (d, *J* = 11.5 Hz, 1H), 3.75 (t, *J* = 10.4 Hz, 1H), 2.44 (dt, *J* = 13.2, 6.7 Hz, 1H), 2.30 – 2.06 (m, 2H), 1.78 – 1.70 (m, 2H), 1.67 (dd, *J* = 6.0, 2.9 Hz, 1H).

^{13}C NMR (101 MHz, CDCl3) δ 147.3, 134.5, 131.6, 129.2, 128.8, 127.5, 89.3, 67.6, 29.5, 24.9, 21.9.

HRMS calc. for $C_{11}H_{13}N_3ONaS$ $(M+Na)^+$, 258.0672; found, 258.0668.



3l

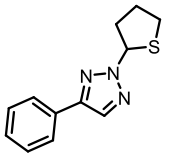
4-phenyl-2-(tetrahydrofuran-2-yl)-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography

using a gradient eluent of PE/EA (10:1-4:1) to provide **3l**. Yield:84%. 36.1mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-d) δ 7.87 (s, 1H), 7.80 (d, J = 8.0 Hz, 2H), 7.42 (t, J = 7.6 Hz, 2H), 7.35 (t, J = 7.6 Hz, 1H), 6.41 – 6.29 (m, 1H), 4.20 (q, J = 7.4 Hz, 1H), 4.06 (q, J = 7.4 Hz, 1H), 2.77 – 2.64 (m, 1H), 2.43 (tq, J = 15.9, 7.5 Hz, 2H), 2.10 (dq, J = 12.3, 7.2, 6.6 Hz,1H).

^{13}C NMR (101 MHz, CDCl3) δ 148.1, 131.5, 130.4, 128.9, 128.5, 126.1, 92.4, 69.6, 31.9, 24.5.

HRMS calc. for $C_{12}H_{13}N_3NaO$ $(M+Na)^+$, 238.0951; found, 238.0953.



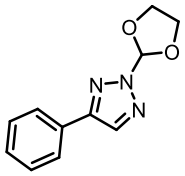
3m

4-phenyl-2-(tetrahydrothiophen-2-yl)-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3m**. Yield:75%. 34.6mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 (s, 1H), 7.82 – 7.76 (m, 2H), 7.47 – 7.38 (m, 2H), 7.38 – 7.31 (m, 1H), 6.31 (dd, *J* = 6.9, 2.6 Hz, 1H), 3.30 (ddd, *J* = 10.6, 7.0, 4.0 Hz, 1H), 3.02 (td, *J* = 9.6, 6.3 Hz, 1H), 2.78 (dd, *J* = 12.5, 6.2 Hz, 1H), 2.72 – 2.52 (m, 1H), 2.49 – 2.23 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.0, 131.4, 130.3, 128.9, 128.5, 126.0, 71.6, 37.5, 33.8, 29.6.

HRMS (ESI) $C_{12}H_{13}N_3NaS$ Calcd. for $(M+Na)^+$ 254.0722, Found: 254.0731.



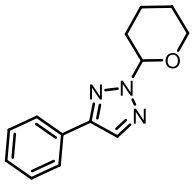
3n

2-(1,3-dioxolan-2-yl)-4-phenyl-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3n**. Yield:51%. 22.1mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 (s, 1H), 7.87 – 7.78 (m, 2H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.38 (t, *J* = 7.3 Hz, 1H), 6.43 (dd, *J* = 6.3, 3.7 Hz, 1H), 5.37 (s, 1H), 5.24 (s, 1H), 4.68 (dd, *J* = 9.3, 3.6 Hz, 1H), 4.40 (dd, *J* = 9.3, 6.2 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.9, 132.4, 129.9, 128.9, 128.9, 126.2, 96.5, 87.8, 69.1.

HRMS calc. for $C_{11}H_{12}N_3O_2$ $(M+H)^+$, 218.0924; found, 218.0917.



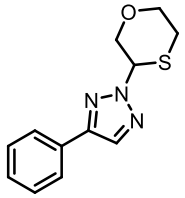
3o

4-phenyl-2-(tetrahydro-2H-pyran-2-yl)-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3o**. Yield:77%. 35.2mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (s, 1H), 7.82 (d, *J* = 7.8 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.36 (t, *J* = 7.0 Hz, 1H), 5.75 (dd, *J* = 9.2, 2.6 Hz, 1H), 4.08 (dt, *J* = 11.9, 3.7 Hz, 1H), 3.77 (dd, *J* = 12.3, 9.2 Hz, 1H), 2.48 (td, *J* = 9.4, 4.0 Hz, 1H), 2.22 – 2.07 (m, 2H), 1.82 – 1.71 (m, 2H), *1.67 (dt, J = 8.0, 4.1 Hz, 1H).*

^{13}C NMR (101 MHz, $CDCl_3$) δ 131.6, 130.2, 128.8, 128.6, 126.3, 126.2, 89.2, 67.5, 29.4, 24.8, 21.9.

HRMS calc. for $C_{13}H_{15}N_3NaO$ $(M+Na)^+$, 252.1107; found, 252.1109.



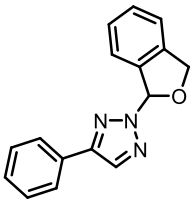
3p

2-(1,4-oxathian-3-yl)-4-phenyl-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3p**. Yield:74%. 36.5mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 (s, 1H), 7.81 (d, *J* = 7.6 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.39 – 7.33 (m, 1H), 5.49 (t, *J* = 3.6 Hz, 1H), 4.51 (dd, *J* = 12.2, 4.2 Hz, 1H), 4.31 (dd, *J* = 12.3, 2.7 Hz, 1H), 4.20 (dt, *J* = 11.9, 4.0 Hz, 1H), 4.07 – 3.96 (m, 1H), 3.46 (ddd, *J* = 13.1, 9.3, 3.1 Hz, 1H), 2.61 (dt, *J* = 13.8, 3.4 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.2, 131.7, 130.1, 128.9, 128.6, 126.1, 71.5, 68.2, 58.9, 25.5.

HRMS calc. for $C_{12}H_{14}N_3OS$ $(M+H)^+$, 248.0852; found, 248.0853.



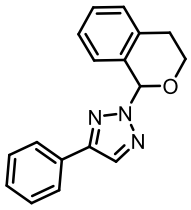
3q

2-(1,3-dihydroisobenzofuran-1-yl)-4-phenyl-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (20:1-4:1) to provide **3q**. Yield:64%. 33.6mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (s, 1H), 7.77 (d, *J* = 7.5 Hz, 2H), 7.45 (t, *J* = 5.0 Hz, 2H), 7.43 – 7.38 (m, 3H), 7.36 (s, 1H), 7.35 – 7.31 (m, 2H), 5.51 (dd, *J* = 12.5, 2.5 Hz, 1H), 5.25 (d, *J* = 12.4 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.5, 140.0, 135.5, 132.4, 130.1, 129.8, 128.9, 128.7, 128.1, 126.1, 122.9, 121.4, 95.6, 74.0.

HRMS calc. for $C_{16}H_{14}N_3O$ $(M+H)^+$, 264.1131; found, 264.1139.



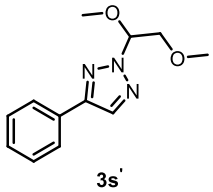
3r

2-(isochroman-1-yl)-4-phenyl-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (20:1-4:1) to provide **3r**. Yield:71%. 39.3mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (s, 1H), 7.80 (d, *J* = 7.6 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.39 – 7.30 (m, 2H), 7.27 (d, *J* = 9.3 Hz, 1H), 7.21 (t, *J* = 7.5 Hz, 1H), 7.06 (s, 1H), 7.03 (d, *J* = 7.8 Hz, 1H), 4.36 (td, *J* = 11.4, 3.4 Hz, 1H), 4.08 (ddd, *J* = 11.5, 5.9, 2.0 Hz, 1H), 3.16 (ddd, *J* = 17.0, 11.4, 5.9 Hz, 1H), 2.86 (dt, *J* = 16.6, 2.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.4, 134.5, 132.0, 130.7, 130.1, 129.0, 128.9, 128.8, 128.7, 127.0, 126.6, 126.2, 86.7, 61.0, 27.8.

HRMS calc. for $C_{17}H_{16}N_3O$ $(M+H)^+$, 278.1288; found, 278.1289.

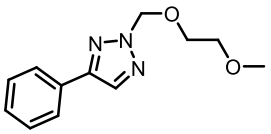


3s'

2-((2-methoxyethoxy) methyl) -4-phenyl-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3s'**. Yield: 45%. Yellow oil. 20.9mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-d) δ 7.96 (s, 1H), 7.88 – 7.79 (m, 2H), 7.44 (t, J = 7.4 Hz, 2H), 7.41 – 7.34 (m, 1H), 5.71 (t, J = 6.0 Hz, 1H), 4.01 (qd, J = 10.4, 6.0 Hz, 2H), 3.40 (s, 3H), 3.37 (s, 3H).

^{13}C NMR (101 MHz, CDCl3) δ 148.5, 132.0, 130.1, 128.9, 128.7, 126.1, 92.2, 72.8, 59.5, 56.9.**HRMS** calc. for $C_{12}H_{15}N_3NaO_2$ $(M+Na)^+$, 256.1056; found, 256.1059.



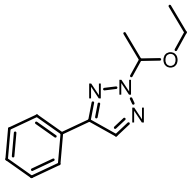
3s

2-(1,2-dimethoxyethyl)-4-phenyl-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3s**. Yield: 31%. 14.4 mg.

^{1}H NMR (400 MHz, Chloroform-d) δ 7.93 (s, 1H), 7.82 (d, J = 7.4 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.37 (t, *J* = 7.4 Hz, 1H), 5.78 (s, 2H), 3.78 (dd, *J* = 5.7, 3.5 Hz, 2H), 3.54 (dd, *J* = 5.7, 3.5 Hz, 2H), 3.37 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.9, 132.3, 130.0, 128.9, 128.8, 126.1, 82.9, 71.4, 69.2, 59.1.

HRMS calc. for $C_{12}H_{15}N_3NaO_2$ $(M+Na)^+$, 256.1056; found, 256.1059.



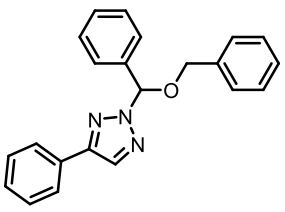
3t

2-(1-ethoxyethyl)-4-phenyl-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3t**. Yield:73%. 31.6mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 (s, 1H), 7.75 (d, *J* = 7.3 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.28 (t, *J* = 7.2 Hz, 1H), 5.73 (q, *J* = 6.0 Hz, 1H), 3.60 – 3.42 (m, 1H), 3.40 – 3.25 (m, 1H), 1.76 (d, *J* = 6.0 Hz, 3H), 1.09 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.9, 131.3, 130.3, 128.9, 128.6, 126.1, 89.5, 64.6, 20.9, 14.8.

HRMS calc. for $C_{12}H_{15}N_3NaO$ $(M+Na)^+$, 240.1107; found, 240.1108.



3u

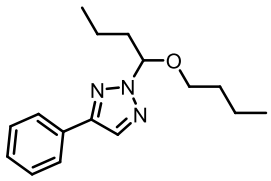
2-((benzyloxy)(phenyl)methyl)-4-phenyl-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography

using a gradient eluent of PE/EA (10:1-4:1) to provide **3u**. Yield:61%. 41.6mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 (d, *J* = 7.7 Hz, 2H), 7.73 (s, 1H), 7.52 – 7.45 (m, 2H), 7.39 (dd, *J* = 8.7, 6.1 Hz, 9H), 7.33 (q, *J* = 7.0, 5.5 Hz, 2H), 6.93 (s, 1H), 4.75 – 4.63 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.3, 136.7, 136.4, 136.0, 132.2, 130.3, 129.4, 128.9, 128.7, 128.4, 128.2, 126.6, 126.2, 125.8, 117.3, 91.9, 88.4, 71.1.

HRMS calc. for $C_{22}H_{20}N_3O$ $(M+H)^+$, 342.1601; found, 342.1609.



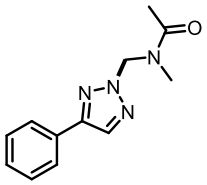
3v

4-phenyl-2-(tetrahydrofuran-2-yl)-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3v.** Yield: 82%. 44.7 mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (s, 1H), 7.83 (d, *J* = 7.6 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.36 (t, *J* = 7.3 Hz, 1H), 5.60 (t, *J* = 6.7 Hz, 1H), 3.48 (dt, *J* = 9.7, 6.7 Hz, 1H), 3.33 (dt, *J* = 9.6, 6.5 Hz, 1H), 2.19 (dddd, *J* = 23.2, 16.4, 10.6, 3.7 Hz, 2H), 1.57 – 1.39 (m, 2H), 1.36 – 1.30 (m, 2H), 1.28 – 1.22 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H), 0.86 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.8, 131.3, 130.4, 128.9, 128.5, 126.1, 93.3, 69.0, 36.7, 31.3, 19.1, 18.1, 13.8, 13.6.

HRMS calc. for $C_{16}H_{23}N_3NaO$ $(M+Na)^+$, 296.1733; found, 296.1737.

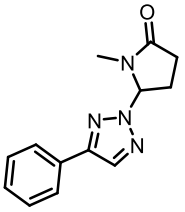


3w

***N*-methyl-*N*-((4-phenyl-2*H*-1,2,3-triazol-2-yl) methyl) acetamide** was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3w.** Yield: 76%. 37.1 mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (s, 1H), 7.78 (d, *J* = 7.0 Hz, 2H), 7.40 (dd, *J* = 28.0, 7.4 Hz, 2H), 5.98 (d, *J* = 2.9 Hz, 1H), 5.84 (d, *J* = 3.1 Hz, 2H), 3.10 (dd, *J* = 25.0, 2.9 Hz, 3H), 2.48 (d, *J* = 2.9 Hz, 2H), 2.18 (d, *J* = 2.9 Hz, 1H).

HRMS calc. for $C_{12}H_{14}N_4ONa$ $(M+Na)^+$, 253.1060; found, 253.1056.



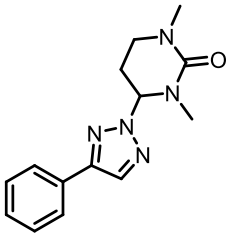
3x

1-methyl-5-(4-phenyl-2*H*-1,2,3-triazol-2-yl) pyrrolidin-2-one was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-0:1) to provide **3s**. Yield:87%. 42.1mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (s, 1H), 7.79 (d, *J* = 7.7 Hz, 2H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.39 (d, *J* = 7.0 Hz, 1H), 6.05 (d, *J* = 7.5 Hz, 1H), 2.98 (dt, *J* = 15.4, 8.4 Hz, 1H), 2.75 (s, 3H), 2.68 – 2.58 (m, 1H), 2.57 – 2.46 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.5, 148.7, 131.9, 129.8, 129.0, 128.9, 126.0, 78.9, 29.0, 27.7, 25.2.

HRMS calc. for $C_{13}H_{15}N_4O$ $(M+H)^+$, 243.1240; found, 243.1234.



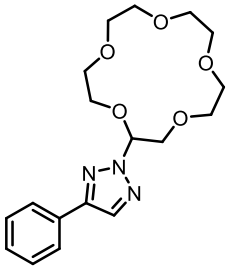
3y

1,3-dimethyl-4-(4-phenyl-2*H*-1,2,3-triazol-2-yl) tetrahydropyrimidin-2(1*H*)-one-methane was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-0:1) to provide **3y**. Yield: 90%. 43.1mg. Yellow oil.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (s, 1H), 7.85 – 7.76 (m, 2H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.41 – 7.32 (m, 1H), 5.90 (dd, *J* = 4.5, 2.7 Hz, 1H), 3.72 (td, *J* = 12.3, 4.0 Hz, 1H), 3.19 (ddd, *J* = 12.0, 6.0, 1.8 Hz, 1H), 3.05 (s, 3H), 2.94 (s, 3H), 2.53 (tt, *J* = 13.2, 5.2 Hz, 1H), 2.40 – 2.22 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.6, 148.1, 131.3, 130.1, 128.9, 128.7, 126.0, 76.1, 43.7, 36.0, 34.3, 27.3.

HRMS calc. for $C_{14}H_{17}N_5NaO$ $(M+Na)^+$, 310.1638; found, 310.1644.



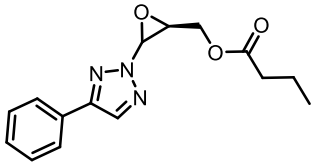
3z

2-(1,4,7,10,13-pentaoxacyclopentadecan-2-yl)-4-phenyl-2*H*-1,2,3-triazole was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-0:1) to provide **3z**. Yield: 74%. Yellow oil. 54.0 mg.

^{1}H NMR (400 MHz, Chloroform-d) δ 7.93 (s, 1H), 7.83 (dd, J = 7.3, 1.6 Hz, 2H), 7.43 (dd, J = 8.3, 6.6 Hz, 2H), 7.38 – 7.32 (m, 1H), 6.15 (t, J = 6.2 Hz, 1H), 4.30 (dd, J = 10.7, 5.9 Hz, 1H), 4.17 (dd, J = 10.9, 6.4 Hz, 1H), 3.92 – 3.57 (m, 16H).

^{13}C NMR (101 MHz, CDCl3) δ 148.3, 131.8, 130.3, 128.8, 128.6, 126.1, 91.6, 71.7, 71.5, 71.1, 70.7, 70.7, 70.6, 70.4, 68.6.

HRMS calc. for $C_{18}H_{26}N_3O_5$ $(M+H)^+$, 364.1867; found, 364.1871.



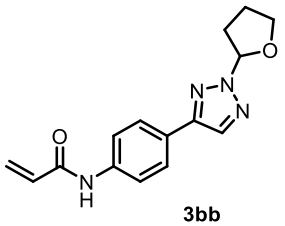
3aa

((2*S*)-3-(4-phenyl-2*H*-1,2,3-triazol-2-yl) oxiran-2-yl) methyl butyrate was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-1:1) to provide **3aa**. Yield: 71%. Yellow oil. 40.7 mg.

^{1}H NMR (400 MHz, Chloroform-d) δ 7.88 (s, 1H), 7.77 (dd, J = 7.1, 1.7 Hz, 2H), 7.50 – 7.40 (m, 2H), 7.40 – 7.34 (m, 1H), 4.69 – 4.53 (m, 2H), 4.43 (dtd, J = 7.1, 5.1, 3.7 Hz, 1H), 4.27 – 4.10 (m, 1H), 2.35 (t, J = 7.4 Hz, 2H), 1.68 (h, J = 7.4 Hz, 2H), 0.96 (t, J = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl3) δ 173.5, 148.3, 131.3, 129.9, 129.0, 128.7, 126.0, 68.7, 65.0, 57.2, 36.0, 18.4, 13.7.

HRMS calc. for $C_{15}H_{17}N_3$ Na O_3 $(M+Na)^+$, 310.1162; found, 309.1172.



3bb

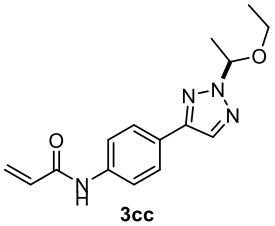
***N*-(4-(2-(tetrahydrofuran-2-yl)-2*H*-1,2,3-triazol-4-yl) phenyl) acrylamide** was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-1:1) to provide **3bb**. Yield: 53%. Yellow oil. 30.1 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 (s, 1H), 7.77 (d, J = 8.4 Hz, 2H), 7.66 (d, J = 8.3 Hz, 2H), 7.43 (s, 1H), 6.46 (d, J = 16.8 Hz, 1H), 6.33 (dd, J = 6.6, 2.5 Hz, 1H), 6.27 (dd, J = 16.8, 10.2 Hz, 1H), 5.86 – 5.76 (m, 1H), 4.20 (q, J = 7.3 Hz, 1H), 4.06 (td,

J = 7.7, 5.8 Hz, 1H), 2.69 (ddd, *J* = 12.6, 7.7, 2.8 Hz, 1H), 2.50 – 2.37 (m, 2H), 2.16 – 2.03 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.5, 147.6, 138.0, 131.2, 131.0, 128.2, 126.8, 126.6, 120.1, 92.3, 69.6, 31.4, 24.5.

HRMS calc. for $C_{15}H_{16}N_4NaO_2$ $(M+Na)^+$, 307.1165; found, 307.1169.



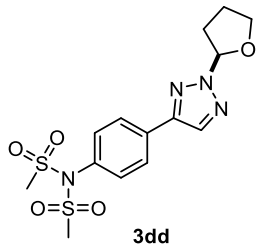
3cc

***N*-(4-(2-(1-ethoxyethyl)-2*H*-1,2,3-triazol-4-yl) phenyl) acrylamide** was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-1:1) to provide **3bb**. Yield: 53%. Yellow oil. 30.1 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (s, 1H), 7.81 (d, *J* = 8.6 Hz, 2H), 7.68 (d, *J* = 8.4 Hz, 2H), 7.40 (s, 1H), 6.47 (dd, *J* = 16.8, 1.3 Hz, 1H), 6.27 (dd, *J* = 16.8, 10.2 Hz, 1H), 5.88 – 5.76 (m, 2H), 3.56 (dq, *J* = 9.4, 7.0 Hz, 1H), 3.39 (dq, *J* = 9.5, 7.1 Hz, 1H), 1.83 (d, *J* = 6.0 Hz, 3H), 1.16 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.4, 147.4, 138.0, 131.1, 131.0, 128.2, 126.8, 120.1, 89.5, 64.7, 29.7, 20.9, 14.8.

HRMS calc. for $C_{15}H_{18}N_4NaO_2$ $(M+Na)^+$, 309.1322; found, 309.1329.



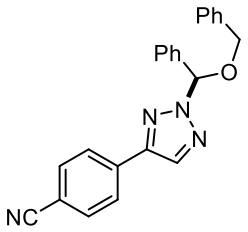
3dd

***N*-(methylsulfonyl)-*N*-(4-(2-(tetrahydrofuran-2-yl)-2*H*-1,2,3-triazol-4-yl) phenyl) methane sulfonamide** was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-1:1) to provide **3bb**. Yield: 58%. Yellow oil. 43.2 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 – 7.79 (m, 3H), 7.35 (d, *J* = 8.3 Hz, 2H), 6.27 (dd, *J* = 6.4, 2.5 Hz, 1H), 4.13 (q, *J* = 7.4 Hz, 1H), 4.00 (td, *J* = 7.8, 5.8 Hz, 1H), 3.35 (s, 6H), 2.61 (ddd, *J* = 12.1, 6.2, 2.7 Hz, 1H), 2.43 – 2.27 (m, 2H), 2.05 (dq, *J* = 13.6, 9.0, 8.5 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 145.6, 132.2, 131.7, 130.7, 130.1, 126.2, 91.5, 68.7, 41.7, 30.4, 23.4.

HRMS calc. for $C_{14}H_{18}N_4O_5NaS_2$ $(M+Na)^+$, 409.0611; found, 409.0607.



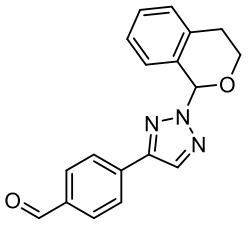
3ee

4-(2-((benzyloxy)(phenyl)methyl)-2H-1,2,3-triazol-4-yl) benzonitrile was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-1:1) to provide **3ee**. Yield: 71%. Yellow oil. 51.9 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 (s, 1H), 7.96 – 7.90 (m, 2H), 7.72 (d, *J* = 8.3 Hz, 2H), 7.58 – 7.50 (m, 2H), 7.43 – 7.28 (m, 8H), 6.78 (s, 1H), 4.71 (d, *J* = 12.0 Hz, 1H), 4.61 (d, *J* = 12.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 146.6, 136.3, 136.2, 134.6, 132.7, 132.6, 129.3, 128.6, 128.5, 128.2, 128.1, 126.6, 126.5, 118.7, 112.1, 92.3, 71.2.

HRMS calc. for $C_{23}H_{18}N_4NaO$ $(M+Na)^+$, 389.1373; found, 389.1379.



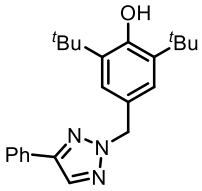
3ff

4-(2-(isochroman-1-yl)-2*H*-1,2,3-triazol-4-yl) benzaldehyde was synthesized by following Procedure B. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **3ff**. Yield: 63%. Yellow oil. 38.4 mg.

^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 10.04 (s, 1H), 7.96 (dd, *J* = 18.8, 8.4 Hz, 5H), 7.39 – 7.28 (m, 2H), 7.23 (t, *J* = 7.3 Hz, 1H), 7.08 (s, 1H), 7.03 (d, *J* = 7.8 Hz, 1H), 4.37 (td, *J* = 11.5, 3.4 Hz, 1H), 4.11 (ddd, *J* = 11.4, 5.9, 2.1 Hz, 1H), 3.18 (ddd, *J* = 17.0, 11.5, 5.8 Hz, 1H), 2.87 (dt, *J* = 16.5, 2.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 191.7, 147.1, 136.2, 135.9, 134.5, 132.6, 130.3, 129.0, 128.9, 127.0, 126.7, 126.6, 87.0, 61.1, 29.7, 27.8.

HRMS calc. for $C_{18}H_{15}N_3O_2Na$ $(M+Na)^+$, 328.1056; found, 328.1055.

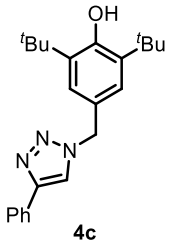


4b

2,6-di-*tert*-butyl-4-((4-phenyl-2*H*-1,2,3-triazol-2-yl) methyl) phenol. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-4:1) to provide **4b**. Yield: 45%. White solid.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 (d, *J* = 1.1 Hz, 1H), 7.82 – 7.77 (m, 2H), 7.47 – 7.38 (m, 2H), 7.36 – 7.31 (m, 1H), 7.21 (s, 2H), 5.53 (s, 2H), 5.23 (d, *J* = 1.1 Hz, 1H), 1.42 (d, *J* = 1.2 Hz, 18H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.2, 148.0, 136.7, 130.8, 128.8, 128.1, 125.7, 125.3, 125.3, 119.4, 54.7, 34.4, 30.2.



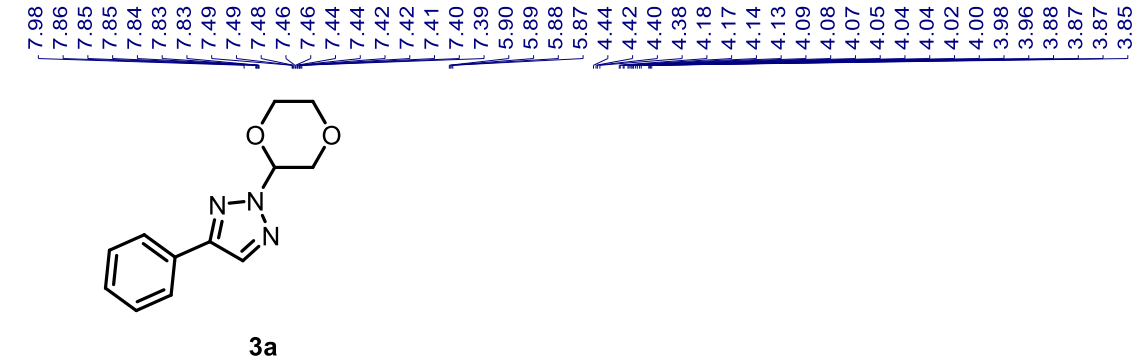
4c

2,6-di-*tert*-butyl-4-((4-phenyl-1*H*-1,2,3-triazol-1-yl) methyl) phenol. The crude material was purified by column chromatography using a gradient eluent of PE/EA (10:1-1:1) to provide **4c**. Yield: 43%. White solid.

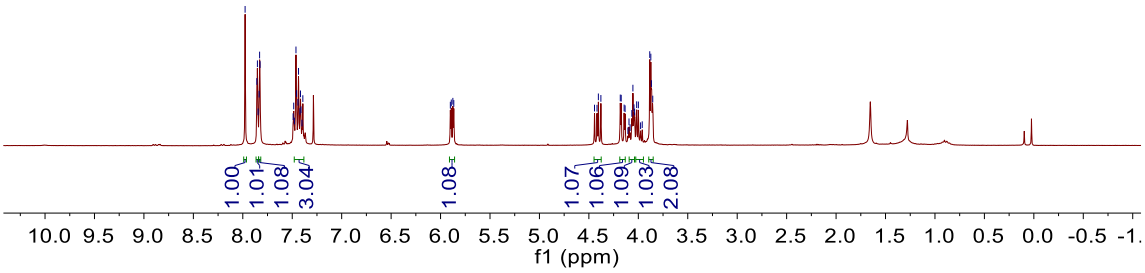
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 (dd, *J* = 7.1, 1.3 Hz, 2H), 7.66 (d, *J* = 1.2 Hz, 1H), 7.44 – 7.35 (m, 2H), 7.35 – 7.27 (m, 1H), 7.15 (s, 2H), 5.46 (s, 2H), 5.32 (s, 1H), 1.42 (d, *J* = 1.1 Hz, 18H).

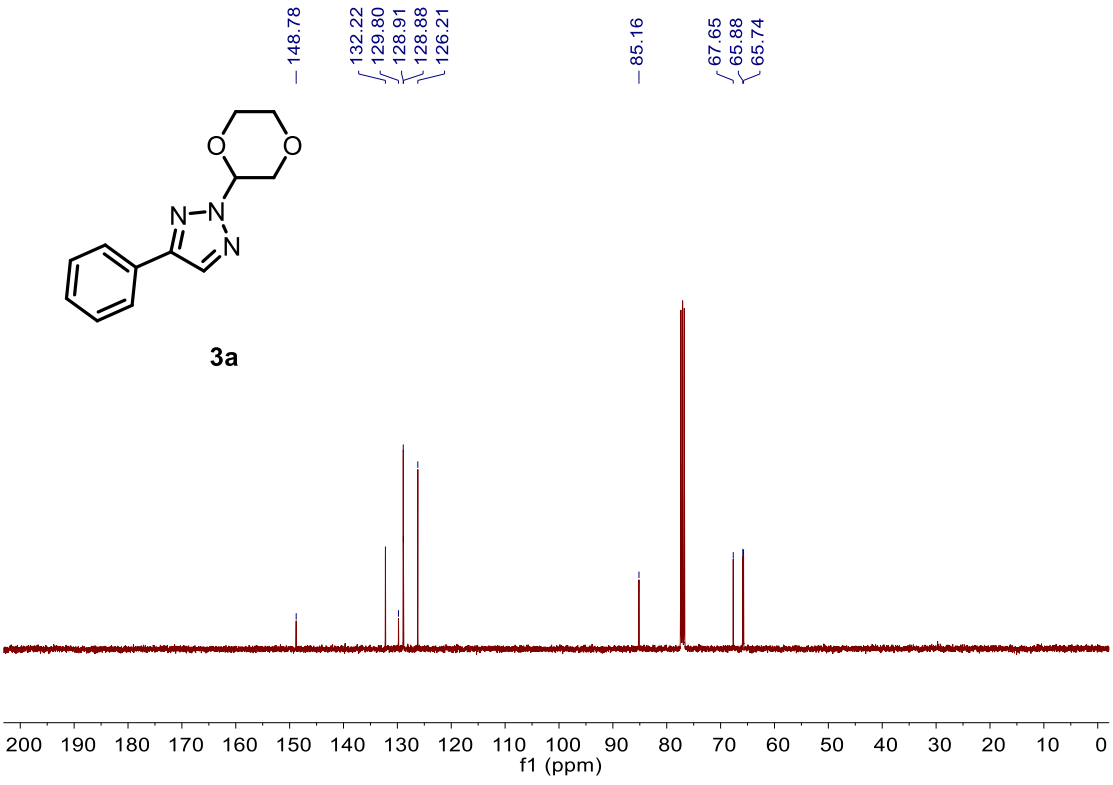
^{13}C NMR (101 MHz, $CDCl_3$) δ 154.2, 148.0, 136.7, 130.8, 128.8, 128.1, 125.7, 125.3, 125.3, 119.4, 54.7, 34.4, 30.2.

8. NMR Spectra of Compounds

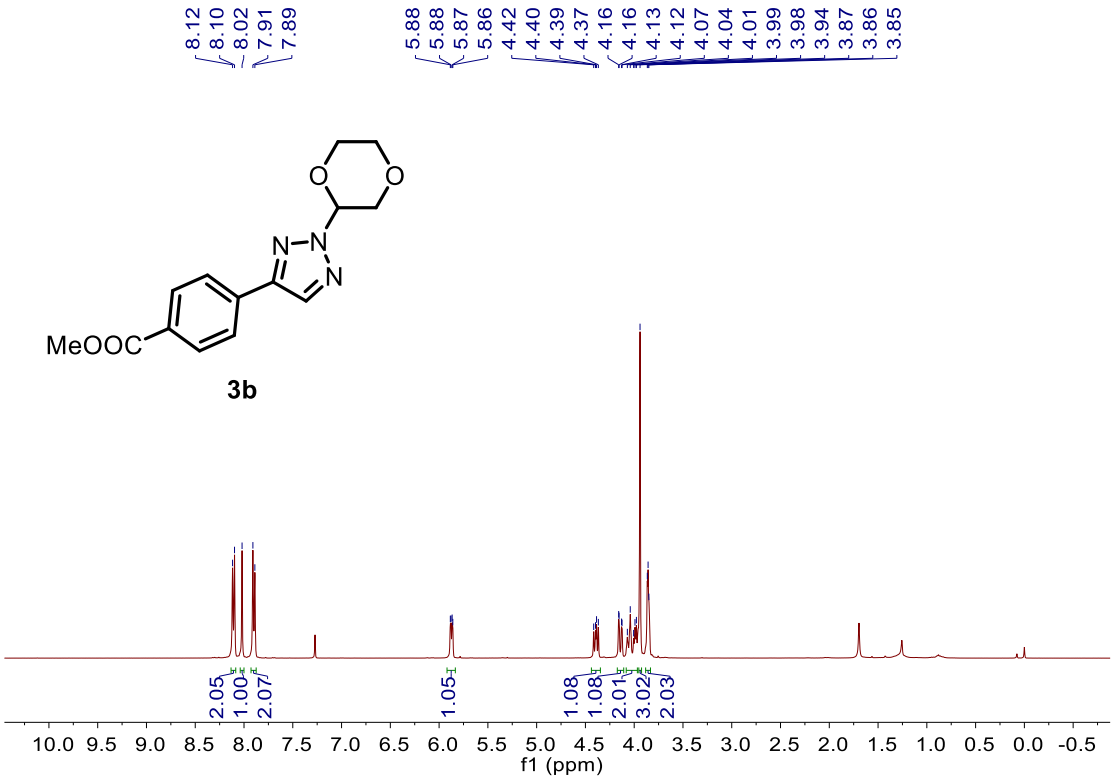


3a





3a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4.01
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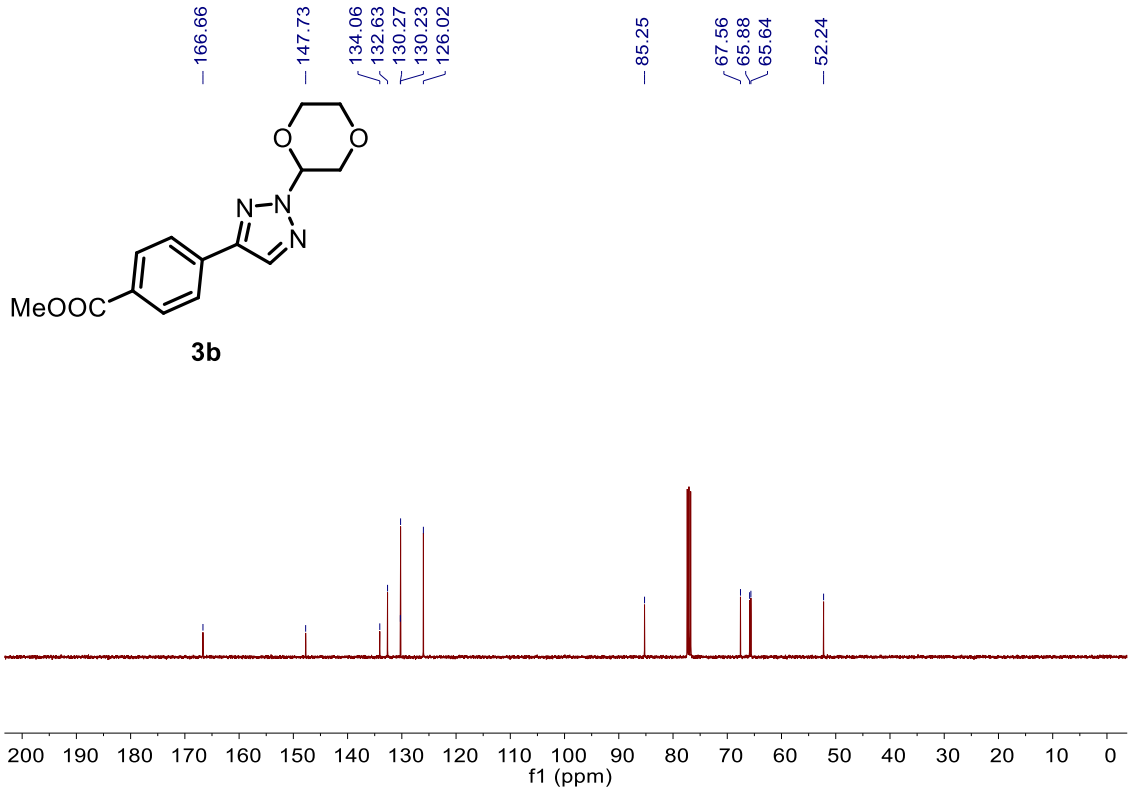
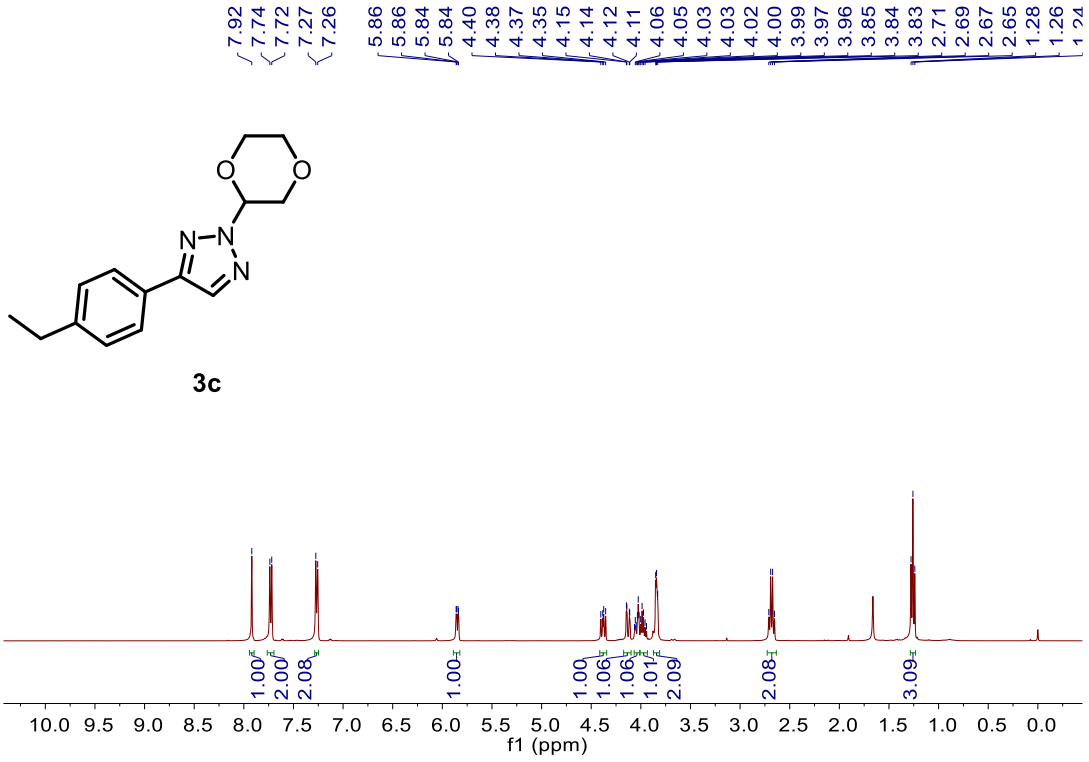
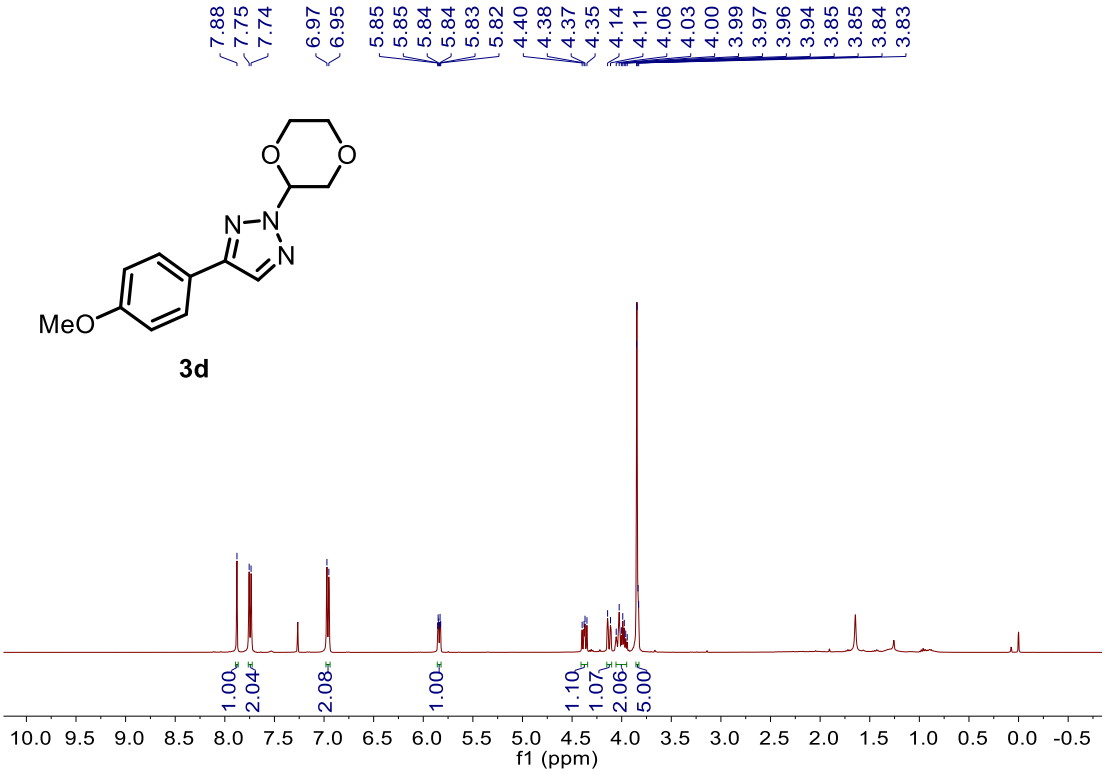
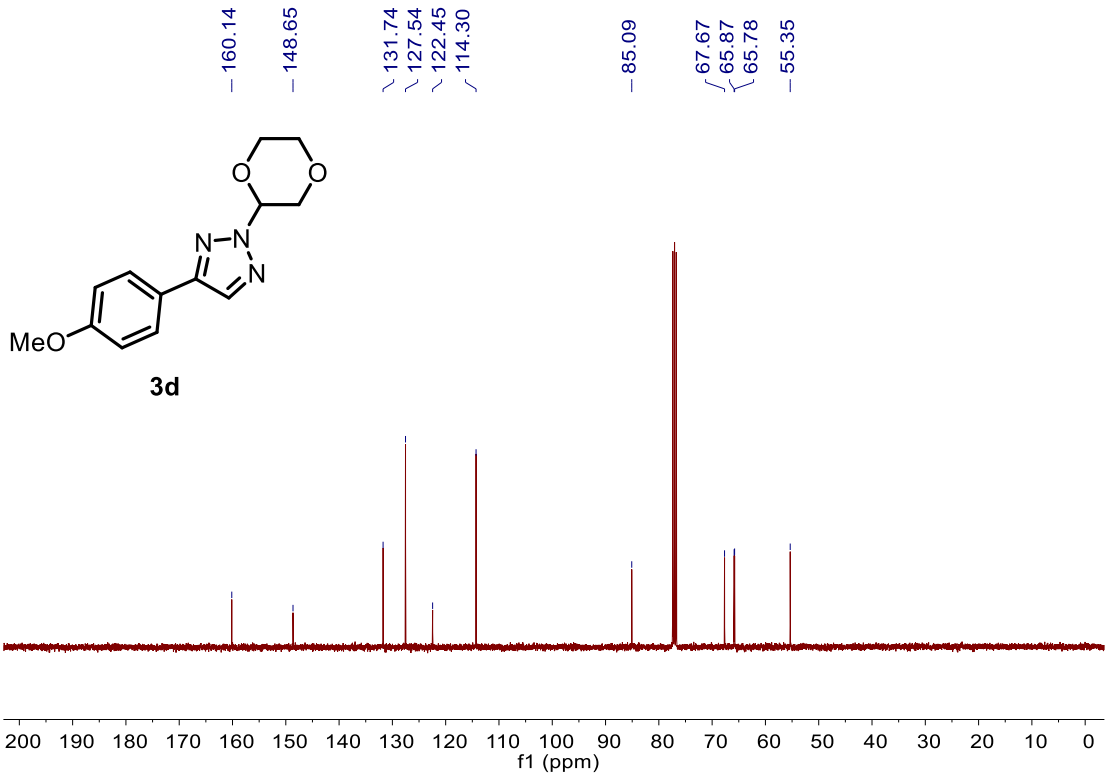
3.98
3.94
3.87
3.86
3.85
MeOOC
3b
2.05
1.00
2.07
1.05
1.08
1.08
2.01
3.02
2.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

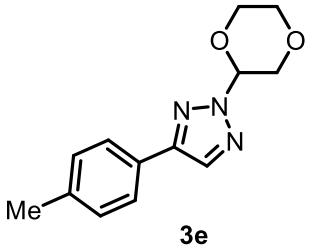

166.66
147.73
134.06
132.63
130.27
130.23
126.02
85.25
67.56
65.88
65.64
52.24
MeOOC
3b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.92
7.74
7.72
7.27
7.26
5.86
5.86
5.84
5.84
4.40
4.38
4.37
4.35
4.15
4.14
4.12
4.11
4.06
4.05
4.03
4.03
4.02
4.00
3.99
3.97
3.96
3.85
3.84
3.83
2.71
2.69
2.67
2.65
1.28
1.26
O
O
N
N
N
3c
1.00
2.00
2.08
1.00
1.00
1.06
1.06
1.01
2.09
2.08
3.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
148.86
145.19
132.08
128.40
127.20
126.20
85.12
67.67
65.87
65.76
28.72
15.48
O
O
N
N
N
3c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

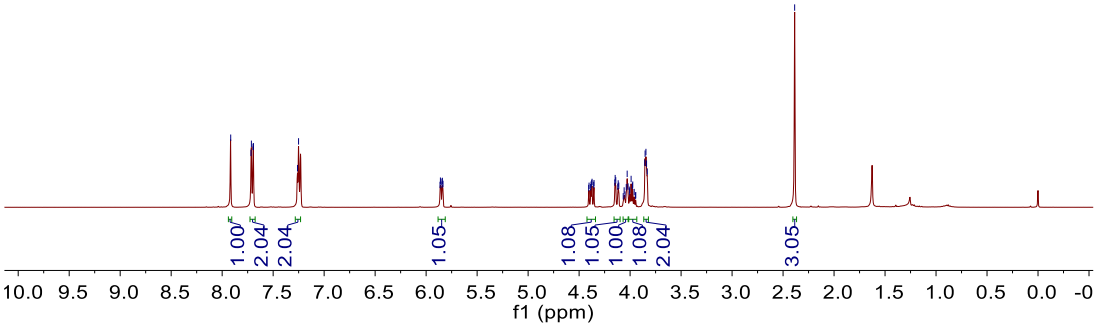

7.88
7.75
7.74
6.97
6.95
5.85
5.85
5.84
5.84
5.83
5.82
4.40
4.38
4.37
4.35
4.14
4.11
4.06
4.03
4.00
3.99
3.97
3.96
3.94
3.85
3.85
3.84
3.83
MeO
3d
1.00
2.04
2.08
1.00
1.10
1.07
2.06
5.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


160.14
148.65
131.74
127.54
122.45
114.30
85.09
67.67
65.87
65.78
55.35
MeO
3d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

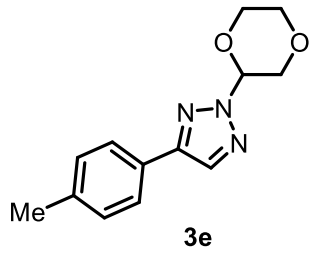

7.92
7.72
7.71
7.70
7.69
7.26
7.25
5.86
5.86
5.85
5.84
5.84
5.83
4.41
4.40
4.39
4.38
4.38
4.37
4.36
4.35
4.15
4.15
4.14
4.12
4.12
4.11
4.06
4.05
4.04
4.03
4.02
4.01
4.00
3.99
3.98
3.97
3.96
3.94
3.86
3.85
3.84
3.83
2.39


O
O
N
N
N
Me

3e

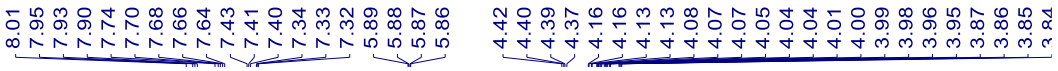

1.00
2.04
2.04
1.05
1.08
1.05
1.00
1.08
2.04
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)


148.85
138.84
132.05
129.59
126.95
126.10
85.12
67.67
65.88
65.77
21.36


O
O
N
N
N
Me

3e

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


8.01
7.95
7.93
7.90
7.74
7.70
7.68
7.66
7.64
7.43
7.41
7.40
7.34
7.33
7.32
5.89
5.88
5.87
5.86
4.42
4.40
4.39
4.37
4.16
4.13
4.13
4.08
4.07
4.07
4.05
4.04
4.04
4.01
4.00
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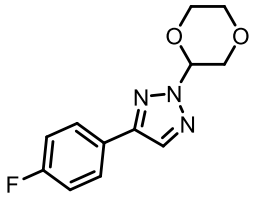
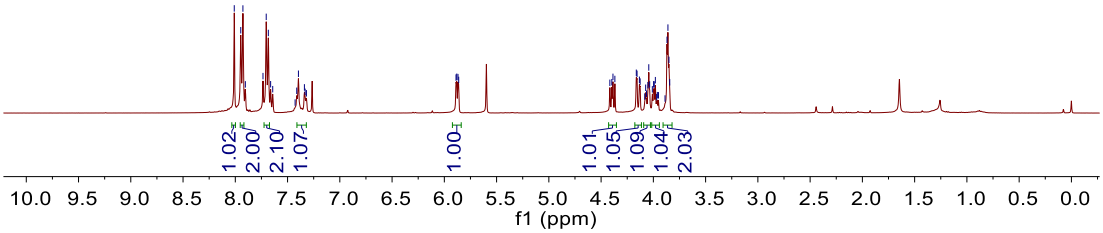
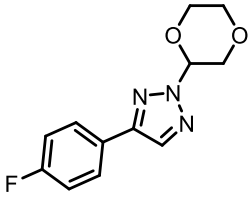
3.98
3.96
3.95
3.87
3.86
3.85


O
O
N
N
N
F

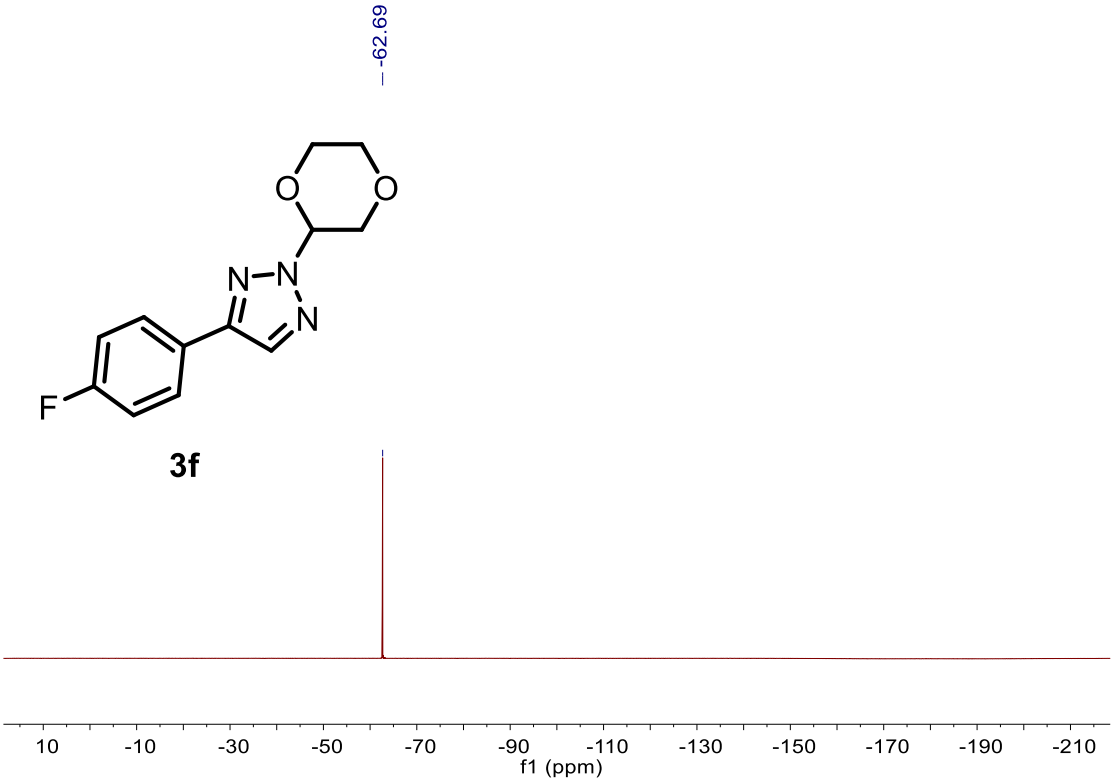
3f


1.02
2.00
2.10
1.07
1.00
1.01
1.05
1.09
1.04
2.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

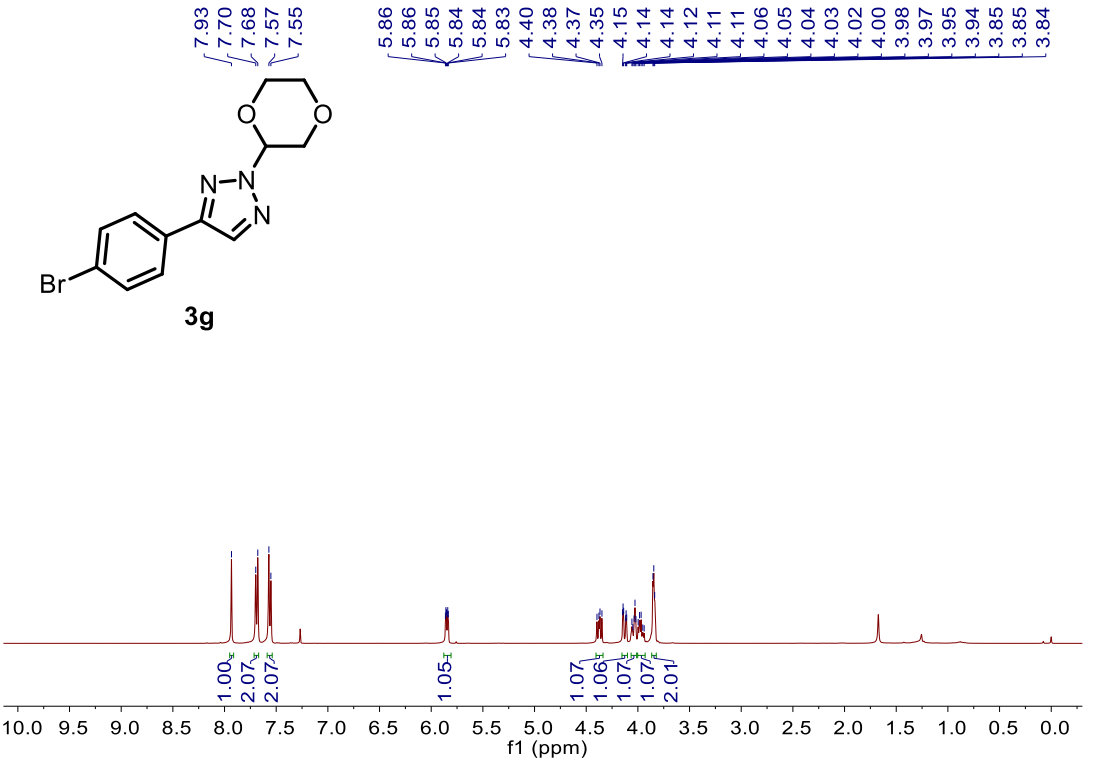

O
O
N
N
N
F

3f

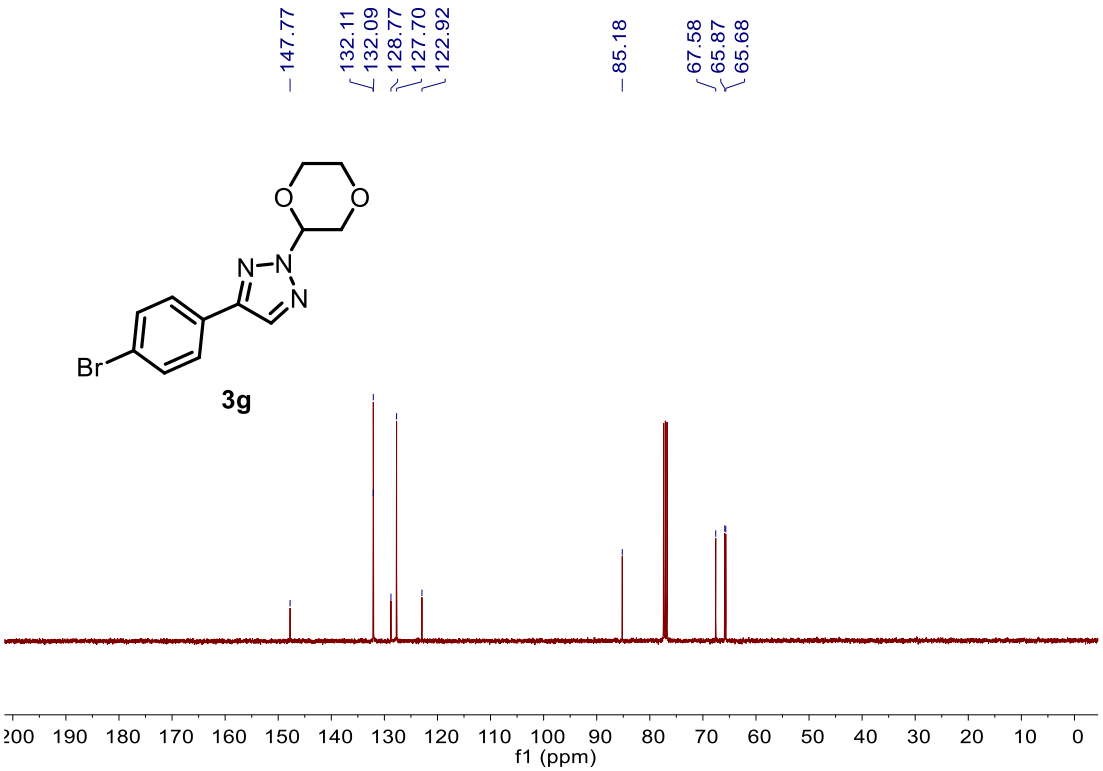
147.40
132.49
129.27
128.98
128.16
126.39
125.92
125.89
125.84
125.83
85.27
67.56
65.88
65.65
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

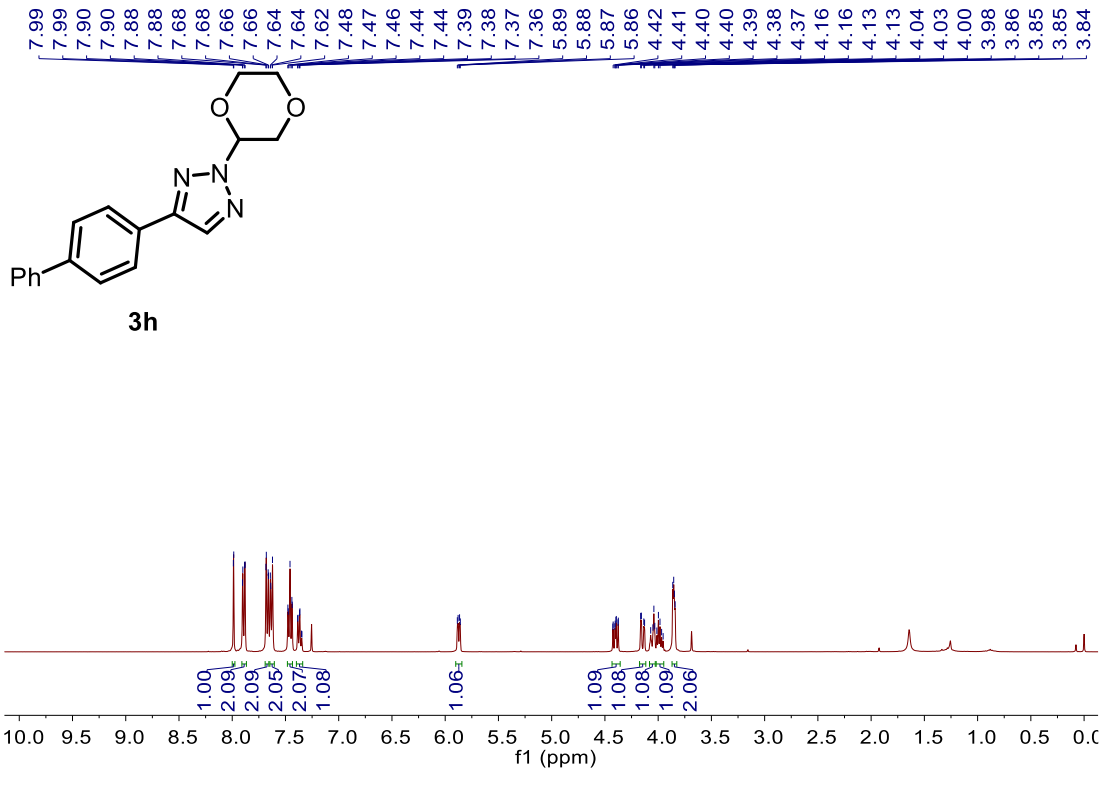

-62.69
F
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

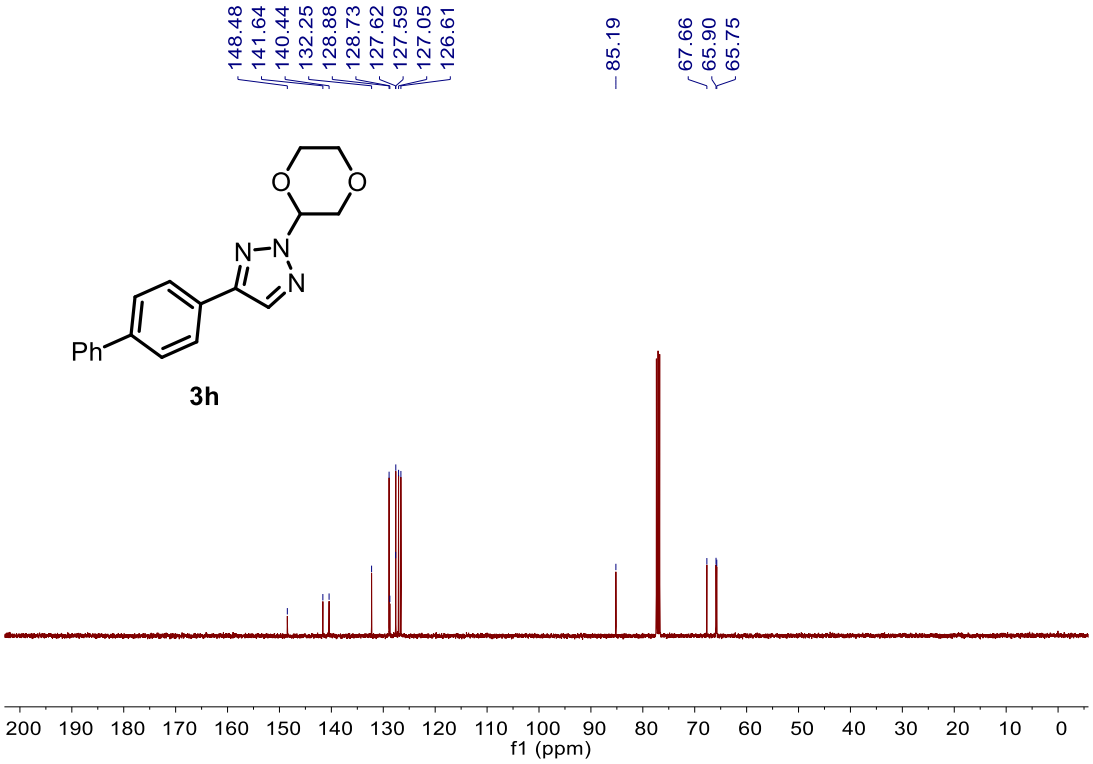
3f


7.93
7.70
7.68
7.57
7.55
5.86
5.86
5.85
5.84
5.84
5.83
4.40
4.38
4.37
4.35
4.15
4.14
4.14
4.12
4.11
4.11
4.06
4.05
4.04
4.03
4.02
4.00
3.98
3.97
3.95
3.94
3.85
3.85
3.84
Br
1.00
2.07
2.07
1.05
1.07
1.06
1.07
1.07
2.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

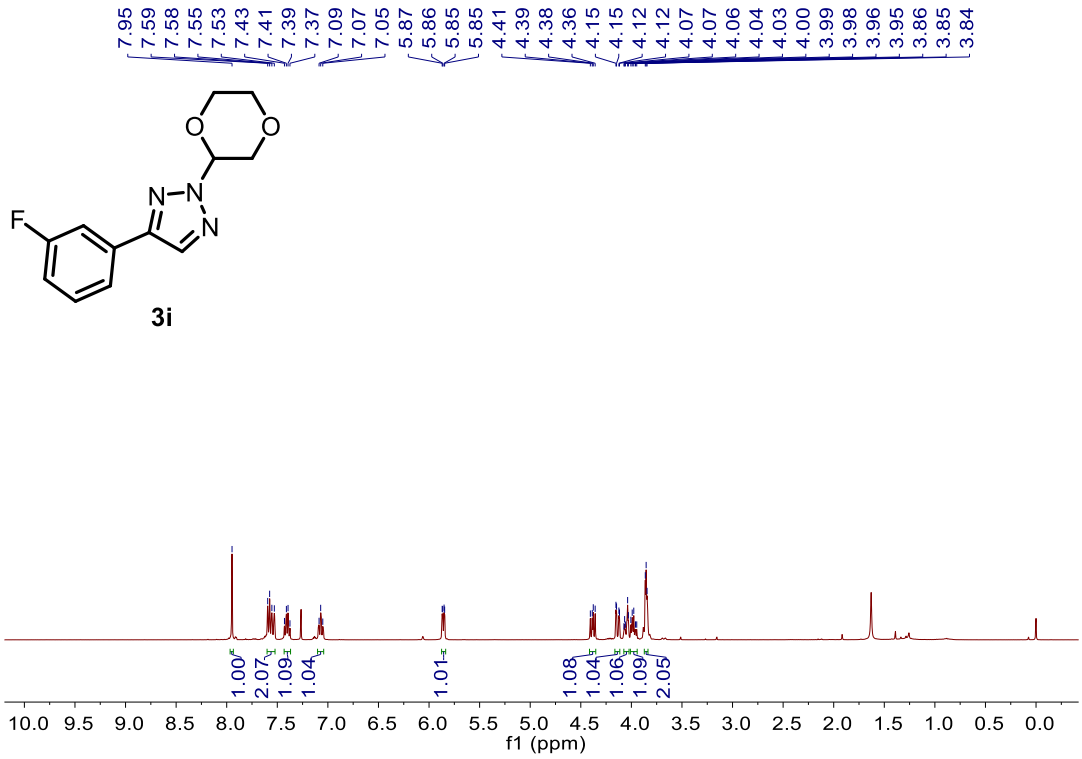
3g


147.77
132.11
132.09
128.77
127.70
122.92
85.18
67.58
65.87
65.68
Br
3g
f1 (ppm)

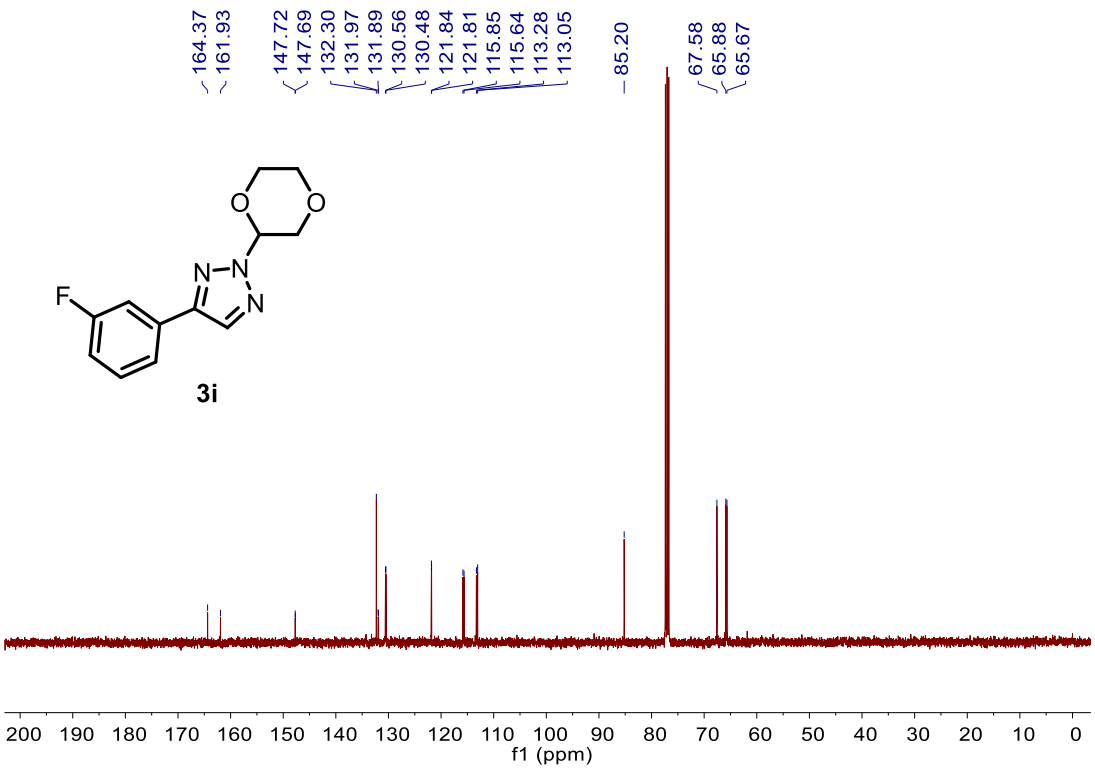

Ph
3h
1.00
2.09
2.09
2.05
2.07
1.08
1.06
1.09
1.08
1.08
1.09
2.06
f1 (ppm)

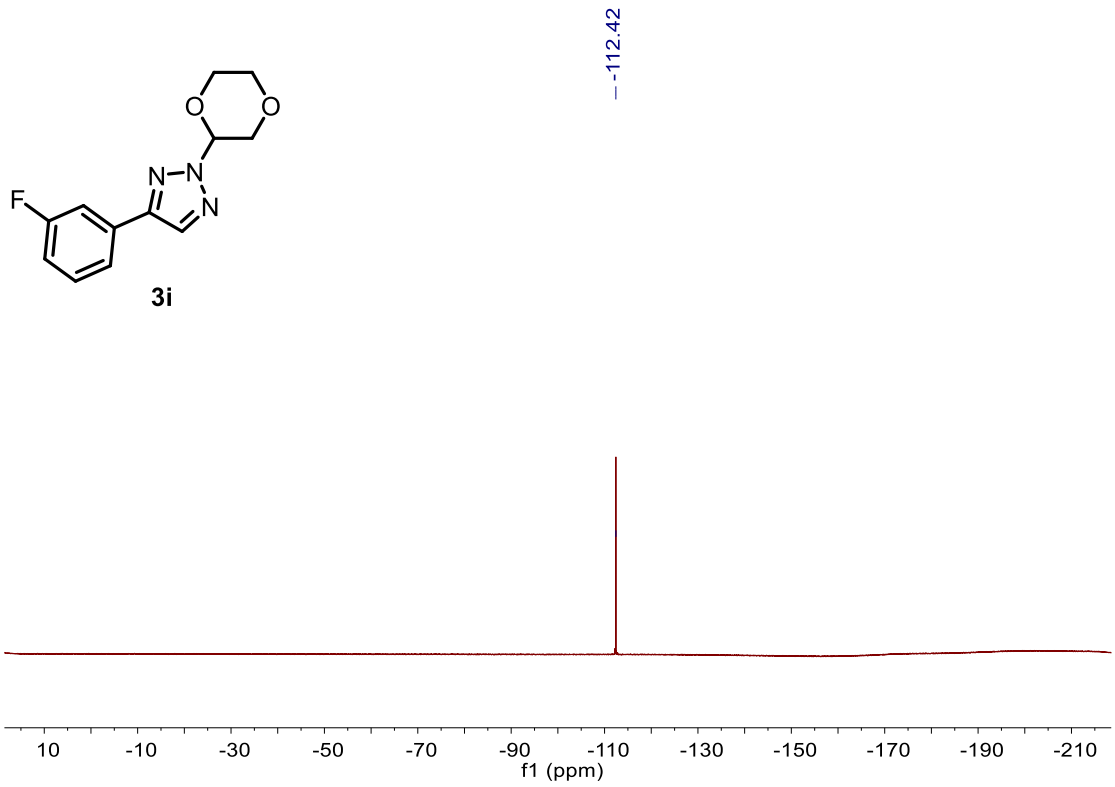

148.48
141.64
140.44
132.25
128.88
128.73
127.62
127.59
127.05
126.61
85.19
67.66
65.90
65.75
O
O
N
N
N
Ph
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

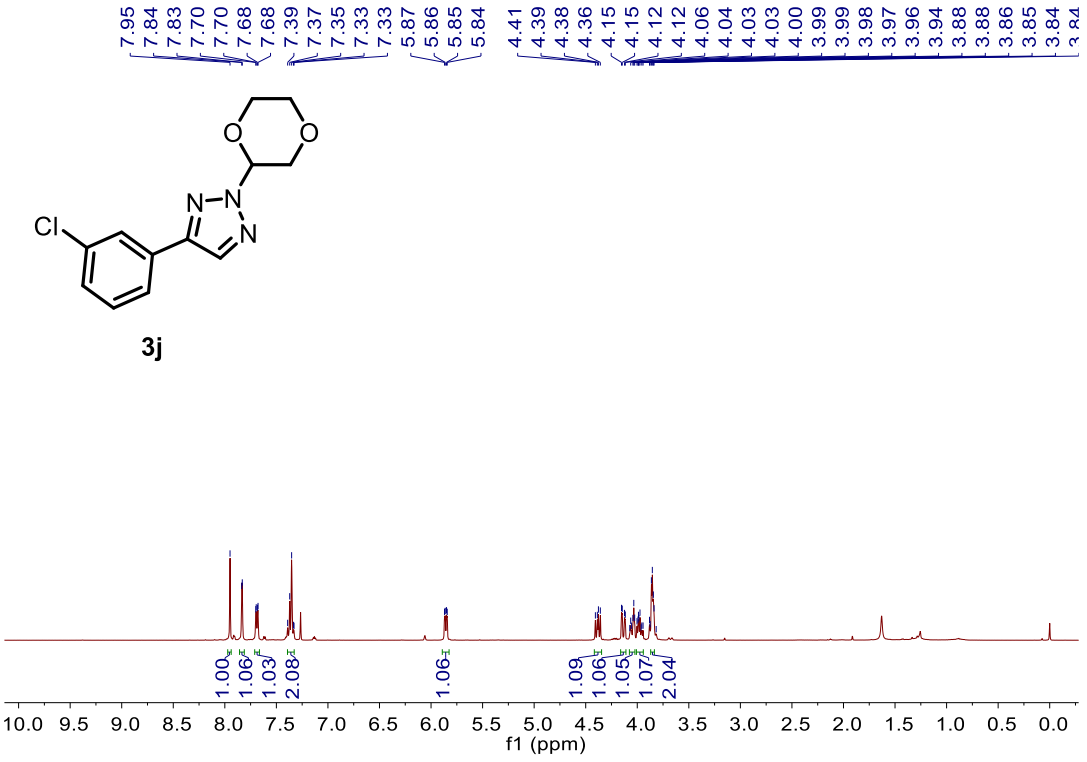
3h

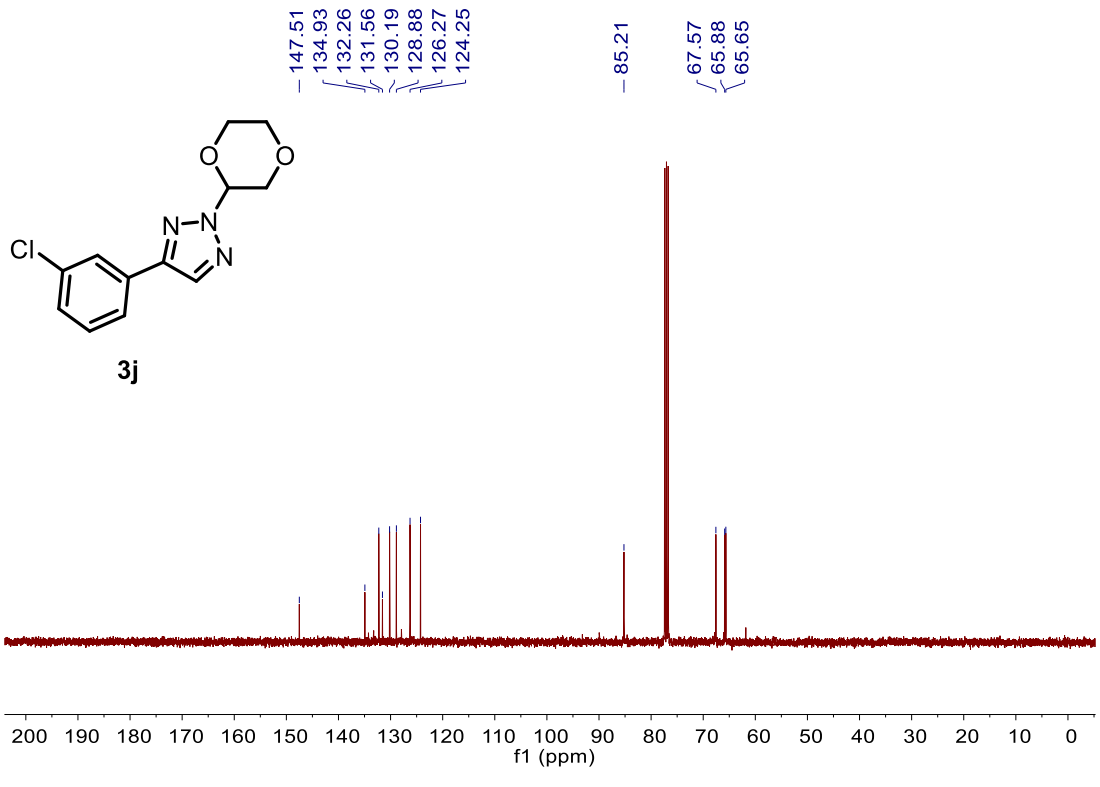

7.95
7.59
7.58
7.55
7.53
7.43
7.41
7.39
7.37
7.09
7.07
7.05
5.87
5.86
5.85
5.85
4.41
4.39
4.38
4.36
4.15
4.15
4.12
4.12
4.07
4.07
4.06
4.04
4.03
4.00
3.99
3.98
3.96
3.95
3.86
3.85
3.84
O
O
N
N
N
F
1.00
2.07
1.09
1.04
1.01
1.08
1.04
1.06
1.09
2.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

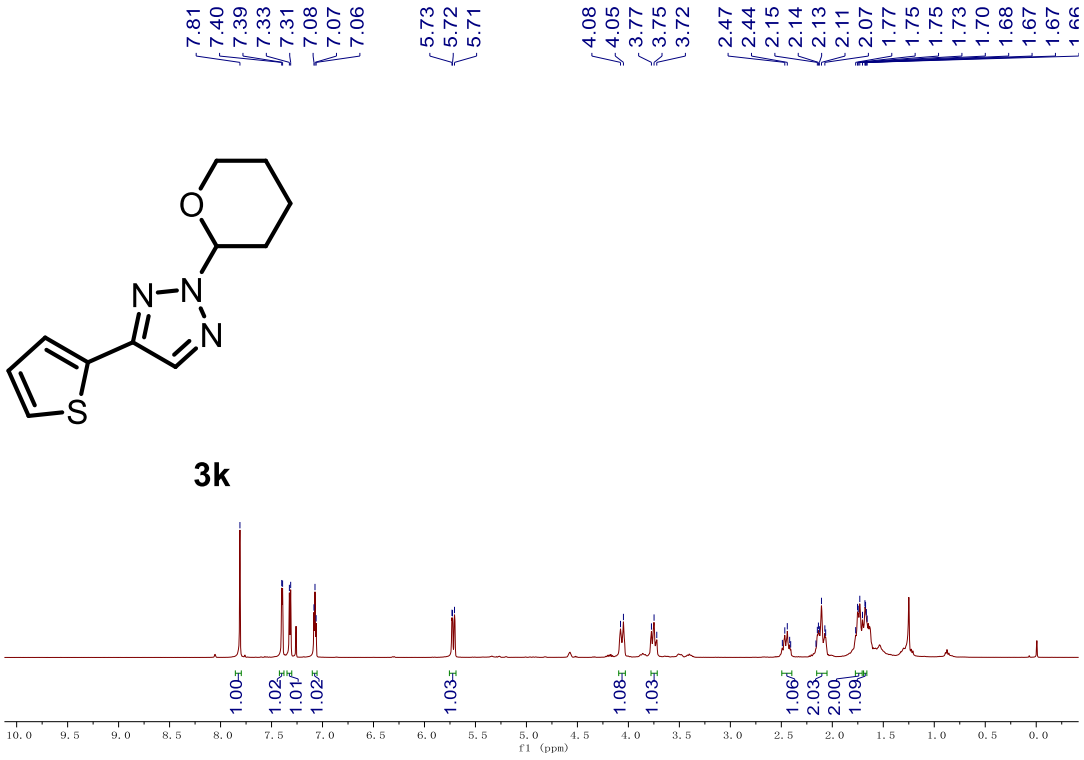
3i

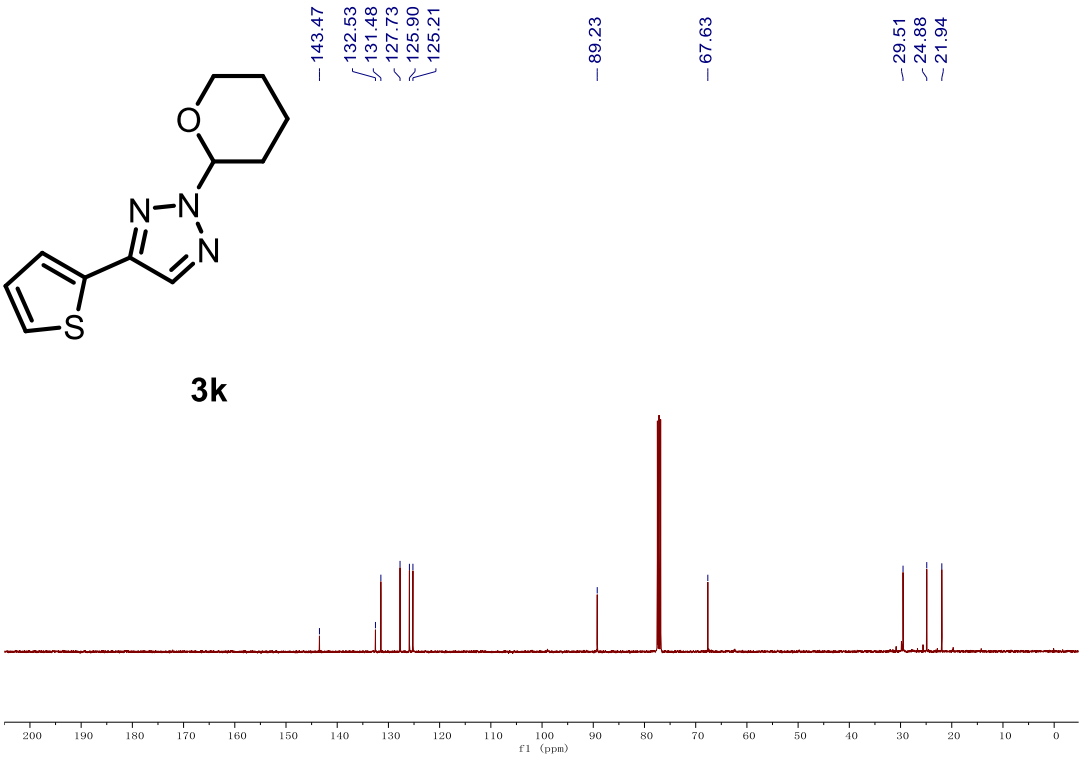

164.37
161.93
147.72
147.69
132.30
131.97
131.89
130.56
130.48
121.84
121.81
115.85
115.64
113.28
113.05
85.20
67.58
65.88
65.67
O
O
N
N
N
F
3i
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

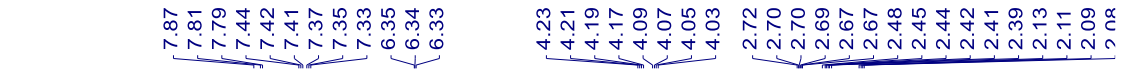

-112.42
O
O
N
N
N
F
3i
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)


7.95
7.84
7.83
7.70
7.70
7.68
7.68
7.39
7.37
7.35
7.33
7.33
5.87
5.86
5.85
5.84
4.41
4.39
4.38
4.36
4.15
4.15
4.12
4.12
4.06
4.04
4.03
4.03
4.00
3.99
3.99
3.98
3.97
3.96
3.94
3.88
3.88
3.86
3.85
3.84
O
O
N
N
N
Cl
3j
1.00
1.06
1.03
2.08
1.06
1.09
1.06
1.05
1.07
2.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


147.51
134.93
132.26
131.56
130.19
128.88
126.27
124.25
85.21
67.57
65.88
65.65
O
O
N
N
N
Cl
3j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.81
7.40
7.39
7.33
7.31
7.08
7.07
7.06
5.73
5.72
5.71
4.08
4.05
3.77
3.75
3.72
2.47
2.44
2.15
2.14
2.13
2.11
2.07
1.77
1.75
1.75
1.73
1.70
1.68
1.67
1.67
O
N
N
N
S
3k
1.00
1.02
1.01
1.02
1.03
1.08
1.03
1.06
2.03
2.00
1.09
f1 (ppm)


143.47
132.53
131.48
127.73
125.90
125.21
89.23
67.63
29.51
24.88
21.94
O
N
N
N
S
3k
f1 (ppm)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7.44
7.42
7.41
7.37
7.35
7.33
6.35
6.34
6.33
4.23
4.21
4.19
4.17
4.09
4.07
4.05
4.03
2.72
2.70
2.70
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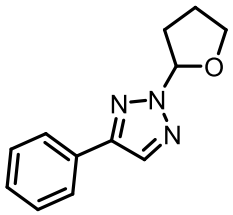
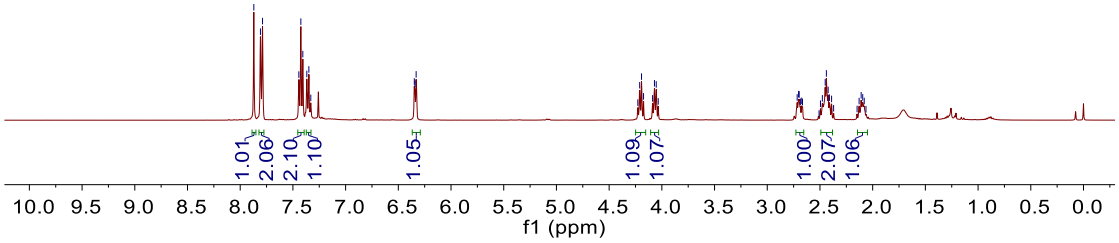
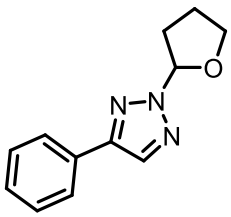
2.42
2.41
2.39
2.13
2.11
2.09



3l

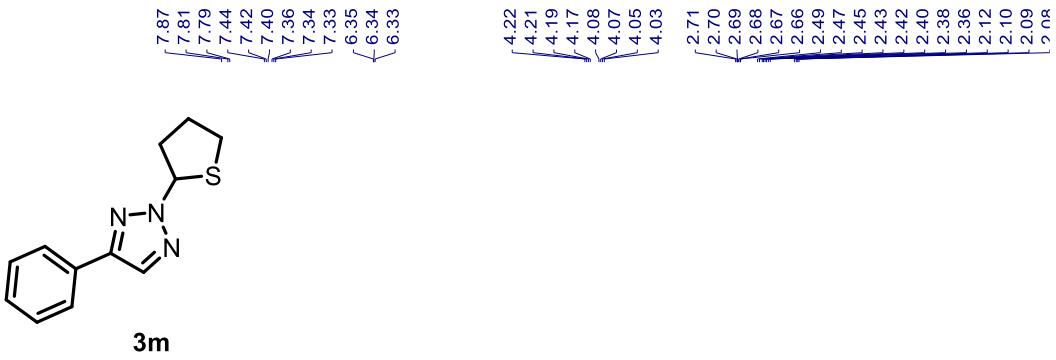

1.01
2.06
2.10
1.10
1.05
1.09
1.07
1.00
2.07
1.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


148.11
131.46
130.35
128.85
128.54
126.06
92.35
69.60
31.38
24.51

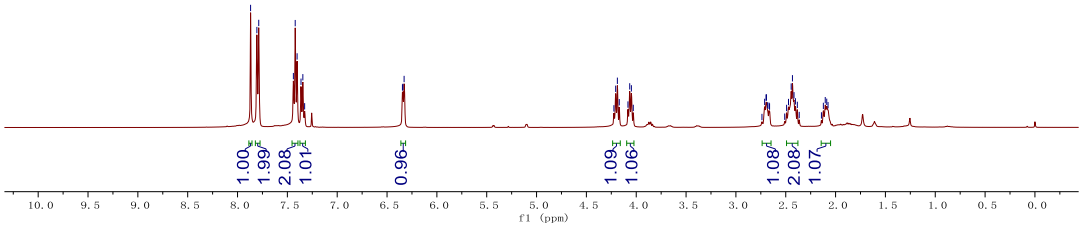


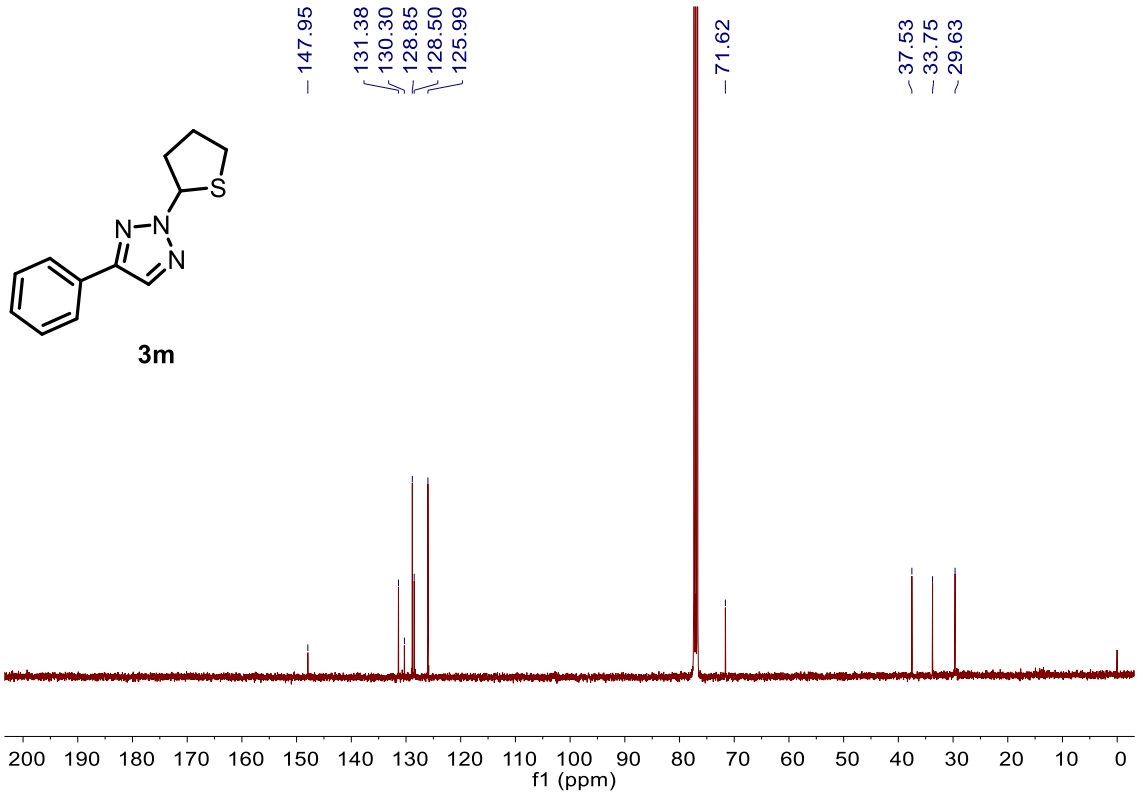
3l

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

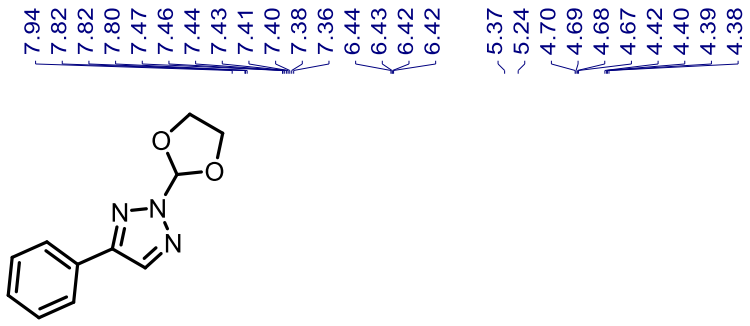

7.87
7.81
7.79
7.44
7.42
7.40
7.36
7.34
7.33
6.35
6.34
6.33
4.22
4.21
4.19
4.17
4.08
4.07
4.05
4.03
2.71
2.70
2.69
2.68
2.67
2.66
2.49
2.47
2.45
2.43
2.42
2.40
2.38
2.36
2.12
2.10
2.09
S
N
N
N

3m

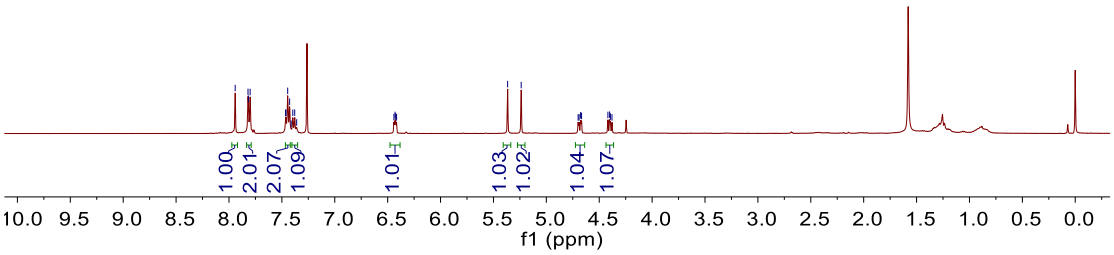

1.00
1.99
2.08
1.01
0.96
1.09
1.06
1.08
2.08
1.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

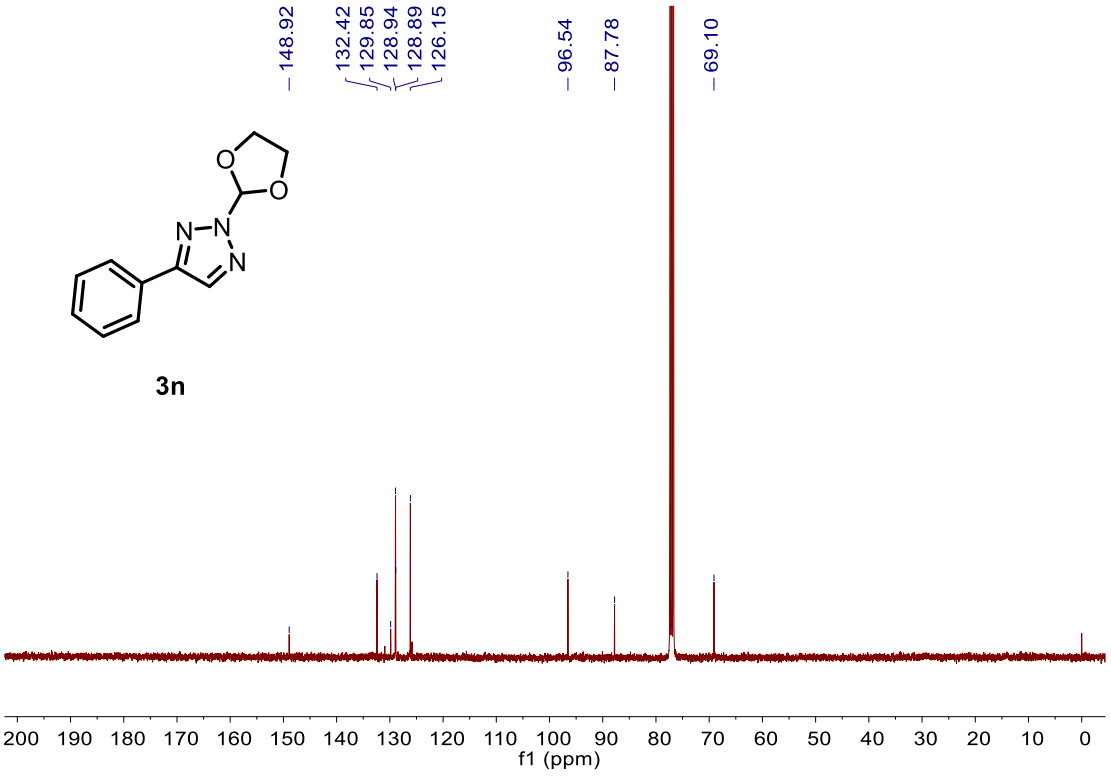

147.95
131.38
130.30
128.85
128.50
125.99
71.62
37.53
33.75
29.63
S
N
N
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3m


7.94
7.82
7.82
7.80
7.47
7.46
7.44
7.43
7.41
7.40
7.38
7.36
6.44
6.43
6.42
6.42
5.37
5.24
4.70
4.69
4.68
4.67
4.42
4.40
4.39
4.38
O
O
N
N
N

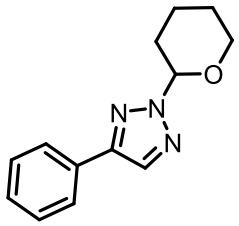
3n


1.00
2.01
2.07
1.09
1.01
1.03
1.02
1.04
1.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

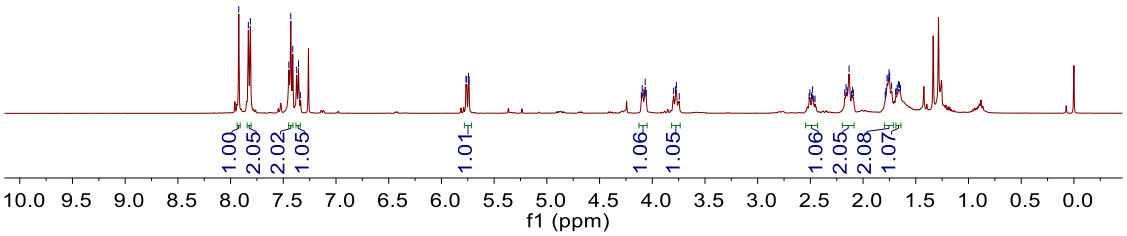

148.92
132.42
129.85
128.94
128.89
126.15
96.54
87.78
69.10
O
O
N
N
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3n

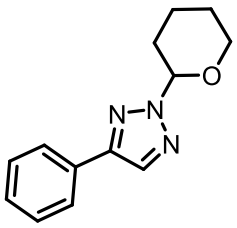

7.92
7.83
7.81
7.45
7.43
7.41
7.37
7.36
7.34
5.77
5.76
5.74
5.74
4.10
4.10
4.09
4.08
4.07
4.06
3.80
3.78
3.77
2.50
2.49
2.48
2.17
2.16
2.15
2.13
2.11
2.10
2.09
1.79
1.78
1.77
1.76
1.75
1.75
1.73
1.69
1.69
1.68
1.67
1.66
1.64



3o


1.00
2.05
2.02
1.05
1.01
1.06
1.05
1.06
2.05
2.08
1.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

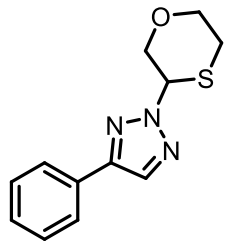

131.64
130.19
128.84
128.62
126.27
126.15
89.17
67.52
29.44
24.82
21.88



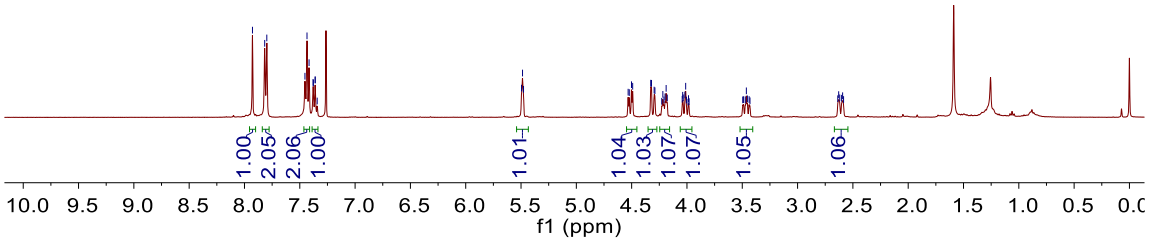
3o

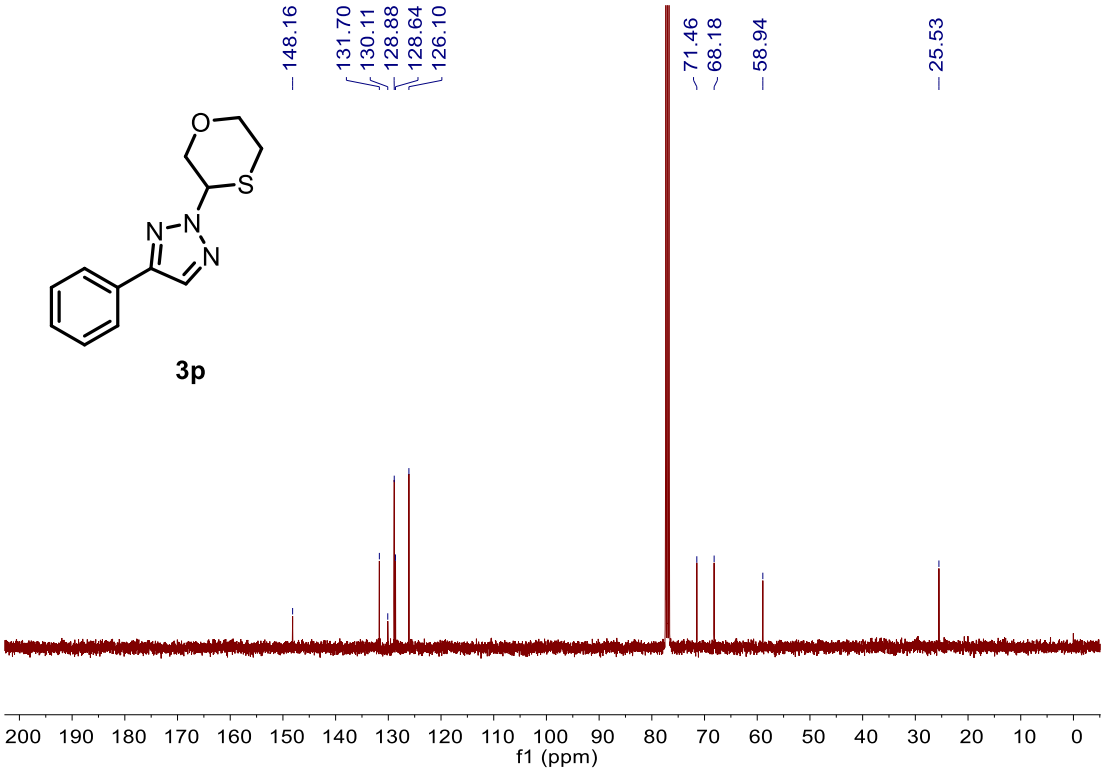
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.93
7.82
7.80
7.45
7.43
7.42
7.38
7.38
7.36
7.36
5.50
5.49
5.48
4.53
4.52
4.50
4.49
4.33
4.32
4.30
4.29
4.22
4.21
4.20
4.19
4.18
4.04
4.04
4.03
4.02
4.01
4.00
3.99
3.50
3.49
3.47
3.46
3.45
3.44
2.64
2.63
2.62
2.60
2.59
2.58

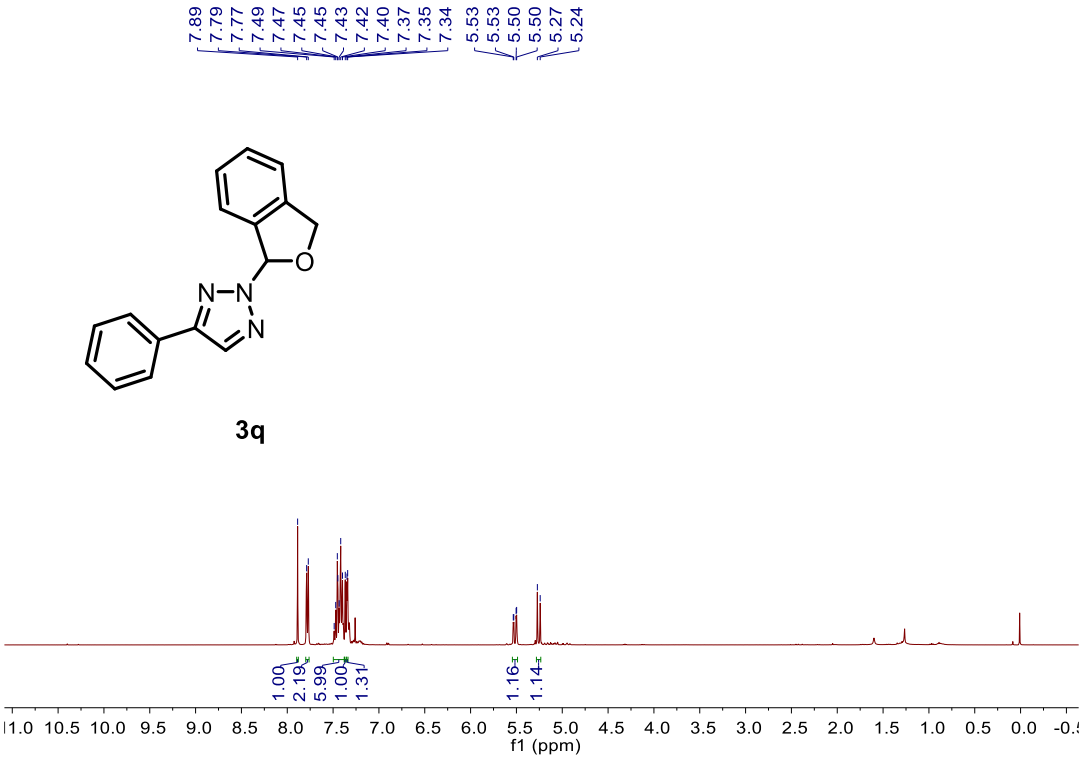


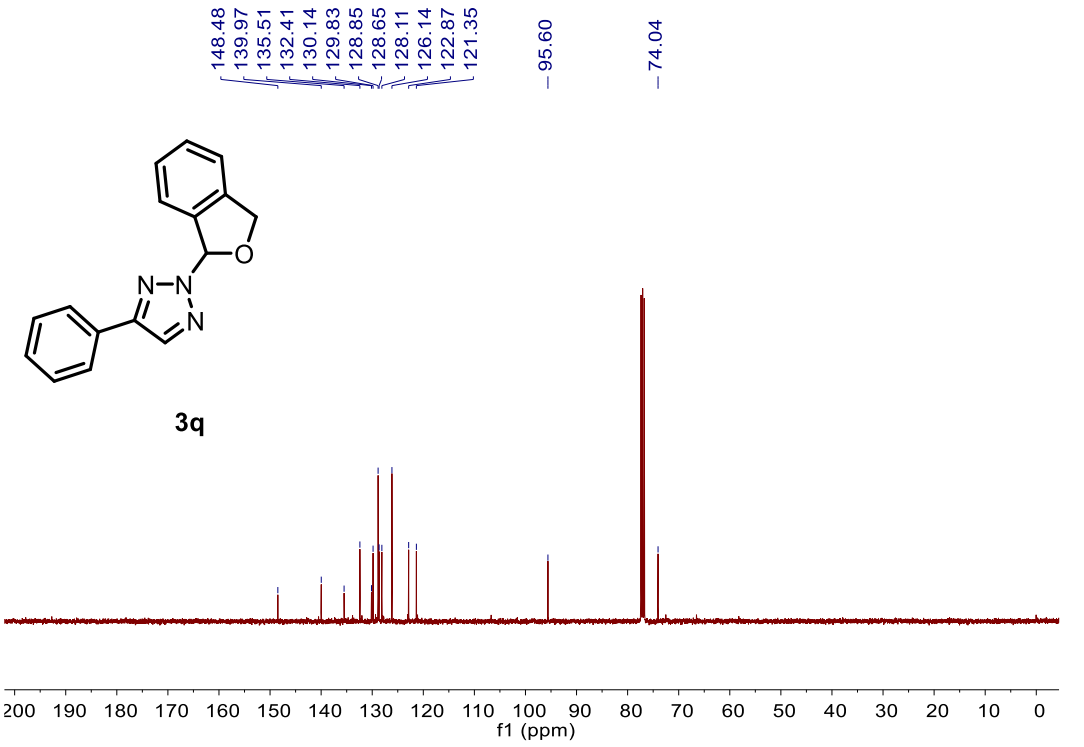
3p


1.00
2.05
2.06
1.00
1.01
1.04
1.03
1.07
1.07
1.05
1.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

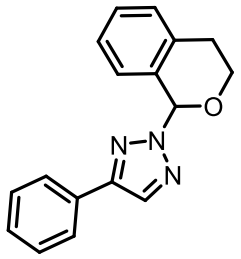

148.16
131.70
130.11
128.88
128.64
126.10
71.46
68.18
58.94
25.53
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3p

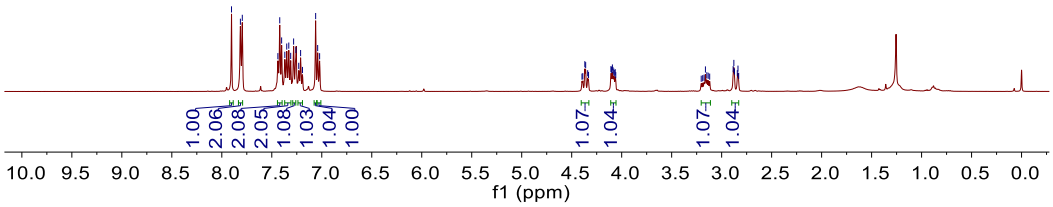

7.89
7.79
7.77
7.49
7.47
7.45
7.45
7.43
7.42
7.40
7.37
7.35
7.34
5.53
5.53
5.50
5.50
5.27
5.24
O
N–N
N
3q
1.00
2.19
5.99
1.00
1.31
1.16
1.14
f1 (ppm)


148.48
139.97
135.51
132.41
130.14
129.83
128.85
128.65
128.11
126.14
122.87
121.35
95.60
74.04
O
N–N
N
3q
f1 (ppm)

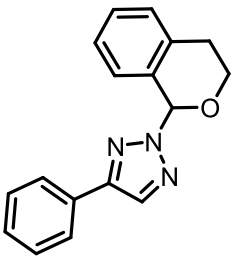

7.90
7.81
7.80
7.44
7.42
7.40
7.37
7.35
7.33
7.31
7.28
7.26
7.23
7.21
7.19
7.06
7.04
7.02
4.40
4.39
4.37
4.36
4.34
4.33
4.11
4.10
4.09
4.09
4.08
4.07
4.06
4.06
3.19
3.18
3.16
3.15
3.13
3.12
2.88
2.88
2.87
2.84
2.84



3r

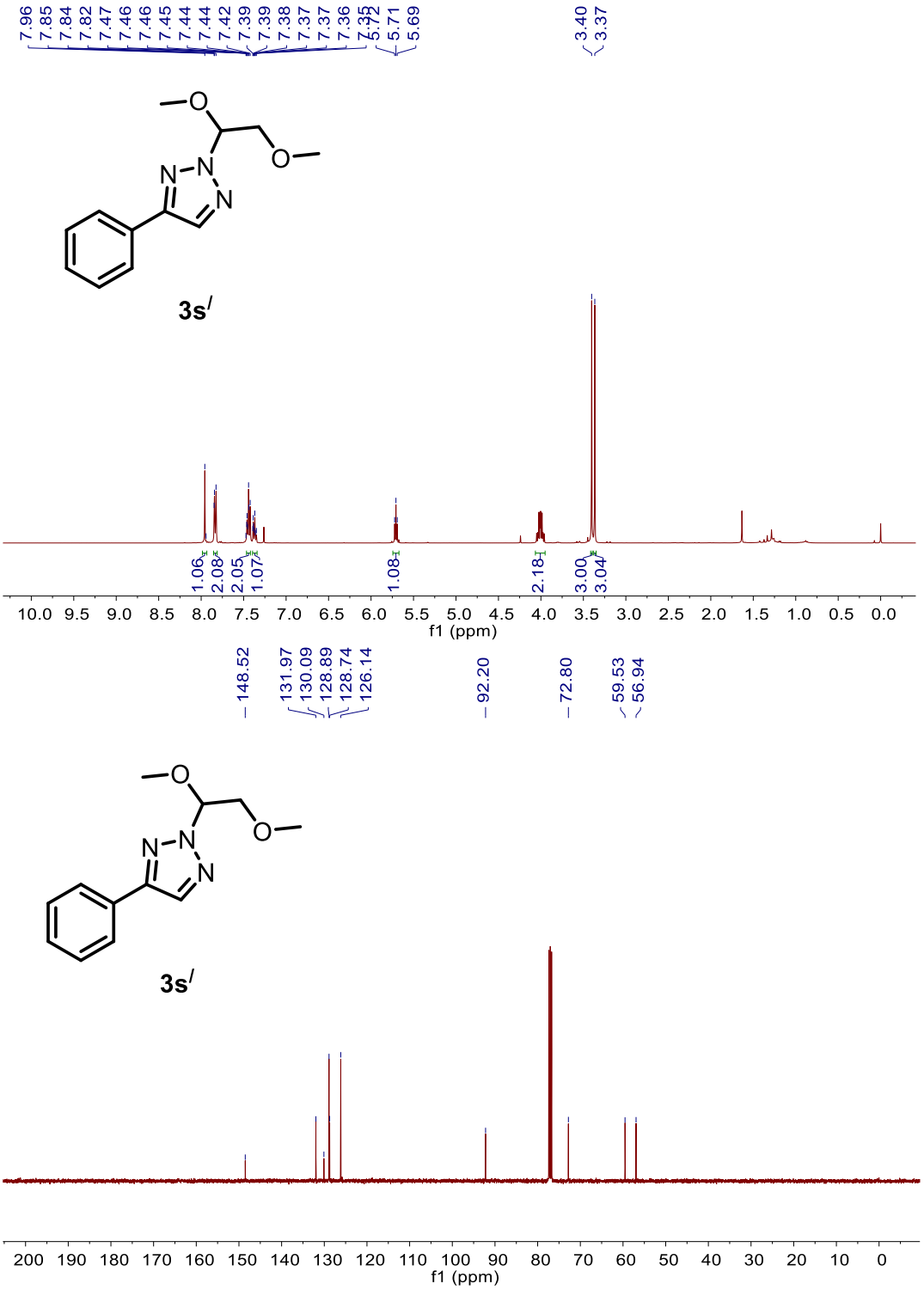

1.00
2.06
2.08
2.05
1.08
1.03
1.04
1.00
1.07
1.04
1.07
1.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

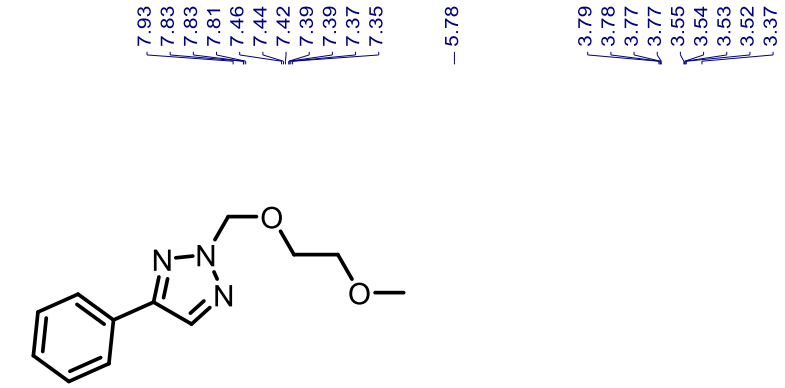

148.41
134.54
131.96
130.65
130.14
128.95
128.86
128.78
128.68
127.03
126.61
126.18
86.69
60.97
27.84



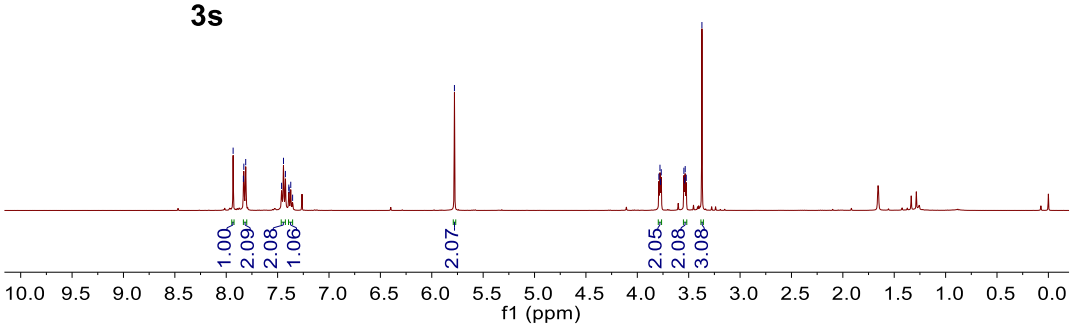
3r

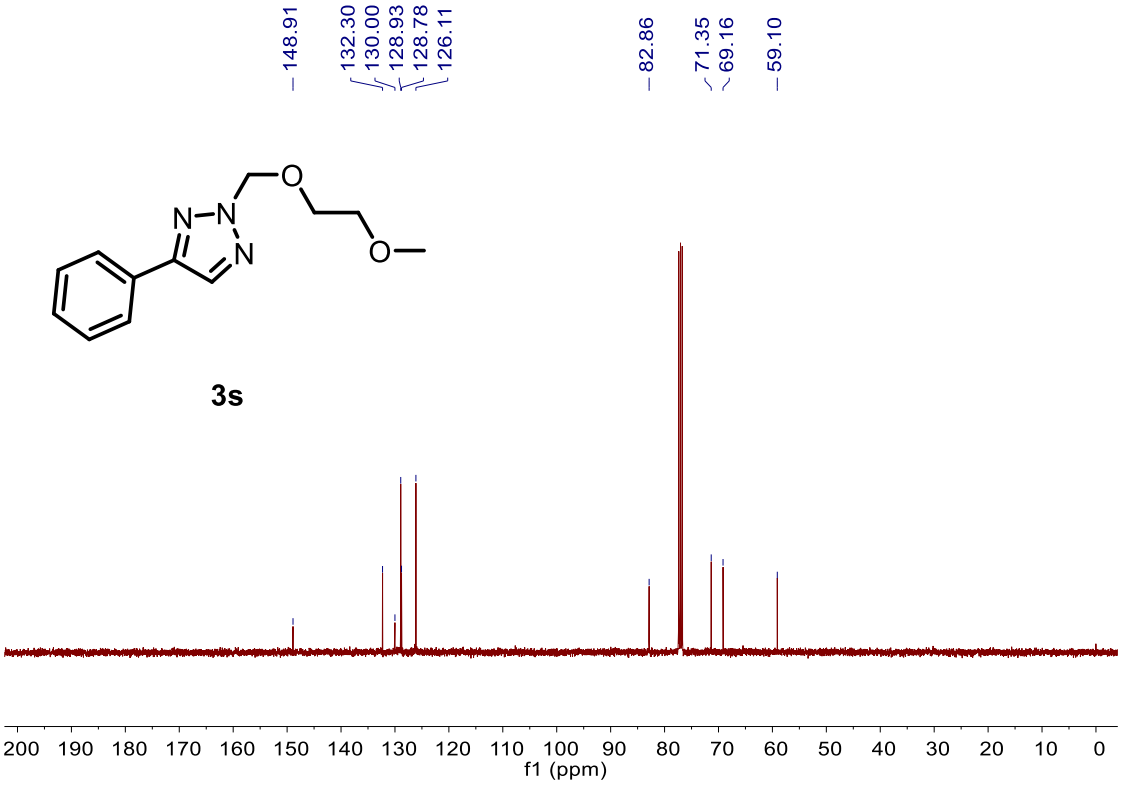
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.96
7.85
7.84
7.82
7.47
7.46
7.46
7.45
7.44
7.44
7.42
7.39
7.39
7.38
7.37
7.37
7.36
7.35
7.32
5.71
5.69
3.40
3.37
O
O
N
N
N
3s/
1.06
2.08
2.05
1.07
1.08
2.18
3.00
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
148.52
131.97
130.09
128.89
128.74
126.14
92.20
72.80
59.53
56.94
O
O
N
N
N
3s/
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.93
7.83
7.83
7.81
7.46
7.44
7.42
7.39
7.39
7.37
7.35
5.78
3.79
3.78
3.77
3.77
3.55
3.54
3.53
3.52
3.37
O
N
N
N
O

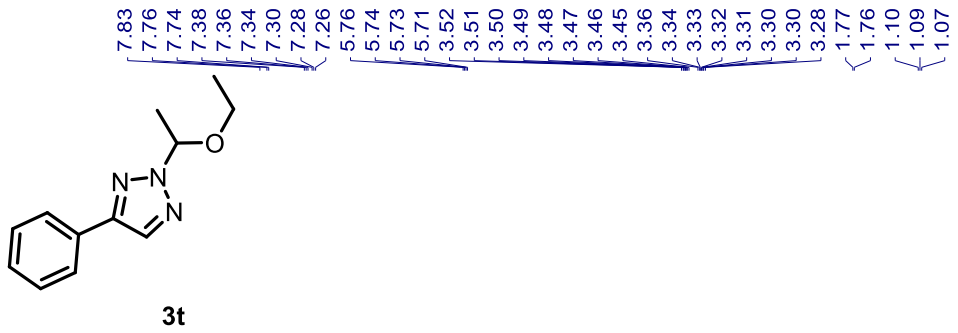
3s


1.00
2.09
2.08
1.06
2.07
2.05
2.08
3.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

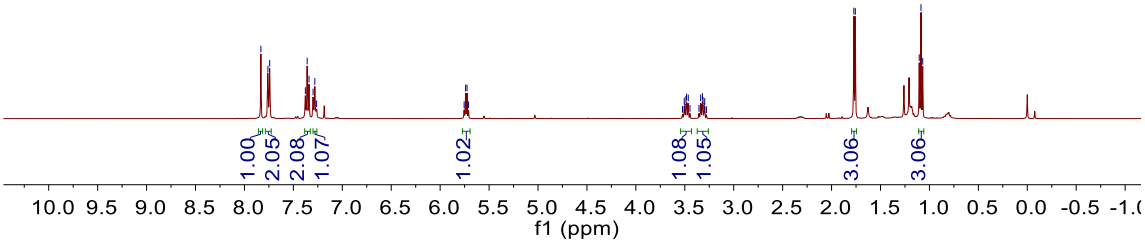

148.91
132.30
130.00
128.93
128.78
126.11
82.86
71.35
69.16
59.10
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

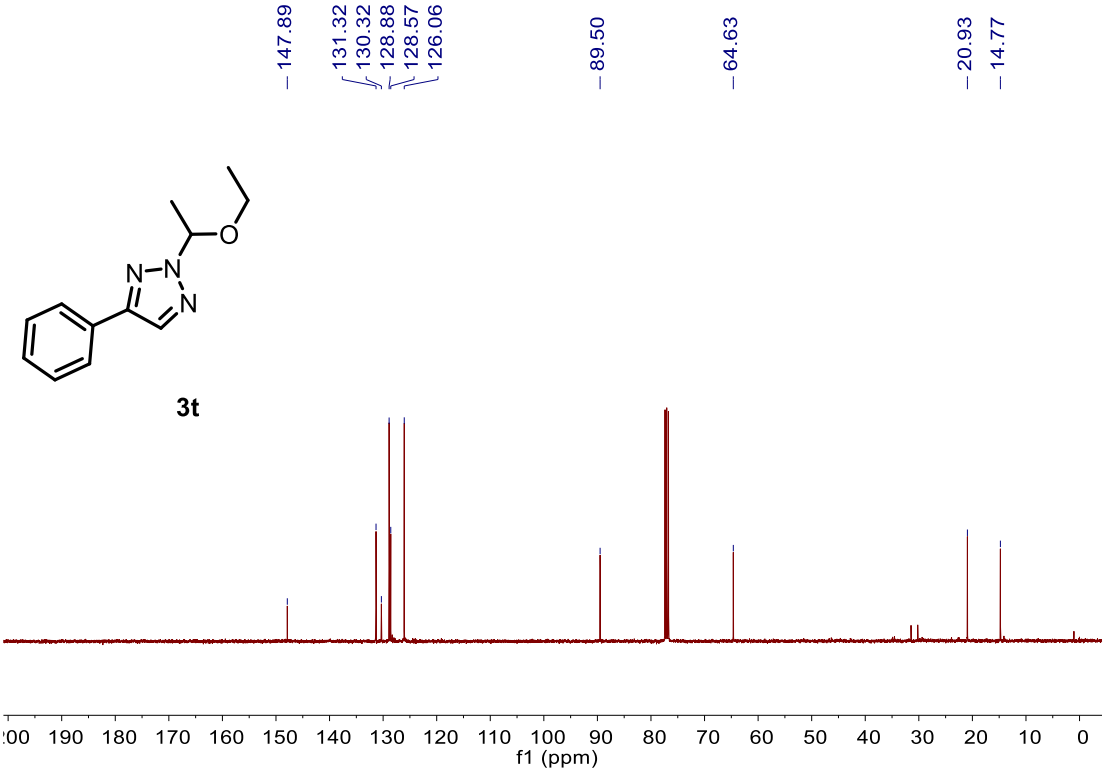
O
N
N
N
O

3s

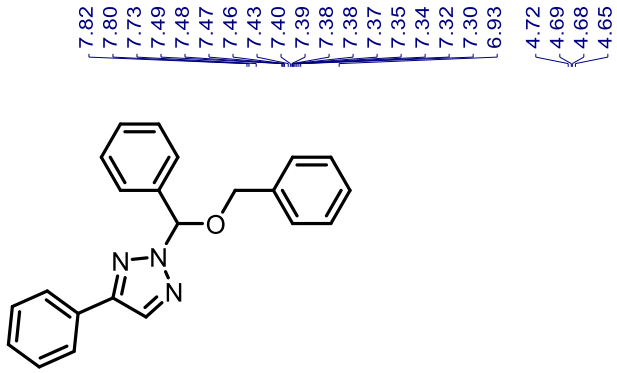

7.83
7.76
7.74
7.38
7.36
7.34
7.30
7.28
7.26
5.76
5.74
5.73
5.71
3.52
3.51
3.50
3.49
3.48
3.47
3.46
3.45
3.36
3.34
3.33
3.32
3.31
3.30
3.30
3.28
1.77
1.76
1.10
1.09
1.07
O
N
N
N

3t

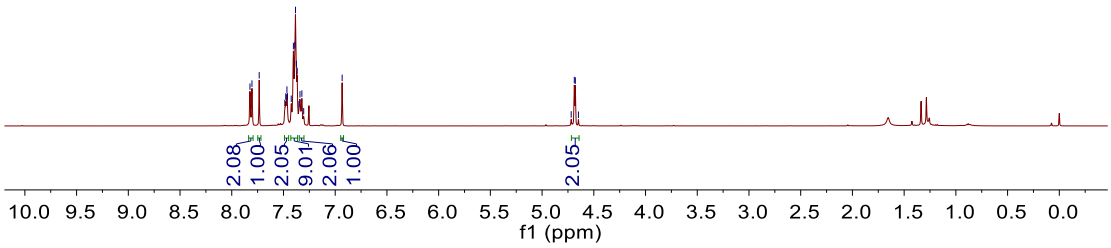

1.00
2.05
2.08
1.07
1.02
1.08
1.05
3.06
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


147.89
131.32
130.32
128.88
128.57
126.06
89.50
64.63
20.93
14.77
O
N
N
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

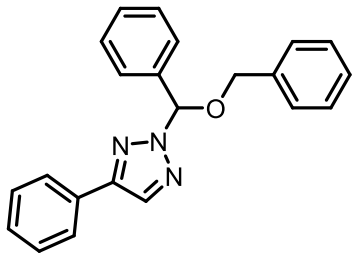
3t


7.82
7.80
7.73
7.49
7.48
7.47
7.46
7.43
7.40
7.39
7.38
7.38
7.37
7.35
7.34
7.32
7.30
6.93
4.72
4.69
4.68
4.65
O
N
N
N

3u

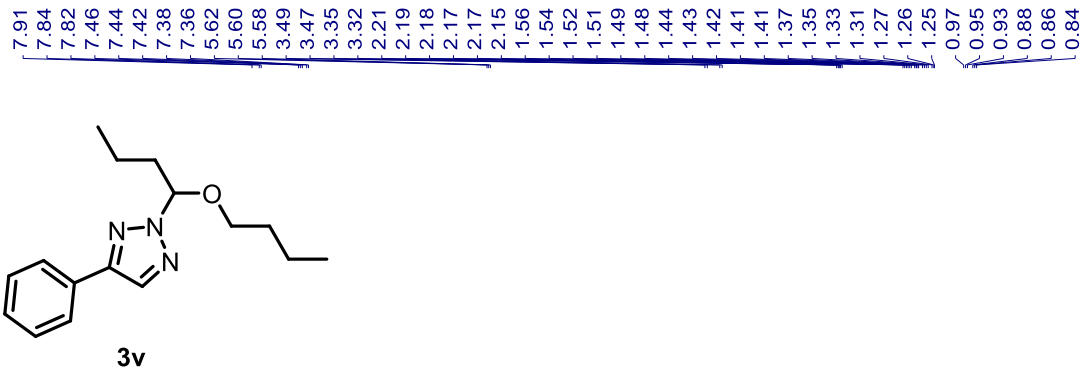

2.08
1.00
2.05
9.01
2.06
1.00
2.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


148.34
136.67
136.43
136.04
132.20
130.34
129.43
128.86
128.66
128.37
128.23
126.59
126.16
125.78
117.34
91.90
88.43
71.06

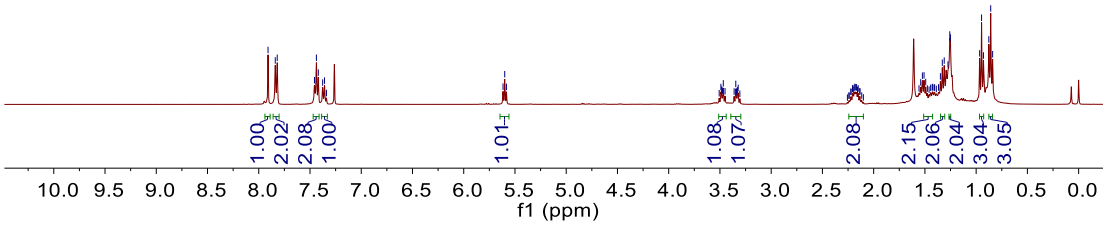

O
N
N
N

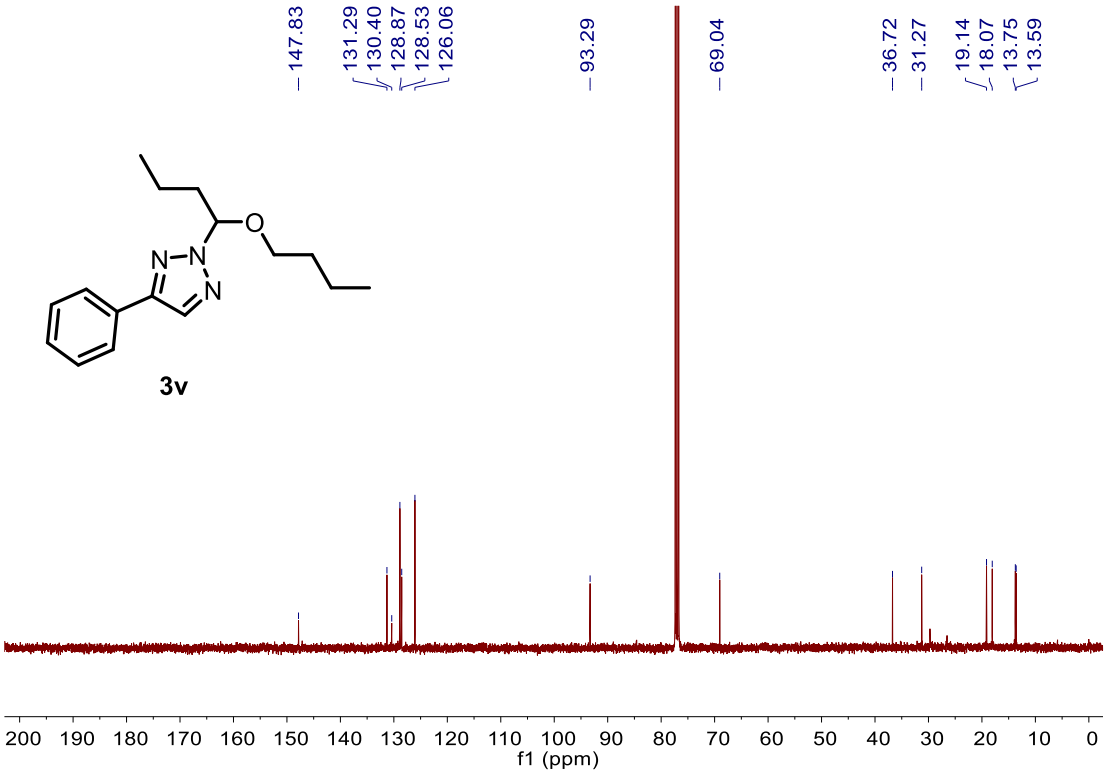
3u

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


7.91
7.84
7.82
7.46
7.44
7.42
7.38
7.36
5.62
5.60
5.58
3.49
3.47
3.35
3.32
2.21
2.19
2.18
2.17
2.17
2.15
1.56
1.54
1.52
1.51
1.49
1.48
1.44
1.43
1.42
1.41
1.41
1.37
1.35
1.33
1.31
1.27
1.26
1.25
0.97
0.95
0.93
0.88
0.86
0.84

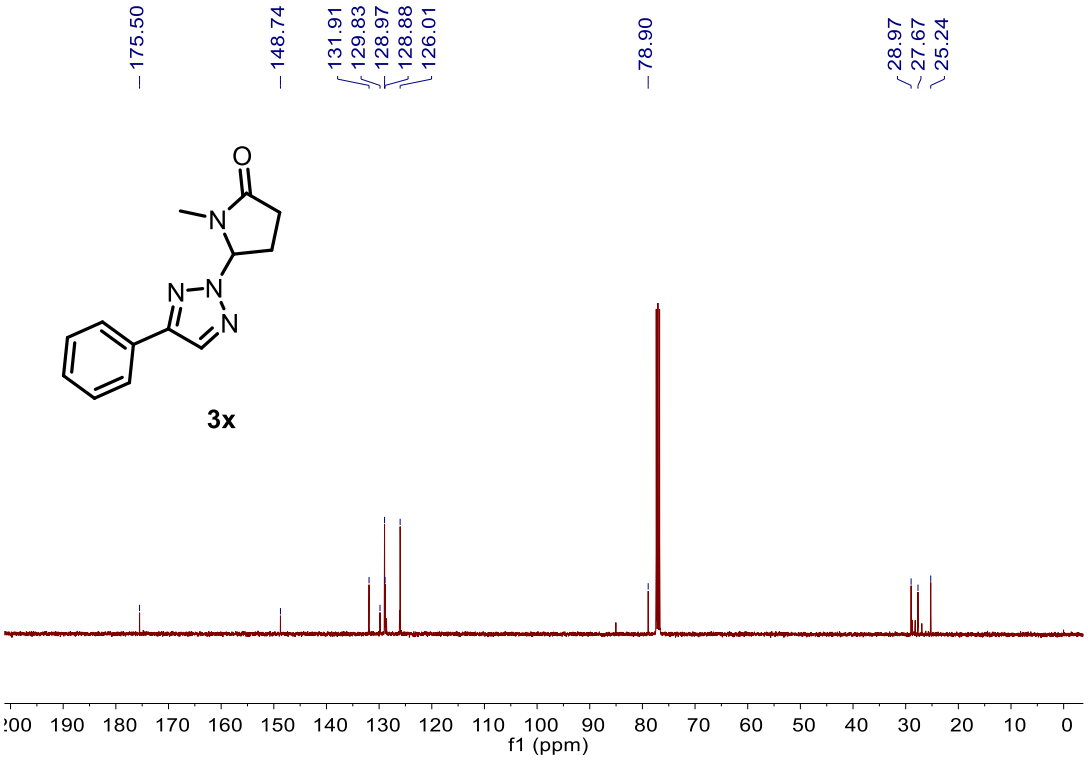
3v

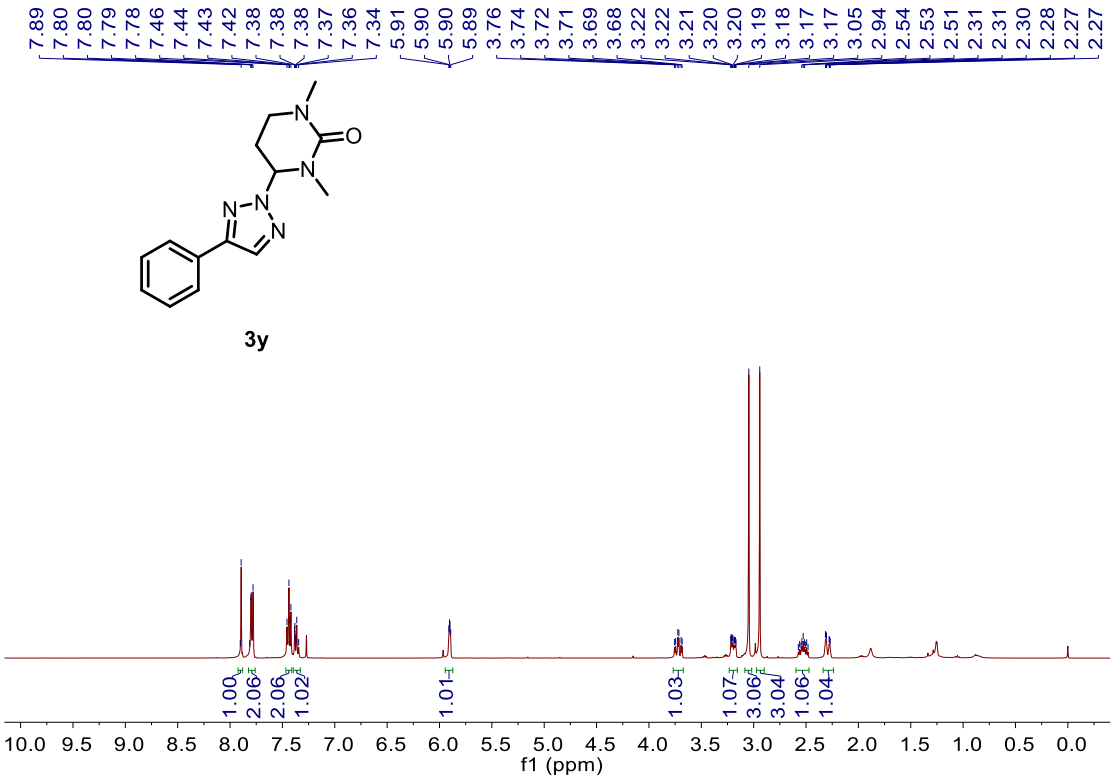

1.00
2.02
2.08
1.00
1.01
1.08
1.07
2.08
2.15
2.06
2.04
3.04
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

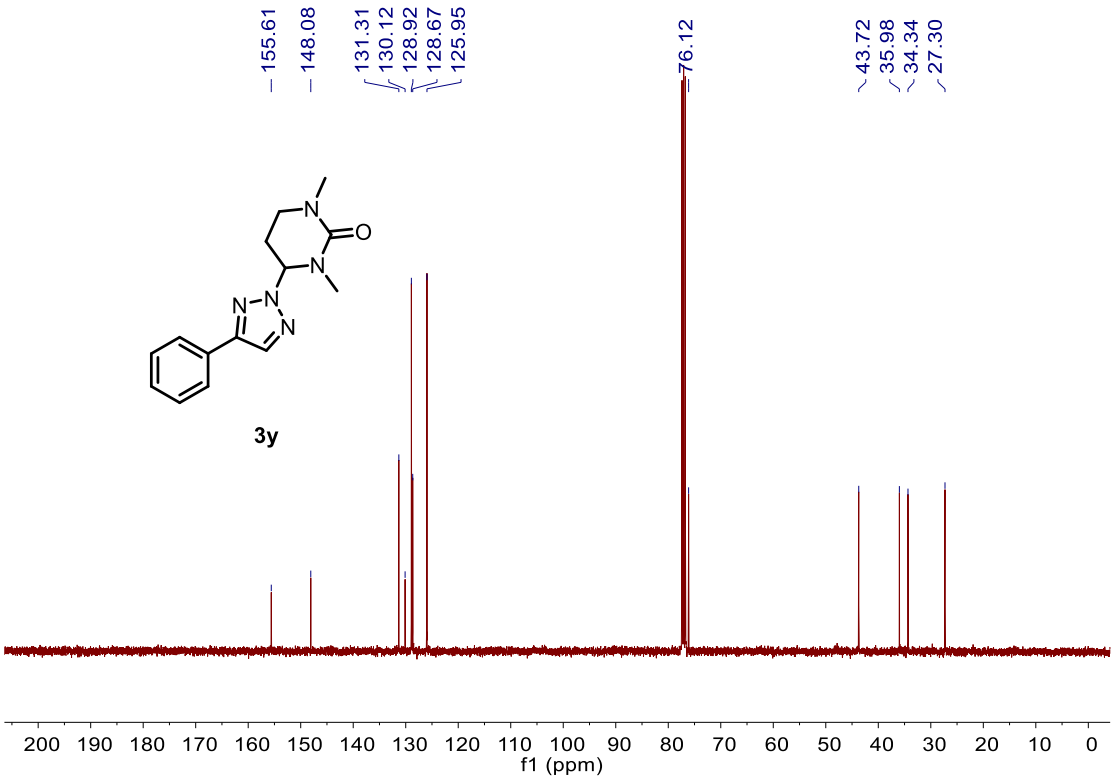

147.83
131.29
130.40
128.87
128.53
126.06
93.29
69.04
36.72
31.27
19.14
18.07
13.75
13.59
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

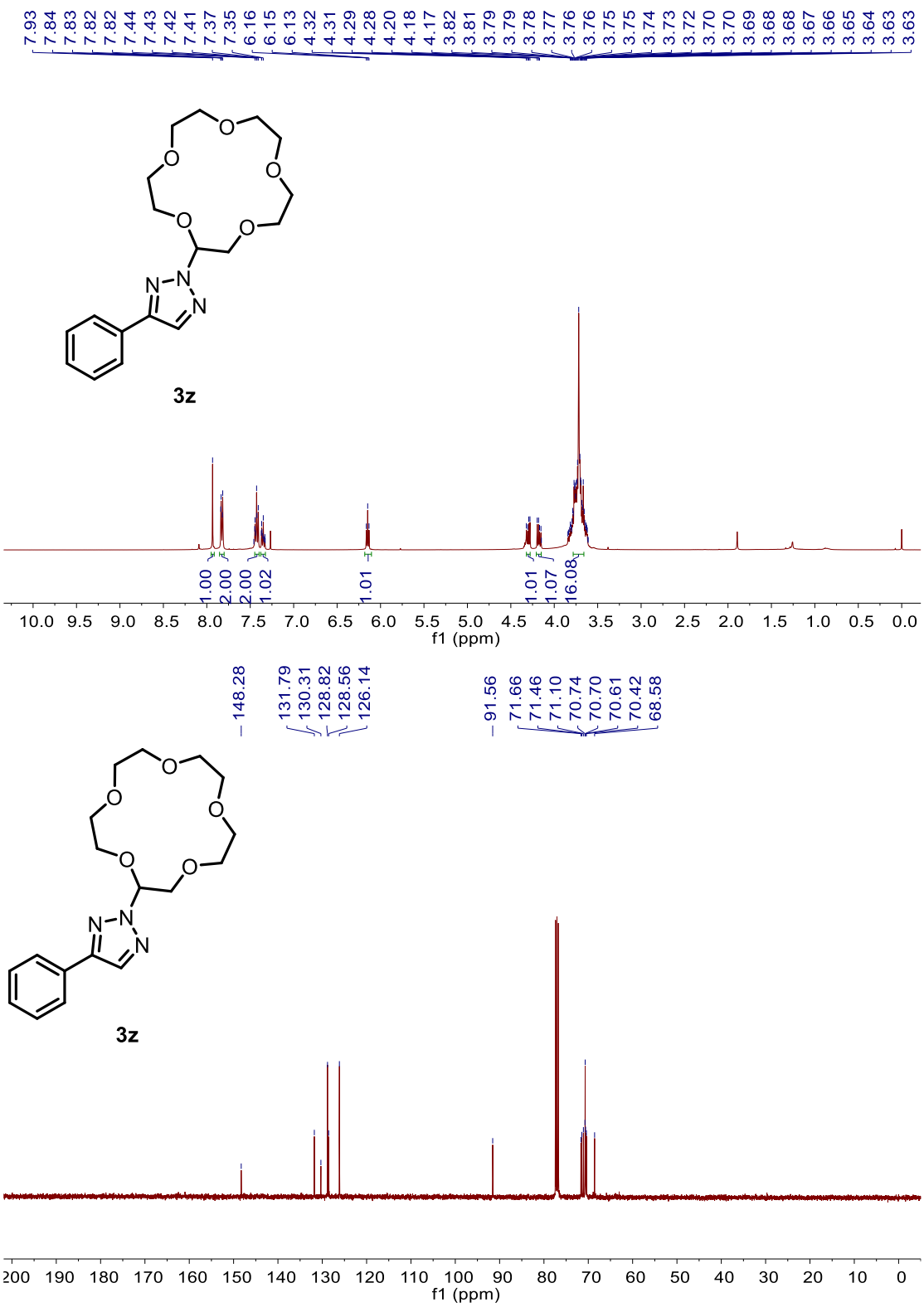
3v


7.89
7.81
7.79
7.78
7.47
7.45
7.43
7.40
7.38
7.36
5.98
5.97
5.84
5.83
3.13
3.12
3.07
3.06
2.48
2.47
2.18
2.17
O
N
N
N
N
3w
1.05
2.06
2.03
1.06
1.00
1.05
3.08
2.00
1.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
7.91
7.80
7.78
7.47
7.45
7.43
7.39
7.38
6.06
6.04
3.02
2.99
2.98
2.96
2.94
2.75
2.66
2.65
2.64
2.63
2.60
2.60
2.59
2.58
2.56
2.54
2.53
2.52
2.51
2.50
2.49
O
N
N
N
N
3x
1.09
2.05
2.09
1.09
1.00
1.04
3.04
1.05
2.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


175.50
148.74
131.91
129.83
128.97
128.88
126.01
78.90
28.97
27.67
25.24
3x
f1 (ppm)


7.89
7.80
7.80
7.79
7.78
7.46
7.44
7.43
7.42
7.38
7.38
7.38
7.37
7.36
7.34
5.91
5.90
5.90
5.89
3.76
3.74
3.72
3.71
3.69
3.68
3.22
3.21
3.20
3.20
3.19
3.18
3.17
3.17
3.05
2.94
2.54
2.53
2.51
2.31
2.31
2.30
2.28
2.27
2.27
3y
1.00
2.06
2.06
1.02
1.01
1.03
1.07
3.06
3.04
1.06
1.04
f1 (ppm)


155.61
148.08
131.31
130.12
128.92
128.67
125.95
76.12
43.72
35.98
34.34
27.30
3y
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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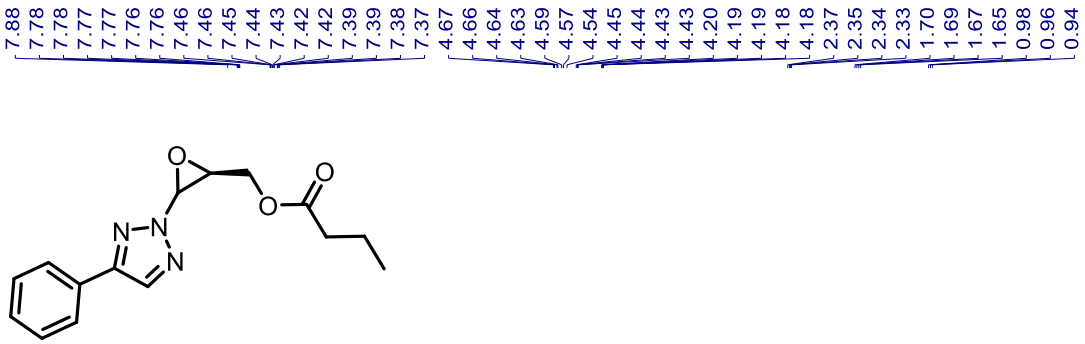
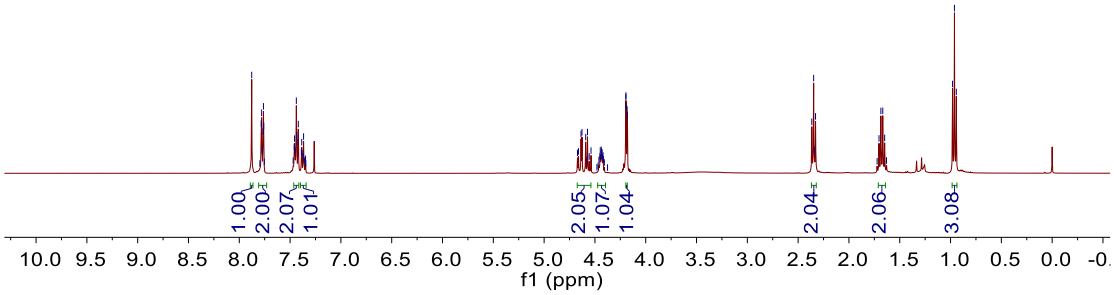
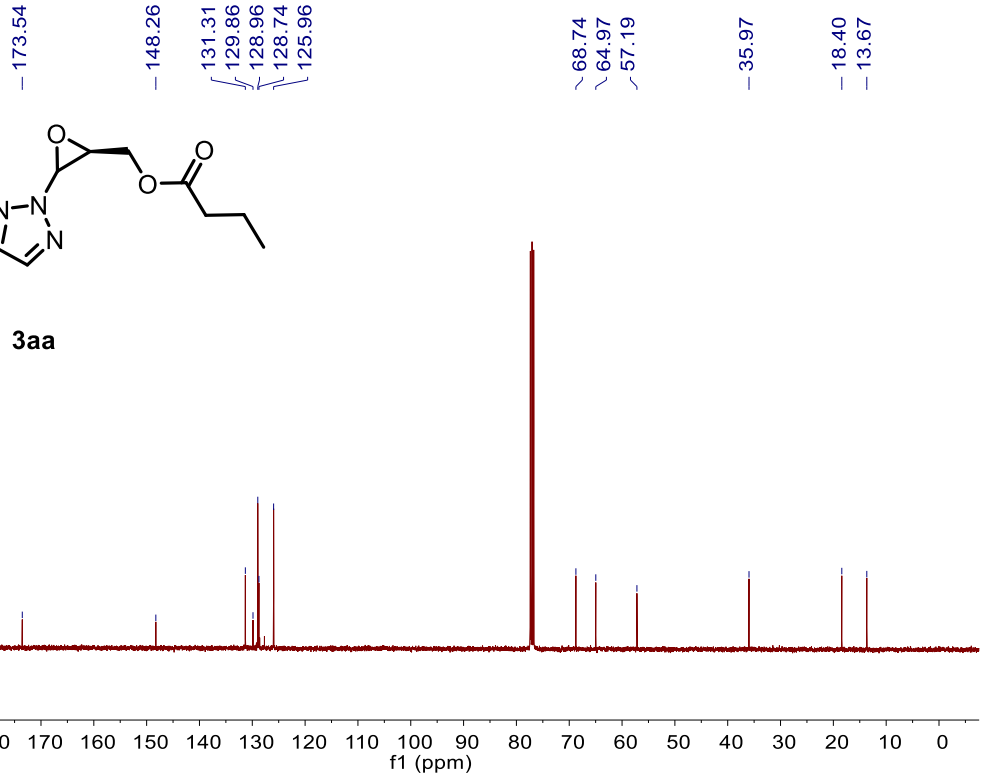
7.84
7.83
7.82
7.82
7.44
7.43
7.42
7.41
7.37
7.35
6.16
6.15
6.13
4.32
4.31
4.29
4.28
4.20
4.18
4.17
3.82
3.81
3.79
3.79
3.78
3.77
3.76
3.76
3.75
3.75
3.74
3.73
3.72
3.70
3.70
3.69
3.68
3.68
3.67
3.66
3.65
3.64
3.63
3.63
3z
1.00
2.00
2.00
1.02
1.01
1.01
1.07
16.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
148.28
131.79
130.31
128.82
128.56
126.14
91.56
71.66
71.46
71.10
70.74
70.70
70.61
70.42
68.58
3z
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

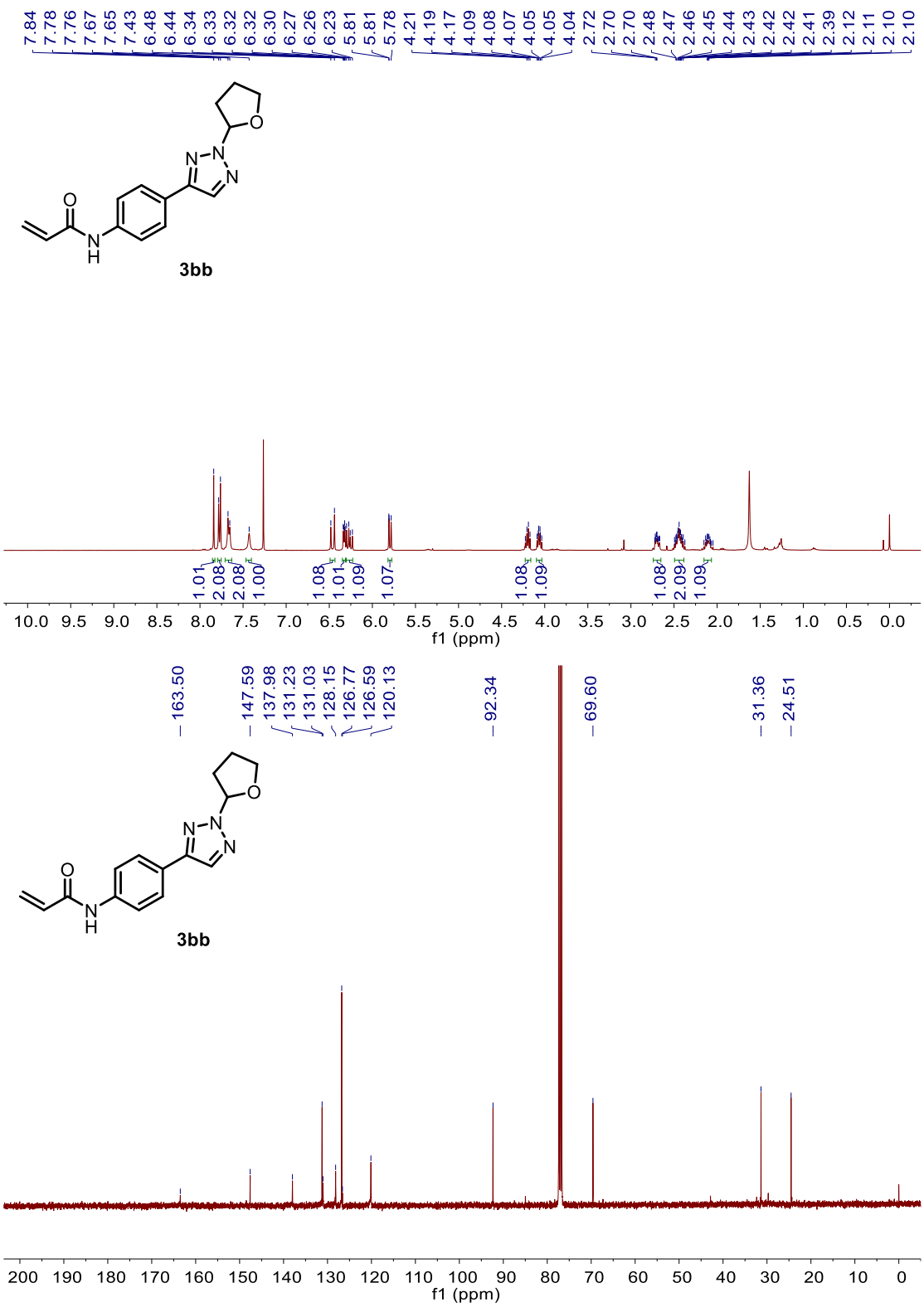

7.88
7.78
7.78
7.77
7.77
7.76
7.76
7.46
7.46
7.45
7.44
7.43
7.42
7.42
7.39
7.39
7.38
7.37
4.67
4.66
4.64
4.63
4.59
4.57
4.54
4.45
4.44
4.43
4.43
4.20
4.19
4.19
4.18
4.18
2.37
2.35
2.34
2.33
1.70
1.69
1.67
1.65
0.98
0.96
0.94

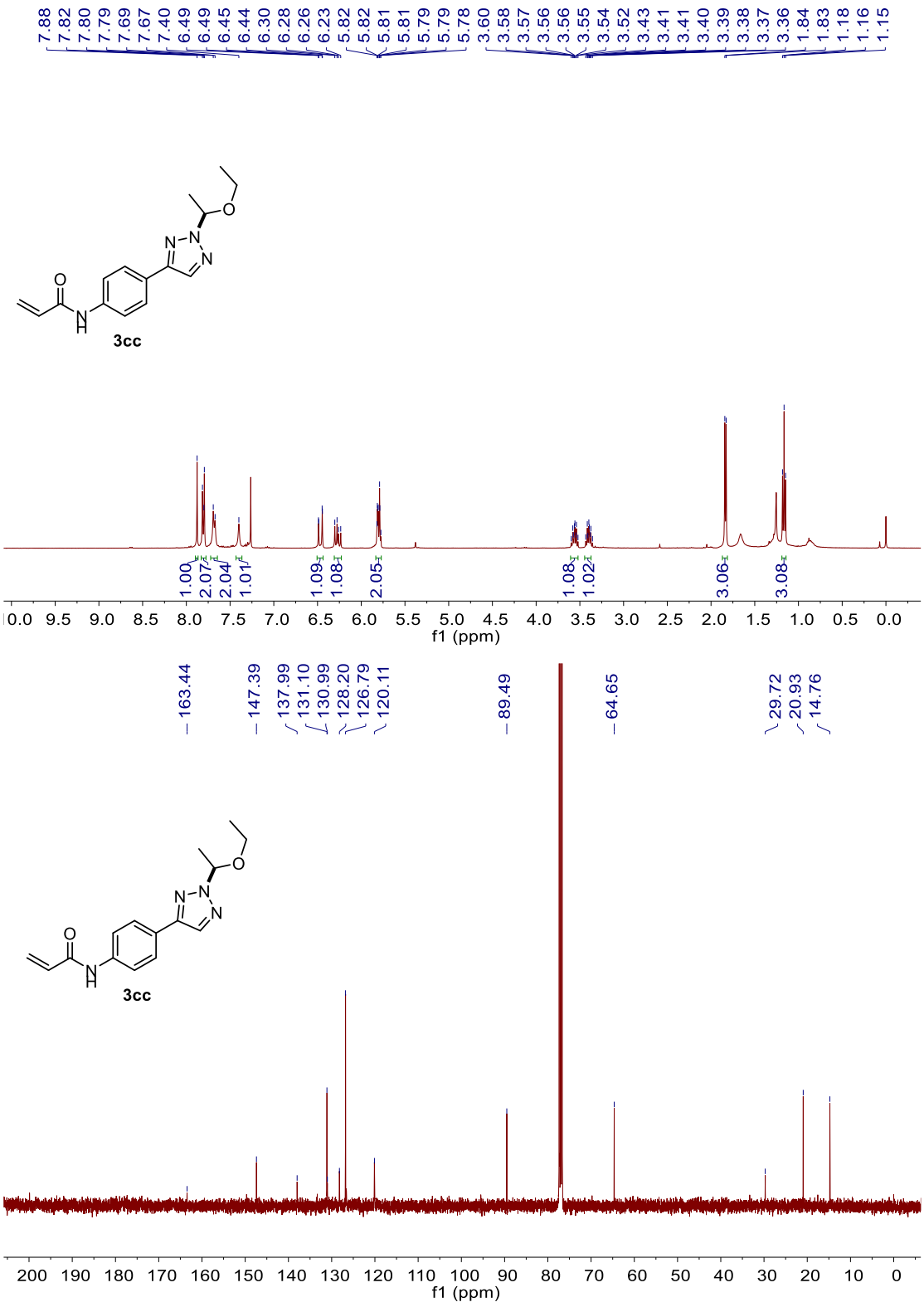
3aa

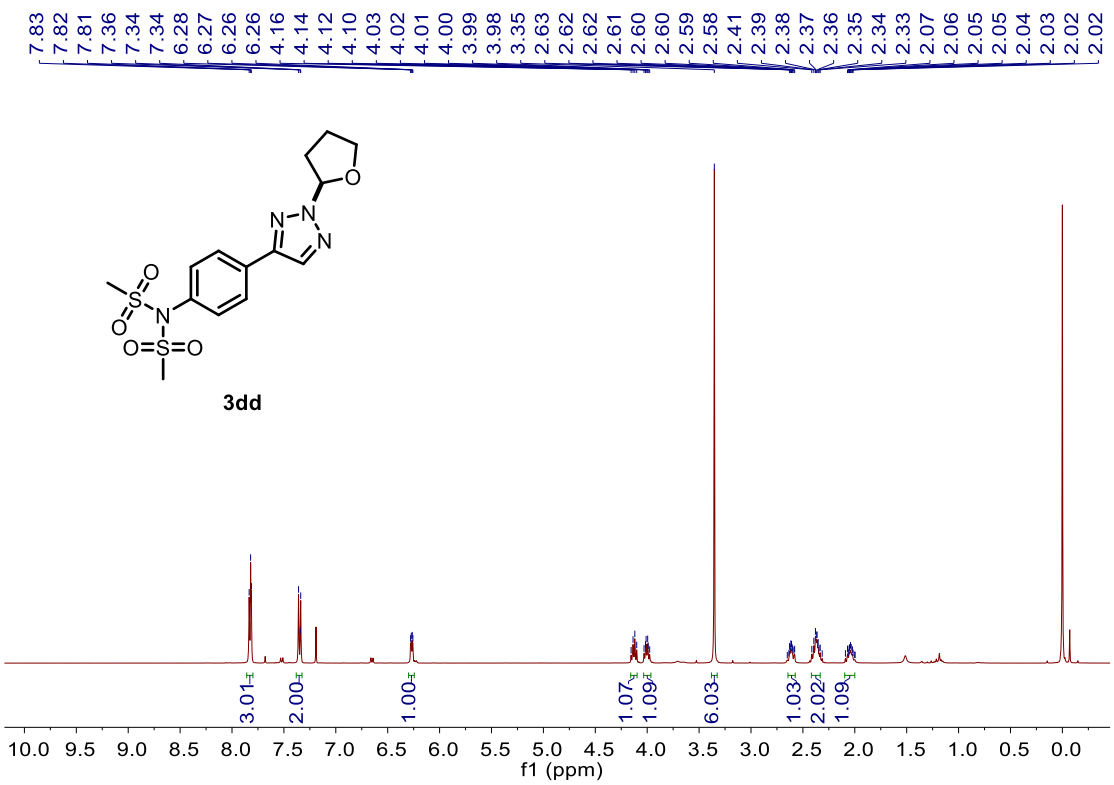

1.00
2.00
2.07
1.01
2.05
1.07
1.04
2.04
2.06
3.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

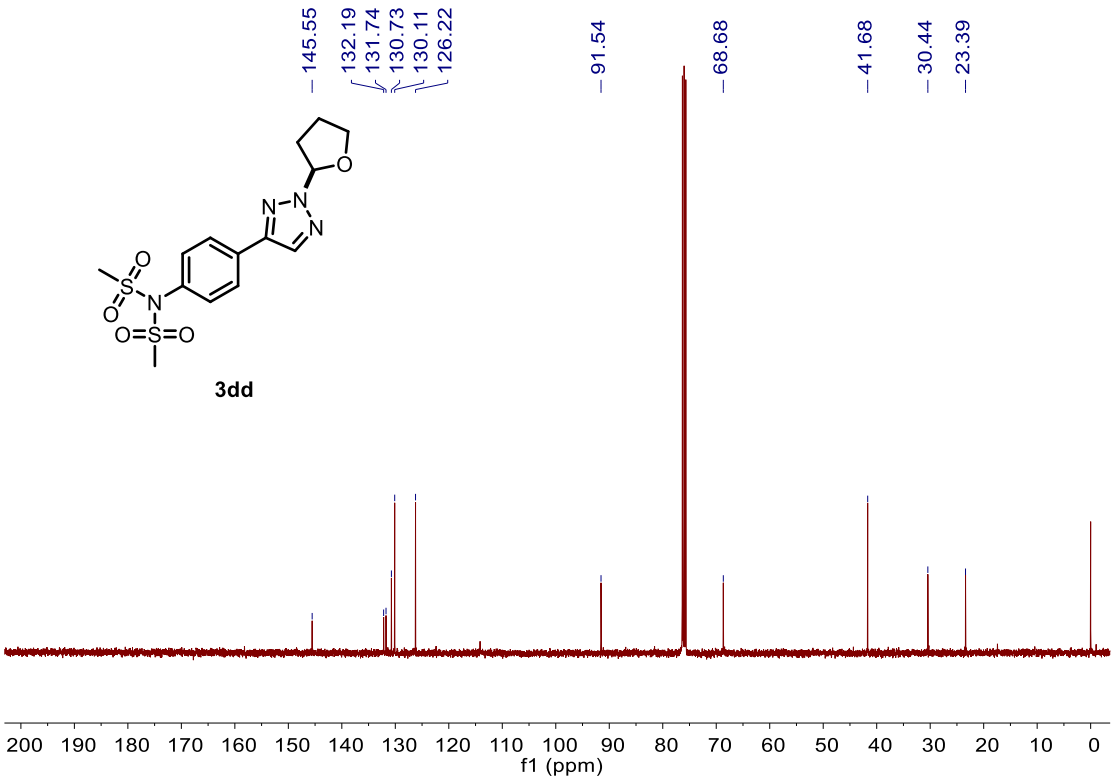

173.54
148.26
131.31
129.86
128.96
128.74
125.96
68.74
64.97
57.19
35.97
18.40
13.67
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3aa

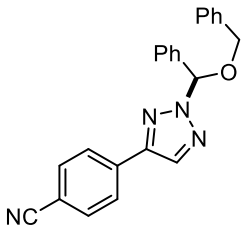

7.84 7.78 7.76 7.67 7.65 7.43 6.48 6.44 6.34 6.33 6.32 6.32 6.30 6.27 6.26 6.23 5.81 5.81 5.78 4.21 4.19 4.17 4.09 4.08 4.07 4.05 4.05 4.04 2.72 2.70 2.70 2.48 2.47 2.46 2.45 2.44 2.43 2.42 2.42 2.41 2.39 2.12 2.11 2.10 2.10
3bb
1.01 2.08 2.08 1.00 1.08 1.01 1.09 1.07 1.08 1.09 1.08 2.09 1.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
163.50 147.59 137.98 131.23 131.03 128.15 126.77 126.59 120.13 92.34 69.60 31.36 24.51
3bb
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.88
7.82
7.80
7.79
7.69
7.67
7.40
6.49
6.49
6.45
6.44
6.30
6.28
6.26
6.23
5.82
5.82
5.81
5.81
5.79
5.79
5.78
3.60
3.58
3.57
3.56
3.56
3.55
3.54
3.52
3.43
3.41
3.41
3.40
3.39
3.38
3.37
3.36
1.84
1.83
1.18
1.16
1.15
3cc
1.00
2.07
2.04
1.01
1.09
1.08
2.05
1.08
1.02
3.06
3.08
f1 (ppm)
163.44
147.39
137.99
131.10
130.99
128.20
126.79
120.11
89.49
64.65
29.72
20.93
14.76
3cc
f1 (ppm)

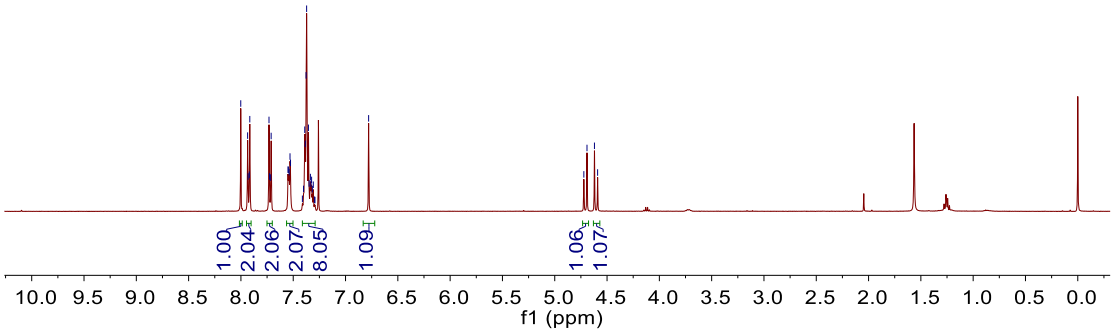

7.83 7.82 7.81 7.36 7.34 7.34 6.28 6.27 6.26 6.26 4.16 4.14 4.12 4.10 4.03 4.02 4.01 4.00 3.99 3.98 3.35 2.63 2.62 2.62 2.61 2.60 2.60 2.59 2.58 2.41 2.39 2.38 2.37 2.36 2.35 2.34 2.33 2.07 2.06 2.05 2.05 2.04 2.03 2.02 2.02
3dd
3.01 2.00 1.00 1.07 1.09 6.03 1.03 2.02 1.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


145.55 132.19 131.74 130.73 130.11 126.22 91.54 68.68 41.68 30.44 23.39
3dd
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

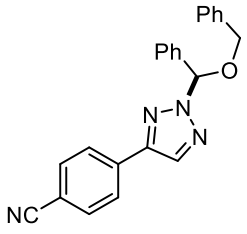

8.00
7.94
7.93
7.92
7.92
7.73
7.73
7.72
7.71
7.55
7.54
7.54
7.53
7.53
7.41
7.40
7.39
7.38
7.38
7.37
7.35
7.35
7.34
7.33
7.32
7.32
7.31
7.30
7.29
6.78
4.72
4.69
4.62
4.59


Ph
Ph
O
N
N
N
NC

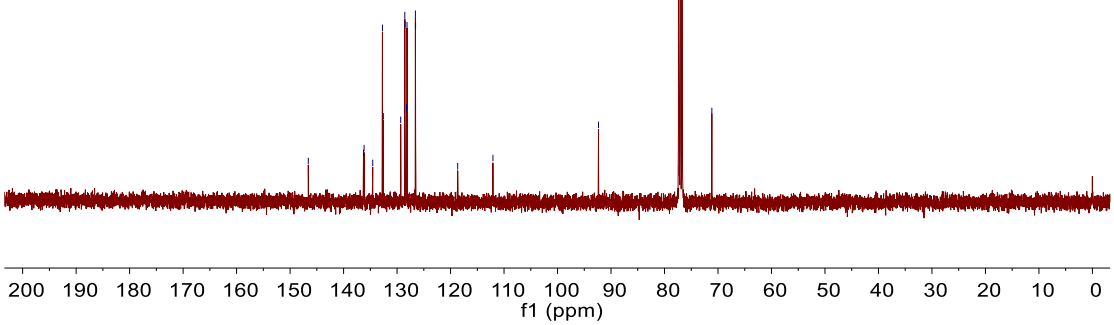
3ee

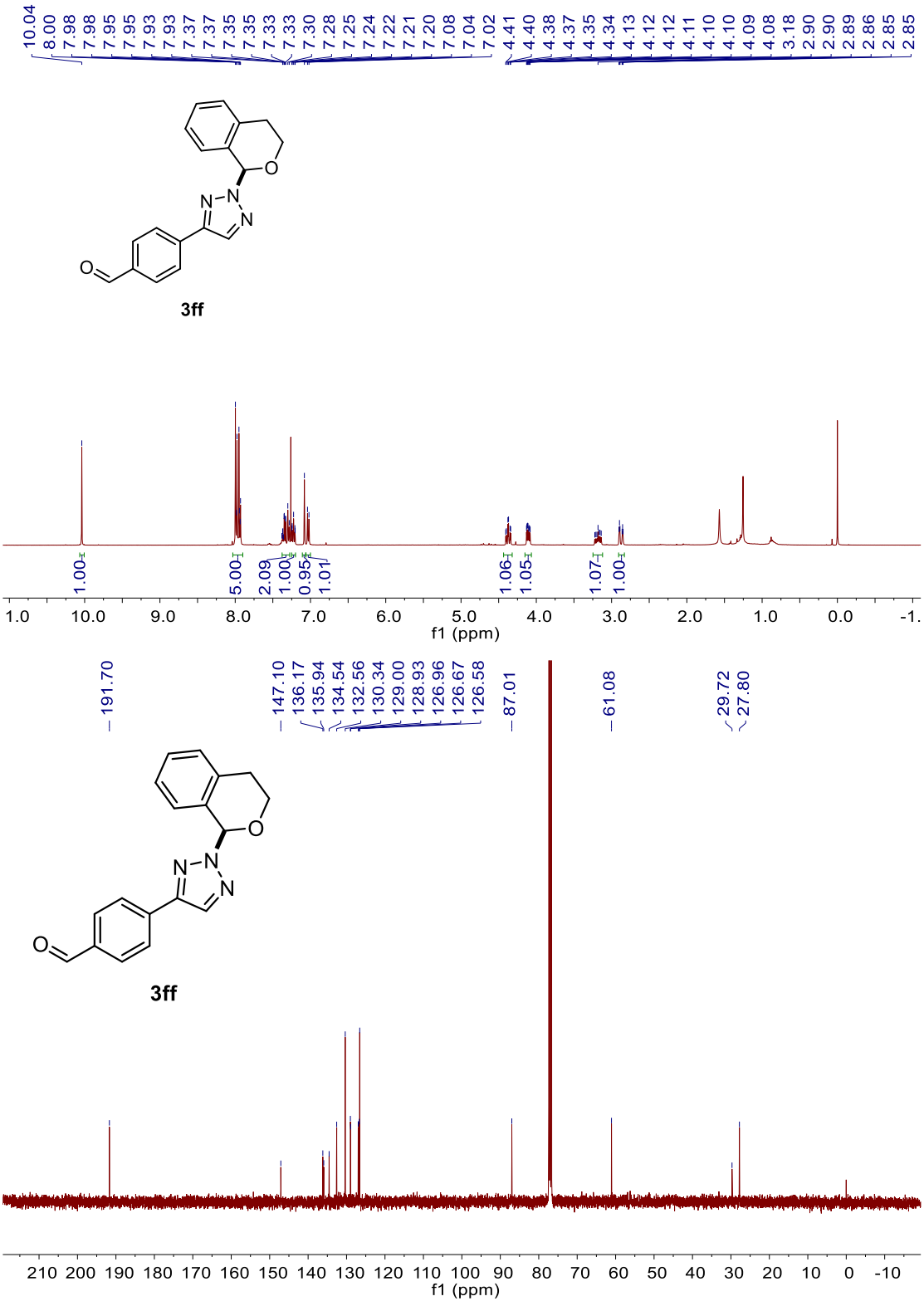

1.00
2.04
2.06
2.07
8.05
1.09
1.06
1.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


146.60
136.28
136.17
134.55
132.73
132.57
129.32
128.55
128.51
128.23
128.14
126.57
126.54
118.67
112.08
92.34
71.15


Ph
Ph
O
N
N
N
NC

3ee


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


10.04
8.00
7.98
7.98
7.95
7.95
7.93
7.93
7.37
7.37
7.35
7.35
7.33
7.33
7.30
7.28
7.25
7.24
7.22
7.21
7.20
7.08
7.04
7.02
4.41
4.40
4.38
4.37
4.35
4.34
4.13
4.12
4.11
4.10
4.10
4.09
4.08
3.18
2.90
2.90
2.89
2.86
2.85
2.85
O
N
N
N
O
3ff
1.00
5.00
2.09
1.00
0.95
1.01
1.06
1.05
1.07
1.00
1.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.
f1 (ppm)
191.70
147.10
136.17
135.94
134.54
132.56
130.34
129.00
128.93
126.96
126.67
126.58
87.01
61.08
29.72
27.80
O
N
N
N
O
3ff
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

9. Supplementary References

1.(a) Garlets, Z. J.; Davies, H. M. L., Harnessing the β-Silicon Effect for Regioselective and Stereoselective Rhodium (II)-Catalyzed C–H Functionalization by Donor/Acceptor Carbenes Derived from 1-Sulfonyl-1,2,3-triazoles. *Org. Lett*., **2018**, 20, 2168–2171. (b) Kwok, S. W.; Zhang, L.; Grimster, N. P.; Fokin, V. V., Catalytic Asymmetric Transannulation of NH-1,2,3-Triazoles with Olefins. *Angew. Chem., Int. Ed*., **2014**, 53, 3452–3456.

2. Bao, Peng. L.; Yue, H. L.; Meng, N.; Zhao, X. H.; Li, J. S.; Wei, Wei. Copper-Catalyzed Three-Component Reaction of Alkynes, $TMSN_3$, and Ethers: Regiocontrollable Synthesis of N^1- and N^2-Oxyalkylated 1,2,3-Triazoles. *Org. Lett.* **2019**, *21*, 18, 7218–7222.