

Supplementary Materials for

**Multi-component Syntheses of Diverse 5-Fluoroalkyl-1,2,3-Triazoles  
Facilitated by the Air Oxidation and Copper catalysis**

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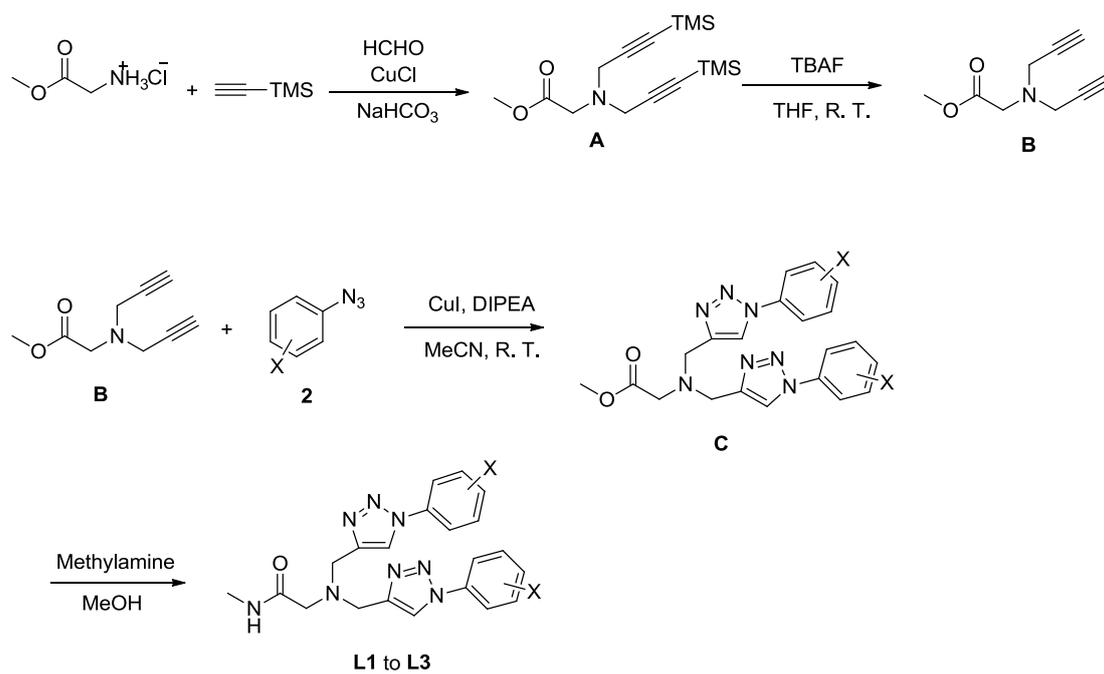
**Materials and Methods.** All reactions were run with anhydrous solvents unless otherwise noted. Tetrahydrofuran (THF) was distilled from sodium and benzophenone immediately before use. CH<sub>3</sub>CN were distilled from CaH<sub>2</sub>. Anhydrous dimethylformamide (DMF) was purchased from Aldrich and used as received. MeOH and EtOH were distilled from Mg turnings and iodine immediately before use. Reactions were monitored by thin-layer chromatography (TLC) on silica gel GF254-precoated plates. Compounds were detected under UV light/or visualized by phosphomolybdic acid in ethanol solution. Solvents were evaporated under reduced pressure and below 50 °C (water bath). Mass spectra were obtained on Bruker APEX. High-resolution MS were performed with Bruker BIFLEX III and Bruker Daltonics, Inc. APEX II. <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR data were recorded with an Avance 400/DPX (Bruker) and Avance III HD600 (Bruker) spectrometer in CDCl<sub>3</sub> solutions using the residual solvent signal or TMS as reference. Chemical shifts are reported in parts per million and coupling constants quoted in Hz. Fluorescence spectra were performed on a Cary Eclipse fluorescence spectrophotometer (Varian, America). Geometries of Copper (I) complexes of TBTA and **L3** were studied at the B3LYP/6-31g(d) level by using Gaussian 09w program package.<sup>[1]</sup>

Alkynes (**1a** to **1g**) were purchased from Alfa Aesar China Co. Ltd. (Tianjin) and used as received. Alkynes (**1h** to **1k**) and organic azides were prepared based on our previous works or the methods in literatures.<sup>[2,3]</sup>

**Table S1** Optimization of supplementary bases, solvent and amount of ligands.

Entry <sup>[a]</sup>	Catalyst (10 mol%)	Oxidant	Base (1 equiv)	Solvent (2 mL)	Product <sup>[b]</sup> (%)	
					<b>3a</b>	<b>4</b>
1	<b>L3</b> .CuCl	air	DIPEA	DMF	50	34
2	<b>L3</b> .CuCl	air	pyridine	DMF	18	66
3	<b>L3</b> .CuCl	air	Na <sub>4</sub> P <sub>2</sub> O <sub>7</sub>	MeCN	59	30
4	<b>L3</b> .CuCl	air	Na <sub>4</sub> P <sub>2</sub> O <sub>7</sub>	CH <sub>2</sub> Cl <sub>2</sub>	64	18
5	<b>L3</b> .CuCl	air	Na <sub>4</sub> P <sub>2</sub> O <sub>7</sub>	THF	69	20
6	<b>L3</b> .CuCl	air	Na <sub>4</sub> P <sub>2</sub> O <sub>7</sub>	DMF	78	10
7 <sup>[c]</sup>	<b>L3</b> .CuCl	air	Na <sub>4</sub> P <sub>2</sub> O <sub>7</sub>	DMF	77	10
8 <sup>[d]</sup>	<b>L3</b> .CuCl	air	Na <sub>4</sub> P <sub>2</sub> O <sub>7</sub>	DMF	65	19

<sup>[a]</sup> 0.20 mmol alkyne (**1a**), 0.22 mmol azide (**2a**) and 0.8 mmol TMSCF<sub>3</sub> were used as substrates. <sup>[b]</sup> Yields of product isolated. <sup>[c]</sup> 20 mol% ligand **L3** was used. <sup>[d]</sup> 5 mol% ligand **L3** was used.



**Scheme S1** Synthetic route of ligand **L1** to **L3**

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## *Syntheses of ligand L1-L3*

### Synthesis of Compound **B**:

According to the general procedure, to a round bottom flask was added glycine methyl ester hydrochloride (3.98 mmol, 500 mg), trimethylsilylacetylene (9.95 mmol, 978.2 mg), 37% formaldehyde (9.95 mmol, 815.6 mg), Sodium Bicarbonate (3.98 mmol, 334.7 mg) and CuCl (0.398 mmol, 39.4 mg). The reaction mixture was stirred for a further 18 h at 35 °C, and the reaction progress was monitored by TLC. Then, the solvent was evaporated and the residue was purified by chromatography over silica gel to give compound **A** (1.13 g, 92%). After that, compound **A** (1.13 g) was dissolved in tetrahydrofuran. Tetrabutylammonium fluoride (3.63 mmol, 2.8 g) was added and the solution was stirred for 3h. The resulted solution was then extracted with ethyl acetate, washed with saturated NaCl solution and dried over anhydrous MgSO<sub>4</sub>. After the solvent was removed under vacuum, the crude product was purified by column chromatography over silica gel to give compound **B** (596 mg, 87%).

To a mixture of compound **B** (1.2 mmol, 200 mg) and azide (2.4 mmol) in acetonitrile (5 mL) was added DIPEA (1.45 mmol, 187 mg) and CuI (0.12 mmol, 23 mg). After the reaction was stirred at room temperature for 10 h, the solution was extracted with ethyl acetate, washed with saturated NaCl solution and dried over anhydrous MgSO<sub>4</sub>. The solvent was removed under vacuum and the product was purified by column chromatography over silica gel to give the product **C**. **C** was then added into methylamine (32.0-34.0 wt% methanol solution), and the reaction was stirred at room temperature for 1 hour. Then, the solution was extracted with ethyl acetate, washed with saturated NaCl solution and dried over anhydrous MgSO<sub>4</sub>. The solvent was removed under vacuum and the product was purified by column chromatography over silica gel to give compound **L1** to **L3**.

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*General synthetic route of compound 5-fluoroalkyl-1,2,3-trizoles*

To a solution of ligand **L3** (10 mol%), CuCl (10 mol%), phenanthroline (20 mol%), and sodium pyrophosphate (0.22 mmol) were sequentially added in a dry round bottom flask. The reaction was cooled to 0 °C and dry DMF (1.0 mL) was added by syringe, then TMSF<sub>3</sub>, TMSF<sub>2</sub>, or TMSF<sub>3</sub> (0.80 mmol) was added dropwise. After two minutes, azide compound (0.22 mmol), terminal alkyne (0.20 mmol), and DMF (1 mL) were added in sequence to transfer the reaction system. After that, the mixture was slowly warmed to room temperature and stirred for 6~10 h. After the reaction was complete shown by TLC plate, water and ethyl acetate were added, and then the organic and aqueous layers were separated. The aqueous layer was extracted with ethyl acetate, and the combined organic layers were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The organic was concentrated in vacuo. Purification of the crude reaction product by column chromatography on silica gel afforded the product.

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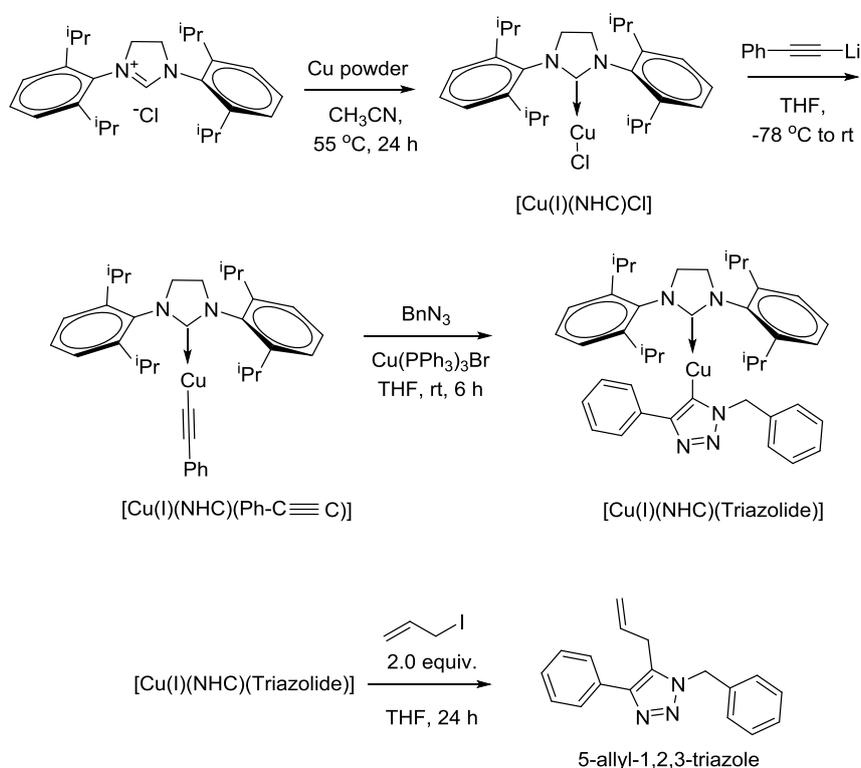
### *Synthesis of [Cu(I)(NHC)(Triazolide)] and testing its reactivity*

The synthesis of [Cu(I)(NHC)(Triazolide)] was based on the methods in literature <sup>[4,5]</sup>. Briefly, To a dry round-bottom flask equipped with a magnetic stirring bar, compound 16 (200 mg, 0.47 mmol) was added followed by Cu powder (150 mg, 2.4 mmol) and acetonitrile (5 mL). The reaction was stirred vigorously at room temperature for 10 min and then at 55 °C for 24 h. The hot reaction mixture was filtered through a silica pad to remove excess copper powder, and the solvent was removed under vacuum to provide ([Cu(I)(NHC)Cl]) (180 mg, 79%, 0.37 mmol) as a white solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.40 (t, *J* = 7.7 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 4H), 4.02 (s, 4H), 3.10-3.03 (m, 4H), 1.37 (d, *J* = 8.0 Hz, 12H), 1.35 (d, *J* = 8.0 Hz, 12H).

To a dry flask charged with N<sub>2</sub> and equipped with a magnetic stirring bar, compound [Cu(I)(NHC)Cl] (110 mg, 0.23 mmol) was suspended in dry THF (2 mL) and cooled to -78 °C in a dry ice/acetone bath. A lithiumphenylacetylide solution in THF (310 μL, 1.0 M in THF, 0.31 mmol) was added dropwise. The cold bath was then removed, and the reaction mixture was stirred vigorously for additional 2 h. The solvent was removed in vacuo to provide a gummy yellow solid. DCM (2 mL) was added to the crude product, and the solution was filtered and then washed with additional DCM (3 × 1 mL). The filtrate was concentrated under vacuum to give a yellow solid, which was redissolved in a minimal amount of DCM and combined with hexanes (5 mL). The flask was capped and placed in a freezer. The precipitate was filtered after 1 hour, washed with hexanes, and dried under high vacuum to afford [Cu(I)(NHC)(Ph-C≡C)] (145 mg, 74%, 0.17 mmol) as a pale yellow powder. <sup>1</sup>H NMR (400 MHz, C<sub>6</sub>D<sub>6</sub>) δ 7.25 – 7.14 (m, 6H), 7.04 (d, *J* = 8.0 Hz, 4H), 6.97 – 6.88 (m, 1H), 3.13 (s, 4H), 2.97–2.91 (m, 4H), 1.42 (d, *J* = 4.0 Hz, 12H), 1.16 (d, *J* = 4.0 Hz, 12H).

To a dry flask charged with N<sub>2</sub> and equipped with a magnetic stirring bar, compound [Cu(I)(NHC)(Ph-C≡C)] (108 mg, 0.19 mmol) and Cu(PPh<sub>3</sub>)<sub>3</sub>Br (9 mg, 0.01 mmol)

were suspended in dry THF (2 mL). Benzyl azide (36  $\mu$ L, 0.29 mmol) was added, and the reaction mixture was stirred vigorously for 6 h. The solvent was removed in vacuo, the crude was dissolved in DCM and then filtered. Hexanes were added to the filtrate, and the solution was placed in a freezer. The precipitate [Cu(I)(NHC)(Triazolide)] was collected for approximately 1 h. The reactivity of [Cu(I)(NHC)(Triazolide)] was tested by added 2.0 equivalent of allyl iodide in to the solution of [Cu(I)(NHC)(Triazolide)] in dry THF. After 24 hour, 5-allyl-1,2,3-triazole could be obtained as white solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.73 – 7.65 (m, 2H), 7.43 (t,  $J = 7.4$  Hz, 2H), 7.39 – 7.30 (m, 4H), 7.23 – 7.16 (m, 2H), 5.84 (ddd,  $J_1 = 22.3$ ,  $J_2 = 10.3$ ,  $J_3 = 5.2$  Hz, 1H), 5.54 (s, 2H), 5.17 (dd,  $J_1 = 10.2$ ,  $J_2 = 1.0$  Hz, 1H), 4.92 (dd,  $J_1 = 17.2$ ,  $J_2 = 1.0$  Hz, 1H), 3.45 (dd,  $J_1 = 3.3$ ,  $J_2 = 1.9$  Hz, 2H). The trapping assay of copper triazolide via allyl iodide proved the reactivity of [Cu(I)(NHC)(Triazolide)]<sup>[5]</sup> enough for the following control experiments shown in Eq-4 and Eq-5 in Scheme 3 in the manuscript.

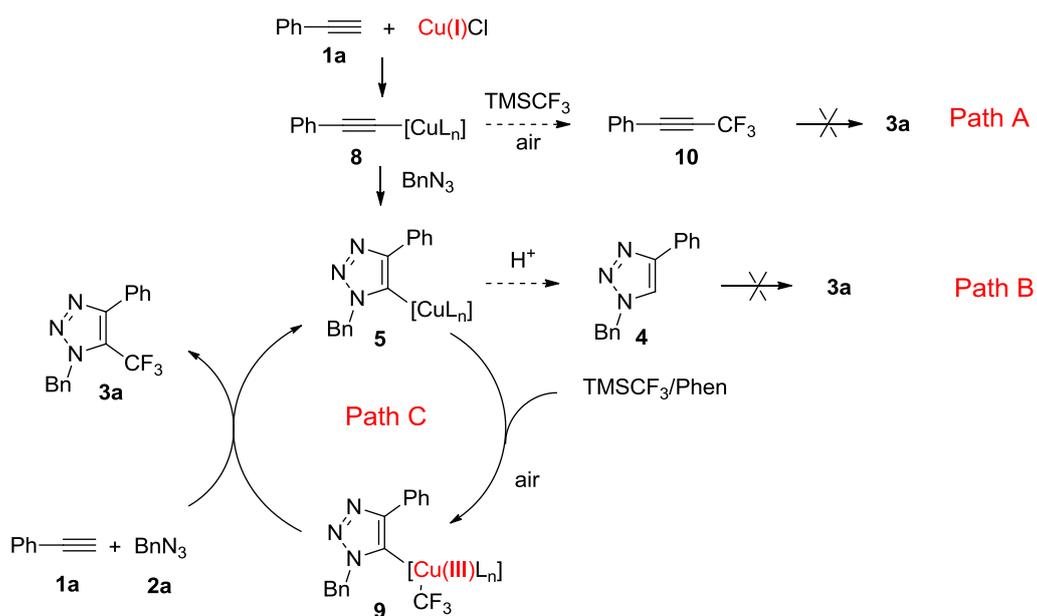


**Scheme S2** Synthesis of [Cu(I)(NHC)(Triazolide)] and testing its reactivity

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### *Discussion of plausible reaction mechanism*

Three possible reaction mechanism of multi-component aerobic oxidative coupling were proposed (Scheme S3): 1) Path A, oxidative coupling of **1a** with  $\text{TMSCF}_3$  to produce  $\text{CF}_3$ -alkyne **10**, followed by cycloaddition with **2a** to give product **3a**. 2) Path B, CuAAC reaction of **1a** and **2a** leads to produce **4**, followed by oxidative coupling with  $\text{TMSCF}_3$  to generate **3a**. 3) Path C, aerobic oxidative coupling of  $\text{TMSCF}_3$  with the in situ formed triazolide **5** to produce **3a**. However, the reaction of triazole **4** or  $\text{CF}_3$ -alkyne **10** with  $\text{TMSCF}_3$  in the presence of  $\text{CuCl}$  and ligand **L3** could not produce product **3a**, and only the starting materials were recovered. This indicate that the reaction did not proceed by either path A or B. Furthermore, when the multi-component reaction was conducted under nitrogen, **3a** could not be detected, and only **4** was obtained in 88% yield. Additionally, the triazolide intermediate **5** could also be trapped to produce 5-allyl-1,2,3-triaole when addition of allyl bromide. Based on these study results, a rational mechanism for the reaction is proposed in Path C in the Scheme S3. The reaction proceeds through a tandem CuAAC and aerobic oxidative coupling, the copper-catalyzed cycloaddition of an azide with alkyne (**1a** to **5**), followed by oxidative coupling of **5** with  $\text{CF}_3^-$  anion (**5** to **3a**). The produce of  $\text{CF}_3^-$  anion from  $\text{TMSCF}_3$  in the presence of phen and  $\text{Cu(I)}$  should be reasonable<sup>[6]</sup>, and the oxidative of  $\text{CF}_3^-$  must take place before the protonation of triazolide **5**.

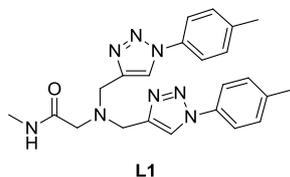


**Scheme S3** Plausible mechanism

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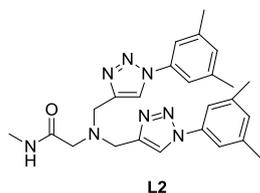
*Characterization data of Ligand L1 to L3*

**2-(bis((1-(p-tolyl)-1H-1,2,3-triazol-4-yl)methyl)amino)-N-methylacetamide (L1)**



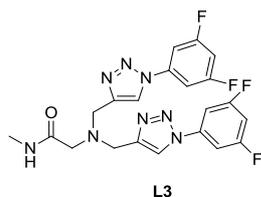
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.00 (s, 2H), 7.66 (s, 1H), 7.60 (d,  $J = 8.4$  Hz, 4H), 7.31 (d,  $J = 8.2$  Hz, 4H), 3.93 (s, 4H), 3.29 (s, 2H), 2.85 (d,  $J = 7.8$  Hz, 3H), 2.42 (s, 6H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  171.0, 144.2, 138.9, 134.6, 130.2, 121.4, 120.2, 57.7, 48.6, 25.8, 21.1. HRMS (ESI)  $m/z$  calculate for  $(\text{M}+\text{H}^+)$   $\text{C}_{23}\text{H}_{27}\text{N}_8\text{O}^+$ : 431.2302, Found: 431.2291.

**2-(bis((1-(2,4-dimethylphenyl)-1H-1,2,3-triazol-4-yl)methyl)amino)-N-methylacetamide(L2)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.97 (s, 2H), 7.70 (s, 1H), 7.32 (s, 4H), 7.05 (s, 2H), 3.91 (s, 4H), 3.29 (s, 2H), 2.86 (s, 3H), 2.38 (s, 12H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  170.8, 143.8, 140.1, 136.9, 131.0, 121.1, 118.0, 57.0, 48.7, 25.0, 21.3. HRMS (ESI)  $m/z$  calculate for  $(\text{M}+\text{H}^+)$   $\text{C}_{25}\text{H}_{31}\text{N}_8\text{O}^+$ : 459.2615, Found: 459.2608.

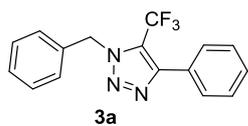
**2-(bis((1-(3,5-difluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)amino)-N-methylacetamide (L3)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (s, 2H), 7.58 - 7.52 (m, 1H), 7.36 (q,  $J = 4.0$  Hz, 4H), 6.94 - 6.89 (m, 2H), 3.92 (s, 4H), 3.28 (s, 2H), 2.87 (d,  $J = 4.8$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  170.9, 164.3 (d,  $J = 216.0$  Hz), 162.3, 145.2, 137.8, 121.4, 103.4 (d,  $J = 63.0$  Hz), 54.4, 51.6, 47.3. HRMS (ESI)  $m/z$  calculate for  $(\text{M}+\text{Na}^+)$   $\text{C}_{21}\text{H}_{18}\text{F}_4\text{N}_8\text{ONa}$ : 497.1432, Found: 497.1428.

### Characterization data of Compound 3a to 3z

#### 1-benzyl-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3a)



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.63 - 7.61 (m, 2 H), 7.45 - 7.44 (m, 3H), 7.37 (t,  $J = 4.0$  Hz, 3H), 7.31 (t,  $J = 4.0$  Hz, 2 H) 5.73 (s, 2 H).  $^{13}\text{C}$  NMR( $\text{CDCl}_3$ , 150 MHz):  $\delta$  148.6, 133.9, 129.4, 129.0, 128.9, 128.8, 128.4, 127.7, 126.1, 123.0 (q,  $J_{\text{CF}} = 55.5$  Hz), 120.8, (q,  $J_{\text{CF}} = 274.5$  Hz), 54.3. HRMS (ESI)  $m/z$  calculate for  $(\text{M}+\text{H}^+)$   $\text{C}_{16}\text{H}_{13}\text{F}_3\text{N}_3$ : 304.1062, Found: 304.1056.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -55.69.

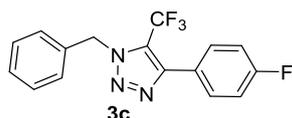
#### 1-benzyl-4-(p-tolyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3b)



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.51 (d,  $J = 8.0$  Hz, 2H), 7.37 (d,  $J = 4.0$  Hz, 3H), 7.30 (t,  $J = 4.0$  Hz, 2H), 7.25 (t,  $J = 4.0$  Hz, 2H), 5.72 (s, 2 H), 2.40 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  148.6, 139.4, 134.0, 129.2, 129.0, 128.9, 128.8, 128.8, 127.7, 124.2

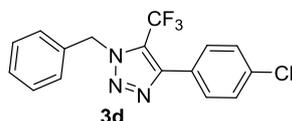
(q,  $J_{CF} = 47.0$  Hz), 120.1 (q,  $J_{CF} = 267.0$  Hz), 54.4, 21.4. HRMS (ESI)  $m/z$  calculate for  $(M+H^+)$   $C_{17}H_{15}F_3N_3$ : 318.1218, Found: 318.1213.  $^{19}F$  NMR (376 MHz,  $CDCl_3$ )  $\delta$  -55.82.

**1-benzyl-4-(4-fluorophenyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3c)**



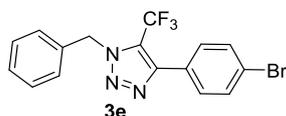
$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.62 – 7.58 (m, 2H), 7.38 (d,  $J = 4.0$  Hz, 3H), 7.31 – 7.30 (m, 2H), 7.14 (t,  $J = 8.0$  Hz, 2H), 5.73 (s, 2H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  163.4 (d,  $J_{CF} = 244.0$  Hz), 147.5, 133.8, 131.0, 130.8, 129.0, 128.9, 127.7, 123.3 (q,  $J_{CF} = 40.00$  Hz), 120.3 (q,  $J_{CF} = 268.0$  Hz), 115.6 (d,  $J_{CF} = 21.0$  Hz), 54.1. HRMS (ESI)  $m/z$  calculate for  $(M+H^+)$   $C_{16}H_{12}F_4N_3$ : 322.0962, Found: 322.0957.

**1-benzyl-4-(4-chlorophenyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3d)**



$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.56 (d,  $J = 8.0$  Hz, 2H), 7.44 – 7.41 (m, 2H), 7.39 – 7.36 (m, 3H), 7.31 (t,  $J = 4.0$  Hz, 2H), 5.73 (s, 2H).  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  147.3, 135.5, 133.7, 130.2, 129.0, 128.9, 128.8, 127.7, 127.3, 123.2 (q,  $J_{CF} = 40.8$  Hz), 120.2 (q,  $J_{CF} = 269.8$  Hz), 54.4. HRMS (ESI)  $m/z$  calculate for  $(M+H^+)$   $C_{16}H_{12}ClF_3N_3$ : 338.0666, Found: 338.0669.

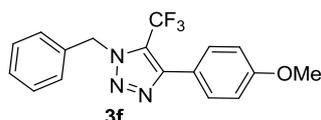
**1-benzyl-4-(4-bromophenyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3e)**



$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.60 – 7.57 (m, 2H), 7.50 (s, 2H), 7.39 – 7.36 (m, 3H),

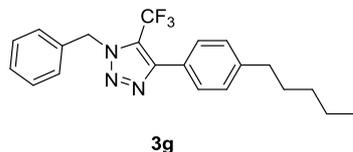
7.31 – 7.30 (m, 2H), 5.73 (s, 2H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  147.4, 133.8, 131.8, 130.5, 129.0, 128.9, 127.9, 127.7, 124.1, 123.1 (q,  $J_{\text{CF}} = 40.5$  Hz), 120.2 (q,  $J_{\text{CF}} = 274.5$  Hz), 54.5. HRMS (ESI)  $m/z$  calculate for  $(\text{M}+\text{H}^+)$   $\text{C}_{16}\text{H}_{12}\text{BrF}_3\text{N}_3$ :382.0161, Found: 382.0155.

**1-benzyl-4-(4-methoxyphenyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3f)**



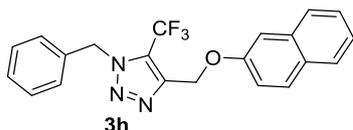
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.56 (d,  $J = 8.0$  Hz, 2H), 7.33 (t,  $J = 8.0$  Hz, 3H), 7.29 – 7.27 (m, 2H), 6.96 (d,  $J = 8.8$  Hz, 2H), 5.69 (s, 2H), 3.81 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.5, 148.4, 134.1, 130.3, 128.9, 127.7, 123.3, 122.3 (q,  $J_{\text{CF}} = 40.0$  Hz), 121.2, 120.5 (q,  $J_{\text{CF}} = 267.0$  Hz), 113.9, 55.3, 54.4. HRMS (ESI)  $m/z$  calculate for  $(\text{M}+\text{H}^+)$   $\text{C}_{17}\text{H}_{15}\text{F}_3\text{N}_3\text{O}$ :334.1162, Found: 334.1161.

**1-benzyl-4-(4-pentylphenyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3g)**



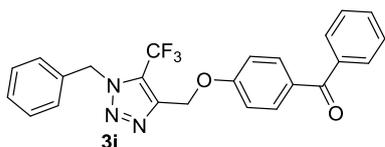
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.53 (d,  $J = 8.0$  Hz, 2H), 7.35 (t,  $J = 8.0$  Hz, 3H), 7.30 – 7.28 (m, 2H), 7.26 (s, 1H), 7.24 (s, 1H), 5.72 (s, 2H), 2.64 (t,  $J = 8.0$  Hz, 2H), 1.64 (t,  $J = 8.0$  Hz, 2H), 1.37 – 1.31 (m, 4H), 0.89 (t,  $J = 8.0$  Hz, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  148.6, 144.4, 134.0, 134.0, 129.4, 128.9, 128.5, 127.7, 126.2, 122.6 (q,  $J_{\text{CF}} = 43.5$  Hz), 120.5 (q,  $J_{\text{CF}} = 267.0$  Hz) 54.6, 36.0, 31.4, 31.0, 22.5, 14.0. HRMS (ESI)  $m/z$  calculate for  $(\text{M}+\text{Na}^+)$   $\text{C}_{21}\text{H}_{22}\text{F}_3\text{N}_3\text{Na}^+$ :396.1658, Found: 396.1658.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -55.83.

**1-benzyl-4-((naphthalen-2-yloxy)methyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3h)**



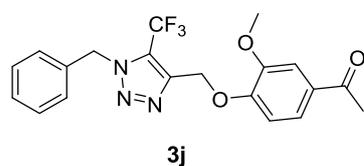
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.17 (d,  $J = 8.2$  Hz, 1H), 7.77 (d,  $J = 7.8$  Hz, 1H), 7.47 – 7.41 (m, 3H), 7.39 – 7.34 (m, 4H), 7.27 (d,  $J = 9.2$  Hz, 2H), 7.00 (d,  $J = 4.8$  Hz, 1H), 5.66 (s, 2H), 5.40 (s, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.9, 144.2, 134.5, 133.5, 129.0, 128.9, 127.8, 127.4, 126.5, 126.0 (q,  $J_{\text{CF}} = 41.0$  Hz), 125.7, 125.6, 125.4, 122.1, 121.2, 120.1 (q,  $J_{\text{CF}} = 268.0$  Hz), 105.5, 61.2, 54.2. HRMS(ESI)  $m/z$  calculate for  $(\text{M}+\text{H}^+)$   $\text{C}_{21}\text{H}_{17}\text{F}_3\text{N}_3\text{O}$ : 384.1279, Found: 384.1268.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -57.52.

**4-((1-benzyl-5-(trifluoromethyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl(phenyl)methanone (3i)**



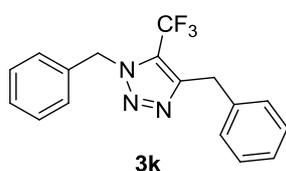
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.83 – 7.81 (m, 2H), 7.76 – 7.74 (m, 2H), 7.58 – 7.55 (m, 1H), 7.47 (t,  $J = 8.0$  Hz, 2H), 7.36 (dd,  $J = 4.2, 1.8$  Hz, 3H), 7.28 (dd,  $J = 7.6, 5.0$  Hz, 2H), 7.07 (d,  $J = 8.0$  Hz, 2H), 5.68 (s, 2H), 5.31 (s, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  195.5, 161.6, 143.5, 138.1, 133.4, 132.5, 132.0, 131.0, 129.8, 129.0, 128.2, 127.8, 126.0 (q,  $J_{\text{CF}} = 41.0$  Hz), 120.0 (q,  $J_{\text{CF}} = 267.0$  Hz), 114.4, 60.8, 54.2. HRMS (ESI)  $m/z$  calculate for  $(\text{M}+\text{H}^+)$   $\text{C}_{24}\text{H}_{19}\text{F}_3\text{N}_3\text{O}_2$ : 438.1385, Found: 438.1376.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -57.76.

**1-(4-((1-benzyl-5-(trifluoromethyl)-1H-1,2,3-triazol-4-yl)methoxy)-3-methoxyphenyl)ethan-1-one (3j)**



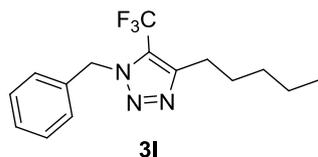
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  7.55 – 7.52 (m, 2H), 7.36 (dd,  $J = 7.8, 4.0$  Hz, 3H), 7.29 – 7.26 (m, 2H), 7.09 (d,  $J = 4.2$  Hz, 1H), 5.65 (s, 2H), 5.34 (s, 2H), 3.87 (s, 3H), 2.56 (s, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  196.8, 152.1, 149.7, 143.2, 132.9, 131.4, 129.9, 128.9, 127.9, 126.1 (q,  $J_{\text{CF}} = 41.0$  Hz), 125.8, 122.8, 120.8, 112.3 (q,  $J_{\text{CF}} = 243.0$  Hz), 111.1, 61.8, 56.1, 26.3. HRMS (ESI)  $m/z$  calculate for  $(\text{M}+\text{H}^+)$   $\text{C}_{20}\text{H}_{19}\text{F}_3\text{N}_3\text{O}_3$ :406.1334, Found: 406.1338.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -57.58.

### 1,4-dibenzyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3k)



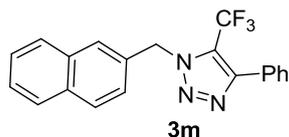
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.29 – 7.24 (m, 3H), 7.22 (d,  $J = 7.4$  Hz, 1H), 7.20 – 7.11 (m, 6H), 5.54 (s, 2H), 4.09 (s, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  146.5, 136.6, 132.8, 127.9, 127.7, 127.6, 127.5, 126.6, 125.7, 124.5 (q,  $J_{\text{CF}} = 40.0$  Hz), 119.4 (q,  $J_{\text{CF}} = 268.0$  Hz), 52.9, 44.9. HRMS (ESI)  $m/z$  calculate for  $(\text{M}+\text{H}^+)$   $\text{C}_{17}\text{H}_{15}\text{F}_3\text{N}_3^+$ :318.1213, Found: 318.1213.  $^{19}\text{F}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  - 56.88.

### 1-benzyl-4-pentyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3l)



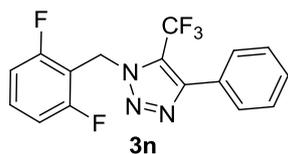
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  7.37 – 7.32 (m, 3H), 7.25 – 7.22 (m, 2H), 5.62 (s, 2H), 2.78 (td,  $J = 6.0, 1.1$  Hz, 2H), 1.72 – 1.67 (m, 2H), 1.35 – 1.32 (m, 4H), 0.91 – 0.87 (m, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  149.4, 134.2, 129.0, 128.8, 127.7, 123.3 (q,  $J_{\text{CF}} = 40.5$  Hz), 120.8 (q,  $J_{\text{CF}} = 267.35$  Hz), 54.0, 31.5, 29.2, 25.5, 22.4, 14.0. HRMS (ESI)  $m/z$  calculate for  $(\text{M}+\text{H}^+)$   $\text{C}_{15}\text{H}_{19}\text{F}_3\text{N}_3^+$ :298.1526, Found: 298.1527.  $^{19}\text{F}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  - 56.88.

### 1-(naphthalen-2-ylmethyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3m)



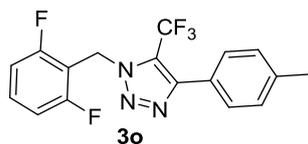
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.88 – 7.83 (m, 3H), 7.77 (s, 1H), 7.65 – 7.63 (m Hz, 2H), 7.52 (dd,  $J = 6.2, 3.2$  Hz, 2H), 7.46 – 7.42 (m, 4H), 5.90 (s, 2H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  148.6, 133.3, 133.2, 131.3, 129.4, 129.0, 128.9, 128.8, 128.5, 128.1, 127.8, 127.2, 126.8, 126.7, 124.9, 123.0 (d,  $J_{\text{CF}} = 39.0$  Hz), 120.4 (d,  $J_{\text{CF}} = 270.0$  Hz), 54.74. HRMS (ESI)  $m/z$  calculate for ( $\text{M}+\text{H}^+$ )  $\text{C}_{20}\text{H}_{15}\text{F}_3\text{N}_3$ : 354.1213, Found: 354.1210.

### 1-(2,6-difluorobenzyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3n)



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (dd,  $J = 4.2, 2.6$  Hz, 2H), 7.44 (dd,  $J = 5.0, 4.2$  Hz, 3H), 7.41 – 7.35 (m, 1H), 6.98 (t,  $J = 8.0$  Hz, 2H), 5.76 (s, 2H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  161.6 (dd,  $J_{\text{CF}} = 250.0, 6.0$  Hz), 148.2, 131.6 (t,  $J_{\text{CF}} = 10.5$  Hz), 129.4 (q,  $J_{\text{CF}} = 39.0$  Hz), 128.9, 128.5, 123.2 (q,  $J_{\text{CF}} = 26.3$  Hz), 120.4 (q,  $J_{\text{CF}} = 268.5$  Hz), 117.7, 111.8 (dd,  $J_{\text{CF}} = 19.5, 3.0$  Hz), 109.6 (t,  $J_{\text{CF}} = 18.0$  Hz), 42.6 (d,  $J_{\text{CF}} = 3.0$  Hz). HRMS (ESI)  $m/z$  calculate for ( $\text{M}+\text{H}^+$ )  $\text{C}_{16}\text{H}_{11}\text{F}_5\text{N}_3$ : 340.0828, Found: 340.0817.  $^{19}\text{F}$  NMR (376MHz,  $\text{CDCl}_3$ )  $\delta$  -56.31, -113.79.

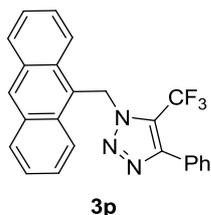
### 1-(2,6-difluorobenzyl)-4-(p-tolyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3o)



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.50 (d,  $J = 8.0$  Hz, 2H), 7.41 – 7.34 (m, 1H), 7.25 (d,  $J = 8.0$  Hz, 2H), 6.96 (t,  $J = 8.0$  Hz, 2H), 5.74 (s, 2H), 2.39 (s, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  161.6 (dd,  $J_{\text{CF}} = 250.5, 6.0$  Hz), 148.2, 139.4, 131.5 (t,  $J_{\text{CF}} = 12.0$

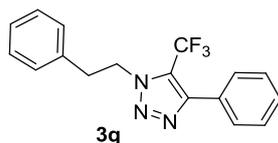
Hz), 129.2, 129.0 (d,  $J_{CF} = 1.5$  Hz), 126.0, 123.1 (q,  $J_{CF} = 39.0$  Hz), 120.4 (q,  $J_{CF} = 270.0$  Hz), 111.7 (dd,  $J_{CF} = 19.5, 4.5$  Hz), 109.6 (t,  $J_{CF} = 12.0$  Hz), 42.5, 21.2. HRMS (ESI)  $m/z$  calculate for (M+H<sup>+</sup>) C<sub>17</sub>H<sub>13</sub>F<sub>5</sub>N<sub>3</sub>: 354.1024, Found: 354.1017.

### 1-(anthracen-9-ylmethyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3p)



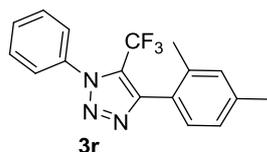
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.60 (s, 1H), 8.16 (d,  $J = 8.8$  Hz, 2H), 8.07 (d,  $J = 12.4$  Hz, 2H), 7.61 – 7.52 (m, 4H), 7.52 – 7.48 (m, 2H), 7.44 – 7.42 (m, 3H), 6.55 (s, 2H).  
<sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 148.3, 131.4, 131.3, 130.1, 129.5, 129.3, 129.2, 128.9, 128.3, 127.4, 125.2, 123.1 (q,  $J_{CF} = 42.0$  Hz), 123.0, 122.4, 120.8 (q,  $J_{CF} = 262.5$  Hz), 47.5. HRMS (ESI)  $m/z$  calculate for (M+H<sup>+</sup>) C<sub>24</sub>H<sub>17</sub>F<sub>3</sub>N<sub>3</sub>: 404.1375, Found: 404.1369.  
<sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -54.91.

### 1-phenethyl-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3q)



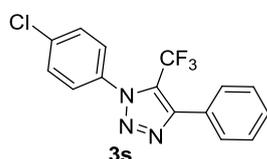
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.61 (dd,  $J = 6.2, 2.6$  Hz, 2H), 7.49 – 7.43 (m, 3H), 7.37 – 7.31 (m, 2H), 7.31 – 7.26 (m, 1H), 7.24 – 7.20 (m, 2H), 4.76 – 4.70 (m, 2H), 3.35 – 3.28 (m, 2H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 148.2, 139.3, 136.3, 129.2, 128.9, 128.8, 127.3, 126.1, 124.0, 122.9 (q,  $J_{CF} = 40.5$  Hz), 120.6 (q,  $J_{CF} = 268.5$  Hz) 51.7, 36.8. HRMS (ESI)  $m/z$  calculate for (M+H<sup>+</sup>) C<sub>17</sub>H<sub>15</sub>F<sub>3</sub>N<sub>3</sub>: 318.1213, Found: 318.1205.

### 1-(2,4-dimethylphenyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3r)



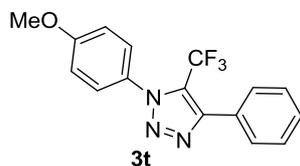
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d,  $J = 4.2$  Hz, 2H), 7.52 – 7.47 (m, 3H), 7.25 (d,  $J = 6.2$  Hz, 1H), 7.21 – 7.15 (m, 2H), 2.43 (s, 3H), 2.09 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  132.6, 131.8, 129.5, 129.1, 128.8, 128.6, 127.3, 126.9, 125.7 (q,  $J_{\text{CF}} = 39.0$  Hz), 120.9 (q,  $J_{\text{CF}} = 268.0$  Hz), 116.0, 21.3, 17.0. HRMS (ESI)  $m/z$  calculate for ( $\text{M}+\text{H}^+$ )  $\text{C}_{17}\text{H}_{15}\text{F}_3\text{N}_3$ : 318.1213, Found: 318.1210.

### 1-(2-chlorophenyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3s)



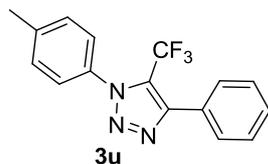
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.78 (d,  $J = 8.0$  Hz, 2H), 7.63 (d,  $J = 8.0$  Hz, 1H), 7.58 (d,  $J = 7.8$ , 1H), 7.55 – 7.46 (m, 5H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  147.7, 133.7, 132.3, 130.6, 129.6, 129.0, 128.7, 128.4, 127.7, 125.25 (q,  $J_{\text{CF}} = 40.0$  Hz), 119.54 (q,  $J_{\text{CF}} = 269.0$  Hz). HRMS (ESI)  $m/z$  calculate for ( $\text{M}+\text{H}^+$ )  $\text{C}_{15}\text{H}_{10}\text{ClF}_3\text{N}_3$ : 324.0510, Found: 324.0509.

### 1-(4-methoxyphenyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3t)



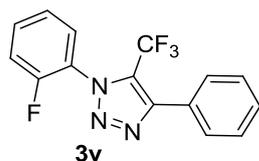
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 – 7.70 (m, 2H), 7.51 – 7.46 (m, 5H), 7.06 (d,  $J = 8.8$  Hz, 2H), 3.90 (s, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  161.2, 148.3, 129.5, 129.0, 128.9, 128.6, 127.0, 124.2 (q,  $J_{\text{CF}} = 37.5$  Hz), 120.1 (q,  $J_{\text{CF}} = 270.0$  Hz), 118.2, 114.5, 55.7. HRMS (ESI)  $m/z$  calculate for ( $\text{M}+\text{H}^+$ )  $\text{C}_{16}\text{H}_{13}\text{F}_3\text{N}_3\text{O}$ : 320.1005, Found: 320.1011.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -54.76.

**4-phenyl-1-(p-tolyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3u)**



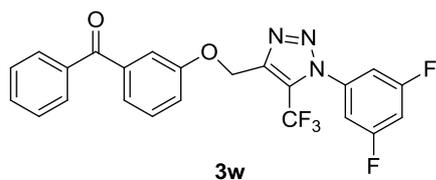
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 – 7.71 (m, 2H), 7.52 – 7.47 (m, 3H), 7.44 (d,  $J$  = 8.4 Hz, 2H), 7.37 (d,  $J$  = 8.2 Hz, 2H), 2.47 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  148.2, 141.1, 133.6, 130.0, 129.5, 129.1, 128.8, 128.6, 125.4, 124.2 (q,  $J_{\text{CF}}$  = 50.0 Hz), 120.0 (q,  $J_{\text{CF}}$  = 268.0 Hz), 21.4. HRMS (ESI)  $m/z$  calculate for ( $\text{M}+\text{H}^+$ )  $\text{C}_{16}\text{H}_{13}\text{F}_3\text{N}_3$ : 304.1056, Found: 304.1044.

**1-(2-fluorophenyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3v)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 – 7.74 (m, 2H), 7.65 – 7.49 (m, 5H), 7.36 (q,  $J$  = 8.0 Hz, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.7 (d,  $J_{\text{CF}}$  = 261.0 Hz), 148.0, 133.0 (d,  $J_{\text{CF}}$  = 12.0 Hz), 129.7, 129.0 (d,  $J_{\text{CF}}$  = 2.0 Hz), 128.7, 128.6, 128.4, 124.8 (d,  $J_{\text{CF}}$  = 4.0 Hz), 124.1 (q,  $J_{\text{CF}}$  = 51.0 Hz), 120.0, 119.9 (q,  $J_{\text{CF}}$  = 272.0 Hz), 116.9 (d,  $J_{\text{CF}}$  = 25.0 Hz). HRMS (ESI)  $m/z$  calculate for ( $\text{M}+\text{H}^+$ )  $\text{C}_{15}\text{H}_{10}\text{F}_4\text{N}_3$ : 308.0805, Found: 308.0804.

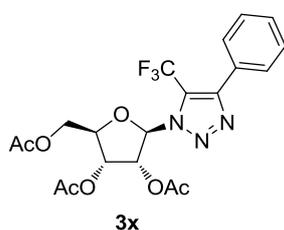
**4-(((1-(3,5-difluorophenyl)-5-(trifluoromethyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl)(phenyl)methanone (3w)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (d,  $J$  = 8.8 Hz, 2H), 7.77 (d,  $J$  = 7.4 Hz, 2H), 7.57 (t,  $J$  = 12.4 Hz, 1H), 7.53 – 7.46 (m, 4H), 7.29 – 7.25 (m, 1H), 7.13 (d,  $J$  = 8.8 Hz,

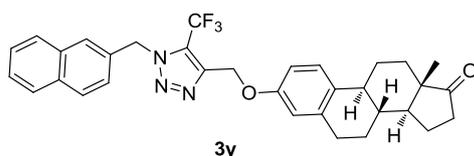
2H), 5.41 (s, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  195.5, 163.8 (d,  $J_{\text{CF}} = 254.0$  Hz), 161.4, 143.5, 138.0, 132.6, 132.0, 131.4 (d,  $J_{\text{CF}} = 4.0$  Hz), 131.1, 129.8, 128.3, 127.8 (d,  $J_{\text{CF}} = 9.0$  Hz), 127.3 (q,  $J_{\text{CF}} = 41.0$  Hz), 119.6 (q,  $J_{\text{CF}} = 272.0$  Hz), 116.8 (d,  $J_{\text{CF}} = 23.0$  Hz), 114.4, 60.8. HRMS (ESI)  $m/z$  calculate for  $(\text{M}+\text{H}^+)$   $\text{C}_{23}\text{H}_{15}\text{F}_5\text{N}_3\text{O}_2$ : 460.1079, Found: 460.1070.

**2-(acetoxymethyl)-5-(4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-3,4-diyl diacetate (3x)**



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.56 – 7.54 (m, 2H), 7.41 – 7.39 (m, 3H), 6.23 – 6.21 (m, 1H), 6.14 (d,  $J = 2.8$  Hz, 1H), 5.75 (t,  $J = 5.8$  Hz, 1H), 4.48 – 4.44 (m, 1H), 4.34 (dd,  $J = 4.0, 3.2$  Hz, 1H), 4.11 (dd,  $J = 4.8, 4.2$  Hz, 1H), 2.10 (s, 3H), 2.07 (s, 3H), 1.94 (s, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  170.5, 169.4, 169.3, 148.5, 129.7, 129.0, 128.6, 128.2, 123.7 (q,  $J_{\text{CF}} = 40.5$  Hz), 120.1 (q,  $J_{\text{CF}} = 262.5$  Hz), 89.8, 81.4, 74.0, 70.9, 62.3, 58.2, 20.2, 18.4. HRMS (ESI)  $m/z$  calculate for  $(\text{M}+\text{Na}^+)$   $\text{C}_{20}\text{H}_{20}\text{F}_3\text{N}_3\text{O}_7\text{Na}$ : 494.1146, Found: 494.1156.  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -55.76.

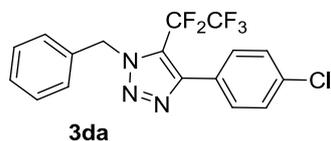
**1,3-methyl-3-((1-(naphthalen-2-ylmethyl)-5-(trifluoromethyl)-1H-1,2,3-triazol-4-yl)methoxy)-6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one (3y)**



$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  7.85 – 7.80 (m, 3H), 7.72 (s, 1H), 7.52 – 7.50 (m, 2H), 7.40 (d,  $J = 6.2$  Hz, 1H), 7.20 (d,  $J = 12.0$  Hz, 1H), 6.81 (d,  $J = 4.0$  Hz, 1H), 6.74 (s, 1H), 5.83 (s, 2H), 5.19 (s, 2H), 2.90 – 2.86 (m, 2H), 2.50 (dd,  $J = 6.8, 6.0$  Hz, 1H),

2.41 – 2.36 (m, 1H), 2.27 – 2.22 (m, 1H), 2.17 – 2.11 (m, 1H), 2.08 – 2.02 (m, 1H), 2.02 – 1.97 (m, 1H), 1.95 (d,  $J = 11.4$  Hz, 1H), 1.65 – 1.57 (m, 2H), 1.53 – 1.47 (m, 3H), 1.43 – 1.41 (m, 1H), 0.90 (s, 3H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  214.7, 156.0, 144.4, 137.9, 133.3, 133.1, 133.0, 130.8, 129.0, 128.1, 127.7, 127.2, 126.8, 126.7, 126.4, 125.9 (q,  $J_{\text{CF}} = 40.5\text{Hz}$ ), 125.0, 119.9 (q,  $J_{\text{CF}} = 270.0\text{Hz}$ ), 115.0, 112.5, 61.0, 54.1, 50.4, 47.8, 44.0, 38.4, 35.7, 31.5, 29.4, 26.7, 25.8, 21.6, 13.9. HRMS (ESI)  $m/z$  calculate for ( $\text{M}+\text{H}^+$ )  $\text{C}_{33}\text{H}_{33}\text{F}_3\text{N}_3\text{O}_2$ : 560.2519, Found: 560.2510.  $^{19}\text{F}$  NMR (565 MHz,  $\text{CDCl}_3$ )  $\delta$  - 57.48.

### 1-benzyl-4-(4-chlorophenyl)-5-(perfluoroethyl)-1H-1,2,3-triazole (3da)



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.49 (d,  $J = 8.0$  Hz, 2H), 7.43 – 7.36 (m, 5H), 7.31 – 7.29 (m, 2H), 5.69 (s, 2H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  149.1, 135.8, 133.7, 130.6, 128.7, 127.4, 121.5 (t,  $J_{\text{CF}} = 37.5$  Hz), 119.4 (t,  $J_{\text{CF}} = 51.0$  Hz), 117.5 (t,  $J_{\text{CF}} = 28.5$  Hz), 112.4 (d,  $J_{\text{CF}} = 46.5$  Hz), 110.7 (d,  $J_{\text{CF}} = 40.5$  Hz), 109.3, 54.8. HRMS (ESI)  $m/z$  calculate for ( $\text{M}+\text{H}^+$ )  $\text{C}_{17}\text{H}_{12}\text{ClF}_5\text{N}_3$ : 388.0634, Found: 388.0630.  $^{19}\text{F}$  NMR (565 MHz,  $\text{CDCl}_3$ )  $\delta$  -83.95, - 107.94.

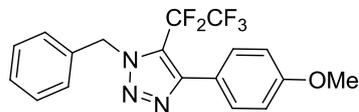
### 1-benzyl-4-(4-bromophenyl)-5-(perfluoroethyl)-1H-1,2,3-triazole (3ea)



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.59 – 7.56 (m, 2H), 7.44 – 7.36 (m, 5H), 7.31 – 7.29 (m, 2H), 5.69 (s, 2H).  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  149.1, 133.9, 131.6, 131.0, 128.6, 127.4, 124.2, 121.7 (t,  $J_{\text{CF}} = 34.5$  Hz), 119.4 (t,  $J_{\text{CF}} = 39.0$  Hz), 117.5 (t,  $J_{\text{CF}} = 36.0$  Hz), 112.5 (d,  $J_{\text{CF}} = 37.5$  Hz), 110.8 (d,  $J_{\text{CF}} = 39.0$  Hz), 54.8. HRMS (ESI)  $m/z$  calculate for ( $\text{M}+\text{H}^+$ )  $\text{C}_{17}\text{H}_{12}\text{BrF}_5\text{N}_3$ : 432.0129, Found: 432.0121.  $^{19}\text{F}$  NMR (565 MHz,

CDCl<sub>3</sub>)  $\delta$  -83.94, - 107.93.

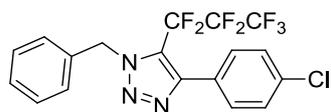
**1-benzyl-4-(4-methoxyphenyl)-5-(perfluoroethyl)-1H-1,2,3-triazole (3fa)**



**3fa**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.74 (d,  $J$  = 8.0 Hz, 2H), 7.23 – 7.15 (m, 7H), 5.54 (s, 2H), 2.29 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  160.4, 148.6, 134.1, 130.5, 129.1, 128.6, 127.2, 122.5 (t,  $J_{CF}$  = 37.5 Hz), 121.4, 121.3, 119.6, 113.7, 58.5, 54.9. HRMS (ESI)  $m/z$  calculate for (M+H<sup>+</sup>) C<sub>18</sub>H<sub>15</sub>F<sub>5</sub>N<sub>3</sub>O: 384.1130, Found: 384.1129. <sup>19</sup>F NMR (565 MHz, CDCl<sub>3</sub>)  $\delta$  - 83.95, - 107.86.

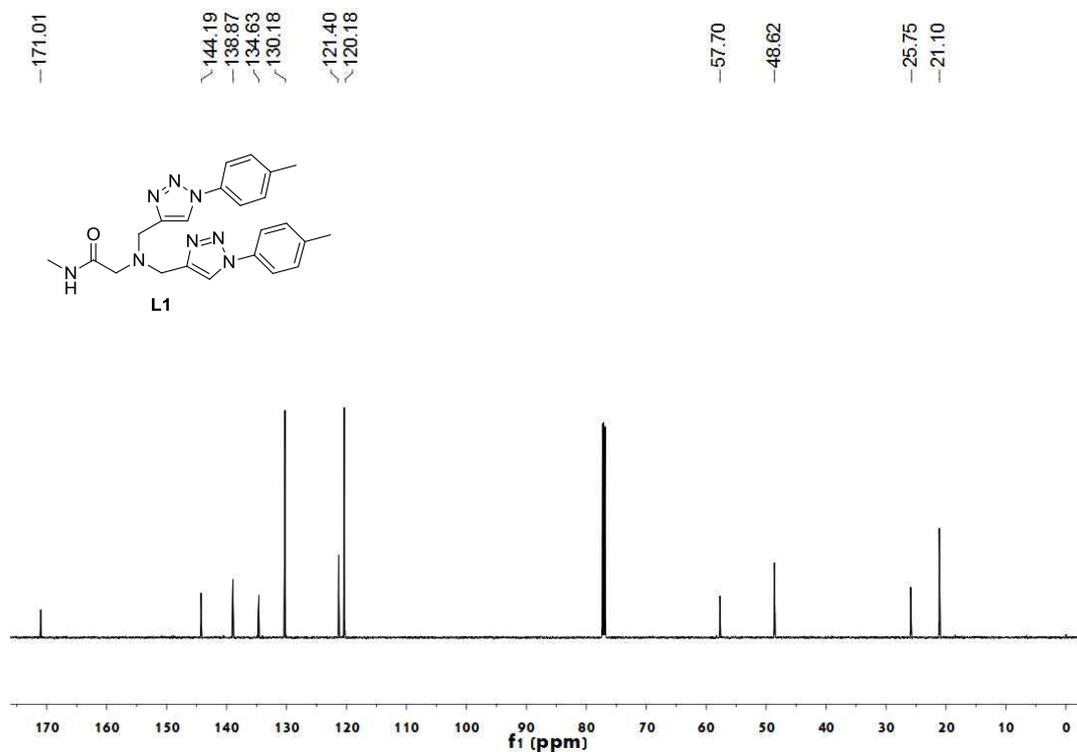
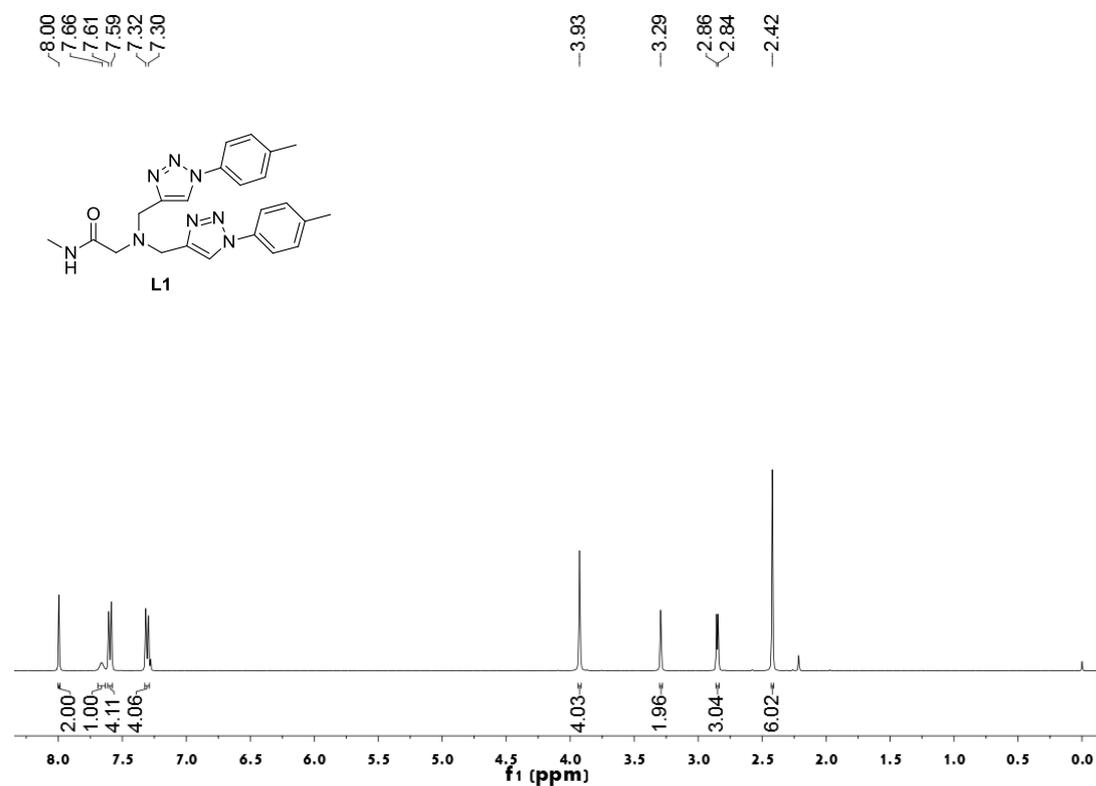
**1- benzyl-4-(4-chlorophenyl)-5-(perfluoropropyl)-1H-1,2,3-triazole (3db)**



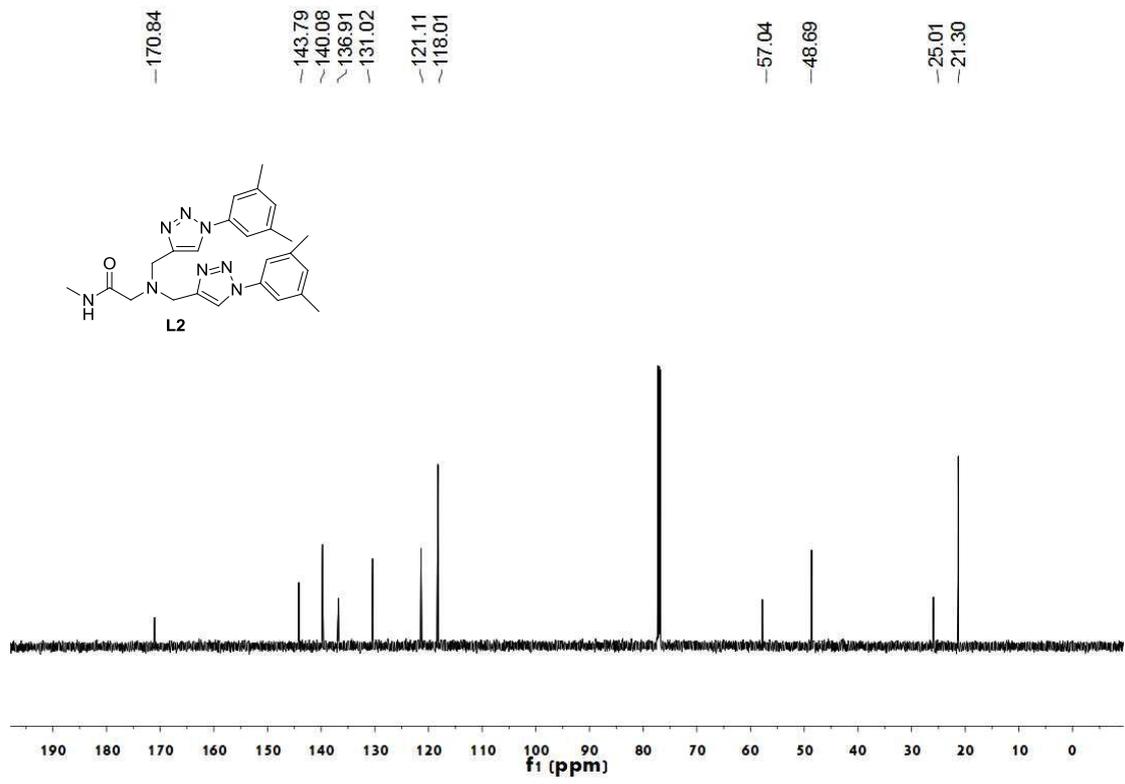
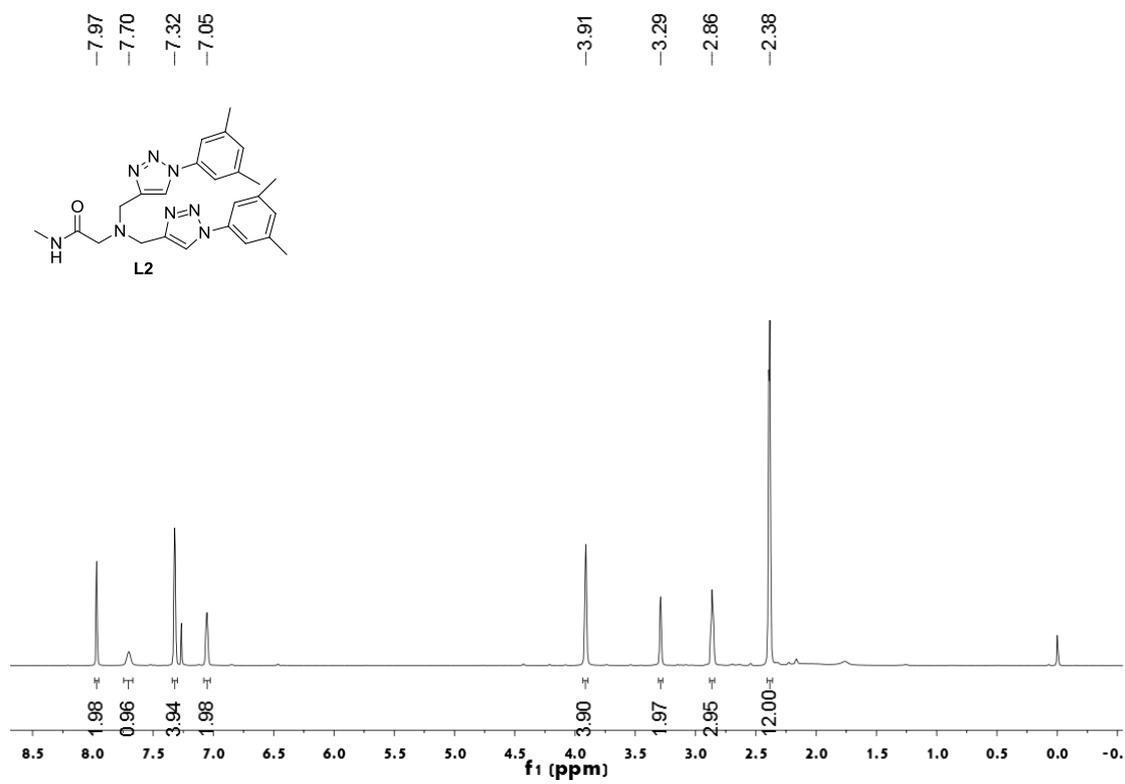
**3db**

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.42 (d,  $J$  = 8.4 Hz, 2H), 7.37 – 7.28 (m, 5H), 7.26 – 7.21 (m, 2H), 5.62 (s, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  148.3, 134.6, 133.1, 129.8, 128.9 (m), 127.9, 127.8, 127.6, 126.6, 120.6 (d,  $J_{CF}$  = 38.0 Hz), 53.9. HRMS (ESI)  $m/z$  calculate for (M+H<sup>+</sup>) C<sub>18</sub>H<sub>12</sub>ClF<sub>7</sub>N<sub>3</sub><sup>+</sup>:438.0602, Found: 438.0601. <sup>19</sup>F NMR (565 MHz, CDCl<sub>3</sub>):  $\delta$  -124.83 (s, 2F),  $\delta$  -104.63 (q,  $J$  = 6.4 Hz, 2F),  $\delta$  -79.89 (t,  $J$  = 9.8 Hz, 3F).

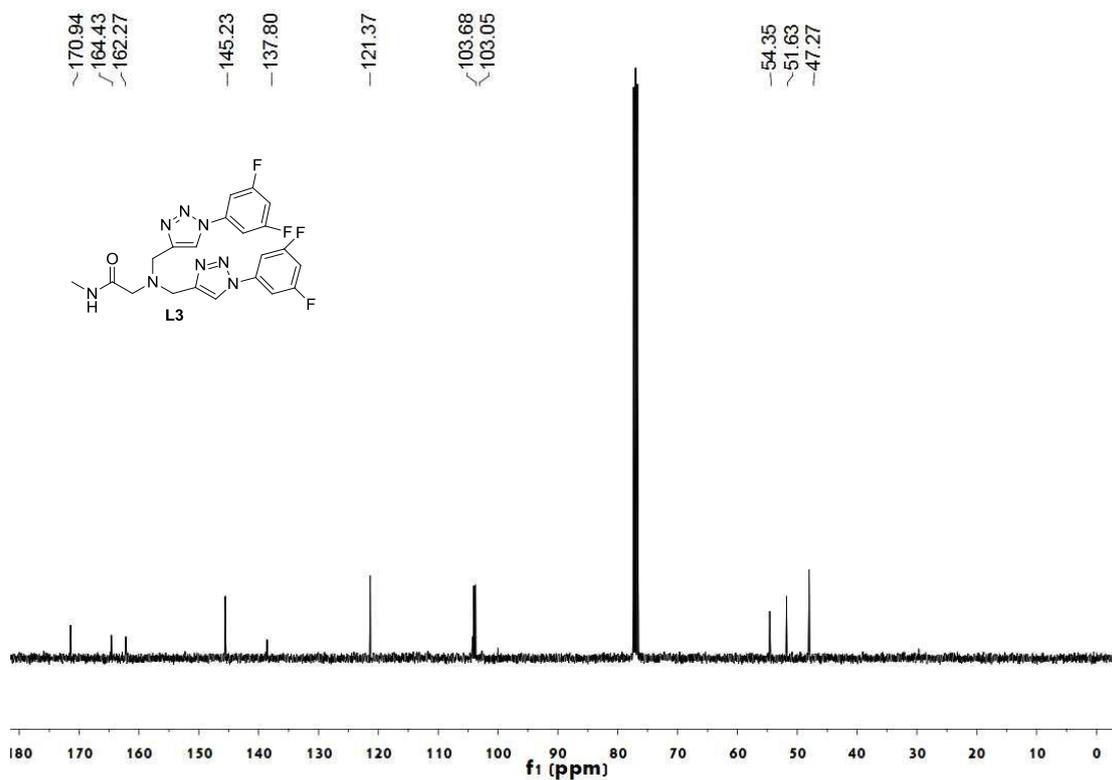
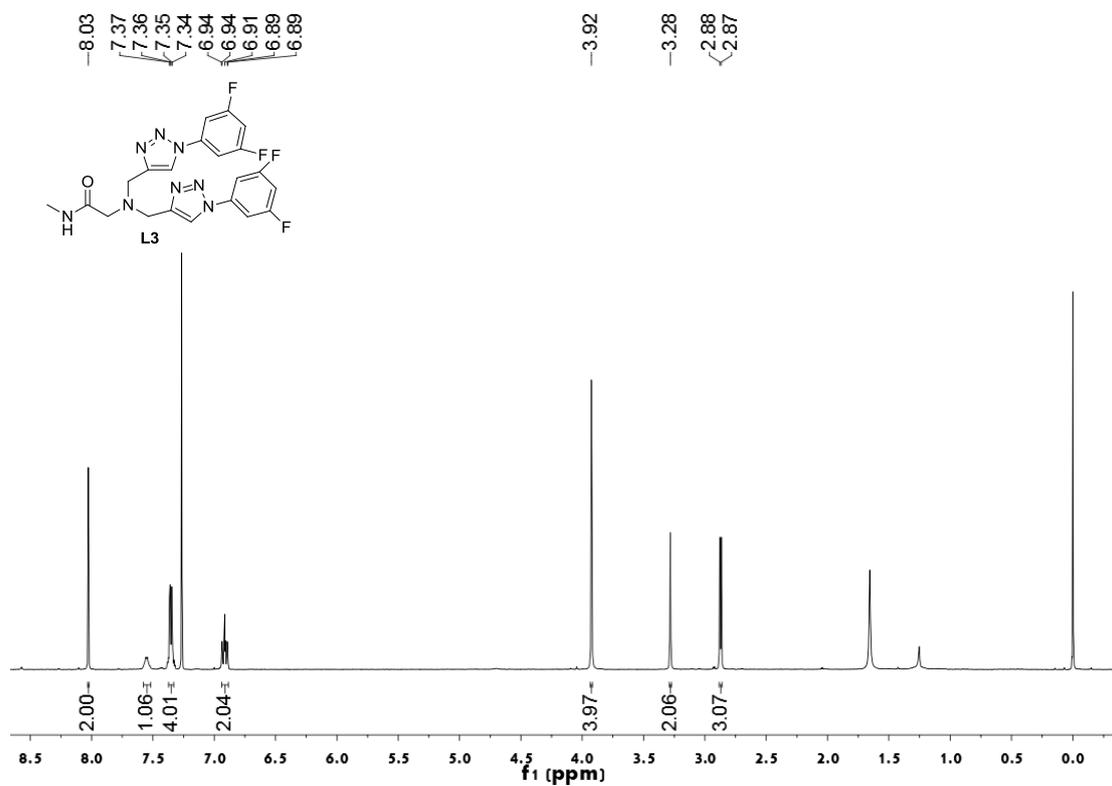
## 2-(bis((1-(p-*tolyl*)-1H-1,2,3-triazol-4-yl)methyl)amino)-N-methylacetamide (L1)



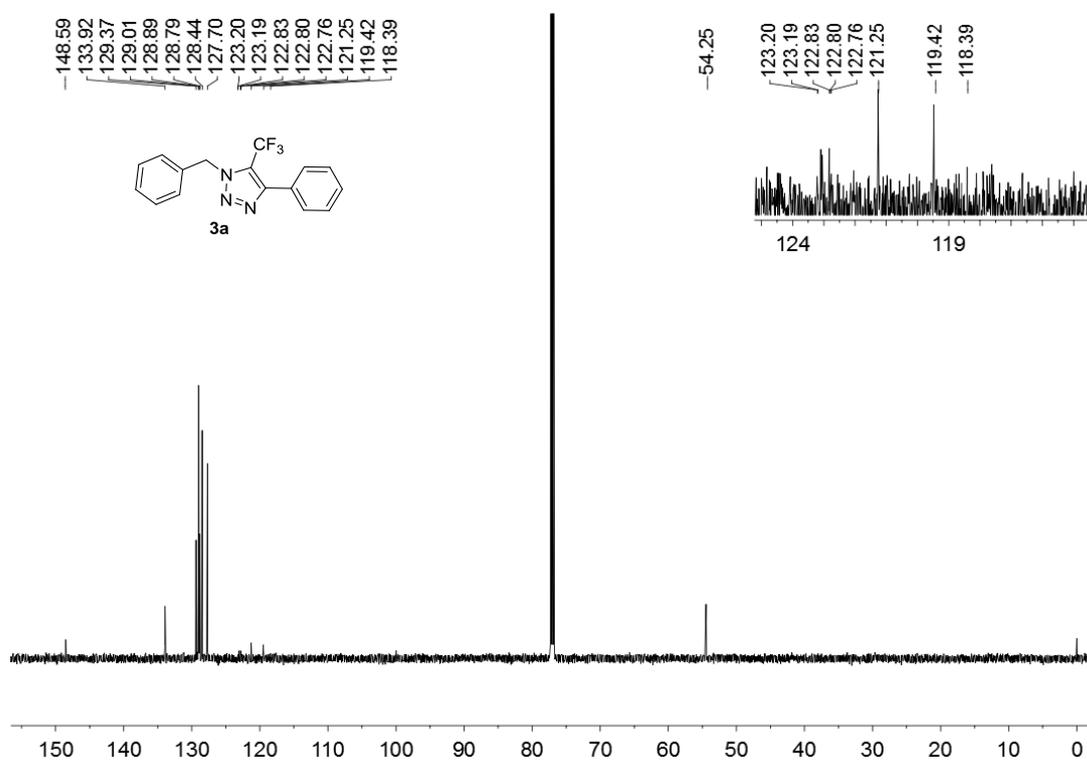
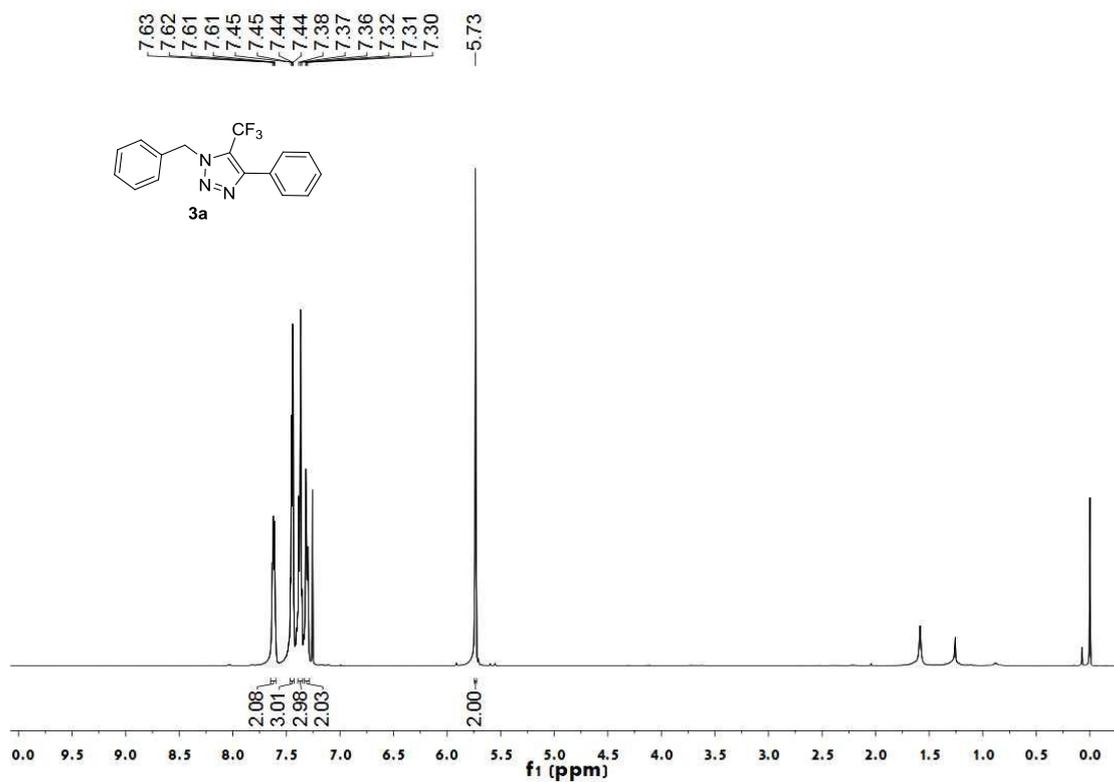
**2-(bis((1-(2,4-dimethylphenyl)-1H-1,2,3-triazol-4-yl)methyl)amino)-N-methylacetamide (L2)**



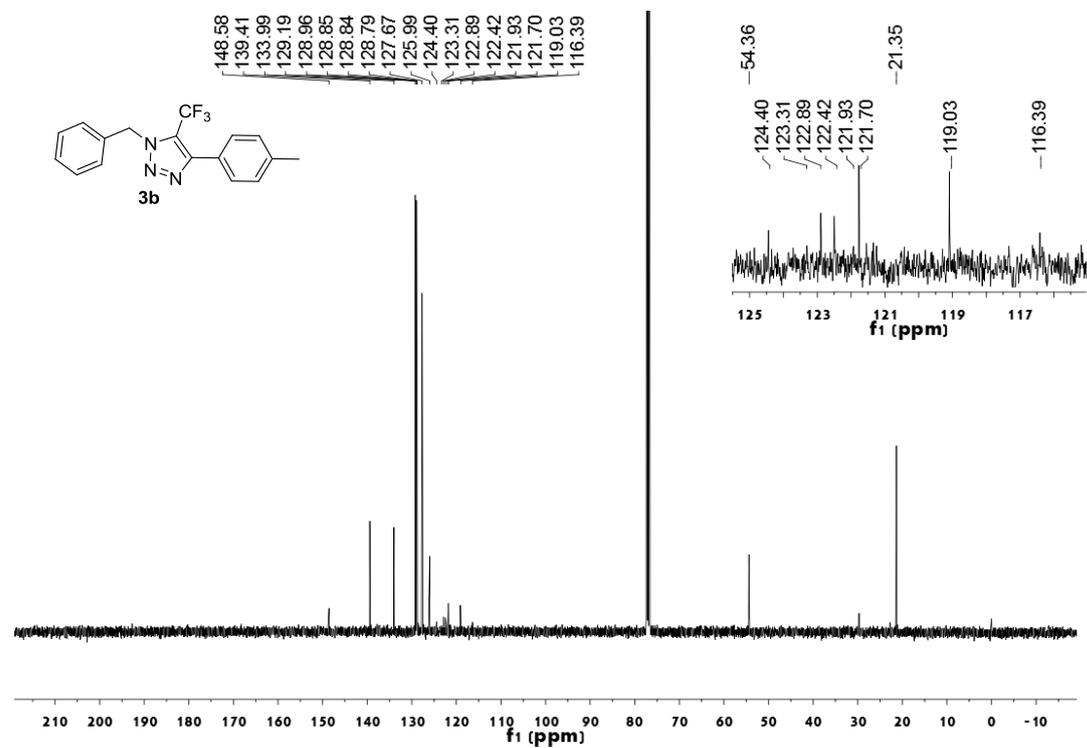
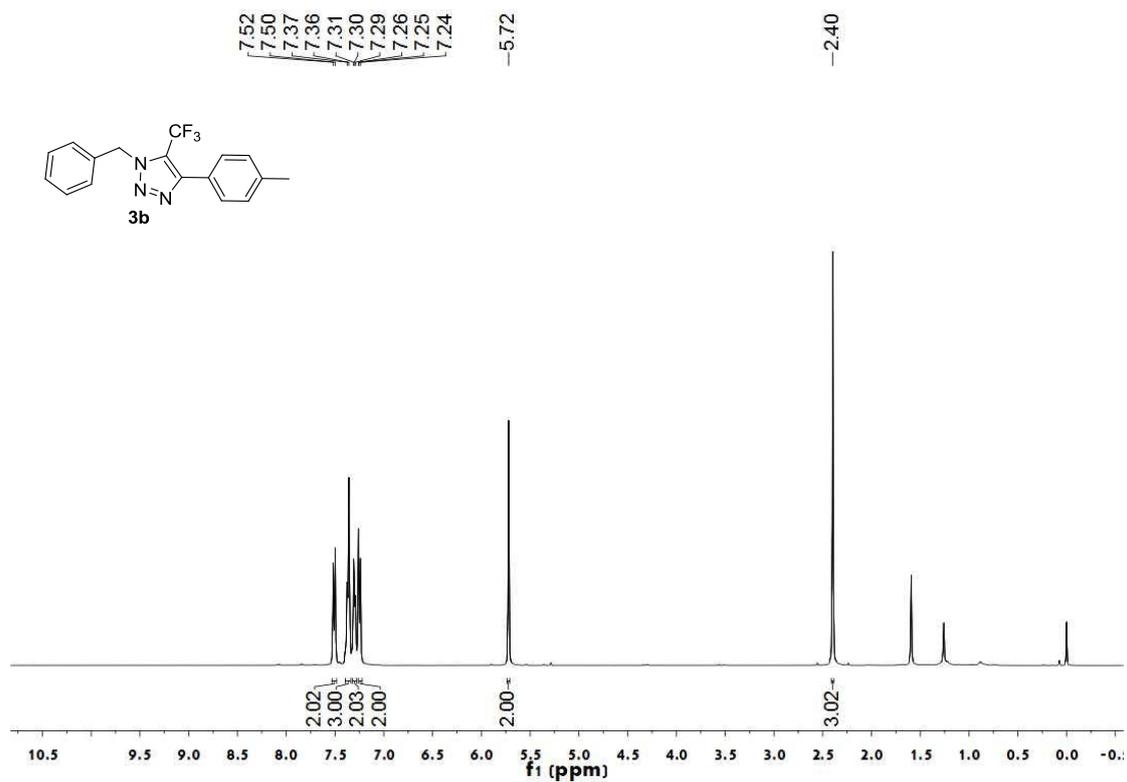
**2-(bis((1-(3,5-difluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)amino)-N-methylacetamide (L3)**



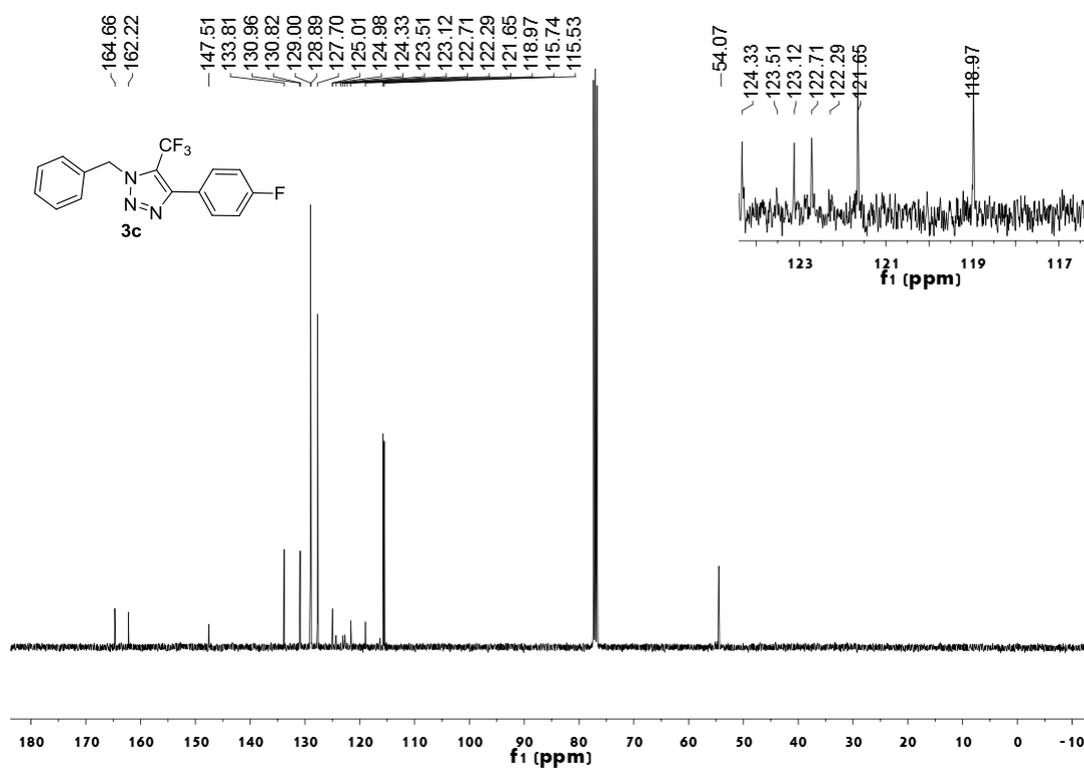
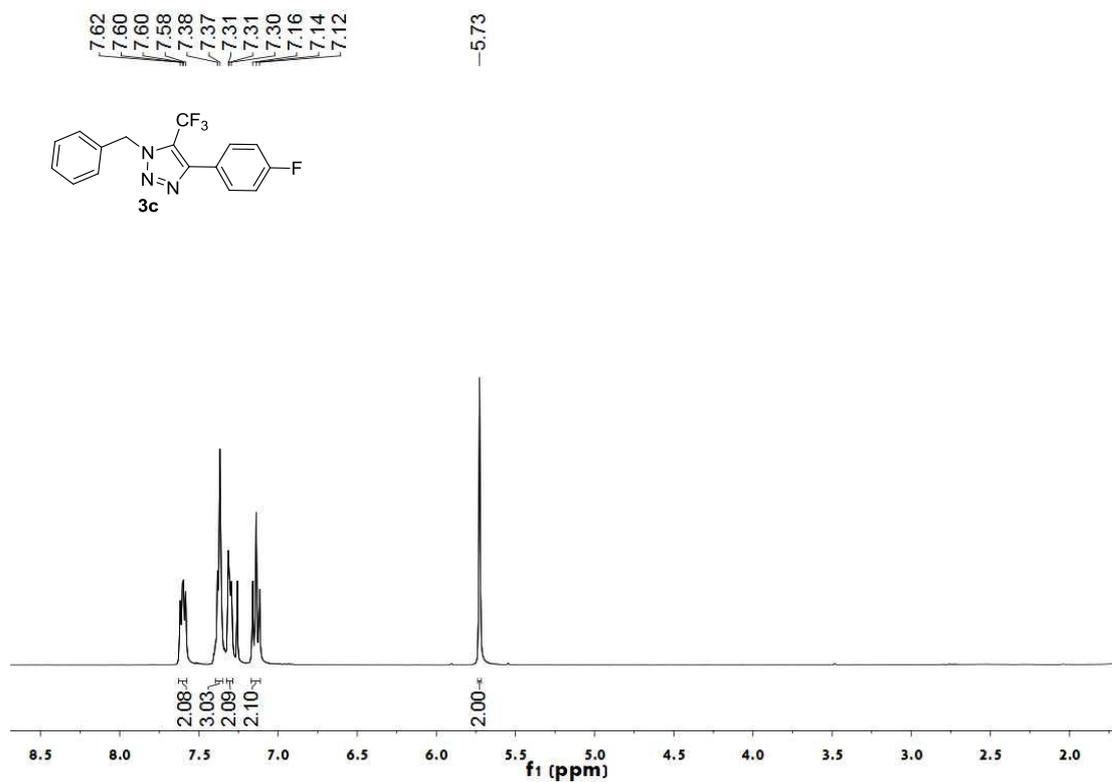
# 1-benzyl-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3a)



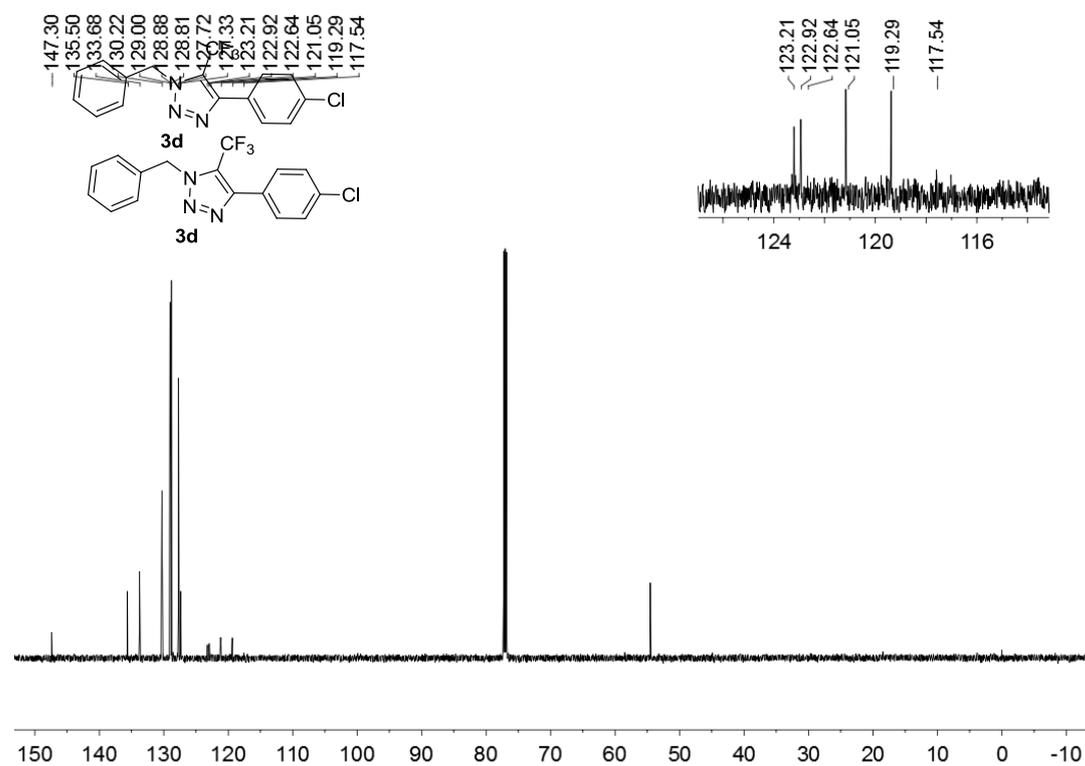
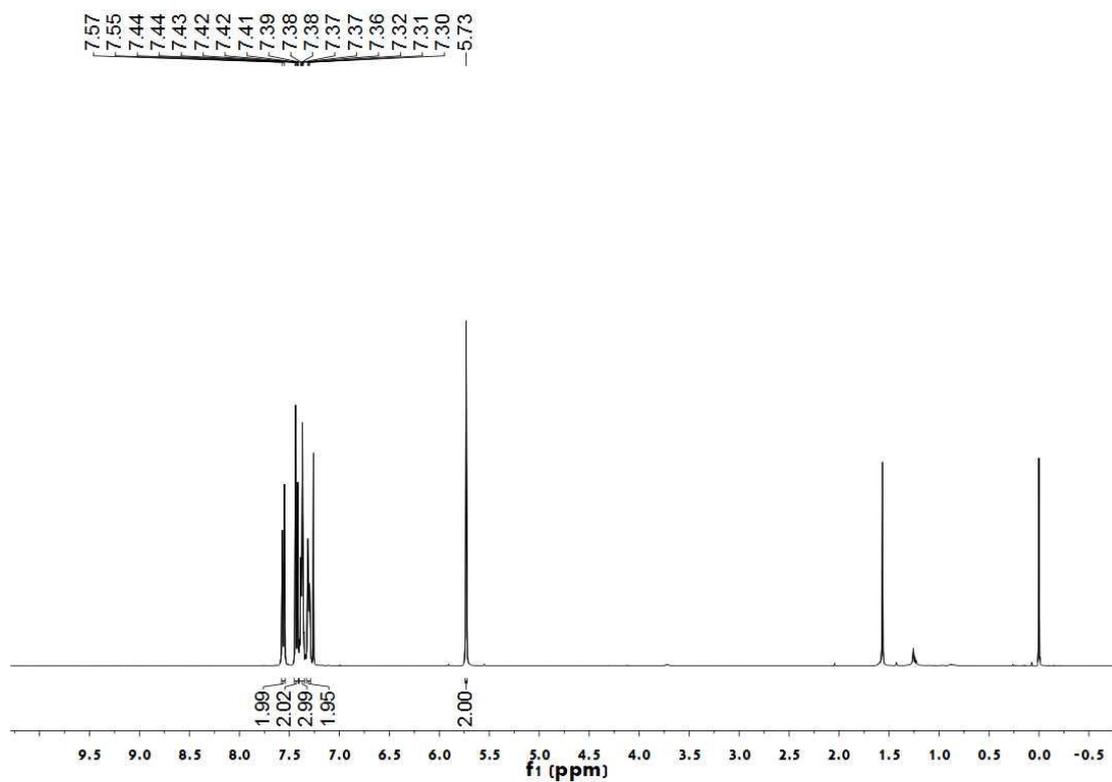
# 1-benzyl-4-(p-tolyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3b)



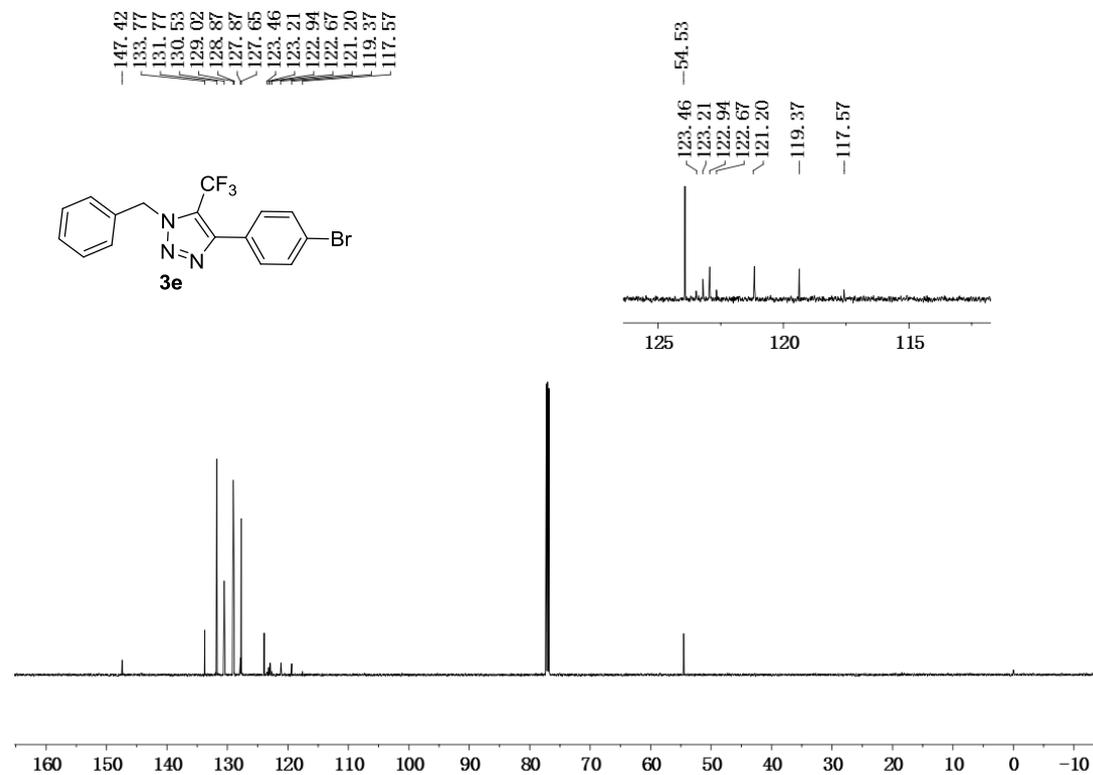
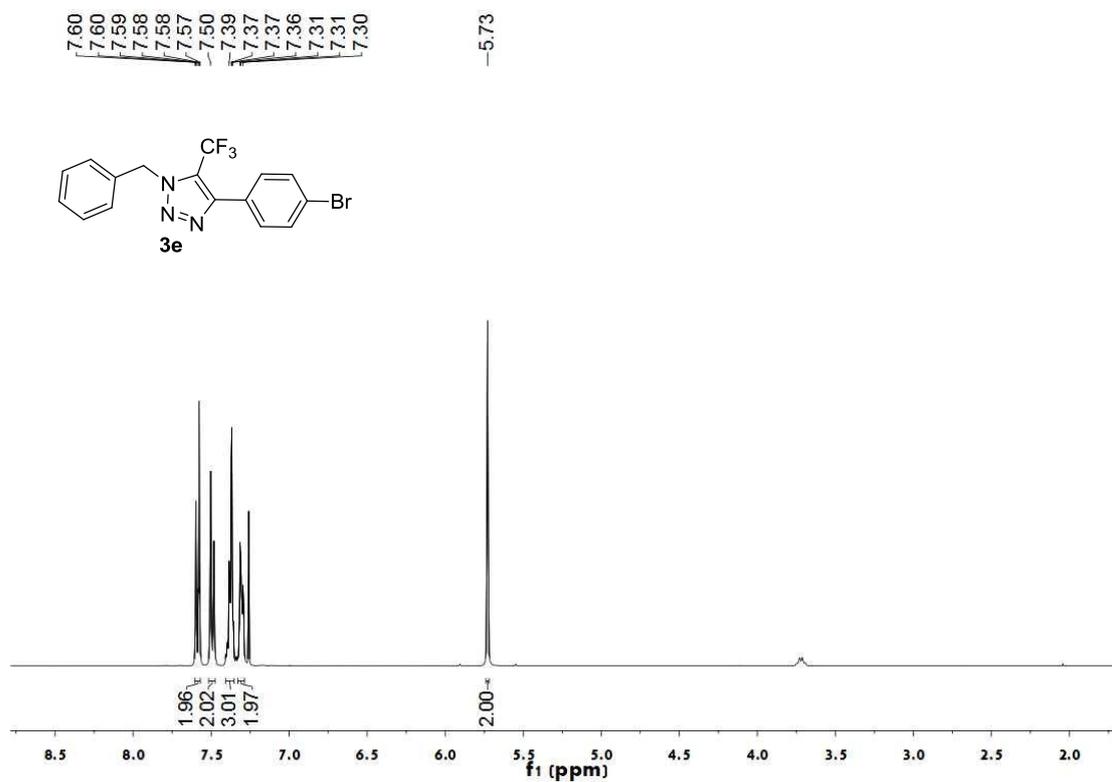
# 1-benzyl-4-(4-fluorophenyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3c)



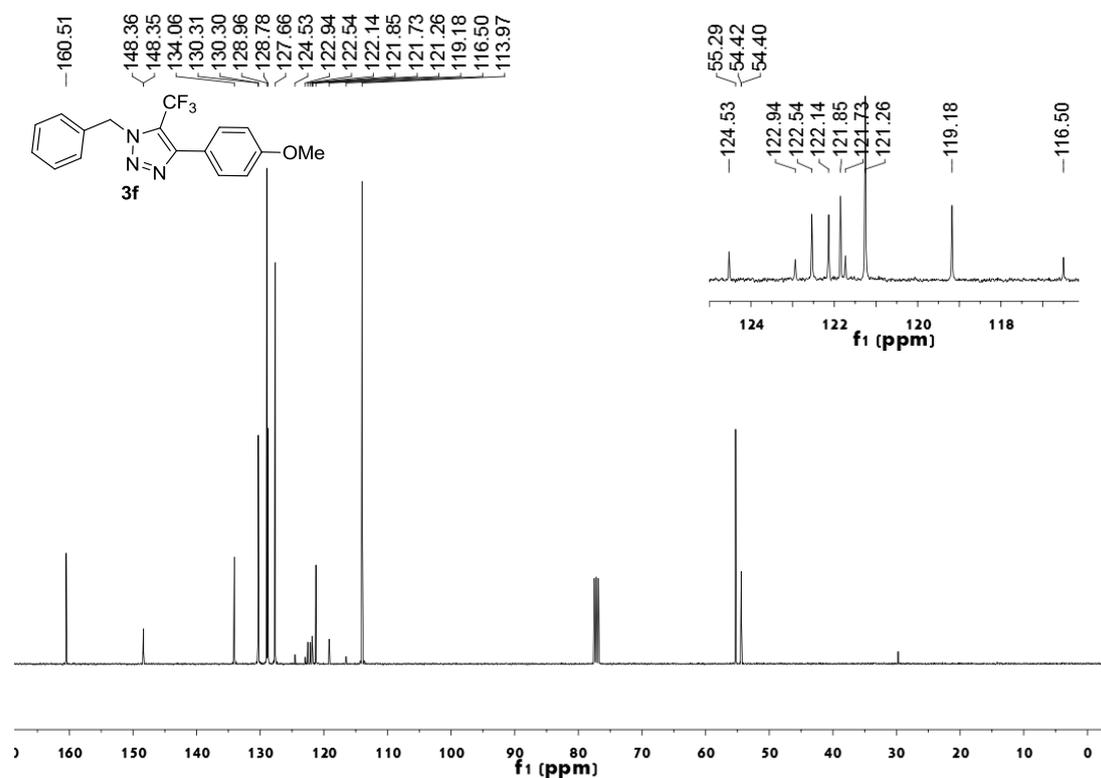
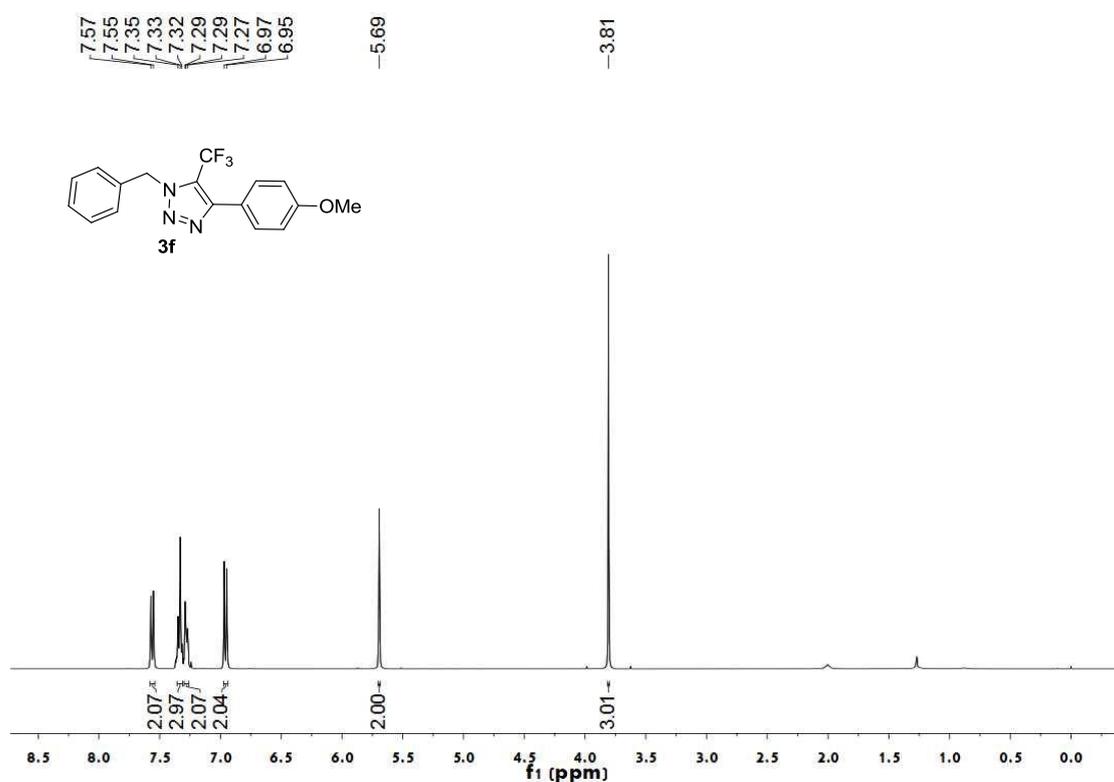
**1-benzyl-4-(4-chlorophenyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3d)**



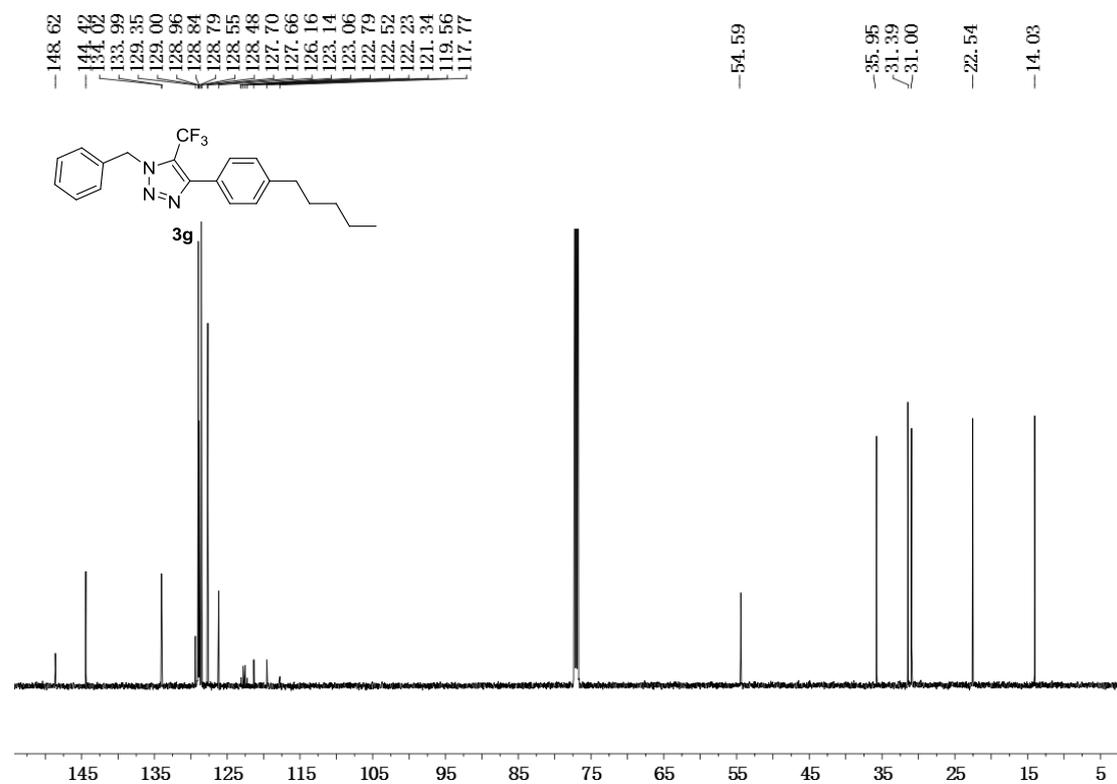
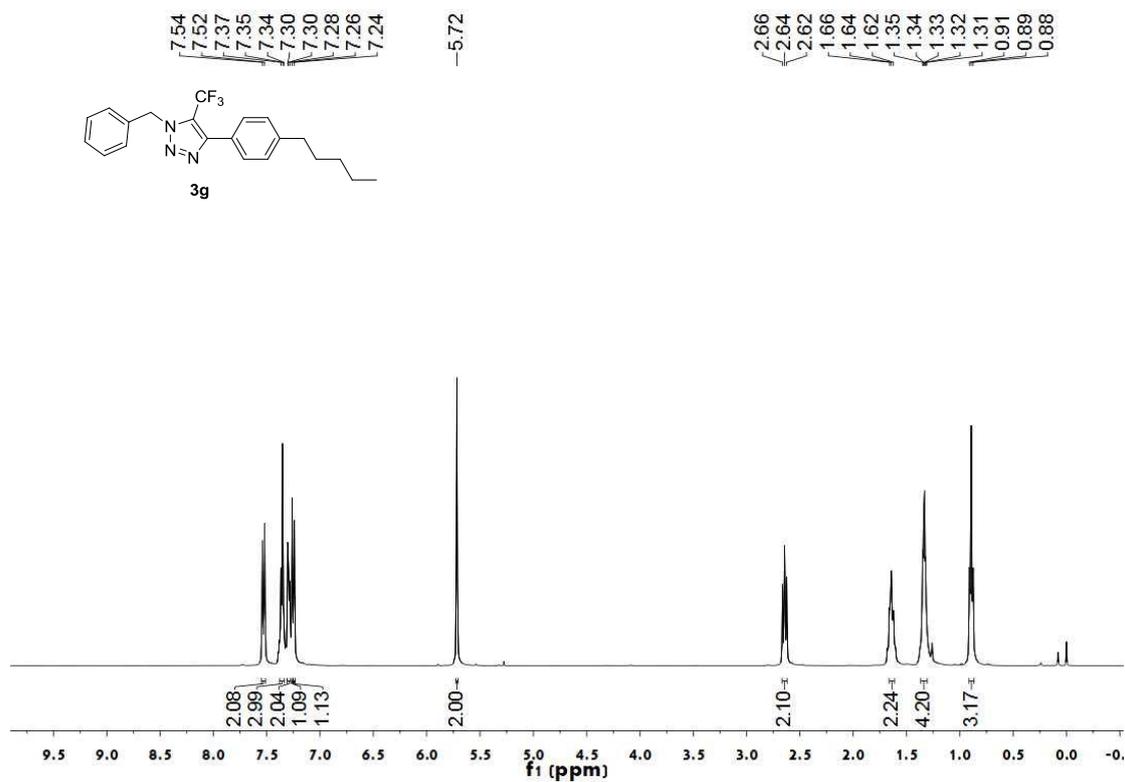
# 1-benzyl-4-(4-bromophenyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3e)



### 1-benzyl-4-(4-methoxyphenyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3f)

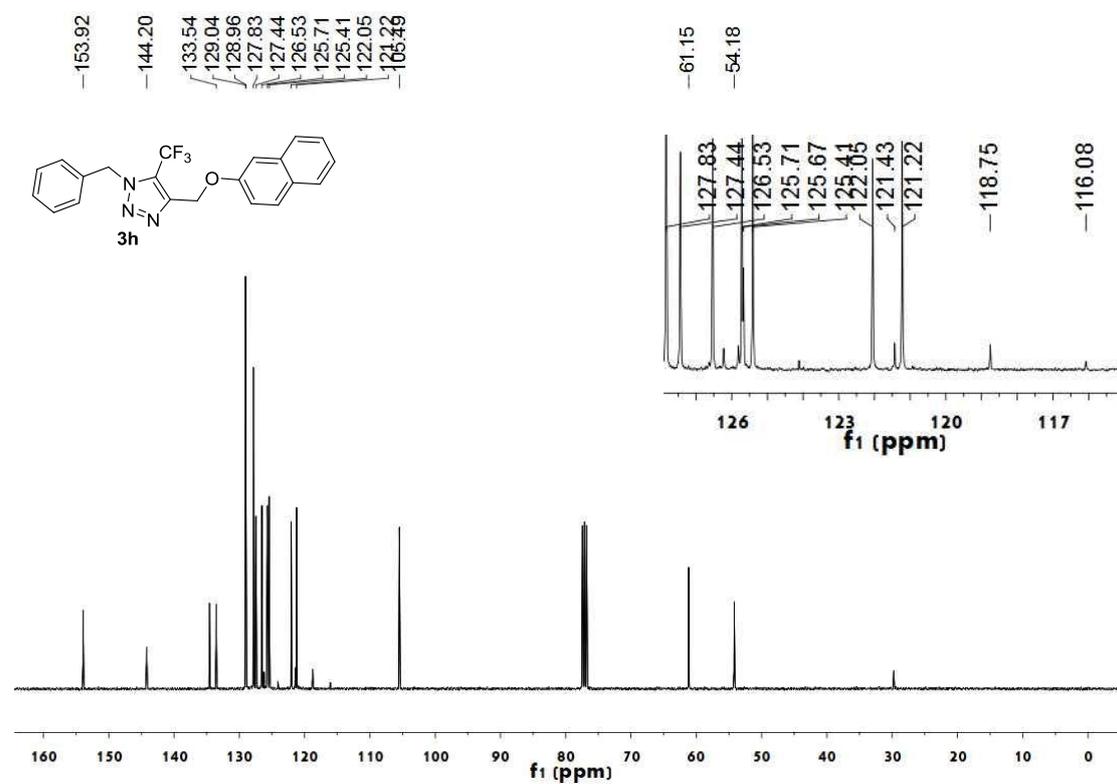
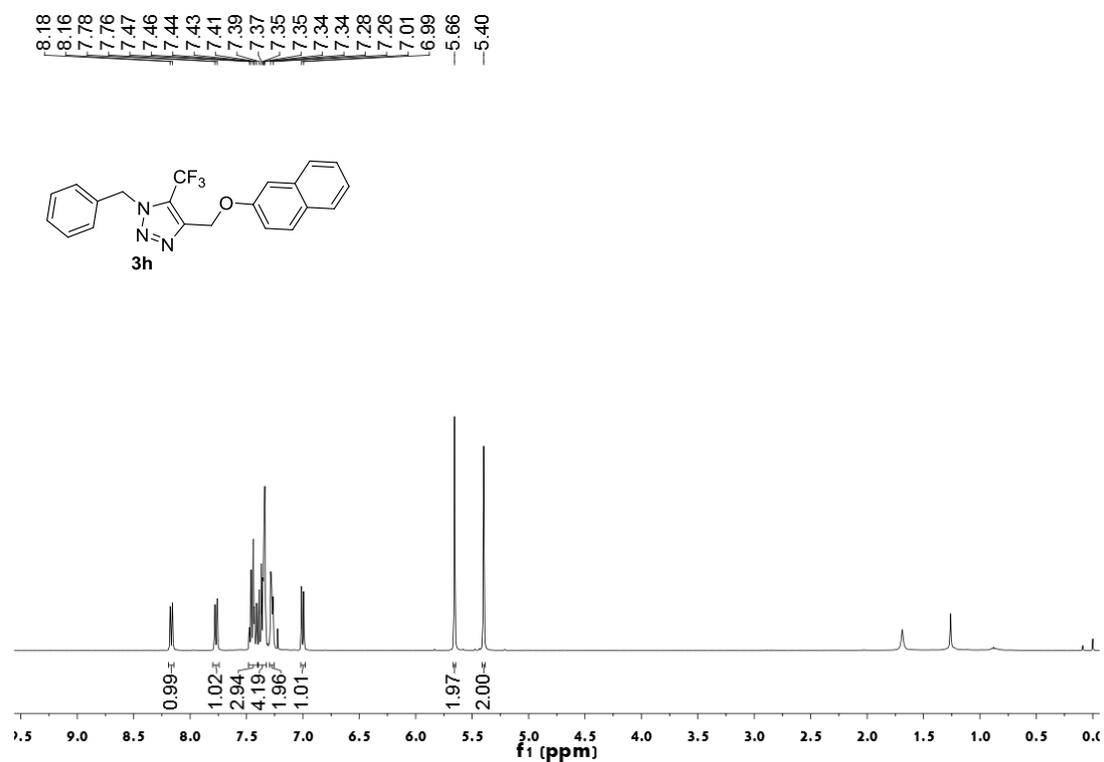


# 1-benzyl-4-(4-pentylphenyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3g)

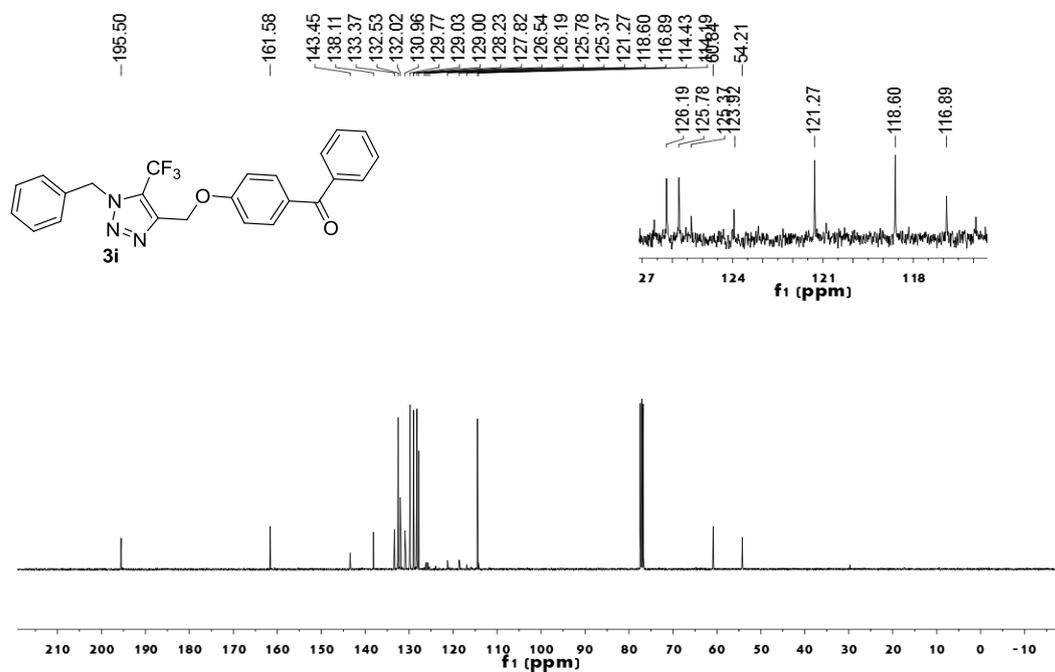
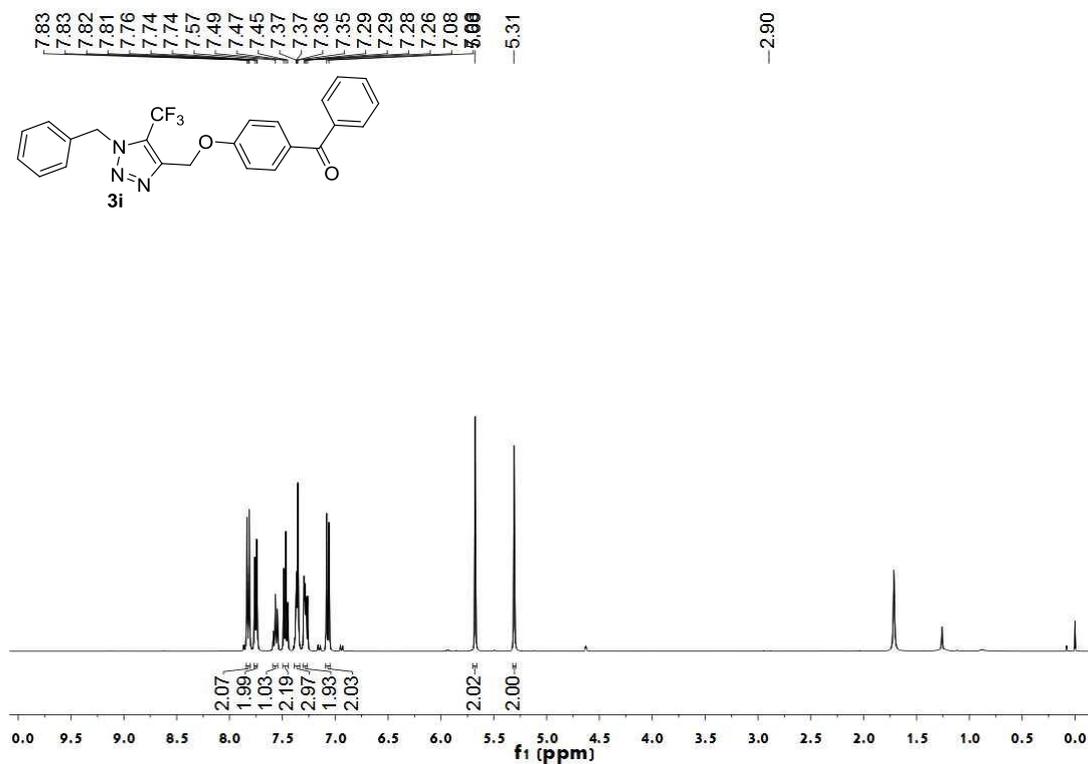


# 1-benzyl-4-((naphthalen-2-yloxy)methyl)-5-(trifluoromethyl)-1H-1,2,3-triazole

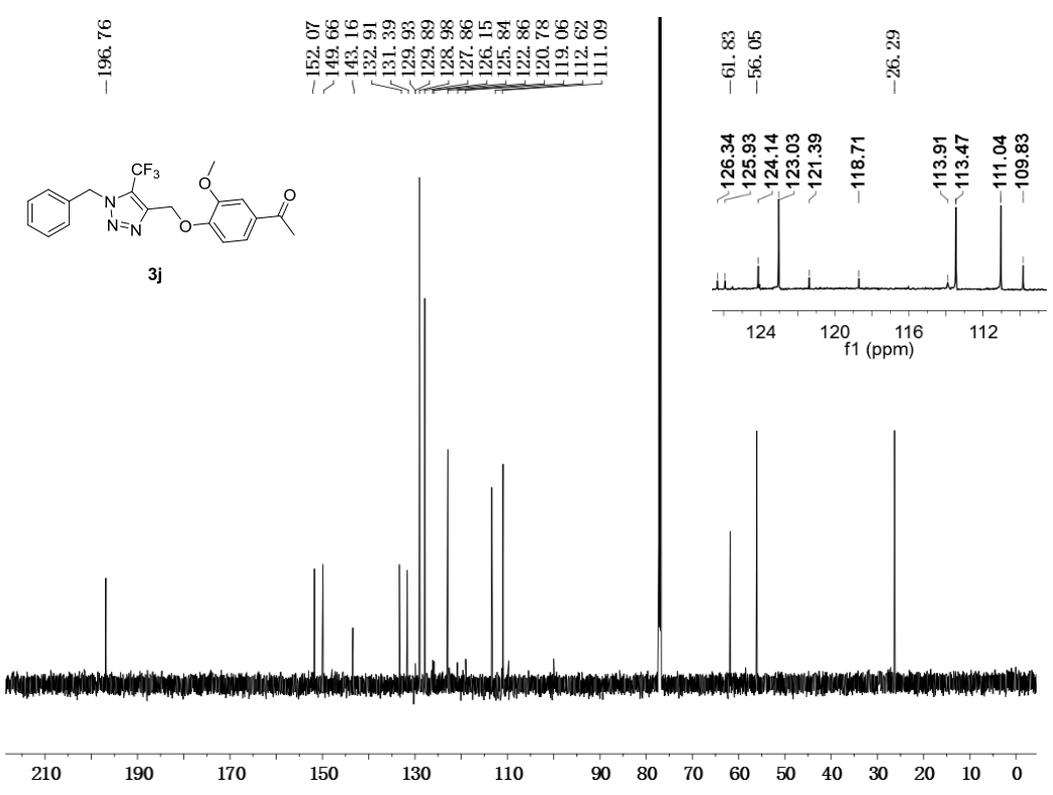
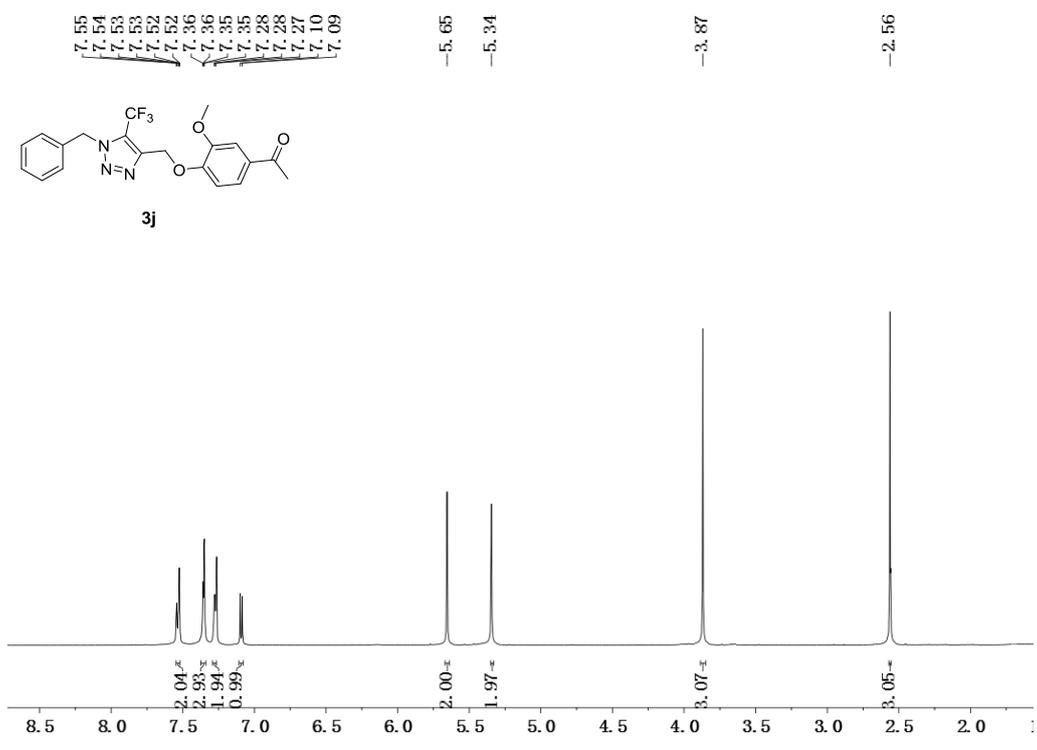
(3h)



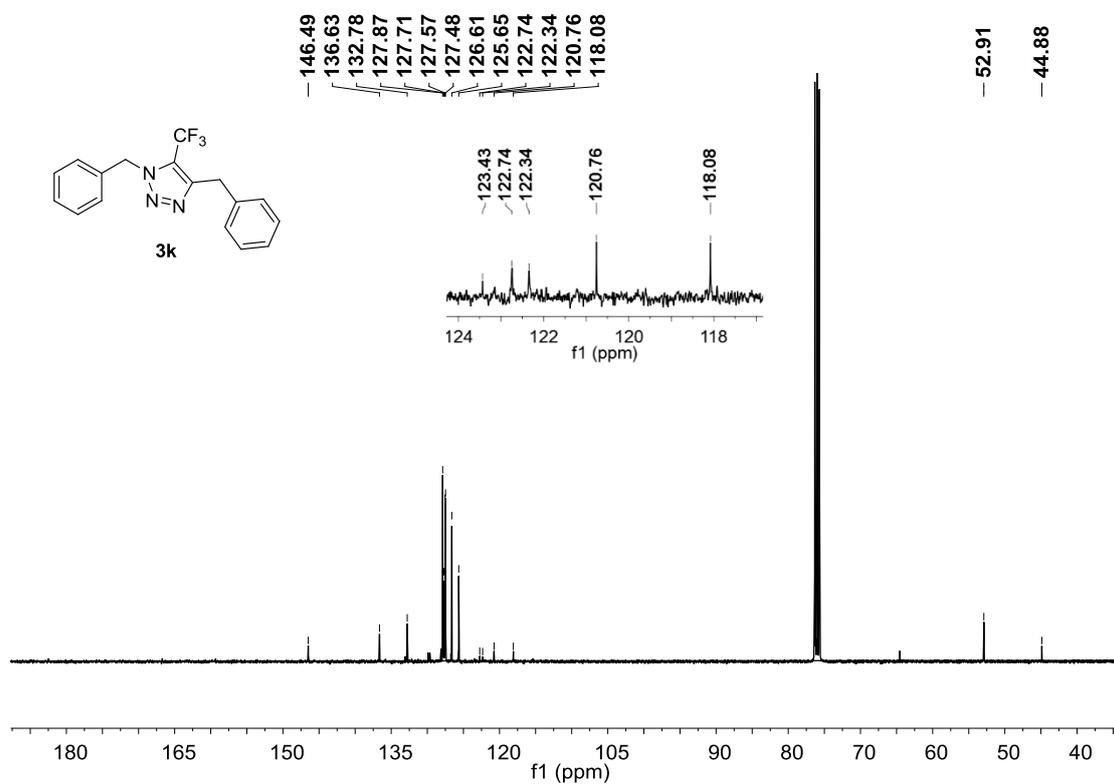
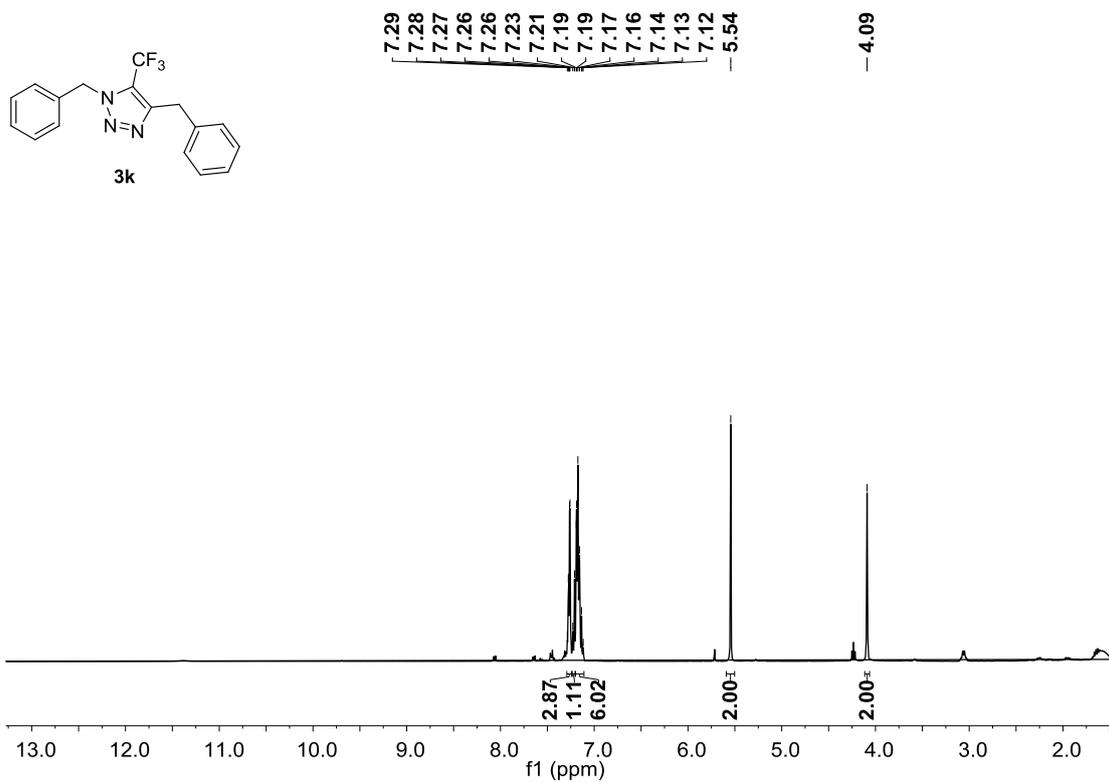
**(4-((1-benzyl-5-(trifluoromethyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl)(phenyl) methanone (3i)**



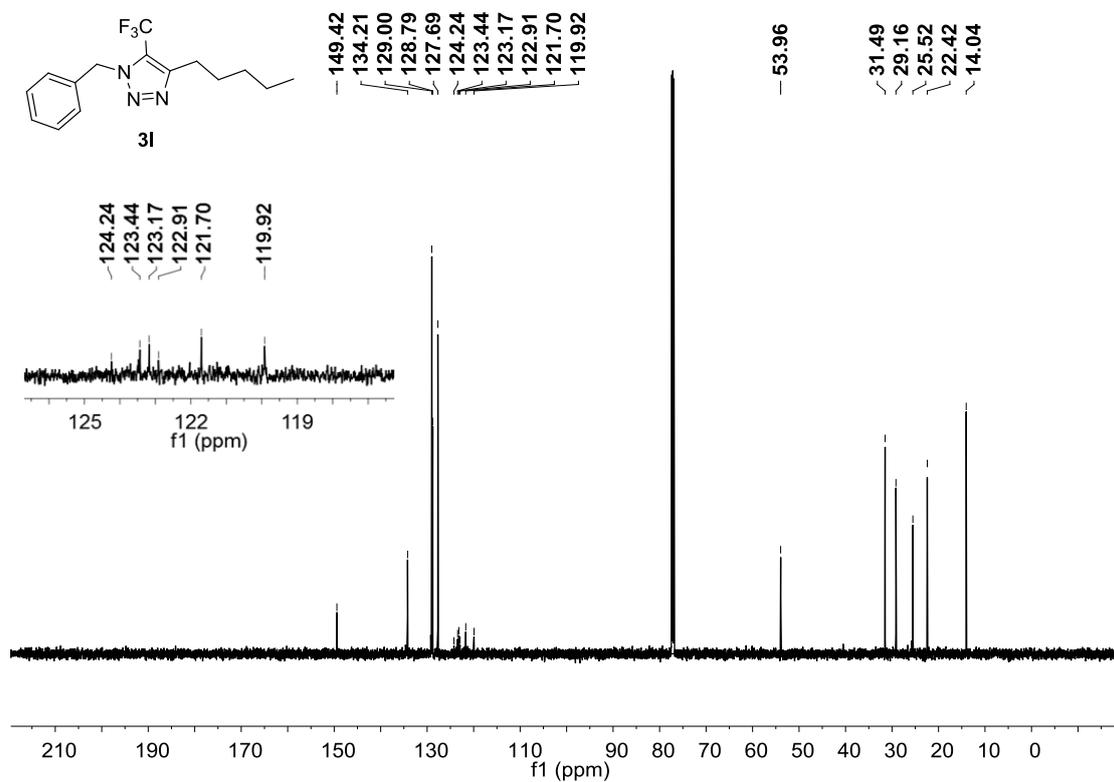
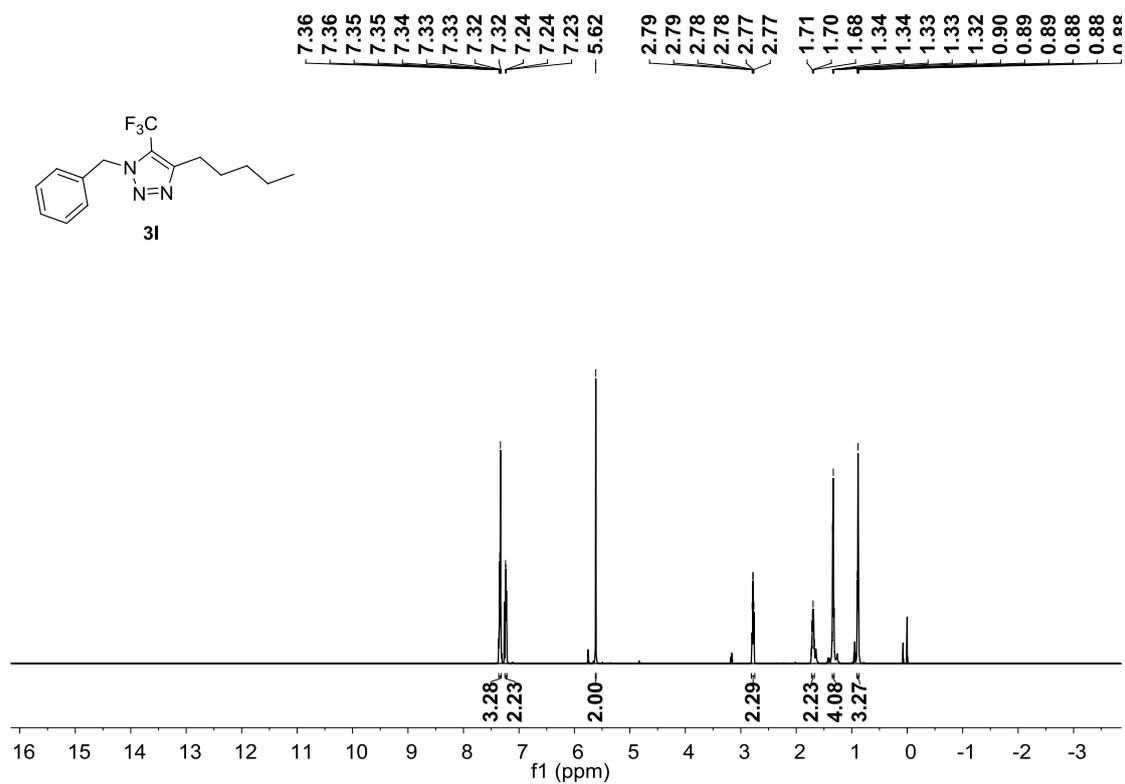
**1-(4-((1-benzyl-5-(trifluoromethyl)-1H-1,2,3-triazol-4-yl)methoxy)-3-methoxyphenyl)ethan-1-one (3j)**



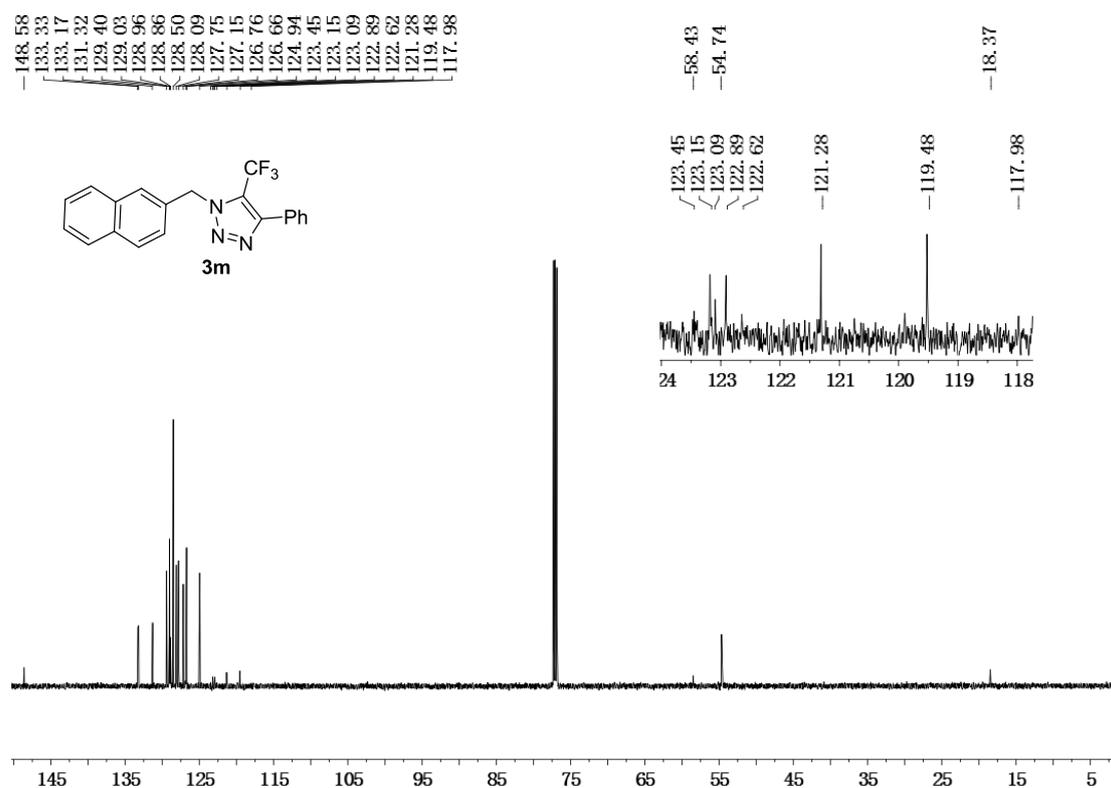
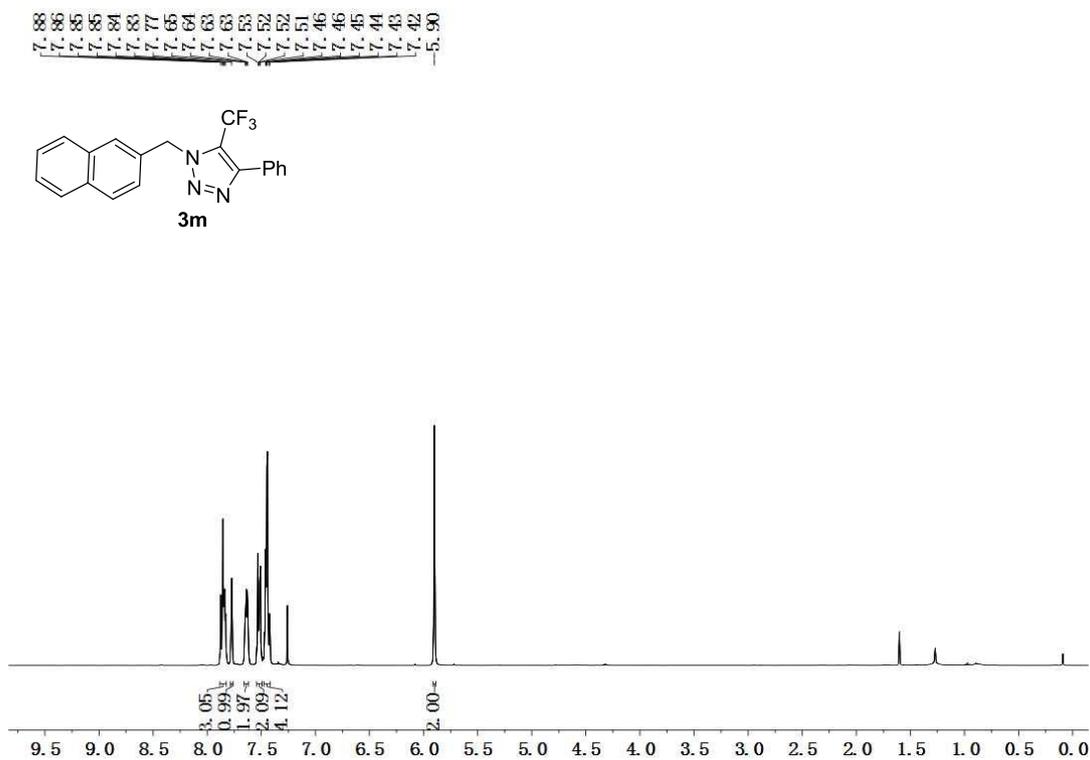
# 1,4-dibenzyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3k)



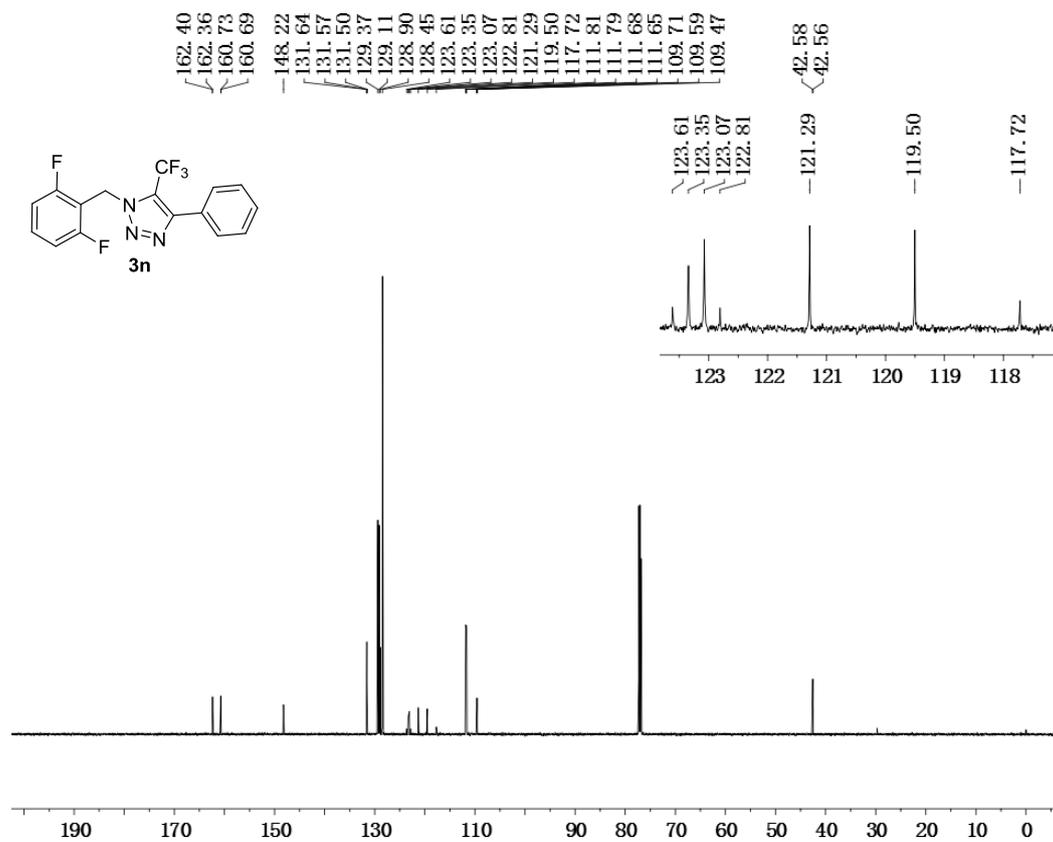
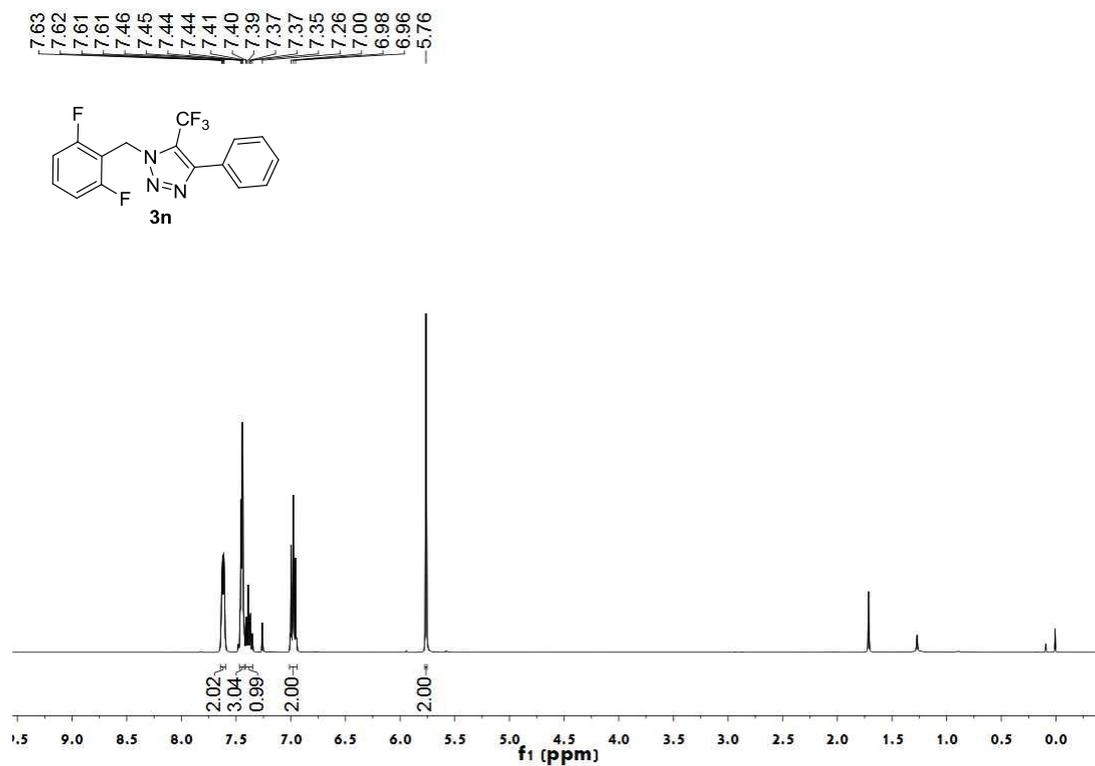
# 1-benzyl-4-pentyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3I)



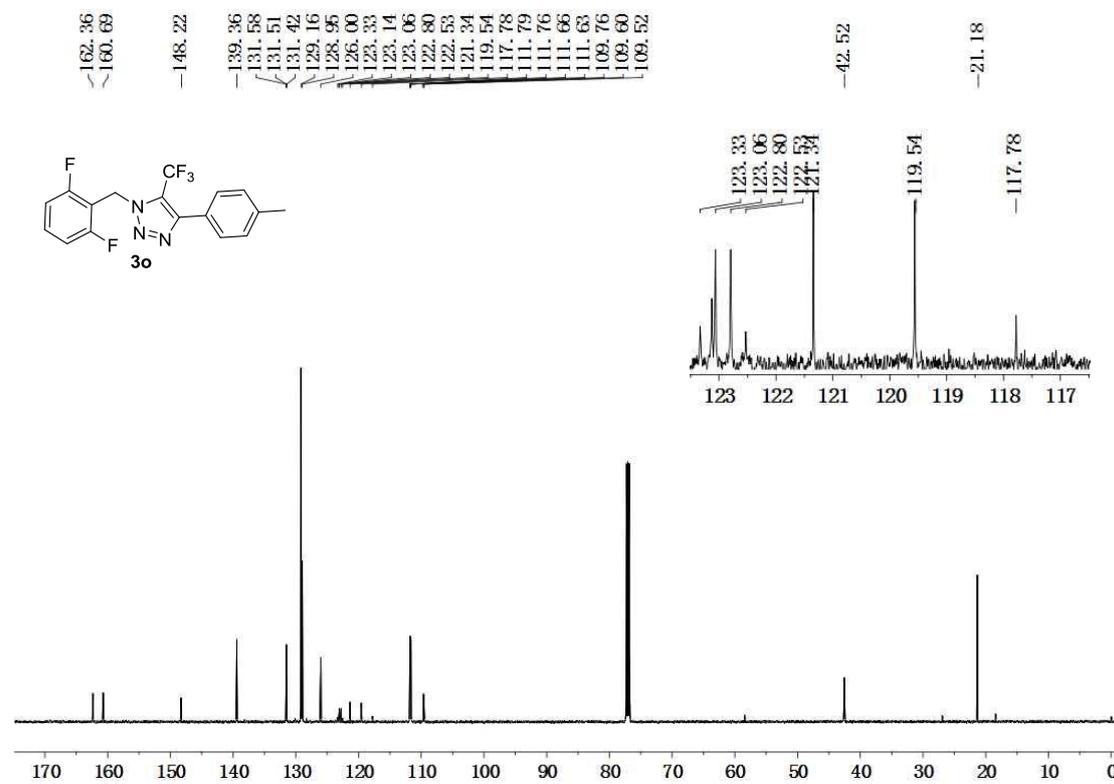
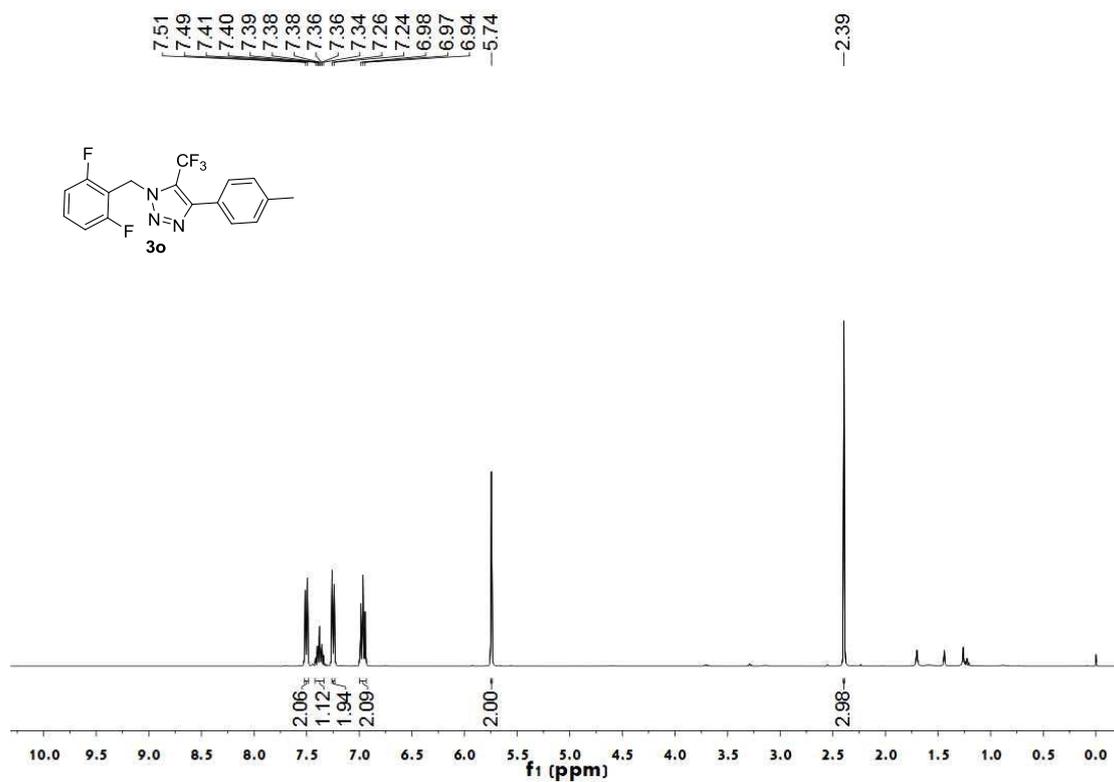
# 1-(naphthalen-2-ylmethyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3m)



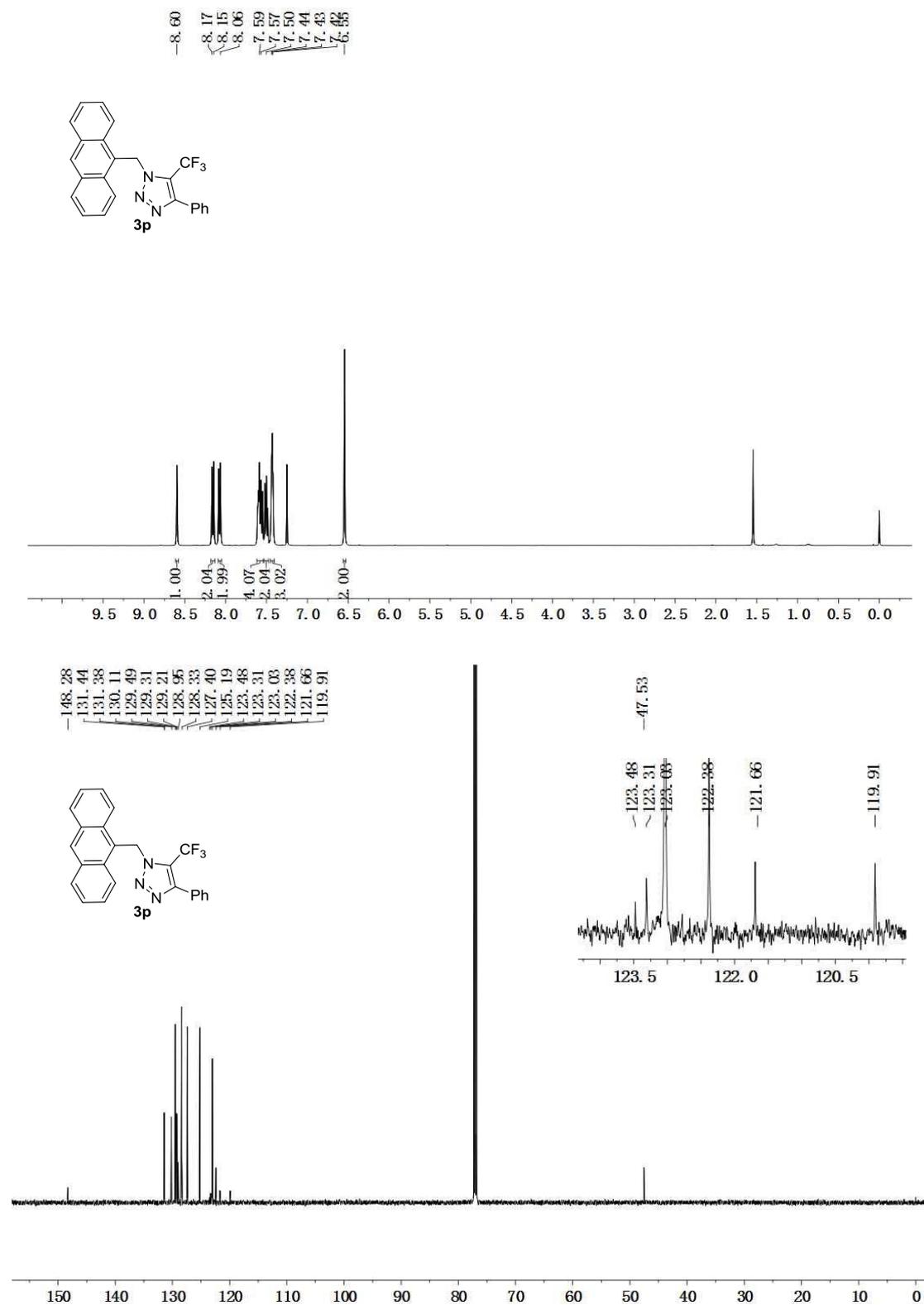
# 1-(2,6-difluorobenzyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3n)



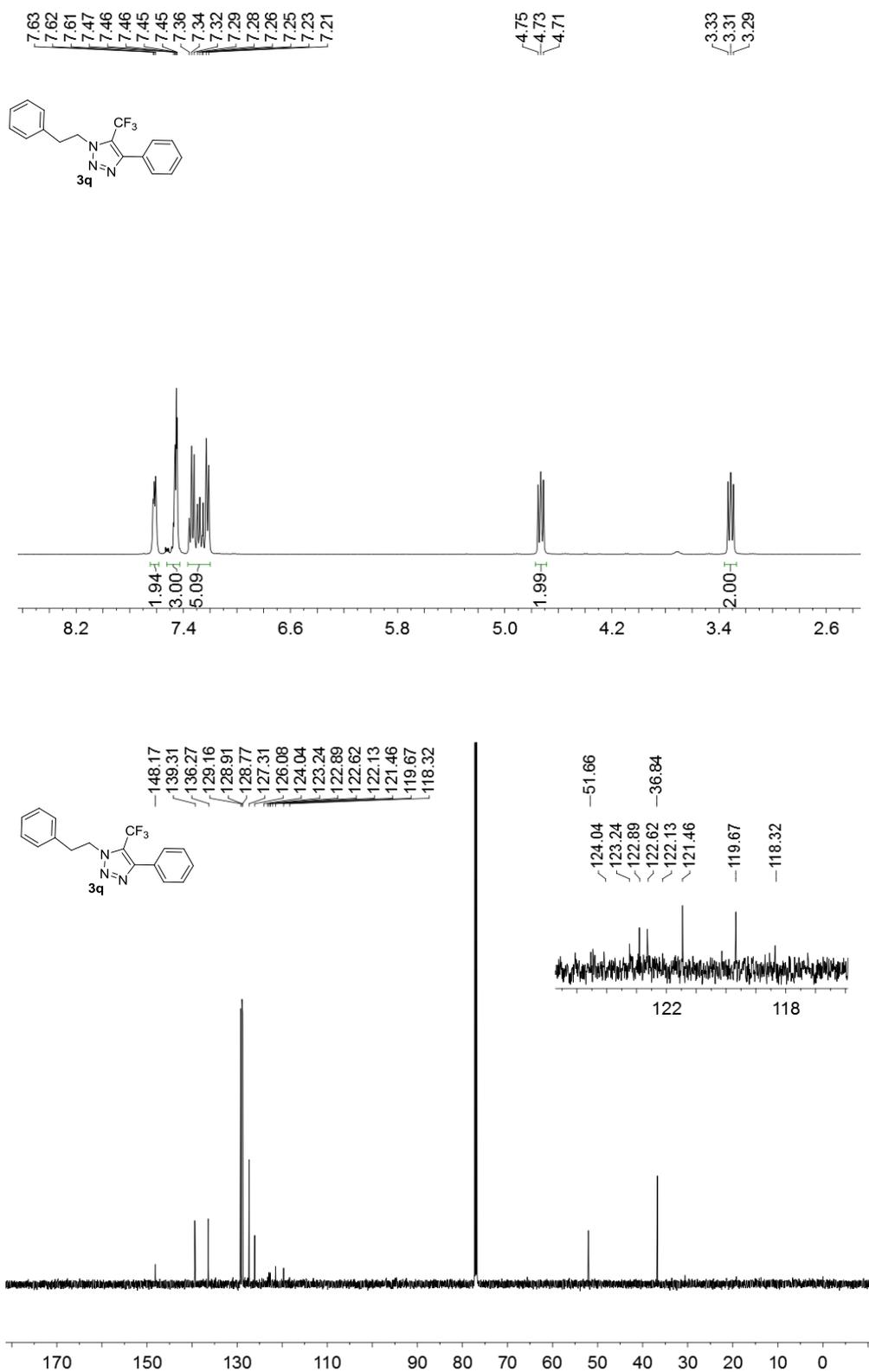
**1-(2,6-difluorobenzyl)-4-(p-tolyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3o)**



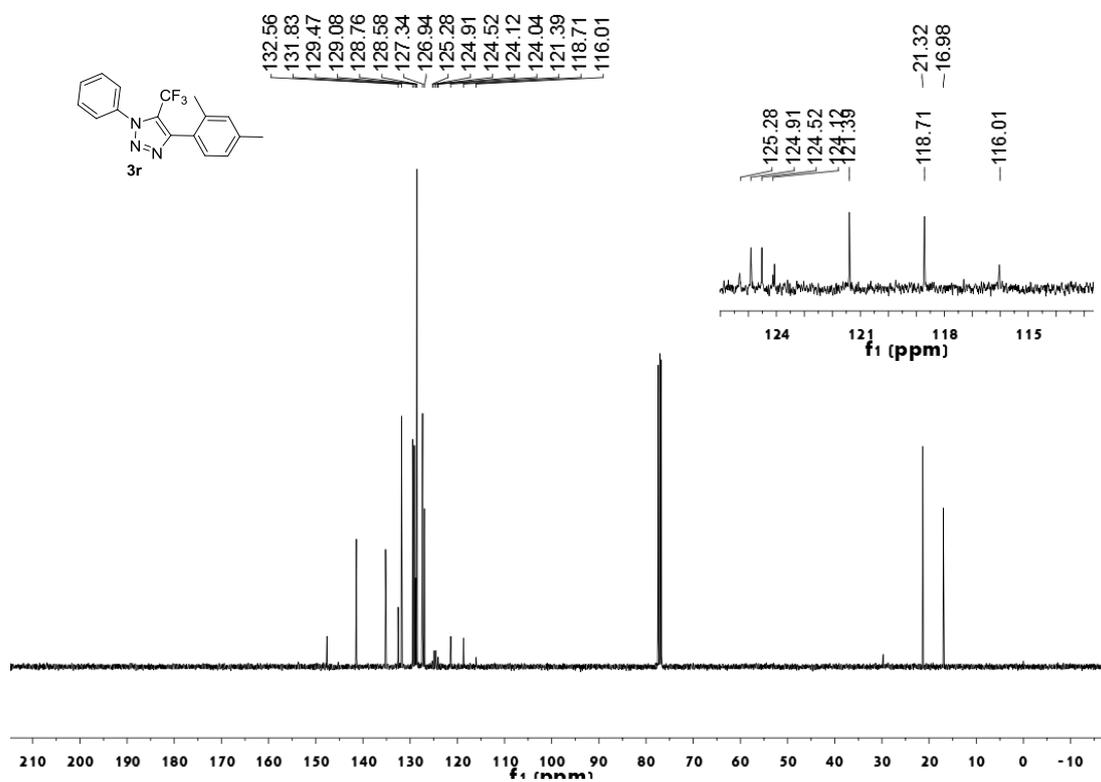
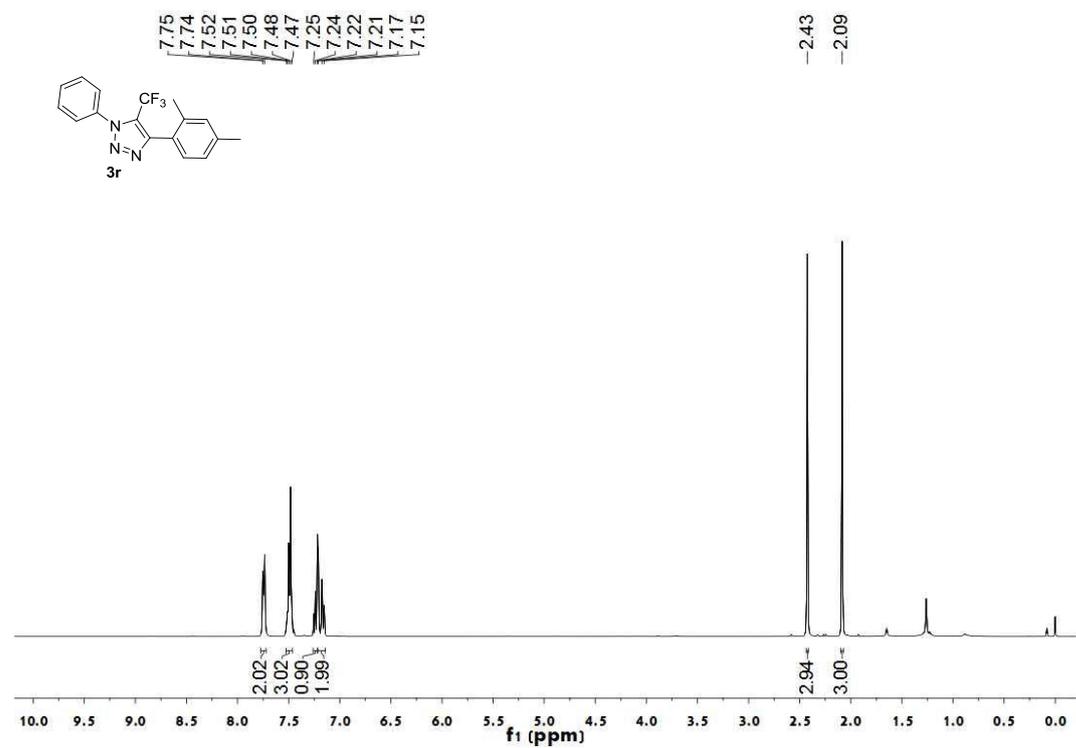
# 1-(anthracen-9-ylmethyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3p)



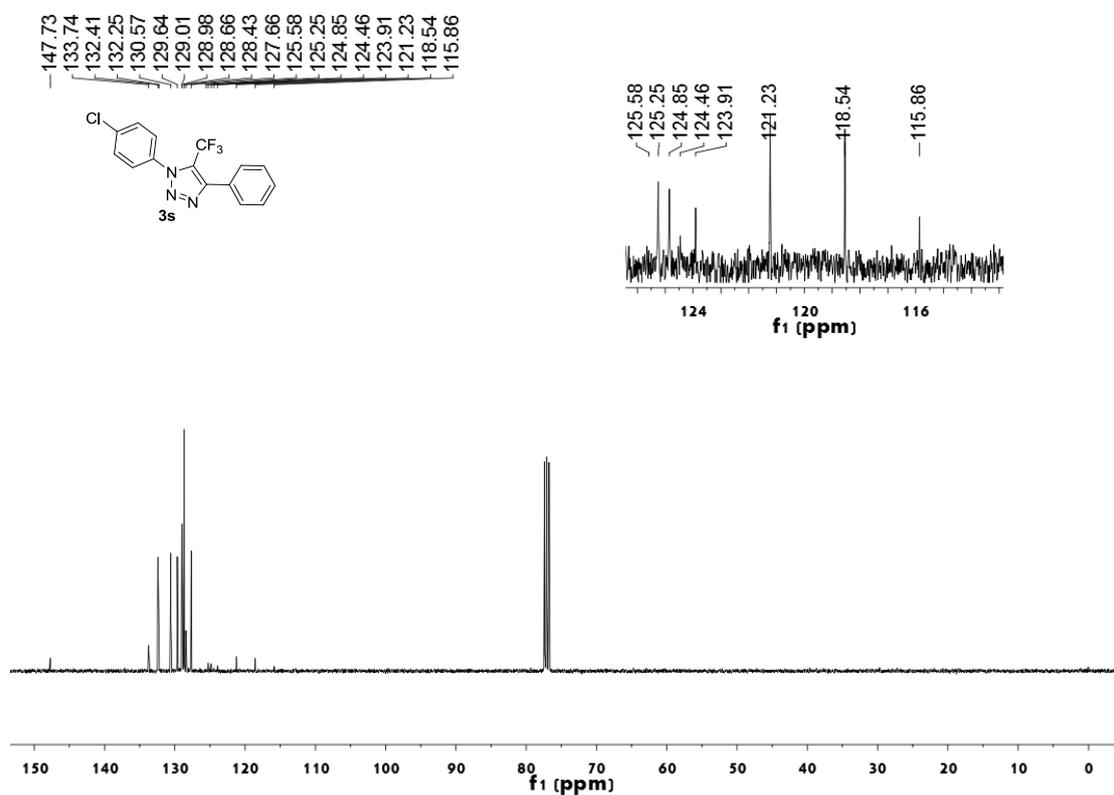
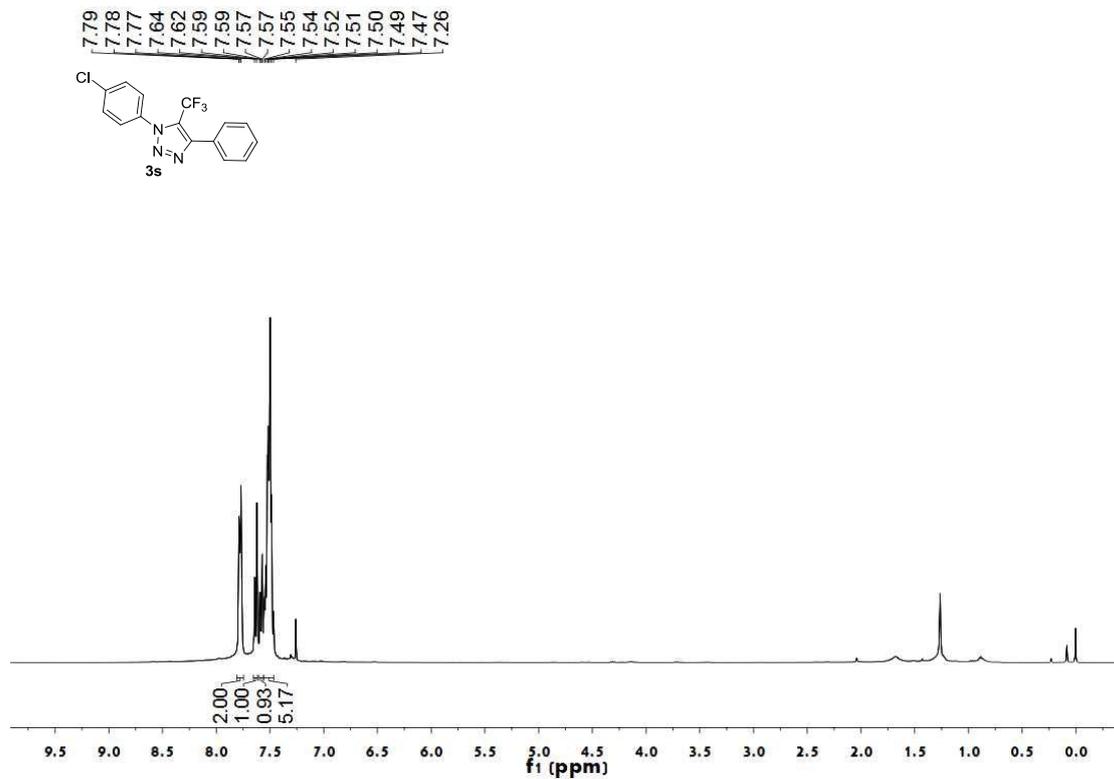
# 1-phenethyl-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3q)



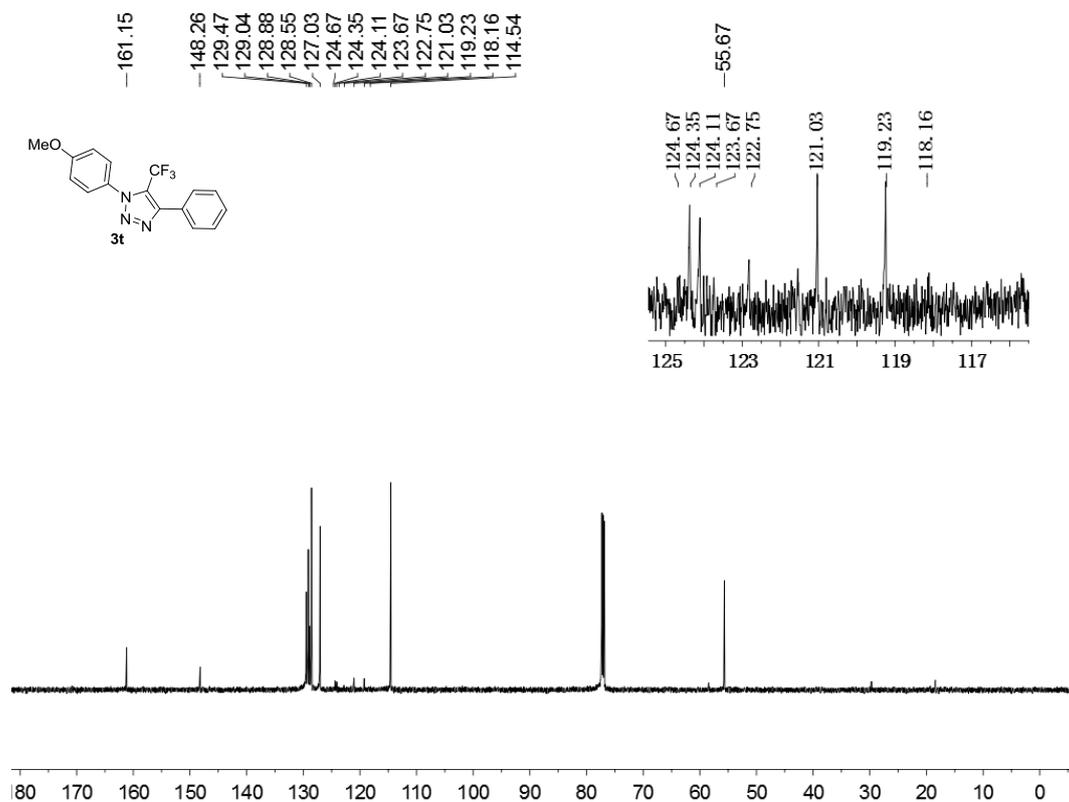
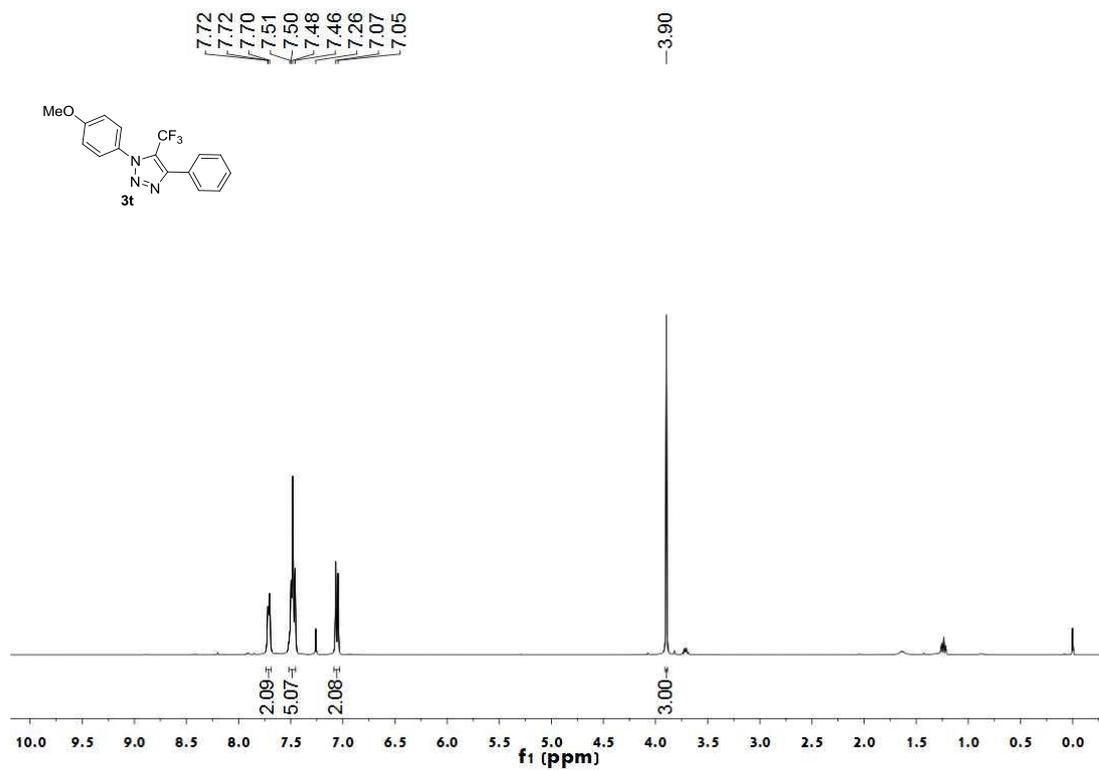
# 1-(2,4-dimethylphenyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3r)



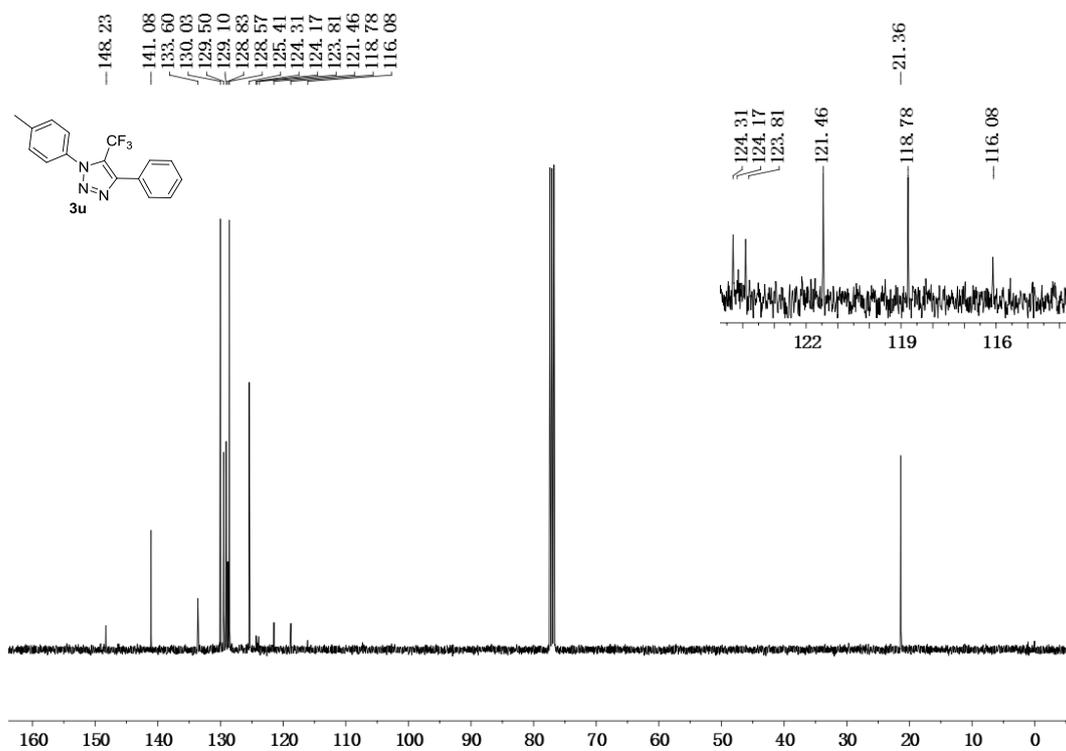
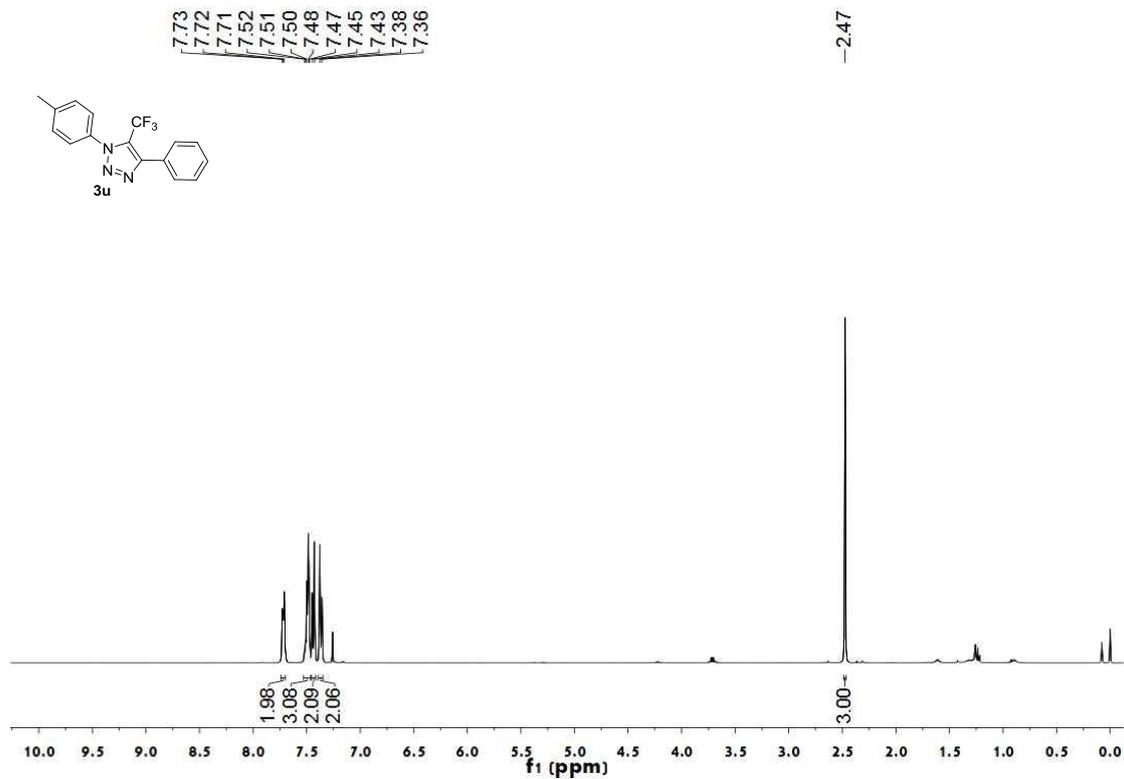
# 1-(2-chlorophenyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3s)



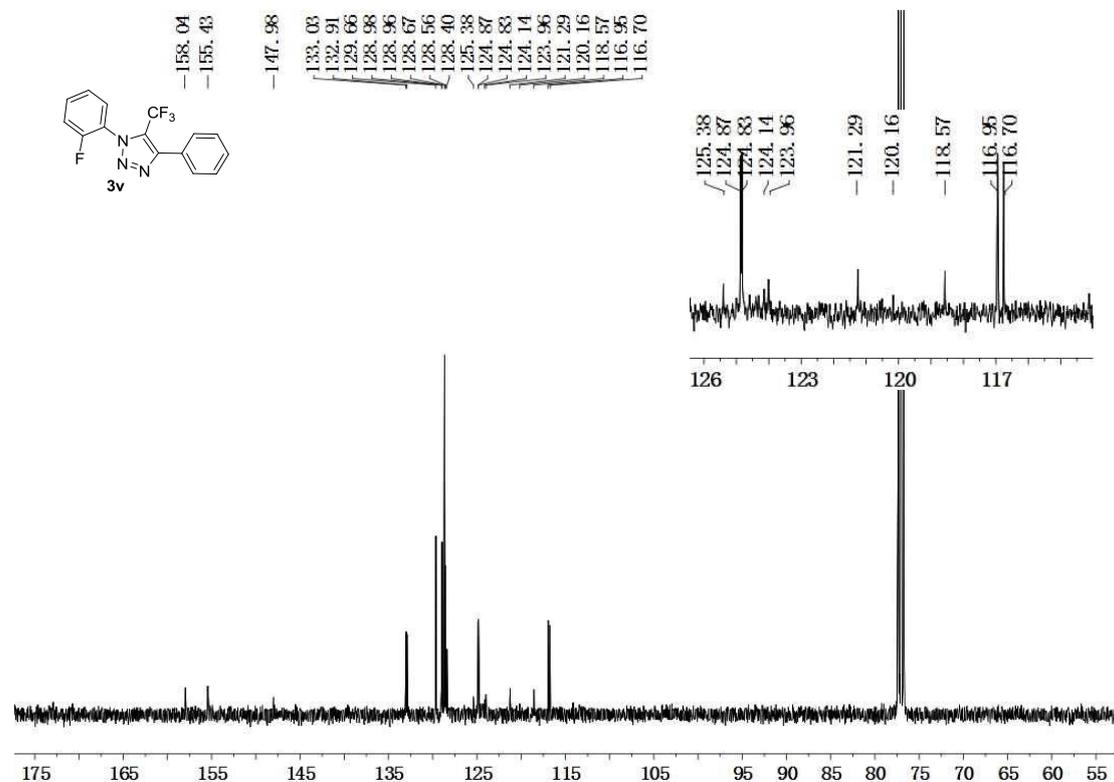
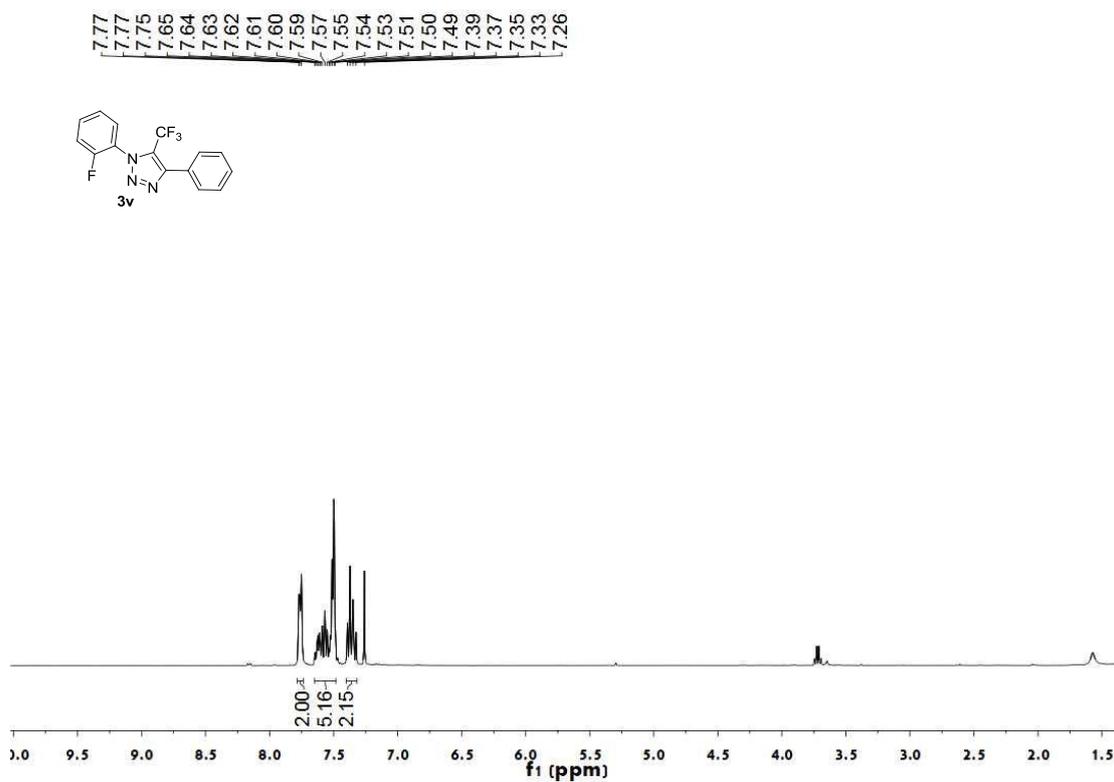
# 1-(4-methoxyphenyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3t)



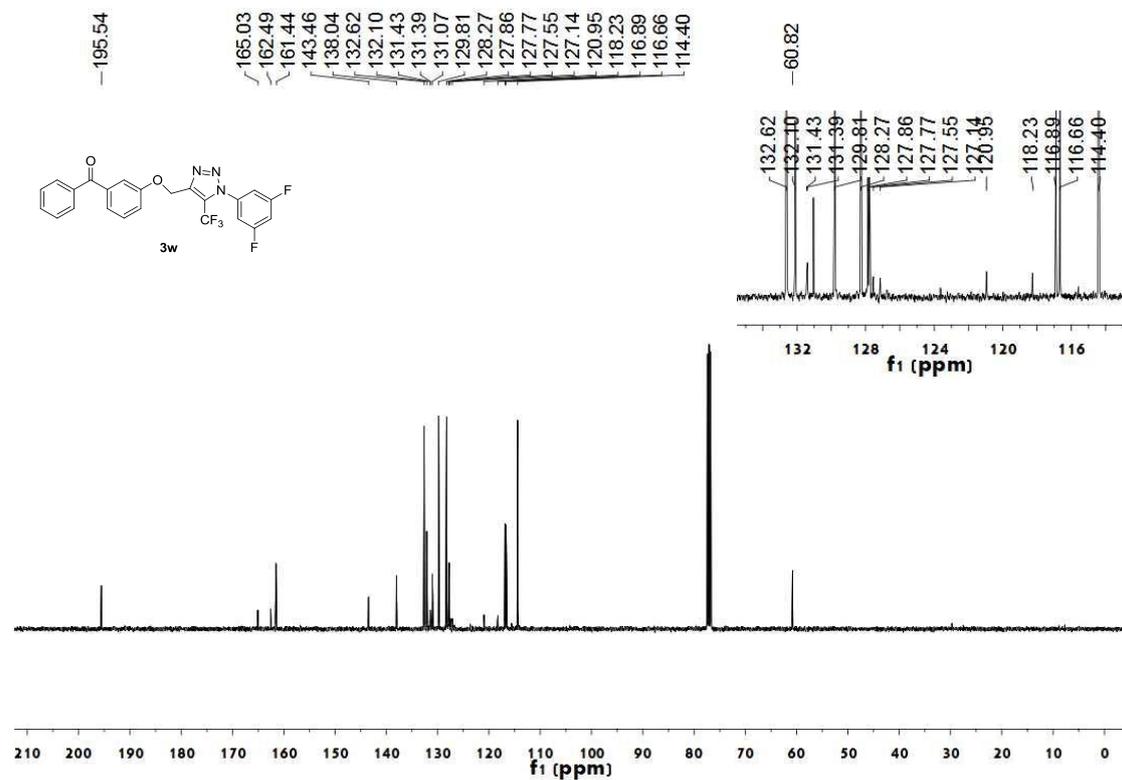
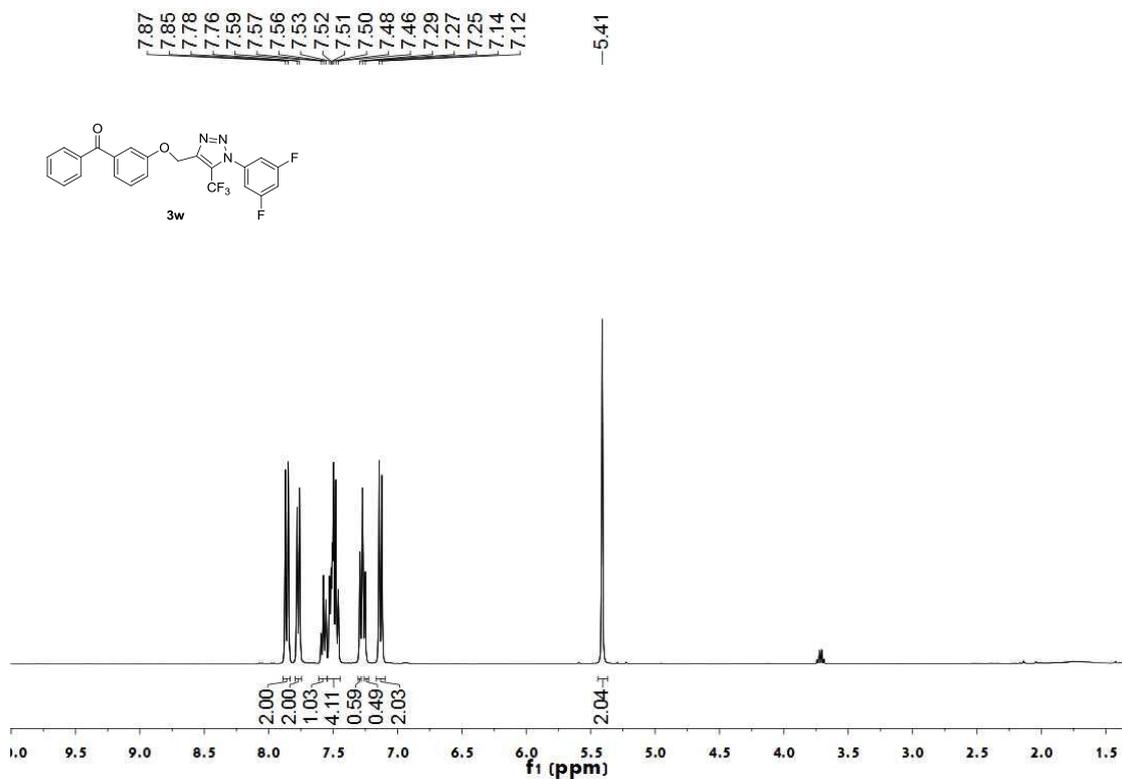
4-phenyl-1-(p-tolyl)-5-(trifluoromethyl)-1H-1,2,3-triazole (3u)



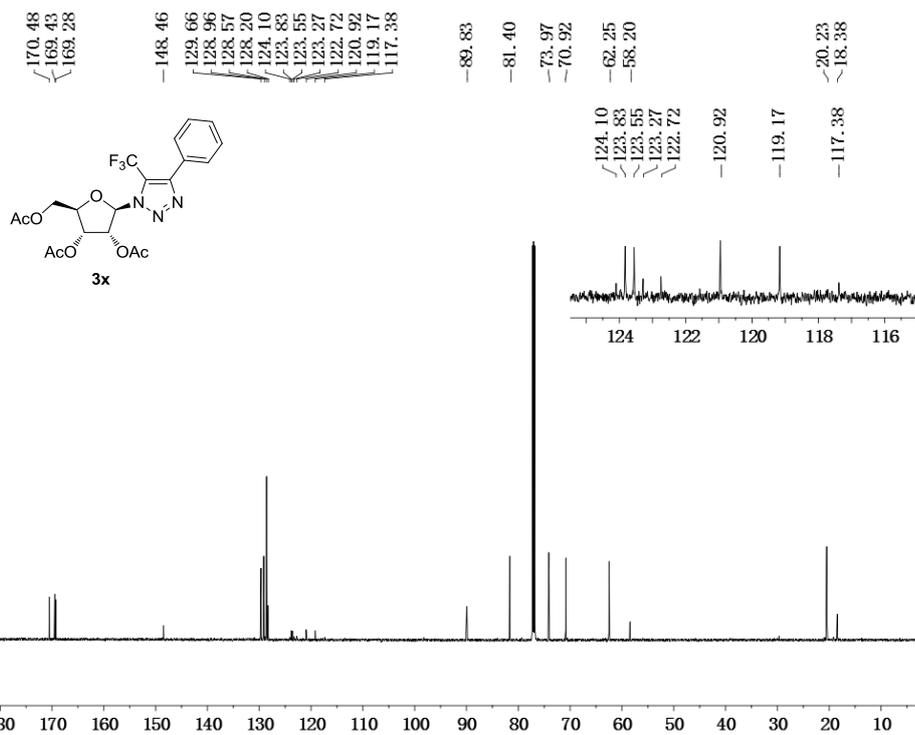
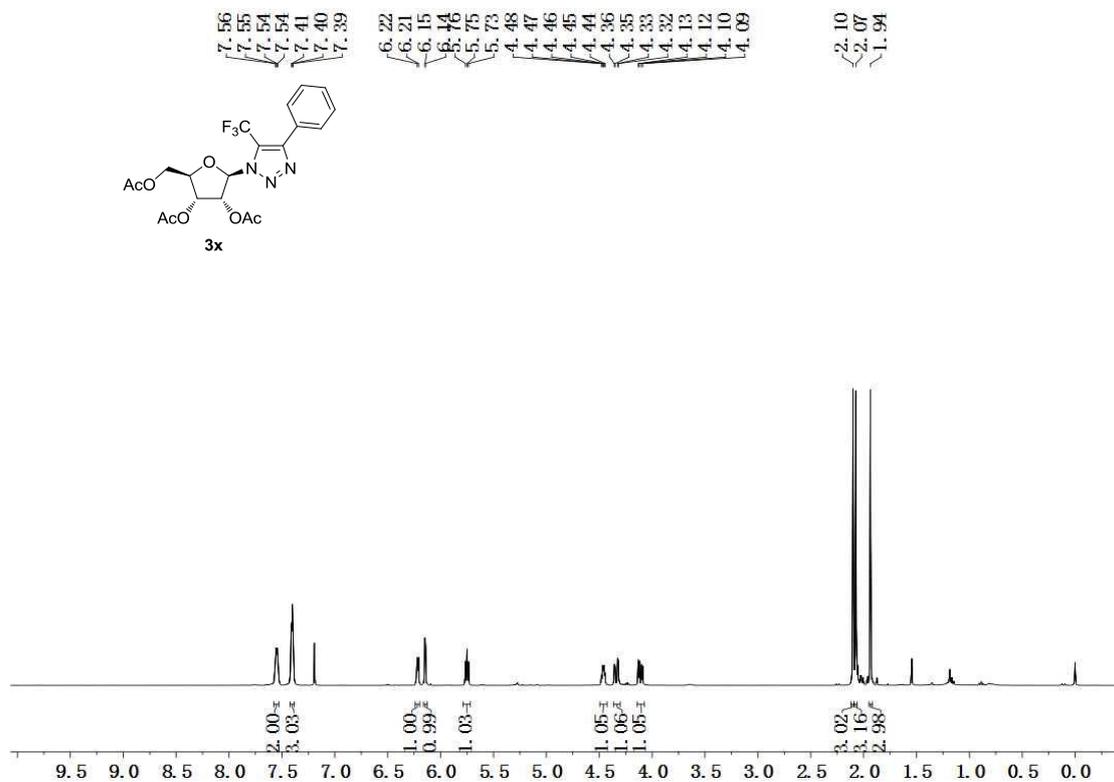
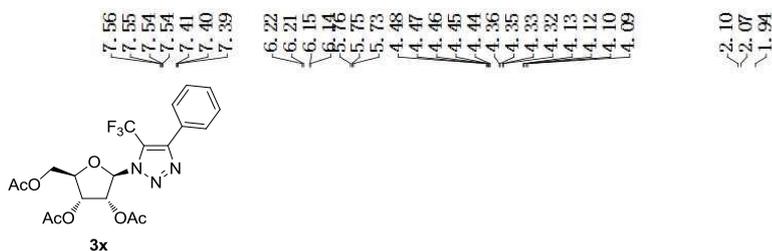
# 1-(2-fluorophenyl)-4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazole (3v)



**(4-((1-(3,5-difluorophenyl)-5-(trifluoromethyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl)(phenyl)methanone (3w)**

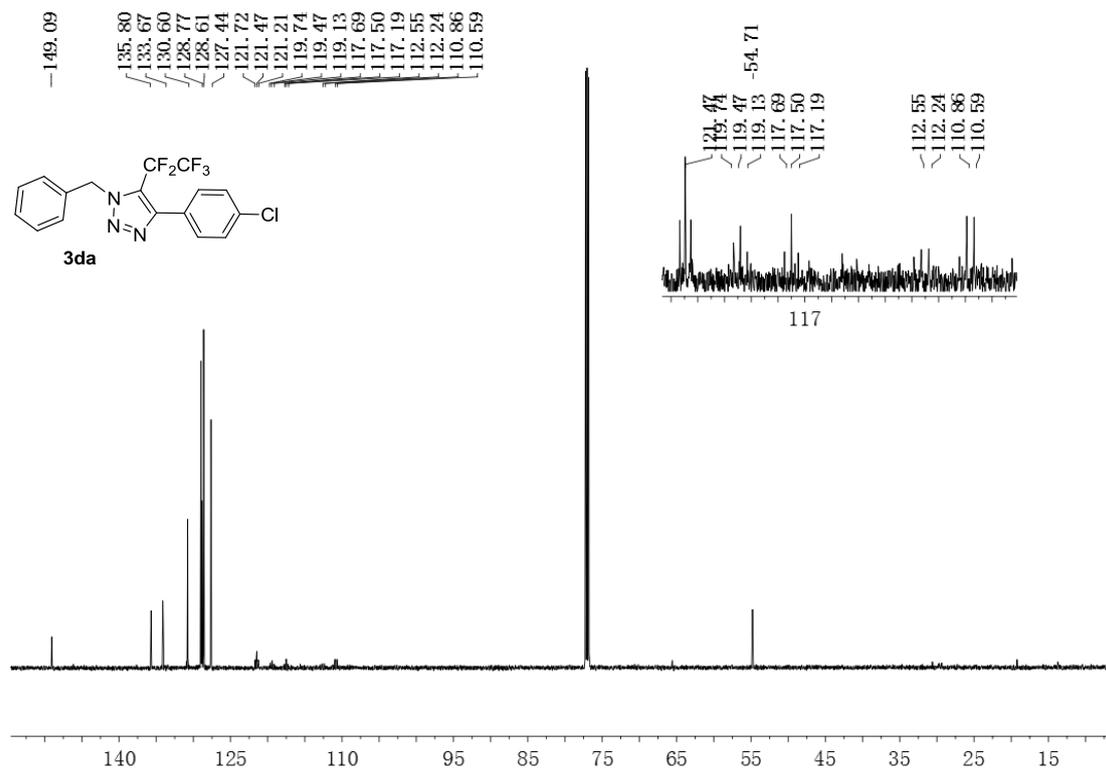
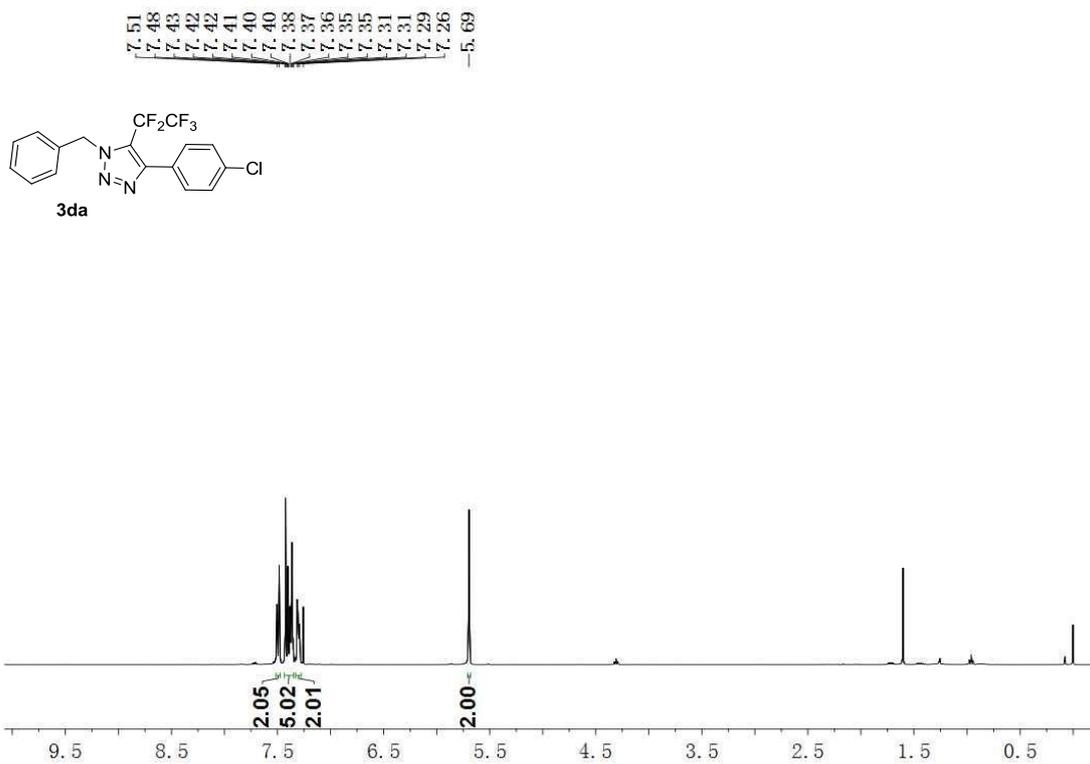


**2-(acetoxymethyl)-5-(4-phenyl-5-(trifluoromethyl)-1H-1,2,3-triazol-1-yl)tetrahy  
(3x)**

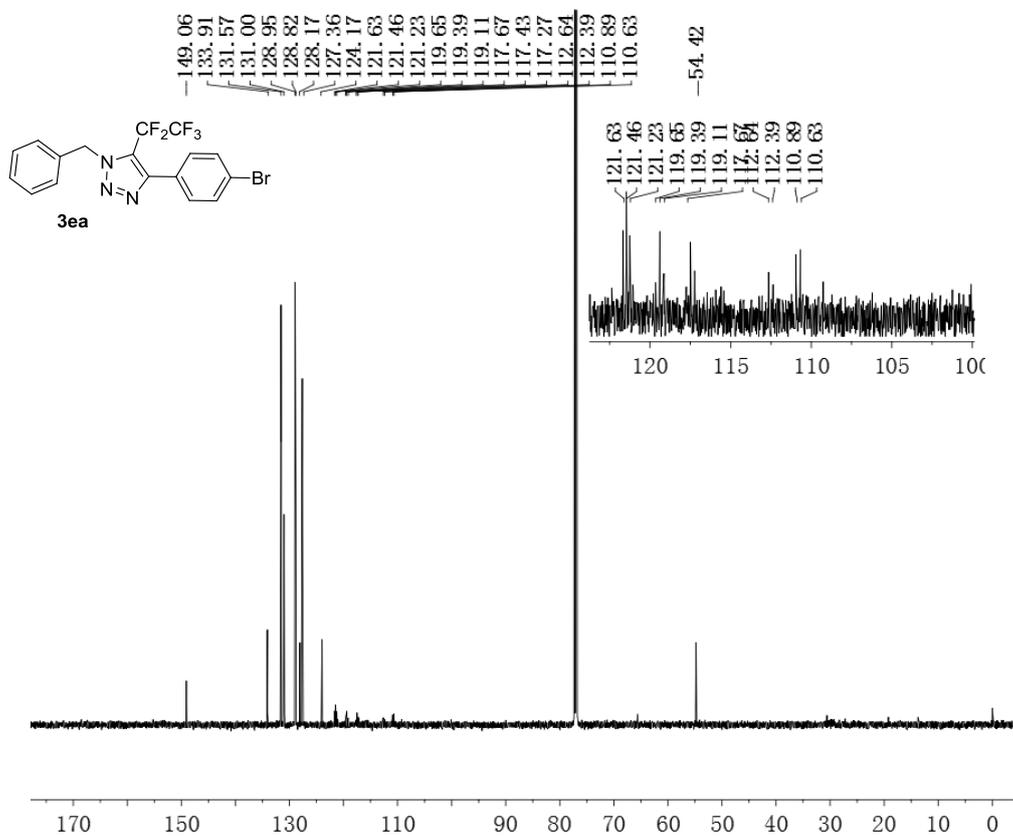
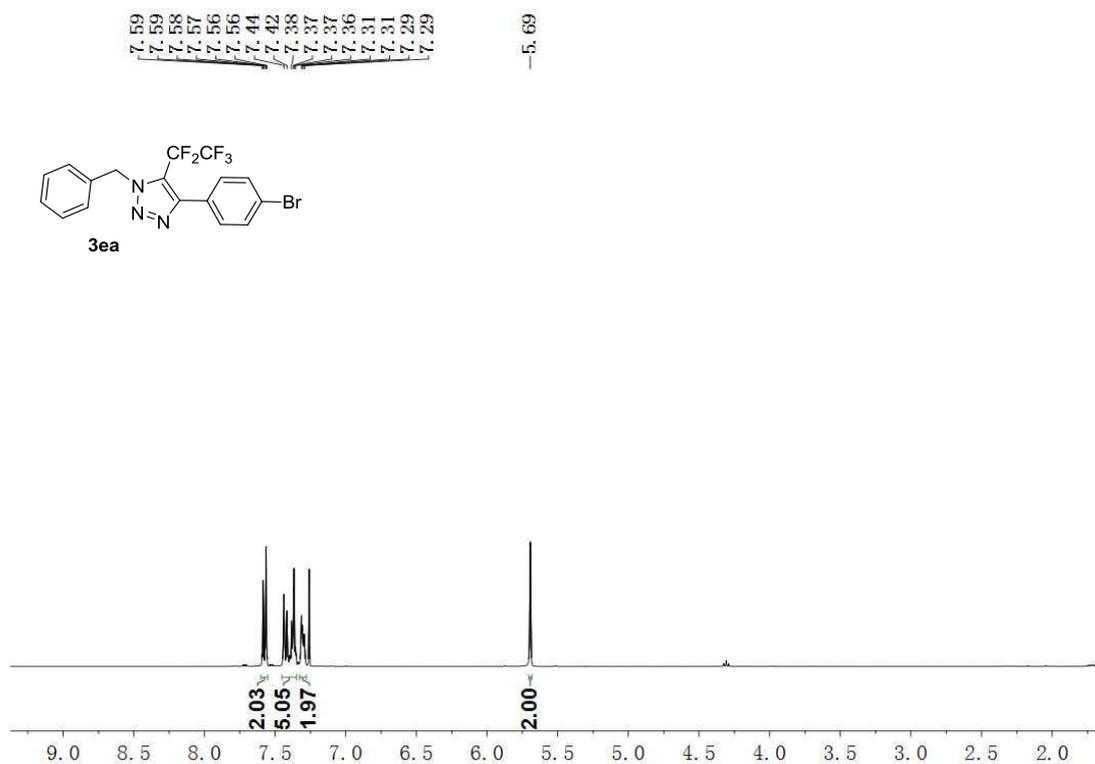




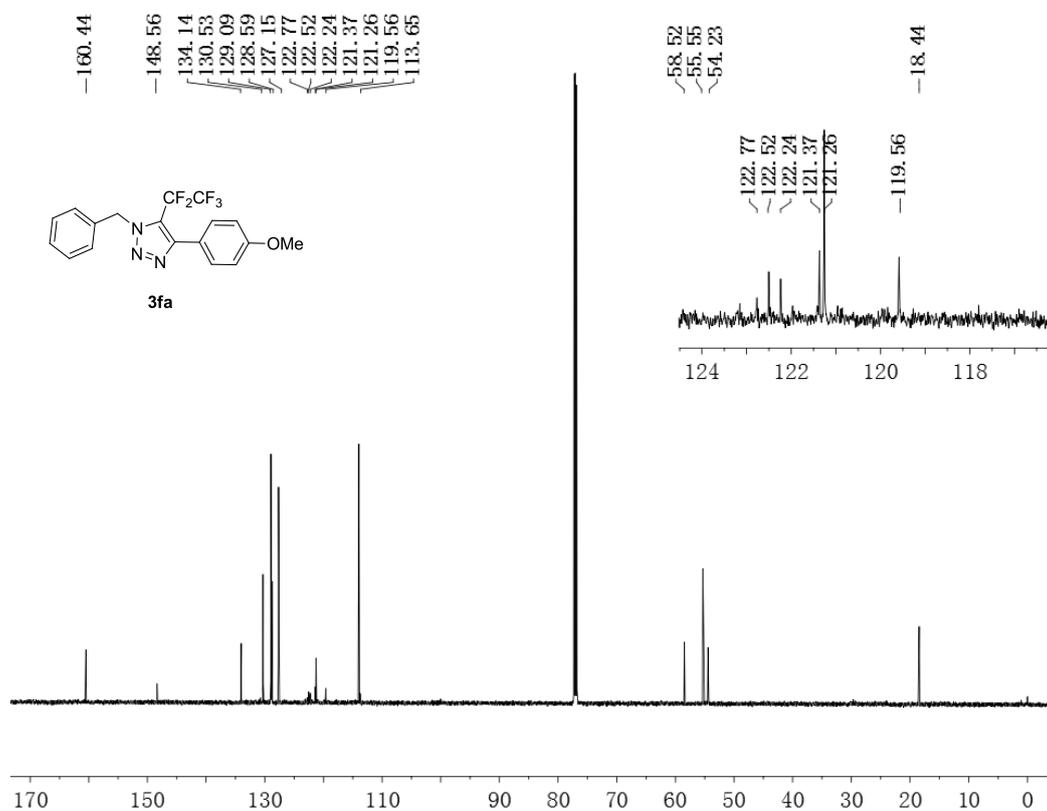
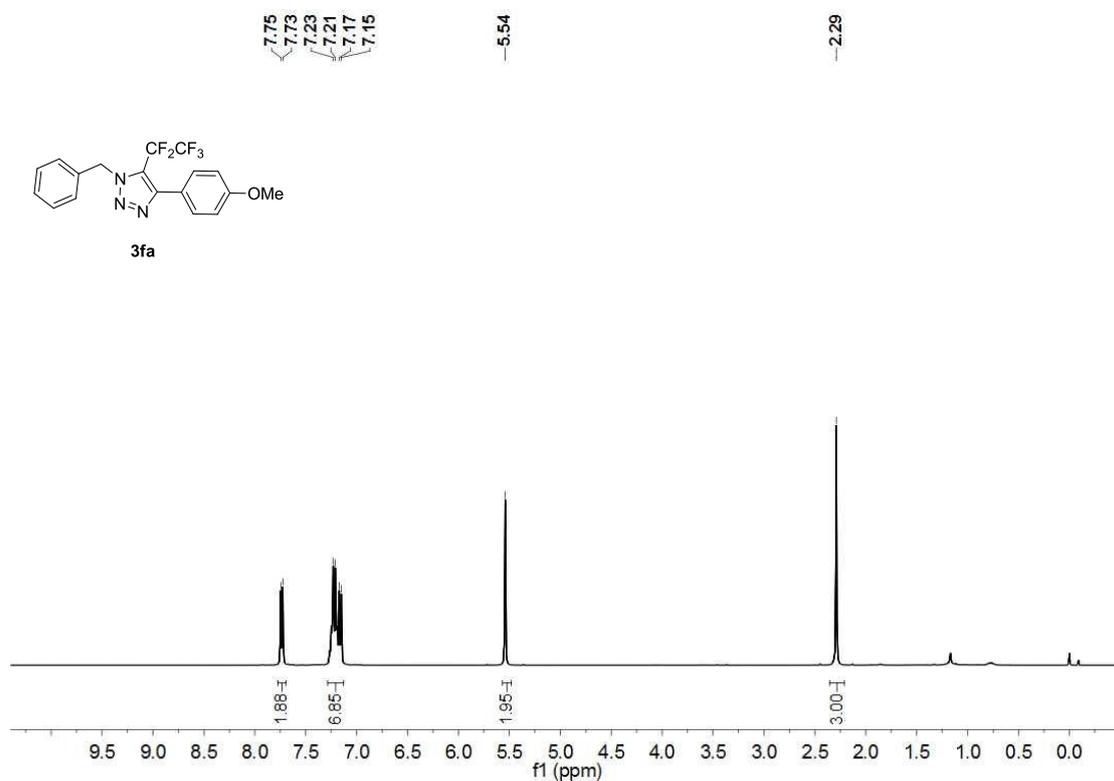
# 1-benzyl-4-(4-chlorophenyl)-5-(perfluoroethyl)-1H-1,2,3-triazole (3da)



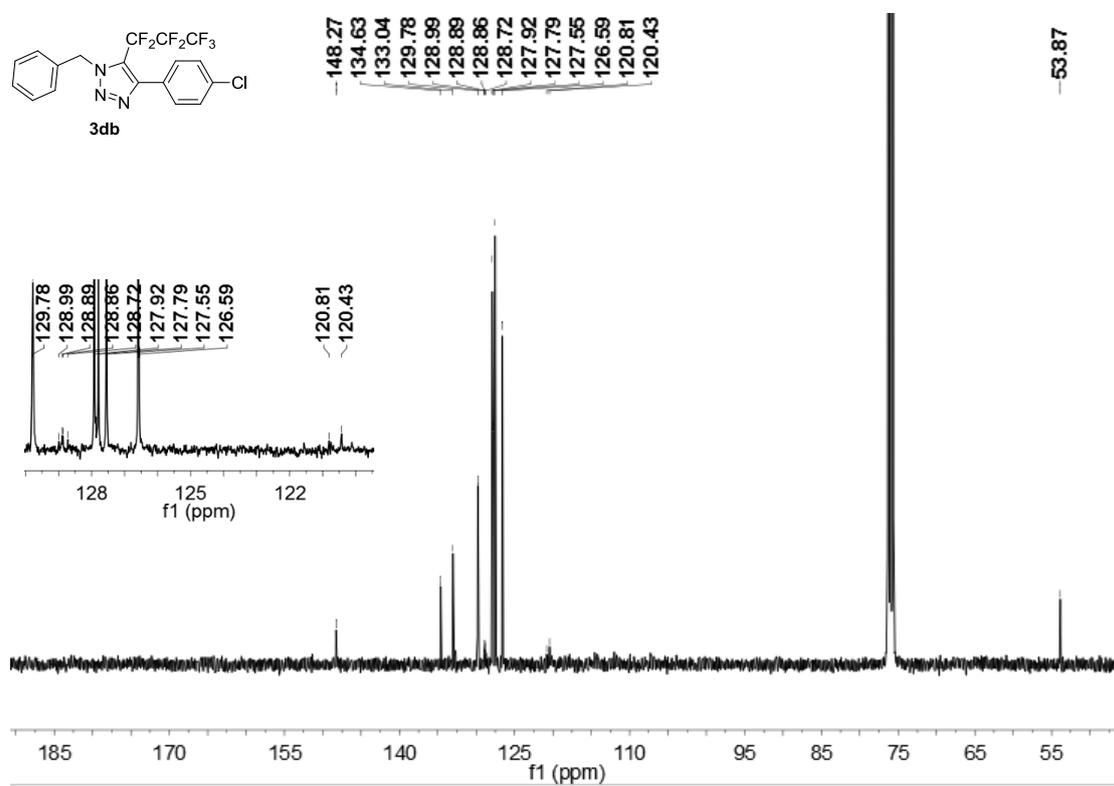
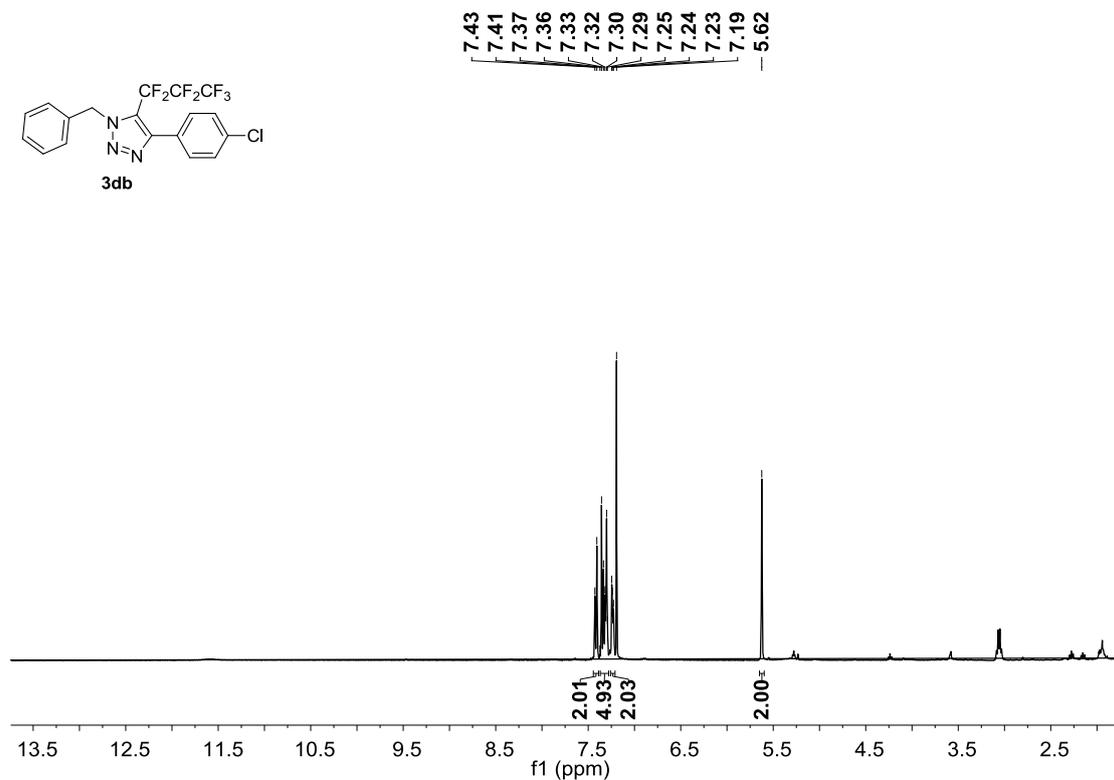
# 1-benzyl-4-(4-bromophenyl)-5-(perfluoroethyl)-1H-1,2,3-triazole (3ea)



# 1-benzyl-4-(4-methoxyphenyl)-5-(perfluoroethyl)-1H-1,2,3-triazole (3fa)



**1-benzyl-4-(4-chlorophenyl)-5-(perfluoropropyl)-1H-1,2,3-triazole (3db)**



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## Reference

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