

*Supporting Information*

**Cascade C-C Bond Cleavage/Reformation and Cycloaddition for the  
Synthesis of 4-Acyl 1,2,3-Triazoles from  $\beta$ -Alkyl Nitroalkenes and  
Organic Azides**

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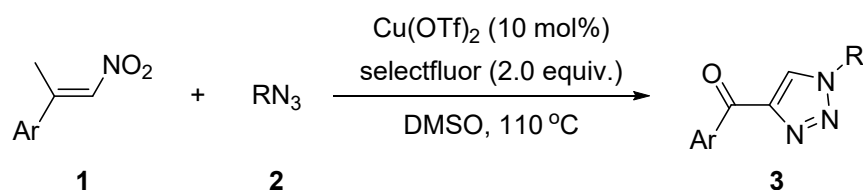
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## 1. General information

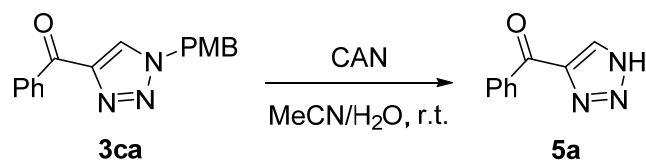
All reactions are basically carried out under air atmosphere. Unless otherwise noted, all commercial reagents and solvents were obtained from the commercial provider and used without further purification. TLC was performed with the detection of compounds with UV light. Flash column chromatography purification of the products was accomplished on silica gel (200–300 or 300–400 mesh). petroleum ether (PE) (60–90 °C) and ethyl acetate (EA) were used as eluents for silica gel chromatography.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded at 22 °C on a Bruker AV 400 and 100 MHz spectrometers with tetramethylsilane (TMS) as an internal standard.  $^1\text{H}$  and  $^{13}\text{C}$  chemical shifts in NMR spectra were referenced relative to signals of  $\text{CDCl}_3$  ( $\delta$  7.26 ppm for  $^1\text{H}$  and 77.0 ppm for  $^{13}\text{C}$ ). High-resolution mass spectra (HRMS) were acquired on Waters Acquity UPLC Class I/Xevo G2Q-TOF.

## 2. General procedures for 4-acyl-1,2,3-triazoles



To a solution of  $\beta$ -alkyl nitroolefins (1 mmol), organic azides (1.5 mmol), Cu(OTf)<sub>2</sub> (0.1 mmol) in DMSO (5.0 mL, 0.2 M) was added selectfluor (2 mmol) in one portion. The reaction mixture was stirred at 110 °C for 8 h. After completion of the reaction, the mixture was poured into water, extracted by ethyl acetate, and dried with anhydrous Na<sub>2</sub>SO<sub>4</sub>. Removal of the organic solvent in a vacuum followed by flash silica gel column chromatographic purification (petroleum/ethyl acetate) afforded 1,2,3-triazole product.

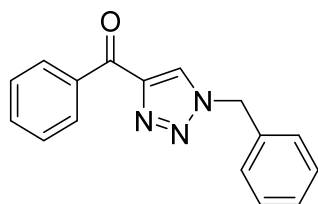
### 3. Deprotection of the $N^1$ -PMB Group in **3ca**



To a solution of **3ca** (0.15 mmol) in MeCN (1.5 mL) was added dropwise a solution of ceric ammonium nitrate (CAN) (0.75 mmol) in H<sub>2</sub>O (0.5 mL) at 0 °C. After 15 min, the solution was stirred at r.t. for 10 h. After completion of the reaction, water was added. The solution was extracted by ethyl acetate, and dried with anhydrous Na<sub>2</sub>SO<sub>4</sub>, and evaporated. The crude was purified with chromatography on silica gel using gradient eluent petroleum/ethyl acetate (v:v = 1:5) to afford **5a** as white solid. 24 mg, 92% yield, <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.37 (s, 1H), 8.29 (d, *J* = 7.6 Hz, 2H), 7.64 (d, *J* = 7.3 Hz, 1H), 7.54 (t, *J* = 7.7 Hz, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 185.8, 136.4, 134.5, 133.6, 130.2, 128.6. Spectral data match those previously reported in the literature.<sup>[1]</sup>

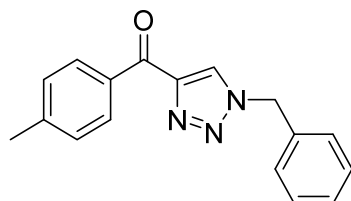
### 4. Compounds characterization

#### (1-benzyl-1H-1,2,3-triazol-4-yl)(phenyl)methanone (**3a**)



Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3a** as a white solid. 210.6 mg, 80% yield, m.p. 116–117 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.41 (d, *J* = 8.2 Hz, 2H), 8.17 (s, 1H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 2H), 7.40 (d, *J* = 6.6 Hz, 3H), 7.33 (d, *J* = 7.8 Hz, 2H), 5.60 (s, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 185.6, 148.3, 136.4, 133.6, 133.2, 130.5, 129.2, 129.1, 128.3, 128.2, 54.4. Spectral data match those previously reported in the literature.<sup>[2]</sup>

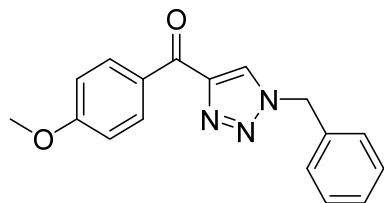
#### (1-benzyl-1H-1,2,3-triazol-4-yl)(*p*-tolyl)methanone (**3b**)



Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3b** as a white solid. 202.5 mg, 73% yield, m.p. 130–132 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.36 (d, *J* = 8.2 Hz, 2H), 8.17 (s, 1H), 7.40 – 7.44 (m, 3H), 7.37 – 7.31 (m, 4H), 5.62 (s, 2H),

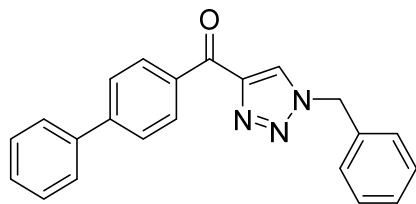
2.45 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , ppm)  $\delta$  185.2, 148.6, 144.2, 134.0, 133.8, 130.8, 129.3, 129.2, 128.4, 128.2, 54.5, 21.8. Spectral data match those previously reported in the literature.<sup>[3]</sup>

**(1-benzyl-1H-1,2,3-triazol-4-yl)(4-methoxyphenyl)methanone (3c)**



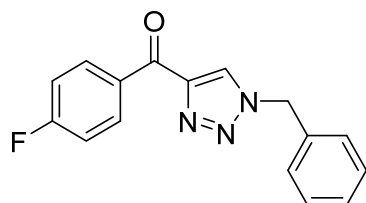
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3c** as a white solid. 202.3 mg, 69% yield, m.p. 129–131 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , ppm)  $\delta$  8.52 – 8.49 (m, 2H), 8.14 (s, 1H), 7.42 – 7.38 (m, 3H), 7.36 – 7.31 (m, 2H), 7.02 – 6.97 (m, 2H), 5.60 (s, 2H), 3.89 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , ppm)  $\delta$  183.9, 163.8, 148.8, 133.7, 133.1, 129.3, 129.1, 128.4, 128.1, 113.6, 55.5, 54.4. Spectral data match those previously reported in the literature.<sup>[4]</sup>

**[1,1'-biphenyl]-4-yl(1-benzyl-1H-1,2,3-triazol-4-yl)methanone (3d)**



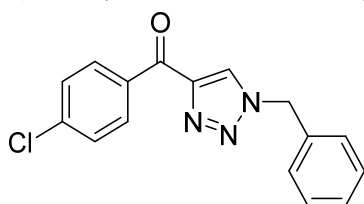
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3d** as a white solid. 224.0 mg, 66% yield, m.p. 146–147 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , ppm)  $\delta$  8.53 (d,  $J$  = 8.0 Hz, 2H), 8.19 (s, 1H), 7.80 – 7.71 (m, 2H), 7.69 – 7.62 (m, 2H), 7.48 (t,  $J$  = 8.0 Hz, 2H), 7.42 – 7.33 (m, 6H), 5.63 (s, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , ppm)  $\delta$  185.2, 148.6, 146.0, 140.1, 135.2, 133.7, 131.2, 129.4, 129.2, 129.0, 128.4, 128.3, 128.2, 127.4, 127.1, 54.5. Spectral data match those previously reported in the literature.<sup>[3]</sup>

**(1-benzyl-1H-1,2,3-triazol-4-yl)(4-fluorophenyl)methanone (3e)**



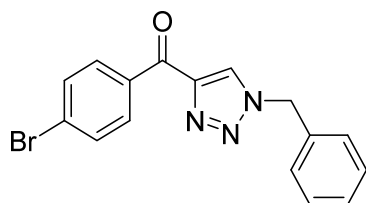
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3e** as a white solid. 281.3 mg, 78% yield, m.p. 145–146 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , ppm)  $\delta$  8.59 – 8.50 (m, 2H), 8.18 (s, 1H), 7.43 – 7.37 (m, 3H), 7.31 – 7.35 m, 2H), 7.17 (t,  $J$  = 8.7 Hz, 2H), 5.61 (s, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , ppm)  $\delta$  183.8, 165.9 (d,  $J$  = 255.3 Hz), 148.3, 133.6, 133.4, 133.4, 132.7 (d,  $J$  = 2.9 Hz), 129.3, 129.2, 128.3, 115.5 (d,  $J$  = 21.7 Hz), 54.5. Spectral data match those previously reported in the literature.<sup>[4]</sup>

**(1-benzyl-1H-1,2,3-triazol-4-yl)(4-chlorophenyl)methanone (3f)**



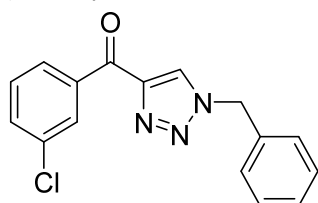
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3f** as a white solid. 241.2 mg, 81% yield, m.p. 158–160 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.43 (d, *J* = 8.7 Hz, 2H), 8.17 (s, 1H), 7.48 (d, *J* = 8.7 Hz, 2H), 7.42 – 7.38 (m, 3H), 7.36 – 7.32 (m, 2H), 5.61 (s, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 184.2, 148.2, 139.8, 134.7, 133.5, 132.1, 129.4, 129.2, 128.7, 128.4, 54.5. Spectral data match those previously reported in the literature.<sup>[5]</sup>

**(1-benzyl-1H-1,2,3-triazol-4-yl)(4-bromophenyl)methanone (3g)**



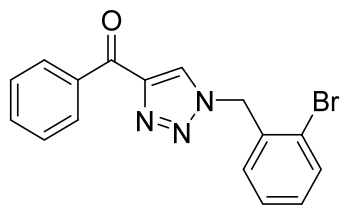
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3g** as a white solid. 270.3 mg, 79% yield, m.p. 149–151 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.36 (d, *J* = 8.5 Hz, 2H), 8.17 (s, 1H), 7.66 (d, *J* = 8.3 Hz, 2H), 7.42 – 7.31 (m, 5H), 5.62 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 184.3, 148.2, 135.1, 133.6, 132.0, 131.6, 129.2, 129.1, 128.5, 128.2, 54.4. Spectral data match those previously reported in the literature.<sup>[4]</sup>

**(1-benzyl-1H-1,2,3-triazol-4-yl)(3-chlorophenyl)methanone (3h)**



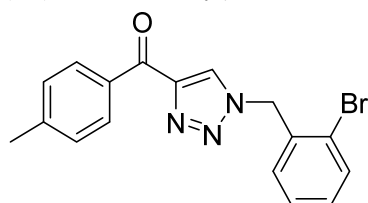
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3h** as a white solid. 223.3 mg, 75% yield, m.p. 93–86 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.37 (t, *J* = 1.9 Hz, 1H), 8.31 – 8.35 (m, 1H), 8.22 (s, 1H), 7.50 – 7.54 (m, 1H), 7.40 (t, *J* = 7.9 Hz, 1H), 7.28 – 7.37 (m, 5H), 5.58 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 184.1, 147.9, 138.0, 134.5, 133.7, 133.2, 130.4, 129.7, 129.3, 129.2, 128.9, 128.7, 128.4, 54.5. Spectral data match those previously reported in the literature.<sup>[5]</sup>

**(1-(2-bromobenzyl)-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3i)**



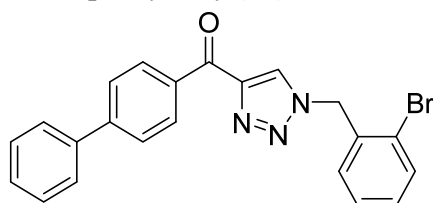
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3i** as a white solid. 256.6 mg, 75% yield, m.p. 103–106 °C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>, ppm) δ 8.42 (d, *J* = 7.8 Hz, 2H), 8.26 (s, 1H), 7.59 – 7.67 (m, 2H), 7.52 (t, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 1H), 7.32 – 7.27 (m, 2H), 5.75 (s, 2H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>, ppm): δ 184.4, 148.1, 135.1, 133.6, 133.1, 132.2, 131.7, 131.0, 128.7, 128.4, 128.0, 124.8, 54.3. Spectral data match those previously reported in the literature.<sup>[5]</sup>

**(1-(2-bromobenzyl)-1H-1,2,3-triazol-4-yl)(p-tolyl)methanone (3j)**



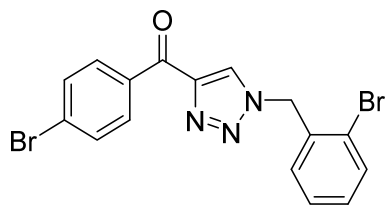
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3j** as a white solid. 245.8 mg, 69% yield, m.p. 97–100 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.35 (d, *J* = 8.3 Hz, 2H), 8.24 (s, 1H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.38 – 7.27 (m, 5H), 5.74 (s, 2H), 2.43 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 185.2, 148.5, 144.2, 134.0, 133.5, 133.3, 130.9, 130.8, 129.1, 128.4, 128.3, 123.9, 54.2, 21.8. Spectral data match those previously reported in the literature.<sup>[5]</sup>

**[1,1'-biphenyl]-4-yl(1-(2-bromobenzyl)-1H-1,2,3-triazol-4-yl)methanone (3k)**



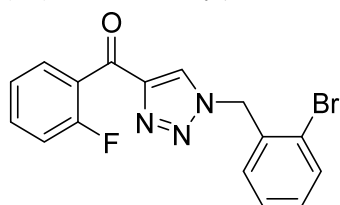
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3k** as a white solid. 267.7 mg, 64% yield, m.p. 164–168 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.53 (d, *J* = 8.4 Hz, 2H), 8.29 (s, 1H), 7.76 – 7.72 (m, 2H), 7.63 – 7.69 (m, 4H), 7.44 – 7.50 (m, 3H), 7.43 – 7.26 (m, 5H), 5.76 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 185.1, 148.4, 146.0, 140.0, 135.2, 133.5, 133.3, 131.3, 130.9 (d, *J* = 2.9 Hz), 129.0, 128.6, 128.4, 128.2, 127.4, 127.1, 124.0, 54.2, 1.1. HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd for C<sub>22</sub>H<sub>17</sub>BrN<sub>3</sub>O: 418.0550; found: 418.0546.

**(1-(2-bromobenzyl)-1H-1,2,3-triazol-4-yl)(4-bromophenyl)methanone (3l)**



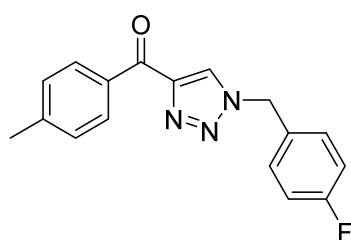
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3l** as a white solid. 320.0 mg, 76% yield, m.p. 106–108 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.38 – 8.33 (m, 2H), 8.27 (s, 1H), 7.65 (d, *J* = 8.3 Hz, 3H), 7.27 – 7.39 (m, 3H), 5.75 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 184.3, 148.1, 135.1, 133.5, 133.1, 132.2, 131.7, 131.0 (d, *J* = 4.2 Hz), 128.7, 128.4, 124.0, 54.2. Spectral data match those previously reported in the literature.<sup>[4]</sup>

**(1-(2-bromobenzyl)-1H-1,2,3-triazol-4-yl)(2-fluorophenyl)methanone (3m)**



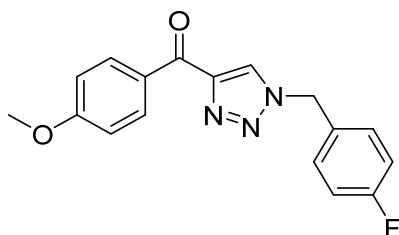
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3m** as a white solid. 252.1 mg, 70% yield, m.p. 60–62 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.22 (s, 1H), 7.86 (t, *J* = 7.4 Hz, 1H), 7.67 (d, *J* = 8.3 Hz, 1H), 7.59 – 7.52 (m, 1H), 7.41 – 7.34 (m, 1H), 7.32 – 7.27 (m, 3H), 7.19 (t, *J* = 9.7 Hz, 1H), 5.76 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 184.8, 160.7 (d, *J* = 255.7 Hz), 147.9, 133.8 (d, *J* = 8.6 Hz), 133.5, 133.2, 131.3 (d, *J* = 1.9 Hz), 130.9, 130.8, 128.4, 127.7, 126.2 (d, *J* = 12.8 Hz), 124.0 (d, *J* = 3.8 Hz), 123.9, 116.5 (d, *J* = 21.7 Hz), 54.2. Spectral data match those previously reported in the literature.<sup>[5]</sup>

**(1-(4-fluorobenzyl)-1H-1,2,3-triazol-4-yl)(p-tolyl)methanone (3n)**



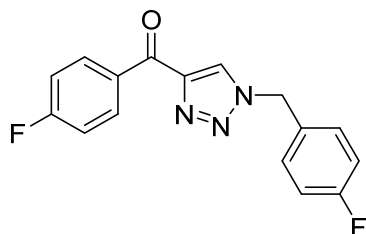
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3n** as a white solid. 218.5 mg, 74% yield, m.p. 145–147 °C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>, ppm) δ 8.36 – 8.31 (m, 2H), 8.16 – 8.14 (m, 1H), 7.36 – 7.30 (m, 4H), 7.12 – 7.06 (m, 2H), 5.57 (s, 2H), 2.43 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>, ppm) δ 185.1, 163.1 (d, *J* = 248.9 Hz), 148.7, 144.2, 133.9, 130.7, 130.3 (d, *J* = 8.4 Hz), 129.7 (d, *J* = 3.1 Hz), 129.1, 128.0, 116.3 (d, *J* = 21.9 Hz), 53.6, 21.7. Spectral data match those previously reported in the literature.<sup>[4]</sup>

**(1-(4-fluorobenzyl)-1H-1,2,3-triazol-4-yl)(4-methoxyphenyl)methanone (3o)**



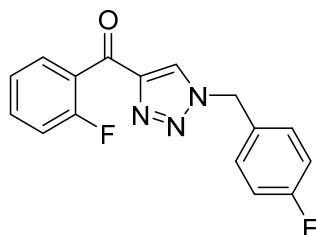
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3o** as a white solid. 221.0 mg, 71% yield, m.p. 131–132 °C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>, ppm) δ 8.53 – 8.49 (m, 2H), 8.15 (s, 1H), 7.36 – 7.31 (m, 2H), 7.10 (t, *J* = 8.6 Hz, 2H), 7.02 – 6.97 (m, 2H), 5.58 (s, 2H), 3.90 (s, 3H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>, ppm) δ 183.8, 163.8, 163.0 (d, *J* = 248.8 Hz), 148.9, 133.1, 130.3 (d, *J* = 8.4 Hz), 129.6 (d, *J* = 3.4 Hz), 129.3, 128.0, 116.4 (d, *J* = 21.8 Hz), 113.7, 55.5, 53.6. Spectral data match those previously reported in the literature.<sup>[4]</sup>

**(1-(4-fluorobenzoyl)-1H-1,2,3-triazol-4-yl)(4-fluorophenyl)methanone (3p)**



Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3p** as a white solid. 236.4 mg, 79% yield, m.p. 165–168 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.59 – 8.49 (m, 2H), 8.18 (s, 1H), 7.38 – 7.30 (m, 2H), 7.18 (t, *J* = 8.7 Hz, 2H), 7.09 (t, *J* = 8.5 Hz, 2H), 5.58 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 183.7, 166.0 (d, *J* = 255.5 Hz), 163.1 (d, *J* = 249.1 Hz), 148.4, 133.4 (d, *J* = 9.4 Hz), 132.7 (d, *J* = 2.9 Hz), 130.3 (d, *J* = 8.4 Hz), 129.5 (d, *J* = 3.4 Hz), 128.2, 116.4 (d, *J* = 21.9 Hz), 115.5 (d, *J* = 21.8 Hz), 53.7. Spectral data match those previously reported in the literature.<sup>[5]</sup>

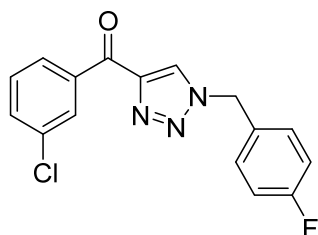
**(1-(2-fluorophenyl)-1H-1,2,3-triazol-4-yl)(4-fluorophenyl)methanone (3q)**



Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3q** as a white solid. 218.5 mg, 73% yield, m.p. 134–137 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.15 (s, 1H), 7.82 – 7.92 (m, 1H), 7.52 – 7.62 (m, 1H), 7.42 – 7.06 (m, 6H), 5.61 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 184.7, 163.1 (d, *J* = 232.6 Hz), 160.6 (d, *J* = 239.1 Hz), 148.0, 133.8 (d, *J* = 8.7 Hz), 131.2 (d, *J* = 2.1 Hz), 130.3 (d, *J* = 8.5 Hz), 129.5 (d, *J* = 3.4 Hz), 127.3, 126.1 (d, *J* = 12.6 Hz), 124.0 (d, *J* = 3.7 Hz), 116.5 (d, *J* = 21.7 Hz), 116.3 (d, *J* = 21.9 Hz), 53.6. HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd for C<sub>16</sub>H<sub>12</sub>F<sub>2</sub>N<sub>3</sub>O: 300.0943; found: 300.0940.

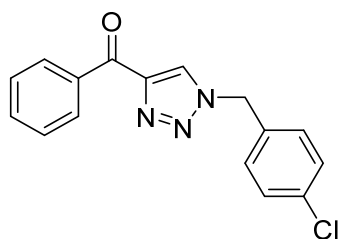


**(3-chlorophenyl)(1-(4-fluorobenzyl)-1H-1,2,3-triazol-4-yl)methanone (3r)**



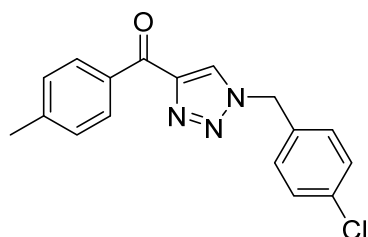
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3r** as a white solid. 233.6 mg, 74% yield, m.p. 123–125 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.44 – 8.30 (m, 2H), 8.19 (s, 1H), 7.55 – 7.59 (m, 1H), 7.45 (t, *J* = 7.9 Hz, 1H), 7.38 – 7.29 (m, 2H), 7.09 (t, *J* = 8.5 Hz, 2H), 5.58 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 184.1, 163.1 (d, *J* = 249.0 Hz), 148.0, 137.8, 134.6, 133.2, 130.4, 130.3 (d, *J* = 8.5 Hz), 129.7, 129.5 (d, *J* = 3.3 Hz), 128.8, 128.3, 116.4 (d, *J* = 21.9 Hz), 53.7. Spectral data match those previously reported in the literature.<sup>[5]</sup>

**(1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3s)**



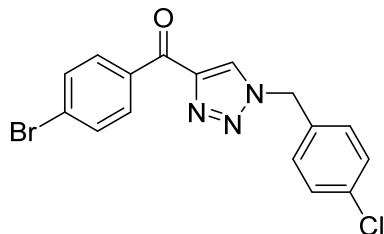
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3s** as a white solid. 244.2 mg, 82% yield, m.p. 150–152 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.41 (d, *J* = 7.2 Hz, 2H), 8.18 (s, 1H), 7.64 – 7.59 (m, 1H), 7.52 (t, *J* = 8.5 Hz, 2H), 7.41 – 7.36 (m, 2H), 7.28 (d, *J* = 9.0 Hz, 3H), 5.58 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 185.6, 136.4, 135.3, 133.4, 132.2, 131.5, 130.6, 129.7, 129.6, 128.9, 128.4, 128.2, 53.7. Spectral data match those previously reported in the literature.<sup>[5]</sup>

**(1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)(p-tolyl)methanone (3t)**



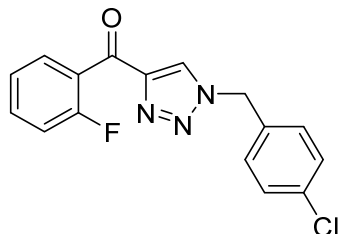
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3t** as a white solid. 205.8 mg, 66% yield, m.p. 178–180 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.34 (d, *J* = 8.1 Hz, 2H), 8.16 (s, 1H), 7.41 – 7.36 (m, 2H), 7.33 – 7.27 (m, 4H), 5.57 (s, 2H), 2.44 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 185.1, 148.7, 144.3, 135.3, 133.9, 132.3, 130.8, 129.7, 129.6, 129.1, 128.1, 53.7, 21.8. Spectral data match those previously reported in the literature.<sup>[4]</sup>

**(4-bromophenyl)(1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)methanone (3u)**



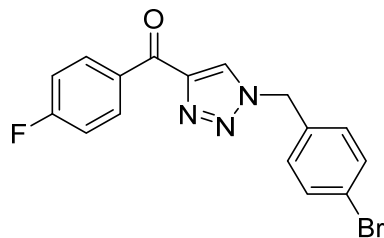
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3u** as a white solid. 308.8 mg, 82% yield, m.p. 175–177 °C. <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>, ppm) δ 8.37 – 8.34 (m, 2H), 8.19 (s, 1H), 7.70 – 7.65 (m, 2H), 7.43 – 7.38 (m, 2H), 7.30 – 7.28 (m, 2H), 5.59 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 184.3, 148.4, 135.4, 135.0, 132.2, 132.1, 131.8, 129.7, 129.6, 128.8, 128.4, 53.8. Spectral data match those previously reported in the literature.<sup>[5]</sup>

**(1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)(2-fluorophenyl)methanone (3v)**



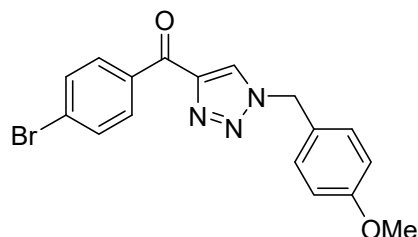
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3v** as a white solid. 246.3 mg, 78% yield, m.p. 175–177 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.20 – 8.12 (m, 1H), 7.87 (t, *J* = 7.5 Hz, 1H), 7.52 – 7.62 (m, 1H), 7.45 – 7.15 (m, 6H), 5.60 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 184.6, 160.7 (d, *J* = 256.2 Hz), 148.1, 135.3, 133.8 (d, *J* = 8.5 Hz), 132.2, 131.2 (d, *J* = 2.1 Hz), 129.6, 129.6, 127.3, 126.2 (d, *J* = 11.6 Hz), 124.1 (d, *J* = 3.3 Hz), 116.5 (d, *J* = 21.8 Hz), 53.7. HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd for C<sub>16</sub>H<sub>12</sub>ClFN<sub>3</sub>O: 316.0647; found: 316.0642.

**(1-(4-bromobenzyl)-1H-1,2,3-triazol-4-yl)(4-fluorophenyl)methanone (3w)**



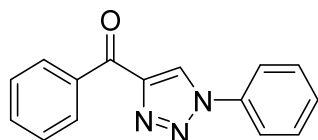
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3w** as a white solid. 277.3 mg, 77% yield, m.p. 195–198 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.53 (m, 2H), 8.19 (s, 1H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.24 – 7.13 (m, 4H), 5.56 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 183.7, 166.0 (d, *J* = 255.0 Hz), 148.5, 133.4 (d, *J* = 9.3 Hz), 132.6, 132.5, 129.9, 128.3, 123.5, 115.6 (d, *J* = 21.8 Hz), 53.8. HRMS (ESI): *m/z* [M + Na]<sup>+</sup> calcd for C<sub>16</sub>H<sub>11</sub>BrFN<sub>3</sub>ONa: 381.9962; found: 381.9957.

**(4-bromophenyl)(1-(4-methoxybenzyl)-1H-1,2,3-triazol-4-yl)methanone (3x)**



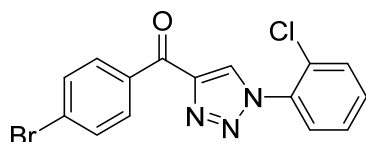
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3x** as a white solid. 234.5 mg, 63% yield, m.p. 145–147 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.40 – 8.28 (m, 2H), 8.13 (s, 1H), 7.68 – 7.60 (m, 2H), 7.33 – 7.23 (m, 2H), 6.97 – 6.86 (m, 2H), 5.53 (s, 2H), 3.81 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 184.4, 160.3, 148.1, 135.2, 132.2, 131.7, 130.0, 128.6, 128.2, 125.5, 114.8, 55.4, 54.1. Spectral data match those previously reported in the literature.<sup>[4]</sup>

**phenyl(1-phenyl-1H-1,2,3-triazol-4-yl)methanone (3y)**



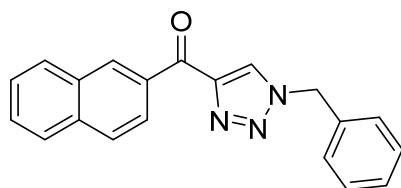
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3y** as a white solid. 179.5 mg, 72% yield, m.p. 126–127 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.74 (s, 1H), 8.51 (d, *J* = 7.3 Hz, 2H), 7.84 (d, *J* = 7.8 Hz, 2H), 7.69 – 7.49 (m, 6H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 185.6, 148.6, 136.5, 133.4, 130.7, 130.0, 129.5, 128.5, 126.4, 120.8. Spectral data match those previously reported in the literature.<sup>[2]</sup>

**(4-bromophenyl)(1-(2-chlorophenyl)-1H-1,2,3-triazol-4-yl)methanone (3z)**



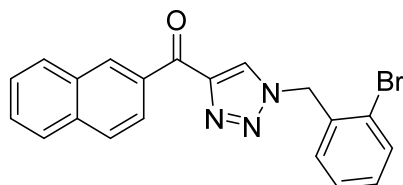
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3z** as a white solid. 257.5 mg, 71% yield, m.p. 120–123 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.71 (s, 1H), 8.45 – 8.41 (m, 2H), 7.74 – 7.62 (m, 4H), 7.48 – 7.56 (m, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 184.2, 135.1, 132.2, 131.8, 131.5, 131.0, 130.6, 128.9, 128.7, 128.1, 127.6. Spectral data match those previously reported in the literature.<sup>[4]</sup>

**(1-benzyl-1H-1,2,3-triazol-4-yl)(naphthalen-2-yl)methanone (3aa)**



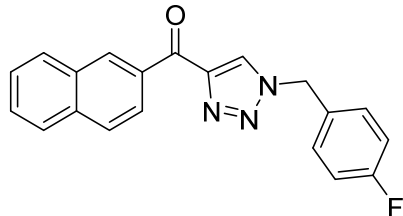
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3aa** as a white solid. 231.9 mg, 74% yield, m.p. 155–157 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 9.23 (s, 1H), 8.33 (d, *J* = 8.4 Hz, 1H), 8.22 (s, 1H), 8.03 (d, *J* = 7.8 Hz, 1H), 7.98 – 7.82 (m, 2H), 7.71 – 7.29 (m, 7H), 5.62 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 185.3, 148.7, 135.7, 133.7, 133.5, 132.5, 132.0, 130.1, 129.4, 129.2, 128.7, 128.4, 128.2, 127.7, 126.6, 125.5, 54.5. Spectral data match those previously reported in the literature.<sup>[4]</sup>

**(1-(2-bromobenzyl)-1H-1,2,3-triazol-4-yl)(naphthalen-2-yl)methanone (3ab)**



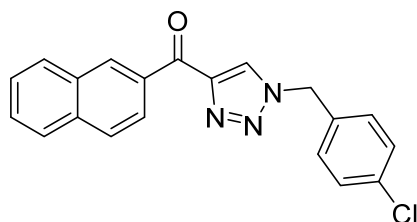
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3ab** as a white solid. 278.5 mg, 71% yield, m.p. 106–108 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.45 (d, *J* = 8.1 Hz, 1H), 8.29 (s, 1H), 8.16 (t, *J* = 6.0 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 7.9 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.62 – 7.25 (m, 6H), 5.77 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 188.4, 148.8, 133.9, 133.5, 133.3, 132.7, 130.9, 130.3, 128.4, 127.7, 126.4, 125.5, 124.4, 123.9, 54.2. HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd for C<sub>20</sub>H<sub>15</sub>BrN<sub>3</sub>O: 392.0393; found: 392.0387.

**(1-(4-fluorobenzyl)-1H-1,2,3-triazol-4-yl)(naphthalen-2-yl)methanone (3ac)**



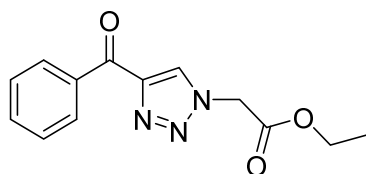
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3ac** as a white solid. 241.9 mg, 73% yield, m.p. 123–124 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.44 (d, *J* = 7.6 Hz, 1H), 8.20 (s, 1H), 8.14 (d, *J* = 7.0 Hz, 1H), 8.07 (d, *J* = 8.1 Hz, 1H), 7.94 (d, *J* = 7.7 Hz, 1H), 7.48 – 7.64 (m, 3H), 7.40 – 7.27 (m, 2H), 7.03 – 7.15 (m, 2H), 5.59 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 188.4, 163.1 (d, *J* = 248.1 Hz), 149.0, 134.3, 133.9, 132.7, 130.8, 130.4, 130.3, 129.7 (d, *J* = 4.0 Hz), 128.5, 128.1, 127.7, 126.4, 125.4, 124.4, 116.4 (d, *J* = 22.0 Hz), 53.7. HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd for C<sub>20</sub>H<sub>15</sub>FN<sub>3</sub>O: 332.1194; found: 332.1190.

**(1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)(naphthalen-2-yl)methanone (3ad)**



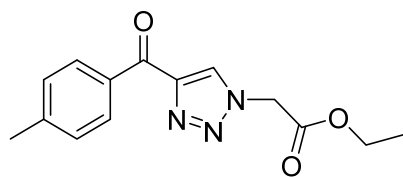
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3ad** as a white solid. 267.8 mg, 77% yield, m.p. 118–121 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.44 (d, *J* = 7.9 Hz, 1H), 8.21 (d, *J* = 4.6 Hz, 1H), 8.17 (s, 1H), 8.06 (t, *J* = 6.4 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.47 – 7.63 (m, 3H), 7.34 – 7.42 (m, 2H), 7.20 – 7.32 (m, 2H), 5.57 (s, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 188.3, 149.1, 135.3, 134.2, 133.9, 132.7, 132.3, 130.8, 130.3, 129.7, 129.6, 128.5, 128.2, 127.7, 126.5, 125.4, 124.4, 53.7. HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd for C<sub>20</sub>H<sub>15</sub>ClN<sub>3</sub>O: 348.0898; found: 348.0894.

**ethyl 2-(4-benzoyl-1H-1,2,3-triazol-1-yl)acetate (3ba)**



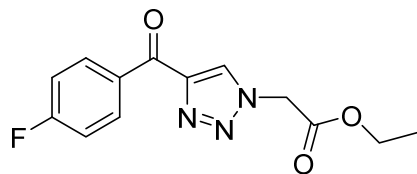
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3ba** as a white solid. 171.1 mg, 66% yield, m.p. 125–126 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.48 – 8.35 (m, 3H), 7.61 – 7.67 (m, 1H), 7.59 – 7.51 (m, 2H), 5.28 (s, 2H), 4.32 (q, *J* = 7.2 Hz, 2H), 1.34 (t, *J* = 7.2 Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 185.5, 165.6, 148.4, 136.5, 133.3, 130.6, 129.9, 128.4, 62.8, 51.0, 14.1. Spectral data match those previously reported in the literature.<sup>[5]</sup>

**ethyl 2-(4-(4-methylbenzoyl)-1H-1,2,3-triazol-1-yl)acetate (3bb)**



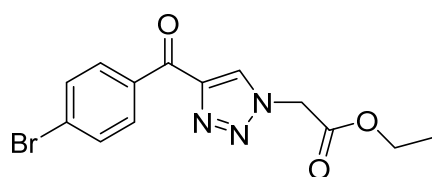
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3v** as a white solid. 169.4 mg, 62% yield, m.p. 148–150 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.40 (s, 1H), 8.35 – 8.28 (m, 2H), 7.27 – 7.33 (m, 2H), 5.24 (s, 2H), 4.21 – 4.31 (m, 2H), 2.42 (q, *J* = 3.1 Hz, 2H), 1.28 (t, *J* = 7.1 Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 185.1, 165.7 (d, *J* = 4.2 Hz), 148.5 (d, *J* = 6.5 Hz), 144.3, 134.0, 130.7 (d, *J* = 1.9 Hz), 129.8, 129.1, 62.7 (d, *J* = 2.4 Hz), 51.0, 21.7, 14.0. Spectral data match those previously reported in the literature.<sup>[5]</sup>

**ethyl 2-(4-(4-fluorobenzoyl)-1H-1,2,3-triazol-1-yl)acetate (3bc)**



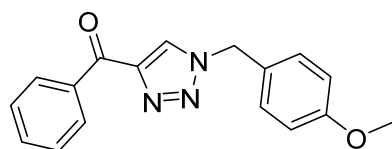
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3v** as a white solid. 194.1 mg, 70% yield, m.p. 160–161 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.61 – 8.50 (m, 2H), 8.45 (s, 1H), 7.21 (t, *J* = 8.7 Hz, 2H), 5.28 (s, 2H), 4.31 (q, *J* = 7.1 Hz, 2H), 1.33 (t, *J* = 7.1 Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 183.6, 166.0 (d, *J* = 255.4 Hz), 165.6, 148.3, 133.4 (d, *J* = 9.4 Hz), 132.7 (d, *J* = 2.9 Hz), 130.0, 115.5 (d, *J* = 21.8 Hz), 62.8, 51.0, 14.0. Spectral data match those previously reported in the literature.<sup>[4]</sup>

**ethyl 2-(4-(4-bromobenzoyl)-1H-1,2,3-triazol-1-yl)acetate (3bd)**



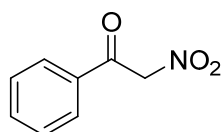
Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3v** as a white solid. 243.5 mg, 72% yield, m.p. 162–164 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.45 (s, 1H), 8.41 – 8.35 (m, 2H), 7.74 – 7.64 (m, 2H), 5.28 (s, 2H), 4.33 (q, *J* = 7.1 Hz, 2H), 1.35 (t, *J* = 7.1 Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 184.2, 165.6, 148.3, 135.1, 132.2, 131.8, 130.0, 128.8, 62.9, 51.0, 14.1. Spectral data match those previously reported in the literature.<sup>[4]</sup>

**(1-(4-methoxybenzyl)-1H-1,2,3-triazol-4-yl)(phenyl)methanone (3ca)**



Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:5) to afford the **3ca** as a white solid. 219.8 mg, 75% yield, m.p. 117–119 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, ppm) δ 8.40 (d, *J* = 7.6 Hz, 2H), 8.12 (s, 1H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 6.94 – 6.90 (m, 2H), 5.54 (s, 2H), 3.82 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, ppm) δ 185.7, 160.2, 148.2, 136.5, 133.2, 130.6, 130.0, 128.4, 128.0, 125.6, 114.7, 55.4, 54.1. Spectral data match those previously reported in the literature.<sup>[3]</sup>

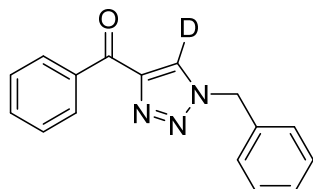
**2-nitro-1-phenylethan-1-one (4)**



Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:5) to afford the **4** as a

pale-yellow solid. 11.7 mg, 7% yield.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ , ppm)  $\delta$  7.93 – 7.87 (m, 2H), 7.74 – 7.68 (m, 1H), 7.56 (t,  $J = 7.8$  Hz, 2H), 5.92 (s, 2H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ , ppm)  $\delta$  185.9, 135.1, 133.4, 129.3, 128.3, 126.9, 81.3. Spectral data match those previously reported in the literature.<sup>[6]</sup>

**(1-benzyl-1H-1,2,3-triazol-4-yl-5-d)(phenyl)methanone (3a')**

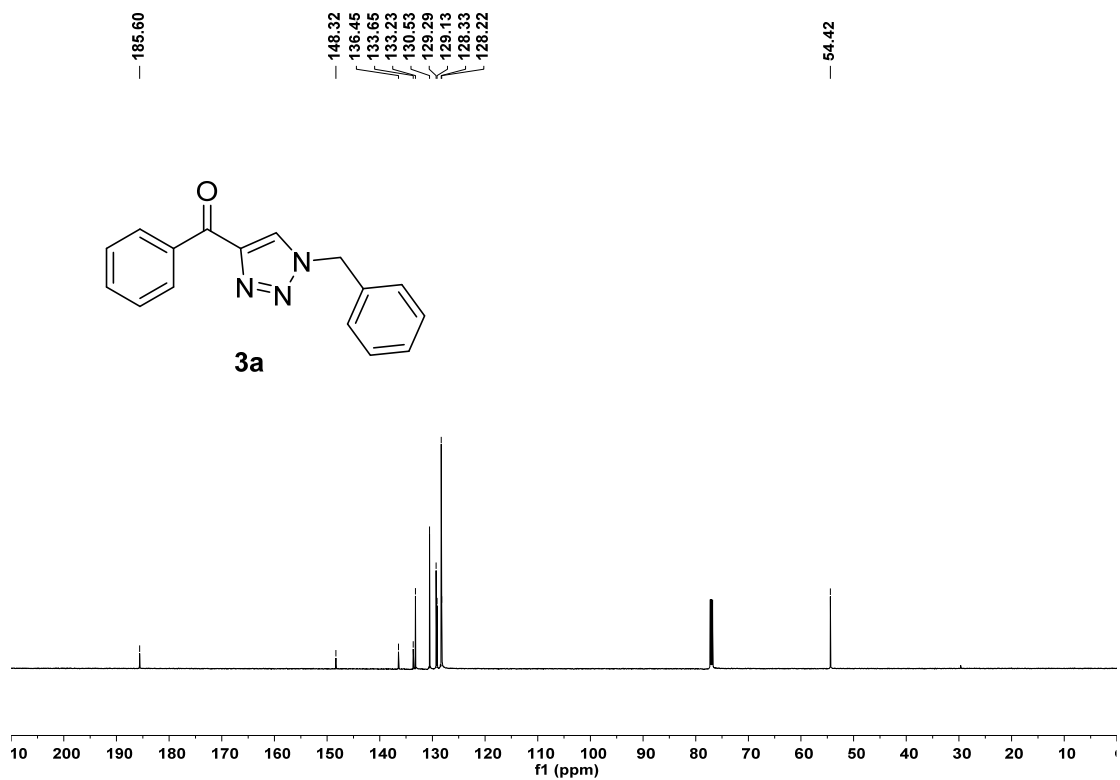
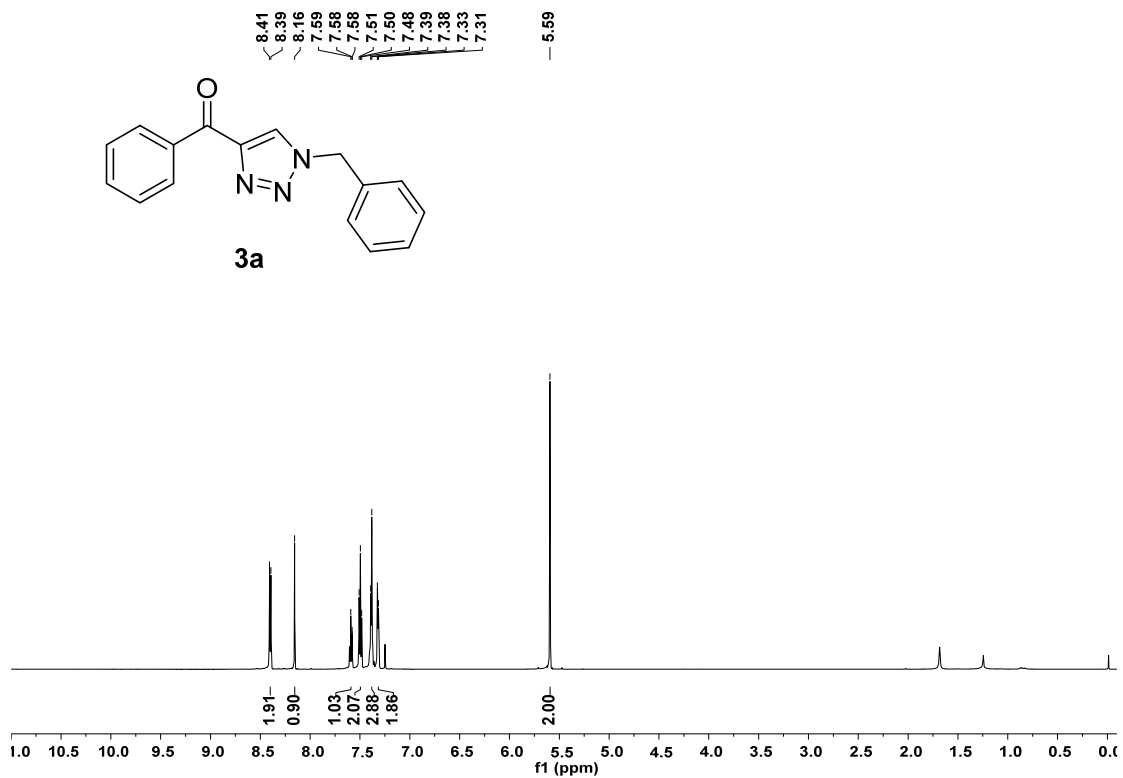


Purified by column chromatography (Ethyl acetate: Petroleum ether = 1:10) to afford the **3a'** as a white solid. 210.6 mg, 80% yield, m.p. 116–117 °C.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ , ppm)  $\delta$  8.42 – 8.41 (m, 2H), 7.63 (t,  $J = 7.8$  Hz, 1H), 7.53 – 7.49 (m, 2H), 7.42 – 7.40 (m, 2H), 7.35 – 7.32 (m, 2H), 5.61 (s, 2H). HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd for  $\text{C}_{16}\text{H}_{13}\text{DN}_3\text{O}$ : 265.1194; found: 265.1192.

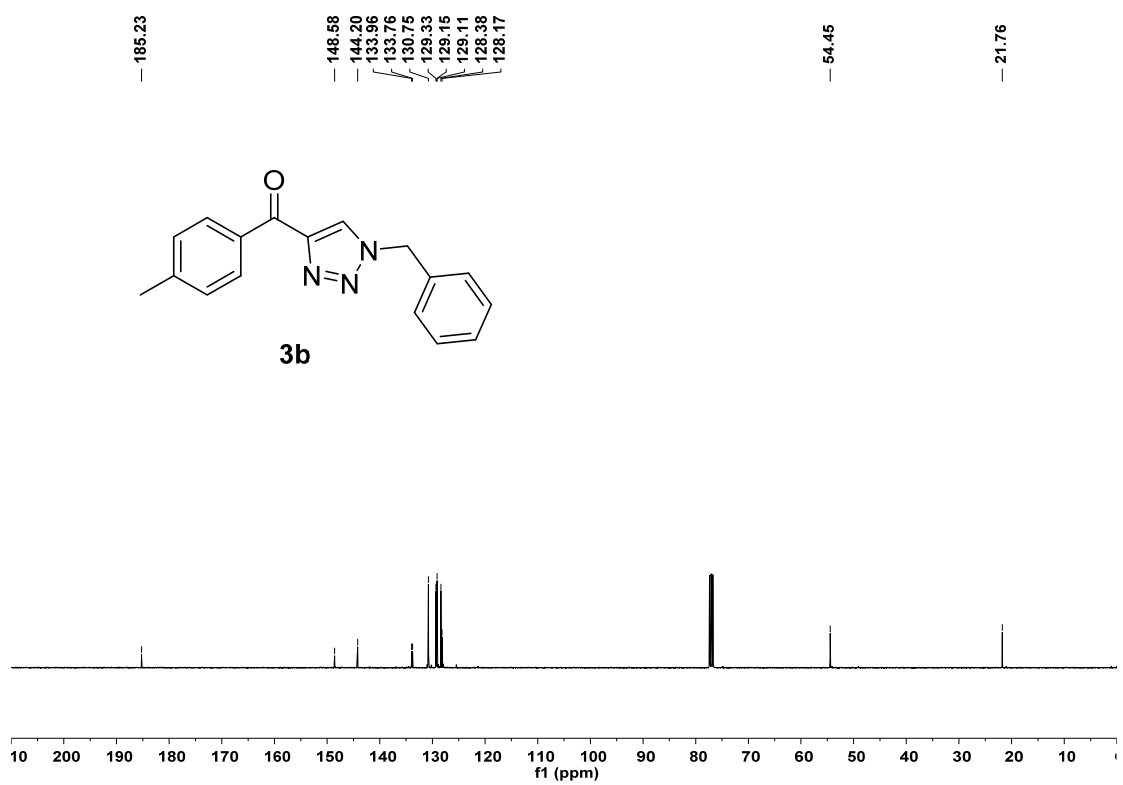
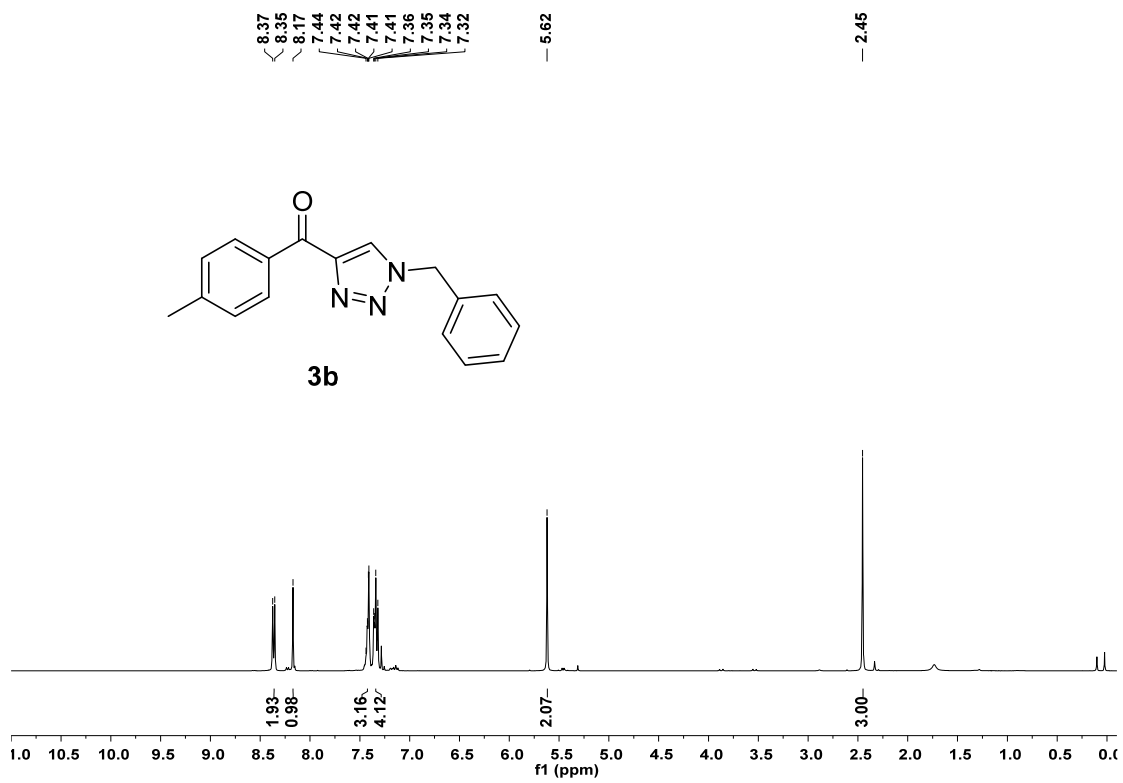
## 5. References

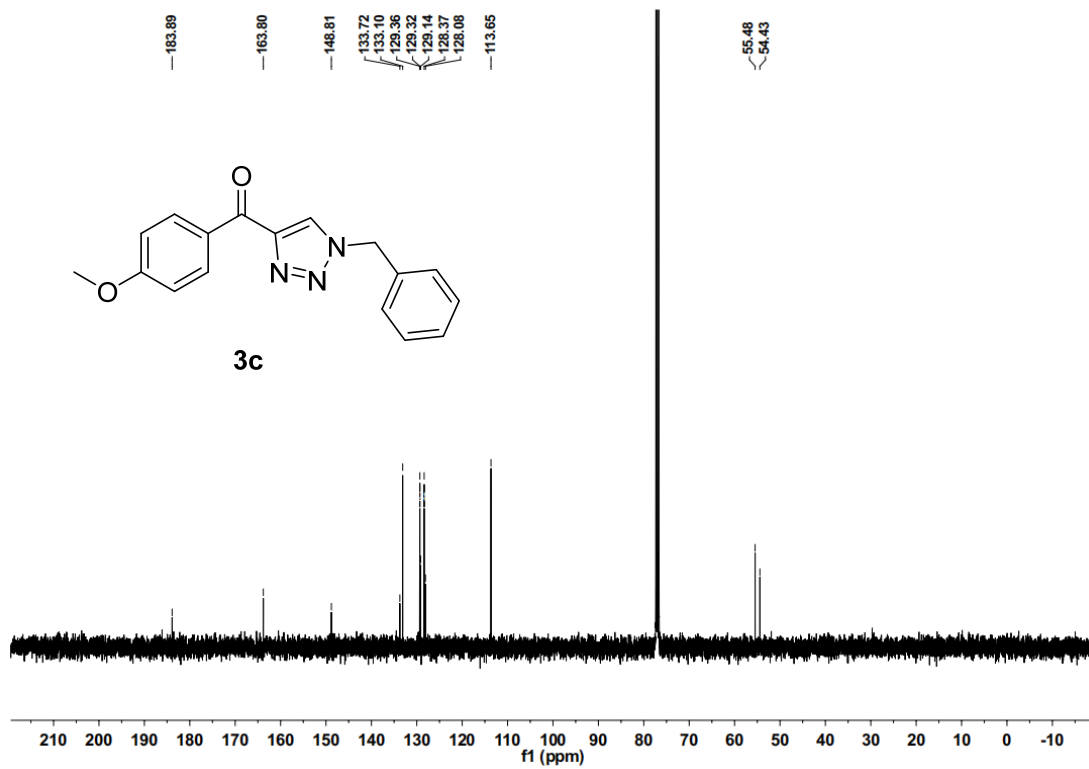
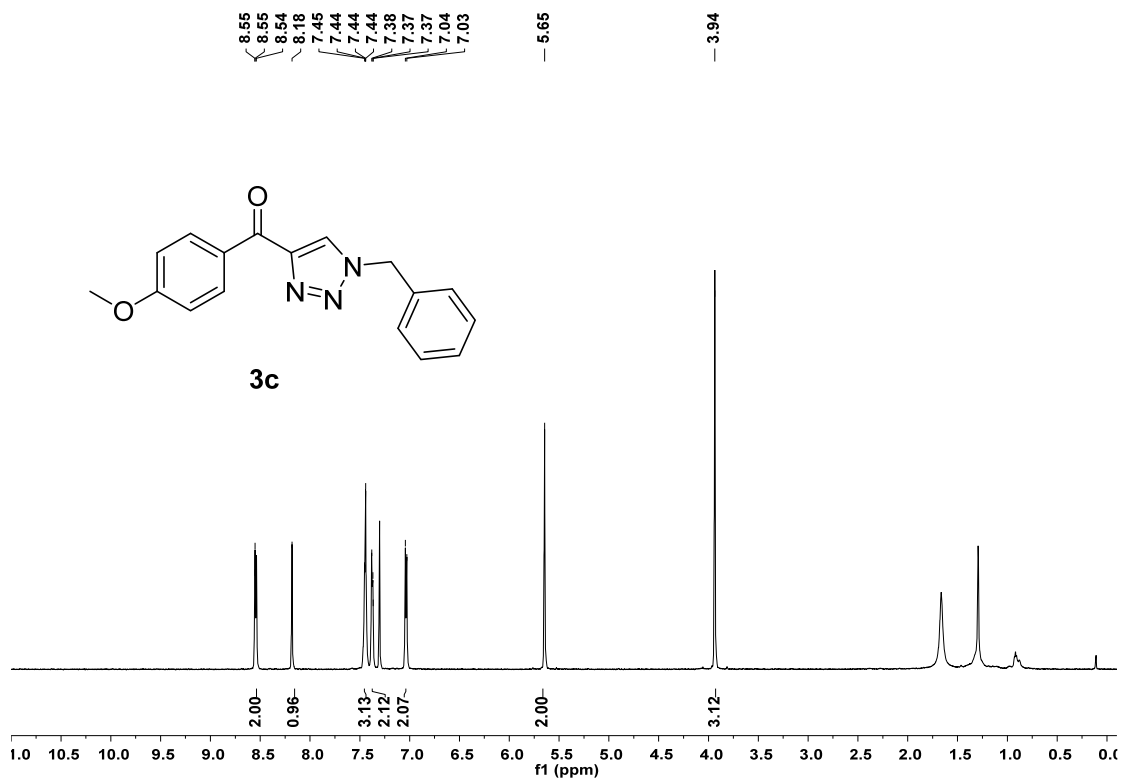
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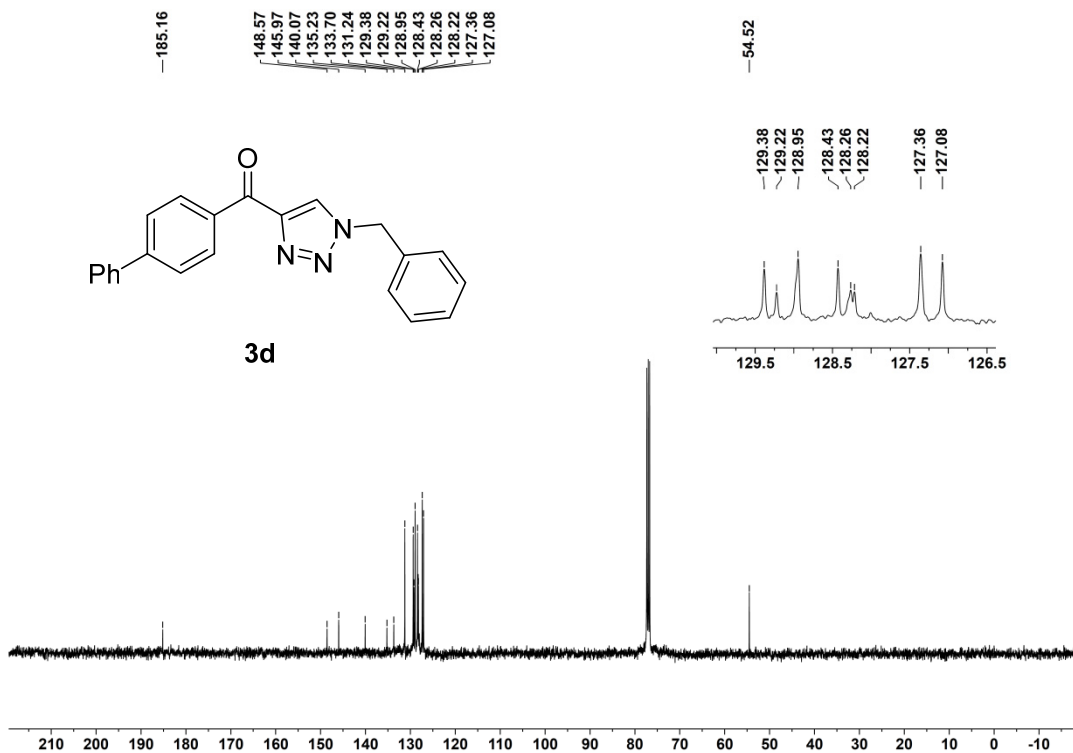
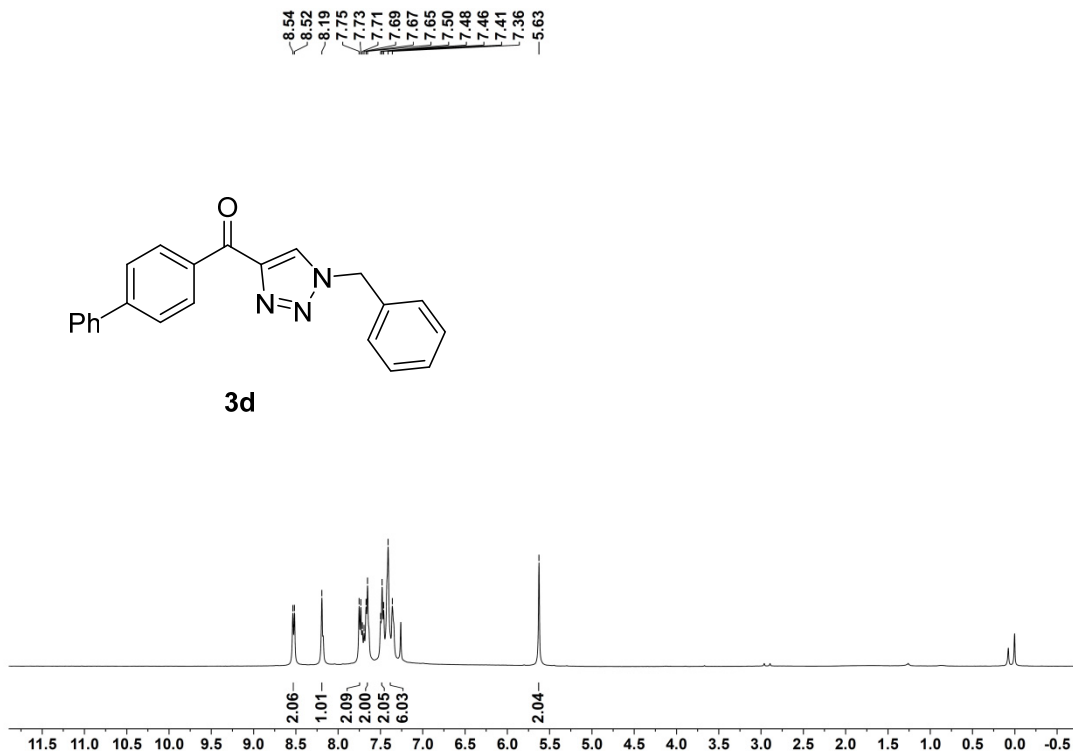
## 6. $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of products

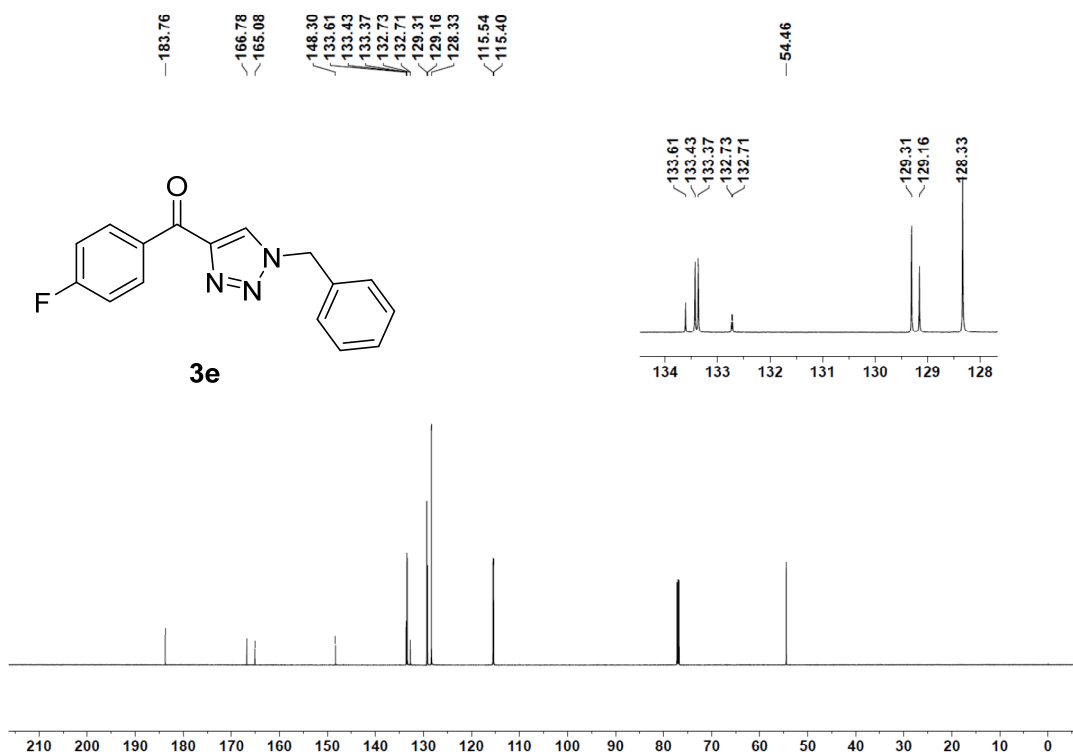
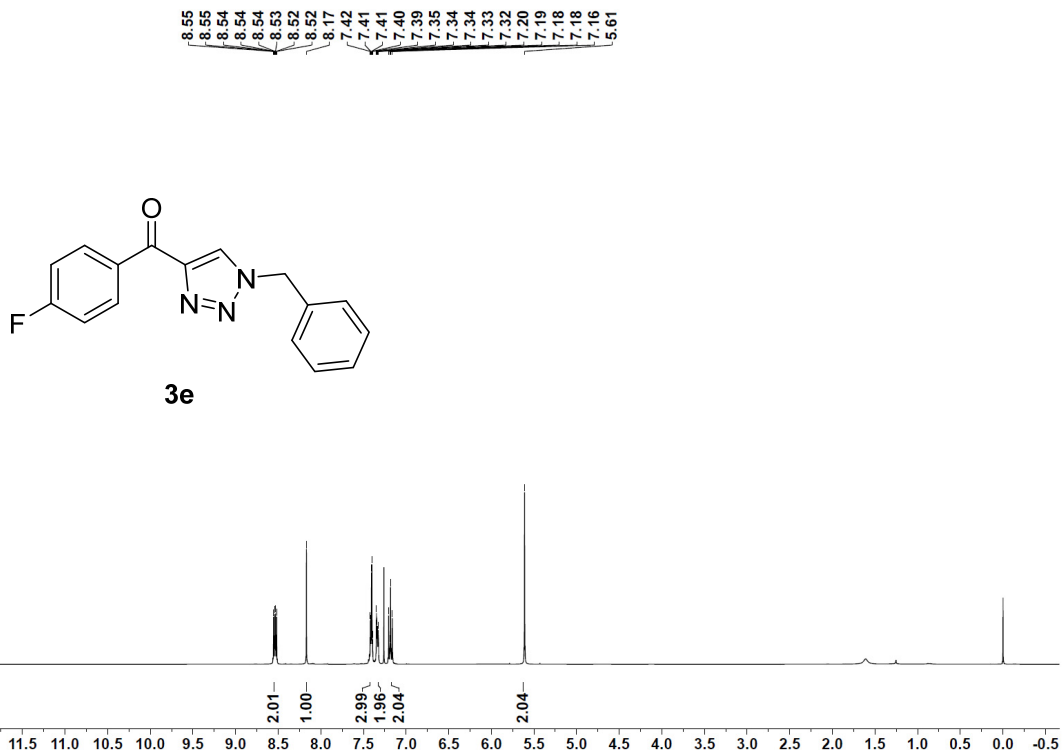


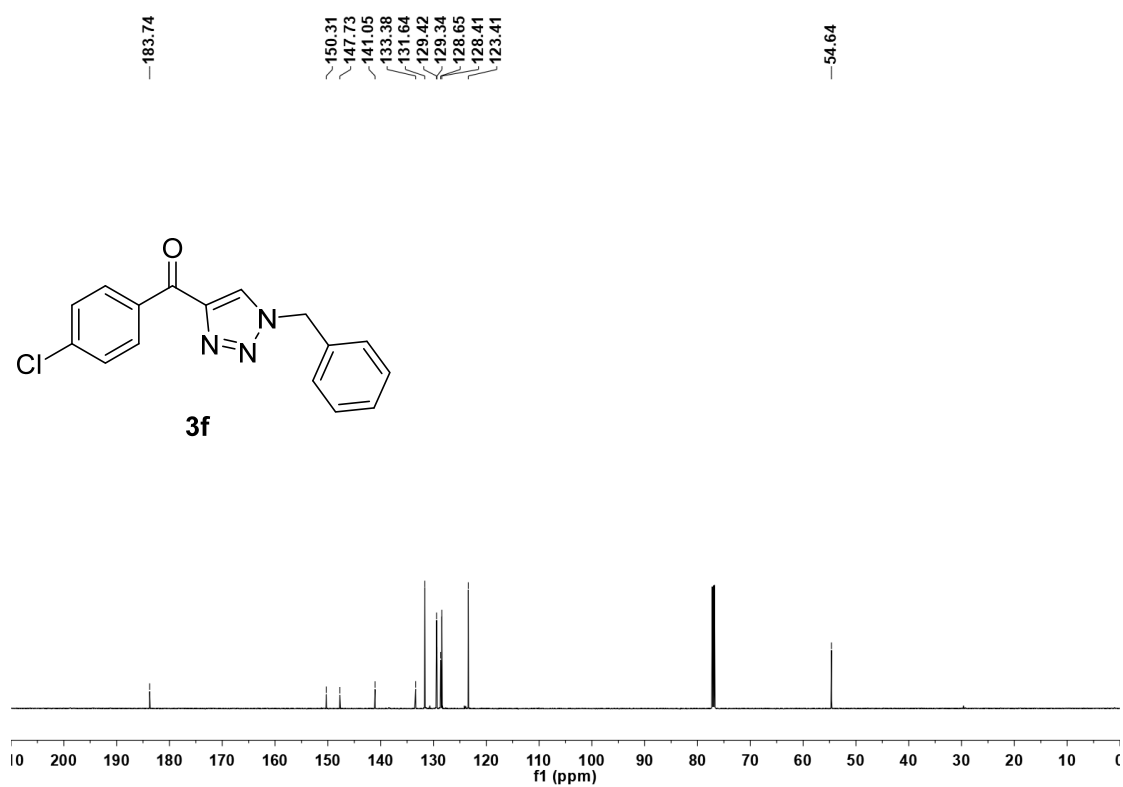
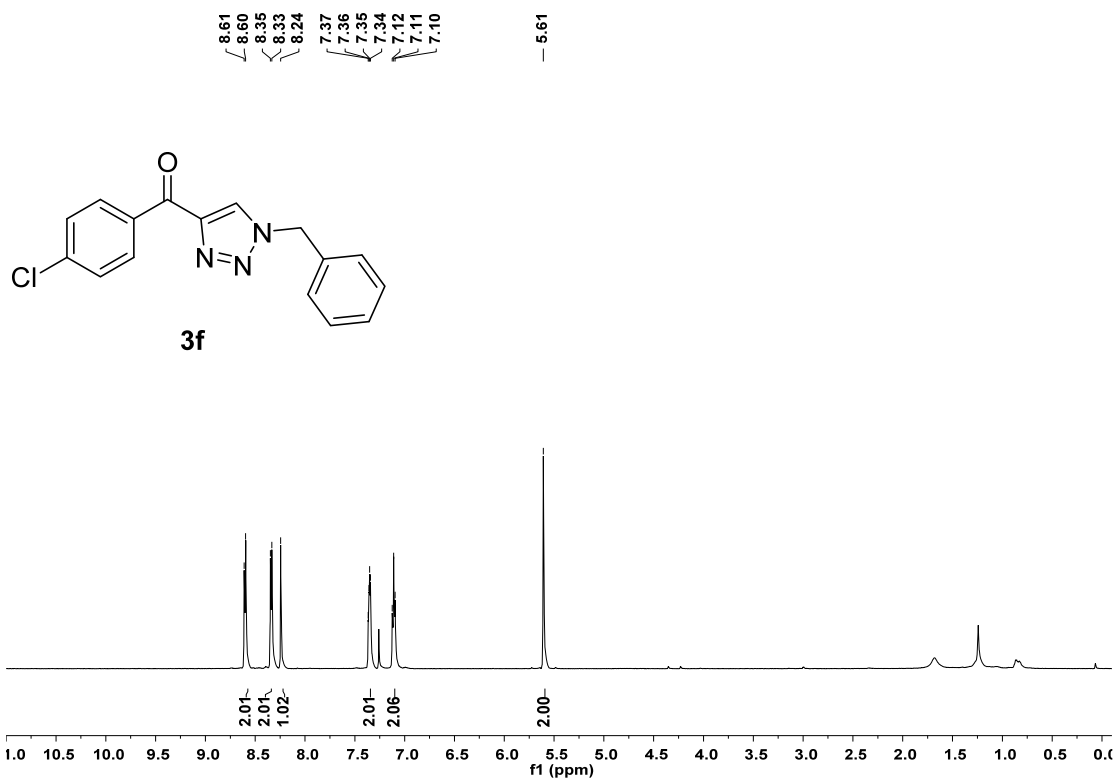


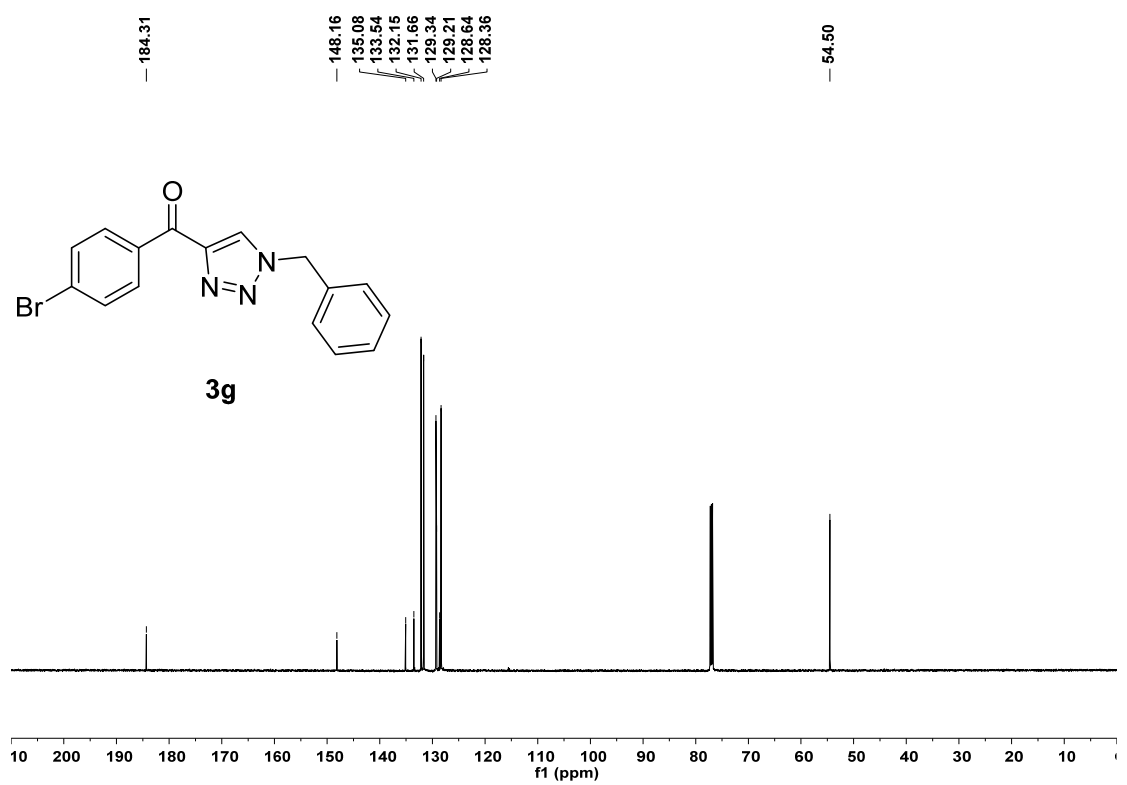
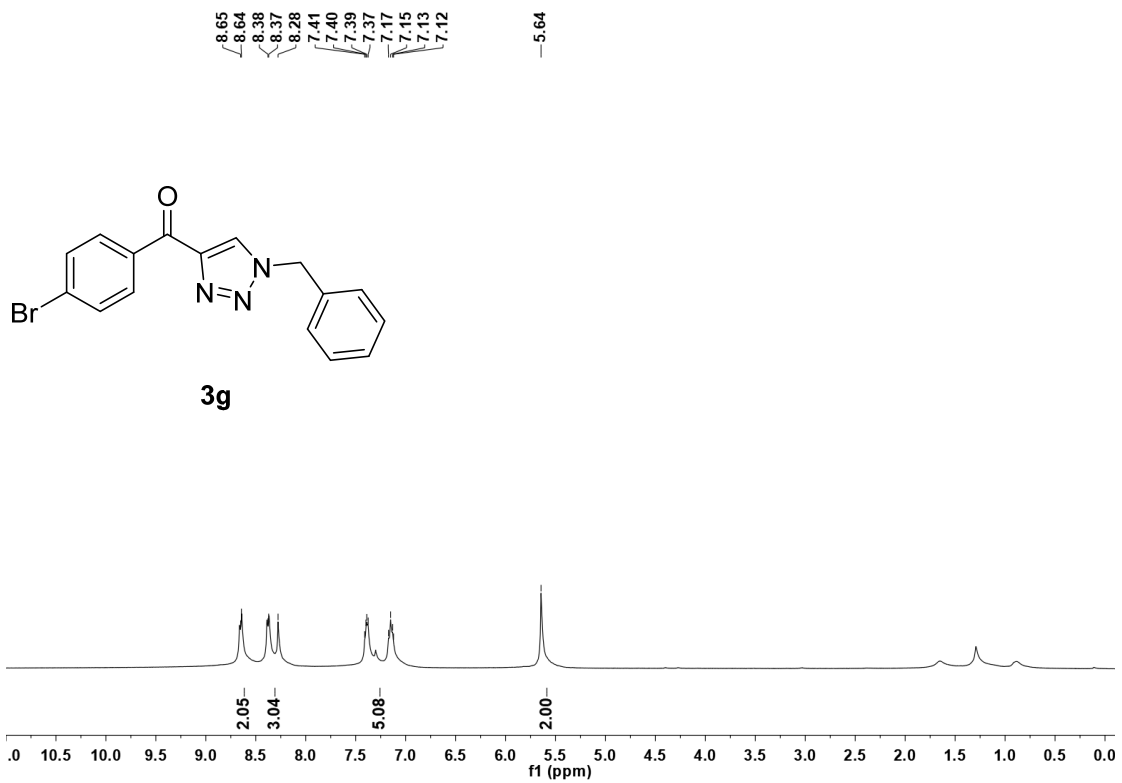


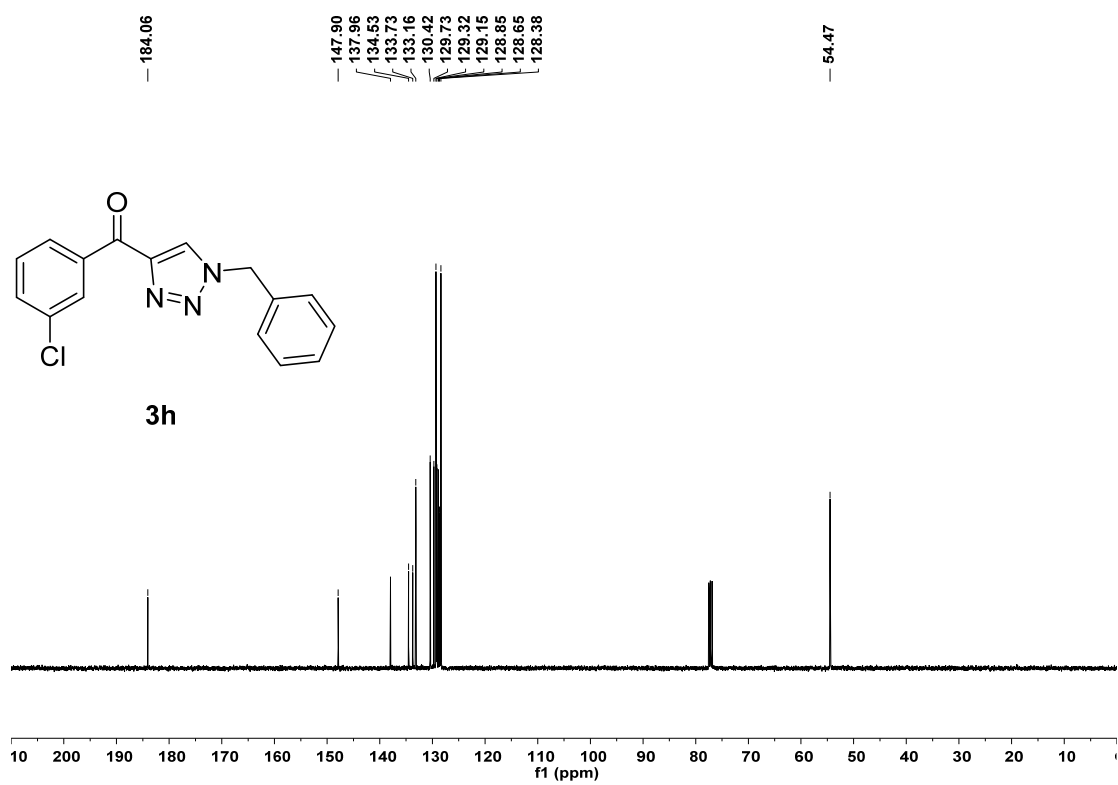
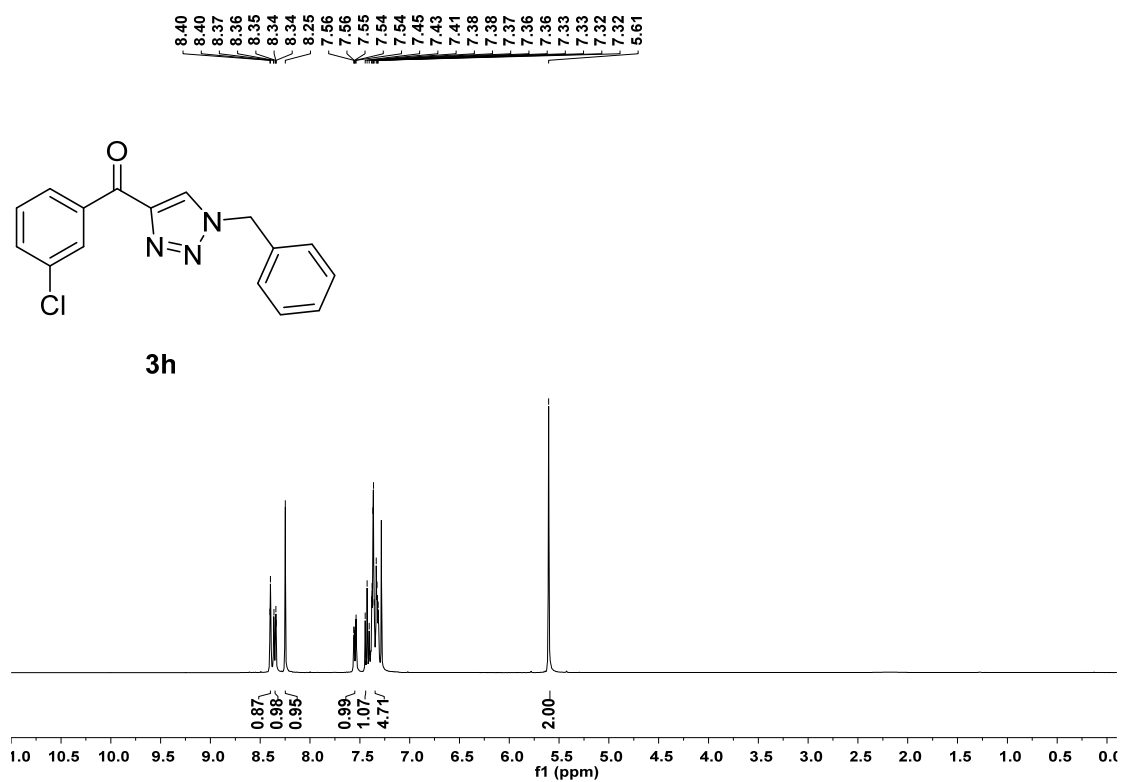


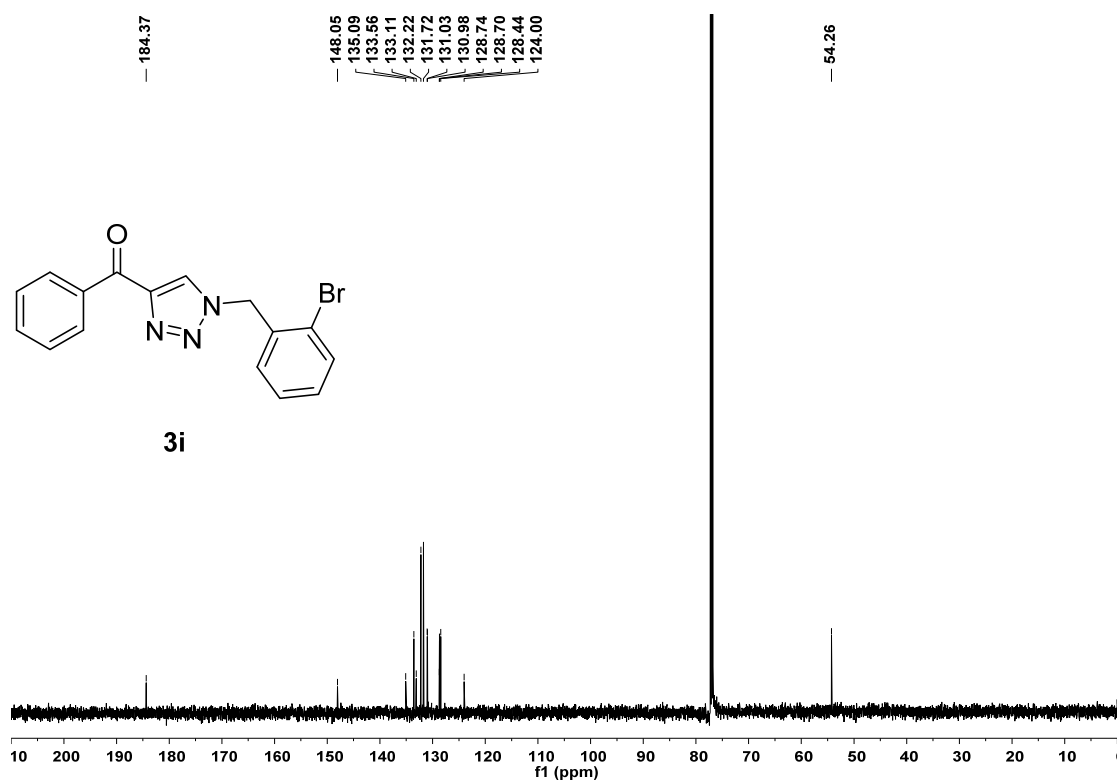
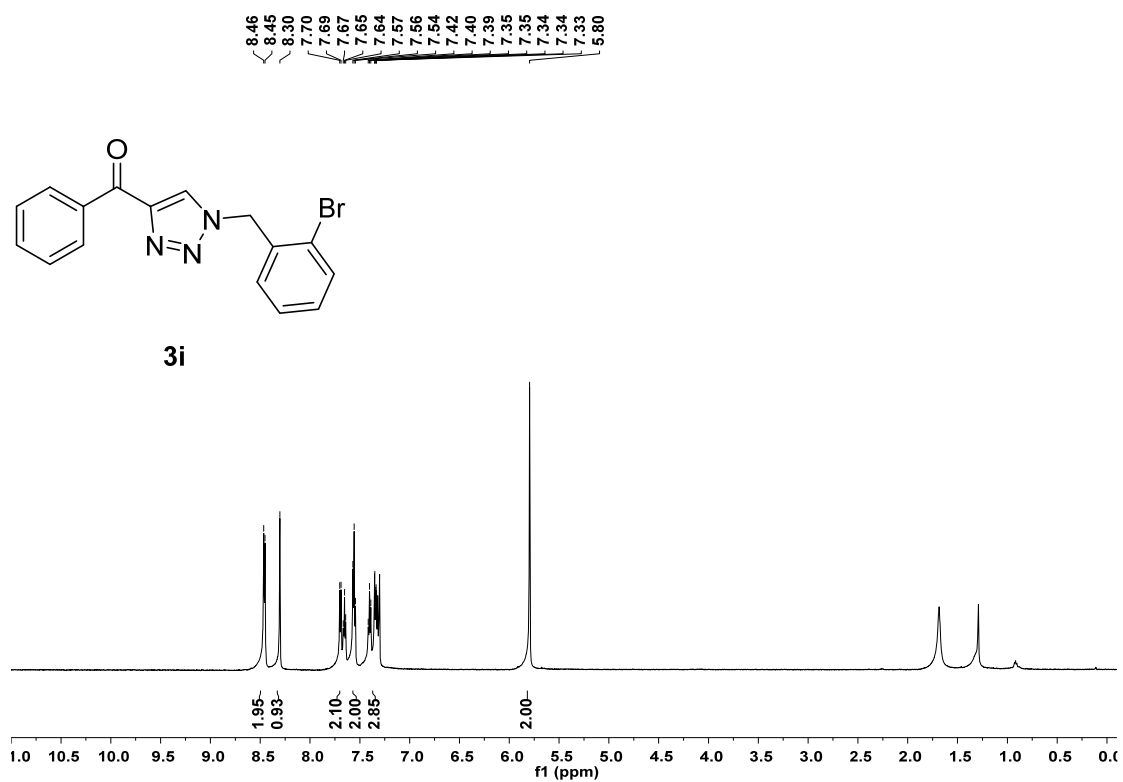




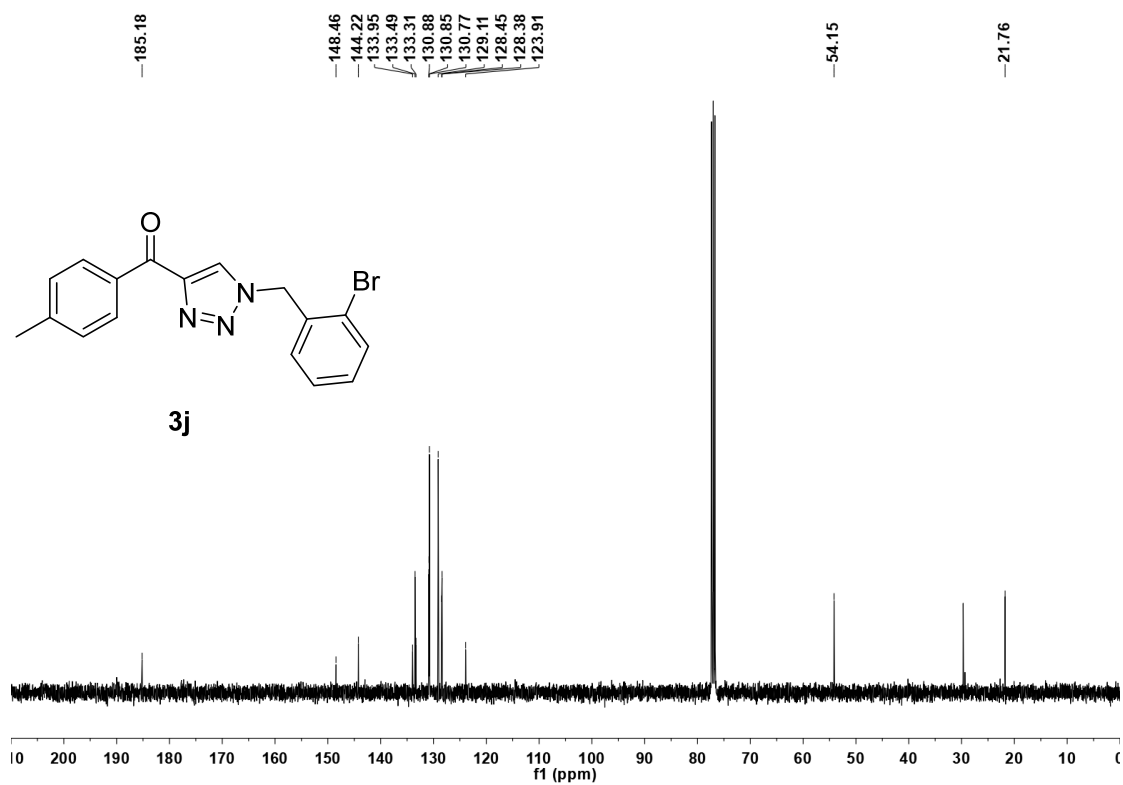
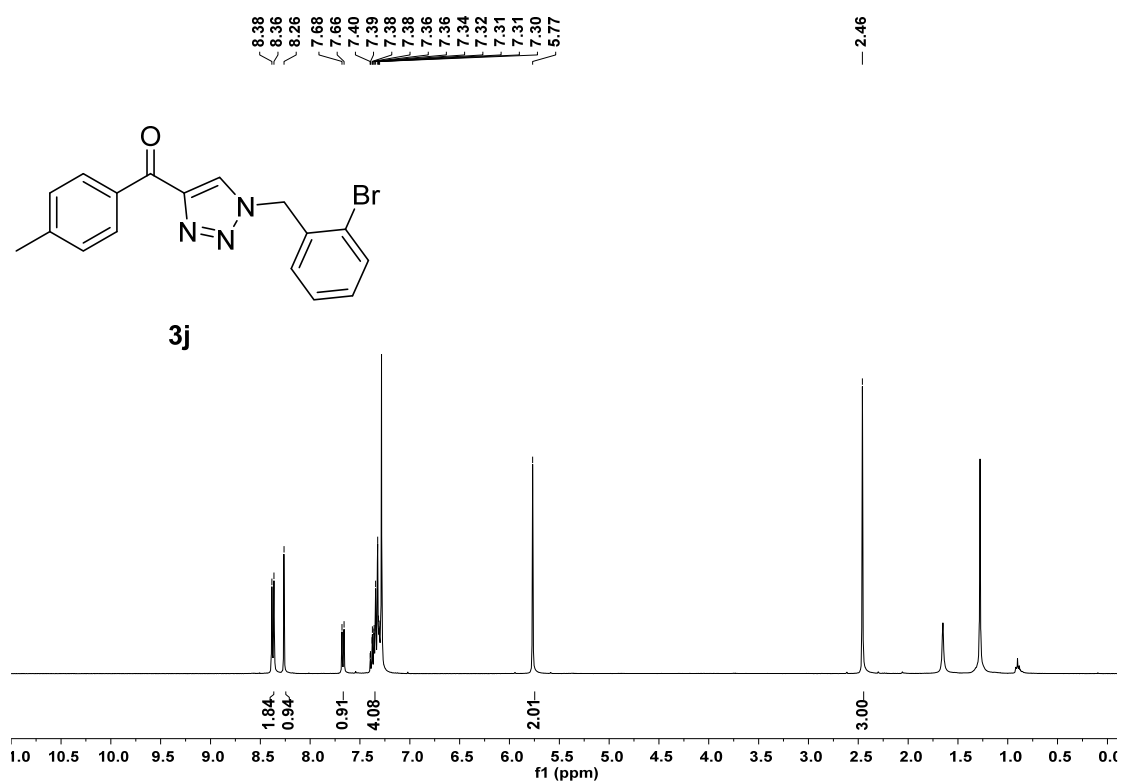


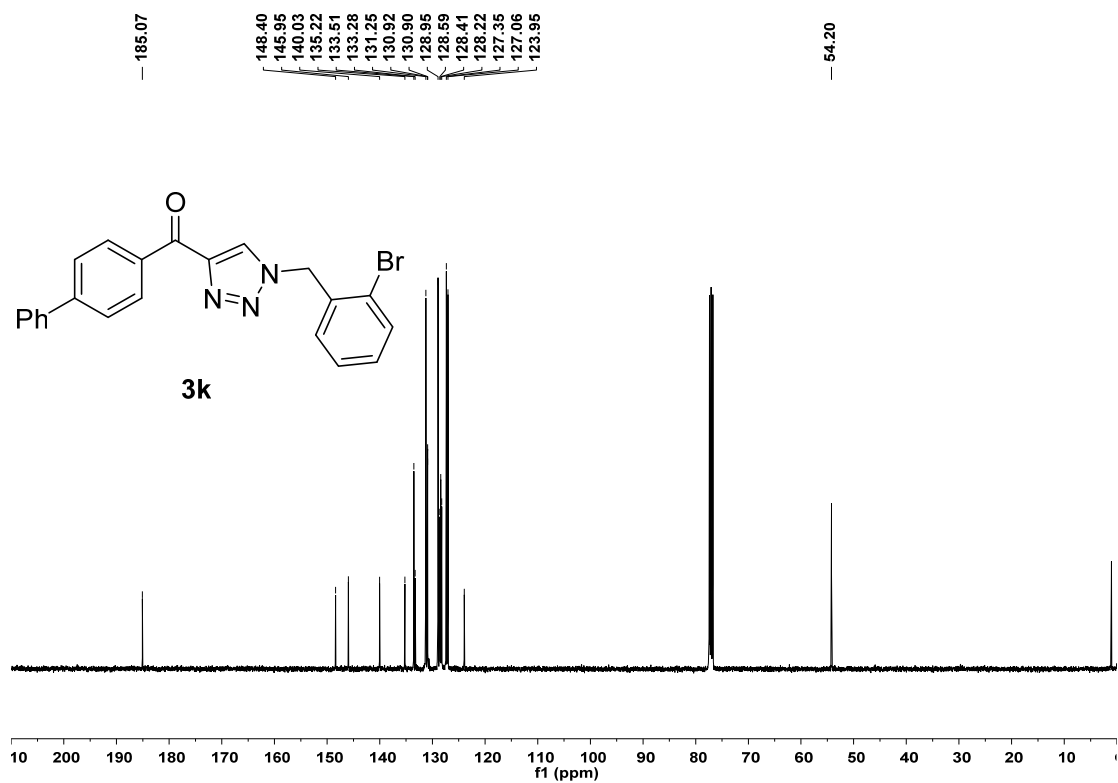
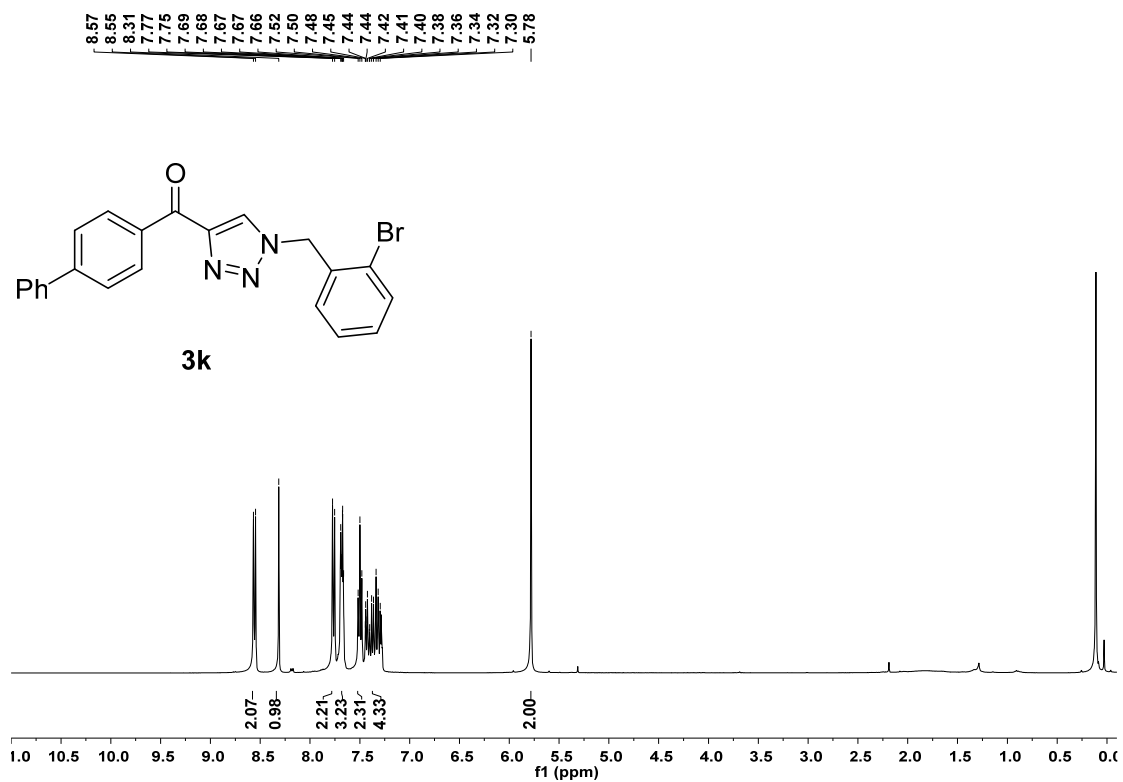


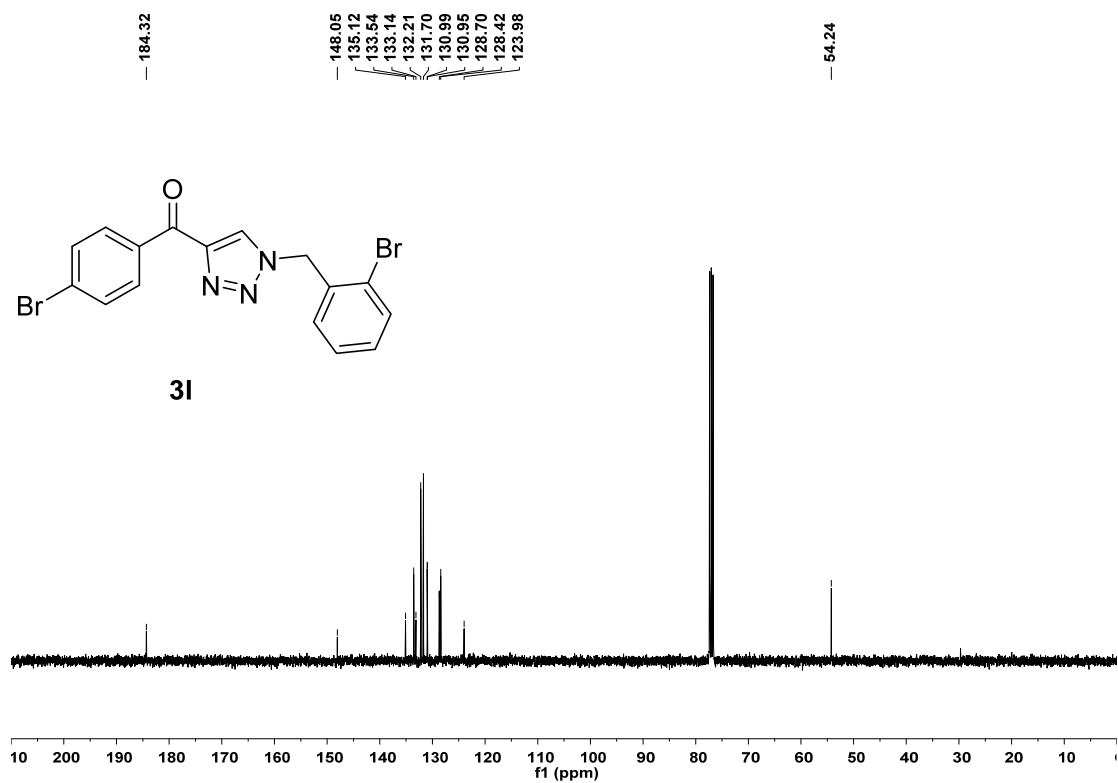
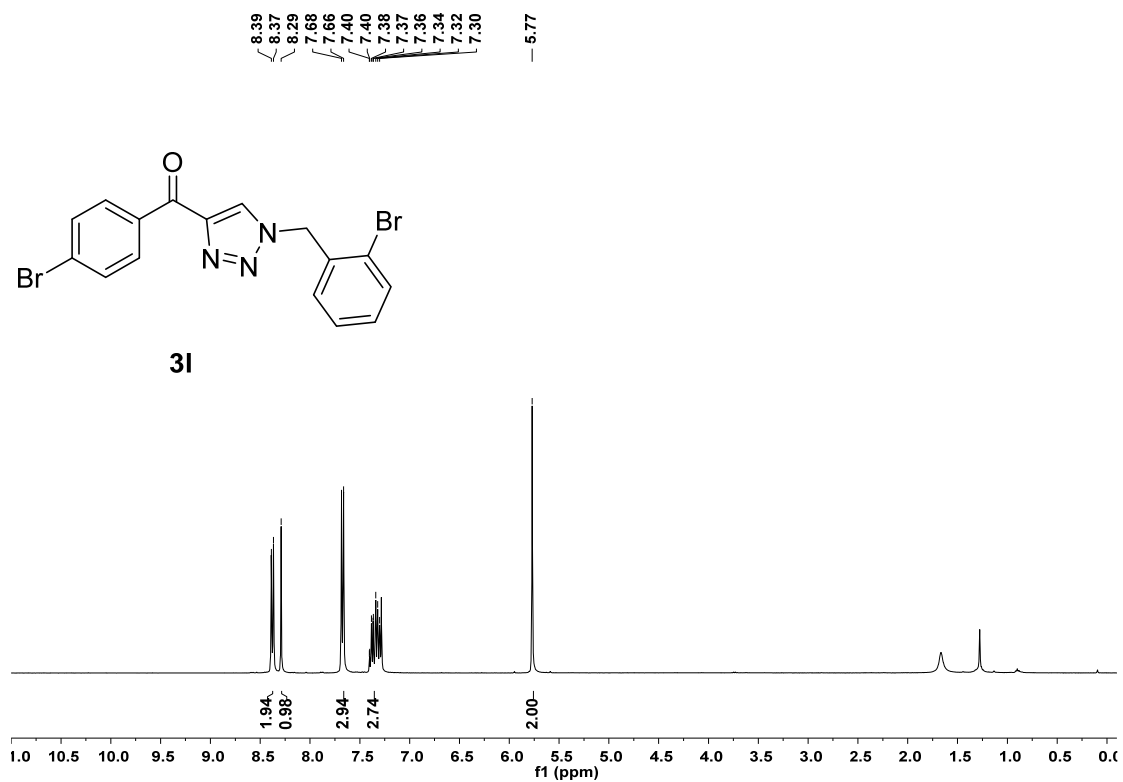


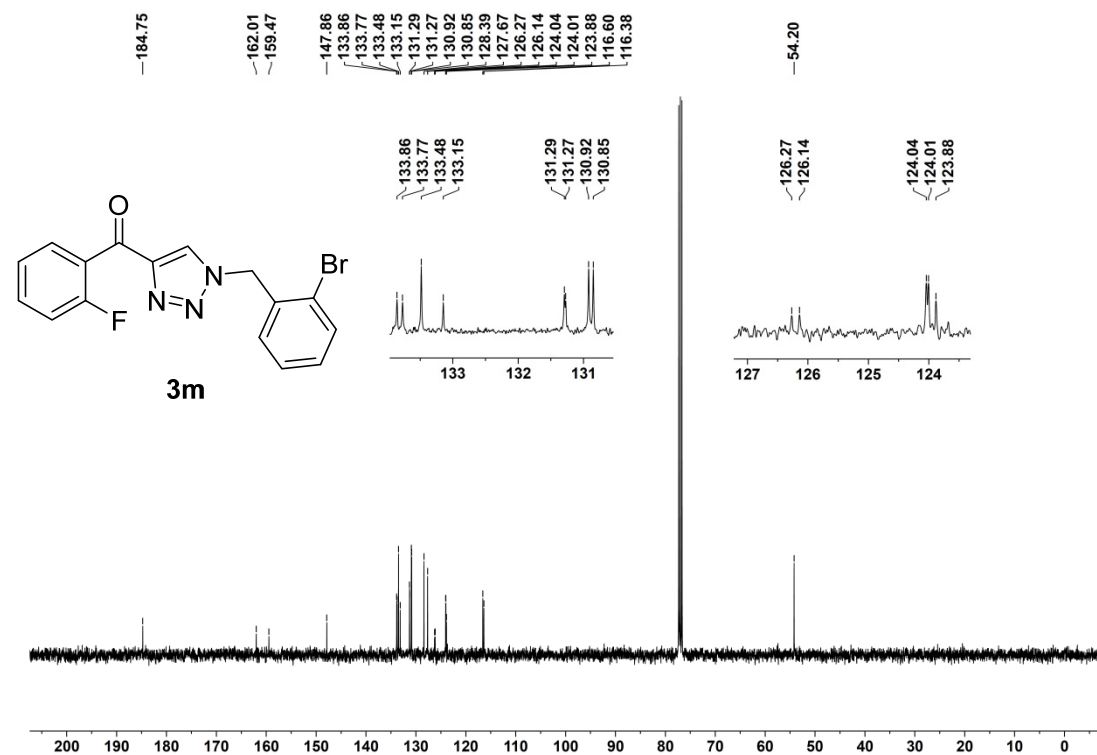
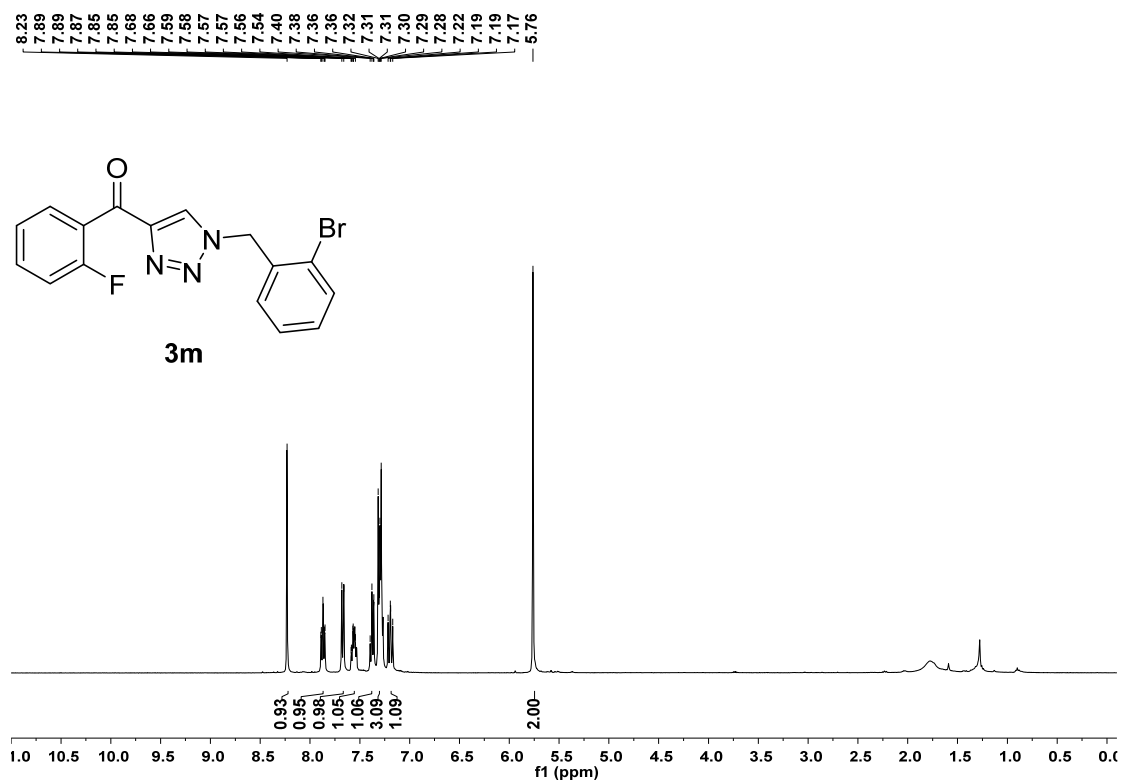


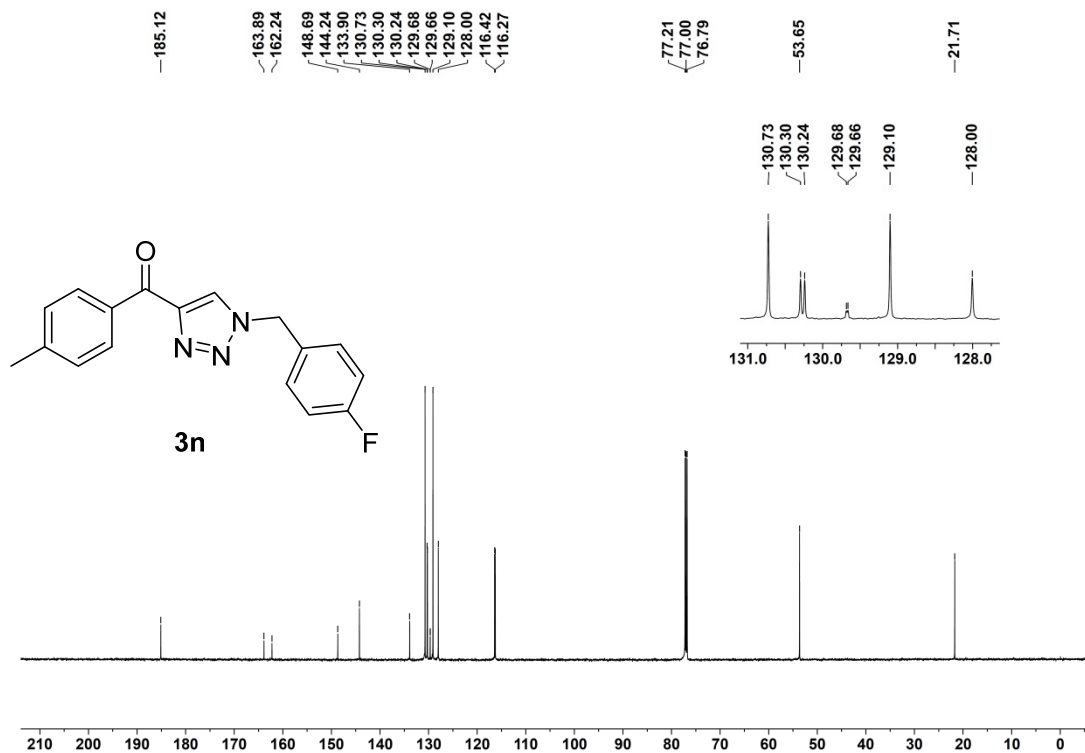
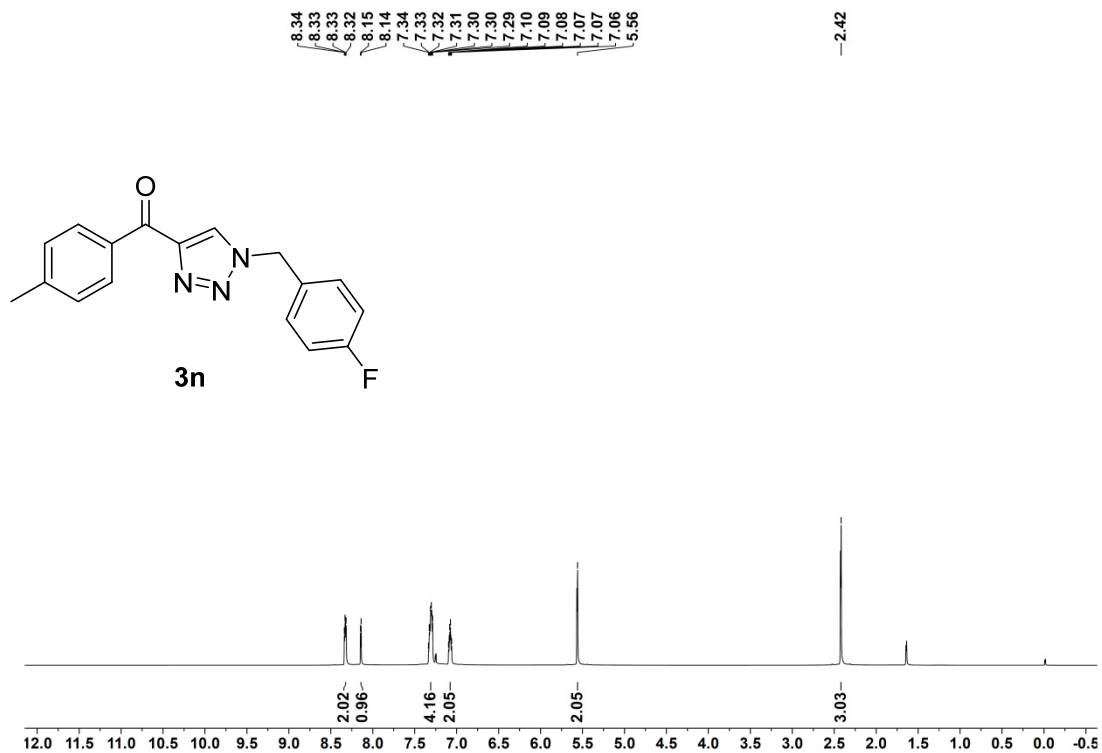


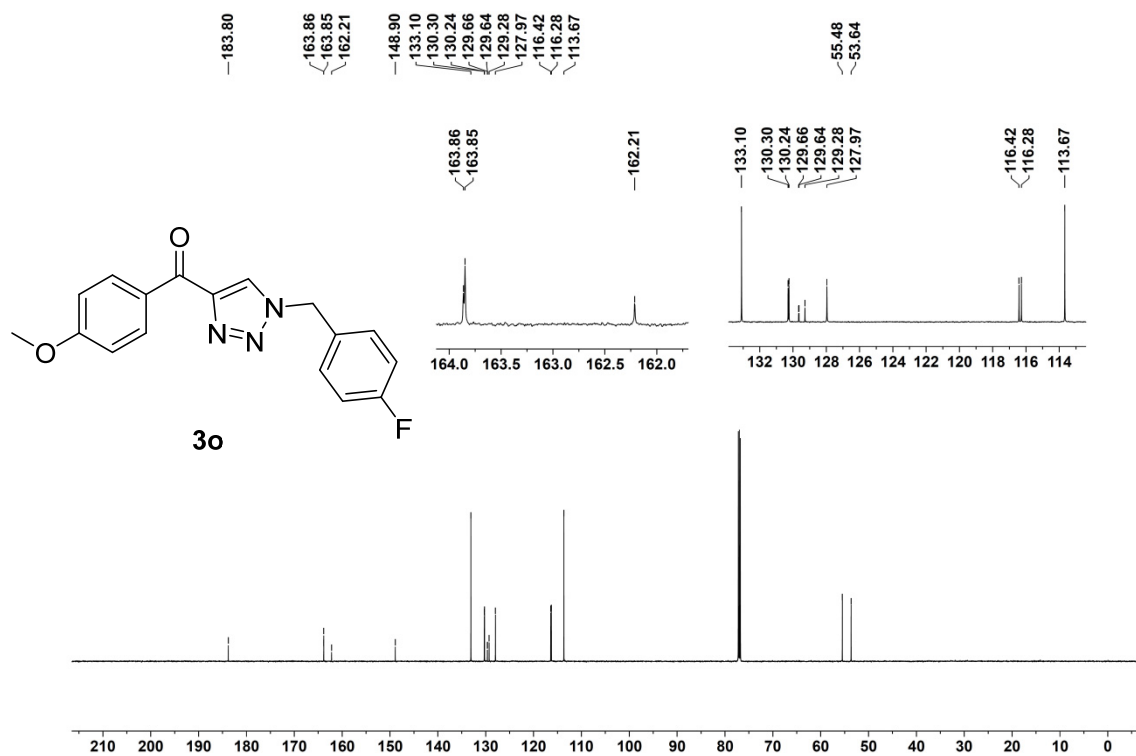
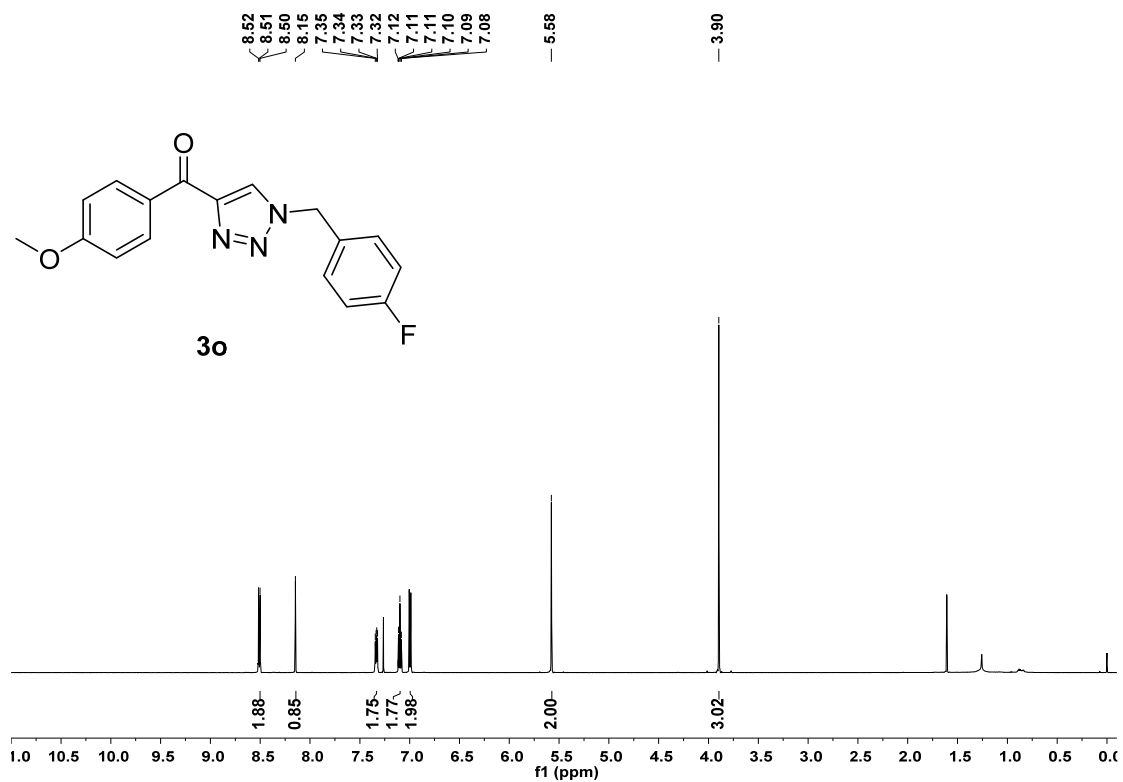


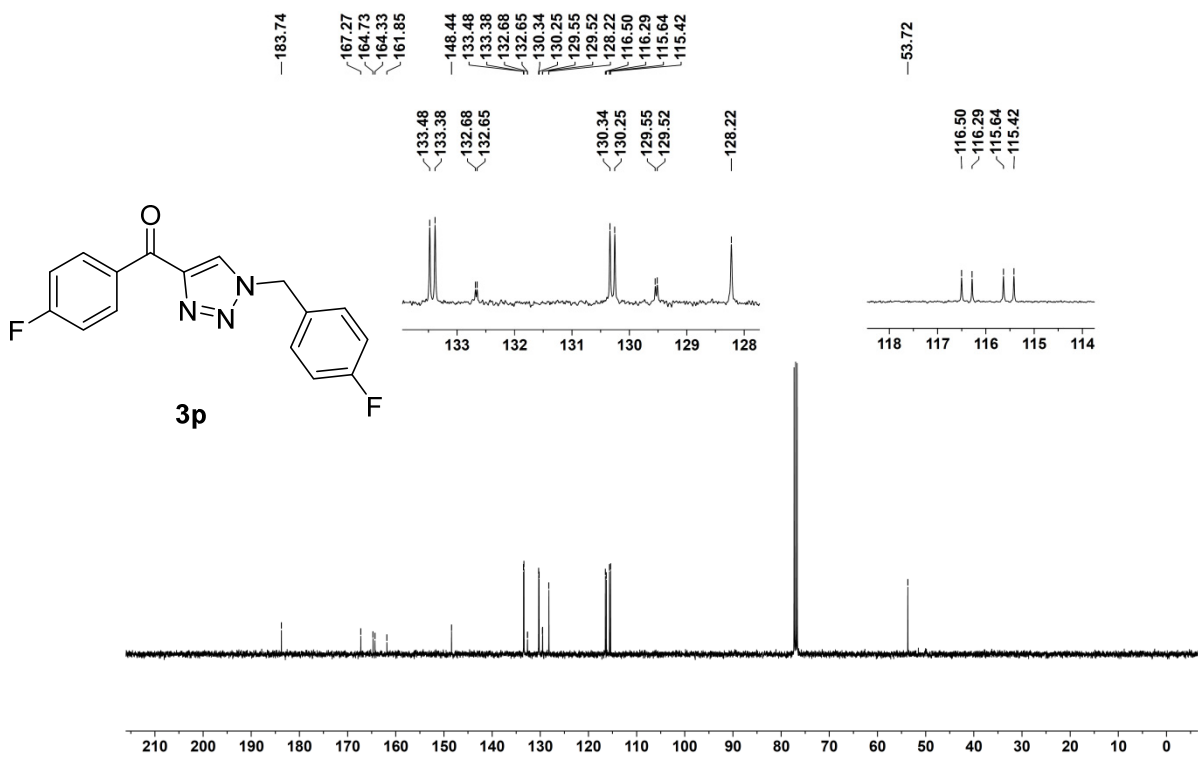
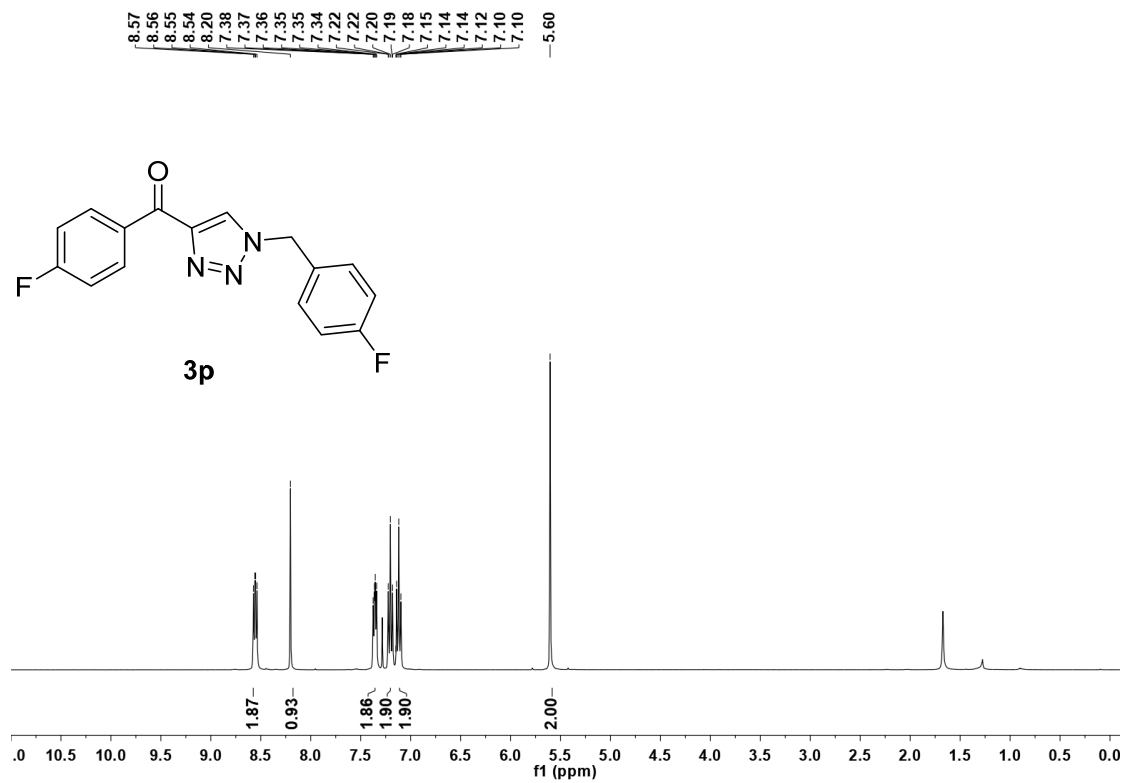


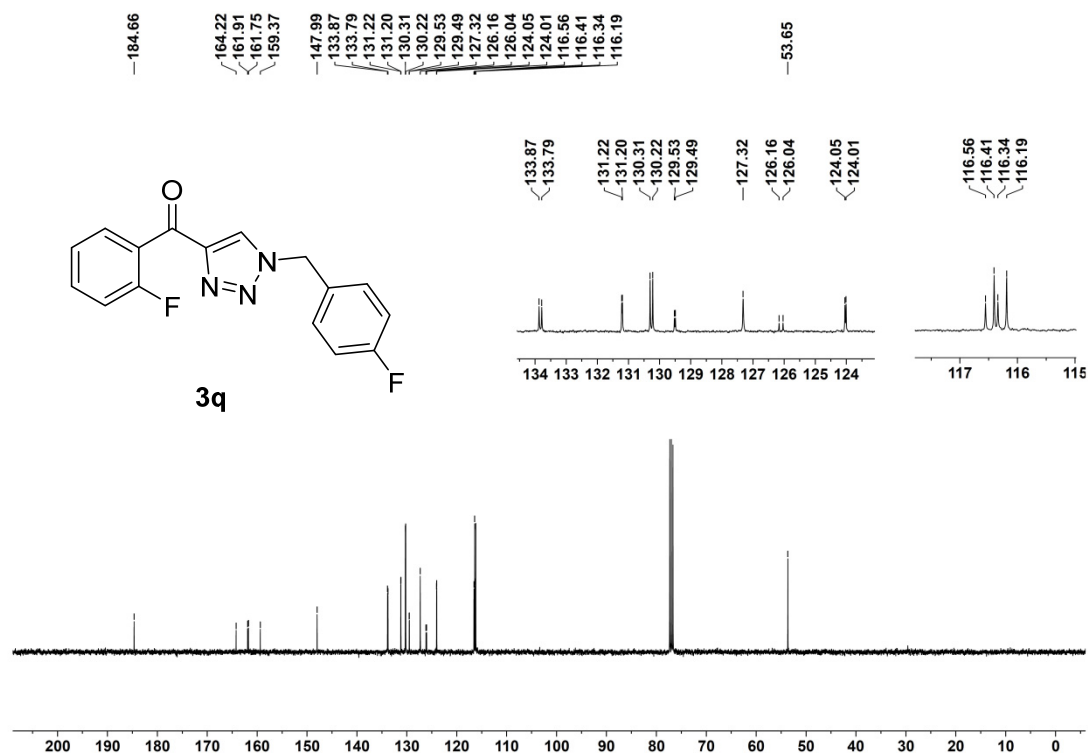
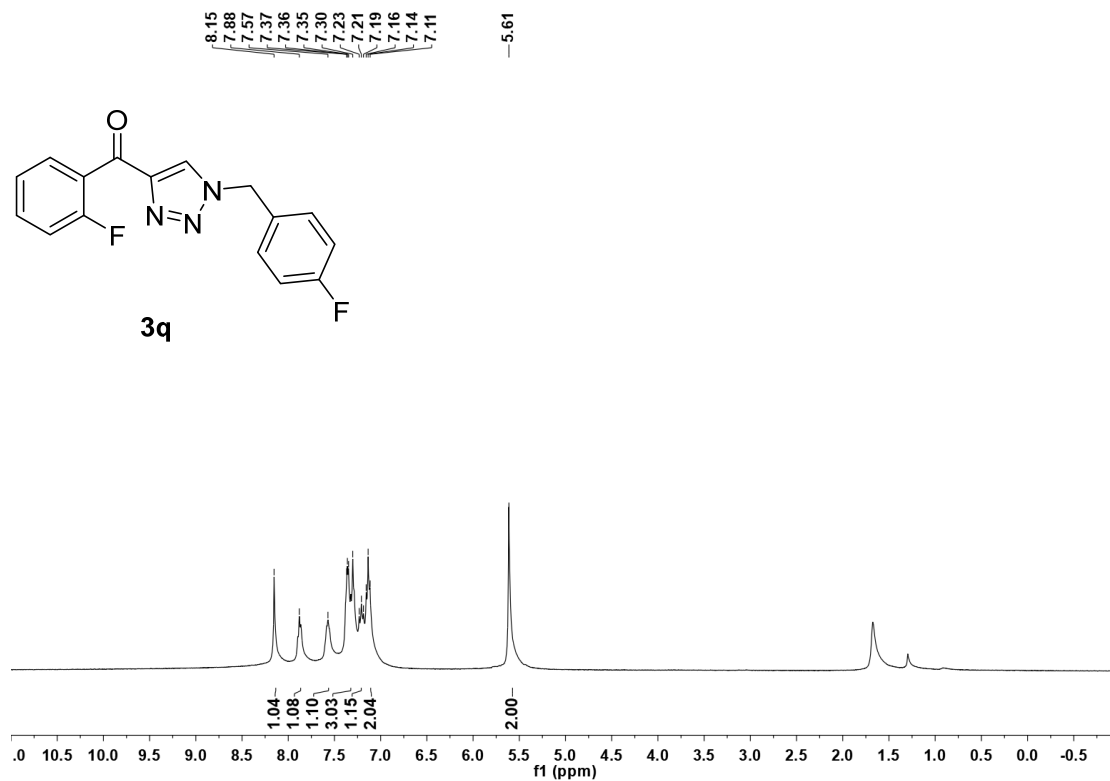




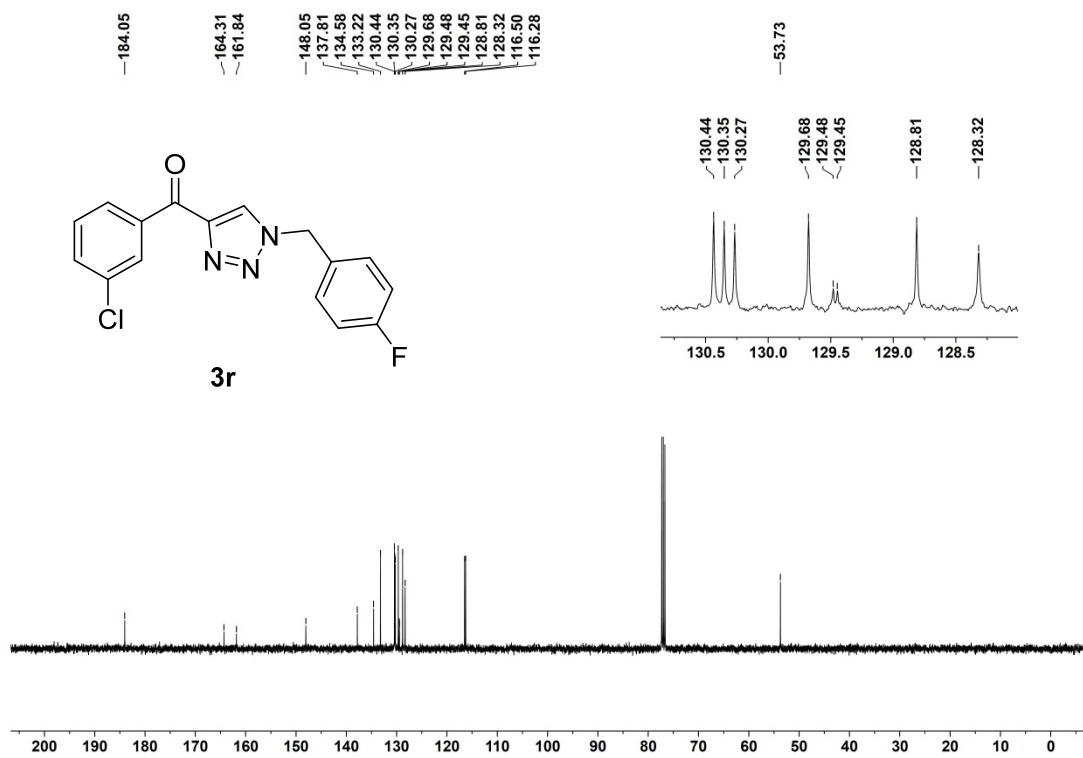
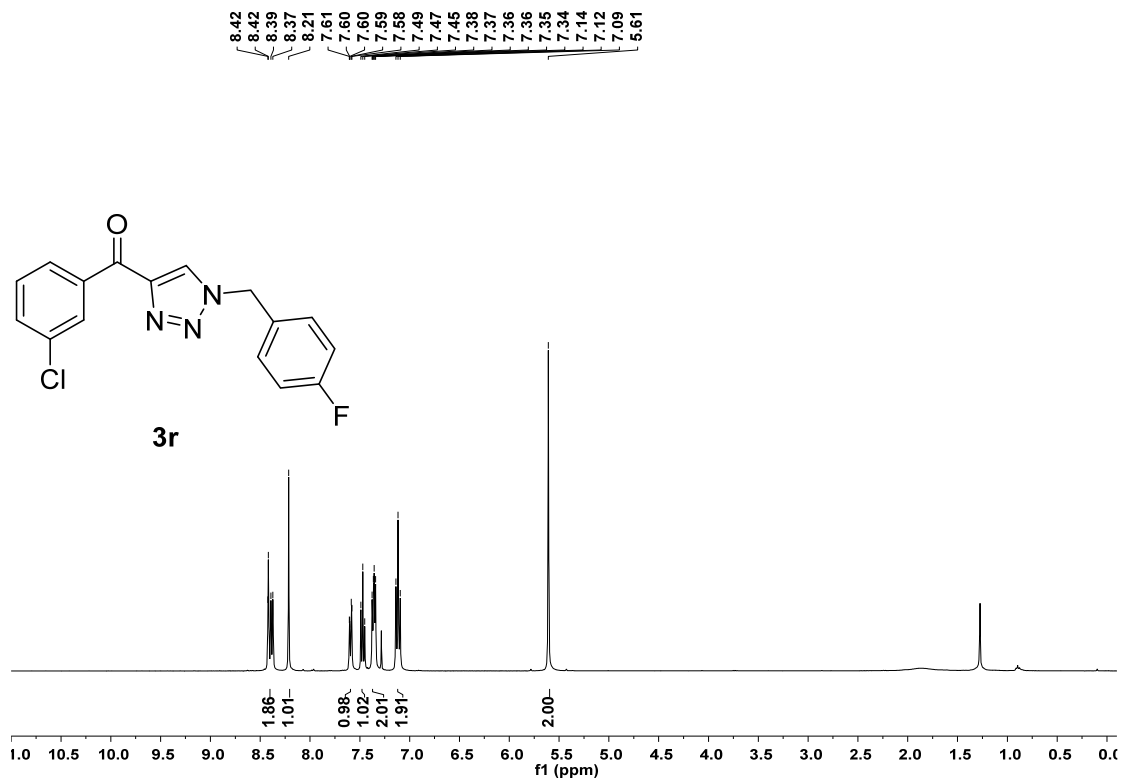


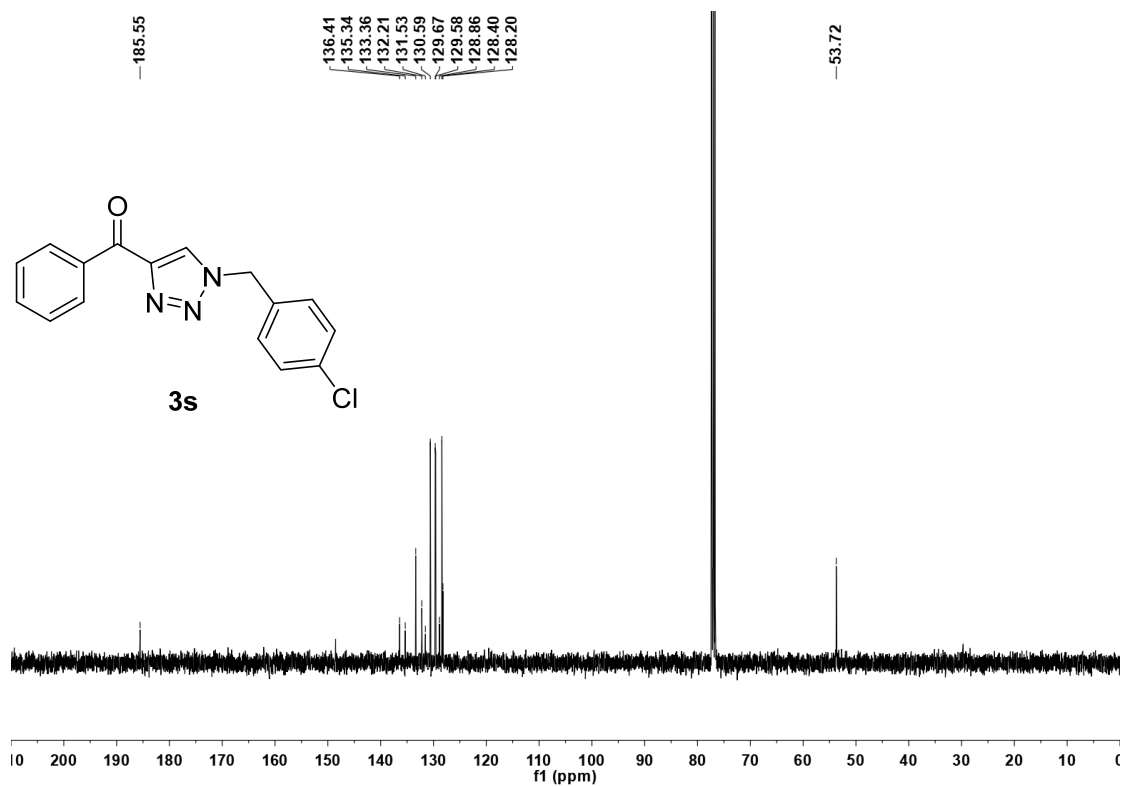
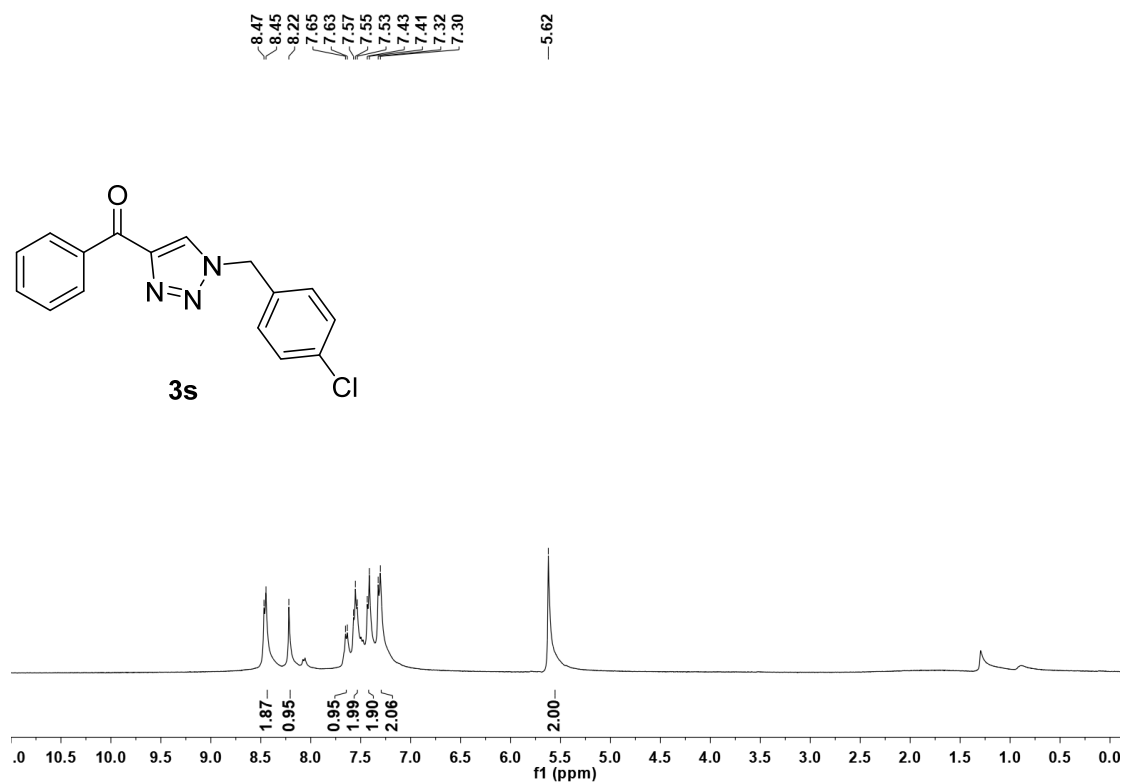


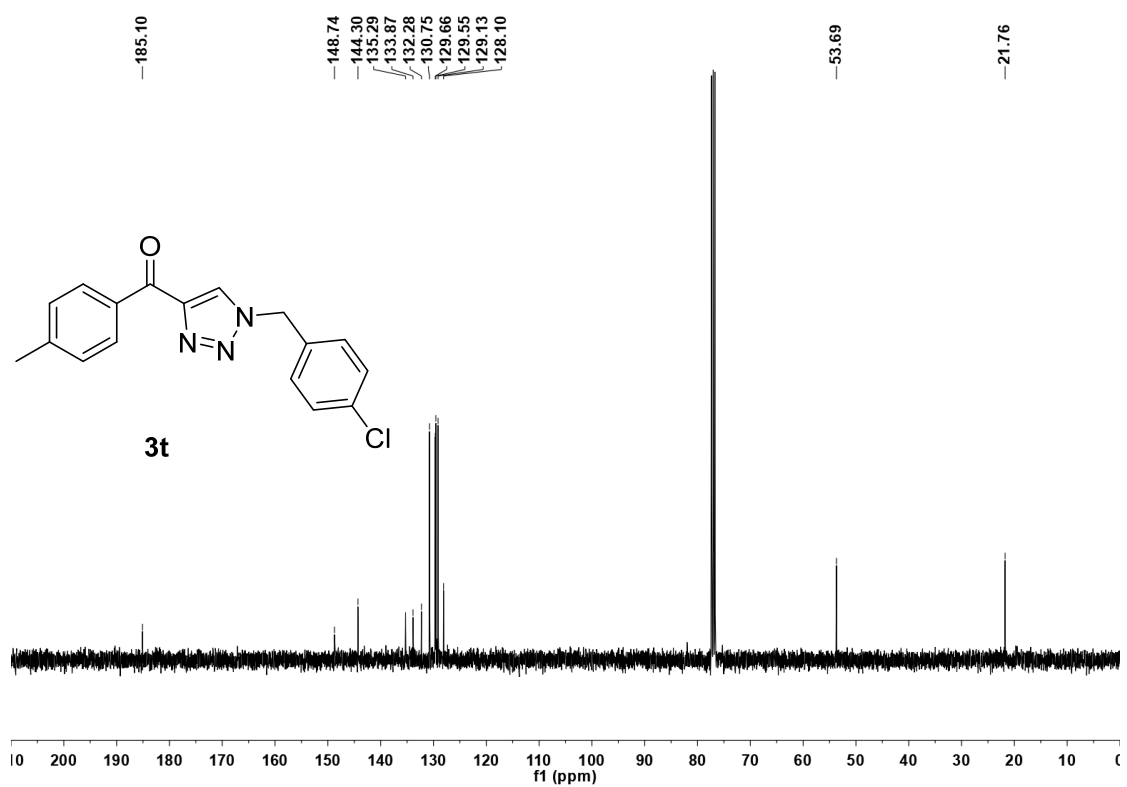
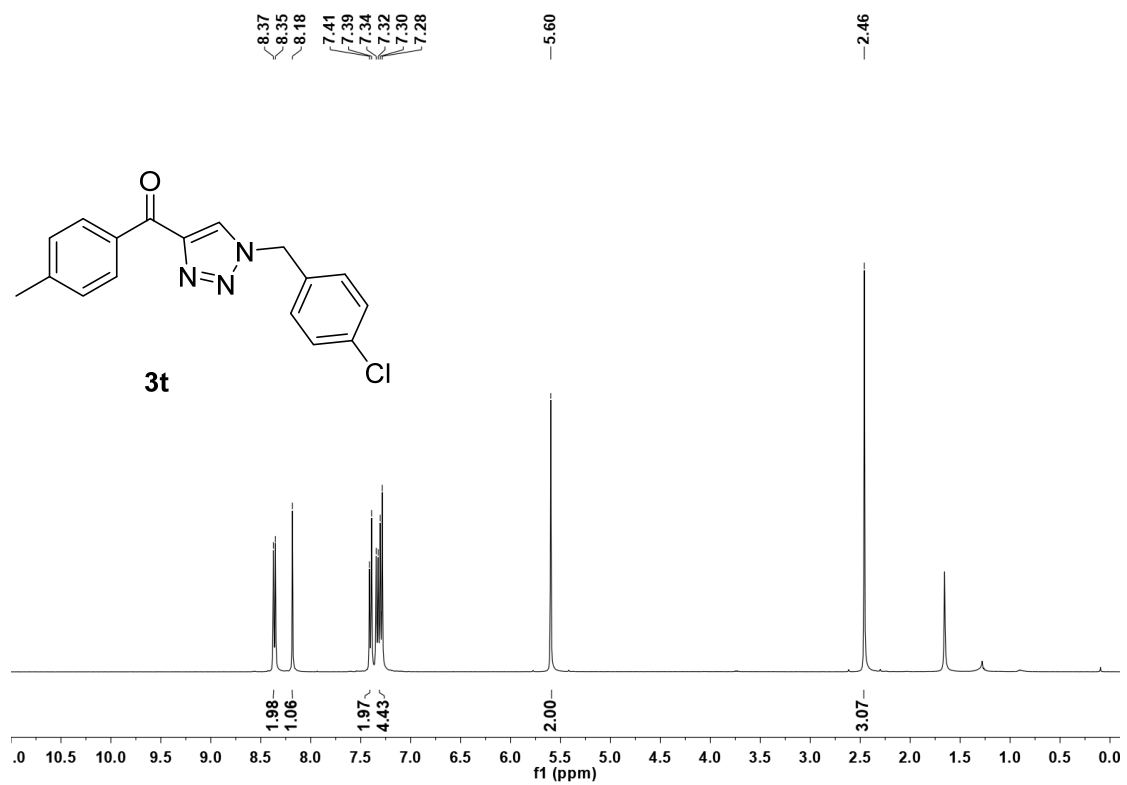


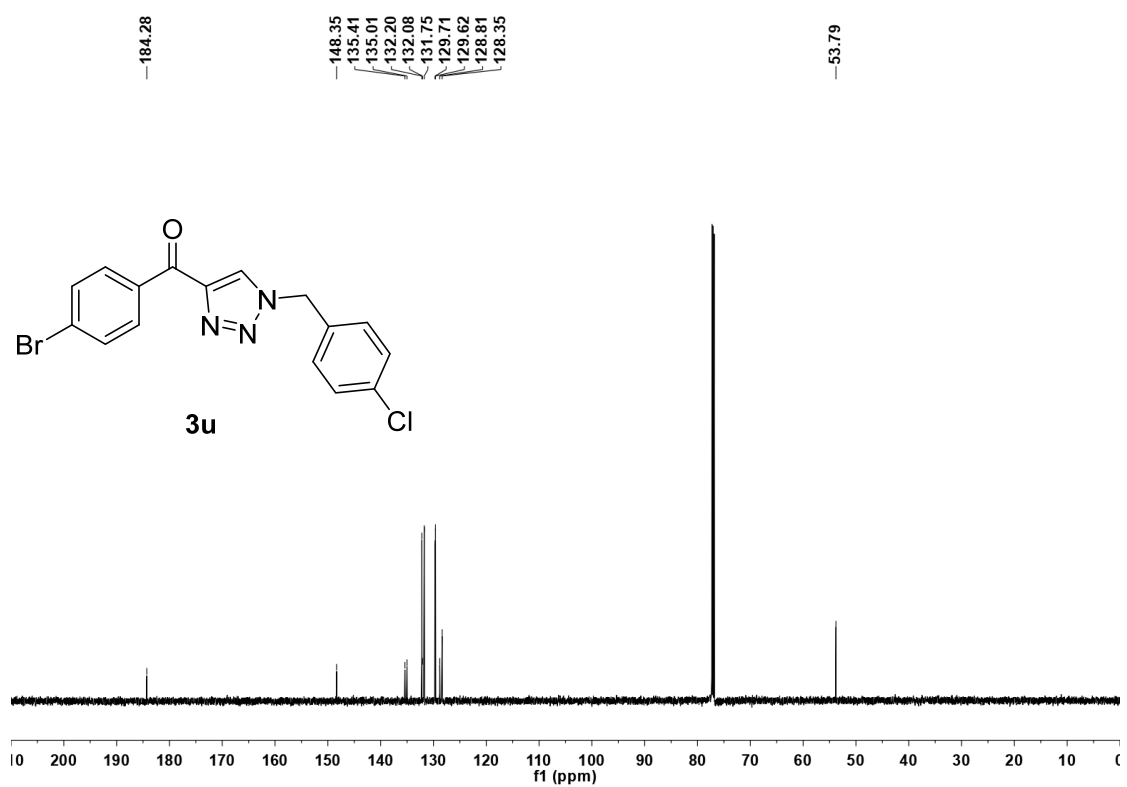
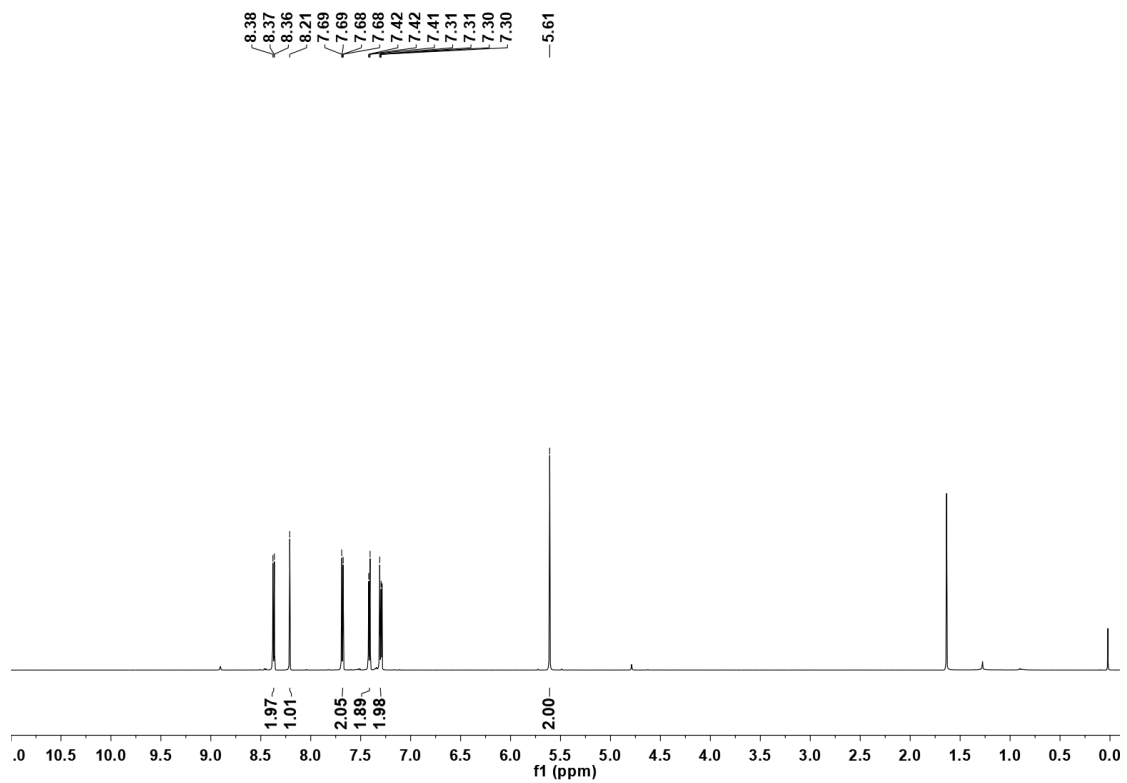


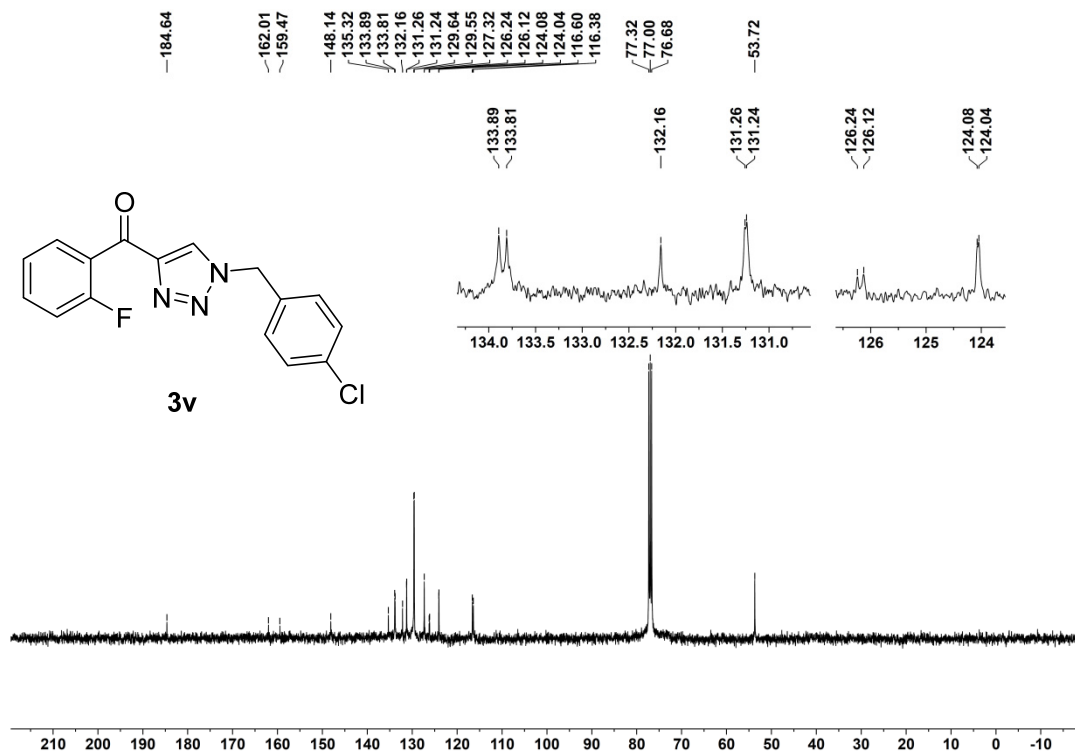
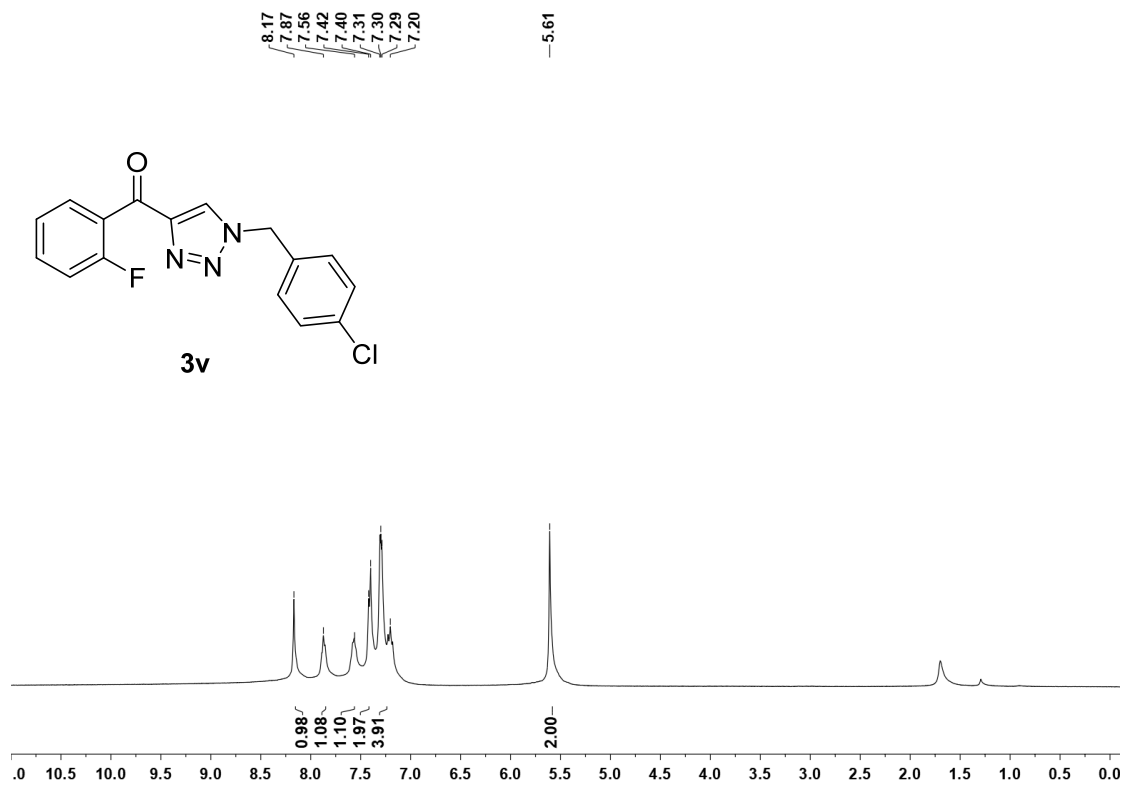


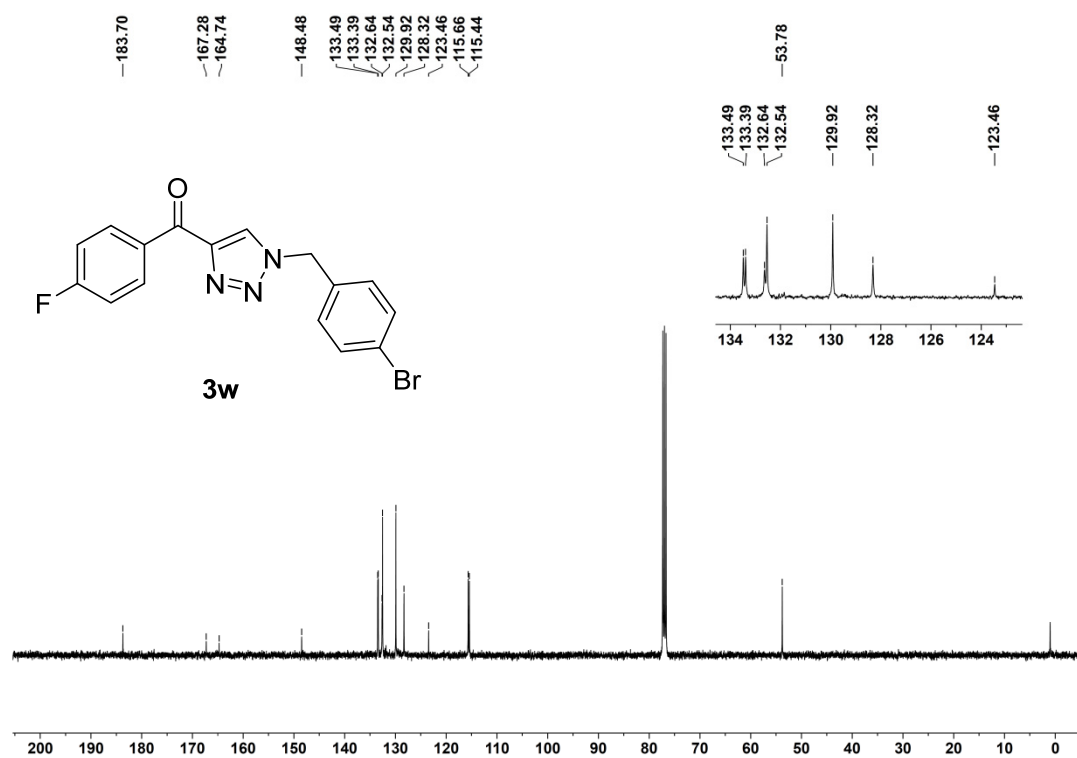
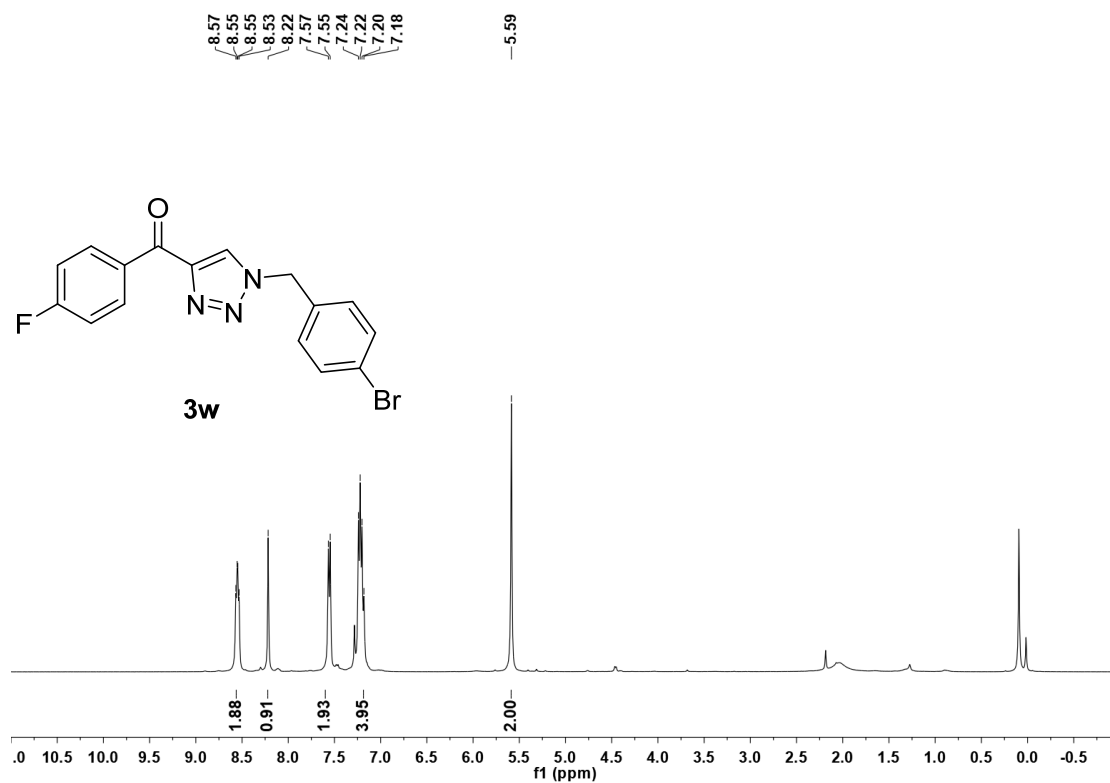


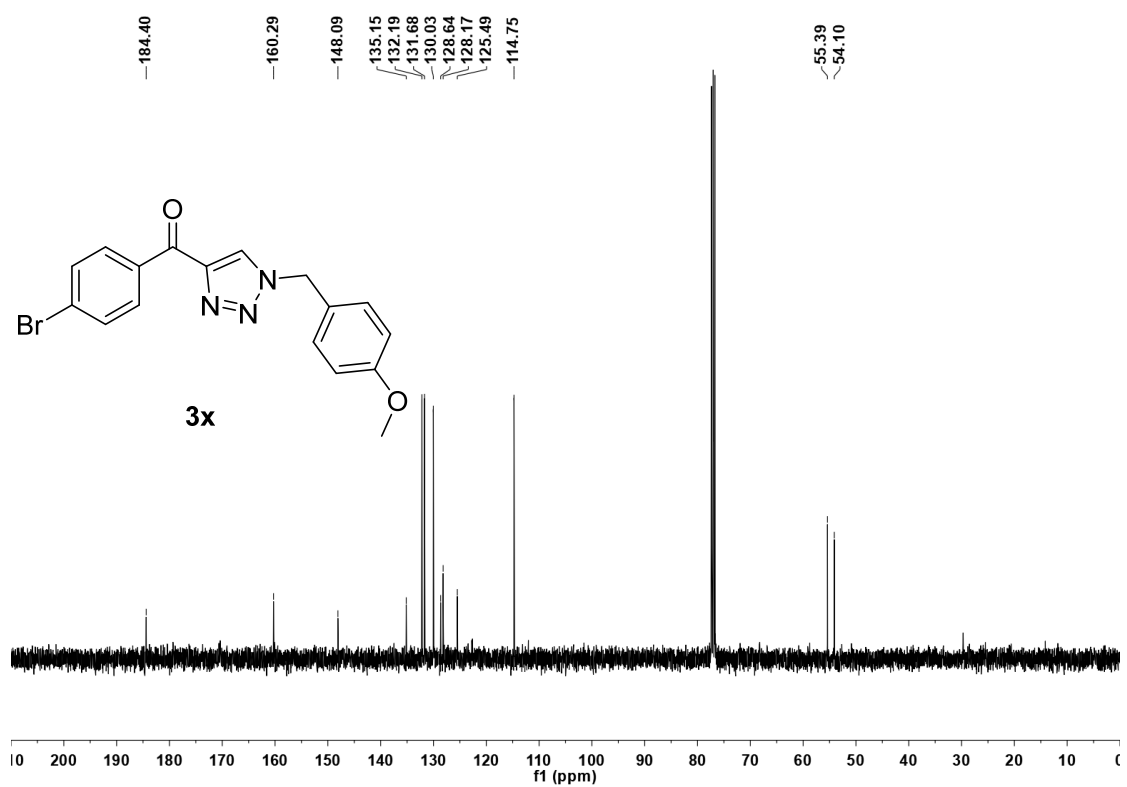
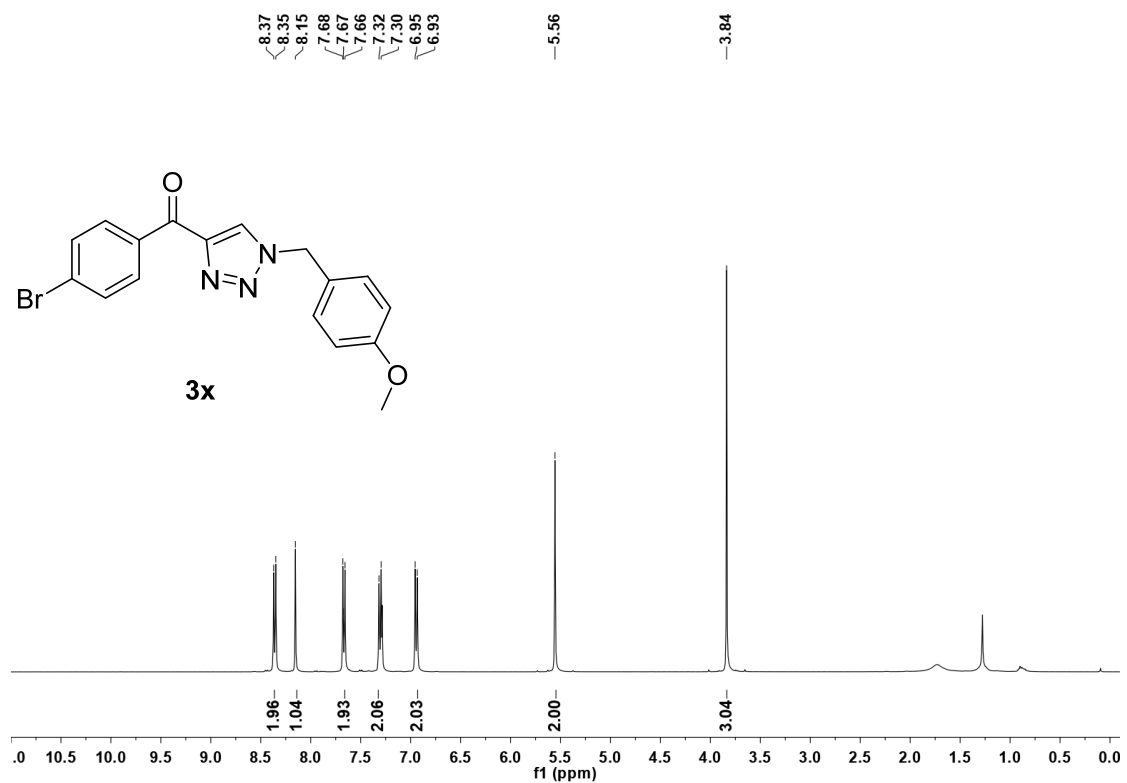


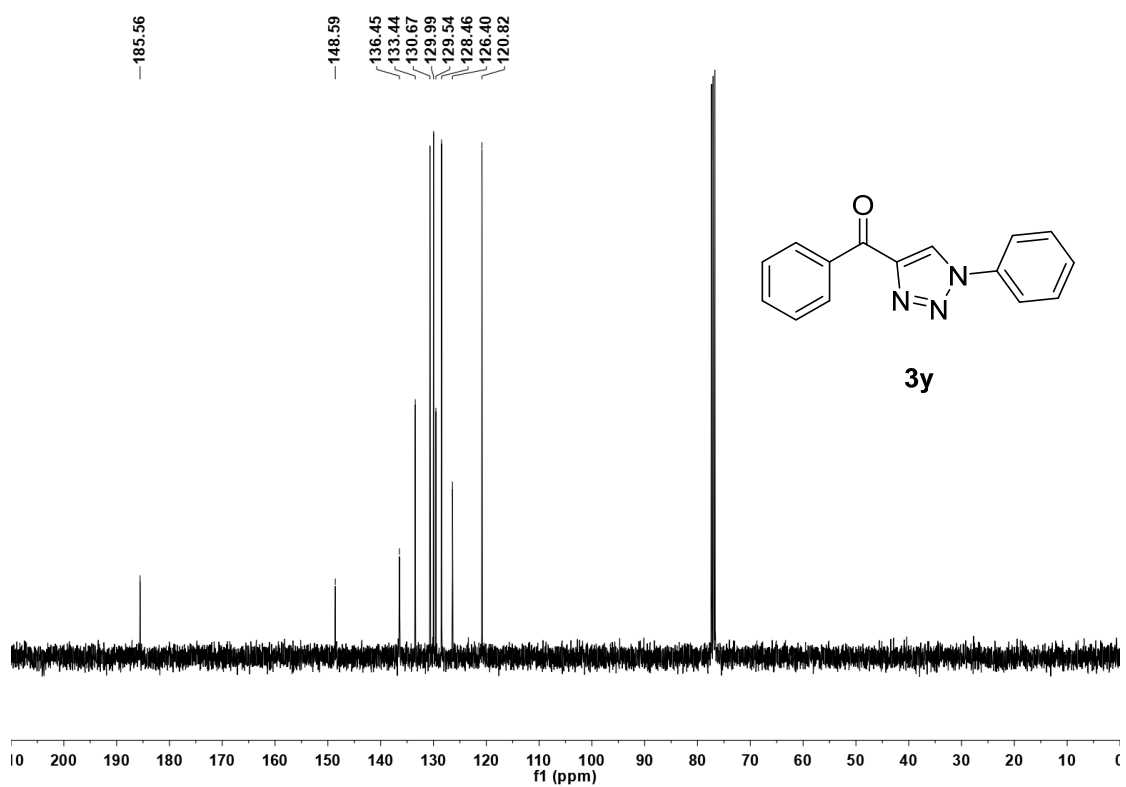
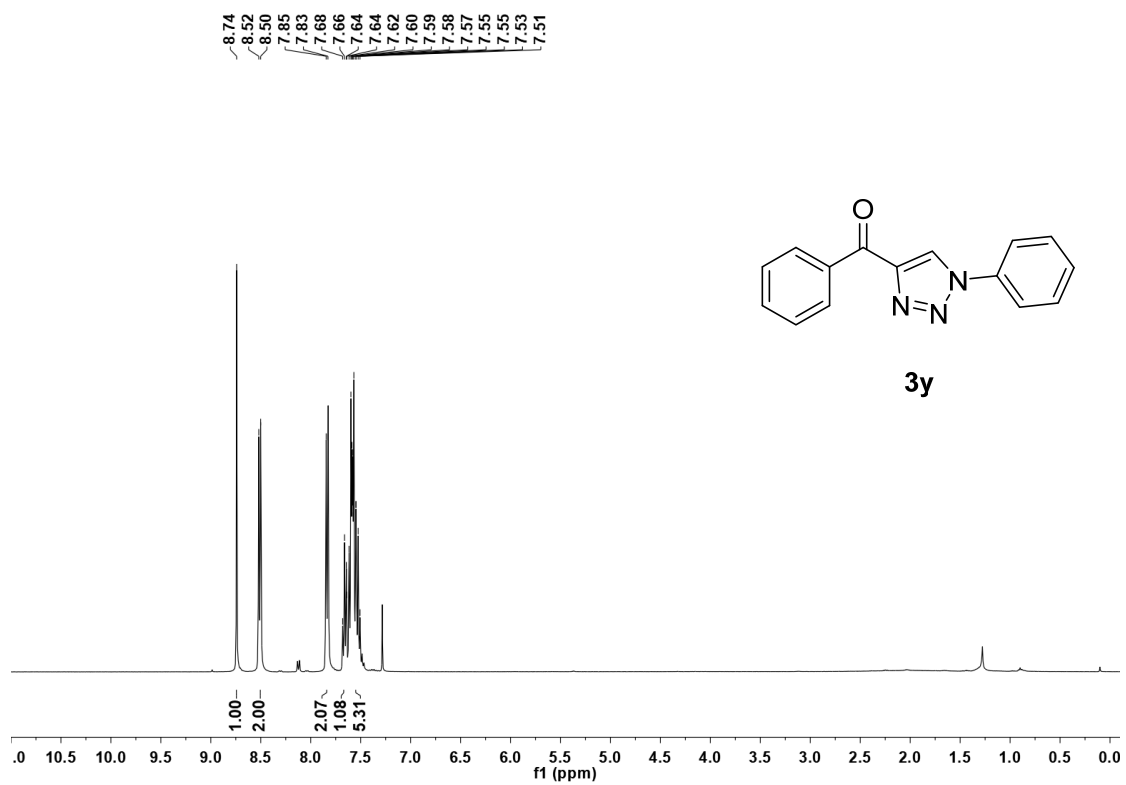




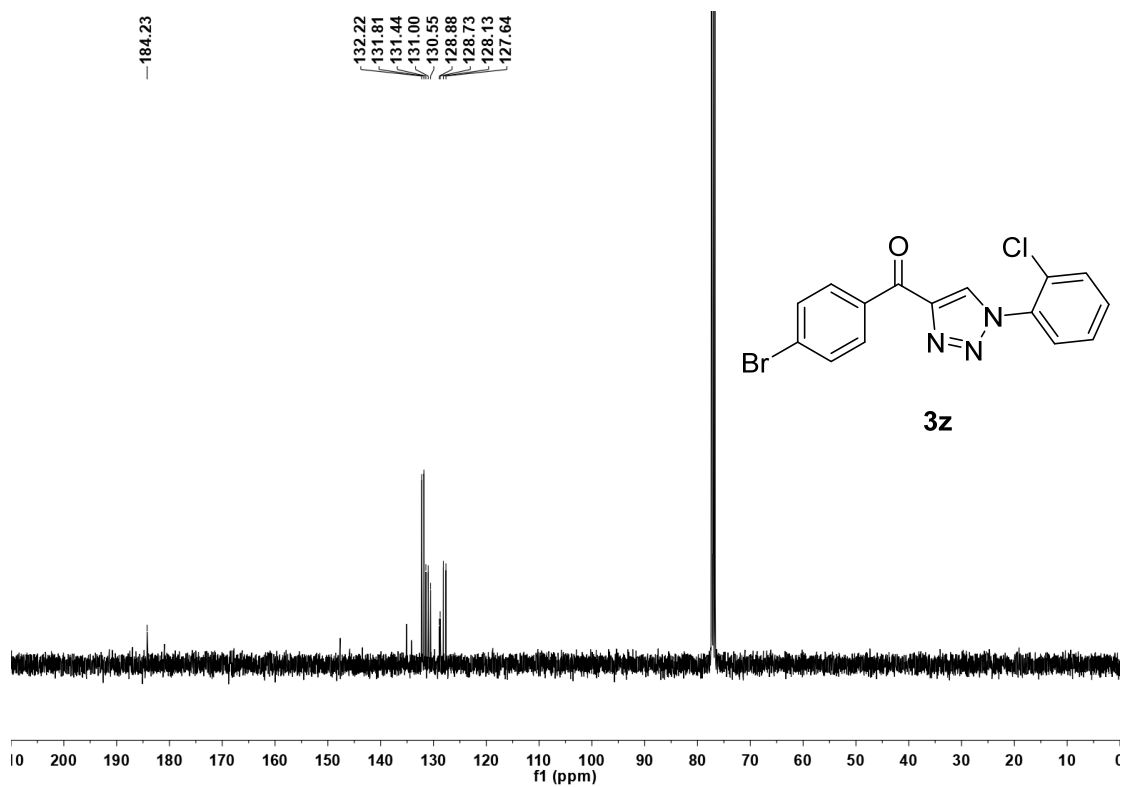
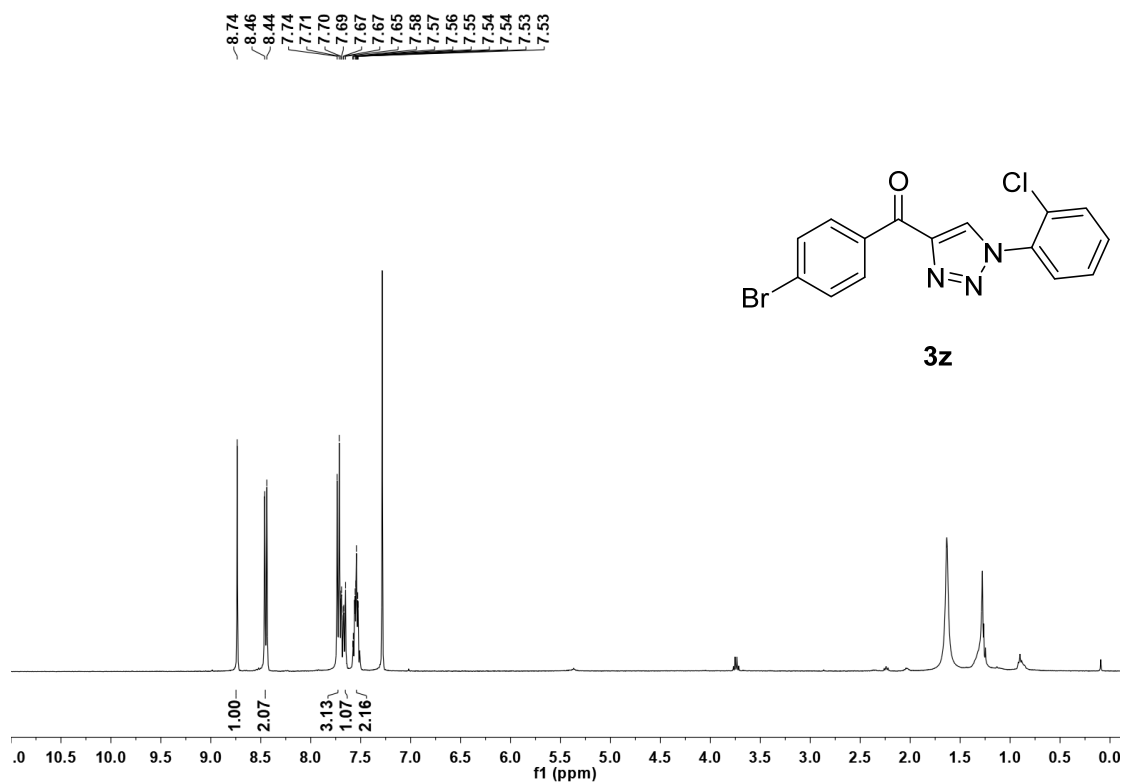


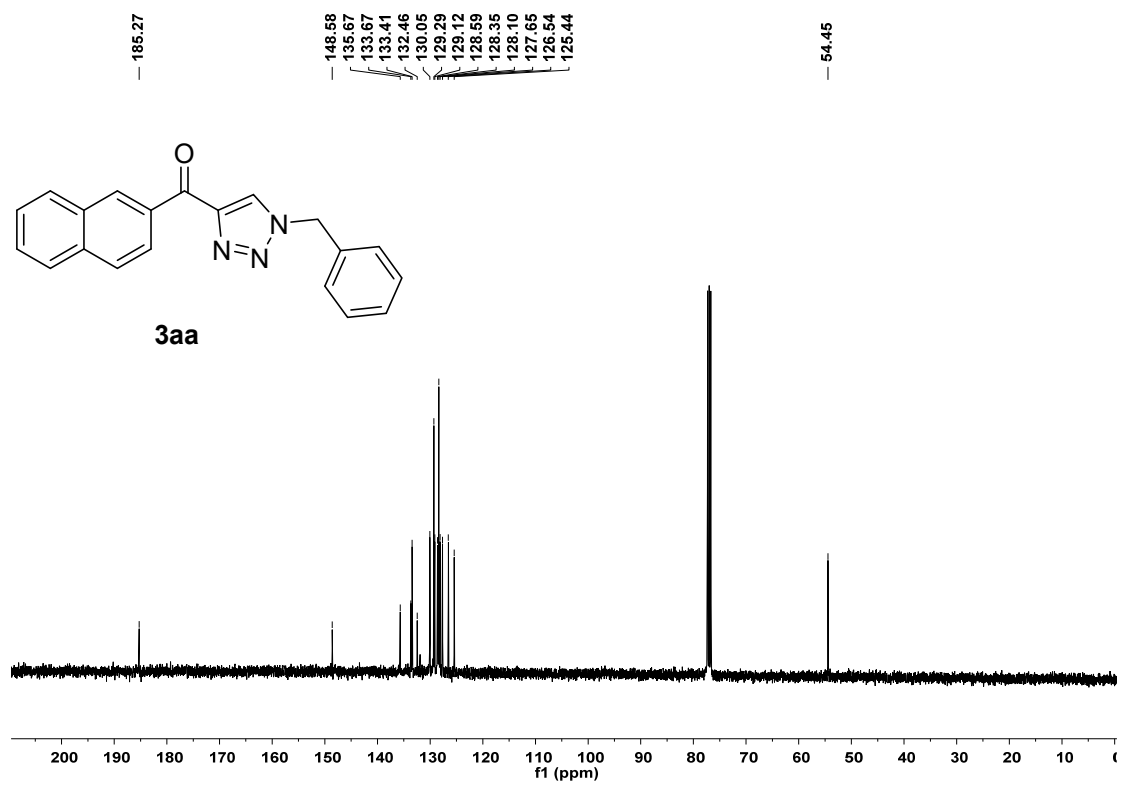
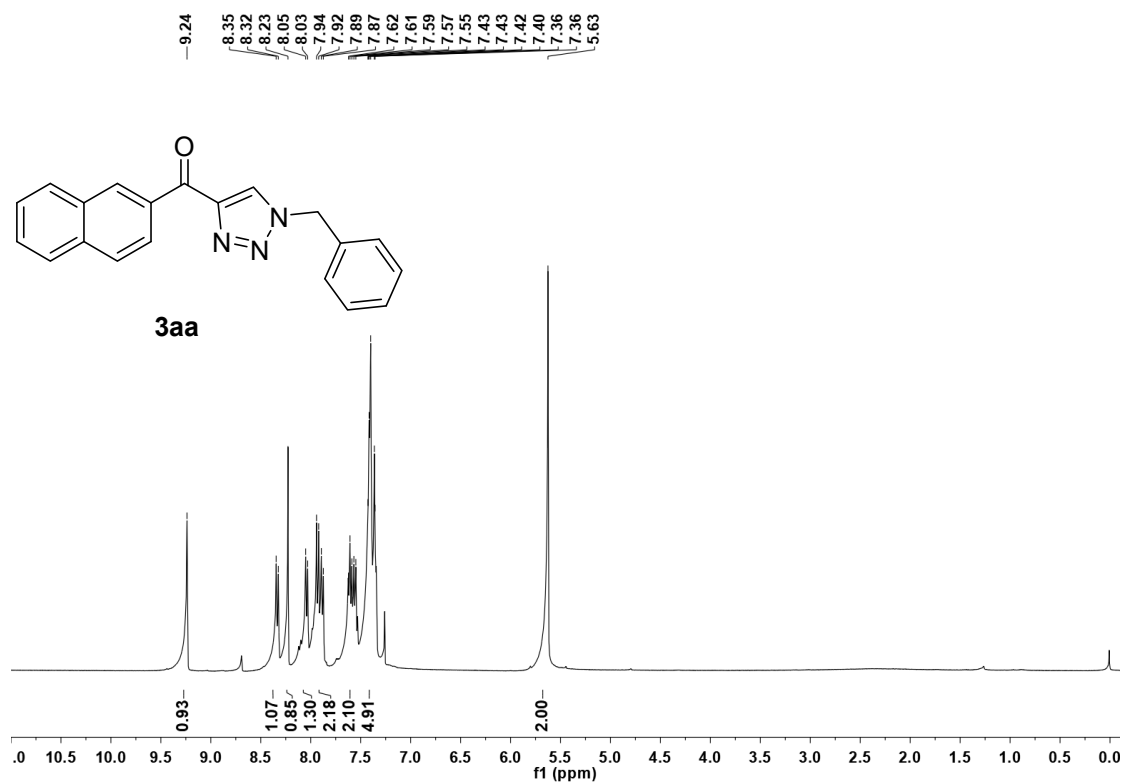


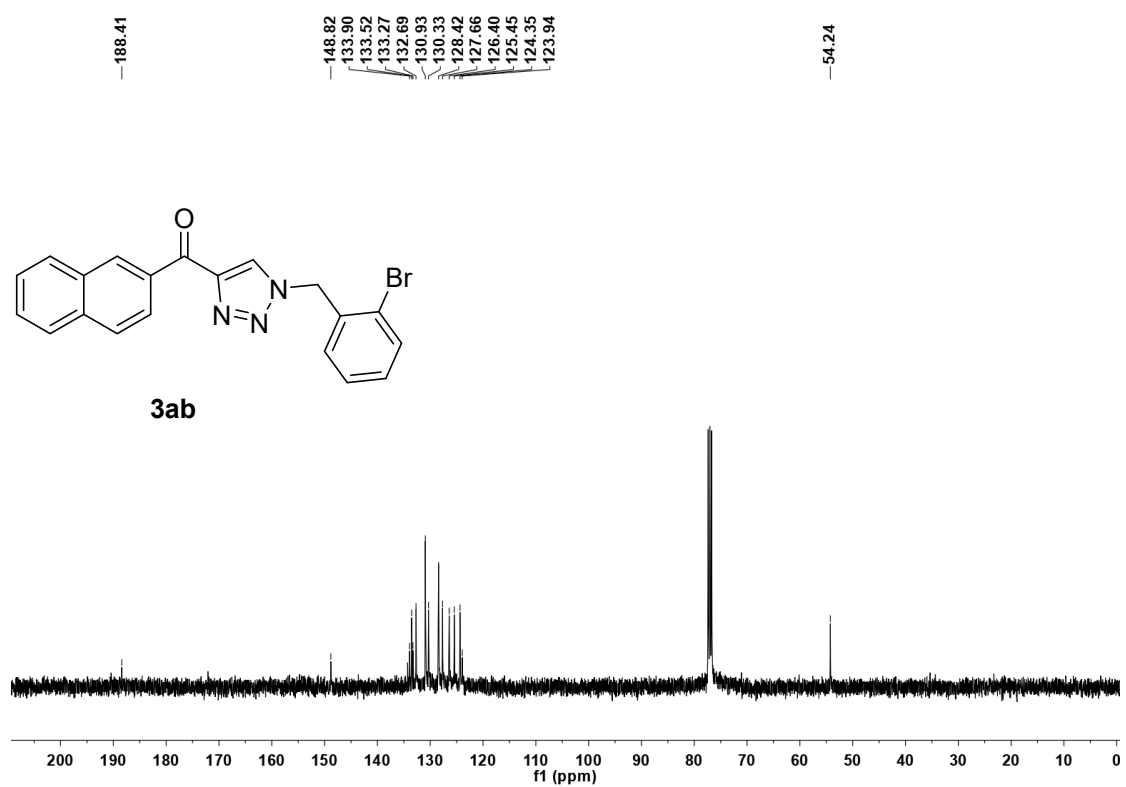
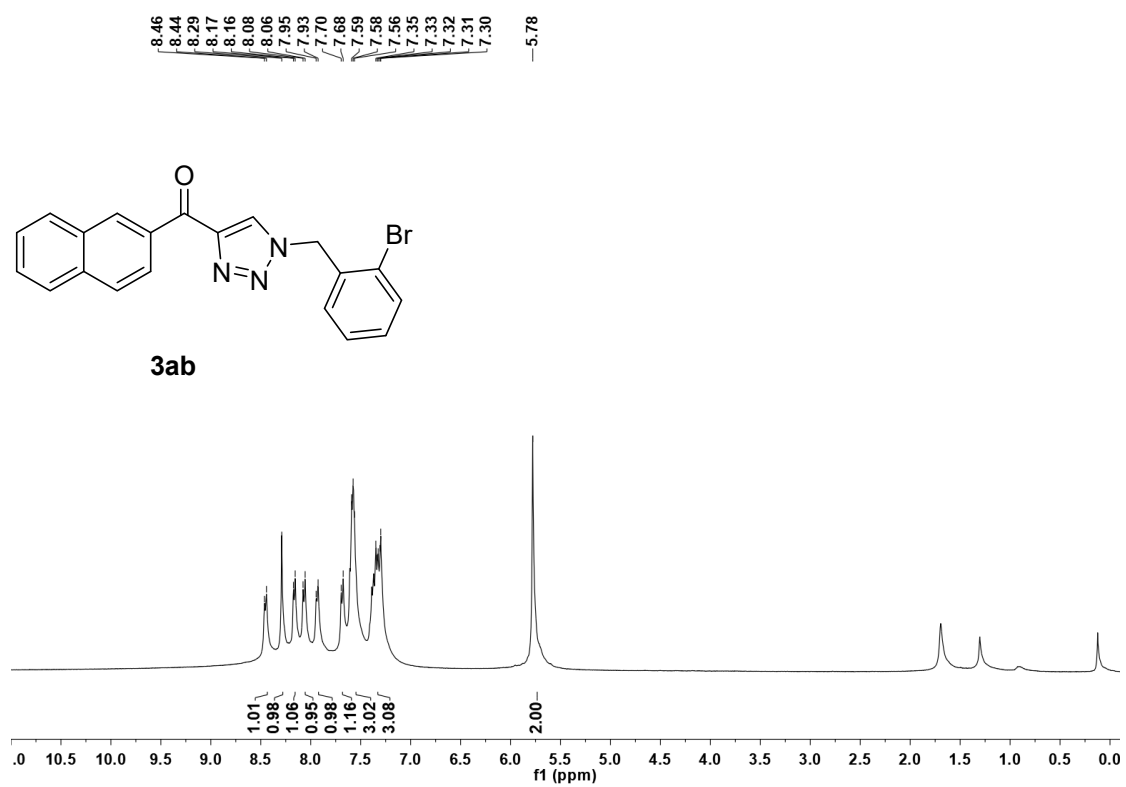


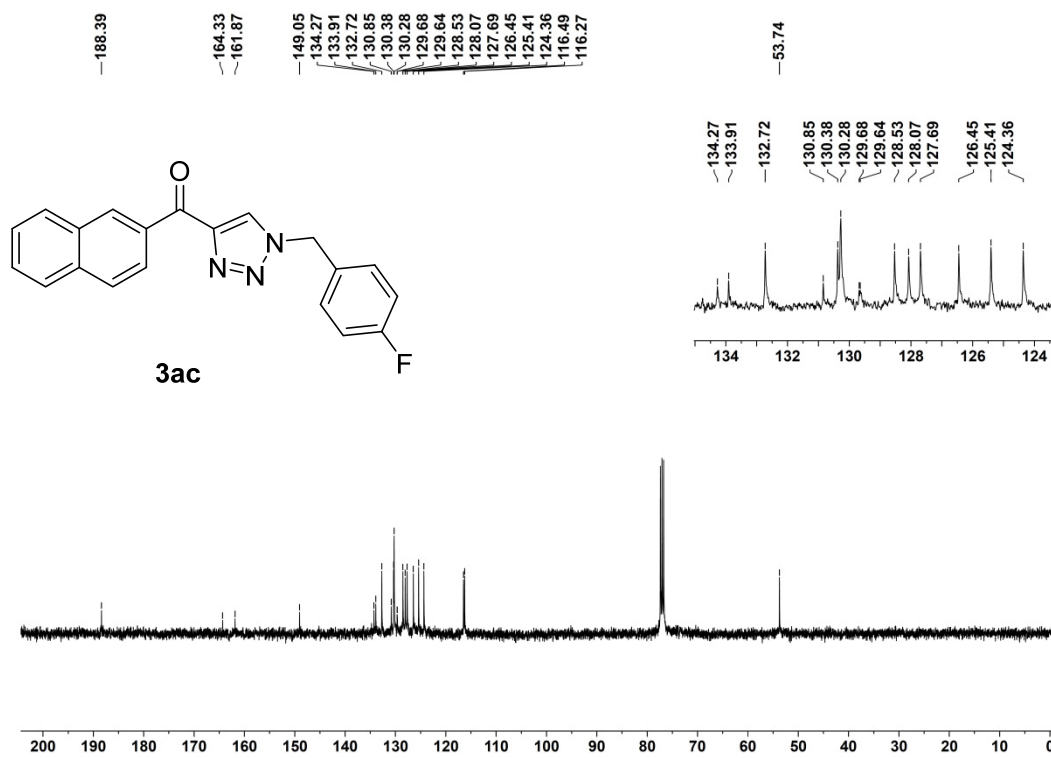
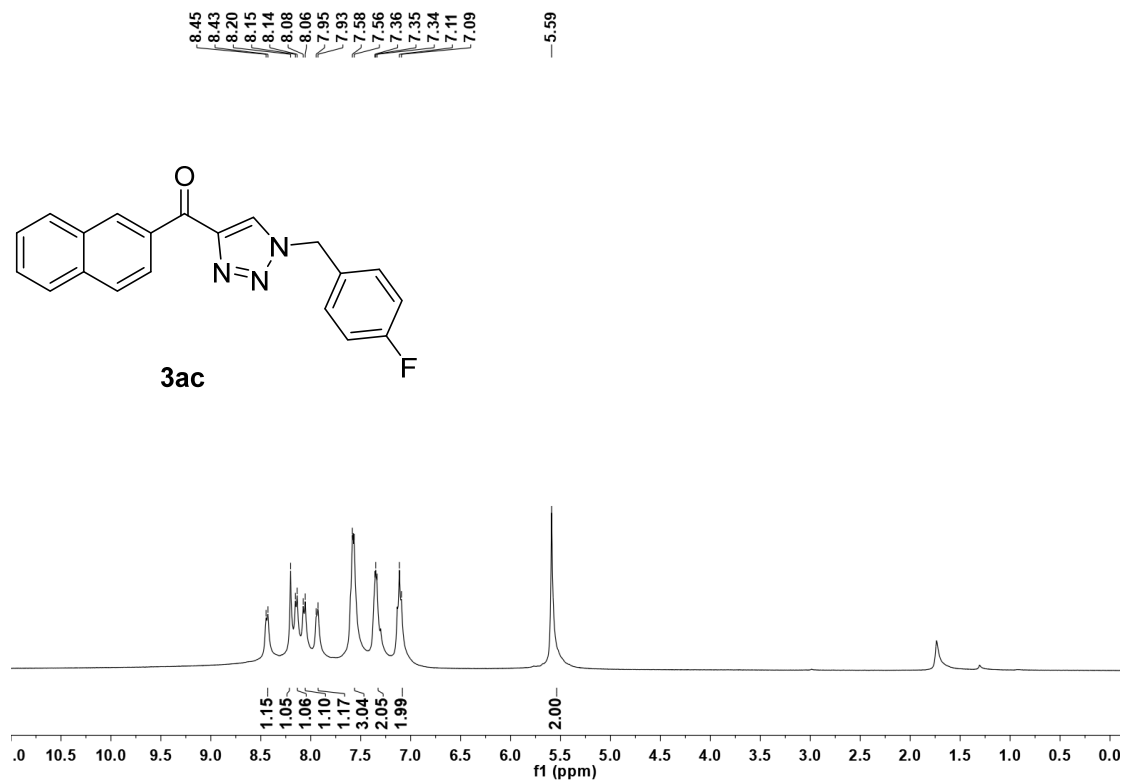


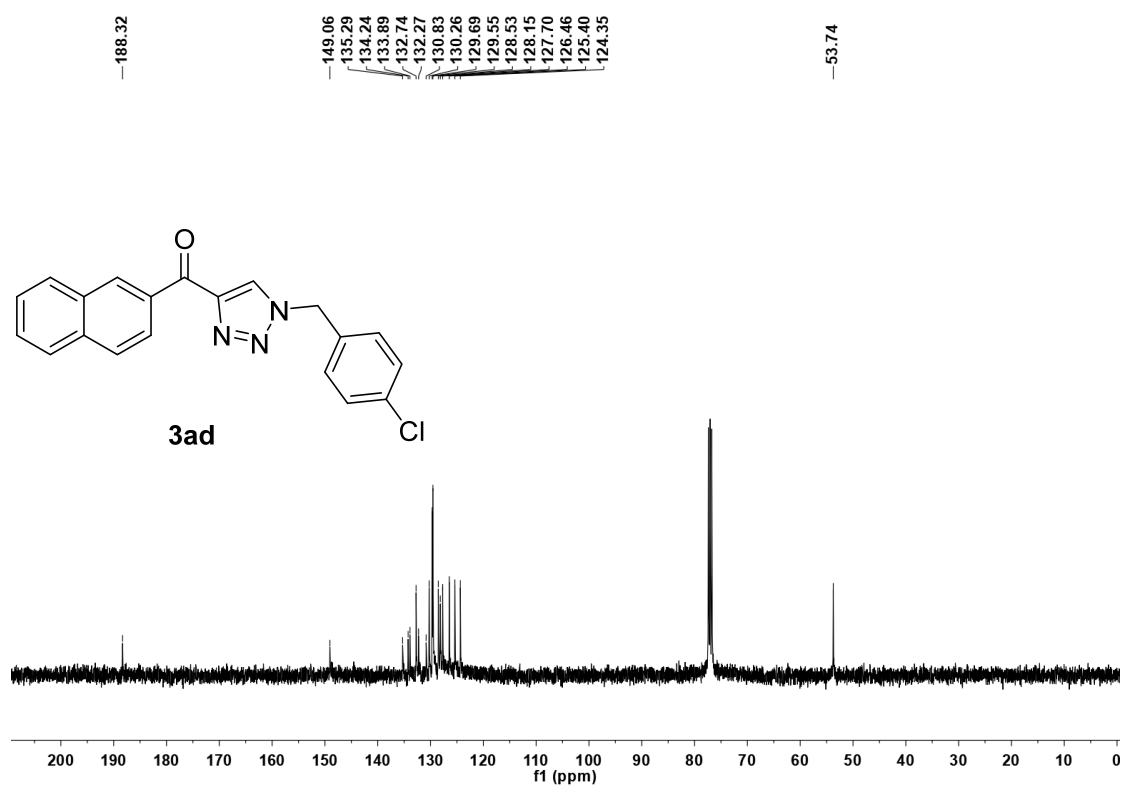
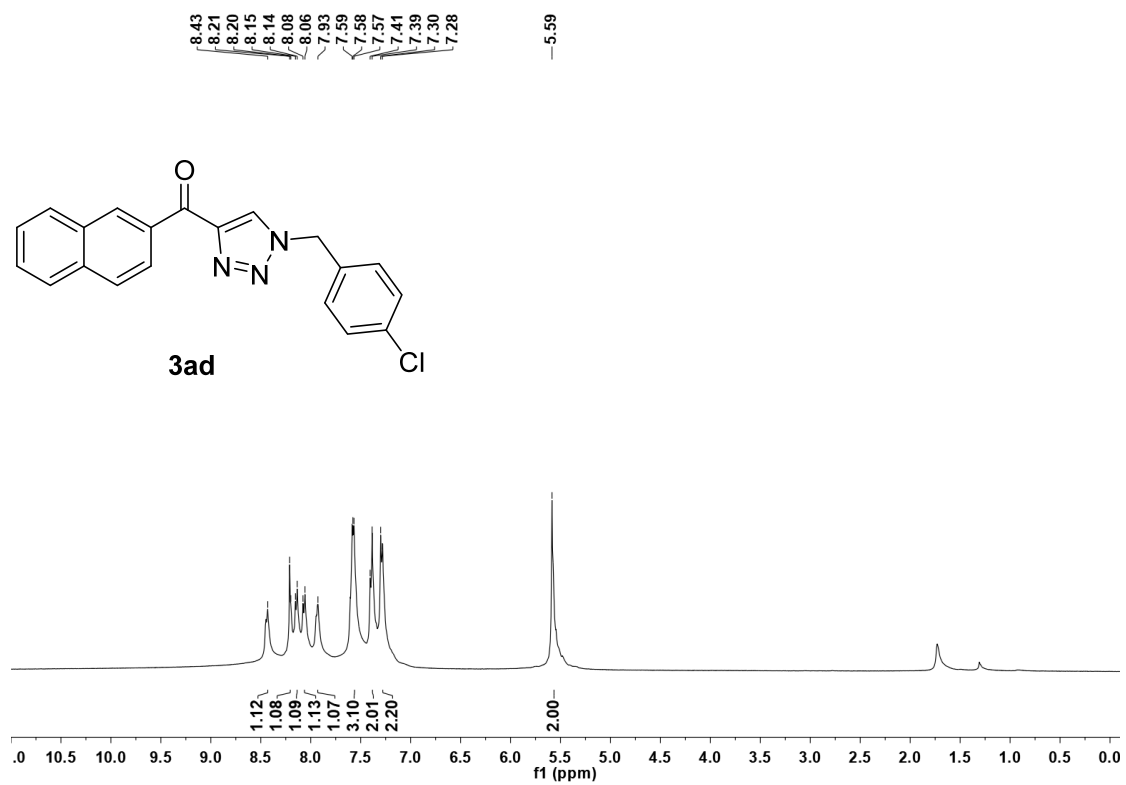


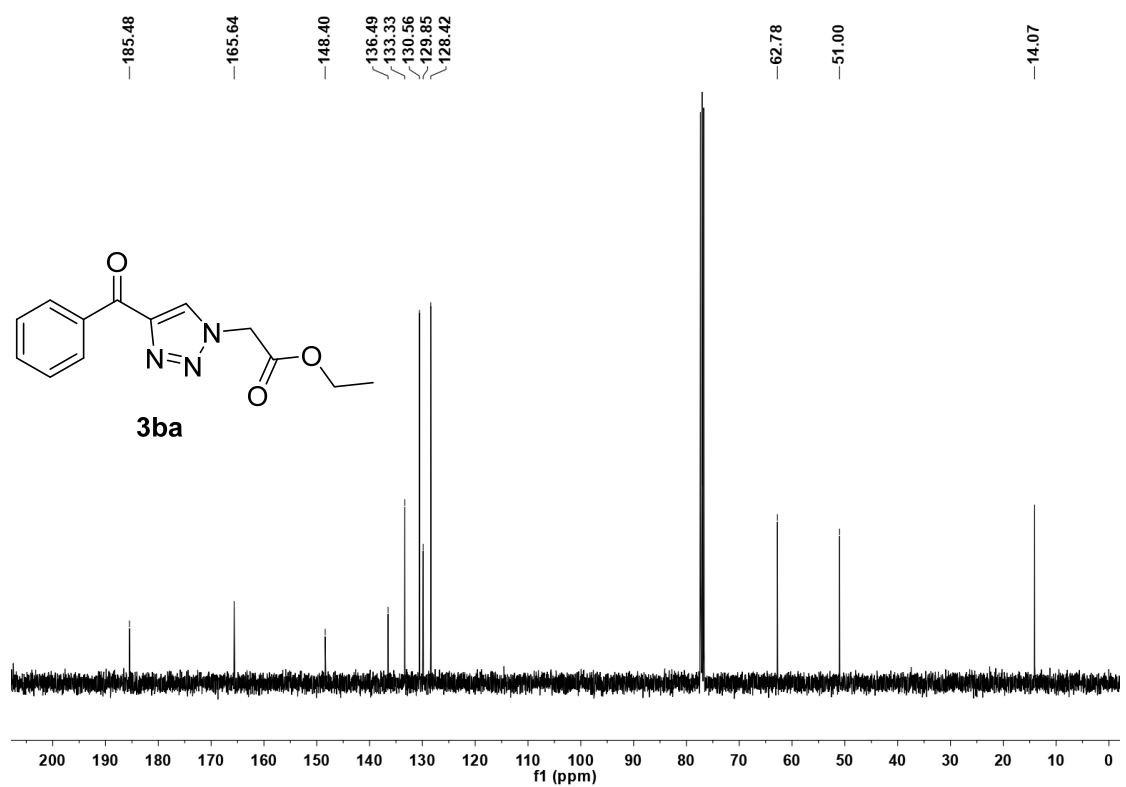
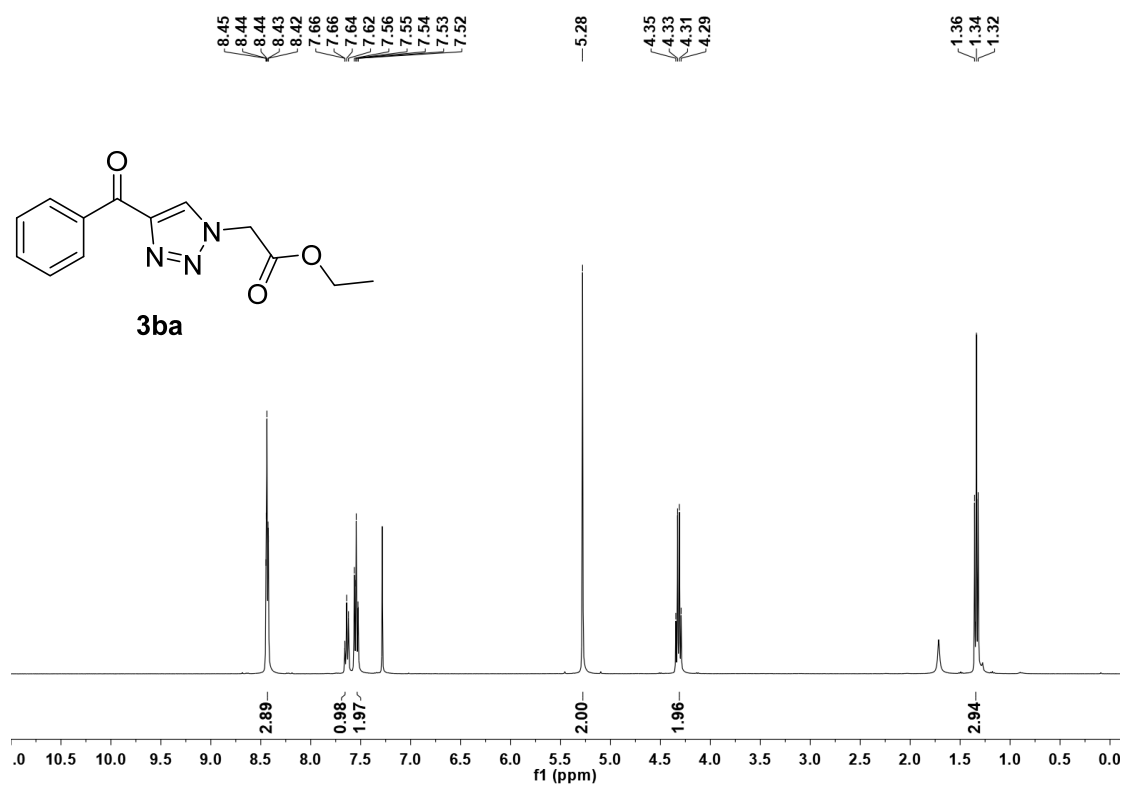


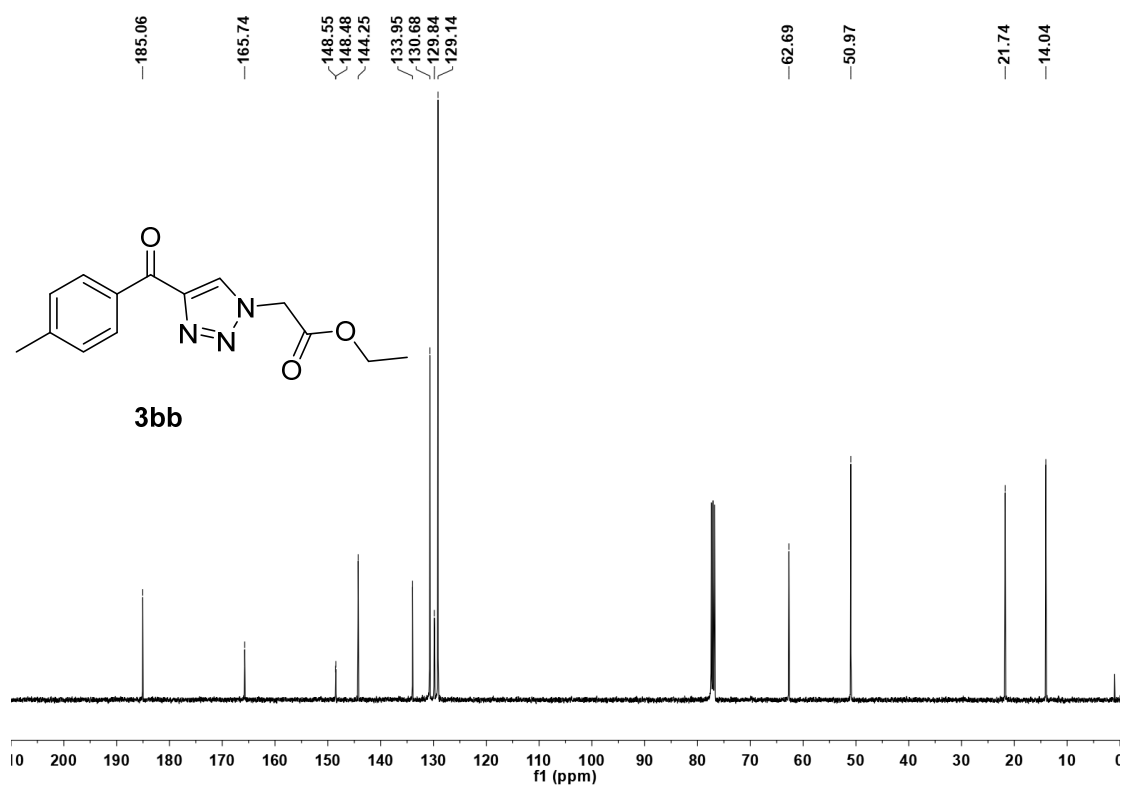
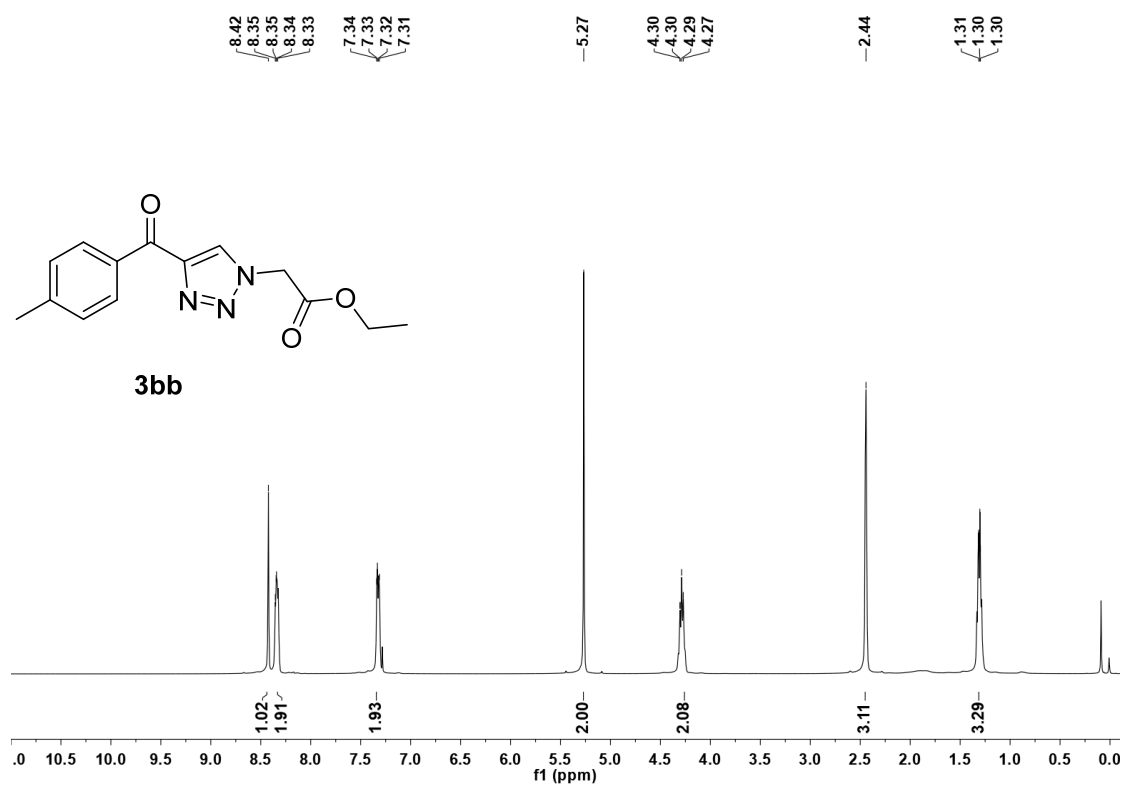


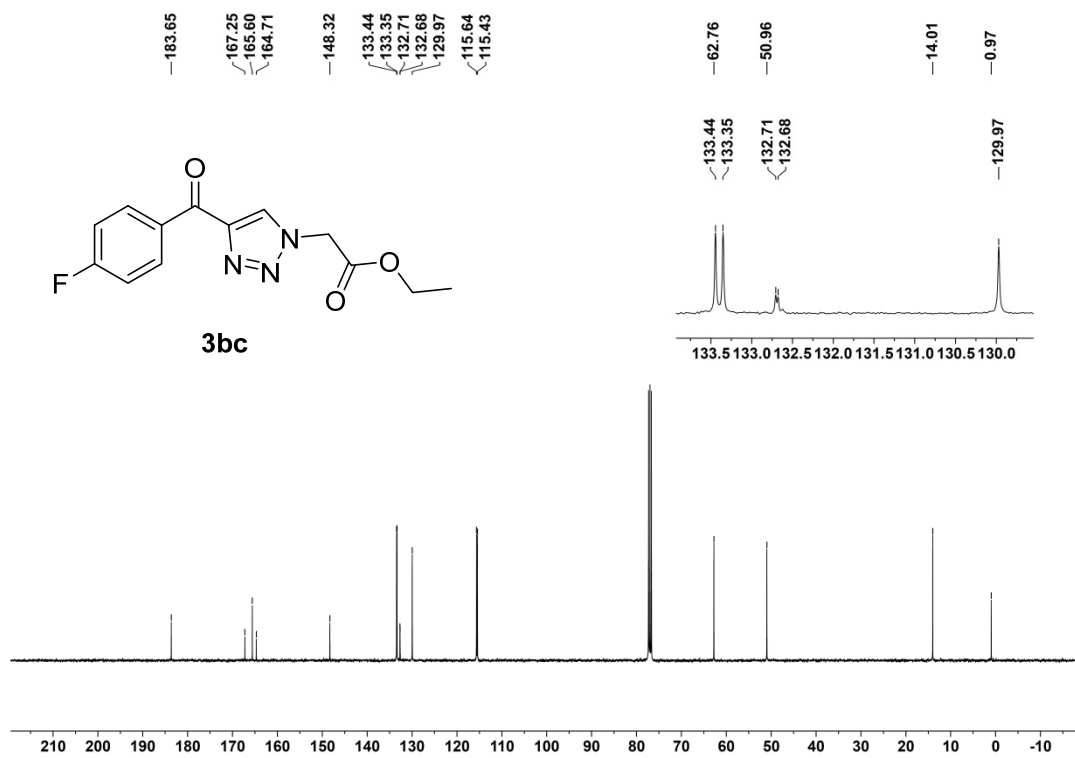
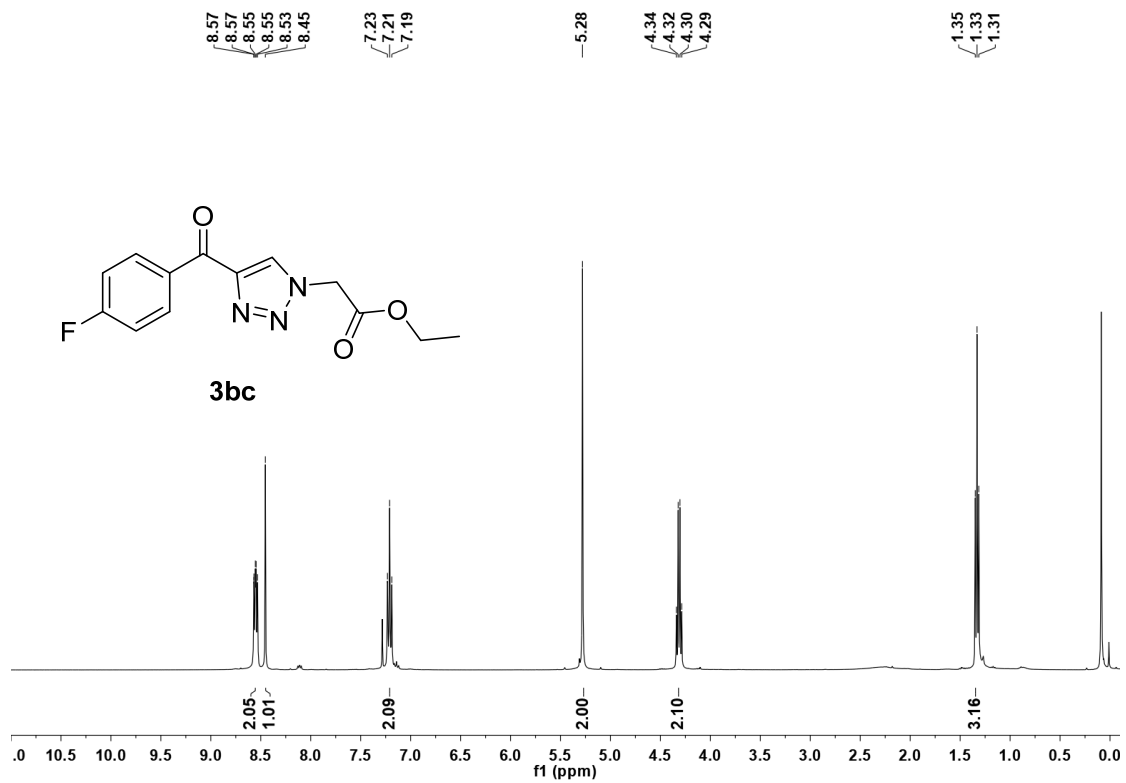




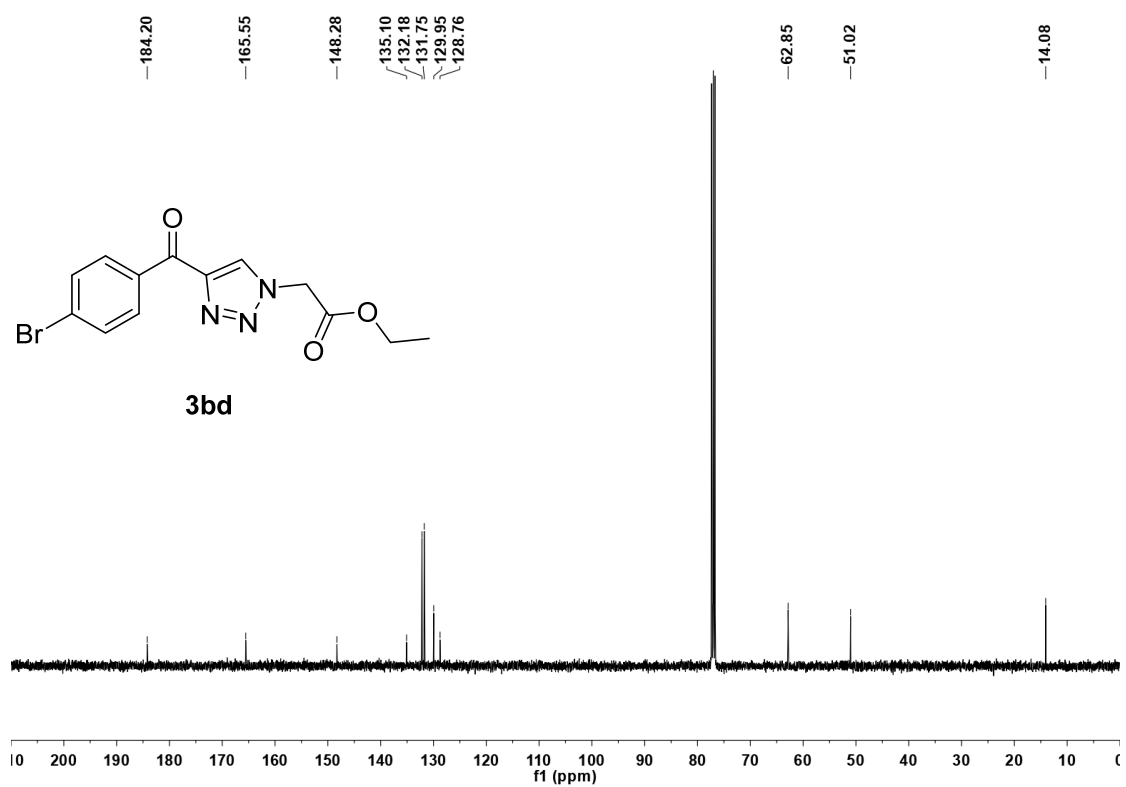
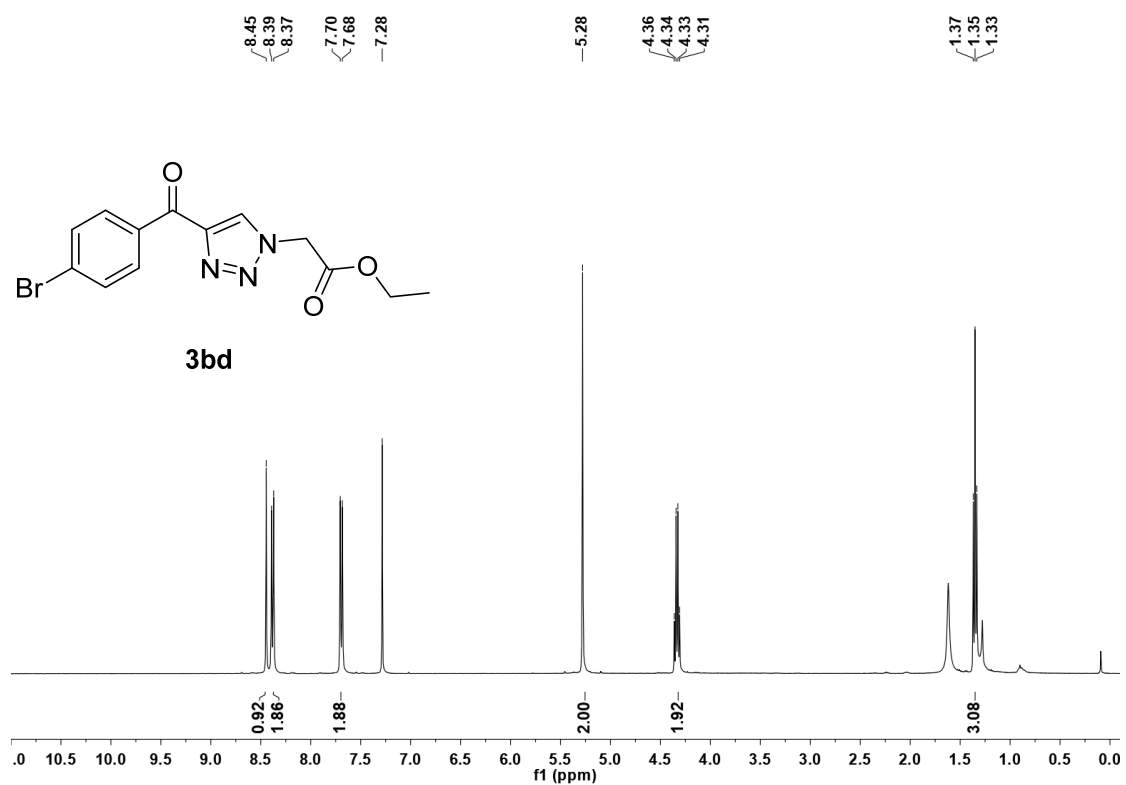


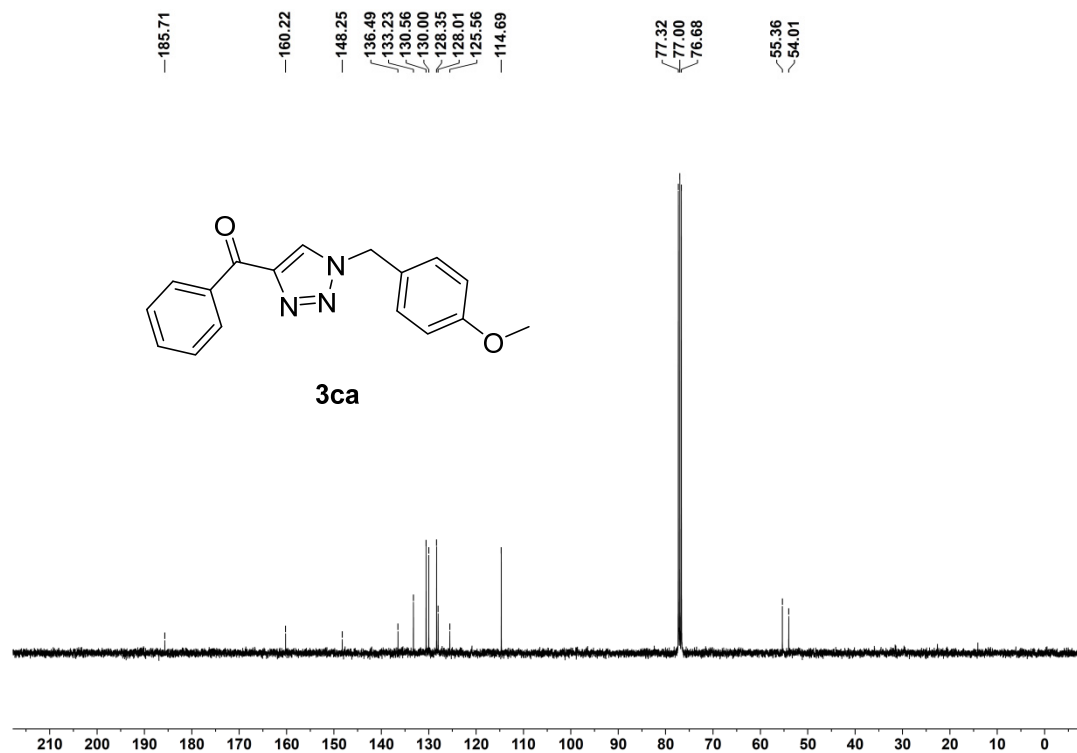
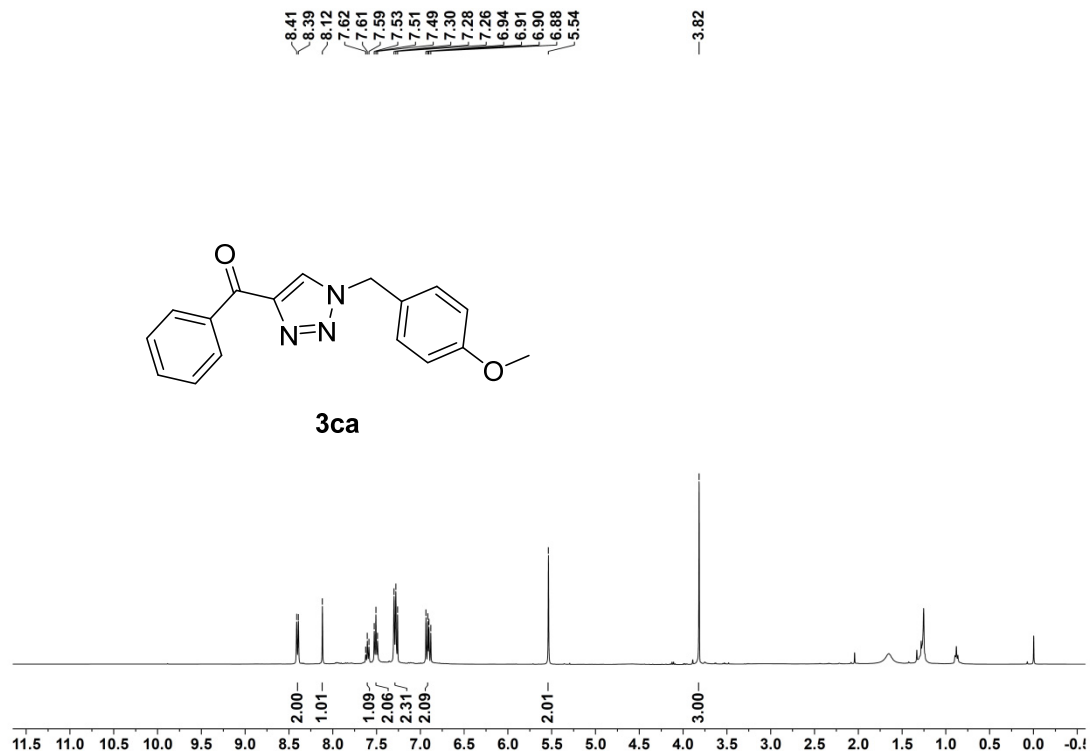


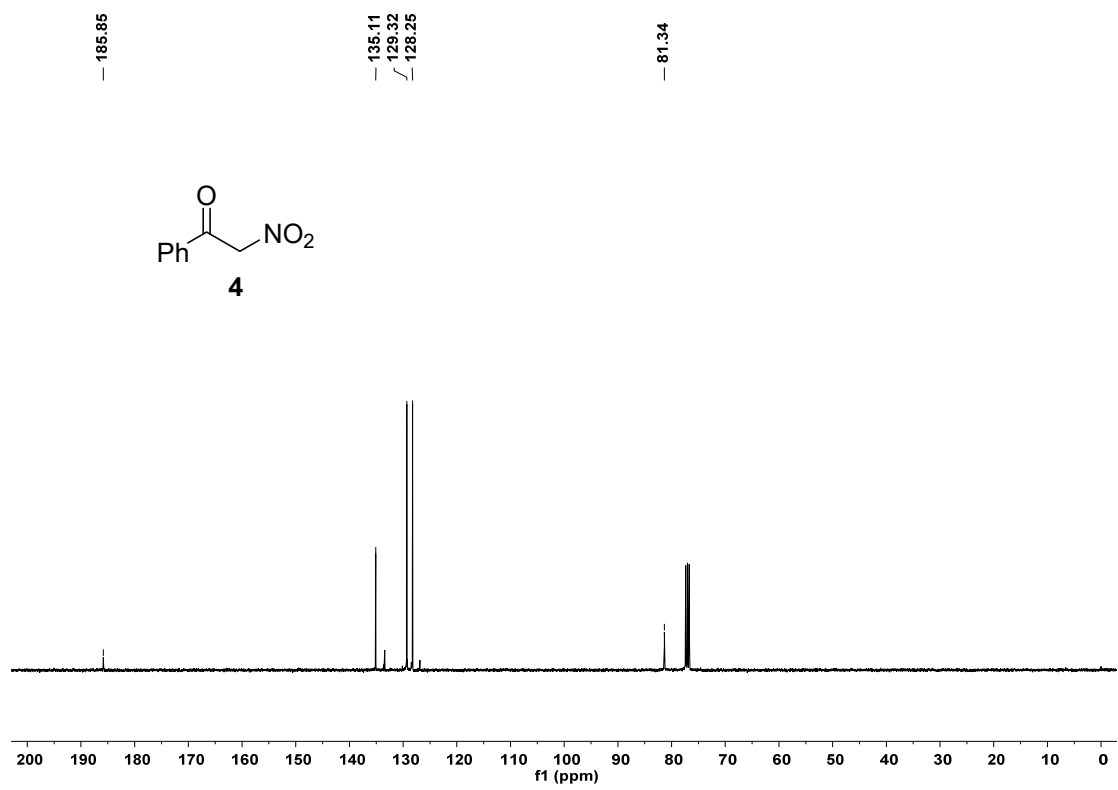
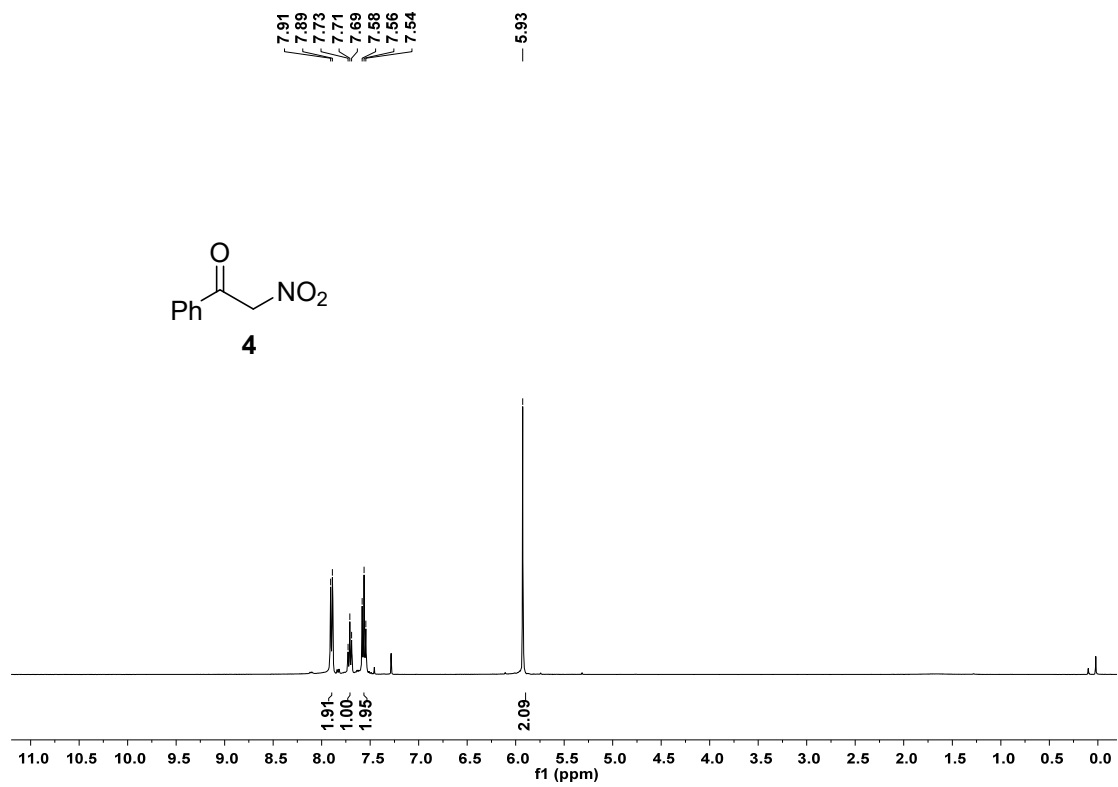


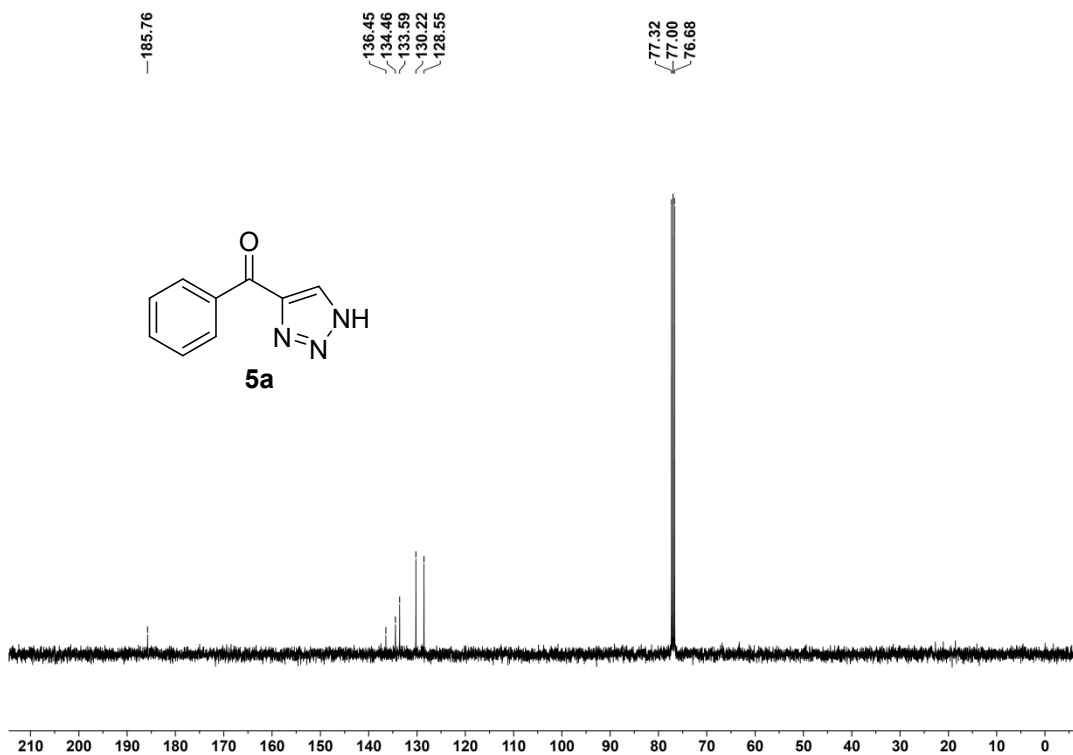
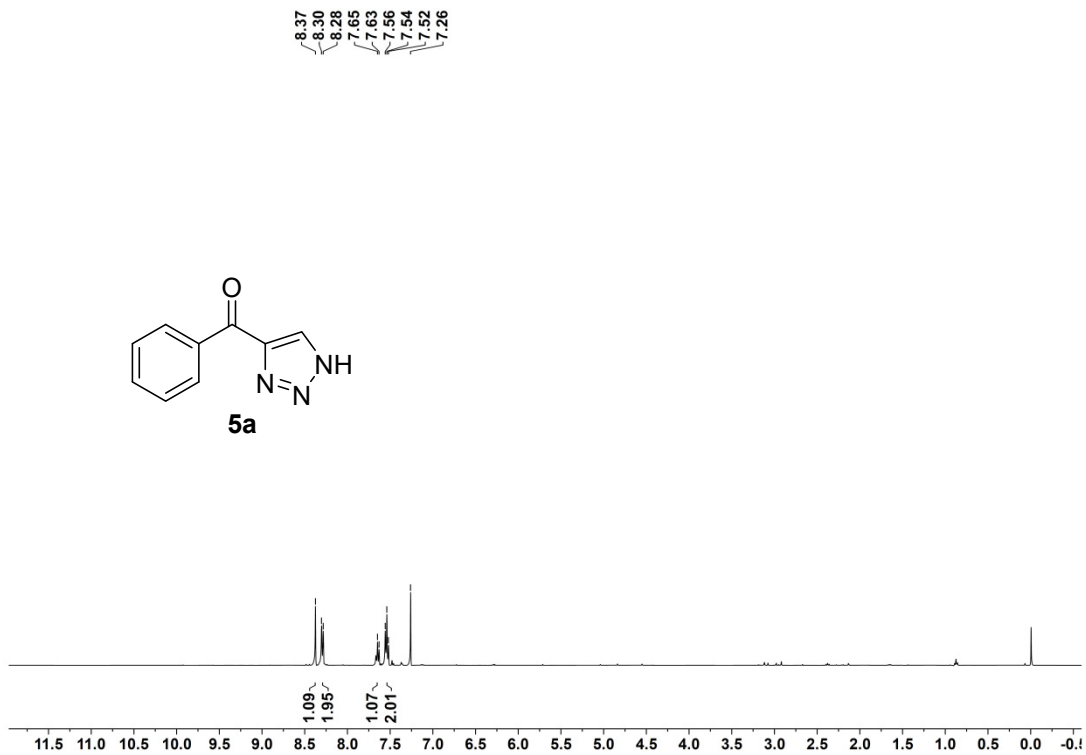












8.42  
8.41  
8.40  
8.16  
7.63  
7.61  
7.61  
7.60  
7.59  
7.59  
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7.35  
7.34  
7.33  
7.32  
-5.61

