

## Electronic Supplementary Information

### Metal-free, highly efficient organocatalytic amination of benzylic C–H bonds

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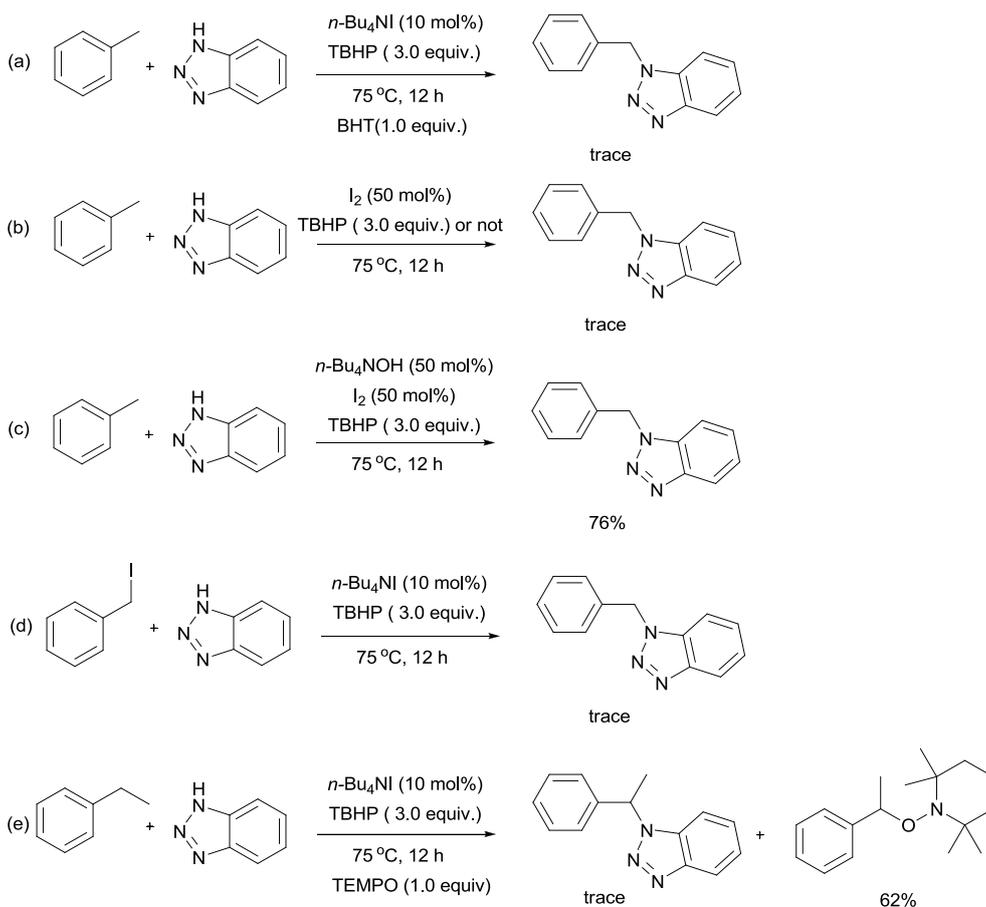
#### Contents:

General Information.....	2
Control experiment on the reaction mechanism .....	2
The regioselectivity for the reaction of 4-isopropyl toluene with 1 <i>H</i> -benzotriazole.....	2
Experimental details of benzotriazole 2n and benzimidazoles 2q .....	3
General procedure of amination of benzylic C–H bonds .....	3
Characterization data of compounds.....	3
Copies <sup>1</sup> H NMR, <sup>13</sup> C NMR.....	8
References:.....	33

## General Information

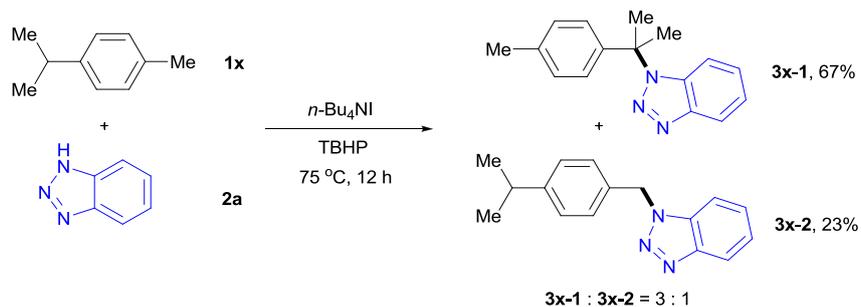
All reactions were carried out under air atmosphere unless otherwise noted. All reagents and solvents were obtained from commercial suppliers and used without further purification. Reactions were monitored by TLC on silica gel plates (GF254).  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded on 400 MHz spectrometer at room temperature. Chemical shifts ( $\delta$ ) are reported in ppm downfield from tetramethylsilane. Abbreviations for signal couplings are: s, singlet; d, doublet; t, triplet; m, multiplet.

## Control experiment on the reaction mechanism



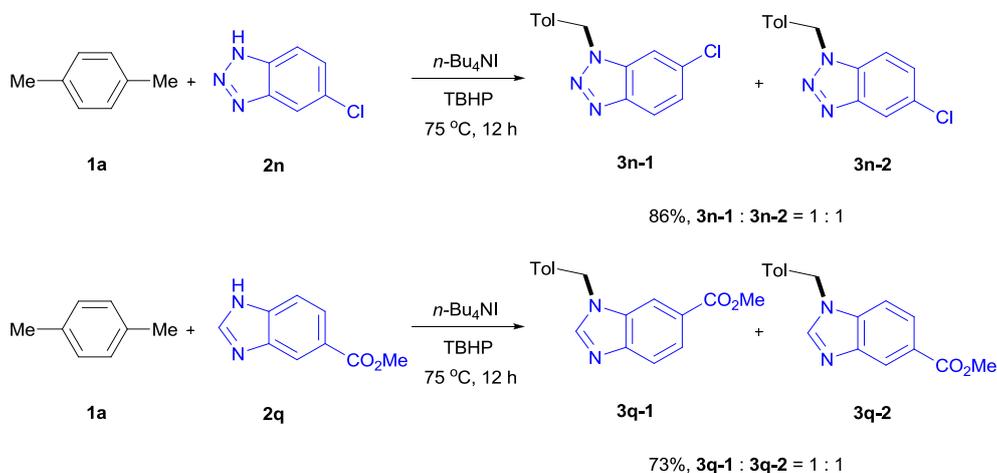
**Scheme 1.** Investigation of the reaction mechanism. Reaction conditions: benzyl C–H substrate (1.5 mmol), **3a** (0.3 mmol).

## The regioselectivity for the reaction of 4-isopropyl toluene with 1H-benzotriazole



**Scheme 2.** Reaction conditions: **1x** (1.5 mmol), **2a** (0.3 mmol), *n*-Bu<sub>4</sub>NI (0.03 mmol), TBHP (0.9 mmol, 70% in water), 75 °C, 12 h, air. Yields are of the isolated products.

### Experimental details of benzotriazole **2n** and benzimidazoles **2q**



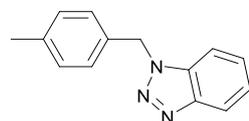
**Scheme 3.** Reaction conditions: **1a** (1.5 mmol), **2** (0.3 mmol), *n*-Bu<sub>4</sub>NI (0.03 mmol), TBHP (0.9 mmol, 70% in water), 75 °C, 12 h, air. Yields are of the isolated products.

### General procedure of amination of benzylic C–H bonds

To the mixture of benzyl C-H substrate **1** (1.5 mmol) and *n*-Bu<sub>4</sub>NI (0.03 mmol, 11.1 mg), the amine **2** (0.3 mmol) and TBHP (0.9 mmol, 70% in water) were successively added into the tube. Then the reaction mixture was stirred at 75 °C under air for 12 hours. After the reaction finished, the reaction mixture was cooled to room temperature and quenched by the addition of a saturated solution of Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> (3 mL). The mixture was extracted with ethyl acetate (3 × 10 mL), the combined organic phases were dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and the solvent was evaporated under vacuum. After removing the solvents in vacuo, the residue was purified by flash column chromatography on silica gel or preparative TLC on GF254 to afford the desired products **3**.

### Characterization data of compounds

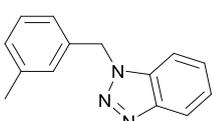
#### 1-(4-methylbenzyl)-1H-benzo[*d*][1,2,3]triazole **3a**<sup>1</sup>



Yield 90%, white solid, mp 97-98 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.08 (d, *J* = 8.4 Hz, 1 H), 7.39-7.29 (m, 3 H), 7.16 (d, *J* = 8.0 Hz, 2 H), 7.11 (d, *J* = 8.0 Hz, 2 H), 5.78 (s, 2 H), 2.30 (s, 3 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 146.2, 138.2, 132.7, 131.6, 129.5, 127.5, 127.2, 123.7, 119.9, 109.7, 52.0, 21.0

ppm.

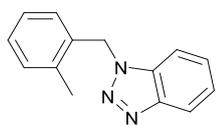
#### 1-(3-methylbenzyl)-1H-benzo[*d*][1,2,3]triazole **3b**<sup>2</sup>



Yield 88%, white solid, mp 119-121 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.06-8.04 (m, 1 H), 7.39-7.30 (m, 3 H), 7.22-7.18 (m, 1 H), 7.11-7.06 (m, 3 H), 5.78 (s, 2 H), 2.30 (s, 3 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 146.2, 138.7, 134.6, 132.7, 129.1, 128.7, 128.2, 127.3, 124.6, 123.8, 119.9, 109.7, 52.1, 21.2

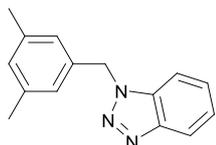
ppm.

1-(2-methylbenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3e**<sup>1</sup>



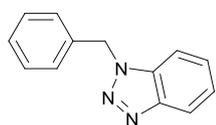
Yield 91%, white solid, mp 80-81 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.06-8.03 (m, 1 H), 7.37-7.12 (m, 6 H), 7.04-7.03 (m, 1 H), 5.82 (s, 2 H), 2.32 (s, 3 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 146.1, 136.4, 132.9, 132.5, 130.8, 128.5, 128.4, 127.2, 126.3, 123.8, 119.9, 109.8, 50.6, 19.1 ppm.

1-(3,5-dimethylbenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3d**



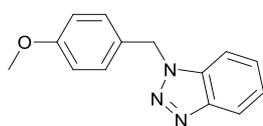
Yield 94%, white solid, mp 97-98 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.06 (d, *J* = 8.0 Hz, 1 H), 7.42-7.31 (m, 3 H), 6.92-6.89 (m, 2 H), 5.75 (s, 2 H), 2.25 (s, 6 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 146.2, 138.6, 134.5, 132.8, 130.0, 127.3, 125.3, 123.8, 119.9, 109.8, 52.2, 21.2 ppm. HRMS (ESI) *m/z* calcd for C<sub>15</sub>H<sub>15</sub>N<sub>3</sub>Na [M+Na]<sup>+</sup> 260.1158; found: 260.1163.

1-benzyl-1*H*-benzo[*d*][1,2,3]triazole **3e**<sup>2</sup>



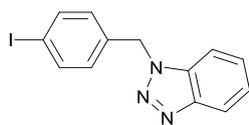
Yield 85%, white solid, mp 110-111 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.07 (d, *J* = 8.0 Hz, 1 H), 7.40-7.26 (m, 8 H), 5.85 (s, 2 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 146.3, 134.7, 132.8, 129.0, 128.4, 127.5, 127.4, 123.9, 120.0, 109.7, 52.2 ppm.

1-(4-methylbenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3f**



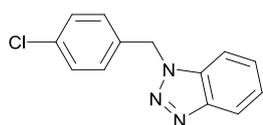
Yield 95%, white solid, mp 80-81 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.04 (d, *J* = 8.4 Hz, 1 H), 7.38-7.22 (m, 5 H), 6.85-6.83 (m, 2 H), 5.76 (s, 2 H), 3.75 (s, 3 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 159.6, 146.2, 132.6, 129.0, 127.2, 126.7, 123.7, 119.9, 114.2, 109.7, 55.2, 51.8 ppm. HRMS (ESI) *m/z* calcd for C<sub>14</sub>H<sub>13</sub>N<sub>3</sub>NaO [M+Na]<sup>+</sup> 262.0951; found: 262.0949.

1-(4-iodobenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3g**



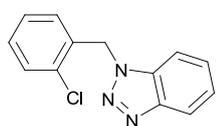
Yield 73%, white solid, mp 136-138 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.07 (d, *J* = 8.4 Hz, 1 H), 7.66 (d, *J* = 8.4 Hz, 2 H), 7.44-7.33 (m, 3 H), 7.01 (d, *J* = 8.0 Hz, 2 H), 5.78 (s, 2 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 146.3, 138.1, 134.4, 132.6, 129.3, 127.6, 124.0, 120.2, 109.4, 94.1, 51.6 ppm. HRMS (ESI) *m/z* calcd for C<sub>13</sub>H<sub>10</sub>IN<sub>3</sub>Na [M+Na]<sup>+</sup> 357.9812; found: 357.9815.

1-(4-chlorobenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3h**<sup>2</sup>



Yield 77%, white solid, mp 87-89 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.08-8.06 (m, 1 H), 7.44-7.29 (m, 5 H), 7.20 (d, *J* = 8.0 Hz, 2 H), 5.81 (s, 2 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 146.3, 134.5, 133.2, 132.7, 129.2, 128.9, 127.6, 124.0, 120.2, 109.4, 51.5 ppm.

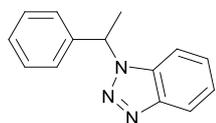
1-(2-chlorobenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3i**<sup>1</sup>



Yield 75%, white solid, mp 80-82 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.09 (d, *J* = 8.4 Hz, 1 H), 7.45-7.42 (m, 3 H), 7.39-7.35 (m, 1 H), 7.28-7.24 (m, 1 H), 7.18-7.14 (m, 1 H), 6.97-6.95 (m, 1 H), 5.98 (s, 2 H) ppm; <sup>13</sup>C NMR (100 MHz,

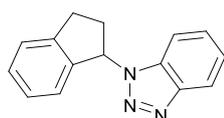
$\text{CDCl}_3$ ):  $\delta = 146.1, 132.9, 132.8, 132.5, 129.8, 129.7, 129.2, 127.6, 127.4, 124.0, 120.1, 109.6, 49.1$  ppm.

1-(1-phenylethyl)-1*H*-benzo[*d*][1,2,3]triazole **3j**<sup>3</sup>



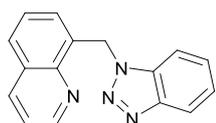
Yield 96%, colorless oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 8.06\text{-}8.04$  (m, 1 H), 7.35-7.24 (m, 8 H), 6.04 (q,  $J = 7.2$  Hz, 1 H), 2.17 (d,  $J = 7.2$  Hz, 3 H) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 146.4, 140.1, 132.4, 128.9, 128.2, 127.0, 126.2, 123.8, 119.9, 110.1, 59.0, 21.1$  ppm.

1-(2,3-dihydro-1*H*-inden-1-yl)-1*H*-benzo[*d*][1,2,3]triazole **3k**



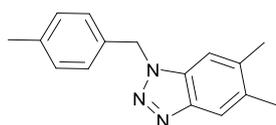
Yield 92%, white solid, mp 94-96 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 8.07\text{-}8.04$  (m, 1 H), 7.42-7.40 (m, 1 H), 7.35-7.21 (m, 3 H), 7.17-7.13 (m, 1 H), 7.00-6.98 (m, 1 H), 6.93-6.91 (m, 1 H), 6.64 (t,  $J = 8.0$  Hz, 1 H), 3.35-3.28 (m, 1 H), 3.18-3.10 (m, 1 H), 2.91-2.82 (m, 1 H), 2.58-2.49 (m, 1 H) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 146.6, 143.4, 139.2, 131.6, 129.0, 127.1, 126.9, 125.2, 124.6, 123.7, 120.1, 110.3, 64.8, 32.5, 30.7$  ppm. HRMS (ESI)  $m/z$  calcd for  $\text{C}_{15}\text{H}_{13}\text{N}_3\text{Na}$   $[\text{M}+\text{Na}]^+$  258.1002; found: 258.1004.

8-((1*H*-benzo[*d*][1,2,3]triazol-1-yl)methyl)quinoline **3l**



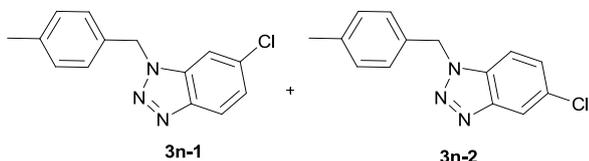
Yield 86%, colorless oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 9.03\text{-}9.01$  (m, 1 H), 8.20-8.17 (m, 1 H), 8.07-8.05 (m, 1 H), 7.78-7.76 (m, 1 H), 7.62-7.60 (m, 1 H), 7.50-7.47 (m, 1 H), 7.44-7.32 (m, 4 H), 6.61 (s, 2 H) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 149.9, 146.1, 145.7, 136.3, 133.5, 133.3, 128.6, 128.3, 127.1, 126.4, 123.7, 121.5, 119.8, 110.4, 47.2$  ppm. HRMS (ESI)  $m/z$  calcd for  $\text{C}_{16}\text{H}_{12}\text{N}_4\text{Na}$   $[\text{M}+\text{Na}]^+$  283.0954; found: 283.0955.

5,6-dimethyl-1-(4-methylbenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3m**



Yield 92%, white solid, mp 144-145 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 7.70$  (s, 1 H), 7.16-7.10 (m, 5 H), 5.73 (s, 2 H), 2.36 (s, 3 H), 2.34 (s, 3 H), 2.30 (s, 3 H) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 145.5, 138.0, 137.6, 133.6, 132.0, 131.8, 129.5, 127.4, 119.0, 109.1, 51.8, 21.1, 20.9, 20.3$  ppm.

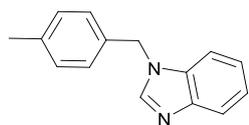
HRMS (ESI)  $m/z$  calcd for  $\text{C}_{16}\text{H}_{17}\text{N}_3\text{Na}$   $[\text{M}+\text{Na}]^+$  274.1315; found: 274.1310.



Chloro-1-(4-methylbenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3n**

Yield 86%, 3n-1 : 3n-2 = 1 : 1.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 8.01\text{-}8.00$  (m, 1 H), 7.96-7.94 (m, 1 H), 7.35-7.24 (m, 4 H), 7.18-7.14 (m, 8 H), 5.77 (s, 2 H), 5.74 (s, 2 H), 2.31 (s, 3 H), 2.30 (s, 3 H) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 146.8, 144.8, 138.5, 133.6, 133.2, 131.3, 131.2, 131.1, 129.7, 129.6, 129.5, 128.2, 127.5, 127.4, 125.0, 120.8, 119.2, 110.7, 109.5, 52.3, 52.1, 21.0$  ppm. HRMS (ESI)  $m/z$  calcd for  $\text{C}_{14}\text{H}_{12}\text{ClN}_3\text{Na}$   $[\text{M}+\text{Na}]^+$  280.0612; found: 280.0607.

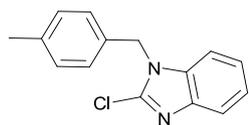
1-(4-methylbenzyl)-1*H*-benzo[*d*]imidazole **3o**<sup>4</sup>



Yield 79%, colorless oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 7.95 (s, 1 H), 7.84-7.82 (m, 1 H), 7.28-7.23 (m, 3 H), 7.13 (d, *J* = 8.0 Hz, 2 H), 7.07 (d, *J* = 8.0 Hz, 2 H), 5.28 (s, 2 H), 2.32 (s, 3 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 143.7, 143.1, 138.0, 133.8, 132.3, 129.6, 127.1, 123.0, 122.2, 120.2, 110.0,

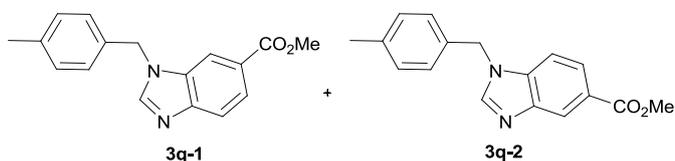
48.6, 21.0 ppm.

2-chloro-1-(4-methylbenzyl)-1*H*-benzo[*d*]imidazole **3p**<sup>5</sup>



Yield 71%, white solid, mp 118-120 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 7.72-7.69 (m, 1 H), 7.27-7.23 (m, 3 H), 7.12 (d, *J* = 8.0 Hz, 2 H), 7.07 (d, *J* = 8.0 Hz, 2 H), 5.34 (s, 2 H), 2.31 (s, 3 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 141.7, 140.7, 138.0, 135.1, 132.0, 129.6, 126.8, 123.3, 122.8, 119.5, 109.9,

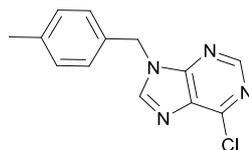
47.7, 21.1 ppm.



Methyl 1-(4-methylbenzyl)-1*H*-benzo[*d*]imidazole-carboxylate **3q**

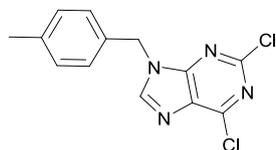
Yield 73%, 3q-1 : 3q-2 = 1 : 1. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.54-8.53 (m, 1 H), 8.11-7.96 (m, 5 H), 7.84-7.81 (m, 1 H), 7.32-7.30 (m, 1 H), 7.16-7.07 (m, 8 H), 5.35 (s, 2 H), 5.32 (s, 2 H), 3.93 (s, 3 H), 3.92 (s, 3 H), 2.33 (s, 6 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 167.4, 167.3, 147.0, 145.5, 144.7, 143.4, 138.3, 137.0, 133.6, 131.8, 131.7, 129.8, 129.7, 127.2, 127.1, 125.0, 124.6, 123.7, 122.7, 119.9, 112.3, 109.8, 52.1, 52.0, 48.8, 48.7, 21.0 ppm. HRMS (ESI) *m/z* calcd for C<sub>17</sub>H<sub>16</sub>N<sub>2</sub>NaO<sub>2</sub> [M+Na]<sup>+</sup> 303.1104; found: 303.1110.

6-chloro-9-(4-methylbenzyl)-9*H*-purine **3r**<sup>6</sup>



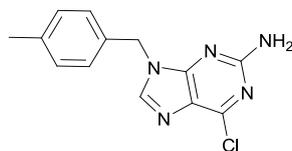
Yield 83%, white solid, mp 130-132 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.78 (s, 1 H), 8.09 (s, 1 H), 7.22 (d, *J* = 8.0 Hz, 2 H), 7.17 (d, *J* = 8.0 Hz, 2 H), 5.41 (s, 2 H), 2.34 (s, 3 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 152.1, 151.8, 151.0, 144.9, 138.8, 131.5, 131.4, 129.9, 127.9, 47.7, 21.1 ppm.

2,6-dichloro-9-(4-methylbenzyl)-9*H*-purine **3s**<sup>6</sup>



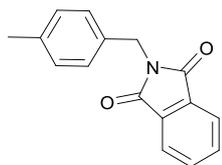
Yield 80%, white solid, mp 142-143 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.04 (s, 1 H), 7.22 (d, *J* = 8.4 Hz, 2 H), 7.18 (d, *J* = 8.4 Hz, 2 H), 5.37 (s, 2 H), 2.35 (s, 3 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 153.1, 153.0, 151.7, 145.5, 139.0, 130.9, 130.6, 129.9, 128.1, 47.8, 21.1 ppm.

6-chloro-9-(4-methylbenzyl)-9*H*-purin-2-amine **3t**<sup>7</sup>



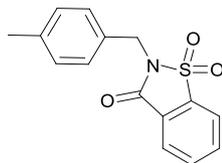
Yield 73%, colorless oil. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 7.74 (s, 1 H), 7.16 (s, 4 H), 5.21 (s, 2 H), 5.07 (bs, 2 H), 2.34 (s, 3 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 159.1, 153.8, 151.3, 142.2, 138.5, 131.9, 129.8, 127.8, 125.1, 47.0, 21.1 ppm.

2-(4-methylbenzyl)isoindoline-1,3-dione **3u**<sup>8</sup>



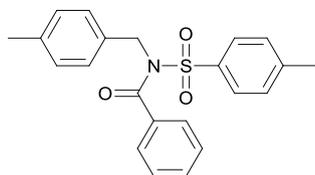
Yield 82%, white solid, mp 115-117 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 7.84-7.82 (m, 2 H), 7.70-7.68 (m, 2 H), 7.33 (d, *J* = 8.0 Hz, 2 H), 7.12 (d, *J* = 8.0 Hz, 2 H), 4.81 (s, 2 H), 2.30 (s, 3 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 168.0, 137.5, 133.9, 133.4, 132.2, 129.3, 128.6, 123.3, 41.3, 21.1 ppm.

*N*-(4-methylbenzyl)saccharine **3v**<sup>9</sup>



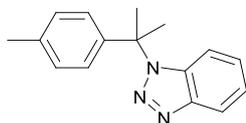
Yield 98%, white solid, mp 112-113 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.05-8.03 (m, 1 H), 7.92-7.90 (m, 1 H), 7.86-7.80 (m, 2 H), 7.40 (d, *J* = 8.0 Hz, 2 H), 7.15 (d, *J* = 8.0 Hz, 2 H), 4.87 (s, 2 H), 2.32 (s, 3 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 158.7, 137.9, 137.7, 134.6, 134.2, 131.4, 129.2, 128.7, 127.2, 125.0, 120.9, 42.4, 21.0 ppm.

*N*-(4-methylbenzyl)-*N*-tosylbenzamide **3w**



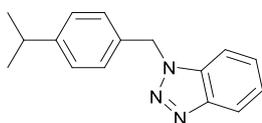
Yield 89%, white solid, mp 113-115 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 7.61-7.58 (m, 2 H), 7.46-7.43 (m, 3 H), 7.34-7.30 (m, 2 H), 7.22-7.20 (m, 2 H), 7.09 (d, *J* = 8.0 Hz, 2 H), 7.05 (d, *J* = 8.0 Hz, 2 H), 4.93 (s, 2 H), 2.41 (s, 3 H), 2.30 (s, 3 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 171.5, 144.6, 137.4, 136.0, 135.1, 133.2, 131.6, 129.3, 129.2, 128.5, 128.2, 128.1, 127.9, 51.0, 21.6, 21.1 ppm. HRMS (ESI) *m/z* calcd for C<sub>22</sub>H<sub>21</sub>NNaO<sub>3</sub>S [M+Na]<sup>+</sup> 402.1134; found: 402.1134.

1-(2-*p*-tolylpropan-2-yl)-1*H*-benzo[*d*][1,2,3]triazole **3x-1**



Yield 67%, white solid, mp 97-98 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.04 (d, *J* = 8.0 Hz, 1 H), 7.27-7.23 (m, 1 H), 7.17-7.06 (m, 5 H), 6.73 (d, *J* = 8.4 Hz, 1 H), 2.33 (s, 3 H), 2.16 (s, 6 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 146.8, 141.1, 137.5, 132.0, 129.5, 126.4, 125.2, 123.5, 119.8, 112.2, 64.6, 29.6, 20.9 ppm. HRMS (ESI) *m/z* calcd for C<sub>16</sub>H<sub>18</sub>N<sub>3</sub> [M+H]<sup>+</sup> 252.1495; found: 252.1492.

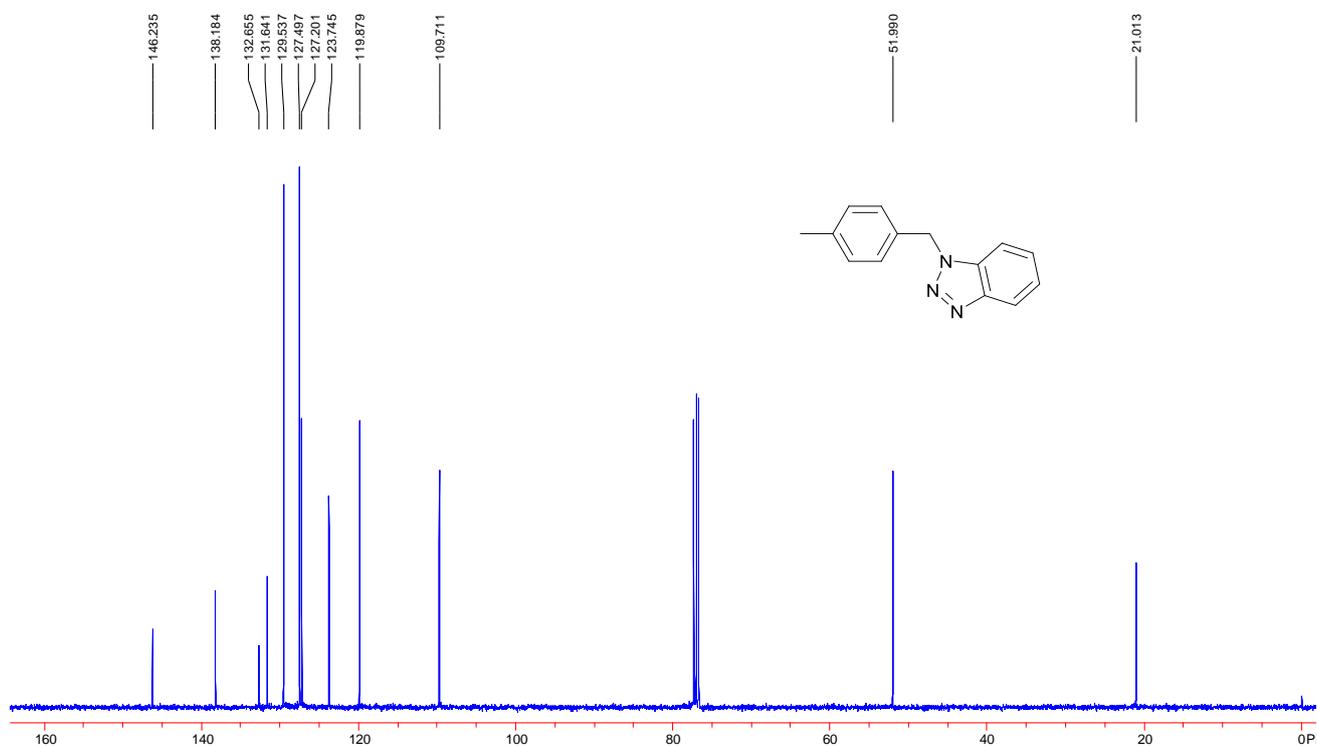
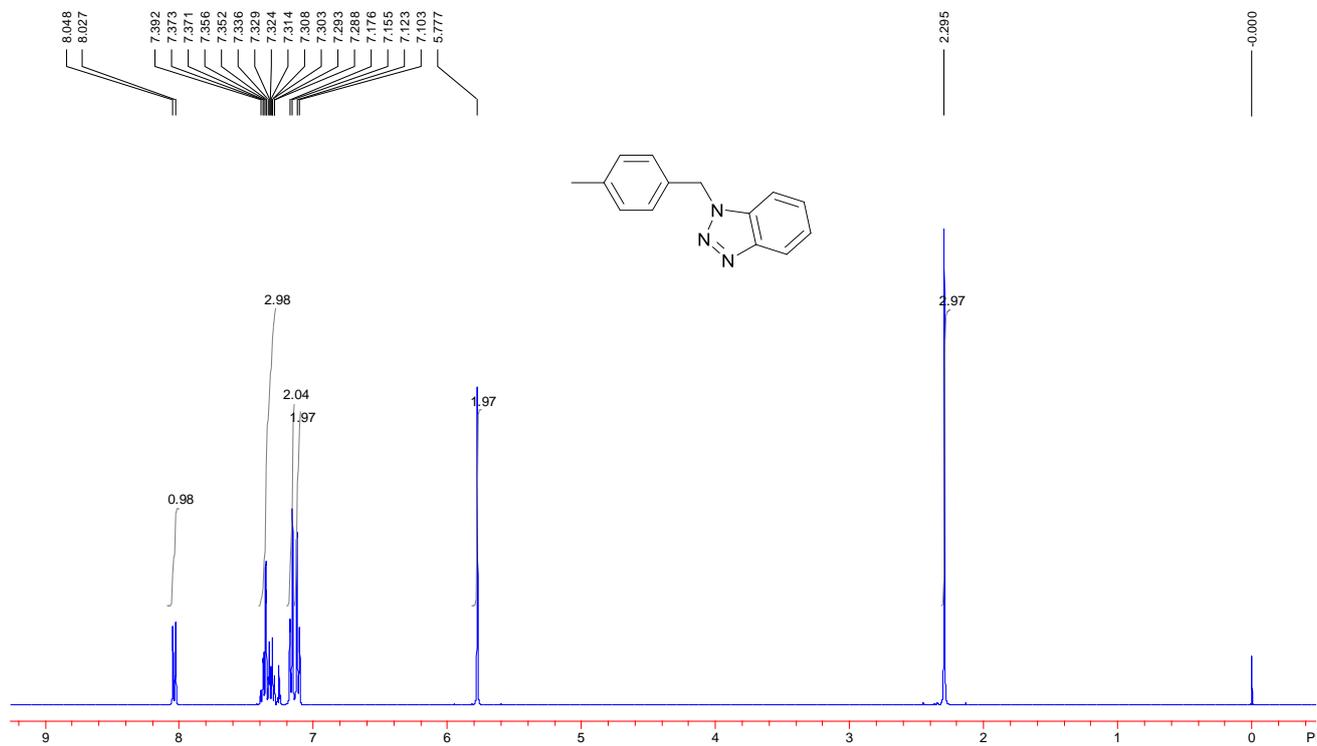
1-(4-isopropylbenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3x-2**



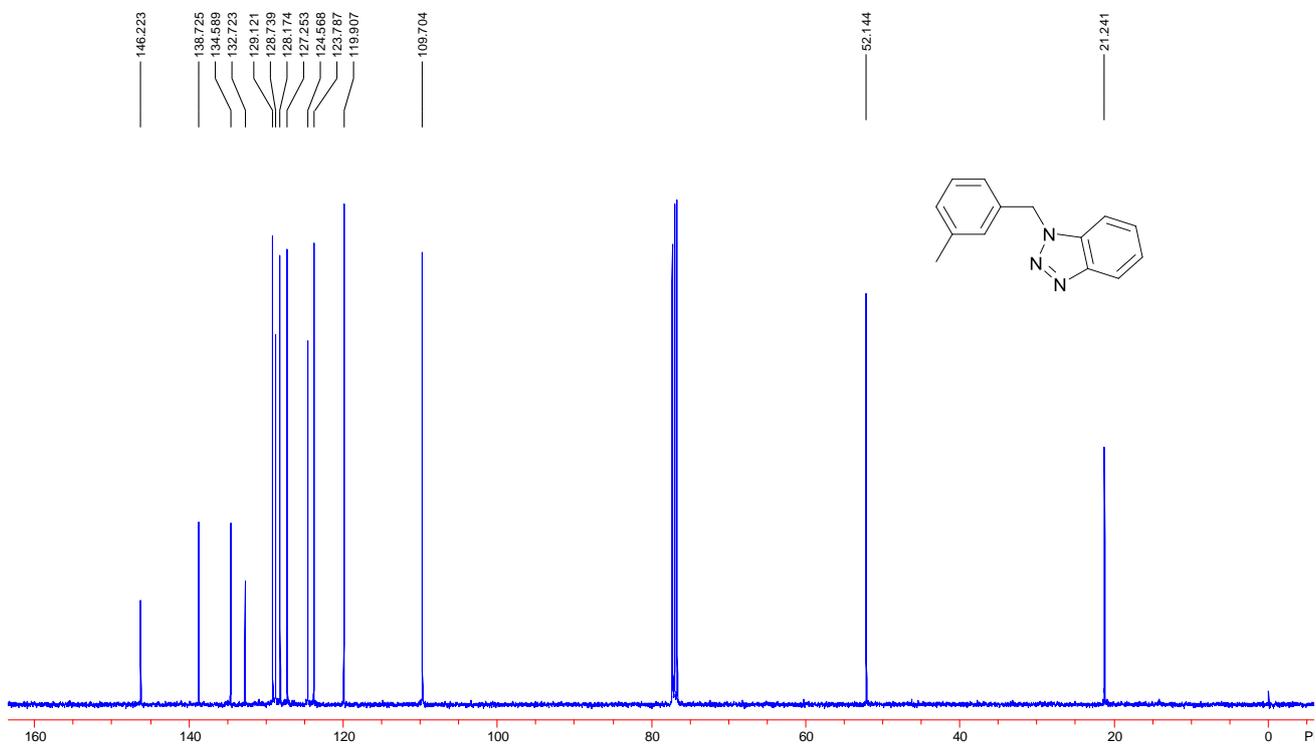
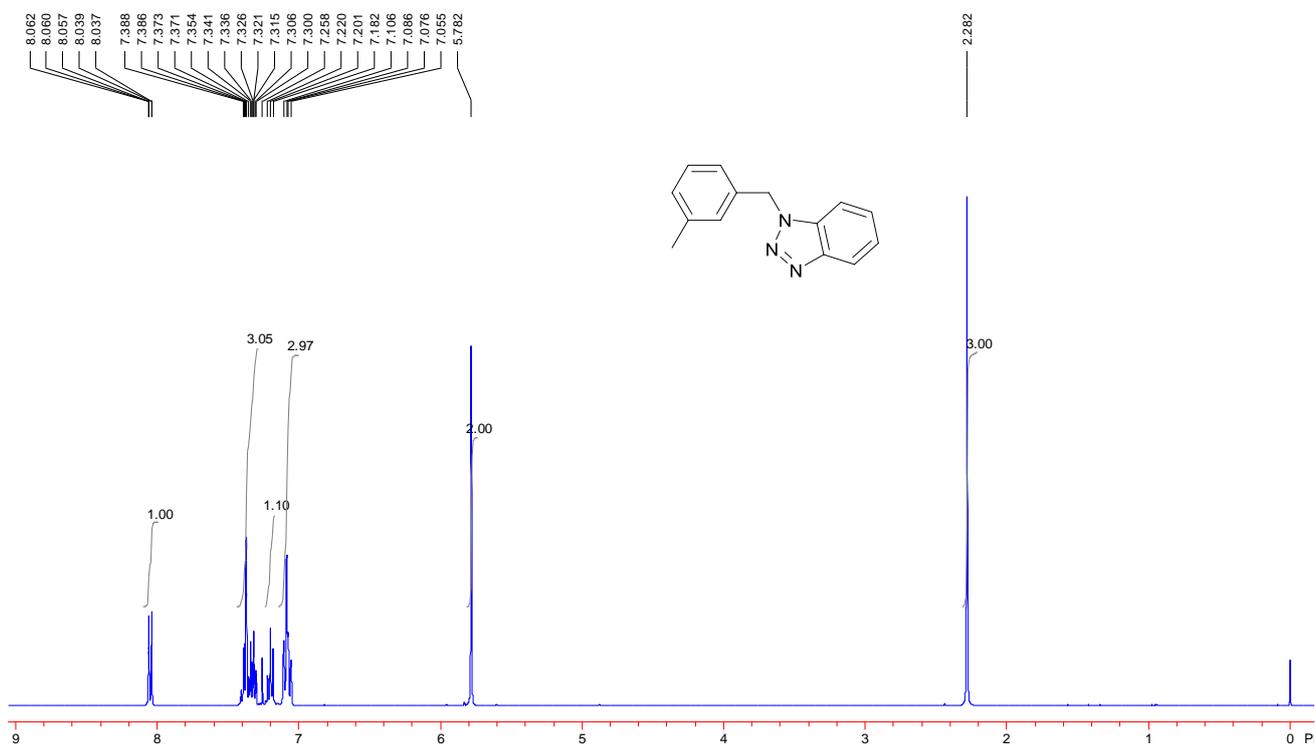
Yield 23%, white solid, mp 110-112 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.05 (d, *J* = 8.0 Hz, 1 H), 7.40-7.37 (m, 2 H), 7.35-7.32 (m, 1 H), 7.22-7.14 (m, 4 H), 5.78 (s, 2 H), 2.92-2.82 (m, 1 H), 1.20 (d, *J* = 6.8 Hz, 6 H) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 149.2, 146.3, 132.8, 132.1, 127.6, 127.2, 126.9, 123.8, 119.9, 109.8, 52.0, 33.7, 23.8 ppm. HRMS (ESI) *m/z* calcd for C<sub>16</sub>H<sub>18</sub>N<sub>3</sub> [M+H]<sup>+</sup> 252.1495; found: 252.1499.

## Copies $^1\text{H}$ NMR, $^{13}\text{C}$ NMR

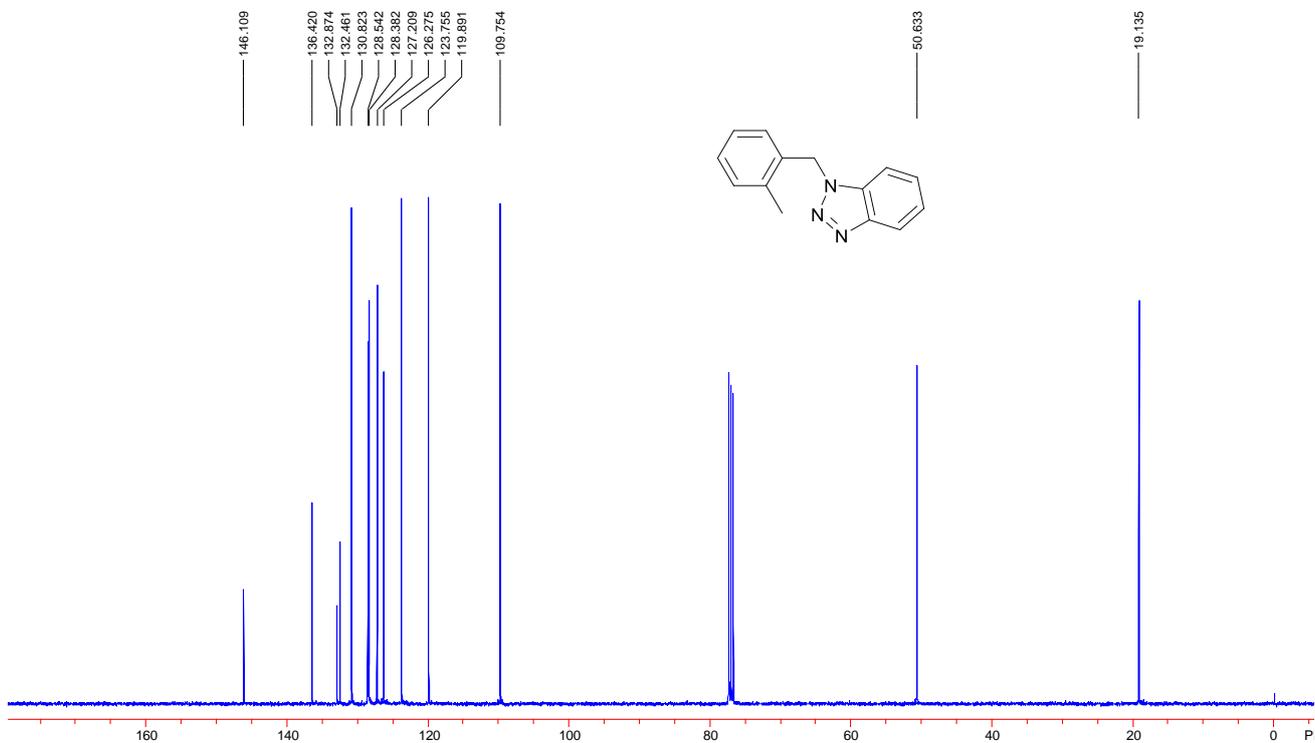
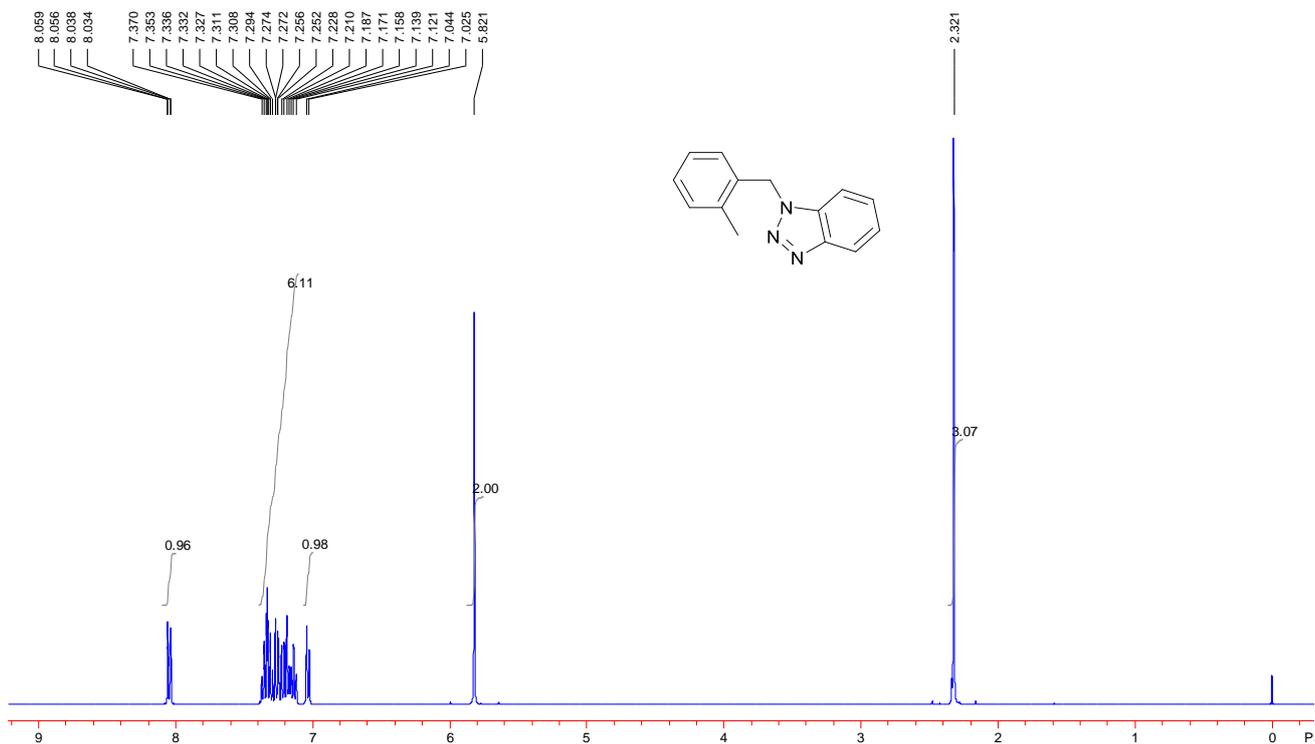
### 1-(4-methylbenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3a**



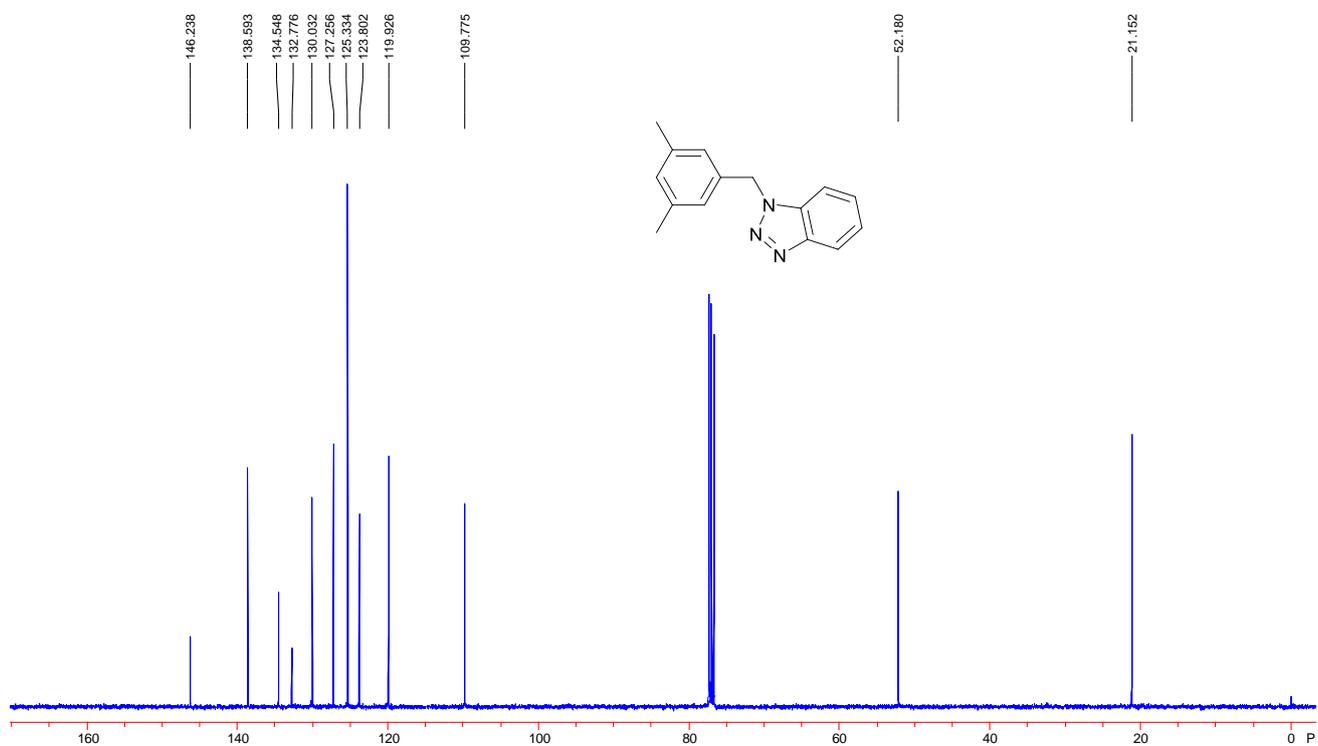
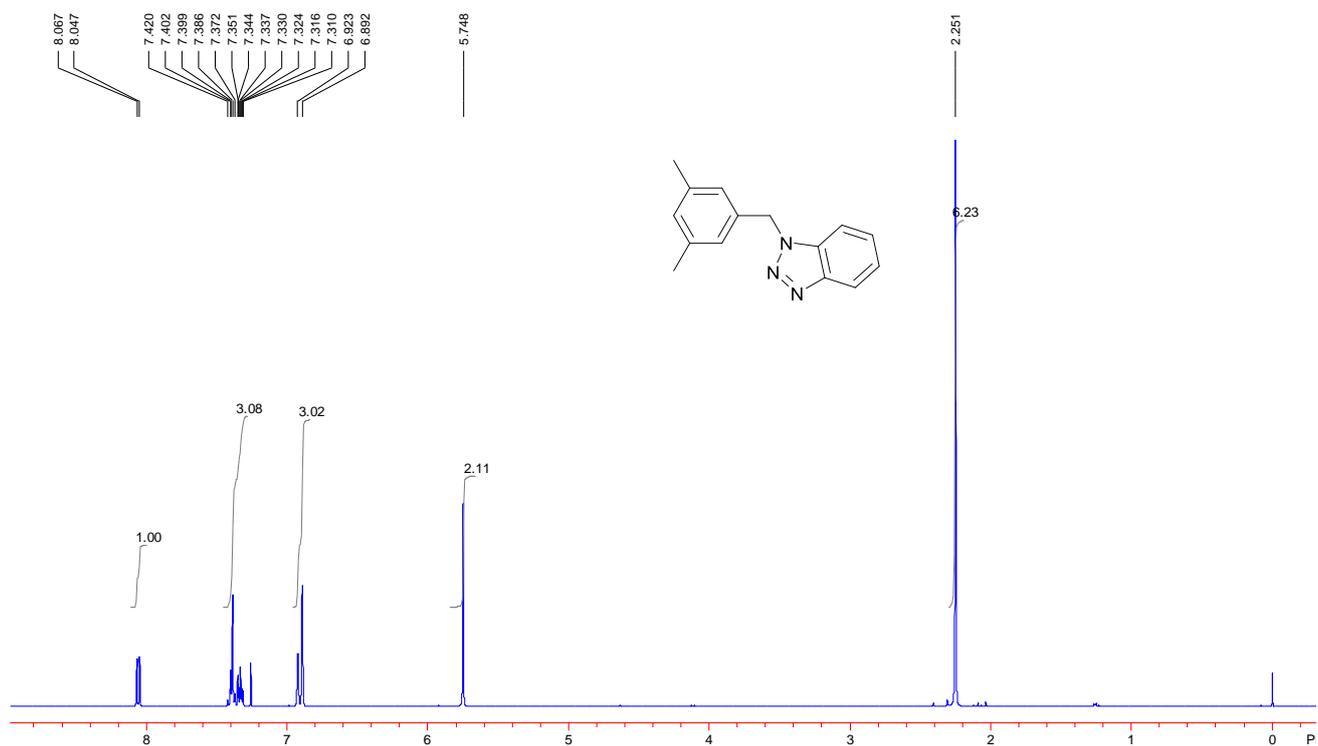
### 1-(3-methylbenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3b**



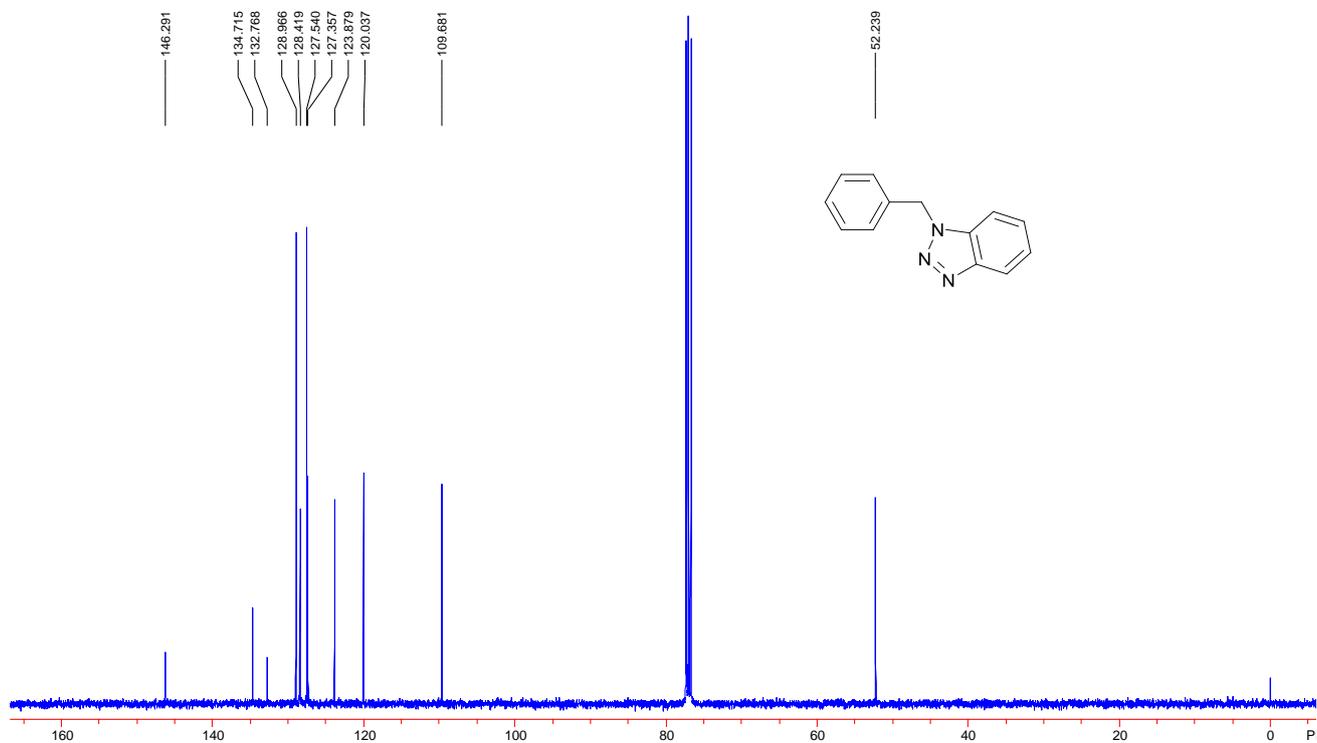
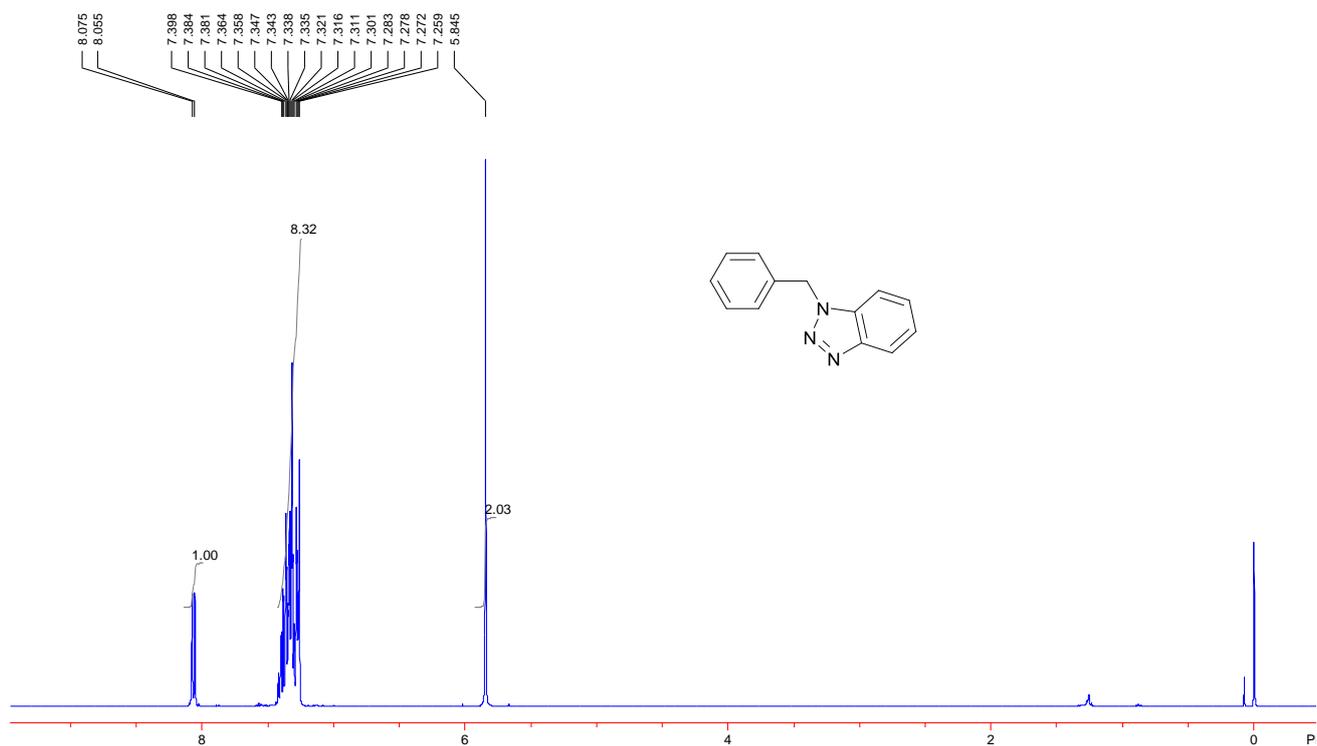
### 1-(2-methylbenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3c**



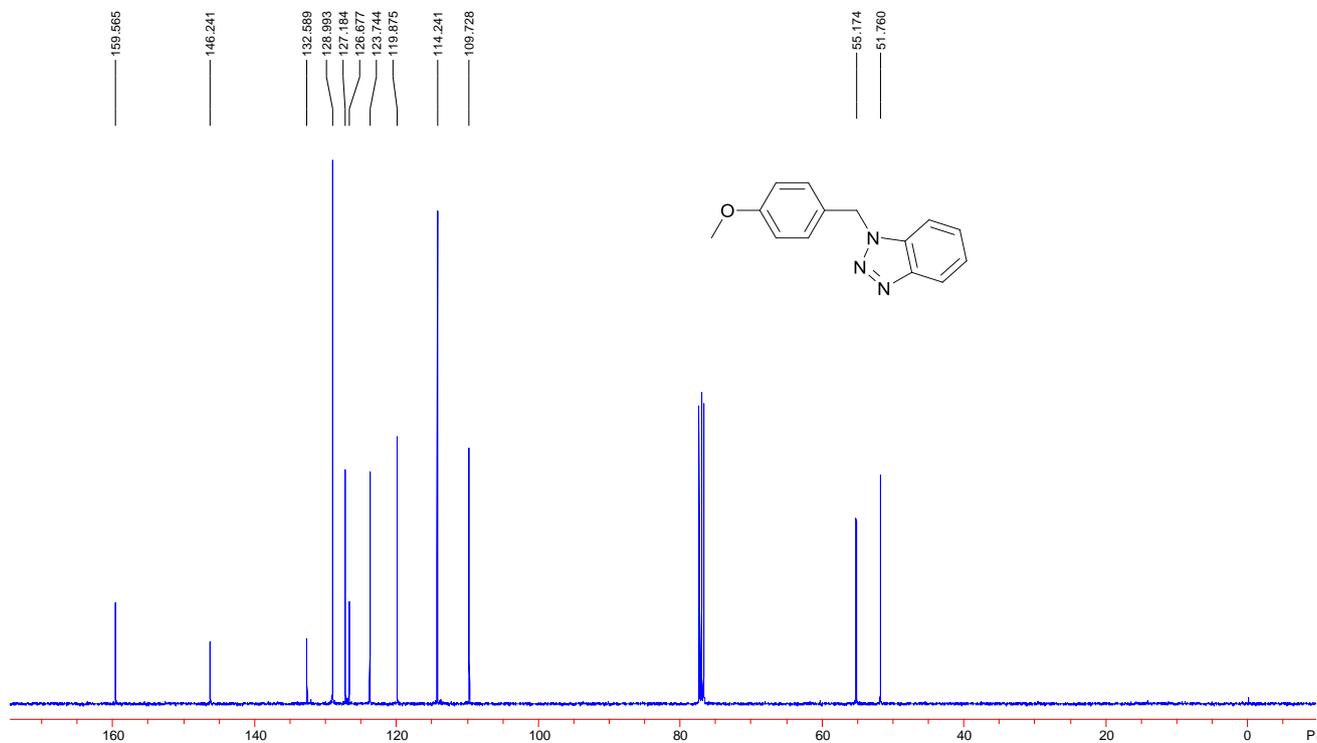
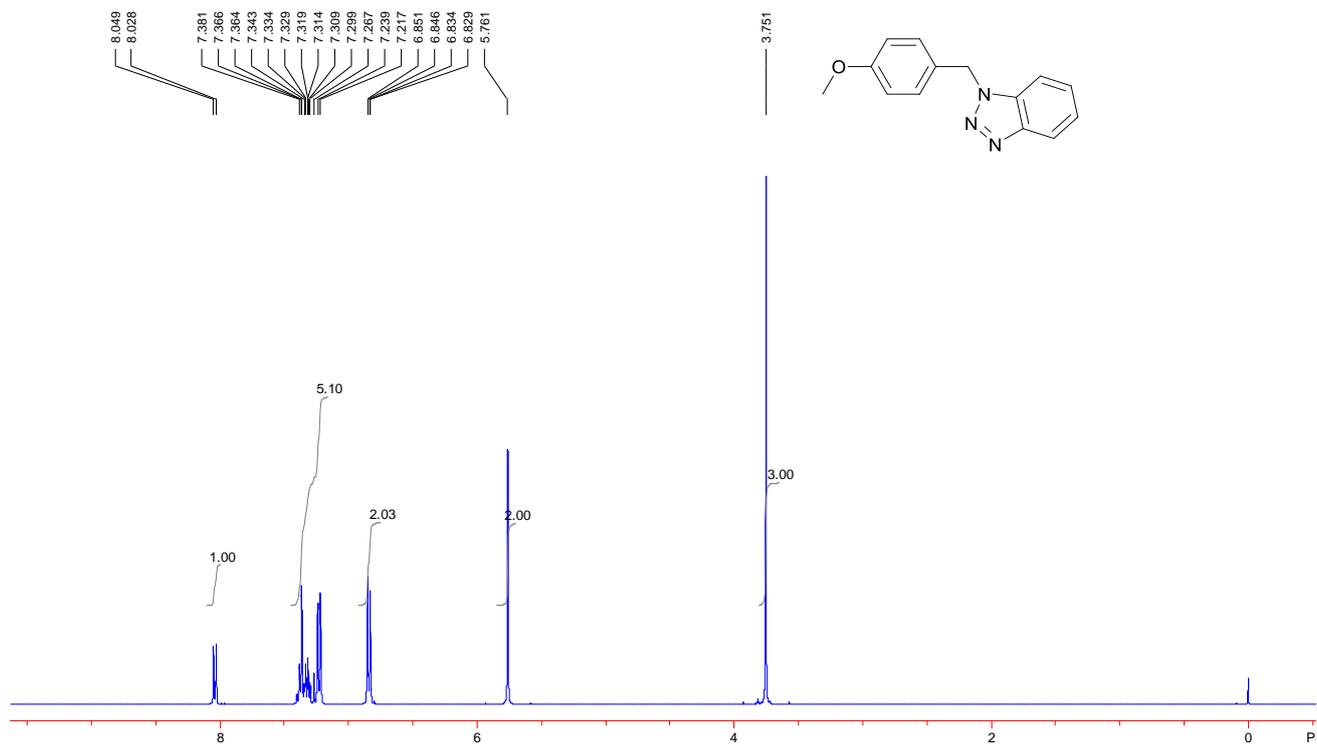
### 1-(3,5-dimethylbenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3d**



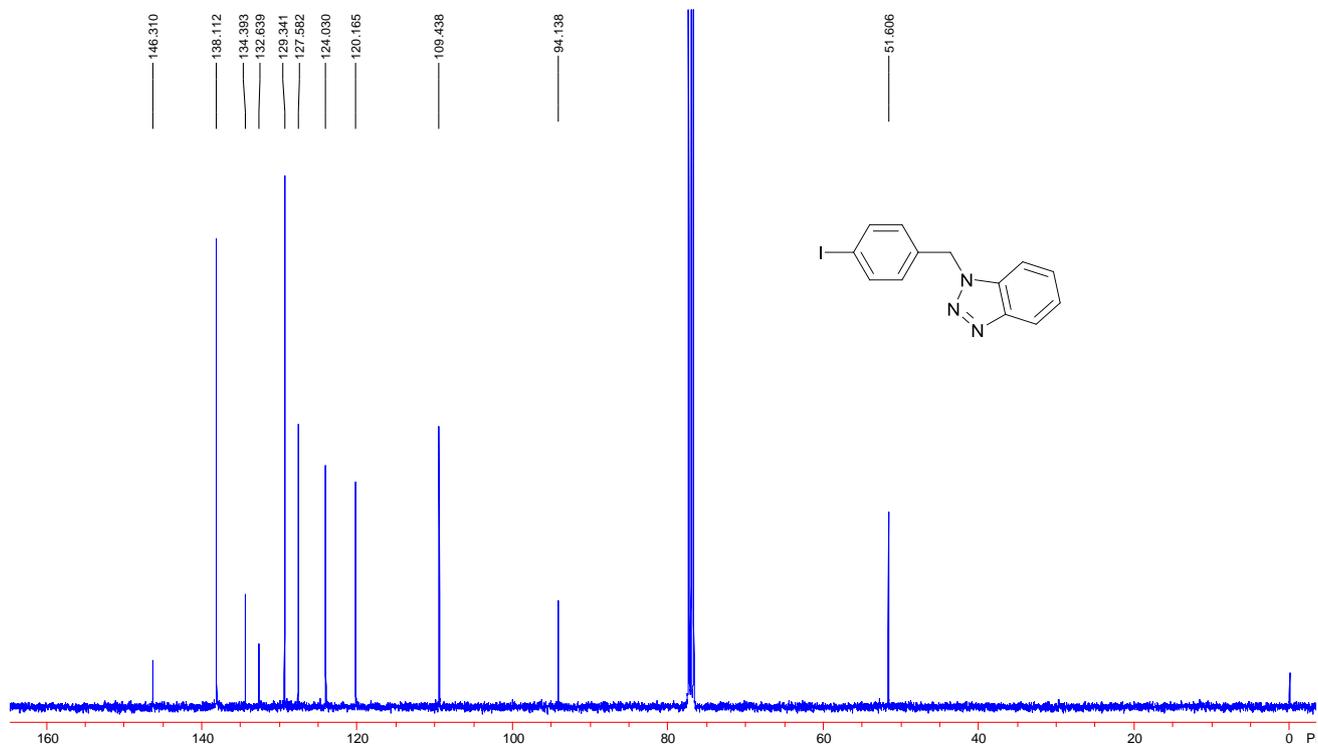
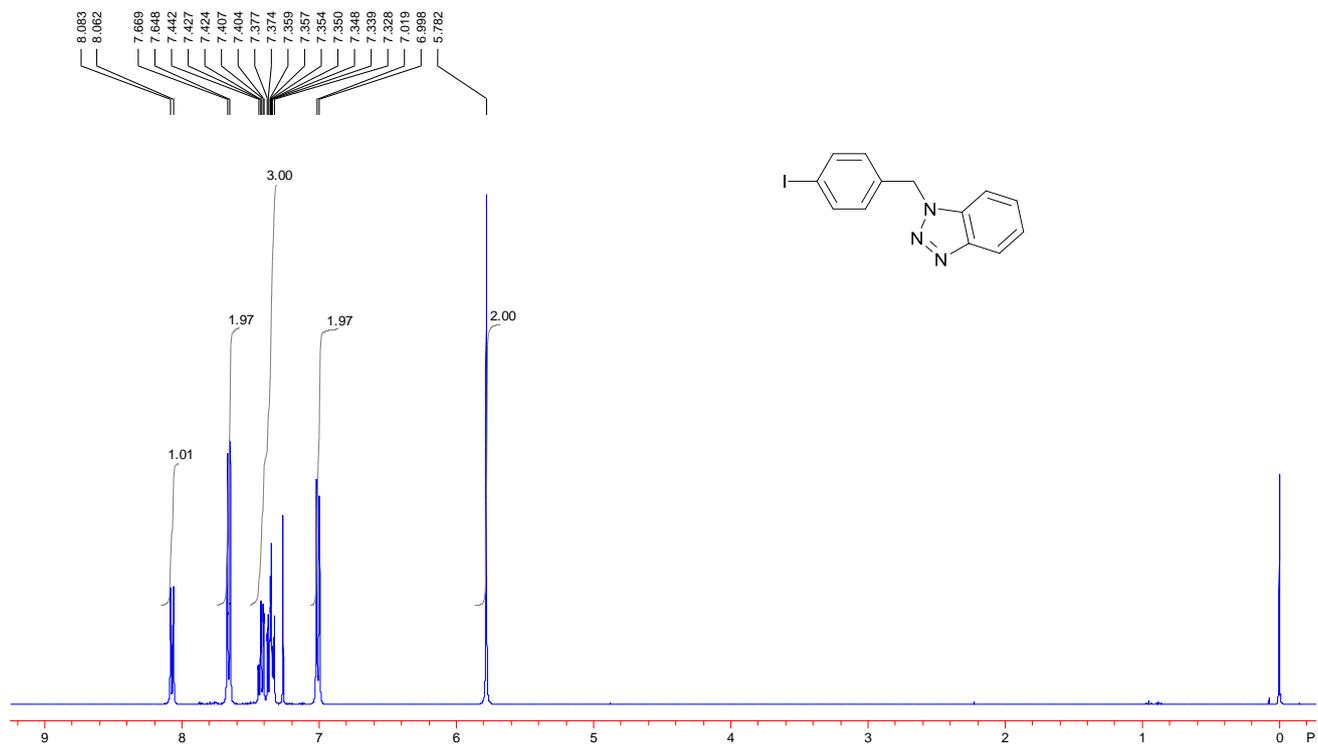
### 1-benzyl-1*H*-benzo[*d*][1,2,3]triazole **3e**



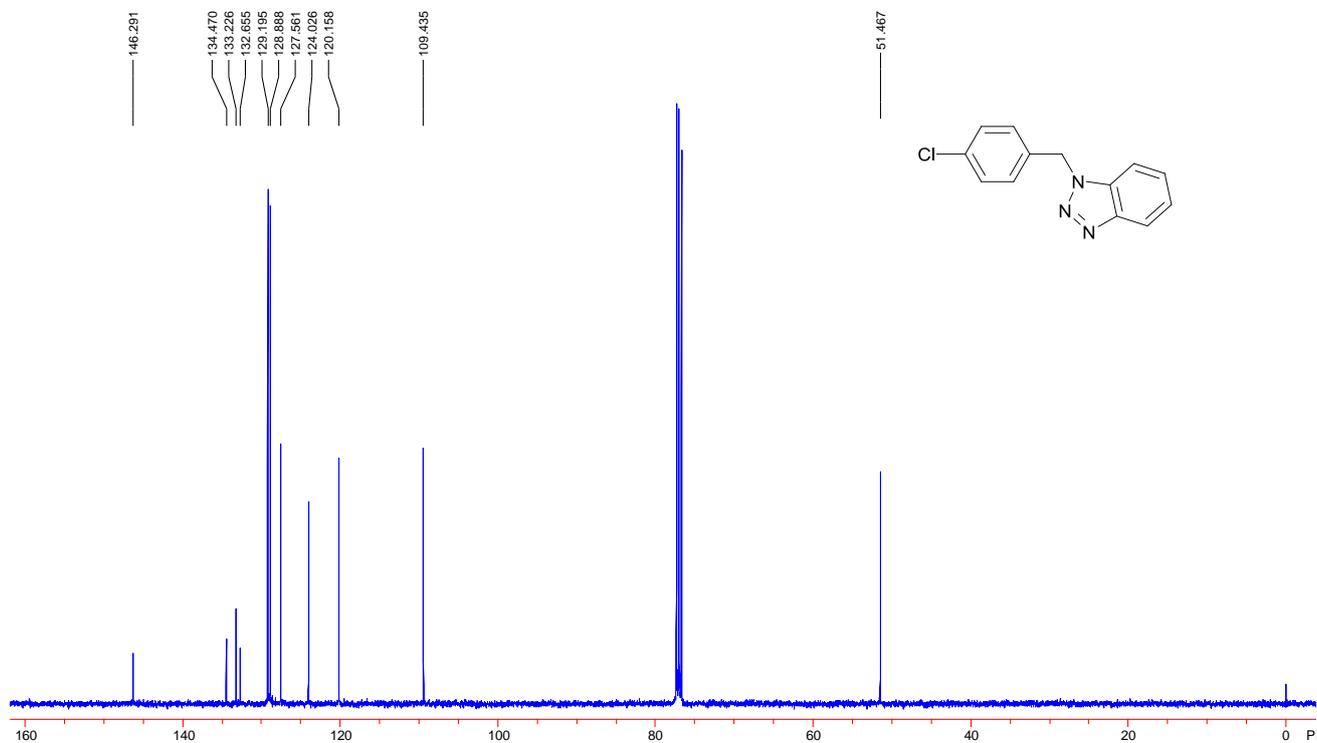
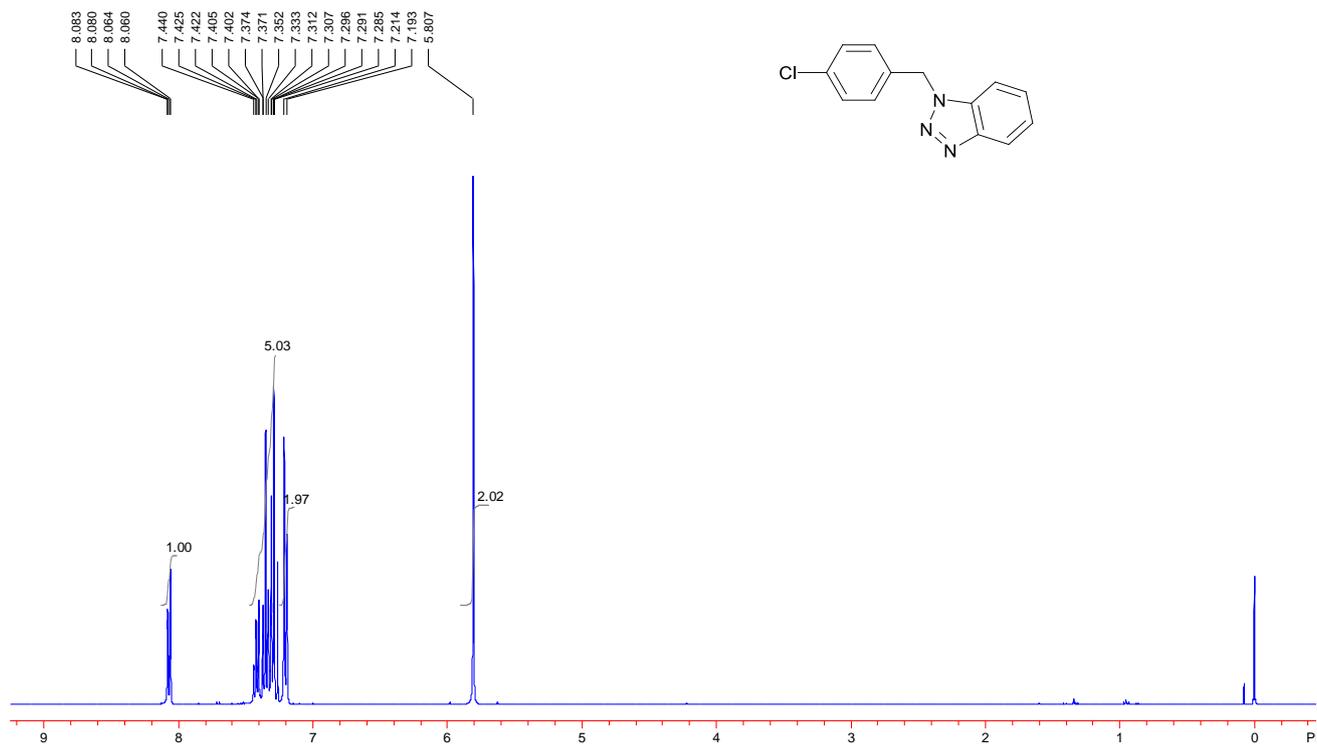
### 1-(4-methylbenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3f**



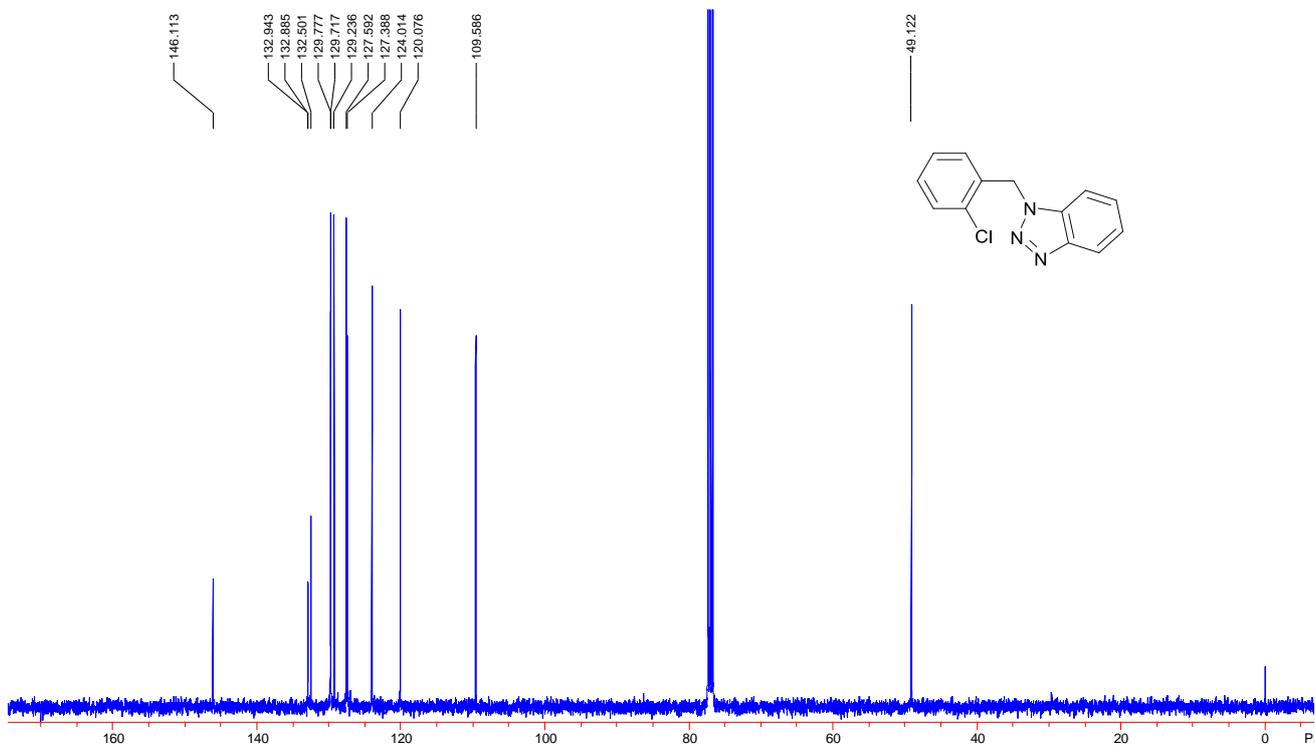
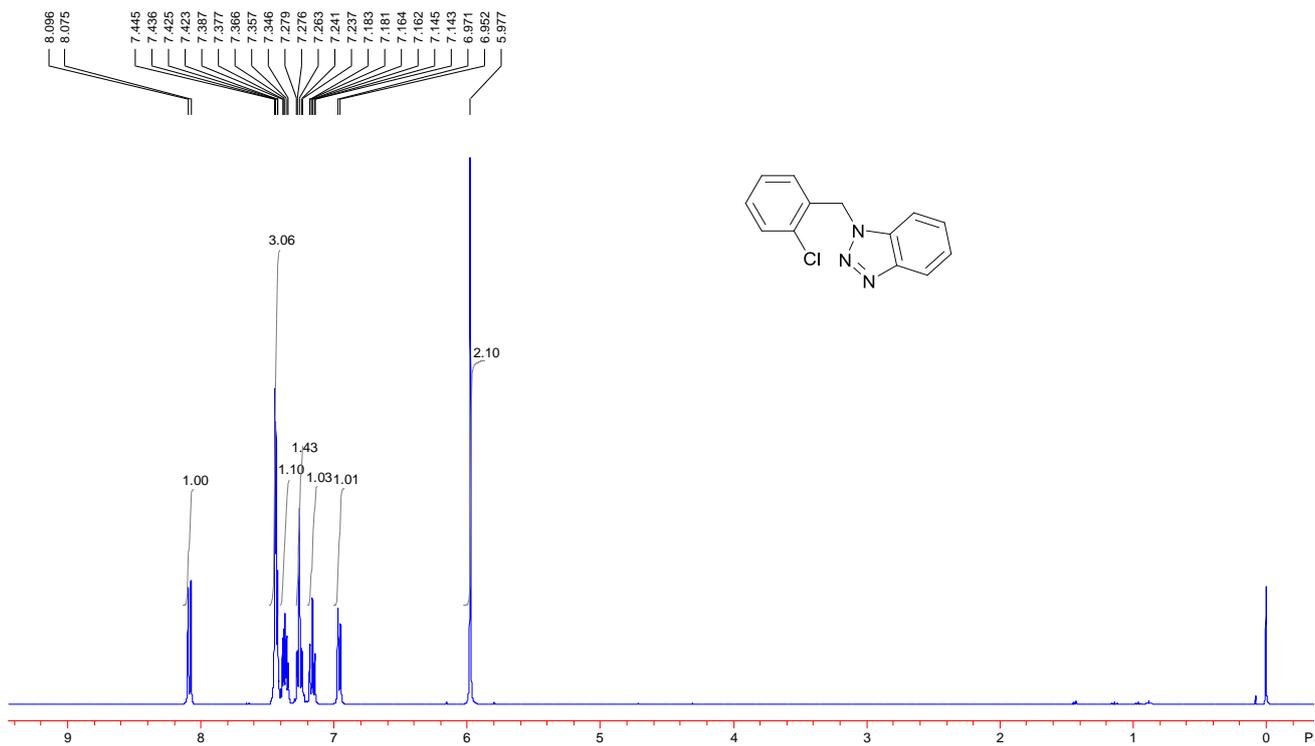
### 1-(4-iodobenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3g**



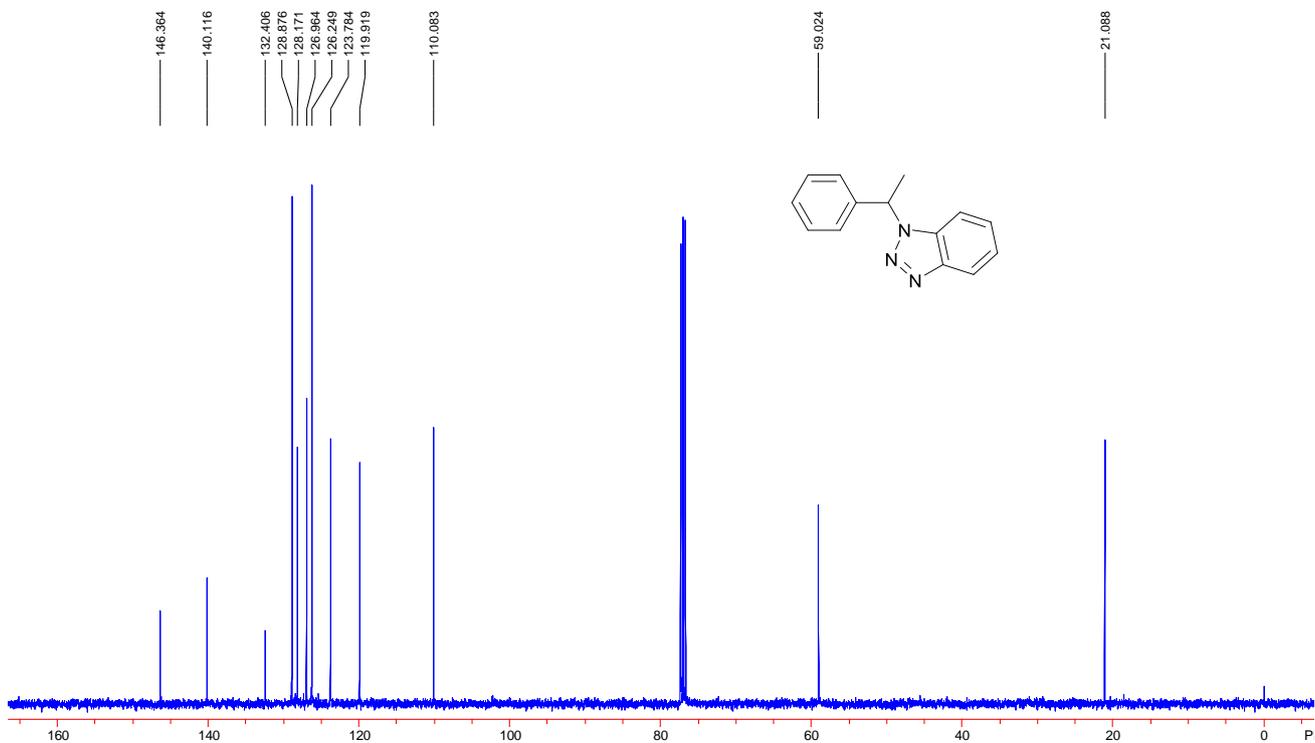
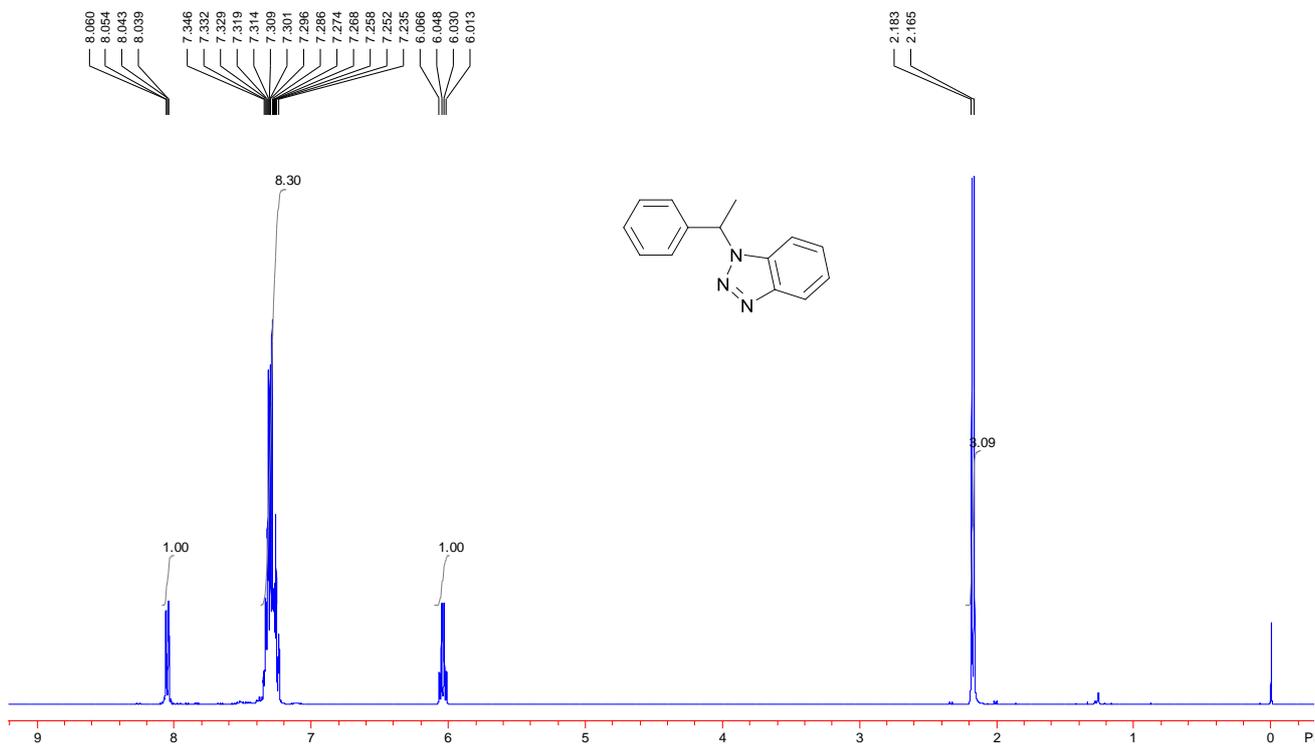
1-(4-chlorobenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3h**



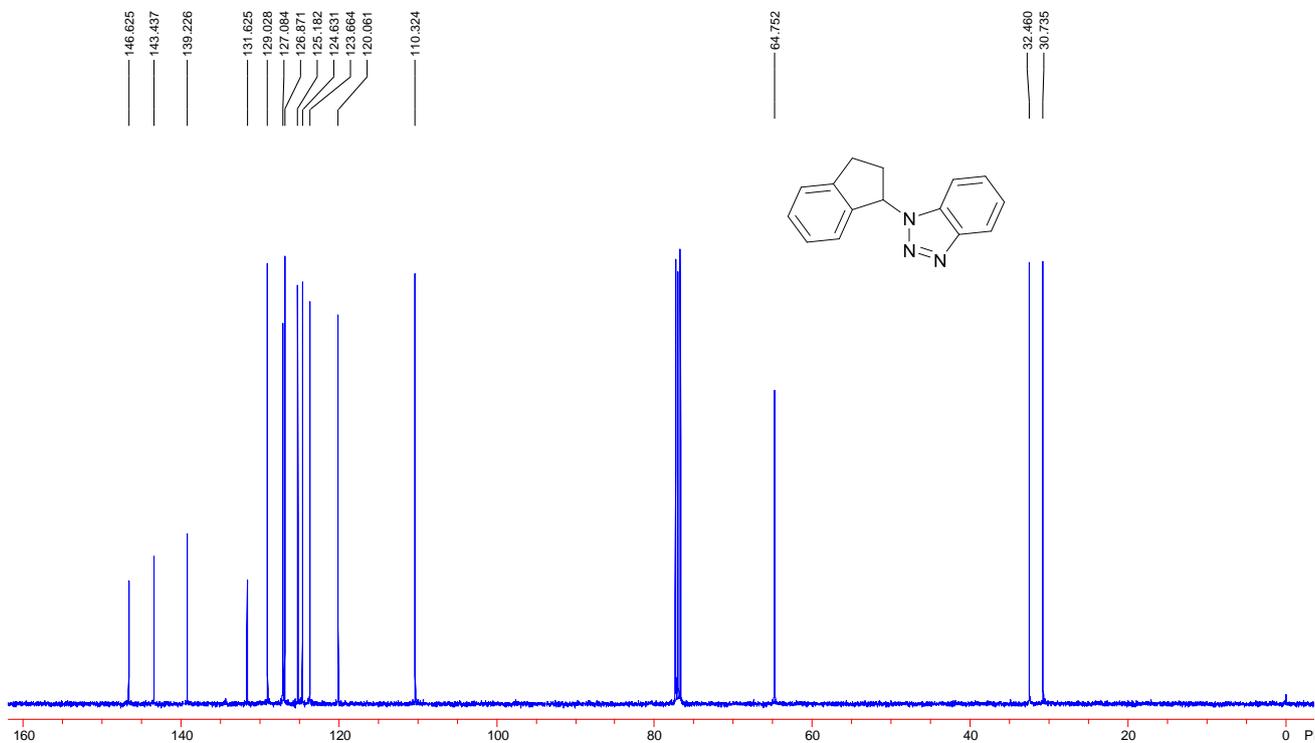
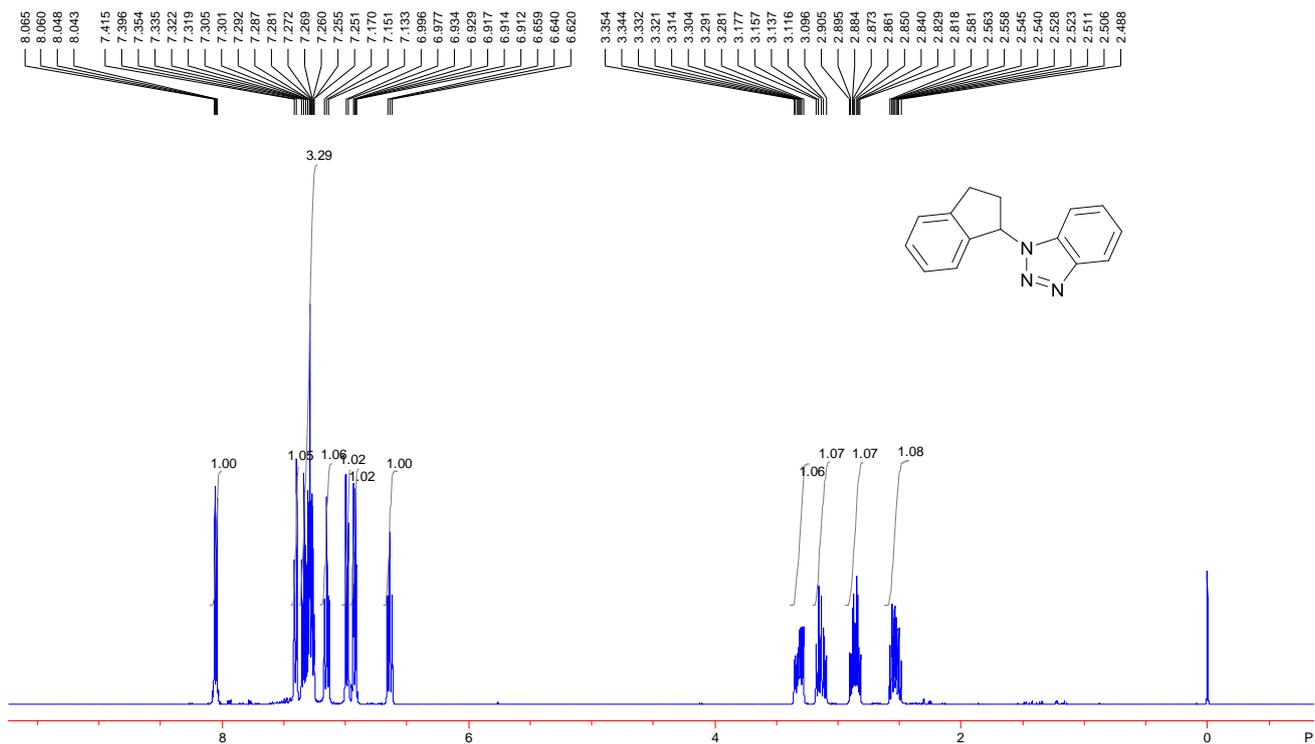
### 1-(2-chlorobenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3i**



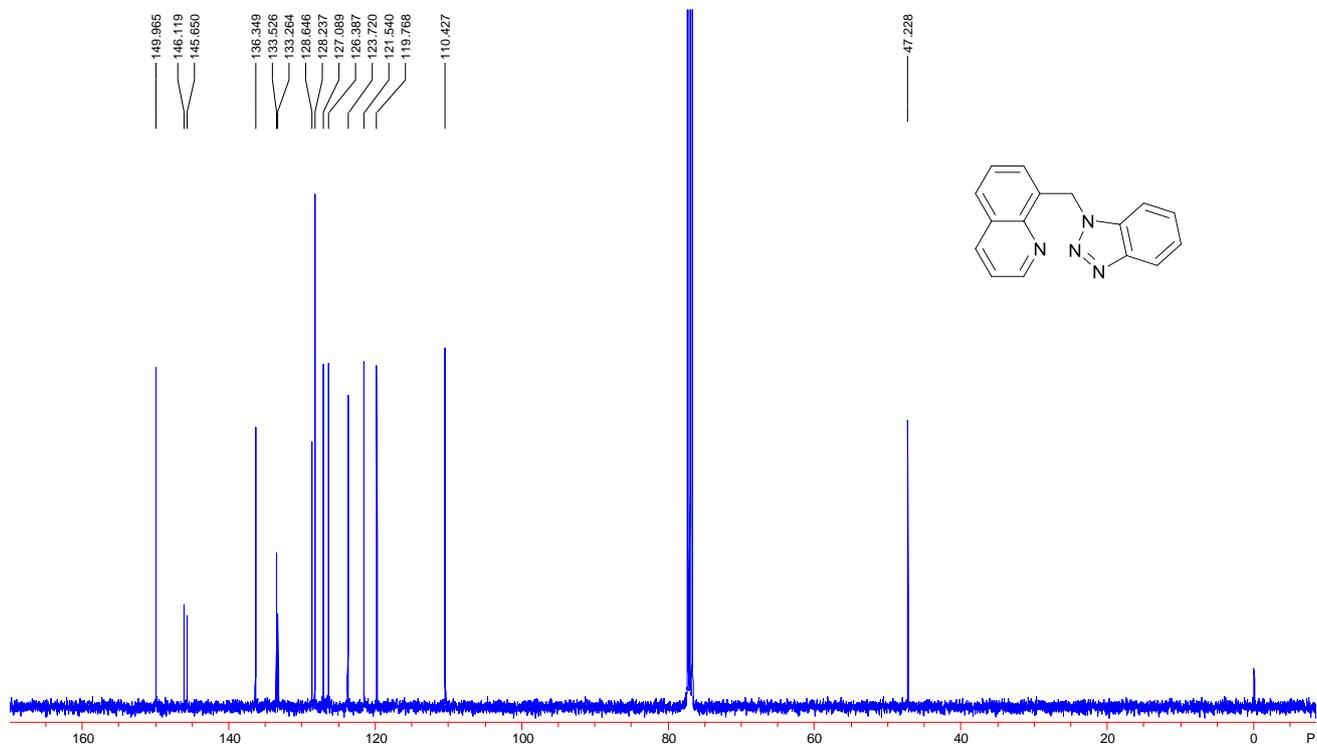
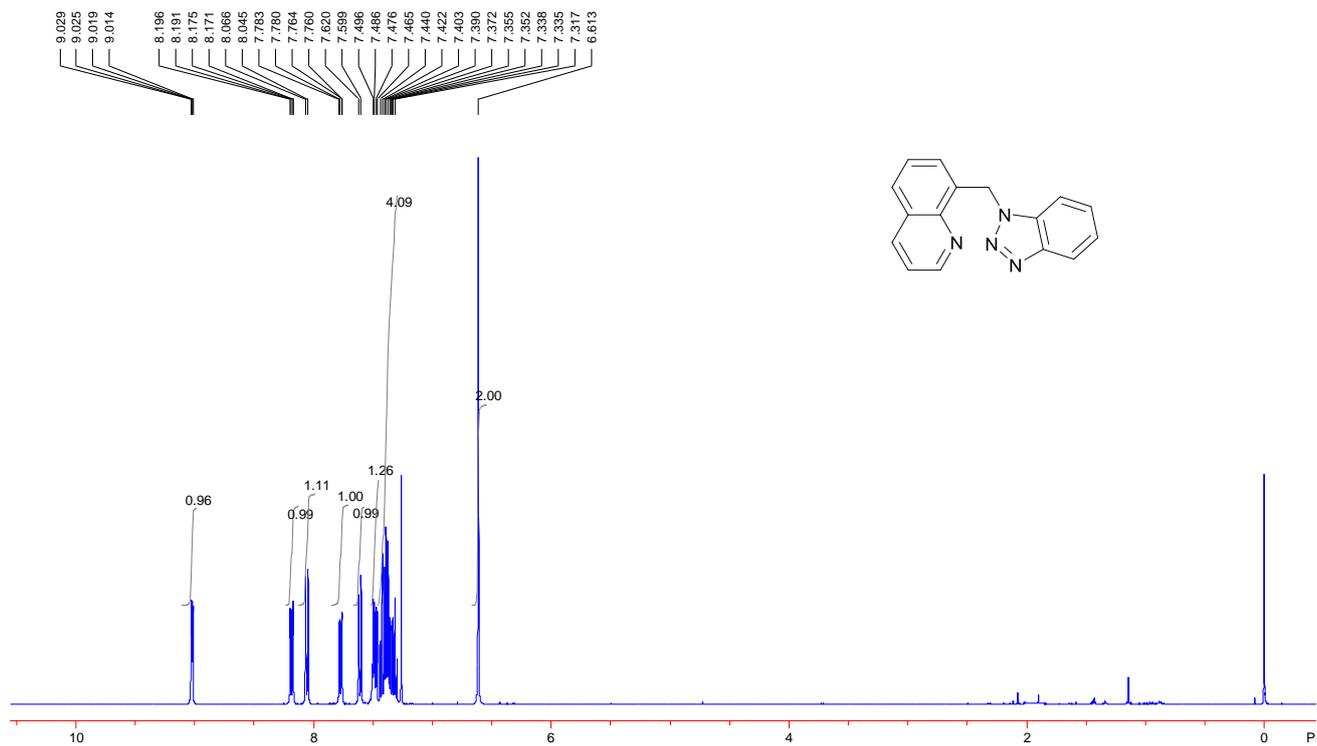
### 1-(1-phenylethyl)-1H-benzo[d][1,2,3]triazole **3j**



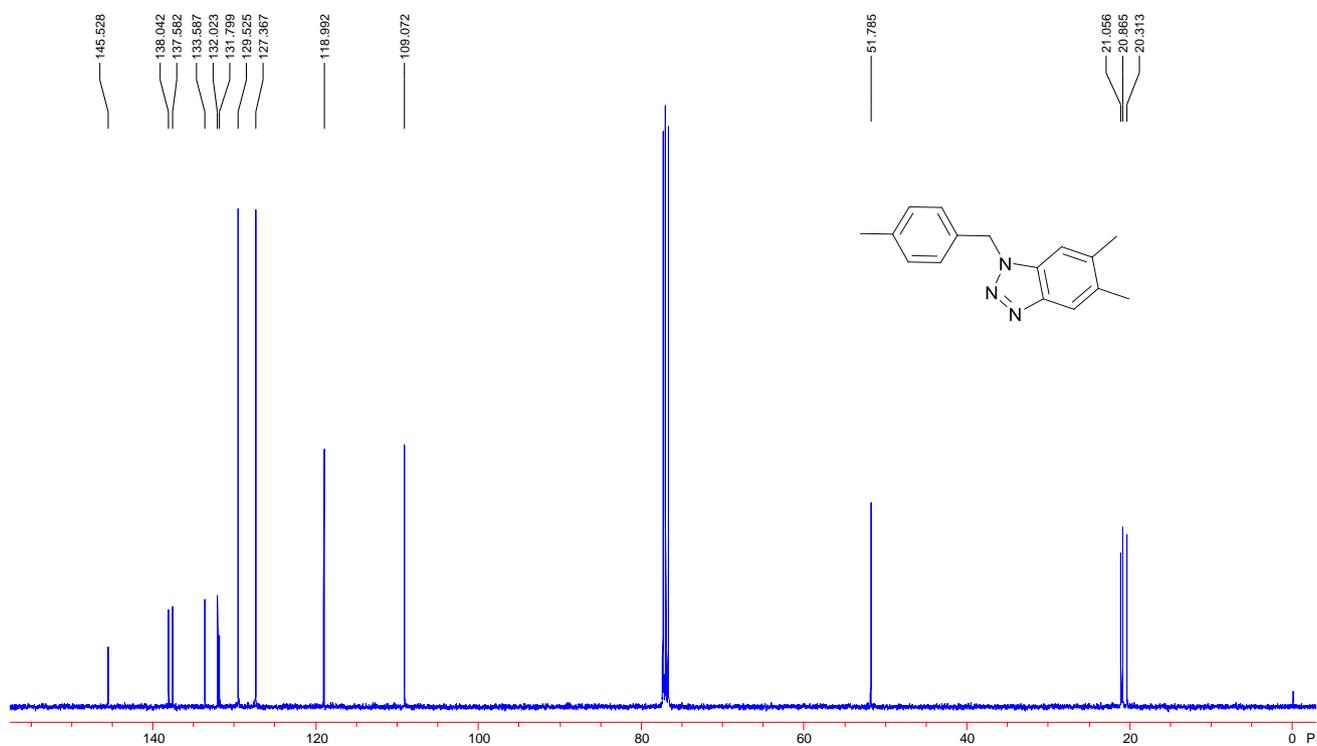
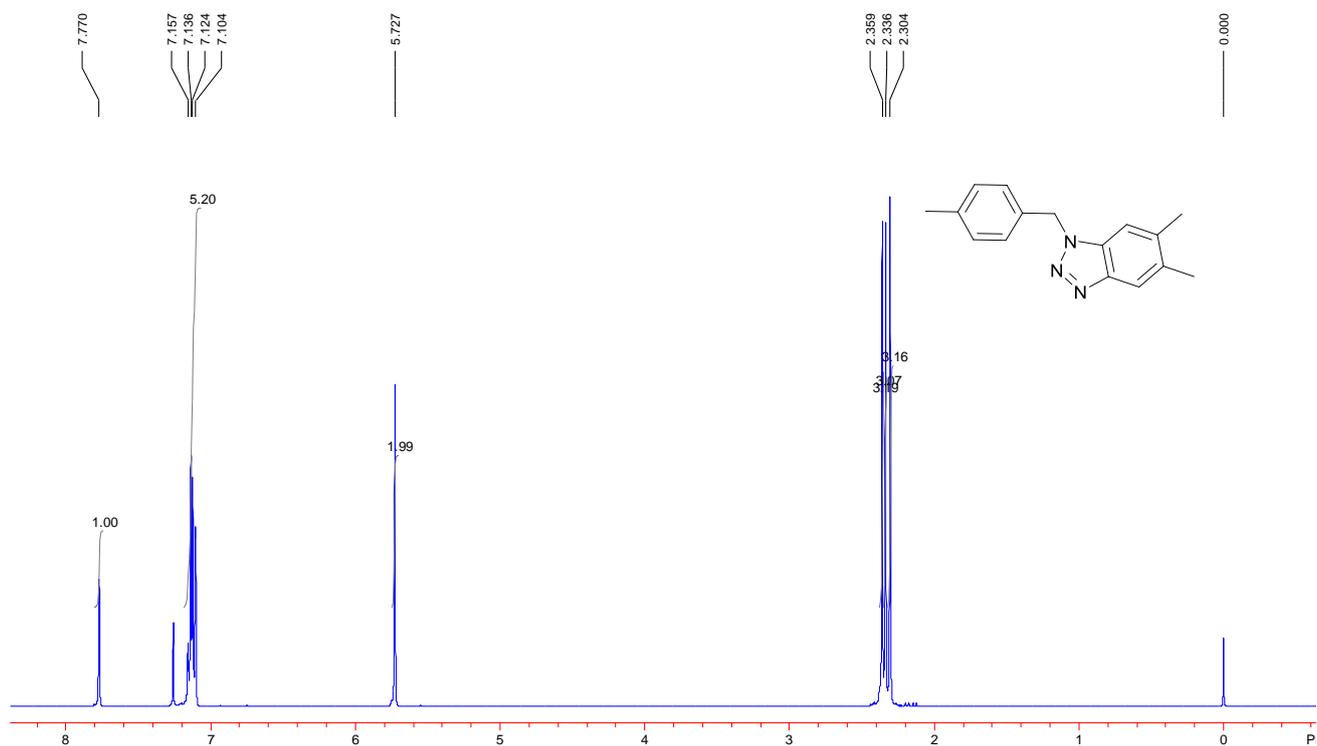
### 1-(2,3-dihydro-1*H*-inden-1-yl)-1*H*-benzo[*d*][1,2,3]triazole **3k**



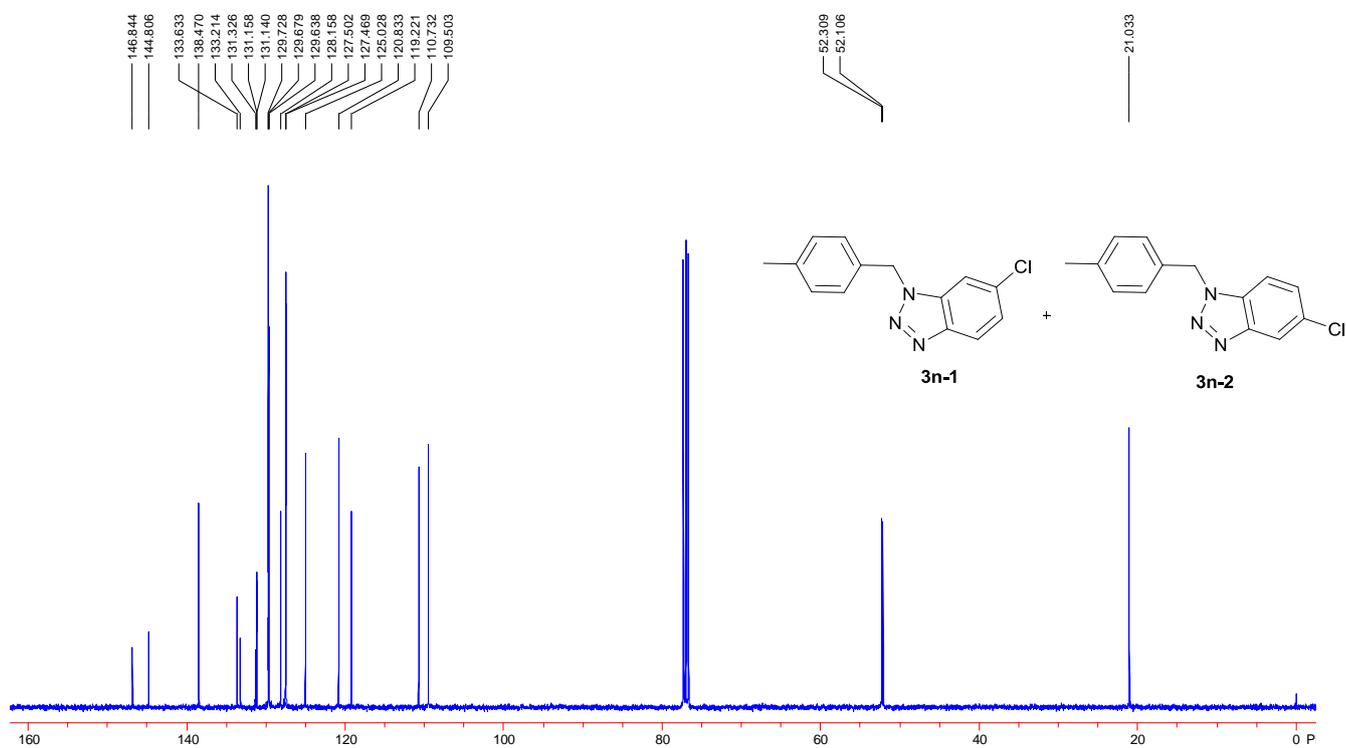
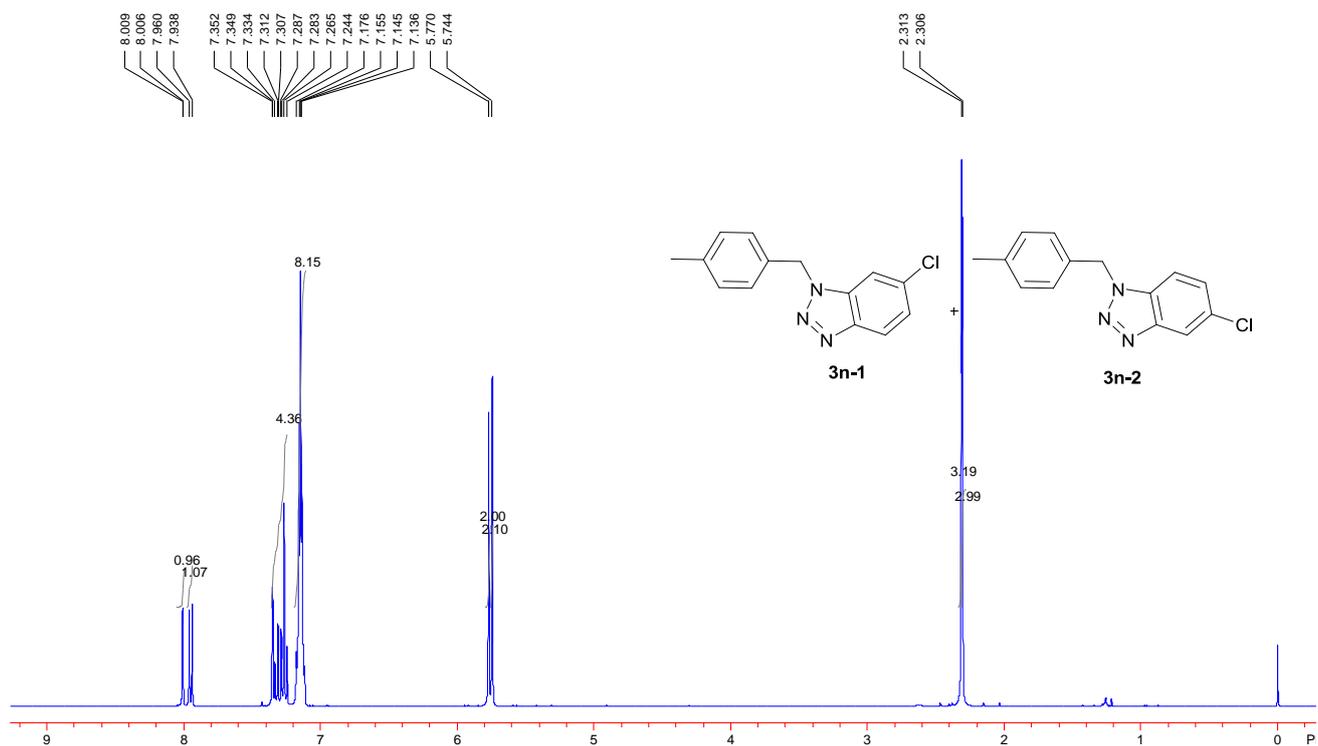
### 8-((1*H*-benzo[*d*][1,2,3]triazol-1-yl)methyl)quinoline **31**



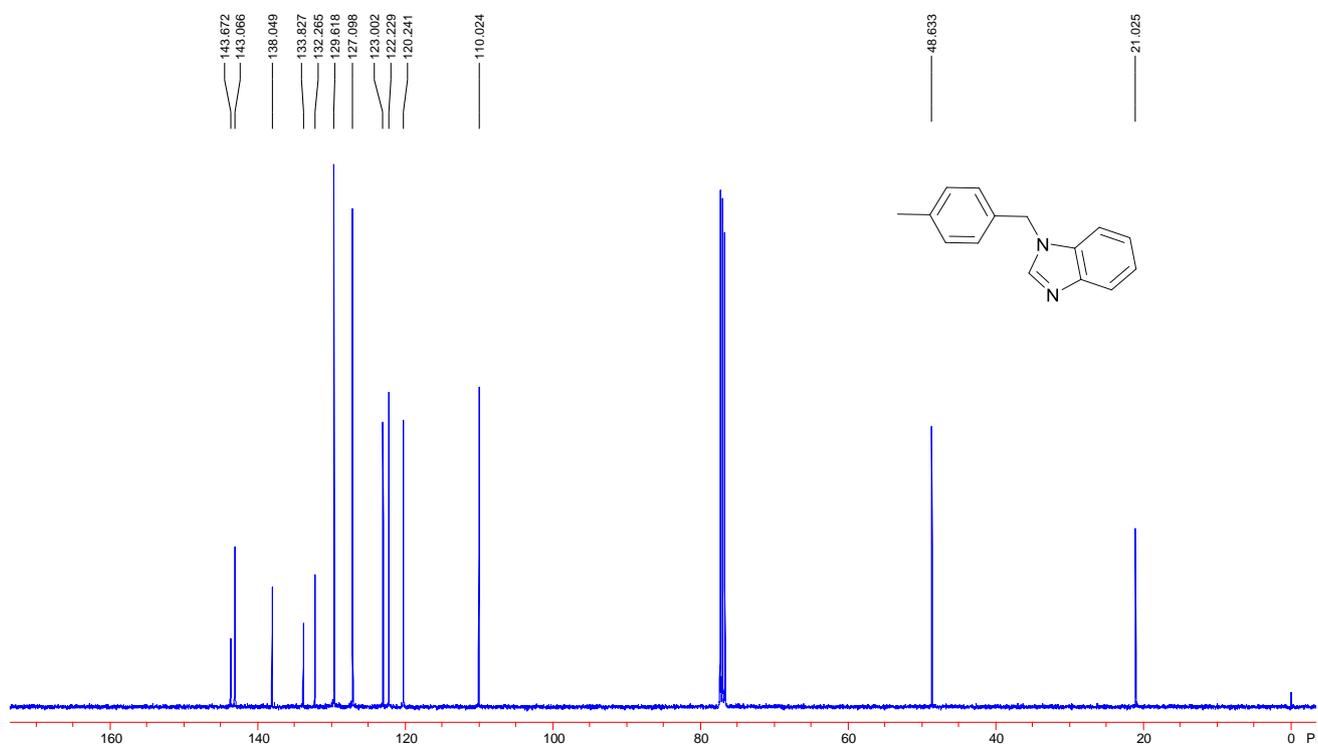
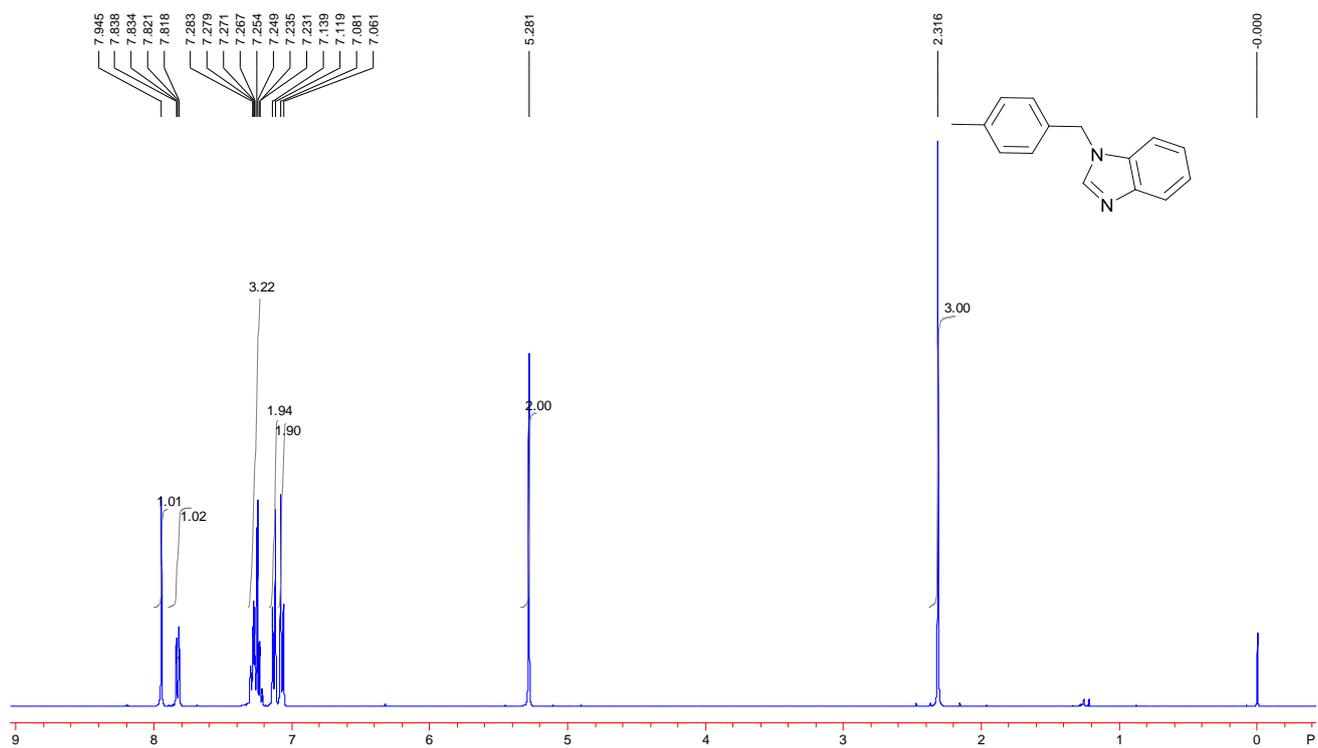
5,6-dimethyl-1-(4-methylbenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3m**



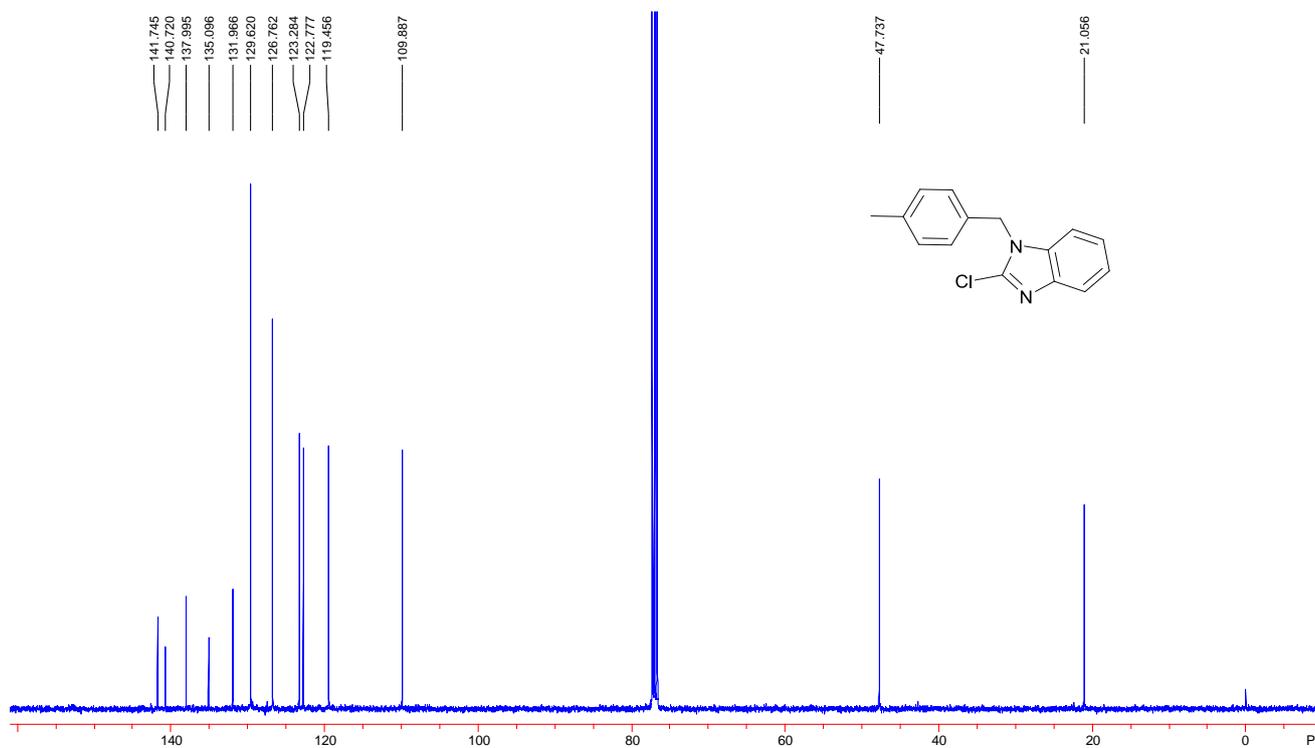
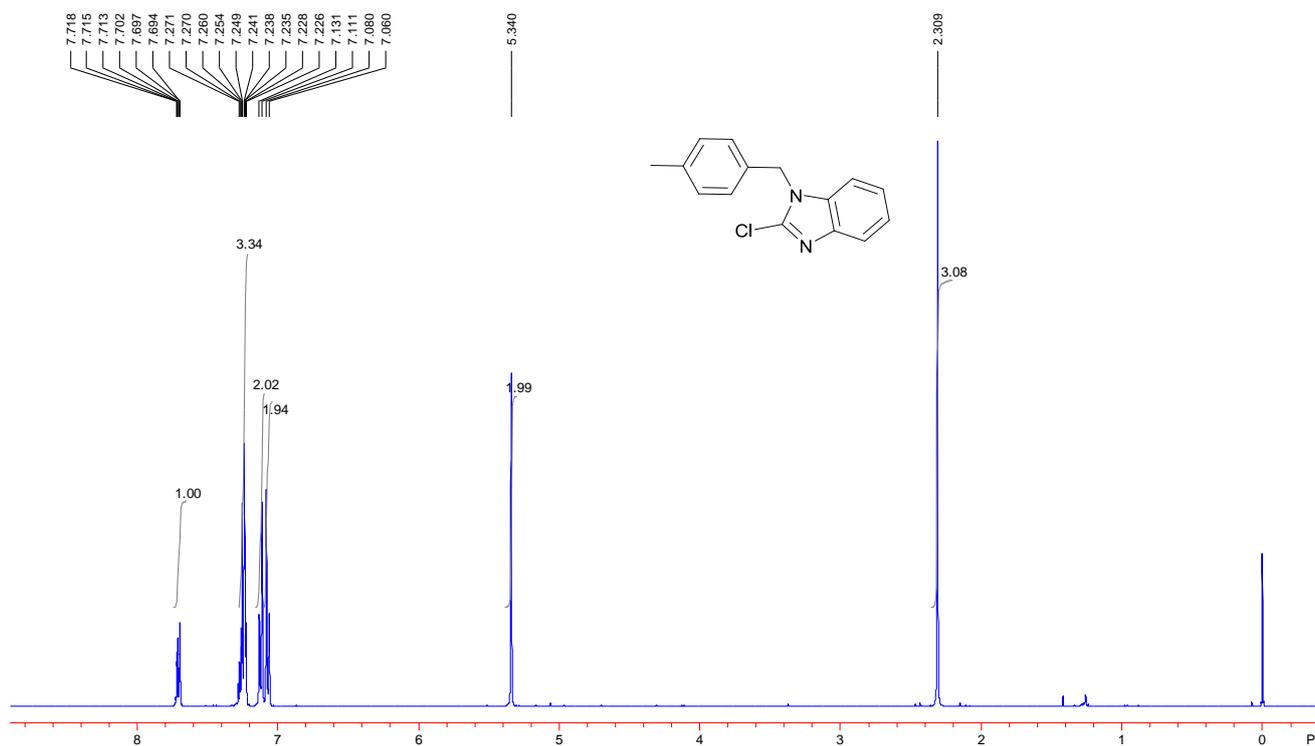
### Chloro-1-(4-methylbenzyl)-1H-benzo[d][1,2,3]triazole **3n**



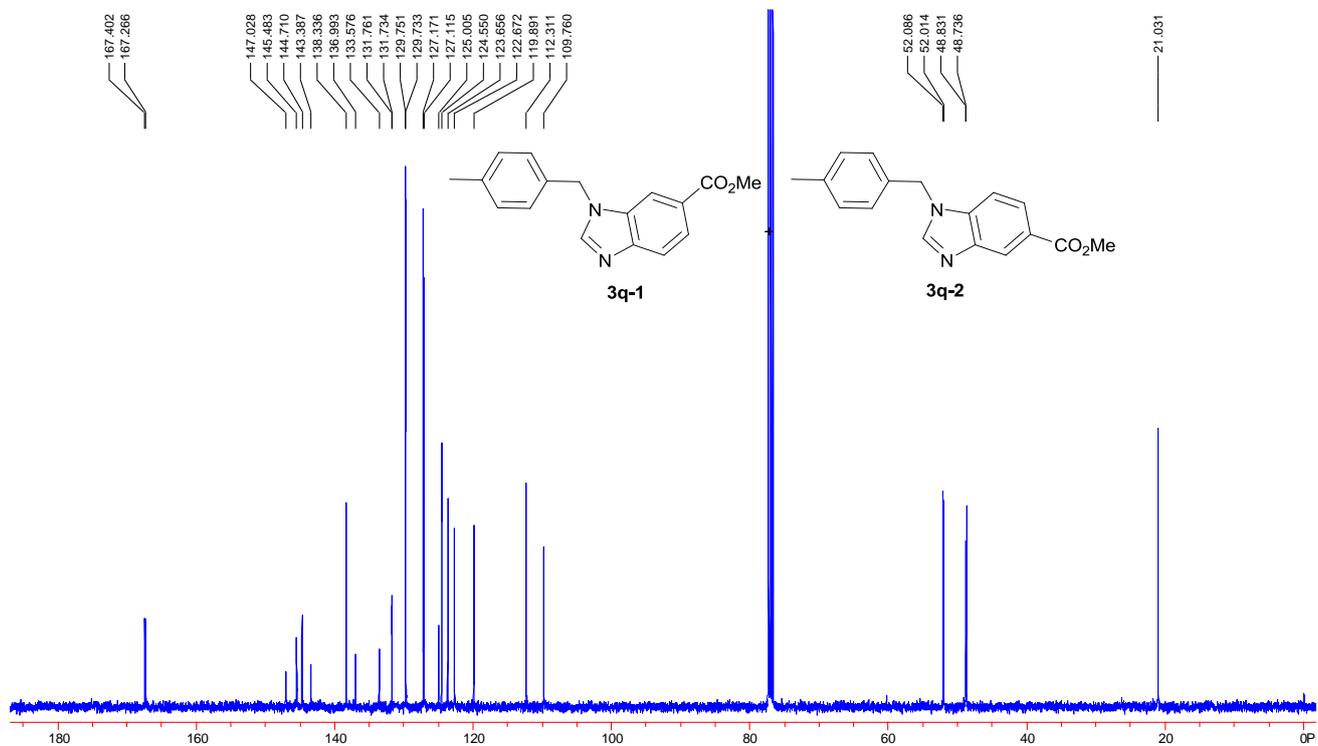
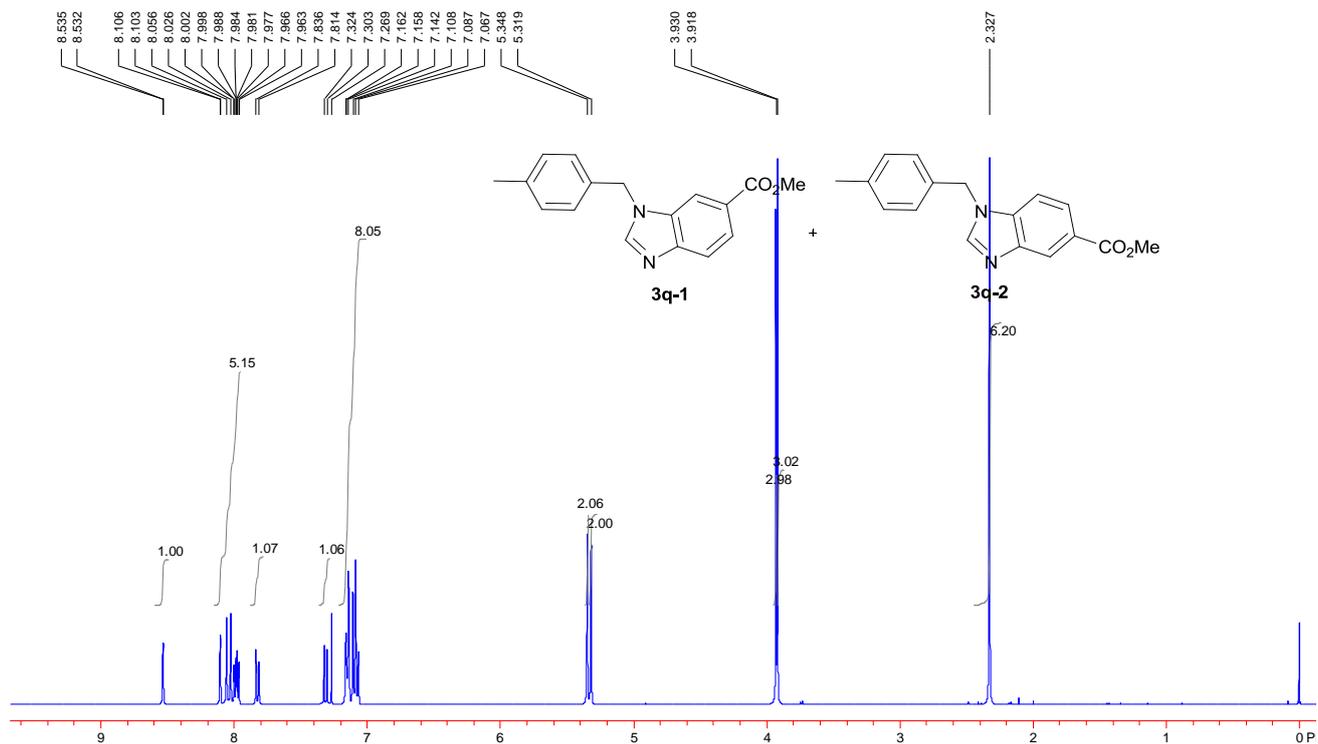
### 1-(4-methylbenzyl)-1*H*-benzo[*d*]imidazole **3o**



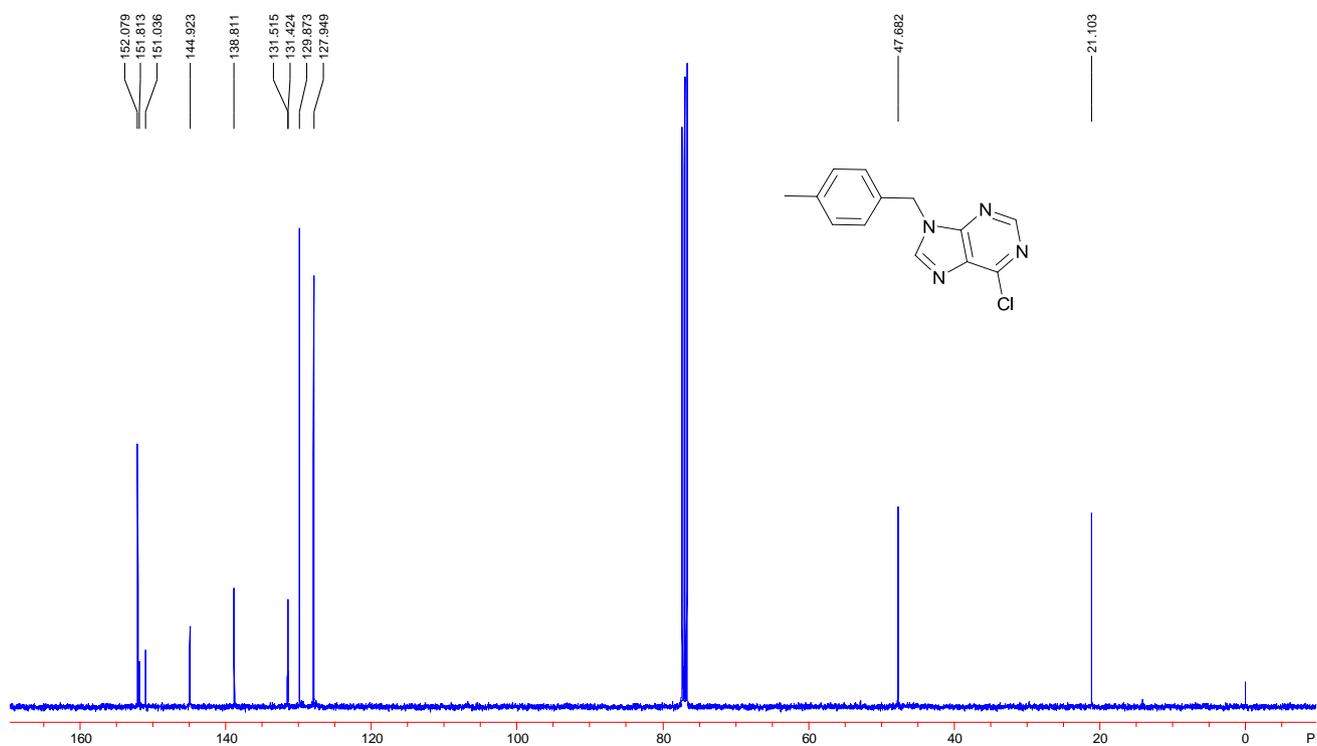
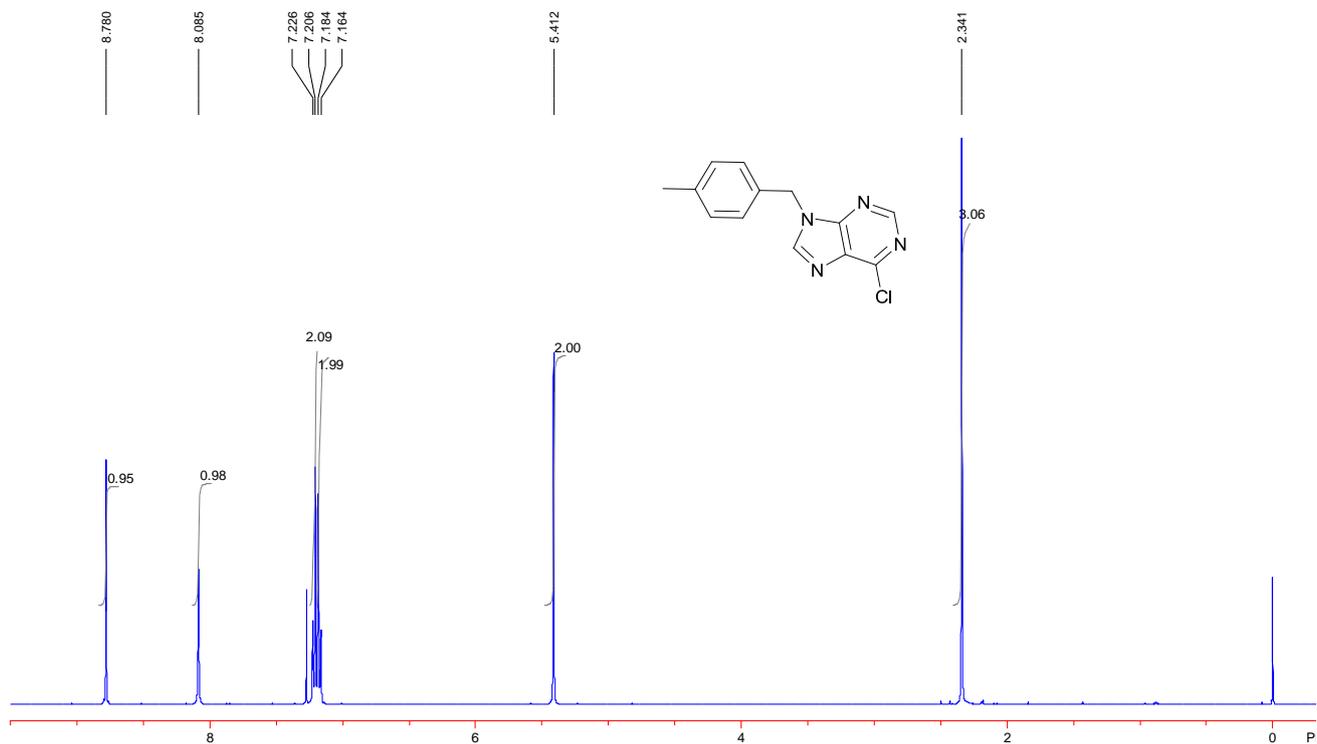
2-chloro-1-(4-methylbenzyl)-1H-benzo[d]imidazole **3p**



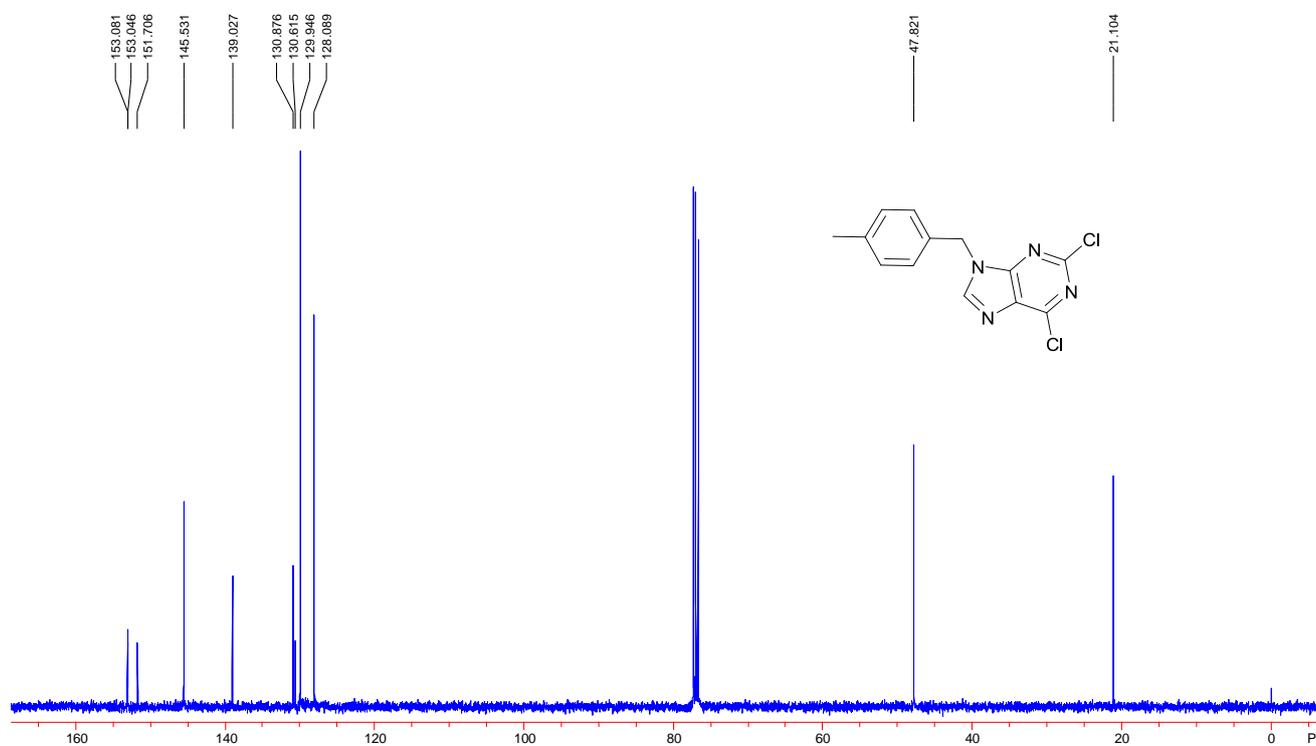
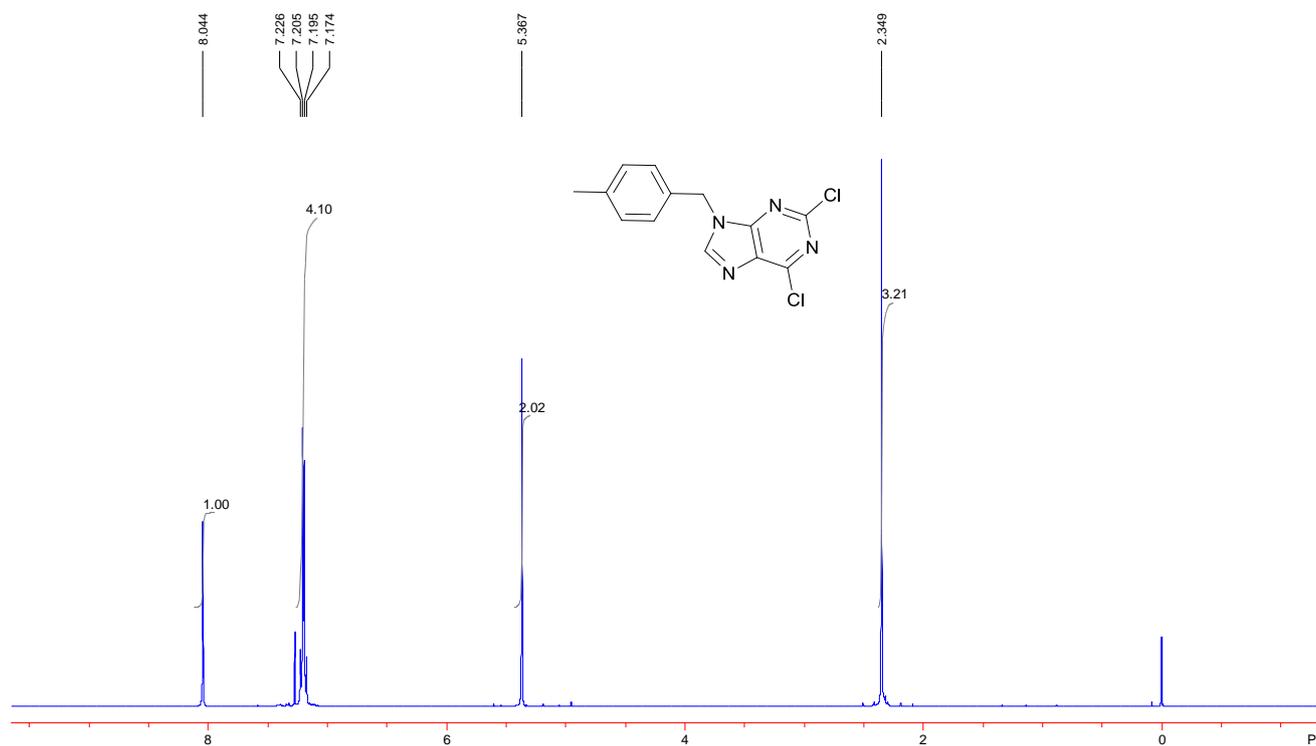
### Methyl 1-(4-methylbenzyl)-1*H*-benzo[*d*]imidazole-carboxylate **3q**



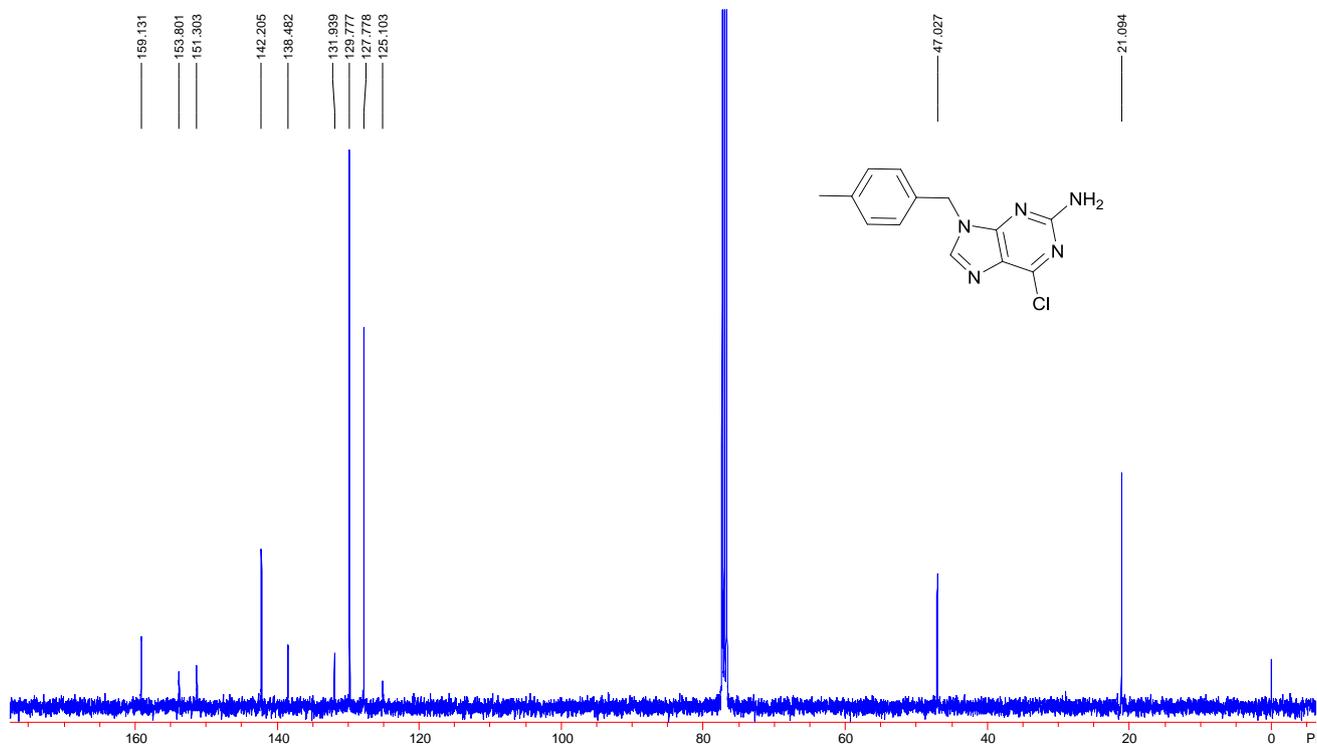
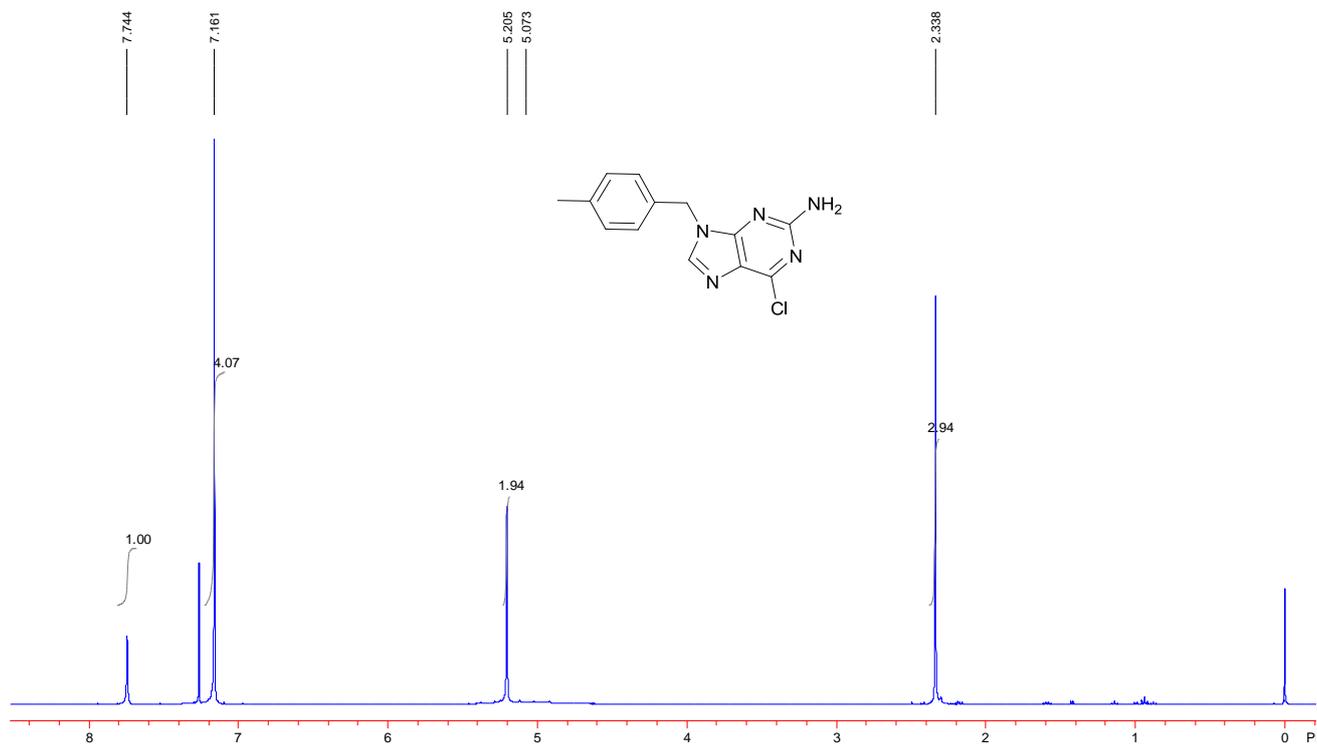
### 6-chloro-9-(4-methylbenzyl)-9H-purine **3r**



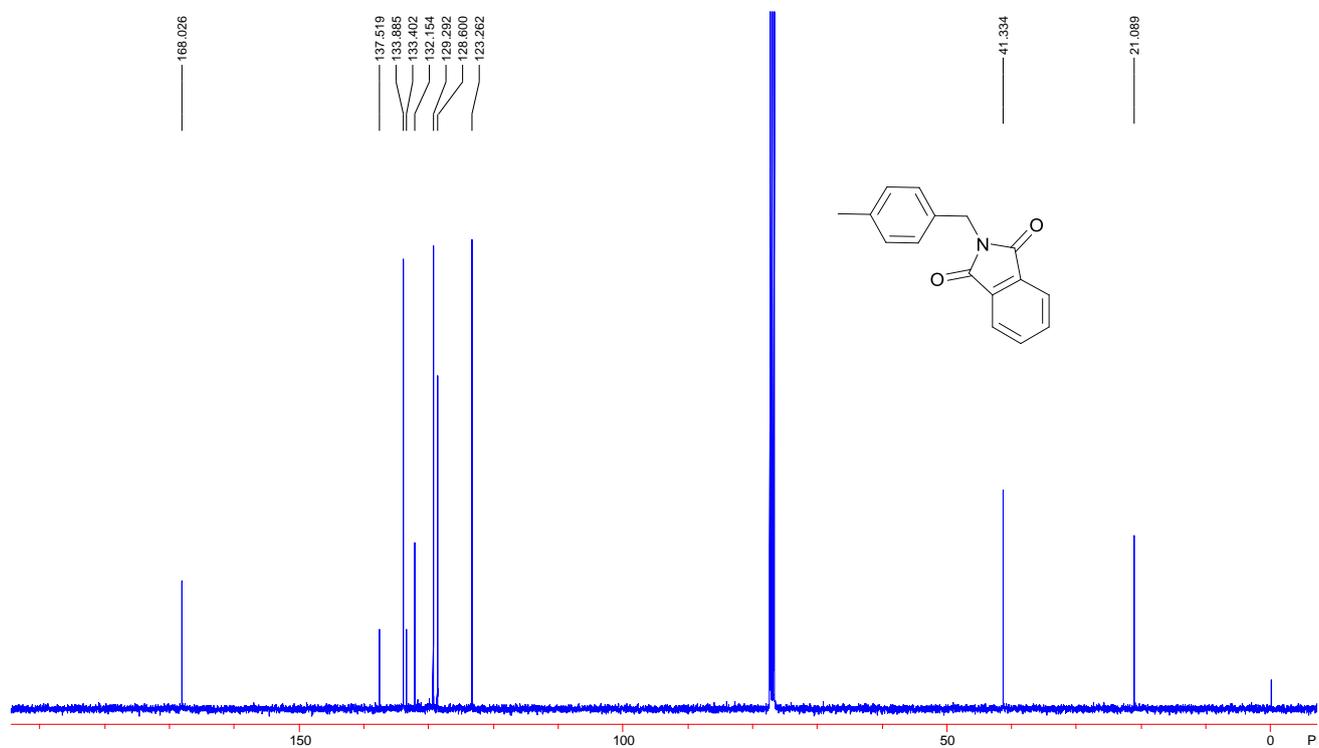
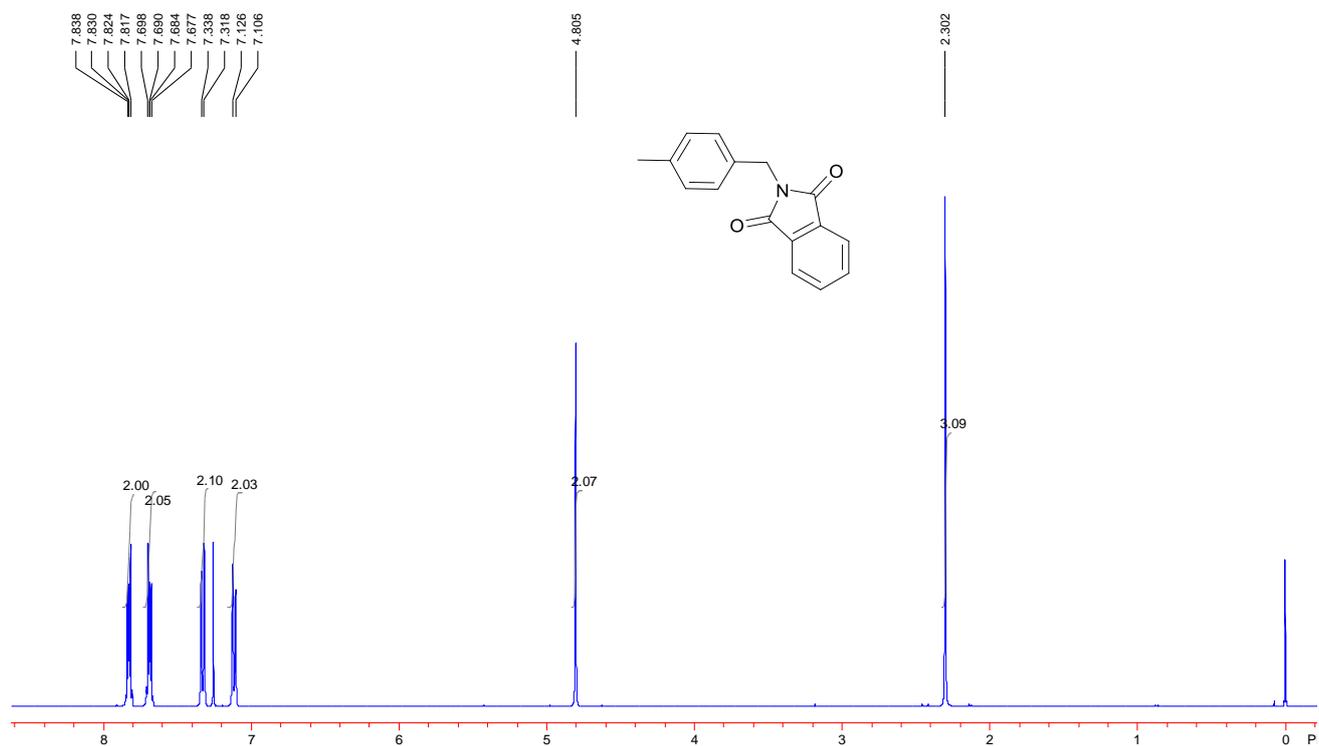
### 2,6-dichloro-9-(4-methylbenzyl)-9H-purine **3s**



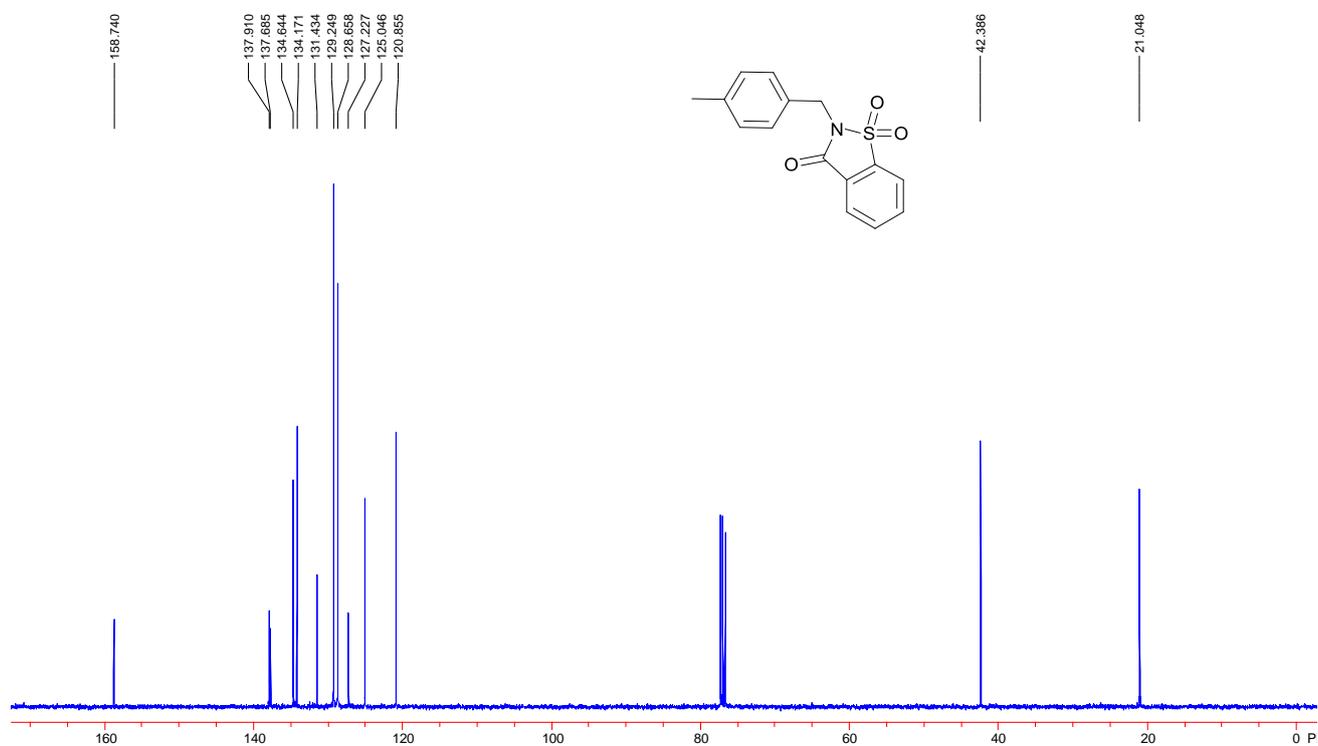
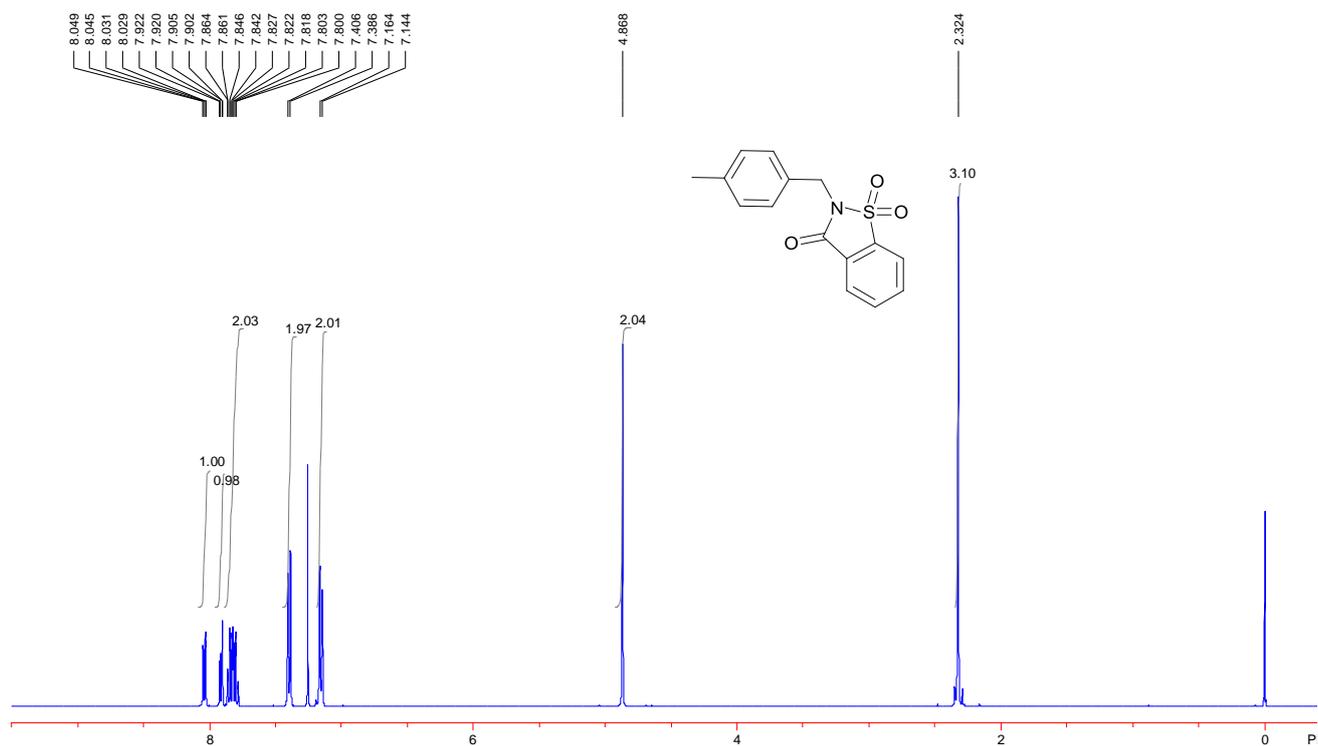
6-chloro-9-(4-methylbenzyl)-9H-purin-2-amine **3t**



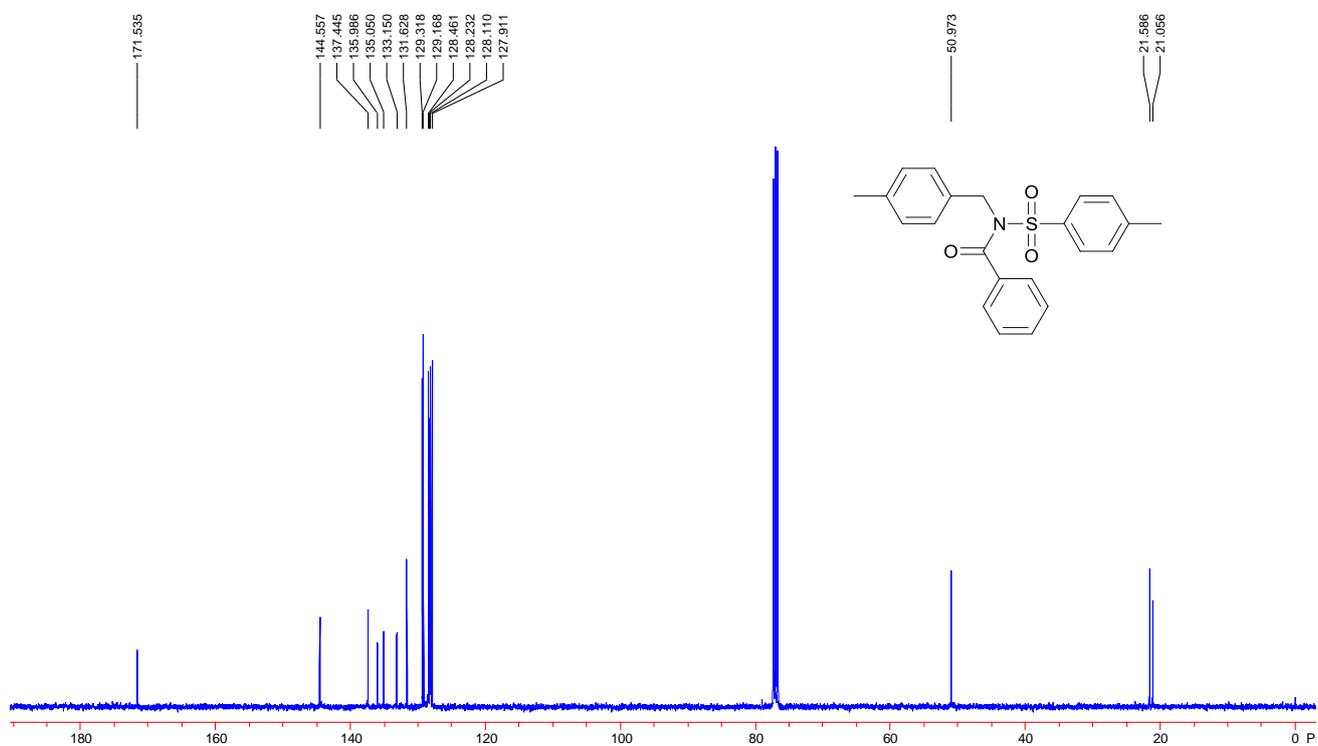
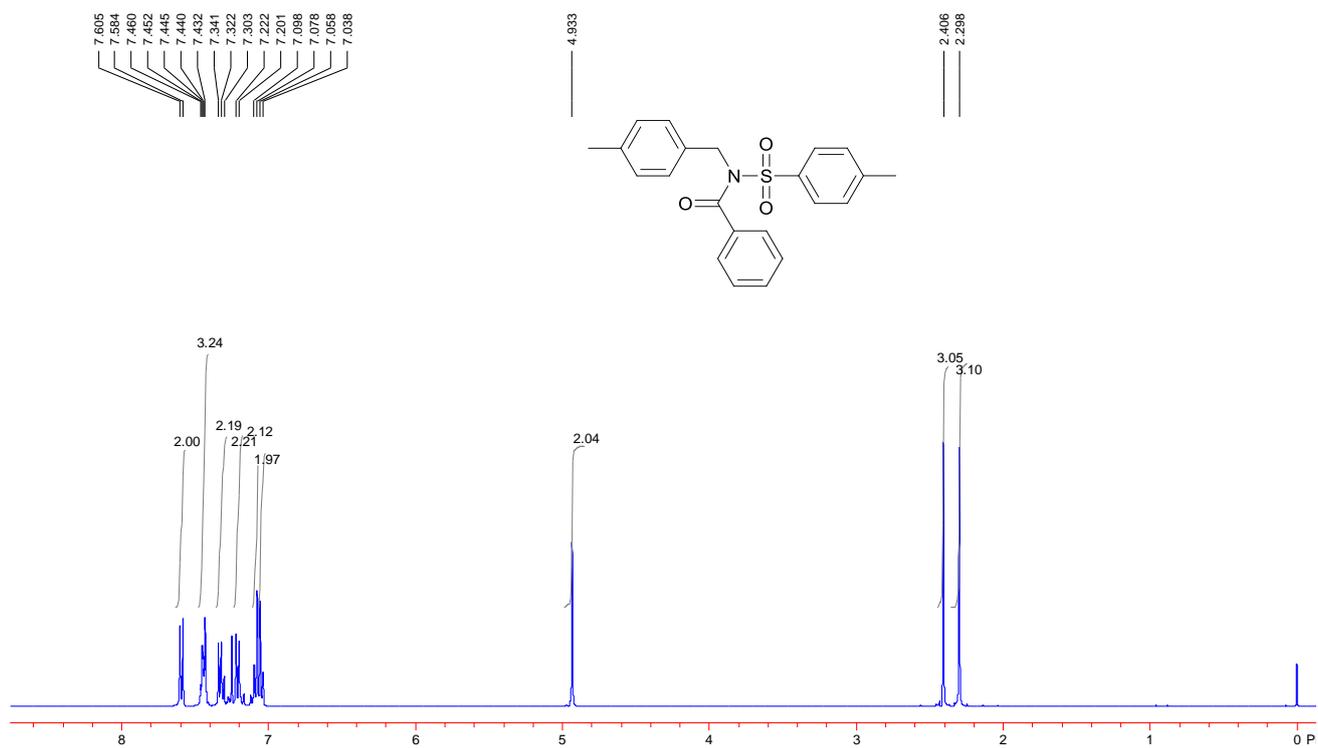
### 2-(4-methylbenzyl)isoindoline-1,3-dione **3u**



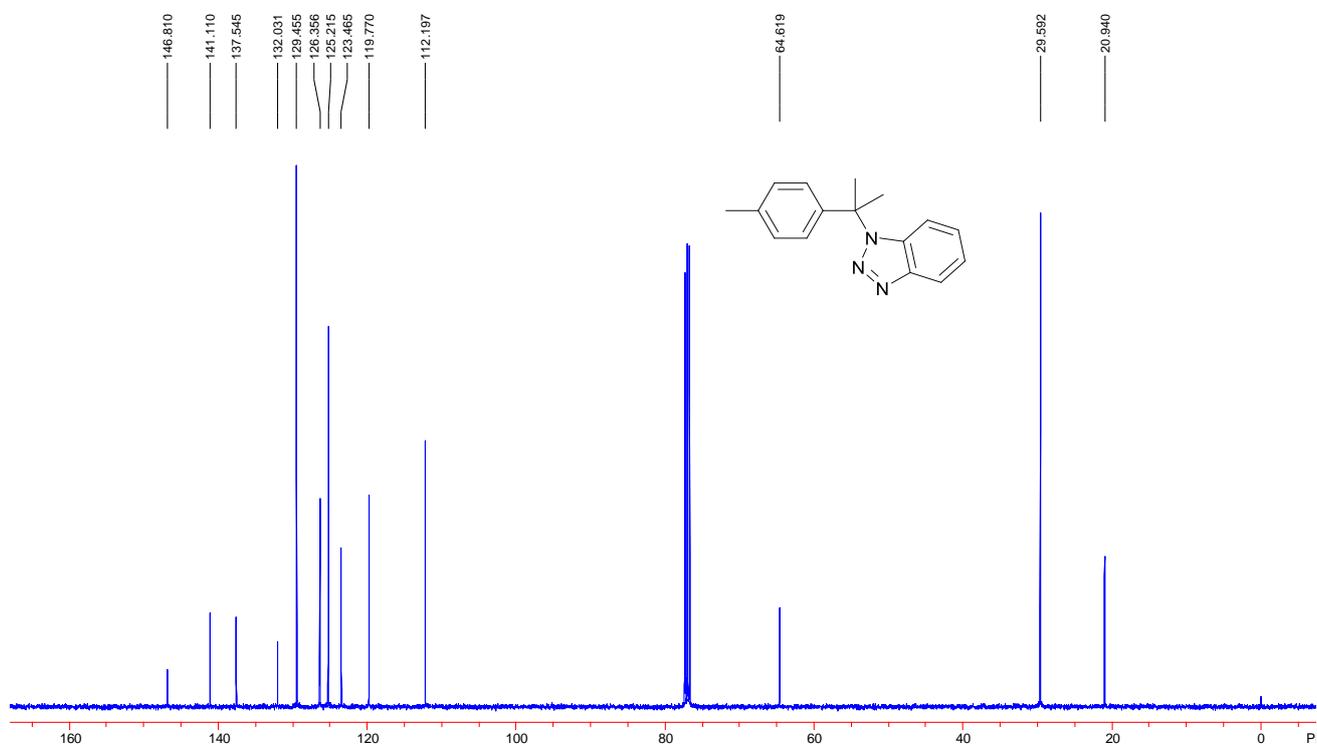
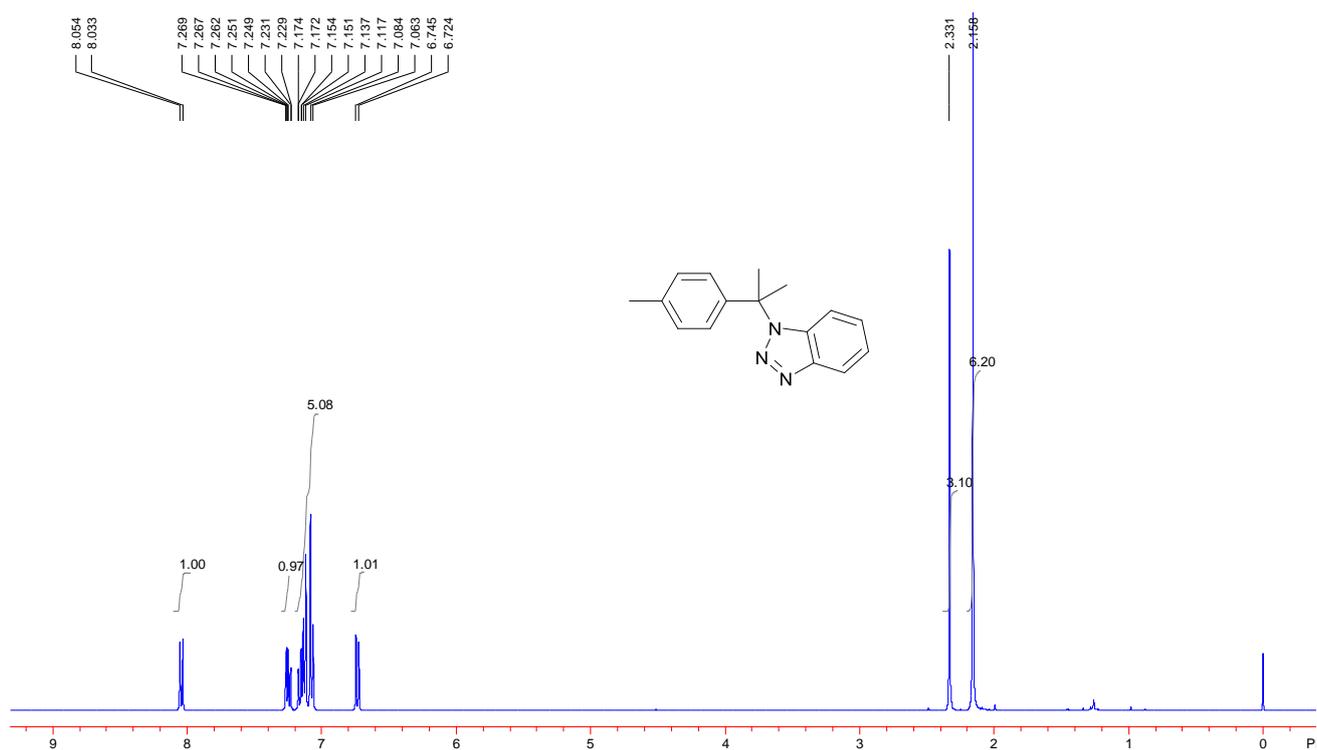
### *N*-(4-methylbenzyl)saccharine **3v**



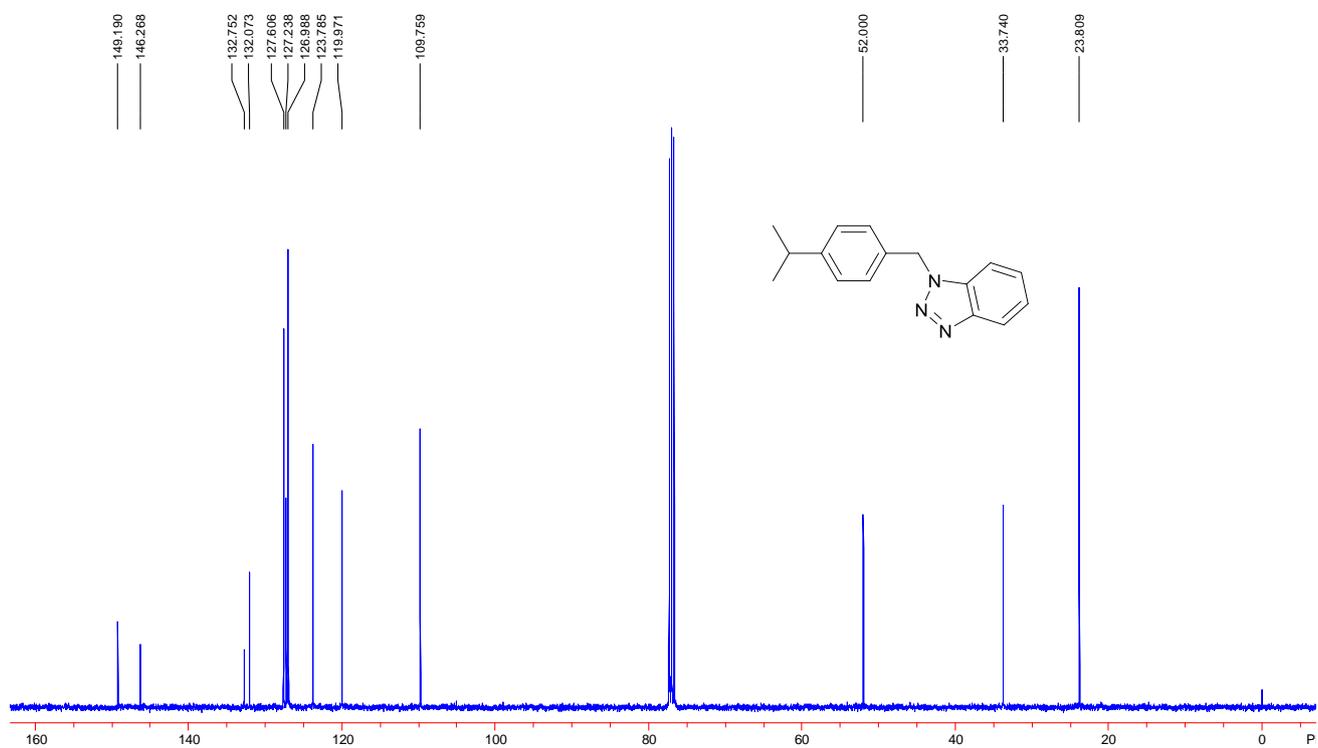
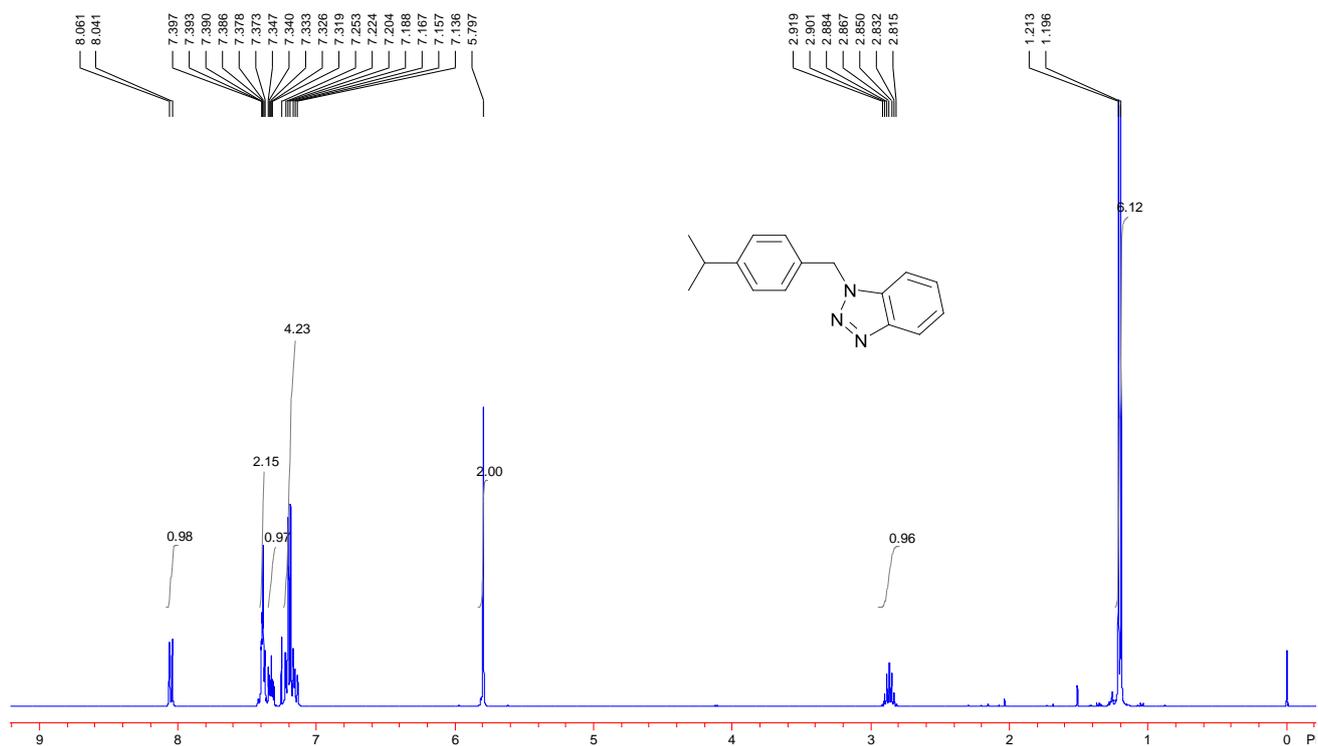
*N*-(4-methylbenzyl)-*N*-tosylbenzamide **3w**



### 1-(2-*p*-tolylpropan-2-yl)-1*H*-benzo[*d*][1,2,3]triazole **3x-1**



### 1-(4-isopropylbenzyl)-1*H*-benzo[*d*][1,2,3]triazole **3x-2**



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