

## Polystyrene resin supported palladium(0) (Pd@PR) nanocomposite mediated regioselective synthesis of 4-aryl-1-alkyl/(2-haloalkyl)-1*H*-1,2,3-triazoles and their *N*-vinyl triazole derivatives from terminal alkynes

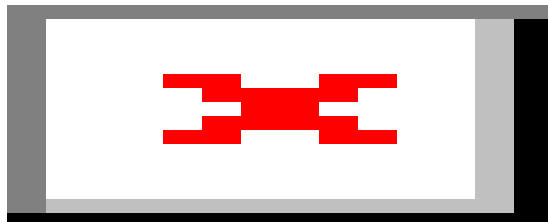
Arun K. Shil<sup>a,b</sup>, Sandeep Kumar<sup>a,b</sup>, Saurabh Sharma<sup>a,b</sup>, Abha Chaudhary<sup>a</sup>, and Pralay Das<sup>\*a,b</sup>

<sup>a</sup>Natural Product Chemistry and Process Development Division, CSIR-Institute of Himalayan Bioresource Technology, Palampur-176061, (H. P.), India, Fax:+91-1894-230433, E-mail: pdas@ihbt.res.in, pdas\_nbu@yahoo.com

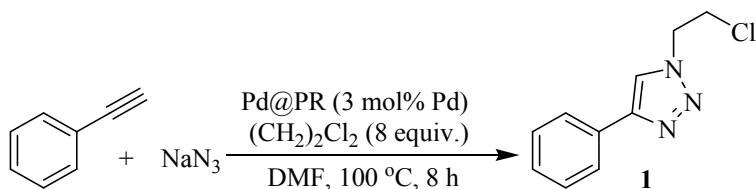
<sup>b</sup>Academy of Scientific & Innovative Research, New Delhi, India

Contents	Page
Preparation of polystyrene resin supported palladium(0) (Pd@PR) nanocomposite.....	S2
Recyclability experiment.....	S2
Typical experimental procedure for the synthesis of 4-aryl-1-alkyl/benzyl-1 <i>H</i> -1,2,3-triazole derivatives ( <b>1-20</b> ) and their characterization data.....	S3
Typical experimental procedure for the synthesis of 4-aryl-1-vinyl-1 <i>H</i> -1,2,3-triazoles ( <b>21-29</b> ) and their characterization data.....	S12
Typical experimental procedure for the synthesis of 4-aryl-1-(2-aryllalkenyl)-1 <i>H</i> -1,2,3-triazoles ( <b>30-37</b> ) and their characterization data.....	S17
2D NMR spectral analysis of product 1-(2-chloroethyl)-4- <i>p</i> -tolyl-1 <i>H</i> -1,2,3-triazole <b>2</b> .....	S21
Copies of <sup>1</sup> H NMR, <sup>13</sup> C NMR and ESI-MS spectra of the synthesized compounds ( <b>1-38</b> ) .....	S23

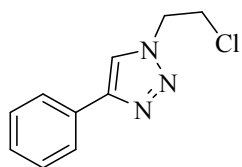
**Preparation of polystyrene resin supported palladium(0) (Pd@PR) nanocomposite:**



**Recyclability experiment:** After each cycle the Pd@PR catalyst was recovered by simple filtration followed by washing with water and acetone until the residual organic or inorganic materials were washed away. The properly washed catalyst was dried in hot air oven and used in next cycle. (1<sup>st</sup> run 68%, 2<sup>nd</sup> run 64%, 3<sup>rd</sup> run 65%, 4<sup>th</sup> run 61% and 5<sup>th</sup> run 58%)

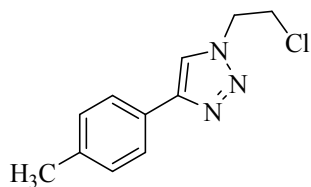


Typical experimental procedure for the synthesis of 4-aryl-1-alkyl/benzyl-1*H*-1,2,3-triazole derivatives (**1-20**) and their characterization data:



1-(2-chloroethyl)-4-phenyl-1*H*-1,2,3-triazole **1** (Table 1, entry 10)

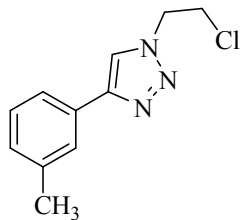
A mixture of phenyl acetylene (100 mg, 0.98 mmol), sodium azide (191.18 mg, 2.94 mmol), 1, 2-dichloroethane (776 mg, 7.84 mmol) and Pd@PR (657 mg, 3 mol% Pd) were taken in an oven dried 40 ml reaction vial with screw cap. Equal volume (as compared to 1, 2-dialoethane) of dry DMF were added into it. The reaction mixture was then stirred under nitrogen in a pre heated oil bath of temperature 100 °C. Progress of the reaction was monitored by TLC. On completion, the cooled reaction mixture was extracted with ethyl acetate (3×5 ml) by addition of 2 ml of water and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. Evaporation of the combined organic layer followed by column chromatography (Hexane:ethylcaetate = 80:20) over silica gel (mesh 60-200) afforded 1-(2-chloroethyl)-4-phenyl-1*H*-1,2,3-triazole **1** as white solid (138.34 mg, 68%), mp 75-77 °C; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 3.92-3.94 (t, *J*=6 Hz, 2H), 4.68-4.70 (t, *J*= 6 Hz, 2H), 7.32-7.34 (m, 1H), 7.40-7.43 (m, 2H), 7.82-7.83 (m, 2H), 7.90 (s, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 42.56, 51.78, 120.81, 125.77 (2C), 128.31, 128.91 (2C), 130.39, 147.76.



1-(2-chloroethyl)-4-*p*-tolyl-1*H*-1,2,3-triazole **2** (Table 2, entry 1)

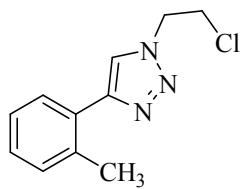
Prepared as described the method for **1**, starting form 1-ethynyl-4-methylbenzene (100 mg, 0.86 mmol), 1, 2-dichloroethane (681.53 mg, 6.88 mmol), sodium azide (167.70 mg, 2.58 mmol) and Pd@PR (577 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylcaetate = 70:30) afforded 1-(2-chloroethyl)-4-*p*-tolyl-1*H*-1,2,3-triazole **2** as white solid (135.50 mg, 71%), mp 103-105 °C; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 2.36 (s, 3H), 3.91-3.93 (t, *J* = 5.4 Hz, 2H), 4.67-4.69 (t, *J* = 6 Hz, 2H), 7.21-7.23 (d, *J* = 7.8 Hz, 2H), 7.70-7.72 (d, *J* = 8.4 Hz,

2H), 7.85 (s, 1H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  21.18, 42.42, 51.61, 120.31, 125.56 (2C), 127.45, 129.45 (2C), 138.04, 147.71. ESIMS data:  $m/z$  calc. for  $[\text{M}+\text{H}]^+$   $\text{C}_{11}\text{H}_{13}\text{ClN}_3$  222.0798, obsd. 222.0731.



1-(2-chloroethyl)-4-*m*-tolyl-1*H*-1,2,3-triazole **3** (Table 2, entry 2)

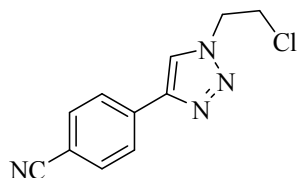
Prepared as described the method for **1**, starting from 1-ethynyl-3-methylbenzene (100 mg, 0.86 mmol), 1, 2-dichloroethane (681.53 mg, 6.88 mmol), sodium azide (167.70 mg, 2.58 mmol) and Pd@PR (577 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 80:20) afforded 1-(2-chloroethyl)-4-*m*-tolyl-1*H*-1,2,3-triazole **3** as colourless semi solid (120.23 mg, 63%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  2.40 (s, 3H), 3.95-3.97 (t,  $J = 6$  Hz, 2H), 4.72-4.73 (t,  $J = 5.4$  Hz, 2H), 7.15-7.16 (d,  $J = 7.2$  Hz, 1H), 7.30-7.33 (t,  $J = 7.8$  Hz, 1H), 7.60-7.62 (d,  $J = 7.8$  Hz, 1H), 7.69 (s, 1H), 7.88 (s, 1H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  21.40, 42.50, 51.77, 120.63, 122.86, 126.44, 128.74, 129.05, 130.19, 138.56, 147.90. ESIMS data:  $m/z$  calc. for  $[\text{M}+\text{H}]^+$   $\text{C}_{11}\text{H}_{13}\text{ClN}_3$  222.0798, obsd. 222.0787.



1-(2-chloroethyl)-4-*o*-tolyl-1*H*-1,2,3-triazole **4** (Table 2, entry 3)

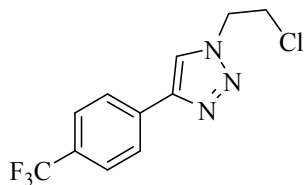
Prepared as described the method for **1**, starting from 1-ethynyl-2-methylbenzene (100 mg, 0.86 mmol), 1, 2-dichloroethane (681.53 mg, 6.88 mmol), sodium azide (167.70 mg, 2.58 mmol) and Pd@PR (577 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 80:20) afforded 1-(2-chloroethyl)-4-*o*-tolyl-1*H*-1,2,3-triazole **4** as colourless semi solid (106.87 mg, 56%);  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  2.50 (s, 3H), 3.99-4.02 (t,  $J = 5.7$  Hz, 2H), 4.76-4.80 (t,  $J = 5.7$  Hz, 2H), 7.28-7.32 (m, 3H), 7.77-7.82 (2H);  $^{13}\text{C}$  NMR (75

MHz, CDCl<sub>3</sub>)  $\delta$  21.30, 42.62, 51.71, 122.88, 126.11, 128.26, 128.94, 129.68, 130.87, 135.57, 147.06. ESIMS data:  $m/z$  calc. for [M+H]<sup>+</sup> C<sub>11</sub>H<sub>13</sub>ClN<sub>3</sub> 222.0798, obsd. 222.0784.



4-(1-(2-chloroethyl)-1*H*-1,2,3-triazol-4-yl)benzonitrile **5** (Table 2, entry 4)

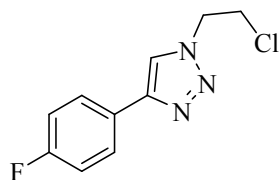
Prepared as described the method for **1**, starting from 4-ethynylbenzonitrile (100 mg, 0.78 mmol), 1, 2-dichloroethane (622.62 mg, 6.29 mmol), sodium azide (152.10 mg, 2.34 mmol) and Pd@PR (523 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 60:40) afforded 4-(1-(2-chloroethyl)-1*H*-1,2,3-triazol-4-yl)benzonitrile **5** as light yellow solid (142.73 mg, 78%); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  3.96-3.98 (t,  $J$  = 2.4 Hz, 2H), 4.74-4.76 (t,  $J$  = 5.4 Hz, 2H), 7.67-7.68 (d,  $J$  = 7.8 Hz, 2H), 7.92-7.94 (d,  $J$  = 8.4 Hz, 2H), 8.04 (s, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  42.42, 51.87, 111.37, 118.66, 121.96, 126.0 (2C), 132.62 (2C), 134.66, 145.76. ESIMS data:  $m/z$  calc. for [M+H]<sup>+</sup> C<sub>11</sub>H<sub>10</sub>ClN<sub>4</sub> 233.0594, obsd. 233.0585.



1-(2-chloroethyl)-4-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazole **6** (Table 2, entry 5)

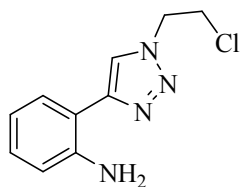
Prepared as described the method for **1a**, starting from 1-ethynyl-4-(trifluoromethyl)benzene (100 mg, 0.58 mmol), 1, 2-dichloroethane (465.3 mg, 4.70 mmol), sodium azide (113.10 mg, 1.74 mmol) and Pd@PR (570 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 70:30) afforded 1-(2-chloroethyl)-4-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazole **6** as white crystalline solid (102.10 mg, 63%), mp 155-157 °C; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  3.97-3.99 (t,  $J$  = 6 Hz, 2H), 4.75-4.77 (t,  $J$  = 6 Hz, 2H), 7.68-7.69 (d,  $J$  = 8.4 Hz, 2H), 7.95-7.96 (d,  $J$  = 8.4, 2H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>)  $\delta$  42.49, 51.94,

121.48, 123.14, 124.95, 125.84 (3C), 130.00, 130.21, 133.78, 146.40. ESIMS data:  $m/z$  calc. for  $[M+H]^+$   $C_{11}H_{10}ClF_3N_3$  276.0515, obsd. 276.0501.



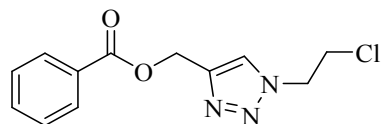
1-(2-chloroethyl)-4-(4-fluorophenyl)-1*H*-1,2,3-triazole **7** (Table 2, entry 6)

Prepared as described the method for **1**, starting from 1-ethynyl-4-fluorobenzene (100 mg, 0.83 mmol), 1, 2-dichloroethane (659 mg, 6.66 mmol), sodium azide (161.90 mg, 2.94 mmol) and Pd@PR (557 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 70:30) afforded 1-(2-chloroethyl)-4-(4-fluorophenyl)-1*H*-1,2,3-triazole **7** as white solid (114.58 mg, 61%);  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  3.95-3.97 (t,  $J$  = 6 Hz, 2H), 4.72-4.74 (t,  $J$  = 6 Hz, 2H), 7.11-7.13 (t,  $J$  = 8.4 Hz, 2H), 7.80-7.82 (t,  $J$  = 6 Hz, 2H), 7.86 (s, 1H);  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  42.51, 51.82, 115.78, 115.92, 120.43, 126.55, 127.47 (2C), 146.93, 161.90, 163.54. ESIMS data:  $m/z$  calc. for  $[M+H]^+$   $C_{10}H_{10}ClFN_3$  226.0547, obsd. 226.0538.



2-(1-(2-chloroethyl)-1*H*-1,2,3-triazol-4-yl)benzenamine **8** (Table 2, entry 7)

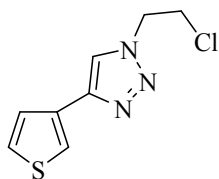
Prepared as described the method for **1**, starting from 2-ethynylbenzenamine (100 mg, 0.85 mmol), 1, 2-dichloroethane (675.80 mg, 6.82 mmol), sodium azide (165.75 mg, 2.55 mmol) and Pd@PR (570 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 60:40) afforded 2-(1-(2-chloroethyl)-1*H*-1,2,3-triazol-4-yl)benzenamine **8** as brown solid (122.74 mg, 64%);  $^1H$  NMR (300 MHz,  $CDCl_3$ )  $\delta$  3.84-3.87 (t,  $J$  = 6 Hz, 2H), 3.94-3.98 (t,  $J$  = 6 Hz, 2H), 6.71-6.79 (m, 2H), 7.10-7.15 (m, 1H), 7.35-7.38 (d,  $J$  = 6.3 Hz, 1H), 7.89 (s, 1H);  $^{13}C$  NMR (75 MHz,  $CDCl_3$ )  $\delta$  42.38, 51.79, 112.58, 116.77, 117.39, 120.86, 129.17, 145.10, 148.43. ESIMS data:  $m/z$  calc. for  $[M+H]^+$   $C_{10}H_{12}ClN_4$  223.0750, obsd. 223.0742.



(1-(2-chloroethyl)-1*H*-1,2,3-triazol-4-yl)methyl benzoate **9** (Table

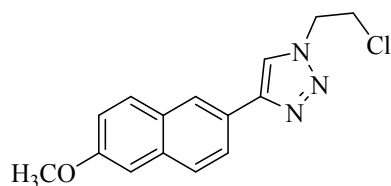
2, entry 8)

Prepared as described the method for **1**, starting from propargyl benzoate (100 mg, 0.62 mmol), 1, 2-dichloroethane (494.25 mg, 4.99 mmol), sodium azide (120.90 mg, 1.86 mmol) and Pd@PR (416 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 70:30) afforded (1-(2-chloroethyl)-1*H*-1,2,3-triazol-4-yl)methyl benzoate **9** as white solid (121 mg, 73%); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 3.90-3.94 (t, *J* = 5.7 Hz, 2H), 4.66-4.70 (t, *J* = 6 Hz, 2H), 5.47 (s, 2H), 7.39-7.46 (m, 2H), 7.54-7.57 (m, 1H), 7.83 (s, 1H), 8.01-8.04 (d, *J* = 8.4 Hz, 2H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 42.27, 51.72, 57.95, 125.02, 128.36 (2C), 129.70 (2C), 133.19, 142.92, 166.41. ESIMS data: *m/z* calc. for [M+H]<sup>+</sup> C<sub>12</sub>H<sub>13</sub>ClN<sub>3</sub>O<sub>2</sub> 266.0696, obsd. 266.0675.



1-(2-chloroethyl)-4-(thiophen-3-yl)-1*H*-1,2,3-triazole **10** (Table 2, entry 9)

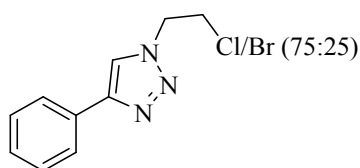
Prepared as described the method for **1**, starting from 3-ethynylthiophene (100 mg, 0.92 mmol), 1, 2-dichloroethane (731.90 mg, 7.39 mmol), sodium azide (179.40 mg, 2.76 mmol) and Pd@PR (617 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 70:30) afforded 1-(2-chloroethyl)-4-(thiophen-3-yl)-1*H*-1,2,3-triazole **10** as white solid (116.55 mg, 59%); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 3.94-3.96 (t, *J* = 5.4 Hz, 2H), 4.70-4.72 (t, *J* = 6 Hz, 2H), 7.38-7.39 (m, 1H), 7.46 (s, 1H), 7.69-7.70 (m, 1H), 7.80 (s, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 42.49, 51.72, 120.45, 121.27 (2C), 125.76 (2C), 126.08 (2C), 131.53, 143.94.



1-(2-chloroethyl)-4-(2-methoxynaphthalen-6-yl)-1*H*-1,2,3-triazole **11**

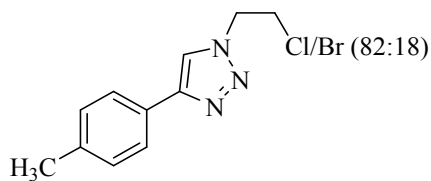
(Table 2, entry 10)

Prepared as described the method for **1**, starting from 2-ethynyl-6-methoxynaphthalene (100 mg, 0.54 mmol), 1,2-dichloroethane (434.44 mg, 4.39 mmol), sodium azide (105.30 mg, 1.62 mmol) and Pd@PR (362 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 70:30) afforded 1-(2-chloroethyl)-4-(2-methoxynaphthalen-6-yl)-1*H*-1,2,3-triazole **11** as brown solid (105.80 mg, 67%), mp 130-132 °C; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 3.93 (s, 3H), 3.96-3.99 (t, *J* = 5.7 Hz, 2H), 4.72-4.76 (t, *J* = 5.7 Hz, 2H), 7.15-7.18 (d, *J* = 10.2 Hz, 2H), 7.77-7.80 (d, *J* = 9 Hz, 2H), 7.88-7.96 (m, 2H), 8.27 (s, 1H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 42.49, 51.79, 55.29, 105.78, 119.30, 120.55, 124.34, 124.39, 125.35, 128.93, 129.67, 134.39, 147.97, 157.95. ESIMS data: *m/z* calc. for [M+H]<sup>+</sup> C<sub>15</sub>H<sub>15</sub>ClN<sub>3</sub>O 288.0903, obsd. 288.0912.



1-(2-chloro/bromoethyl)-4-phenyl-1*H*-1,2,3-triazole **12** (Table 2, entry 11) (The product ratio was calculated on the basis of <sup>1</sup>H NMR)

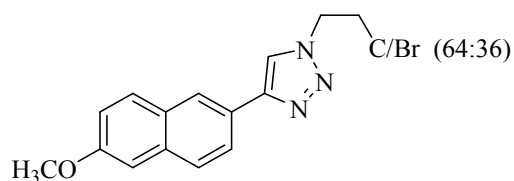
Prepared as described the method for **1**, starting from phenylacetylene (100 mg, 0.98 mmol), 1-bromo-2-chloroethane (1124.33 mg, 7.84 mmol), sodium azide (191.10 mg, 2.94 mmol) and Pd@PR (657 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 70:30) afforded the mixture of 1-(2-chloroethyl)-4-phenyl-1*H*-1,2,3-triazole and 1-(2-bromoethyl)-4-phenyl-1*H*-1,2,3-triazole **12** in ratio 75:25, as white solid (134.11 mg, 63% (combined yield)); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 3.79-3.81 (t, *J* = 6.6 Hz, 2H), 3.95-3.97 (t, *J* = 6 Hz, 2H), 4.73-4.74 (t, *J* = 5.4 Hz, 2H), 4.80-4.82 (t, *J* = 6.6 Hz, 2H), 7.33-7.36 (m, 1H), 7.42-7.45 (m, 2H), 7.83-7.89 (m, 2H), 7.90 (s, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 29.37, 42.50, 51.64, 51.79, 120.41, 125.76 (2C), 128.28, 128.86 (2C), 147.80. ESIMS data: *m/z* calc. for [M+H]<sup>+</sup> C<sub>10</sub>H<sub>11</sub>ClN<sub>3</sub> 208.0641 and C<sub>10</sub>H<sub>11</sub>BrN<sub>3</sub> 252.0136, obsd. 208.0638 and 252.0124 respectively.



1-(2-chloro/bromoethyl)-4-*p*-tolyl-1*H*-1,2,3-triazole **13** (Table 2, entry 12) (The product ratio was calculated on the basis of <sup>1</sup>H NMR)

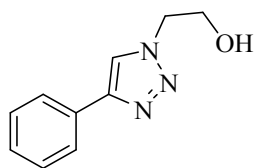


Prepared as described the method for **1**, starting from 1-ethynyl-4-methylbenzene (100 mg, 0.86 mmol), 1-bromo-2-chloroethane (986.66 mg, 6.88 mmol), sodium azide (167.70 mg, 2.58 mmol) and Pd@PR (577 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 70:30) afforded the mixture of 1-(2-chloroethyl)-4-p-tolyl-1*H*-1,2,3-triazole and 1-(2-bromoethyl)-4-p-tolyl-1*H*-1,2,3-triazole **13** in ratio 82:18, as white solid (125.82 mg, 64% (combined yield)); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 2.38 (s, 3H), 3.79-3.80 (m, 2H), 3.95-3.97 (m, 2H), 4.72-4.73 (m, 2H), 4.74-4.82 (m, 2H), 7.24-7.26 (m, 3H), 7.72-7.84 (m, 2H), 7.85 (s, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 21.28, 29.36, 29.69, 51.63, 120.03, 125.69 (2C), 129.54 (2C), 138.18. ESIMS data: m/z calc. for [M+H]<sup>+</sup> C<sub>11</sub>H<sub>13</sub>ClN<sub>3</sub> 222.0798 and C<sub>11</sub>H<sub>13</sub>BrN<sub>3</sub> 266.0292, obsd. 266.0291 and 222.0786 respectively.



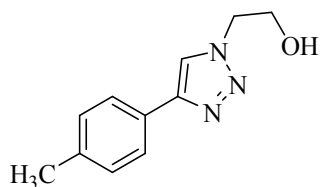
1-(2-chloro/bromoethyl)-4-(2-methoxynaphthalen-6-yl)-1*H*-1,2,3-triazole **14** (Table 2, entry 13) (The product ratio was calculated on the basis of <sup>1</sup>H NMR)

Prepared as described the method for **1**, starting from 2-ethynyl-6-methoxynaphthalene (100 mg, 0.54 mmol), 1-bromo-2-chloroethane (619.53 mg, 4.32 mmol), sodium azide (105.30 mg, 1.62 mmol) and Pd@PR (362 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 70:30) afforded the mixture of 1-(2-chloroethyl)-4-(2-methoxynaphthalen-6-yl)-1*H*-1,2,3-triazole and 1-(2-bromoethyl)-4-(2-methoxynaphthalen-6-yl)-1*H*-1,2,3-triazole **14** in ratio 64:36, as brown solid (98.20 mg, 59% (combined yield)); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 3.81-3.83 (t, *J* = 6.6 Hz, 2H), 3.93 (s, 3H), 3.98-4.00 (t, *J* = 6 Hz, 2H), 4.75-4.77 (t, *J* = 6 Hz, 2H), 4.82-4.84 (t, *J* = 6.6 Hz, 2H), 7.15-7.18 (m, 2H), 7.78-7.80 (m, 2H), 7.89-7.90 (d, *J* = 7.8 Hz, 1H), 7.96-7.97 (d, *J* = 5.4 Hz, 1H), 8.27 (s, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 29.40, 42.54, 51.69, 51.84, 55.33, 105.79, 119.34, 120.29, 120.54, 124.37, 124.43, 125.54, 127.39, 128.96, 129.70, 134.42, 147.96, 157.98. ESIMS data: m/z calc. for [M+H]<sup>+</sup> C<sub>15</sub>H<sub>15</sub>ClN<sub>3</sub>O 288.0903 and C<sub>15</sub>H<sub>15</sub>BrN<sub>3</sub>O 332.0398, obsd. 288.0899 and 332.0394 respectively.



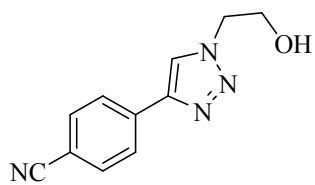
2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethanol **15** (Table 2, entry 14)

Prepared as described the method for **1**, starting from phenylacetylene (100 mg, 0.98 mmol), 2-bromoethanol (612.30 mg, 4.9 mmol), sodium azide (191.10 mg, 2.94 mmol) and Pd@PR (657 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 60:40) afforded 2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethanol **15** as colourless semi solid (137.21 mg, 74%); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 4.07-4.08 (m, 2H), 4.35-4.44 (m, 1H), 4.45-4.46 (t, *J* = 1.5 Hz, 1H), 7.26-7.36 (m, 3H), 7.63-7.64 (m, 2H), 7.80 (s, 1H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 52.96, 60.95, 121.05, 125.49, 128.07, 128.75 (2C), 129.51, 147.26.



2-(4-p-tolyl-1*H*-1,2,3-triazol-1-yl)ethanol **16** (Table 2, entry 15)

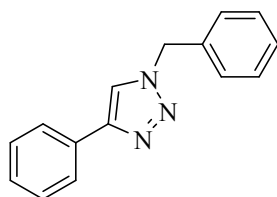
Prepared as described the method for **1**, starting from 1-ethynyl-4-methylbenzene (100 mg, 0.78 mmol), 2-bromoethanol (484.18 mg, 3.9 mmol), sodium azide (152.10 mg, 2.34 mmol) and Pd@PR (523 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 60:40) afforded 2-(4-p-tolyl-1*H*-1,2,3-triazol-1-yl)ethanol **16** as white amorphous solid (134.73 mg, 77%); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 2.36 (s, 3H), 4.07-4.10 (t, *J* = 4.8 Hz, 2H), 4.43-4.46 (t, *J* = 5.4 Hz, 2H), 7.14-7.17 (d, *J* = 8.1 Hz, 2H), 7.52-7.54 (d, *J* = 8.1 Hz, 2H), 7.75 (s, 1H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 21.20, 52.91, 60.97, 120.68, 125.40 (2C), 127.29, 129.39 (2C), 137.93, 147.34; DEPT 135° (600 MHz, CDCl<sub>3</sub>) δ 21.18 (CH<sub>3</sub>), 42.44 (CH<sub>2</sub>), 51.61 (CH<sub>2</sub>), 120.30 (CH), 125.53 (CH), 129.43 (CH). ESIMS data: *m/z* calc. for [M+H]<sup>+</sup> C<sub>11</sub>H<sub>14</sub>N<sub>3</sub>O 204.1136, obsd. 204.1125.



4-(1-(2-hydroxyethyl)-1*H*-1,2,3-triazol-4-yl)benzotrile **17** (Table 2, entry 16)

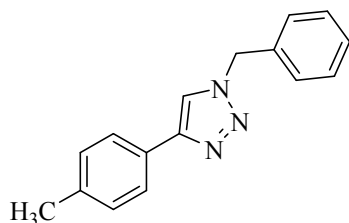
Prepared as described the method for **1**, starting from 4-ethynylbenzotrile (100 mg, 0.78 mmol), 2-bromoethanol (487.34 mg, 3.9 mmol), sodium azide (152.10 mg, 2.34 mmol) and Pd@PR (523 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 50:50) afforded 4-(1-(2-hydroxyethyl)-1*H*-1,2,3-triazol-4-yl)benzotrile

**17** as off white solid (126.36 mg, 75%), mp 86-88 °C; <sup>1</sup>H NMR (300 MHz, MeOD) δ 3.86-3.90 (m, 2H), 4.38-4.47 (m, 2H), 7.67-7.73 (m, 2H), 7.77-7.80 (m, 1H), 7.89-7.92 (d, *J* = 8.4 Hz, 2H), 8.39 (s, 1H); <sup>13</sup>C NMR (75 MHz, MeOD) δ 54.11, 61.52, 112.42, 119.61, 124.38, 127.17 (2C), 131.22, 133.94 (2C), 136.54, 146.84. ESIMS data: *m/z* calc. for [M+H]<sup>+</sup> C<sub>11</sub>H<sub>11</sub>N<sub>4</sub>O 215.0932, obsd. 215.0912.



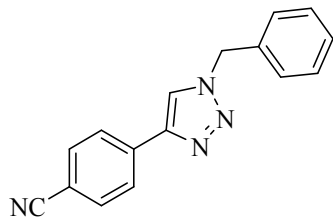
1-benzyl-4-phenyl-1*H*-1,2,3-triazole **18** (Table 2, entry 17)

Prepared as described the method for **1**, starting from phenylacetylene (100 mg, 0.98 mmol), benzyl bromide (502.74 mg, 2.94 mmol), sodium azide (191.10 mg, 2.94 mmol) and Pd@PR (657 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 70:30) afforded 1-benzyl-4-phenyl-1*H*-1,2,3-triazole **18** as white solid (168.38 mg, 73%); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 5.56 (s, 2H), 7.30-7.40 (m, 8H), 7.66 (s, 1H), 7.79-7.80 (d, *J* = 7.8 Hz, 2H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 54.20, 119.44, 125.69 (2C), 128.02 (2C), 128.12, 128.75 (3C), 129.12, 130.03, 134.70, 148.21



1-benzyl-4-*p*-tolyl-1*H*-1,2,3-triazole **19** (Table 2, entry 18)

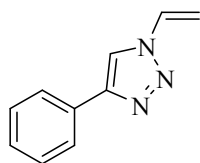
Prepared as described the method for **1**, starting from 1-ethynyl-4-methylbenzene (100 mg, 0.78 mmol), benzyl bromide (400.14 mg, 2.34 mmol), sodium azide (152.10 mg, 2.34 mmol) and Pd@PR (523 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 70:30) afforded 1-benzyl-4-*p*-tolyl-1*H*-1,2,3-triazole **19** as white solid (158.83 mg, 74%); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 2.36 (s, 3H), 5.56 (s, 2H), 7.19-7.21 (d, *J* = 7.8 Hz, 2H), 7.29-7.31 (d, *J* = 7.8 Hz, 2H), 7.32-7.39 (m, 3H), 7.61 (s, 1H), 7.67-7.69 (d, *J* = 7.8 Hz, 2H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 21.23, 54.17, 119.07, 125.56 (2C), 127.67 (2C), 128.71, 129.10, 129.43 (2C), 134.70, 137.97, 148.28. ESIMS data: *m/z* calc. for [M+H]<sup>+</sup> C<sub>16</sub>H<sub>16</sub>N<sub>3</sub> 250.1344, obsd. 250.1334.



4-(1-benzyl-1*H*-1,2,3-triazol-4-yl)benzonitrile **20** (Table 2, entry 19)

Prepared as described the method for **1**, starting from 4-ethynylbenzonitrile (100 mg, 0.78 mmol), benzyl bromide (403.56 mg, 2.36 mmol), sodium azide (152 mg, 2.34 mmol) and Pd@PR (523 mg, 3 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 60:40) afforded 4-(1-benzyl-1*H*-1,2,3-triazol-4-yl)benzonitrile **20** as light yellow solid (142.73 mg, 78%), mp 135-137 °C; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 5.59 (s, 2H), 7.31-7.41 (m, 5H), 7.66-7.69 (d, *J* = 6 Hz, 2H), 7.75 (s, 1H), 7.89-7.91 (d, *J* = 6 Hz, 2H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 54.42, 111.47, 118.70, 120.59, 126.03 (2C), 128.14 (2C), 129.0, 129.26 (2C), 132.65 (2C), 134.19, 134.88, 146.34. ESIMS data: *m/z* calc. for [M+H]<sup>+</sup> 261.1140, obsd. 261.1125.

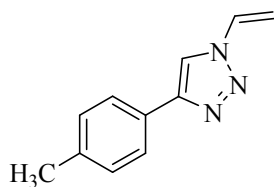
Typical experimental procedure for the synthesis of 4-aryl-1-vinyl-1*H*-1,2,3-triazoles (**21-29**) and their characterization data:



4-phenyl-1-vinyl-1*H*-1,2,3-triazole **21** (Table 3)

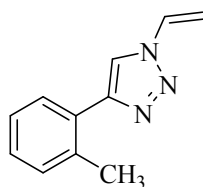
To a mixture of 1-(2-chloroethyl)-4-phenyl-1*H*-1,2,3-triazole (100 mg, 0.48 mmol) and K<sub>2</sub>CO<sub>3</sub> (132.91 mg, 0.96 mmol) in an oven dried 40 ml reaction vial was added 2 ml of dry DMF. The reaction mixture was then stirred under nitrogen in a pre heated oil bath of temperature 110 °C for 2 hours. Progress of the reaction was monitored by TLC. On completion, the cooled reaction mixture was extracted with ethyl acetate (3×3 ml) by addition of 2 ml of water and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. Evaporation of the combined organic layer followed by column chromatography (Hexane:ethylacetate = 90:10) over silica gel (mesh 60-200) afforded 4-phenyl-1-vinyl-1*H*-1,2,3-triazole **21** as white solid (70.89 mg, 86%), mp 85-87 °C; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 5.18-5.19 (dd, *J* = 7.8, 1.2 Hz, 1H), 5.69-5.72 (dd, *J* = 14.4, 1.8 Hz, 1H), 7.34-7.45 (m, 4H), 7.85-7.86 (d, *J* = 7.8 Hz, 2H), 8.01 (s, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 104.63, 116.10,

125.87 (2C), 128.47, 128.87 (2C), 130.01, 130.32, 147.98. ESIMS data:  $m/z$  calc. for  $[M+H]^+$   $C_{10}H_{10}N_3$  172.0874, obsd. 172.0812.



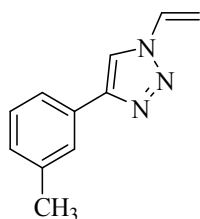
4-*p*-tolyl-1-vinyl-1*H*-1,2,3-triazole, **22** (Table 3)

Prepared as described the method for **21**, starting from 1-(2-chloroethyl)-4-*m*-tolyl-1*H*-1,2,3-triazole (100 mg, 0.45 mmol) and  $K_2CO_3$  (124.50 mg, 0.90 mmol) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethyl acetate = 95:5) afforded 4-*p*-tolyl-1-vinyl-1*H*-1,2,3-triazole **22** as white solid (68.51 mg, 82%);  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  2.39 (s, 3H), 5.17-5.19 (dd,  $J = 7.2, 1.8$  Hz, 1H), 5.67-5.70 (dd,  $J = 14.4, 1.8$  Hz, 1H), 7.24-7.26 (d,  $J = 9$  Hz, 2H), 7.37-7.41 (q,  $J = 9$  Hz, 1H), 7.74-7.75 (d,  $J = 7.8$  Hz, 2H), 7.97 (s, 1H);  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  21.30, 104.42, 115.65, 125.78 (2C), 127.18, 129.57, 130.40 (2C), 138.42, 148.07. ESIMS data:  $m/z$  calc. for  $[M+H]^+$   $C_{11}H_{12}N_3$  186.1031, obsd. 186.1025



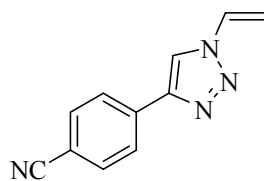
4-*o*-tolyl-1-vinyl-1*H*-1,2,3-triazole, **23** (Table 3)

Prepared as described the method for **21**, starting from 1-(2-chloroethyl)-4-*o*-tolyl-1*H*-1,2,3-triazole (100 mg, 0.45 mmol) and  $K_2CO_3$  (124.50 mg, 0.90 mmol) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethyl acetate = 90:10) afforded 4-*o*-tolyl-1-vinyl-1*H*-1,2,3-triazole **23** as colourless semi solid (72.69 mg, 87%);  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  2.50 (s, 3H), 5.19-5.21 (dd,  $J = 7.2, 1.8$  Hz, 1H), 5.71-5.74 (dd,  $J = 14.4, 1.8$  Hz, 1H), 7.293-7.297 (m, 3H), 7.40-7.44 (q,  $J = 9$  Hz, 1H), 7.77 (s, 1H), 7.88 (s, 1H);  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  21.33, 104.58, 118.32, 126.14, 128.47, 129.04, 129.36, 130.35, 130.93, 135.72, 147.41. ESIMS data:  $m/z$  calc. for  $[M+H]^+$   $C_{11}H_{12}N_3$  186.1031, obsd. 186.1021.



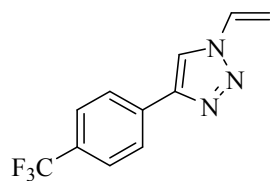
4-m-tolyl-1-vinyl-1*H*-1,2,3-triazole, **24** (Table 3)

Prepared as described the method for **21**, starting from 1-(2-chloroethyl)-4-m-tolyl-1*H*-1,2,3-triazole (100 mg, 0.45 mmol) and K<sub>2</sub>CO<sub>3</sub> (124.50 mg, 0.90 mmol) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethyl acetate = 95:5) afforded 4-m-tolyl-1-vinyl-1*H*-1,2,3-triazole **24** as colourless liquid (68.51 mg, 82%); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 2.41 (s, 3H), 5.18-5.19 (dd, *J* = 6.6, 1.8 Hz, 1H), 5.68-5.71 (dd, *J* = 13.8, 2.4 Hz, 1H), 7.17-7.18 (d, *J* = 7.2 Hz, 1H), 7.31-7.34 (q, *J* = 7.8 Hz, 2H), 7.37-7.43 (q, *J* = 8.4 Hz, 1H), 7.62-7.63 (d, *J* = 7.2 Hz, 1H), 7.71 (s, 1H), 8.00 (s, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 21.40, 104.53, 116.01, 122.97, 126.56, 128.78, 129.27, 129.86, 130.38, 138.61, 148.10. ESIMS data: *m/z* calc. for [M+H]<sup>+</sup> C<sub>11</sub>H<sub>12</sub>N<sub>3</sub> 186.1031, obsd. 186.1013.



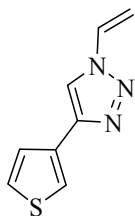
4-(1-vinyl-1*H*-1,2,3-triazol-4-yl)benzonitrile, **25** (Table 3)

Prepared as described the method for **21**, starting from 4-(1-(2-chloroethyl)-1*H*-1,2,3-triazol-4-yl)benzonitrile (100 mg, 0.42 mmol) and K<sub>2</sub>CO<sub>3</sub> (118.62 mg, 0.85 mmol) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethyl acetate = 85:15) afforded 4-(1-vinyl-1*H*-1,2,3-triazol-4-yl)benzonitrile **25** as white solid (71.67 mg, 85%); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 5.25-5.27 (dd, *J* = 6.6, 2.4 Hz, 1H), 5.76-5.79 (dd, *J* = 13.8, 1.8 Hz, 1H), 7.38-7.42 (q, *J* = 9 Hz, 1H), 7.72-7.72 (d, *J* = 8.4 Hz, 2H), 7.97-7.98 (d, *J* = 8.4 Hz, 2H), 8.11 (s, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 105.65, 111.84, 117.38, 118.63, 126.21 (2C), 130.05, 132.75 (2C), 134.09, 146.10.



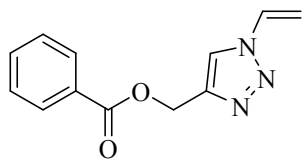
4-(4-(trifluoromethyl)phenyl)-1-vinyl-1*H*-1,2,3-triazole, **26** (Table 3)

Prepared as described the method for **21**, starting from 1-(2-chloroethyl)-4-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazole (100 mg, 0.36 mmol) and  $K_2CO_3$  (100.12 mg, 0.72 mmol) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 90:10) afforded 4-(4-(trifluoromethyl)phenyl)-1-vinyl-1*H*-1,2,3-triazole **26** as white solid (67.68 mg, 78%);  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  5.23-5.25 (dd,  $J = 7.2, 1.8$  Hz, 1H), 5.74-5.77 (dd,  $J = 13.8, 1.8$  Hz, 1H), 7.38-7.42 (q,  $J = 9$  Hz, 1H), 7.69-7.79 (d,  $J = 8.4$  Hz, 2H), 7.97-7.98 (d,  $J = 8.4$  Hz, 2H), 8.09 (s, 1H);  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  105.33, 166.97, 123.12, 124.93, 125.87, 125.90, 125.92, 125.94, 126.01, 130.17, 130.25, 125.45, 133.45, 146.60. ESIMS data:  $m/z$  calc. for  $[M+H]^+$   $C_{11}H_9F_3N_3$  240.0748, obsd. 240.0739.



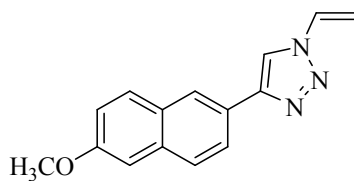
4-(thiophen-3-yl)-1-vinyl-1*H*-1,2,3-triazole, **27** (Table 3)

Prepared as described the method for **21**, starting from 1-(2-chloroethyl)-4-(thiophen-3-yl)-1*H*-1,2,3-triazole (100 mg, 0.46 mmol) and  $K_2CO_3$  (129.16 mg, 0.93 mmol) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethylacetate = 90:10) afforded 4-(thiophen-3-yl)-1-vinyl-1*H*-1,2,3-triazole **27** as white solid (63.86 mg, 77%);  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  5.17-5.19 (dd,  $J = 6.6, 1.8$  Hz, 1H), 5.67-5.70 (dd,  $J = 13.8, 2.4$  Hz, 1H), 7.36-7.40 (m, 2H), 7.46-7.47 (m, 1H), 7.73-7.74 (m, 1H), 7.91 (s, 1H);  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  104.56, 115.82, 121.72, 125.75, 126.49, 130.00, 131.22, 144.14. ESIMS data:  $m/z$  calc. for  $[M+H]^+$   $C_8H_8N_3S$  178.0438, obsd. 178.0422.



(1-vinyl-1*H*-1,2,3-triazol-4-yl)methyl benzoate, **28** (Table 3)

Prepared as described the method for **21**, starting from 1-(2-chloroethyl)-1*H*-1,2,3-triazol-4-yl)methyl benzoate (100 mg, 0.37 mmol) and  $K_2CO_3$  (103.88 mg, 0.75 mmol) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethyl acetate = 90:10) afforded (1-vinyl-1*H*-1,2,3-triazol-4-yl)methyl benzoate **28** as white solid (69 mg, 80%);  $^1H$  NMR (600 MHz,  $CDCl_3$ )  $\delta$  5.17-5.19 (dd,  $J = 7.2, 1.8$  Hz, 1H), 5.68-5.71 (dd,  $J = 14.4, 1.8$  Hz, 1H), 7.31-7.35 (q,  $J = 8.4$  Hz, 1H), 7.41-7.46 (m, 2H), 7.54-7.56 (m, 1H), 7.94 (s, 1H), 8.03-8.04 (d,  $J = 7.2$  Hz, 2H);  $^{13}C$  NMR (150 MHz,  $CDCl_3$ )  $\delta$  57.86, 105.36, 120.93, 128.39, 129.61 (2C), 129.72, 133.25, 143.25, 166.43. ESIMS data:  $m/z$  calc. for  $[M+H]^+$   $C_{12}H_{12}N_3O_2$  230.0929, obsd. 230.0918.

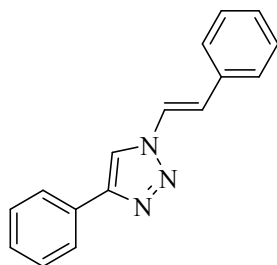


4-(2-methoxynaphthalen-6-yl)-1-vinyl-1*H*-1,2,3-triazole, **29** (Table 3)

Prepared as described the method for **21**, starting from 1-(2-chloroethyl)-4-(2-methoxynaphthalen-6-yl)-1*H*-1,2,3-triazole (100 mg, 0.34 mmol) and  $K_2CO_3$  (95.91 mg, 0.69 mmol) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethyl acetate = 90:10) afforded 4-(2-methoxynaphthalen-6-yl)-1-vinyl-1*H*-1,2,3-triazole as light brown crystalline solid (70.73 mg, 81%), mp 135-137 °C;  $^1H$  NMR (300 MHz,  $CDCl_3$ )  $\delta$  3.94 (s, 3H), 5.19-5.22 (dd,  $J = 7.2, 1.8$  Hz, 1H), 5.70-5.76 (dd,  $J = 14.1, 1.8$  Hz, 1H), 7.16-7.20 (m, 2H), 7.32-7.40 (q,  $J = 9$  Hz, 1H), 7.84-7.87 (d,  $J = 9.3$  Hz, 2H), 7.89-7.92 (m, 1H), 8.08 (s, 1H), 8.30 (s, 1H);  $^{13}C$  NMR (75 MHz,  $CDCl_3$ )  $\delta$  55.31, 104.52, 105.80, 115.92, 119.36, 124.32, 124.63, 125.18, 127.42, 128.91, 129.71, 130.37, 134.51, 148.17, 158.06. ESIMS data:  $m/z$  calc. for  $[M+H]^+$   $C_{15}H_{14}N_3O$  252.1136, obsd. 252.1112.

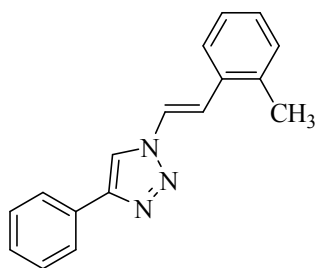


Typical experimental procedure for the synthesis of 4-aryl-1-(2-arylalkenyl)-1*H*-1,2,3-triazoles (**30-37**) and their characterization data:



4-phenyl-1-styryl-1*H*-1,2,3-triazole **30**

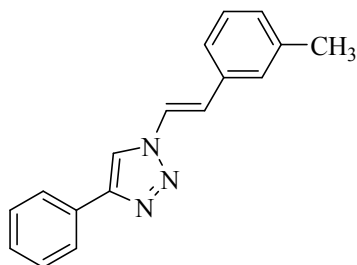
To a mixture of 4-phenyl-1-vinyl-1*H*-1,2,3-triazole (100 mg, 0.58 mmol), iodobenzene (178.74 mg, 0.87 mmol), K<sub>2</sub>CO<sub>3</sub> (160 mg, 1.16 mmol) and Pd@PR (648 mg, 5 mol% Pd) in an oven dried 40 ml reaction vial was added 2 ml of dry DMF. The reaction mixture was then stirred under nitrogen in a pre heated oil bath of temperature 120 °C for 20 hours. Progress of the reaction was monitored by TLC. On completion, the cooled reaction mixture was extracted with ethyl acetate (3×5 ml) by addition of 2 ml of water and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. Evaporation of the combined organic layer followed by column chromatography (Hexane:ethyl acetate = 90:10) over silica gel (mesh 60-200) afforded 4-phenyl-1-styryl-1*H*-1,2,3-triazole **30** as pale yellow solid (78 mg, 54%), mp 93-95 °C; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 7.18-7.20 (d, *J* = 14.4 Hz, 1H), 7.35-7.50 (m, 9H), 7.80-7.83 (d, *J* = 15 Hz, 1H), 7.88-7.90 (d, *J* = 8.4 Hz, 2H), 8.09 (s, 1H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 116.48, 121.57, 123.07, 125.88 (2C), 126.72 (2C), 128.51, 128.80, 128.92, 129.04 (2C), 130.04, 133.58, 148.04. ESIMS data: *m/z* calc. for [M+H]<sup>+</sup> C<sub>16</sub>H<sub>14</sub>N<sub>3</sub> 248.1187, obsd. 248.1178.



1-(2-methylstyryl)-4-phenyl-1*H*-1,2,3-triazole, **31** (Table 4)

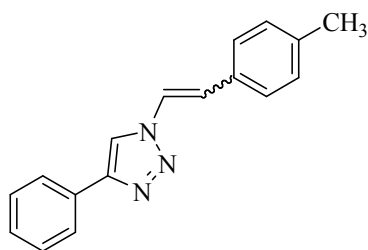
Prepared as described the method for **30**, starting from 4-phenyl-1-vinyl-1*H*-1,2,3-triazole (100 mg, 0.58 mmol), 2-iodotoluene (189.66 mg, 0.87 mmol), K<sub>2</sub>CO<sub>3</sub> (160 mg, 1.16 mmol) and Pd@PR (648 mg, 5 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethyl acetate = 95:5) afforded 1-(2-methylstyryl)-4-phenyl-1*H*-1,2,3-triazole **31** as white solid (82.43 mg, 54%), mp 132-134 °C; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 2.46 (s, 3H), 7.24-7.27 (m, 3H),

7.38-7.70 (m, 5H), 7.65-7.70 (d,  $J = 14.4$  Hz, 1H), 7.90-7.92 (d,  $J = 6.9$  Hz, 2H), 8.10 (s, 1H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  19.92, 116.77, 119.74, 123.74, 125.63, 125.84 (2C), 126.46, 128.43, 128.72, 128.86 (2C), 130.05, 130.69, 132.57, 136.40, 147.96. ESIMS data:  $m/z$  calc. for  $[\text{M}+\text{H}]^+$   $\text{C}_{17}\text{H}_{16}\text{N}_3$  262.1344, obsd. 262.1335.



1-(3-methylstyryl)-4-phenyl-1*H*-1,2,3-triazole, **32** (Table 4)

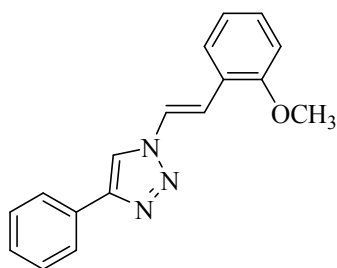
Prepared as described the method for **30**, starting from 4-phenyl-1-vinyl-1*H*-1,2,3-triazole (100 mg, 0.58 mmol), 3-iodotoluene (189.66 mg, 0.87 mmol),  $\text{K}_2\text{CO}_3$  (160 mg, 1.16 mmol) and Pd@PR (648 mg, 5 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethyl acetate = 95:5) afforded 1-(3-methylstyryl)-4-phenyl-1*H*-1,2,3-triazole **32** as colourless liquid (88.53 mg, 58%);  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  2.41 (s, 3H), 7.14-7.19 (d,  $J = 14.7$  Hz, 2H), 7.28-7.50 (m, 6H), 7.79-7.84 (d,  $J = 14.7$  Hz, 1H), 7.89-7.92 (d,  $J = 6.9$  Hz, 2H), 8.10 (s, 1H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  116.47, 121.67, 122.90, 123.88, 125.87 (2C), 127.39, 128.48, 128.91(3C), 129.62, 130.07, 133.50, 138.71, 147.99. ESIMS data:  $m/z$  calc. for  $[\text{M}+\text{H}]^+$   $\text{C}_{17}\text{H}_{16}\text{N}_3$  262.1344, obsd. 262.1337.



1-(4-methylstyryl)-4-phenyl-1*H*-1,2,3-triazole, **33** (Table 4) (*cis:trans* = 50:50; detected by  $^1\text{H}$  NMR spectra)

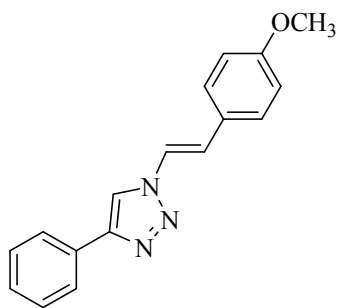
Prepared as described the method for **30**, starting from 4-phenyl-1-vinyl-1*H*-1,2,3-triazole (100 mg, 0.58 mmol), 4-iodotoluene (189.66 mg, 0.87 mmol),  $\text{K}_2\text{CO}_3$  (160 mg, 1.16 mmol) and Pd@PR (648 mg, 5 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethyl acetate = 90:10) afforded 1-(4-methylstyryl)-4-phenyl-1*H*-1,2,3-triazole **33** as white solid (87 mg, 57%), mp 127-129 °C;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  2.39 (s, 3H), 2.44 (s, 3H), 7.10-

7.41 (m, 13H), 7.61-7.64 (m, 2H), 7.78 (s, 1H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  21.18, 21.35, 118.63, 120.53, 125.77 (2C), 127.54 (2C), 128.14, 128.75 (2C), 129.33 (3C), 130.00 (2C), 130.31, 133.88, 135.60, 136.32, 138.80, 146.81. ESIMS data:  $m/z$  calc. for  $[\text{M}+\text{H}]^+$   $\text{C}_{17}\text{H}_{16}\text{N}_3$  262.1344, obsd. 262.1338.



1-(2-methoxystyryl)-4-phenyl-1*H*-1,2,3-triazole, **34** (Table 4)

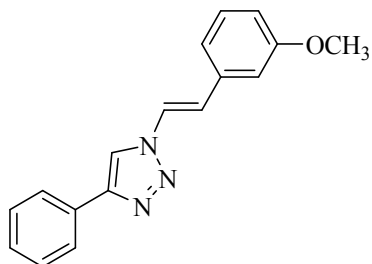
Prepared as described the method for **30**, starting from 4-phenyl-1-vinyl-1*H*-1,2,3-triazole (100 mg, 0.58 mmol), 2-iodoanisole (203.58 mg, 0.87 mmol),  $\text{K}_2\text{CO}_3$  (160 mg, 1.16 mmol) and Pd@PR (648 mg, 5 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethyl acetate = 90:10) afforded 1-(2-methoxystyryl)-4-phenyl-1*H*-1,2,3-triazole **34** as white solid (70.37 mg, 53%);  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  3.93 (s, 3H), 6.94-7.00 (m, 2H), 7.31-7.49 (m, 6H), 7.90-7.92 (d,  $J = 7.2$  Hz, 1H), 7.93-8.01 (d,  $J = 25.5$  Hz, 1H), 8.06 (s, 1H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  55.47, 111.45, 116.31, 117.62, 120.93, 122.40, 124.17, 125.86 (2C), 128.38 (2C), 128.87 (2C), 129.79, 130.22, 147.87, 157.40



1-(4-methoxystyryl)-4-phenyl-1*H*-1,2,3-triazole, **35** (Table 4)

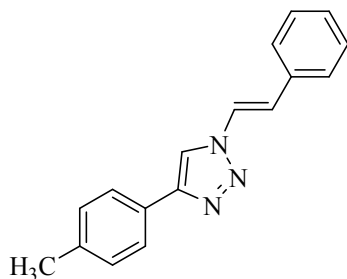
Prepared as described the method for **30**, starting from 4-phenyl-1-vinyl-1*H*-1,2,3-triazole (100 mg, 0.58 mmol), 4-iodoanisole (203.58 mg, 0.87 mmol),  $\text{K}_2\text{CO}_3$  (160 mg, 1.16 mmol) and Pd@PR (648 mg, 5 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethyl acetate = 90:10) afforded 1-(4-methoxystyryl)-4-phenyl-1*H*-1,2,3-triazole **35** as white crystalline solid (67.72 mg, 51%);  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  3.86 (s, 3H), 6.94-6.97 (d,  $J = 8.7$

Hz, 2H), 7.11-7.16 (d,  $J = 14.7$  Hz, 1H), 7.26-7.29 (m, 2H), 7.43-7.46 (d,  $J = 8.7$  Hz, 2H), 7.68-7.73 (d,  $J = 14.7$  Hz, 1H), 7.77-7.80 (d,  $J = 8.1$  Hz, 2H), 8.04 (s, 1H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  55.36, 114.49, 116.02, 121.20, 121.40, 125.75, 126.16, 127.32, 128.03, 129.58, 138.34, 147.98, 160.12. ESIMS data:  $m/z$  calc. for  $[\text{M}+\text{H}]^+$   $\text{C}_{17}\text{H}_{16}\text{N}_3\text{O}$  278.1293, obsd. 278.3284.



1-(3-methoxystyryl)-4-phenyl-1*H*-1,2,3-triazole, **36** (Table 4)

Prepared as described the method for **30**, starting from 4-phenyl-1-vinyl-1*H*-1,2,3-triazole (100 mg, 0.58 mmol), 3-iodoanisole (203.58 mg, 0.87 mmol),  $\text{K}_2\text{CO}_3$  (160 mg, 1.16 mmol) and Pd@PR (648 mg, 5 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethyl acetate = 90:10) afforded 1-(3-methoxystyryl)-4-phenyl-1*H*-1,2,3-triazole **36** as white solid (82.37 mg, 62%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  3.85 (s, 3H), 6.89-6.91 (m, 1H), 7.01 (s, 1H), 7.08-7.09 (d,  $J = 7.8$  Hz, 1H), 7.14-7.16 (d,  $J = 15$  Hz, 1H), 7.31-7.38 (m, 2H), 7.44-7.47 (t,  $J = 7.8$ , 2H), 7.79-7.82 (d,  $J = 14.4$  Hz, 1H), 7.88-7.89 (d,  $J = 7.2$  Hz, 2H), 8.09 (s, 1H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  55.30, 112.07, 114.40, 116.48, 119.30, 121.44, 123.32 (2C), 128.52, 128.93 (3C), 130.01, 134.96, 148.05, 160.04



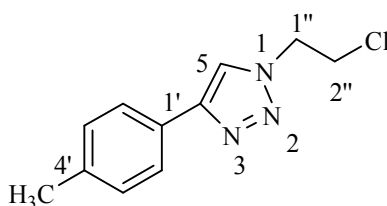
1-styryl-4-*p*-tolyl-1*H*-1,2,3-triazole, **37** (Table 4)

Prepared as described the method for **30**, starting from 4-*p*-tolyl-1-vinyl-1*H*-1,2,3-triazole (100 mg, 0.53 mmol), iodobenzene (165.20 mg, 0.80 mmol),  $\text{K}_2\text{CO}_3$  (146.28 mg, 1.06 mmol) and Pd@PR (592 mg, 5 mol% Pd) gave, after purification with silica gel (mesh 60-200) column chromatography (Hexane:ethyl acetate = 90:10) afforded 1-styryl-4-*p*-tolyl-1*H*-1,2,3-triazole **37** as white solid (67.60 mg, 48%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ :MeOD)  $\delta$  2.35 (s, 3H), 7.22-7.24 (d,  $J = 7.8$  Hz, 2H), 7.30-7.32 (m, 2H), 7.36-7.38 (m, 2H), 7.50-7.51 (d,  $J = 7.8$  Hz, 2H), 7.70-7.71 (d,  $J = 7.8$  Hz, 2H), 7.82-7.84

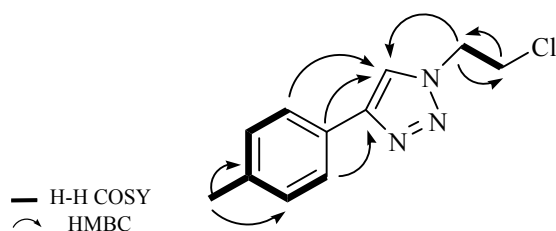
(d,  $J = 14.4$  Hz, 1H), 8.37 (s, 1H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3:\text{MeOD}$ )  $\delta$  20.32, 116.92, 116.96, 121.78, 122.45, 125.21, 126.26 (2C), 126.48, 128.25, 128.43 (2C), 129.08 (2C), 133.24, 138.10, 147.66. ESIMS data:  $m/z$  calc. for  $[\text{M}+\text{H}]^+$   $\text{C}_{17}\text{H}_{16}\text{N}_3$  262.1344, obsd. 262.1284.

## 2D NMR spectral interpretation of product 1-(2-Chloroethyl)-4-*p*-tolyl-1*H*-1,2,3-triazole **2**

1-(2-Chloroethyl)-4-*p*-tolyl-1*H*-1,2,3-triazole, **2**



**Figure 1.** Structure of compound **2**



**Figure 2.** Selected HMBC and COSY correlations of **2**

**Table 1.**  $^1\text{H}$ -NMR (600 MHz) and  $^{13}\text{C}$ -NMR (150 MHz) data of compounds **1** in  $\text{CDCl}_3$  ( $\delta$  values)

Position	$\delta_{\text{C}}$ (ppm)	$\delta_{\text{H}}$ (ppm) m ( $J$ Hz)
1	-	-
2	-	-

3	-	-
4	147.8	-
5	120.4	7.82 s
1'	127.5	-
2'	125.7	7.67-7.68 d (7.8)
3'	129.5	7.18-7.19 d (7.8)
4'	138.1	-
5'	129.5	7.18-7.19 d (7.8)
6'	125.7	7.67-7.68 d (7.8)
1''	51.7	4.63 m
2''	42.5	3.87 m
4'-CH <sub>3</sub>	21.3	2.33 s

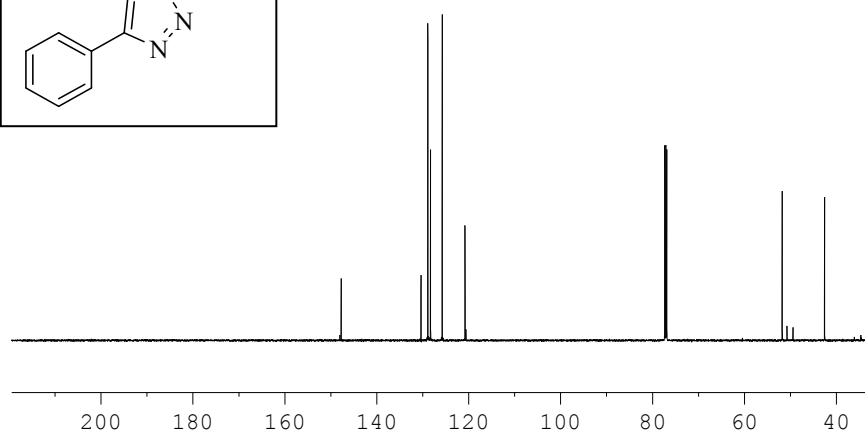
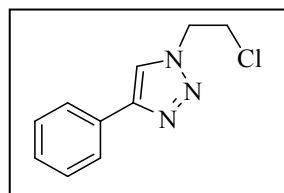
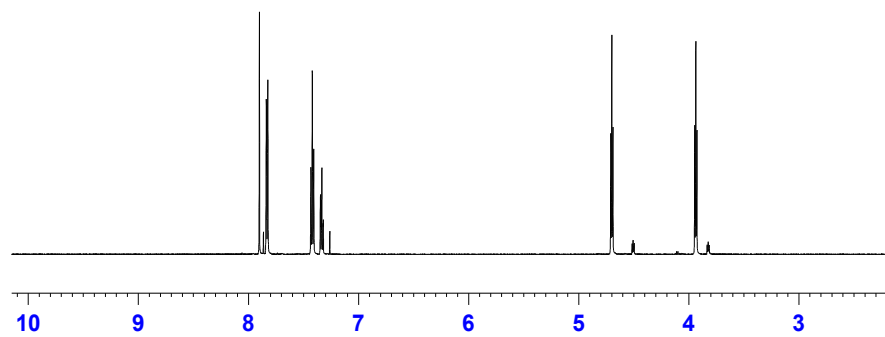
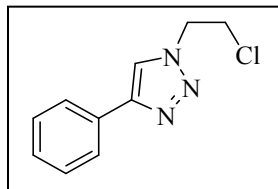
The <sup>1</sup>H, <sup>13</sup>C-NMR spectra revealed 11 carbon signals which were constituted of one methyls, two methylenes, one methines, and three quaternary carbons as evident from the DEPT spectra.

The two methane singlets were found at  $\delta$  4.63 and 3.87 corresponding to carbons at  $\delta$  51.7 (CH<sub>2</sub>) and 42.5 (CH<sub>2</sub>), respectively, one methyl singlet at  $\delta$  2.33 (4'-CH<sub>3</sub>), and one hydroxymethine signal at  $\delta$  3.59 (C-1) (1'' Table 1). One carbonyl moiety at  $\delta$  194.3 was assignable to C-9, the characteristic signal of an  $\alpha,\beta$ -unsaturated ketone moiety. Aromatic carbons were found at  $\delta$  138.1, 129.5, 125.7 and 127.5. Two olefinic signals at  $\delta$  147.8 and 120.4 revealed the position of one double bond at C-4 and C-5 in the triazole ring.

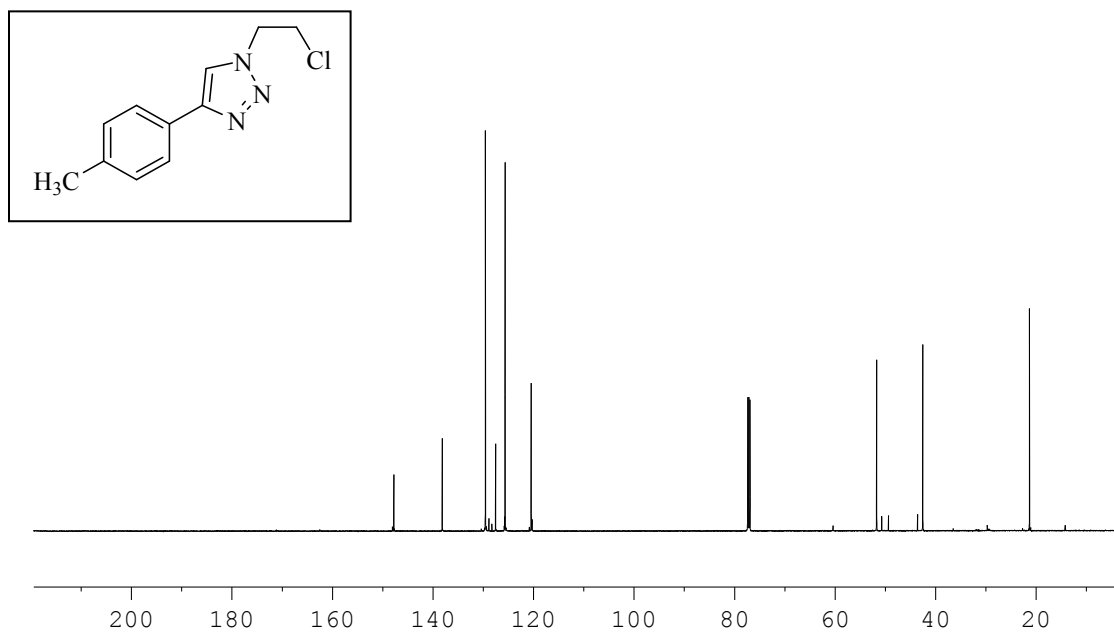
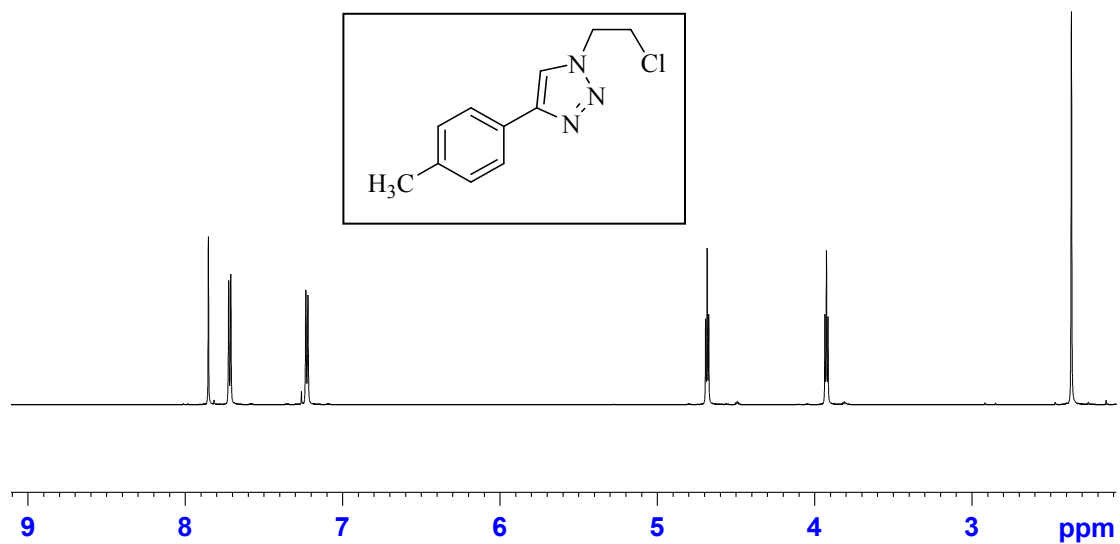
Analysis of its COSY data disclosed two proton-proton networks corresponding to H-2, H-2', H-3', H-5', H-6' and H<sub>3</sub>-4', as well as H-1'' and H-2'' (Fig. 2). Long-range proton-carbon correlations observed in the HMBC spectrum of **2** (Fig. 2) provided corroborative evidence to support these subunits deduced from COSY data. The HMBC spectrum showed the linkage of chloroethane moiety near to C-5 of triazole ring evident from H<sub>2</sub>-1''/C-5 correlation. The other HMBC correlations were as following: H<sub>1</sub>-5/C-4; H<sub>1</sub>-2'/C-4, C-5, C-1', H<sub>1</sub>-6'/C-4, C-5, C-1'; H<sub>3</sub>-4'/C-3', C-4', C-5'; H<sub>1</sub>-5'/4'-CH<sub>3</sub>; H<sub>1</sub>-3'/4'-CH<sub>3</sub>; H<sub>2</sub>-1''/C-2'' and H<sub>2</sub>-2''/C-1''.

Copies of  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and ESI-MS spectra of the synthesized compounds (1-38):

1-(2-chloroethyl)-4-phenyl-1*H*-1,2,3-triazole **1** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )

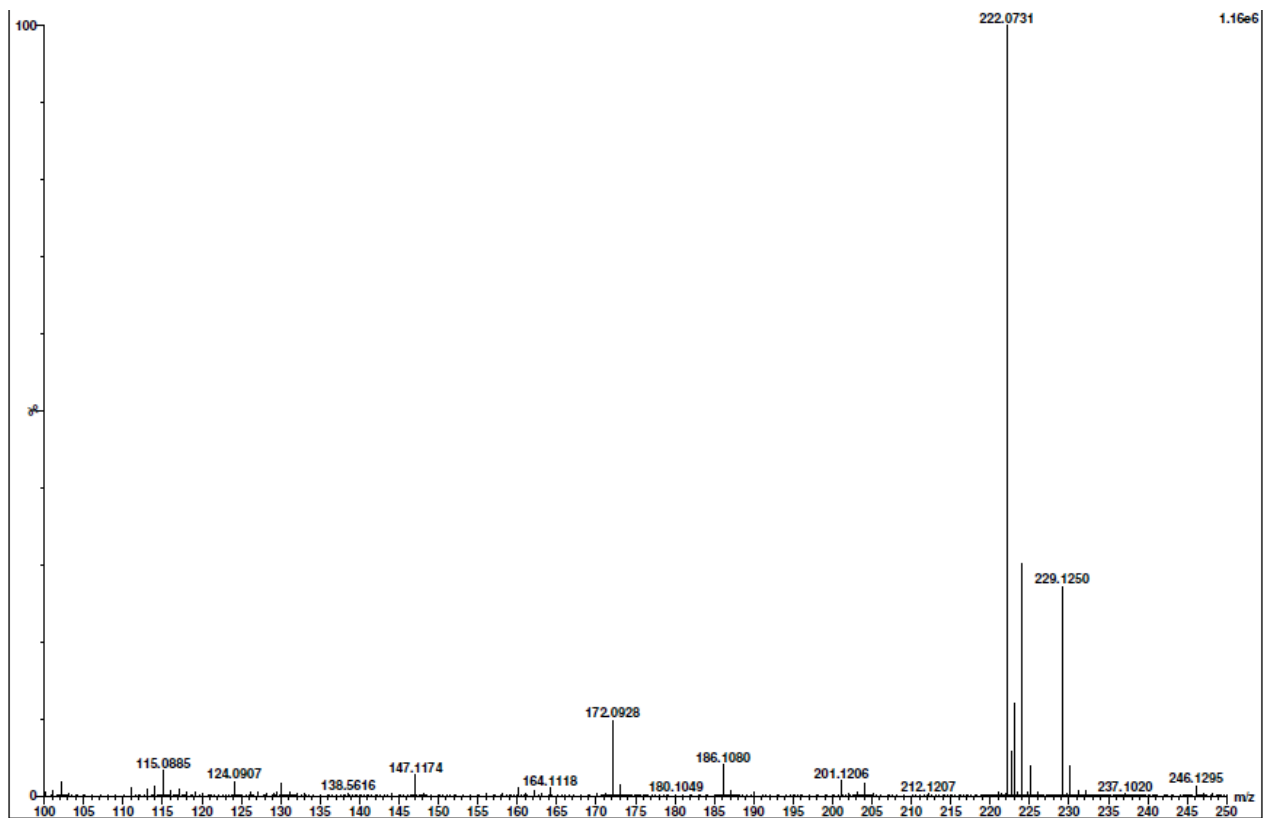


1-(2-chloroethyl)-4-*p*-tolyl-1*H*-1,2,3-triazole **2** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )



1-(2-chloroethyl)-4-*p*-tolyl-1*H*-1,2,3-triazole **2** (ESI MS in  $\text{MeCN}:\text{H}_2\text{O}$  (1:1))

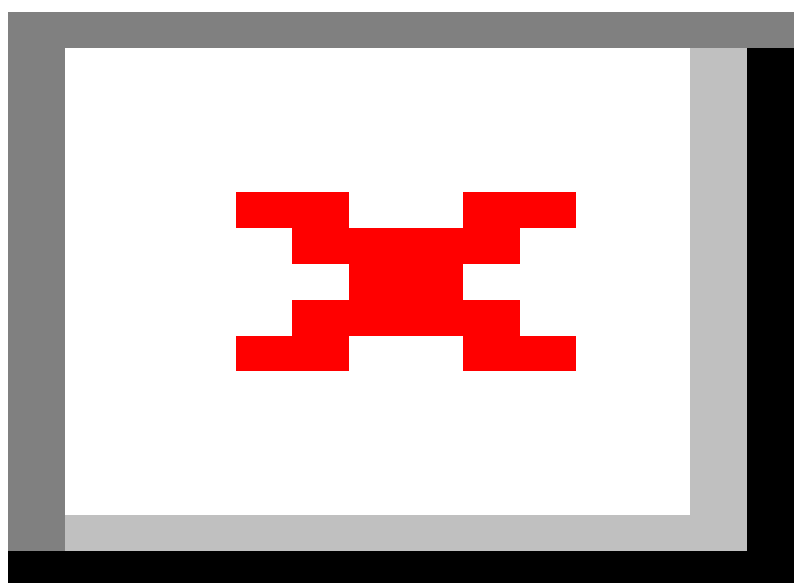
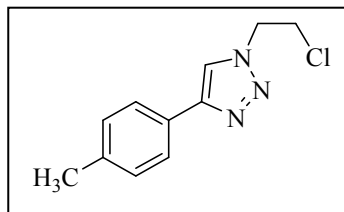




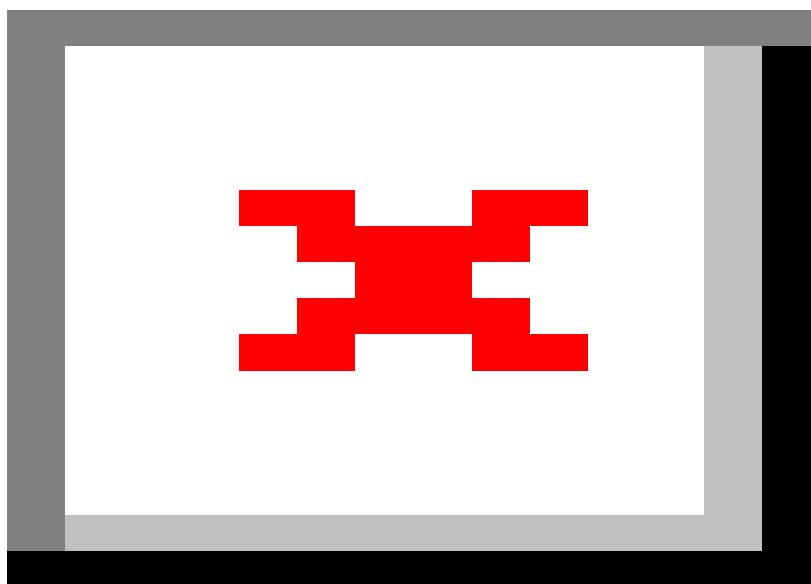
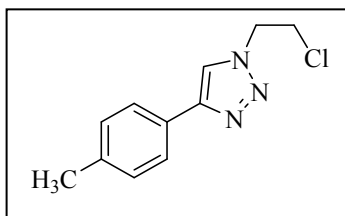
1-(2-chloroethyl)-4-*p*-tolyl-1*H*-1,2,3-triazole **2** (DEPT 135 ° in CDCl<sub>3</sub>)



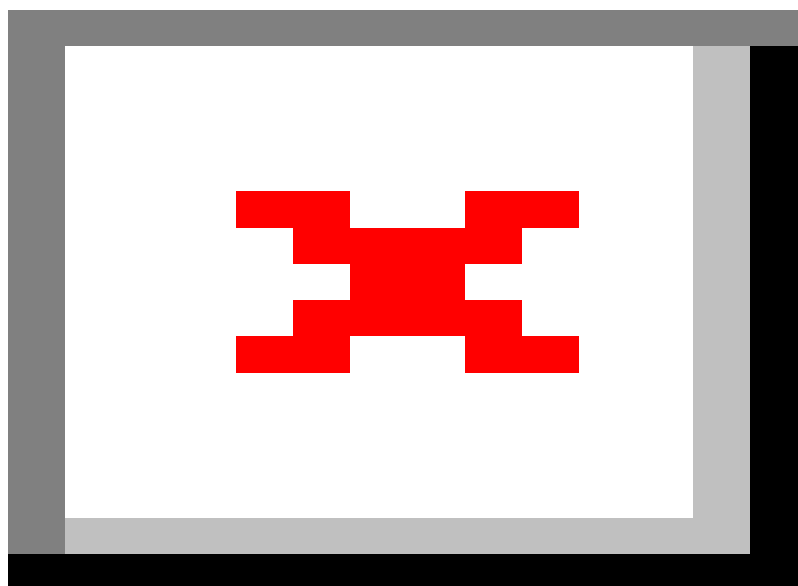
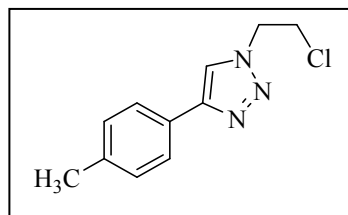
1-(2-chloroethyl)-4-*p*-tolyl-1*H*-1,2,3-triazole **2** (HMQC in CDCl<sub>3</sub>)



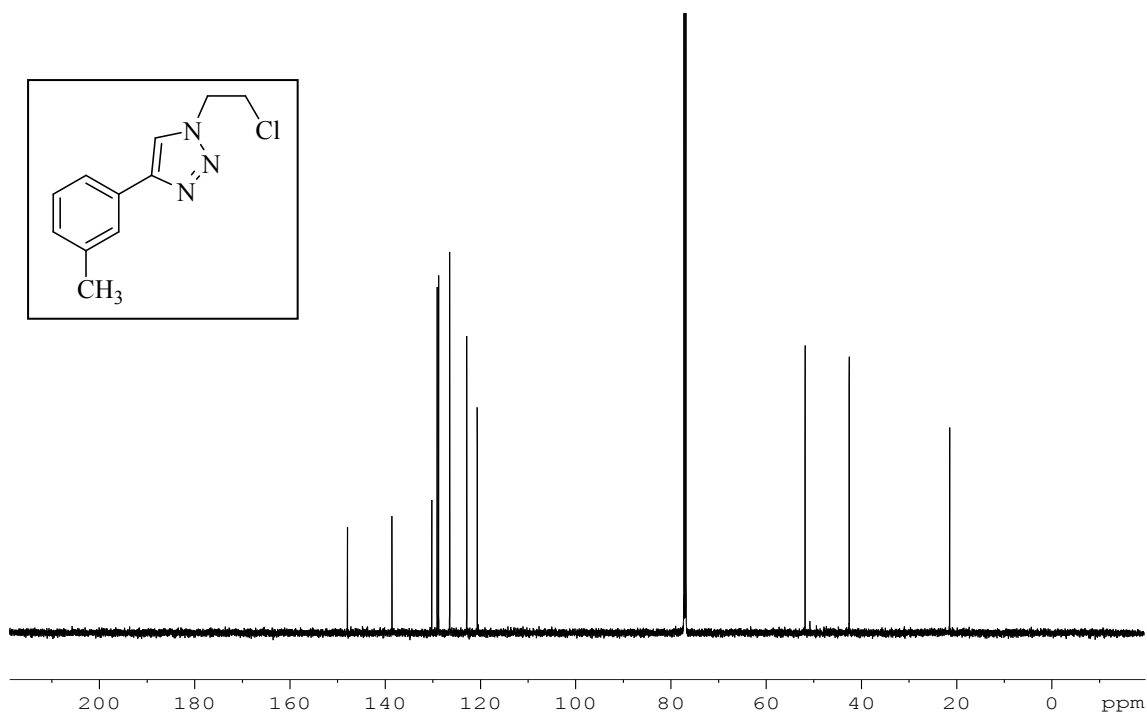
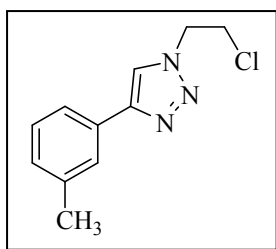
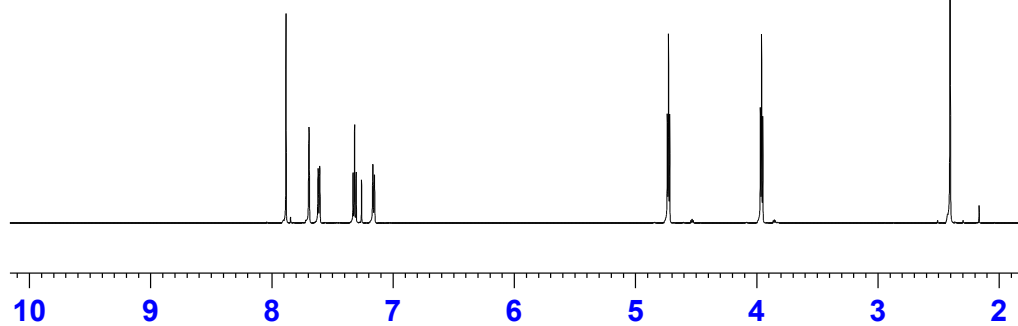
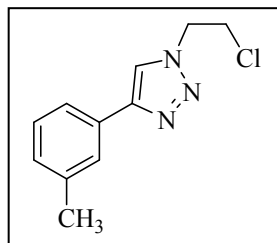
1-(2-chloroethyl)-4-*p*-tolyl-1*H*-1,2,3-triazole **2** (HMBC in CDCl<sub>3</sub>)



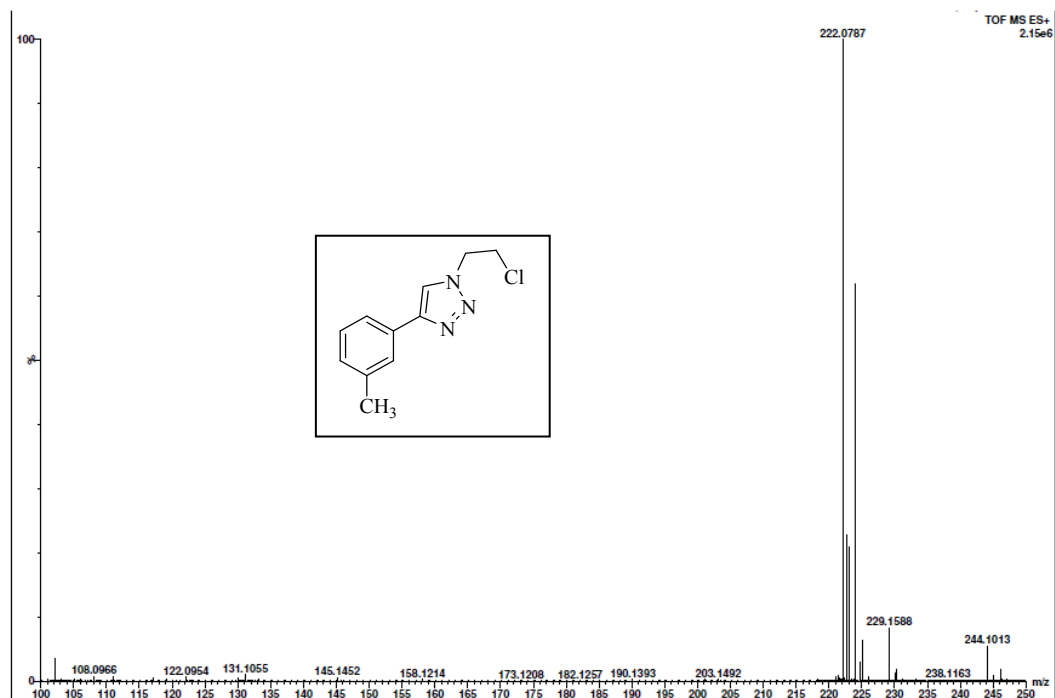
1-(2-chloroethyl)-4-*p*-tolyl-1*H*-1,2,3-triazole **2** (COSY in CDCl<sub>3</sub>)



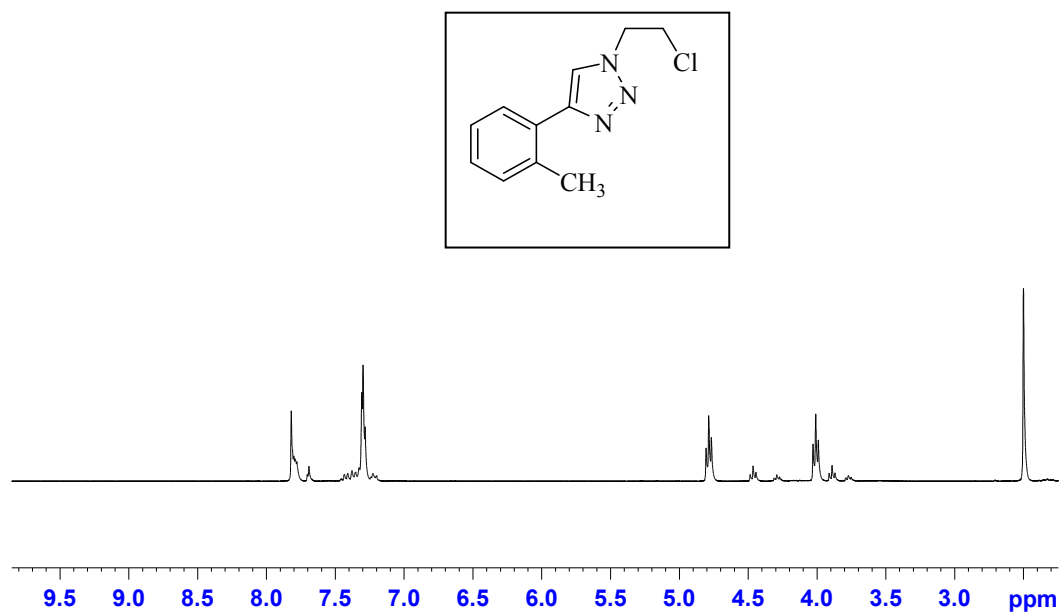
1-(2-chloroethyl)-4-*m*-tolyl-1*H*-1,2,3-triazole **3** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )

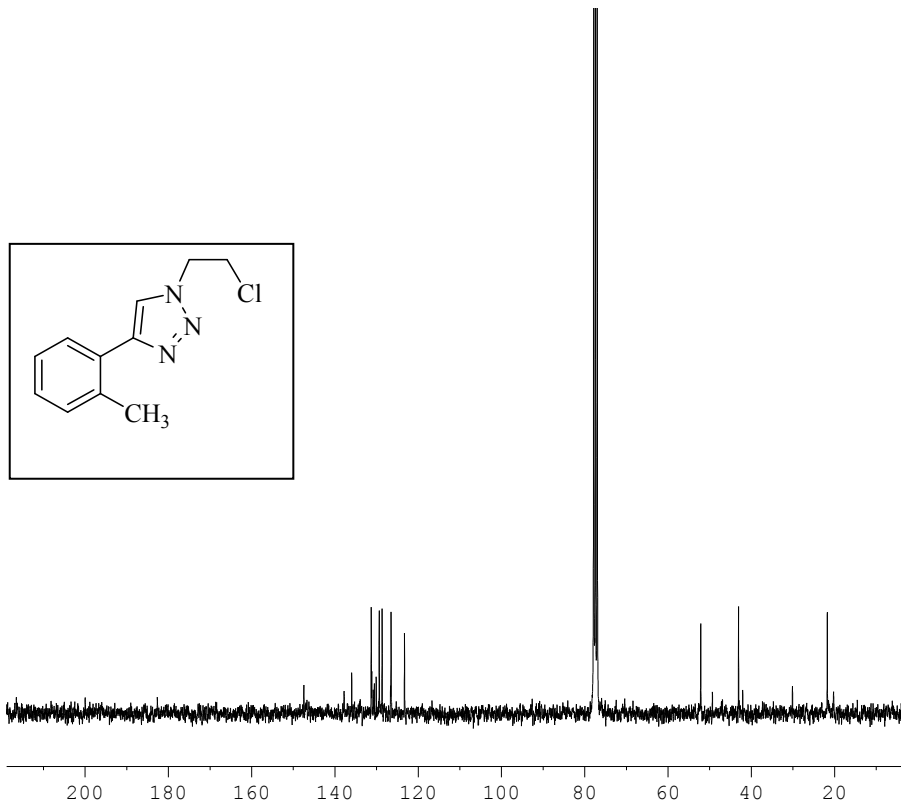


1-propyl-4-*m*-tolyl-1*H*-1,2,3-triazole **3** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

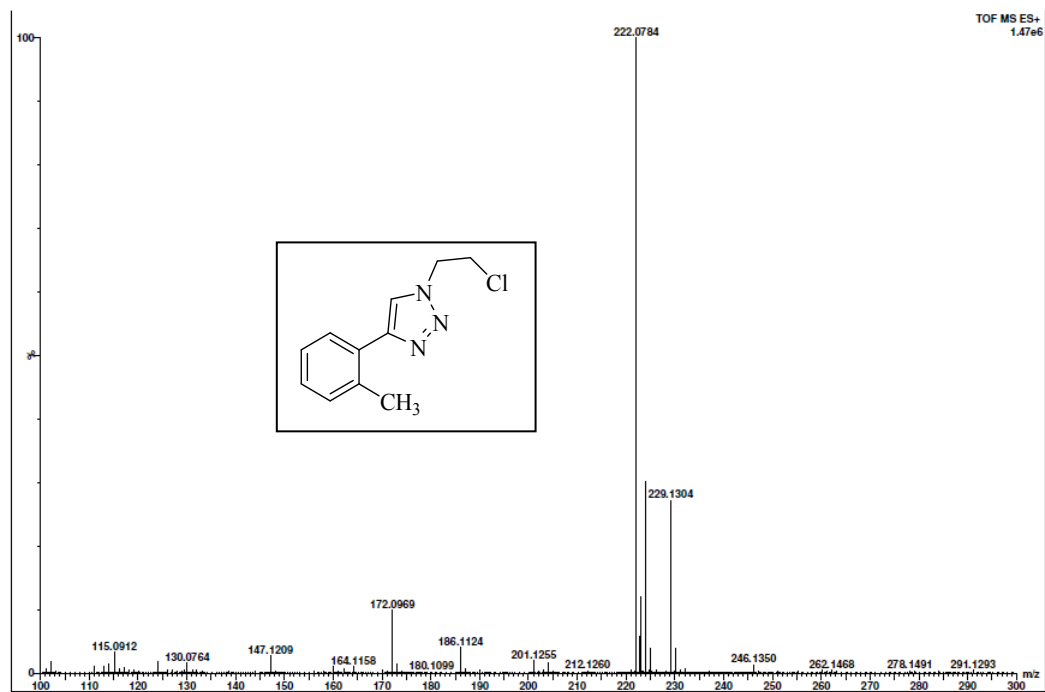


1-(2-chloroethyl)-4-*o*-tolyl-1*H*-1,2,3-triazole **4** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)



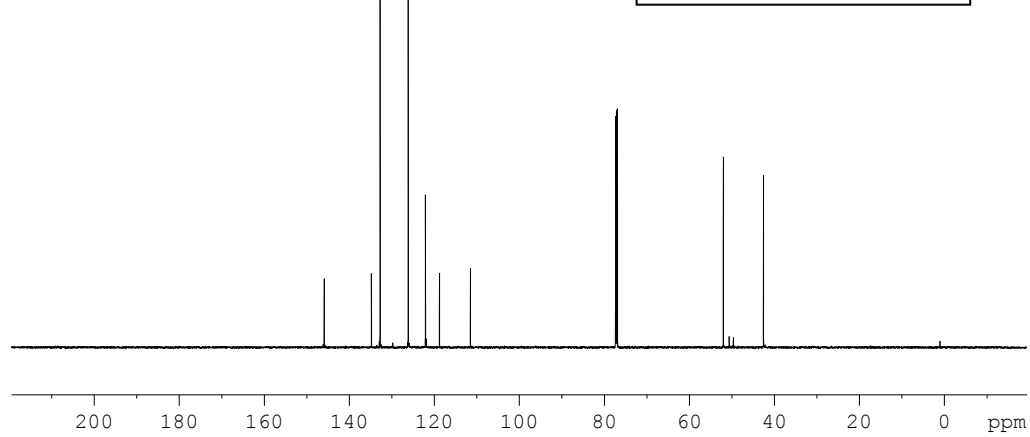
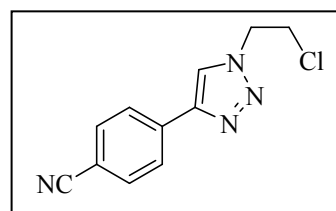
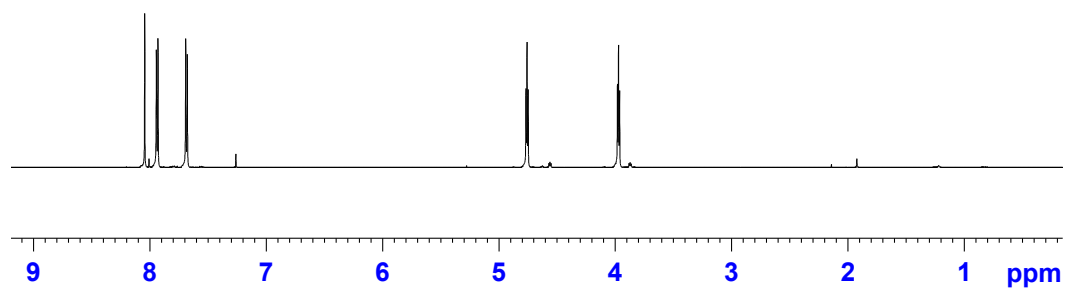
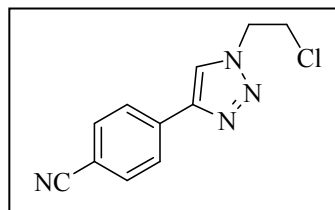


1-(2-chloroethyl)-4-*o*-tolyl-1H-1,2,3-triazole **4** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

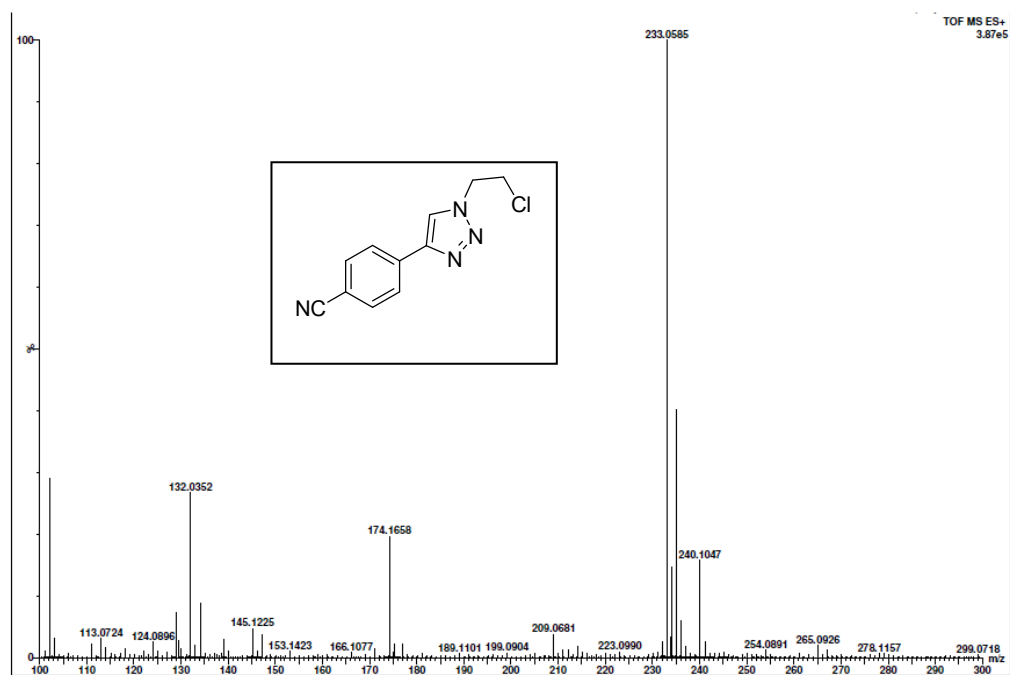




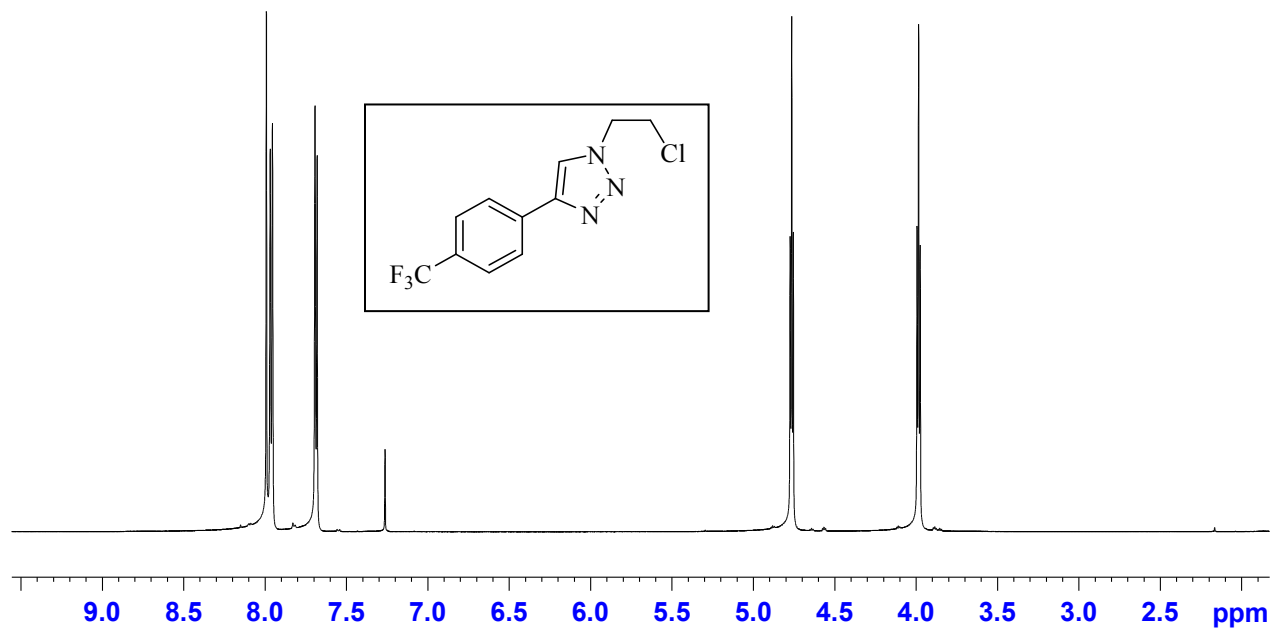
4-(1-(2-chloroethyl)-1H-1,2,3-triazol-4-yl)benzonitrile **5** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )

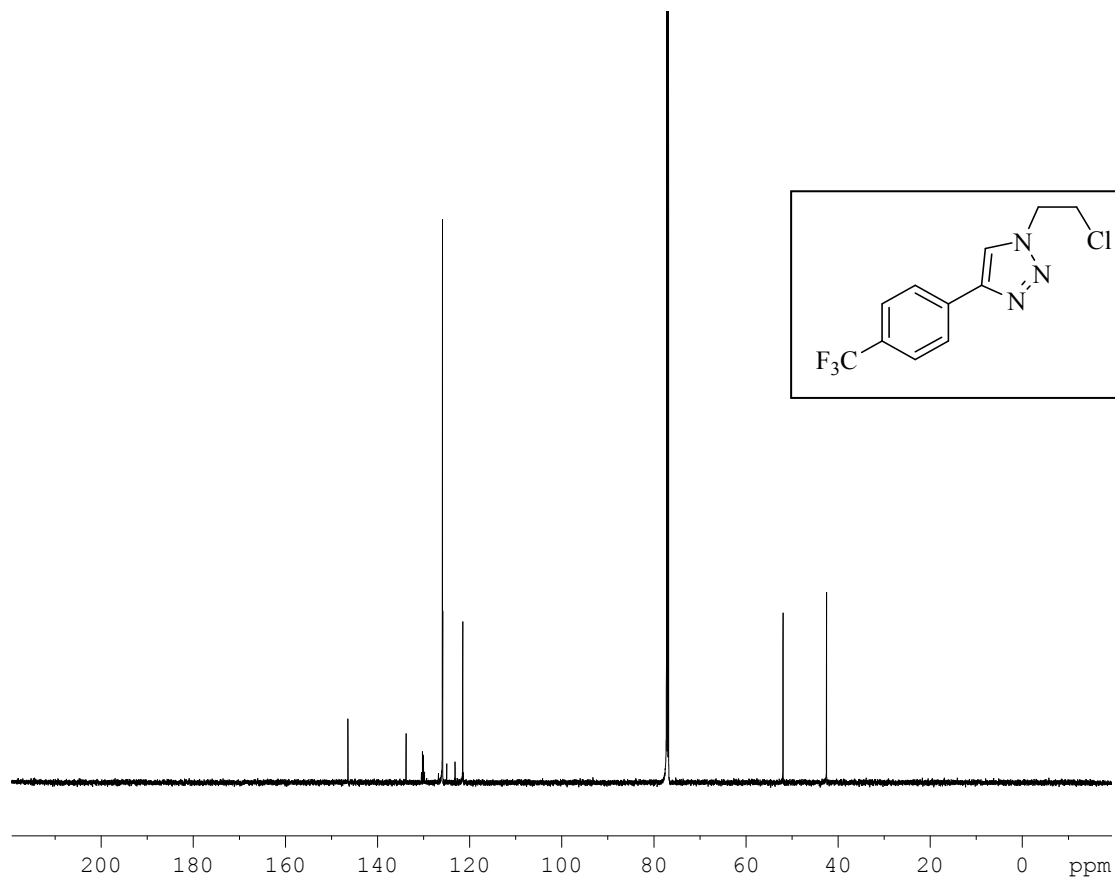


4-(1-(2-chloroethyl)-1*H*-1,2,3-triazol-4-yl)benzonitrile **5** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

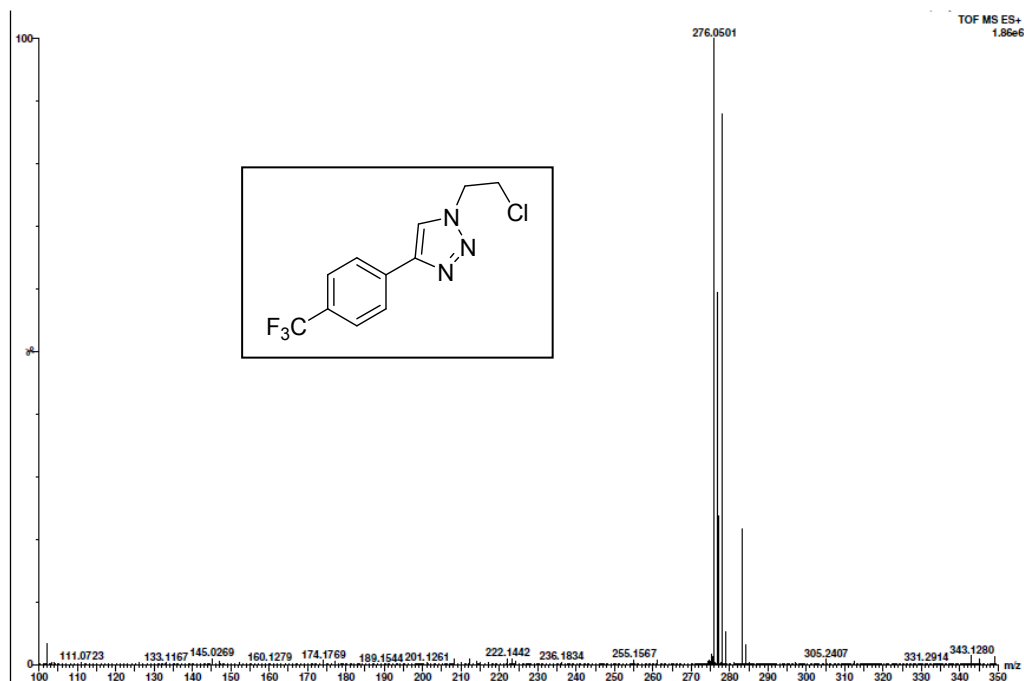


1-(2-chloroethyl)-4-(4-(trifluoromethyl)phenyl)-1*H*-1,2,3-triazole **6** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)

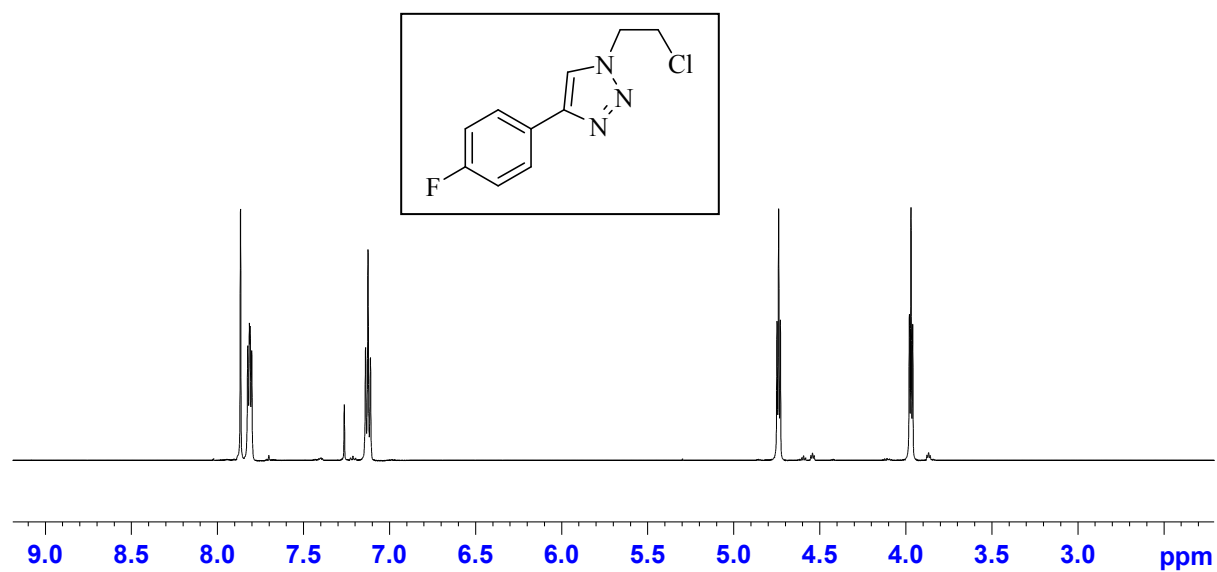




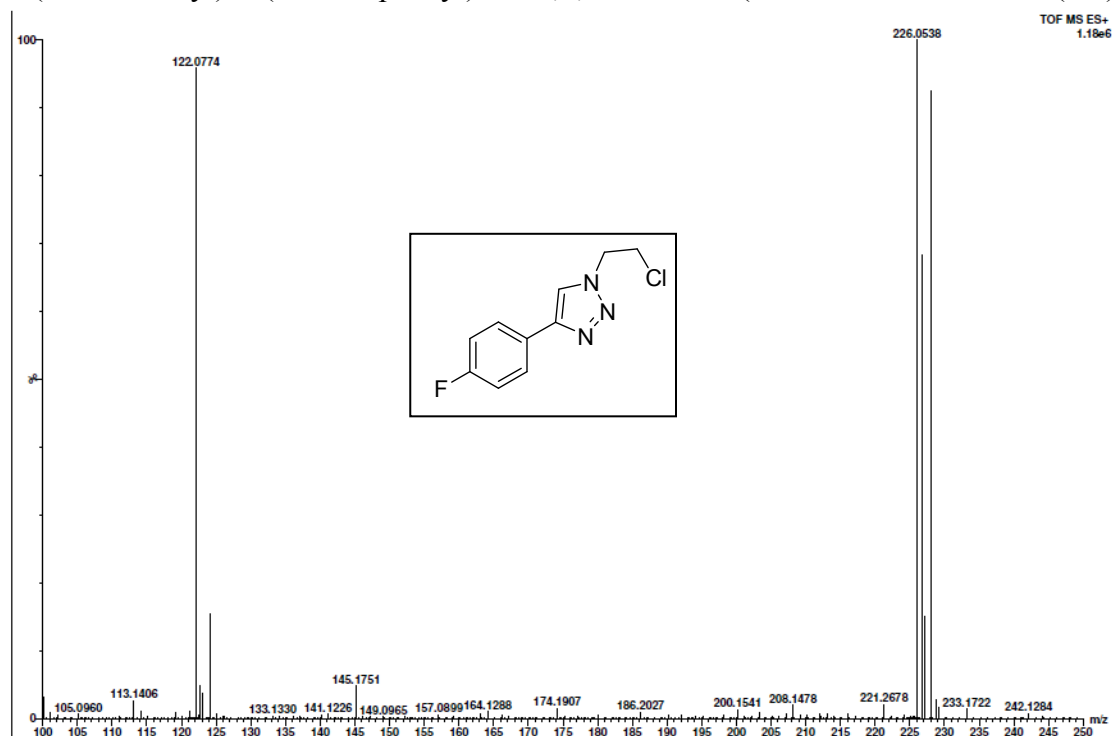
1-(2-chloroethyl)-4-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazole **6** (ESI MS in MeCN:H<sub>2</sub>O (1:1))



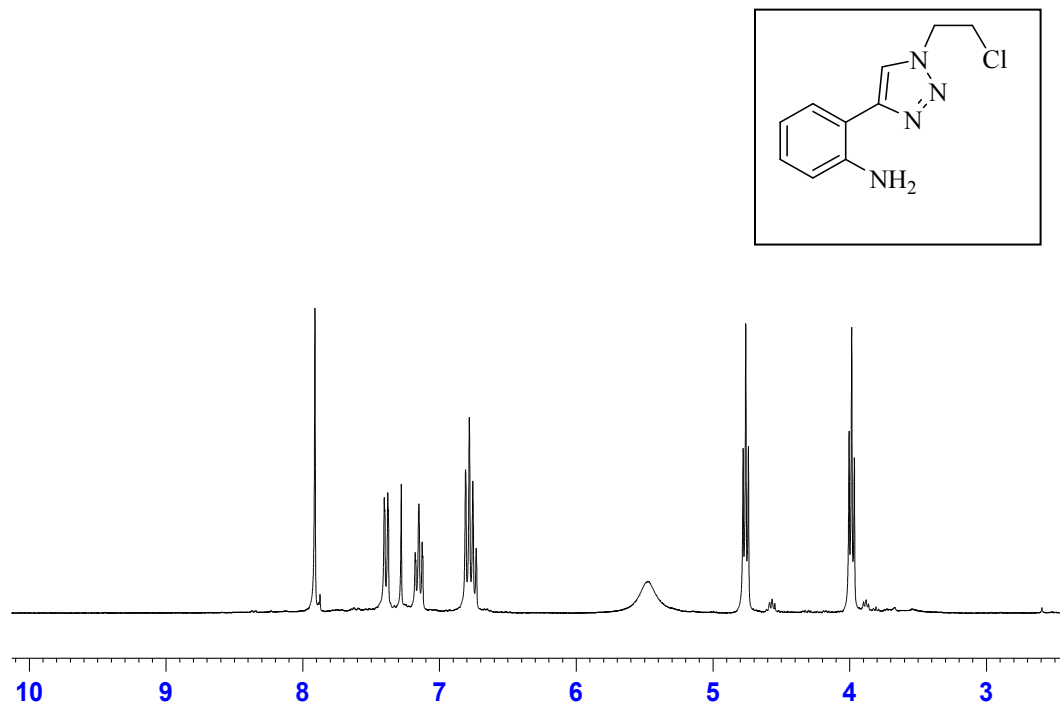
1-(2-chloroethyl)-4-(4-fluorophenyl)-1*H*-1,2,3-triazole **7** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)

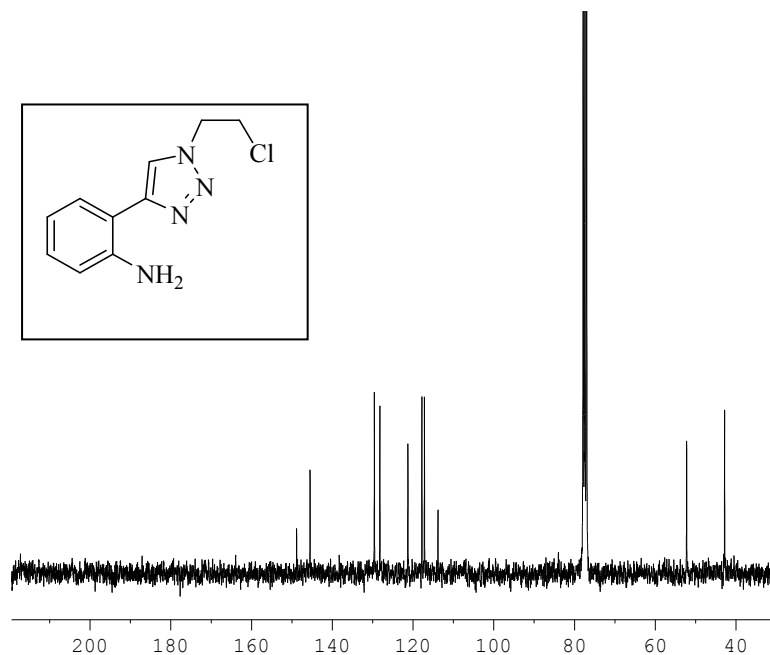


1-(2-chloroethyl)-4-(4-fluorophenyl)-1*H*-1,2,3-triazole **7** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

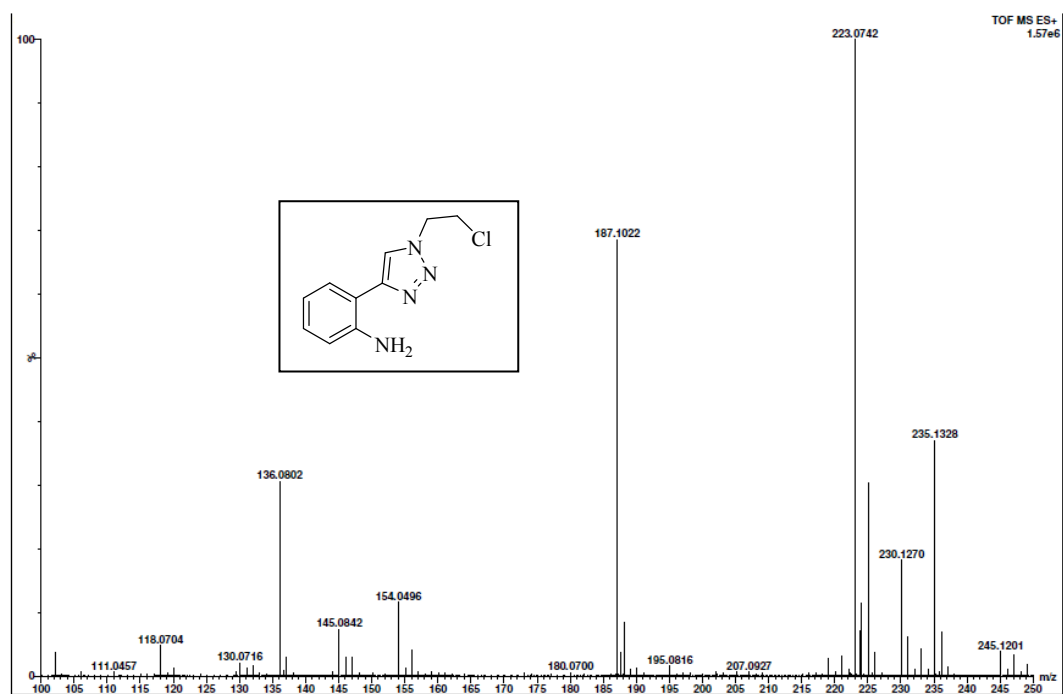


2-(1-(2-chloroethyl)-1*H*-1,2,3-triazol-4-yl)benzenamine **8** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)

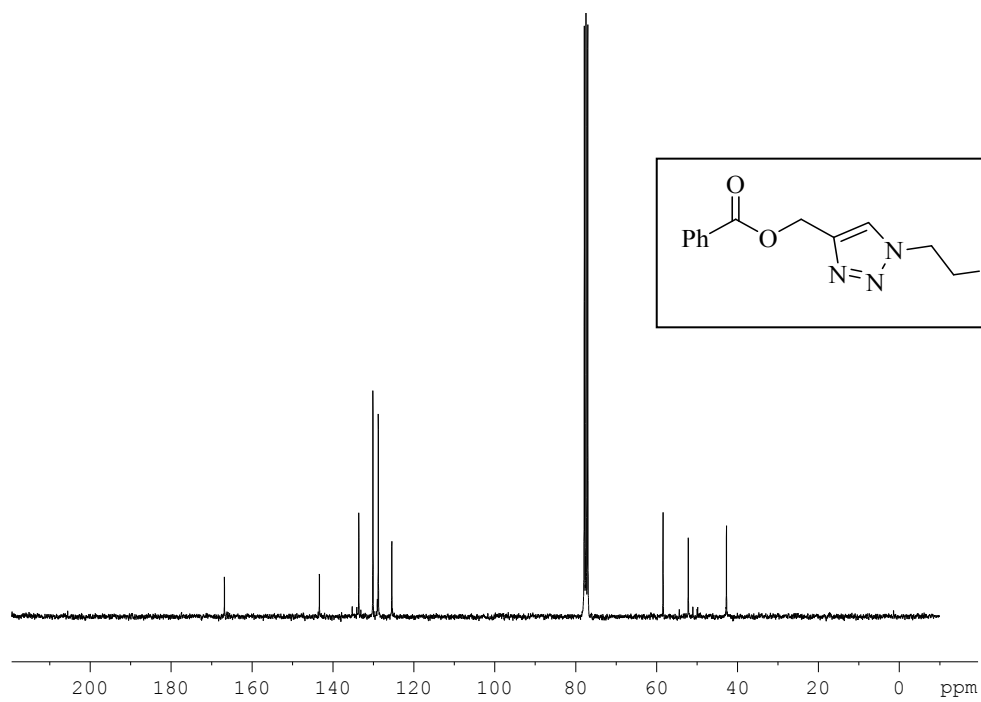
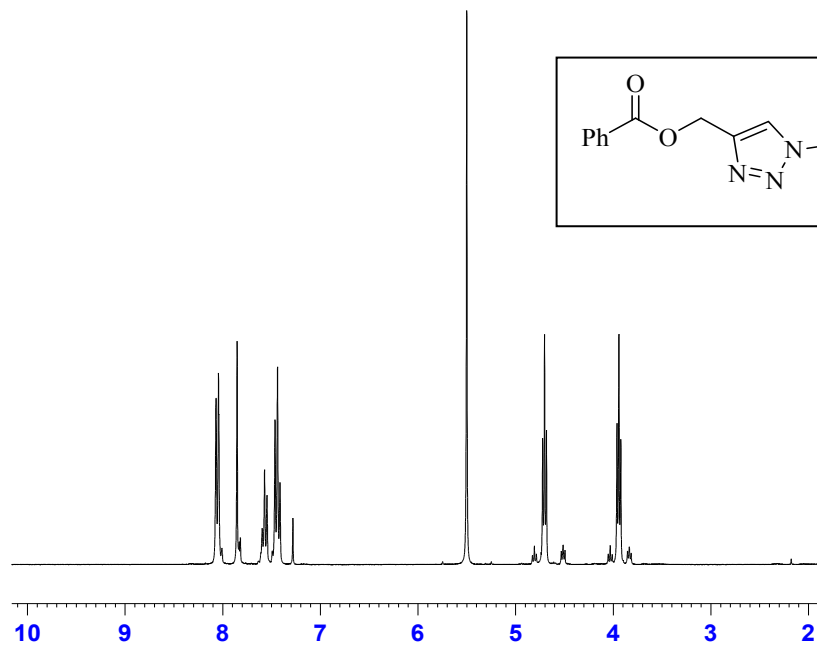




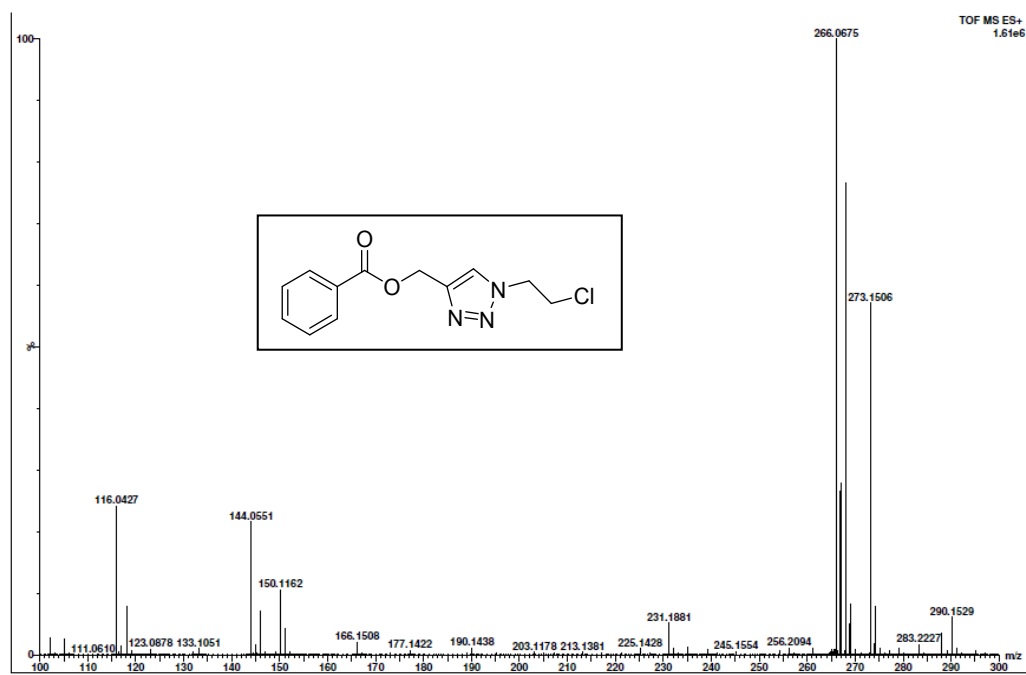
2-(1-(2-chloroethyl)-1H-1,2,3-triazol-4-yl)benzenamine **8** (ESI MS in MeCN:H<sub>2</sub>O (1:1))



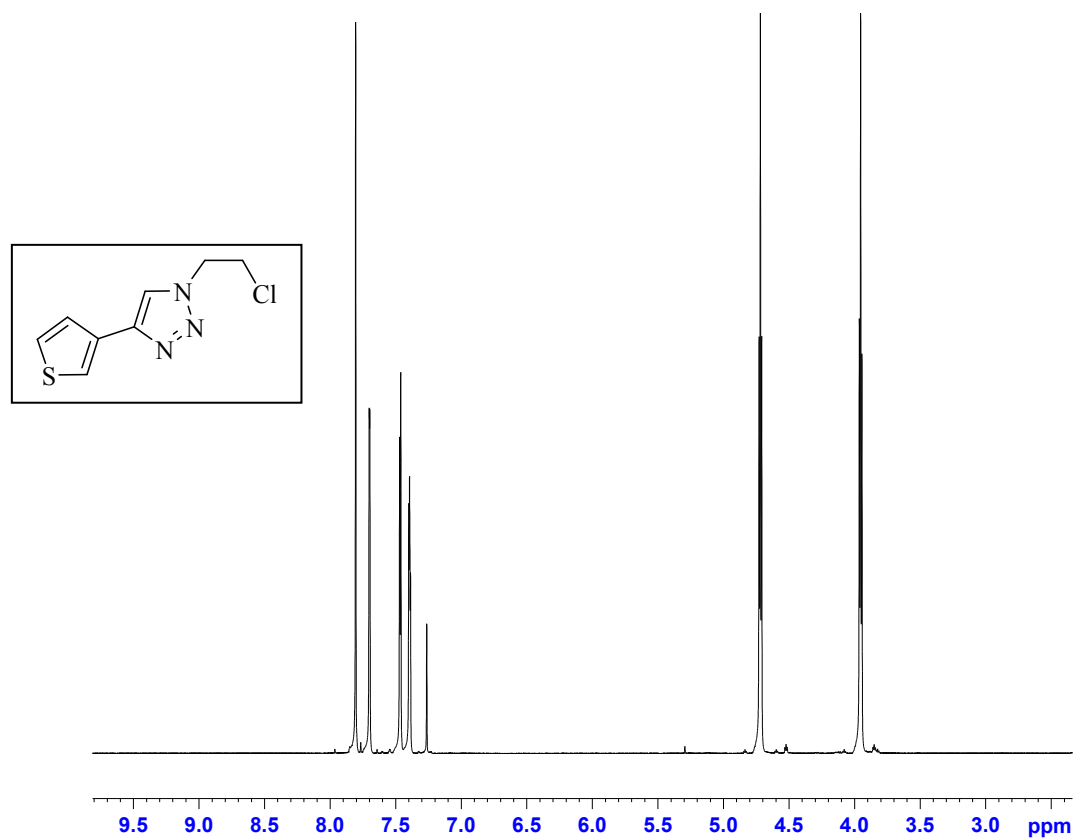
(1-(2-chloroethyl)-1*H*-1,2,3-triazol-4-yl)methyl benzoate **9** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )



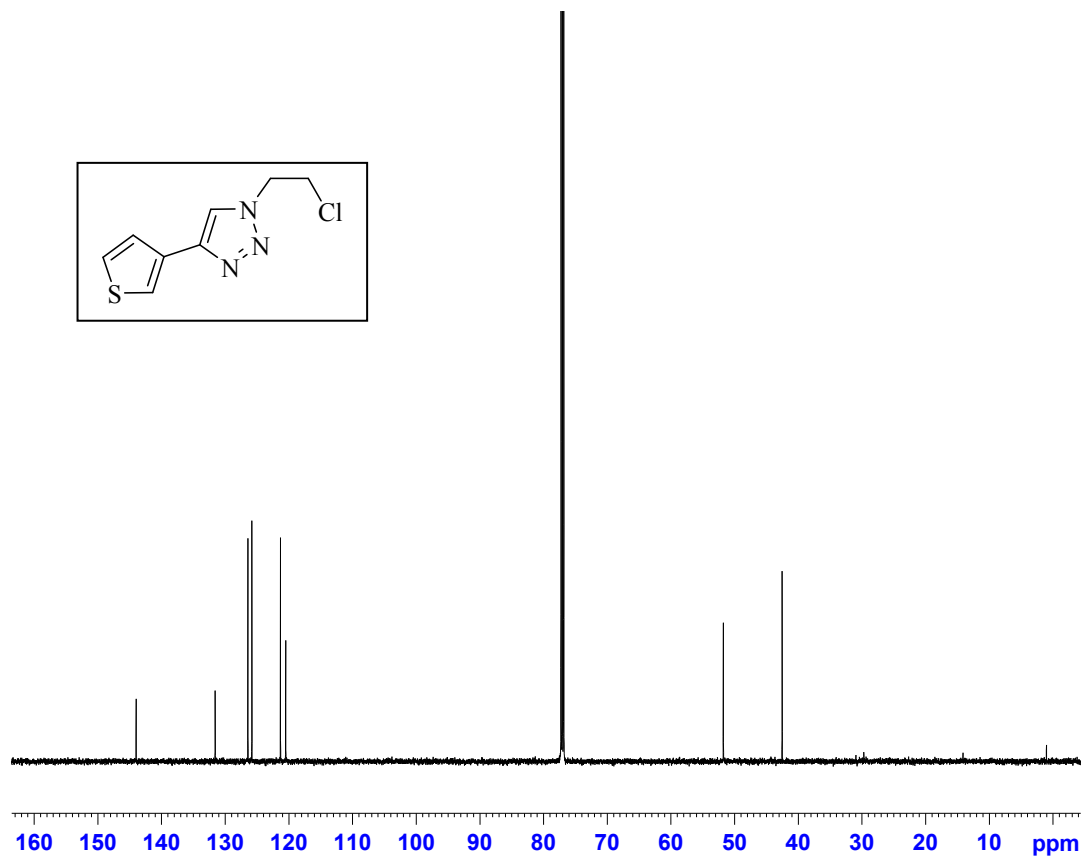
(1-(2-chloroethyl)-1*H*-1,2,3-triazol-4-yl)methyl benzoate **9** (ESI MS in MeCN:H<sub>2</sub>O (1:1))



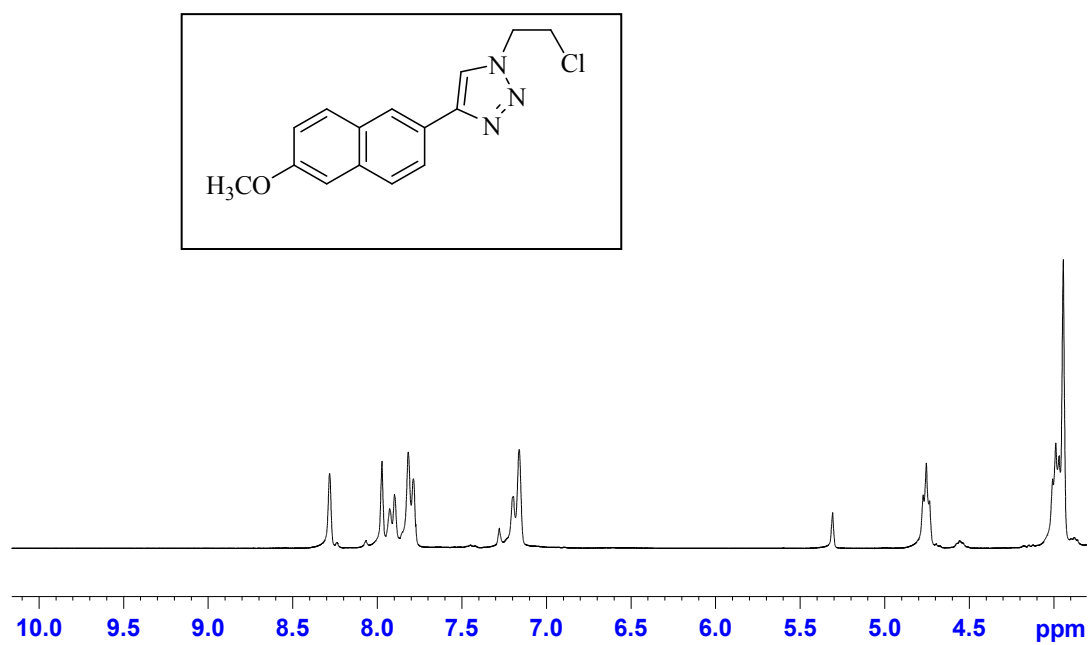
1-(2-chloroethyl)-4-(thiophen-3-yl)-1*H*-1,2,3-triazole **10** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)

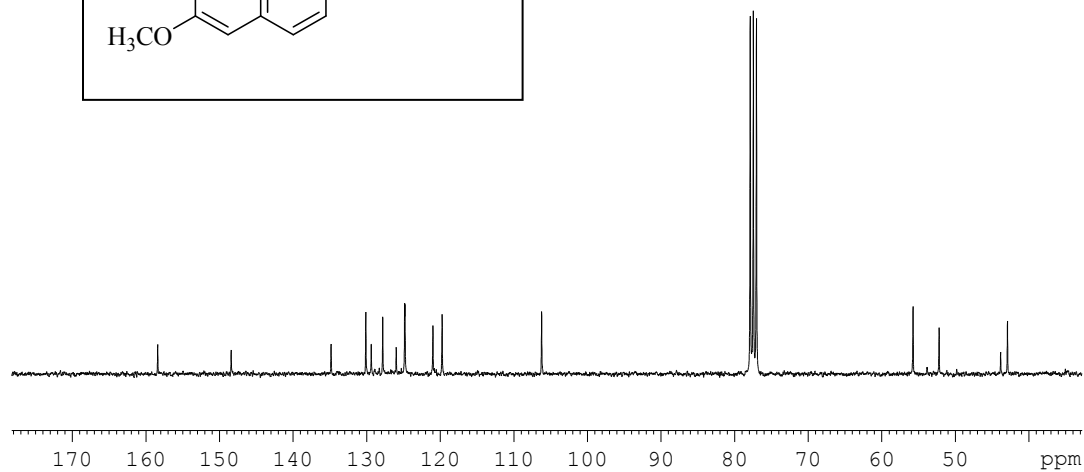
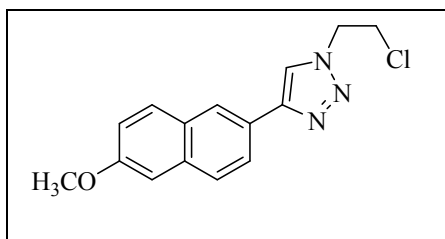




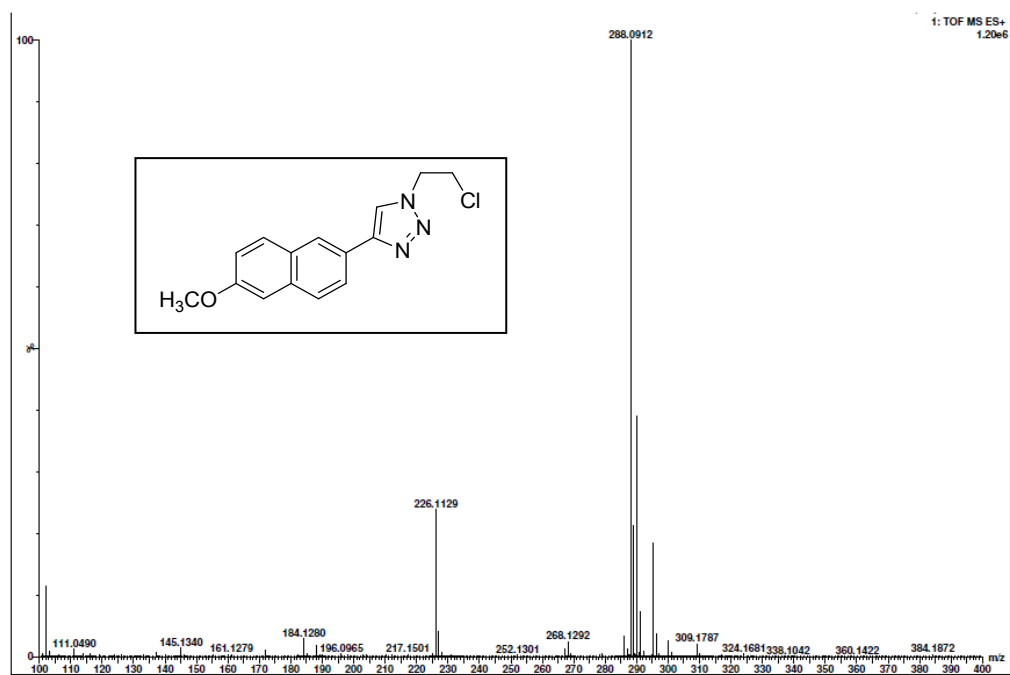


1-(2-chloroethyl)-4-(2-methoxynaphthalen-6-yl)-1H-1,2,3-triazole **11** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )

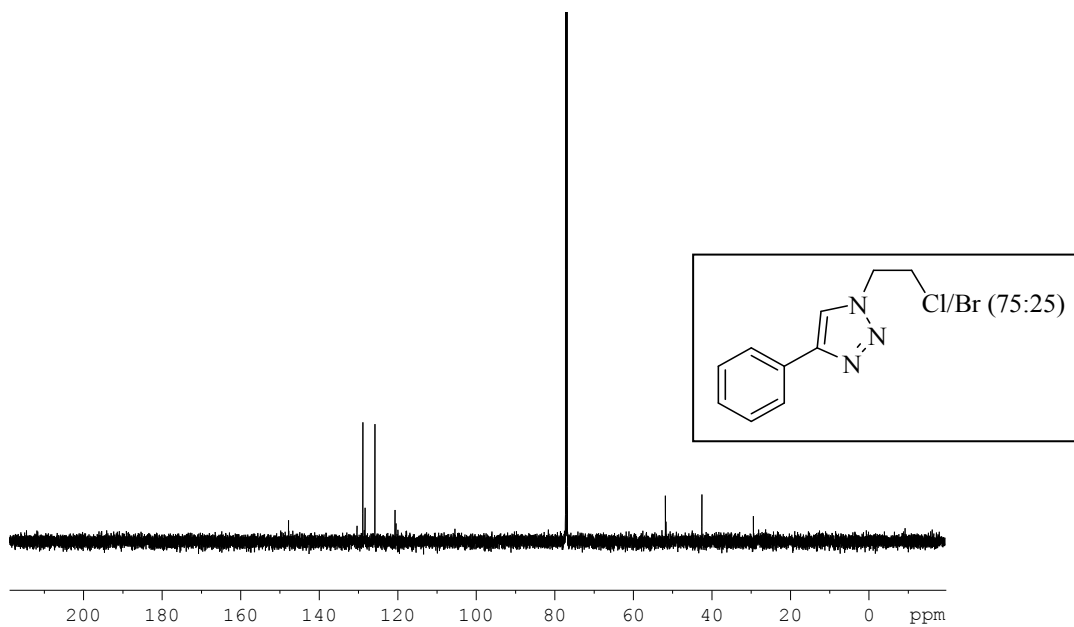
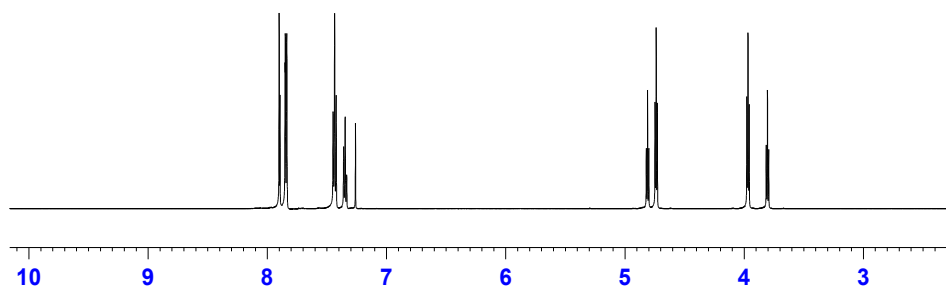
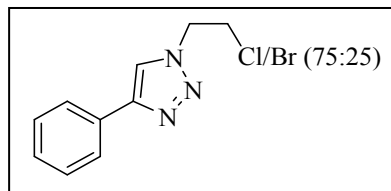




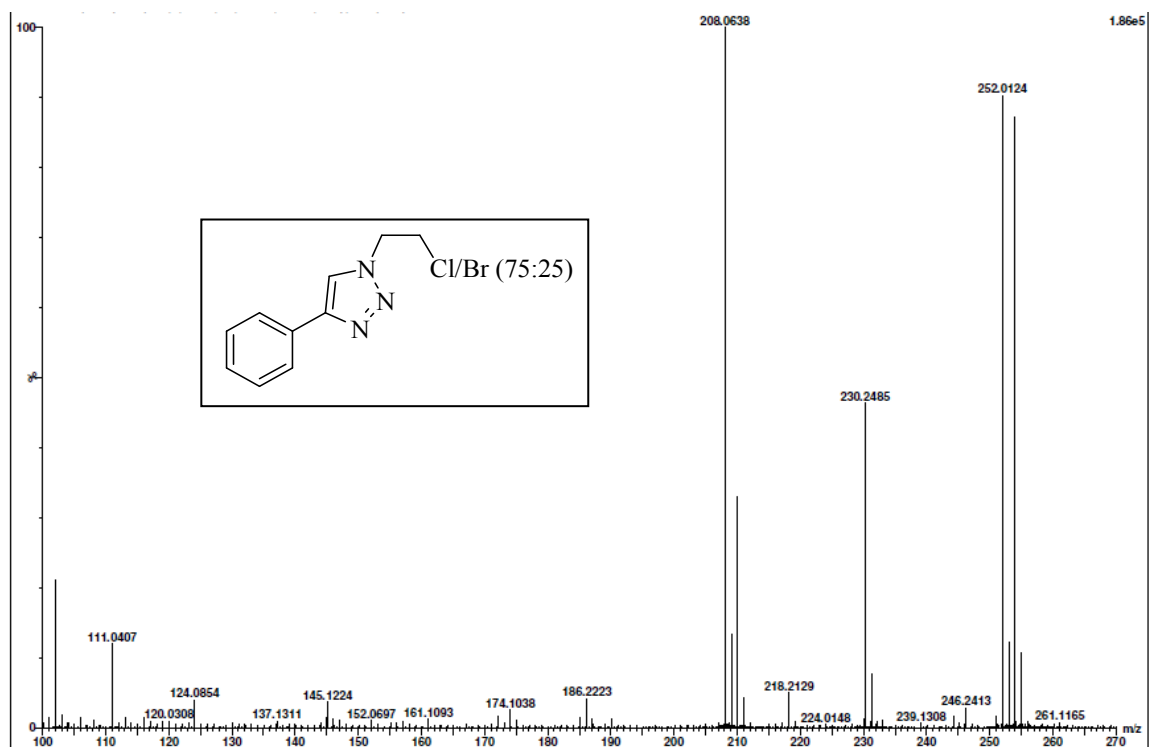
1-(2-chloroethyl)-4-(2-methoxynaphthalen-6-yl)-1H-1,2,3-triazole **11** (ESI MS in MeCN:H<sub>2</sub>O (1:1))



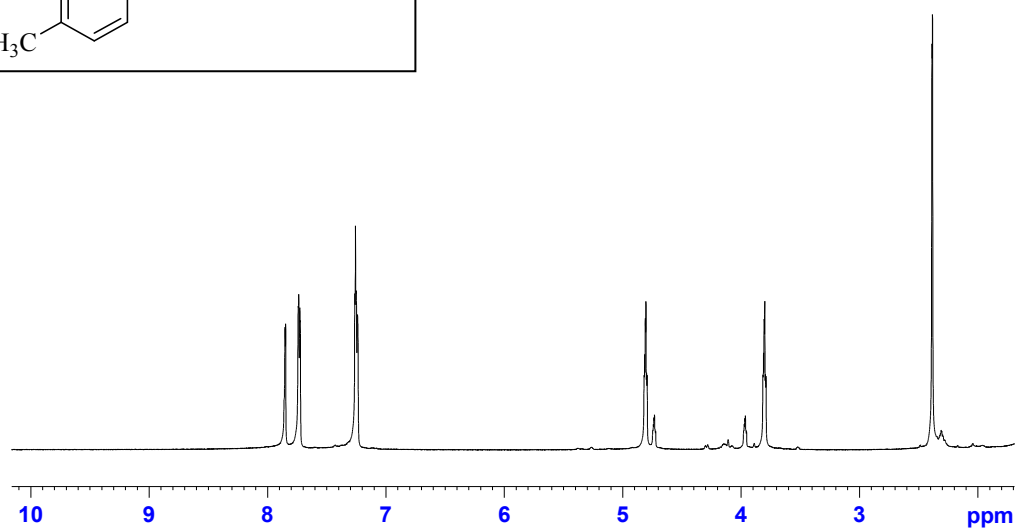
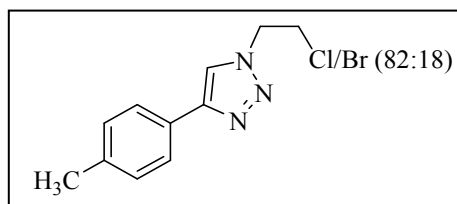
1-(2-chloro/bromoethyl)-4-phenyl-1*H*-1,2,3-triazole **12** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)

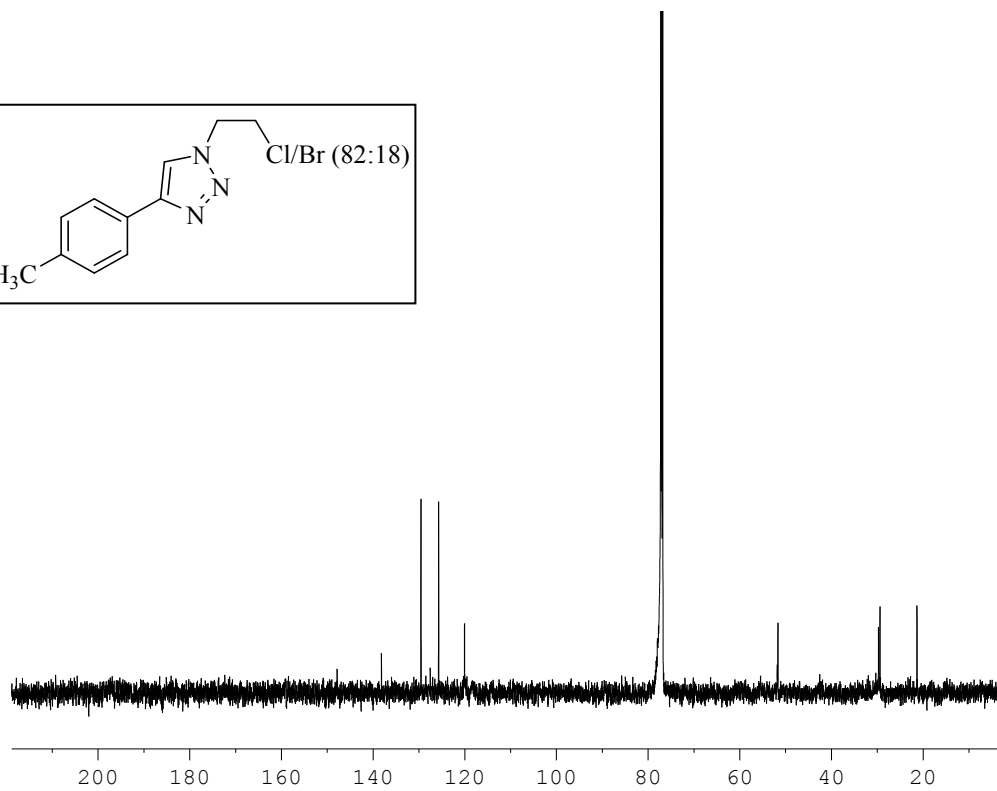
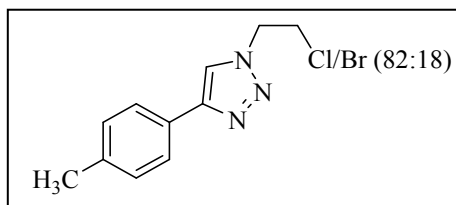


1-(2-chloro/bromoethyl)-4-phenyl-1*H*-1,2,3-triazole **12** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

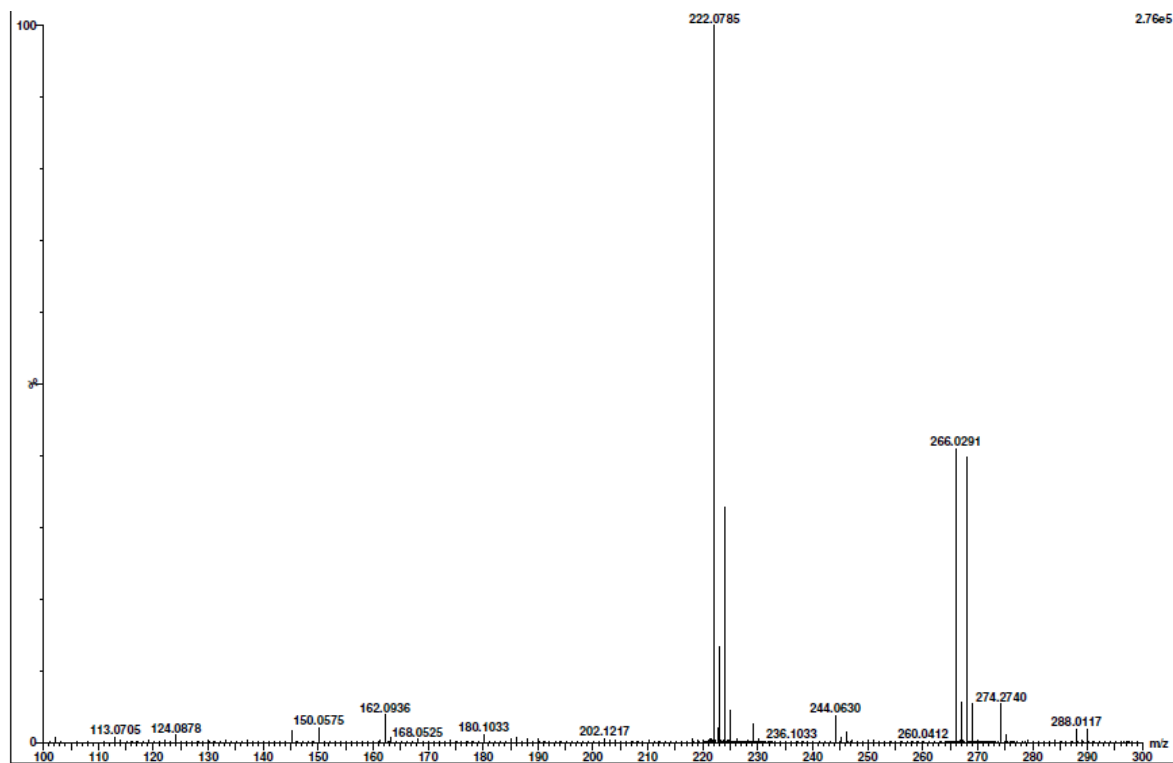


1-(2-chloro/bromoethyl)-4-*p*-tolyl-1*H*-1,2,3-triazole **13** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)

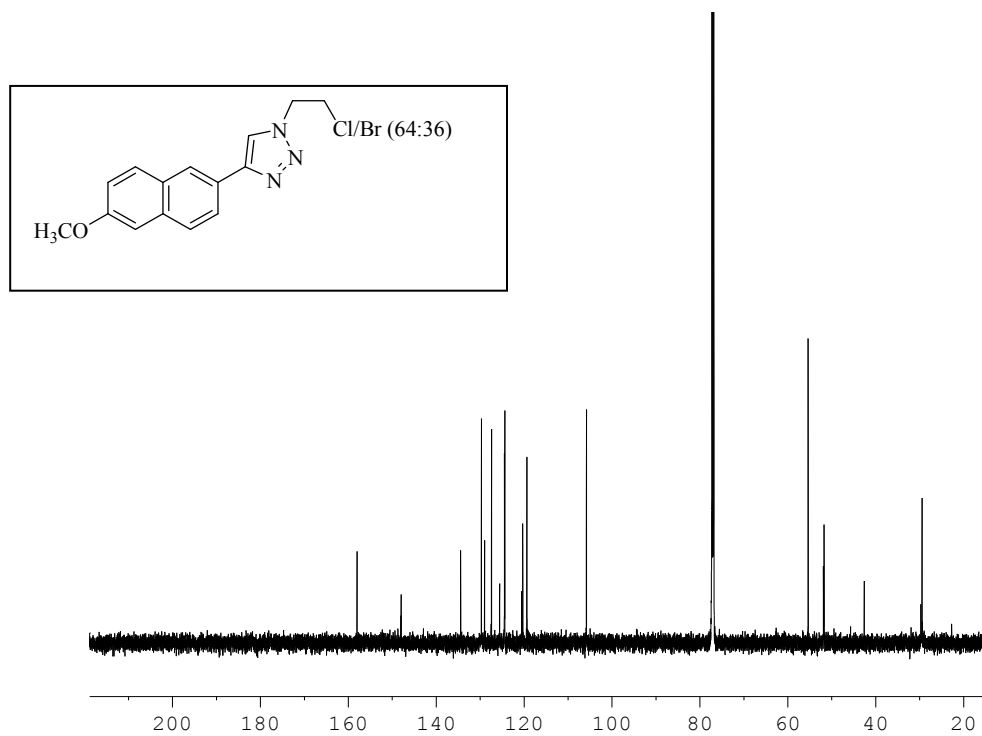
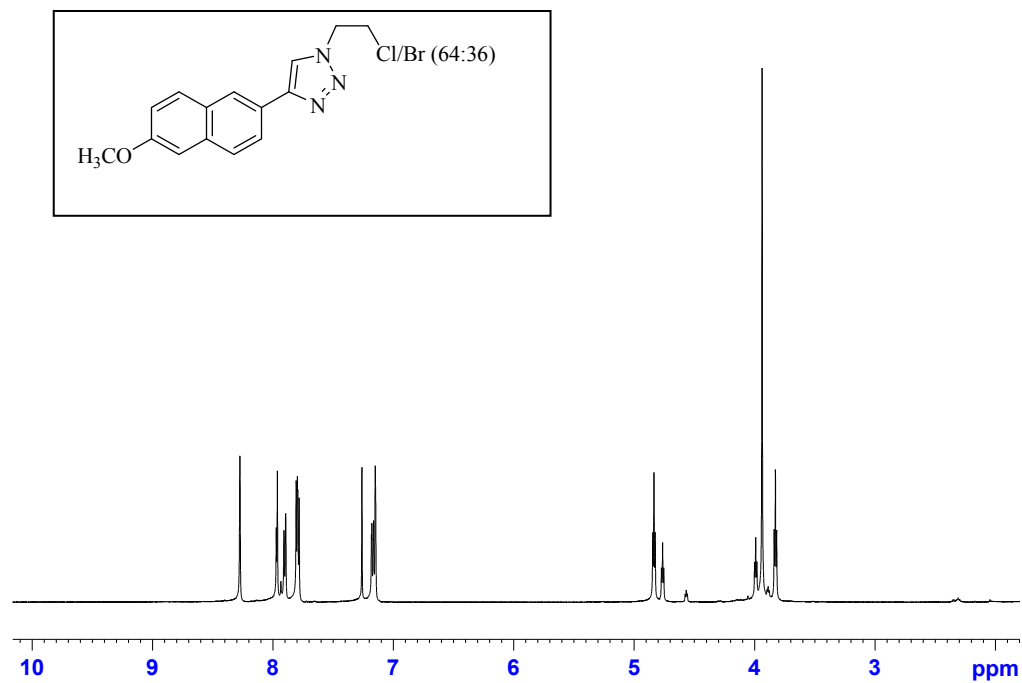




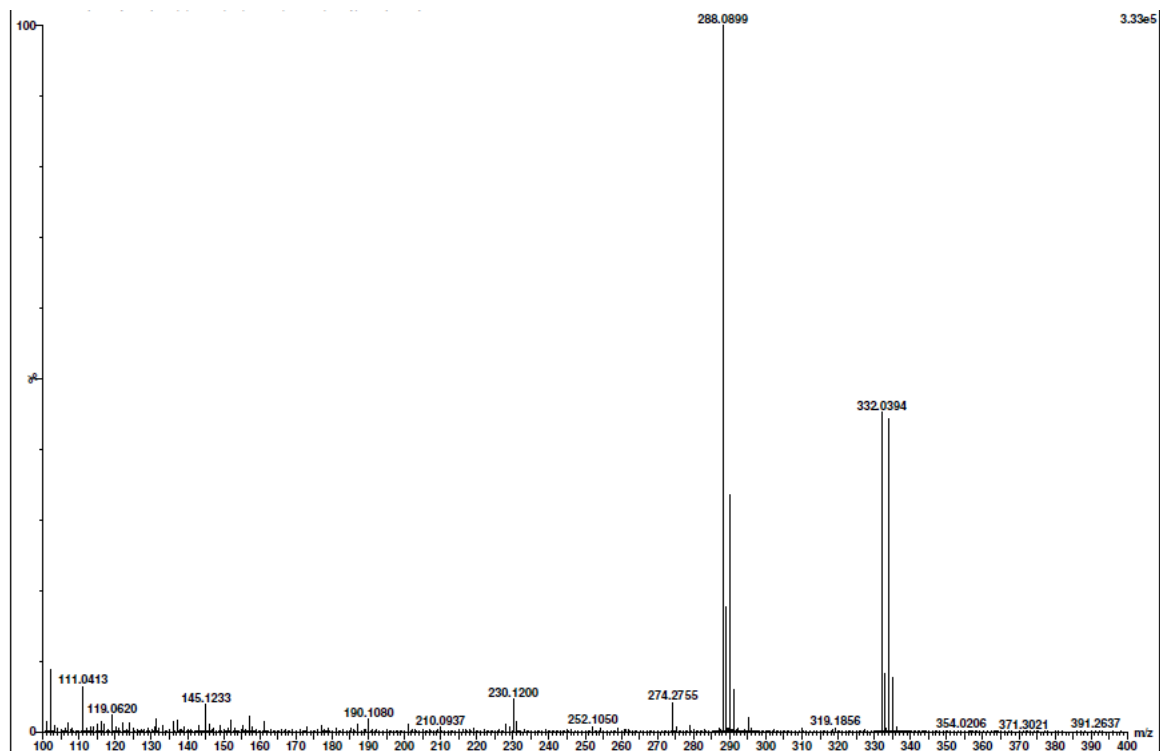
1-(2-chloro/bromoethyl)-4-*p*-tolyl-1*H*-1,2,3-triazole **13** (ESI MS in MeCN:H<sub>2</sub>O (1:1))



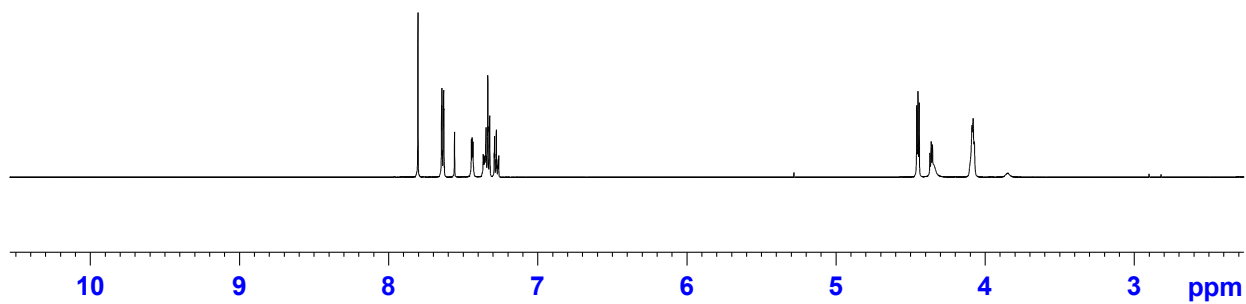
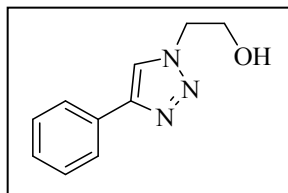
1-(2-chloro/bromoethyl)-4-(2-methoxynaphthalen-6-yl)-1*H*-1,2,3-triazole **14** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )

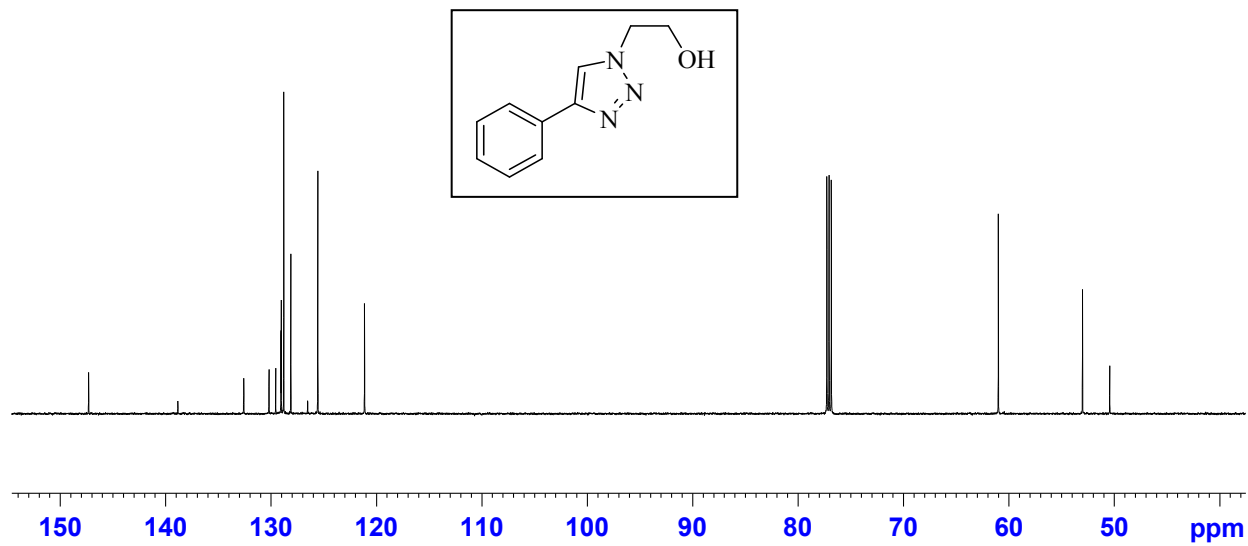


1-(2-chloro/bromoethyl)-4-(2-methoxynaphthalen-6-yl)-1*H*-1,2,3-triazole **14** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

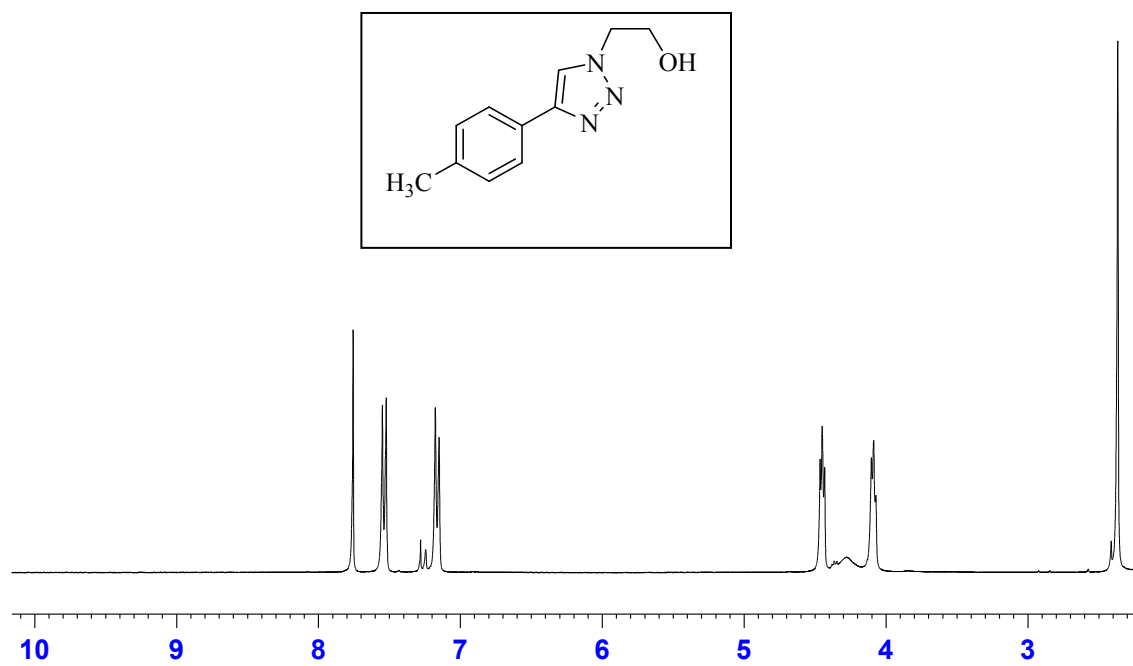


2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethanol **15** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)

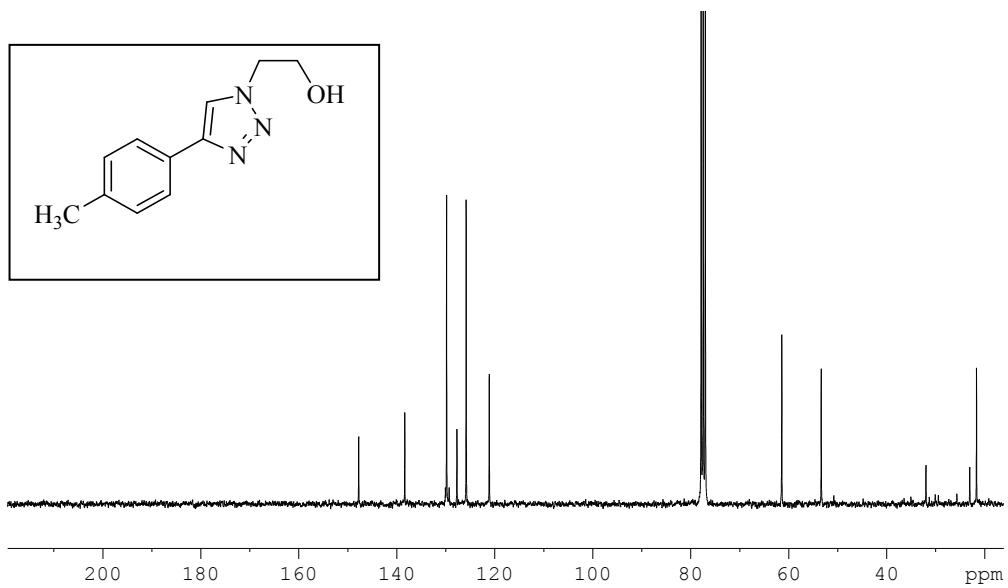




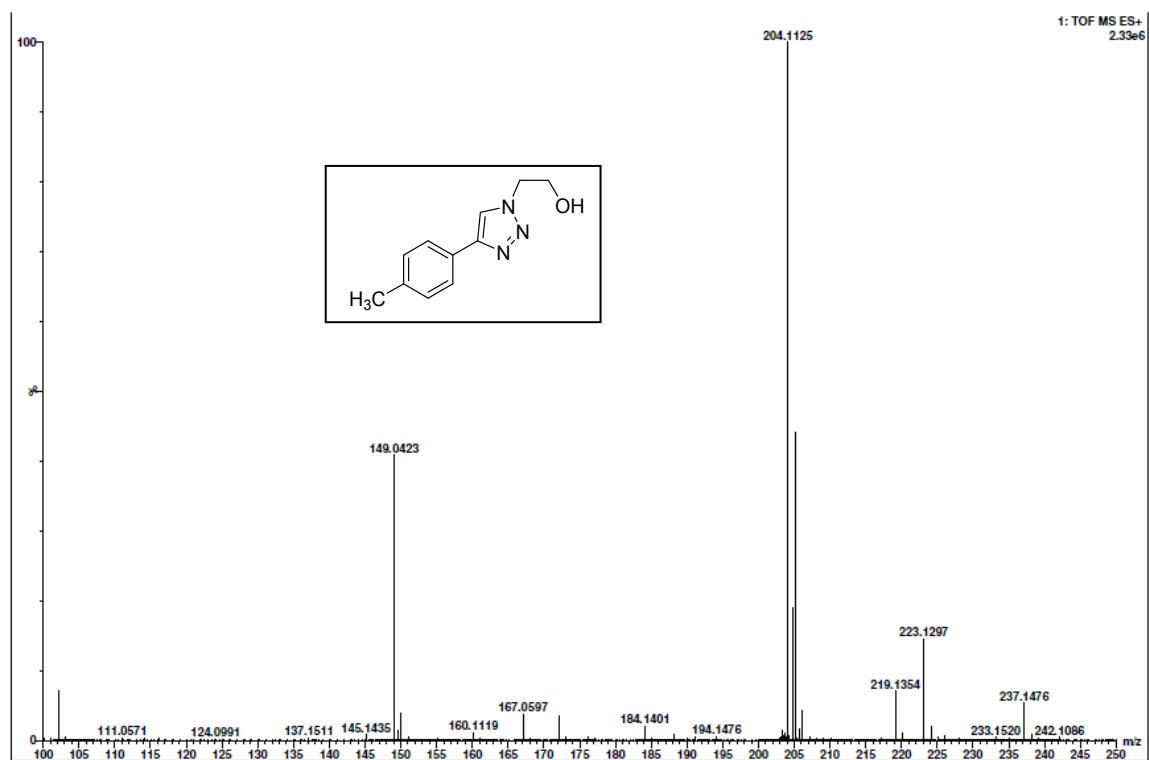
2-(4-p-tolyl-1H-1,2,3-triazol-1-yl)ethanol **16** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)



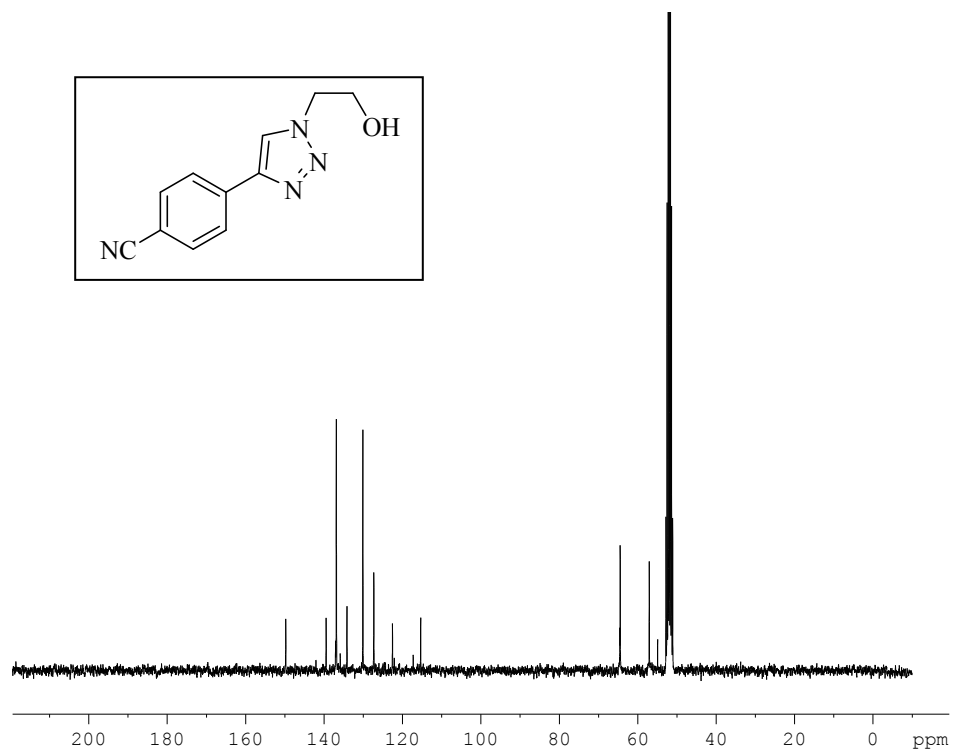
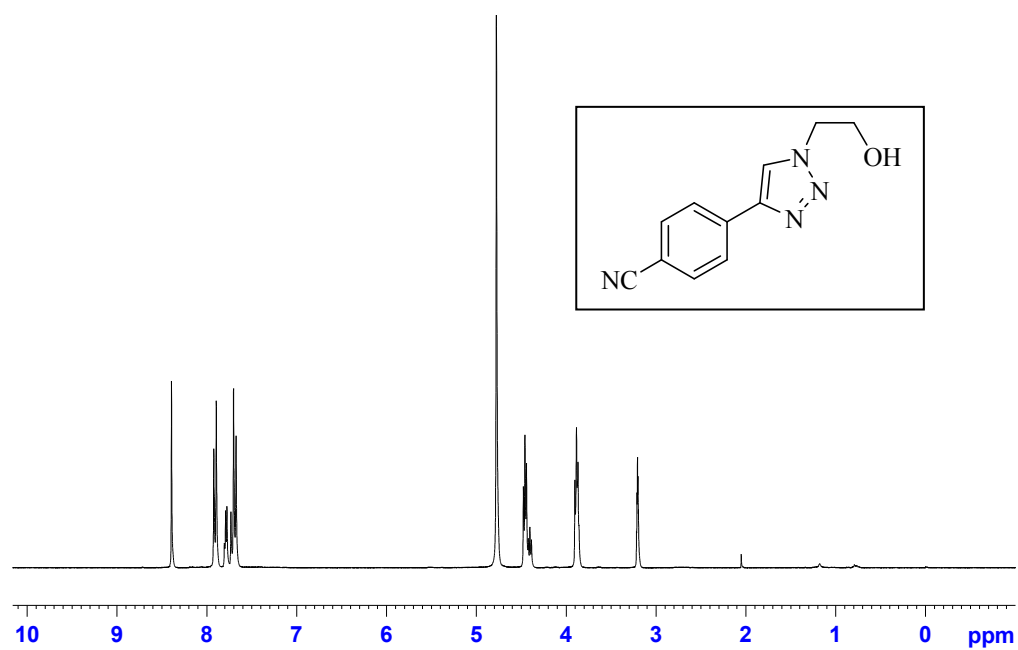




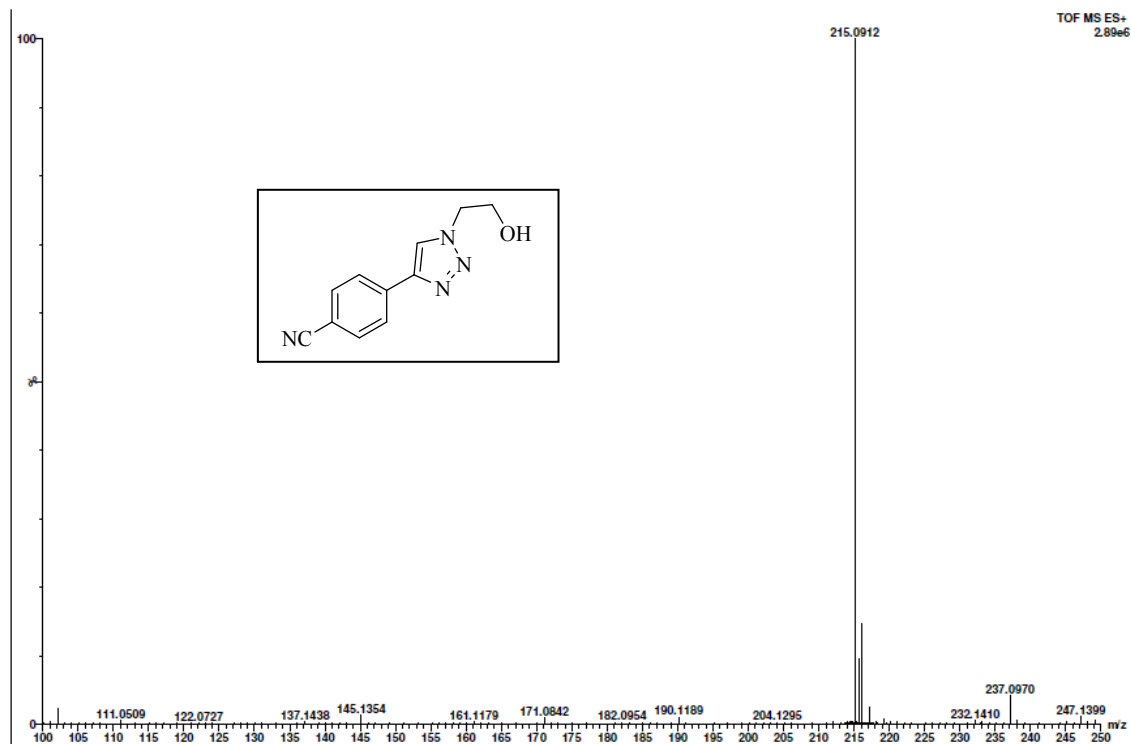
2-(4-p-tolyl-1H-1,2,3-triazol-1-yl)ethanol (ESI MS in MeCN:H<sub>2</sub>O (1:1))



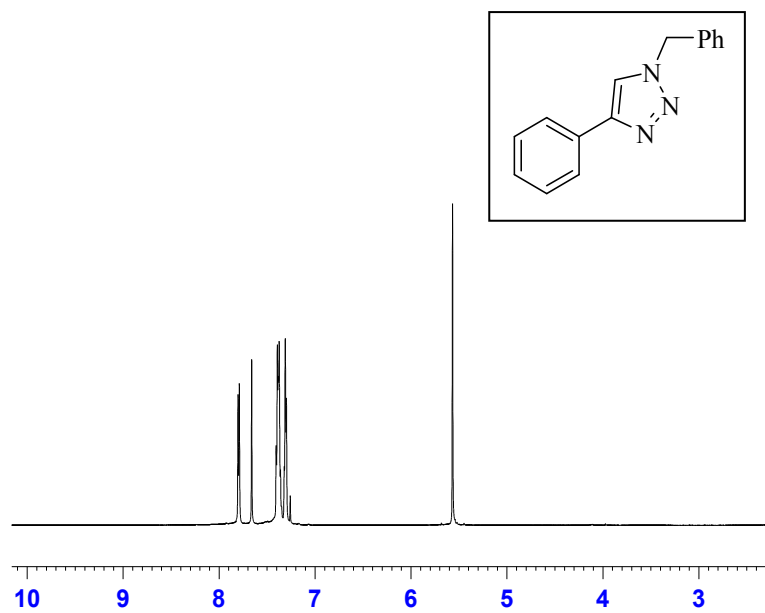
4-(1-(2-hydroxyethyl)-1*H*-1,2,3-triazol-4-yl)benzonitrile **17** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in MeOD)

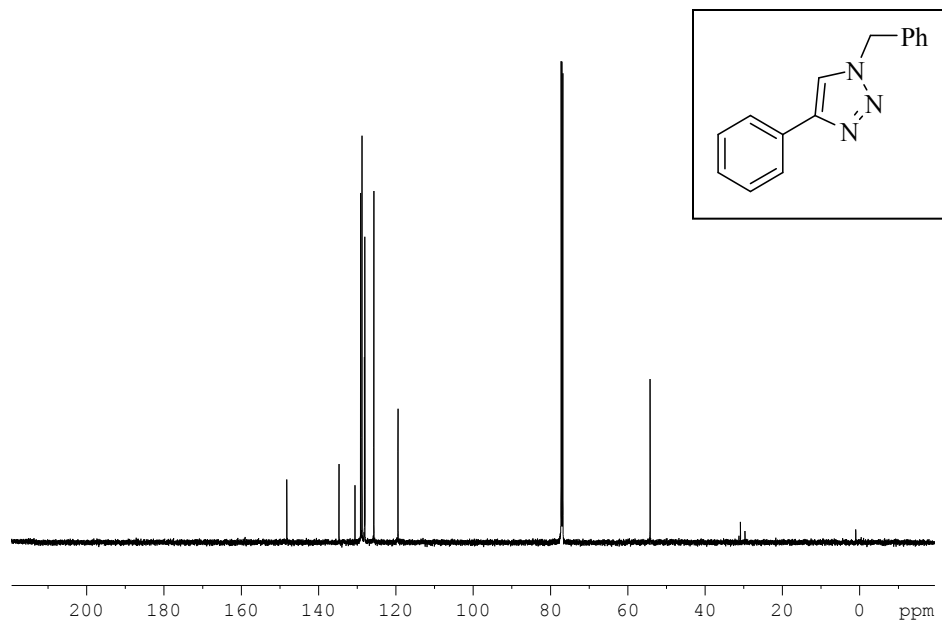


4-(1-(2-hydroxyethyl)-1*H*-1,2,3-triazol-4-yl)benzotrile **17** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

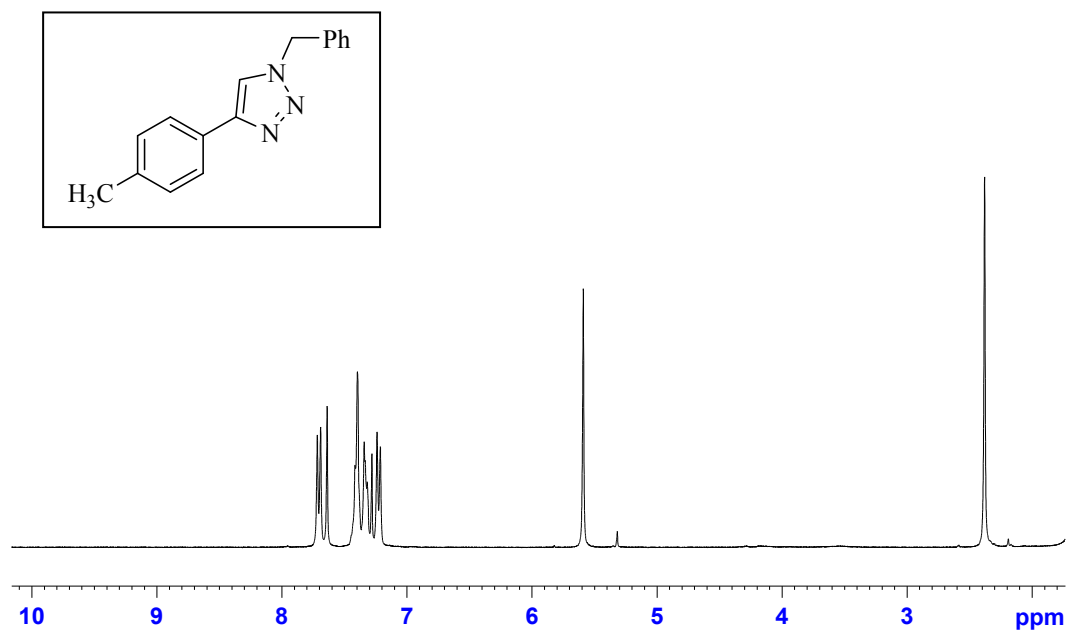


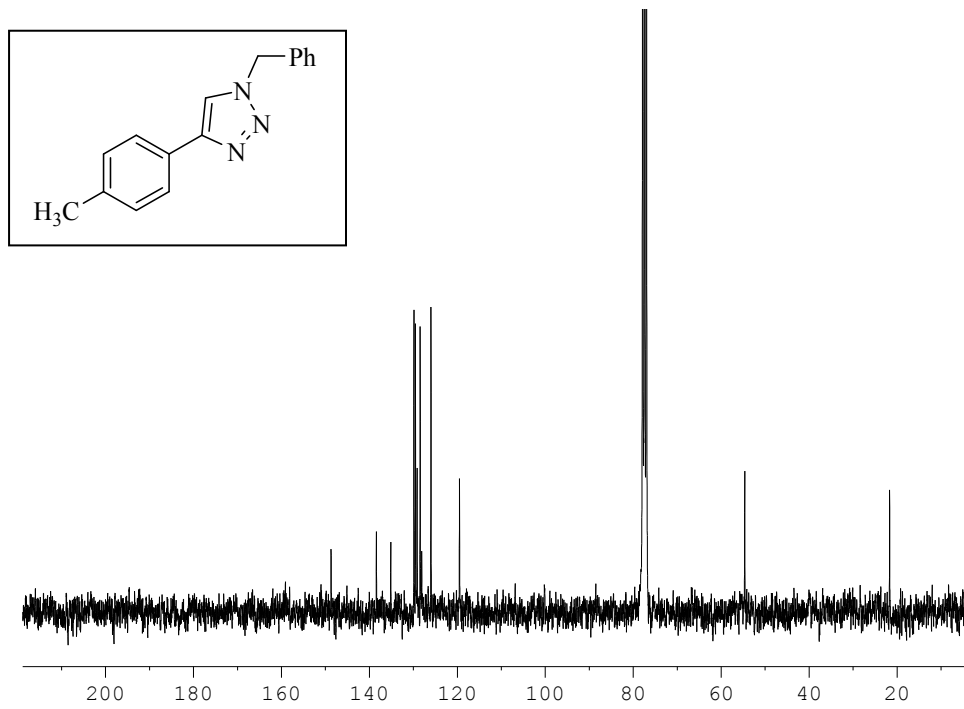
1-benzyl-4-phenyl-1*H*-1,2,3-triazole **18** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)



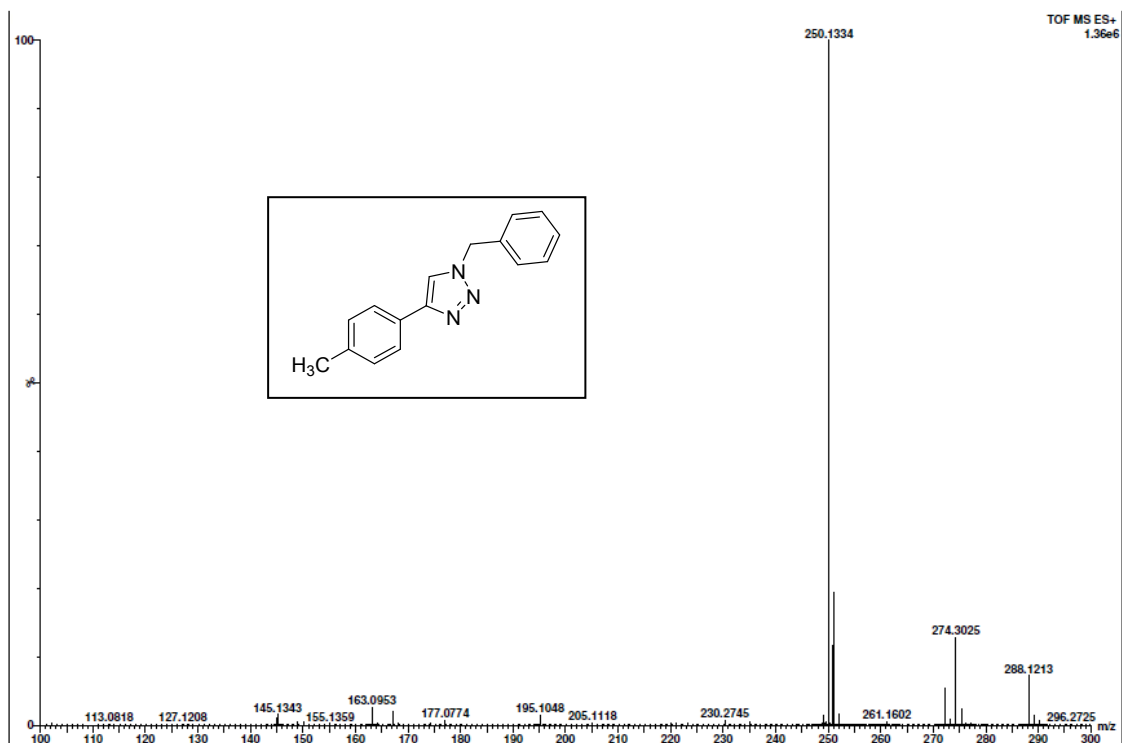


1-benzyl-4-p-tolyl-1H-1,2,3-triazole **19** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)

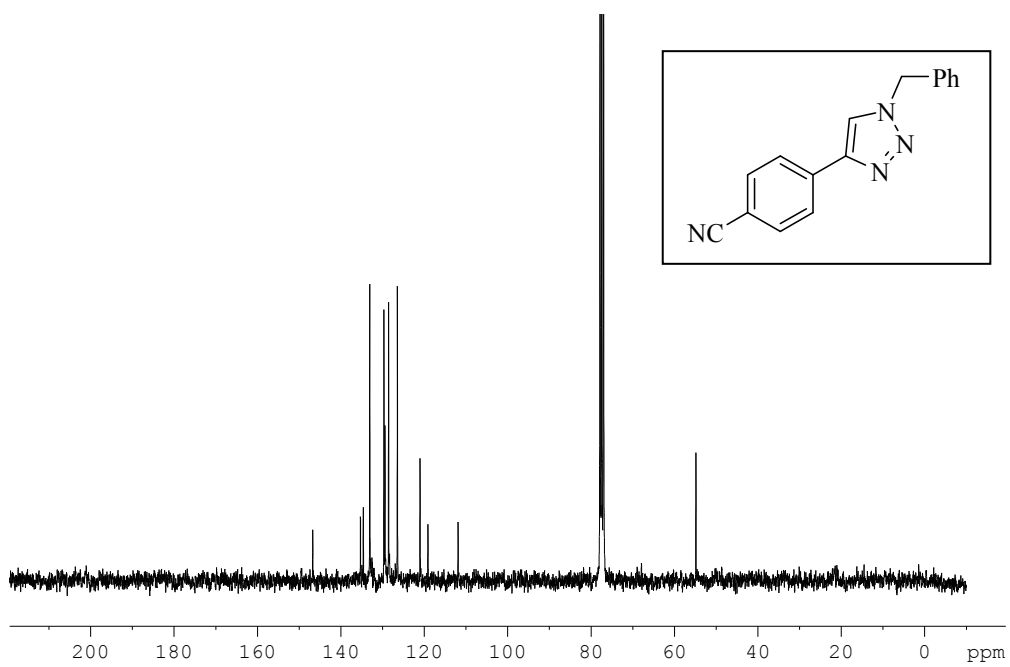
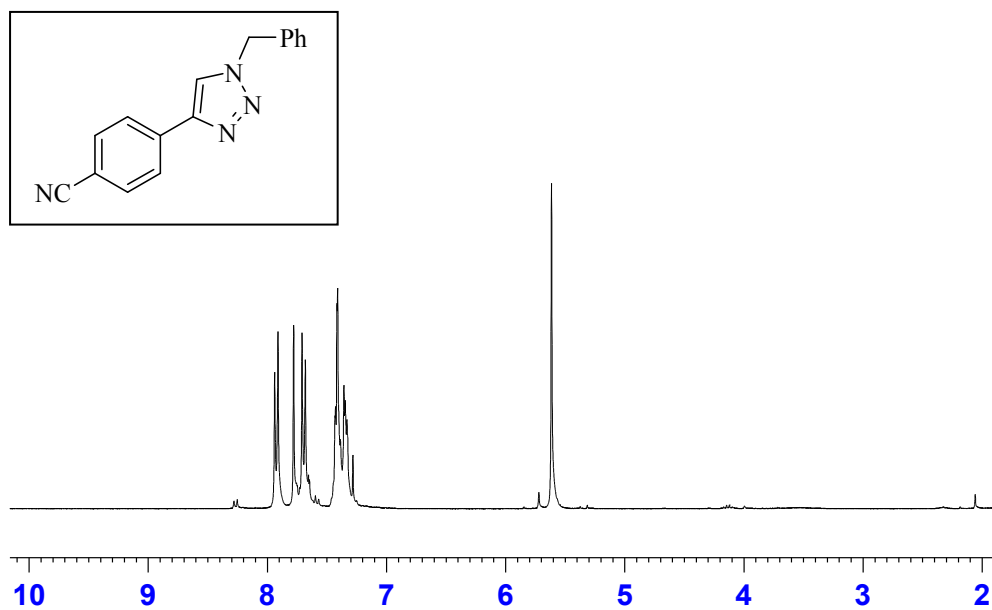




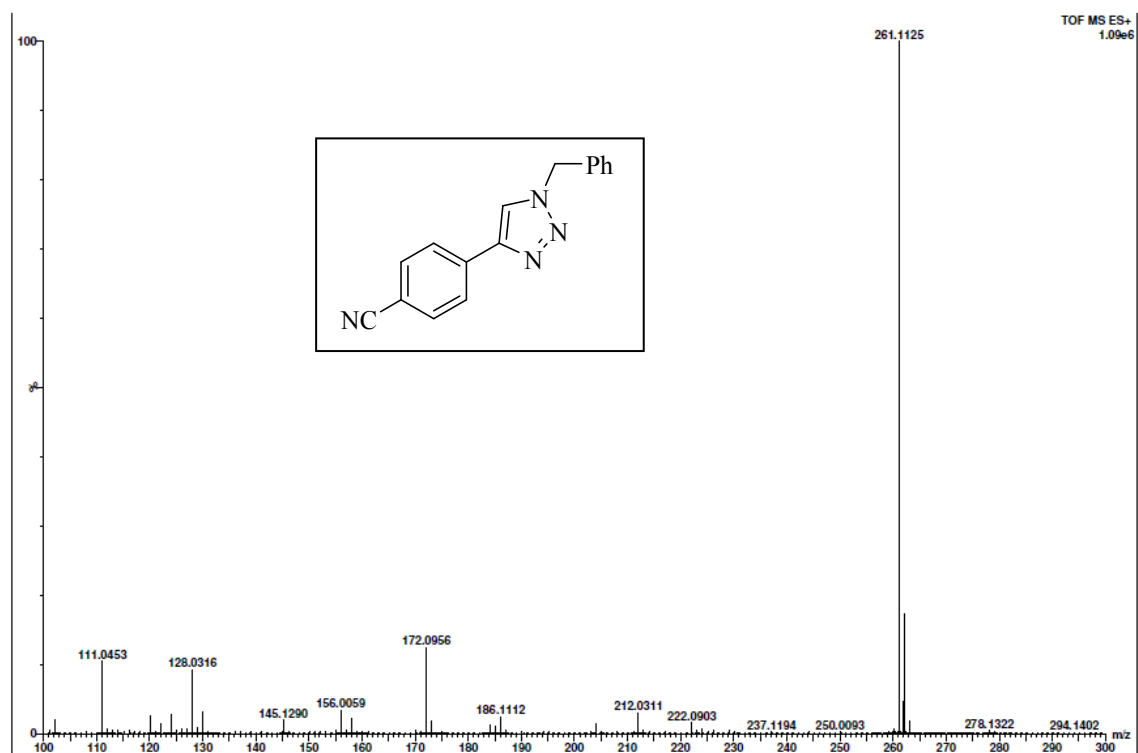
1-benzyl-4-*p*-tolyl-1*H*-1,2,3-triazole **19** (ESI MS in MeCN:H<sub>2</sub>O (1:1))



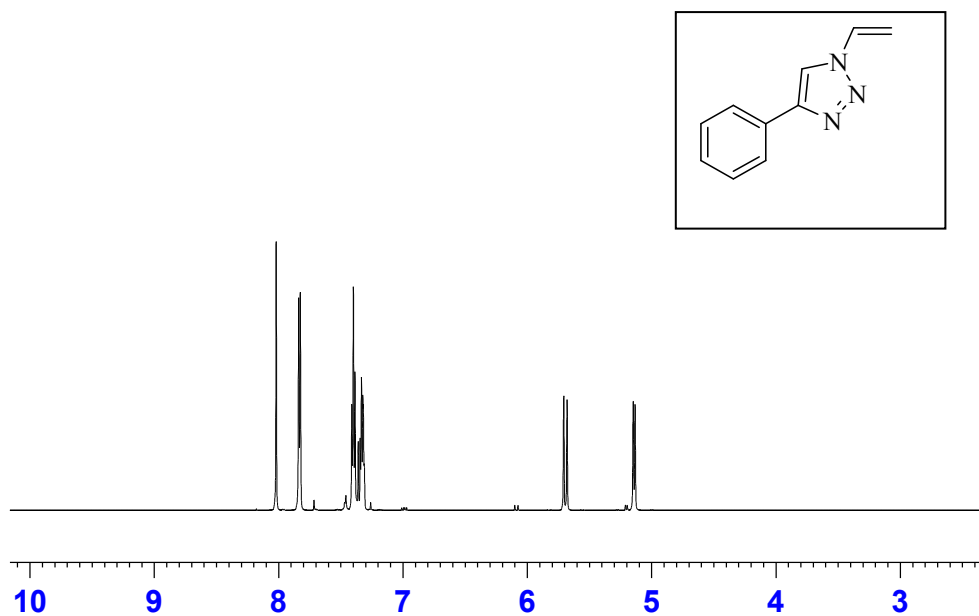
4-(1-benzyl-1*H*-1,2,3-triazol-4-yl)benzonitrile **20** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )

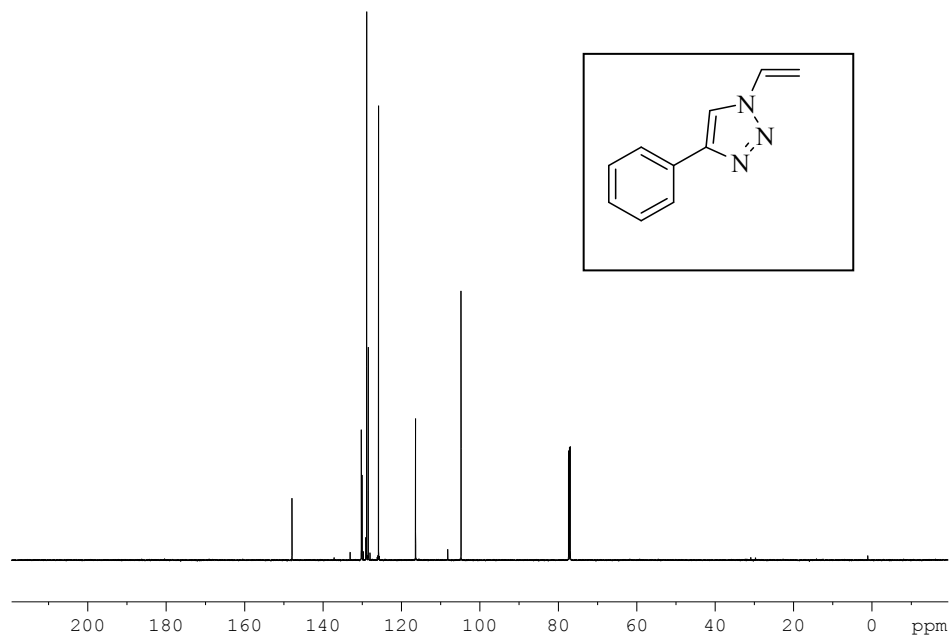


4-(1-benzyl-1*H*-1,2,3-triazol-4-yl)benzonitrile **20** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

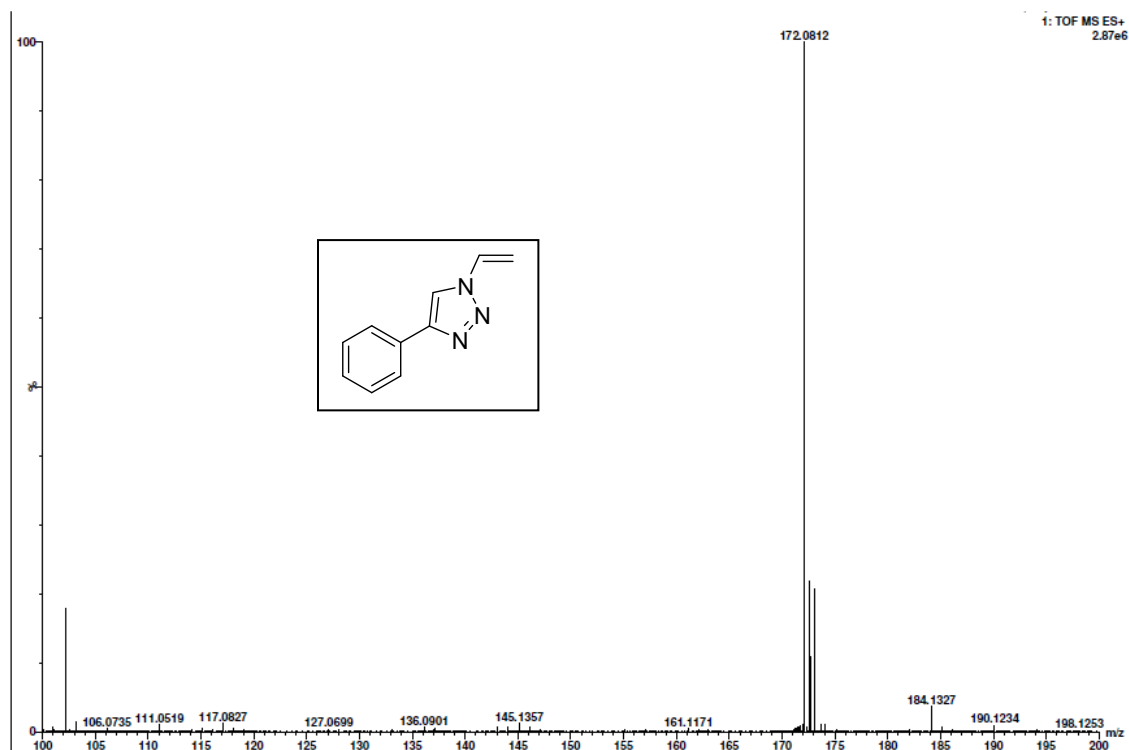


4-phenyl-1-vinyl-1*H*-1,2,3-triazole **21** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)



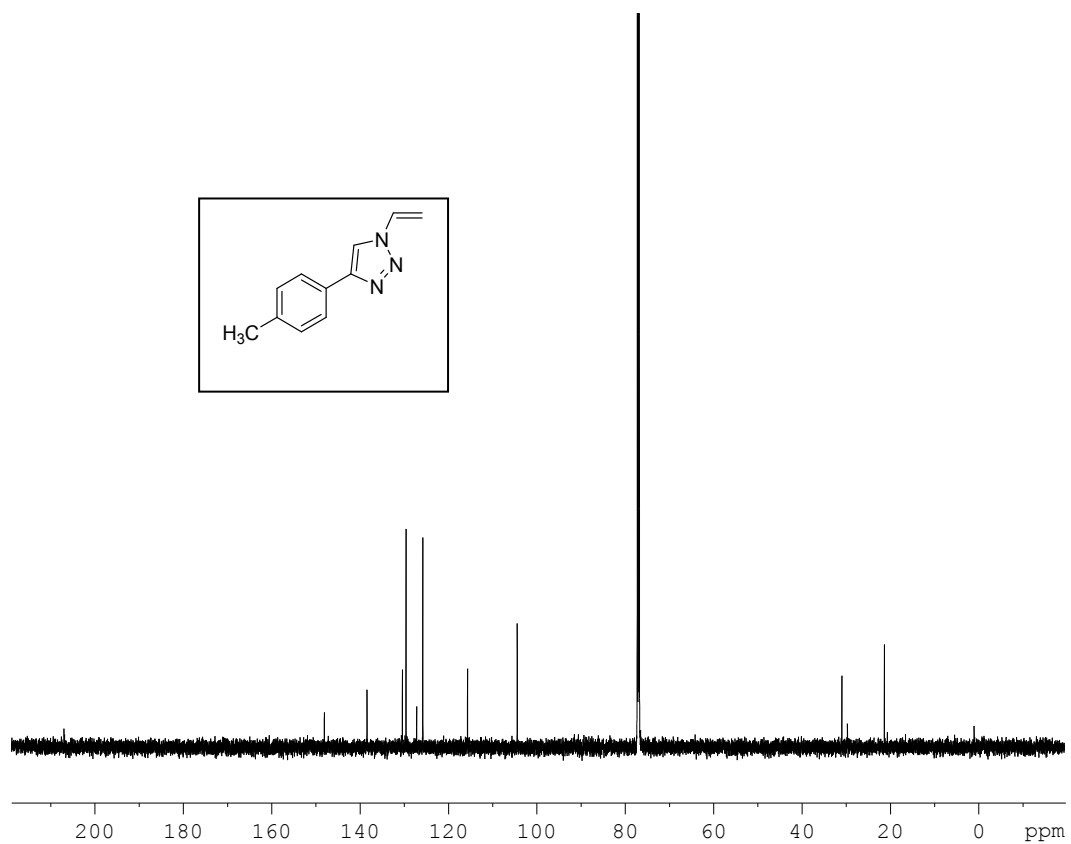
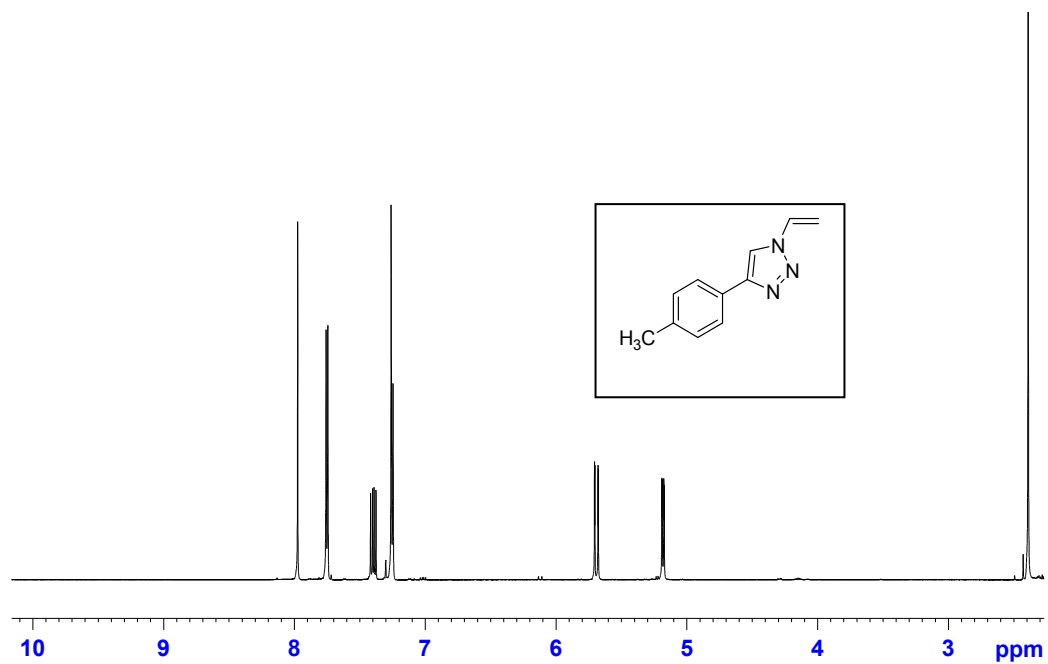


4-phenyl-1-vinyl-1H-1,2,3-triazole **21** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

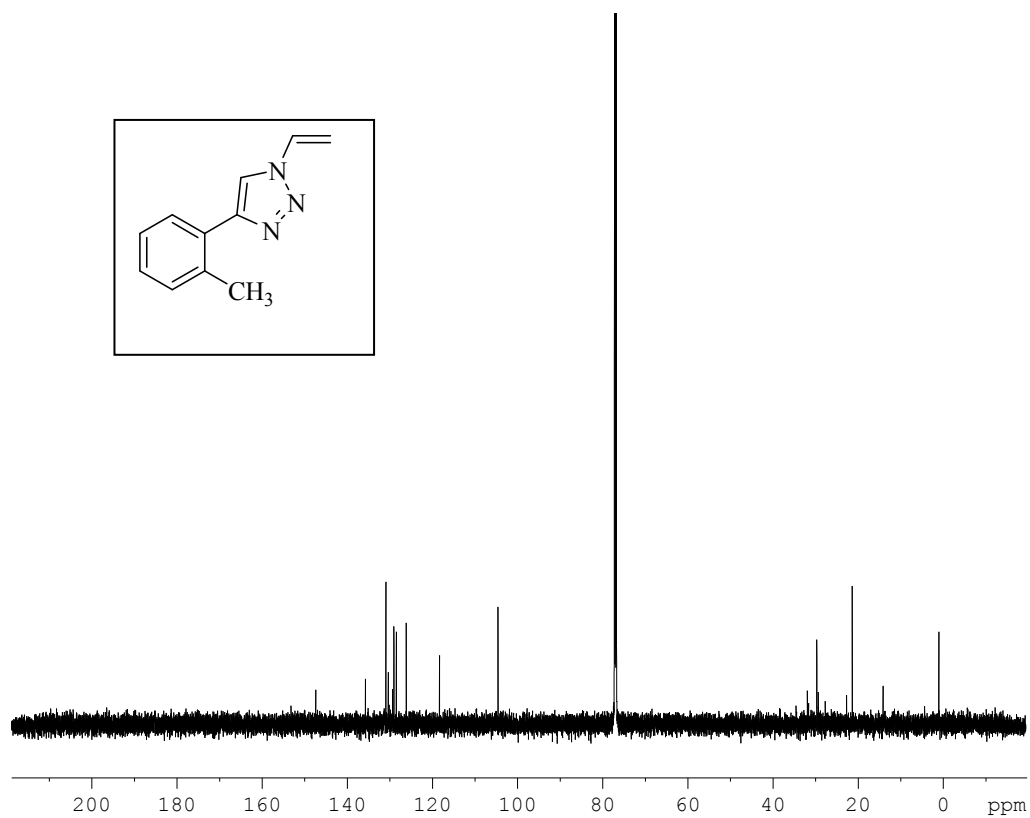




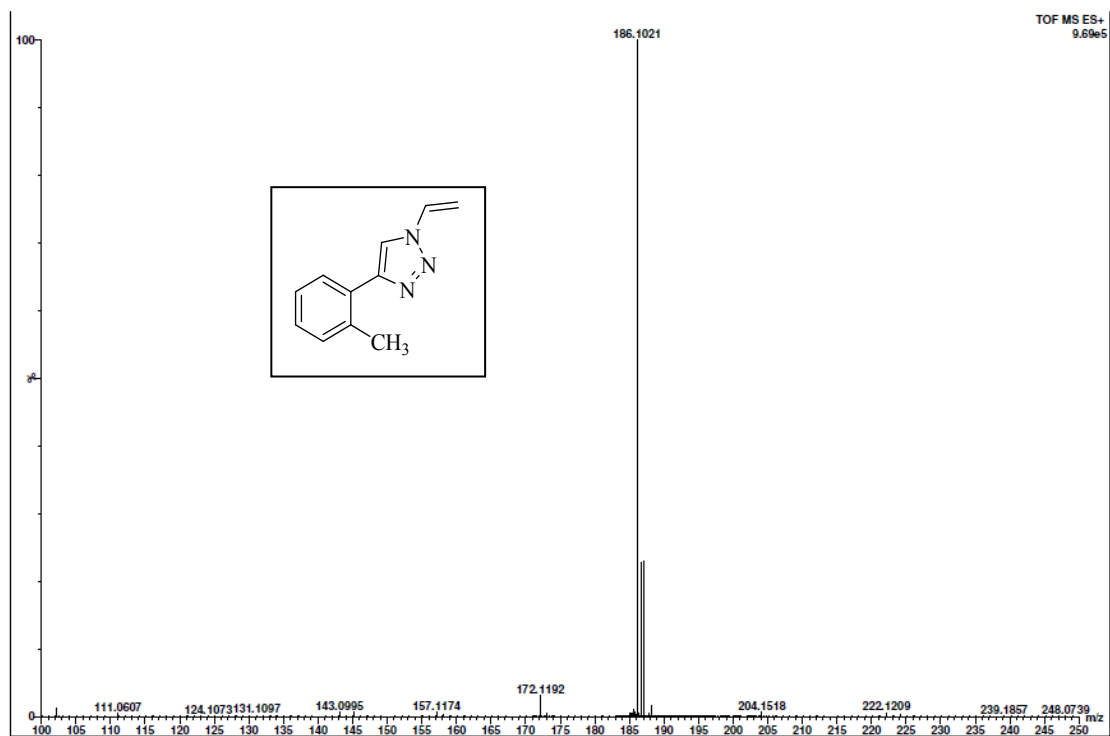
4-p-tolyl-1-vinyl-1*H*-1,2,3-triazole **22** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )



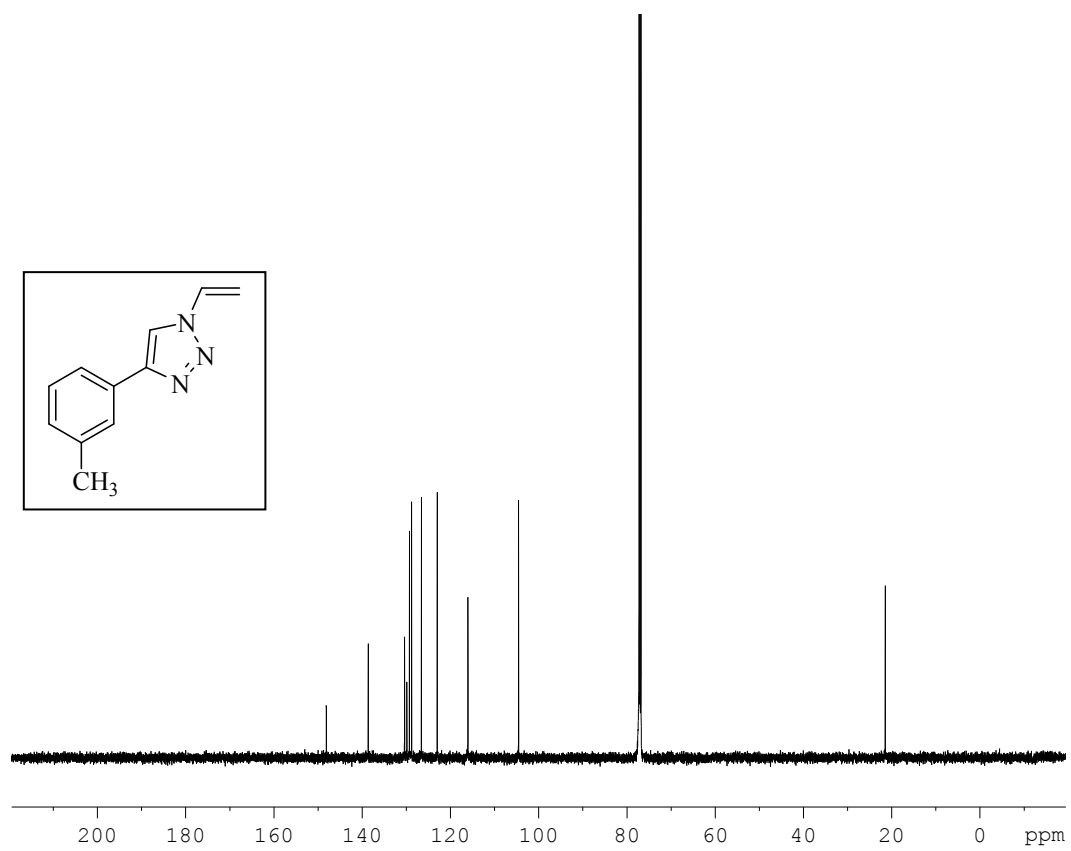
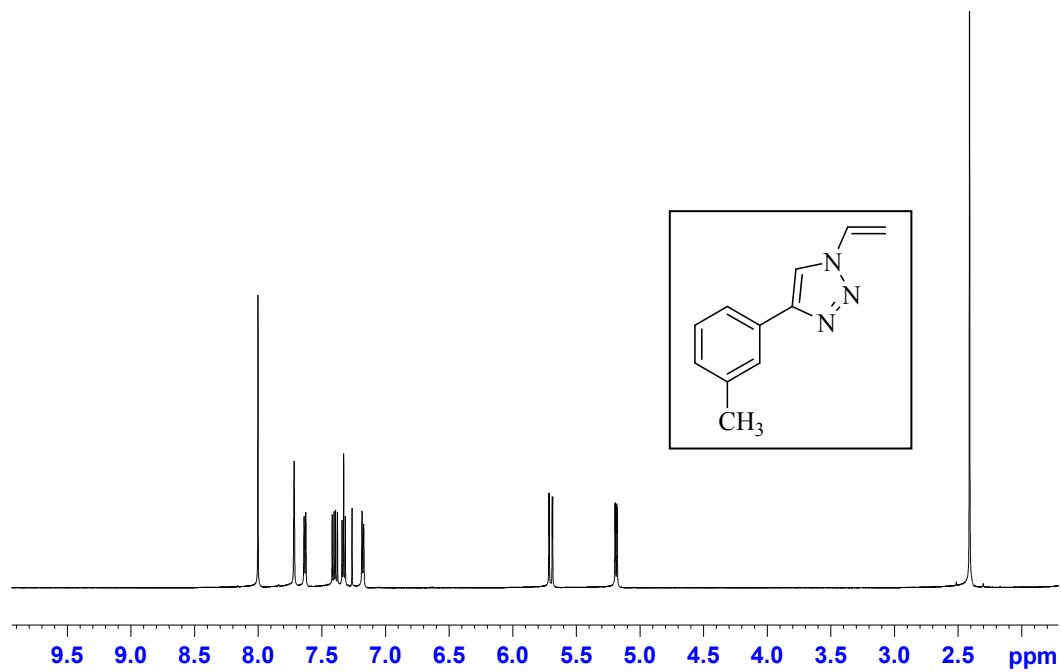




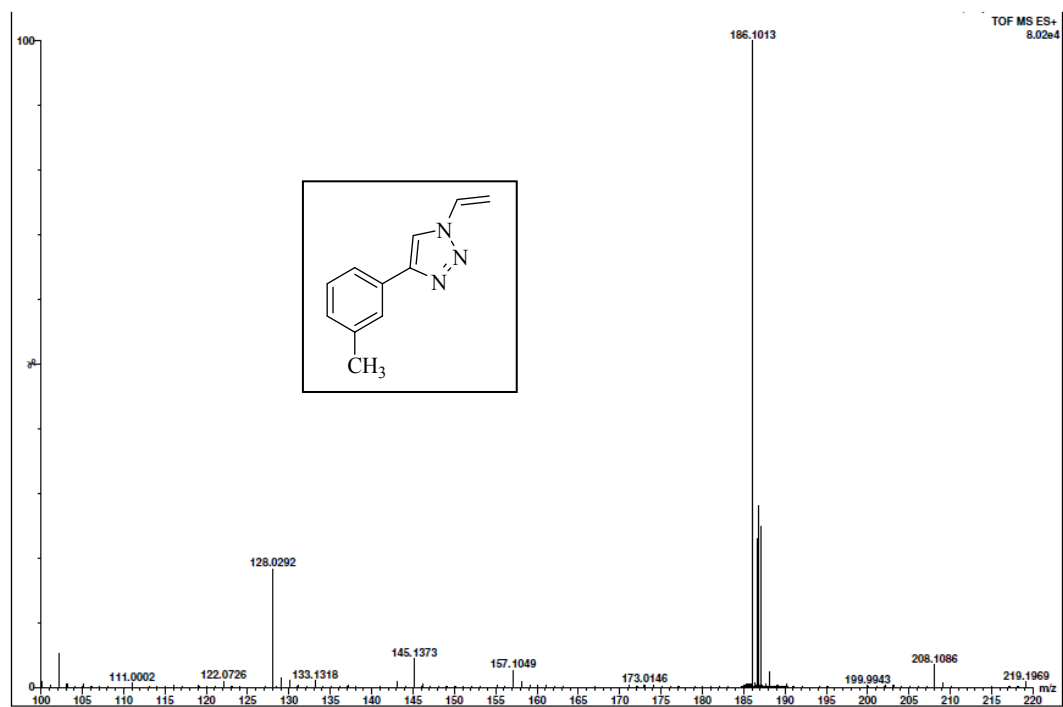
4-*o*-tolyl-1-vinyl-1*H*-1,2,3-triazole **23** (ESI MS in MeCN:H<sub>2</sub>O (1:1))



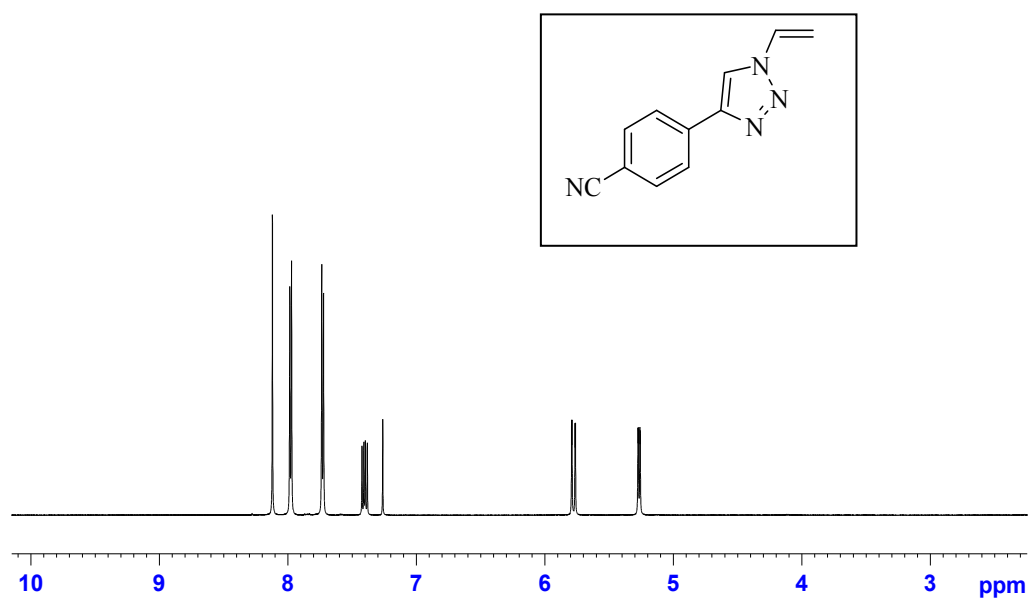
4-*m*-tolyl-1-vinyl-1*H*-1,2,3-triazole **24** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )

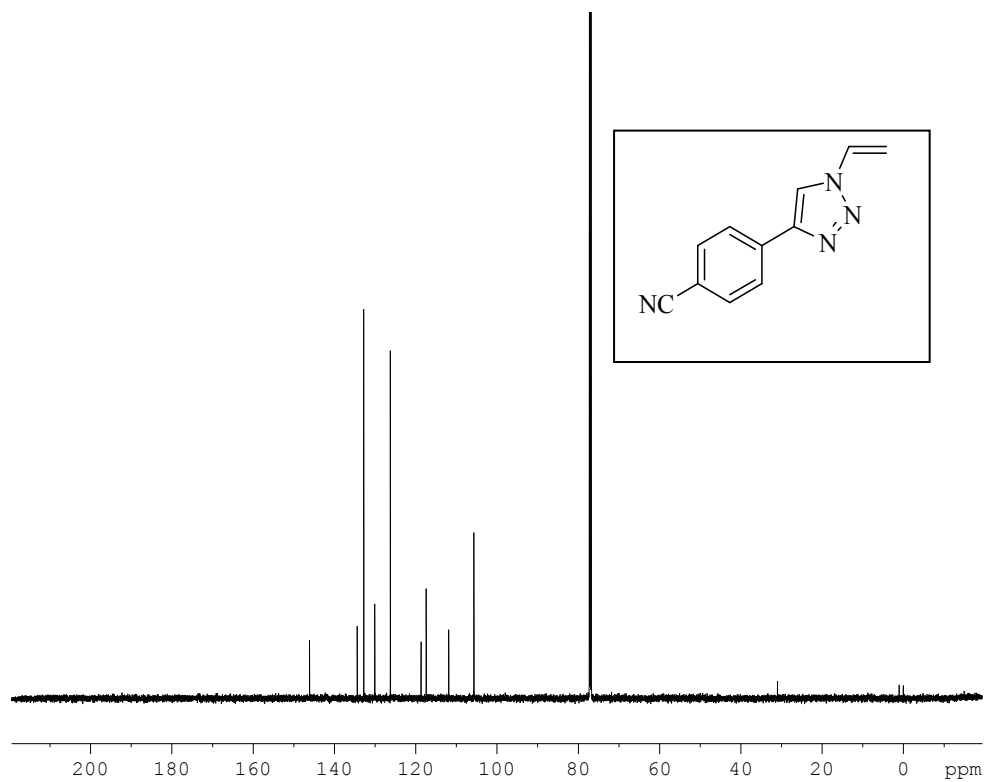


4-*m*-tolyl-1-vinyl-1*H*-1,2,3-triazole **24** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

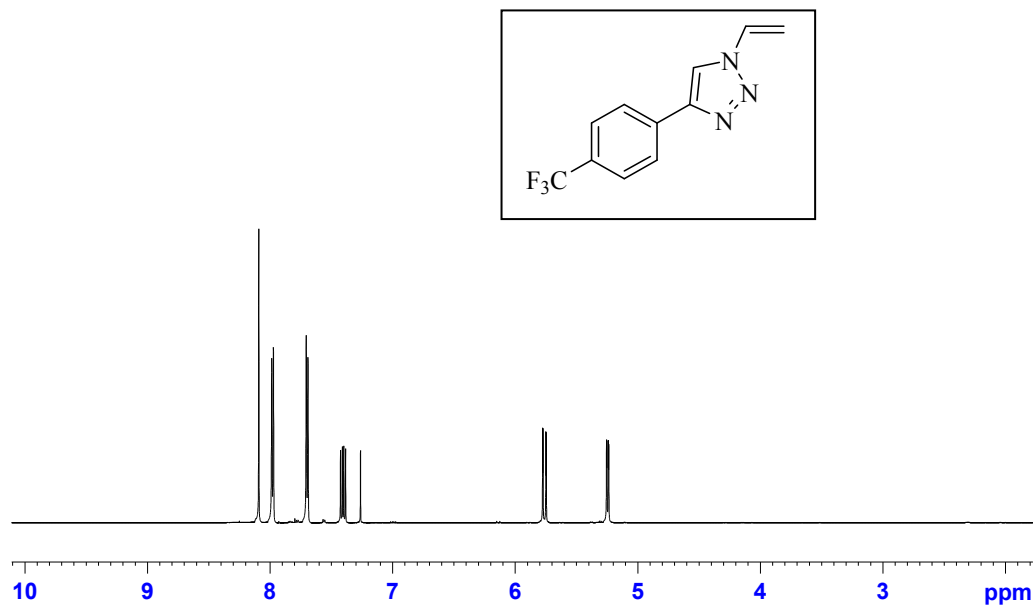


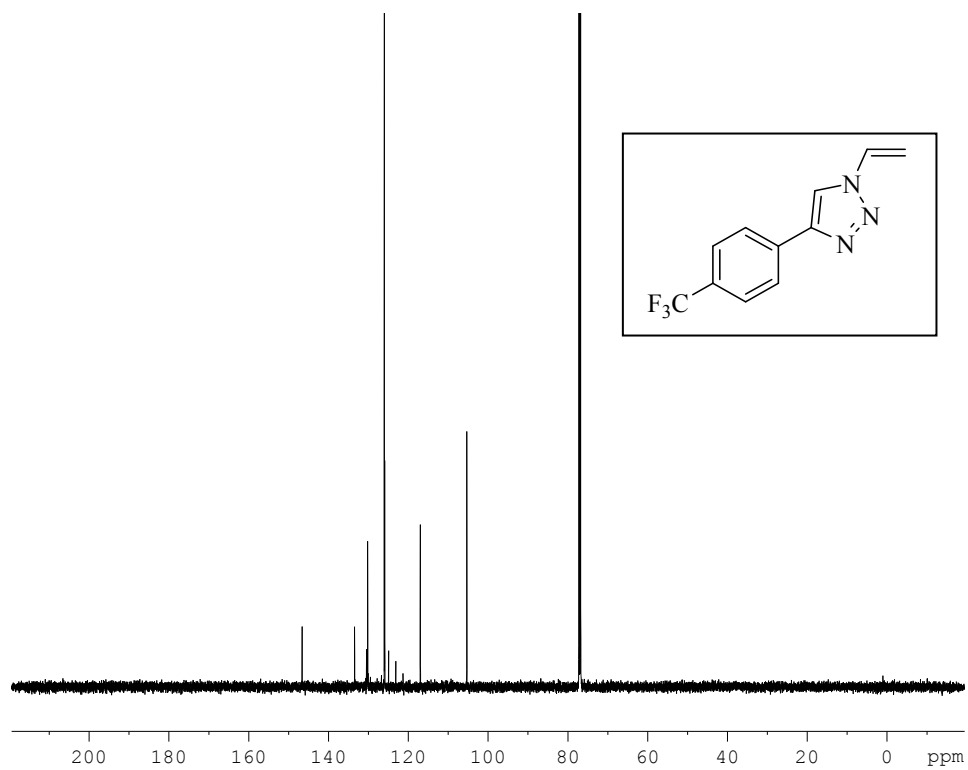
4-(1-vinyl-1*H*-1,2,3-triazol-4-yl)benzonitrile **25** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)



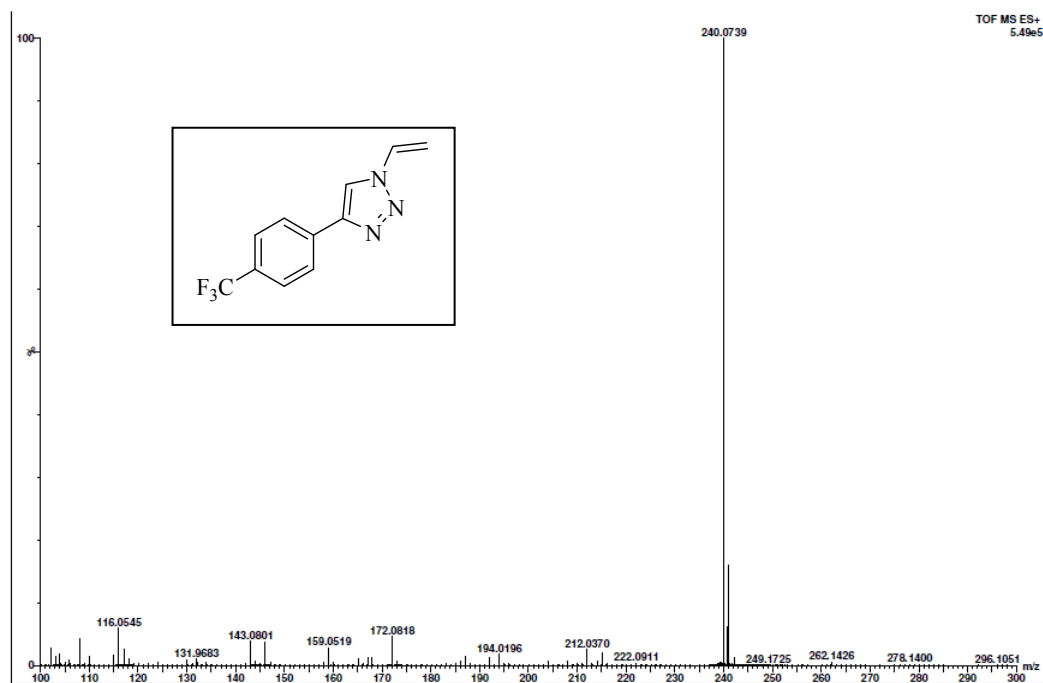


4-(4-(trifluoromethyl)phenyl)-1-vinyl-1H-1,2,3-triazole **26** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )

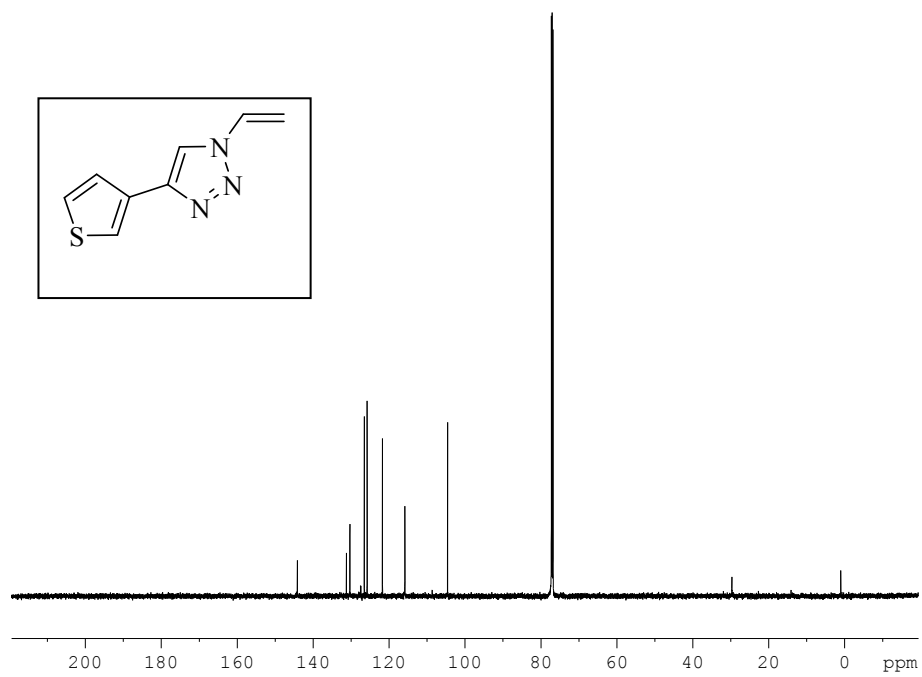
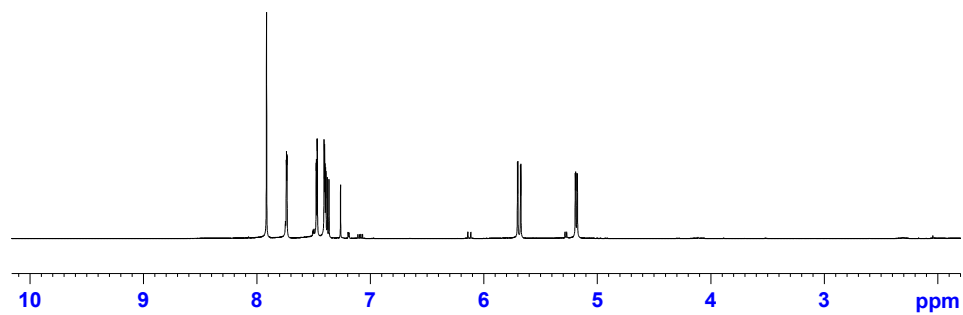
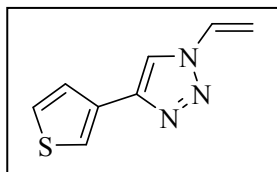




4-(4-(trifluoromethyl)phenyl)-1-vinyl-1H-1,2,3-triazole **26** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

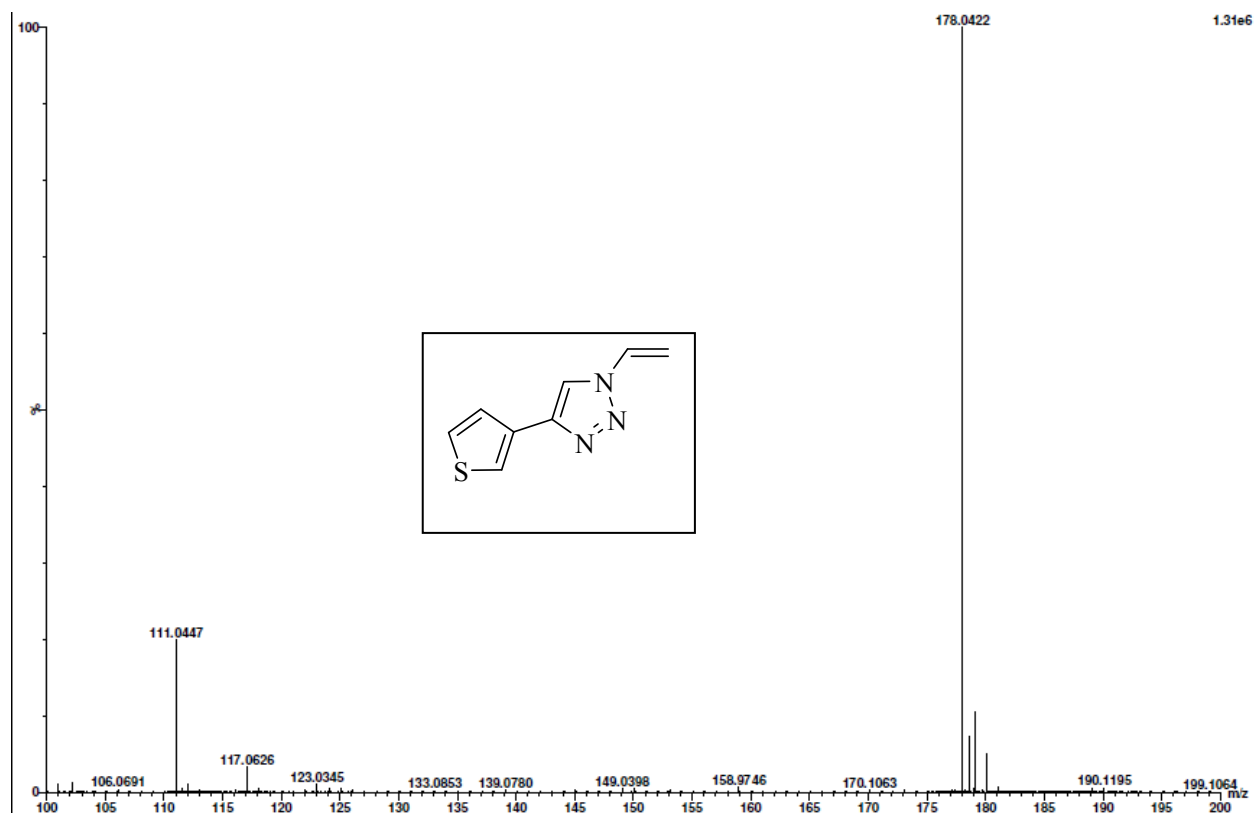


4-(thiophen-3-yl)-1-vinyl-1*H*-1,2,3-triazole **27** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)

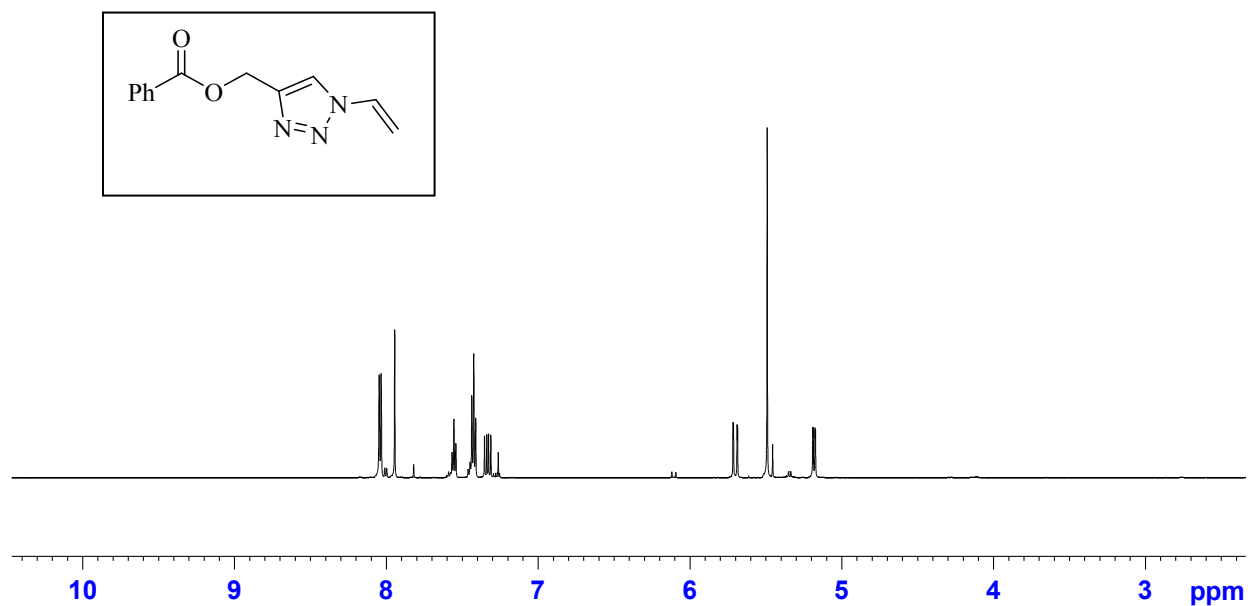


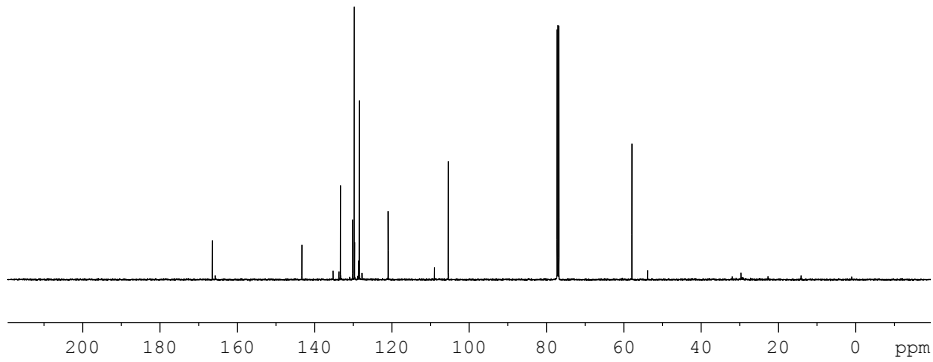
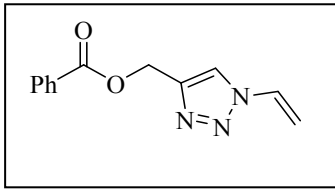


4-(thiophen-3-yl)-1-vinyl-1*H*-1,2,3-triazole **27** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

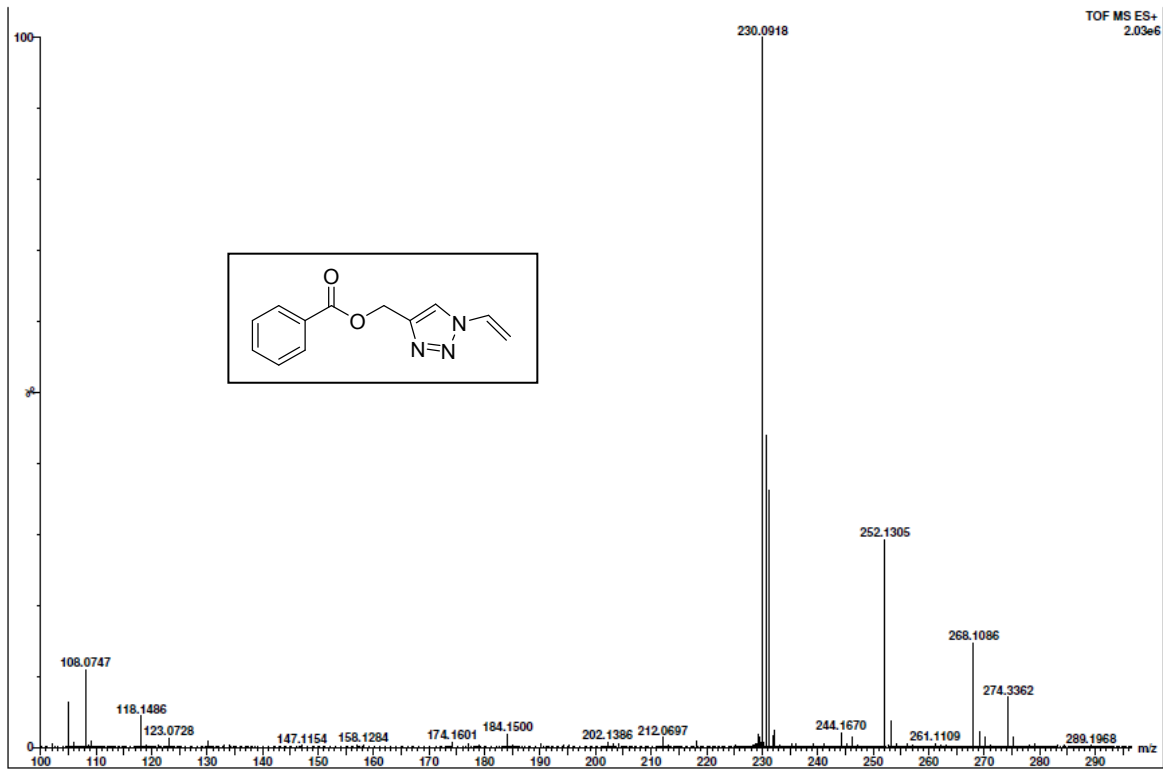


(1-vinyl-1*H*-1,2,3-triazol-4-yl)methyl benzoate **28** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)

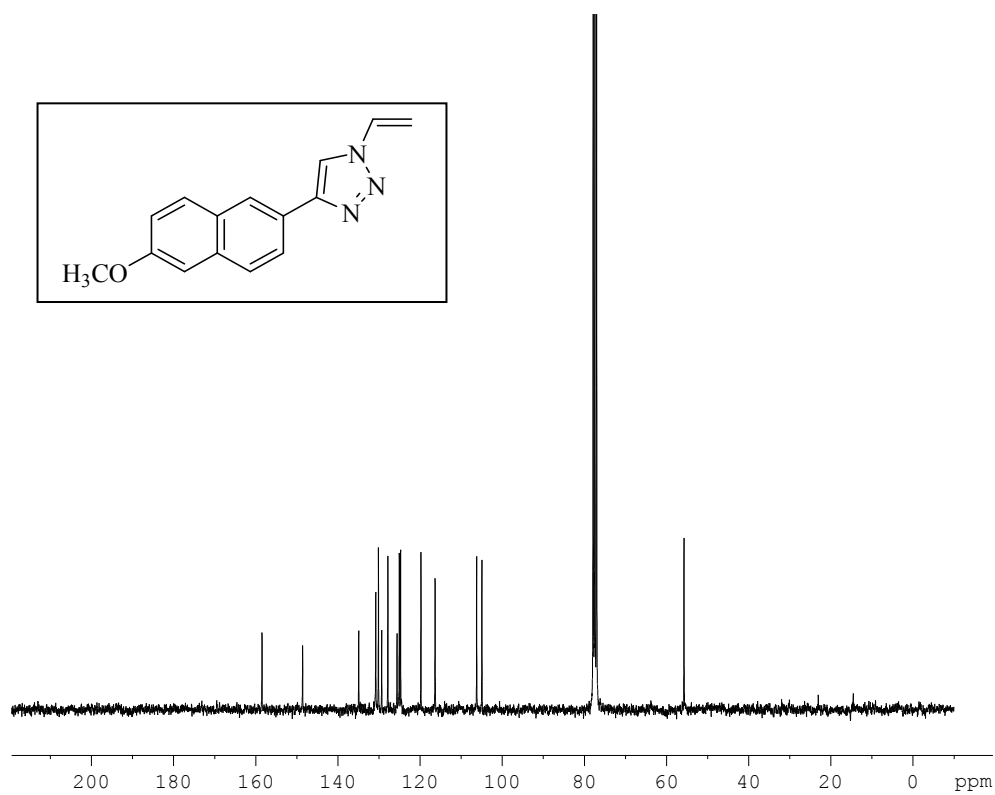
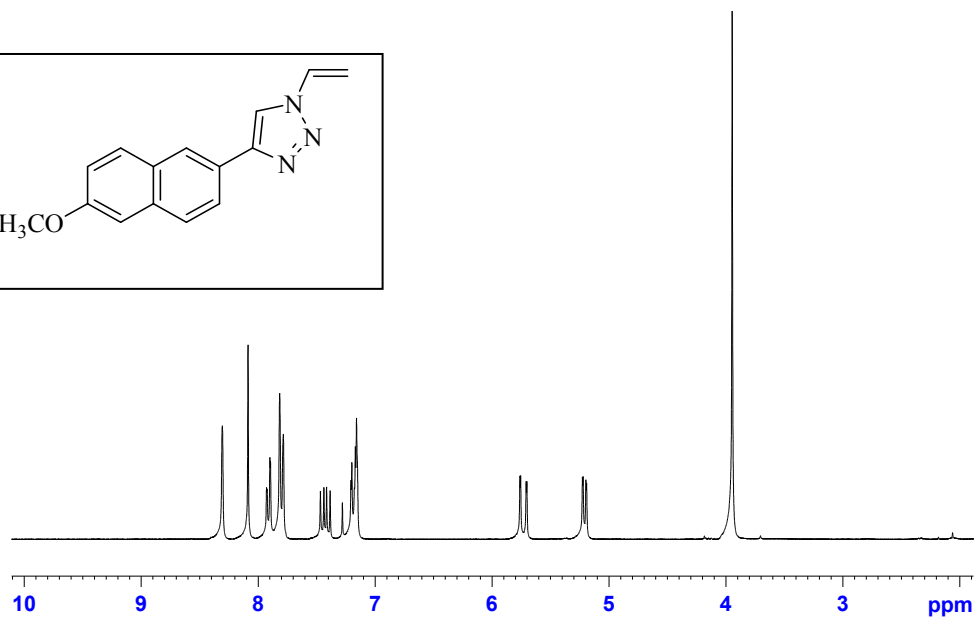
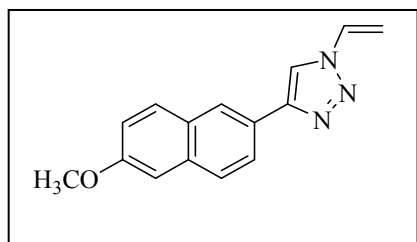




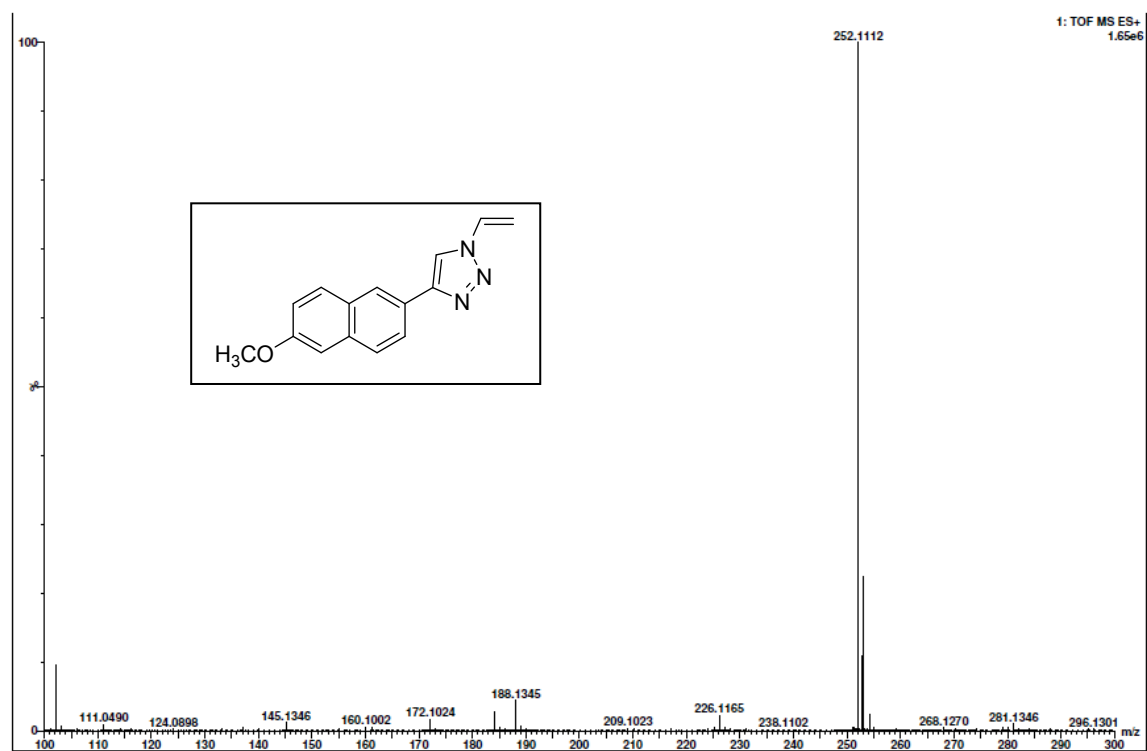
(1-vinyl-1H-1,2,3-triazol-4-yl)methyl benzoate **28** (ESI MS in MeCN:H<sub>2</sub>O (1:1))



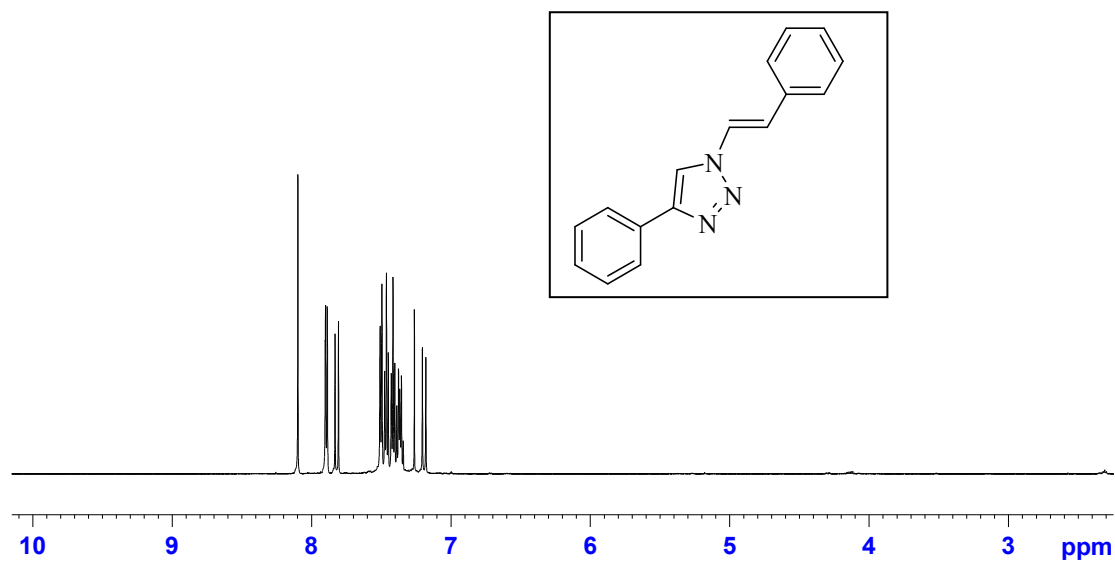
4-(2-methoxynaphthalen-6-yl)-1-vinyl-1*H*-1,2,3-triazole **29** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )

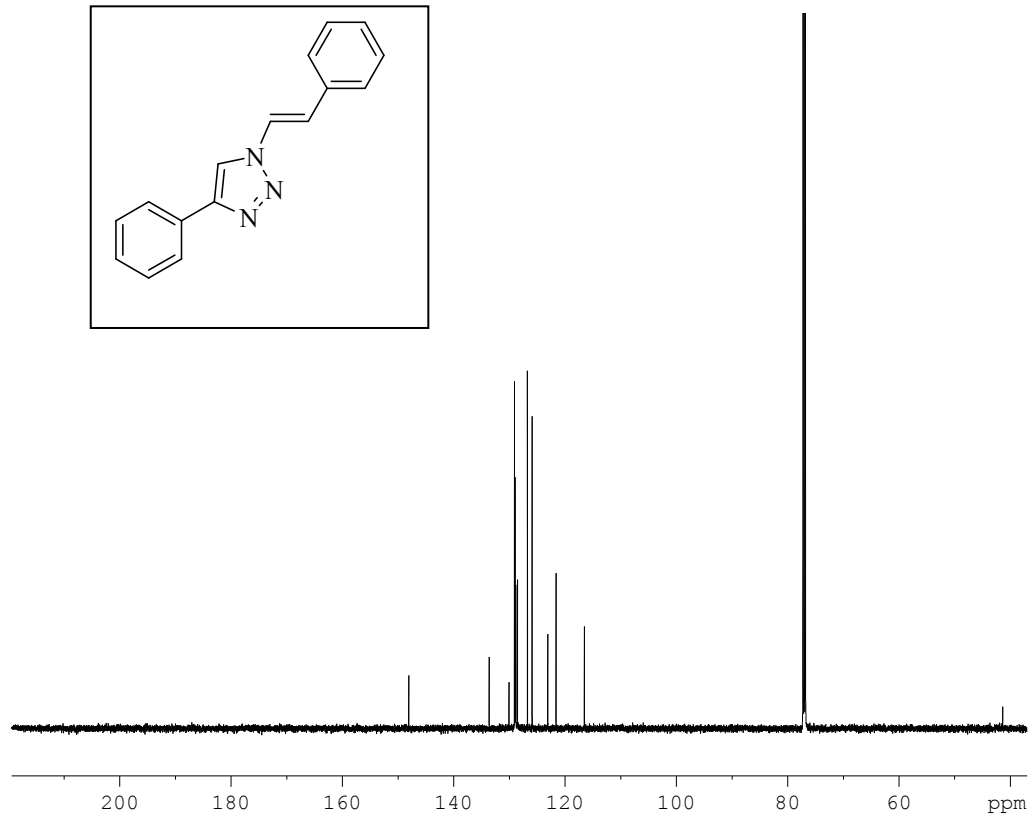
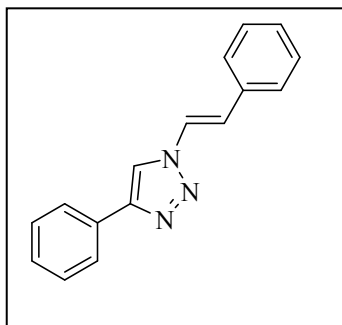


4-(2-methoxynaphthalen-6-yl)-1-vinyl-1*H*-1,2,3-triazole **29** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

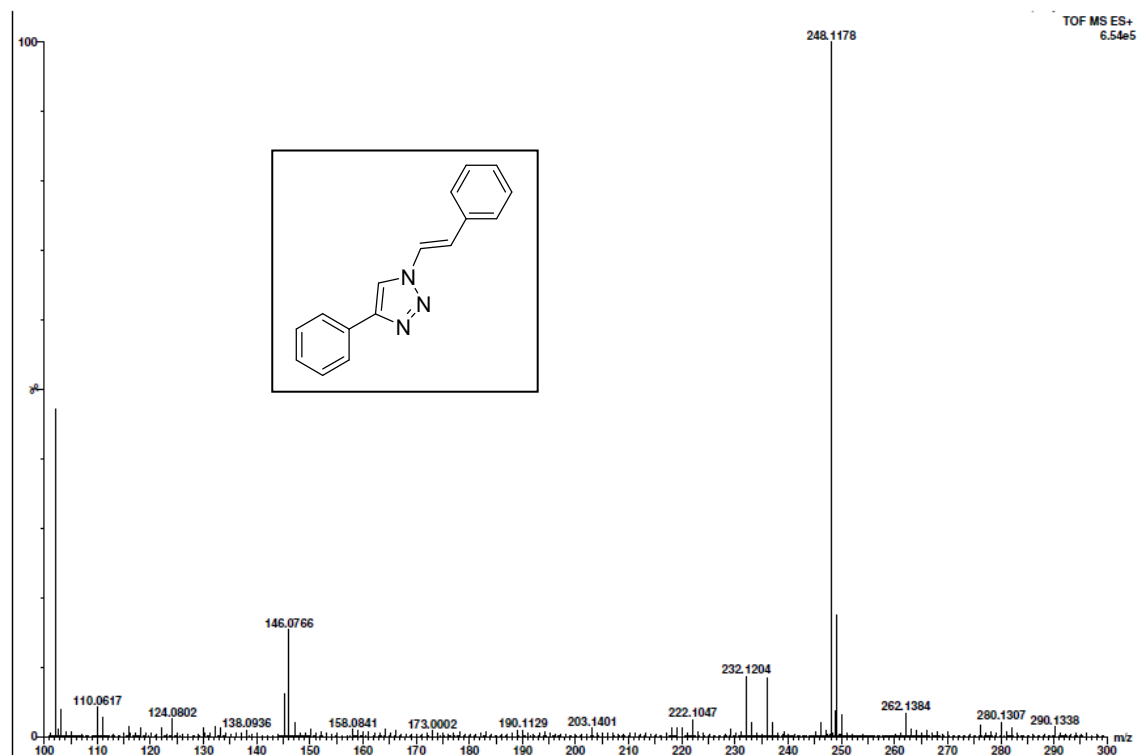


4-phenyl-1-styryl-1*H*-1,2,3-triazole **30** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)

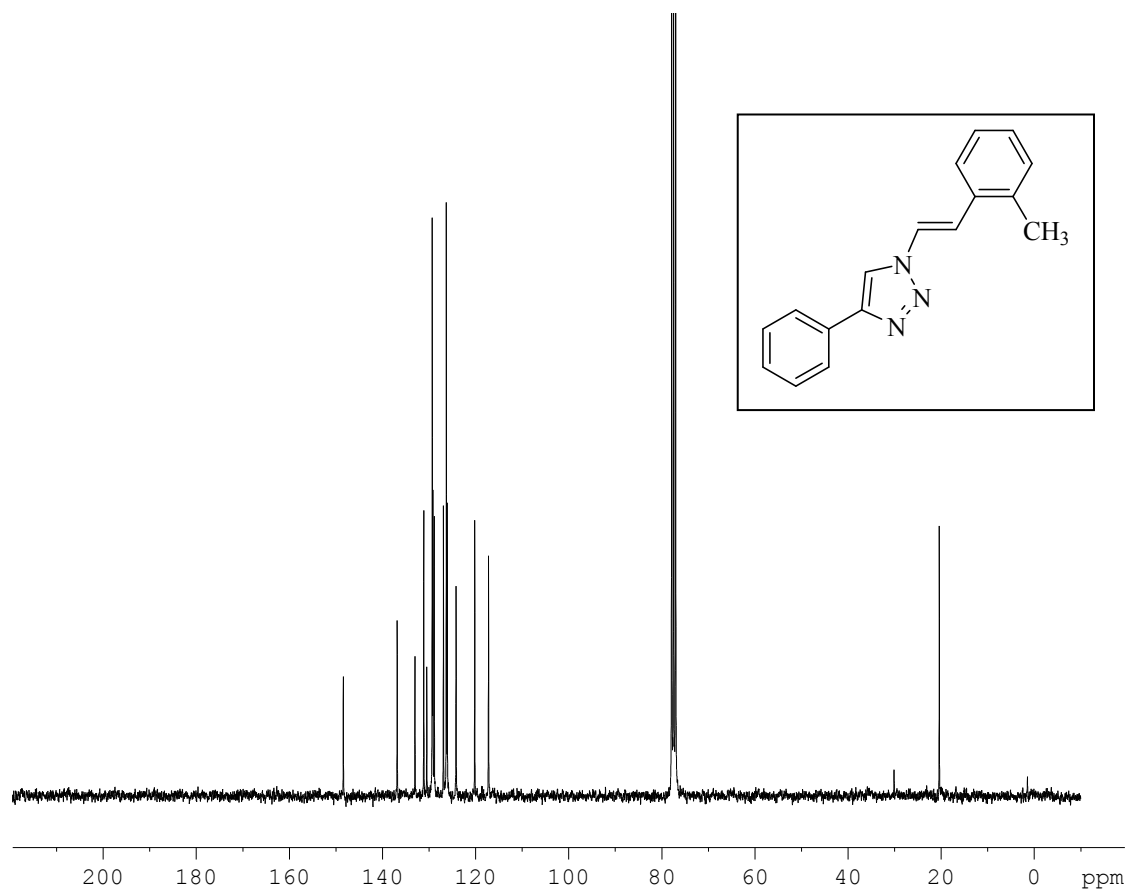
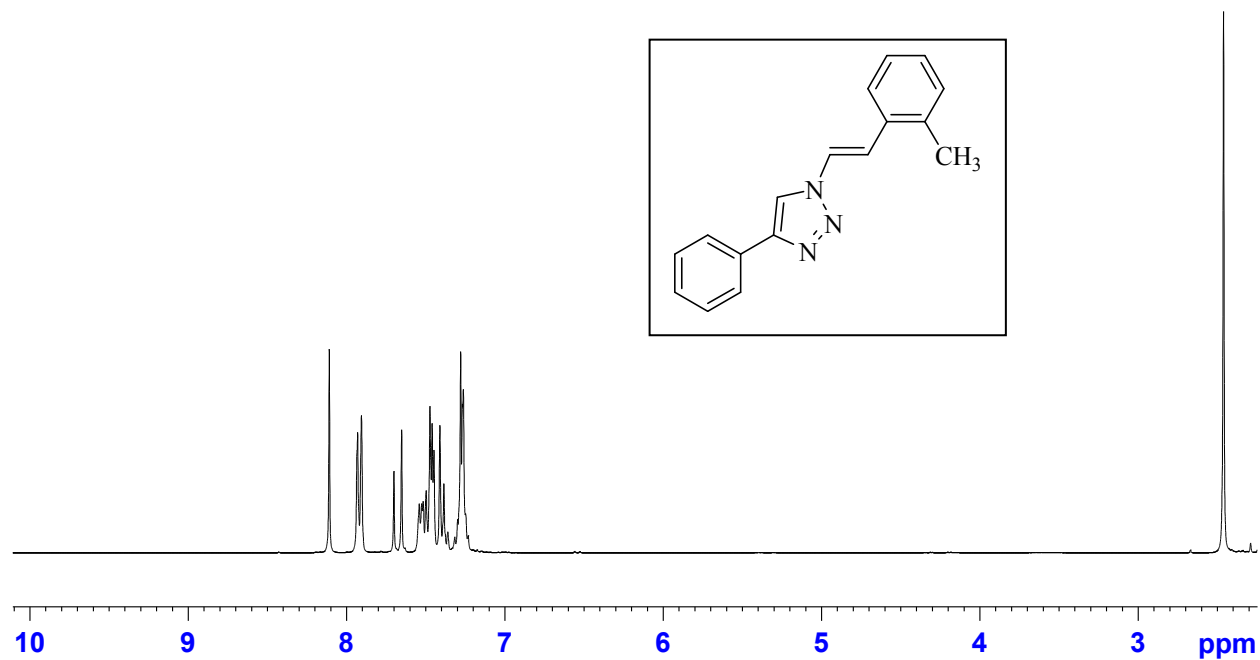




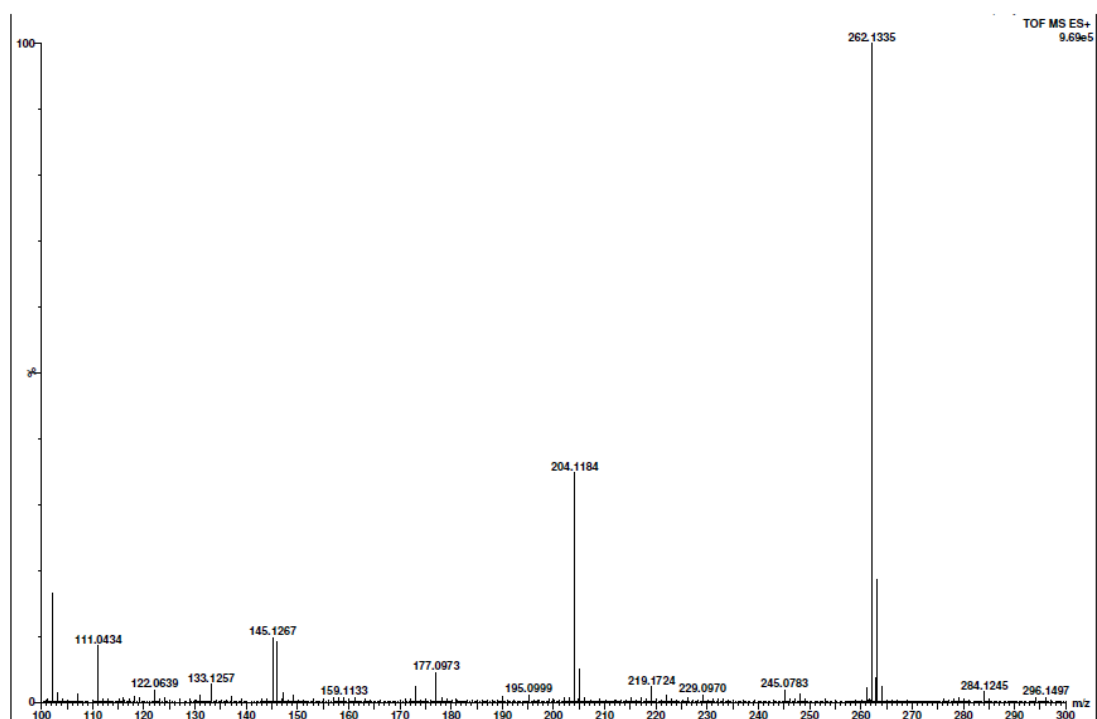
4-phenyl-1-styryl-1*H*-1,2,3-triazole **30** (ESI MS in MeCN:H<sub>2</sub>O (1:1))



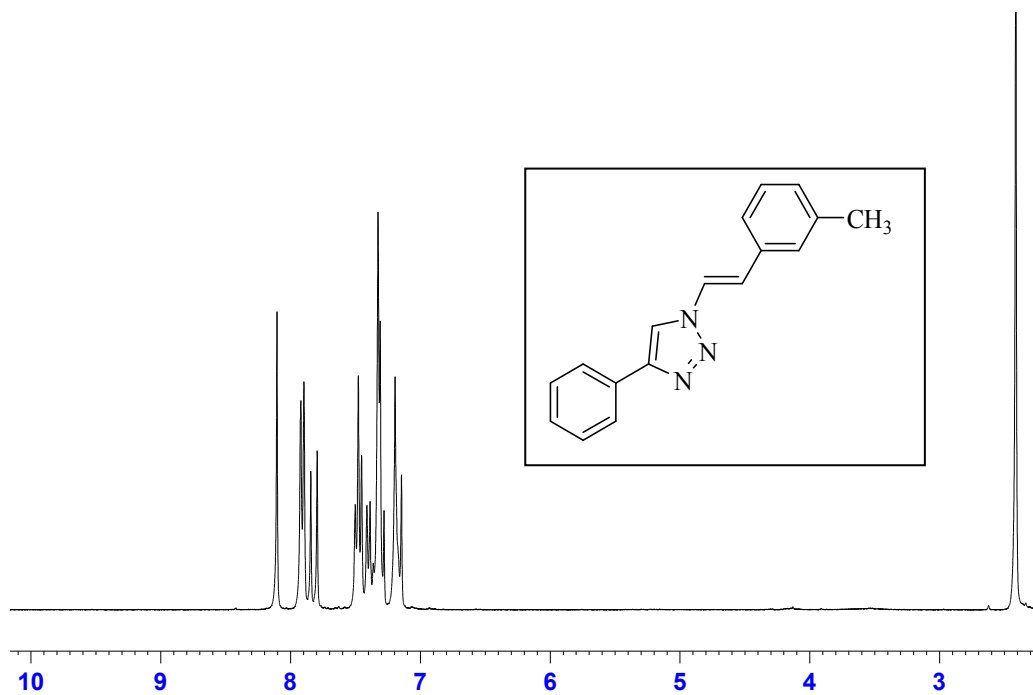
1-(2-methylstyryl)-4-phenyl-1*H*-1,2,3-triazole **31** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )

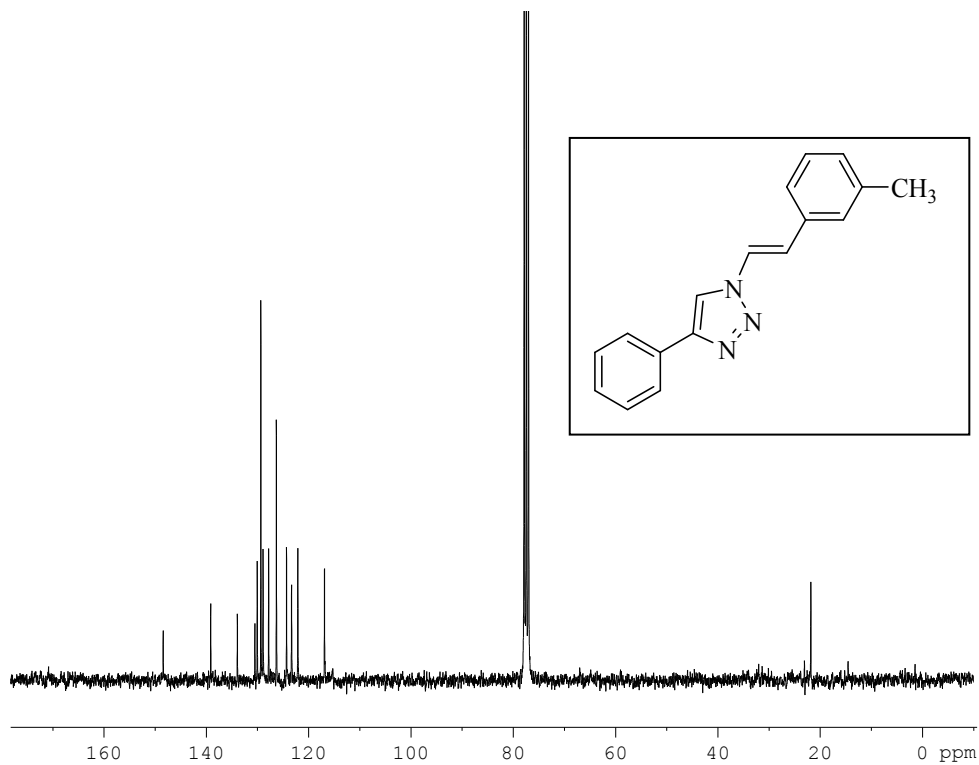


4-phenyl-1-(2-methylstyryl)-1*H*-1,2,3-triazole **31** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

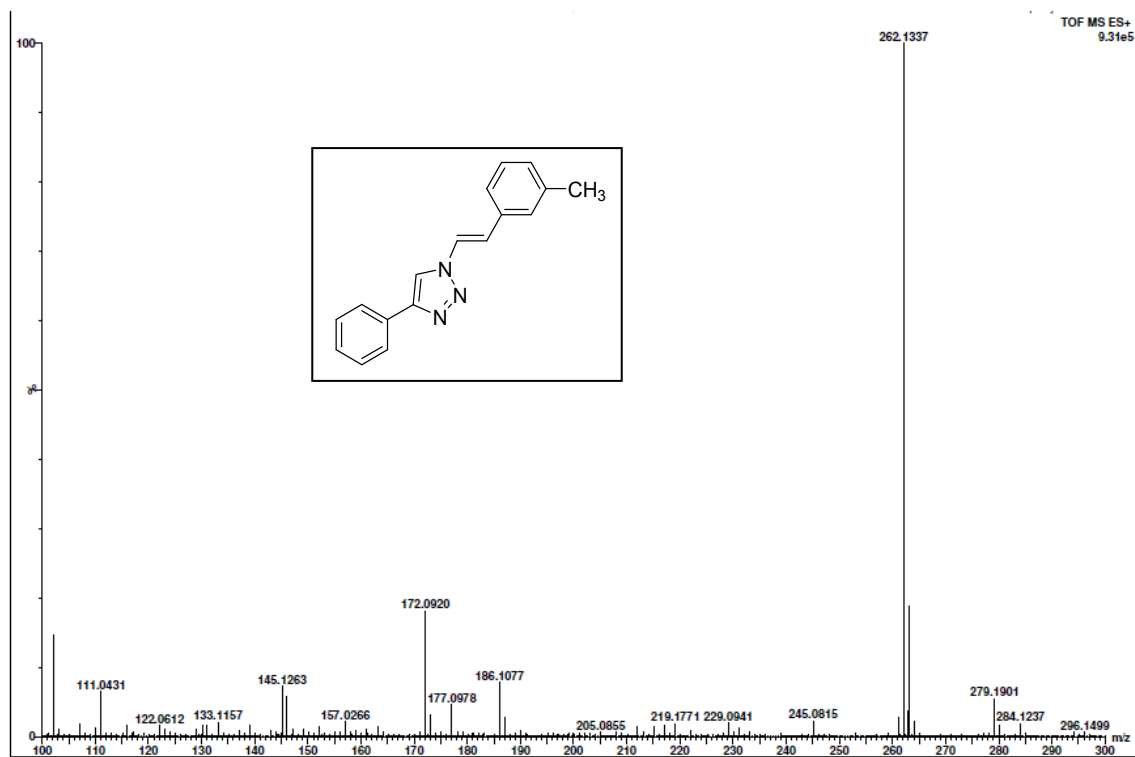


1-(3-methylstyryl)-4-phenyl-1*H*-1,2,3-triazole **32** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)



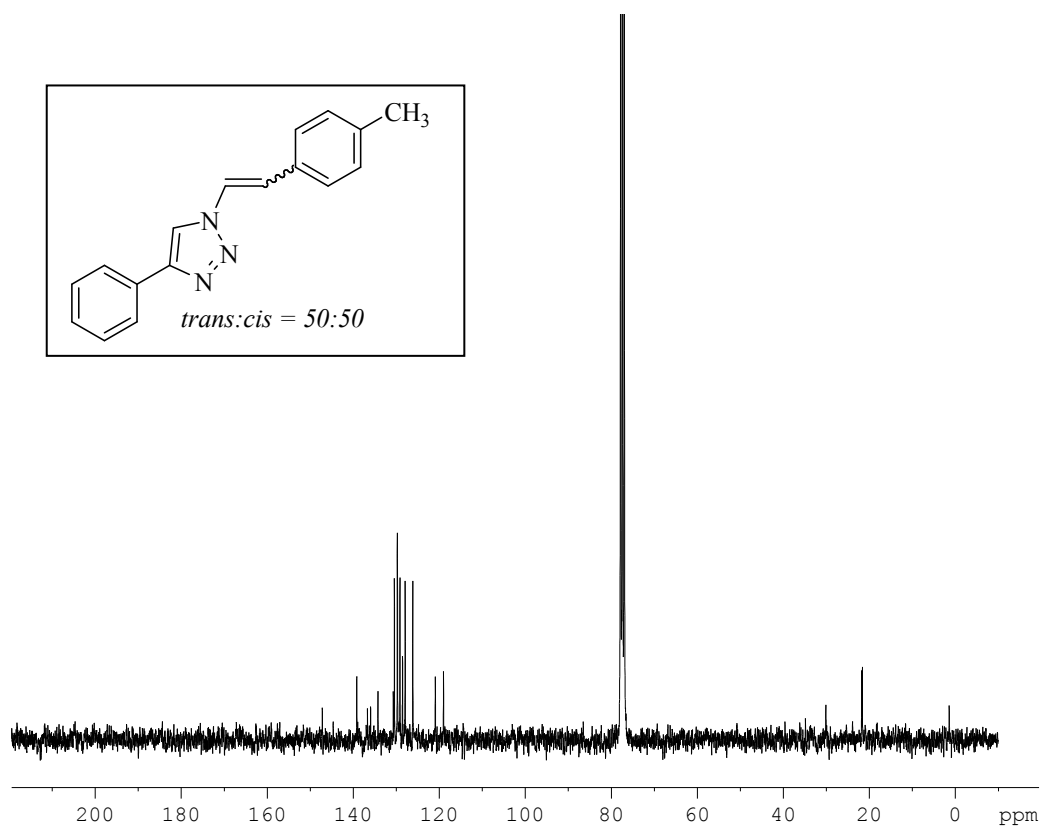
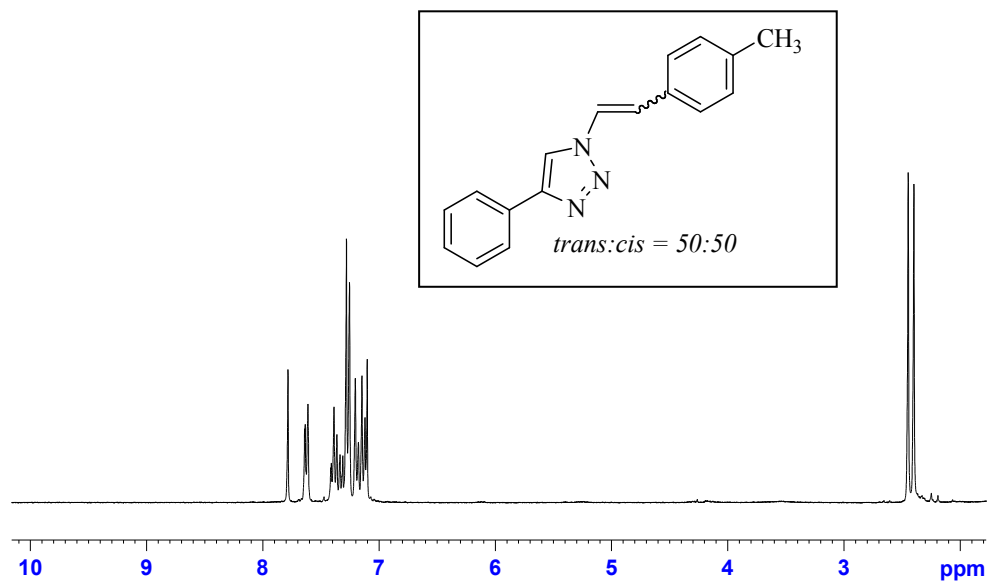


4-phenyl-1-(3-methylstyryl)-1H-1,2,3-triazole **32** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

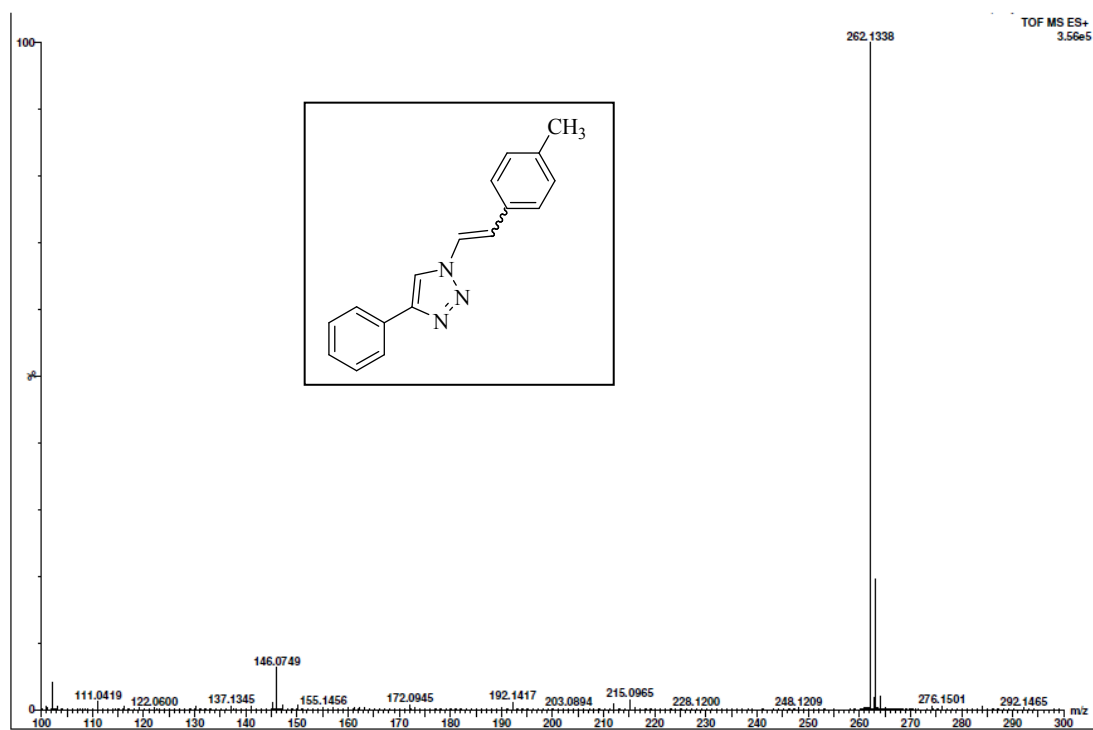




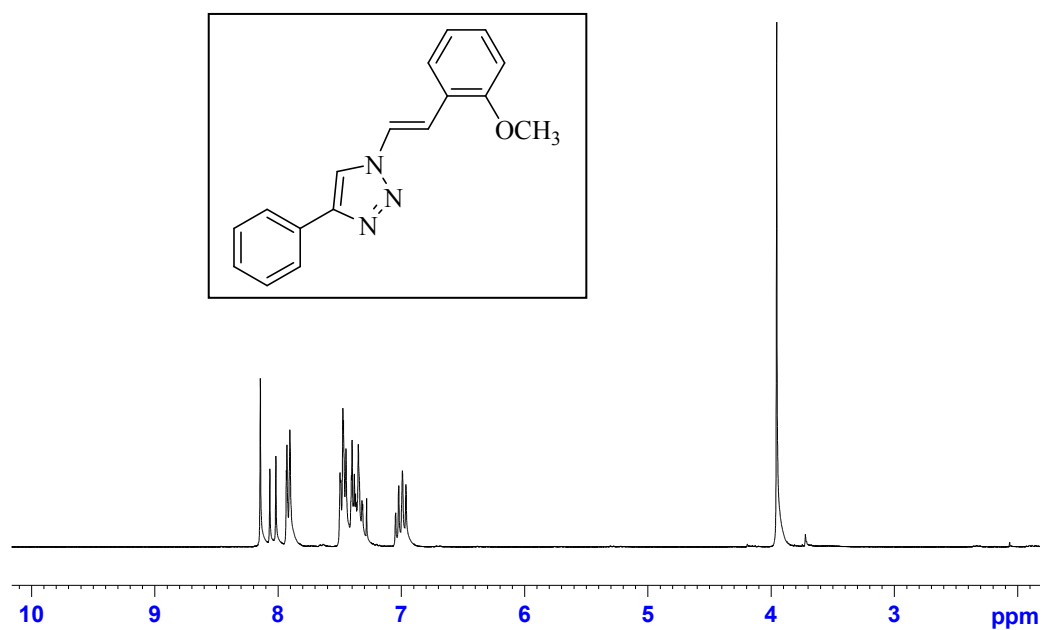
1-(4-methylstyryl)-4-phenyl-1H-1,2,3-triazole **33** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )

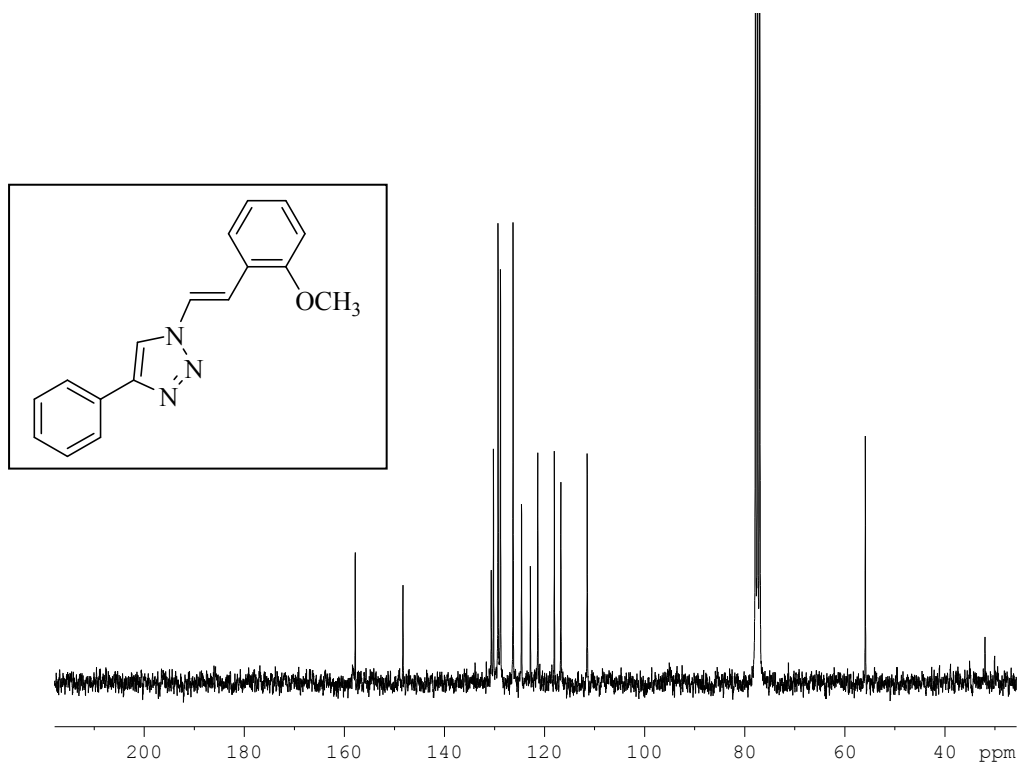


1-(2-methylstyryl)-4-phenyl-1*H*-1,2,3-triazole **33** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

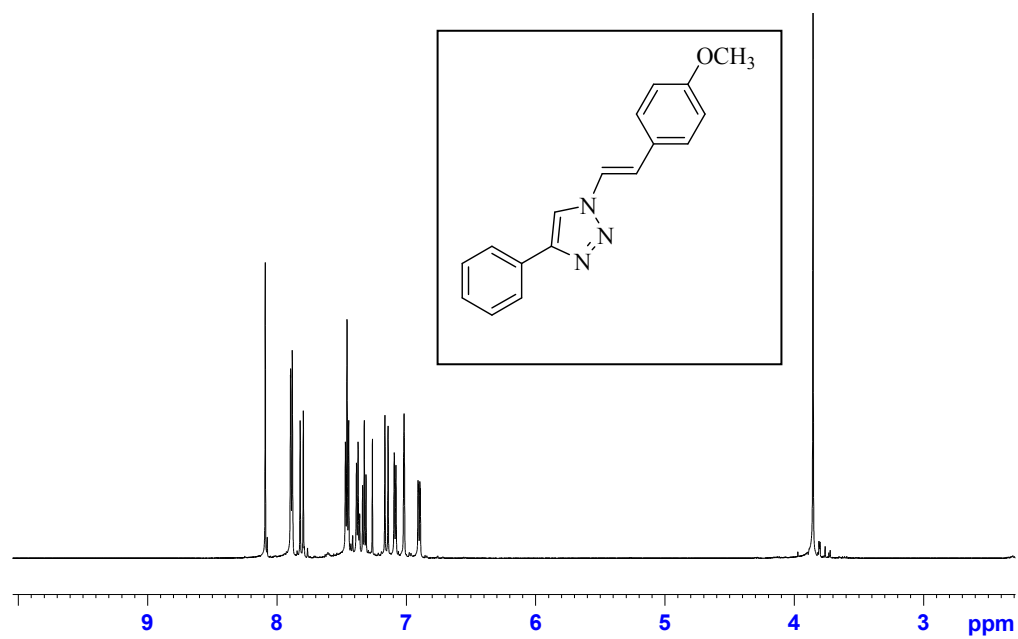


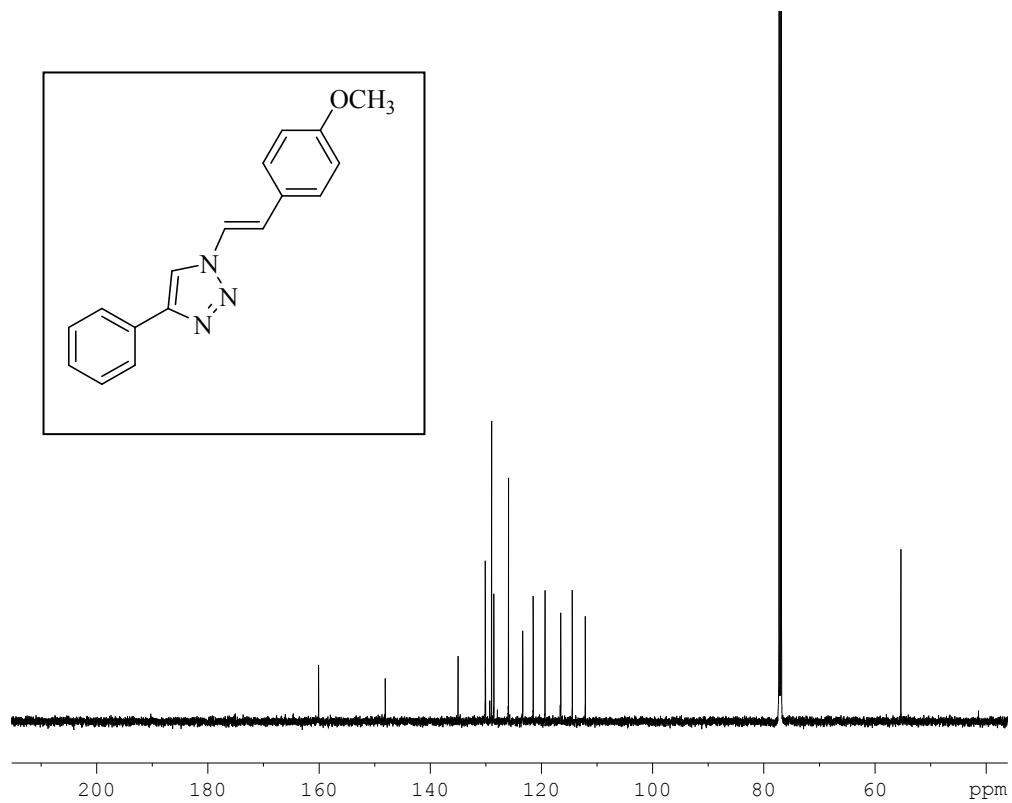
1-(2-methoxystyryl)-4-phenyl-1*H*-1,2,3-triazole **34** (<sup>1</sup>H & <sup>13</sup>C NMR in CDCl<sub>3</sub>)



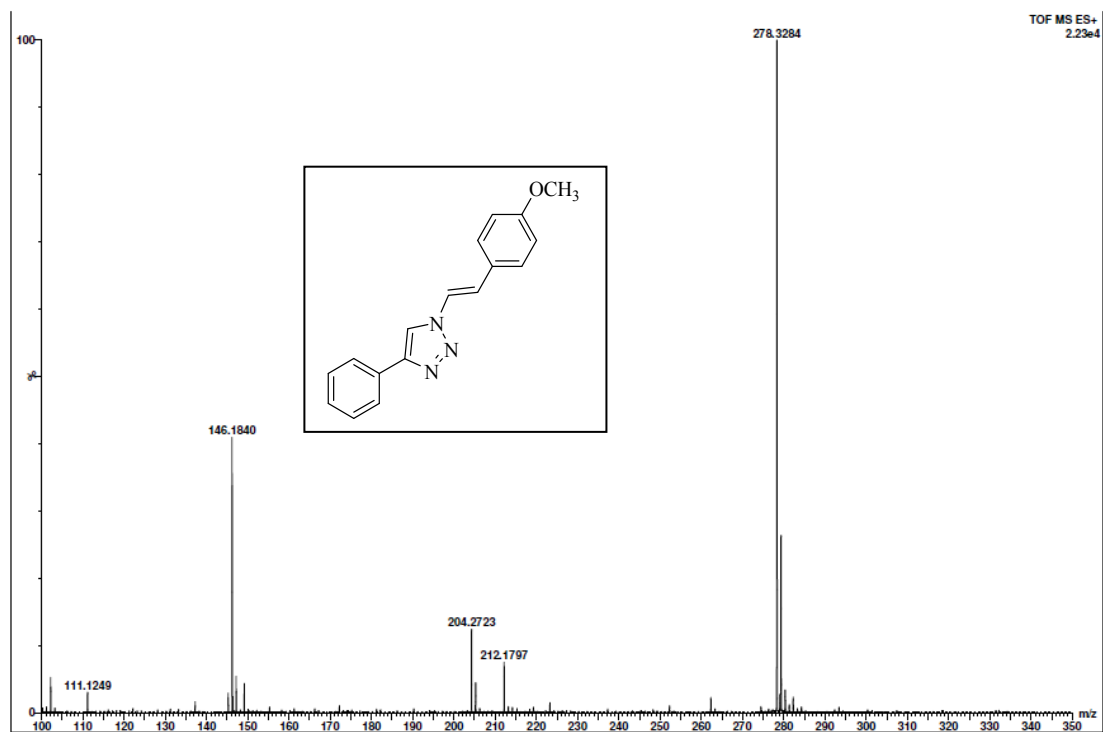


1-(4-methoxystyryl)-4-phenyl-1H-1,2,3-triazole **35** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )

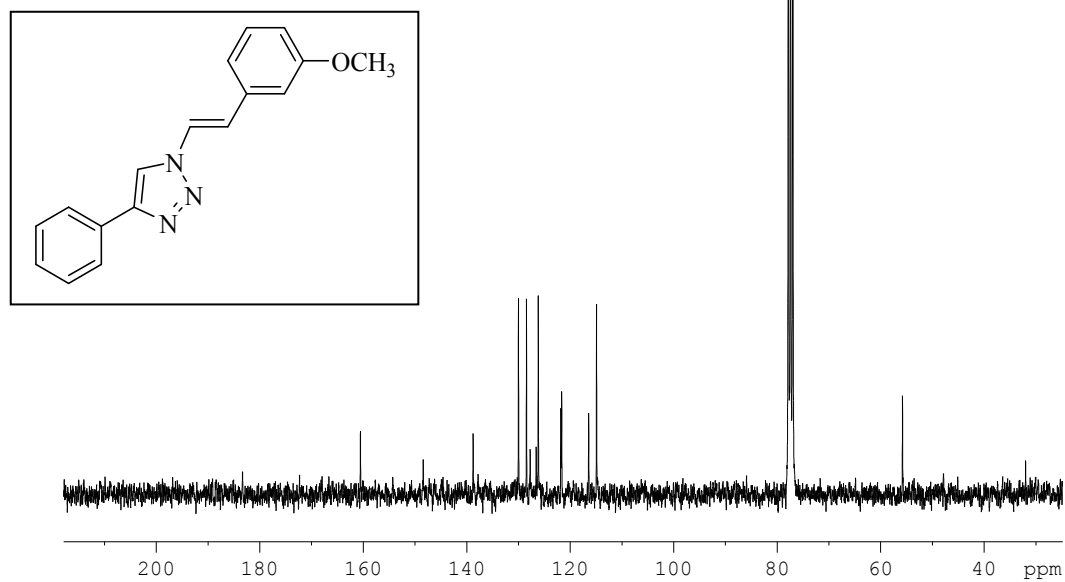
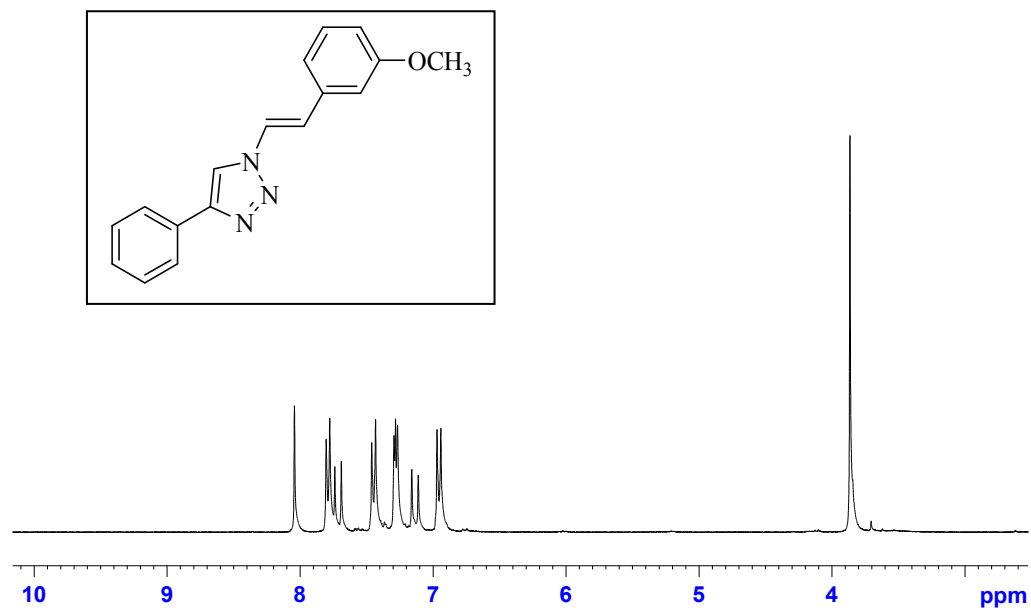




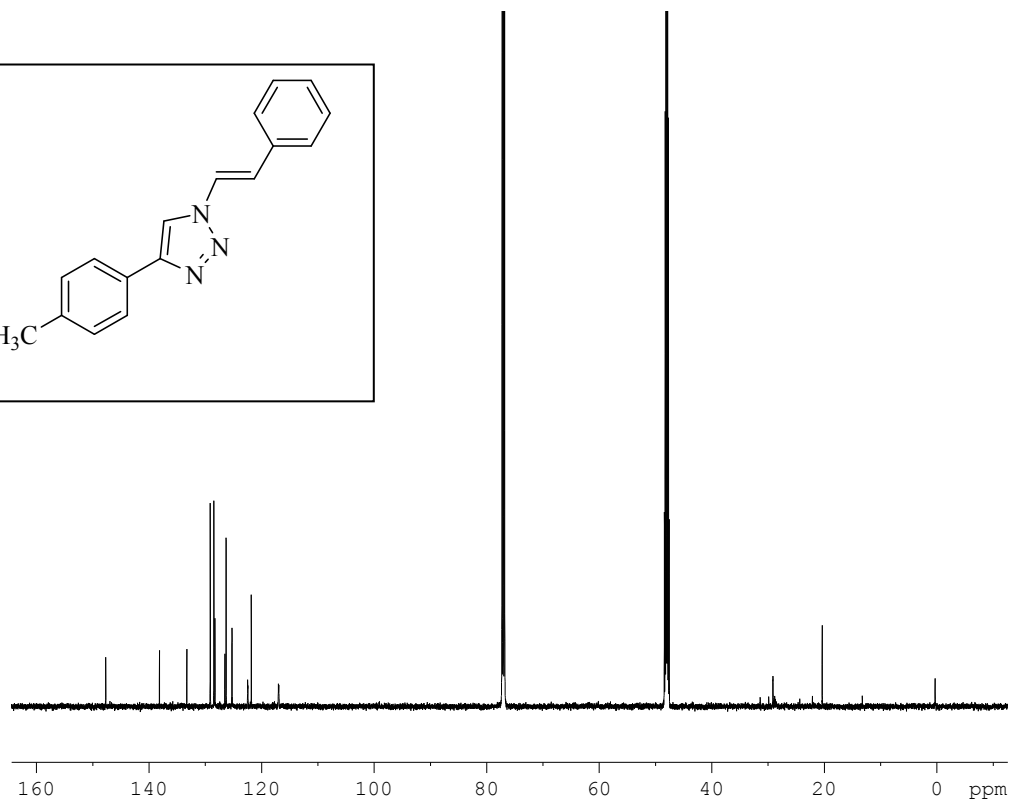
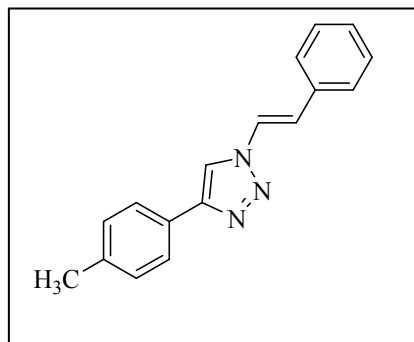
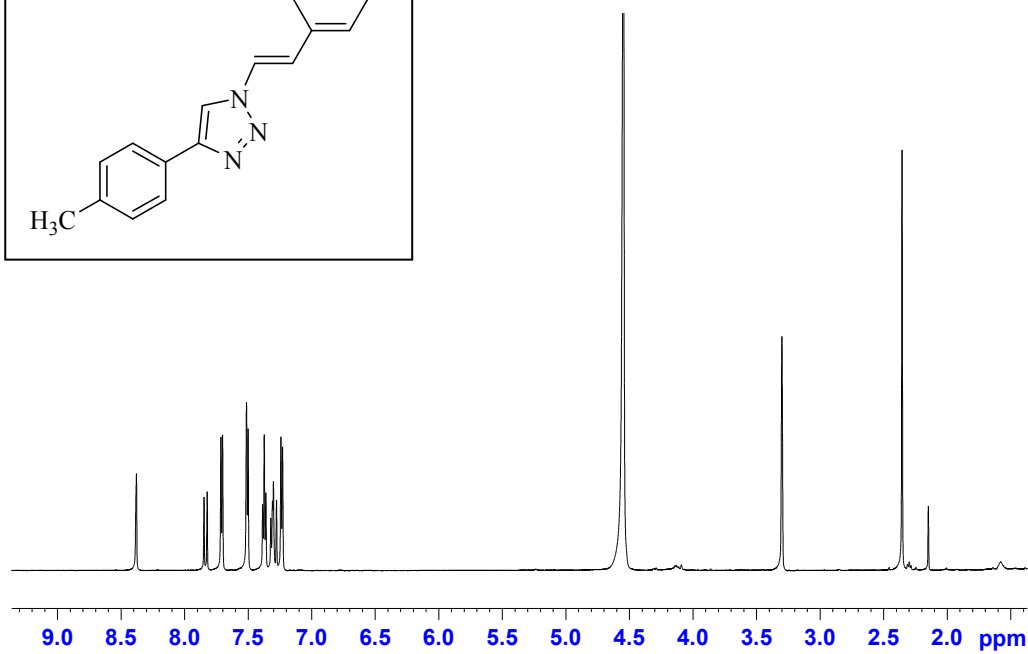
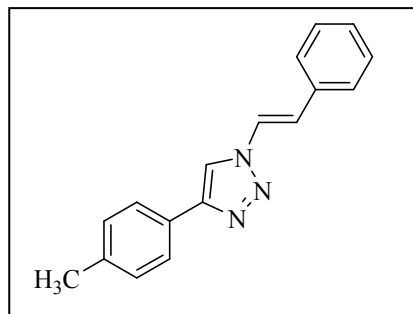
1-(4-methoxystyryl)-4-phenyl-1H-1,2,3-triazole **35** (ESI MS in MeCN:H<sub>2</sub>O (1:1))



1-(3-methoxystyryl)-4-phenyl-1*H*-1,2,3-triazole **36** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ )



1-styryl-4-*p*-tolyl-1*H*-1,2,3-triazole **37** ( $^1\text{H}$  &  $^{13}\text{C}$  NMR in  $\text{CDCl}_3$ :MeOD (1:1))



1-styryl-4-*p*-tolyl-1*H*-1,2,3-triazole **37** (ESI MS in MeCN:H<sub>2</sub>O (1:1))

