

## Supporting Information

### A Facile Metal-Free One-Pot Synthesis of 3-Aminoisoquinolines by Intramolecular Transannulation of 1-Sulfonyl-4-(2- aminomethylphenyl)-1,2,3-triazoles

Hai Shang,<sup>a, b</sup> Ling-Yu Li,<sup>a</sup> Yu Tian,<sup>a</sup> Hong-mei Jia<sup>a</sup> and Zhong-Mei Zou\*<sup>a</sup>

<sup>a</sup> Institute of Medicinal Plant Development, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100193, P. R. China.

<sup>b</sup> State Key Laboratory of Bioactive Substance and Function of Natural Medicines, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, P. R. China

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## 1. General Information

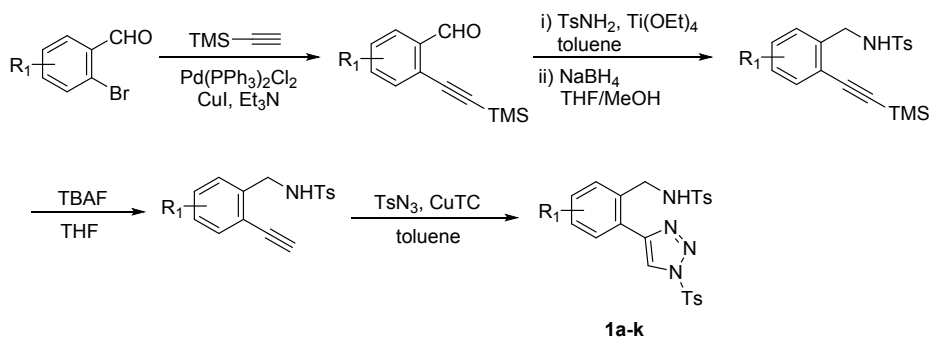
NMR spectra were recorded on Bruker AV III 600 NMR spectrometer and Bruker AV 400 instrument. Solvent signal was used as reference for  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 7.26 ppm;  $\text{DMSO-}d_6$ , 2.50 ppm) and  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 77.16 ppm;  $\text{DMSO-}d_6$ , 39.52 ppm). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, td = triple doublet, m = multiplet. Infrared (IR) spectra were recorded on a FTIR-8400S spectrometer. High-resolution mass spectra (HRMS) were recorded on a Waters SYNAPT G2 HDMS.

Reactions were monitored by Thin Layer Chromatography on plates ( $\text{GF}_{254}$ ) supplied by Yantai Chemicals (China). If not specially mentioned, flash column chromatography uses silica gel (200–300 mesh) supplied by Tsingtao Haiyang Chemicals (China). Solvent purification was conducted according to Purification of Laboratory Chemicals (D. D. Perrin, W. L. Armarego and D. R. Perrins, Pergamon Press, Oxford, 1980).

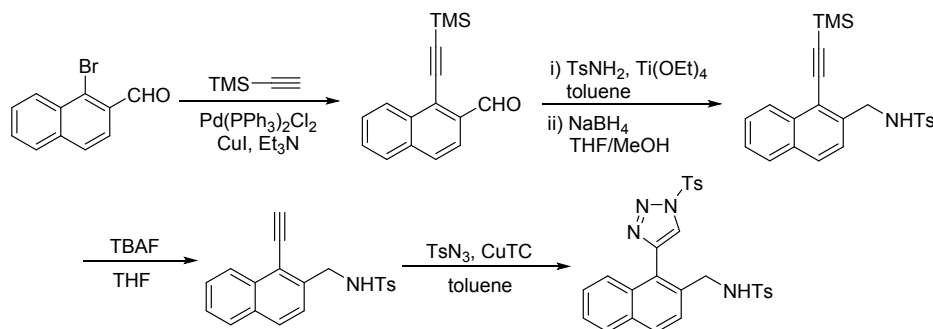
## 2. Procedure for the Preparation of Triazole Substrates

**Procedure A:** Triazoles **1a-k**, **1o** and **1p** were prepared referring to the literature procedures<sup>[1-3]</sup> as described below.

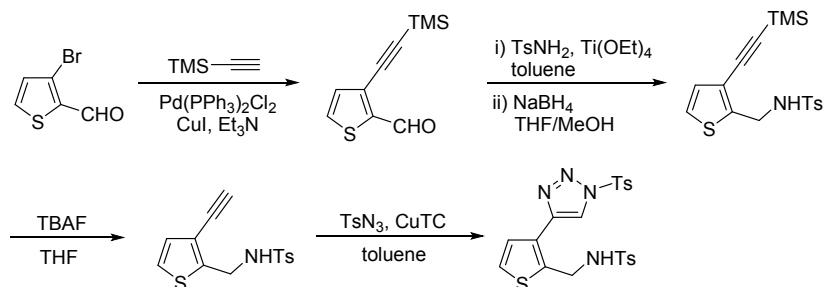
triazoles **a-k**:



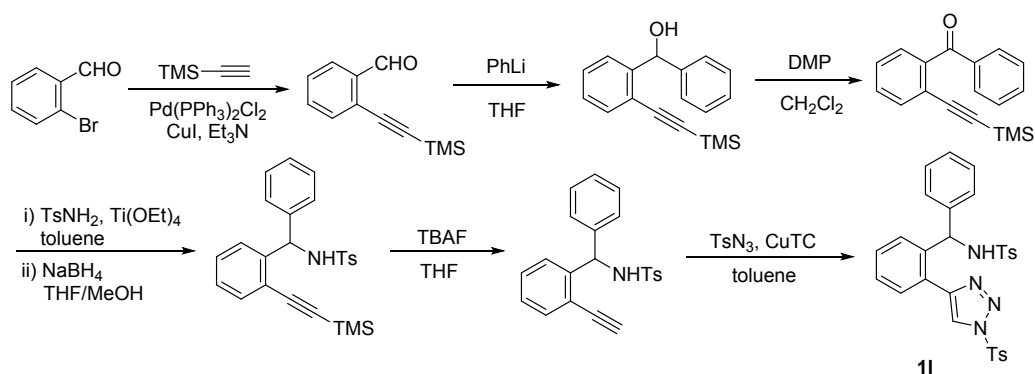
triazole **1o**:



triazole **1p**:

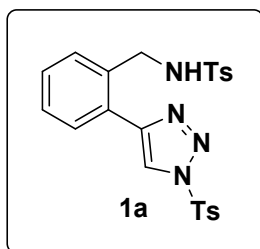


**Procedure B:** Triazole **11** was prepared referring to the literature procedures<sup>[1-4]</sup> as described below.

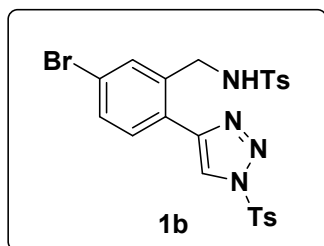


- [1]. Ze. F. Xu, X. Yu, D. Yang, C. Y. Li, *Org. Biomol. Chem.*, 2017, **15**, 3161-3164.
- [2]. M. Bandini, A. Gualandi, M. Monari, A. Romaniello, D. Savoia, M Tragni, *J. Organomet. Chem.* 2011, **696**, 337-347.
- [3]. J. Raushel, V. V. Fokin, *Org. Lett.*, 2010, **12**, 4952-4955.
- [4]. E. H. Ryu, H. K. Cho, Y. Zhao, *Org. Lett.*, 2007, **9**, 5147-5150.

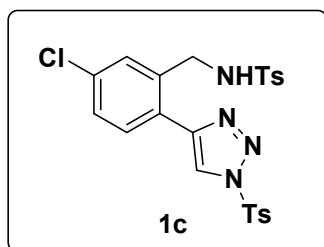
### 3. Analysis Data of Triazole Substrates



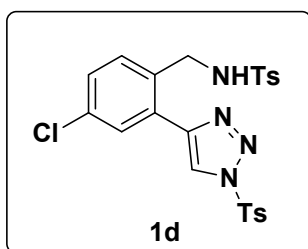
**4-methyl-N-(2-(1-tosyl-1H-1,2,3-triazol-4-yl)benzyl)benzenesulfonamide (1a):** Yield: 81%;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  8.32 (s, 1H), 8.05 (d,  $J = 8.5$  Hz, 2H), 7.65 (d,  $J = 8.3$  Hz, 2H), 7.43 (d,  $J = 8.2$  Hz, 2H), 7.41 (dd,  $J = 7.7$  Hz, 1.3 Hz, 1H), 7.33 (dd,  $J = 7.2$  Hz, 1.6 Hz, 1H), 7.30-7.24 (m, 2H), 7.17 (d,  $J = 8.0$  Hz, 2H), 6.23 (t,  $J = 6.9$  Hz, 1H), 4.10 (d,  $J = 6.9$  Hz, 2H), 2.47 (s, 3H), 2.36 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  147.9, 146.8, 143.1, 137.4, 134.6, 132.6, 131.8, 130.7, 129.6, 129.5, 129.3, 128.9, 128.5, 128.0, 127.0, 121.3, 46.5, 22.0, 21.5; IR  $\nu_{\text{max}}$  (KBr): 3256, 3158, 1593, 1387, 1321, 1194, 1095, 990  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $\text{C}_{23}\text{H}_{23}\text{N}_4\text{O}_4\text{S}_2$   $[\text{M}+\text{H}]^+$ : 483.1161; found: 483.1161.



**N-(5-bromo-2-(1-tosyl-1H-1,2,3-triazol-4-yl)benzyl)-4-methylbenzenesulfonamide (1b):** Yield: 56%;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.33 (s, 1H), 8.08 (d,  $J = 8.4$  Hz, 2H), 7.64 (d,  $J = 8.3$  Hz, 2H), 7.47 (d,  $J = 8.2$  Hz, 2H), 7.43-7.37 (m, 2H), 7.28 (d,  $J = 1.1$  Hz, 1H), 7.19 (d,  $J = 8.0$  Hz, 2H), 6.27 (t,  $J = 6.9$  Hz, 1H), 4.13 (d,  $J = 6.9$  Hz, 2H), 2.51 (s, 3H), 2.39 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  148.1, 146.0, 143.3, 137.6, 136.6, 134.7, 132.5, 131.5, 130.8, 130.6, 129.6, 129.1, 127.1, 126.9, 123.5, 121.3, 46.1, 22.1, 21.6; IR  $\nu_{\text{max}}$  (KBr): 2957, 2852, 1729, 1595, 1399, 1159, 1091, 1007  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $\text{C}_{23}\text{H}_{22}\text{BrN}_4\text{O}_4\text{S}_2$   $[\text{M}+\text{H}]^+$ : 561.0266; found: 561.0266.



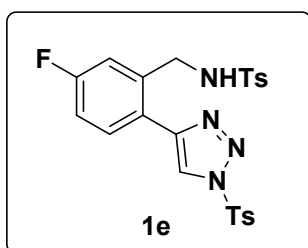
**N-(5-chloro-2-(1-tosyl-1H-1,2,3-triazol-4-yl)benzyl)-4-methylbenzenesulfonamide (1c):** Yield: 81%;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  8.29 (s, 1H), 8.06 (d,  $J = 8.3$  Hz, 2H), 7.63 (d,  $J = 8.1$  Hz, 2H), 7.45 (d,  $J = 8.3$  Hz, 2H), 7.32 (d,  $J = 8.9$  Hz, 1H), 7.25-7.22 (m, 2H), 7.17 (d,  $J = 8.1$  Hz, 2H), 6.21 (t,  $J = 6.9$  Hz, 1H), 4.11 (d,  $J = 6.9$  Hz, 2H), 2.48 (s, 3H), 2.37 (s, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  148.1, 146.0, 143.3, 137.6, 136.5, 135.3, 132.6, 131.9, 130.8, 130.5, 129.6, 129.1, 128.6, 127.1, 126.5, 121.3, 46.2, 22.1, 21.6; IR  $\nu_{\text{max}}$  (KBr): 3287, 2920, 2849, 1594, 1396, 1333, 1155, 1094, 986  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $\text{C}_{23}\text{H}_{22}\text{ClN}_4\text{O}_4\text{S}_2$   $[\text{M}+\text{H}]^+$ : 517.0771; found: 517.0771.



***N*-(4-chloro-2-(1-tosyl-1*H*-1,2,3-triazol-4-yl)benzyl)-4-**

**methylbenzenesulfonamide (1d):** Yield: 77%; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.32 (s, 1H), 8.06 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 8.2 Hz, 2H), 7.45 (d, *J* = 8.2 Hz, 2H), 7.39 (d, *J* = 2.1 Hz, 1H), 7.29 (d, *J* = 8.2 Hz, 1H), 7.23 (dd, *J* = 8.2 Hz, 2.1 Hz, 1H), 7.18 (d, *J* = 8.0 Hz,

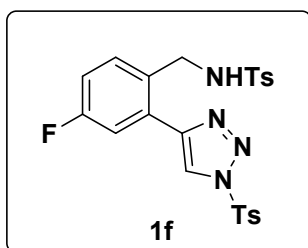
2H), 6.13 (t, *J* = 6.9 Hz, 1H), 4.11 (d, *J* = 6.9 Hz, 2H), 2.48 (s, 3H), 2.38 (s, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 148.1, 145.6, 143.3, 137.6, 134.3, 133.4, 133.4, 132.6, 130.8, 129.6, 129.5, 129.1, 129.0, 127.1, 121.5, 46.0, 22.1, 21.6; IR ν<sub>max</sub> (KBr): 3315, 3166, 1594, 1394, 1335, 1157, 1092, 997 cm<sup>-1</sup>; HRMS *m/z* calcd for C<sub>23</sub>H<sub>22</sub>ClN<sub>4</sub>O<sub>4</sub>S<sub>2</sub> [M+H]<sup>+</sup>: 517.0771; found: 517.0776.



***N*-(5-fluoro-2-(1-tosyl-1*H*-1,2,3-triazol-4-yl)benzyl)-4-**

**methylbenzenesulfonamide (1e):** Yield: 72%; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.26 (s, 1H), 8.05 (d, *J* = 8.5 Hz, 2H), 7.65 (d, *J* = 8.3 Hz, 2H), 7.44 (d, *J* = 8.2 Hz, 2H), 7.37 (dd, *J* = 8.6 Hz, 5.5 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.04 (dd, *J* = 9.1 Hz, 2.6 Hz, 1H), 6.98 (td,

*J* = 8.2 Hz, 2.7 Hz, 1H), 6.17 (t, *J* = 6.9 Hz, 1H), 4.10 (d, *J* = 6.9 Hz, 2H), 2.48 (s, 3H), 2.38 (s, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 162.9 (d, *J* = 251.0 Hz), 148.0, 146.1, 143.3, 137.6, 137.5 (d, *J* = 7.6 Hz), 132.7, 131.2 (d, *J* = 8.6 Hz), 130.8, 129.7, 129.1, 127.1, 124.2 (d, *J* = 3.2 Hz), 121.1, 118.7 (d, *J* = 22.0 Hz), 115.6 (d, *J* = 21.3 Hz), 46.2, 22.1, 21.6; IR ν<sub>max</sub> (KBr): 3355, 3148, 2920, 1596, 1487, 1398, 1332, 1156, 1094, 989 cm<sup>-1</sup>; HRMS *m/z* calcd for C<sub>23</sub>H<sub>22</sub>FN<sub>4</sub>O<sub>4</sub>S<sub>2</sub> [M+H]<sup>+</sup>: 501.1066; found: 501.10670.

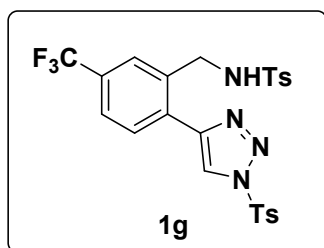


***N*-(4-fluoro-2-(1-tosyl-1*H*-1,2,3-triazol-4-yl)benzyl)-4-**

**methylbenzenesulfonamide (1f):** Yield: 69%; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.32 (s, 1H), 8.06 (d, *J* = 8.3 Hz, 2H), 7.65 (d, *J* = 8.1 Hz, 2H), 7.45 (d, *J* = 8.3 Hz, 2H), 7.33 (dd, *J* = 8.4 Hz, 5.7 Hz, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.13 (dd, *J* = 9.1 Hz, 2.6 Hz, 1H), 6.97 (td,

*J* = 8.2 Hz, 2.6 Hz, 1H), 6.08 (t, *J* = 6.9 Hz, 1H), 4.11 (d, *J* = 6.9 Hz, 2H), 2.48 (s, 3H), 2.38 (s, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 162.3 (d, *J* = 248.4 Hz), 148.1, 145.9 (d, *J* = 2.0 Hz), 143.3, 137.6, 134.0 (d, *J* = 8.3 Hz), 132.6, 130.9, 130.8, 130.0 (d, *J* = 8.4 Hz), 129.7, 129.1, 127.1, 121.6, 116.4 (d, *J* = 20.9 Hz), 115.9 (d, *J* = 23.1 Hz), 45.9, 22.1, 21.6; IR ν<sub>max</sub> (KBr): 3249, 3134, 1592, 1500, 1394, 1194, 1159, 1001, 811 cm<sup>-1</sup>; HRMS *m/z* calcd for C<sub>23</sub>H<sub>22</sub>FN<sub>4</sub>O<sub>4</sub>S<sub>2</sub> [M+H]<sup>+</sup>: 501.1066;

found: 501.1068.

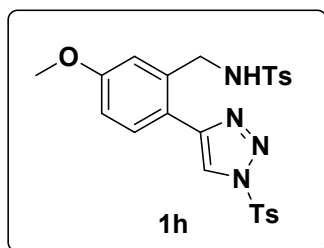


**4-methyl-N-(2-(1-tosyl-1H-1,2,3-triazol-4-yl)-5-**

**(trifluoromethyl)benzyl)benzenesulfonamide (1g):** Yield: 53%;

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  8.39 (s, 1H), 8.08 (d,  $J = 8.4$  Hz, 2H), 7.61 (d,  $J = 8.2$  Hz, 2H), 7.55-7.50 (m, 2H), 7.49 (s, 1H), 7.46 (d,  $J = 8.2$  Hz, 2H), 7.15 (d,  $J = 8.1$  Hz, 2H), 6.23 (t,  $J = 6.9$

Hz, 1H), 4.23 (d,  $J = 6.9$  Hz, 2H), 2.49 (s, 3H), 2.35 (s, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  148.2, 145.6, 143.4, 137.6, 135.6, 132.5, 131.6, 131.3 (q,  $J = 32.9$  Hz), 130.9, 129.7, 129.6, 129.2, 128.7 (q,  $J = 3.4$  Hz), 127.0, 125.3 (q,  $J = 3.4$  Hz), 123.5 (q,  $J = 272.6$  Hz), 122.0, 46.3, 22.1, 21.5; IR  $\nu_{\text{max}}$  (KBr): 3281, 2924, 1595, 1395, 1325, 1170, 1155, 996  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $\text{C}_{24}\text{H}_{22}\text{F}_3\text{N}_4\text{O}_4\text{S}_2$   $[\text{M}+\text{H}]^+$ : 551.1035; found: 551.1039.

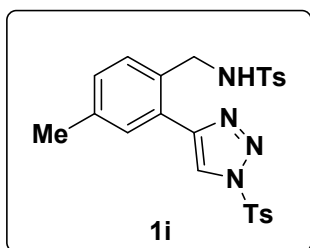


**N-(5-methoxy-2-(1-tosyl-1H-1,2,3-triazol-4-yl)benzyl)-4-**

**methylbenzenesulfonamide (1h):** Yield: 93%;  $^1\text{H}$  NMR (600

MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 (s, 1H), 8.04 (d,  $J = 8.4$  Hz, 2H), 7.65 (d,  $J = 8.2$  Hz, 2H), 7.43 (d,  $J = 8.3$  Hz, 2H), 7.30 (d,  $J = 8.5$  Hz, 1H), 7.17 (d,  $J = 8.1$  Hz, 2H), 6.82 (d,  $J = 2.6$  Hz, 1H), 6.80 (dd,  $J = 8.5$

Hz, 2.6 Hz, 1H), 6.26 (t,  $J = 6.8$  Hz, 1H), 4.08 (d,  $J = 6.8$  Hz, 2H), 3.77 (s, 3H), 2.47 (s, 3H), 2.36 (s, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  160.3, 147.8, 146.9, 143.1, 137.7, 136.3, 132.8, 130.7, 130.7, 129.6, 129.0, 127.1, 120.4, 120.4, 116.6, 114.4, 55.5, 46.8, 22.0, 21.6; IR  $\nu_{\text{max}}$  (KBr): 3274, 2921, 1615, 1495, 1397, 1196, 1159, 977  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $\text{C}_{24}\text{H}_{25}\text{N}_4\text{O}_5\text{S}_2$   $[\text{M}+\text{H}]^+$ : 513.1266; found: 513.1271.

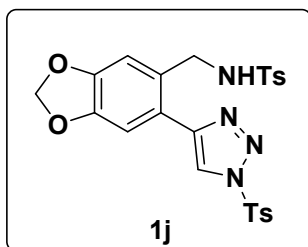


**4-methyl-N-(4-methyl-2-(1-tosyl-1H-1,2,3-triazol-4-**

**yl)benzyl)benzenesulfonamide (1i):** Yield: 98%;  $^1\text{H}$  NMR (600

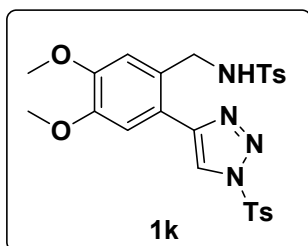
MHz,  $\text{CDCl}_3$ )  $\delta$  8.29 (s, 1H), 8.05 (d,  $J = 8.4$  Hz, 2H), 7.66 (d,  $J = 8.2$  Hz, 2H), 7.43 (d,  $J = 8.2$  Hz, 2H), 7.24-7.20 (m, 2H), 7.18 (d,  $J = 8.0$  Hz, 2H), 7.08 (d,  $J = 7.7$  Hz, 1H), 6.12 (t,  $J = 6.7$  Hz, 1H),

4.06 (d,  $J = 6.7$  Hz, 2H), 2.48 (s, 3H), 2.38 (s, 3H), 2.32 (s, 3H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$  147.9, 147.0, 143.0, 138.5, 137.6, 132.8, 131.9, 131.8, 130.7, 130.4, 129.9, 129.6, 129.0, 127.9, 127.1, 121.1, 46.3, 22.0, 21.6, 21.1; IR  $\nu_{\text{max}}$  (KBr): 3146, 2923, 1596, 1328, 1161, 1093, 1009, 814  $\text{cm}^{-1}$ ; HRMS  $m/z$  calcd for  $\text{C}_{24}\text{H}_{25}\text{N}_4\text{O}_4\text{S}_2$   $[\text{M}+\text{H}]^+$ : 497.1317; found: 497.1322.



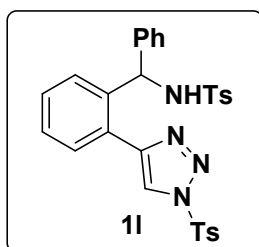
**4-methyl-N-((6-(1-tosyl-1*H*-1,2,3-triazol-4-yl)benzo[d][1,3]dioxol-5-yl)methyl)benzenesulfonamide (1j):**

Yield: 93%; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) δ 8.19 (s, 1H), 8.05 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.44 (d, *J* = 8.3 Hz, 2H), 7.21 (d, *J* = 8.1 Hz, 2H), 6.82 (s, 1H), 6.79 (s, 1H), 6.08 (t, *J* = 6.8 Hz, 1H), 5.97 (s, 2H), 3.98 (d, *J* = 6.8 Hz, 2H), 2.48 (s, 3H), 2.39 (s, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 148.6, 147.9, 147.8, 146.8 143.1, 137.7, 132.8, 130.8, 129.6, 129.5, 129.1, 127.2, 121.7, 120.7, 111.9, 109.0, 101.9, 46.4, 22.1, 21.6; IR ν<sub>max</sub> (KBr): 3268, 3171, 1595, 1506, 1391, 1158, 1031, 985 cm<sup>-1</sup>; HRMS *m/z* calcd for C<sub>24</sub>H<sub>23</sub>N<sub>4</sub>O<sub>6</sub>S<sub>2</sub> [M+H]<sup>+</sup>: 527.1059; found: 527.1055.



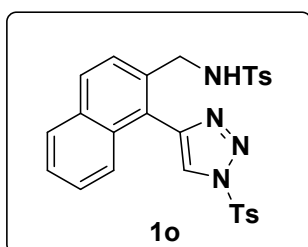
**N-(4,5-dimethoxy-2-(1-tosyl-1*H*-1,2,3-triazol-4-yl)benzyl)-4-methylbenzenesulfonamide (1k):** Yield: 85%; <sup>1</sup>H NMR (600 MHz,

CDCl<sub>3</sub>) δ 8.25 (s, 1H), 8.06 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.43 (d, *J* = 8.2 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 6.86 (s, 1H), 6.77 (s, 1H), 6.08 (t, *J* = 6.8 Hz, 1H), 4.04 (d, *J* = 6.8 Hz, 2H), 3.86 (s, 3H), 3.83 (s, 3H), 2.48 (s, 3H), 2.37 (s, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) δ 149.6, 148.8, 147.9, 146.7, 143.2, 137.6, 132.8, 130.7, 129.6, 129.0, 127.7, 127.1, 120.6, 120.5, 114.4, 112.0, 56.3, 56.1, 46.4, 22.1, 21.6; IR ν<sub>max</sub> (KBr): 3341, 3156, 1593, 1501, 1461, 1332, 1156, 2083, 973 cm<sup>-1</sup>; HRMS *m/z* calcd for C<sub>25</sub>H<sub>27</sub>N<sub>4</sub>O<sub>6</sub>S<sub>2</sub> [M+H]<sup>+</sup>: 543.1372; found: 543.1378.



**4-methyl-N-(phenyl(2-(1-tosyl-1*H*-1,2,3-triazol-4-yl)phenyl)methyl)benzenesulfonamide (1l):** Yield: 82%; <sup>1</sup>H NMR

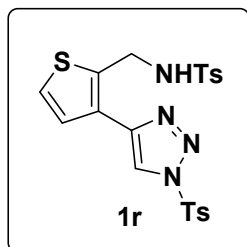
(600 MHz, CDCl<sub>3</sub>) δ 7.92 (d, *J* = 8.5 Hz, 2H), 7.72 (s, 1H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.42 (d, *J* = 8.1 Hz, 2H), 7.30-7.27 (m, 1H), 7.26-7.21 (m, 3H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.93-6.82 (m, 5H), 6.71 (d, *J* = 8.8 Hz, 1H), 5.90 (d, *J* = 9.0 Hz, 1H), 2.49 (s, 3H), 2.33 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 147.6, 146.7, 143.0, 140.1, 134.0, 138.0, 132.8, 131.0, 130.7, 130.6, 129.5, 129.3, 128.9, 128.0, 127.8, 127.6, 127.0, 126.9, 126.4, 121.3, 59.8, 22.0, 21.6; IR ν<sub>max</sub> (KBr): 3274, 3134, 1593, 1449, 1396, 1318, 1195, 1165, 1095, 983 cm<sup>-1</sup>; HRMS *m/z* calcd for C<sub>29</sub>H<sub>27</sub>N<sub>4</sub>O<sub>4</sub>S<sub>2</sub> [M+H]<sup>+</sup>: 559.1474; found: 559.1476.



**4-methyl-N-((1-(1-tosyl-1*H*-1,2,3-triazol-4-yl)naphthalen-2-yl)methyl)benzenesulfonamide (1o):** Yield: 90%; <sup>1</sup>H NMR (400



MHz, CDCl<sub>3</sub>)  $\delta$  8.29 (s, 1H), 8.11 (d,  $J$  = 8.4 Hz, 2H), 7.86-7.79 (m, 2H), 7.63 (d,  $J$  = 8.3 Hz, 2H), 7.52-7.40 (m, 6H), 7.16 (d,  $J$  = 8.1 Hz, 2H), 5.62 (t,  $J$  = 6.6 Hz, 1H), 3.90 (d,  $J$  = 6.6 Hz, 2H), 2.50 (s, 3H), 2.36 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  147.9, 143.4, 142.9, 137.0, 134.4, 133.1, 132.8, 132.2, 130.8, 130.3, 129.7, 129.1, 128.5, 127.8, 127.3, 127.1, 126.5, 125.5, 124.9, 123.8, 46.4, 22.1, 21.6; IR  $\nu_{\max}$  (KBr): 3137, 1594, 1399, 1319, 1198, 1153, 1091, 1025, 995 cm<sup>-1</sup>; HRMS  $m/z$  calcd for C<sub>27</sub>H<sub>25</sub>N<sub>4</sub>O<sub>4</sub>S<sub>2</sub> [M+H]<sup>+</sup>: 533.1317; found: 533.1321.

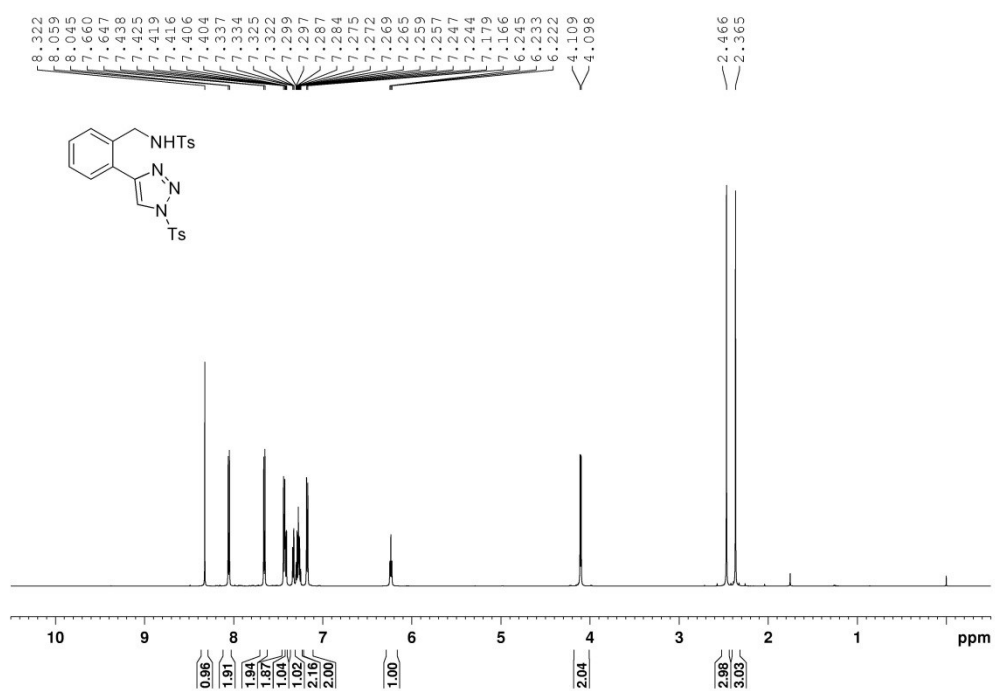


**4-methyl-N-((3-(1-tosyl-1H-1,2,3-triazol-4-yl)thiophen-2-**

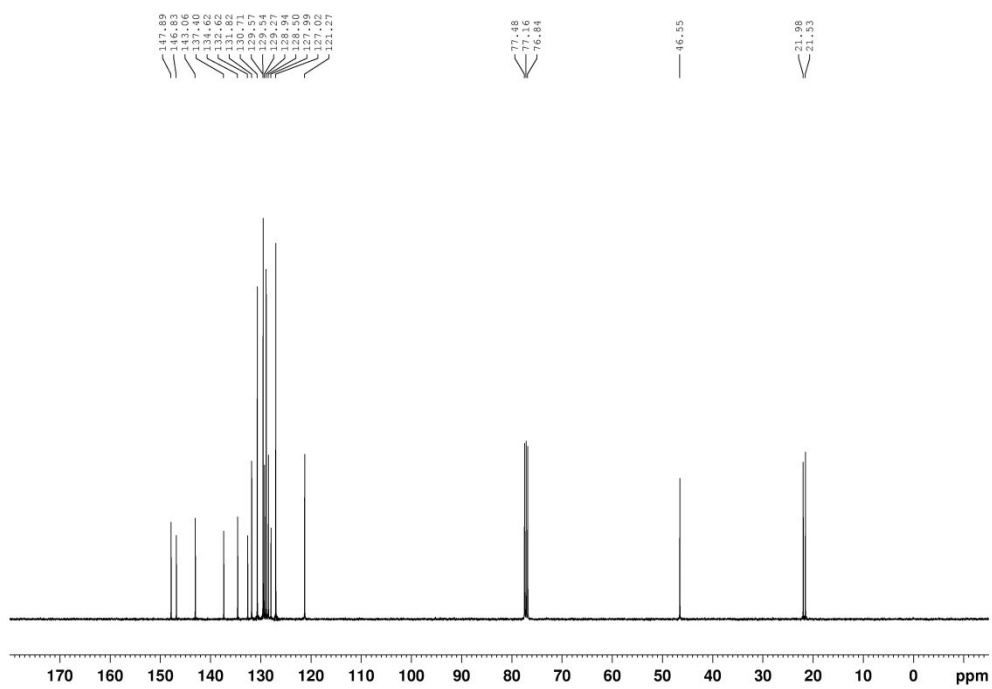
**yl)methyl)benzenesulfonamide (1r):** Yield: 84%; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.20 (s, 1H), 8.04 (d,  $J$  = 8.4 Hz, 2H), 7.66 (d,  $J$  = 8.3 Hz, 2H), 7.44 (d,  $J$  = 8.2 Hz, 2H), 7.20-7.15 (m, 3H), 7.07 (d,  $J$  = 5.3 Hz, 1H), 6.19 (t,  $J$  = 6.8 Hz, 1H), 4.41 (d,  $J$  = 6.8 Hz, 2H), 2.48 (s, 3H), 2.38 (s,

3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  147.9, 143.3, 143.2, 137.6, 136.6, 132.9, 130.8, 129.6, 129.0, 127.1, 127.1, 127.0, 125.3, 119.8, 40.7, 22.1, 21.6; IR  $\nu_{\max}$  (KBr): 3231, 1928, 1595, 1431, 1392, 1194, 1091, 987 cm<sup>-1</sup>; HRMS  $m/z$  calcd for C<sub>21</sub>H<sub>21</sub>N<sub>4</sub>O<sub>4</sub>S<sub>3</sub> [M+H]<sup>+</sup>: 489.0725; found: 489.0728.

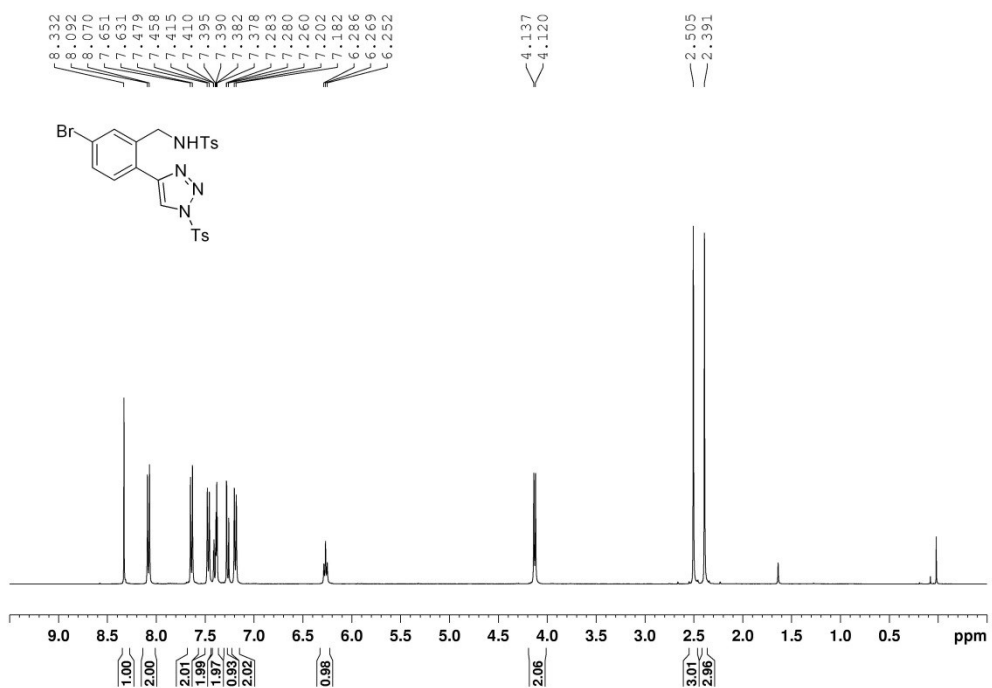
## 4. NMR spectrum



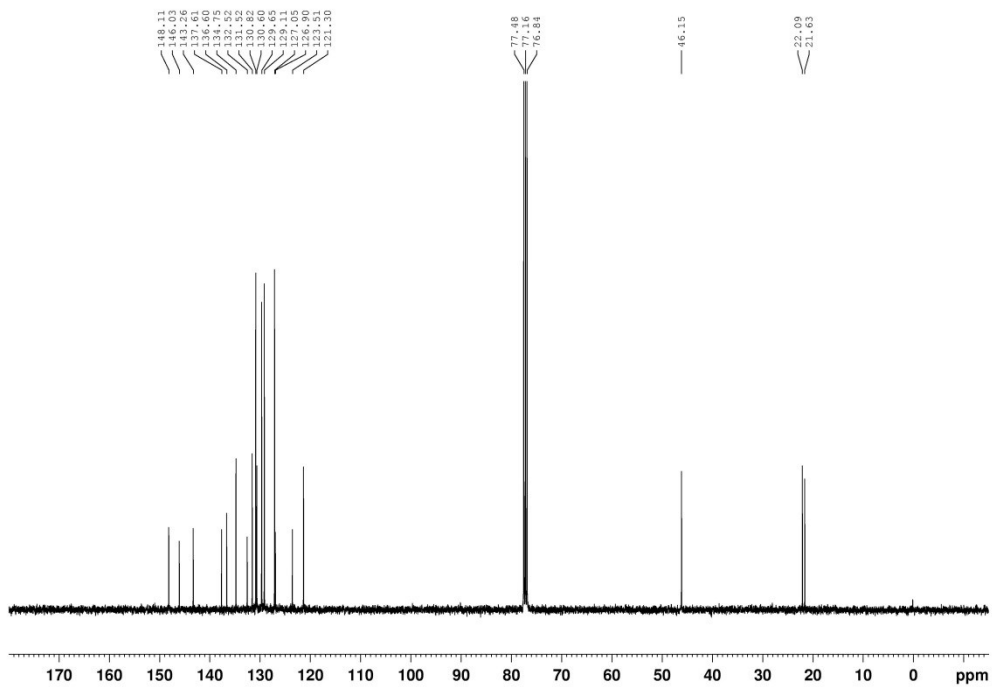
<sup>1</sup>H NMR Spectrum for **1a** (CDCl<sub>3</sub>, 600 MHz)



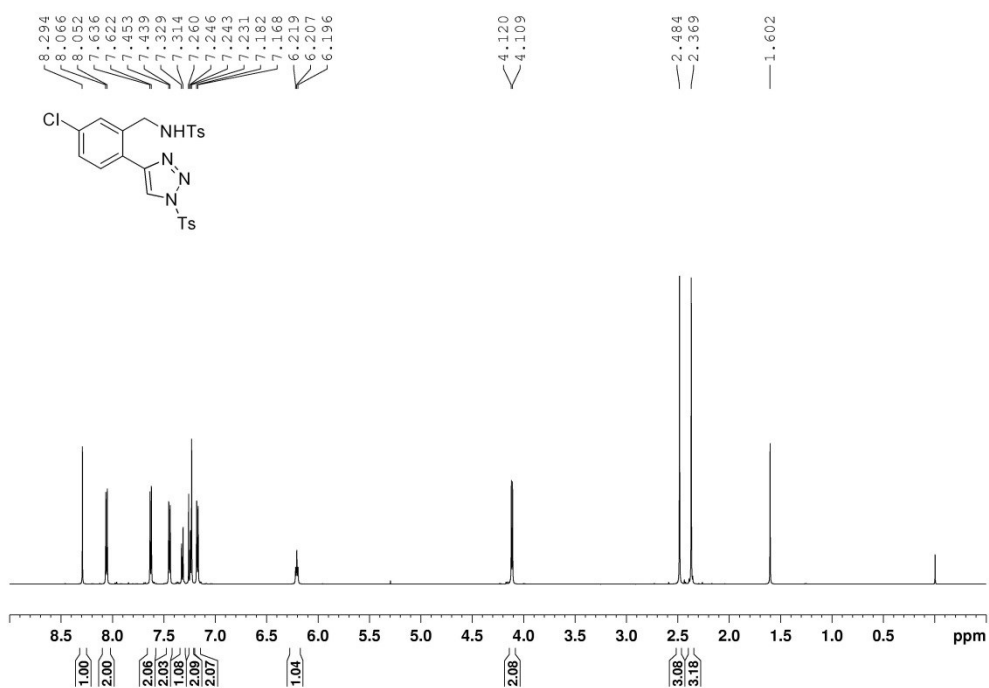
<sup>13</sup>C NMR Spectrum for **1a** (CDCl<sub>3</sub>, 100 MHz)



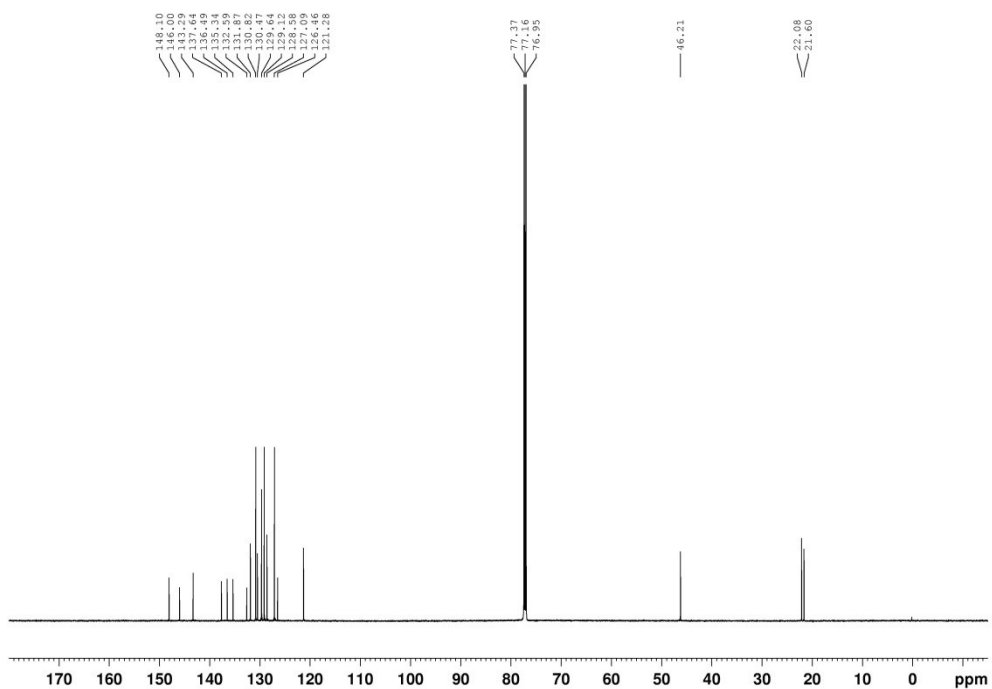
<sup>1</sup>H NMR Spectrum for **1b** (CDCl<sub>3</sub>, 400 MHz)



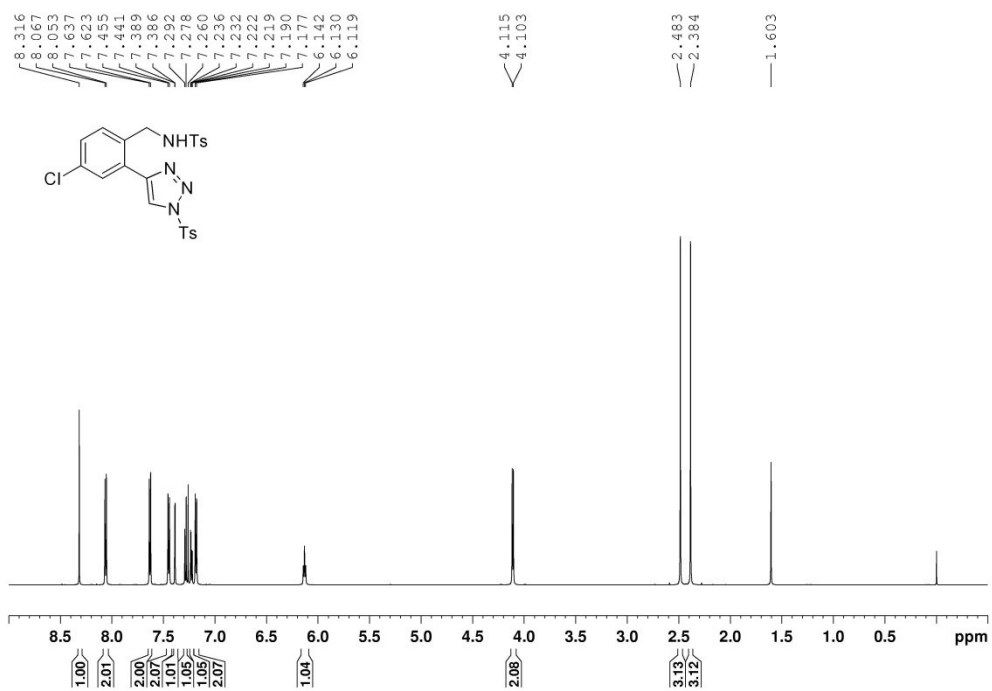
<sup>13</sup>C NMR Spectrum for **1b** (CDCl<sub>3</sub>, 100 MHz)



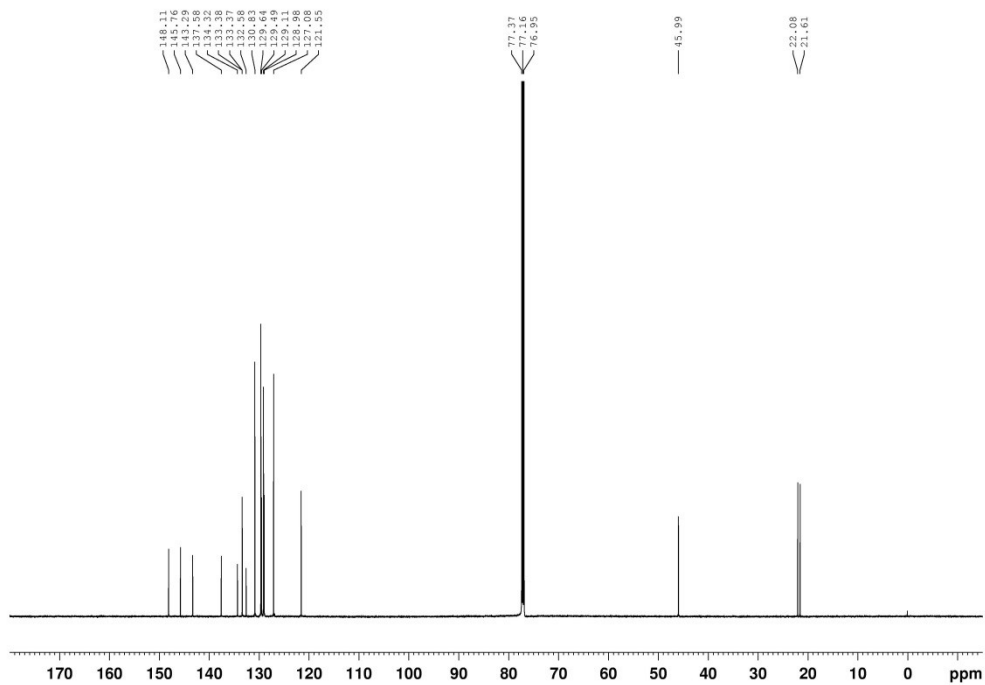
<sup>1</sup>H NMR Spectrum for 1c (CDCl<sub>3</sub>, 600 MHz)



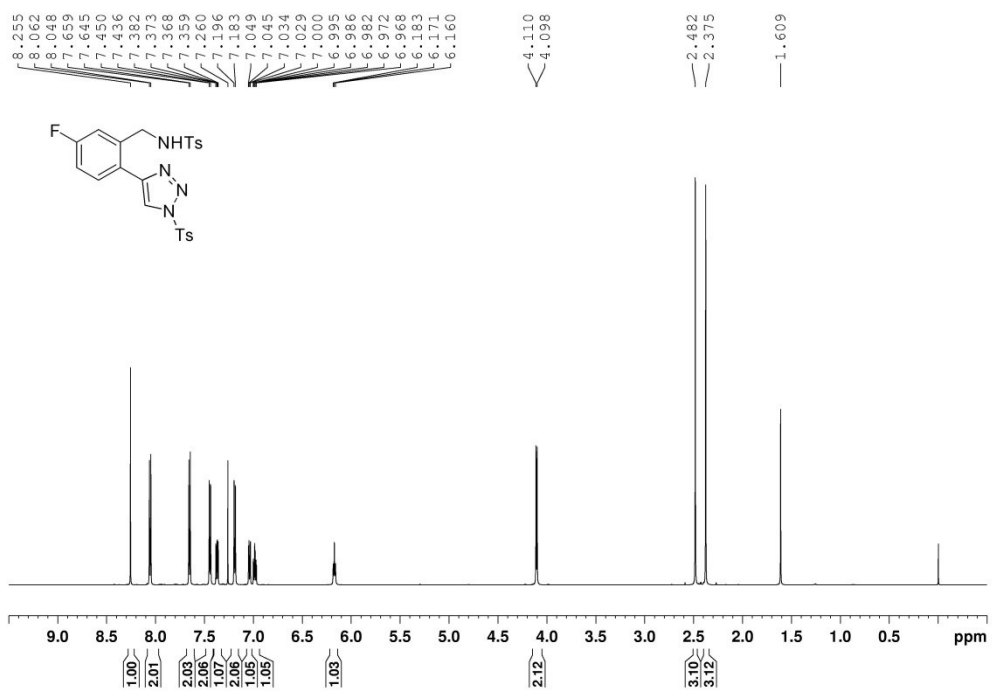
<sup>13</sup>C NMR Spectrum for 1c (CDCl<sub>3</sub>, 150 MHz)



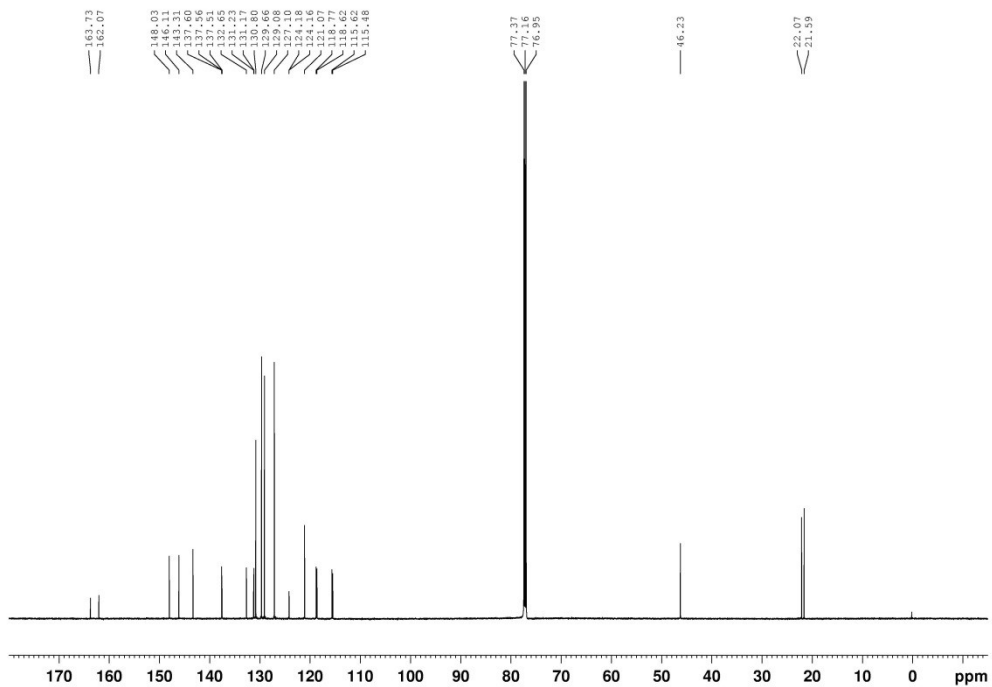
**<sup>1</sup>H NMR Spectrum for **1d** (CDCl<sub>3</sub>, 600 MHz)**



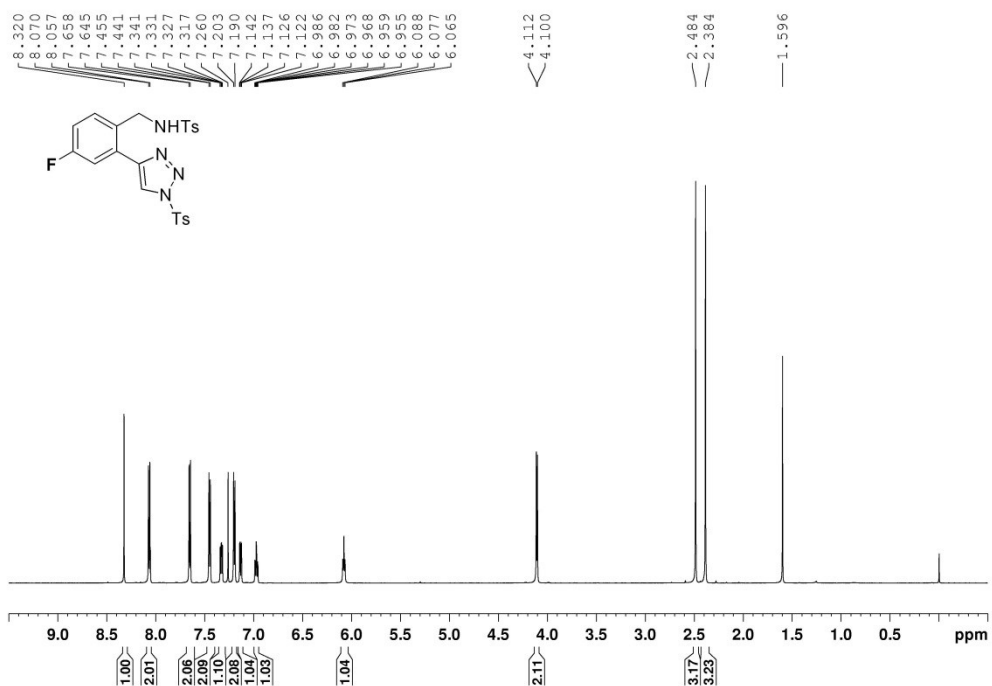
**<sup>13</sup>C NMR Spectrum for **1d** (CDCl<sub>3</sub>, 150 MHz)**



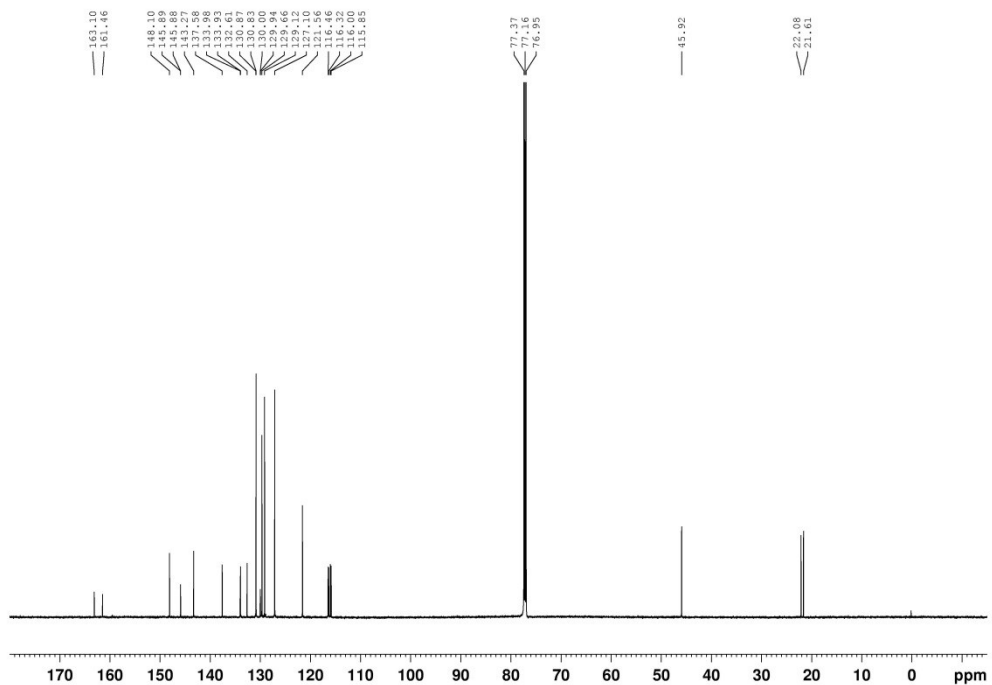
**<sup>1</sup>H NMR Spectrum for 1e (CDCl<sub>3</sub>, 600 MHz)**



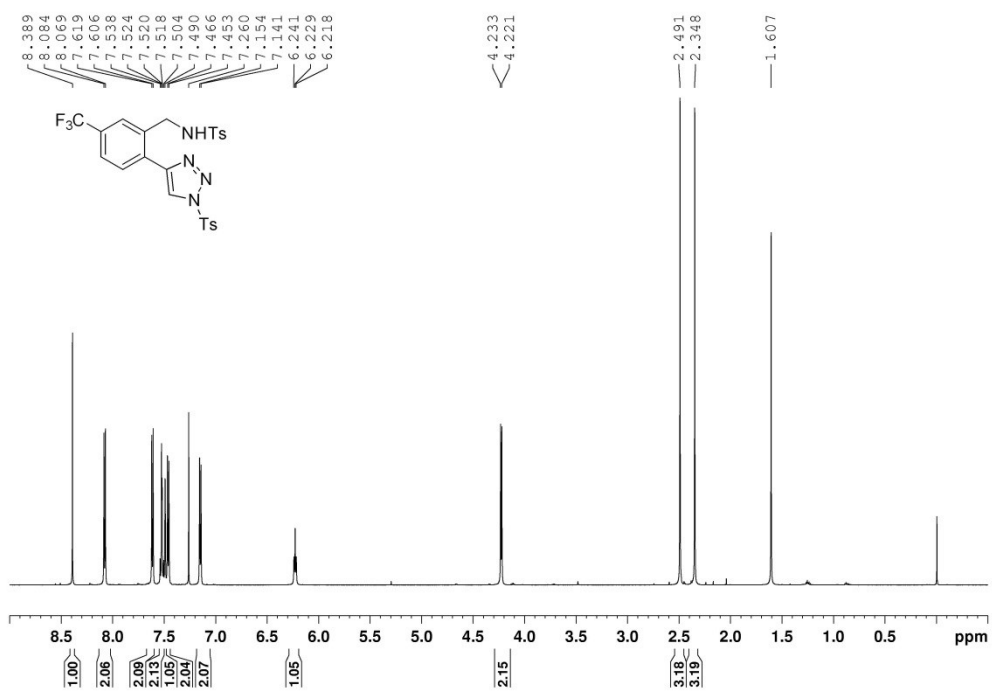
**<sup>13</sup>C NMR Spectrum for 1e (CDCl<sub>3</sub>, 150 MHz)**



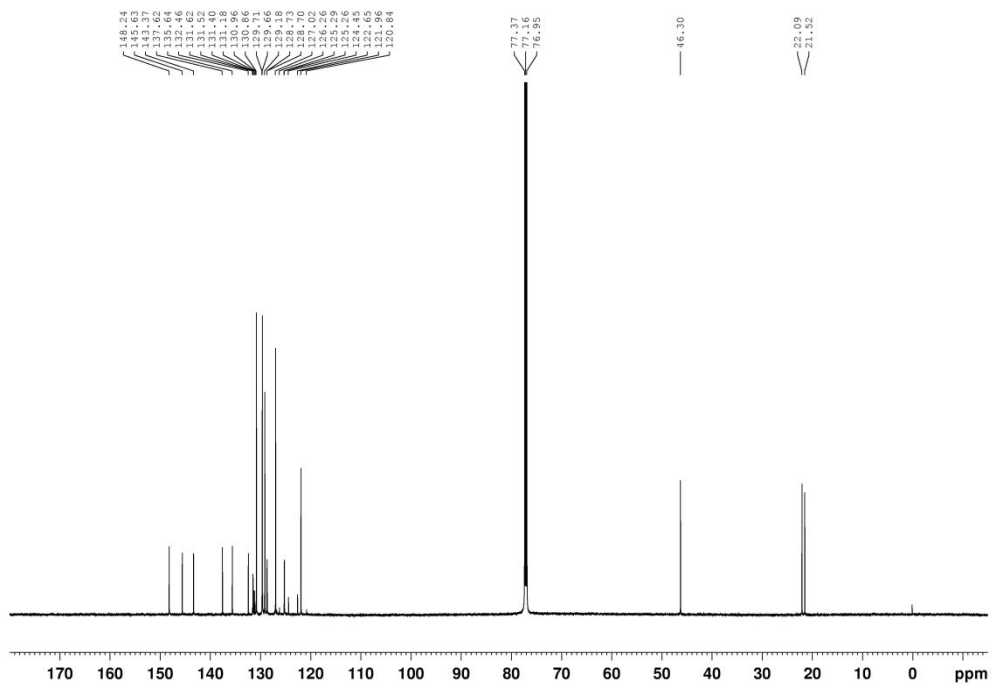
<sup>1</sup>H NMR Spectrum for **1f** (CDCl<sub>3</sub>, 600 MHz)



<sup>13</sup>C NMR Spectrum for **1f** (CDCl<sub>3</sub>, 150 MHz)

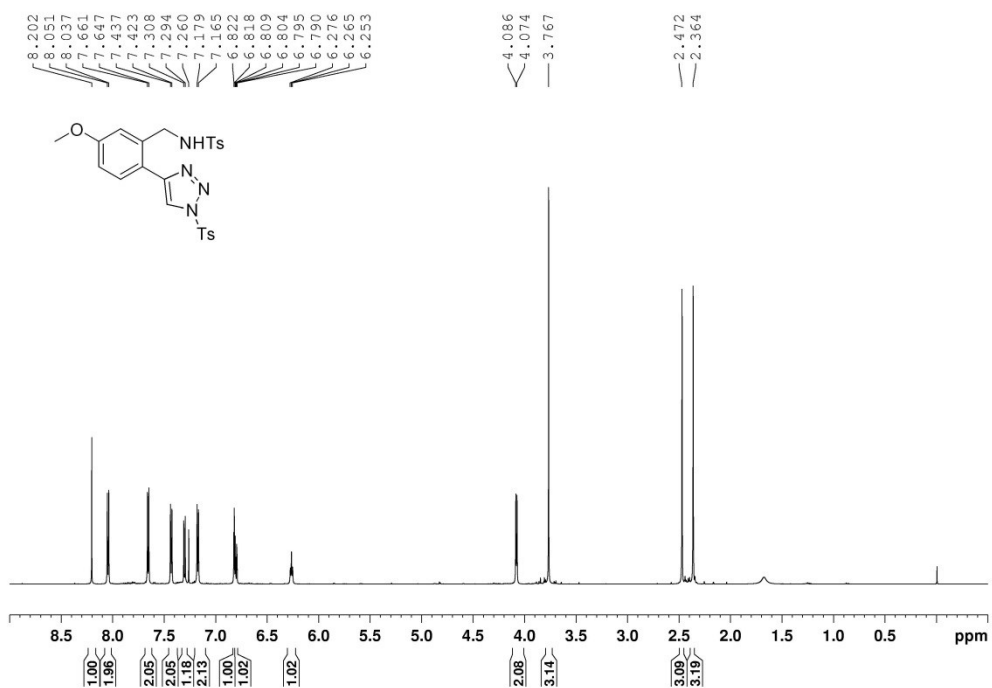


<sup>1</sup>H NMR Spectrum for **1g** (CDCl<sub>3</sub>, 600 MHz)

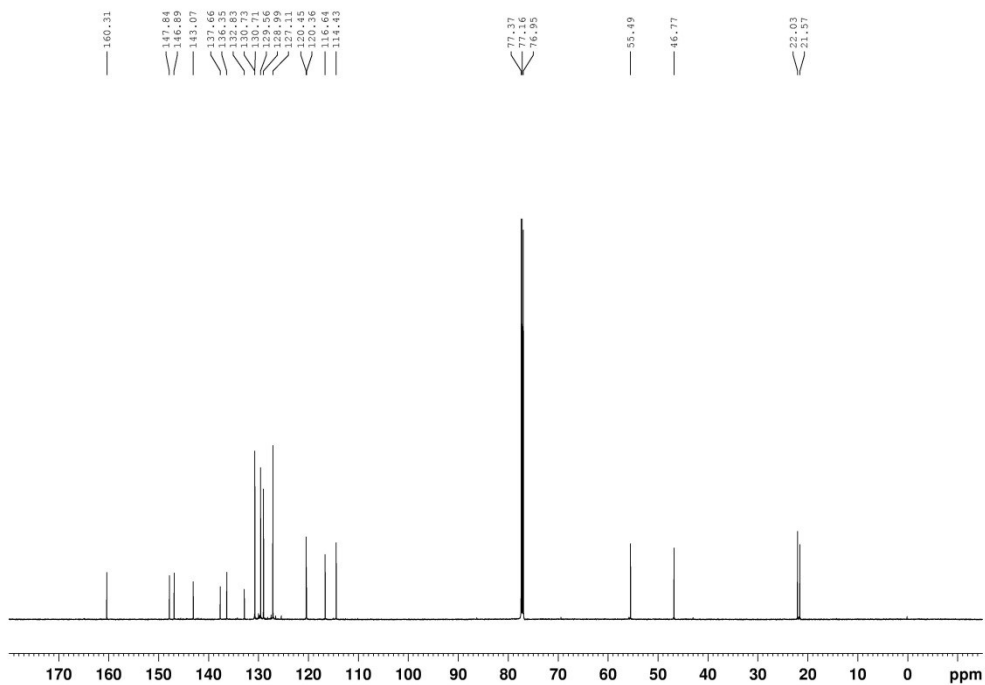


<sup>13</sup>C NMR Spectrum for **1g** (CDCl<sub>3</sub>, 150 MHz)

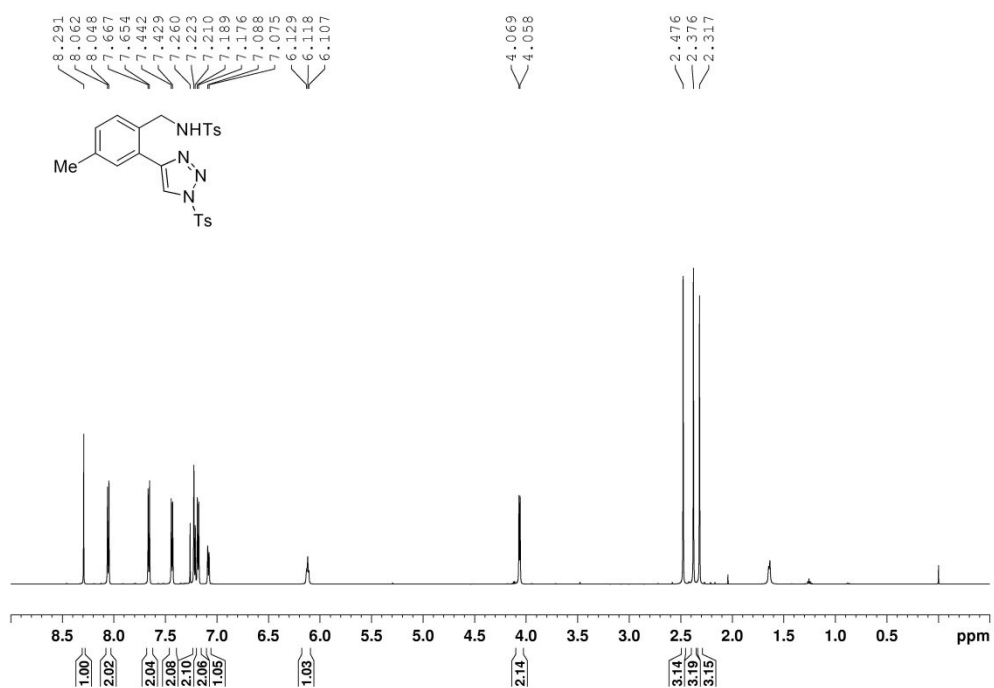




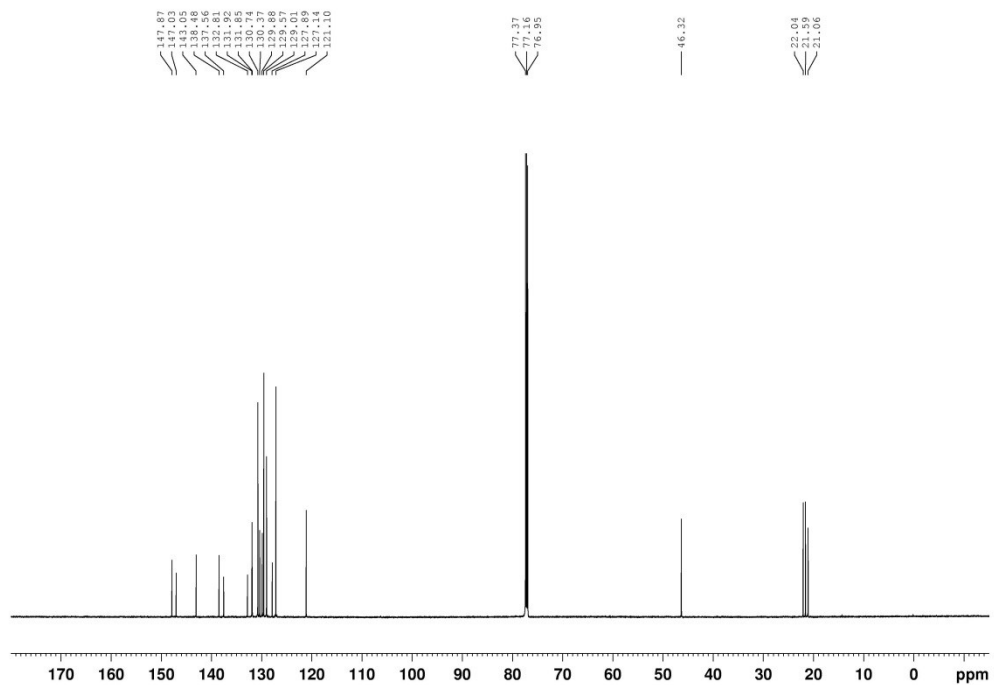
**<sup>1</sup>H NMR Spectrum for **1h** (CDCl<sub>3</sub>, 600 MHz)**



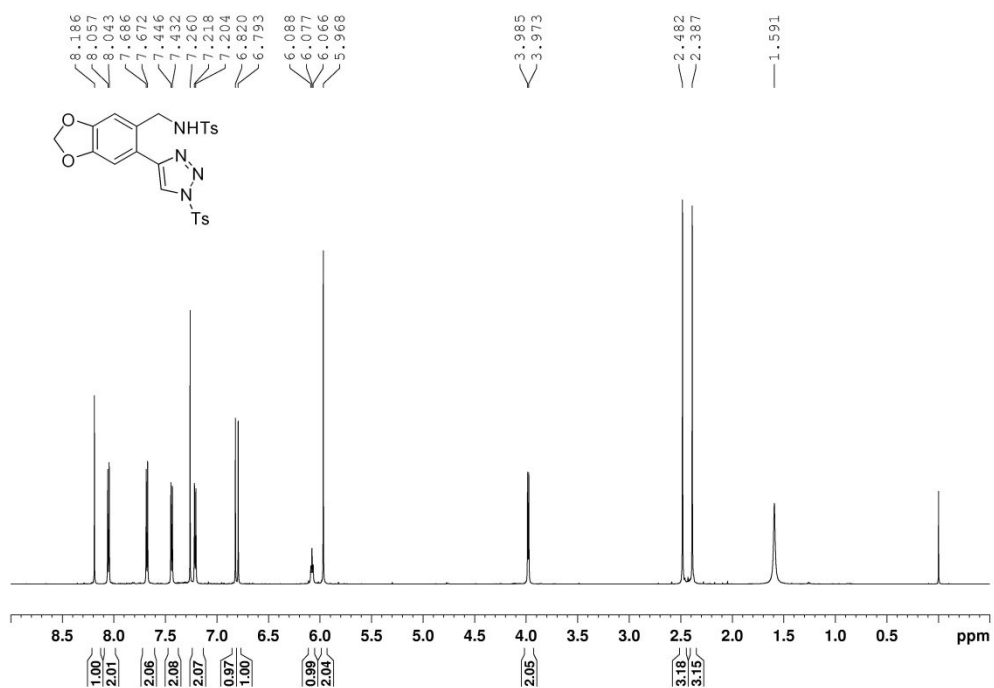
**<sup>13</sup>C NMR Spectrum for **1h** (CDCl<sub>3</sub>, 150 MHz)**



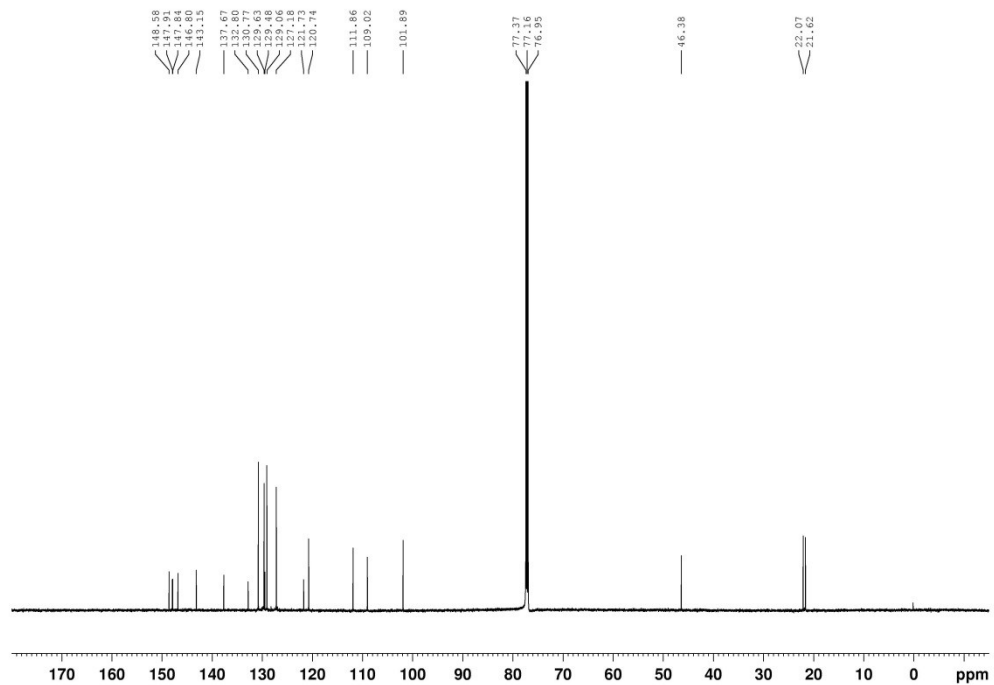
**<sup>1</sup>H NMR Spectrum for **1i** (CDCl<sub>3</sub>, 600 MHz)**



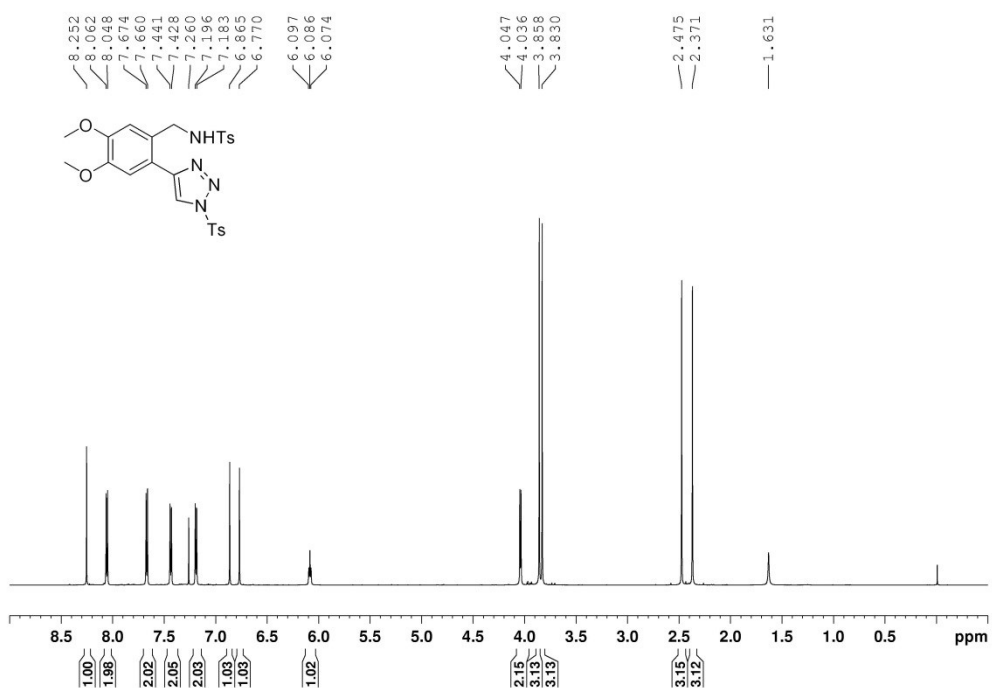
**<sup>13</sup>C NMR Spectrum for **1i** (CDCl<sub>3</sub>, 150 MHz)**



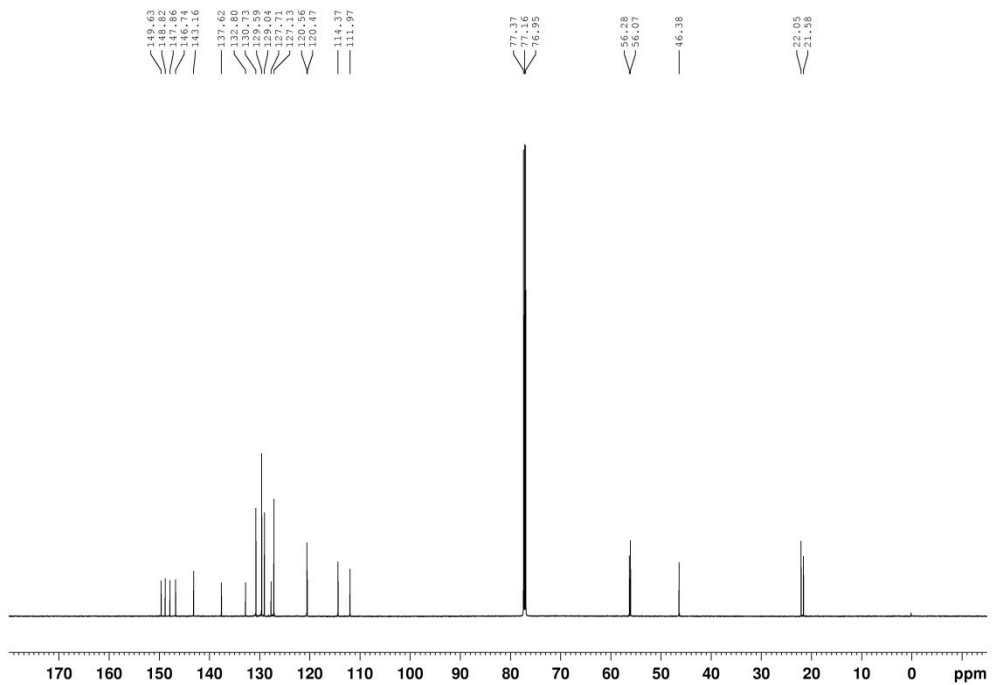
**<sup>1</sup>H NMR Spectrum for **1j** (CDCl<sub>3</sub>, 600 MHz)**



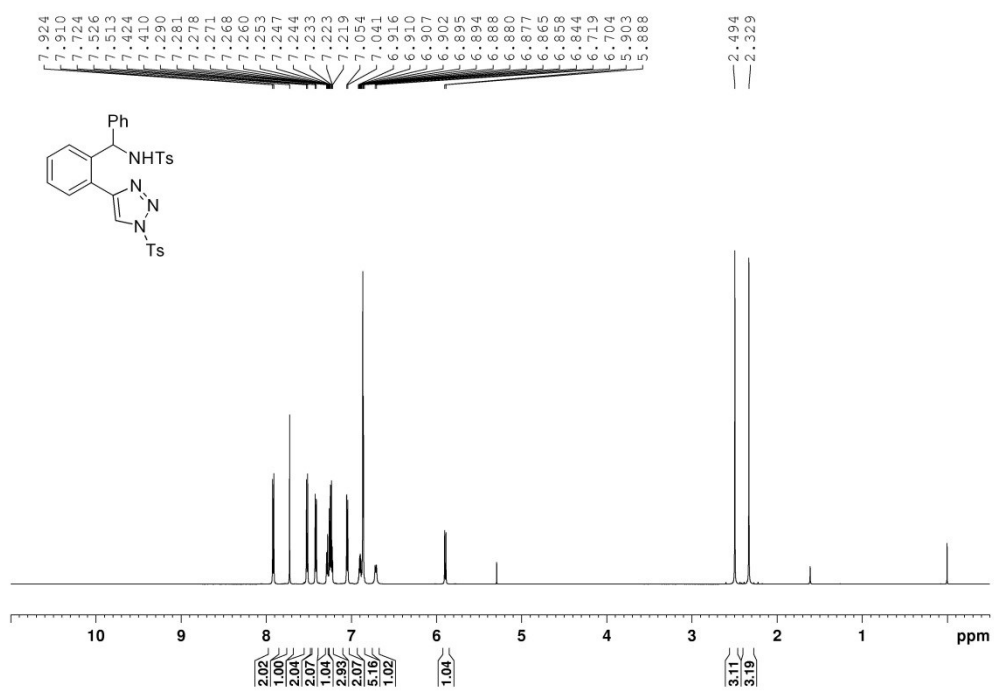
**<sup>13</sup>C NMR Spectrum for **1j** (CDCl<sub>3</sub>, 150 MHz)**



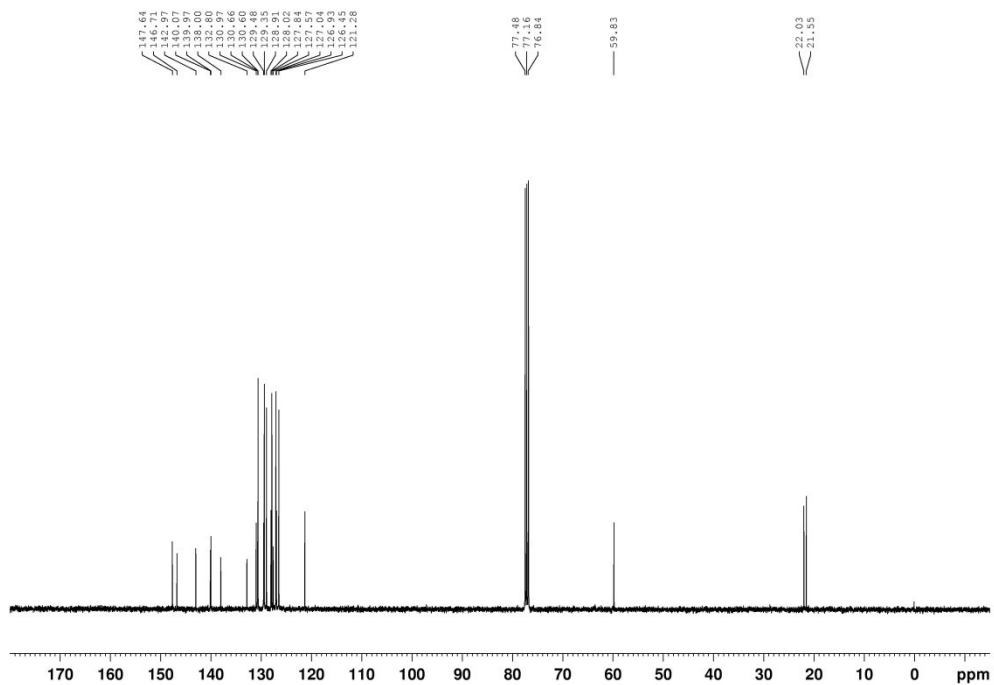
<sup>1</sup>H NMR Spectrum for **1k** (CDCl<sub>3</sub>, 600 MHz)



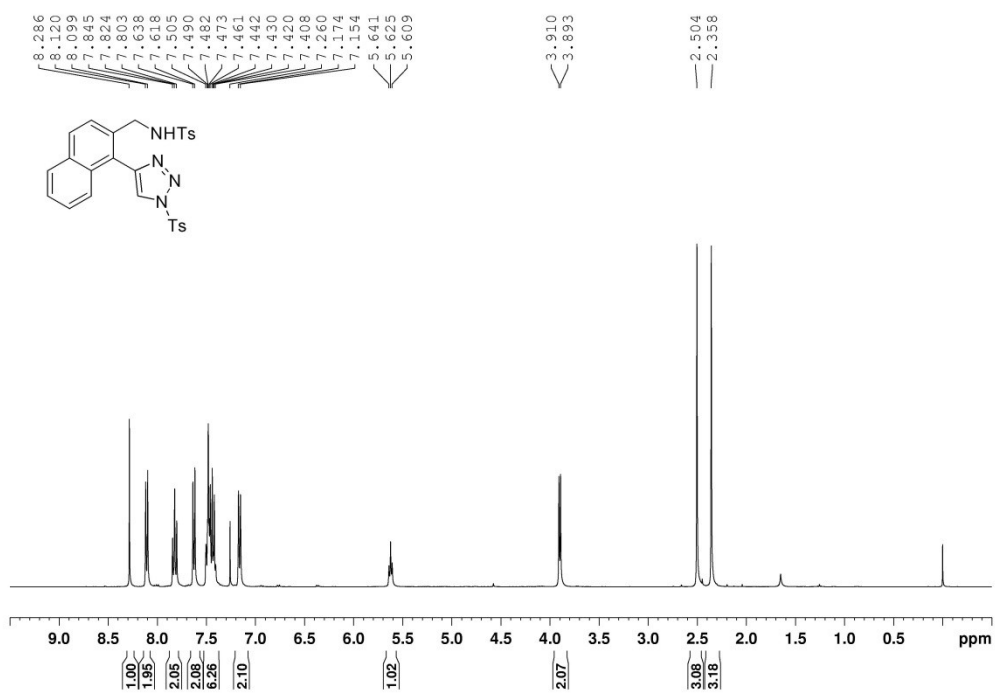
<sup>13</sup>C NMR Spectrum for **1k** (CDCl<sub>3</sub>, 150 MHz)



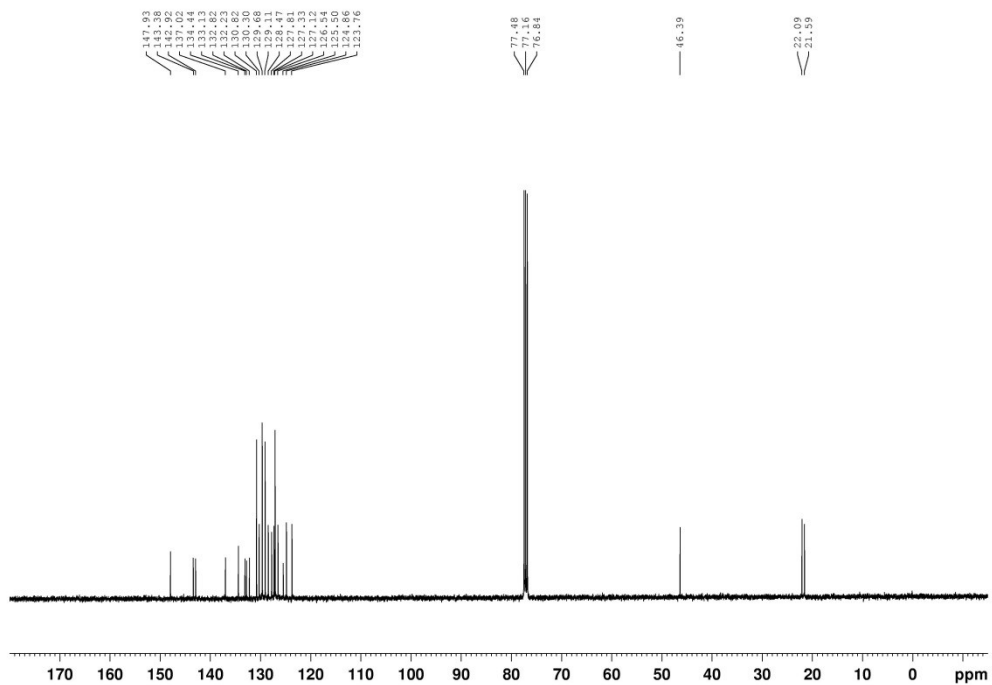
<sup>1</sup>H NMR Spectrum for **11** (CDCl<sub>3</sub>, 600 MHz)



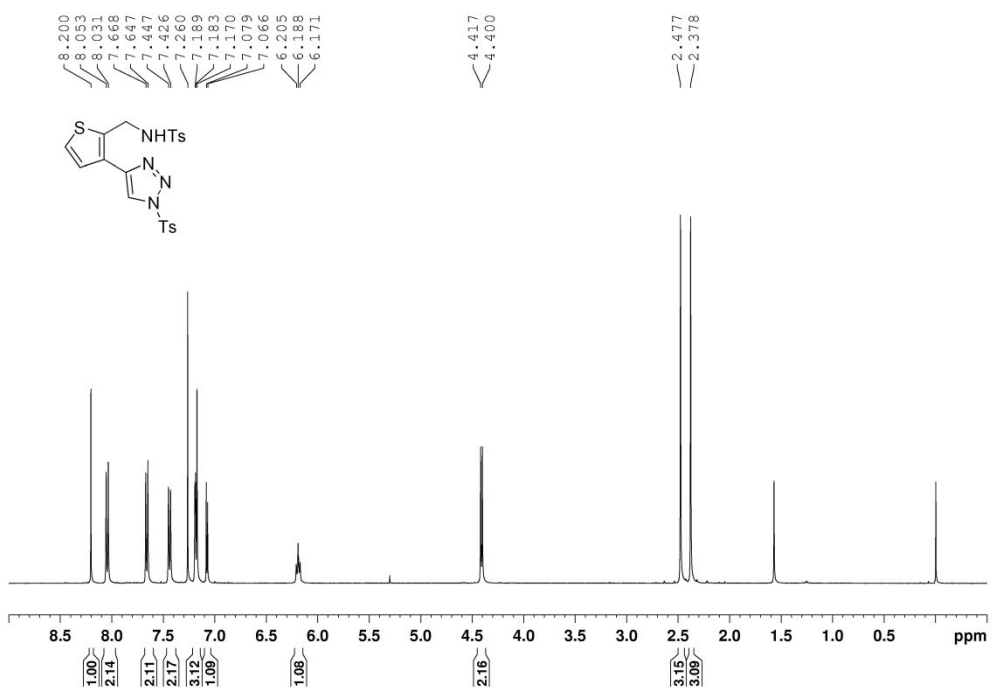
<sup>13</sup>C NMR Spectrum for **11** (CDCl<sub>3</sub>, 100 MHz)



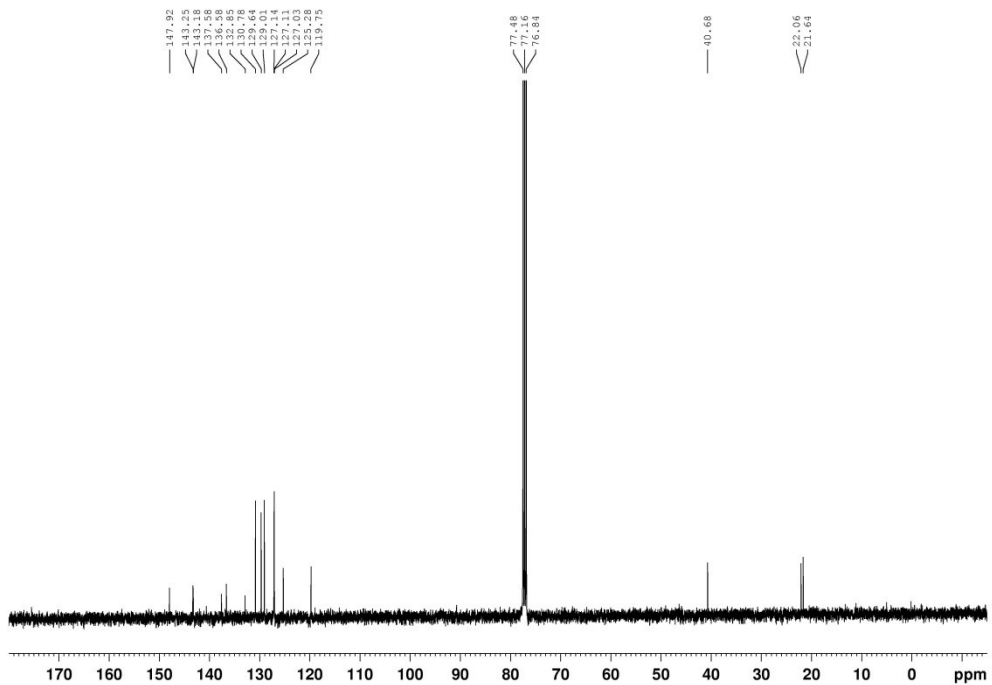
<sup>1</sup>H NMR Spectrum for **1o** (CDCl<sub>3</sub>, 400 MHz)



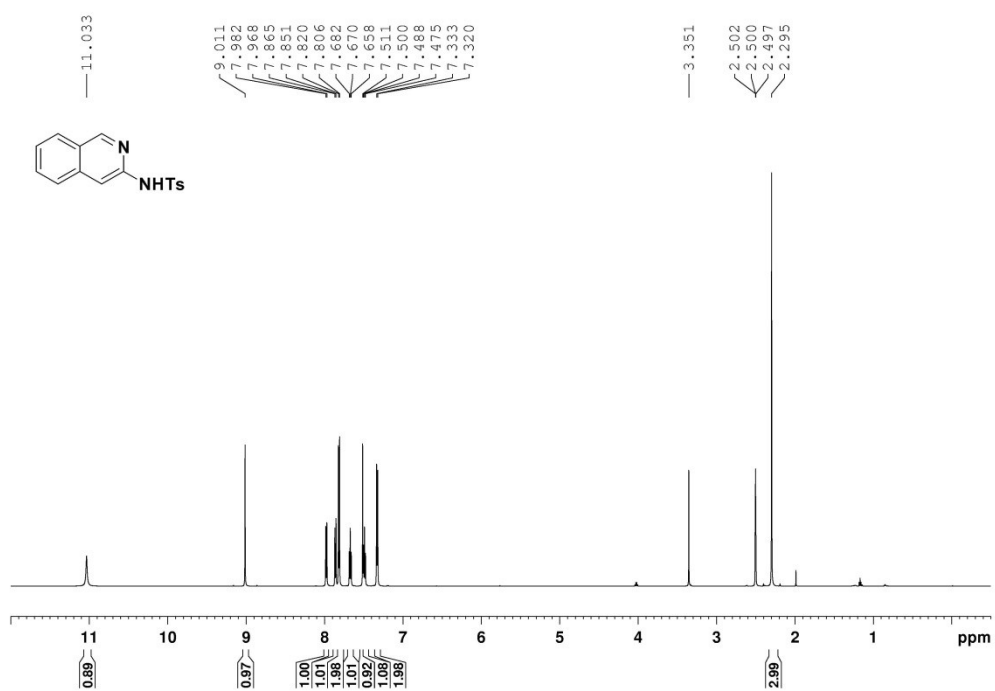
<sup>13</sup>C NMR Spectrum for **1o** (CDCl<sub>3</sub>, 100 MHz)



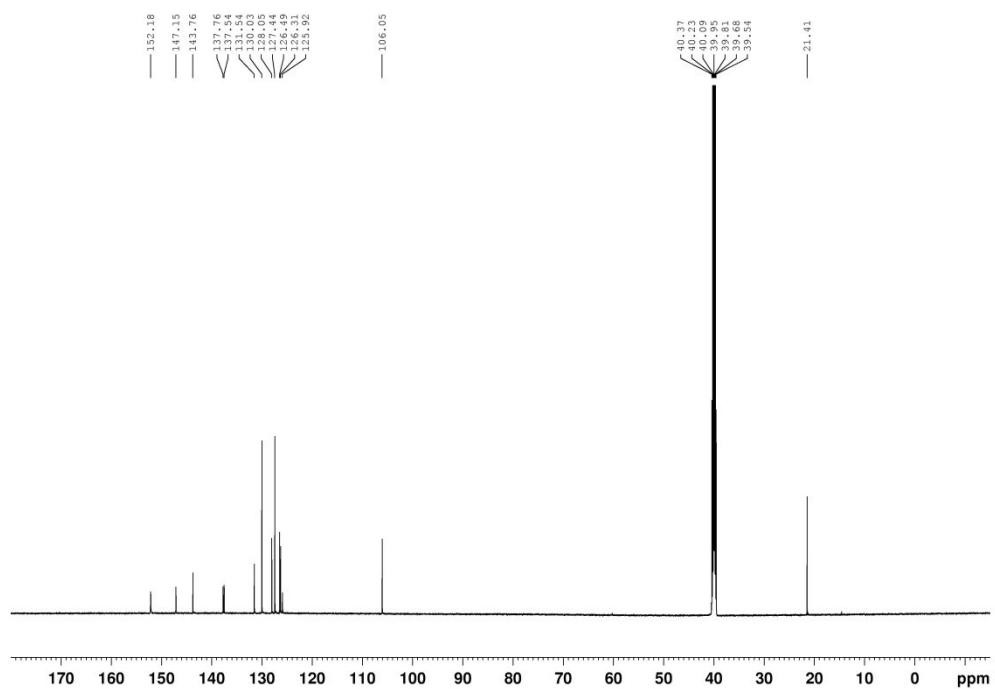
<sup>1</sup>H NMR Spectrum for **1p** (CDCl<sub>3</sub>, 400 MHz)



<sup>13</sup>C NMR Spectrum for **1p** (CDCl<sub>3</sub>, 100 MHz)

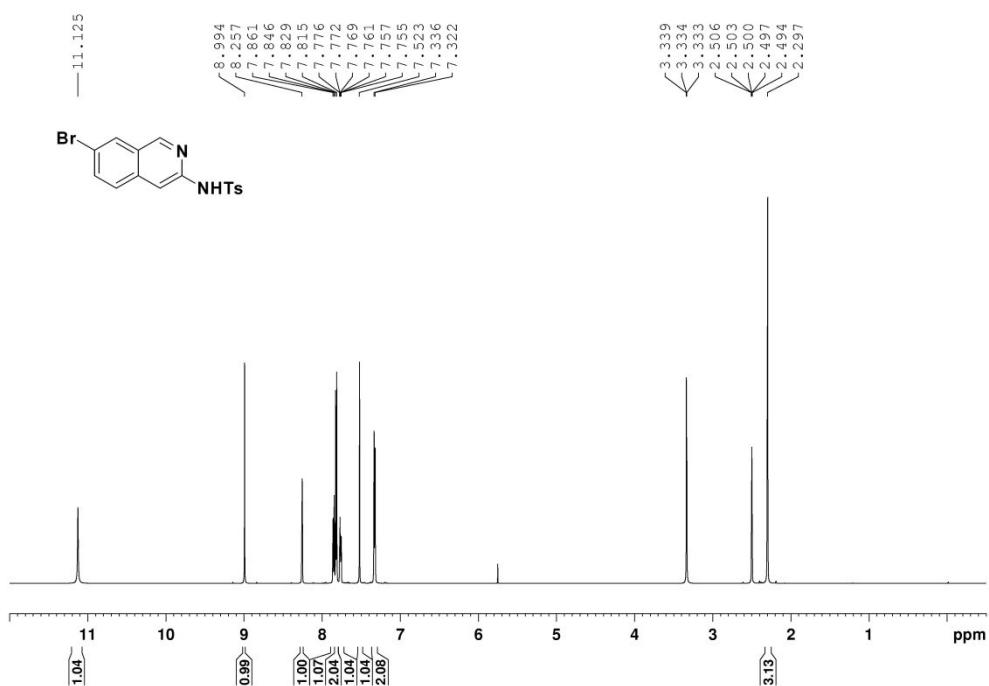


<sup>1</sup>H NMR Spectrum for **3a** (DMSO-*d*<sub>6</sub>, 600 MHz)

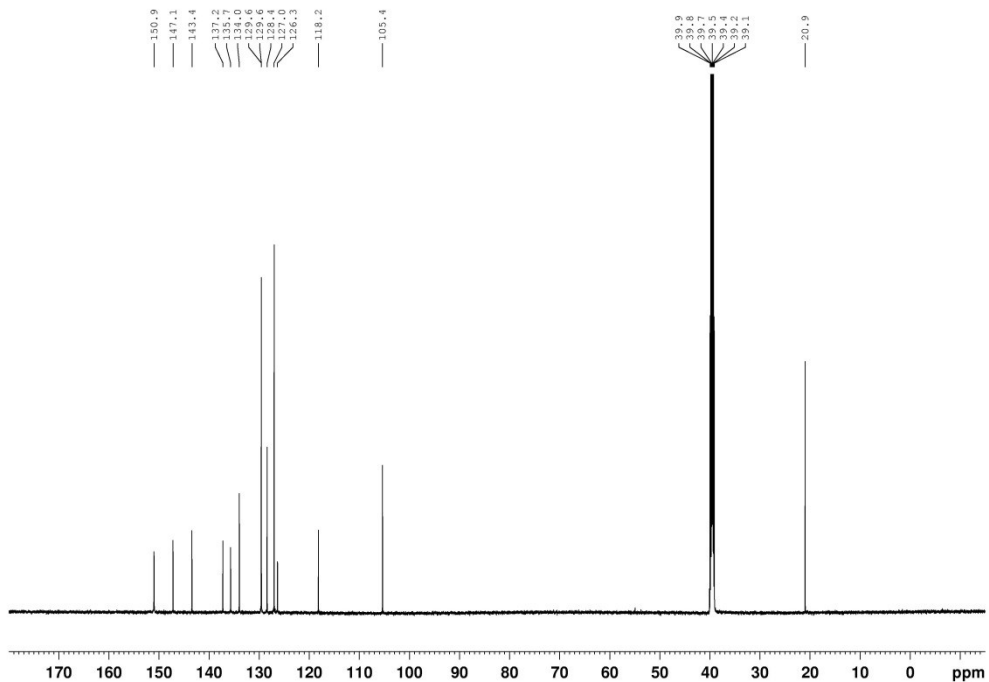


<sup>13</sup>C NMR Spectrum for **3a** (DMSO-*d*<sub>6</sub>, 150 MHz)

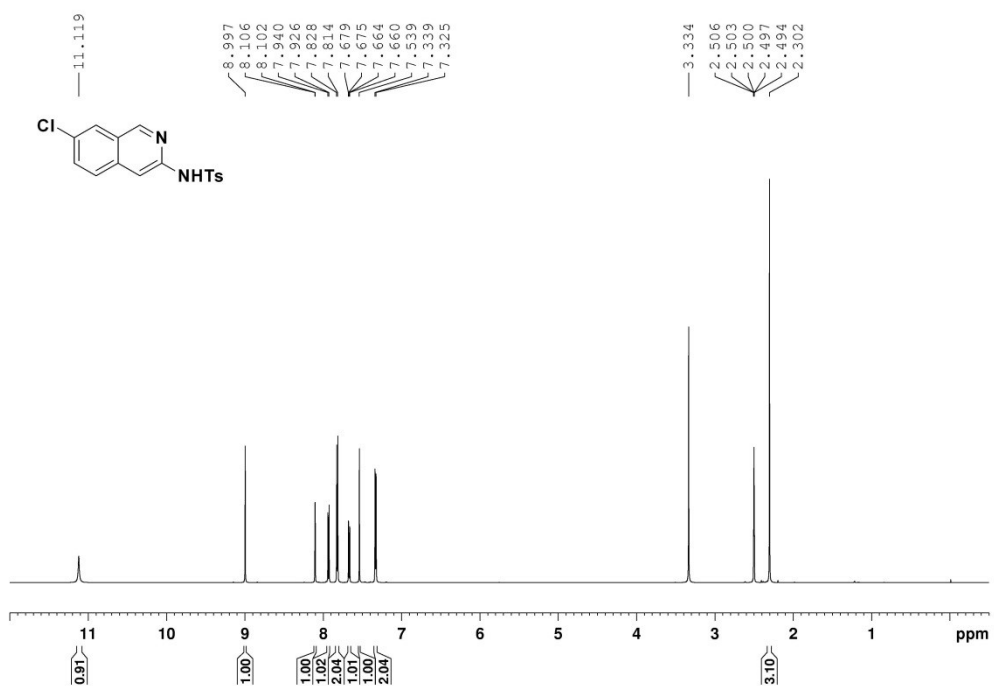




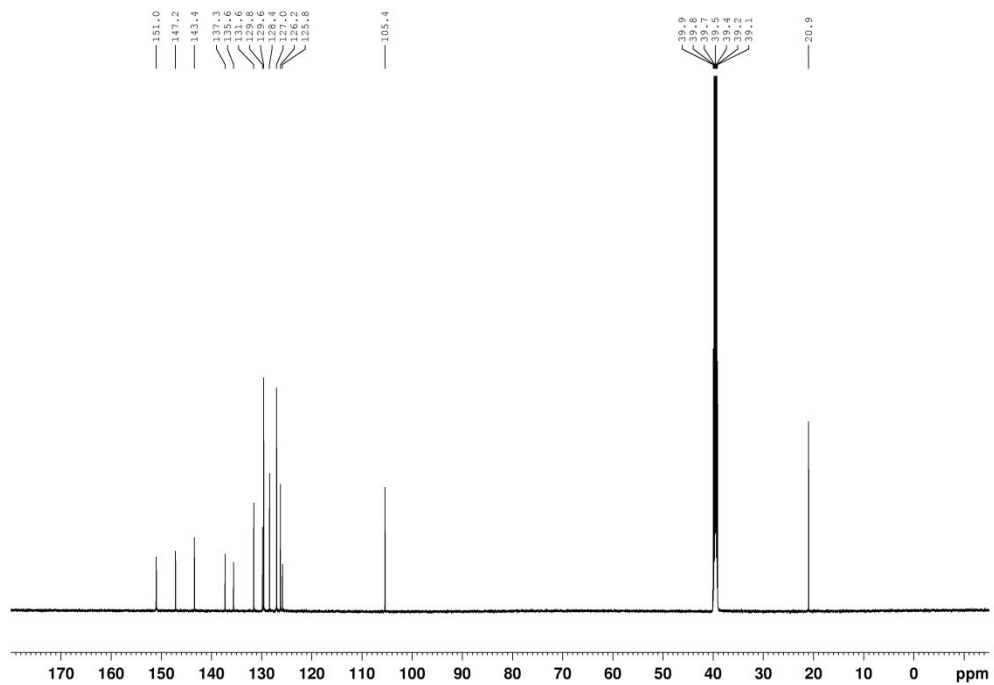
<sup>1</sup>H NMR Spectrum for **3b** (DMSO-*d*<sub>6</sub>, 600 MHz)



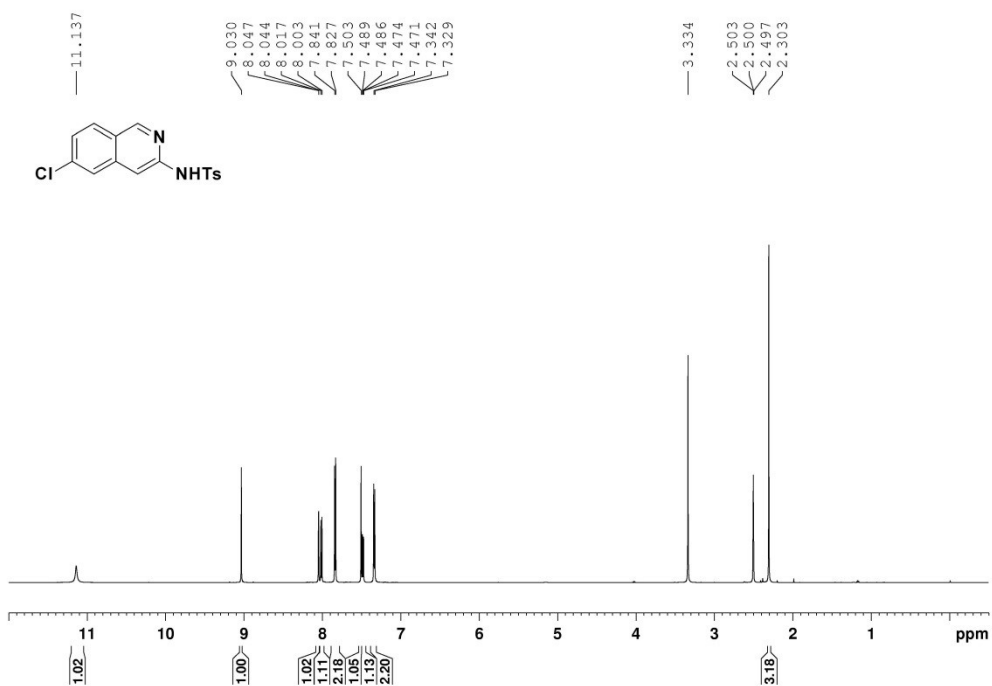
<sup>13</sup>C NMR Spectrum for **3b** (DMSO-*d*<sub>6</sub>, 150 MHz)



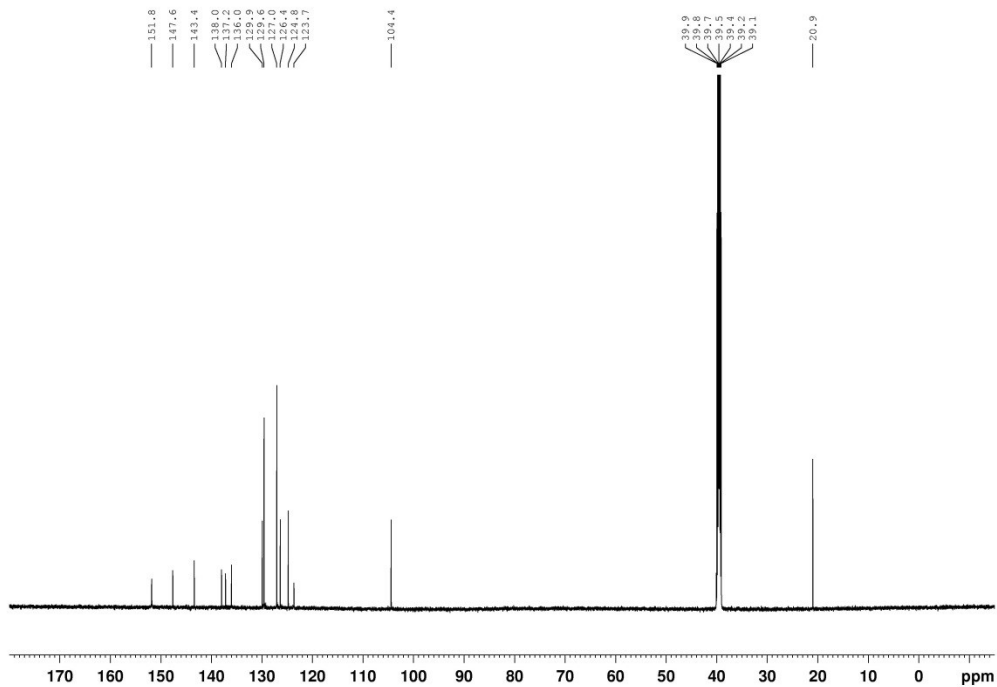
<sup>1</sup>H NMR Spectrum for **3c** (DMSO-*d*<sub>6</sub>, 600 MHz)



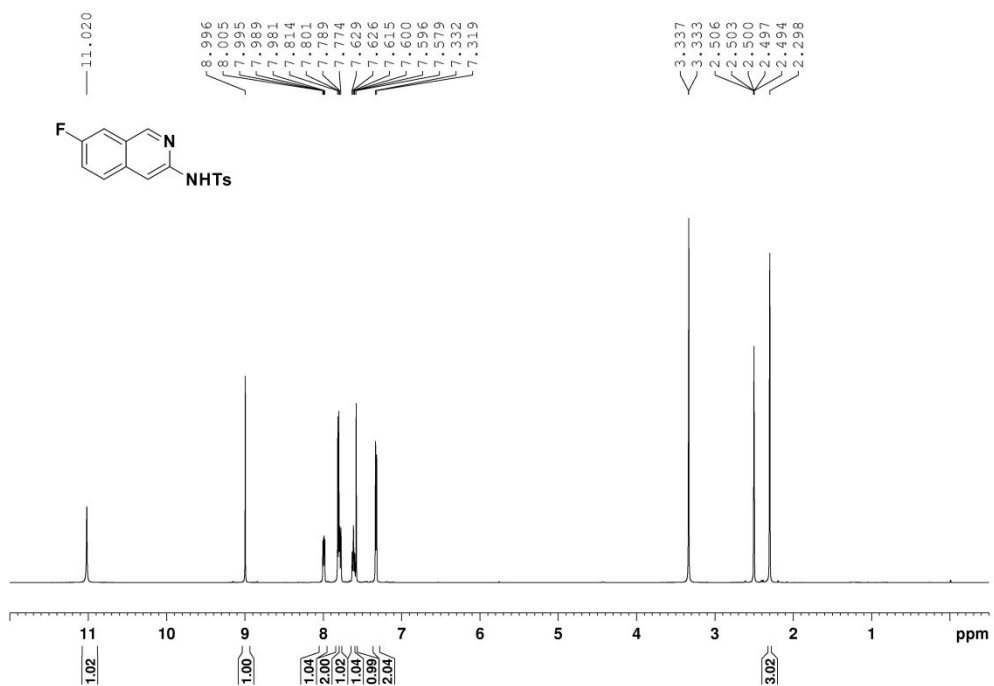
<sup>13</sup>C NMR Spectrum for **3c** (DMSO-*d*<sub>6</sub>, 150 MHz)



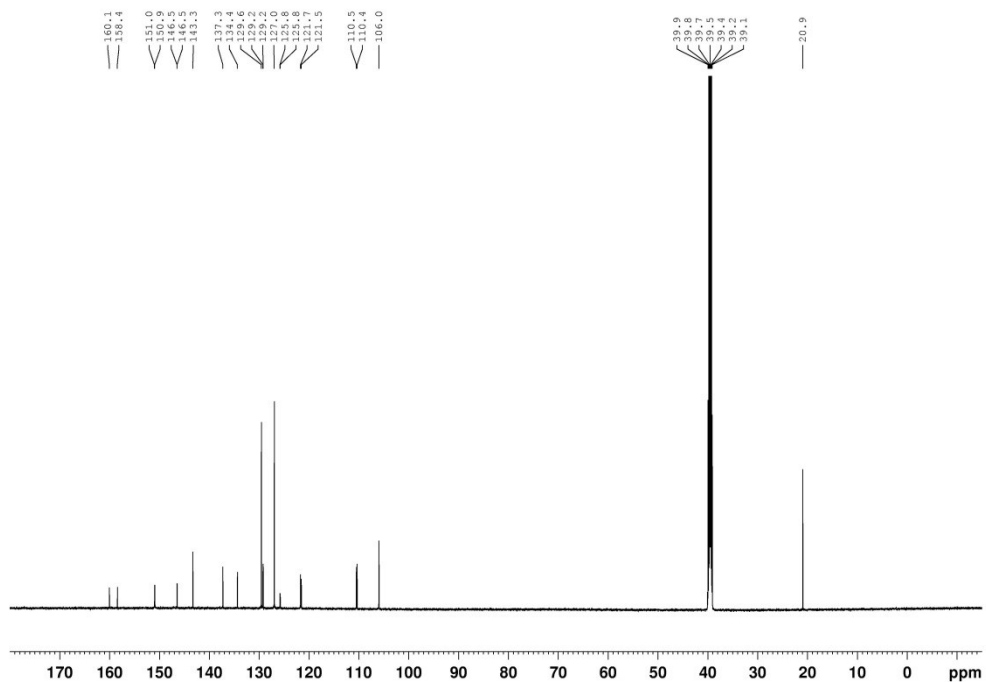
<sup>1</sup>H NMR Spectrum for **3d** (DMSO-*d*<sub>6</sub>, 600 MHz)



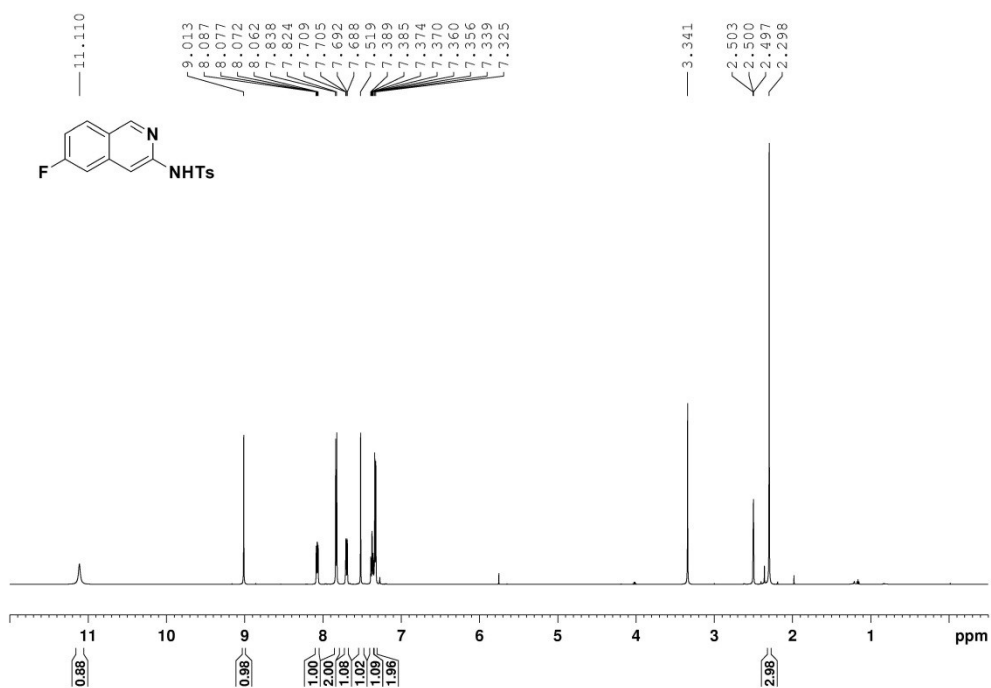
<sup>13</sup>C NMR Spectrum for **3d** (DMSO-*d*<sub>6</sub>, 150 MHz)



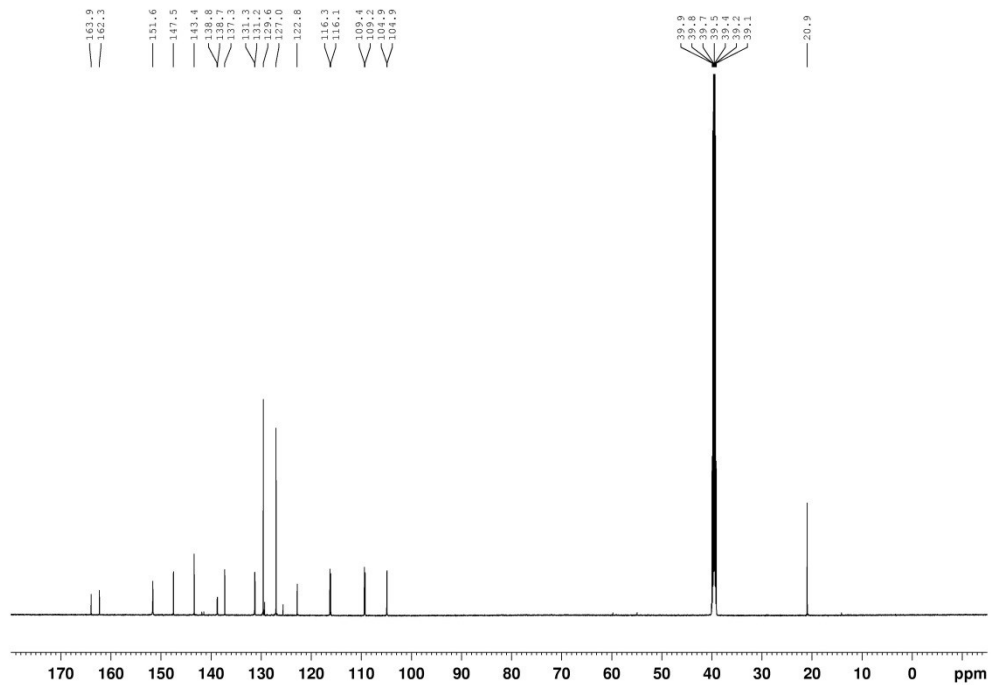
<sup>1</sup>H NMR Spectrum for 3e (DMSO-*d*<sub>6</sub>, 600 MHz)



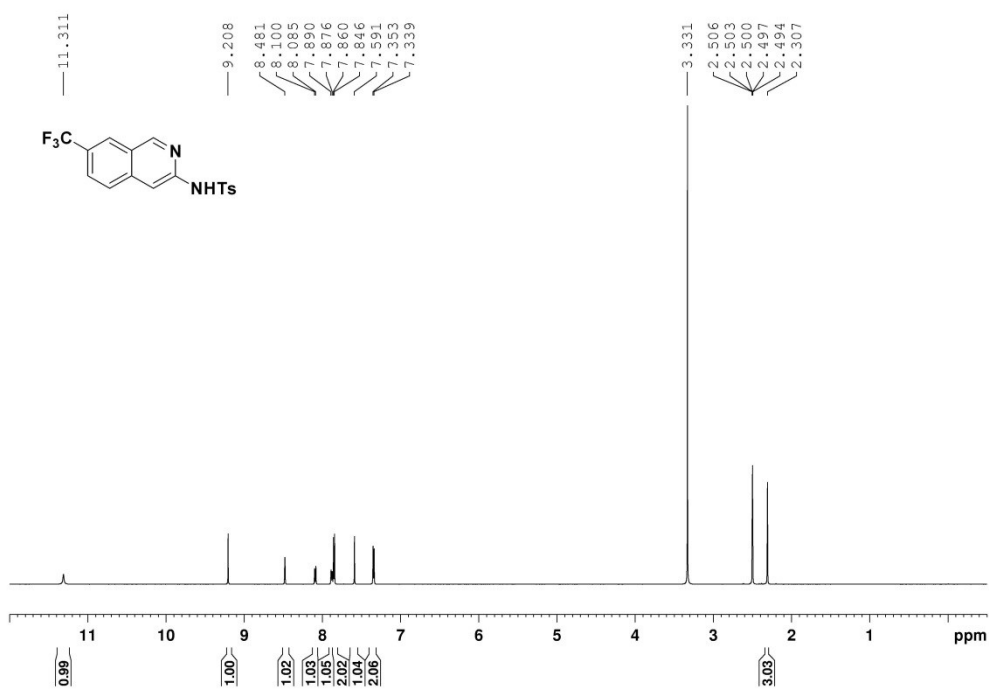
<sup>13</sup>C NMR Spectrum for 3e (DMSO-*d*<sub>6</sub>, 150 MHz)



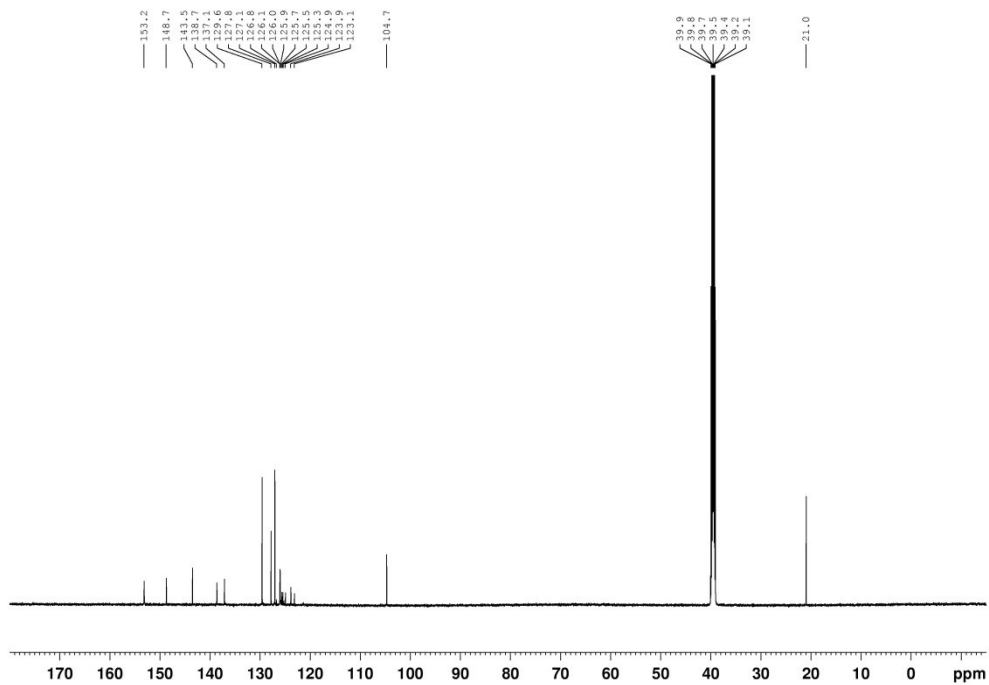
<sup>1</sup>H NMR Spectrum for **3f** (DMSO-*d*<sub>6</sub>, 600 MHz)



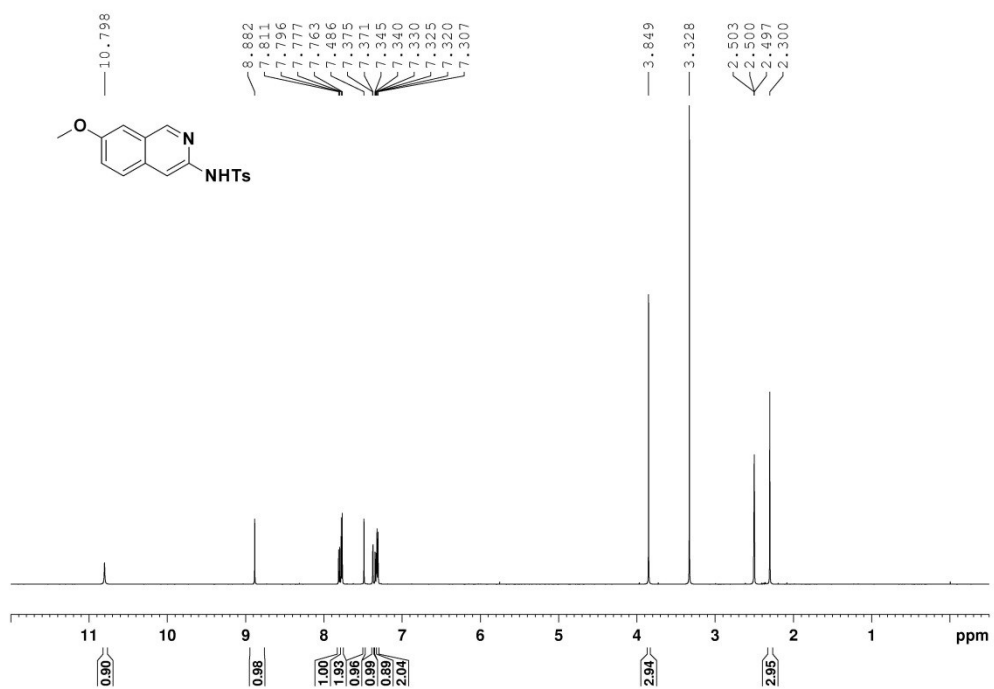
<sup>13</sup>C NMR Spectrum for **3f** (DMSO-*d*<sub>6</sub>, 150 MHz)



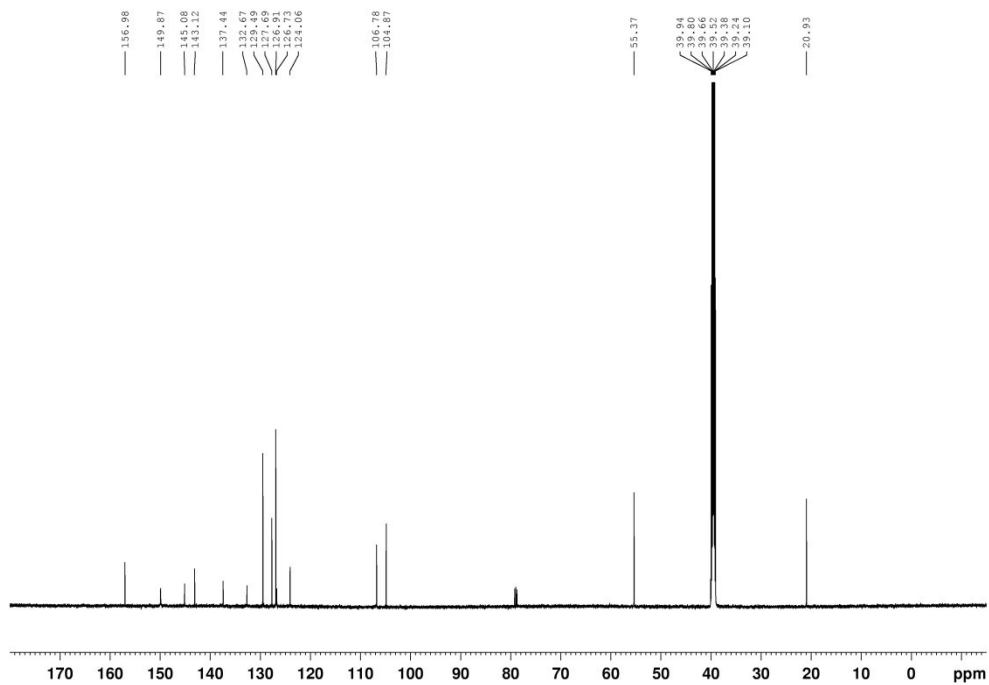
**<sup>1</sup>H NMR Spectrum for 3g (DMSO-*d*<sub>6</sub>, 600 MHz)**



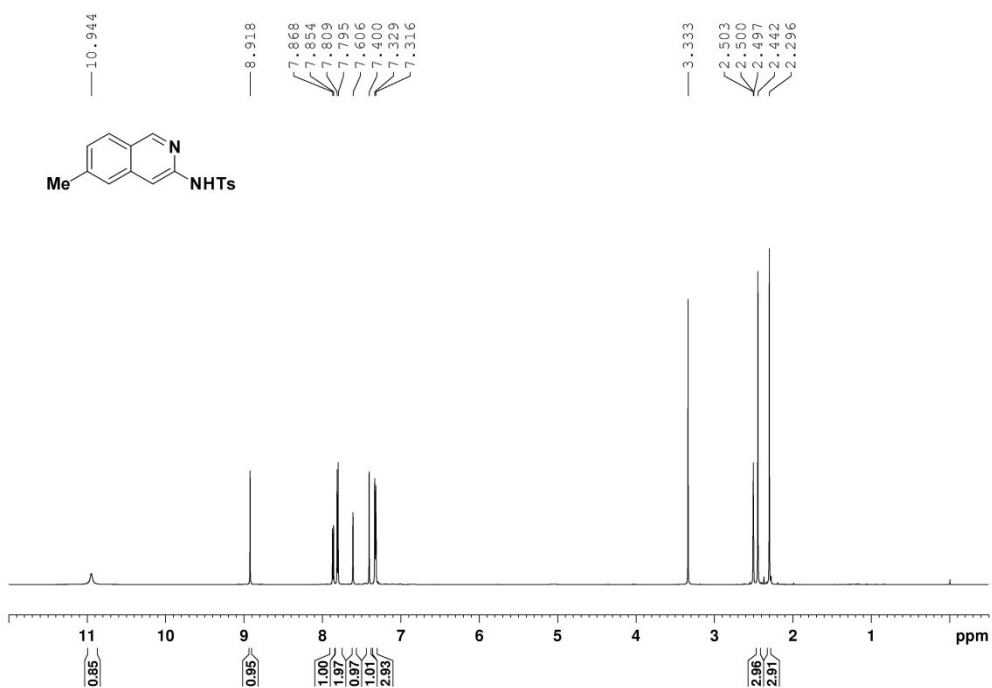
**<sup>13</sup>C NMR Spectrum for 3g (DMSO-*d*<sub>6</sub>, 150 MHz)**



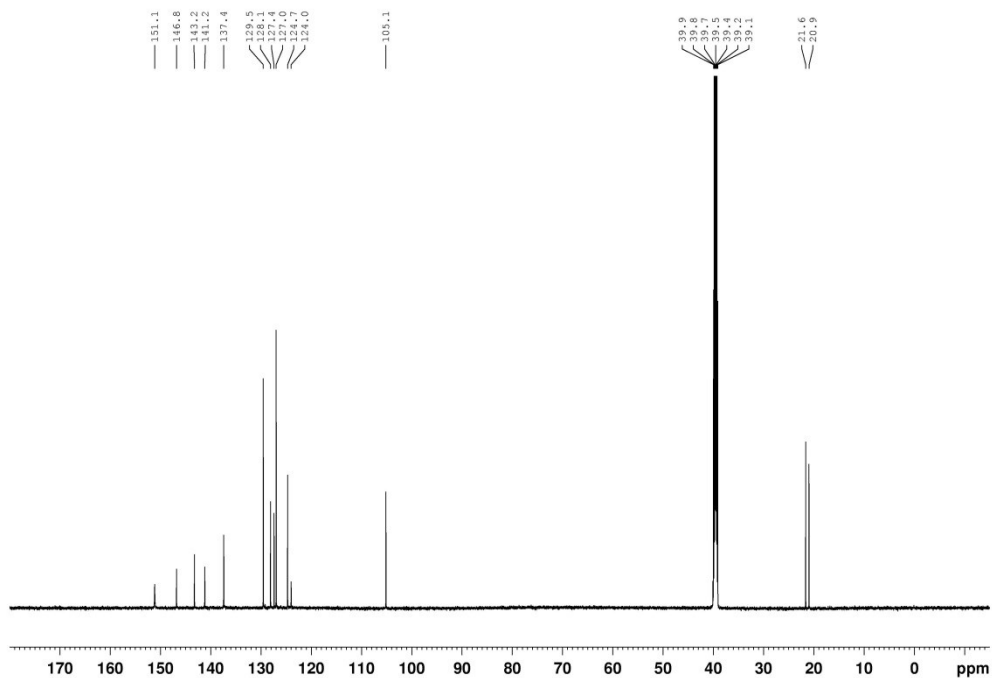
<sup>1</sup>H NMR Spectrum for **3h** (DMSO-*d*<sub>6</sub>, 600 MHz)



<sup>13</sup>C NMR Spectrum for **3h** (DMSO-*d*<sub>6</sub>, 150 MHz)

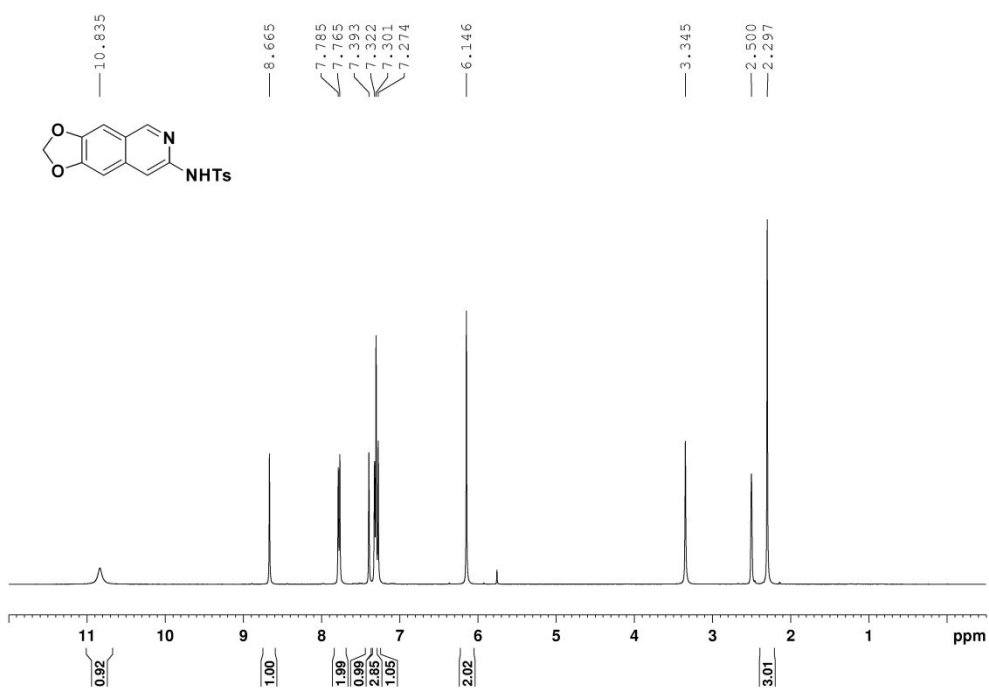


<sup>1</sup>H NMR Spectrum for **3i** (DMSO-*d*<sub>6</sub>, 600 MHz)

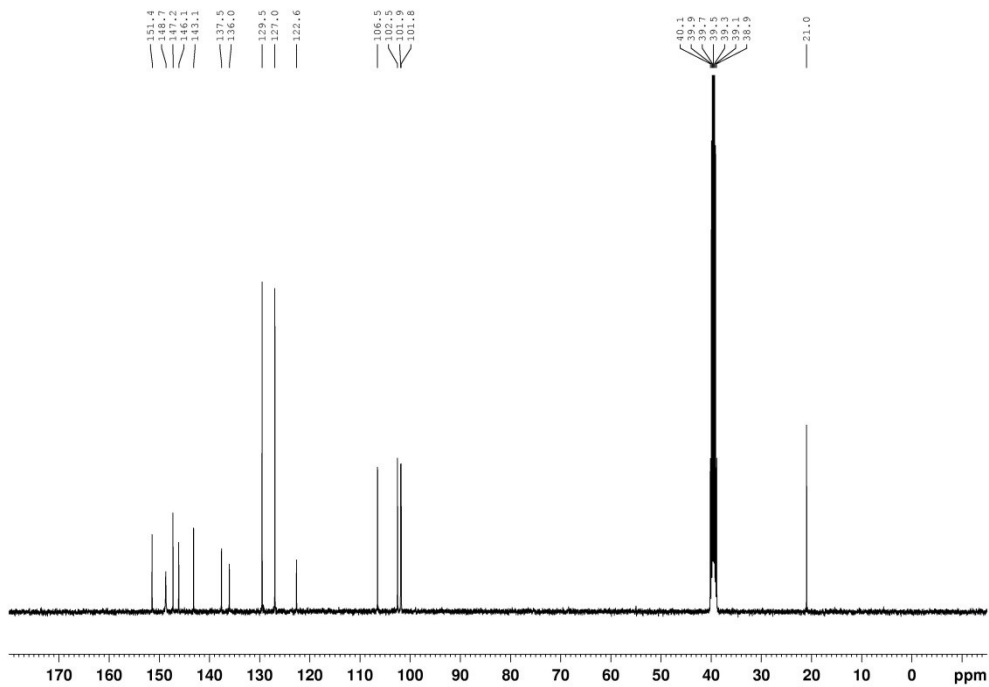


<sup>13</sup>C NMR Spectrum for **3i** (DMSO-*d*<sub>6</sub>, 150 MHz)

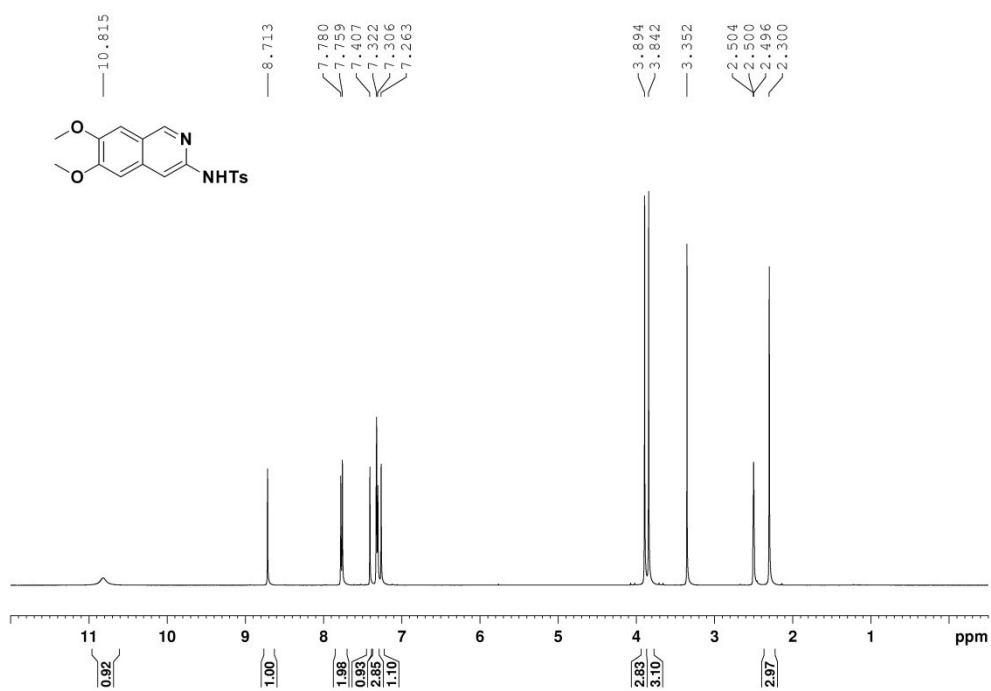




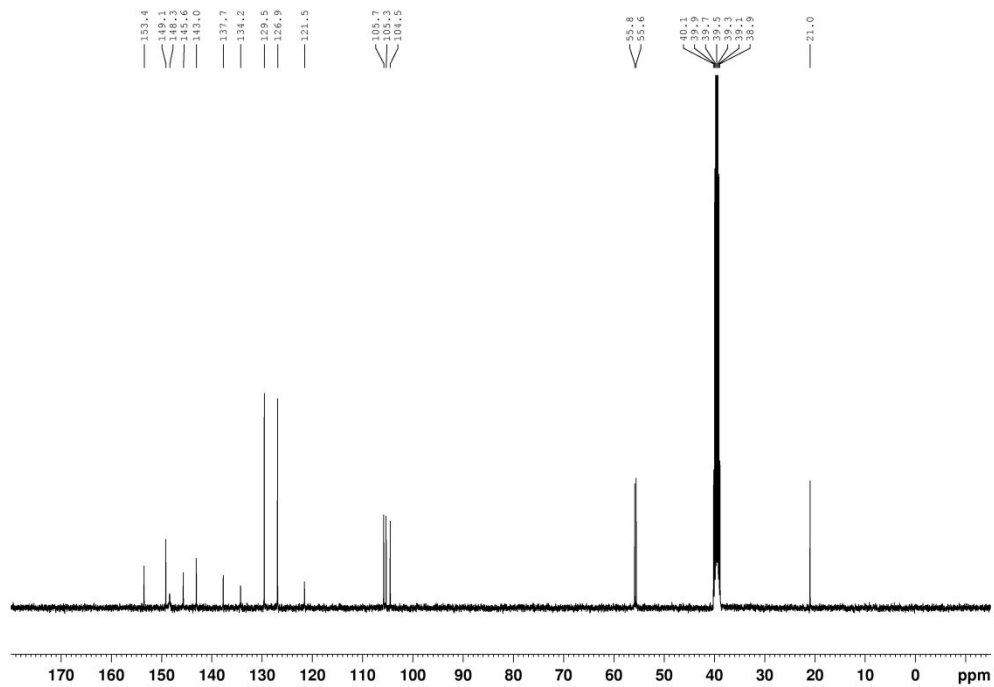
<sup>1</sup>H NMR Spectrum for **3j** (DMSO-*d*<sub>6</sub>, 400 MHz)



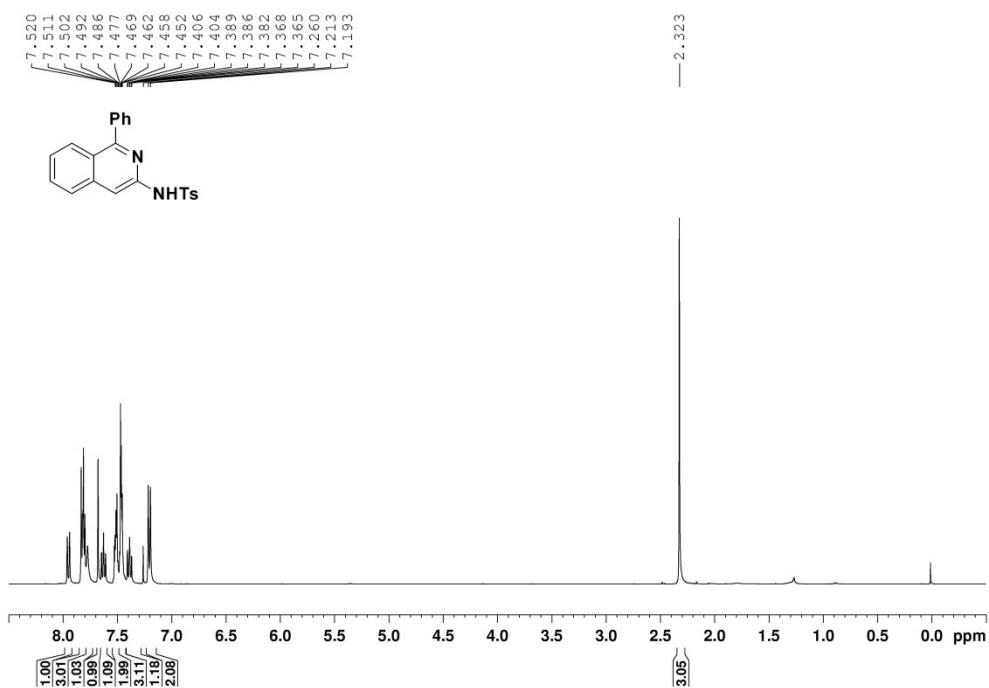
<sup>13</sup>C NMR Spectrum for **3j** (DMSO-*d*<sub>6</sub>, 100 MHz)



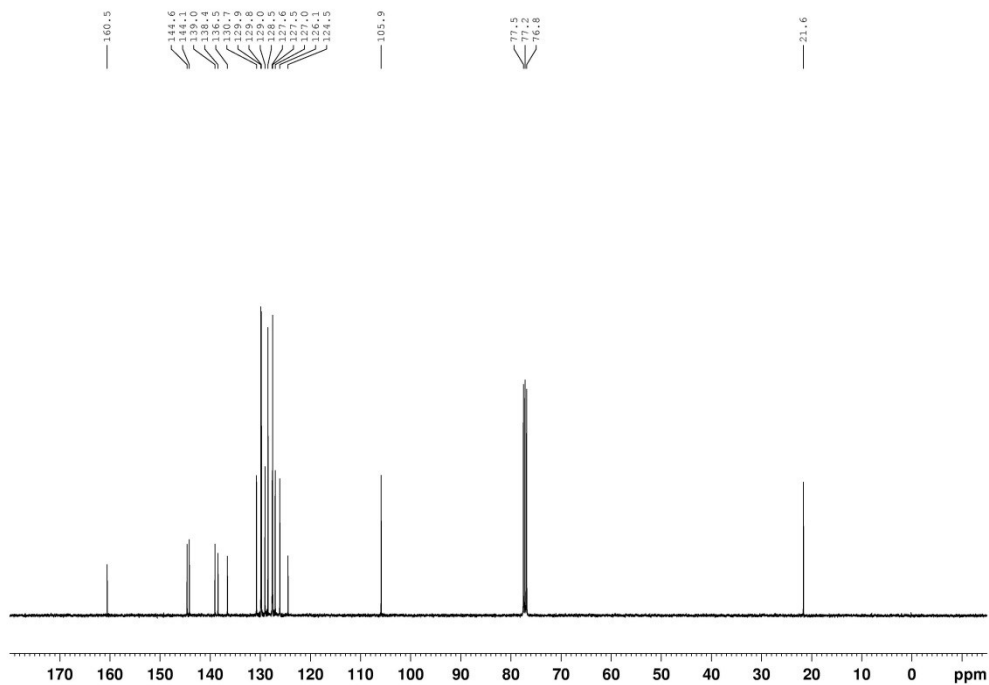
<sup>1</sup>H NMR Spectrum for **3k** (DMSO-*d*<sub>6</sub>, 400 MHz)



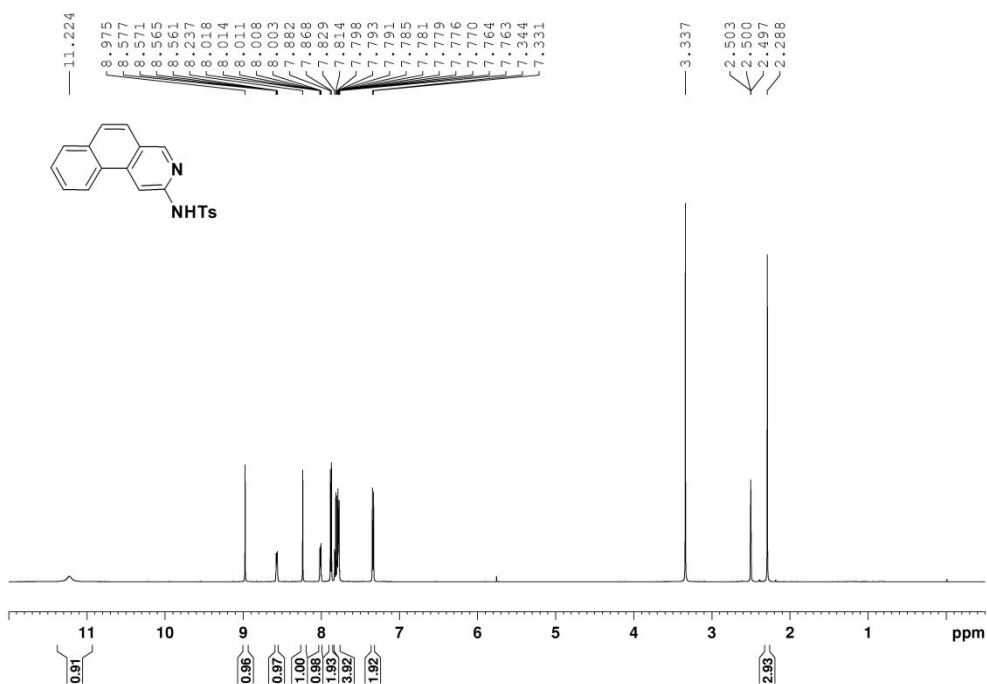
<sup>13</sup>C NMR Spectrum for **3k** (DMSO-*d*<sub>6</sub>, 100 MHz)



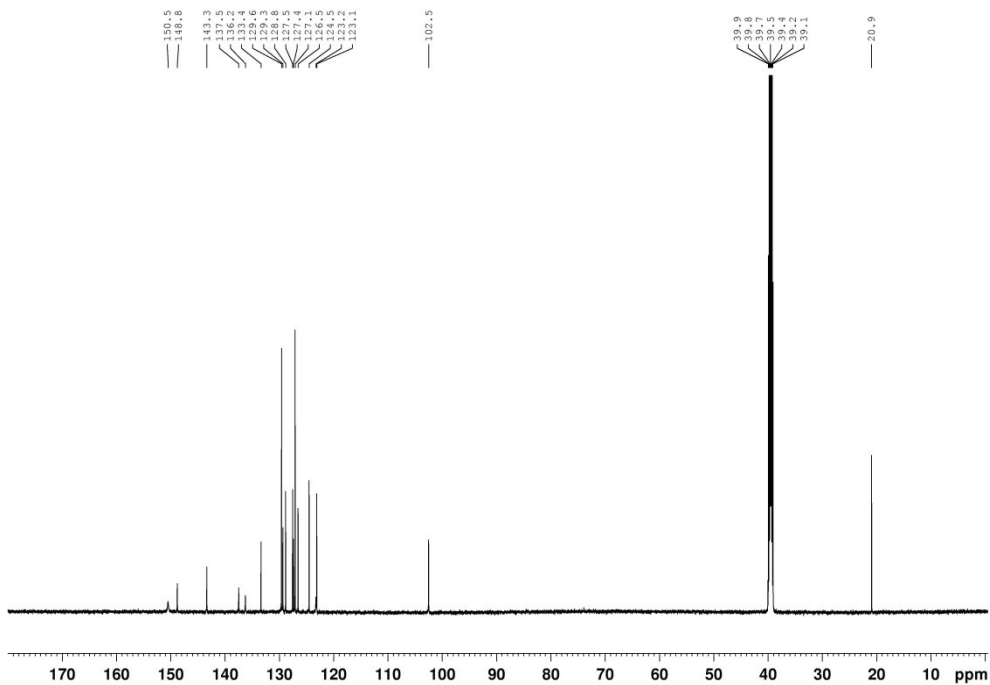
<sup>1</sup>H NMR Spectrum for **31** (CDCl<sub>3</sub>, 400 MHz)



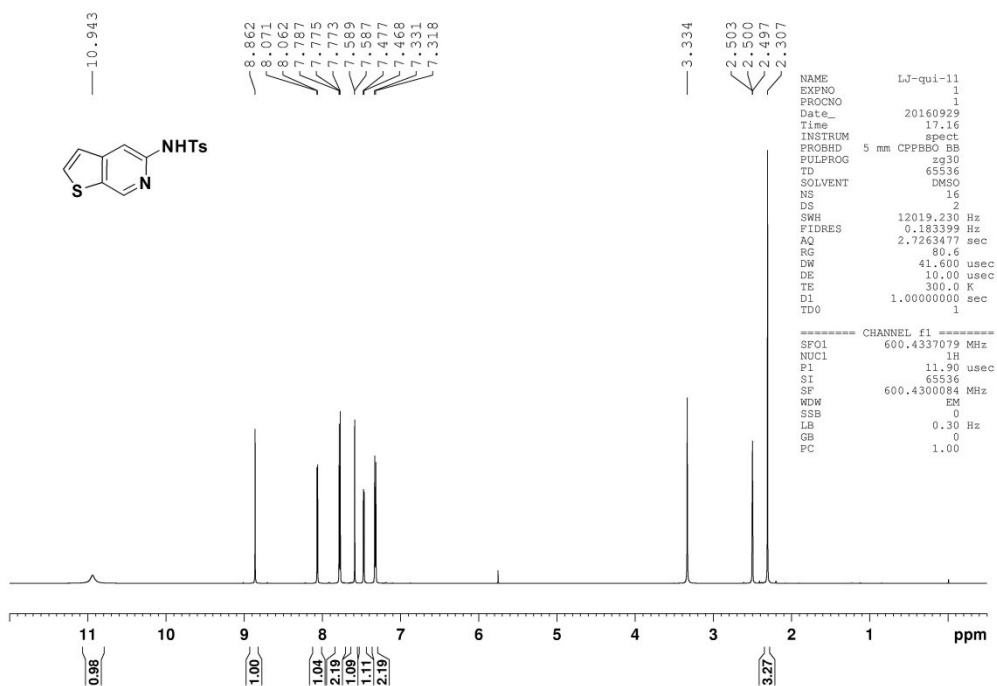
<sup>13</sup>C NMR Spectrum for **31** (CDCl<sub>3</sub>, 100 MHz)



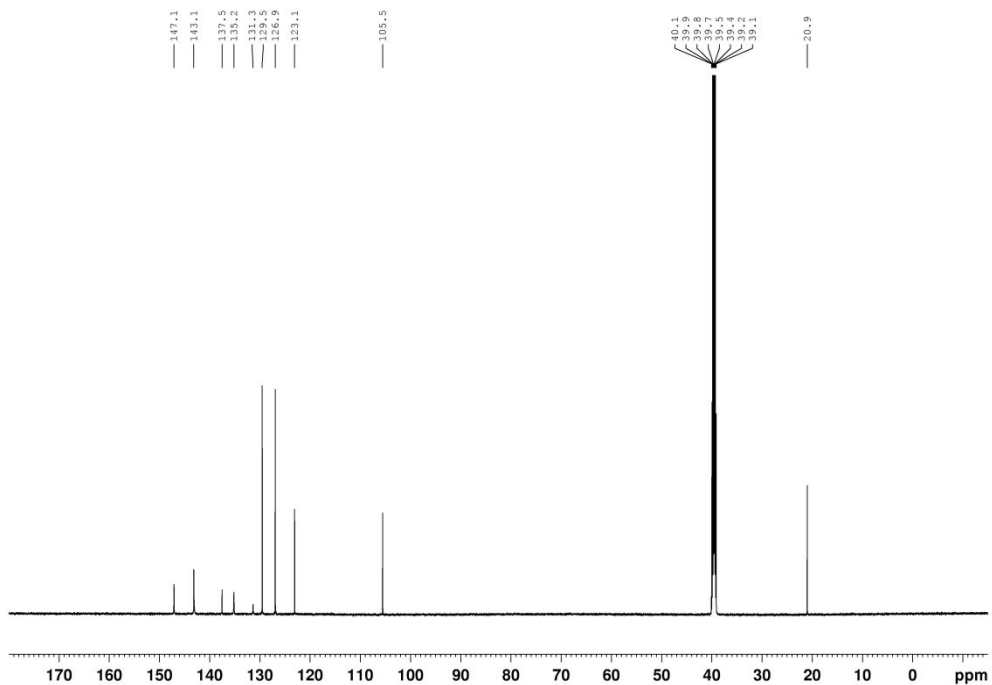
**<sup>1</sup>H NMR Spectrum for 3o (DMSO-*d*<sub>6</sub>, 600 MHz)**



**<sup>13</sup>C NMR Spectrum for 3o (DMSO-*d*<sub>6</sub>, 150 MHz)**



<sup>1</sup>H NMR Spectrum for **3p** (DMSO-*d*<sub>6</sub>, 600 MHz)



<sup>13</sup>C NMR Spectrum for **3p** (DMSO-*d*<sub>6</sub>, 150 MHz)