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Supporting Information

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Copper-Catalyzed Synthesis of *N*-Sulfonyl-1,2,3-triazoles: Controlling Selectivity

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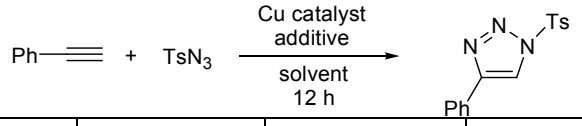
General Methods. Unless otherwise stated, all commercial reagents and solvents were used without additional purification. Analytical thin layer chromatography (TLC) was performed on Merck precoated silica gel 60 F_{254} plates. Visualization on TLC was achieved by use of UV light (254 nm) and treatment with phosphomolybdic acid and anisaldehyde stain followed by heating. Flash column chromatography was undertaken on silica gel (Merck Kieselgel 60 F_{254} 400-630 mesh). ^{1}H NMR was recorded on Bruker FT AM 400 (400 MHz). Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants, *J*, were reported in hertz unit (Hz). ^{13}C NMR was recorded on Bruker FT AM 400 (100 MHz) and was fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the center line of a triplet at 77.0 ppm of chloroform-*d*. Infrared (IR) spectra were recorded neat in 0.5 mm path length using a sodium chloride cell on Bruker EQUINOX 55. Frequencies are given in reciprocal centimeters (cm^{-1}) and only selected absorbance is reported. High resolution mass spectra were recorded on VG AUTOSPEC ULTIMA by using EI method.

Experimental Procedure for the Optimization Studies (*Table S1*). To a stirred mixture of phenylacetylene (61.3 mg, 0.6 mmol), *p*-toluenesulfonyl azide (98.6 mg, 0.5 mmol), CuI (9.5 mg, 0.05 mmol) in a solvent (1.0 mL) was slowly added an additive (0.6 mmol except entries 1, 14, and 15). After stirring the reaction mixture for 12 h at the indicated temperature, it was diluted by adding CH_2Cl_2

(2 mL) and saturated NH_4Cl solution (3 mL). The mixture was stirred for an additional 30 min and two layers were separated. The aqueous layer was extracted with CH_2Cl_2 (3 mL x 3). The combined organic layers were dried over $MgSO_4$, filtered, and concentrated in *vacuo*. The NMR yield of desired product, 1-(4-methylbenzenesulfonyl)-4-phenyl-1,2,3-triazole, was determined by integration using an internal standard (1,3-benzodioxole).

Table S1: Cu-catalyzed N-sulfonyl triazole formation under the various conditions.[a]



Entry	Catalyst	Additive	Solvent	Temp (°C)	Yield (%)[b]
1	$CuSO_4 \cdot 5H_2O$	Na-ascorbate[c]	H_2O/*t*-BuOH[d]	25	12
2	CuI	2,6-lutidine	H_2O/*t*-BuOH[d]	25	15
3	CuI	2,6-lutidine	*t*-BuOH	25	25
4	Cu(OAc)	2,6-lutidine	$CHCl_3$	25	<1
5	Cu_2O	2,6-lutidine	$CHCl_3$	25	15
6	Cu_2O	2,6-lutidine	$CHCl_3$	0	51
7	CuBr	2,6-lutidine	$CHCl_3$	0	55
8	$(Ph_3P)_3CuCl$	2,6-lutidine	$CHCl_3$	0	<1
9	CuI	2,6-lutidine	CH_3CN	0	12
10	CuI	2,6-lutidine	toluene	0	75
11	CuI	2,6-lutidine	$CHCl_3$	0	80
12	CuI	2,6-lutidine	$CHCl_3$	25	37
13	CuI	2,6-lutidine	$CHCl_3$	70	4
14	CuI	-	$CHCl_3$	0	3
15	CuI	2,6-lutidine[e]	$CHCl_3$	0	73
16	CuI	pyridine	$CHCl_3$	0	6
17	CuI	DIPEA	$CHCl_3$	0	<1
18	CuI	Et_3N	$CHCl_3$	0	<1
19	CuI	*N,N*-dimethylaniline	$CHCl_3$	0	<1
20	CuI	K_2CO_3	$CHCl_3$	0	<1
21	CuI	MgO	$CHCl_3$	0	<1

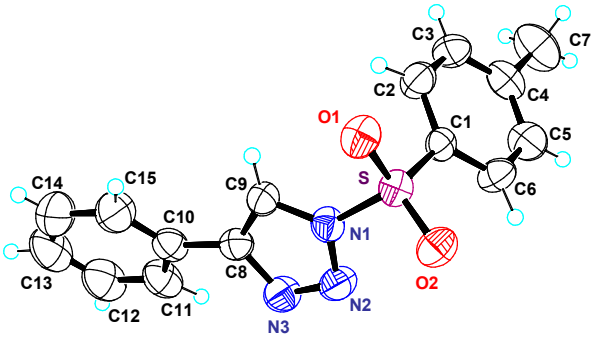
[a] A solution of phenylacetylene (0.60 mmol), *p*-toluenesulfonyl azide (0.50 mmol), additive (0.60 mmol except entries 1, 14, and 15), and CuI (0.05 mmol) in solvent (1.0 mL) was stirred for 12 h at the indicated temperature. [b] NMR yield based on an internal standard (1,3-benzodioxole). [c] 0.1 Equiv of sodium ascorbate was employed. [d] Ratio of H_2O/*t*-BuOH was 1:2. [e] 0.2 Equiv of 2,6-lutidine was used.

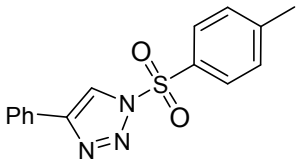
Representative Procedure for the Preparation of triazoles (*Table 2*). To a stirred mixture of phenylacetylene (61.3 mg, 0.6 mmol), *p*-toluenesulfonyl azide (98.6 mg, 0.5 mmol), and CuI (9.5 mg, 0.05 mmol) in $CHCl_3$ (1.0 mL) was slowly added 2,6-lutidine (0.070 mL, 0.6 mmol) at 0 ^oC. After stirring the reaction mixture for 12 h at room temperature, it was diluted with CH_2Cl_2 (2 mL) and then with aqueous NH_4Cl solution (3 mL). The mixture was stirred for an additional 30 min at room temperature and two layers were separated. The aqueous layer was extracted with CH_2Cl_2 (3 mL x 3) and the combined organic layers were dried over $MgSO_4$, filtered, and concentrated in *vacuo*. The crude residue was purified by flash column chromatography (EtOAc/*n*-Hx, 1:5) to give the desired product, 1-(4-methylbenzenesulfonyl)-4-phenyl-1,2,3-triazole (249 mg, 83%), as a white solid.

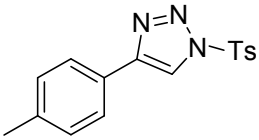
Representative Experimental Procedure of the Scale-up Reactions. To a stirred mixture of phenylacetylene (1.3 mL, 12.0 mmol), *p*-toluenesulfonyl azide (1.5 mL, 10.0 mmol), and CuI (95.2 mg, 0.5 mmol) in chloroform (20 mL) was slowly added 2,6-lutidine (1.4 mL, 12.0 mmol) at 0 ^oC. After stirring the reaction mixture for 12 h at 0 ^oC, it was diluted by adding CH_2Cl_2 (20 mL) and aqueous NH_4Cl solution (50 mL). The mixture was stirred for an additional 30 min and two layers were separated. The aqueous layer was extracted with CH_2Cl_2 (50 mL x 3). The combined organic layers were dried over $MgSO_4$, filtered, and concentrated in *vacuo*. The crude residue was crystallized (CH_2Cl_2/*n*-hexane) to give the desired product, 1-(4-methylbenzenesulfonyl)-4-phenyl-1,2,3-triazole (2.57 g, 86%).

1-(4-Methylbenzenesulfonyl)-4-phenyl-1,2,3-triazole (***Table 2***, entry 1): white solid; m.p. 107-108 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 8.01 (d, *J* = 8.4 Hz, 2H), 7.82-7.79 (m, 2H), 7.43-7.35 (m, 5H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 130.4, 129.1, 129.0, 128.7, 126.1, 118.9, 21.8; IR (KBr) ν 3142, 1594, 1393, 1196, 1176, 987, 670, 587, 543, 447 cm^{-1}.

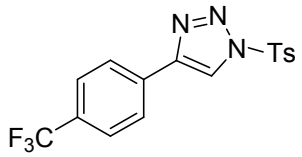
Figure S1. ORTEP plot of **1-(4-Methylbenzenesulfonyl)-4-phenyl-1,2,3-triazole** (***Table 2***, entry 1)



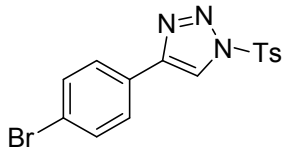




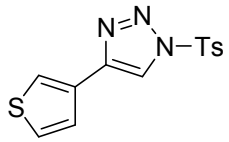
1-(4-Methylbenzenesulfonyl)-4-(4-methylphenyl)-1,2,3-triazole (***Table 2***, entry 2): white solid; m.p. 158-159 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 8.00 (d, *J* = 8.3 Hz, 2H), 7.69 (d, *J* = 8.1 Hz, 2H), 7.36 (d, *J* = 8.2 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 2.42 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.4, 147.3, 139.1, 133.1, 130.4, 129.6, 128.6, 126.0 ,125.9, 118.5, 21.8, 21.3; IR (KBr) ν 3146, 2923, 1594, 1450, 1195, 1179, 989, 812, 672, 583, 543 cm^{-1}; HRMS (EI) m/z calcd. for $C_{16}H_{15}N_3O_2S$ $[M]^+$: 313.0885, found: 313.0885.



1-(4-Methylbenzenesulfonyl)-4-(4-trifluoromethylphenyl)-1,2,3-triazole (***Table 2***, entry 3): white solid; white solid; m.p. 159-160 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 8.02 (d, *J* = 8.3 Hz, 2H), 7.93 (d, *J* = 8.1 Hz, 2H), 7.66 (d, *J* = 8.2 Hz, 2H), 7.38 (d, *J* = 8.2 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 145.9, 132.8, 132.3, 131.4, 131.0, 130.7, 130.5, 130.4, 128.8, 127.9, 126.3, 126.0, 126.0, 125.9, 125.9, 125.2, 122.5, 119.8, 21.8; IR (KBr) ν 3103, 2924, 1397, 1325, 1192, 1172, 1109, 992, 674, 592 cm^{-1}; HRMS (EI) m/z calcd. for $C_{16}H_{12}F_3N_3O_2S$ $[M]^+$: 367.0602, found: 367.0616.

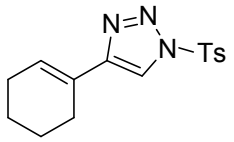


4-(4-Bromophenyl)-1-(4-methylbenzenesulfonyl)-1,2,3-triazole (***Table 2***, entry 4): white solid; m.p. 159-160 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 8.00 (dd, *J* = 6.9, 1.6 Hz, 2H), 7.68 (dd, *J* = 6.6, 1.9 Hz, 2H), 7.54 (dd, *J* = 6.7, 1.9 Hz, 2H), 7.37 (d, *J* = 8.1 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.5, 146.3, 133.0, 132.2, 130.5, 128.7, 127.9, 127.5, 123.1, 119.0, 21.8; IR (KBr) ν 3141, 1594, 1479, 1394, 1196, 1175, 988, 812, 671, 588, 543 cm^{-1}; HRMS (EI) m/z calcd. for $C_{15}H_{12}BrN_3O_2S$ $[M]^+$: 376.9834, found: 376.9843.

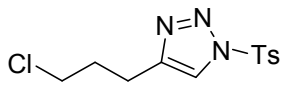


1-(4-Methylbenzenesulfonyl)-4-(thien-3-yl)-1,2,3-triazole (***Table 2***, entry 5): white solid; m.p. 140-141 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.99 (d, *J* = 8.4 Hz, 2H), 7.74-7.73 (m, 1H), 7.40-7.35 (m, 4H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 143.5, 133.1, 130.4, 130.0, 128.7,

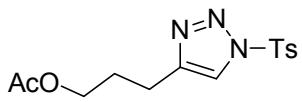
126.8, 125.6, 122.8, 118.5, 21.8; IR (KBr) ν 3108, 2924, 1594, 1392, 1195, 1176, 1030, 786, 671, 587 cm^{-1}; HRMS (EI) m/z calcd. for $C_{13}H_{11}N_3O_2S_2$ $[M]^+$: 305.0293, found: 305.0293.



4-(Cyclohex-1-enyl)-1-(4-methylbenzenesulfonyl)-1,2,3-triazole (***Table 2***, entry 6): white solid; m.p. 102-103 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.4 Hz, 2H), 7.87 (s, 1H), 7.33 (d, *J* = 8.4 Hz, 2H), 6.64-6.62 (m, 1H), 2.41 (s, 3H), 2.29-2.28 (m, 2H), 2.18-2.15 (m, 2H), 1.74-1.71 (m, 2H), 1.64-1.61 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 147.0, 133.3, 130.3, 128.5, 127.6, 125.8, 117.3, 26.1, 25.2, 22.2, 21.9, 21.8; IR (KBr) ν 3144, 2929, 1655, 1493, 1196, 1177, 1093, 1019, 990, 813, 671, 593, 543, 458 cm^{-1}; HRMS (EI) m/z calcd. for $C_{15}H_{17}N_3O_2S$ $[M]^+$: 303.1041, found: 303.1044

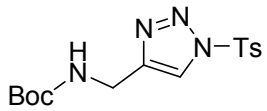


4-(3-Chloropropyl)-1-(4-methylbenzenesulfonyl)-1,2,3-triazole (***Table 2***, entry 7): yellowish liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.85 (s, 1H), 7.35 (d, *J* = 8.4 Hz, 2H), 3.53-3.50 (m, 2H), 2.73-2.72 (m, 2H), 2.42 (s, 3H), 1.81-1.78 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.4, 147.1, 133.2, 130.4, 128.6, 120.4, 44.5, 31.8, 26.1, 24.6, 21.8; IR (KBr) ν 3148, 2927, 1391, 1194, 1179, 1010, 967, 813, 670, 542, 474 cm^{-1}; HRMS (EI) m/z calcd. for $C_{12}H_{14}ClN_3O_2S$ $[M]^+$: 299.0495, found: 299.0480.

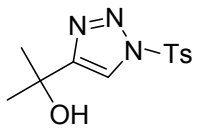


4-(Acetyloxypropyl)-1-(4-methylbenzenesulfonyl)-1,2,3-triazole (***Table 2***, entry 8): white solid; m.p. 74-75 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 6.7, 1.7 Hz, 2H), 7.87 (s, 1H), 7.35 (d, *J* = 8.0 Hz,

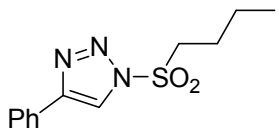
2H), 4.06 (t, J = 6.3 Hz, 2H), 2.77 (t, J = 7.4 Hz, 2H), 2.41 (s, 3H), 2.02-1.96 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 147.1, 146.8, 133.2, 130.4, 128.6, 120.5, 63.3, 27.8, 22.0, 21.8, 20.8; IR (KBr) ν 2925, 1737, 1391, 1241, 1194, 1180, 673, 584, 542 cm^{-1}; HRMS (EI) m/z calcd. for $C_{14}H_{17}N_3O_4S$ $[M]^+$: 323.0940, found: 323.0940.



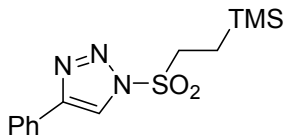
4-(*tert*-Butyloxycarbamidomethyl)-1-(4-methylbenzenesulfonyl)-1,2,3-triazol (***Table 2***, entry 9): white solid; m.p. 117-118 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.95 (d, J = 8.2 Hz, 2H), 7.35 (d, J = 8.1 Hz, 2H), 5.09 (br, 1H), 4.35 (d, J = 6.0 Hz, 2H), 2.41 (s, 3H), 1.39 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 147.3, 145.4, 133.0, 130.4, 128.7, 121.7, 80.0, 35.8, 28.3, 21.8; IR (KBr) ν 3341, 2980, 2931, 1705, 1514, 1392, 1196, 1176, 670, 585 cm^{-1}; HRMS (EI) m/z calcd. for $C_{15}H_{20}N_4O_4S$ $[M]^+$: 352.1205, found: 352.1210.



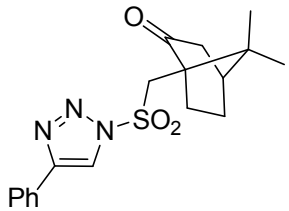
4-(1-Hydroxy-1-methylethyl)-1-(4-methylbenzenesulfonyl)-1,2,3-triazole (***Table 2***, entry 10): white solid; m.p. 122-123 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.95 (d, J = 8.4 Hz, 2H), 7.35 (d, J = 8.4 Hz, 2H), 2.74 (s, 1H), 2.41 (s, 3H), 1.57 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.2, 147.3, 132.9, 130.4, 128.6, 119.1, 68.5, 30.1, 21.8; IR (KBr) ν 3407, 3151, 2980, 2931, 1595, 1558, 1492, 1210, 1195, 1042, 1007, 814, 673, 627, 544 cm^{-1}; HRMS (EI) m/z calcd. for $C_{12}H_{15}N_3O_3S$ $[M]^+$: 281.0834, found: 281.0827.



1-(Butanesulfonyl)-4-phenyl-1,2,3-triazole (***Table 2***, entry 11): white solid; m.p. 55-56 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.87-7.85 (m, 2H), 7.47-7.38 (m, 2H), 3.66-3.62 (m, 2H), 1.80-1.72 (m, 2H), 1.48-1.39 (m, 2H), 0.93-0.89 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 129.2, 129.0, 128.7, 126.1, 119.5, 55.0, 24.7, 21.0, 13.2; IR (KBr) ν 3145, 2964, 2876, 1483, 1453, 1388, 1358, 1236, 1173, 1104, 1025, 988, 952, 916, 765, 691, 609, 554 cm^{-1}; HRMS (EI) m/z calcd. for $C_{12}H_{15}N_3O_2S$ $[M]^+$: 265.0885, found: 265.0885.



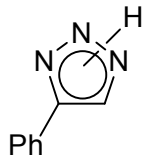
4-Phenyl-1-[2-(trimethylsilyl)ethanesulfonyl]-1,2,3-triazole (***Table 2***, entry 12): white solid; m.p. 122-123 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.88-7.86 (m, 2H), 7.47-7.39 (m, 3H), 3.60-3.55 (m, 2H), 0.99-0.94 (m, 2H), 0.05 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.2, 129.2, 129.0, 128.8, 126.1, 119.8, 52.6, 9.7, -2.1; IR (KBr) ν 3134, 2926, 1369, 1253, 1184, 1163, 991, 849, 833, 763, 742, 691, 553, 532 cm^{-1}; HRMS (EI) m/z calcd. for $C_{13}H_{19}N_3O_2SSi$ $[M]^+$: 309.0967, found: 309.0968.



1-[(7,7-Dimethylbicyclo[2.2.1]heptan-1-yl)methanesulfonyl]-4-phenyl-1,2,3-triazole (***Table 2***, entry 13): yellowish liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.86-7.84 (m, 2H), 7.45-7.35 (m, 4H), 3.98 (d, J = 14.8, 1H), 3.62 (d, J = 14.8, 1H), 2.54 (s, 3H), 2.40-2.33 (m, 2H), 2.15-2.07 (m, 2H), 1.97 (s, 1H), 1.92-1.84 (m, 1H), 1.50-1.46 (m, 1H), 1.23 (s, 3H), 0.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 213.1, 147.3, 129.1, 129.0, 128.8, 128.7, 126.1, 126.0, 119.4, 58.8, 53.6, 48.4, 42.7, 42.3, 26.9, 25.2,

19.6; IR (KBr) ν 3143, 2962, 1748, 1389, 1180, 1105, 1053, 1026, 987, 765, 691 cm^{-1}; HRMS (EI) m/z calcd. for $C_{18}H_{21}N_3O_3S$ $[M]^+$: 359.1304, found: 359.1303.

Typical Procedure for the Deprotection of 1-(*N*-sulfonyl)-1,2,3-tiazole. The solution of Mg (24.3 mg, 1.0 mmol) in MeOH (3 mL) was added 1-(4-methylbenzensulfonyl)-4-phenyl-1,2,3-triazole (60.0 mg, 0.2 mmol) at 25 ^oC. The reaction mixture was stirred at the same temperature for 2 h. and then quenched by adding NH_4Cl (1 mL). The aqueous layer was extracted with CH_2Cl_2 (3 mL x 3) and the combined organic layers were dried over $MgSO_4$, filtered, and concentrated in *vacuo*. The crude residue was purified by flash column chromatograph with EtOAc/n-hexane = 1:3 to give the desired product, 4-phenyl-*N*H-1,2,3-triazole (26.7 mg, 92%), as a white solid.

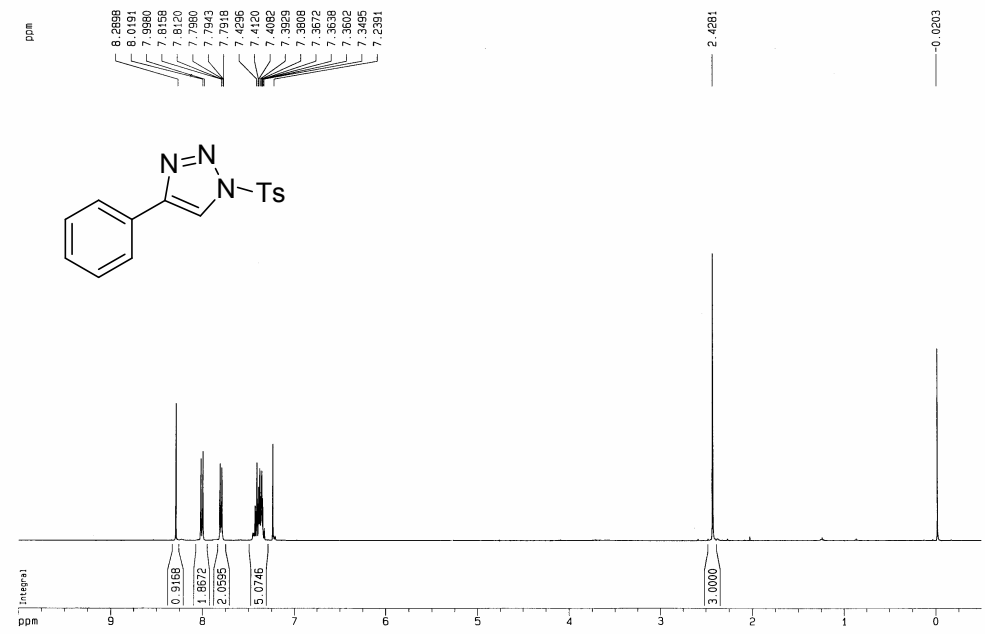


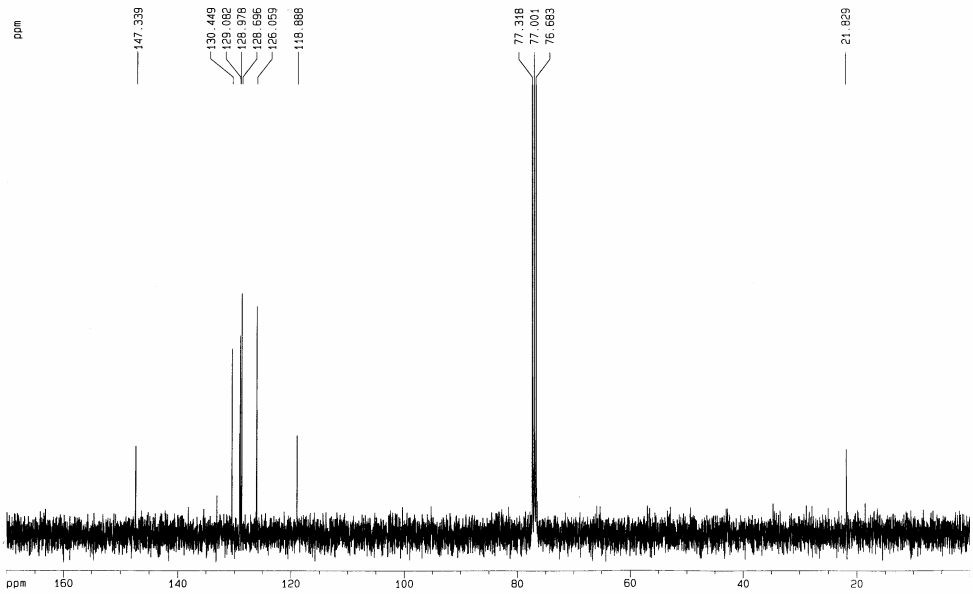
4-Phenyl-*N*H-1,2,3-triazole: white solid; m.p. 146-147 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 12.3 (s, 1H), 7.97 (s, 1H), 7.37-7.80 (m, 2H), 7.46-7.43 (m, 2H), 7.39-7.35 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 129.8, 129.0, 128.8, 126.1, 77.2; IR (KBr) ν 3152, 3116, 2944, 2850, 1454, 1083, 978, 914, 874, 765, 745, 693 cm^{-1}; HRMS (EI) m/z calcd. for $C_8H_7N_3$ $[M]^+$: 145.0640, found: 145.0640.

Appendix I

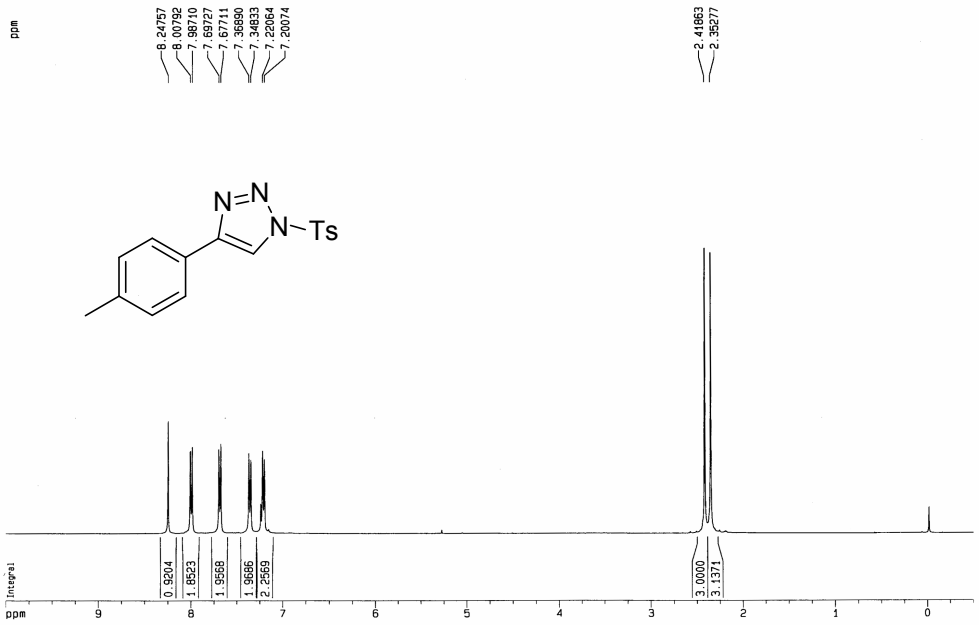
Spectral Copies of ^{1}H and ^{13}C NMR of New Compounds Obtained in this Study

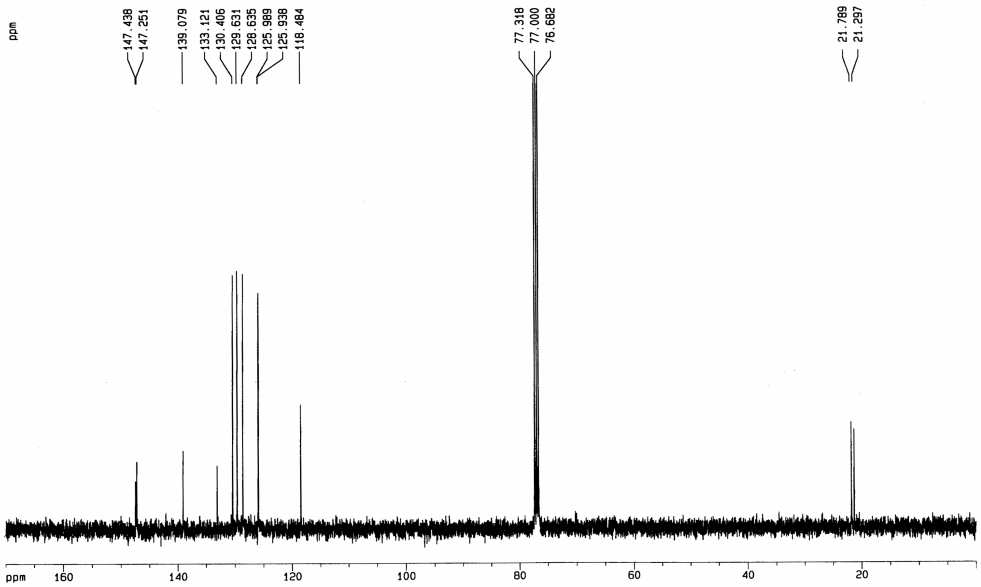
1-(4-Methylbenzenesulfonyl)-4-phenyl-1,2,3-triazole



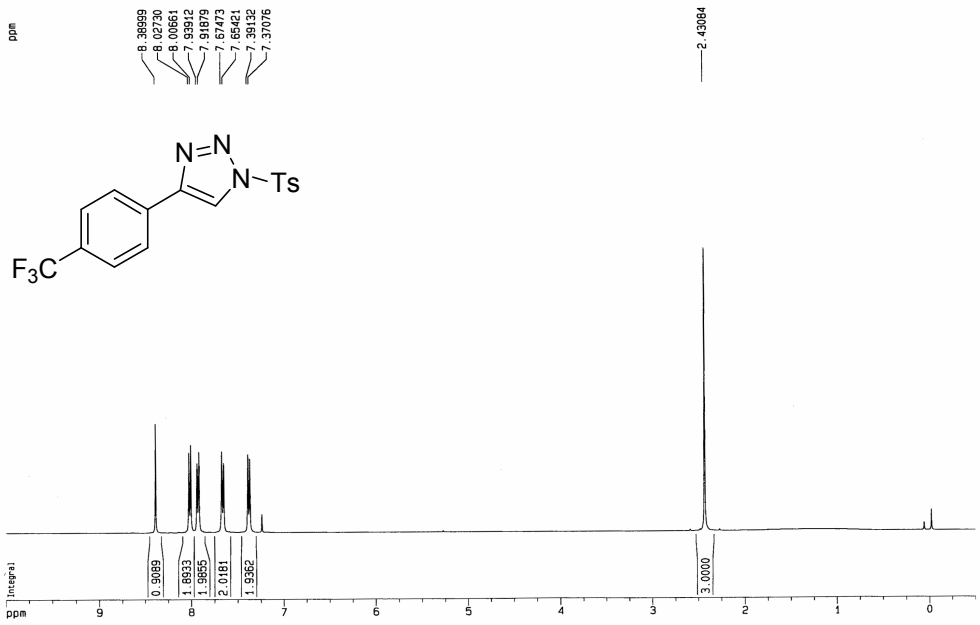


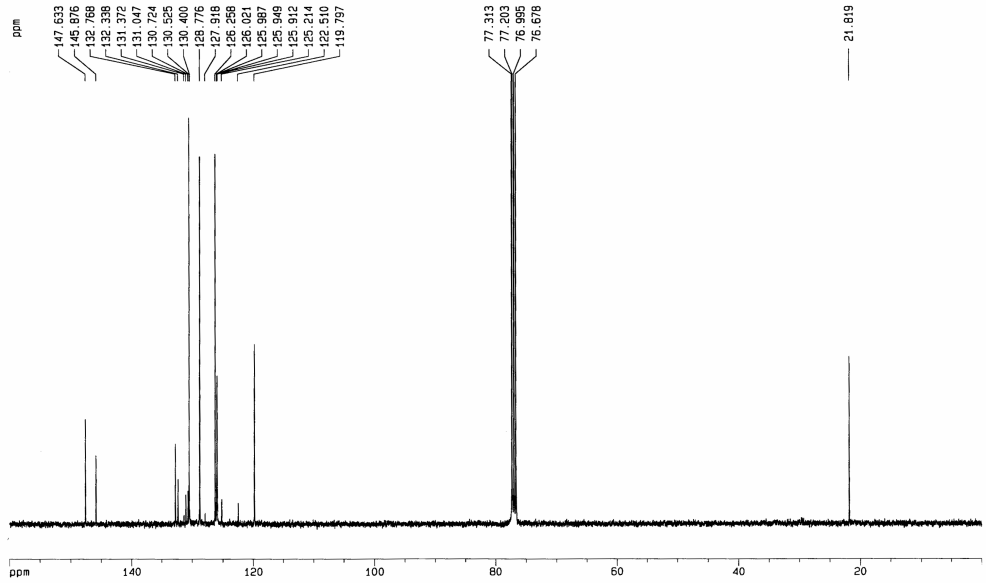
1-(4-Methylbenzenesulfonyl)-4-(4-methylphenyl)-1,2,3-triazole



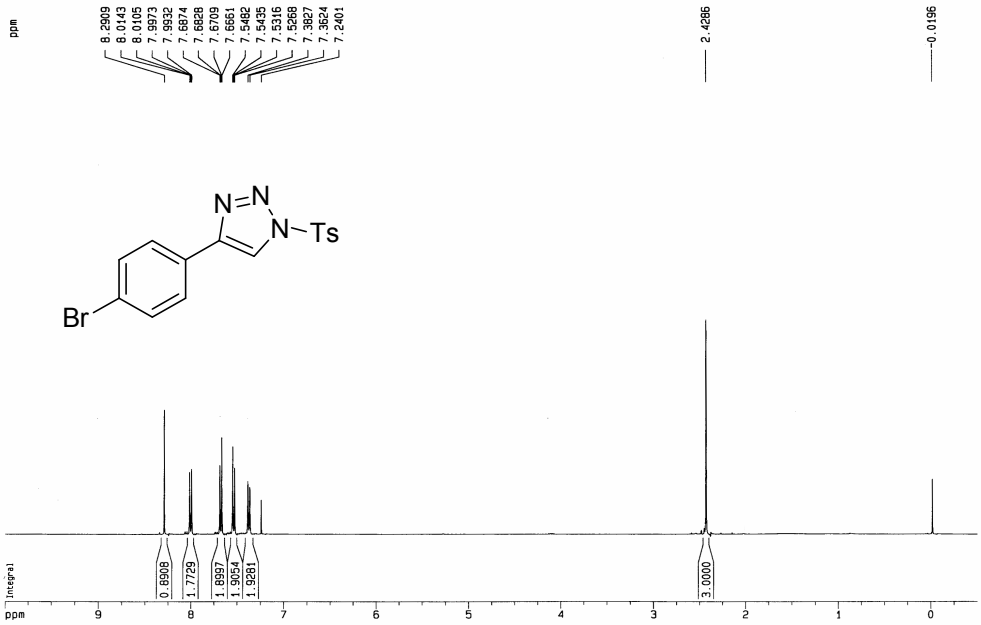


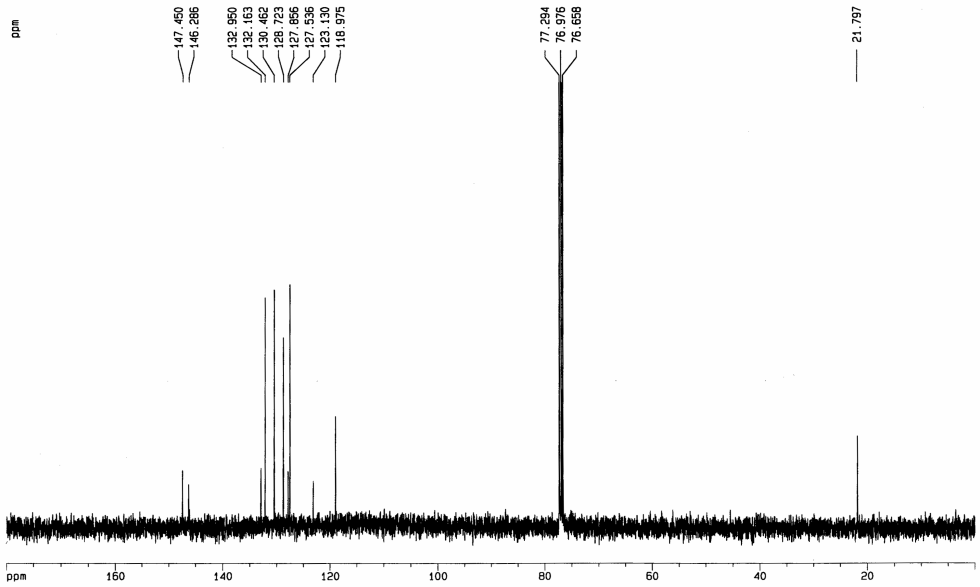
1-(4-Methylbenzenesulfonyl)-4-(4-trifluoromethylphenyl)-1,2,3-triazole



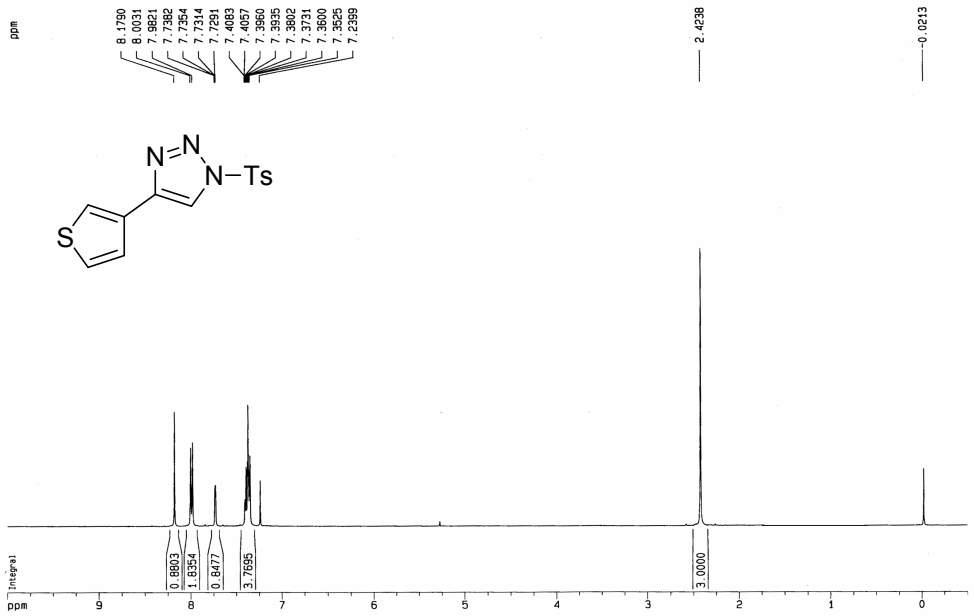


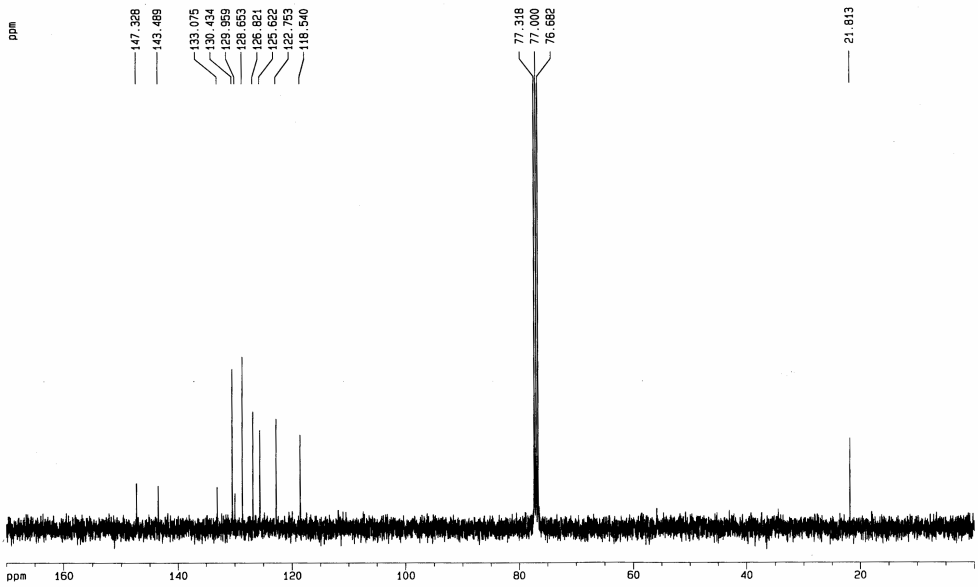
4-(4-Bromophenyl)-1-(4-methylbenzenesulfonyl)-1,2,3-triazole



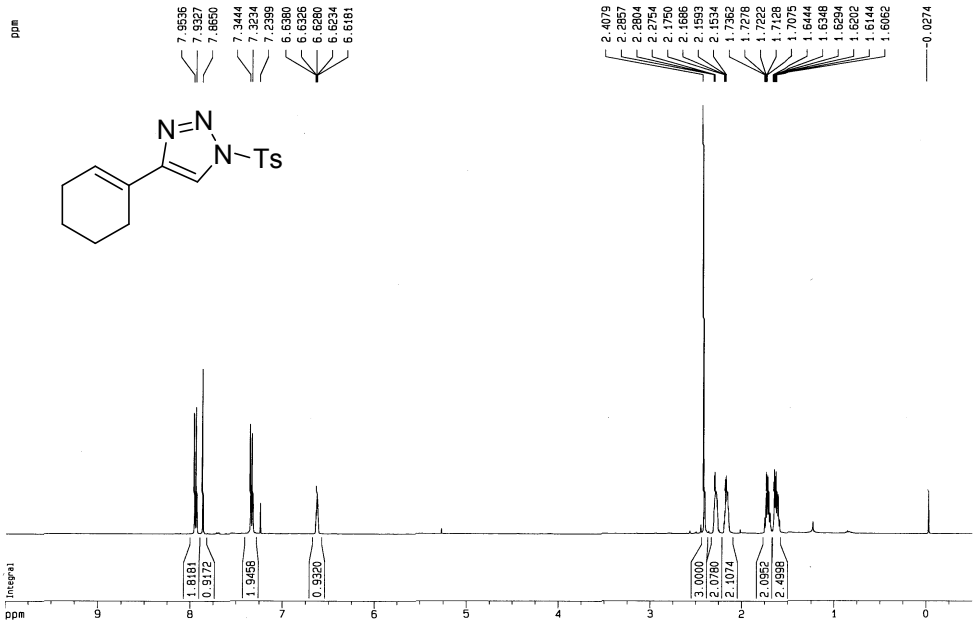


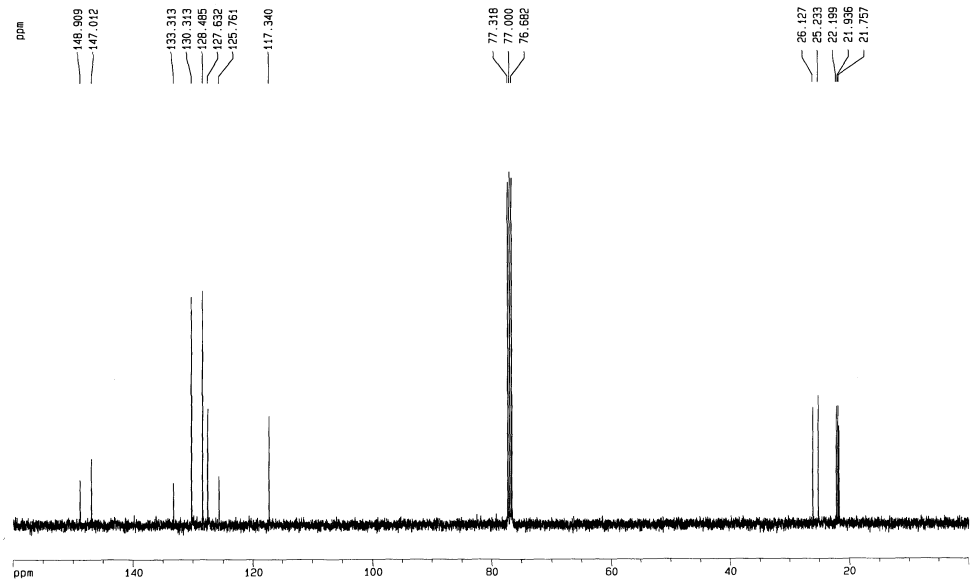
1-(4-Methylbenzensulfonyl)-4-(thien-3-yl)-1,2,3-triazole



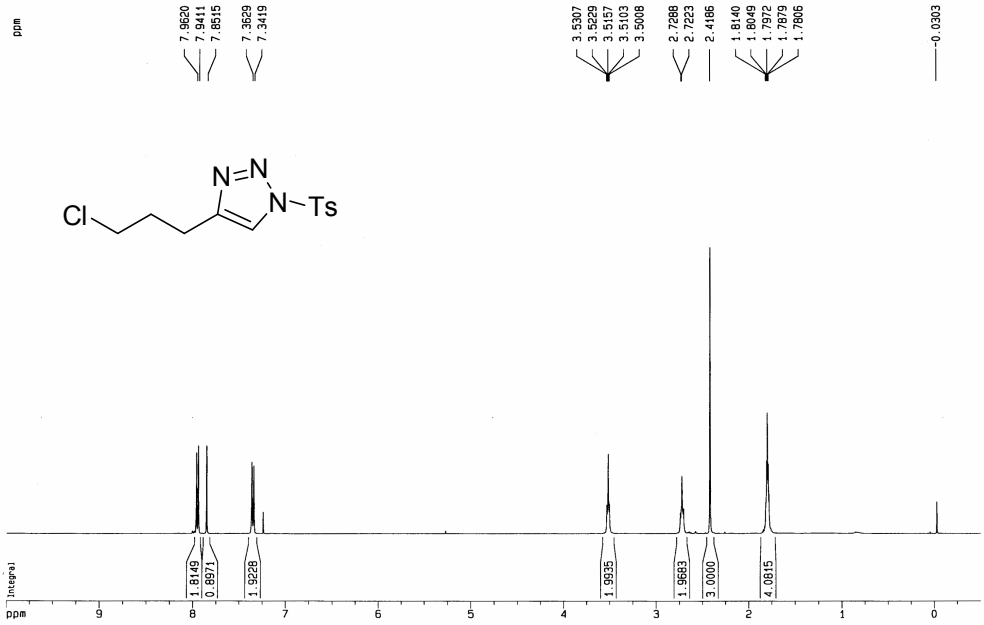


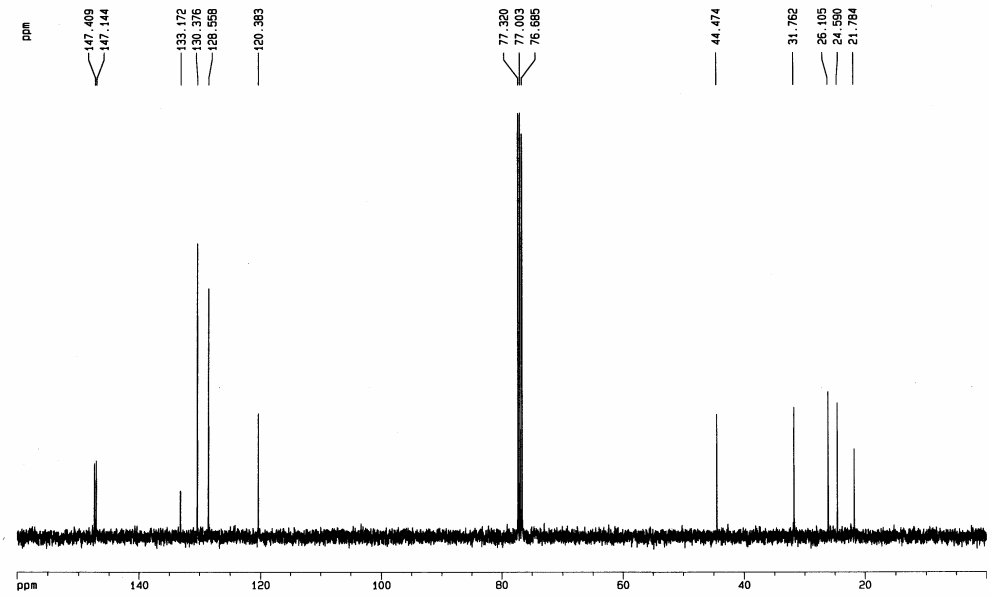
4-(Cyclohex-1-enyl)-1-(4-methylbenzenesulfonyl)-1,2,3-triazole



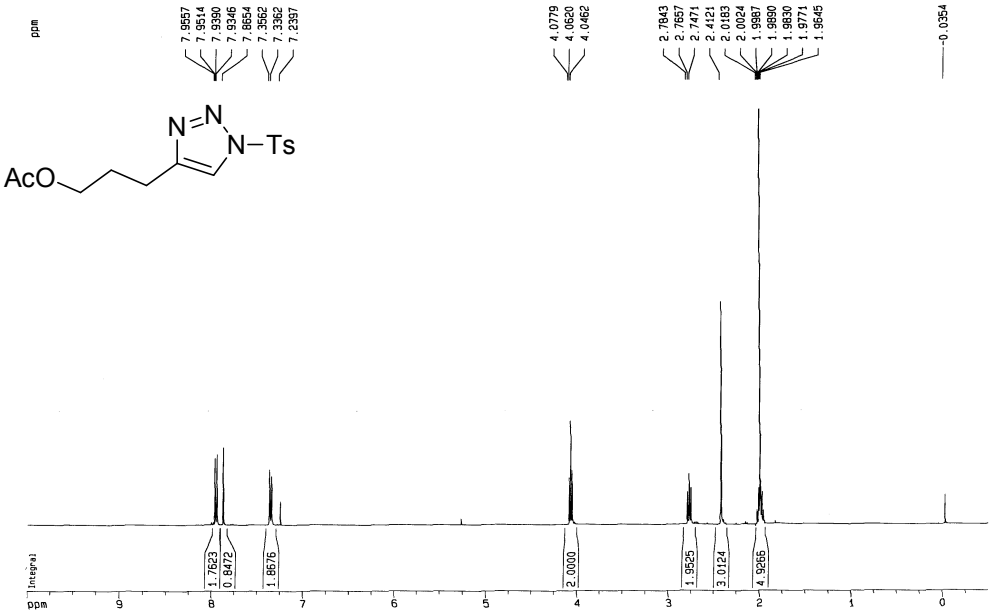


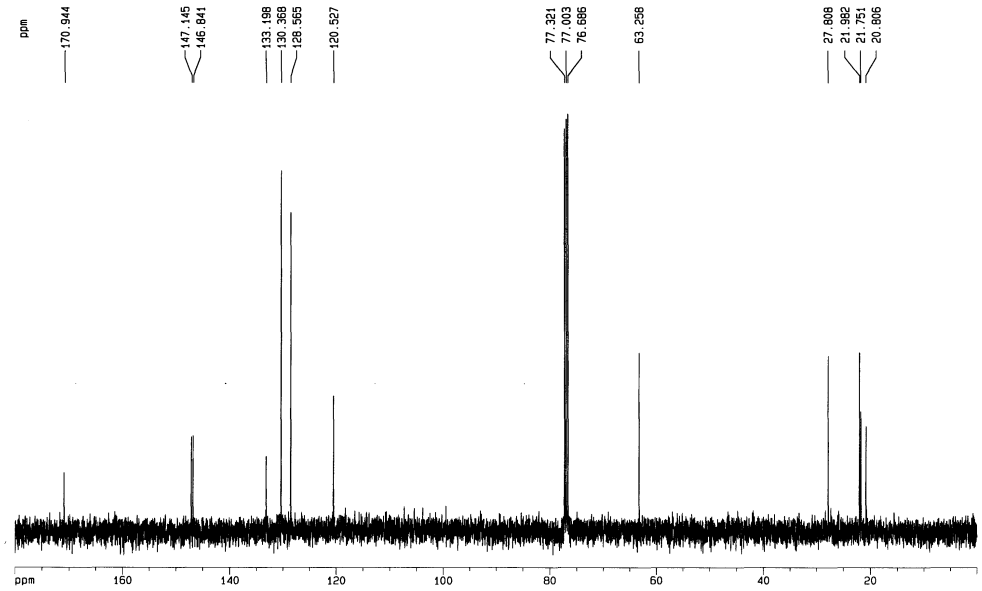
4-(3-Chloropropyl)-1-(4-methylbenzenesulfonyl)-1,2,3-triazole



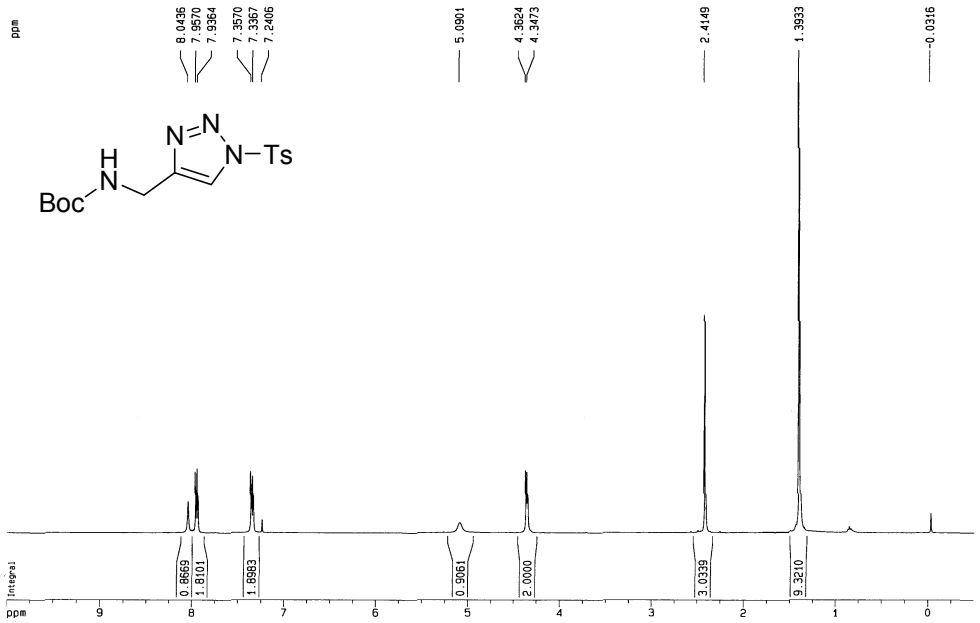


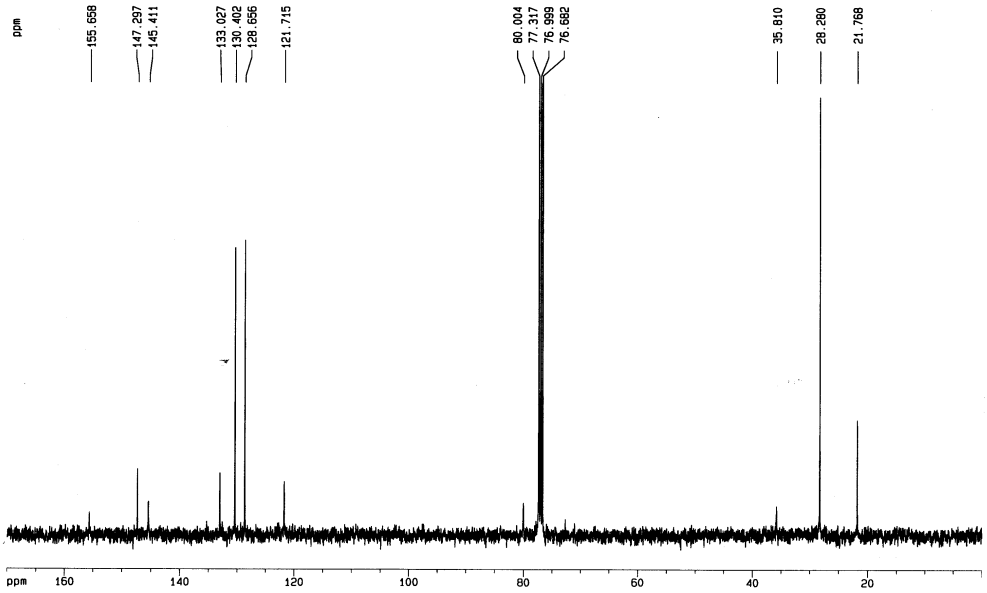
4-(Acetyloxypropyl)-1-(4-methylbenzenesulfonyl)-1,2,3-triazole



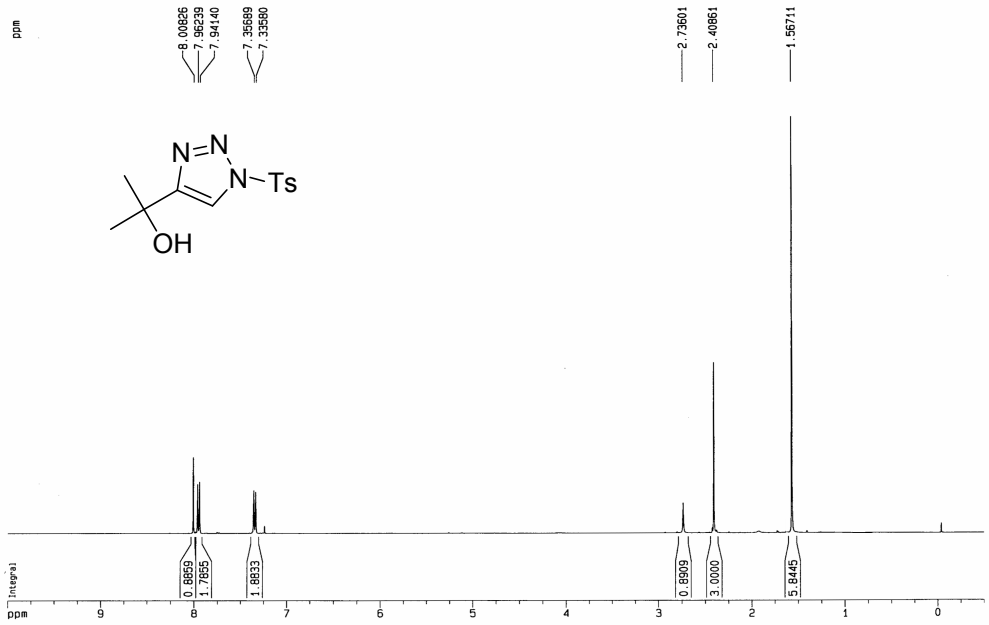


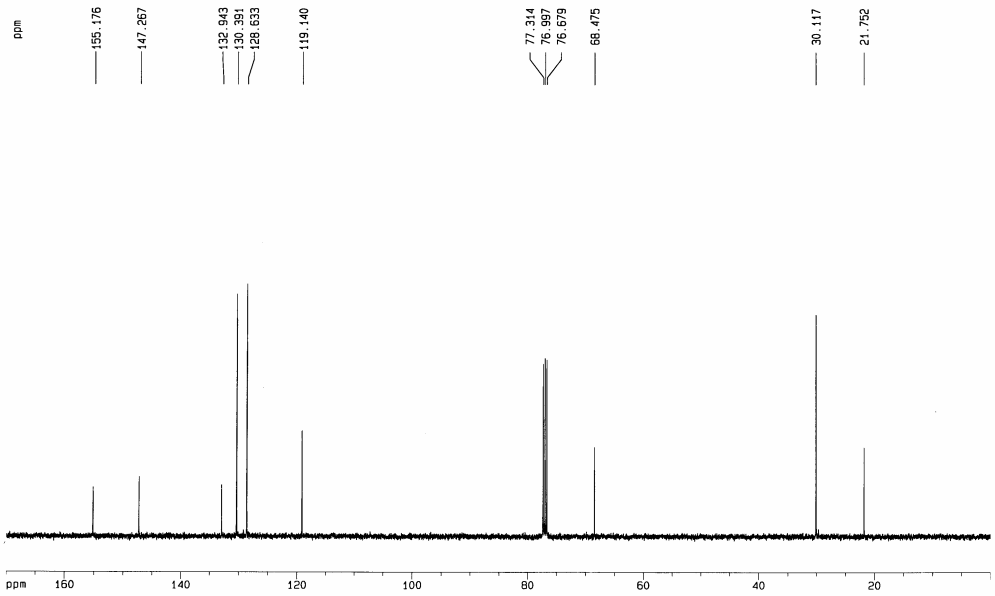
4-(*tert*-Butyloxycarbamidomethyl)-1-(4-methylbenzenesulfonyl)-1,2,3-triazole



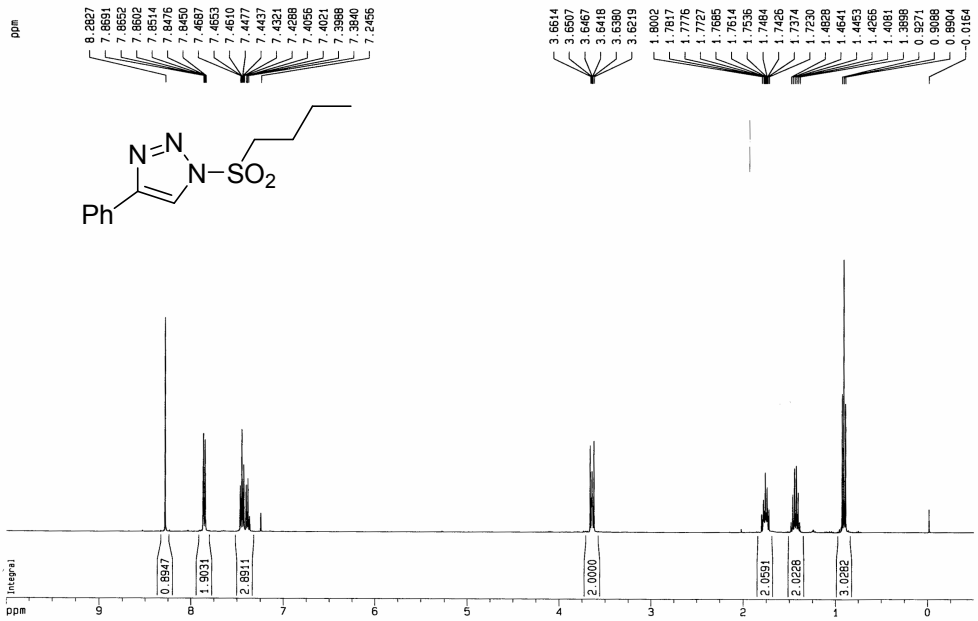


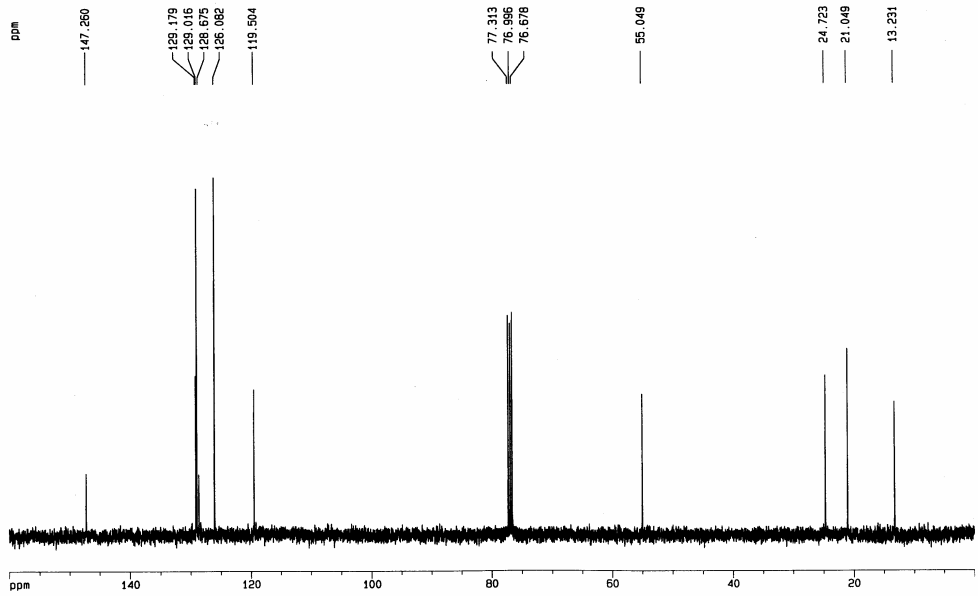
4-(1-Hydroxy-1-methylethyl)-1-(4-methylbenzenesulfonyl)-1,2,3-triazole



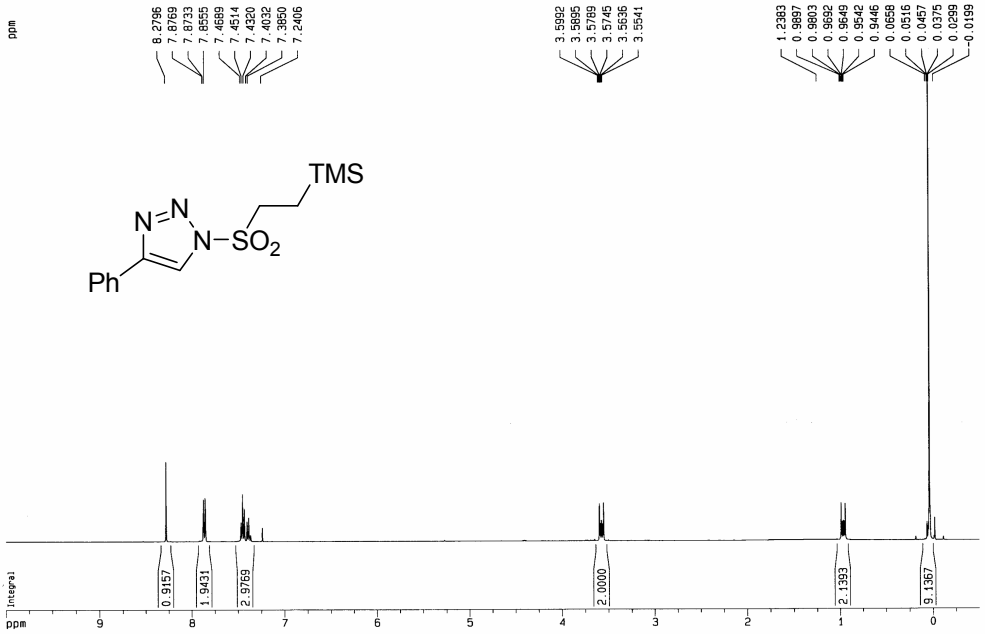


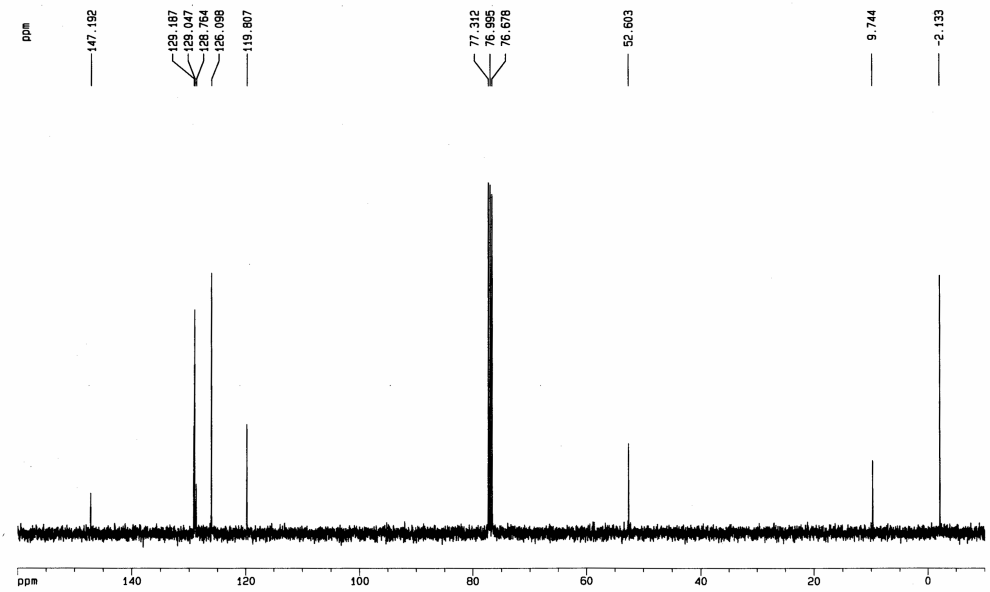
1-(Butanesulfonyl)-4-phenyl-1,2,3-triazole



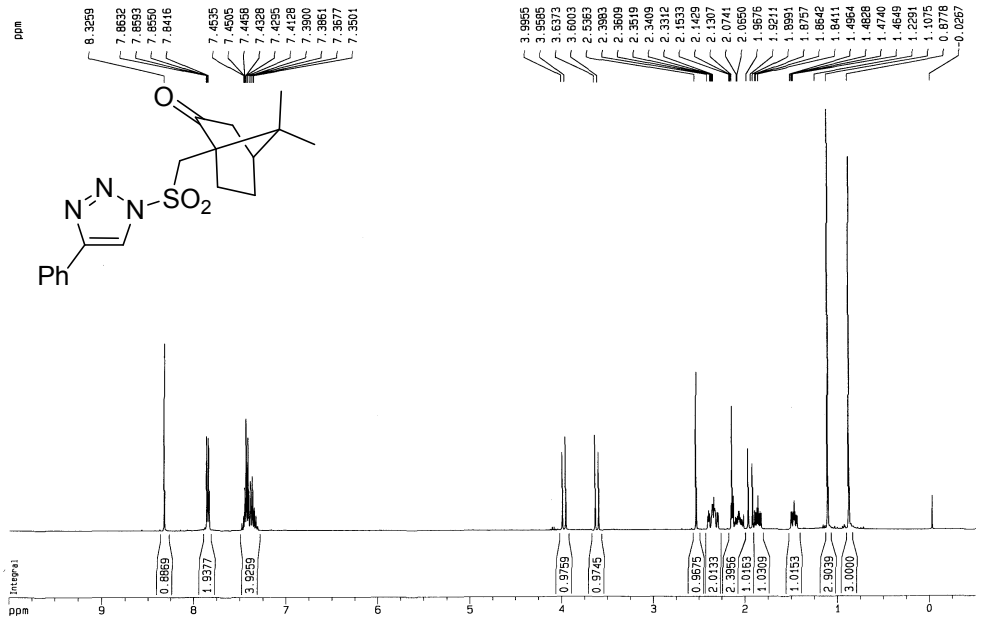


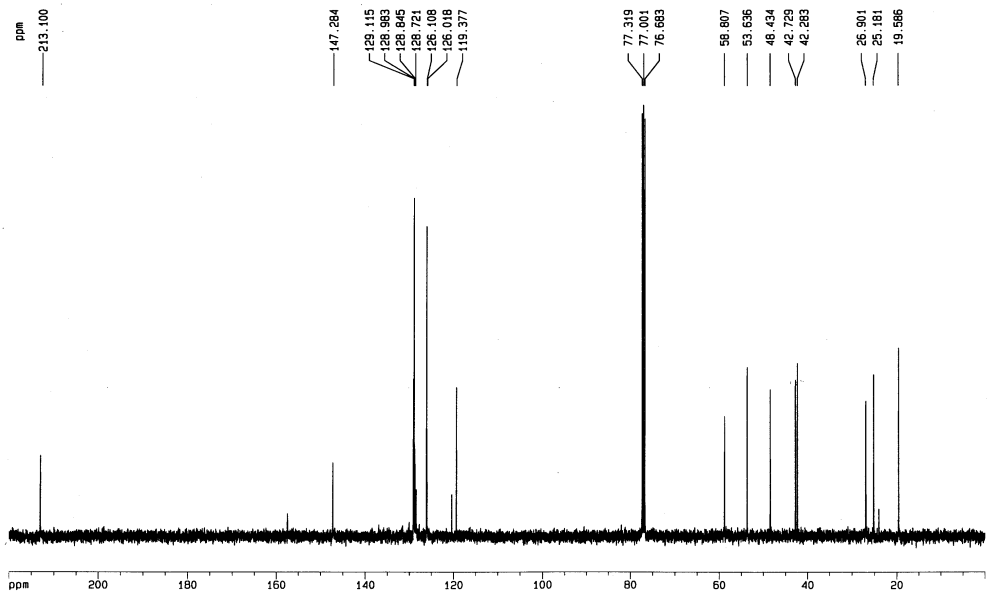
4-Phenyl-1-[2-(trimethylsilyl)ethanesulfonyl]-1,2,3-triazole



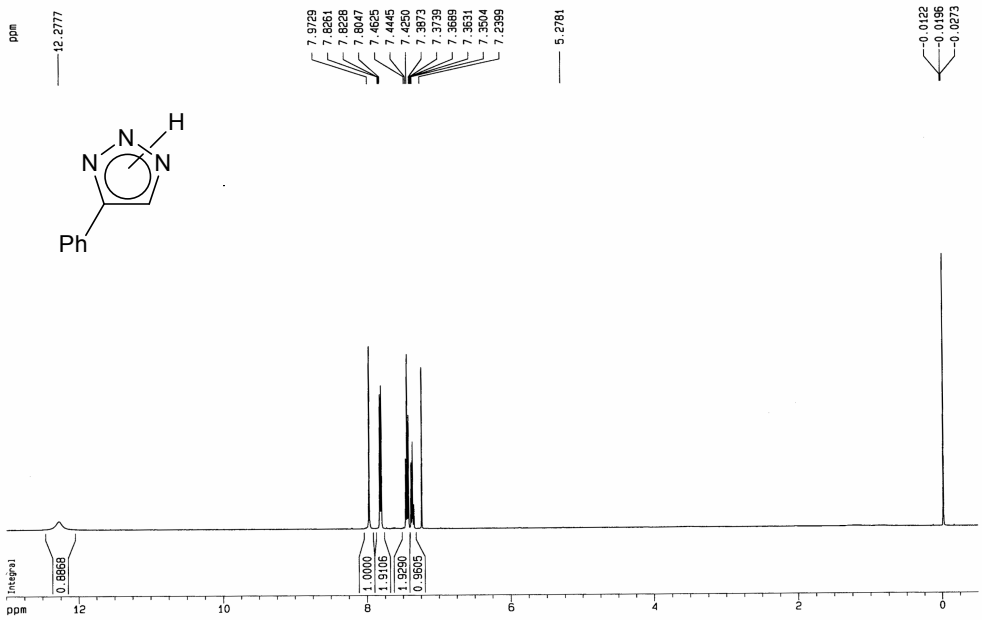


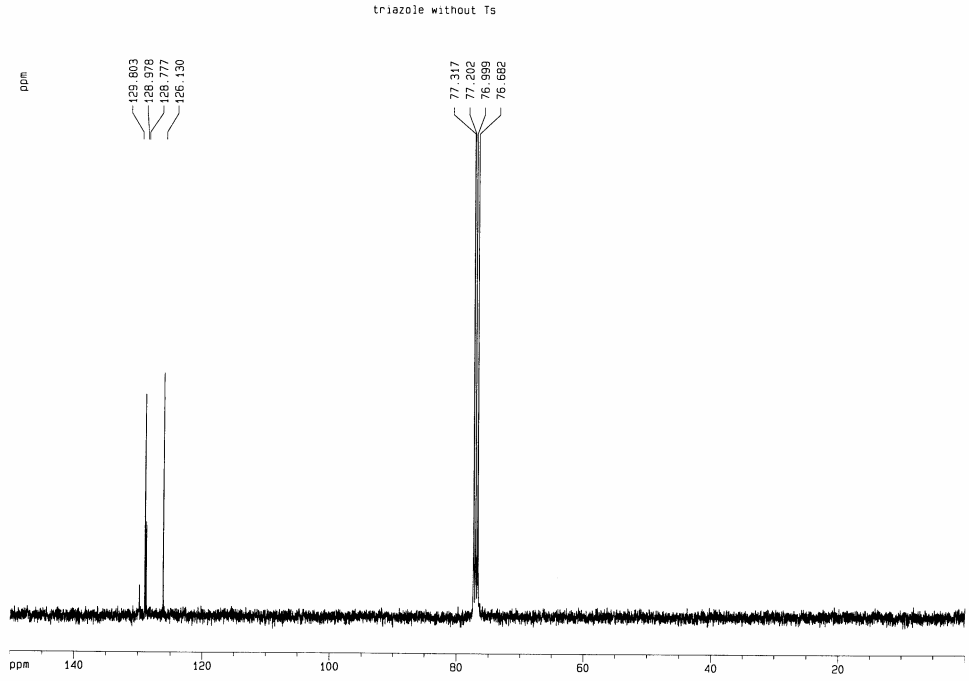
1-[(7,7-Dimethylbicyclo[2.2.1]heptan-1-yl)methanesulfonyl]-4-phenyl-1,2,3-triazole





4-Phenyl-*N*H-1,2,3-triazole





Appendix II

Coordinates, solution phase energies (atomic units) and zero point energy corrections (ZPE) of ground state and transition state geometries (numbered as in article).

Compound **D**

Solution phase energy -1141.661251

ZPE 359.4 kJ/mol

atom	x	y	z
Cu1	3.3811261187	-0.1387326744	0.0927673708
N2	4.9907563645	-3.4480039427	-1.8164387540
N3	4.3552104354	-4.0367026470	-0.8483074009
N4	3.8010689341	-3.0348147314	-0.1157269532
C5	4.0406002001	-1.7738826543	-0.6245631205
C6	4.8329559315	-2.0929949026	-1.7289380471
C7	5.4981151078	-1.2154661052	-2.7421867123
H8	5.1227445922	-0.1923331757	-2.6915698500
H9	6.5831322379	-1.1899407316	-2.5875249200
H10	5.3230580010	-1.5987468787	-3.7531014960
O11	2.7256212523	1.5734915528	0.7426662138
H12	1.7687518407	1.7078970143	0.8136884856
H13	3.1277045888	1.9570243853	1.5356910182
S14	2.7086000600	-3.4966934112	1.1540237858
O15	1.4237673034	-3.8200512848	0.5332195671
O16	2.7461663153	-2.4118852467	2.1316974361
C17	3.4554068283	-4.9809611966	1.8095602331
H18	4.4504666763	-4.7383554939	2.1783022203
H19	2.7950774472	-5.2866767509	2.6235215809
H20	3.4826312366	-5.7313035040	1.0227099814

Transition state $\mathbf{E}_{TS}$

Solution phase energy -1141.636797

ZPE 358.9 kJ/mol

atom	x	y	z
N3	0.0000000000	0.0000000000	0.0000000000
N4	0.0000000000	0.0000000000	2.1103483021
Cu1	2.1806222163	0.0000000000	4.0229872174
N2	1.1626368945	0.0021864862	0.0428570654
C5	1.3172052101	0.0109032902	2.2949069991
C6	2.0464484347	0.0126274224	1.0839182457
C7	3.5161315639	0.0082531239	0.8075876138
H8	4.0690136612	0.1251901915	1.7406440017
H9	3.8410028071	-0.9270905756	0.3384107342
H10	3.7990464030	0.8306001829	0.1423983239
O11	3.0426209040	0.0048141828	5.7771591953
H12	2.7627765208	0.6501465804	6.4429187672
H13	3.1780550845	-0.8368262953	6.2371214846
S14	-1.0849045287	0.0581422201	3.3543702411
O15	-1.1008537034	1.4005293529	3.9785228272
O16	-0.8833779561	-1.0651983898	4.2974824990
C17	-2.6406572676	-0.1849428154	2.5115686224
H18	-2.6317854827	-1.1613238589	2.0303410004
H19	-3.4052399820	-0.1435604441	3.2893614651
H20	-2.7811805636	0.6191503073	1.7916752229

Compound **F**

Solution phase energy -1141.647724

ZPE 351.1 kJ/mol

atom	x	y	z
N3	0.8864298775	-0.0411562252	-0.2742825069
N4	-0.3176941221	-0.0905584541	2.6679846343
Cu1	1.6023493693	-0.1573518061	4.8570367718
N2	1.3876101876	0.0325613792	0.7321853125
C5	0.9617337432	-0.0339377902	3.0323811733
C6	1.9000517632	0.0862899403	1.9490567390
C7	3.3916974011	0.2932886122	2.0266623510

H8	3.6689911054	0.4233796061	3.0736855439
H9	3.9493224159	-0.5585168892	1.6247251514
H10	3.7013947377	1.1892326953	1.4790678534
O11	2.3027747052	-0.3120205295	6.6811190988
H12	1.8555950615	0.1383241414	7.4136638639
H13	2.5820729239	-1.1782932390	7.0105173333
S14	-1.4503731686	-0.2850340848	3.8615763669
O15	-1.1462135800	0.4985887360	5.0866759848
O16	-1.6982152026	-1.7299099287	4.1049628835
C17	-2.9260771777	0.3834828248	3.1043293763
H18	-3.1339302751	-0.1820128439	2.1968608944
H19	-3.7279160938	0.2524057925	3.8323820412
H20	-2.7675012376	1.4385459773	2.8864675241

Compound **G**

Solution phase energy -593.0181329

ZPE 336.8 kJ/mol

atom	x	y	z
Cu1	2.8170891607	-0.4118481394	-0.3000038915
N2	5.5564196883	-3.3095278379	-1.4238153665
N3	5.1068358967	-3.7578937787	-0.2732938182
N4	4.2036112379	-2.8707306091	0.1626608175
C5	4.0383332718	-1.8149000581	-0.6945962996
C6	4.9385111963	-2.1362966127	-1.7197394065
C7	3.5420376138	-3.1340609648	1.4342796320
H8	3.7479866563	-2.3268932930	2.1375652510
H9	2.4666438748	-3.2322309641	1.2838193653
H10	3.9409806763	-4.0689513935	1.8267782746
C11	5.2958265904	-1.4334089191	-2.9936003761
H12	4.7154177024	-0.5199374097	-3.1295884045
H13	6.3594430124	-1.1681318376	-3.0080066736
H14	5.1187235409	-2.0832299658	-3.8585277340
O15	1.5435762621	0.9597000234	0.2309278662
H16	0.6219912372	0.6736828311	0.3180883521
H17	1.7627125781	1.4517195898	1.0358728076

Transition State $\mathbf{H}_{TS}$

Solution phase energy -592.9570155

ZPE 324.8 kJ/mol

atom	x	y	z
N3	0.0000000000	0.0000000000	0.0000000000
N4	0.0000000000	0.0000000000	2.4235428709
Cu1	2.4933164294	0.0000000000	3.9945620916
N2	1.1467741020	0.0003798343	0.2050091276
C5	1.2814884557	0.0046159194	2.4841789846
C6	2.0061169950	0.0021152873	1.2036484334
C7	-0.8919970360	0.0023117151	3.5691202738
H8	-1.5418757566	-0.8795505921	3.5367927638
H9	-0.3603798194	0.0106185359	4.5284434167
H10	-1.5520218083	0.8760737880	3.5259139677
C11	3.4848521416	-0.0004563725	0.9690314667
H12	3.9689519932	-0.8768786245	1.4127037115
H13	3.6886607859	-0.0173115530	-0.1047363431
H14	3.9697229490	0.8892956340	1.3850792254
O15	3.8926722551	-0.0017828954	5.3723182199
H16	4.4722096631	-0.7772780547	5.4091927580
H17	4.4627600679	0.7797878099	5.4258092690

Compound **I**

Solution phase energy -592.9637619

ZPE 325.5 kJ/mol

atom	x	y	z
Cu1	2.9506019115	-0.4683497995	-0.2317585486
N2	5.5421667539	-3.3059871899	-1.8088669580
N3	6.0937397262	-4.3039902583	-1.7759640873
N4	4.0519303167	-3.0218646835	0.3618263837
C5	4.0238635172	-2.0571481271	-0.4998434997
C6	4.8574111768	-2.2081761065	-1.7146384761
C7	3.2627048030	-2.9371433078	1.5792492687
H8	2.6763938754	-2.0085305232	1.6533466970
H9	2.5734830419	-3.7875113592	1.6421398855
H10	3.9156679475	-3.0036706037	2.4576152087

C11	4.9833719915	-1.2193086355	-2.8458492020
H12	4.0207559119	-1.0490225609	-3.3379657278
H13	5.3550326606	-0.2534780799	-2.4902447968
H14	5.6824043180	-1.5865129302	-3.6019289178
O15	1.7998919702	1.0591555899	0.2343375402
H16	0.8473854033	0.8847658089	0.2516731373
H17	2.0122158492	1.5236282676	1.0578803043

Transition State $\mathbf{J}_{TS}$

Solution phase energy -1141.625111

ZPE 343.0 kJ/mol

atom	x	y	z
Cu1	0.0000000000	0.0000000000	0.0000000000
C6	0.0000000000	0.0000000000	2.7983833240
N2	0.9273249544	0.0000000000	4.2251017405
N3	2.0179815210	-0.0310442686	4.4574952828
N4	2.2020565859	0.1481002597	1.8779261183
C5	0.8578040917	0.0556535242	1.7928575798
C7	-1.4263243765	0.0948308130	3.1942065667
H8	-1.6626732966	1.0632647842	3.6492604113
H9	-2.0568226312	-0.0238856555	2.3123520917
H10	-1.6923673928	-0.6880741903	3.9109716792
O11	-0.8941239956	-0.0866028930	-1.7649797296
H12	-0.9052806233	0.7096977237	-2.3158771911
H13	-0.6833975834	-0.8277745853	-2.3512776931
S14	3.0715436177	-0.0836730503	0.5240747414
O15	2.3239476994	0.3528399447	-0.6978565335
O16	3.5884266034	-1.4753262135	0.4281095797
C17	4.4983228864	0.9759486502	0.7375520246
H18	5.0065636196	0.6821338390	1.6555161959
H19	5.1416868830	0.8055076862	-0.1272943322
H20	4.1689852279	2.0125444335	0.7828461586

Compound **K**

Solution phase energy -869.5894953

ZPE 322.0kJ/mol

atom	x	y	z
N1	5.2452726963	-3.1240969195	-1.5971523338
N2	4.7226578810	-3.7013183659	-0.5554095142
N3	3.9707294165	-2.7766001040	0.0627133240
C4	4.0367127516	-1.5723949089	-0.5831526556
C5	4.8585986171	-1.8141339383	-1.6608636879
C10	5.3221481224	-0.9453938141	-2.7821495027
H11	5.0663223643	0.1009883039	-2.6150823799
H12	6.4077311000	-1.0255842939	-2.8940436028
H13	4.8691106089	-1.2677845472	-3.7255235597
H14	3.5124390450	-0.6954431484	-0.2413114952
S11	3.2471425777	-3.1775071007	1.6168248610
O12	2.1645106803	-2.2134285039	1.7616044906
O14	4.3259349839	-3.1825716106	2.5964375373
C14	2.6587795777	-4.8418434128	1.3557607503
H15	3.5141705608	-5.4674108143	1.1066344301
H16	2.2267031564	-5.1336136038	2.3158200795
H17	1.9082320826	-4.8329430486	0.5686830034

Compound **L**

Solution phase energy -869.5887575

ZPE 317.1 kJ/mol

atom	x	y	z
N1	6.1615335637	-2.8112929094	-1.4009537975
N2	7.1801266684	-3.1758368517	-1.1191953181
N3	4.2778561175	-2.7894214927	0.5357795768
C4	3.9912672892	-2.4156650326	-0.6948736111
C5	4.9425406194	-2.3899746370	-1.7286845610
C6	4.7189375233	-1.9425602135	-3.1514147281
H7	3.6614739087	-1.7086748590	-3.2828400718
H8	5.3006882822	-1.0474559946	-3.3878373166
H9	4.9859200768	-2.7269191076	-3.8644998864
H10	2.9863177077	-2.1029826490	-0.9828384689
S11	3.0060552917	-2.9567541526	1.5785486843
O12	2.5334965935	-4.3573818041	1.5171375205
O13	1.9583274886	-1.9423127606	1.3369589239

C14	3.7033262166	-2.7035765862	3.1976086493
H15	4.0648386707	-1.6805070491	3.2774521650
H16	2.8771202310	-2.8821215630	3.8886184562
H17	4.4963535001	-3.4333531352	3.3516241799

Transition Sate $\mathbf{M}_{TS}$

Solution phase energy -869.5425112

ZPE 302.9 kJ/mol

atom	x	y	z
H1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.9303637268
N3	1.5759550648	0.0000000000	3.3769916846
N4	2.3917547744	-0.0698929842	4.1023079506
N5	2.0566145736	0.1558752861	0.6219232058
C6	0.7223981482	0.0534042911	0.8361283633
C7	-1.1770713483	0.1162804353	2.7458860055
H8	-1.2632124067	1.0806747720	3.2550761458
H9	-2.0072875149	0.0579706278	2.0193180948
H10	-1.3057873853	-0.7166781774	3.4416860913
S11	2.5381270766	-0.1896603055	-0.8844545327
O12	1.6632830570	0.4297321964	-1.9156057678
O13	2.6928619315	-1.6568231240	-1.0796438466
C14	4.1686705102	0.5185218760	-1.0195349866
H15	4.8023455678	0.0857788198	-0.2470496274
H16	4.5207605547	0.2270195171	-2.0110370049
H17	4.0984031822	1.6007303739	-0.9346278302