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Supporting Information

Copper-Catalyzed Cascade Reactions of Ynamide Derivatives to Synthesize Medium-Sized Heterocycles

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(A) General Information

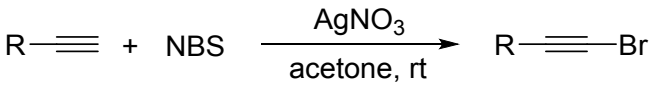
All reagents were obtained from commercial suppliers and used without further purification. A series of substrates **1** were prepared according to the literature procedure.[1-2] 6-chlorohex-1-yne and terminal alkyne are commercially available from TCI. Yields for all products were determined by the silica gel (300-400 mesh) column chromatography (eluent: petroleum ether 60-90/EtOAc), and the reactions were monitored by thin layer chromatography (TLC) on a glass plate coated with silica gel with fluorescent indicator (ZF_7) using UV light. The ^1H; ^{13}C; ^{19}F nuclear magnetic resonance (NMR) spectra were recorded on a Agilent 400 MHz using $CDCl_3$ as solvent with TMS as internal standard. Chemical shifts are given in ppm (δ) referenced to $CDCl_3$ with 7.26 for ^1H and 77.00 for ^{13}C. Signals are abbreviated as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet, and coupling constants are expressed in hertz. Melting points were measured on a YRT-3 and uncorrected. HRMS (ESI) was recorded using Agilent Q-TOF 6540. All calculations were carried out with the Gaussian 09 software.[3] Geometry optimization and frequency analysis were completed at PBE0-D3BJ/def2-SVP level,[4-6] and singlet point energy calculations were performed at PBE0-D3BJ/def2-TZVP level4. The SMD implicit solvation model was used to account for the solvation effect of toluene.[7]

(B) General Experimental Procedures

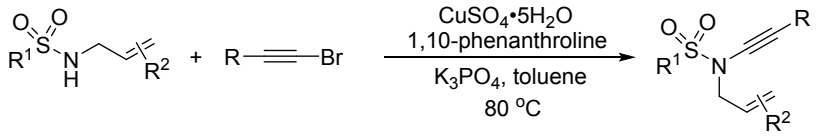
(a) Materias

N-allyl ynamides were prepared according to literature procedures.[1-2]

Preparation of bromoalkynes



To a stirred solution of terminal alkyne (10.0 mmol) in acetone (10.0 mL) was added *N*-bromosuccinimide (NBS) (1.2eq, 12.0 mmol) under N_2 atmosphere. The reaction mixture was stirred at room temperature and stirred for 3 h, then removal of solvent under reduced pressure. The residue was filtered through a pad of Celite with petroleum ether (PE) solvent. If necessary, further purification was performed by column chromatography on silica gel (PE as eluent) to afford bromoalkyne.



Following a slight modification of Hsung's procedure

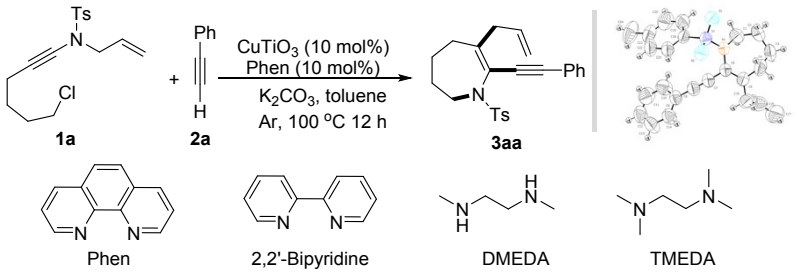
To a stirred solution of bromoalkyne (1.2 eq, 9.6 mmol), *N*-allyl sulfonamide (1 eq, 8.0 mmol), K_3PO_4 (2 eq, 16.0 mmol), $CuSO_4•5H_2O$ (0.1 eq, 0.8 mmol) and 1,10-phenanthroline (0.2 eq, 1.6 mmol) in toluene (16.0 mL) was heated at 80 °C for 48 h. After cooling to room temperature, the mixture was filtered through a short pad of silica gel using CH_2Cl_2 (20 mL) as the eluent, and the filtrate was concentrated in vacuo. Purification of the residue by column chromatography (PE/ EtOAc = 20 : 1) gave the *N*-allyl ynamides.

Copper Titanate ($CuTiO_3$) were prepared according to literature procedures [8] and supplied by Dr. Zhang Y, the co-first author of the report.

(b) General Procedures for Copper-Catalyzed Aza-Claisen Rearrangement/Cross-Coupling/ Cyclization Cascades toward Medium-Sized Heterocycles:

To a Schlenk tube were added **1** (0.2 mmol), **2** (0.6 mmol), $CuTiO_3$ (0.02 mmol), 1,10-phenanthroline (0.02 mmol), K_2CO_3 (0.4 mmol), and toluene (2.0 mL). Then the mixture was stirred at 100 °C (oil bath temperature) under argon atmosphere (1 atm) for 12 h until complete consumption of starting material as monitored by TLC and GC-MS analysis. After the reaction was finished, the reaction mixture was re-extracted with EtOAc. The combined organic extracts were concentrated in vacuum. The residue was purified by silica gel flash column chromatography (PE/ EtOAc = 20 : 1) to afford the desired products **3**.

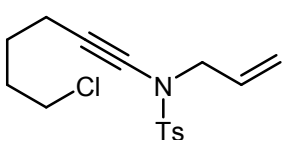
(C) Optimization of reaction conditions



Entry	Variation from the Standard Conditions	Isolated Yield [%]
1	none	62
2	without Phen	0
3	without $CuTiO_3$	0
4	$CuTiO_3$ (5 mol%) and Phen (5 mol%)	45
5	$CuTiO_3$ (20 mol%) and Phen (20 mol%)	66
6	$Cu(OAc)_2$ instead of $CuTiO_3$	31
7	$Cu(TFA)_2$ instead of $CuTiO_3$	28
8	$CuCl_2$ instead of $CuTiO_3$	27
9	$Cu(OTf)_2$ instead of $CuTiO_3$	34
10	$Cu(acac)_2$ instead of $CuTiO_3$	37
11	$Cu(MeCN)_4PF_6$ instead of $CuTiO_3$	29
12	CuCl instead of $CuTiO_3$	24
13	CuBr instead of $CuTiO_3$	25
14	CuI instead of $CuTiO_3$	23
15	2,2'-Bipyridine instead of Phen	0
16	DMEDA instead of Phen	0
17	TMEDA instead of Phen	0
18	Cs_2CO_3 instead of K_2CO_3	43
19	*t*-BuOK instead of K_2CO_3	0
20	KOAc instead of K_2CO_3	0
21	Et_3N instead of K_2CO_3	0
22	without K_2CO_3	0
23	MeCN instead of toluene	46
24	THF instead of toluene	39
25	DMF instead of toluene	0
26	DMSO instead of toluene	0
27	at 80 °C	26
28	at 120 °C	57

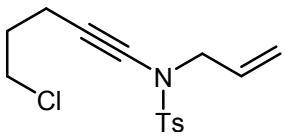
[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.6 mmol), $CuTiO_3$ (10 mol%), Phen (10 mol%), K_2CO_3 (2 equiv), toluene (2 mL), argon, 100 °C and 12 h.

(D) Analytical data



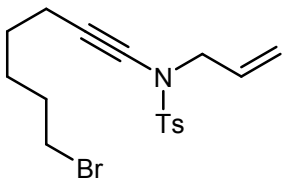
***N*-allyl-*N*-(6-chlorohex-1-yn-1-yl)-4-methylbenzenesulfonamide (1a):**

Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.78 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 5.77-5.67 (m, 1H), 5.25-5.18 (m, 2H), 3.93-3.91 (m, 2H), 3.53 (t, *J* = 6.8Hz, 2H), 2.45 (s, 3H), 2.30 (t, *J* = 6.8 Hz, 2H), 1.86-1.79 (m, 2H), 1.65-1.58 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.5, 134.6, 131.1, 129.6, 127.6, 119.7, 73.6, 69.5, 54.2, 44.5, 31.4, 26.0, 21.6, 17.7; HRMS (ESI) for $C_{16}H_{20}ClNO_2S$ $[M+H]^+$calcd. 326.0976, found. 326.0974.



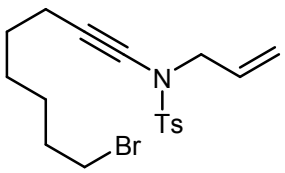
***N*-allyl-*N*-(5-chloropent-1-yn-1-yl)-4-methylbenzenesulfonamide (1b):**

Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.71 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 5.69-5.59 (m, 1H), 5.19-5.11 (m, 2H), 3.86-3.84 (m, 2H), 3.52 (t, *J* = 6.4 Hz, 2H), 2.38 (t, *J* = 6.4 Hz, 2H), 2.37 (s, 3H) , 1.86-1.80 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.4, 134.2, 130.8, 129.5, 127.4, 119.6, 73.8, 68.3, 53.9, 43.3, 31.2, 21.4, 15.6; HRMS (ESI) for $C_{15}H_{18}ClNO_2S$ $[M+H]^+$calcd. 312.0820, found. 312.0817.



***N*-allyl-*N*-(7-bromohept-1-yn-1-yl)-4-methylbenzenesulfonamide (1c):**

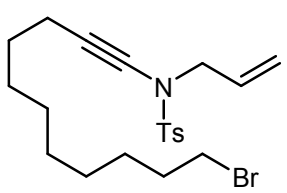
Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.78 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 5.78-5.67 (m, 1H), 5.25-5.17 (m, 2H), 3.93-3.91 (m, 2H), 3.38 (t, *J* = 6.8 Hz, 2H), 2.45 (s, 3H), 2.29-2.25 (m, 2H), 1.86-1.82 (m, 2H), 1.51-1.47 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.4, 134.7, 131.2, 129.6, 127.7, 119.6, 73.4, 69.8, 54.2, 33.6, 32.2, 27.9, 27.2, 21.6, 18.2; HRMS (ESI) for $C_{17}H_{22}BrNO_2S$ $[M+H]^+$calcd. 384.0627, found. 384.0631.



***N*-allyl-N-(8-bromooct-1-yn-1-yl)-4-methylbenzenesulfonamide (1d):**

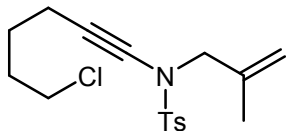
Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.78 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 7.6 Hz, 2H), 5.77-5.67 (m, 1H), 5.25-

5.18 (m, 2H), 3.92 (d, *J* = 6.4 Hz, 2H), 3.40 (t, *J* = 6.8 Hz, 2H), 2.46 (s, 3H), 2.26 (t, *J* = 6.8 Hz, 2H), 1.88-1.81 (m, 2H), 1.51-1.32 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.4, 134.6, 131.1, 129.6, 127.7, 119.6, 73.1, 70.1, 54.2, 33.9, 32.6, 28.6, 27.7, 27.6, 21.6, 18.3; HRMS (ESI) for $C_{18}H_{24}BrNO_2S$ $[M+H]^+$calcd. 398.0784, found. 398.0789.



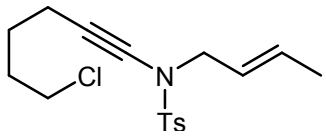
_N_-allyl-_N_-(11-bromoundec-1-yn-1-yl)-4-methylbenzenesulfonamide (1e):

Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.78 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 5.77-5.67 (m, 1H), 5.24-5.17 (m, 2H), 3.91 (d, *J* = 6.4 Hz, 2H), 3.41 (t, *J* = 6.8 Hz, 2H), 2.45 (s, 3H), 2.23 (t, *J* = 6.8 Hz, 2H), 1.89-1.81 (m, 2H), 1.49-1.39 (m, 4H), 1.34-1.28 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.3, 134.7, 131.2, 129.5, 127.7, 119.5, 73.0, 70.4, 54.2, 34.0, 32.8, 29.3, 29.0, 28.8, 28.7, 28.6, 28.1, 21.6, 18.4; HRMS (ESI) for $C_{21}H_{30}BrNO_2S$ $[M+H]^+$calcd. 440.1253, found. 440.1261.



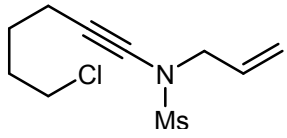
_N_-(6-chlorohex-1-yn-1-yl)-4-methyl-_N_-(2-methylallyl)benzenesulfonamide (1f):

Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.78 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 4.92 (d, *J* = 15.2 Hz, 2H), 3.81 (s, 2H), 3.52 (t, *J* = 6.8 Hz, 2H), 2.45 (s, 3H), 2.29 (t, *J* = 6.8 Hz, 2H), 1.86-1.78 (m, 2H), 1.72 (s, 3H), 1.63-1.56 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.4, 138.9, 134.6, 129.6, 127.6, 115.4, 73.6, 69.3, 57.7, 44.5, 31.3, 26.0, 21.6, 19.6, 17.7; HRMS (ESI) for $C_{17}H_{22}ClNO_2S$ $[M+H]^+$calcd. 340.1133, found. 340.1128.



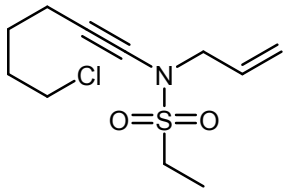
***(E)*-_N_-(but-2-en-1-yl)-_N_-(6-chlorohex-1-yn-1-yl)-4-methylbenzenesulfonamide (1g):**

Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.76 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 5.70-5.61 (m, 1H), 5.40-5.32 (m, 1H), 3.84 (d, *J* = 6.8 Hz, 2H), 3.53 (t, *J* = 6.8 Hz, 2H), 2.45 (s, 3H), 2.31 (t, *J* = 6.8 Hz, 2H), 1.87-1.79 (m, 2H), 1.60-1.65 (m, 3H), 1.63-1.58 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 144.3, 134.6, 131.7, 129.5, 127.7, 123.8, 73.7, 69.3, 53.7, 47.9, 44.5, 31.3, 26.0, 21.5, 17.7; HRMS (ESI) for $C_{17}H_{22}ClNO_2S$ $[M+H]^+$calcd. 340.1133, found. 340.1125.



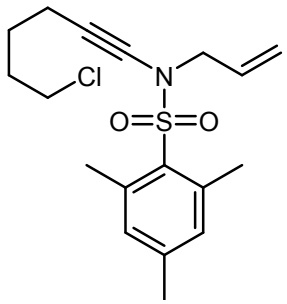
***N*-allyl-*N*-(6-chlorohex-1-yn-1-yl)methanesulfonamide (1h):**

Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 5.97-5.87 (m, 1H), 5.39- 5.31 (m, 2H), 4.02 (d, *J* = 6.0 Hz, 2H), 3.57 (t, *J* = 6.4 Hz, 2H), 3.05 (s, 3H), 2.35 (t, J = 6.8 Hz, 2H), 1.92-1.85 (m, 2H), 1.71-1.64 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 131.0, 120.1, 73.1, 69.9, 54.1, 44.5, 38.3, 31.4, 26.0, 17.7; HRMS (ESI) for $C_{10}H_{16}ClNO_2S$ $[M+H]^+$calcd. 250.0663, found. 250.0667.



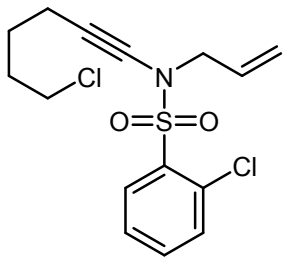
***N*-allyl-*N*-(6-chlorohex-1-yn-1-yl)ethanesulfonamide (1i):**

Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 5.91-5.81 (m, 1H), 5.33-5.25 (m, 2H), 3.98 (d, *J* = 6.4 Hz, 2H), 3.52 (t, *J* = 6.4 Hz, 2H), 3.23-3.17 (m, 2H), 2.29 (t, *J* = 6.8 Hz, 2H), 1.87-1.80 (m, 2H), 1.66-1.58 (m, 2H), 1.37 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 131.5, 119.7, 73.3, 69.3, 54.0, 46.3, 44.4, 31.4, 26.0, 17.7, 7.9; HRMS (ESI) for $C_{11}H_{18}ClNO_2S$ $[M+H]^+$calcd. 264.0820, found. 264.0816.



***N*-allyl-*N*-(6-chlorohex-1-yn-1-yl)-2,4,6-trimethylbenzenesulfonamide (1j):**

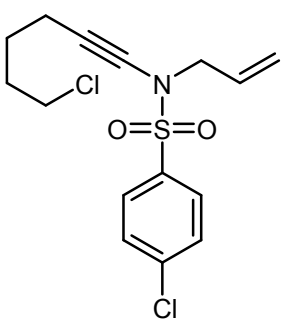
Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.97 (s, 2H), 5.90-5.80 (m, 1H), 5.32-5.24 (m, 2H), 4.01 (d, *J* = 6.0 Hz, 2H), 3.45 (t, *J* = 6.4 Hz, 2H), 2.63 (s, 6H), 2.31 (s, 3H), 2.24 (t, *J* = 6.8 Hz, 2H), 1.72-1.65 (m, 2H), 1.55-1.48 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 143.3, 140.6, 131.8, 131.7, 131.5, 119.6, 73.2, 70.4, 52.5, 44.4, 31.1, 25.8, 22.9, 21.0, 17.7; HRMS (ESI) for $C_{18}H_{24}ClNO_2S$ $[M+H]^+$calcd. 354.1289, found. 354.1287.



***N*-allyl-2-chloro-*N*-(6-chlorohex-1-yn-1-yl)benzenesulfonamide (1k):**

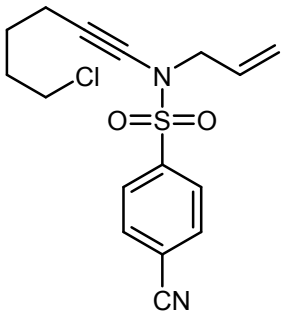
Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.15-8.13 (m, 1H), 7.57-7.55 (m, 2H), 7.46-7.42 (m, 1H), 5.94-5.84 (m, 1H), 5.36-5.27 (m, 2H), 4.17 (d, *J* = 6.0 Hz, 2H), 3.46 (t, *J* = 6.4 Hz, 2H), 2.23 (t, *J* = 6.8 Hz, 2H), 1.75-1.68 (m, 2H), 1.55-1.48 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 135.5, 134.4, 132.7, 132.4, 132.1, 131.6, 126.9, 119.6, 72.5, 70.3,

54.4, 44.5, 31.2, 25.8, 17.6; HRMS (ESI) for $C_{15}H_{17}Cl_2NO_2S$ $[M+H]^+$calcd. 346.0430, found. 346.0434.



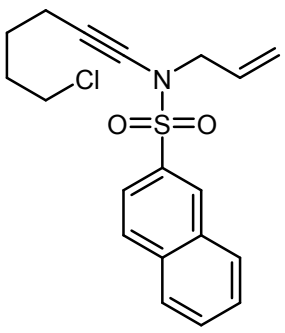
***N*-allyl-4-chloro-*N*-(6-chlorohex-1-yn-1-yl)benzenesulfonamide (1l):**

Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.84 (d, *J* = 8.4 Hz, 2H), 7.54 (d, *J* = 8.4 Hz, 2H), 5.77-5.67 (m, 1H), 5.27-5.21 (m, 2H), 3.94 (d, *J* = 6.4 Hz, 2H), 3.54 (t, *J* = 6.4 Hz, 2H), 2.31 (t, *J* = 6.8 Hz, 2H), 1.87-1.80 (m, 2H), 1.66-1.59 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 140.1, 136.0, 130.7, 129.4, 129.0, 120.1, 73.1, 69.9, 54.3, 44.5, 31.4, 25.9, 17.7; HRMS (ESI) for $C_{15}H_{17}Cl_2NO_2S$ $[M+H]^+$calcd. 346.0430, found. 346.0423.



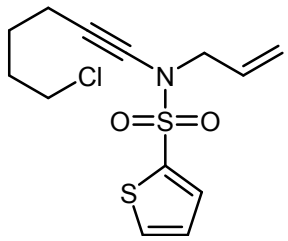
***N*-allyl-*N*-(6-chlorohex-1-yn-1-yl)-4-cyanobenzenesulfonamide (1m):**

Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.02 (d, *J* = 8.8 Hz, 2H), 7.87 (d, *J* = 8.8 Hz, 2H), 5.75-5.65 (m, 1H), 5.27-5.22 (m, 2H), 3.98 (d, *J* = 6.4 Hz, 2H), 3.55 (t, *J* = 6.4 Hz, 2H), 2.32 (t, *J* = 6.8 Hz, 2H), 1.87-1.80 (m, 2H), 1.67-1.60 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.6, 132.9, 130.3, 128.2, 120.4, 117.2, 117.1, 72.6, 70.3, 54.5, 44.4, 31.4, 25.9, 17.7; HRMS (ESI) for $C_{16}H_{17}ClN_2O_2S$ $[M+H]^+$calcd. 337.0772, found. 337.0775.



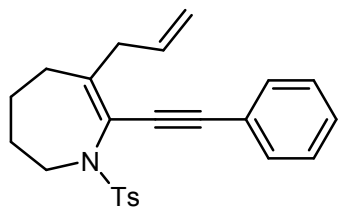
***N*-allyl-*N*-(6-chlorohex-1-yn-1-yl)naphthalene-2-sulfonamide (1n):**

Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.46 (s, 1H), 8.00 (d, *J* = 8.4 Hz, 2H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.90-7.87 (m, 1H), 7.70-7.62 (m, 2H), 5.78-5.68 (m, 1H), 5.26-5.17 (m, 2H), 4.00-3.98 (m, 2H), 3.47 (t, *J* = 6.4 Hz, 2H), 2.30 (t, *J* = 6.8 Hz, 2H), 1.82-1.75 (m, 2H), 1.61-1.56 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 135.1, 134.4, 131.9, 131.0, 129.3, 129.3, 129.3, 129.1, 127.9, 127.7, 122.6, 119.9, 73.5, 69.7, 54.3, 44.5, 31.3, 25.9, 17.7; HRMS (ESI) for $C_{19}H_{20}ClNO_2S$ $[M+H]^+$calcd. 362.0976, found. 362.0982.



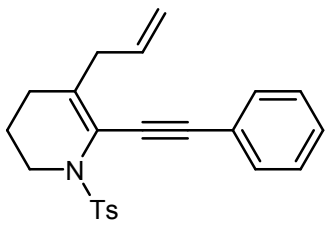
_N_-allyl-_N_-(6-chlorohex-1-yn-1-yl)thiophene-2-sulfonamide (1o):

Colourless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.69-7.67 (m, 2H), 7.17-7.14 (m, 1H), 5.80-5.70 (m, 1H), 5.28-5.21 (m, 2H), 3.96-3.94 (m, 2H), 3.54 (t, J = 6.4 Hz, 2H), 2.33 (t, J = 6.8 Hz, 2H), 1.89-1.82 (m, 2H), 1.68-1.61 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 137.0, 133.2, 133.0, 130.6, 127.4, 119.9, 73.0, 70.5, 54.4, 44.5, 31.3, 25.9, 17.6; HRMS (ESI) for $C_{13}H_{16}ClNO_2S_2$ $[M+H]^+$calcd. 318.0384, found. 318.0387.



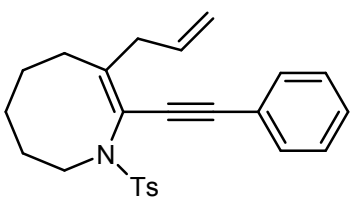
6-Allyl-7-(phenylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3aa):

Isolated yield 62%, 48.5 mg; Light yellow solid, mp 105-107 ^{o}C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.87 (d, J = 8.4 Hz, 2H), 7.29-7.26 (m, 3H), 7.21-7.18 (m, 4H), 5.82-5.72 (m, 1H), 5.19-5.08 (m, 2H), 3.44-3.42 (m, 2H), 3.18 (d, J = 6.8 Hz, 2H), 2.43-2.41 (m, 2H), 2.36 (s, 3H), 1.94-1.89 (m, 2H), 1.51-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.5, 142.8, 138.2, 133.8, 131.3, 129.2, 128.2, 128.1, 127.5, 122.8, 120.4, 117.4, 93.6, 84.8, 49.7, 40.6, 32.1, 31.0, 23.7, 21.4; HRMS (ESI) for $C_{24}H_{25}NO_2S$ $[M+H]^+$calcd. 392.1679, found. 392.1682.



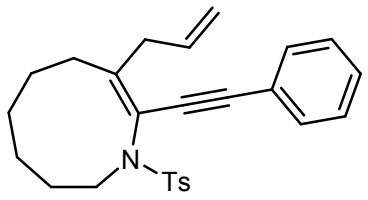
5-Allyl-6-(phenylethynyl)-1-tosyl-1,2,3,4-tetrahydropyridine (3ba):

Isolated yield 72%, 54.2 mg. Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.80 (d, J = 8.4 Hz, 2H), 7.36-7.29 (m, 5H), 7.23 (d, J = 8.0 Hz, 2H), 5.82-5.71 (m, 1H), 5.07-5.01 (m, 2H), 3.69-3.67 (m, 2H), 3.09 (d, J = 6.8 Hz, 2H), 2.39 (s, 3H), 2.11 (t, J = 6.8 Hz, 2H), 1.75-1.68 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 143.2, 137.8, 134.9, 134.5, 131.3, 129.4, 128.3, 128.2, 127.5, 123.0, 117.1, 116.3, 94.3, 84.0, 45.9, 39.4, 26.9, 21.8, 21.5; HRMS (ESI) for $C_{23}H_{23}NO_2S$ $[M+H]^+$calcd. 378.1522, found. 378.1523.



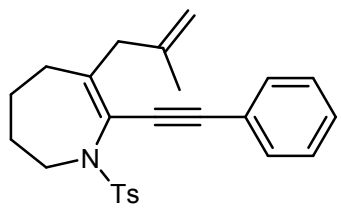
(*E*)-7-Allyl-8-(phenylethynyl)-1-tosyl-1,2,3,4,5,6-hexahydroazocine (3ca):

Isolated yield 47%, 38.1 mg. Light yellow solid, mp 112-114 ^{o}C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.79 (d, J = 8.4 Hz, 2H), 7.26-7.17 (m, 5H), 7.00- 6.98 (m, 2H), 5.91-5.81 (m, 1H), 5.24-5.10 (m, 2H), 3.75 (brs, 2H), 3.20-3.18 (m, 2H), 3.00 (brs, 2H), 2.32 (s, 3H), 1.70 (brs, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.8, 142.9, 136.7, 134.1, 131.2, 129.2, 128.1, 128.0, 122.6, 117.3, 115.5, 93.3, 83.1, 49.9, 39.1, 31.4, 29.1, 27.1, 27.0, 21.4; HRMS (ESI) for $C_{25}H_{27}NO_2S$ $[M+H]^+$calcd. 406.1835, found. 406.1838.



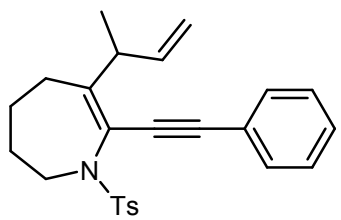
(*E*)-8-Allyl-9-(phenylethynyl)-1-tosyl-2,3,4,5,6,7-hexahydro-1*H*-azonine (3da):

Isolated yield 32%, 26.8 mg. Light yellow solid, mp 117-119 ^{o}C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.77 (d, J = 8.0 Hz, 2H), 7.26-7.18 (m, 5H), 6.93-6.91 (m, 2H), 5.92-5.81 (m, 1H), 5.26-5.11 (m, 2H), 3.65-3.59 (m, 1H), 3.29-3.21 (m, 2H), 3.07-3.01 (m, 2H), 2.30 (s, 3H), 2.14-2.08 (m, 1H), 1.88-1.66 (m, 4H), 1.62-1.56 (m, 1H), 1.51-1.37 (m, 2H), 1.33-1.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 154.8, 143.1, 135.3, 134.2, 131.1, 129.1, 128.3, 128.07, 128.0, 122.5, 117.3, 117.1, 93.2, 83.4, 48.2, 39.2, 30.0, 26.1, 25.5, 25.3, 23.7, 21.4; HRMS (ESI) for $C_{26}H_{29}NO_2S$ $[M+H]^+$calcd. 420.1992, found. 420.1994.



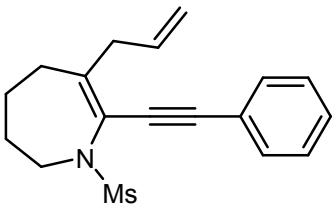
6-(2-Methylallyl)-7-(phenylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3fa):

Isolated yield 60%, 48.6 mg. Light yellow solid, mp 116-118 ^{o}C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.87 (d, J = 8.4 Hz, 2H), 7.29-7.26 (m, 3H), 7.21-7.17 (m, 4H), 4.83 (d, J = 6.0 Hz, 2H), 3.45-3.43 (m, 2H), 3.13 (s, 2H), 2.41-2.38 (m, 2H), 2.36 (s, 3H), 1.96-1.90 (m, 2H), 1.75 (s, 3H), 1.49-1.47 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.5, 142.8, 142.0, 138.3, 131.2, 129.2, 128.2, 128.1, 127.5, 122.8, 121.0, 113.1, 93.3, 85.1, 49.7, 44.6, 31.8, 31.2, 23.7, 22.0, 21.4; HRMS (ESI) for $C_{25}H_{27}NO_2S$ $[M+H]^+$calcd. 406.1835, found. 406.1830.



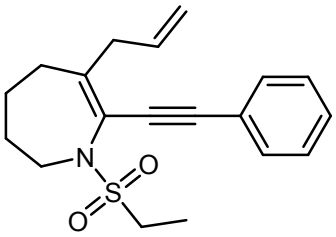
6-(But-3-en-2-yl)-7-(phenylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ga):

Isolated yield 52%, 42.1 mg. Light yellow solid, mp 122-124 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.86 (d, *J* = 8.4 Hz, 2H), 7.29-7.26 (m, 3H), 7.22-7.18 (m, 4H), 5.86-5.78 (m, 1H), 5.15-5.08 (m, 2H), 3.88-3.82 (m, 1H), 3.44-3.42 (m, 2H), 2.36 (s, 3H), 2.30-2.38 (m, 2H), 1.90 (t, *J* = 6.0 Hz, 2H), 1.48-1.42 (m, 2H), 1.17 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.0, 142.8, 139.3, 138.2, 131.3, 129.2, 128.2, 128.1, 127.5, 122.8, 119.6, 114.9, 93.6, 84.6, 49.5, 41.2, 31.0, 27.4, 24.4, 21.4, 16.2; HRMS (ESI) for $C_{25}H_{27}NO_2S$ $[M+H]^+$calcd. 406.1835, found. 406.1828.



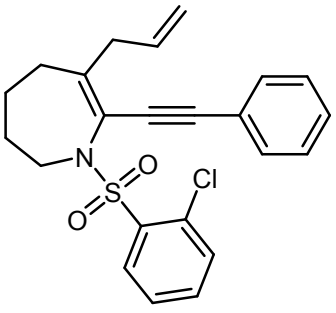
6-Allyl-1-(methylsulfonyl)-7-(phenylethynyl)-2,3,4,5-tetrahydro-1*H*-azepine (3ha):

Isolated yield 74%, 46.6 mg. Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.44-7.42 (m, 2H), 7.35-7.32 (m, 3H), 5.84-5.74 (m, 1H), 5.21-5.10 (m, 2H), 3.41-3.39 (m, 2H), 3.18 (d, *J* = 6.8 Hz, 2H), 3.14 (s, 3H), 2.46-2.43 (m, 2H), 1.92-1.86 (m, 2H), 1.53-1.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.9, 133.8, 131.2, 128.6, 128.4, 122.5, 120.1, 117.5, 93.9, 84.2, 49.5, 40.6, 39.6, 32.2, 31.5, 23.7; HRMS (ESI) for $C_{18}H_{21}NO_2S$ $[M+H]^+$calcd. 316.1366, found. 316.1363.



6-Allyl-1-(ethylsulfonyl)-7-(phenylethynyl)-2,3,4,5-tetrahydro-1*H*-azepine (3ia):

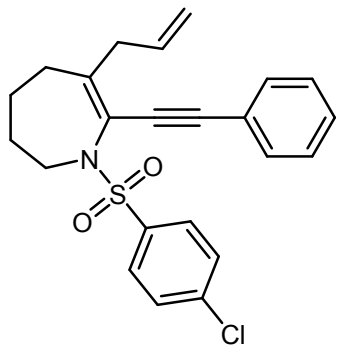
Isolated yield 68%, 44.7 mg. Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.42-7.38 (m, 2H), 7.35-7.31 (m, 3H), 5.84-5.74 (m, 1H), 5.21-5.10 (m, 2H), 3.47-3.45 (m, 2H), 3.38-3.32 (m, 2H), 3.19 (d, *J* = 6.8 Hz, 2H), 2.48-2.45 (m, 2H), 1.92-1.87 (m, 2H), 1.53-1.51 (m, 2H), 1.45 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.8, 133.7, 131.2, 128.6, 128.4, 122.6, 120.0, 117.4, 93.3, 84.6, 50.5, 47.7, 40.8, 32.3, 31.9, 23.7, 8.2; HRMS (ESI) for $C_{19}H_{23}NO_2S$ $[M+H]^+$calcd. 330.1522, found. 330.1527.



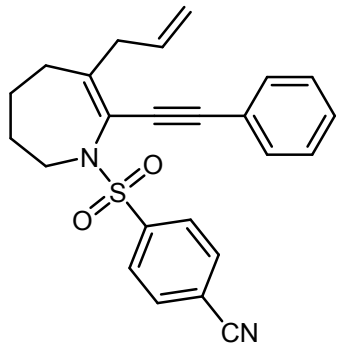
6-Allyl-1-((2-chlorophenyl)sulfonyl)-7-(phenylethynyl)-2,3,4,5-tetrahydro-1*H*-azepine (3ka):

Isolated yield 49%, 40.3 mg. Light yellow solid, mp 126-128 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.12-8.09 (m, 1H), 7.44-7.42 (m, 1H), 7.29-7.15 (m, 5H), 6.95-

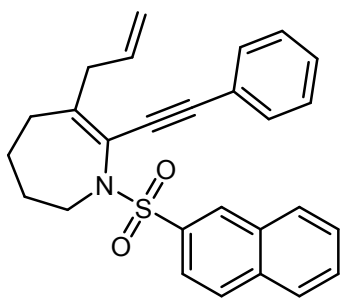
6.93 (m, 2H), 5.81-5.71 (m, 1H), 5.19-5.09 (m, 2H), 3.78-3.76 (m, 2H), 3.14 (d, J = 6.8 Hz, 2H), 2.56-2.53 (m, 2H), 2.01-1.96 (m, 2H), 1.59-1.54 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 152.2, 139.0, 133.5, 133.0, 132.2, 132.0, 131.5, 131.1, 128.2, 127.9, 126.6, 122.3, 119.4, 117.5, 93.5, 83.8, 51.2, 40.8, 32.4, 32.1, 23.6; HRMS (ESI) for $C_{23}H_{22}ClNO_2S$ $[M+H]^+$calcd. 412.1133, found. 412.1136.



6-Allyl-1-((4-chlorophenyl)sulfonyl)-7-(phenylethynyl)-2,3,4,5-tetrahydro-1*H*-azepine (3la): Isolated yield 54%, 44.3 mg. Light yellow solid, mp 132-134 ^{o}C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.91 (d, J = 8.8 Hz, 2H), 7.38-7.34 (m, 2H), 7.32-7.29 (m, 3H), 7.18-7.16 (m, 2H), 5.82-5.72 (m, 1H), 5.20-5.09 (m, 2H), 3.44-3.42 (m, 2H), 3.18 (d, J = 6.8 Hz, 2H), 2.45-2.42 (m, 2H), 1.96-1.91 (m, 2H), 1.53-1.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.0, 139.5, 138.6, 133.6, 131.2, 128.9, 128.8, 128.5, 128.3, 122.4, 120.0, 117.5, 93.9, 84.4, 49.8, 40.6, 32.1, 31.2, 23.6; HRMS (ESI) for $C_{23}H_{22}ClNO_2S$ $[M+H]^+$calcd. 412.1133, found. 412.1132.

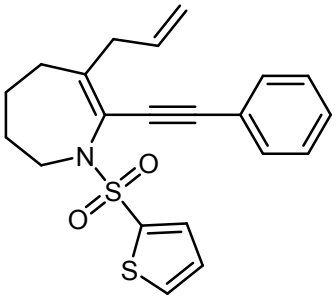


4-((A-allyl-7-(phenylethynyl)-2,3,4,5-tetrahydro-1*H*-azepin-1-yl)sulfonyl)benzonitrile (3ma): Isolated yield 41%, 33.0 mg. Light yellow solid, mp 137-139 ^{o}C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 1H NMR (400 MHz, Chloroform-d) δ 8.07 (d, J = 8.4 Hz, 2H), 7.66 (d, J = 8.4 Hz, 2H), 7.37-7.32 (m, 3H), 7.14-7.12 (m, 2H), 5.81-5.71 (m, 1H), 5.20-5.10 (m, 2H), 3.48-3.46 (m, 2H), 3.17 (d, J = 6.8 Hz, 2H), 2.47-2.44 (m, 2H), 1.99-1.93 (m, 2H), 1.55-1.53 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.4, 145.1, 133.3, 132.4, 131.1, 128.8, 128.4, 128.0, 122.1, 119.6, 117.7, 117.4, 115.7, 94.1, 84.0, 50.1, 40.5, 32.0, 31.3, 23.5; HRMS (ESI) for $C_{24}H_{22}N_2O_2S$ $[M+H]^+$calcd. 403.1475, found. 403.1473.



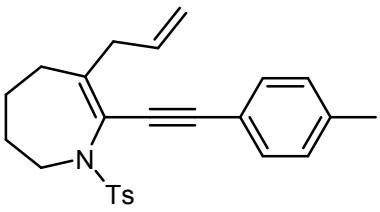
6-Allyl-1-(naphthalen-2-ylsulfonyl)-7-(phenylethynyl)-2,3,4,5-tetrahydro-1*H*-azepine (3na): Isolated yield 56%, 47.8 mg. Light yellow solid, mp 131-133 ^{o}C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.51

(s, 1H), 8.02-7.99 (m, 1H), 7.87-7.83 (m, 2H), 7.76-7.74 (m, 1H), 7.60-7.56 (m, 1H), 7.50-7.46 (m, 1H), 7.22-7.18 (m, 1H), 7.13-7.09 (m, 2H), 6.97-6.95 (m, 2H), 5.82-5.72 (m, 1H), 5.20-5.08 (m, 2H), 3.50-3.49 (m, 2H), 3.19 (d, J = 6.8 Hz, 2H), 2.46-2.44 (m, 2H), 1.98-1.94(m, 2H), 1.52-1.50 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.6, 137.9, 134.6, 133.7, 132.0, 131.1, 129.2, 128.8, 128.7, 128.4, 128.1, 128.0, 127.6, 127.0, 122.8, 122.4, 120.2, 117.4, 93.7, 84.4, 49.8, 40.6, 32.1, 31.1, 23.6; HRMS (ESI) for $C_{27}H_{25}NO_2S$ $[M+H]^+$calcd. 428.1679, found. 428.1686.



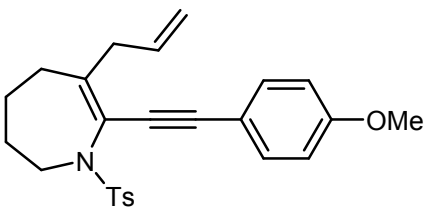
6-Allyl-7-(phenylethynyl)-1-(thiophen-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-azepine (3oa):

Isolated yield 65%, 49.8 mg. Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.71-7.70 (m, 1H), 7.53-7.52 (m, 1H), 7.31-7.29 (m, 5H), 7.01-6.99 (m, 1H), 5.83-5.73 (m, 1H), 5.20-5.09 (m, 2H), 3.45-3.43 (m, 2H), 3.19 (d, J = 6.8 Hz, 2H), 2.43-2.40 (m, 2H), 1.96-1.90 (m, 2H), 1.52-1.50 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.5, 142.8, 138.2, 133.8, 131.3, 129.2, 128.2, 128.1, 127.5, 122.8, 120.4, 117.4, 93.6, 84.8, 49.7, 40.6, 32.1, 31.0, 23.7, 21.4; HRMS (ESI) for $C_{21}H_{21}NO_2S_2$ $[M+H]^+$calcd. 384.1086, found. 384.1084.



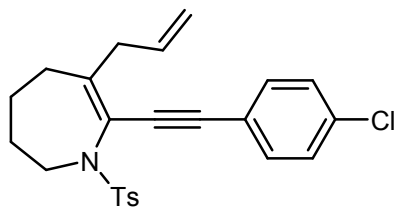
6-Allyl-7-(*p*-tolylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ab):

Isolated yield 68%, 55.1 mg. Light yellow solid, mp 118-120 ^{o}C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.87 (d, J = 8.4 Hz, 2H), 7.20 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 8.8 Hz, 2H), 6.81 (d, J = 8.8 Hz, 2H), 5.82-5.72 (m, 1H), 5.18-5.07 (m, 2H), 3.82 (s, 3H), 3.43-3.41 (m, 2H), 3.16 (d, J = 6.8 Hz, 2H), 2.42-2.39 (m, 2H), 2.38 (s, 3H), 1.94-1.88 (m, 2H), 1.51-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.6, 149.5, 142.8, 138.3, 134.0, 132.8, 129.2, 127.5, 120.6, 117.3, 115.0, 113.8, 93.6, 83.5, 55.3, 49.7, 40.6, 32.0, 31.1, 23.8, 21.5; HRMS (ESI) for $C_{25}H_{27}NO_2S$ $[M+H]^+$calcd. 406.1835, found. 406.1831.



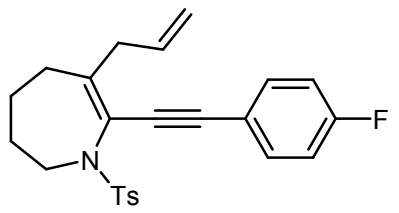
6-Allyl-7-((4-methoxyphenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ac):

Isolated yield 76%, 64.0 mg. Light yellow solid, mp 127-129 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.87 (d, *J* = 8.4 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 8.8 Hz, 2H), 6.81 (d, *J* = 8.8 Hz, 2H), 5.82-5.72 (m, 1H), 5.18-5.07(m, 2H), 3.82 (s, 3H), 3.43-3.41 (m, 2H), 3.16 (d, *J* = 6.8 Hz, 2H), 2.42-2.39 (m, 2H), 2.38 (s, 3H), 1.94-1.88 (m, 2H), 1.51-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.6, 149.5, 142.8, 138.3, 134.0, 132.8, 129.2, 127.5, 120.6, 117.3, 115.0, 113.8, 93.6, 83.5, 55.3, 49.7, 40.6, 32.0, 31.1, 23.8, 21.5; HRMS (ESI) for $C_{25}H_{27}NO_3S$ $[M+H]^+$calcd. 422.1784, found. 422.1788.



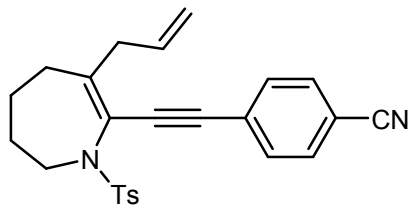
6-Allyl-7-((4-chlorophenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ad):

Isolated yield 64%, 54.4 mg. Light yellow solid, mp 124-126 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.84 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.4 Hz, 2H), 5.81-5.71 (m, 1H), 5.18-5.08 (m, 2H), 3.44-3.42 (m, 2H), 3.16 (d, *J* = 7.2 Hz, 2H), 2.45-2.39 (m, 2H), 2.37 (s, 3H), 1.93-1.87 (m, 2H), 1.51-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.0, 142.9, 138.2, 134.2, 133.6, 132.4, 129.2, 128.4, 127.4, 121.3, 120.1, 117.5, 92.4, 85.8, 49.7, 40.6, 32.1, 31.0, 23.6, 21.4; HRMS (ESI) for $C_{24}H_{24}ClNO_2S$ $[M+H]^+$calcd. 426.1289, found. 426.1293.



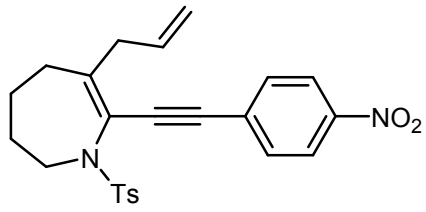
6-Allyl-7-((4-fluorophenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ae):

Isolated yield 53%, 43.3 mg. Light yellow solid, mp 116-118 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.85 (d, *J* = 8.0 Hz, 2H), 7.21-7.16 (m, 4H), 6.97 (t, *J* = 8.8 Hz, 2H), 5.81-5.71 (m, 1H), 5.18- 5.08 (m, 2H), 3.44-3.42 (m, 2H), 3.16 (d, *J* = 6.8 Hz, 2H), 2.42-2.39 (m, 2H), 2.37 (s, 3H), 1.92-1.88 (m, 2H), 1.51-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.7, 161.2, 150.6, 142.9, 138.3, 133.8, 133.2, 133.1, 129.2, 127.5, 120.3, 118.9, 117.4, 115.6, 115.3, 92.5, 84.5, 84.5, 49.7, 40.7, 32.1, 31.0, 23.7, 21.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -110.8; HRMS (ESI) for $C_{24}H_{24}FNO_2S$ $[M+H]^+$calcd. 410.1585, found. 410.1591.



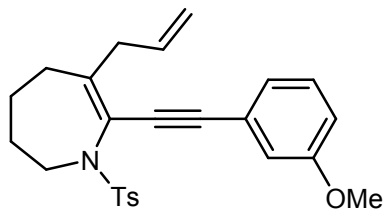
4-((3-Allyl-1-tosyl-4,5,6,7-tetrahydro-1*H*-azepin-2-yl)ethynyl)benzonitrile (3af):

Isolated yield 42%,35.0 mg. Light yellow solid, mp 133-135 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.83 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 5.80-5.70 (m, 1H), 5.19-5.11 (m, 2H), 3.47-3.45 (m, 2H), 3.17 (d, *J* = 6.8 Hz, 2H), 2.40-2.38 (m, 2H), 2.39 (s, 3H), 1.93-1.87 (m, 2H), 1.51-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 152.9, 143.1, 138.3, 133.3, 131.8, 131.7, 129.3, 127.7, 127.4, 119.9, 118.4, 117.8, 111.4, 91.8, 89.4, 49.8, 40.7, 32.2, 30.8, 23.5, 21.5; HRMS (ESI) for $C_{25}H_{24}N_2O_2S$ $[M+H]^+$calcd. 417.1631, found. 417.1626.



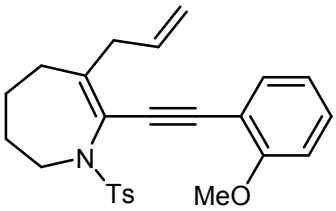
6-Allyl-7-((4-nitrophenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ag):

Isolated yield 34%, 29.7 mg. Light yellow solid, mp 141-143 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.15 (d, *J* = 8.8 Hz, 2H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.8 Hz, 2H), 7.24 (d, *J* = 7.6 Hz, 2H), 5.81-5.71 (m, 1H), 5.20-5.12 (m, 2H), 3.48-3.46 (m, 2H), 3.18 (d, *J* = 6.8 Hz, 2H), 2.41-2.38 (m, 2H), 2.40 (s, 3H), 1.93-1.88 (m, 2H), 1.52-1.50 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.4, 146.9, 143.2, 138.3, 133.3, 131.8, 129.7, 129.3, 127.4, 123.4, 119.8, 117.8, 91.6, 90.3, 49.8, 40.8, 32.3, 30.8, 23.5, 21.5; HRMS (ESI) for $C_{24}H_{24}N_2O_4S$ $[M+H]^+$calcd. 437.1530, found. 437.1539.



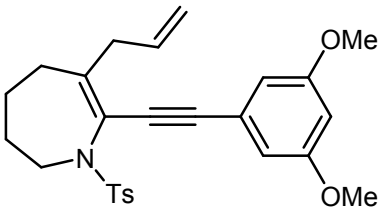
6-Allyl-7-((3-methoxyphenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ah):

Isolated yield 72%, 60.6 mg. Light yellow solid, mp 122-124 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.86 (d, *J* = 8.4 Hz, 2H), 7.22-7.17 (m, 3H), 6.87-6.79 (m, 2H), 6.78-6.72 (m, 1H), 5.82-5.72 (m, 1H), 5.19-5.08 (m, 2H), 3.79 (s, 3H), 3.44-3.42 (m, 2H), 3.18 (d, *J* = 6.8 Hz, 2H), 2.44-2.40 (m, 2H), 2.37 (s, 3H), 1.94-1.88 (m, 2H), 1.51-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.1, 150.6, 142.9, 138.2, 133.8, 129.2, 129.2, 127.5, 123.9, 123.8, 120.3, 117.4, 116.3, 114.5, 93.5, 84.5, 55.2, 49.7, 40.6, 32.1, 31.0, 23.7, 21.4; HRMS (ESI) for $C_{25}H_{27}NO_3S$ $[M+H]^+$calcd. 422.1784, found. 422.1786.



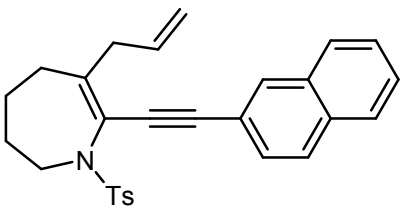
6-Allyl-7-((2-methoxyphenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ai):

Isolated yield 60%, 50.5 mg. Light yellow solid, mp 114-116 (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.92 (d, *J* = 8.4 Hz, 2H), 7.28-7.20 (m, 3H), 7.07-7.05 (m, 1H), 6.88-6.83 (m, 2H), 5.86-5.76 (m, 1H), 5.21-5.06 (m, 2H), 3.82 (s, 3H), 3.40-3.38 (m, 2H), 3.25 (d, *J* = 6.8 Hz, 2H), 2.44-2.41 (m, 2H), 2.38 (s, 3H), 1.94-1.88(m, 2H), 1.51-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.9, 150.4, 142.7, 138.1, 134.2, 132.7, 129.6, 129.2, 127.7, 120.6, 120.2, 117.1, 112.3, 110.5, 90.1, 89.0, 55.6, 49.5, 40.7, 32.1, 31.0, 23.8, 21.5; HRMS (ESI) for $C_{25}H_{27}NO_3S$ $[M+H]^+$calcd. 422.1784, found. 422.1781.



6-Allyl-7-((3,5-dimethoxyphenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3aj):

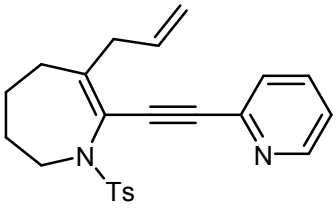
Isolated yield 67%, 60.5 mg. Light yellow solid, mp 136-138 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.86 (d, *J* = 8.4 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 6.42 (t, *J* = 2.4 Hz, 1H), 6.36 (d, *J* = 2.4 Hz, 2H), 5.82-5.72 (m, 1H), 5.19-5.09 (m, 2H), 3.77 (s, 6H), 3.43-3.41 (m, 2H), 3.17 (d, *J* = 6.8 Hz, 2H), 2.43-2.40 (m, 2H), 2.37 (s, 3H), 1.94-1.88 (m, 2H), 1.51-1.49 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 160.4, 150.7, 142.9, 138.2, 133.8, 129.2, 127.5, 124.1, 120.3, 117.4, 109.2, 101.4, 93.6, 84.3, 55.4, 49.7, 40.6, 32.1, 31.0, 23.7, 21.4; HRMS (ESI) for $C_{26}H_{29}NO_4S$ $[M+H]^+$calcd. 452.1890, found. 452.1895.



6-Allyl-7-(naphthalen-2-ylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ak):

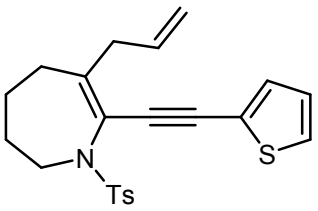
Isolated yield 52%, 45.9 mg. Light yellow solid, mp 128-130 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.90 (d, *J* = 8.4 Hz, 2H), 7.81-7.79 (m, 1H), 7.75-7.72 (m, 2H), 7.68 (s, 1H), 7.50-7.47 (m, 2H), 7.25-7.20 (m, 3H), 5.86-5.75 (m, 1H), 5.22-5.10 (m, 2H), 3.48-3.46 (m, 2H), 3.23 (d, *J* = 6.8 Hz, 2H), 2.46-2.43 (m, 2H), 2.35 (s, 3H), 1.96-1.91 (m, 2H), 1.53-1.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.6, 142.9, 138.4, 133.9, 132.8, 132.7, 131.2, 129.3, 128.0, 127.7, 127.6, 127.5, 126.7, 126.6, 120.4, 120.1, 117.4,

110.0, 94.0, 85.1, 49.8, 40.7, 32.1, 31.1, 23.7, 21.5; HRMS (ESI) for $C_{28}H_{27}NO_2S$ $[M+H]^+$calcd. 442.1835, found. 442.1833.



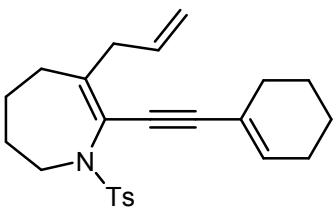
6-Allyl-7-(pyridin-2-ylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3al):

Isolated yield 48%, 37.7 mg. Light yellow solid, mp 113-115 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.58-8.57 (m, 1H), 7.91 (d, *J* = 8.4 Hz, 2H), 7.64-7.60 (m, 1H), 7.22-7.19 (m, 4H), 5.81-5.71 (m, 1H), 5.19-5.09 (m, 2H), 3.41-3.39 (m, 2H), 3.22 (d, *J* = 6.8 Hz, 2H), 2.40-2.37 (m, 2H), 2.35 (s, 3H), 1.92-1.87 (m, 2H), 1.49-1.47 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 152.8, 149.9, 143.1, 143.0, 137.8, 135.9, 133.6, 129.3, 127.7, 127.1, 122.7, 119.8, 117.6, 92.5, 84.7, 49.5, 40.7, 32.1, 30.8, 23.6, 21.4; HRMS (ESI) for $C_{23}H_{24}N_2O_2S$ $[M+H]^+$calcd. 393.1631, found. 393.1627.



6-Allyl-7-(thiophen-2-ylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3am):

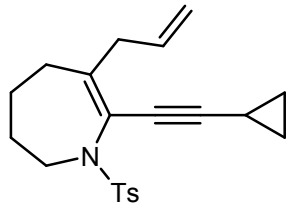
Isolated yield 70%, 55.6 mg. Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.86 (d, *J* = 8.4 Hz, 2H), 7.27-7.25 (m, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.04-7.03 (m, 1H), 6.98-6.95 (m, 1H), 5.81-5.71 (m, 1H), 5.19-5.08 (m, 2H), 3.40-3.38 (m, 2H), 3.15 (d, *J* = 6.8 Hz, 2H), 2.44-2.41 (m, 2H), 2.38 (s, 3H), 1.94-1.89 (m, 2H), 1.51-1.49(m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.9, 143.0, 138.0, 133.7, 131.8, 129.3, 127.5, 127.4, 126.9, 122.8, 120.2, 117.5, 88.3, 86.8, 49.6, 40.7, 32.2, 31.0, 23.7, 21.5; HRMS (ESI) for $C_{22}H_{23}NO_2S_2$ $[M+H]^+$calcd. 398.1243, found. 398.1238.



6-Allyl-7-(cyclohex-1-en-1-ylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3an):

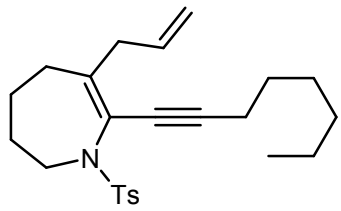
Isolated yield 55%, 43.4 mg. Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.86 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 5.91-5.89 (m, 1H), 5.78-5.68 (m, 1H), 5.15-5.05 (m, 2H), 3.35-3.33 (m, 2H), 3.09 (d, *J* = 6.8 Hz, 2H), 2.41 (s, 3H), 2.37-2.35 (m, 2H), 2.10-2.07 (m, 2H), 2.01-1.98 (m, 2H), 1.90-1.84 (m, 2H), 1.63-1.55 (m, 4H), 1.47-1.45 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.0, 142.7, 138.2, 134.9, 134.0, 129.1, 127.5, 120.6, 120.4, 117.1,

95.5, 82.2, 49.5, 40.6, 31.9, 30.9, 28.8, 25.7, 23.7, 22.2, 21.4, 21.4; HRMS (ESI) for $C_{24}H_{29}NO_2S$ $[M+H]^+$calcd. 396.1992, found. 396.1988.



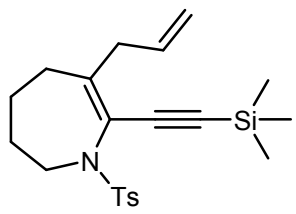
6-Allyl-7-(cyclopropylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ao):

Isolated yield 48%, 34.0 mg. Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.84 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 5.76-5.66 (m, 1H), 5.13-5.04 (m, 2H), 3.33-3.31 (m, 2H), 3.05 (d, *J* = 6.8 Hz, 2H), 2.42 (s, 3H), 2.33-2.30 (m, 2H), 1.88-1.82 (m, 2H), 1.45-1.43 (m, 2H), 1.28-1.21 (m, 1H), 0.78-0.73 (m, 2H), 0.59-0.55 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.4, 142.8, 138.3, 134.2, 129.1, 127.6, 120.6, 117.0, 97.8, 71.2, 49.5, 40.4, 31.8, 30.9, 23.7, 21.5, 8.4, 0.1; HRMS (ESI) for $C_{21}H_{25}NO_2S$ $[M+H]^+$calcd. 356.1679, found. 356.1680.



6-Allyl-7-(oct-1-yn-1-yl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ap):

Isolated yield 53%, 42.3 mg. Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.84 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 5.77-5.67 (m, 1H), 5.14-5.04 (m, 2H), 3.34-3.32 (m, 2H), 3.06 (d, *J* = 6.8 Hz, 2H), 2.41 (s, 3H), 2.34-2.31 (m, 2H), 2.17 (t, *J* = 7.2 Hz, 2H), 1.89-1.83 (m, 2H), 1.45-1.38 (m, 4H), 1.34-1.23 (m, 6H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.0, 142.7, 138.3, 134.2, 129.0, 127.6, 120.7, 116.9, 94.9, 75.8, 49.5, 40.4, 31.7, 31.3, 31.0, 28.6, 28.4, 23.7, 22.5, 21.5, 19.5, 14.0; HRMS (ESI) for $C_{24}H_{33}NO_2S$ $[M+H]^+$calcd. 400.2305, found. 400.2299.



6-Allyl-1-tosyl-7-((trimethylsilyl)ethynyl)-2,3,4,5-tetrahydro-1*H*-azepine (3aq):

Isolated yield 45%, 34.8 mg. Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.88 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.0 Hz, 2H), 5.79-5.69 (m, 1H), 5.16-5.06 (m, 2H), 3.31-3.29 (m, 2H), 3.11 (d, *J* = 6.8 Hz, 2H), 2.42 (s, 3H), 2.40-2.38 (m, 2H), 1.91-1.85 (m, 2H), 1.48-1.46 (m, 2H), 0.13 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.7, 142.9, 138.0, 133.7, 129.1, 127.7, 120.4, 117.3,

99.7, 98.8, 49.3, 40.8, 32.1, 30.9, 23.7, 21.5, -0.2; HRMS (ESI) for $C_{21}H_{29}NO_2SSi$ $[M+H]^+$calcd. 388.1761, found. 388.1768.

(E) Reference

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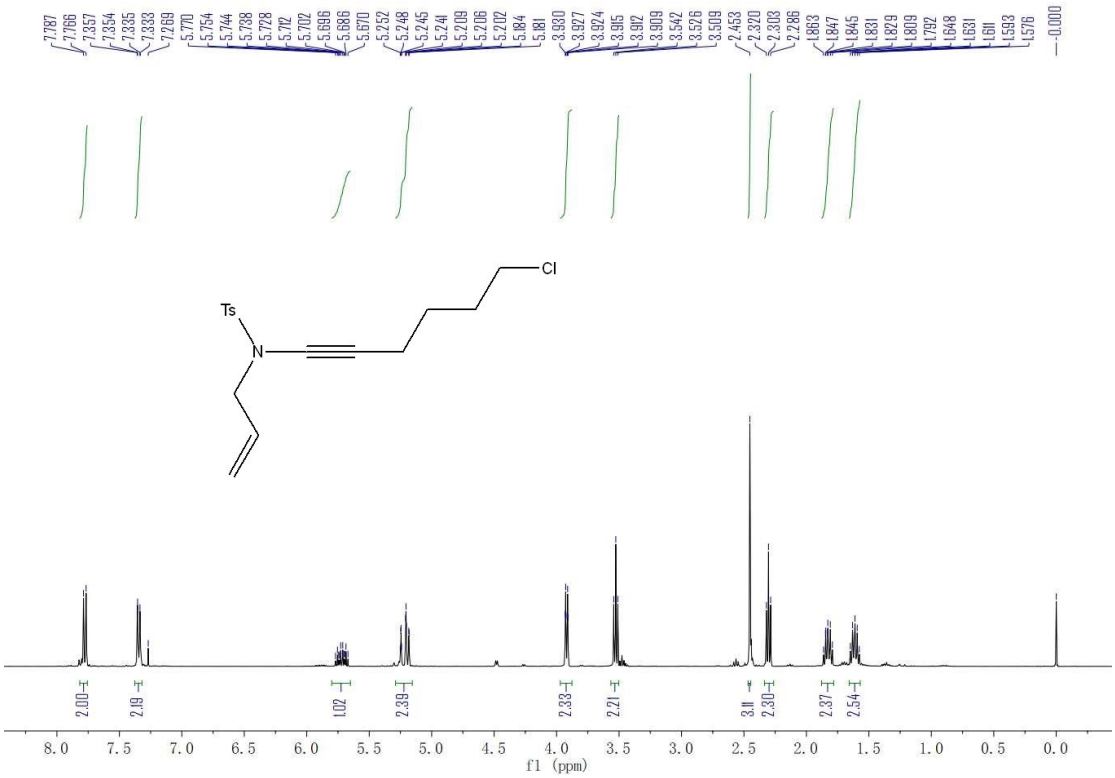
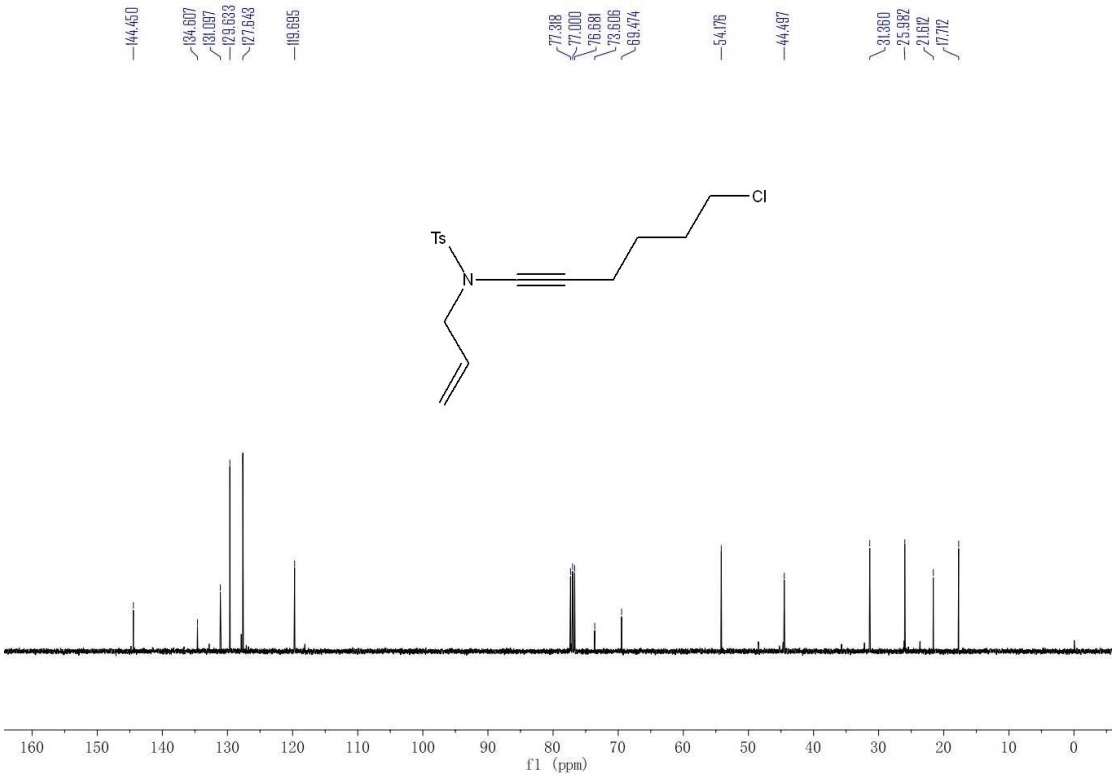
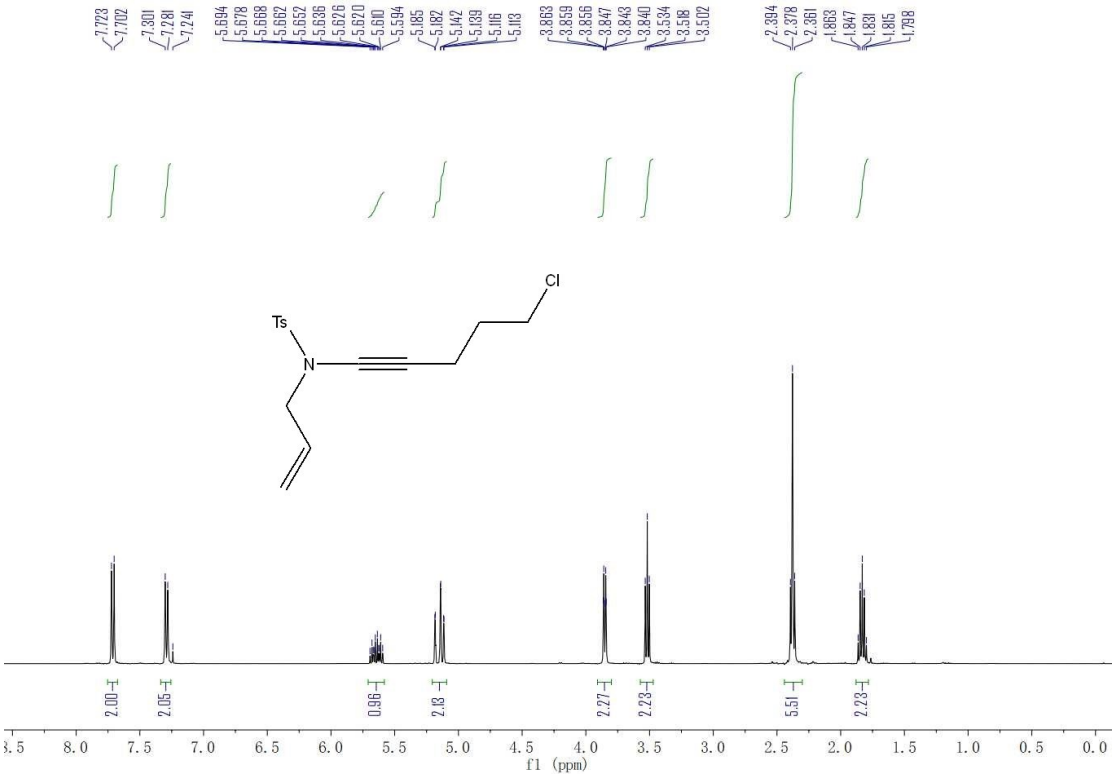
(F) Spectra

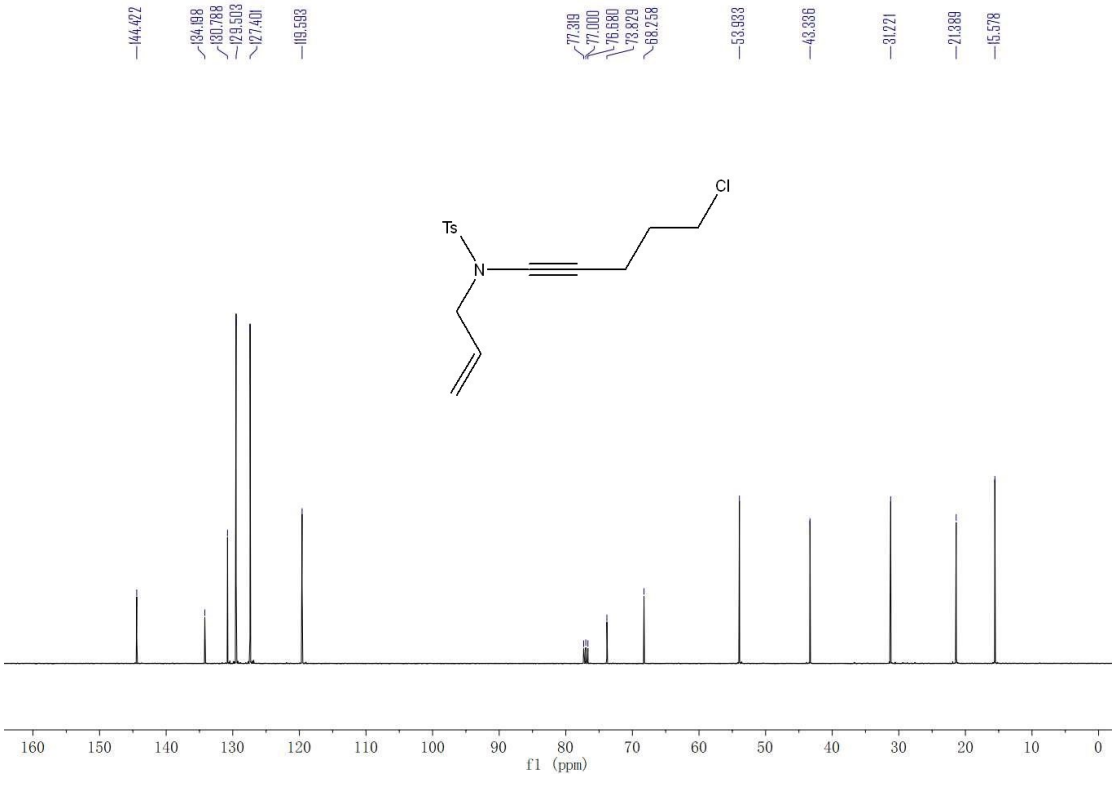
N-allyl-*N*-(6-chlorohex-1-yn-1-yl)-4-methylbenzenesulfonamide (1a)



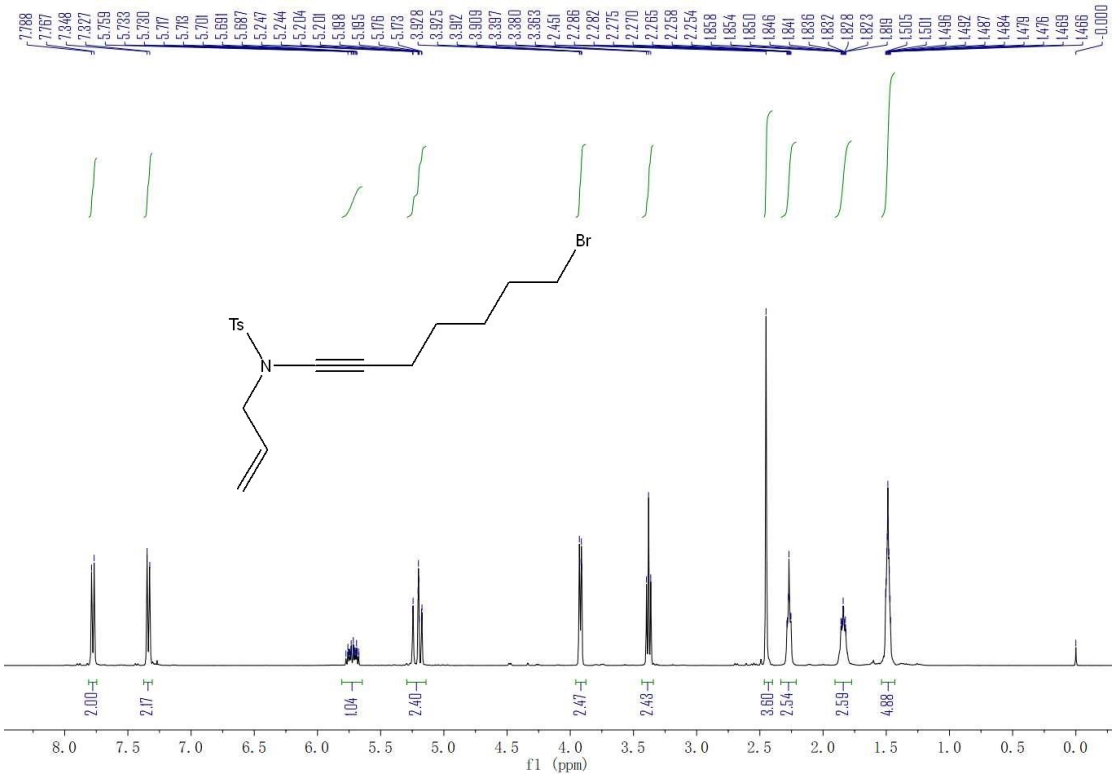


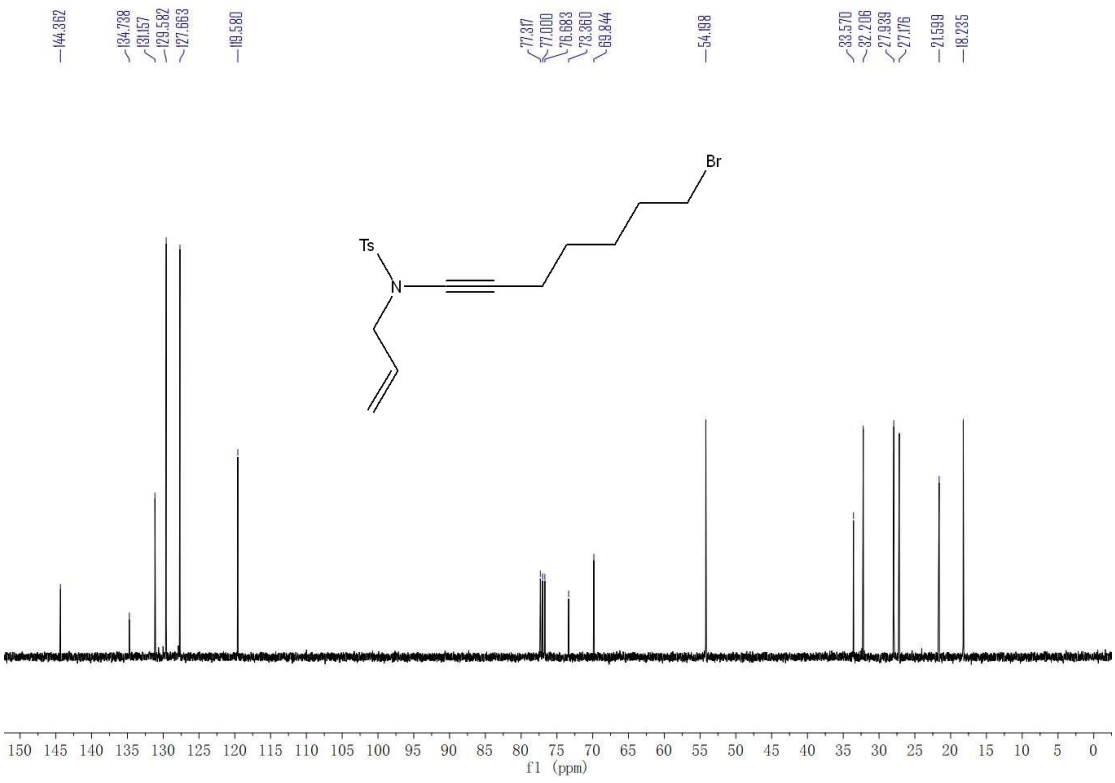
N-allyl-*N*-(5-chloropent-1-yn-1-yl)-4-methylbenzenesulfonamide (1b)



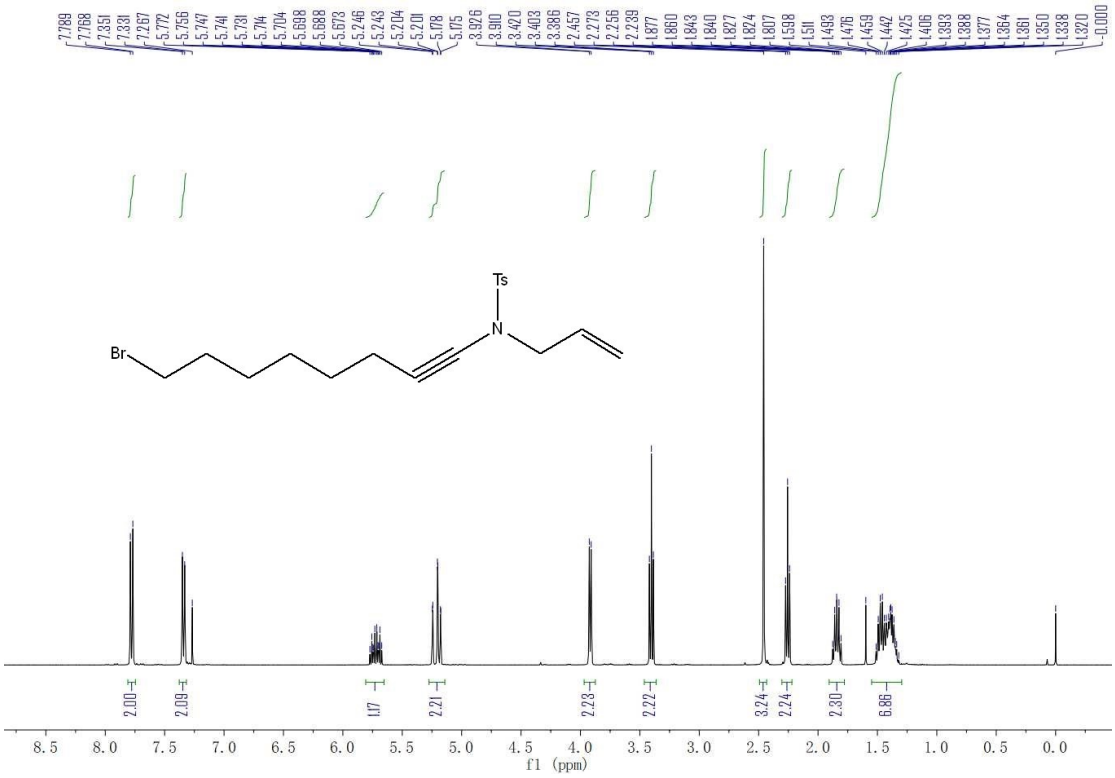


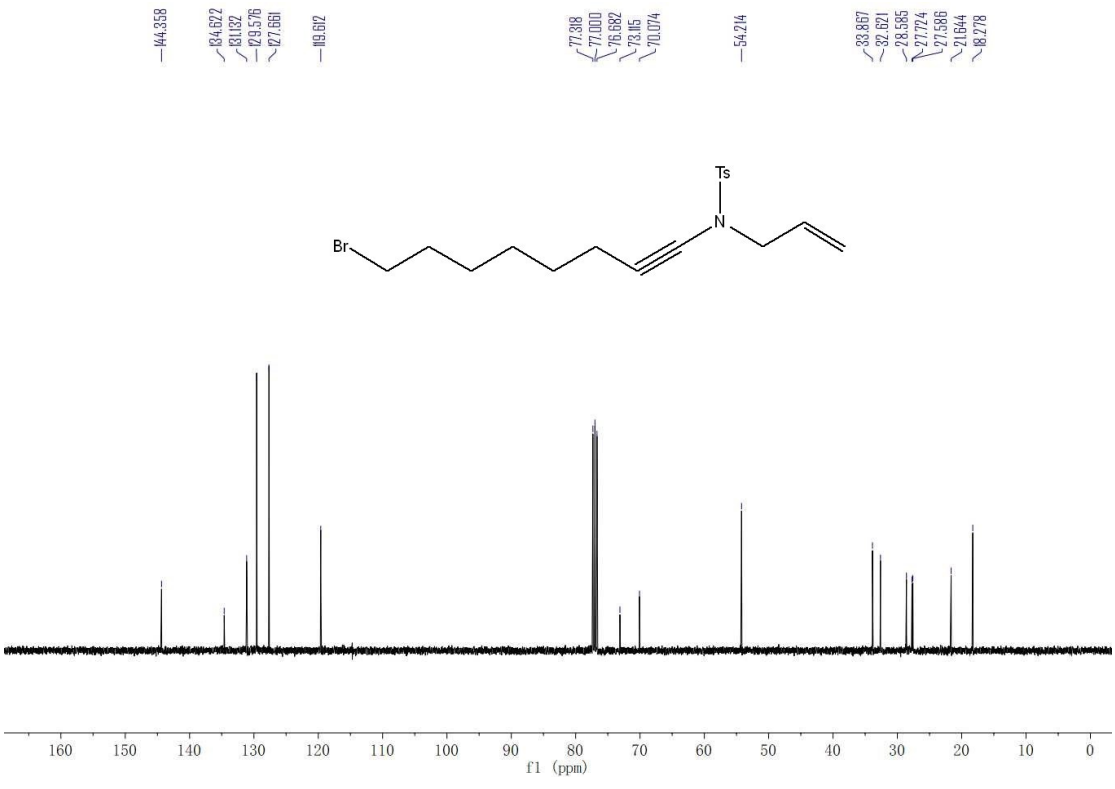
N-allyl-*N*-(7-bromohept-1-yn-1-yl)-4-methylbenzenesulfonamide (1c)



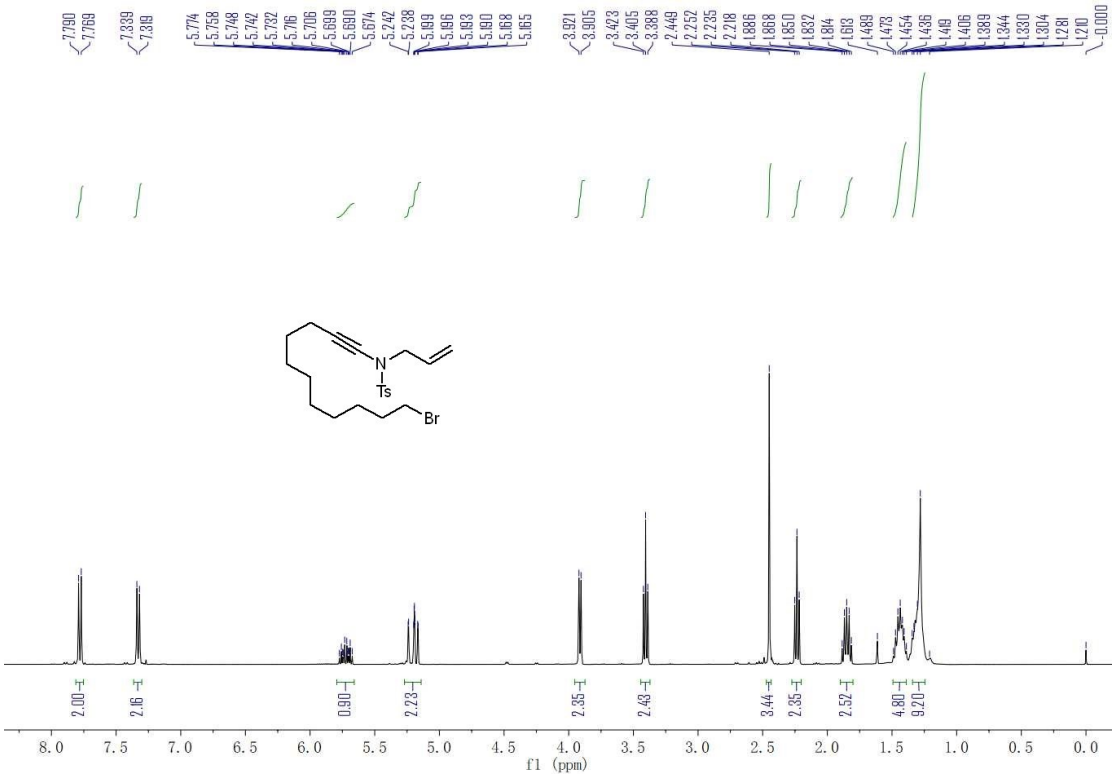


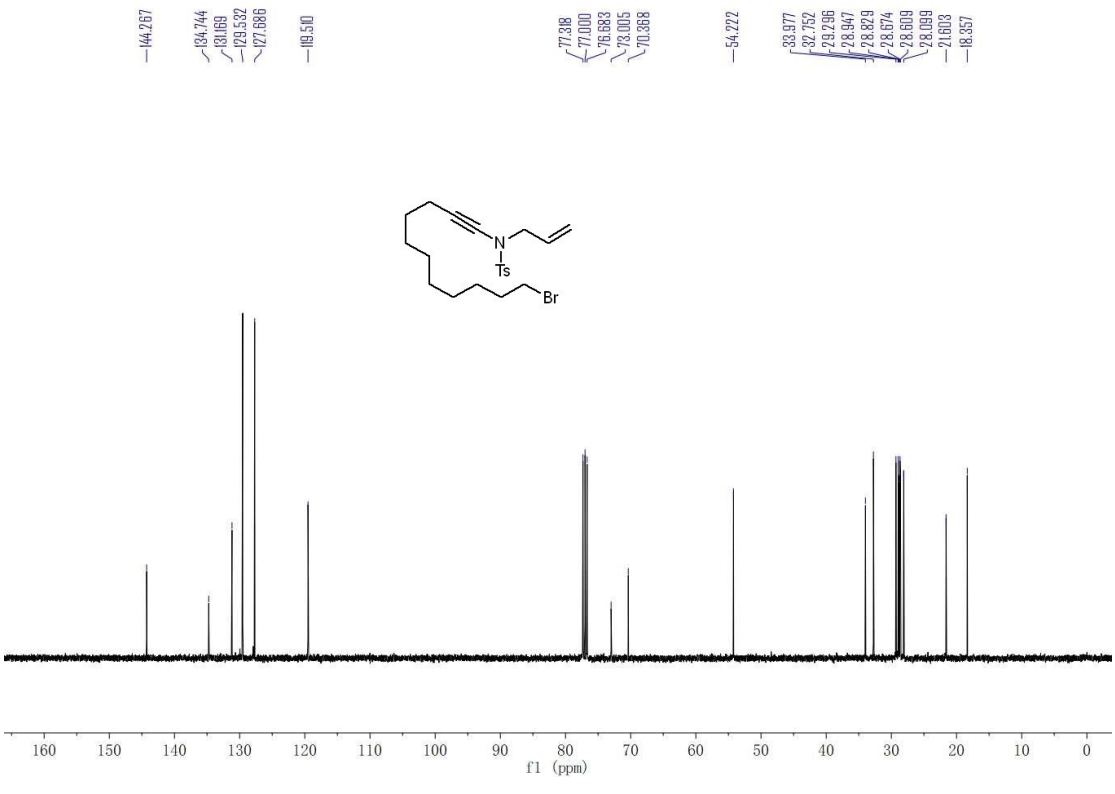
N-allyl-N-(8-bromooct-1-yn-1-yl)-4-methylbenzenesulfonamide (1d)



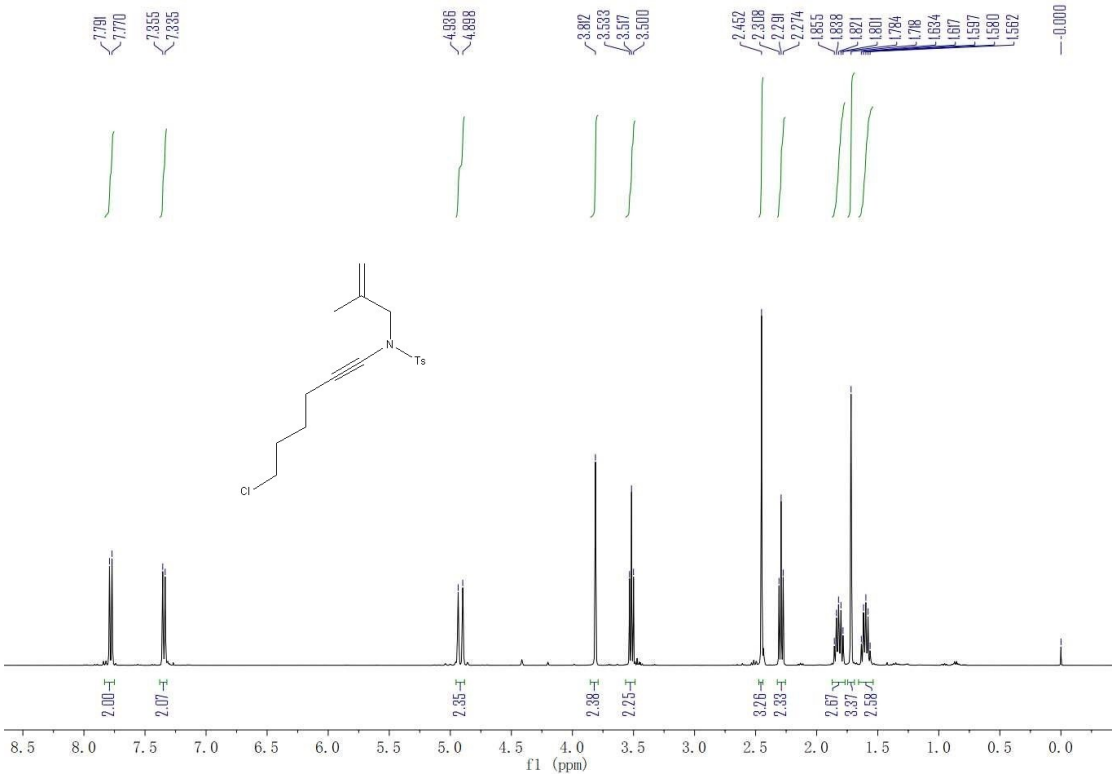


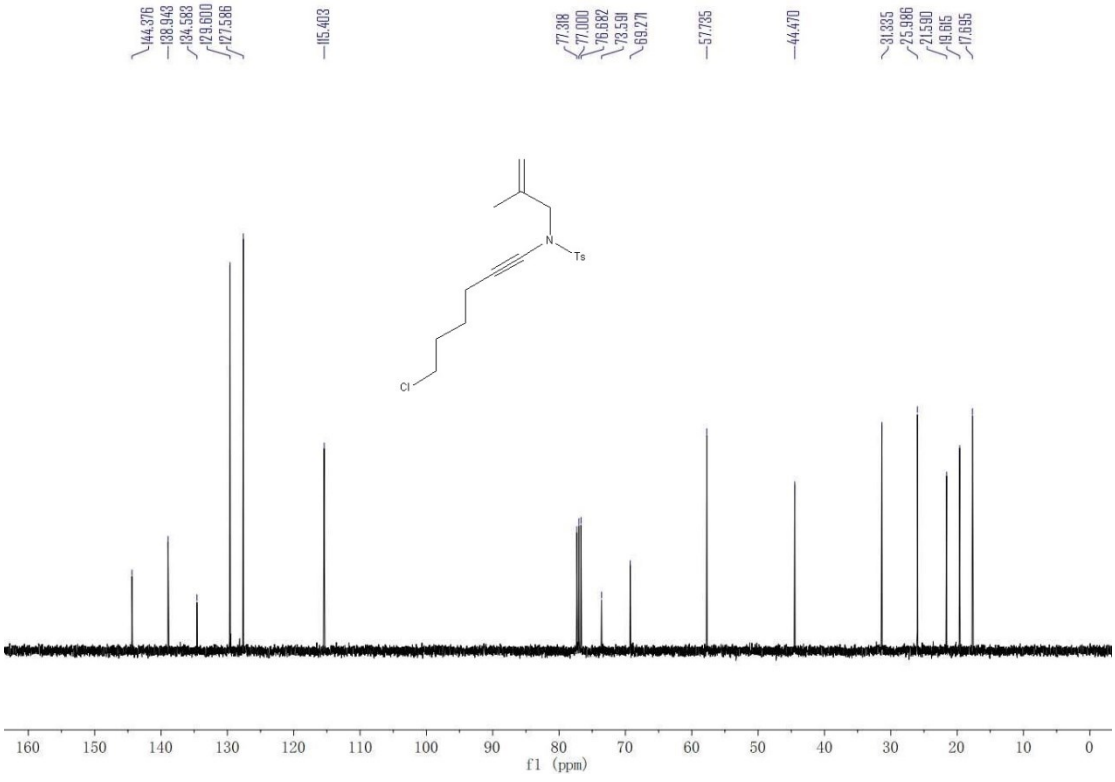
N-allyl-*N*-(11-bromoundec-1-yn-1-yl)-4-methylbenzenesulfonamide (1e)



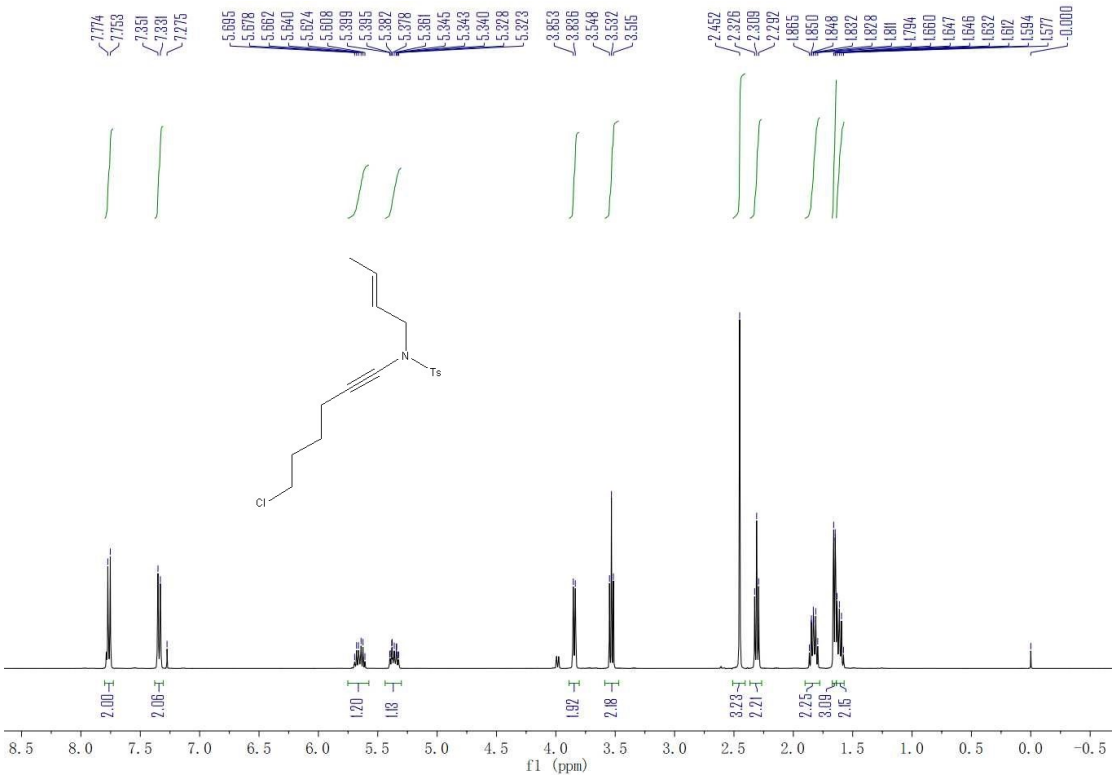


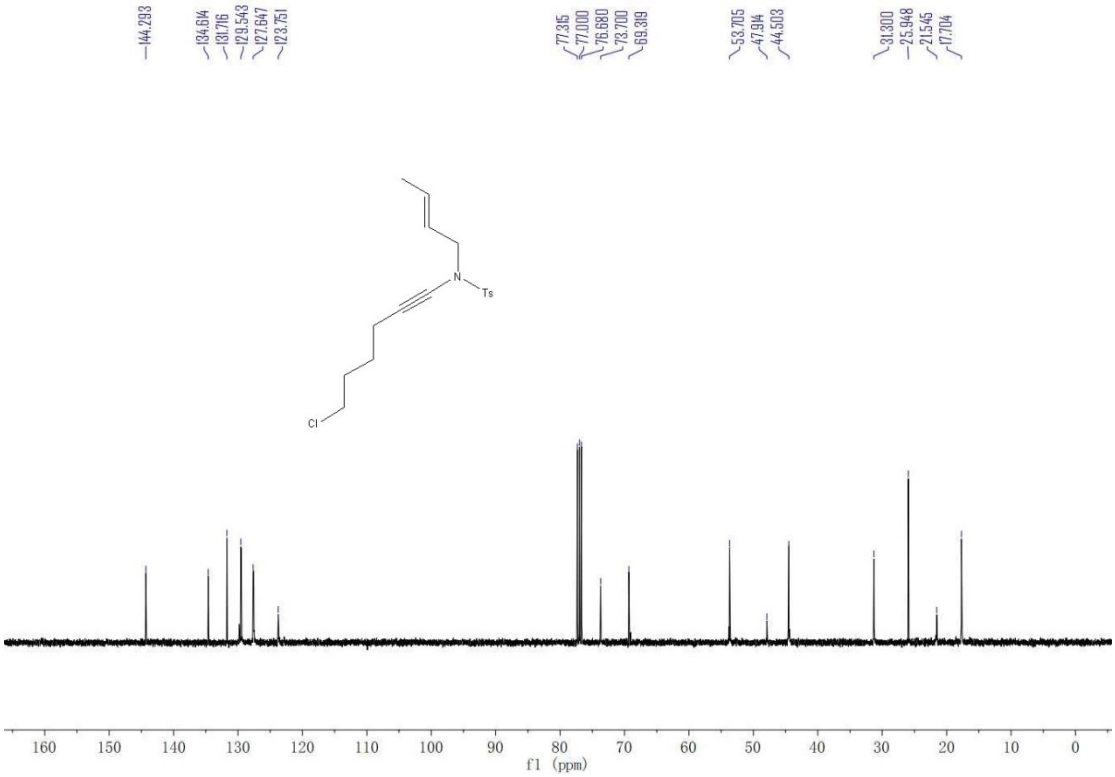
N-(6-chlorohex-1-yn-1-yl)-4-methyl-*N*-(2-methylallyl)benzenesulfonamide (1f)



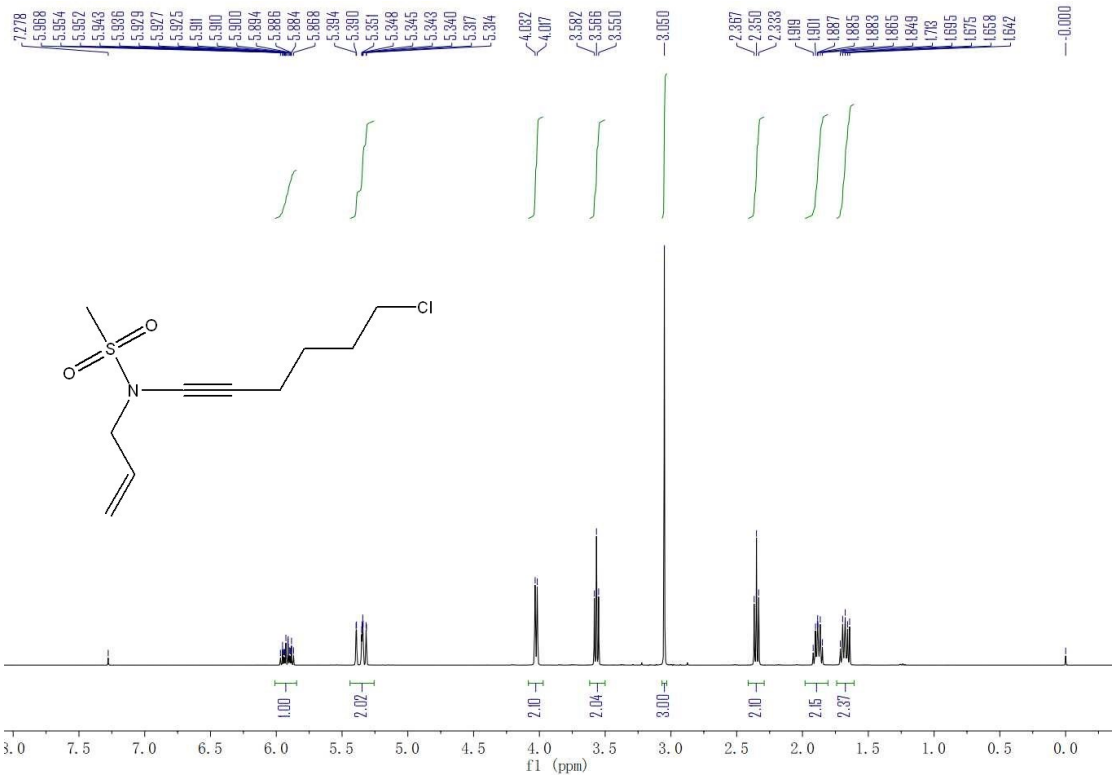


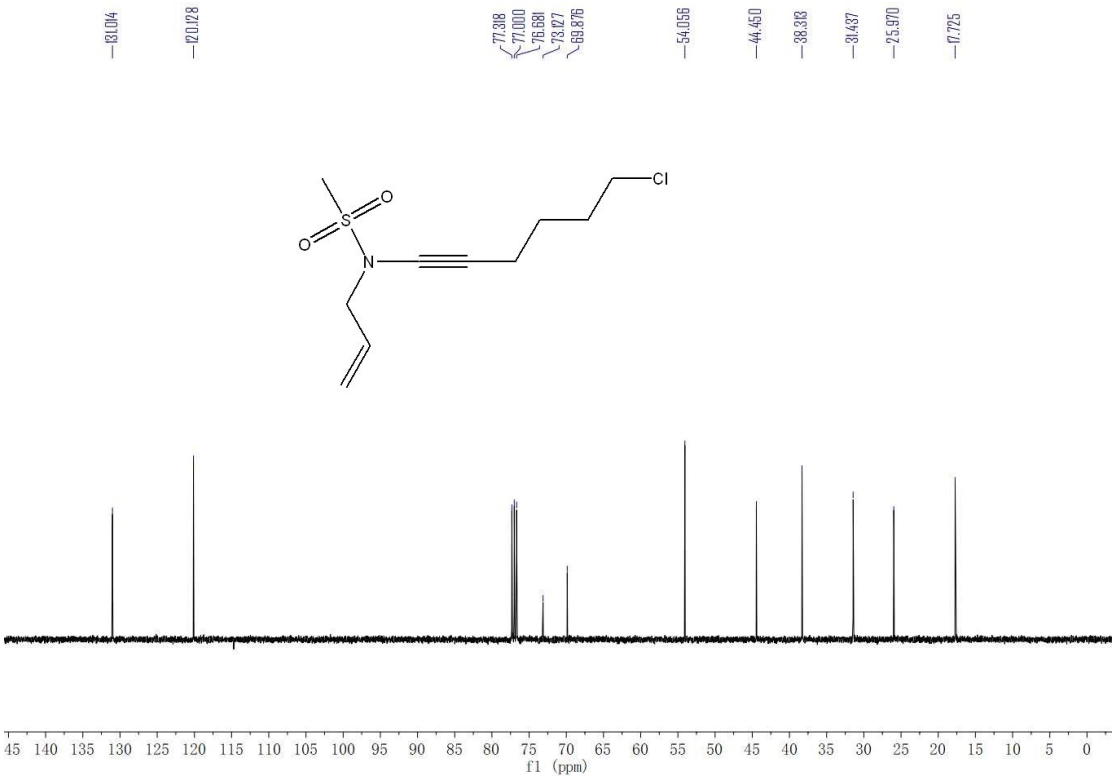
***(E)*-*N*-(but-2-en-1-yl)-*N*-(6-chlorohex-1-yn-1-yl)-4-methylbenzenesulfonamide (1g)**



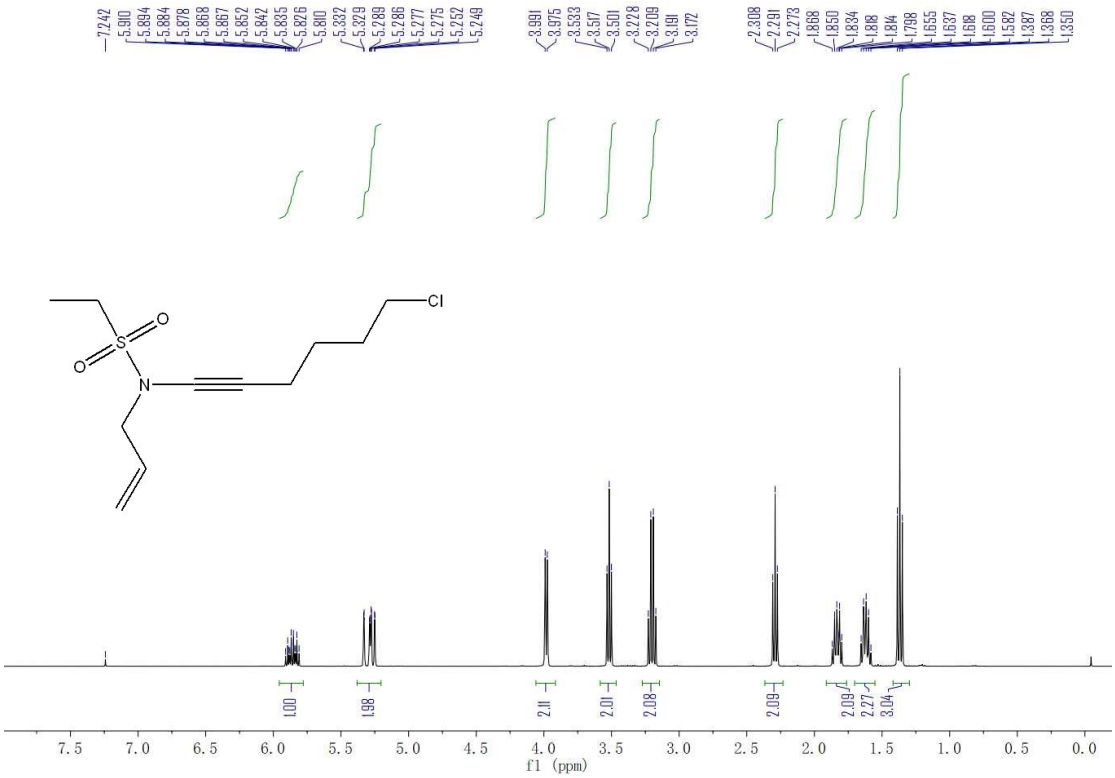


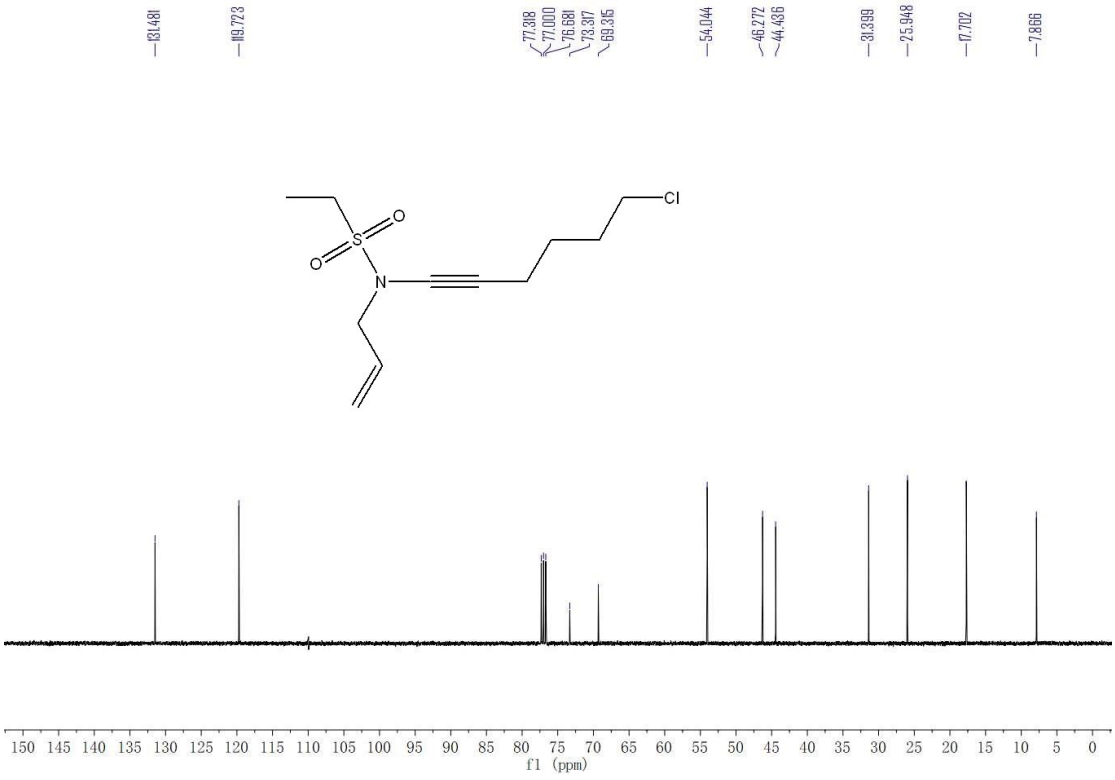
***N*-allyl-*N*-(6-chlorohex-1-yn-1-yl)methanesulfonamide (1h)**



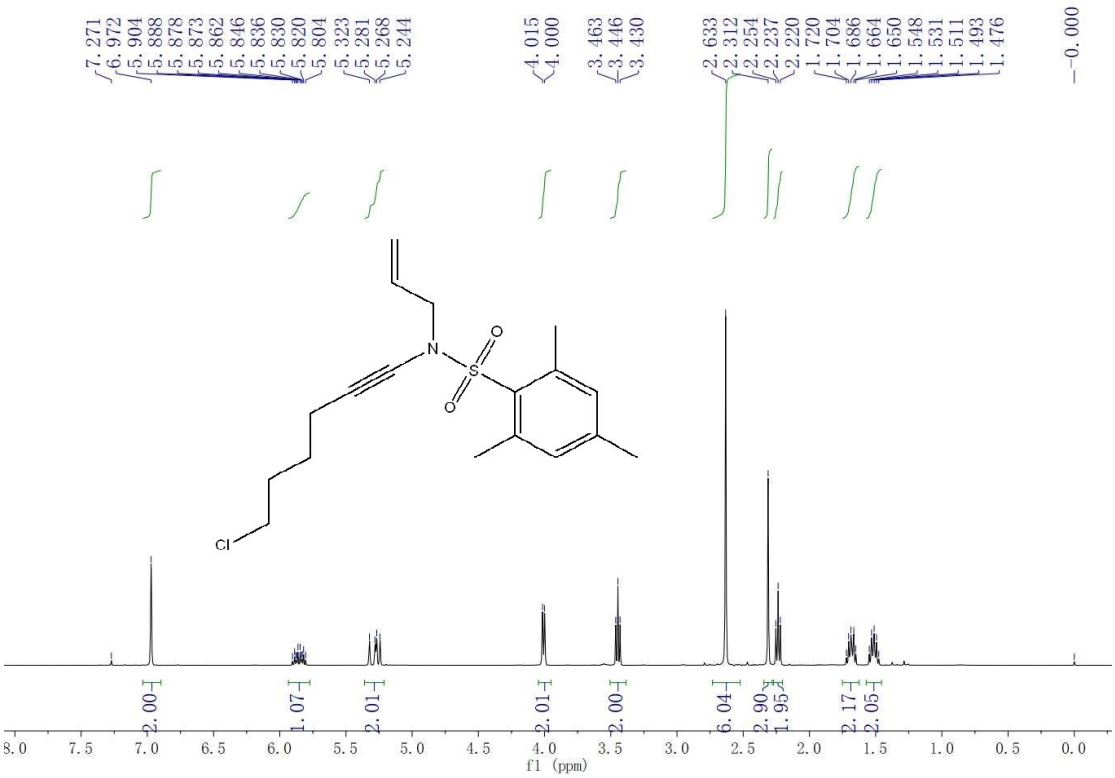


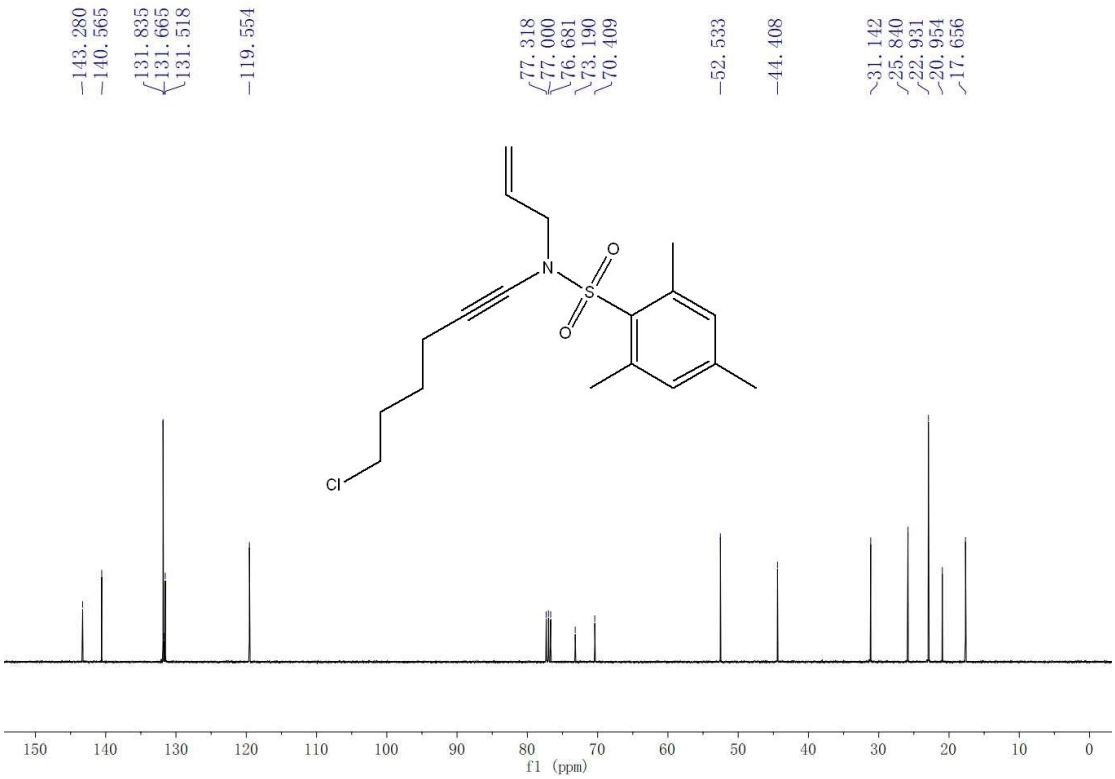
_N_-allyl-_N_-(6-chlorohex-1-yn-1-yl)ethanesulfonamide (1i)



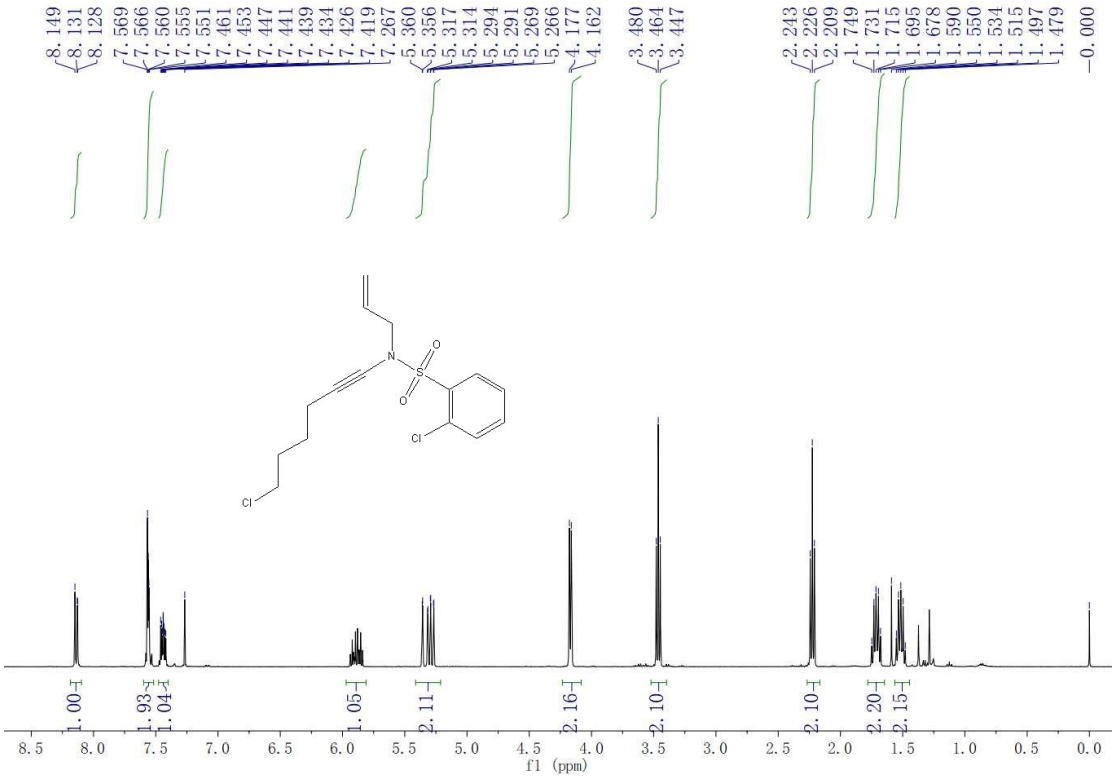


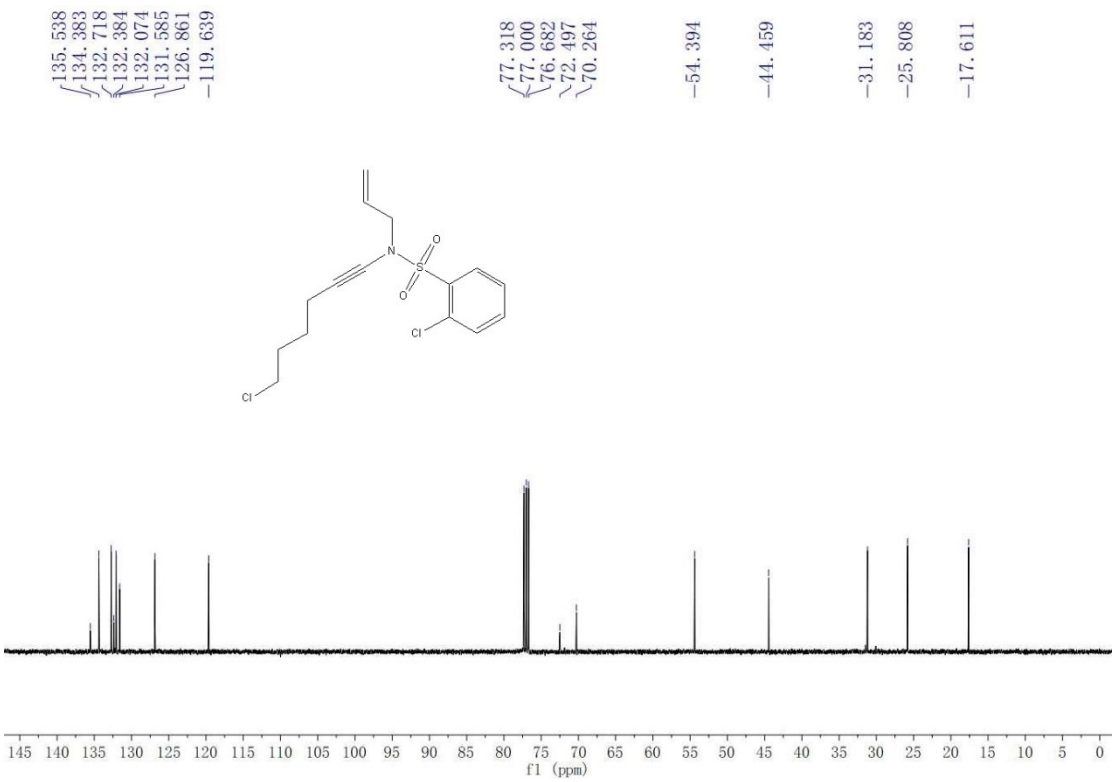
_N_-allyl-_N_-(6-chlorohex-1-yn-1-yl)-2,4,6-trimethylbenzenesulfonamide (1j)



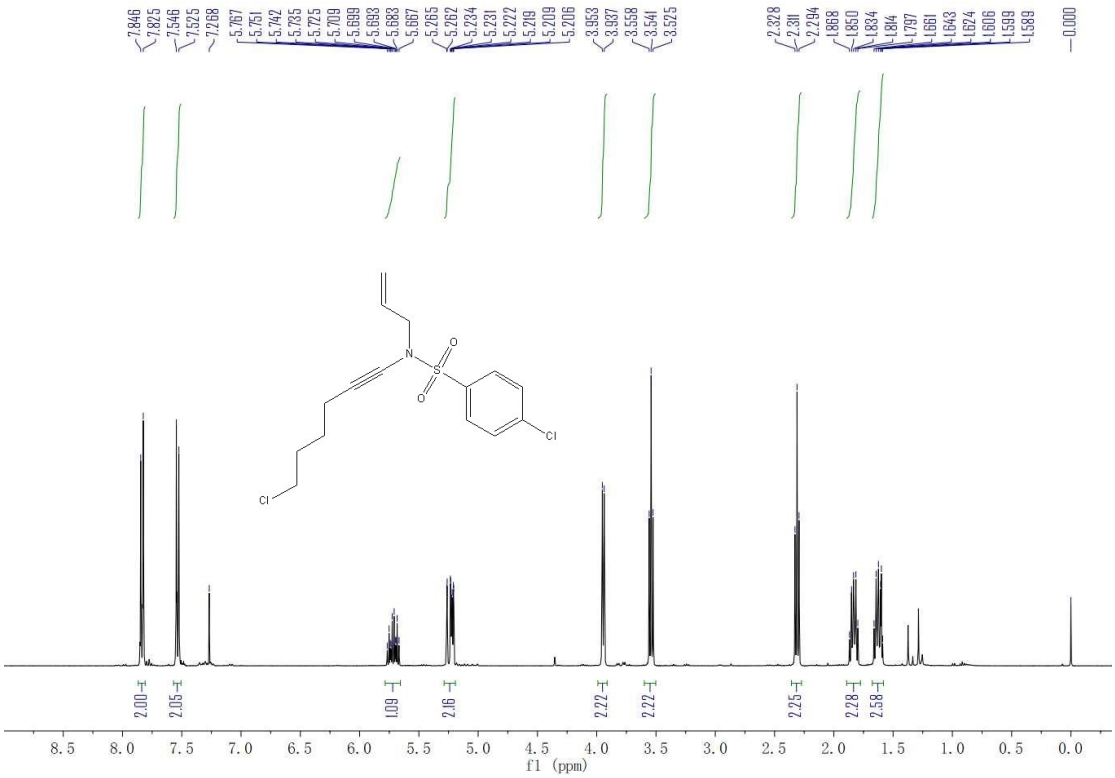


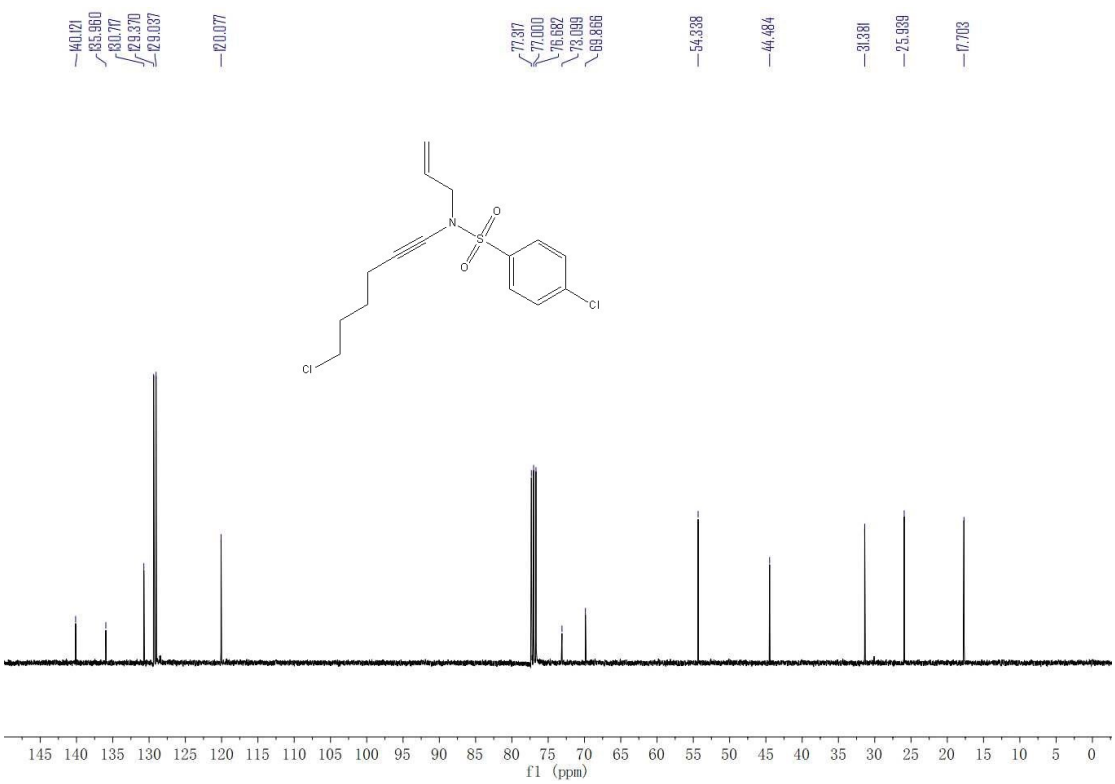
_N_-allyl-2-chloro-_N_-(6-chlorohex-1-yn-1-yl)benzenesulfonamide (1k)



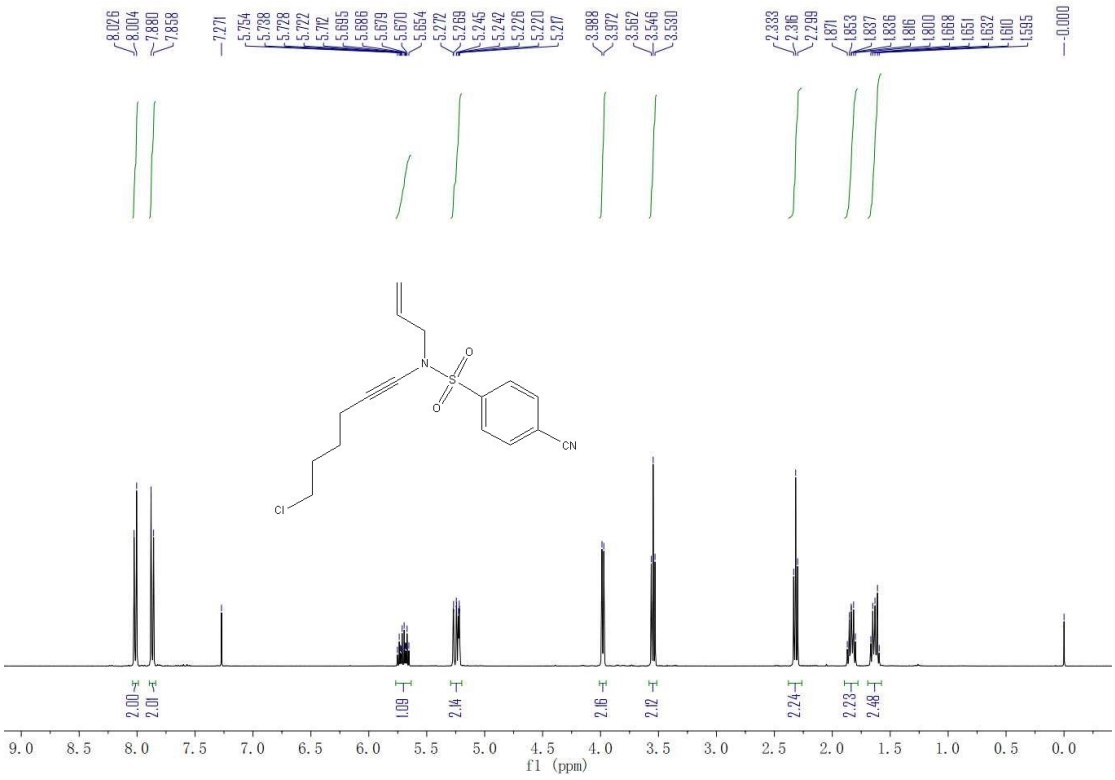


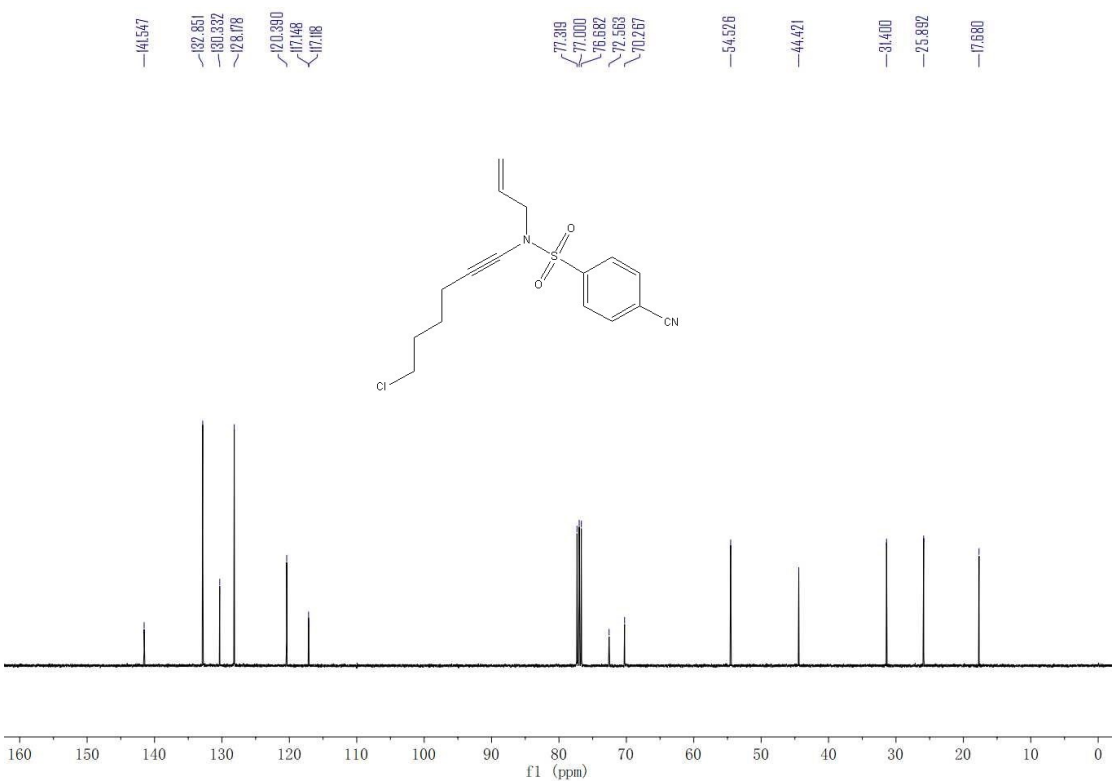
_N_-allyl-4-chloro-_N_-(6-chlorohex-1-yn-1-yl)benzenesulfonamide (1l)



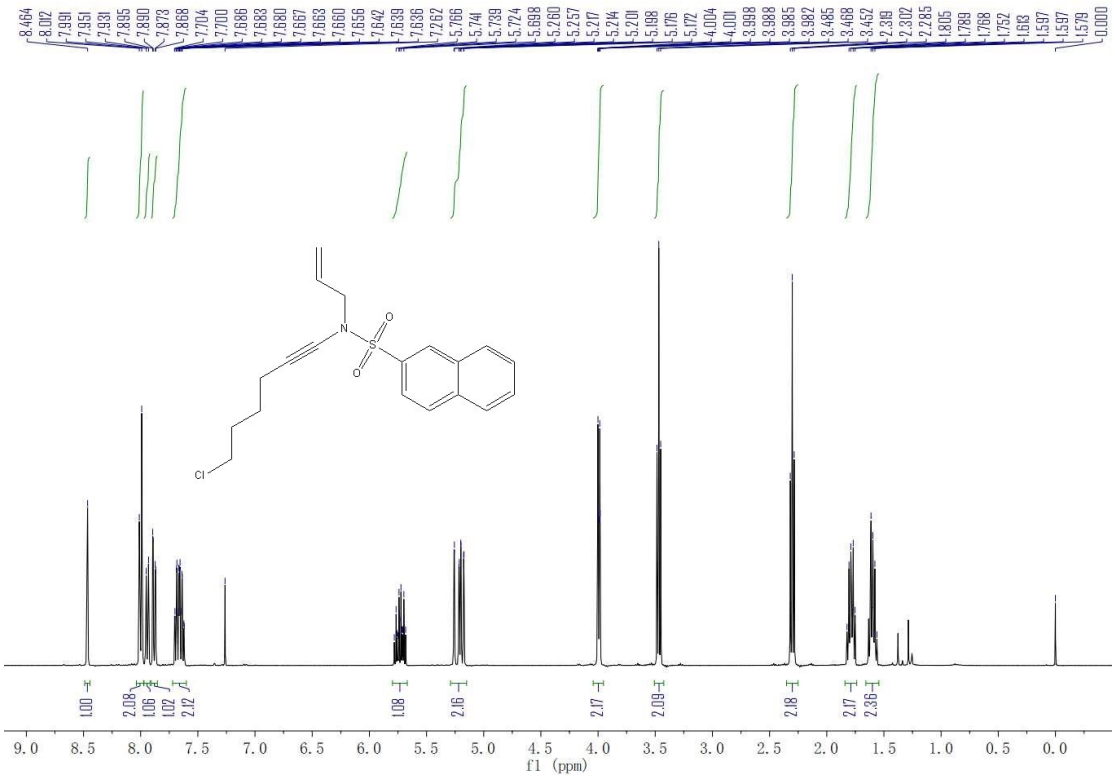


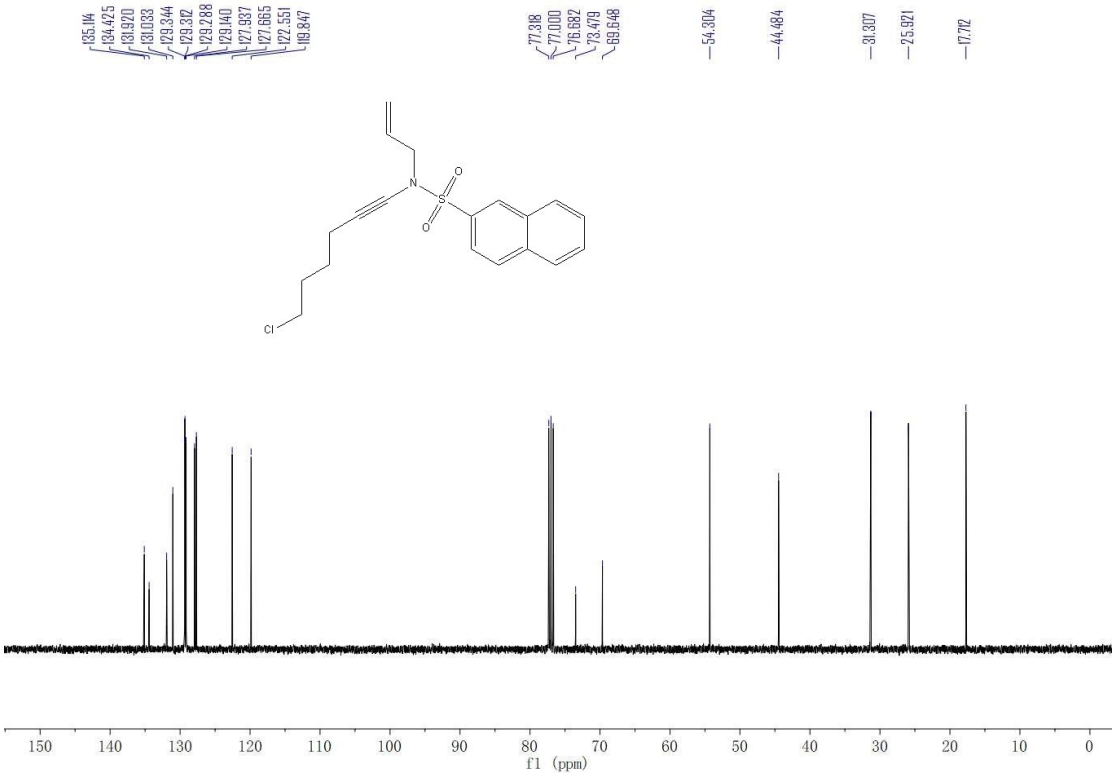
_N_-allyl-_N_-(6-chlorohex-1-yn-1-yl)-4-cyanobenzenesulfonamide (1m)



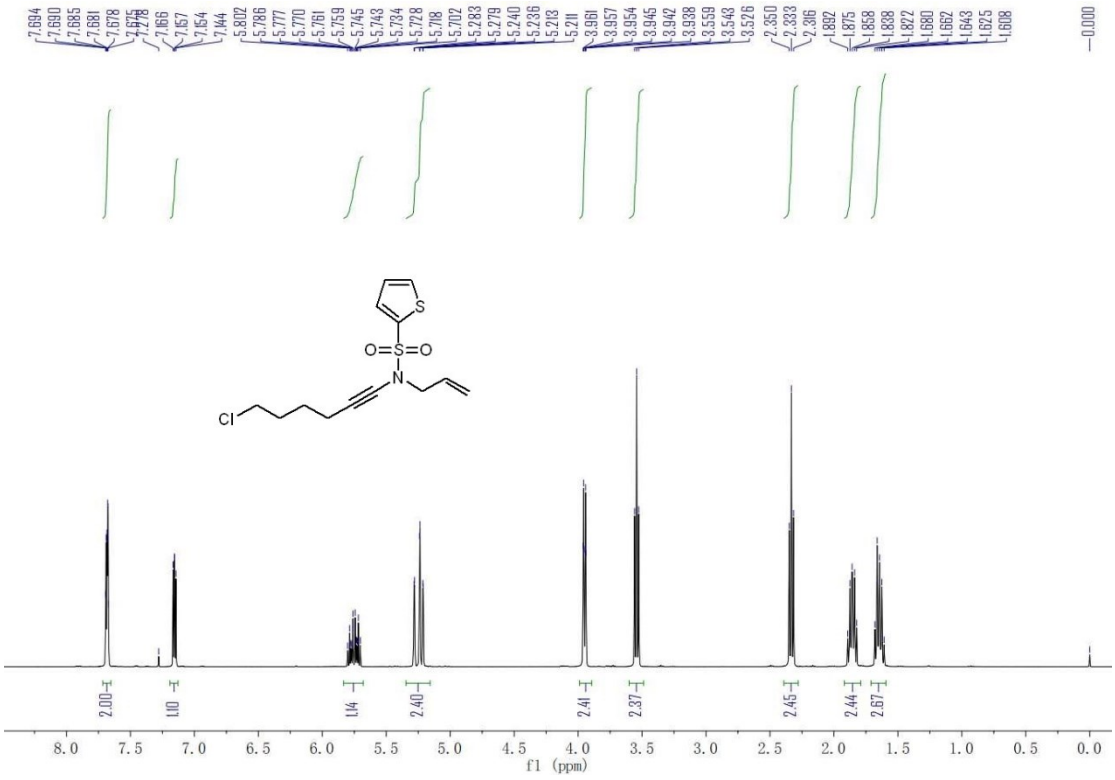


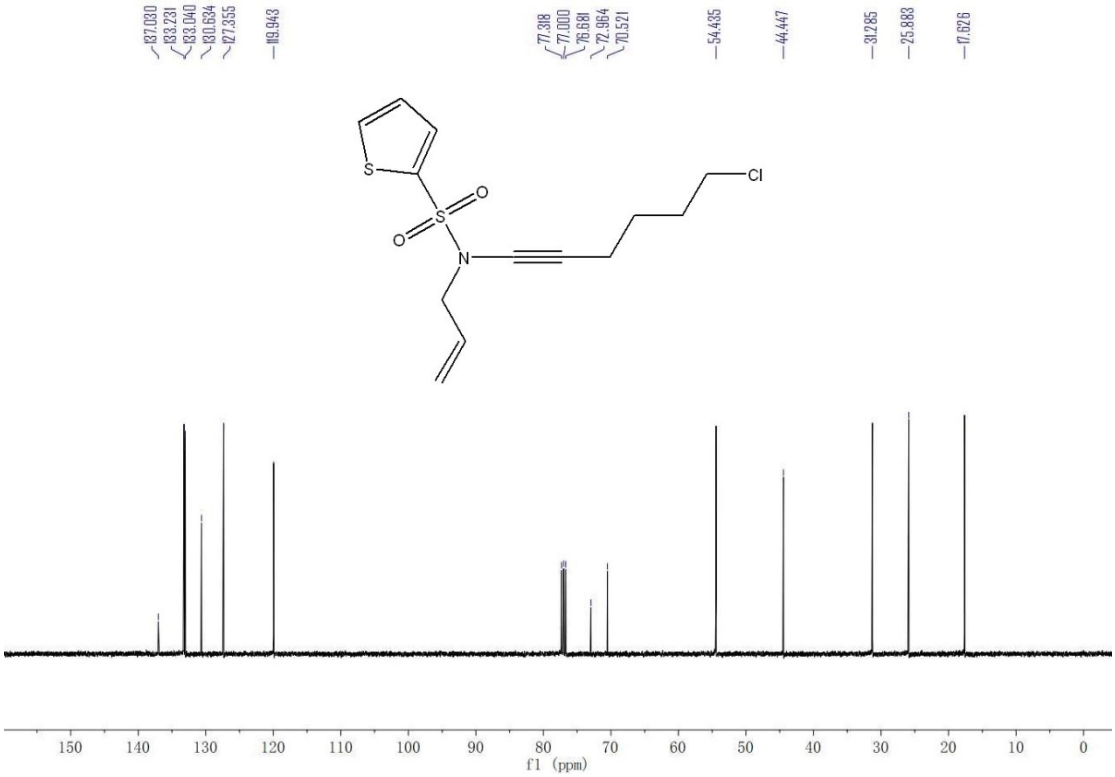
_N_-allyl-_N_-(6-chlorohex-1-yn-1-yl)naphthalene-2-sulfonamide (1n)



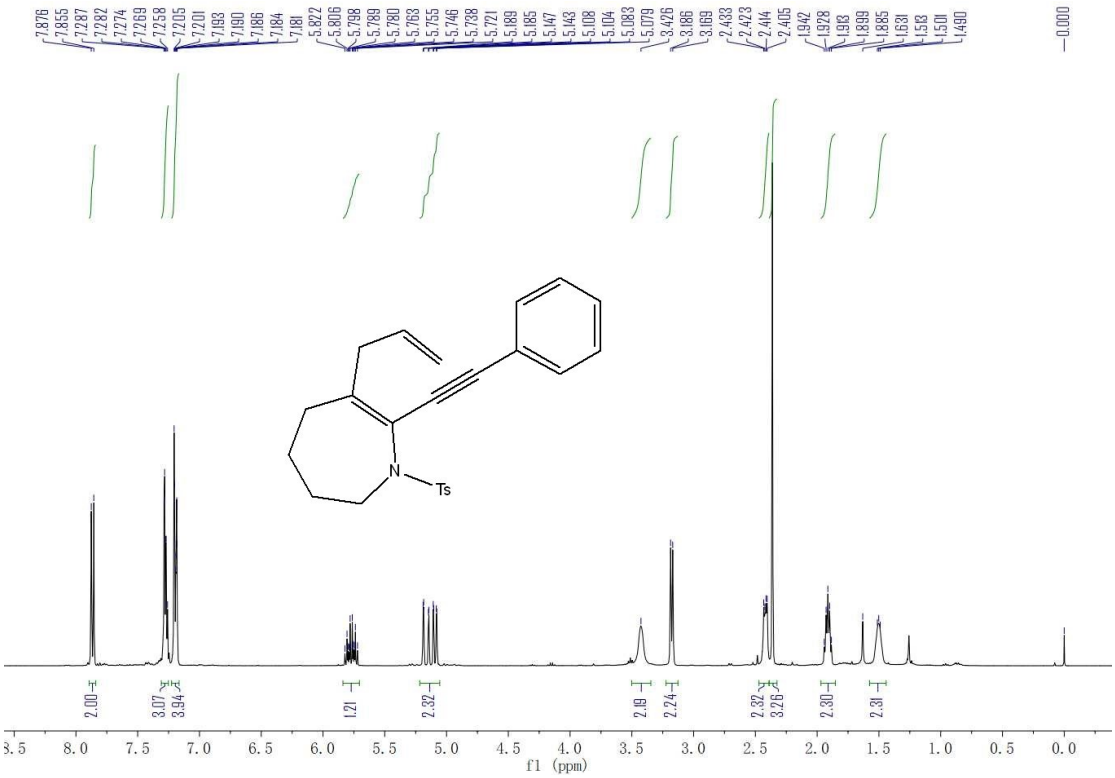


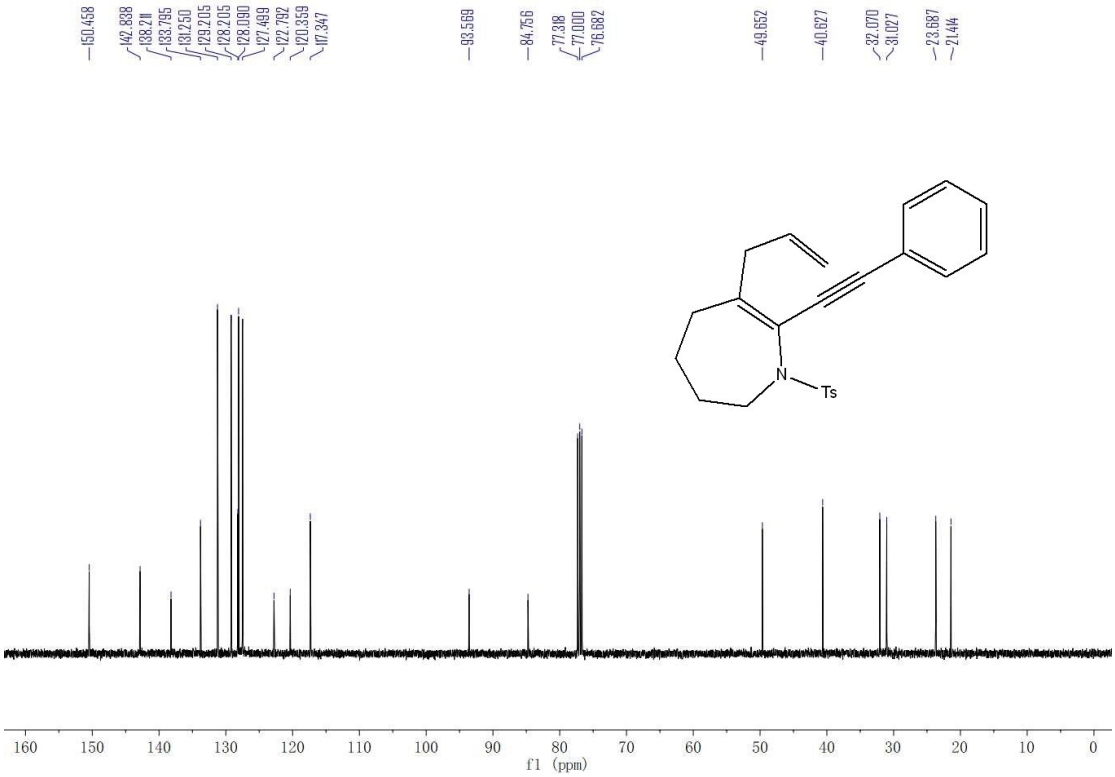
_N_-allyl-_N_-(6-chlorohex-1-yn-1-yl)thiophene-2-sulfonamide (1o)



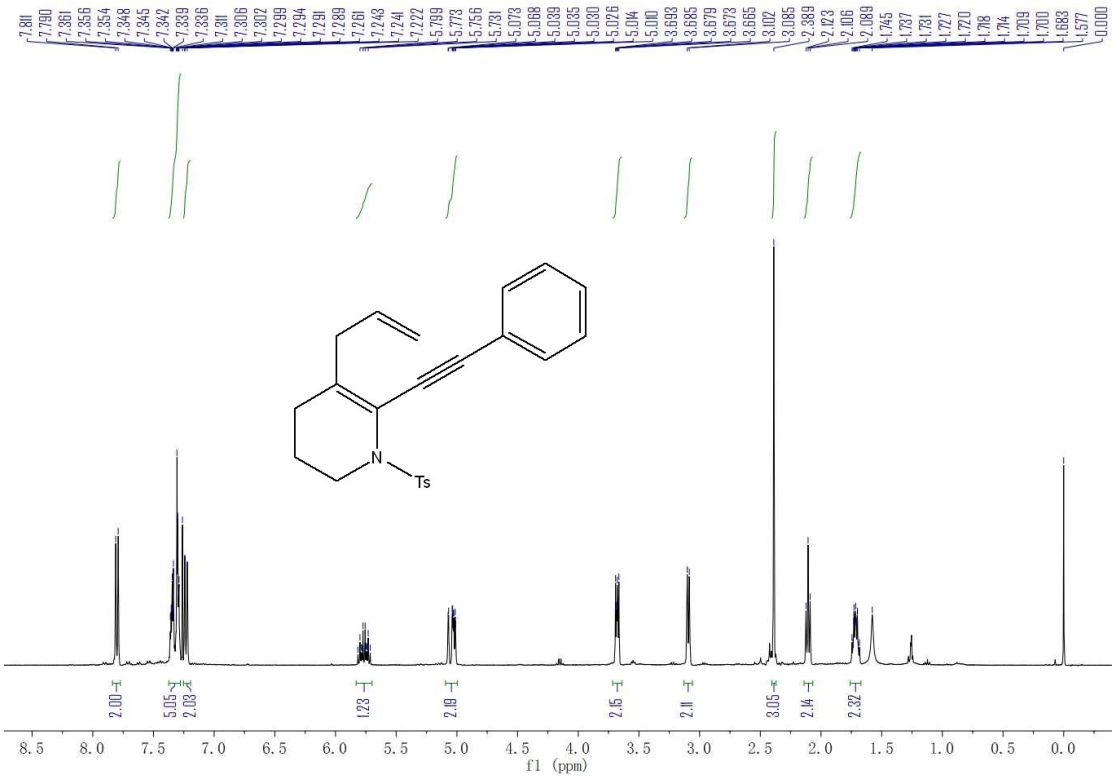


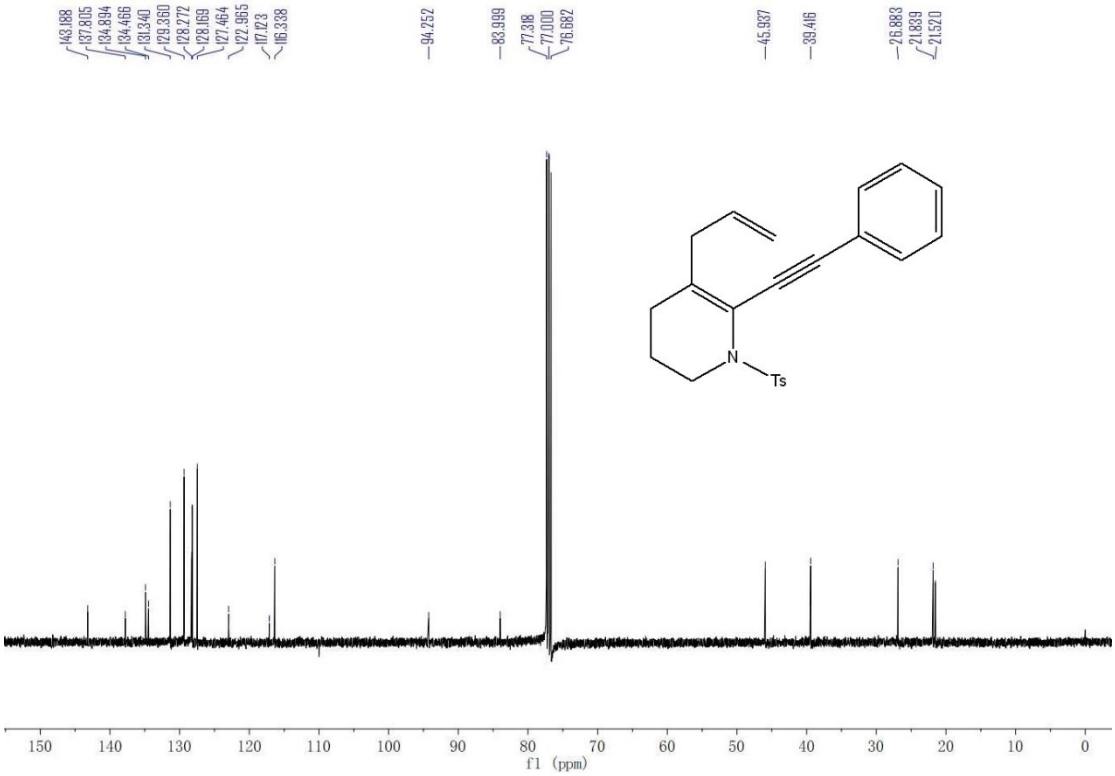
6-Allyl-7-(phenylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3aa)



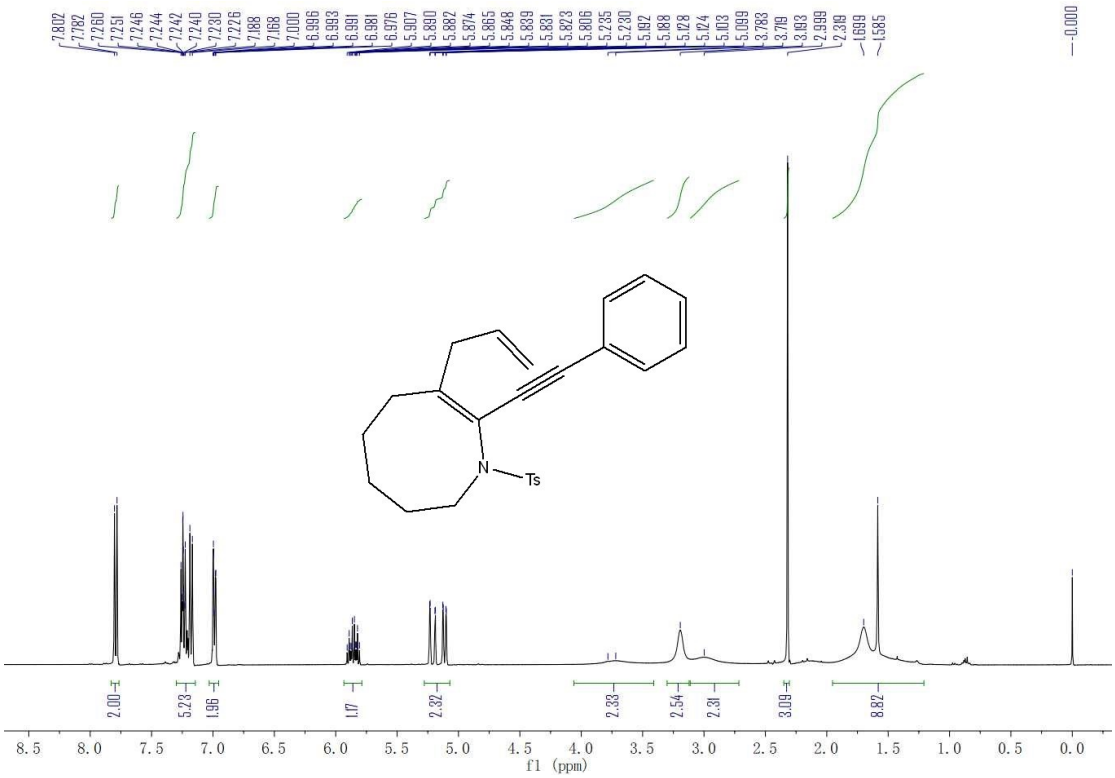


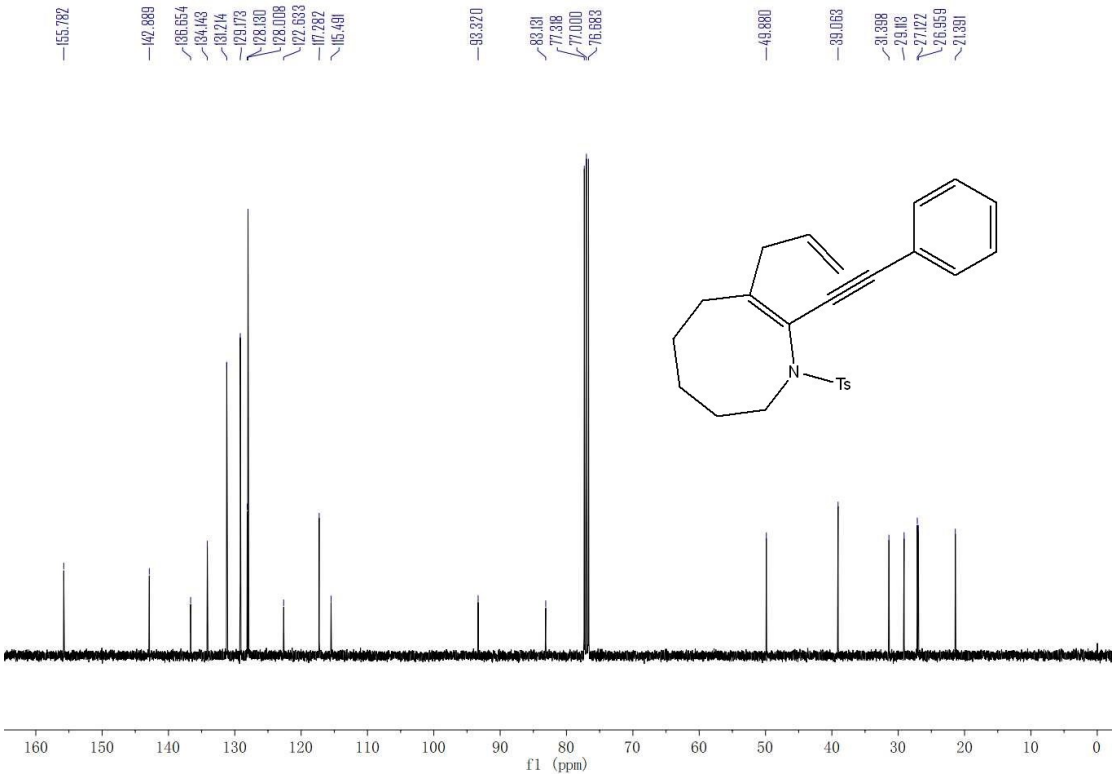
5-Allyl-6-(phenylethynyl)-1-tosyl-1,2,3,4-tetrahydropyridine (3ba)





(*E*)-7-Allyl-8-(phenylethynyl)-1-tosyl-1,2,3,4,5,6-hexahydroazocine (3ca)





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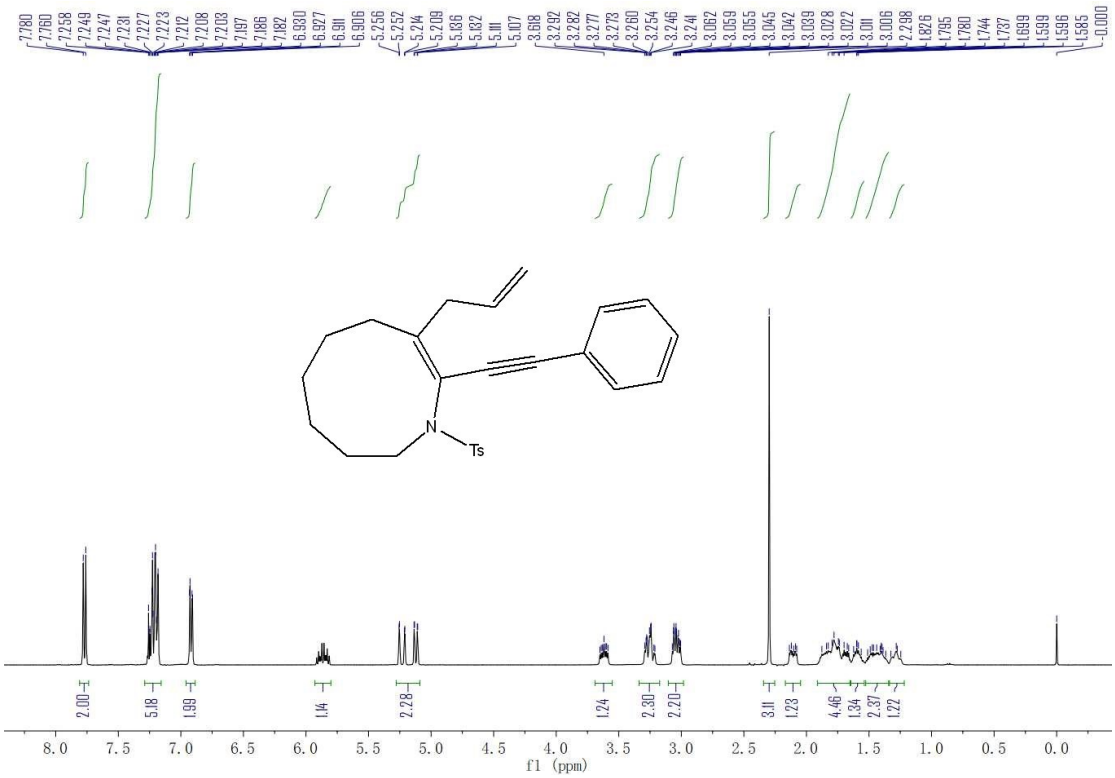
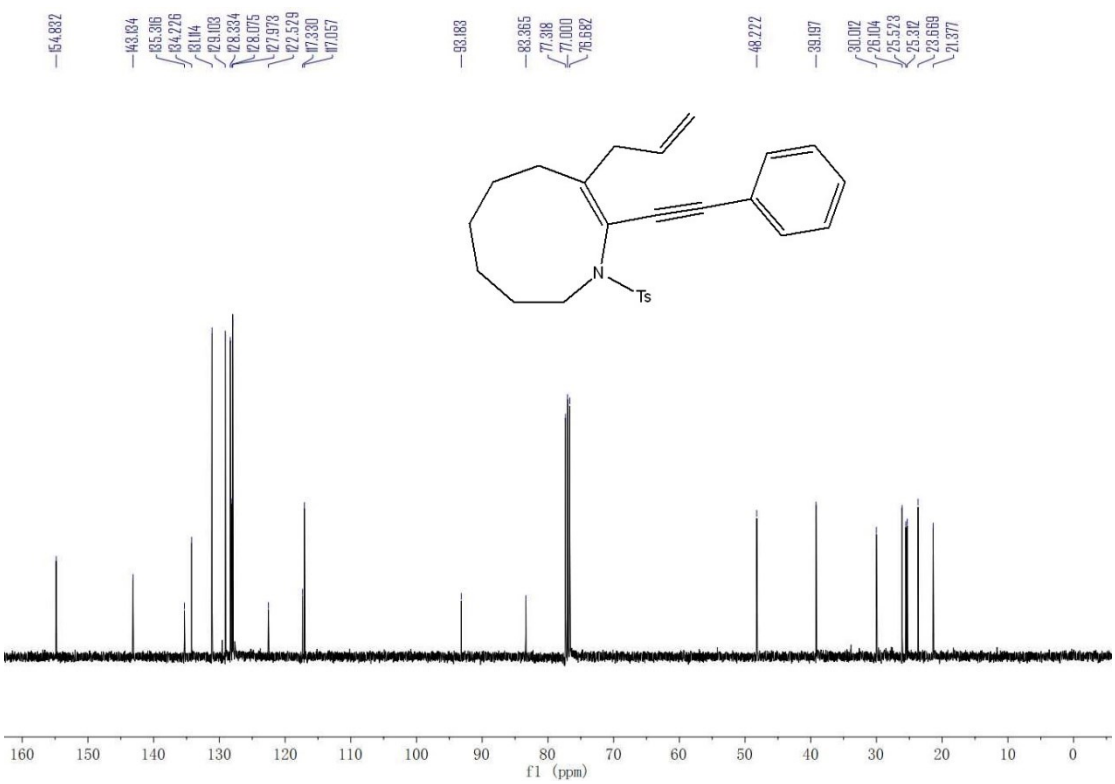
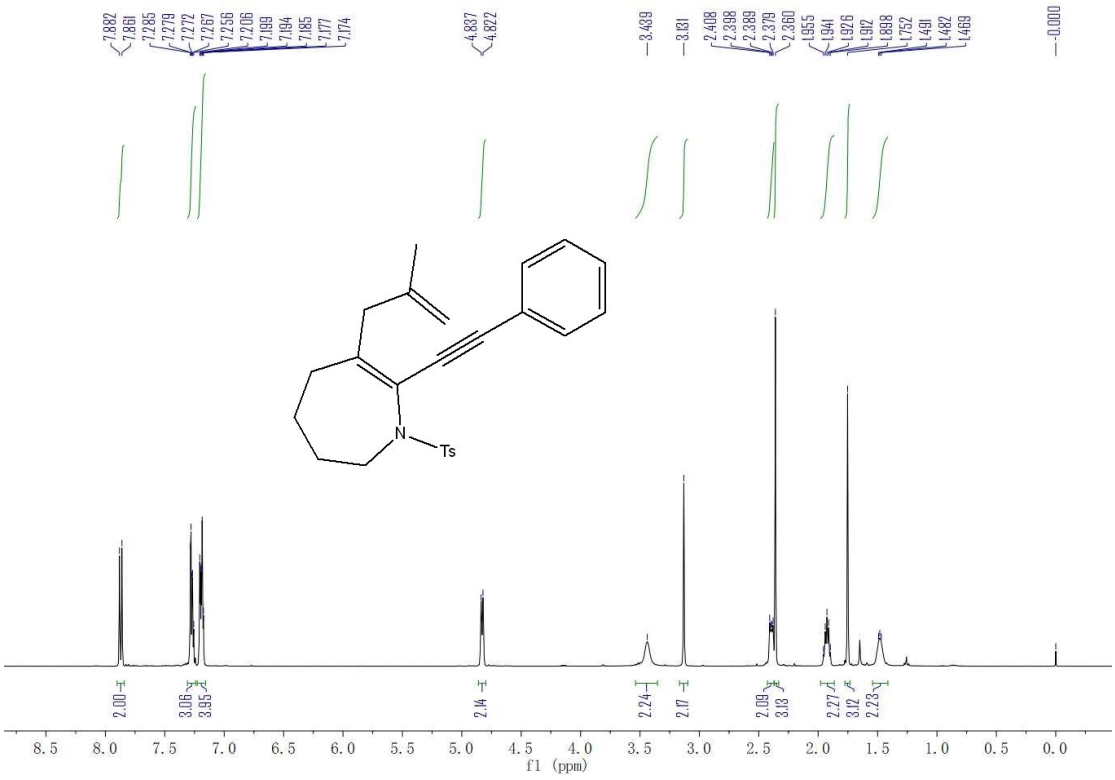
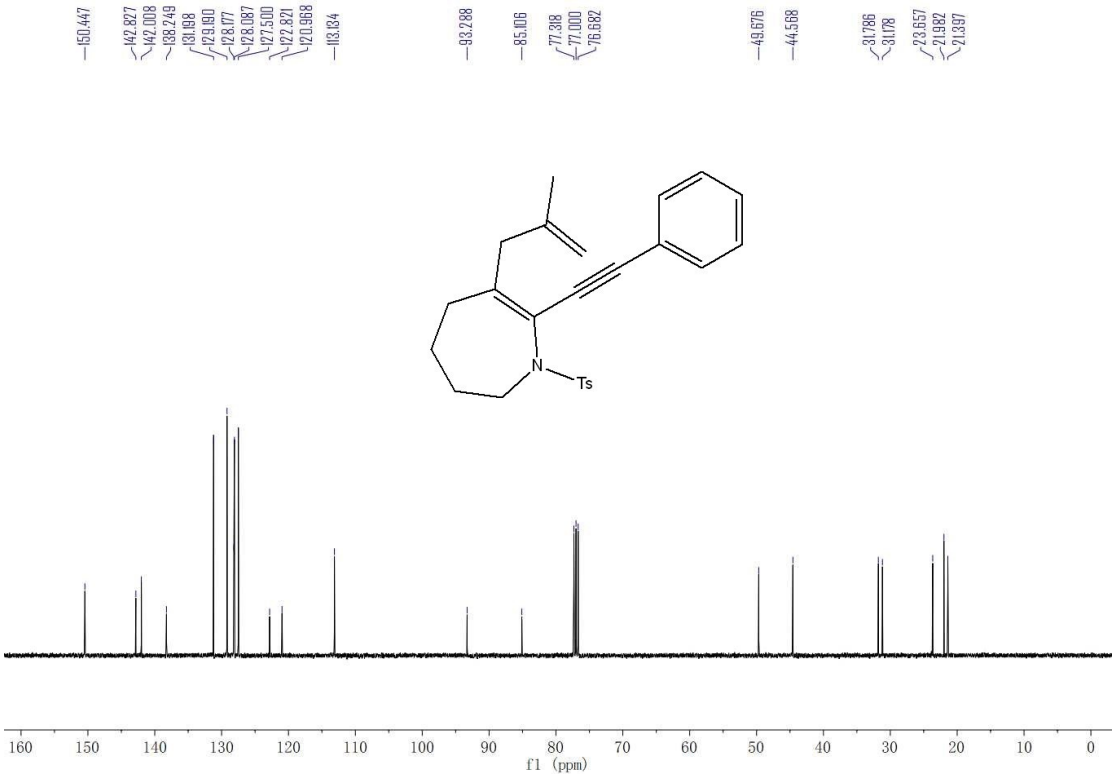


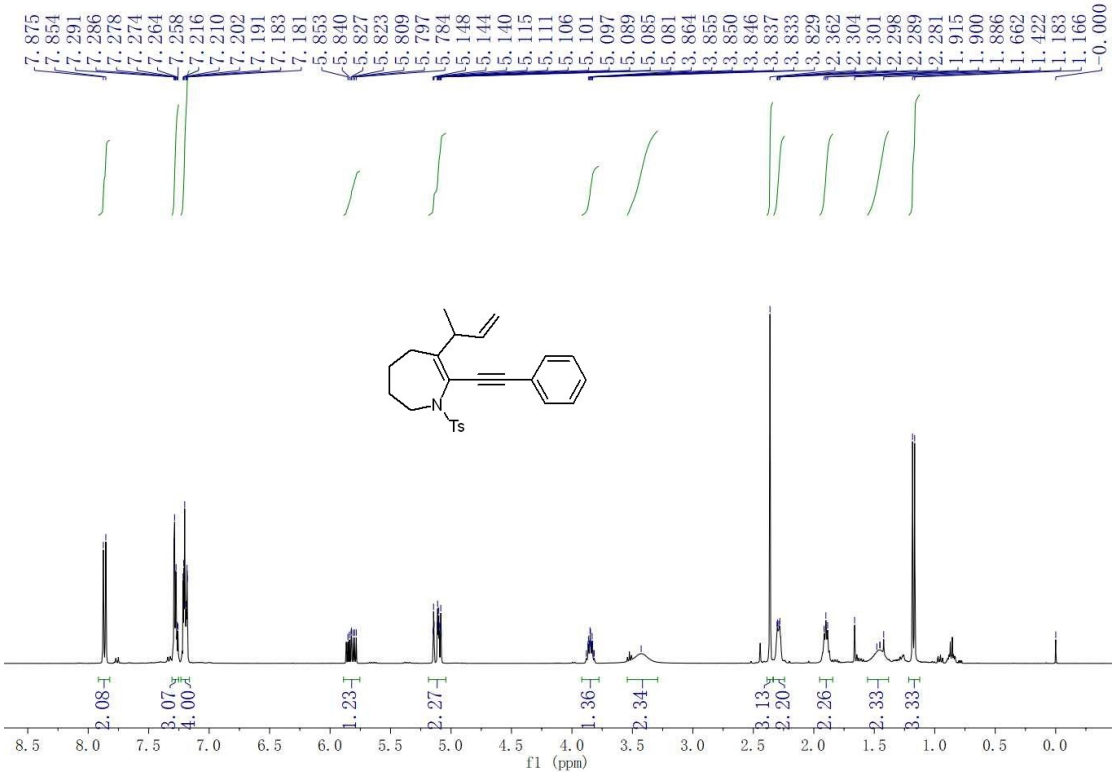


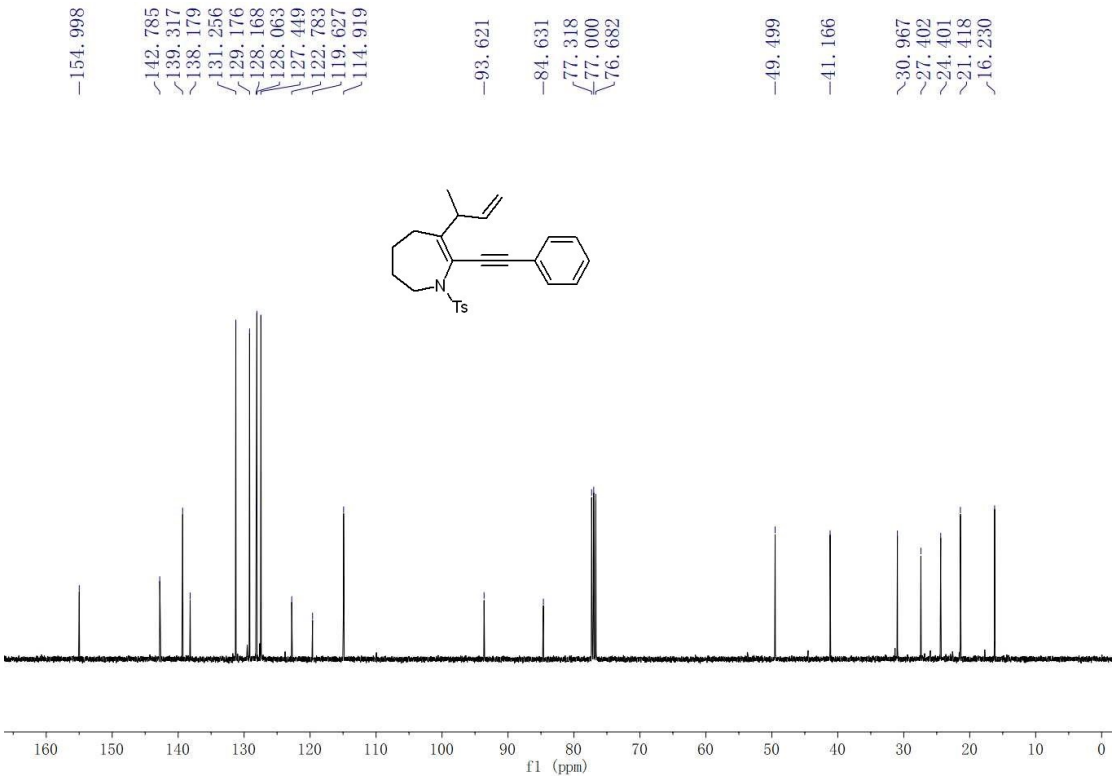
6-(2-Methylallyl)-7-(phenylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3fa)



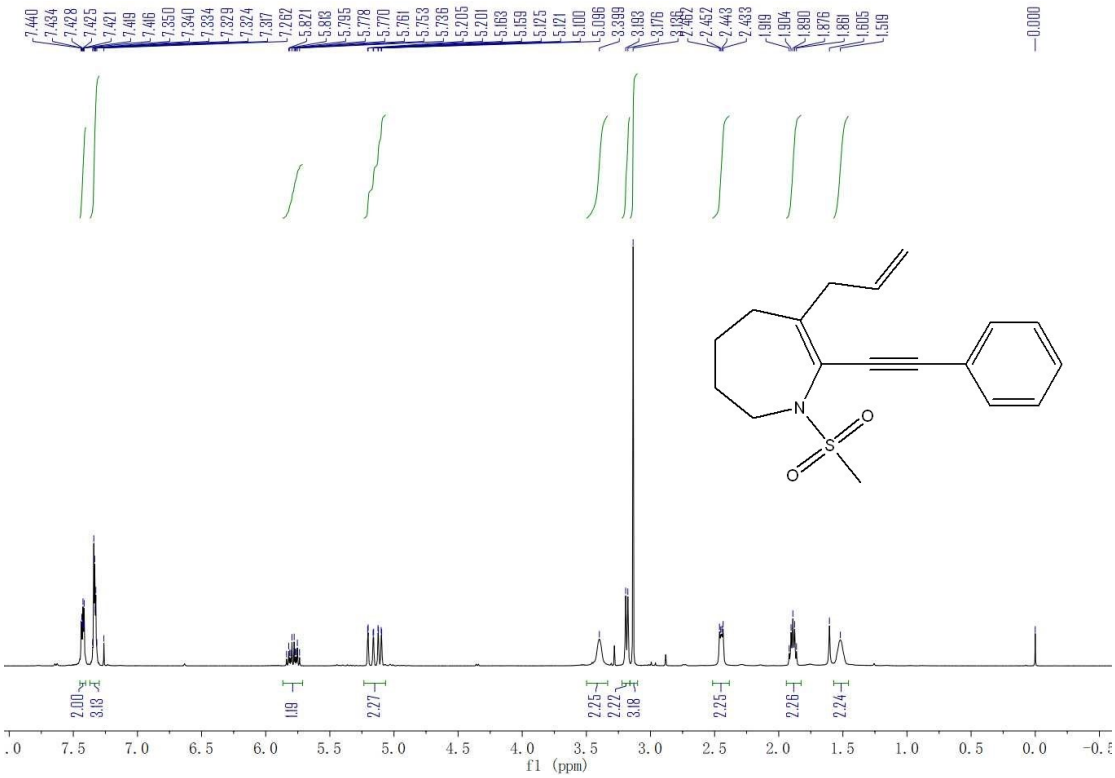


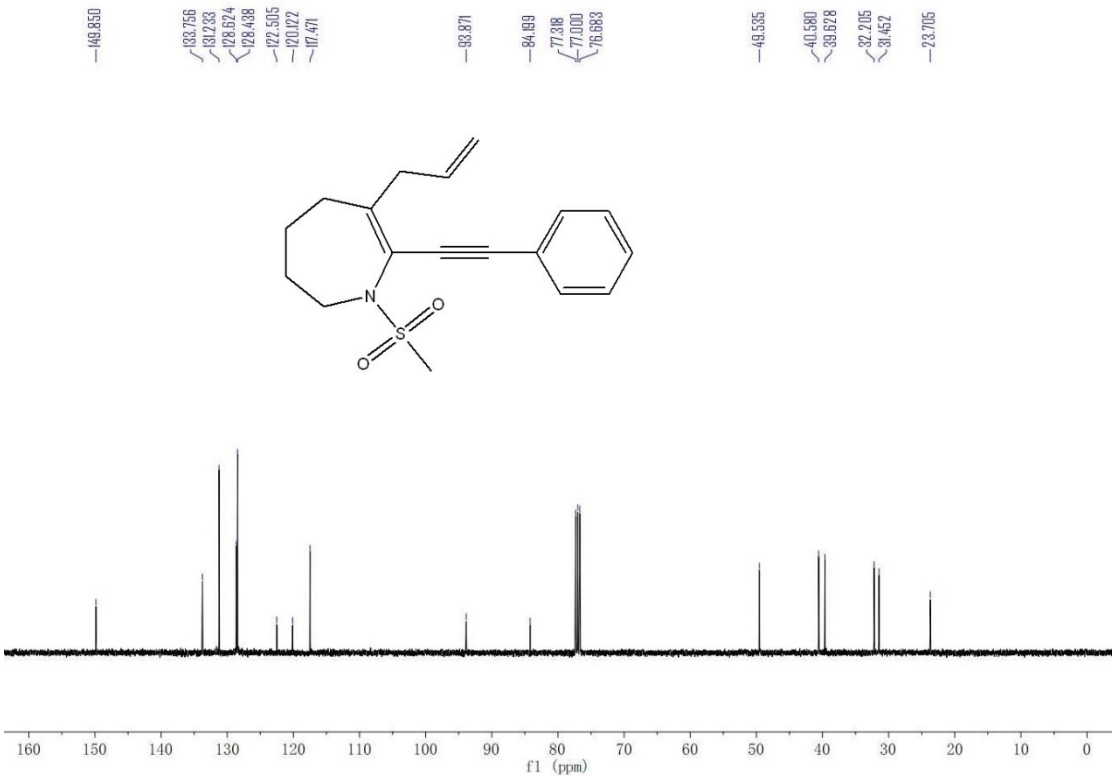
6-(But-3-en-2-yl)-7-(phenylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ga)



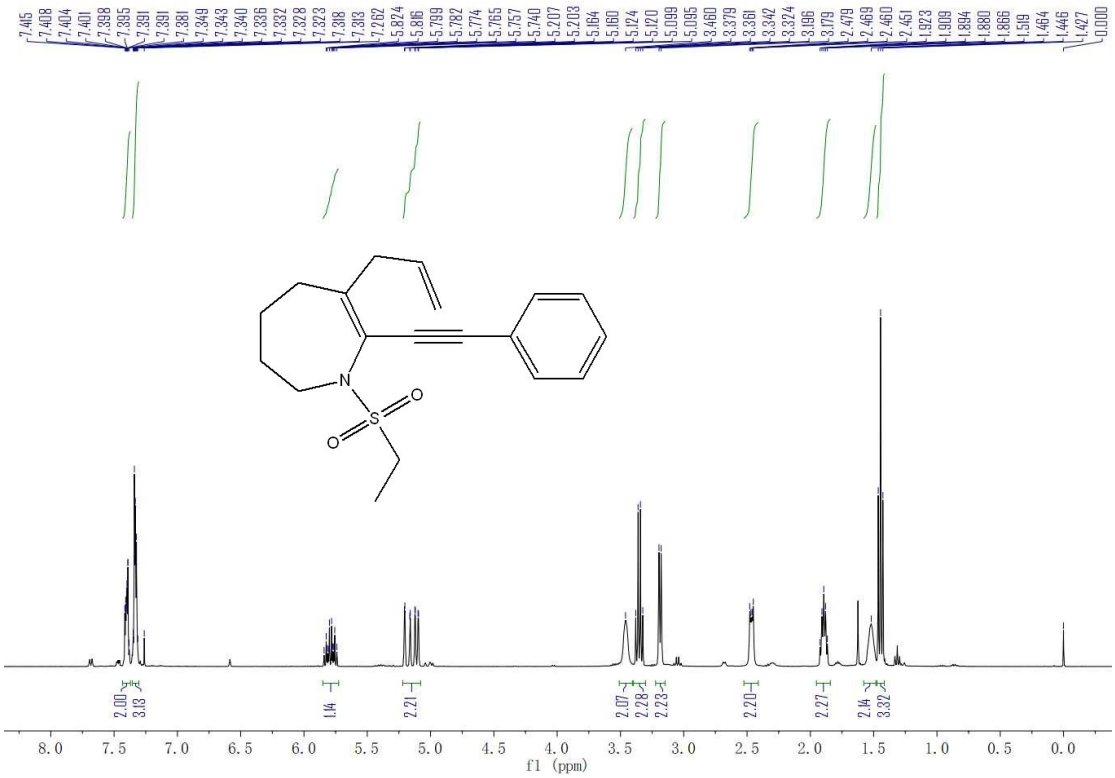


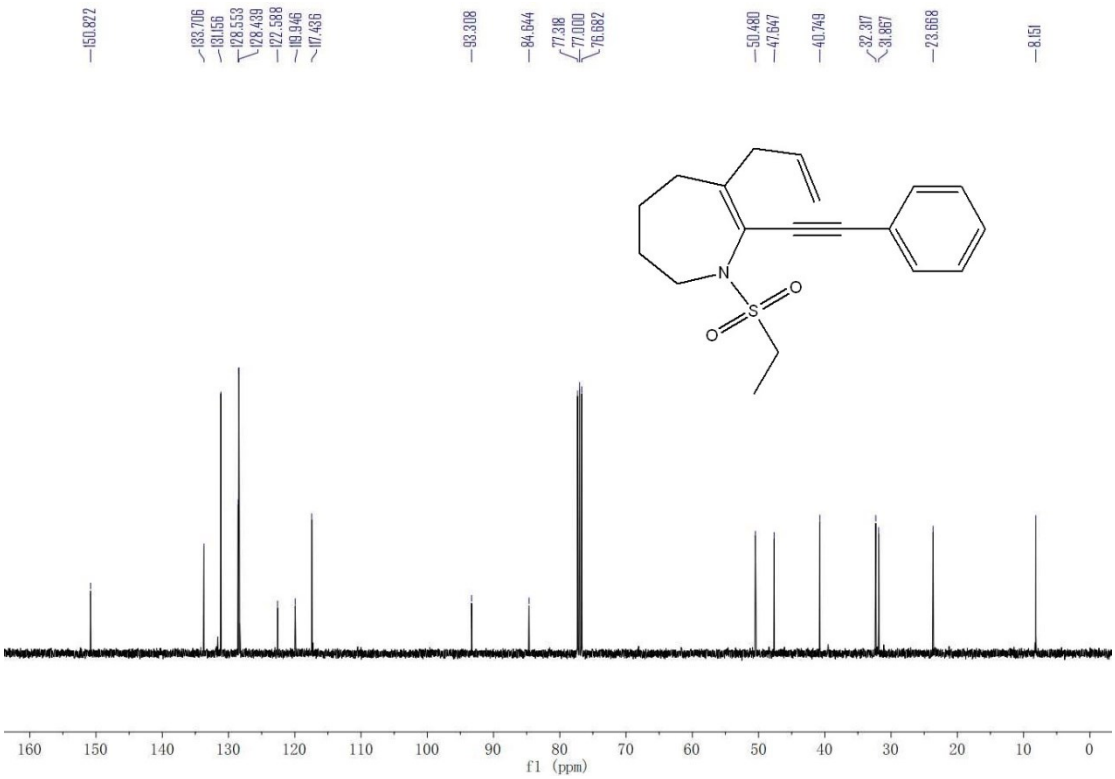
6-Allyl-1-(methylsulfonyl)-7-(phenylethynyl)-2,3,4,5-tetrahydro-1*H*-azepine (3ha)





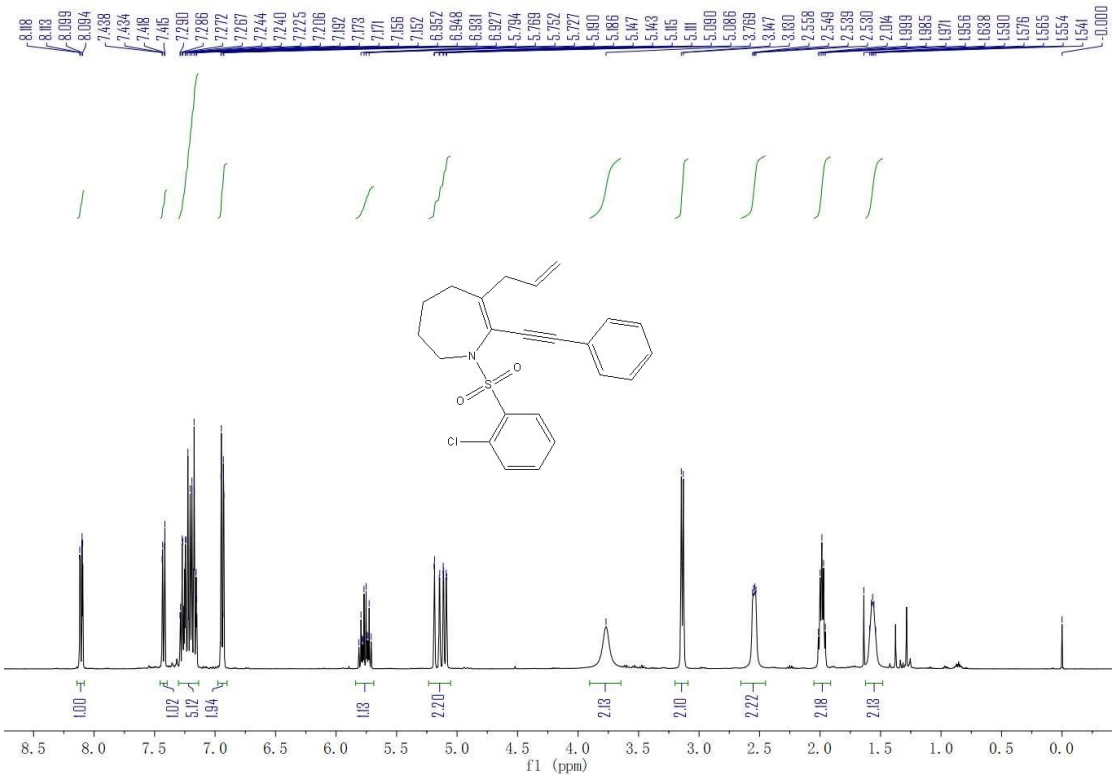
6-Allyl-1-(ethylsulfonyl)-7-(phenylethynyl)-2,3,4,5-tetrahydro-1*H*-azepine (3ia)

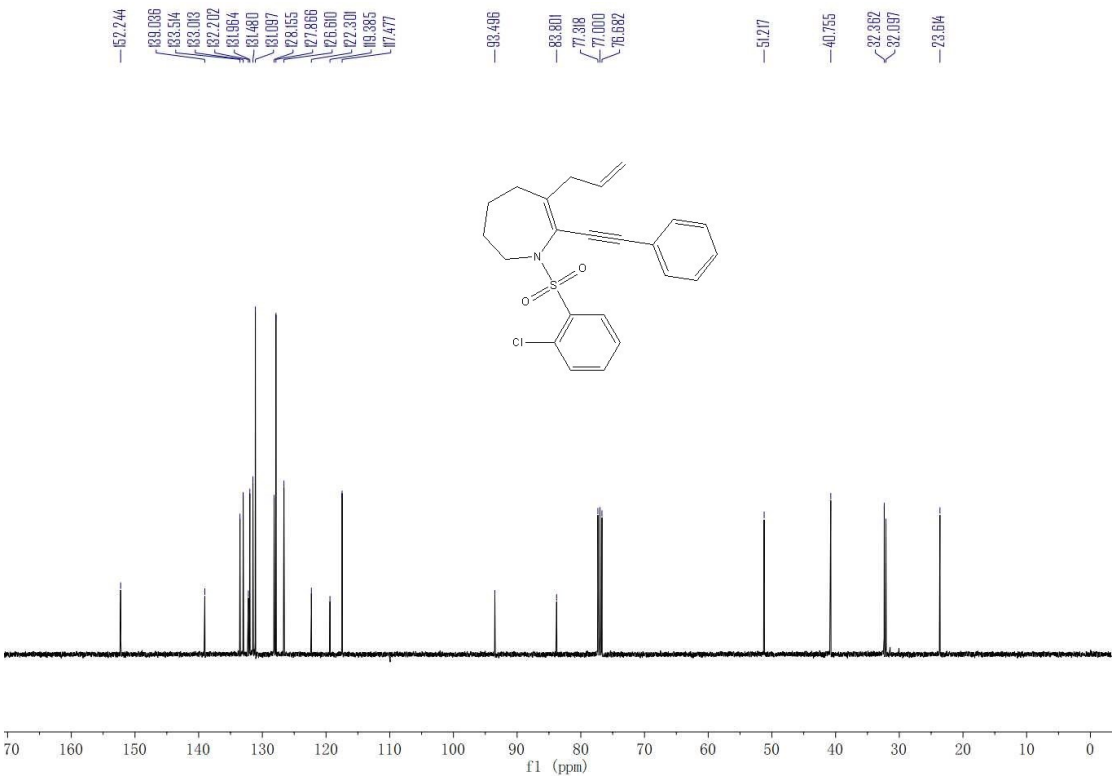




6-Allyl-1-((2-chlorophenyl)sulfonyl)-7-(phenylethynyl)-2,3,4,5-tetrahydro-1*H*-

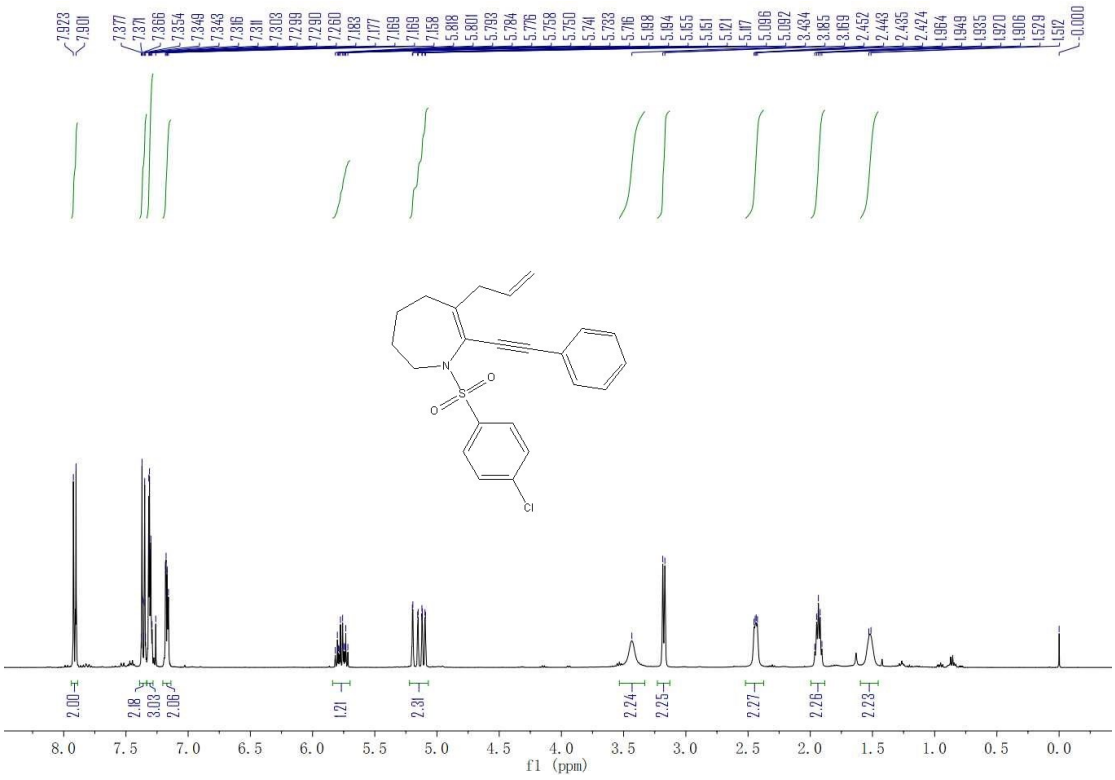
azepine (3ka)

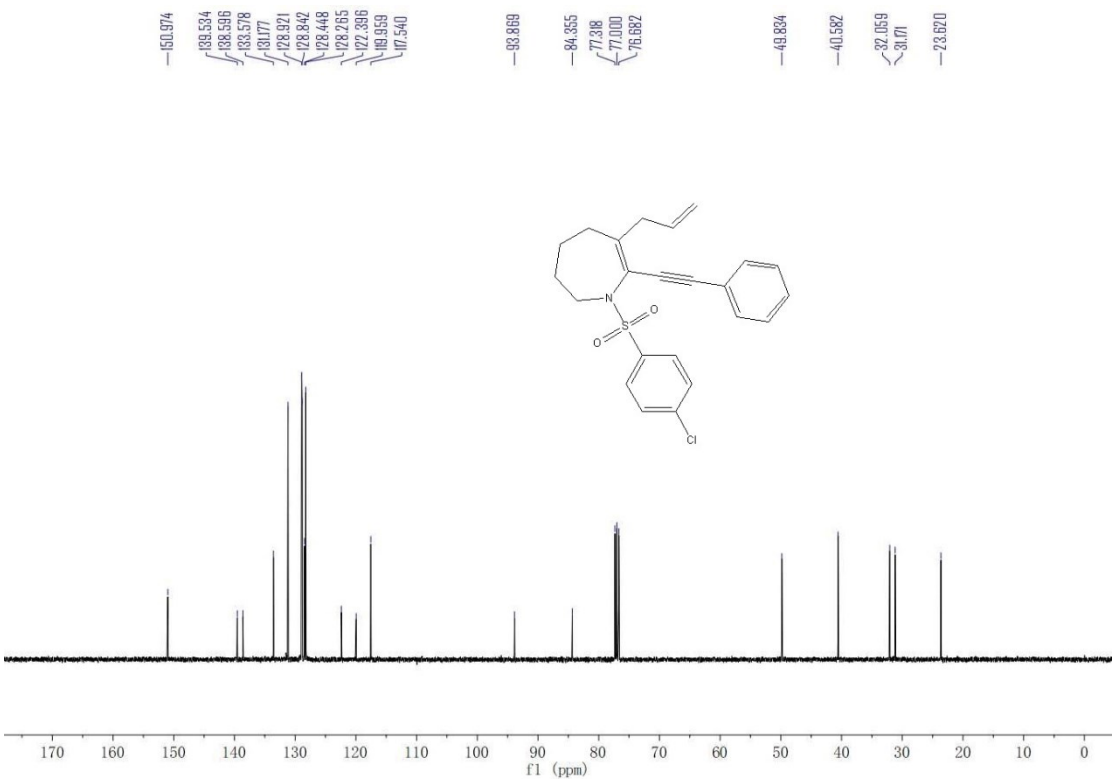




6-Allyl-1-((4-chlorophenyl)sulfonyl)-7-(phenylethynyl)-2,3,4,5-tetrahydro-1*H*-

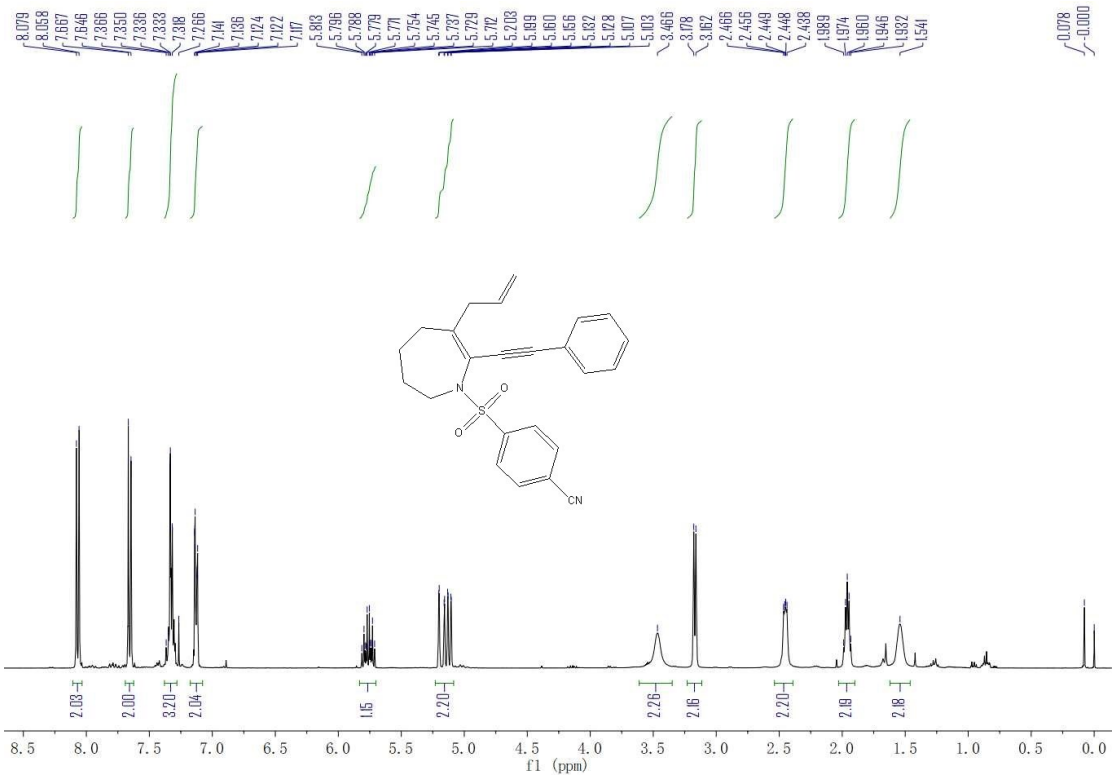
azepine (3la)

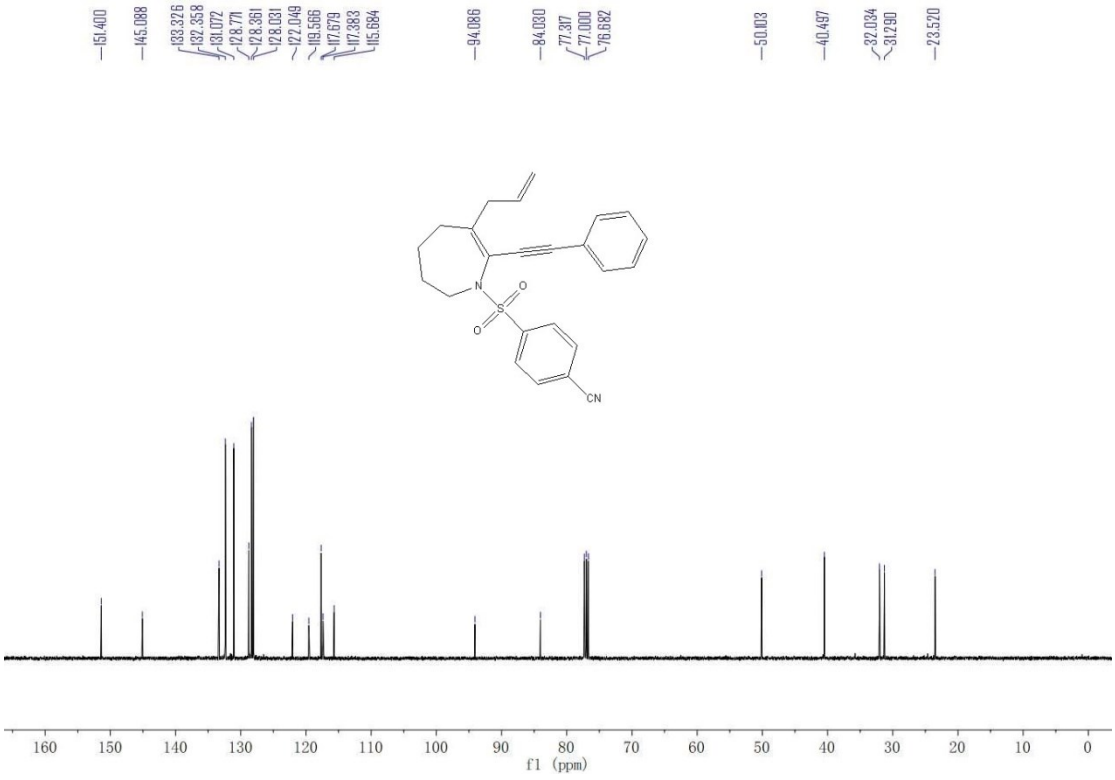




4-((A-allyl-7-(phenylethynyl)-2,3,4,5-tetrahydro-1*H*-azepin-1-

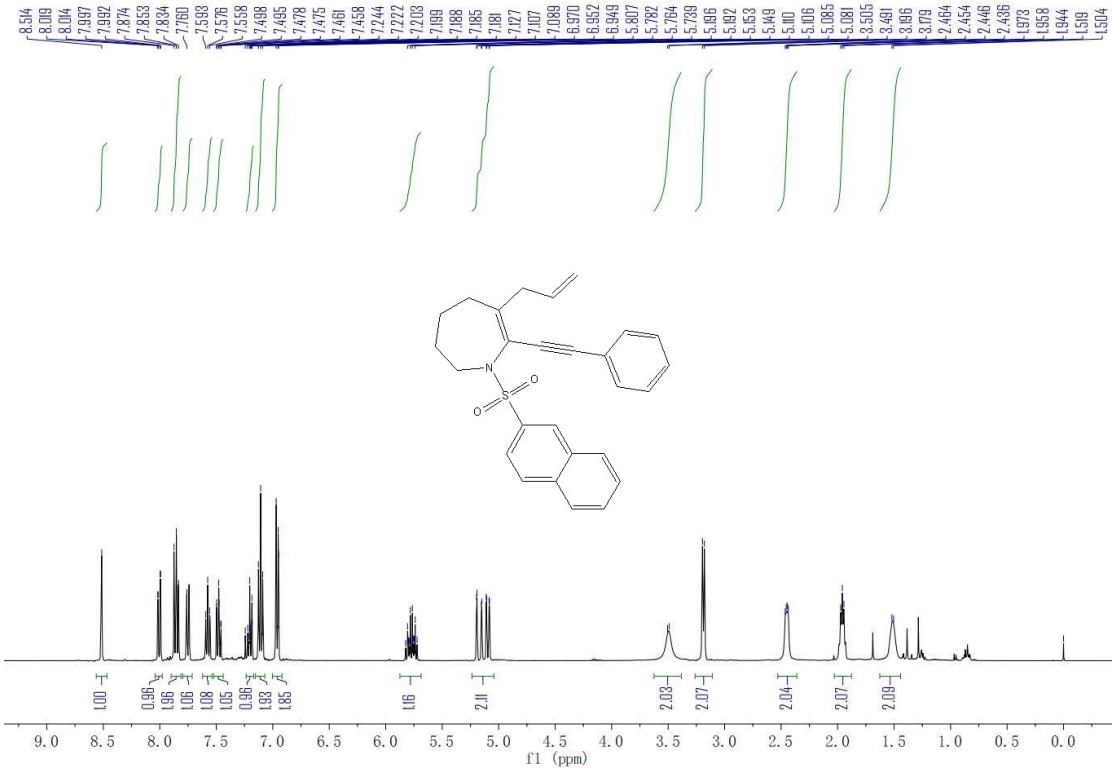
yl)sulfonyl)benzonitrile (3ma)

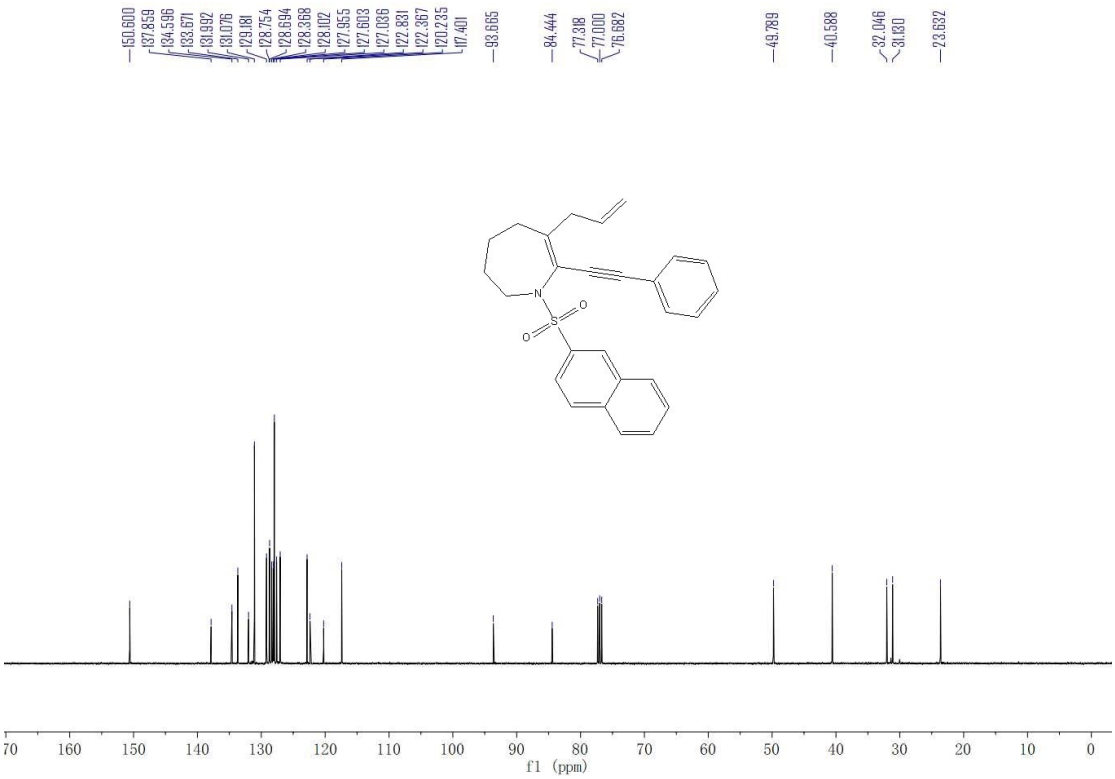




6-Allyl-1-(naphthalen-2-ylsulfonyl)-7-(phenylethynyl)-2,3,4,5-tetrahydro-1*H*-

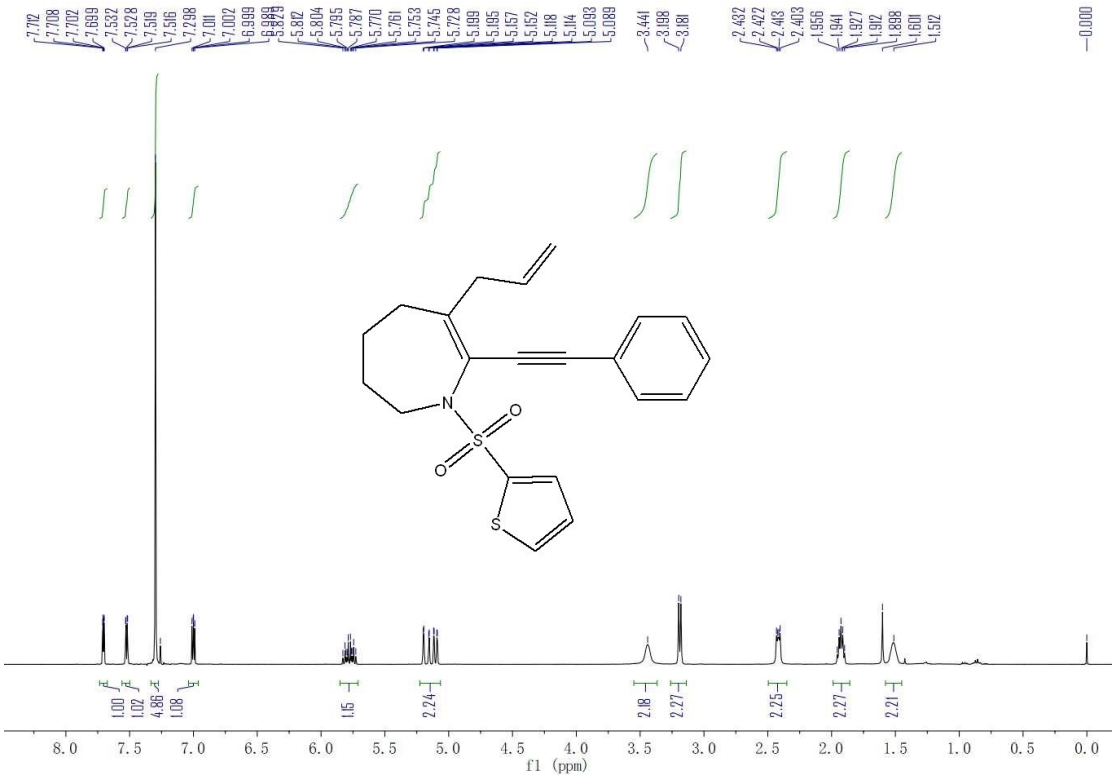
azepine (3na)

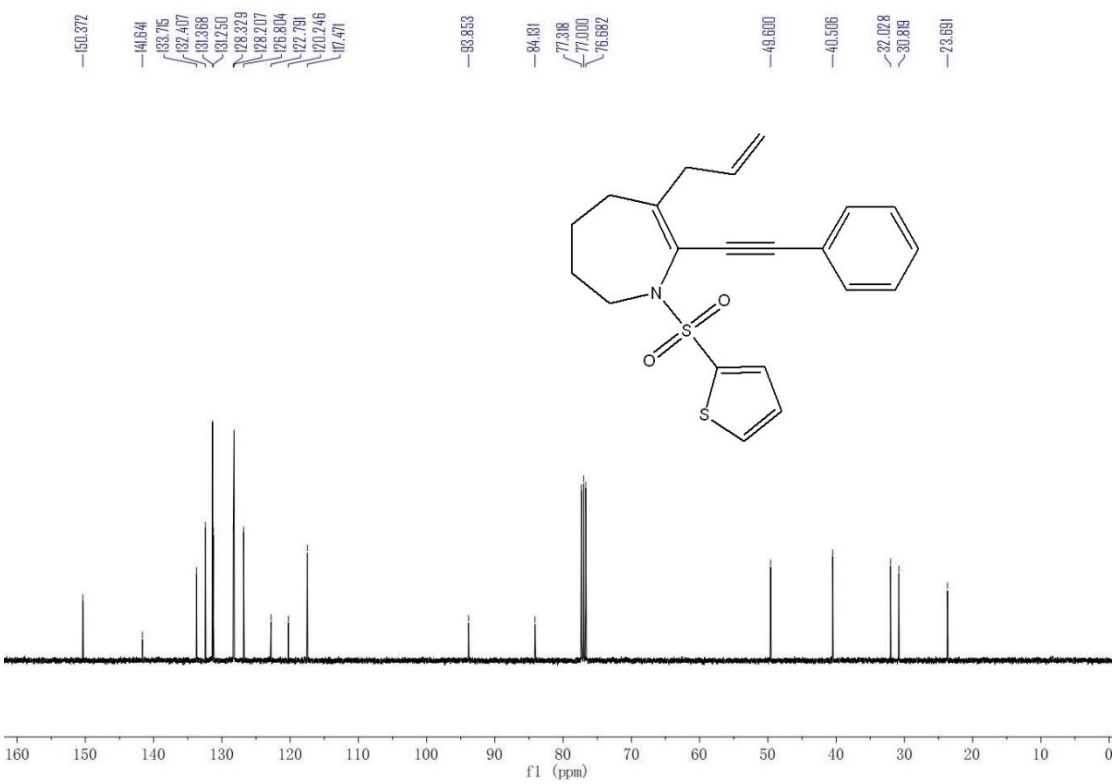




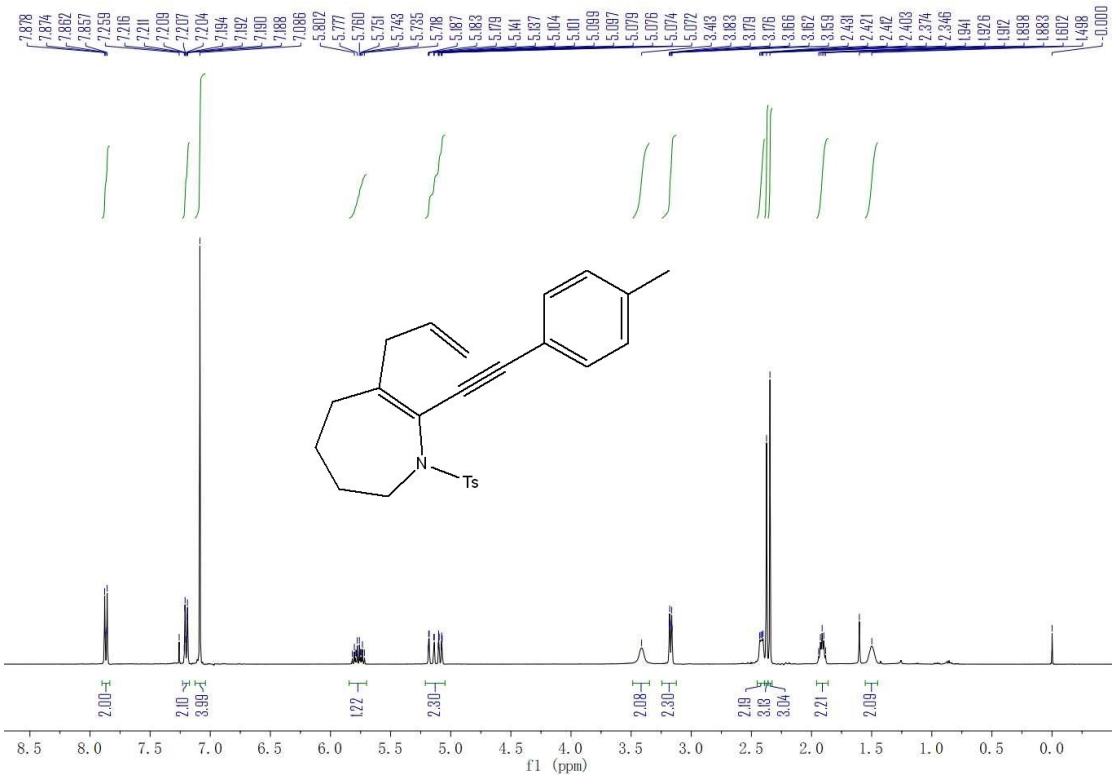
6-Allyl-7-(phenylethynyl)-1-(thiophen-2-ylsulfonyl)-2,3,4,5-tetrahydro-1*H*-

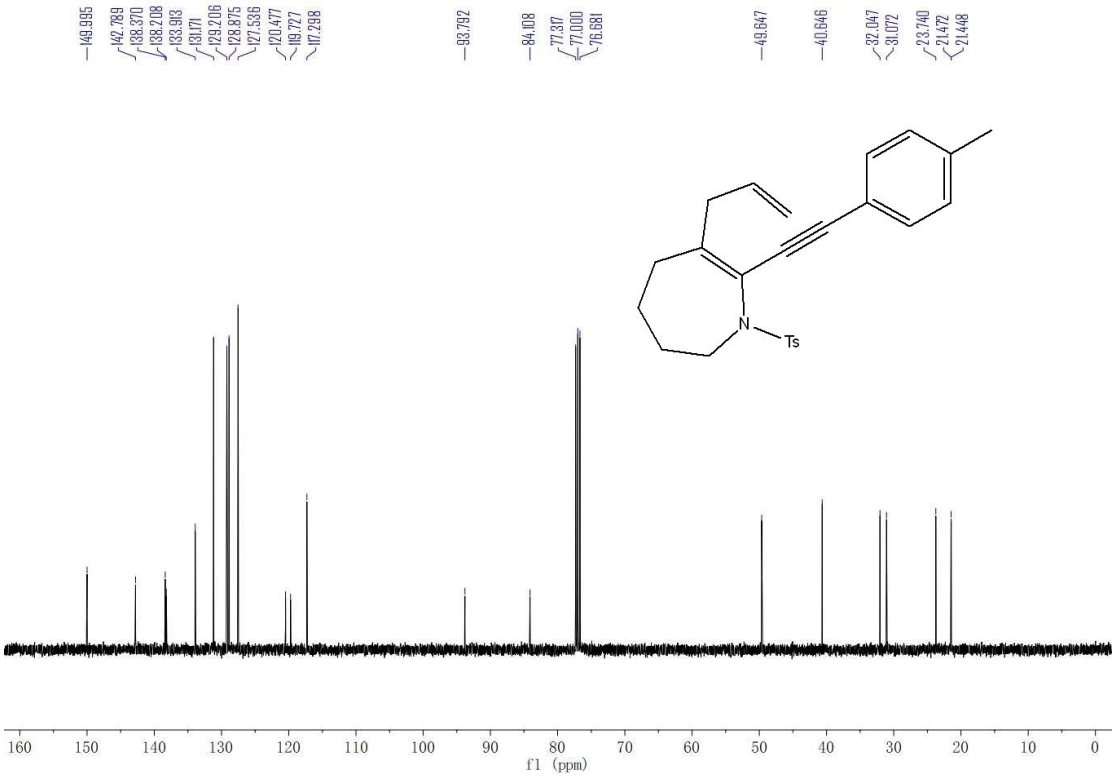
azepine (3oa)



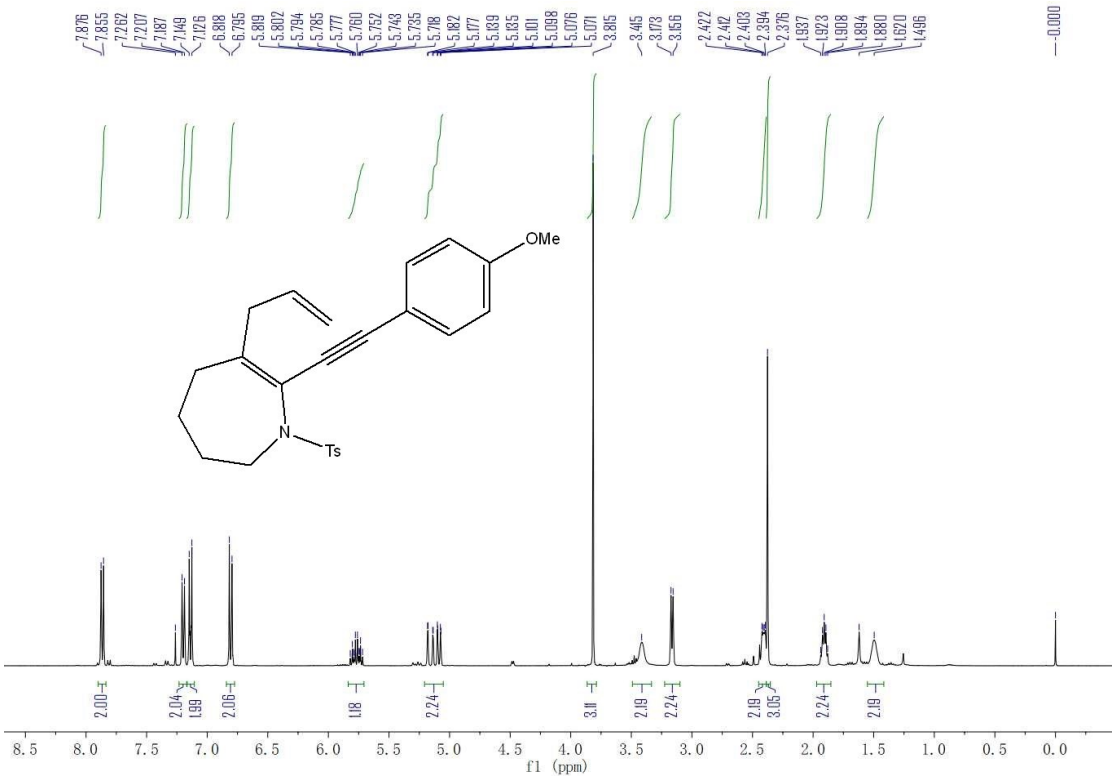


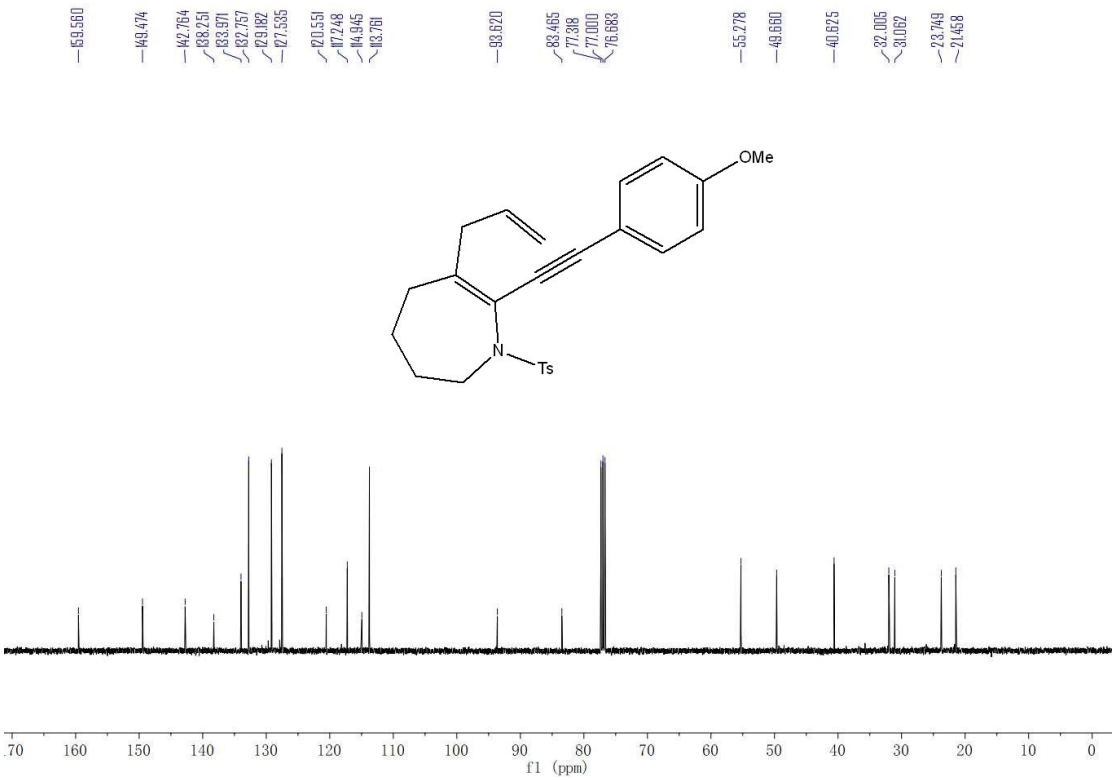
6-Allyl-7-(*p*-tolylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ab)



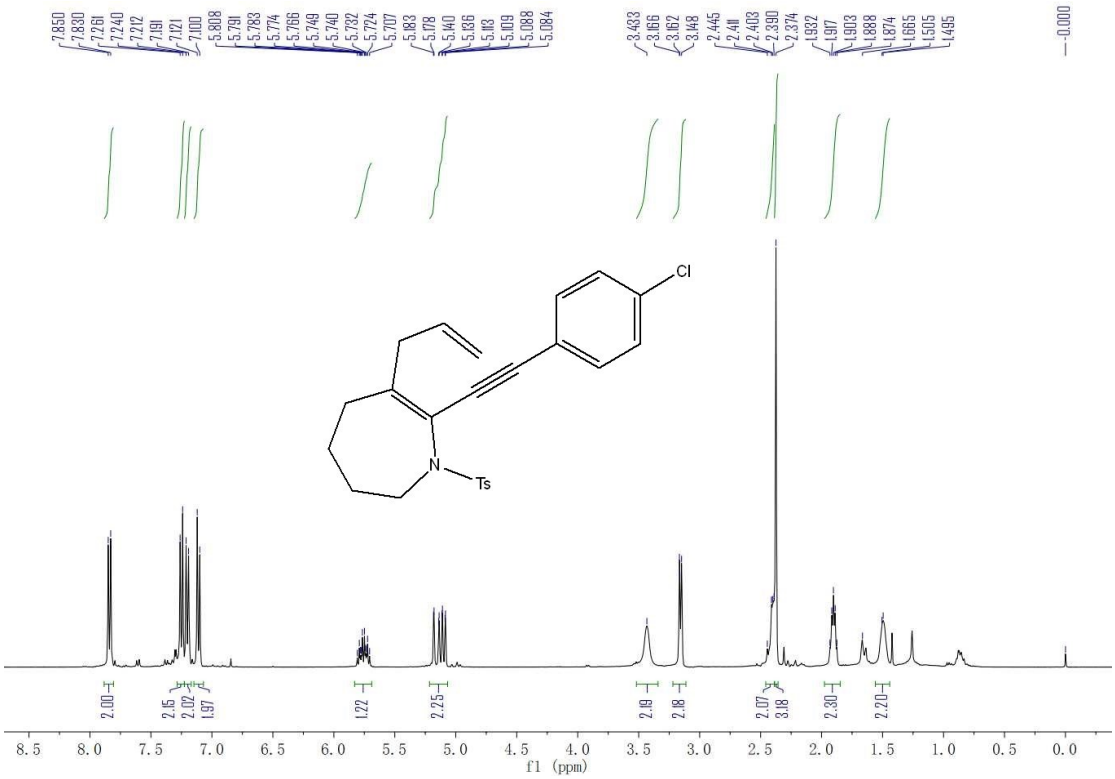


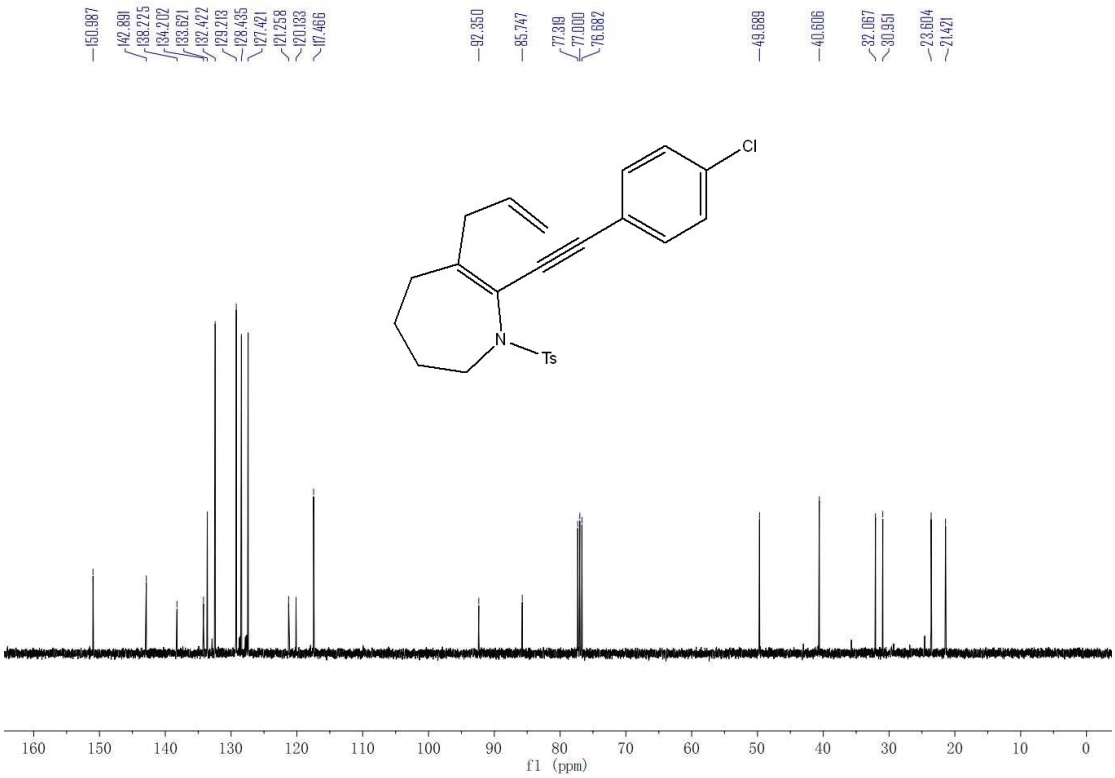
6-Allyl-7-((4-methoxyphenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ac)



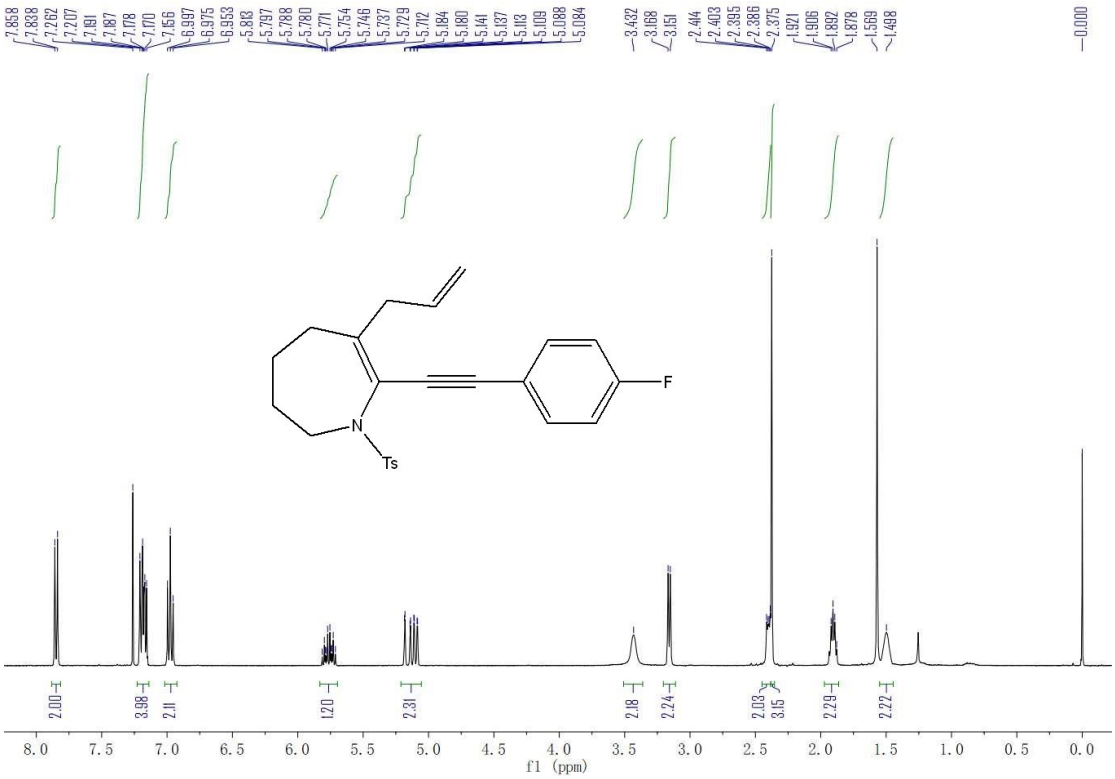


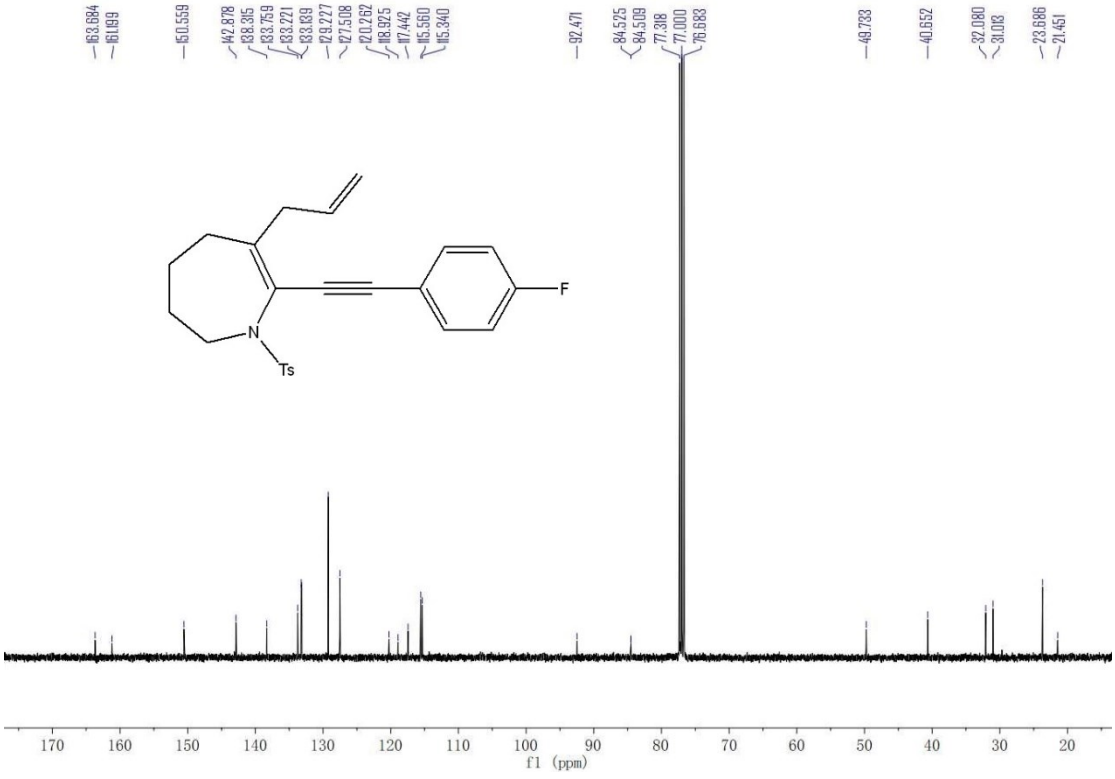
6-Allyl-7-((4-chlorophenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ad)



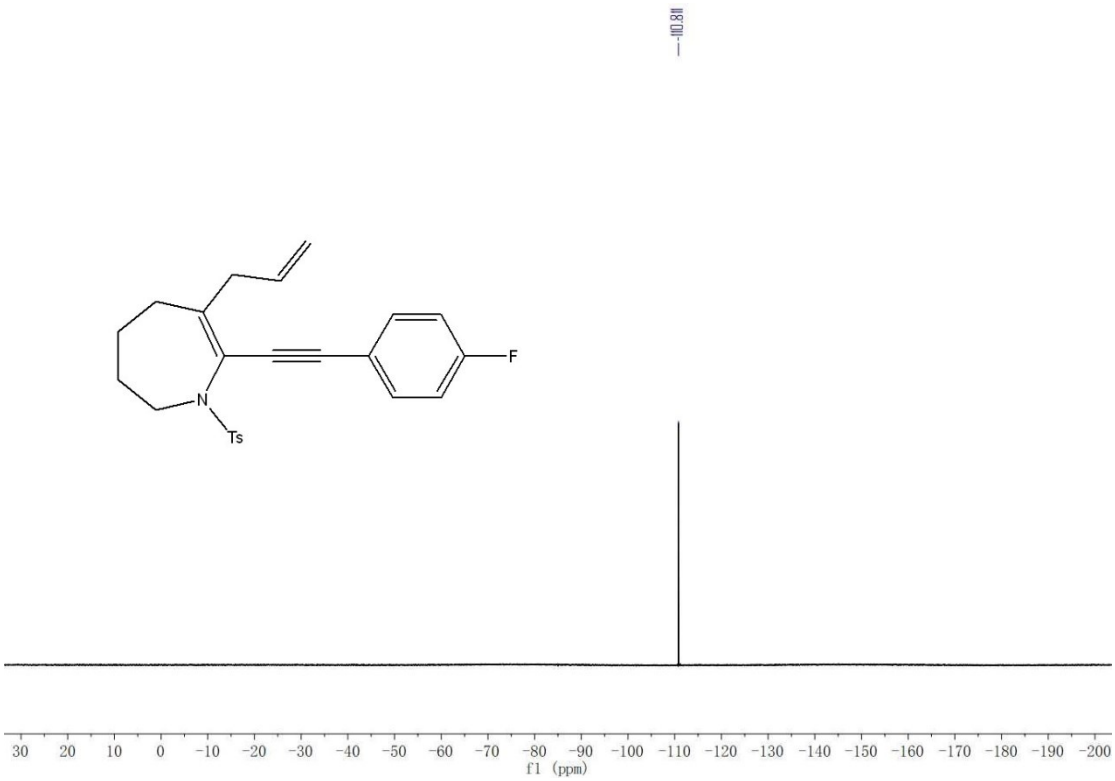


6-Allyl-7-((4-fluorophenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ae)

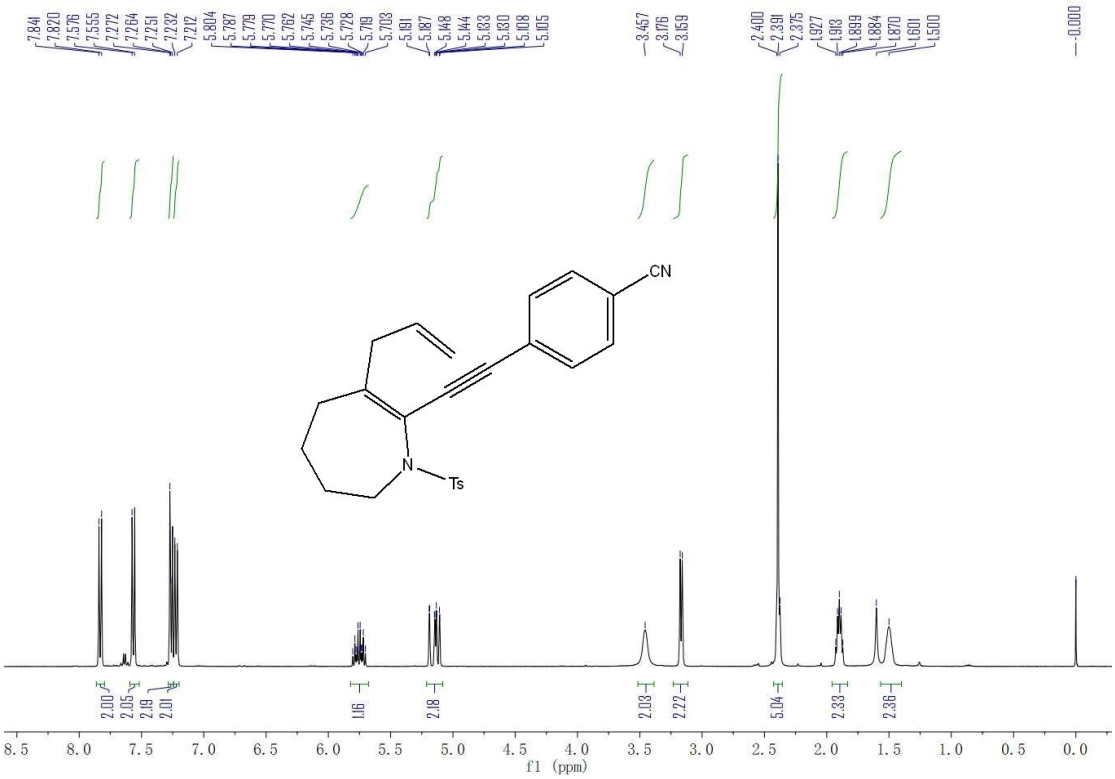


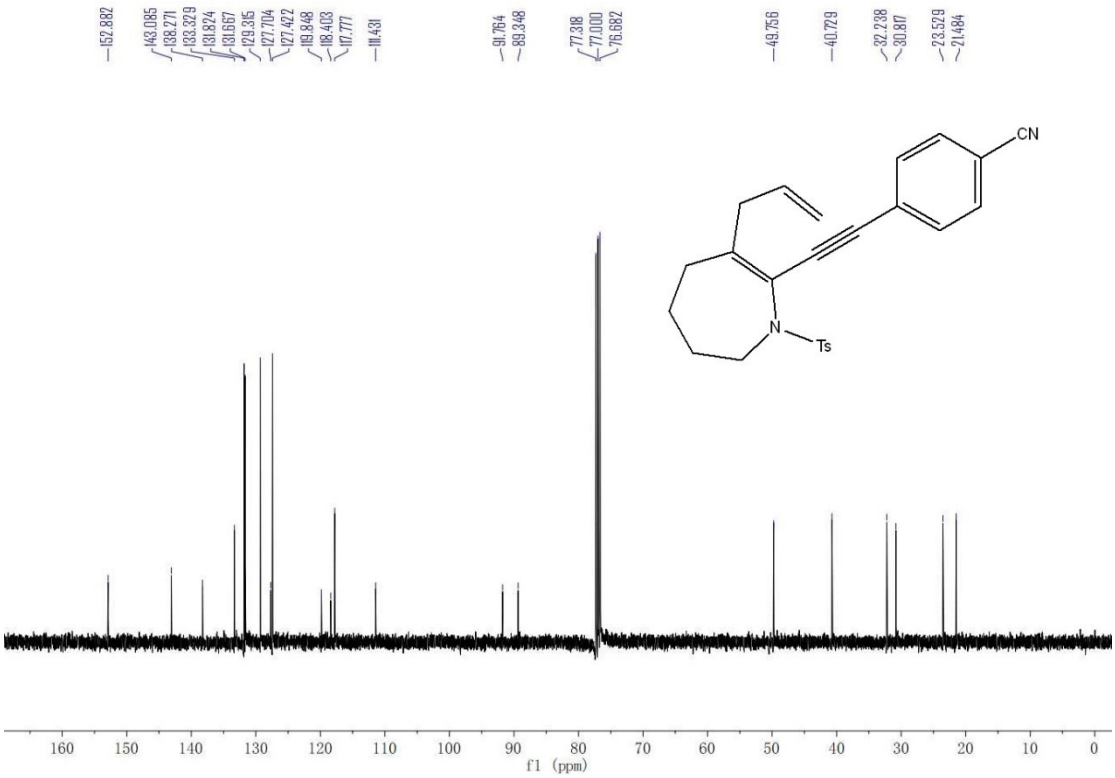


6-Allyl-7-((4-fluorophenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ae)

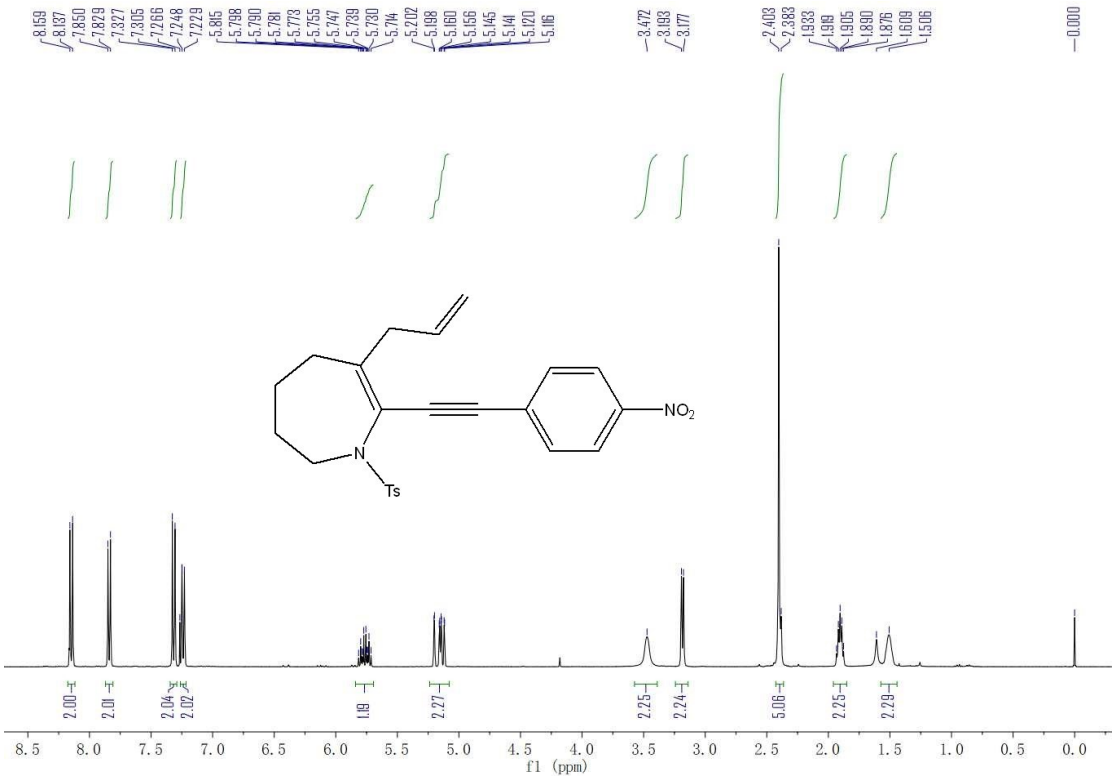


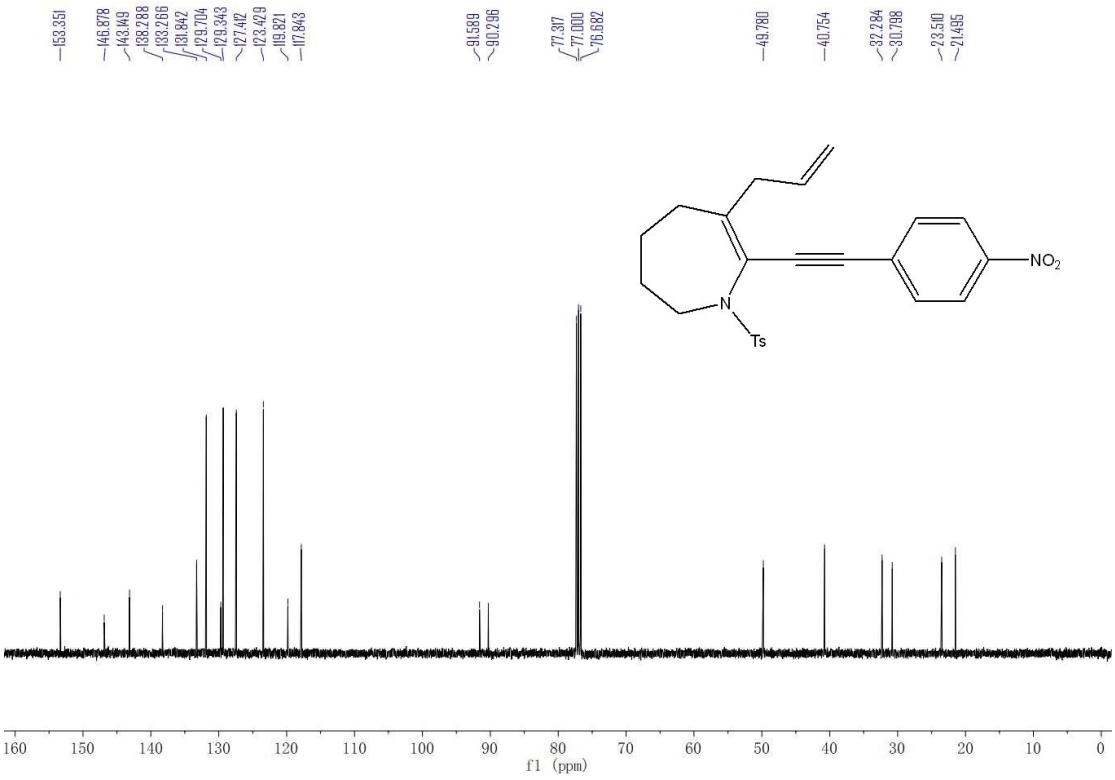
4-((3-Allyl-1-tosyl-4,5,6,7-tetrahydro-1*H*-azepin-2-yl)ethynyl)benzonitrile (3af)



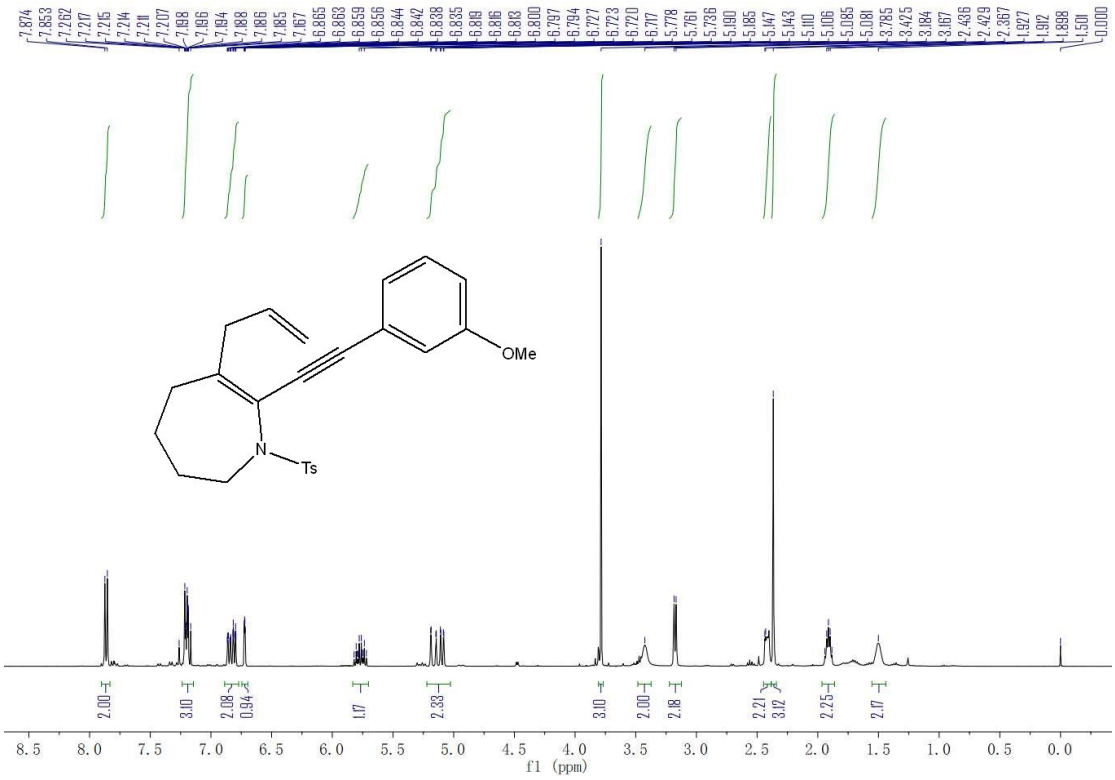


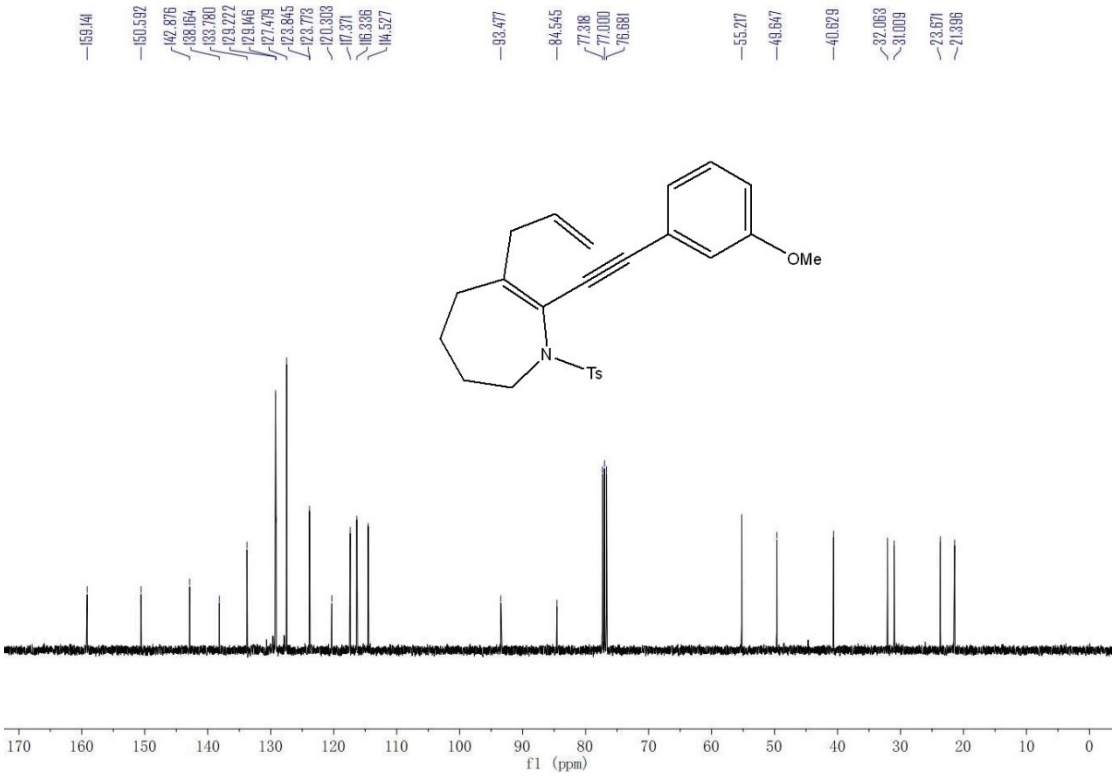
6-Allyl-7-((4-nitrophenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ag)



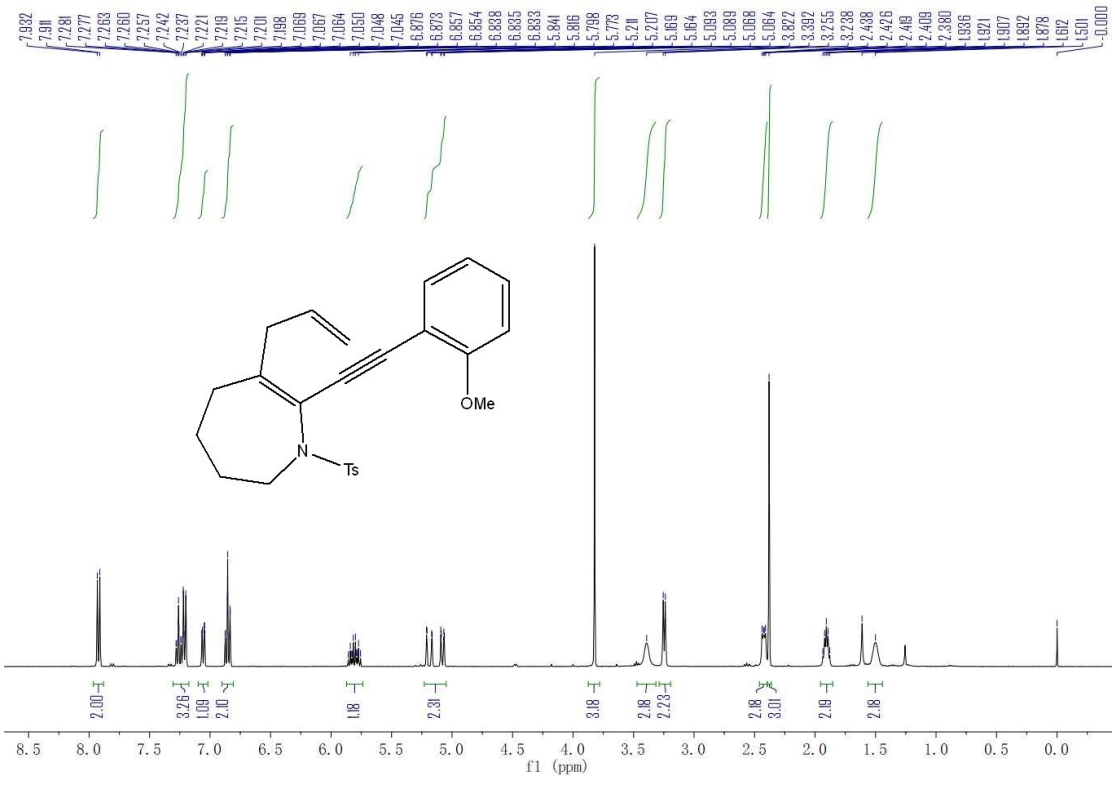


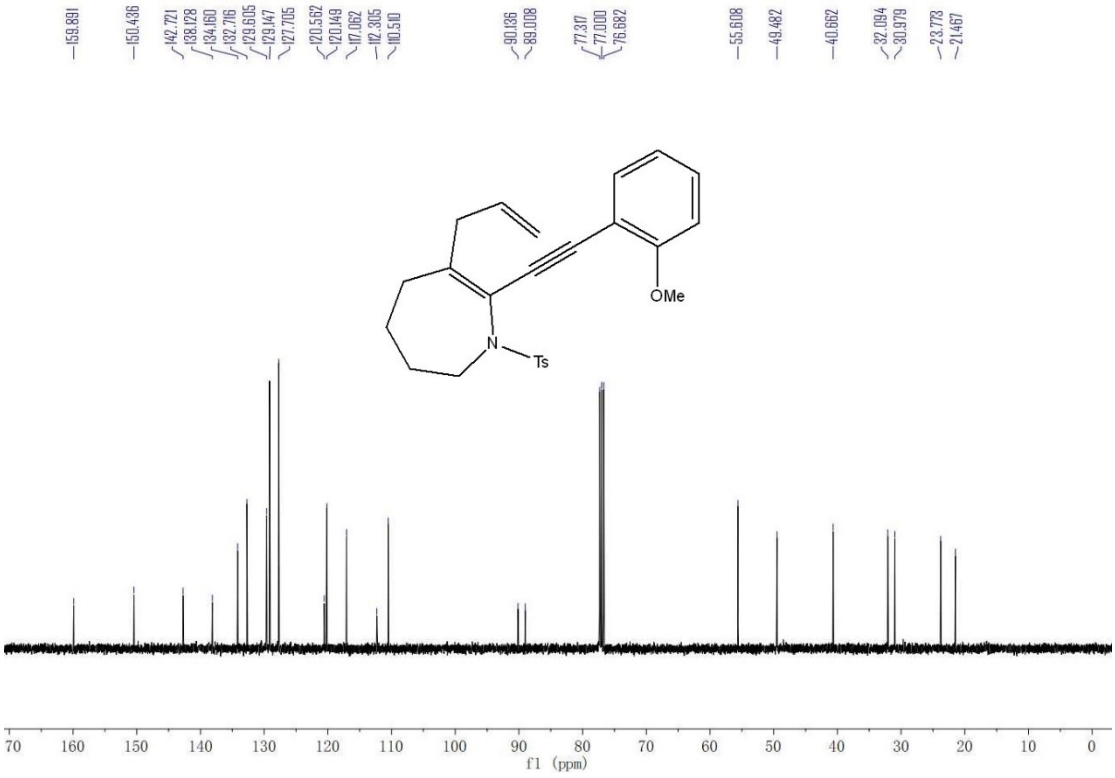
6-Allyl-7-((3-methoxyphenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ah)



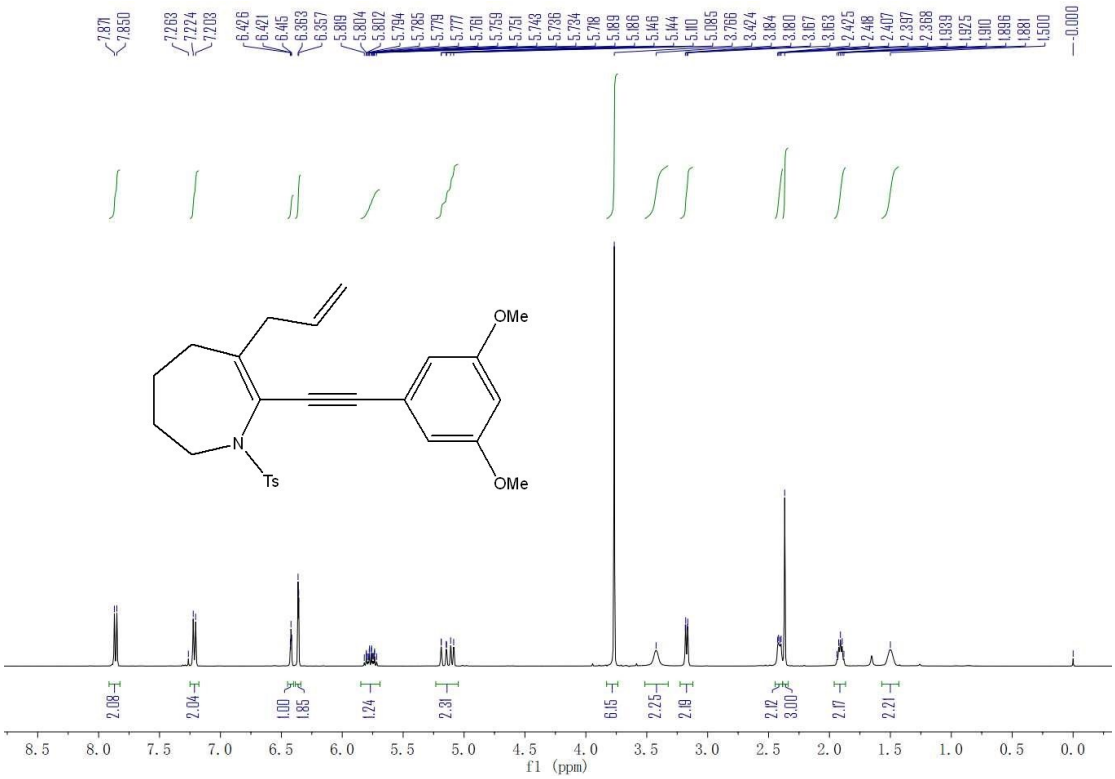


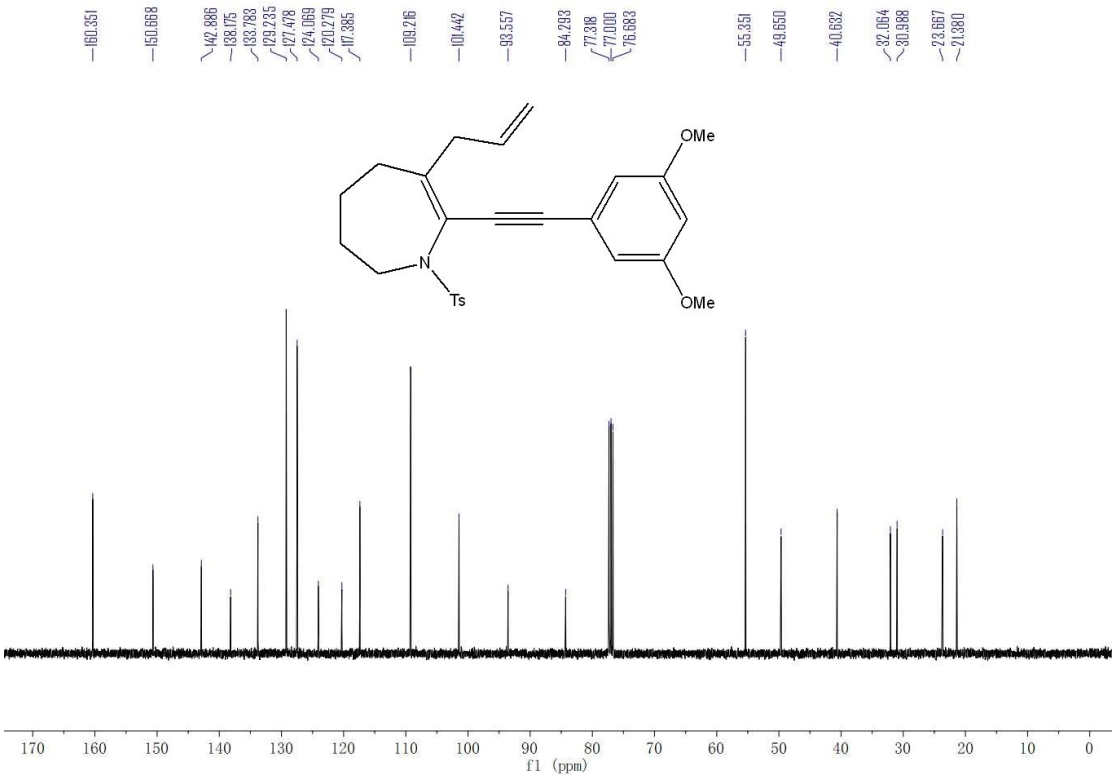
6-Allyl-7-((2-methoxyphenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ai)



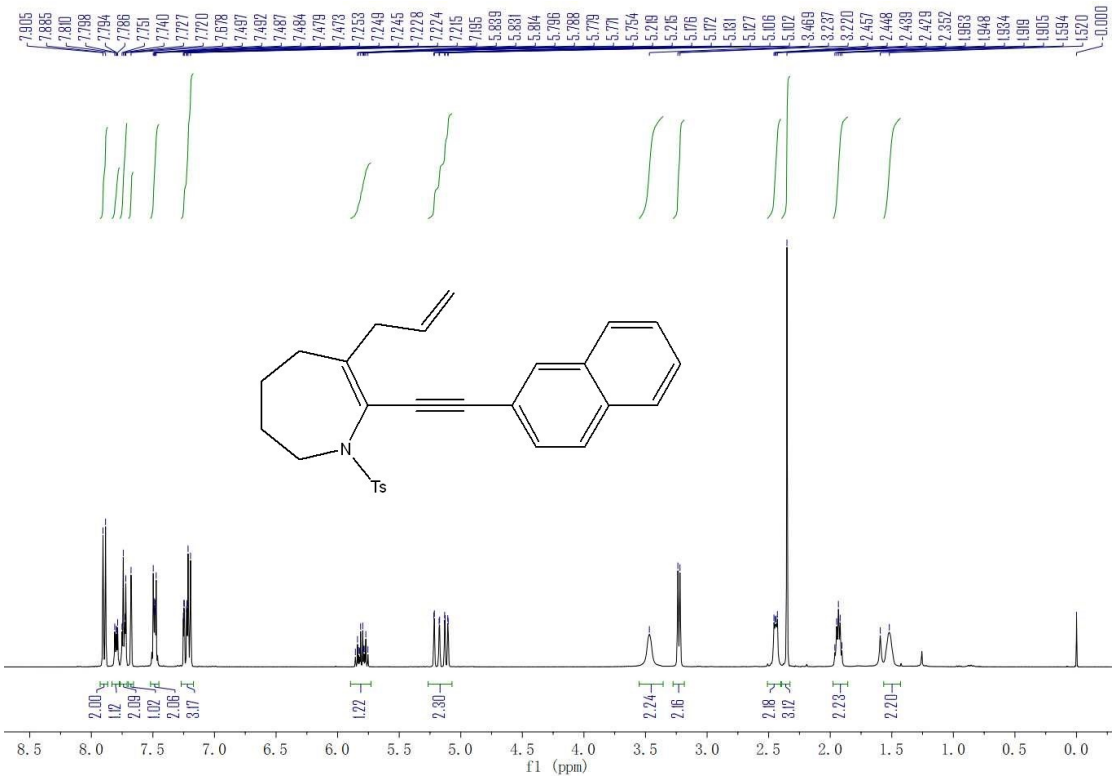


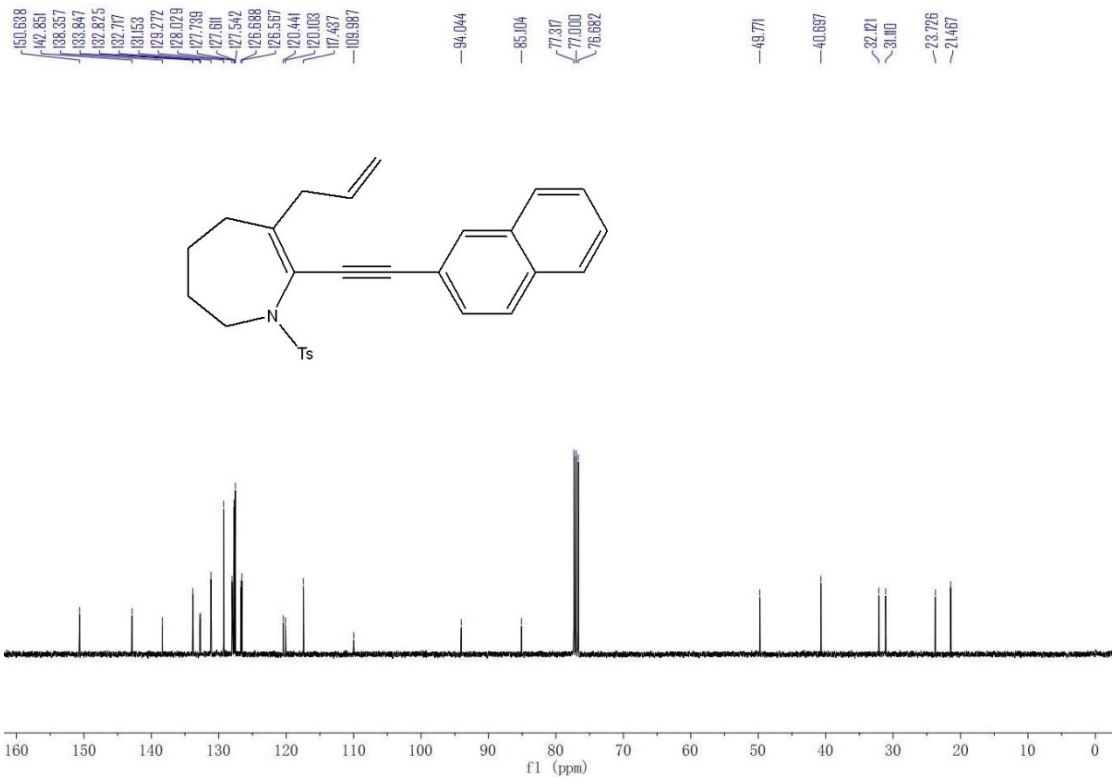
6-Allyl-7-((3,5-dimethoxyphenyl)ethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3aj)





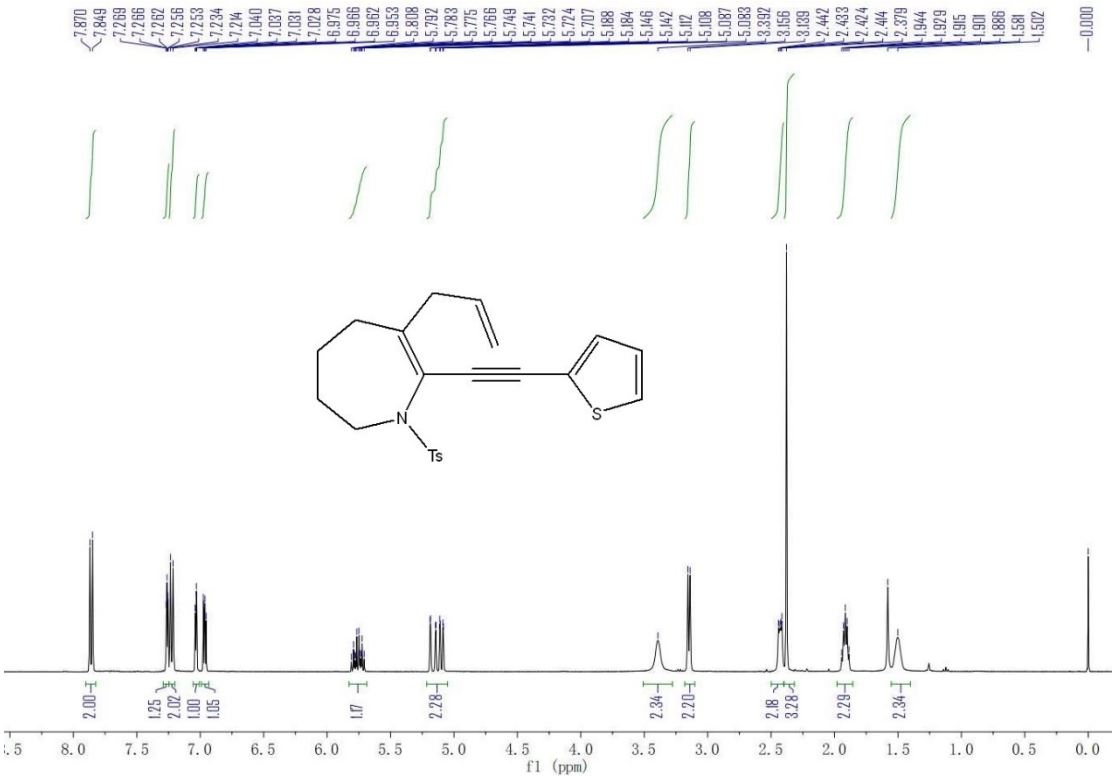
6-Allyl-7-(naphthalen-2-ylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ak)

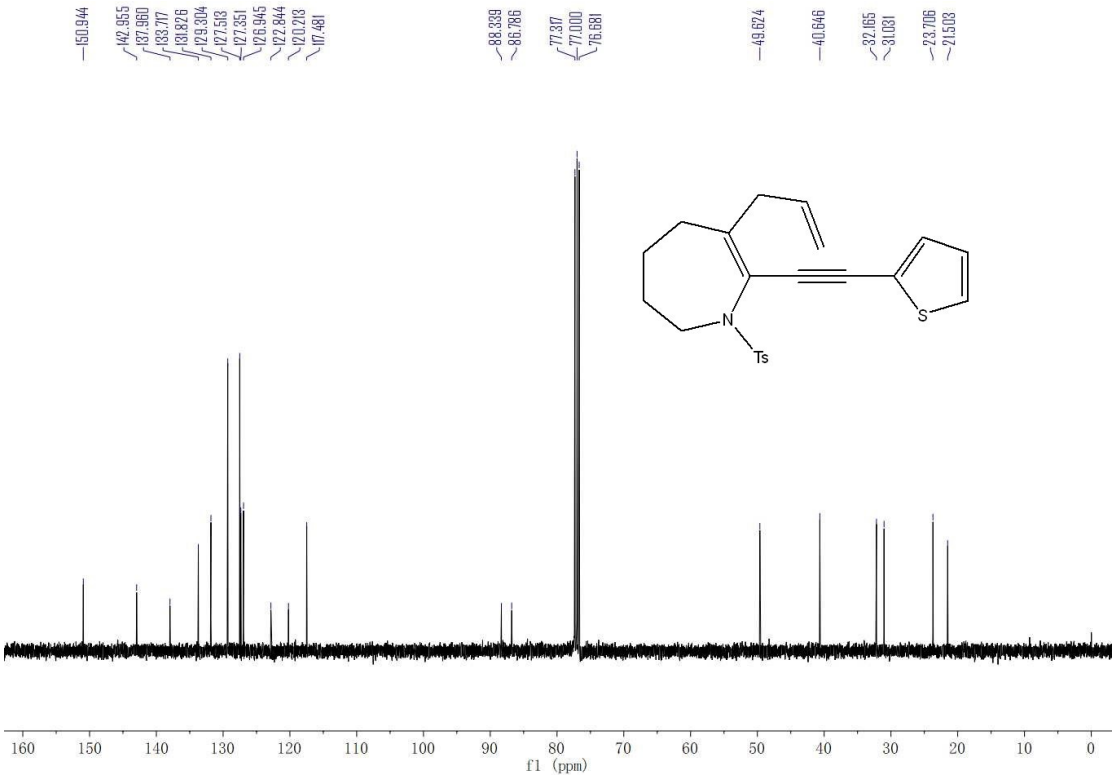




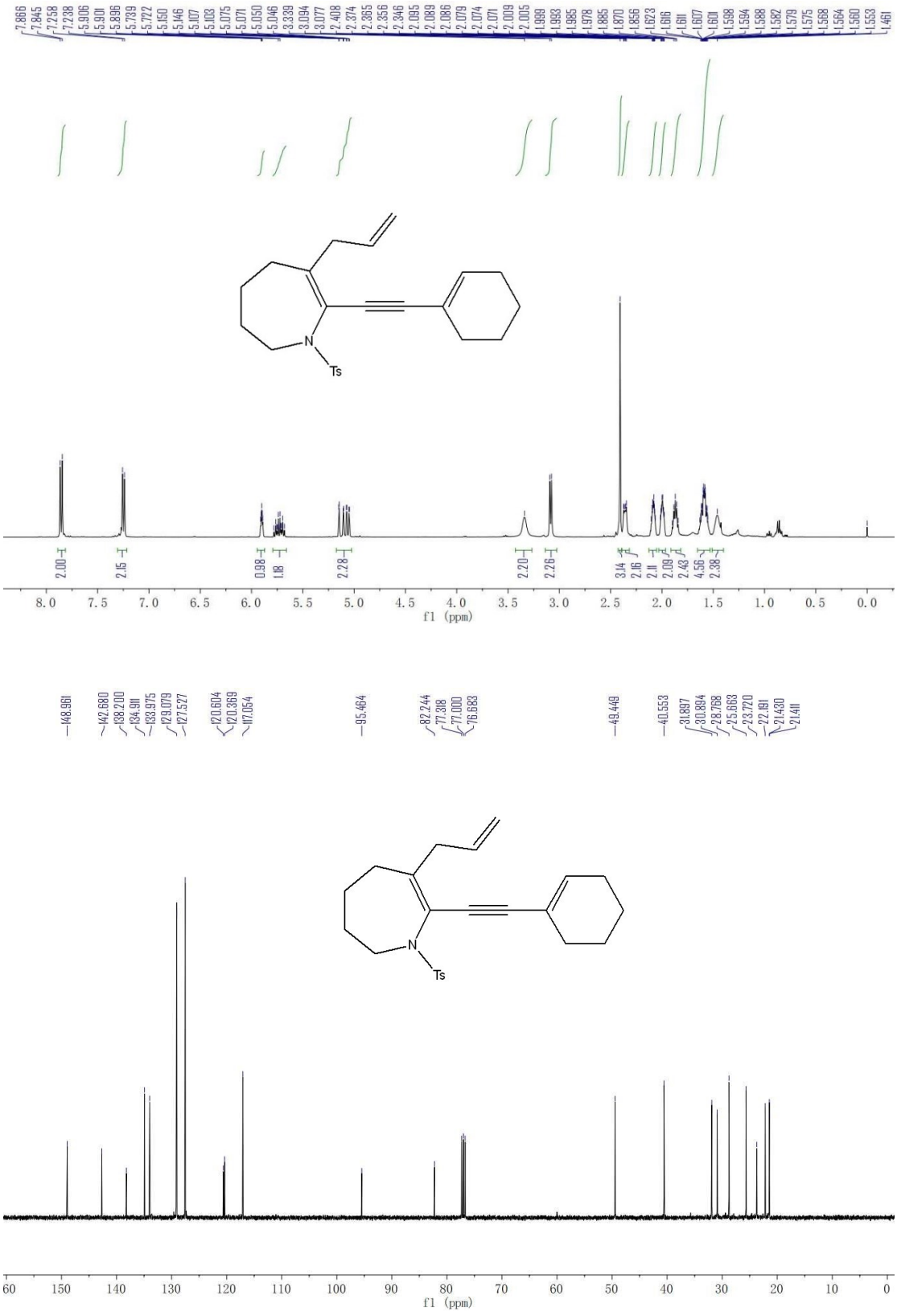
6-Allyl-7-(pyridin-2-ylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3al)

6-Allyl-7-(thiophen-2-ylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3am)

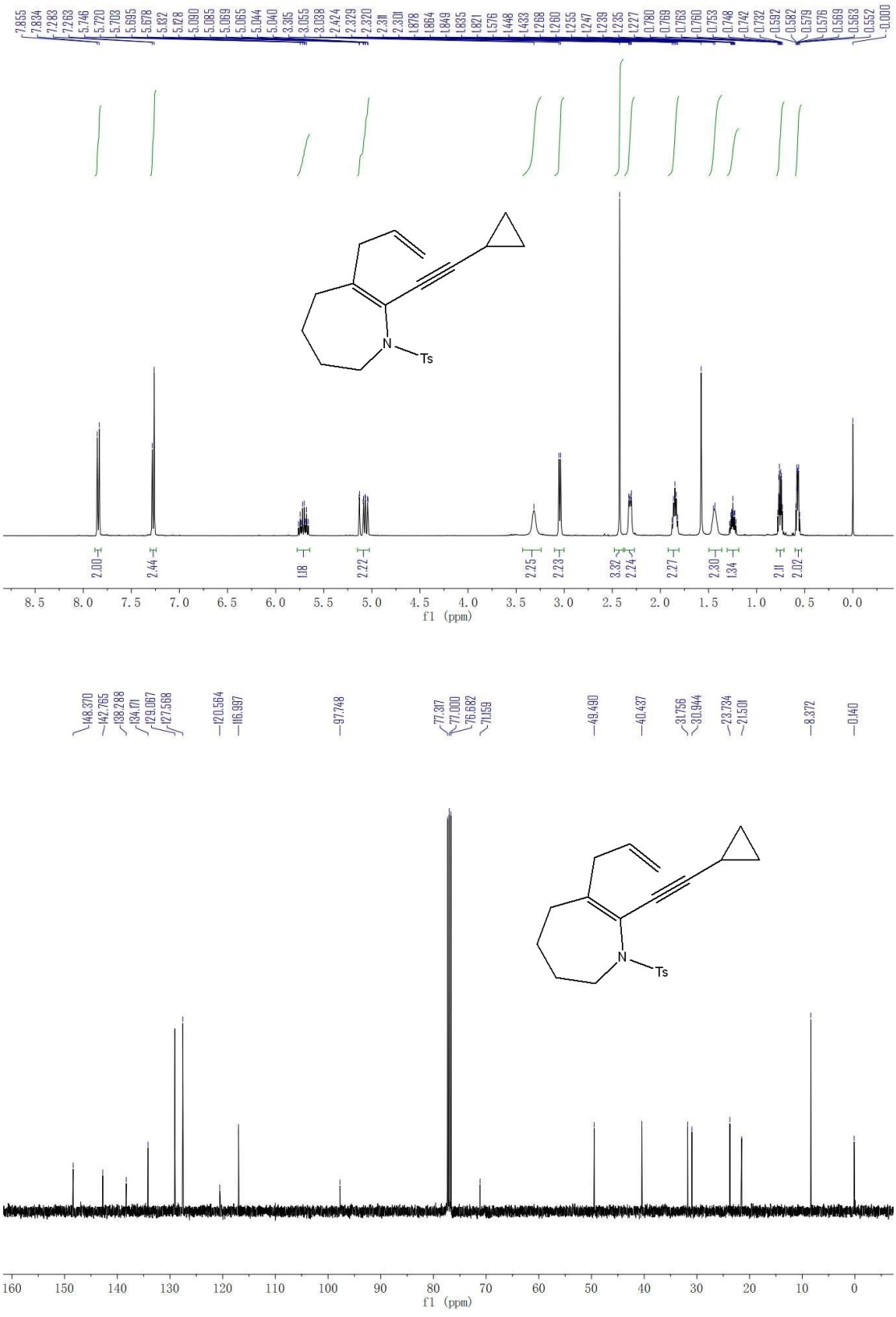




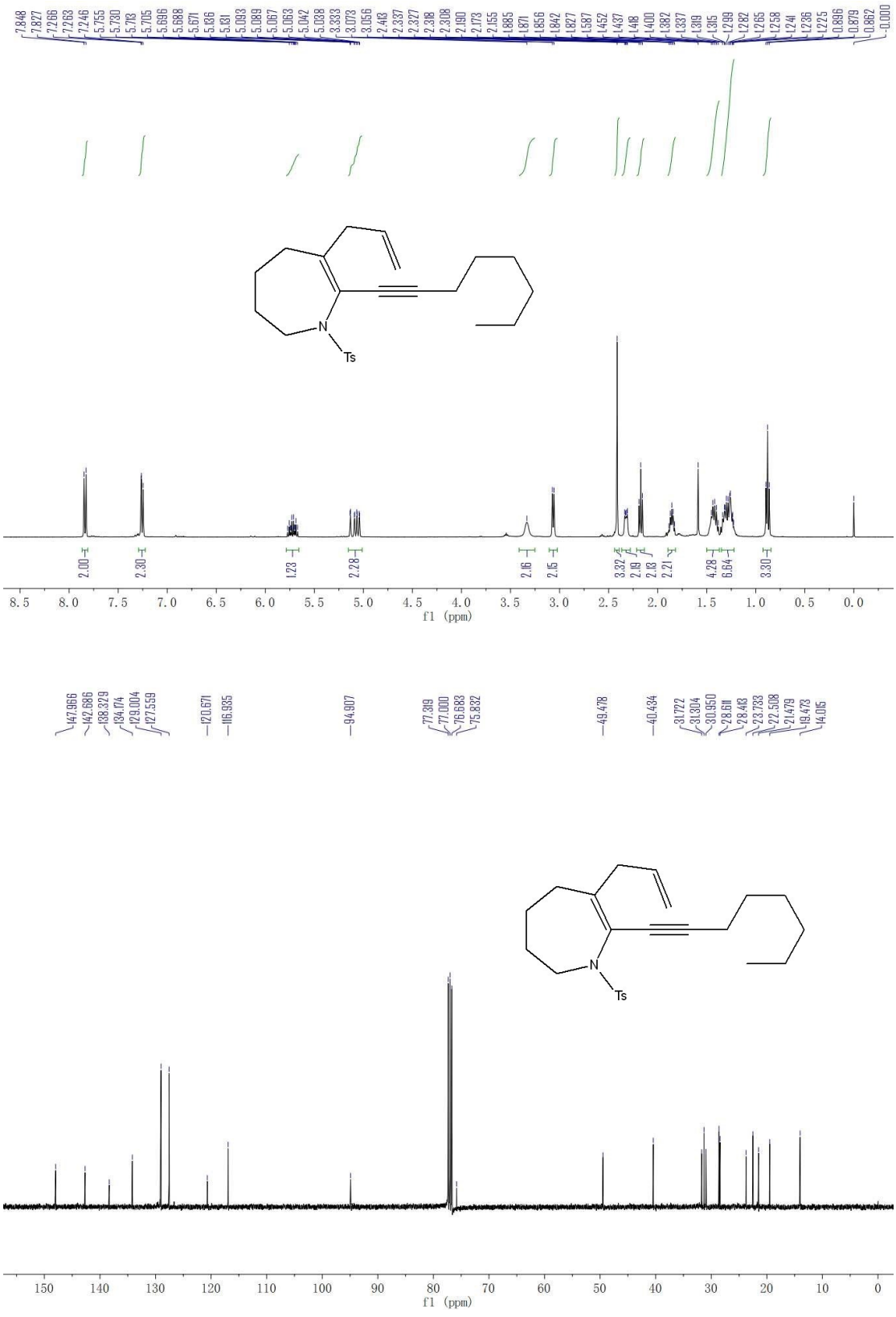
6-Allyl-7-(cyclohex-1-en-1-ylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3an)



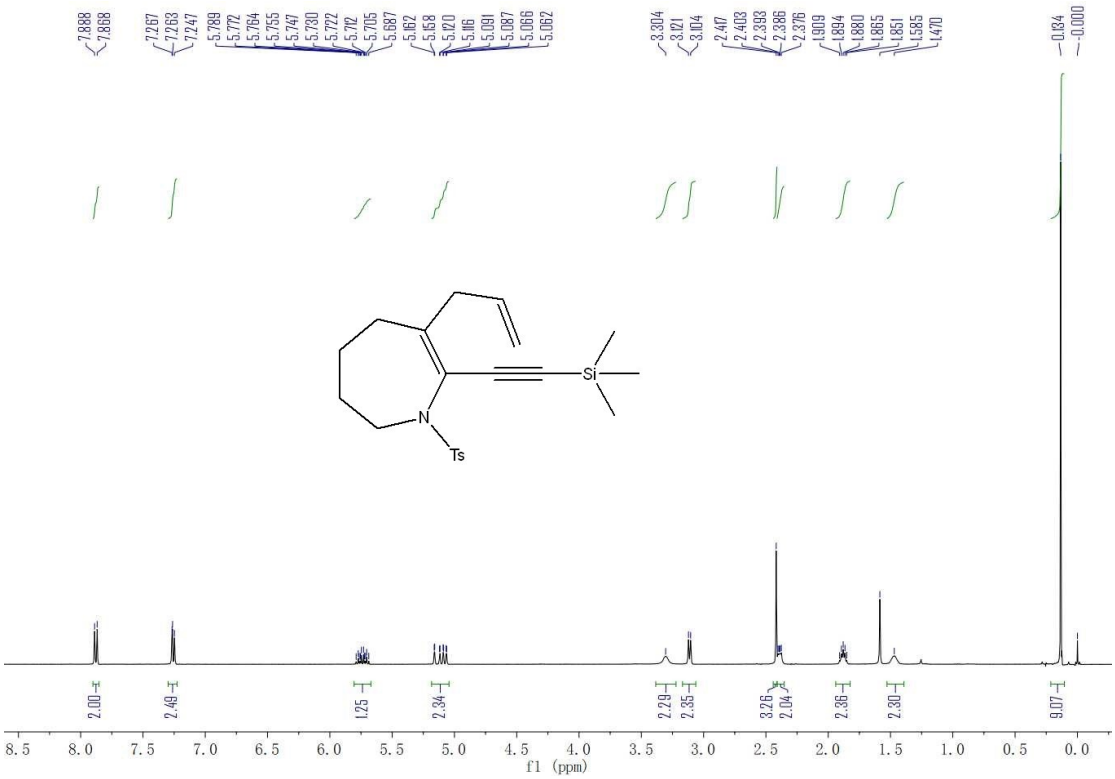
6-Allyl-7-(cyclopropylethynyl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ao)

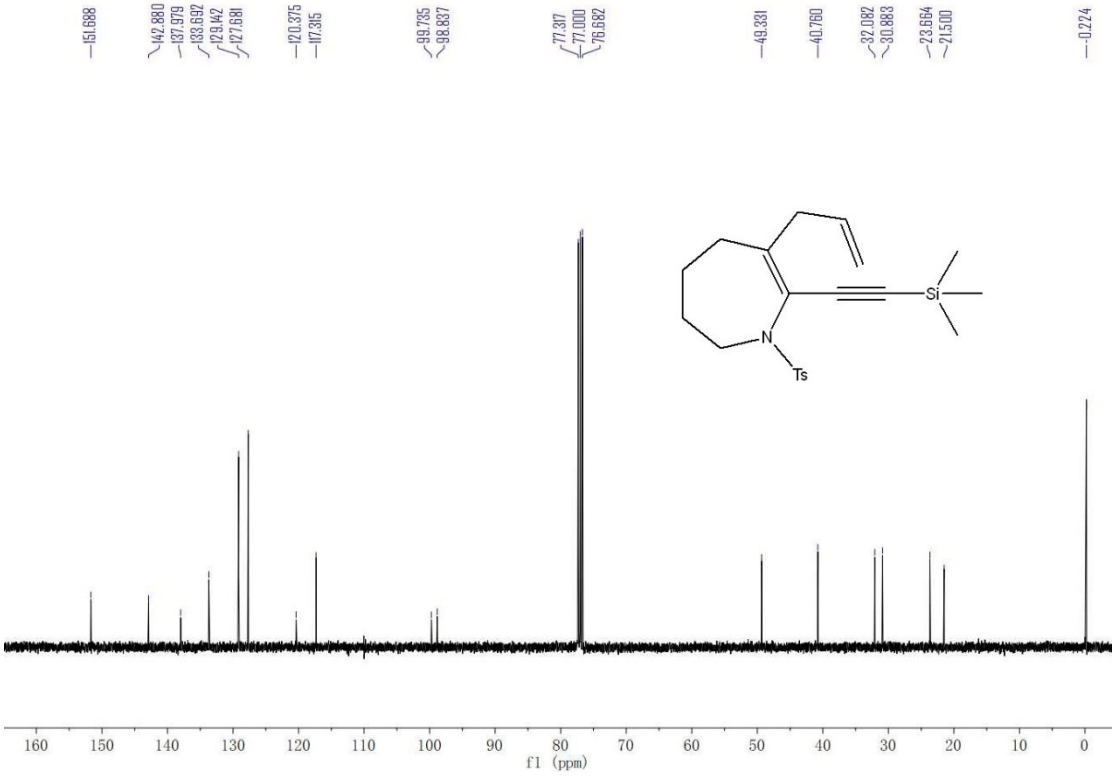


6-Allyl-7-(oct-1-yn-1-yl)-1-tosyl-2,3,4,5-tetrahydro-1*H*-azepine (3ap)

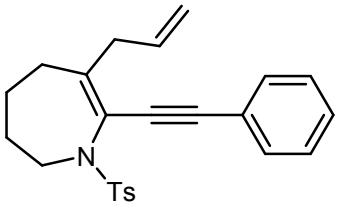


6-Allyl-1-tosyl-7-((trimethylsilyl)ethynyl)-2,3,4,5-tetrahydro-1*H*-azepine (3aq)





(G) X-ray crystallographic data of compound 3aa



CCDC 1910929

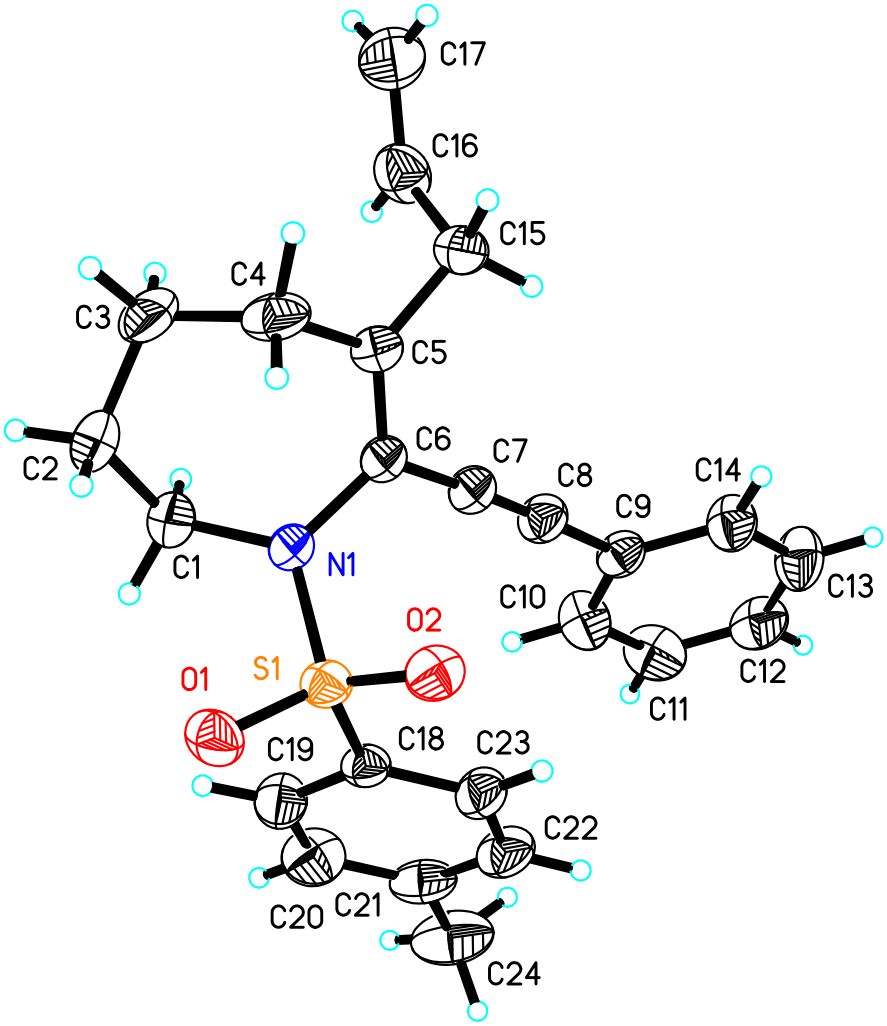


Table 1. Crystal data and structure refinement for d8v18637.

Identification code	d8v18637	
Empirical formula	C24 H25 N O2 S	
Formula weight	391.51	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.3035(4) Å	α= 85.085(2)°.
	b = 9.6639(6) Å	β= 70.963(2)°.
	c = 13.7416(7) Å	γ = 67.2140(10)°.
Volume	1075.59(10) $Å^3$	
Z	2	
Density (calculated)	1.209 Mg/m^3	
Absorption coefficient	0.169 mm^{-1}	
F(000)	416	
Crystal size	0.200 x 0.170 x 0.130 mm^3	
Theta range for data collection	2.835 to 25.995°.	
Index ranges	-11<=h<=11, -11<=k<=11, -16<=l<=16	
Reflections collected	17792	
Independent reflections	4181 [R(int) = 0.0389]	
Completeness to theta = 25.242°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6846	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4181 / 0 / 263	
Goodness-of-fit on F^2	1.013	
Final R indices [I>2sigma(I)]	R1 = 0.0438, wR2 = 0.1045	
R indices (all data)	R1 = 0.0571, wR2 = 0.1145	
Extinction coefficient	0.061(9)	
Largest diff. peak and hole	0.195 and -0.274 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d8v18637. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	2779(1)	5236(1)	8486(1)	52(1)
O(1)	1190(2)	6029(2)	9203(1)	70(1)
O(2)	3737(2)	6037(1)	7876(1)	63(1)
N(1)	2496(2)	4299(2)	7683(1)	53(1)
C(1)	1158(3)	3736(3)	8011(2)	74(1)
C(2)	-226(3)	4634(4)	7579(2)	100(1)
C(3)	250(3)	4604(3)	6416(2)	92(1)
C(4)	1577(3)	5201(2)	5889(2)	71(1)
C(5)	3281(2)	4145(2)	5837(1)	51(1)
C(6)	3716(2)	3771(2)	6691(1)	49(1)
C(7)	5329(2)	2781(2)	6683(1)	54(1)
C(8)	6670(2)	1976(2)	6707(2)	59(1)
C(9)	8253(2)	1007(2)	6771(2)	54(1)
C(10)	8361(3)	70(2)	7586(2)	74(1)
C(11)	9879(3)	-859(3)	7665(2)	82(1)
C(12)	11281(3)	-864(3)	6946(2)	77(1)
C(13)	11193(3)	50(3)	6135(2)	82(1)
C(14)	9687(2)	990(2)	6046(2)	68(1)
C(15)	4458(3)	3434(2)	4802(2)	62(1)
C(16)	4113(3)	2179(3)	4507(2)	76(1)
C(17)	3835(4)	2037(5)	3664(3)	108(1)
C(18)	3965(2)	3943(2)	9182(1)	49(1)
C(19)	3257(3)	3165(2)	9945(2)	68(1)
C(20)	4212(3)	2139(3)	10468(2)	83(1)
C(21)	5843(3)	1885(2)	10264(2)	72(1)
C(22)	6502(3)	2712(3)	9526(2)	74(1)
C(23)	5583(2)	3738(2)	8975(2)	64(1)
C(24)	6879(4)	741(3)	10839(2)	109(1)

Table 3. Bond lengths [Å] and angles [°] for d8v18637.

S(1)-O(2)	1.4247(14)
S(1)-O(1)	1.4305(14)
S(1)-N(1)	1.6293(15)
S(1)-C(18)	1.7629(17)
N(1)-C(6)	1.437(2)
N(1)-C(1)	1.471(2)
C(1)-C(2)	1.519(3)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(3)	1.513(3)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.509(3)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.499(3)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(6)	1.340(2)
C(5)-C(15)	1.505(3)
C(6)-C(7)	1.430(2)
C(7)-C(8)	1.197(2)
C(8)-C(9)	1.434(2)
C(9)-C(14)	1.375(3)
C(9)-C(10)	1.384(3)
C(10)-C(11)	1.383(3)
C(10)-H(10)	0.9300
C(11)-C(12)	1.354(3)
C(11)-H(11)	0.9300
C(12)-C(13)	1.366(3)
C(12)-H(12)	0.9300
C(13)-C(14)	1.382(3)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(16)	1.486(3)
C(15)-H(15A)	0.9700

C(15)-H(15B)	0.9700
C(16)-C(17)	1.295(4)
C(16)-H(16)	0.9300
C(17)-H(17A)	0.95(4)
C(17)-H(17B)	1.02(3)
C(18)-C(23)	1.373(3)
C(18)-C(19)	1.377(3)
C(19)-C(20)	1.380(3)
C(19)-H(19)	0.9300
C(20)-C(21)	1.373(3)
C(20)-H(20)	0.9300
C(21)-C(22)	1.371(3)
C(21)-C(24)	1.515(3)
C(22)-C(23)	1.387(3)
C(22)-H(22)	0.9300
C(23)-H(23)	0.9300
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600

O(2)-S(1)-O(1)	120.29(9)
O(2)-S(1)-N(1)	106.48(8)
O(1)-S(1)-N(1)	106.28(8)
O(2)-S(1)-C(18)	107.53(8)
O(1)-S(1)-C(18)	107.38(8)
N(1)-S(1)-C(18)	108.43(8)
C(6)-N(1)-C(1)	117.58(15)
C(6)-N(1)-S(1)	120.35(11)
C(1)-N(1)-S(1)	121.16(13)
N(1)-C(1)-C(2)	111.8(2)
N(1)-C(1)-H(1A)	109.3
C(2)-C(1)-H(1A)	109.3
N(1)-C(1)-H(1B)	109.3
C(2)-C(1)-H(1B)	109.3
H(1A)-C(1)-H(1B)	107.9
C(3)-C(2)-C(1)	115.4(2)
C(3)-C(2)-H(2A)	108.4
C(1)-C(2)-H(2A)	108.4

C(3)-C(2)-H(2B)	108.4
C(1)-C(2)-H(2B)	108.4
H(2A)-C(2)-H(2B)	107.5
C(4)-C(3)-C(2)	114.49(19)
C(4)-C(3)-H(3A)	108.6
C(2)-C(3)-H(3A)	108.6
C(4)-C(3)-H(3B)	108.6
C(2)-C(3)-H(3B)	108.6
H(3A)-C(3)-H(3B)	107.6
C(5)-C(4)-C(3)	114.65(19)
C(5)-C(4)-H(4A)	108.6
C(3)-C(4)-H(4A)	108.6
C(5)-C(4)-H(4B)	108.6
C(3)-C(4)-H(4B)	108.6
H(4A)-C(4)-H(4B)	107.6
C(6)-C(5)-C(4)	121.27(17)
C(6)-C(5)-C(15)	120.83(17)
C(4)-C(5)-C(15)	117.77(16)
C(5)-C(6)-C(7)	123.44(17)
C(5)-C(6)-N(1)	119.51(15)
C(7)-C(6)-N(1)	116.92(15)
C(8)-C(7)-C(6)	177.7(2)
C(7)-C(8)-C(9)	178.2(2)
C(14)-C(9)-C(10)	118.35(18)
C(14)-C(9)-C(8)	121.86(18)
C(10)-C(9)-C(8)	119.79(18)
C(11)-C(10)-C(9)	120.5(2)
C(11)-C(10)-H(10)	119.7
C(9)-C(10)-H(10)	119.7
C(12)-C(11)-C(10)	120.5(2)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(11)-C(12)-C(13)	119.6(2)
C(11)-C(12)-H(12)	120.2
C(13)-C(12)-H(12)	120.2
C(12)-C(13)-C(14)	120.7(2)
C(12)-C(13)-H(13)	119.7
C(14)-C(13)-H(13)	119.7

C(9)-C(14)-C(13)	120.3(2)
C(9)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8
C(16)-C(15)-C(5)	111.13(17)
C(16)-C(15)-H(15A)	109.4
C(5)-C(15)-H(15A)	109.4
C(16)-C(15)-H(15B)	109.4
C(5)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0
C(17)-C(16)-C(15)	126.3(3)
C(17)-C(16)-H(16)	116.9
C(15)-C(16)-H(16)	116.9
C(16)-C(17)-H(17A)	120(2)
C(16)-C(17)-H(17B)	114.7(19)
H(17A)-C(17)-H(17B)	125(3)
C(23)-C(18)-C(19)	120.24(18)
C(23)-C(18)-S(1)	119.85(15)
C(19)-C(18)-S(1)	119.90(14)
C(18)-C(19)-C(20)	119.0(2)
C(18)-C(19)-H(19)	120.5
C(20)-C(19)-H(19)	120.5
C(21)-C(20)-C(19)	122.1(2)
C(21)-C(20)-H(20)	119.0
C(19)-C(20)-H(20)	119.0
C(22)-C(21)-C(20)	117.68(19)
C(22)-C(21)-C(24)	120.9(2)
C(20)-C(21)-C(24)	121.4(2)
C(21)-C(22)-C(23)	121.7(2)
C(21)-C(22)-H(22)	119.1
C(23)-C(22)-H(22)	119.1
C(18)-C(23)-C(22)	119.2(2)
C(18)-C(23)-H(23)	120.4
C(22)-C(23)-H(23)	120.4
C(21)-C(24)-H(24A)	109.5
C(21)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(21)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5

H(24B)-C(24)-H(24C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for d8v18637. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	50(1)	54(1)	49(1)	4(1)	-22(1)	-14(1)
O(1)	55(1)	73(1)	61(1)	-7(1)	-17(1)	-3(1)
O(2)	76(1)	60(1)	63(1)	16(1)	-31(1)	-32(1)
N(1)	44(1)	72(1)	47(1)	3(1)	-19(1)	-22(1)
C(1)	62(1)	105(2)	67(1)	2(1)	-16(1)	-46(1)
C(2)	51(1)	163(3)	91(2)	-15(2)	-23(1)	-42(2)
C(3)	57(1)	131(2)	90(2)	-20(2)	-40(1)	-19(1)
C(4)	74(1)	68(1)	67(1)	-4(1)	-44(1)	-6(1)
C(5)	55(1)	51(1)	51(1)	2(1)	-23(1)	-19(1)
C(6)	44(1)	54(1)	50(1)	4(1)	-19(1)	-18(1)
C(7)	49(1)	61(1)	56(1)	4(1)	-21(1)	-20(1)
C(8)	53(1)	61(1)	64(1)	2(1)	-25(1)	-17(1)
C(9)	50(1)	50(1)	64(1)	1(1)	-26(1)	-13(1)
C(10)	65(1)	66(1)	77(2)	14(1)	-19(1)	-16(1)
C(11)	86(2)	64(1)	78(2)	15(1)	-36(1)	-6(1)
C(12)	63(1)	68(1)	93(2)	-1(1)	-42(1)	-3(1)
C(13)	50(1)	88(2)	102(2)	12(1)	-24(1)	-19(1)
C(14)	56(1)	71(1)	76(1)	17(1)	-27(1)	-20(1)
C(15)	69(1)	70(1)	51(1)	2(1)	-19(1)	-30(1)
C(16)	79(2)	70(1)	71(1)	-11(1)	-8(1)	-31(1)
C(17)	110(2)	131(3)	96(2)	-35(2)	-21(2)	-62(2)
C(18)	52(1)	53(1)	45(1)	3(1)	-22(1)	-17(1)
C(19)	66(1)	78(1)	66(1)	18(1)	-27(1)	-30(1)
C(20)	106(2)	82(2)	75(2)	31(1)	-44(1)	-42(1)
C(21)	95(2)	58(1)	68(1)	1(1)	-51(1)	-14(1)
C(22)	64(1)	81(2)	80(2)	1(1)	-42(1)	-16(1)
C(23)	59(1)	77(1)	64(1)	11(1)	-29(1)	-28(1)
C(24)	146(3)	76(2)	112(2)	12(2)	-92(2)	-12(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for d8v18637.

	x	y	z	U(eq)
H(1A)	726	3792	8758	89
H(1B)	1591	2690	7781	89
H(2A)	-1097	4253	7847	120
H(2B)	-670	5671	7832	120
H(3A)	622	3576	6163	110
H(3B)	-722	5192	6224	110
H(4A)	1554	5442	5193	85
H(4B)	1325	6127	6250	85
H(10)	7406	64	8084	89
H(11)	9936	-1486	8215	98
H(12)	12298	-1486	7005	92
H(13)	12156	39	5637	99
H(14)	9644	1615	5494	82
H(15A)	4362	4186	4286	74
H(15B)	5576	3057	4824	74
H(16)	4094	1424	4972	91
H(19)	2150	3329	10104	82
H(20)	3737	1603	10976	100
H(22)	7594	2583	9392	89
H(23)	6057	4281	8472	77
H(24A)	7145	1251	11283	163
H(24B)	7875	82	10353	163
H(24C)	6274	165	11244	163
H(17A)	3600(40)	1200(40)	3550(30)	139(12)
H(17B)	3840(40)	2900(40)	3180(30)	132(13)

Table 6. Torsion angles [°] for d8v18637.

O(2)-S(1)-N(1)-C(6)	30.77(15)
O(1)-S(1)-N(1)-C(6)	160.15(13)
C(18)-S(1)-N(1)-C(6)	-84.68(15)
O(2)-S(1)-N(1)-C(1)	-160.36(15)
O(1)-S(1)-N(1)-C(1)	-30.99(18)
C(18)-S(1)-N(1)-C(1)	84.19(17)
C(6)-N(1)-C(1)-C(2)	-83.8(2)
S(1)-N(1)-C(1)-C(2)	106.99(19)
N(1)-C(1)-C(2)-C(3)	61.1(3)
C(1)-C(2)-C(3)-C(4)	-59.5(3)
C(2)-C(3)-C(4)-C(5)	76.5(3)
C(3)-C(4)-C(5)-C(6)	-66.7(2)
C(3)-C(4)-C(5)-C(15)	109.2(2)
C(4)-C(5)-C(6)-C(7)	-179.40(17)
C(15)-C(5)-C(6)-C(7)	4.8(3)
C(4)-C(5)-C(6)-N(1)	4.8(3)
C(15)-C(5)-C(6)-N(1)	-170.99(16)
C(1)-N(1)-C(6)-C(5)	65.8(2)
S(1)-N(1)-C(6)-C(5)	-124.98(16)
C(1)-N(1)-C(6)-C(7)	-110.31(19)
S(1)-N(1)-C(6)-C(7)	58.9(2)
C(14)-C(9)-C(10)-C(11)	-0.1(3)
C(8)-C(9)-C(10)-C(11)	-179.2(2)
C(9)-C(10)-C(11)-C(12)	0.1(4)
C(10)-C(11)-C(12)-C(13)	-0.4(4)
C(11)-C(12)-C(13)-C(14)	0.7(4)
C(10)-C(9)-C(14)-C(13)	0.4(3)
C(8)-C(9)-C(14)-C(13)	179.5(2)
C(12)-C(13)-C(14)-C(9)	-0.7(4)
C(6)-C(5)-C(15)-C(16)	98.3(2)
C(4)-C(5)-C(15)-C(16)	-77.6(2)
C(5)-C(15)-C(16)-C(17)	125.3(3)
O(2)-S(1)-C(18)-C(23)	-7.81(18)
O(1)-S(1)-C(18)-C(23)	-138.59(16)
N(1)-S(1)-C(18)-C(23)	106.95(16)
O(2)-S(1)-C(18)-C(19)	170.83(16)

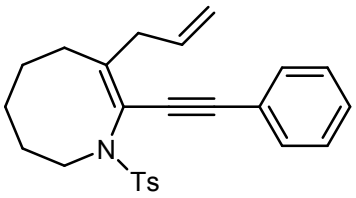
O(1)-S(1)-C(18)-C(19)	40.05(18)
N(1)-S(1)-C(18)-C(19)	-74.41(17)
C(23)-C(18)-C(19)-C(20)	-2.4(3)
S(1)-C(18)-C(19)-C(20)	178.92(17)
C(18)-C(19)-C(20)-C(21)	1.0(4)
C(19)-C(20)-C(21)-C(22)	1.3(4)
C(19)-C(20)-C(21)-C(24)	-179.3(2)
C(20)-C(21)-C(22)-C(23)	-2.1(3)
C(24)-C(21)-C(22)-C(23)	178.4(2)
C(19)-C(18)-C(23)-C(22)	1.6(3)
S(1)-C(18)-C(23)-C(22)	-179.76(16)
C(21)-C(22)-C(23)-C(18)	0.7(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for d8v18637 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

(H) X-ray crystallographic data of compound 3ca



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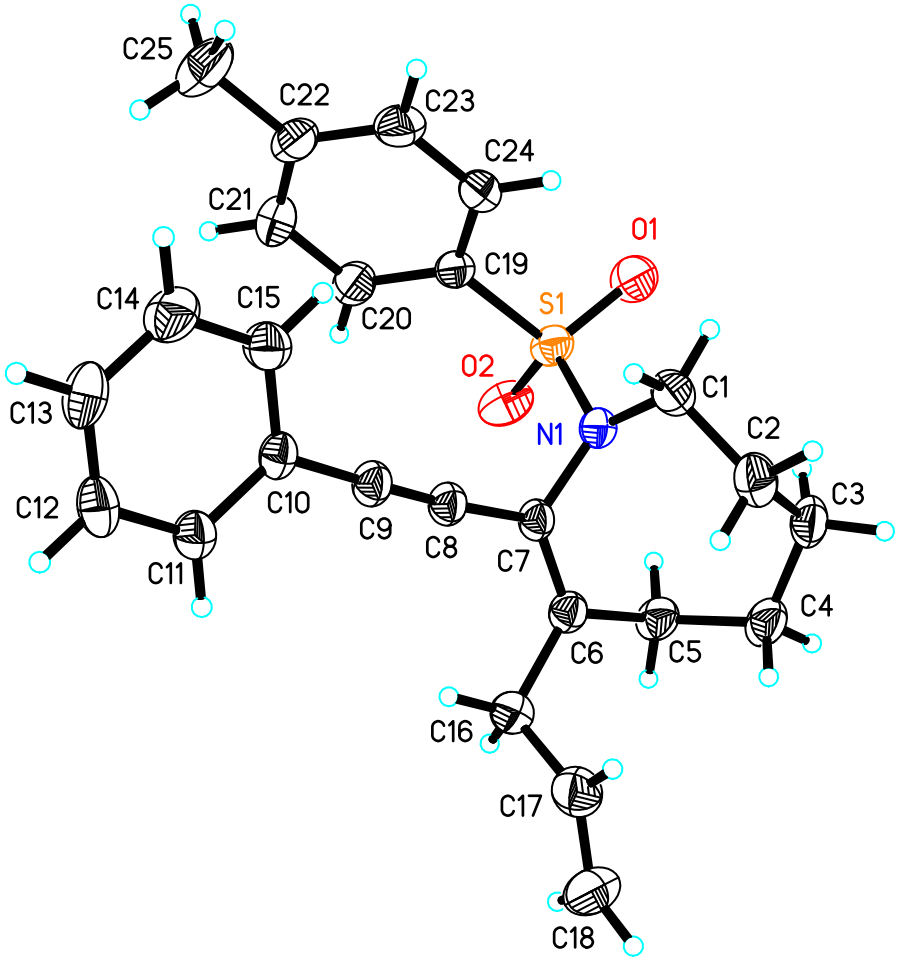


Table 1. Crystal data and structure refinement for mo_dd18203_0m.

Identification code	mo_dd18203_0m	
Empirical formula	C25 H27 N O2 S	
Formula weight	405.53	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.1582(2) Å	α= 113.1630(10)°.
	b = 11.9799(3) Å	β= 109.3030(10)°.
	c = 12.0459(3) Å	γ = 97.3560(10)°.
Volume	1094.87(5) $Å^3$	
Z	2	
Density (calculated)	1.230 Mg/m^3	
Absorption coefficient	0.168 mm^{-1}	
F(000)	432	
Crystal size	0.200 x 0.180 x 0.140 mm^3	
Theta range for data collection	2.468 to 25.998°.	
Index ranges	-11<=h<=11, -14<=k<=14, -14<=l<=14	
Reflections collected	16240	
Independent reflections	4273 [R(int) = 0.0299]	
Completeness to theta = 25.242°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6550	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4273 / 0 / 272	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2sigma(I)]	R1 = 0.0420, wR2 = 0.1100	
R indices (all data)	R1 = 0.0516, wR2 = 0.1182	
Extinction coefficient	0.051(11)	
Largest diff. peak and hole	0.267 and -0.311 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_dd18203_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	1764(1)	7641(1)	3180(1)	53(1)
O(1)	2522(2)	8479(1)	2818(1)	76(1)
O(2)	168(2)	6791(1)	2314(1)	70(1)
N(1)	2948(2)	6764(1)	3382(1)	46(1)
C(1)	4716(2)	7333(2)	4017(2)	60(1)
C(2)	5550(2)	6388(2)	3448(2)	66(1)
C(3)	4890(3)	5751(2)	1929(2)	67(1)
C(4)	3699(3)	4426(2)	1188(2)	65(1)
C(5)	2043(2)	4305(2)	1242(2)	55(1)
C(6)	2032(2)	4510(2)	2558(2)	47(1)
C(7)	2388(2)	5675(2)	3542(2)	43(1)
C(8)	2422(2)	5954(2)	4823(2)	47(1)
C(9)	2481(2)	6261(2)	5913(2)	49(1)
C(10)	2571(2)	6661(2)	7231(2)	45(1)
C(11)	1980(2)	5792(2)	7590(2)	52(1)
C(12)	2078(2)	6196(2)	8863(2)	62(1)
C(13)	2754(2)	7456(2)	9778(2)	68(1)
C(14)	3340(3)	8319(2)	9429(2)	71(1)
C(15)	3255(2)	7933(2)	8167(2)	59(1)
C(16)	1600(2)	3350(2)	2732(2)	59(1)
C(17)	2763(3)	2612(2)	2692(2)	73(1)
C(18)	2424(6)	1394(3)	1953(4)	106(1)
C(19)	1741(2)	8597(2)	4717(2)	47(1)
C(20)	379(2)	8356(2)	4937(2)	61(1)
C(21)	365(3)	9126(2)	6131(2)	69(1)
C(22)	1694(3)	10138(2)	7127(2)	61(1)
C(23)	3054(3)	10359(2)	6894(2)	66(1)
C(24)	3091(2)	9602(2)	5702(2)	62(1)
C(25)	1680(4)	10972(3)	8437(2)	94(1)

Table 3. Bond lengths [Å] and angles [°] for mo_dd18203_0m.

S(1)-O(2)	1.4264(14)
S(1)-O(1)	1.4304(14)
S(1)-N(1)	1.6301(14)
S(1)-C(19)	1.7618(16)
N(1)-C(7)	1.4471(19)
N(1)-C(1)	1.469(2)
C(1)-C(2)	1.514(3)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(3)	1.532(3)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.517(3)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.530(3)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(6)	1.510(2)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-C(7)	1.336(2)
C(6)-C(16)	1.508(2)
C(7)-C(8)	1.433(2)
C(8)-C(9)	1.195(2)
C(9)-C(10)	1.437(2)
C(10)-C(15)	1.387(2)
C(10)-C(11)	1.388(2)
C(11)-C(12)	1.382(2)
C(11)-H(11)	0.9300
C(12)-C(13)	1.371(3)
C(12)-H(12)	0.9300
C(13)-C(14)	1.371(3)
C(13)-H(13)	0.9300
C(14)-C(15)	1.375(3)
C(14)-H(14)	0.9300

C(15)-H(15)	0.9300
C(16)-C(17)	1.470(3)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.303(4)
C(17)-H(17)	0.9300
C(18)-H(18A)	0.99(3)
C(18)-H(18B)	0.96(4)
C(19)-C(20)	1.376(2)
C(19)-C(24)	1.383(2)
C(20)-C(21)	1.375(3)
C(20)-H(20)	0.9300
C(21)-C(22)	1.380(3)
C(21)-H(21)	0.9300
C(22)-C(23)	1.380(3)
C(22)-C(25)	1.505(3)
C(23)-C(24)	1.378(3)
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600

O(2)-S(1)-O(1)	120.55(9)
O(2)-S(1)-N(1)	106.68(7)
O(1)-S(1)-N(1)	105.68(8)
O(2)-S(1)-C(19)	107.50(8)
O(1)-S(1)-C(19)	106.89(8)
N(1)-S(1)-C(19)	109.21(7)
C(7)-N(1)-C(1)	114.70(13)
C(7)-N(1)-S(1)	119.18(11)
C(1)-N(1)-S(1)	119.95(11)
N(1)-C(1)-C(2)	111.28(15)
N(1)-C(1)-H(1A)	109.4
C(2)-C(1)-H(1A)	109.4
N(1)-C(1)-H(1B)	109.4
C(2)-C(1)-H(1B)	109.4
H(1A)-C(1)-H(1B)	108.0

C(1)-C(2)-C(3)	114.11(17)
C(1)-C(2)-H(2A)	108.7
C(3)-C(2)-H(2A)	108.7
C(1)-C(2)-H(2B)	108.7
C(3)-C(2)-H(2B)	108.7
H(2A)-C(2)-H(2B)	107.6
C(4)-C(3)-C(2)	116.21(16)
C(4)-C(3)-H(3A)	108.2
C(2)-C(3)-H(3A)	108.2
C(4)-C(3)-H(3B)	108.2
C(2)-C(3)-H(3B)	108.2
H(3A)-C(3)-H(3B)	107.4
C(3)-C(4)-C(5)	117.23(16)
C(3)-C(4)-H(4A)	108.0
C(5)-C(4)-H(4A)	108.0
C(3)-C(4)-H(4B)	108.0
C(5)-C(4)-H(4B)	108.0
H(4A)-C(4)-H(4B)	107.2
C(6)-C(5)-C(4)	115.87(15)
C(6)-C(5)-H(5A)	108.3
C(4)-C(5)-H(5A)	108.3
C(6)-C(5)-H(5B)	108.3
C(4)-C(5)-H(5B)	108.3
H(5A)-C(5)-H(5B)	107.4
C(7)-C(6)-C(16)	120.61(14)
C(7)-C(6)-C(5)	121.62(15)
C(16)-C(6)-C(5)	117.77(14)
C(6)-C(7)-C(8)	125.21(14)
C(6)-C(7)-N(1)	118.78(13)
C(8)-C(7)-N(1)	115.70(13)
C(9)-C(8)-C(7)	176.12(18)
C(8)-C(9)-C(10)	178.64(19)
C(15)-C(10)-C(11)	119.05(15)
C(15)-C(10)-C(9)	119.91(15)
C(11)-C(10)-C(9)	121.03(15)
C(12)-C(11)-C(10)	120.14(17)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9

C(13)-C(12)-C(11)	120.20(17)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(14)	119.91(16)
C(12)-C(13)-H(13)	120.0
C(14)-C(13)-H(13)	120.0
C(13)-C(14)-C(15)	120.64(19)
C(13)-C(14)-H(14)	119.7
C(15)-C(14)-H(14)	119.7
C(14)-C(15)-C(10)	120.06(17)
C(14)-C(15)-H(15)	120.0
C(10)-C(15)-H(15)	120.0
C(17)-C(16)-C(6)	114.16(16)
C(17)-C(16)-H(16A)	108.7
C(6)-C(16)-H(16A)	108.7
C(17)-C(16)-H(16B)	108.7
C(6)-C(16)-H(16B)	108.7
H(16A)-C(16)-H(16B)	107.6
C(18)-C(17)-C(16)	126.4(3)
C(18)-C(17)-H(17)	116.8
C(16)-C(17)-H(17)	116.8
C(17)-C(18)-H(18A)	109.7(17)
C(17)-C(18)-H(18B)	126(2)
H(18A)-C(18)-H(18B)	125(3)
C(20)-C(19)-C(24)	119.81(16)
C(20)-C(19)-S(1)	120.33(13)
C(24)-C(19)-S(1)	119.86(13)
C(21)-C(20)-C(19)	119.74(18)
C(21)-C(20)-H(20)	120.1
C(19)-C(20)-H(20)	120.1
C(20)-C(21)-C(22)	121.54(18)
C(20)-C(21)-H(21)	119.2
C(22)-C(21)-H(21)	119.2
C(21)-C(22)-C(23)	117.95(17)
C(21)-C(22)-C(25)	121.4(2)
C(23)-C(22)-C(25)	120.6(2)
C(24)-C(23)-C(22)	121.44(18)
C(24)-C(23)-H(23)	119.3

C(22)-C(23)-H(23)	119.3
C(23)-C(24)-C(19)	119.52(18)
C(23)-C(24)-H(24)	120.2
C(19)-C(24)-H(24)	120.2
C(22)-C(25)-H(25A)	109.5
C(22)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(22)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_dd18203_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	74(1)	51(1)	42(1)	24(1)	28(1)	24(1)
O(1)	127(1)	70(1)	73(1)	49(1)	64(1)	43(1)
O(2)	74(1)	65(1)	48(1)	17(1)	11(1)	29(1)
N(1)	56(1)	46(1)	44(1)	22(1)	28(1)	16(1)
C(1)	61(1)	56(1)	60(1)	25(1)	28(1)	8(1)
C(2)	53(1)	79(1)	77(1)	41(1)	33(1)	19(1)
C(3)	77(1)	82(1)	78(1)	47(1)	56(1)	37(1)
C(4)	88(1)	72(1)	59(1)	33(1)	49(1)	37(1)
C(5)	70(1)	56(1)	41(1)	19(1)	26(1)	21(1)
C(6)	51(1)	50(1)	44(1)	23(1)	24(1)	18(1)
C(7)	48(1)	49(1)	41(1)	24(1)	24(1)	16(1)
C(8)	52(1)	51(1)	45(1)	25(1)	26(1)	18(1)
C(9)	56(1)	56(1)	46(1)	27(1)	27(1)	20(1)
C(10)	47(1)	57(1)	41(1)	26(1)	23(1)	21(1)
C(11)	55(1)	59(1)	50(1)	28(1)	26(1)	18(1)
C(12)	61(1)	88(1)	57(1)	47(1)	31(1)	24(1)
C(13)	71(1)	99(2)	40(1)	32(1)	27(1)	29(1)
C(14)	84(1)	68(1)	45(1)	15(1)	24(1)	18(1)
C(15)	74(1)	56(1)	51(1)	26(1)	28(1)	16(1)
C(16)	71(1)	51(1)	63(1)	28(1)	36(1)	20(1)
C(17)	79(1)	77(1)	85(1)	52(1)	40(1)	33(1)
C(18)	163(4)	80(2)	128(3)	56(2)	99(3)	68(2)
C(19)	60(1)	40(1)	47(1)	20(1)	27(1)	16(1)
C(20)	56(1)	56(1)	62(1)	17(1)	28(1)	13(1)
C(21)	71(1)	74(1)	75(1)	32(1)	48(1)	30(1)
C(22)	86(1)	54(1)	54(1)	25(1)	37(1)	33(1)
C(23)	79(1)	46(1)	56(1)	13(1)	26(1)	8(1)
C(24)	72(1)	48(1)	63(1)	19(1)	38(1)	6(1)
C(25)	132(2)	93(2)	65(1)	26(1)	54(1)	55(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for mo_dd18203_0m.

	x	y	z	U(eq)
H(1A)	5106	7619	4965	72
H(1B)	4984	8067	3885	72
H(2A)	5437	5734	3724	80
H(2B)	6697	6823	3821	80
H(3A)	4364	6292	1623	80
H(3B)	5800	5705	1689	80
H(4A)	4205	3900	1537	78
H(4B)	3523	4074	263	78
H(5A)	1596	4915	1010	66
H(5B)	1327	3463	568	66
H(11)	1517	4936	6971	63
H(12)	1685	5610	9101	74
H(13)	2816	7726	10633	82
H(14)	3800	9174	10053	86
H(15)	3656	8526	7941	71
H(16A)	1523	3617	3578	71
H(16B)	540	2802	2037	71
H(17)	3848	3059	3249	87
H(20)	-528	7676	4280	73
H(21)	-561	8960	6270	83
H(23)	3965	11033	7555	79
H(24)	4017	9766	5563	74
H(25A)	1132	11584	8346	141
H(25B)	2774	11407	9098	141
H(25C)	1125	10458	8702	141
H(18A)	1260(40)	1040(30)	1350(30)	112(11)
H(18B)	3190(40)	920(30)	1960(30)	154(13)

Table 6. Torsion angles [°] for mo_dd18203_0m.

O(2)-S(1)-N(1)-C(7)	-40.57(13)
O(1)-S(1)-N(1)-C(7)	-170.01(11)
C(19)-S(1)-N(1)-C(7)	75.33(13)
O(2)-S(1)-N(1)-C(1)	168.48(12)
O(1)-S(1)-N(1)-C(1)	39.05(14)
C(19)-S(1)-N(1)-C(1)	-75.62(13)
C(7)-N(1)-C(1)-C(2)	60.70(18)
S(1)-N(1)-C(1)-C(2)	-147.12(13)
N(1)-C(1)-C(2)-C(3)	52.3(2)
C(1)-C(2)-C(3)-C(4)	-99.5(2)
C(2)-C(3)-C(4)-C(5)	67.6(2)
C(3)-C(4)-C(5)-C(6)	-71.7(2)
C(4)-C(5)-C(6)-C(7)	83.0(2)
C(4)-C(5)-C(6)-C(16)	-97.17(19)
C(16)-C(6)-C(7)-C(8)	0.8(3)
C(5)-C(6)-C(7)-C(8)	-179.37(15)
C(16)-C(6)-C(7)-N(1)	174.10(14)
C(5)-C(6)-C(7)-N(1)	-6.0(2)
C(1)-N(1)-C(7)-C(6)	-98.05(17)
S(1)-N(1)-C(7)-C(6)	109.54(15)
C(1)-N(1)-C(7)-C(8)	75.91(17)
S(1)-N(1)-C(7)-C(8)	-76.50(16)
C(15)-C(10)-C(11)-C(12)	-0.1(2)
C(9)-C(10)-C(11)-C(12)	-179.98(16)
C(10)-C(11)-C(12)-C(13)	0.3(3)
C(11)-C(12)-C(13)-C(14)	-0.2(3)
C(12)-C(13)-C(14)-C(15)	0.1(3)
C(13)-C(14)-C(15)-C(10)	0.0(3)
C(11)-C(10)-C(15)-C(14)	0.0(3)
C(9)-C(10)-C(15)-C(14)	179.85(17)
C(7)-C(6)-C(16)-C(17)	-115.4(2)
C(5)-C(6)-C(16)-C(17)	64.7(2)
C(6)-C(16)-C(17)-C(18)	-128.4(3)
O(2)-S(1)-C(19)-C(20)	6.28(17)
O(1)-S(1)-C(19)-C(20)	137.03(16)
N(1)-S(1)-C(19)-C(20)	-109.08(16)

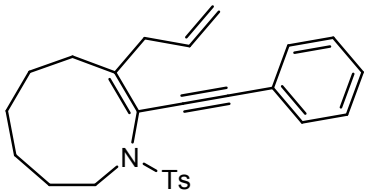
O(2)-S(1)-C(19)-C(24)	-173.06(14)
O(1)-S(1)-C(19)-C(24)	-42.31(17)
N(1)-S(1)-C(19)-C(24)	71.57(16)
C(24)-C(19)-C(20)-C(21)	0.7(3)
S(1)-C(19)-C(20)-C(21)	-178.68(15)
C(19)-C(20)-C(21)-C(22)	-0.4(3)
C(20)-C(21)-C(22)-C(23)	-0.2(3)
C(20)-C(21)-C(22)-C(25)	-179.5(2)
C(21)-C(22)-C(23)-C(24)	0.4(3)
C(25)-C(22)-C(23)-C(24)	179.8(2)
C(22)-C(23)-C(24)-C(19)	-0.1(3)
C(20)-C(19)-C(24)-C(23)	-0.4(3)
S(1)-C(19)-C(24)-C(23)	178.91(15)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo_dd18203_0m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

(I) X-ray crystallographic data of compound 3da



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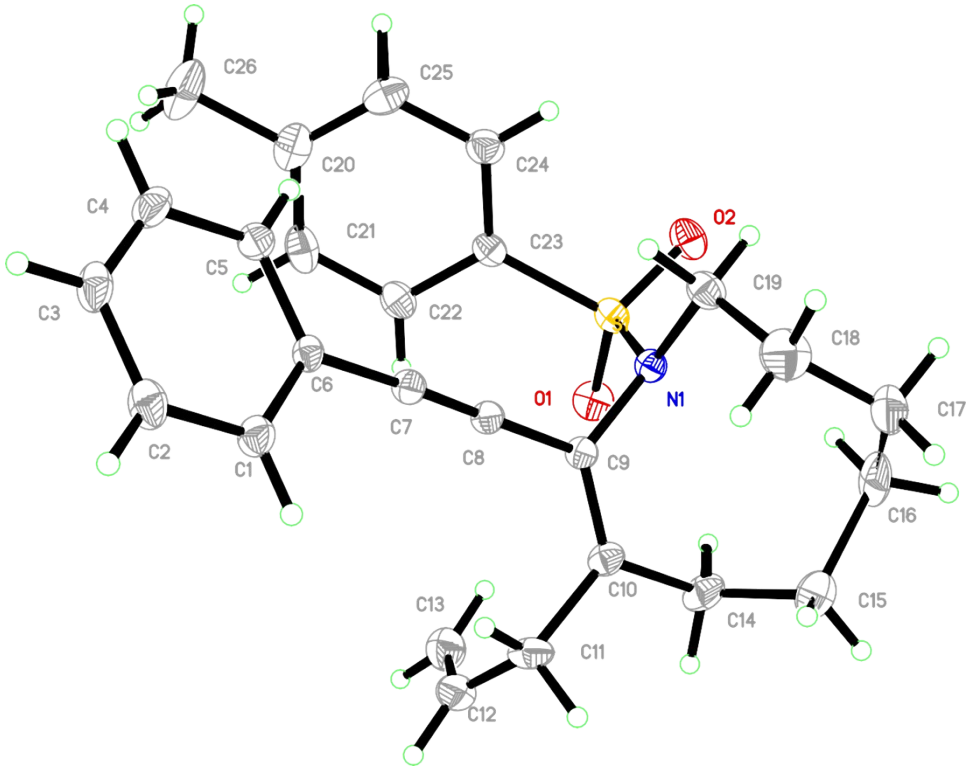

Table 1. Crystal data and structure refinement for 2010226ZH_ZNZ7828_0m_a.

Identification code	2010226ZH_ZNZ7828_0m_a	
Empirical formula	C26 H29 N O2 S	
Formula weight	419.56	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.161(3) Å	α= 90°.
	b = 20.083(6) Å	β= 92.934(4)°.
	c = 12.559(3) Å	γ = 90°.
Volume	2307.8(11) $Å^3$	
Z	4	
Density (calculated)	1.208 Mg/m^3	
Absorption coefficient	0.162 mm^{-1}	
F(000)	896	
Crystal size	0.220 x 0.190 x 0.160 mm^3	
Theta range for data collection	1.914 to 25.003°.	
Index ranges	-10<=h<=7, -23<=k<=22, -13<=l<=14	
Reflections collected	11777	
Independent reflections	4055 [R(int) = 0.0277]	
Completeness to theta = 25.003°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4055 / 0 / 281	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0536, wR2 = 0.1333	
R indices (all data)	R1 = 0.0792, wR2 = 0.1500	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.414 and -0.258 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2010226ZH_ZNZ7828_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3327(3)	3551(2)	4164(2)	59(1)
C(2)	3547(4)	3719(2)	3119(2)	69(1)
C(3)	4694(4)	4120(2)	2877(2)	67(1)
C(4)	5614(3)	4362(2)	3669(3)	66(1)
C(5)	5419(3)	4200(1)	4716(2)	55(1)
C(6)	4266(3)	3790(1)	4975(2)	44(1)
C(7)	4051(3)	3607(1)	6054(2)	48(1)
C(8)	3852(3)	3432(1)	6942(2)	46(1)
C(9)	3544(3)	3241(1)	8006(2)	44(1)
C(10)	2746(3)	2709(1)	8229(2)	53(1)
C(11)	2222(3)	2241(2)	7351(2)	69(1)
C(12)	3127(4)	1630(2)	7274(3)	76(1)
C(13)	4335(4)	1500(2)	7801(3)	88(1)
C(14)	2333(4)	2534(2)	9332(3)	75(1)
C(15)	1060(5)	2924(2)	9739(3)	105(1)
C(16)	1568(7)	3585(4)	10316(4)	90(2)
C(17)	1250(5)	4196(3)	9811(5)	120(2)
C(18)	1909(4)	4406(2)	8762(4)	102(1)
C(19)	3536(3)	4376(1)	8755(2)	63(1)
C(20)	8805(3)	3949(2)	6673(3)	80(1)
C(21)	8428(4)	3314(2)	6941(3)	80(1)
C(22)	7497(3)	3189(2)	7747(2)	65(1)
C(23)	6947(3)	3713(1)	8308(2)	51(1)
C(24)	7305(3)	4354(2)	8051(3)	67(1)
C(25)	8224(4)	4466(2)	7233(3)	82(1)
C(26)	9826(5)	4081(3)	5781(4)	128(2)
C(15')	1060(5)	2924(2)	9739(3)	105(1)
C(16')	667(10)	3541(5)	9676(10)	89(3)
C(17')	1250(5)	4196(3)	9811(5)	120(2)
N(1)	4077(2)	3685(1)	8843(2)	46(1)
O(1)	5863(2)	2871(1)	9595(2)	70(1)
O(2)	6005(2)	4049(1)	10138(2)	74(1)

S(1)	5748(1)	3558(1)	9332(1)	54(1)

Table 3. Bond lengths [Å] and angles [°] for 2010226ZH_ZNZ7828_0m_a.

C(1)-C(2)	1.380(4)
C(1)-C(6)	1.384(4)
C(1)-H(1)	0.9300
C(2)-C(3)	1.371(4)
C(2)-H(2)	0.9300
C(3)-C(4)	1.361(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.375(4)
C(4)-H(4)	0.9300
C(5)-C(6)	1.390(4)
C(5)-H(5)	0.9300
C(6)-C(7)	1.428(3)
C(7)-C(8)	1.193(3)
C(8)-C(9)	1.432(3)
C(9)-C(10)	1.331(3)
C(9)-N(1)	1.444(3)
C(10)-C(14)	1.497(4)
C(10)-C(11)	1.509(4)
C(11)-C(12)	1.487(5)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.287(5)
C(12)-H(12)	0.9300
C(13)-H(13A)	0.9300
C(13)-H(13B)	0.9300
C(14)-C(15')	1.515(5)
C(14)-C(15)	1.515(5)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-C(16)	1.570(9)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-C(17)	1.405(8)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.537(6)

C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-C(19)	1.493(5)
C(18)-C(17')	1.537(6)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-N(1)	1.475(3)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(20)-C(21)	1.368(5)
C(20)-C(25)	1.375(5)
C(20)-C(26)	1.520(5)
C(21)-C(22)	1.379(5)
C(21)-H(21)	0.9300
C(22)-C(23)	1.376(4)
C(22)-H(22)	0.9300
C(23)-C(24)	1.371(4)
C(23)-S(1)	1.762(3)
C(24)-C(25)	1.380(5)
C(24)-H(24)	0.9300
C(25)-H(25)	0.9300
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(15')-C(16')	1.290(10)
C(15')-H(15C)	0.9700
C(15')-H(15D)	0.9700
C(16')-C(17')	1.427(11)
C(16')-H(16C)	0.9700
C(16')-H(16D)	0.9700
C(17')-H(17C)	0.9700
C(17')-H(17D)	0.9700
N(1)-S(1)	1.641(2)
O(1)-S(1)	1.420(2)
O(2)-S(1)	1.424(2)

C(2)-C(1)-C(6)	120.0(3)
C(2)-C(1)-H(1)	120.0

C(6)-C(1)-H(1)	120.0
C(3)-C(2)-C(1)	120.3(3)
C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8
C(4)-C(3)-C(2)	120.1(3)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(3)-C(4)-C(5)	120.5(3)
C(3)-C(4)-H(4)	119.7
C(5)-C(4)-H(4)	119.7
C(4)-C(5)-C(6)	120.1(3)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(1)-C(6)-C(5)	118.9(2)
C(1)-C(6)-C(7)	119.9(2)
C(5)-C(6)-C(7)	121.2(2)
C(8)-C(7)-C(6)	177.6(3)
C(7)-C(8)-C(9)	177.0(3)
C(10)-C(9)-C(8)	123.2(2)
C(10)-C(9)-N(1)	120.8(2)
C(8)-C(9)-N(1)	115.9(2)
C(9)-C(10)-C(14)	123.4(3)
C(9)-C(10)-C(11)	120.3(2)
C(14)-C(10)-C(11)	116.3(2)
C(12)-C(11)-C(10)	113.9(2)
C(12)-C(11)-H(11A)	108.8
C(10)-C(11)-H(11A)	108.8
C(12)-C(11)-H(11B)	108.8
C(10)-C(11)-H(11B)	108.8
H(11A)-C(11)-H(11B)	107.7
C(13)-C(12)-C(11)	127.0(3)
C(13)-C(12)-H(12)	116.5
C(11)-C(12)-H(12)	116.5
C(12)-C(13)-H(13A)	120.0
C(12)-C(13)-H(13B)	120.0
H(13A)-C(13)-H(13B)	120.0
C(10)-C(14)-C(15')	115.2(3)
C(10)-C(14)-C(15)	115.2(3)

C(10)-C(14)-H(14A)	108.5
C(15)-C(14)-H(14A)	108.5
C(10)-C(14)-H(14B)	108.5
C(15)-C(14)-H(14B)	108.5
H(14A)-C(14)-H(14B)	107.5
C(14)-C(15)-C(16)	112.2(4)
C(14)-C(15)-H(15A)	109.2
C(16)-C(15)-H(15A)	109.2
C(14)-C(15)-H(15B)	109.2
C(16)-C(15)-H(15B)	109.2
H(15A)-C(15)-H(15B)	107.9
C(17)-C(16)-C(15)	118.7(5)
C(17)-C(16)-H(16A)	107.6
C(15)-C(16)-H(16A)	107.6
C(17)-C(16)-H(16B)	107.6
C(15)-C(16)-H(16B)	107.6
H(16A)-C(16)-H(16B)	107.1
C(16)-C(17)-C(18)	123.1(4)
C(16)-C(17)-H(17A)	106.6
C(18)-C(17)-H(17A)	106.6
C(16)-C(17)-H(17B)	106.6
C(18)-C(17)-H(17B)	106.6
H(17A)-C(17)-H(17B)	106.5
C(19)-C(18)-C(17')	115.4(4)
C(19)-C(18)-C(17)	115.4(4)
C(19)-C(18)-H(18A)	108.4
C(17)-C(18)-H(18A)	108.4
C(19)-C(18)-H(18B)	108.4
C(17)-C(18)-H(18B)	108.4
H(18A)-C(18)-H(18B)	107.5
N(1)-C(19)-C(18)	111.7(3)
N(1)-C(19)-H(19A)	109.3
C(18)-C(19)-H(19A)	109.3
N(1)-C(19)-H(19B)	109.3
C(18)-C(19)-H(19B)	109.3
H(19A)-C(19)-H(19B)	107.9
C(21)-C(20)-C(25)	118.0(3)
C(21)-C(20)-C(26)	121.1(4)

C(25)-C(20)-C(26)	120.9(4)
C(20)-C(21)-C(22)	121.5(3)
C(20)-C(21)-H(21)	119.2
C(22)-C(21)-H(21)	119.2
C(21)-C(22)-C(23)	119.6(3)
C(21)-C(22)-H(22)	120.2
C(23)-C(22)-H(22)	120.2
C(24)-C(23)-C(22)	119.9(3)
C(24)-C(23)-S(1)	120.2(2)
C(22)-C(23)-S(1)	119.8(2)
C(23)-C(24)-C(25)	119.4(3)
C(23)-C(24)-H(24)	120.3
C(25)-C(24)-H(24)	120.3
C(20)-C(25)-C(24)	121.6(3)
C(20)-C(25)-H(25)	119.2
C(24)-C(25)-H(25)	119.2
C(20)-C(26)-H(26A)	109.5
C(20)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(20)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(16')-C(15')-C(14)	133.8(5)
C(16')-C(15')-H(15C)	103.8
C(14)-C(15')-H(15C)	103.8
C(16')-C(15')-H(15D)	103.8
C(14)-C(15')-H(15D)	103.8
H(15C)-C(15')-H(15D)	105.4
C(15')-C(16')-C(17')	140.9(9)
C(15')-C(16')-H(16C)	101.8
C(17')-C(16')-H(16C)	101.8
C(15')-C(16')-H(16D)	101.8
C(17')-C(16')-H(16D)	101.8
H(16C)-C(16')-H(16D)	104.7
C(16')-C(17')-C(18)	108.2(6)
C(16')-C(17')-H(17C)	110.1
C(18)-C(17')-H(17C)	110.1
C(16')-C(17')-H(17D)	110.1

C(18)-C(17')-H(17D)	110.1
H(17C)-C(17')-H(17D)	108.4
C(9)-N(1)-C(19)	115.3(2)
C(9)-N(1)-S(1)	116.71(16)
C(19)-N(1)-S(1)	118.56(17)
O(1)-S(1)-O(2)	119.96(13)
O(1)-S(1)-N(1)	107.17(11)
O(2)-S(1)-N(1)	105.96(12)
O(1)-S(1)-C(23)	107.48(13)
O(2)-S(1)-C(23)	108.06(13)
N(1)-S(1)-C(23)	107.66(11)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 2010226ZH_ZNZ7828_0m_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	63(2)	73(2)	42(2)	2(1)	3(1)	-7(1)
C(2)	88(2)	79(2)	39(2)	2(2)	-3(2)	8(2)
C(3)	94(2)	63(2)	45(2)	14(1)	18(2)	21(2)
C(4)	77(2)	59(2)	64(2)	17(2)	23(2)	-1(2)
C(5)	64(2)	50(2)	51(2)	4(1)	5(1)	1(1)
C(6)	54(1)	43(1)	36(1)	5(1)	5(1)	8(1)
C(7)	54(1)	48(2)	40(2)	3(1)	-2(1)	-1(1)
C(8)	49(1)	49(2)	39(2)	3(1)	-2(1)	-3(1)
C(9)	51(1)	45(1)	37(1)	5(1)	-2(1)	0(1)
C(10)	57(2)	56(2)	48(2)	12(1)	1(1)	-5(1)
C(11)	69(2)	66(2)	69(2)	7(2)	-12(2)	-25(2)
C(12)	84(2)	76(2)	69(2)	-9(2)	5(2)	-16(2)
C(13)	82(2)	91(3)	92(3)	-9(2)	11(2)	5(2)
C(14)	79(2)	81(2)	66(2)	24(2)	12(2)	-16(2)
C(15)	119(3)	118(4)	83(3)	1(3)	40(2)	-19(3)
C(16)	78(4)	160(7)	31(3)	-19(4)	7(3)	5(4)
C(17)	91(3)	136(4)	138(4)	-62(4)	48(3)	-16(3)
C(18)	82(2)	86(3)	136(4)	5(3)	-2(2)	26(2)
C(19)	74(2)	51(2)	62(2)	1(1)	-1(2)	7(1)
C(20)	54(2)	127(3)	60(2)	4(2)	-5(2)	1(2)
C(21)	74(2)	106(3)	58(2)	-19(2)	-5(2)	21(2)
C(22)	72(2)	67(2)	56(2)	-7(2)	-7(2)	5(2)
C(23)	47(1)	55(2)	49(2)	-6(1)	-12(1)	1(1)
C(24)	59(2)	64(2)	77(2)	-7(2)	1(2)	-4(1)
C(25)	63(2)	87(3)	96(3)	12(2)	1(2)	-15(2)
C(26)	81(3)	217(6)	87(3)	15(3)	25(2)	-9(3)
C(15')	119(3)	118(4)	83(3)	1(3)	40(2)	-19(3)
C(16')	74(6)	89(7)	106(8)	0(6)	26(6)	-8(5)
C(17')	91(3)	136(4)	138(4)	-62(4)	48(3)	-16(3)
N(1)	53(1)	49(1)	37(1)	3(1)	1(1)	0(1)
O(1)	79(1)	70(1)	59(1)	18(1)	-13(1)	9(1)
O(2)	86(1)	87(2)	46(1)	-18(1)	-13(1)	-2(1)

S(1)	61(1)	59(1)	40(1)	0(1)	-11(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2010226ZH_ZNZ7828_0m_a.

	x	y	z	U(eq)
H(1)	2549	3278	4324	71
H(2)	2915	3558	2576	83
H(3)	4843	4228	2171	80
H(4)	6381	4640	3502	79
H(5)	6059	4364	5251	66
H(11A)	1223	2111	7470	82
H(11B)	2217	2476	6676	82
H(12)	2783	1307	6794	92
H(13A)	4728	1807	8291	106
H(13B)	4816	1100	7691	106
H(14A)	3177	2603	9817	90
H(14B)	2092	2064	9348	90
H(15A)	546	2649	10233	126
H(15B)	384	3033	9145	126
H(16A)	1138	3593	11006	107
H(16B)	2619	3560	10448	107
H(17A)	1506	4541	10328	144
H(17B)	196	4213	9689	144
H(18A)	1505	4122	8195	122
H(18B)	1602	4859	8599	122
H(19A)	3853	4572	8100	75
H(19B)	3955	4635	9346	75
H(21)	8809	2958	6572	96
H(22)	7243	2754	7910	78
H(24)	6933	4710	8425	80
H(25)	8456	4901	7055	99
H(26A)	10436	3699	5689	192
H(26B)	10427	4461	5960	192
H(26C)	9261	4167	5131	192
H(15C)	208	2684	9456	126
H(15D)	1110	2835	10499	126
H(16C)	-149	3551	10139	107

H(16D)	221	3563	8960	107
H(17C)	1998	4200	10387	144
H(17D)	482	4503	9989	144

Table 6. Torsion angles [°] for 2010226ZH_ZNZ7828_0m_a.

C(6)-C(1)-C(2)-C(3)	0.1(5)
C(1)-C(2)-C(3)-C(4)	-0.7(5)
C(2)-C(3)-C(4)-C(5)	1.0(5)
C(3)-C(4)-C(5)-C(6)	-0.7(4)
C(2)-C(1)-C(6)-C(5)	0.2(4)
C(2)-C(1)-C(6)-C(7)	-178.9(3)
C(4)-C(5)-C(6)-C(1)	0.1(4)
C(4)-C(5)-C(6)-C(7)	179.2(2)
C(8)-C(9)-C(10)-C(14)	-175.6(3)
N(1)-C(9)-C(10)-C(14)	0.4(4)
C(8)-C(9)-C(10)-C(11)	5.2(4)
N(1)-C(9)-C(10)-C(11)	-178.8(2)
C(9)-C(10)-C(11)-C(12)	99.4(3)
C(14)-C(10)-C(11)-C(12)	-79.8(3)
C(10)-C(11)-C(12)-C(13)	-6.6(5)
C(9)-C(10)-C(14)-C(15')	79.5(4)
C(11)-C(10)-C(14)-C(15')	-101.3(4)
C(9)-C(10)-C(14)-C(15)	79.5(4)
C(11)-C(10)-C(14)-C(15)	-101.3(4)
C(10)-C(14)-C(15)-C(16)	-88.9(5)
C(14)-C(15)-C(16)-C(17)	108.9(6)
C(15)-C(16)-C(17)-C(18)	-65.4(8)
C(16)-C(17)-C(18)-C(19)	-53.4(7)
C(17')-C(18)-C(19)-N(1)	66.4(4)
C(17)-C(18)-C(19)-N(1)	66.4(4)
C(25)-C(20)-C(21)-C(22)	-0.1(5)
C(26)-C(20)-C(21)-C(22)	-179.7(3)
C(20)-C(21)-C(22)-C(23)	-1.0(5)
C(21)-C(22)-C(23)-C(24)	1.1(4)
C(21)-C(22)-C(23)-S(1)	179.6(2)
C(22)-C(23)-C(24)-C(25)	-0.3(4)
S(1)-C(23)-C(24)-C(25)	-178.8(2)
C(21)-C(20)-C(25)-C(24)	0.9(5)
C(26)-C(20)-C(25)-C(24)	-179.4(3)
C(23)-C(24)-C(25)-C(20)	-0.8(5)
C(10)-C(14)-C(15')-C(16')	-40.7(10)

C(14)-C(15')-C(16')-C(17')	-47(2)
C(15')-C(16')-C(17')-C(18)	85.5(16)
C(19)-C(18)-C(17')-C(16')	-103.2(6)
C(10)-C(9)-N(1)-C(19)	-118.0(3)
C(8)-C(9)-N(1)-C(19)	58.3(3)
C(10)-C(9)-N(1)-S(1)	95.9(3)
C(8)-C(9)-N(1)-S(1)	-87.9(2)
C(18)-C(19)-N(1)-C(9)	59.3(3)
C(18)-C(19)-N(1)-S(1)	-155.2(3)
C(9)-N(1)-S(1)-O(1)	-50.2(2)
C(19)-N(1)-S(1)-O(1)	164.7(2)
C(9)-N(1)-S(1)-O(2)	-179.44(18)
C(19)-N(1)-S(1)-O(2)	35.5(2)
C(9)-N(1)-S(1)-C(23)	65.1(2)
C(19)-N(1)-S(1)-C(23)	-79.9(2)
C(24)-C(23)-S(1)-O(1)	-165.9(2)
C(22)-C(23)-S(1)-O(1)	15.7(2)
C(24)-C(23)-S(1)-O(2)	-35.1(3)
C(22)-C(23)-S(1)-O(2)	146.5(2)
C(24)-C(23)-S(1)-N(1)	79.0(2)
C(22)-C(23)-S(1)-N(1)	-99.5(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 2010226ZH_ZNZ7828_0m_a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)