

Supporting Information

Photoredox-catalyzed cascade [2+2+1] cyclization of 1,6-enynes with thiols

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Table of Contents

1.	General remarks.....	S2
2.	General procedures for the synthesis of substrates 1	S3
3.	Optimization of reaction conditions	S8
4.	General procedure for the synthesis of 3	S12
5.	Mechanistic studies.....	S13
6.	Gram scale reaction	S17
7.	Transformation of product 3a	S18
8.	Spectroscopic data of substrates 1	S19
9.	Spectroscopic data of products 3, 4, 5	S65
10.	Computational studies	S124
11.	X-Ray structures.....	S135
12.	References	S136

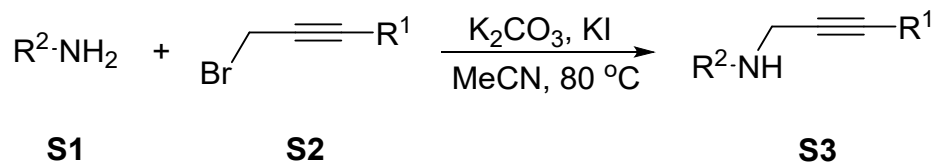
1. General remarks

^1H , ^{13}C and ^{19}F NMR spectra were recorded at 400 MHz or 600 MHz, 100 MHz or 150 MHz and 376 MHz or 564 MHz, respectively. HRMS spectra were recorded by EI, ESI, FI method. Infrared spectra were recorded on a Perkin-Elmer PE-983 spectrometer with absorption in cm^{-1} . Mass spectra were recorded by EI, ESI, and HRMS was measured on an Agilent Technologies 6224 TOF LC/MS instrument and a Waters Micromass GCT Premier. Melting points were determined on a digital melting point apparatus and temperatures were uncorrected. X-ray structure was determined on a Bruker Smart-1000 X-ray Diffraction meter. The employed solvents were dried up by standard methods when necessary. Commercially obtained reagents were used without further purification. All reactions were monitored by TLC plate analysis with silica gel coated plates (Huanghai GF254). Flash column chromatography was performed by using 300-400 mesh silica gel eluting with ethyl acetate and petroleum ether at increased pressure. Substrates **1ab** and **1ad** contain trace of impurity.

2. General procedures for the synthesis of substrates 1

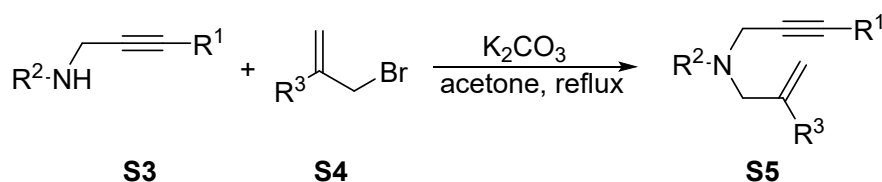
Synthesis of substrates 1

Step 1



To a solution of **S1** (60 mmol) in MeCN (100 mL) was added K_2CO_3 (90 mmol), KI (6.0 mmol) and **S2** (90 mmol) and the resulting solution was allowed to stir at 80 °C for 12 h. After filtration, the organic phase was concentrated under reduced pressure and the residue was purified by a flash column chromatography on silica gel to give the desired products **S3** (PE:EA = 4:1).

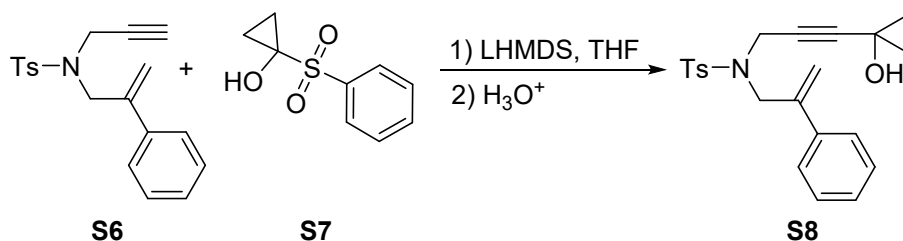
Step 2



To a solution of **S3** (50 mmol) in acetone (100 mL) was added K_2CO_3 (1.5 equiv.) and **S4** (1.5 equiv.) and the resulting solution was allowed to stir at 70 °C for 12 h. After filtration, the organic phase was concentrated under reduced pressure and the residue was purified by a flash column chromatography on silica gel to give the desired products **S5** (PE:EA = 10:1).

Synthesis of substrate 1ab^[1]

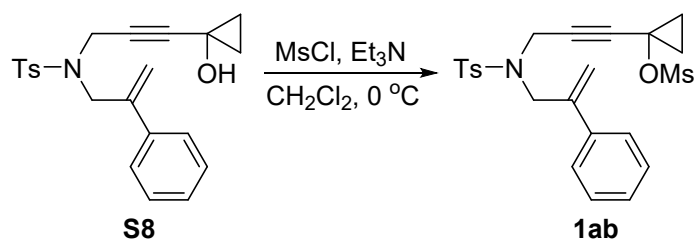
Step 1



To a solution of compounds **S6** (20 mmol) in THF (30 mL) was slowly added LHMDS (24 mmol, 1.0 M in THF) at -78 °C under the protection of argon and the resulting solution was allowed to stir

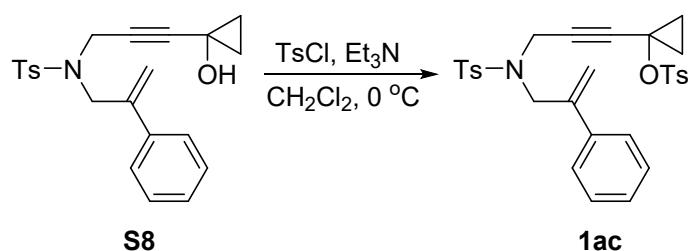
at -78 °C for 30 min before a solution of **S7** (10 mmol) in THF (10 mL) was added into the above mixture. Consequently, the reaction mixture was allowed to warm up to room temperature and the mixture was left standing overnight. Then, saturated NH₄Cl solution was added to quench the reaction. Extracted with ethyl acetate, dried over anhydrous Na₂SO₄, and filtered, the organic phase was concentrated under reduce pressure and the residue was purified by a flash column chromatography on silica gel to give the desired product **S8** (PE:EA = 4:1~2:1).

Step 2



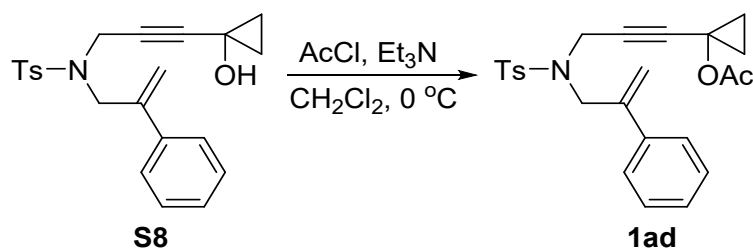
To a solution of **S8** (5.0 mmol) and anhydrous Et₃N (2.0 equiv.) in CH₂Cl₂ (20 mL) was added MsCl (2.0 equiv.) at 0 °C under the protection of argon and the resulting solution was allowed to stir at 0 °C for 1.0 h before some amounts of water were added to quench the reaction. Extracted with CH₂Cl₂ (20 mL × 3), dried over anhydrous Na₂SO₄, and filtered, the organic phase was concentrated under reduce pressure and the residue purified by a flash column chromatography on silica gel to give the desired product **1ab** (PE:EA = 2:1).

Synthesis of substrate 1ac



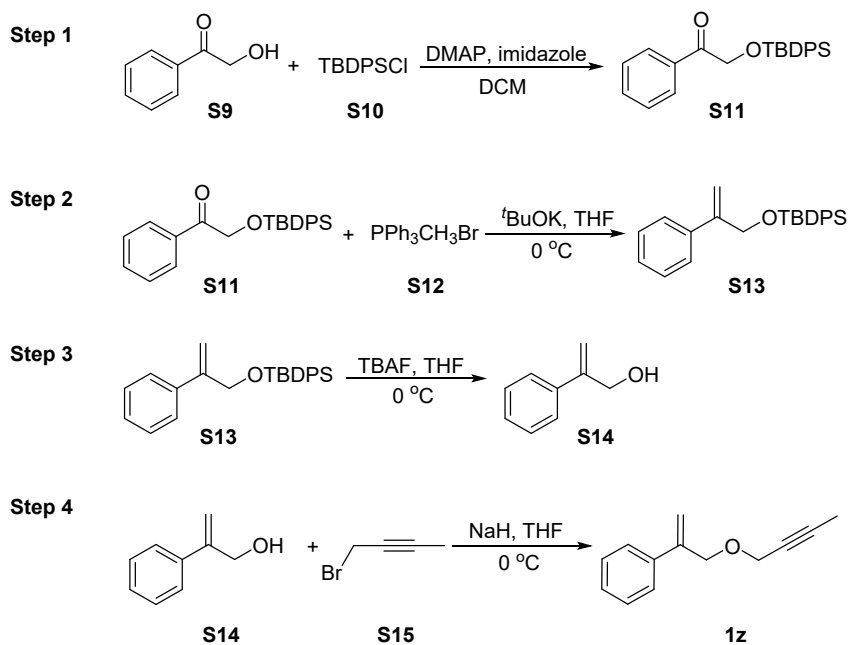
To a solution of **S8** (5.0 mmol) and anhydrous Et₃N (2.0 equiv.) in CH₂Cl₂ (20 mL) was added TsCl (2.0 equiv.) at 0 °C under the protection of argon and the resulting solution was allowed to stir at 0 °C for 1.0 h before some amounts of water were added to quench the reaction. Extracted with CH₂Cl₂ (20 mL × 3), dried over anhydrous Na₂SO₄, and filtered, the organic phase was concentrated under reduce pressure and the residue purified by a flash column chromatography on silica gel to give the desired product **1ac** (PE:EA = 2:1).

Synthesis of substrate 1ad



To a solution of **S8** (5.0 mmol) and anhydrous Et₃N (2.0 equiv.) in CH₂Cl₂ (20 mL) was added AcCl (2.0 equiv.) at 0 °C under the protection of argon and the resulting solution was allowed to stir at 0 °C for 1.0 h before some amounts of water were added to quench the reaction. Extracted with CH₂Cl₂ (20 mL × 3), dried over anhydrous Na₂SO₄, and filtered, the organic phase was concentrated under reduce pressure and the residue purified by a flash column chromatography on silica gel to give the desired product **1ad** (PE:EA = 2:1).

Synthesis of substrate 1z.



Step 1: To a flame dried 100 mL flask was added **S9** (10.0 mmol), DMAP (0.6 equiv.), imidazole (1.1 equiv.) and the solvent DCM (30.0 mL) under the protection of argon and then, the flask was cooled to 0 °C before **S10** (11.0 mmol) was added dropwise into the flask under argon. The reaction mixture was stirred at ambient temperature for 12 h before water was added to quench the reaction.

Extracted with EA, dried over anhydrous Na₂SO₄, and filtered, the organic phase was concentrated under reduce pressure and the residue was purified by a flash column chromatography on silica gel to give the desired product **S11** (PE:EA = 10:1).

Step 2: To a flame dried 100 mL flask was added ^tBuOK (11.0mmol), **S12** (10.0 mmol) and the solvent THF (30 mL) under the protection of argon and then, the reaction mixture was stirred at 0 °C for 30 min. The solution of **S11** (10.0 mmol) in THF was added slowly and the reaction mixture was warmed to room temperature overnight before water was added to quench the reaction. Extracted with EA, dried over anhydrous Na₂SO₄, and filtered, the organic phase was concentrated under reduce pressure and the residue was purified by a flash column chromatography on silica gel to give the desired product **S13** (PE:EA = 20:1).

Step 3: To a flame dried 50 mL flask was added **S13** (5.0 mmol), and the solvent THF (15 mL) under the protection of argon and then, the flask was cooled to 0 °C before the solution of TBAF (1.0 M, 10.0 mL) was added dropwise into the flask. The resulting solution was allowed to stir at 0 °C for 8.0 h before water was added to quench the reaction. Extracted with EA, dried over anhydrous Na₂SO₄, and filtered, the organic phase was concentrated under reduce pressure and the residue was purified by a flash column chromatography on silica gel to give the desired products **S14** (PE:EA = 4:1).

Step 4: To a flame dried 50 mL flask was added NaH (60% dispersion in mineral oil, 3.0 mmol, 2.0 equiv.), and the solvent THF (10 mL) under the protection of argon and then, the flask was cooled to 0 °C before the solution of **S14** (1.5 mmol) in THF was added dropwise into the flask. The reaction mixture was stirred at 0 °C for 30 min. The **S15** (3.0 mmol, 2.0 equiv.) was added slowly and the reaction was heated to room temperature overnight before water was added to quench the reaction. Extracted with EA, dried over anhydrous Na₂SO₄, and filtered, the organic phase was concentrated under reduce pressure and the residue was purified by a flash column chromatography on silica gel to give the desired product **1z** (PE:EA = 50:1).

Unsuccessful substrates

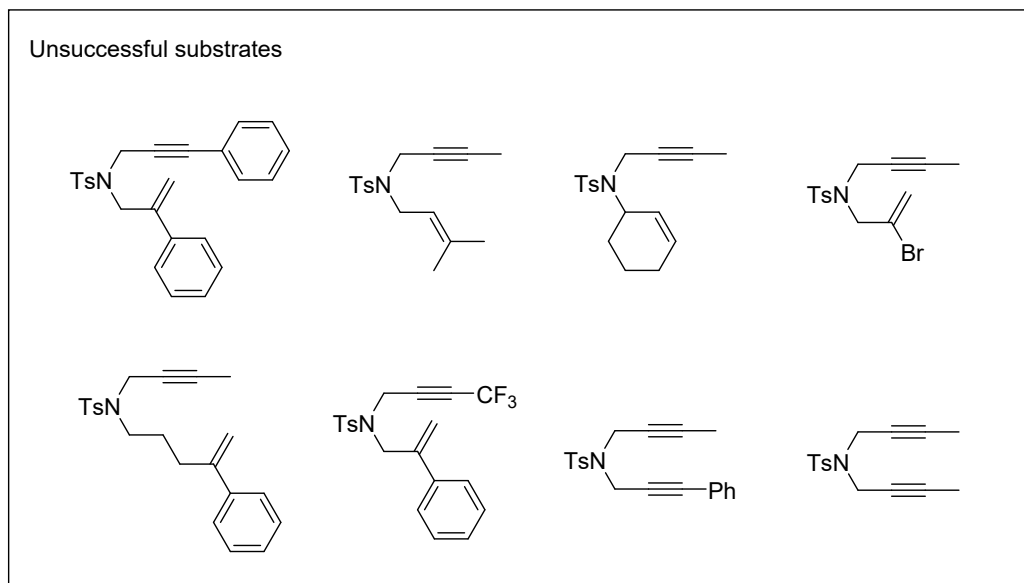


Figure S1. Unsuccessful substrates.

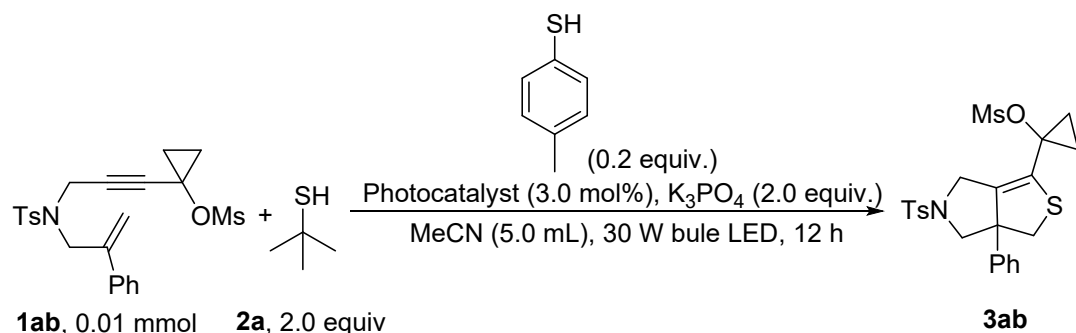
3. Optimization of reaction conditions

Table S1. Optimization of reaction conditions using **1a** as a template substrate.^a

Reaction scheme showing the synthesis of **3a** from **1a** and **2a**. **1a** (0.01 mmol) reacts with **2a** (2.0 equiv.) in the presence of K_2CO_3 (2.0 equiv.), $[Ir(dFCF_3ppy)_2(dtbbpy)]PF_6$ (3.0 mol%), and *p*-toluenethiol (0.2 equiv.) in DCE (5 mL) under 30 W blue LED irradiation for 12 h to yield **3a**.

entry ^a	variation from the standard condition	3a , yield ^b [%]
1	none	95
2	<i>fac</i> -Ir(ppy) ₃ as PC	15
3	Ir(dtbbpy)ppy ₂ as PC	50
4	Cs ₂ CO ₃ instead of K ₂ CO ₃	72
5	NEt ₃ instead of K ₂ CO ₃	0
6	Na ₂ CO ₃ instead of K ₂ CO ₃	77
7	DCM instead of DCE	58
8	MeCN instead of DCE	60
9	1.0 mL DCE instead of 5.0 mL DCE	59
10	Without base	40
11	Without <i>p</i> -MePhSH	67
12	Without light or PC	0

^a Reaction was carried out with **1a** (0.1 mmol), **2a** (2.0 equiv.), K_2CO_3 (2.0 equiv.), *p*-toluenethiol (0.2 equiv.), $[Ir(dFCF_3ppy)_2(dtbbpy)]PF_6$ (3.0 mol%) in DCE (5.0 mL) at ambient temperature using 30 W blue LEDs irradiation. ^b ¹H NMR yield using dimethyl terephthalate as an internal standard.

Table S2. Optimization of reaction conditions using **1ab** as a template substrate (PC).^a

entry ^a	Photocatalyst	3ab , yield ^b [%]
1	[Ir(dFCF ₃ ppy) ₂ dtbpy]PF ₆	65
2	[Ir(dFCF ₃ ppy) ₂ dCF ₃ bpy]PF ₆	NR
3	PC1	NR
4	Eosin Y	55
5	PC2	NR
6	PC3	NR
7	Ru(bpy) ₃	32
8	Ir(ppy) ₃	NR
9	Ir[(dtbpy)ppy ₂]PF ₆	60
10	4CzIPN	63

^a Reaction was carried out with **1ab** (0.1 mmol), **2a** (2.0 equiv.), K₃PO₄ (2.0 equiv.), *p*-toluenethiol (0.2 equiv.), photocatalyst (3.0 mol%) in MeCN (5.0 mL) at ambient temperature using 30 W blue LEDs irradiation. ^b ¹H NMR yield using dimethyl terephthalate as an internal standard.

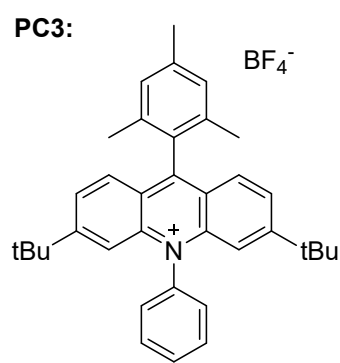
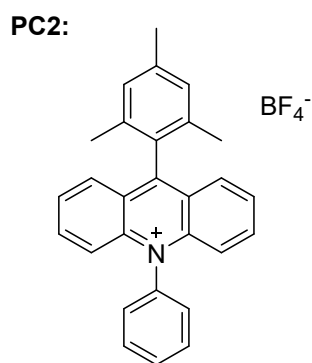
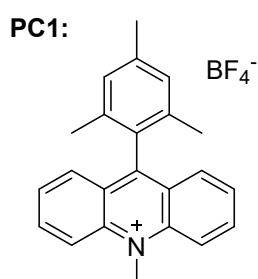


Table S3. Optimization of reaction conditions using **1ab** as a template substrate (solvent).^a

1ab, 0.01 mmol **2a**, 2.0 equiv. **3ab**

entry ^a	solvent	3ab , yield ^b [%]
1	DCM	64
2	DMF	NR
3	DCE	70
4	DMA	NR
5	MeOH	58
6	MeCN	65

^a Reaction was carried out with **1ab** (0.1 mmol), **2a** (2.0 equiv.), K₃PO₄ (2.0 equiv.), *p*-toluenethiol (0.2 equiv.), [Ir(dFCF₃ppy)₂dtbpy]PF₆ (3.0 mol%) in solvent (5.0 mL) at ambient temperature using 30 W blue LEDs irradiation. ^b ¹H NMR yield using dimethyl terephthalate as an internal standard.

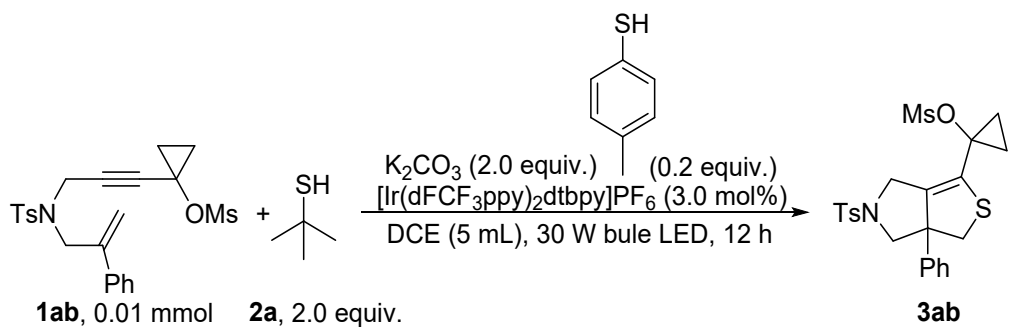
Table S4. Optimization of reaction conditions using **1ab** as a template substrate (base).^a

1ab, 0.01 mmol **2a**, 2.0 equiv. **3ab**

entry ^a	base	3ab , yield ^b [%]
1	K ₂ CO ₃	82
2	Na ₂ CO ₃	73
3	Cs ₂ CO ₃	79
4	K ₃ PO ₄	70
5	KH ₂ PO ₄	56
6	NEt ₃	complex

^a Reaction was carried out with **1ab** (0.1 mmol), **2a** (2.0 equiv.), base (2.0 equiv.), *p*-toluenethiol (0.2 equiv.), [Ir(dFCF₃ppy)₂dtbpy]PF₆ (3.0 mol%) in DCE (5.0 mL) at ambient temperature using 30 W blue LEDs irradiation. ^b ¹H NMR yield using dimethyl terephthalate as an internal standard.

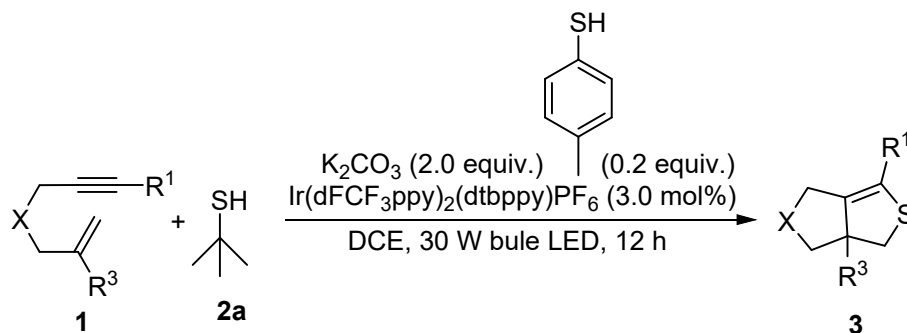
Table S5. Optimization of reaction conditions using **1ab** as a template substrate (control experiment).^a



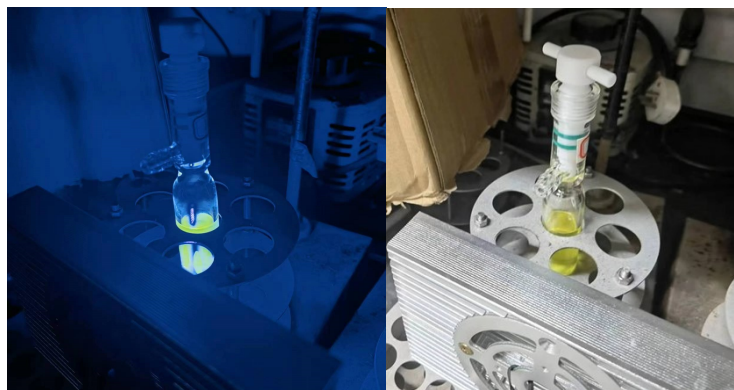
entry ^a	variation from standard condition	3ab , yield ^b [%]
1	No K_2CO_3	41
2	No <i>p</i> -MePhSH	70
3	No light/No PC	NR

^a Reaction was carried out with **1ab** (0.1 mmol), **2a** (2.0 equiv.), K_2CO_3 (2.0 equiv.), *p*-toluenethiol (0.2 equiv.), $[\text{Ir}(\text{dFCF}_3\text{ppy})_2\text{dtbpy}]\text{PF}_6$ (3.0 mol%) in DCE (5.0 mL) at ambient temperature using 30 W blue LEDs irradiation. ^b ¹H NMR yield using dimethyl terephthalate as an internal standard.

4. General procedure for the synthesis of **3**



Substrates **1** (0.1 mmol, 1.0 equiv.), K_2CO_3 (2.0 equiv.), *p*-toluenethiol (0.2 equiv.) and $[Ir(dFCF_3ppy)_2(dtbbpy)]PF_6$ (3.0 mol%) were added in a flame dried 15 mL Schlenk tube. The reaction tube was placed under vacuum and backfilled with argon three times. Then, DCE (5.0 mL) and **2a** (2.0 equiv.) were added in the Schlenk tube via a syringe. Next, the tube was placed 5.0 cm away from blue LEDs (30 W), and stirred vigorously under the irradiation of blue light for 12 h. After completion, the solvent was removed under reduced pressure. The crude product residue was purified by a column chromatography on silica gel (PE/EA = 10/1 to 4/1) to afford the purified product **3**.



5. Mechanistic studies

(a) Luminescence quenching experiments (Stern-Volmer Studies).^[2]

Emission intensities were recorded using Varian Cary Eclipse spectrometer for all experiments. All Ir[(dFCF₃ppy)₂(dtbpy)]PF₆ solutions were excited at 380 nm and the emission intensity was collected at 540 nm. Solutions of different concentration of **1a** and **2a** were prepared and introduced to a 1.0 cm path length quartz cuvette equipped with a Teflon® septum. In a typical experiment, to a 1*10⁻⁶ M solution of photocatalyst in DCE was added the appropriate amount of **1a** in a screw-top quartz cuvette under Ar atmosphere and the emission of the sample was collected. Subsequently, to a 1*10⁻⁶ M solution of photocatalyst in DCE was added the appropriate amount of **2a** in screw-top quartz cuvette under Ar atmosphere and the emission of the sample was collected

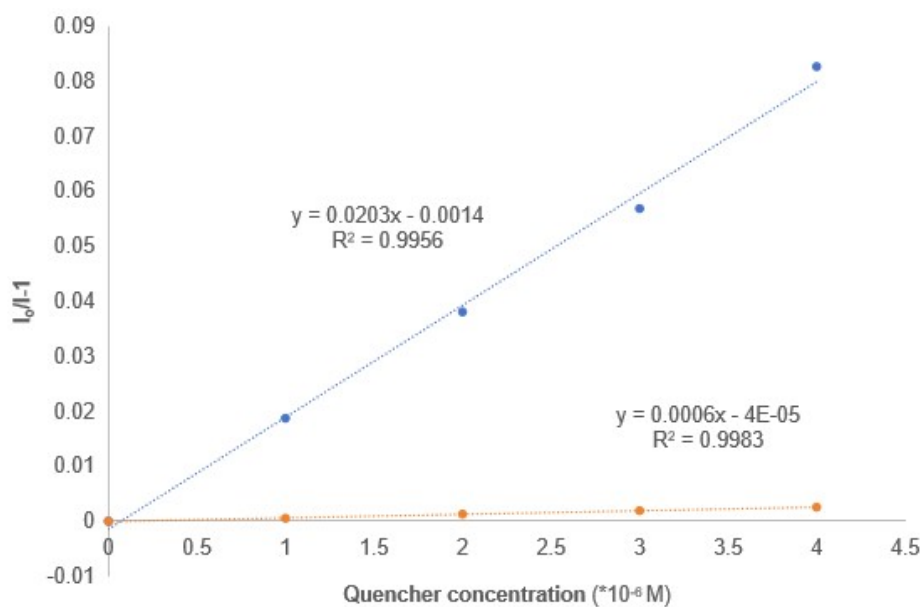


Figure S2. Stern-Volmer plot for the quenching studies above.

(b) Light on/off experiment and quantum yield.^[2]

To study the necessity of continuous irradiation with visible light for the progress of the reaction, the reaction proceeding was monitored by ¹H NMR spectroscopy using dimethyl terephthalate as an internal standard before and after light irradiation and dark periods.

The control experiments shown below with successive intervals of irradiation and dark periods did result in interruption of the reaction progress in the absence of light, demonstrating that light is a necessary component for the reaction after triggering the reaction in the first part.

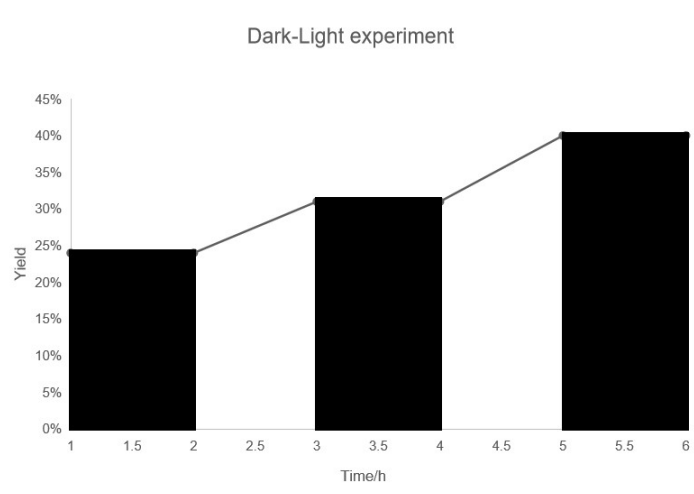
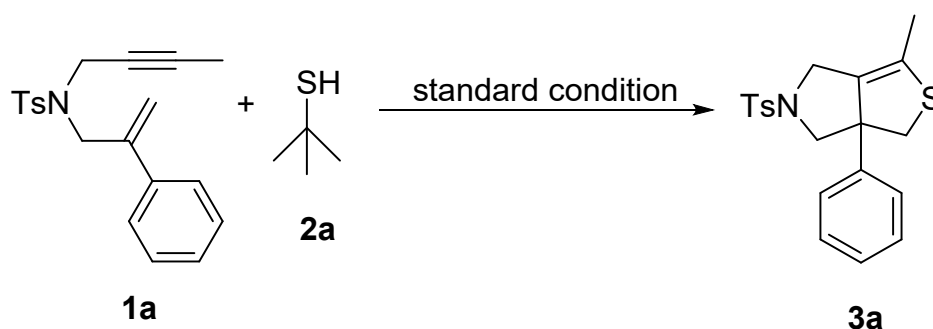


Figure S3. Light on-off experiment.

To further investigate whether the chain process is involved upon light irradiation, we measured the quantum yield of the template reaction of 1.0 h.

$$\phi = \frac{n_x}{n_p} = \frac{n_x}{\frac{\Delta E \times S \times t}{N_A h \nu}} = \frac{n_x \times N_A \times h \times c}{\Delta E \times S \times t \times \lambda}$$

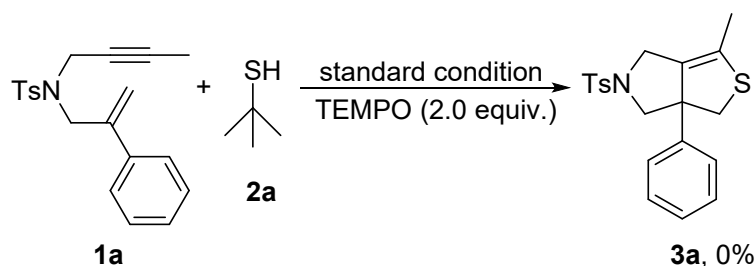
$$= \frac{0.045 \times 10^{-3} \text{ mol} \times 6.022 \times 10^{23} \times 6.626 \times 10^{-34} \text{ J}\cdot\text{s} \times 2.998 \times 10^8 \text{ m}\cdot\text{s}^{-1}}{(14.0 \times 10^{-3} \text{ W}\cdot\text{cm}^2 \times 2 \times 3600 \text{ s} \times 415 \times 10^{-9} \text{ m})}$$

$$= 0.13$$

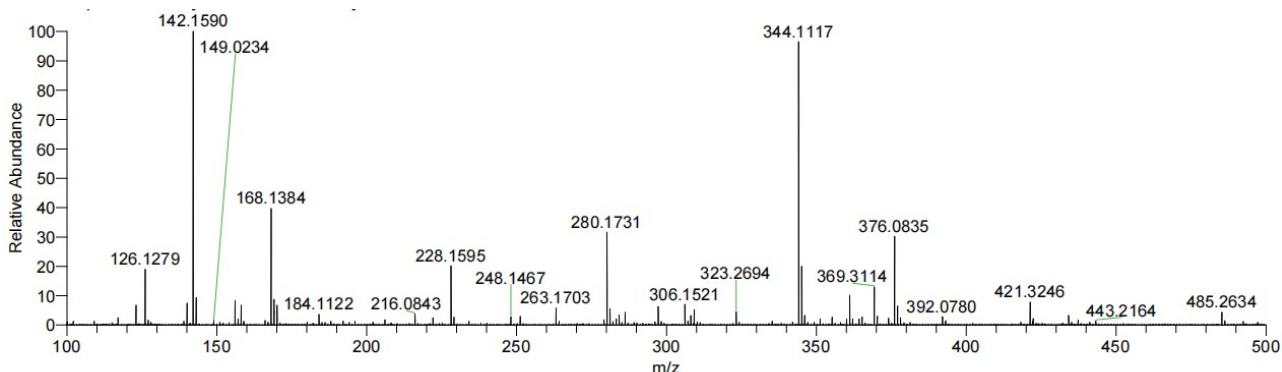
n_x is the amount of photochemical or photophysical events x occurred during irradiation, n_p is the number of photons absorbed by the reactant. E is the radiant power. S is the irradiated area: 2 cm²; t is the irradiated time: 3600 s; N_A is the Avogadro constant: 6.022×10^{23} /mol; h is the Planck constant: 6.626×10^{-34} J·s; ν is the frequency of incident light; c is velocity of light 2.998×10^8 m/s). λ is the wavelength: 415 nm; n_x was analyzed by ¹H NMR, ΔE was measured by ILT1400 Portable Radiometer/Photometer.

Substrate **1a** (0.04 mmol, 1.0 equiv.), K₂CO₃ (2.0 equiv.), *p*-toluenethiol (0.2 equiv.) and Ir(dFCF₃ppy)₂(dtbpy)PF₆ (3.0 mol%) were added in a cuvette equipped with a magnetic stir bar. The reaction cuvette was placed under vacuum and backfilled with argon three times. Then, DCE (5.0 mL) and **2a** (2.0 equiv.) were added in the Schlenk tube via a syringe. Next, the tube was placed 5.0 cm away from blue LEDs (30 W), and stirred vigorously under the irradiation of blue light for 1.0 h. The reaction mixture was concentrated in *vacuo* and analyzed by ¹H NMR spectrum using dimethyl terephthalate as an internal standard. The quantum yield is calculated to be 0.13.

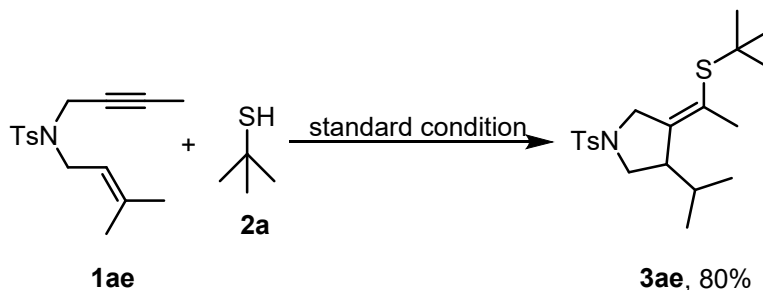
(c) Radical trapping experiments.^[3]



Substrate **1a** (0.1 mmol, 1.0 equiv.), K_2CO_3 (2.0 equiv.), *p*-toluenethiol (0.2 equiv.), TEMPO (2.0 equiv.) and $\text{Ir}(\text{dFCF}_3\text{ppy})_2(\text{dtbpy})\text{PF}_6$ (3.0 mol%) were added in a flame dried 15 mL Schlenk tube. The reaction tube was placed under vacuum and backfilled with argon three times. Then, **2a** (2.0 equiv.) and DCE (5.0 mL) were added in the Schlenk tube via a syringe. Next, the tube was placed 5.0 cm away from blue LEDs (30 W), and stirred vigorously under the irradiation of blue light for 12 h. When the reaction finished up, the mixture was concentrated in vacuo. The yield of product **3a** was determined by ^1H NMR spectroscopy using dimethyl terephthalate as an internal standard. However, the TEMPO-trapped adduct can not be characterized by HRMS spectrometry.

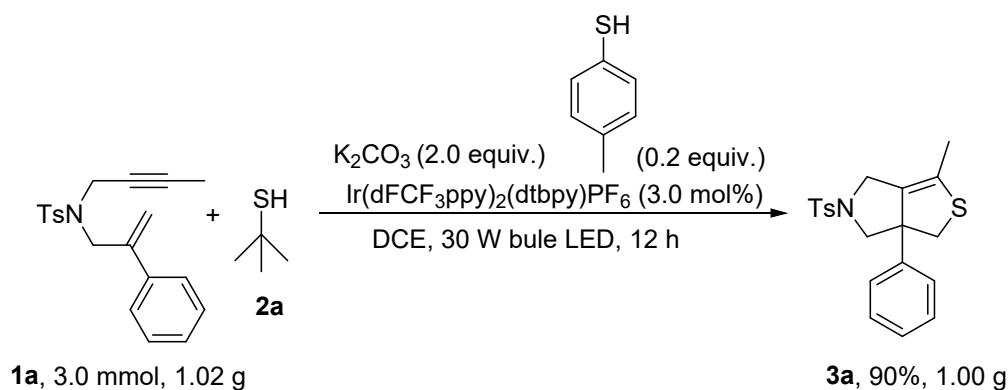


(d) Control experiments.



Substrate **1ae** (0.1 mmol, 1.0 equiv.), K₂CO₃ (2.0 equiv.), *p*-toluenethiol (0.2 equiv.), and Ir(dFCF₃ppy)₂(dtbpy)PF₆ (3.0 mol%) were added in a flame dried 15 mL Schlenk tube. The reaction tube was placed under vacuum and backfilled with argon three times. Then, **2a** (2.0 equiv.) and DCE (5.0 mL) were added in the Schlenk tube via a syringe. Next, the tube was placed 5.0 cm away from blue LEDs (30 W), and stirred vigorously under the irradiation of blue light for 12 h. When the reaction finished up, the mixture was concentrated in vacuo. The yield of product **3ae** was determined by ¹H NMR spectroscopy using dimethyl terephthalate as an internal standard.

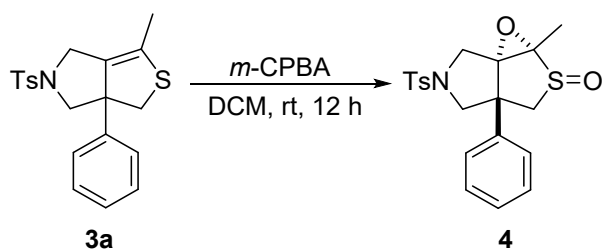
6. Gram scale reaction



Substrate **1a** (3.0 mmol, 1.0 equiv.), K_2CO_3 (2.0 equiv.), *p*-toluenethiol (0.2 equiv.) and $Ir(dFCF_3ppy)_2(dtbbpy)PF_6$ (3.0 mol%) were added in a flame dried 50 mL Schlenk tube. The reaction tube was placed under vacuum and backfilled with argon three times. Then, **2a** (2.0 equiv.) and DCE (30.0 mL) was added in the Schlenk flask via a syringe. Next, the tube was placed 5.0 cm away from blue LEDs (30 W), and stirred vigorously under the irradiation of blue light for 12 h. After completion, the solvent was removed under reduced pressure. The crude product residue was purified by a column chromatography on silica gel (PE/EA = 10/1) to afford the purified product **3a** in 90% yield (1.00 g).

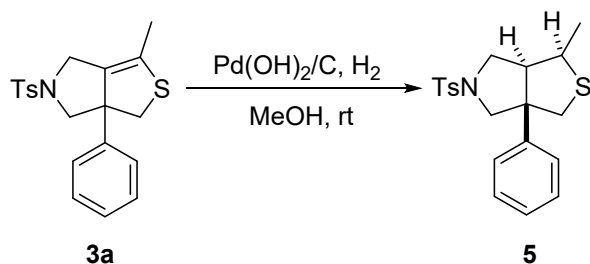
7. Transformation of product **3a**.^[3]

A. Oxidation reaction



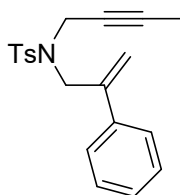
To a flask was added substrate **3a** (0.1 mmol, 1.0 equiv.), 3-chloroperoxybenzoic acid (0.5 mmol, 5.0 equiv.), and DCM (10 mL). After the reaction mixture was stirred at room temperature for 12 hours, the resulting mixture was filtered with a pad of celite. The filtrate was concentrated and the residue was purified with a silica gel column chromatography (PE/EA = 4/1) to give product **6** as a colorless oil (93% yield).

B. Hydrogenative reduction reaction



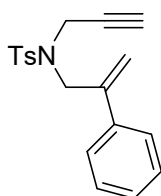
To a flask was added substrate **3a** (0.1 mmol, 1.0 equiv), Pd(OH)₂/C (16 mg) and MeOH (8.0 mL). After the reaction mixture was stirred at room temperature for 12 hours under 1.0 atm H₂, the resulting mixture was filtered with a pad of celite. The filtrate was concentrated under reduced pressure and the residue was purified with a silica gel column chromatography (PE/EA = 4/1) to give product **5** as a colorless oil (70% yield).

8. Spectroscopic data of substrates 1



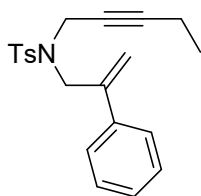
N-(but-2-yn-1-yl)-4-methyl-*N*-(2-phenylallyl)benzenesulfonamide (**1a**)

This is a known compound and its spectroscopic data are consistent with those reported in the previous literature,^[4] 83% yield, 390.0 mg. ¹H NMR (300 MHz, CDCl₃, TMS) δ 7.76 (d, *J* = 8.4 Hz, 2H), 7.52 (dd, *J* = 8.4, 1.8 Hz, 2H), 7.38-7.29 (m, 5H), 5.56 (s, 1H), 5.33 (s, 1H), 4.23 (s, 2H), 3.93 (q, *J* = 2.1 Hz, 2H), 2.44 (s, 3 H), 1.51 (t, *J* = 2.4 Hz, 3H). ¹³C NMR (75.5 MHz CDCl₃, TMS) δ 143.4, 141.7, 138.0, 136.0, 129.3, 128.5, 128.2, 126.5, 117.0, 82.0, 71.5, 50.1, 36.2, 21.6, 3.3.



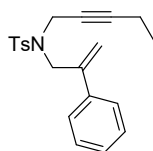
4-methyl-*N*-(2-phenylallyl)-*N*-(prop-2-yn-1-yl)benzenesulfonamide (**1b**)

This is a known compound and its spectroscopic data are consistent with those reported in the previous literature,^[5] 87% yield, 375.0 mg. ¹H NMR (600 MHz, CDCl₃, TMS) δ 7.75 (d, *J* = 8.2 Hz, 2H), 7.53 (d, *J* = 7.3 Hz, 2H), 7.35 (t, *J* = 7.3 Hz, 2H), 7.33 – 7.29 (m, 3H), 5.59 (s, 1H), 5.36 (s, 1H), 4.28 (s, 2H), 4.00 (d, *J* = 2.3 Hz, 2H), 2.44 (s, 3H), 1.99 (t, *J* = 2.3 Hz, 1H). ¹³C NMR (151 MHz, CDCl₃, TMS) δ 143.7, 141.3, 137.7, 135.6, 129.5, 128.5, 128.2, 128.0, 126.4, 117.3, 76.2, 74.2, 50.0, 35.6, 21.6

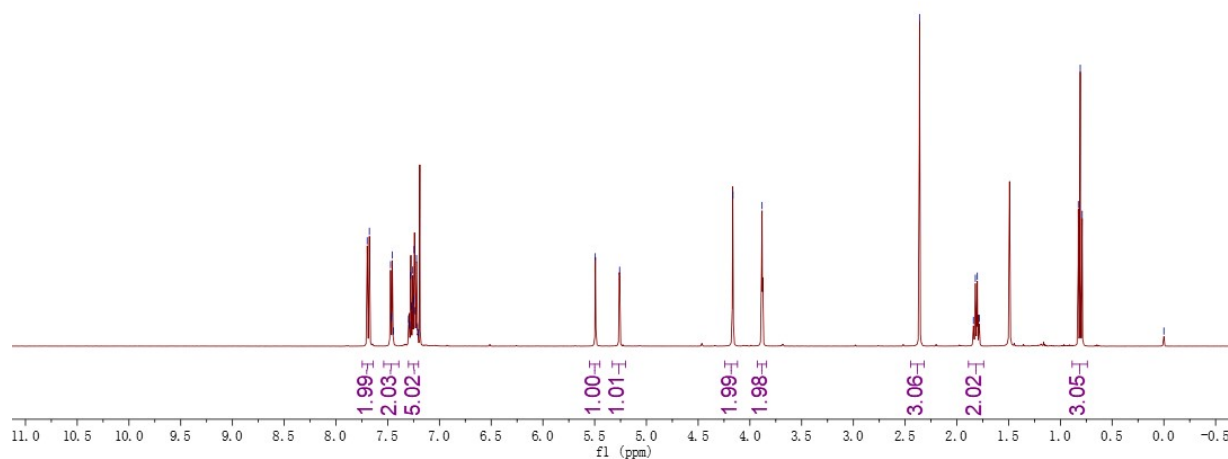


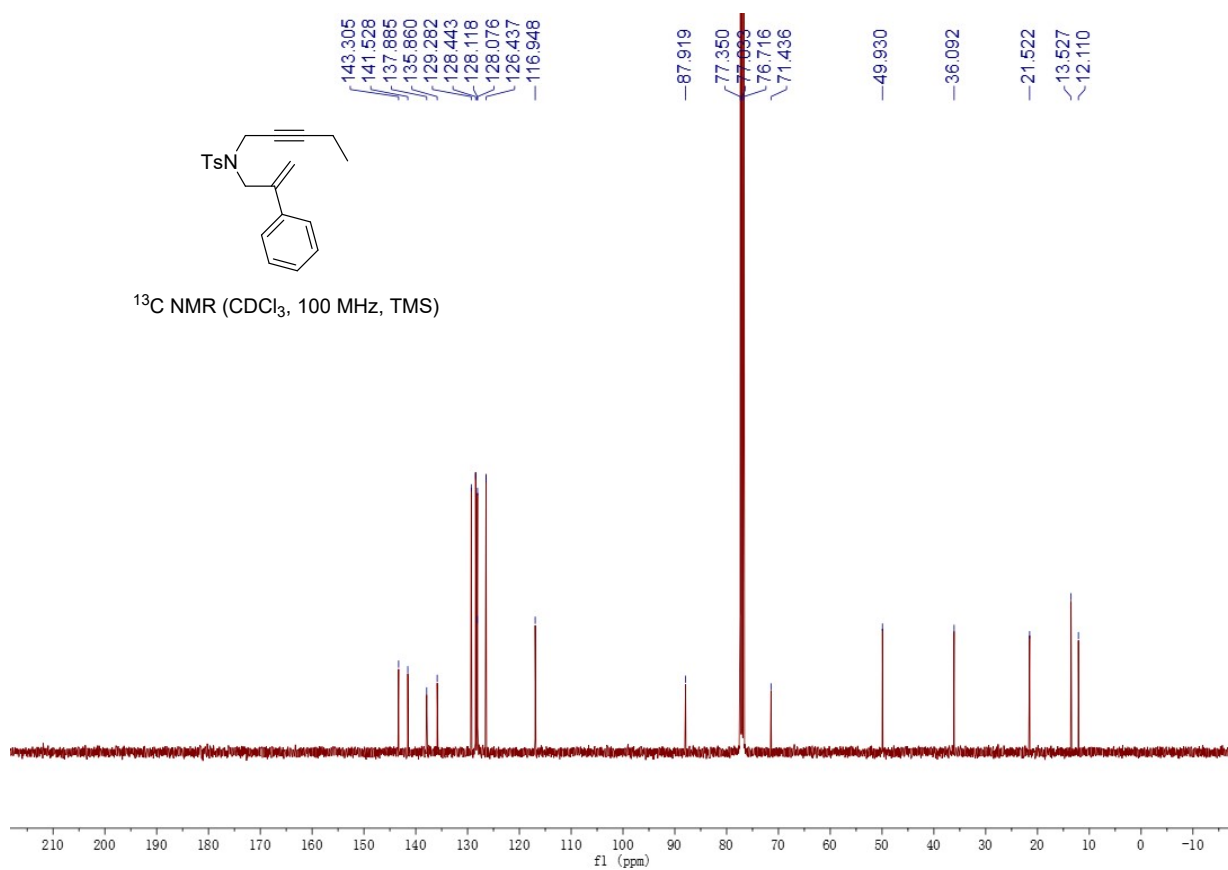
4-methyl-N-(pent-2-yn-1-yl)-N-(2-phenylallyl)benzenesulfonamide (1c)

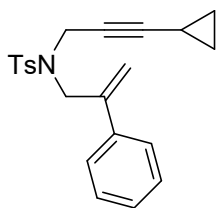
A colorless oil, 48% yield, 239.0 mg. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.69 (d, $J = 8.3$ Hz, 2H), 7.54 – 7.39 (m, 2H), 7.30 – 7.20 (m, 5H), 5.49 (s, 1H), 5.26 (s, 1H), 4.16 (s, 2H), 3.88 (s, 2H), 2.36 (s, 3H), 1.81 (q, $J = 7.5$ Hz, 2H), 0.81 (t, $J = 7.5$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 143.3, 141.5, 137.9, 135.9, 129.3, 128.4, 128.12, 128.08, 126.4, 116.9, 87.9, 71.4, 49.9, 36.1, 21.5, 13.5, 12.1. IR (Acetone) ν 762, 1093, 1160, 1348, 2203, 2953 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{21}\text{H}_{24}\text{O}_2\text{NS}$ (M+H): 354.1522, Found: 354.1509.



^1H NMR (CDCl_3 , 400 MHz, TMS)

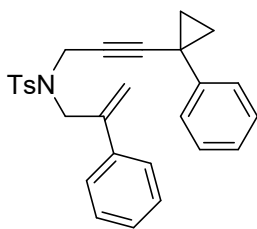






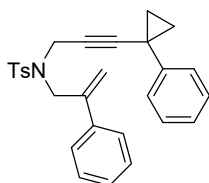
***N*-(3-cyclopropylprop-2-yn-1-yl)-4-methyl-*N*-(2-phenylallyl)benzenesulfonamide (1d)**

This is a known compound and its spectroscopic data are consistent with those reported in the previous literature,^[6] 70% yield, 260.0 mg. ¹H NMR (300 MHz, CDCl₃, TMS) δ 7.74 (d, *J* = 8.1 Hz, 2H), 7.53 (d, *J* = 6.8 Hz, 2H), 7.25 – 7.37 (m, 5H), 5.56 (s, 1H), 5.32 (s, 1H), 4.22 (s, 2H), 3.93 (s, 2H), 2.45 (s, 3H), 0.89 – 0.95 (m, 1H), 0.57 – 0.63 (m, 2H), 0.25 – 0.30 (m, 2H). ¹³C NMR (75.5 MHz, CDCl₃, TMS) δ 187.8, 142.8, 142.7, 139.2, 137.4, 129.4, 128.2, 127.7, 127.3, 126.5, 115.8, 108.0, 79.7, 50.6, 48.8, 38.2, 32.1, 26.3, 26.2, 21.4, 6.9.

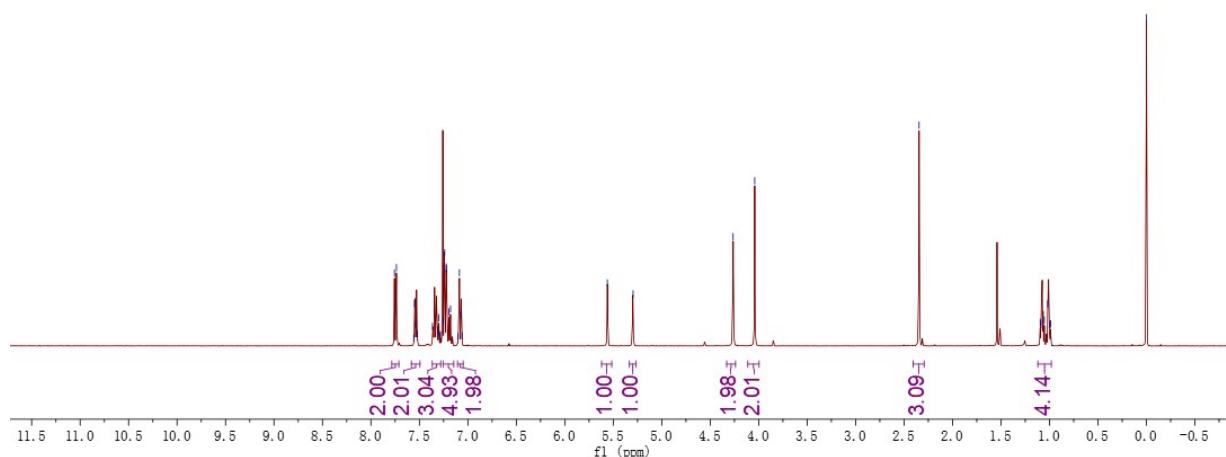


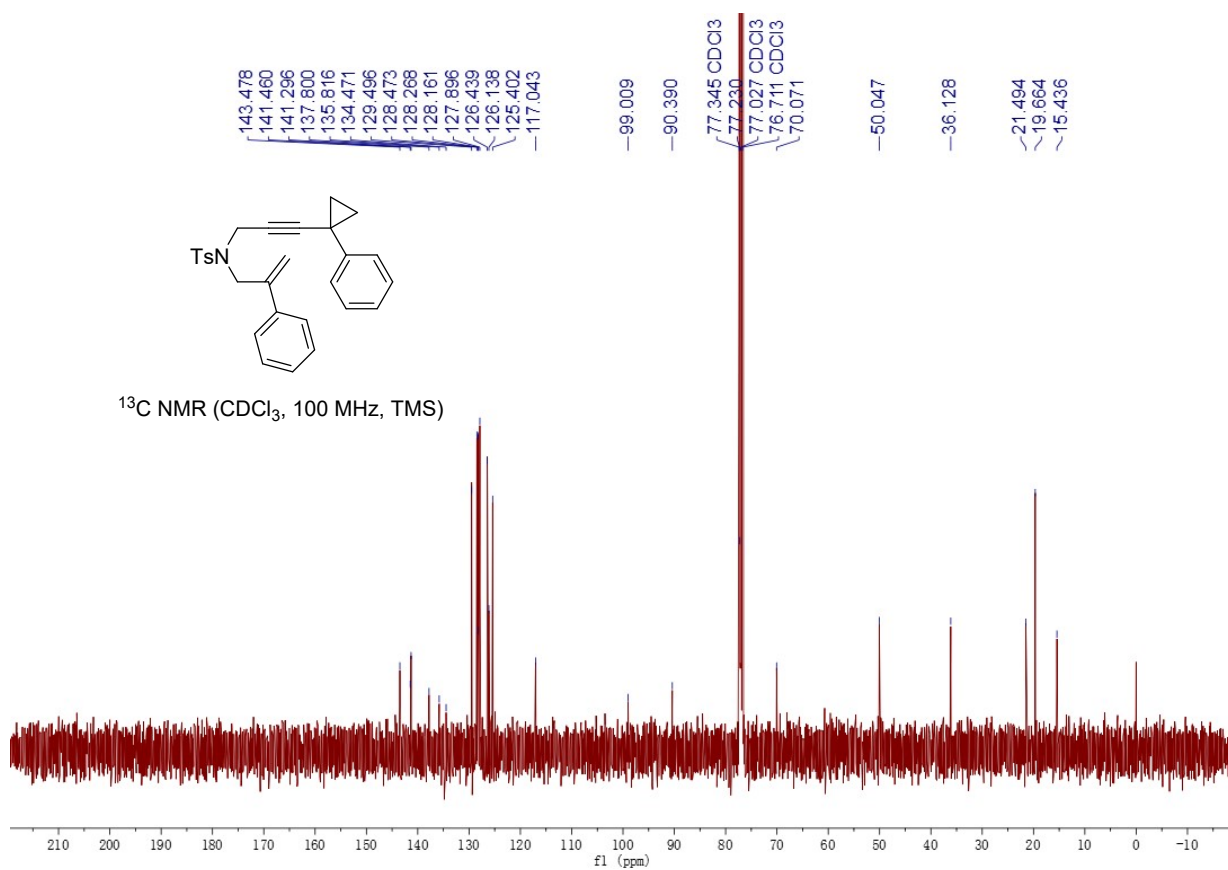
4-methyl-N-(2-phenylallyl)-N-(3-(1-phenylcyclopropyl)prop-2-yn-1-yl)benzenesulfonamide (1e)

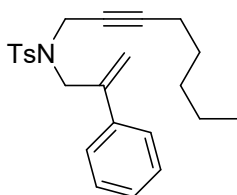
A colorless oil, 60% yield, 285.6 mg. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.75 (d, $J = 8.3$ Hz, 2H), 7.58-7.49 (m, 2H), 7.37 – 7.28 (m, 3H), 7.26 – 7.15 (m, 5H), 7.11-7.05 (m, 2H), 5.56 (s, 1H), 5.30 (s, 1H), 4.26 (s, 2H), 4.04 (s, 2H), 2.35 (s, 3H), 1.12 – 0.98 (m, 4H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 143.5, 141.5, 141.3, 137.8, 135.8, 134.5, 129.5, 128.5, 128.3, 128.2, 127.9, 126.4, 126.1, 125.4, 117.0, 99.0, 90.4, 70.1, 50.0, 36.1, 21.5, 19.7, 15.4. IR (Acetone) ν 659, 1092, 1161, 1348, 1491, 2987 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{28}\text{H}_{28}\text{O}_2\text{NS}$ ($\text{M}+\text{H}$): 442.1835, Found: 442.1823.



^1H NMR (CDCl_3 , 400 MHz, TMS)

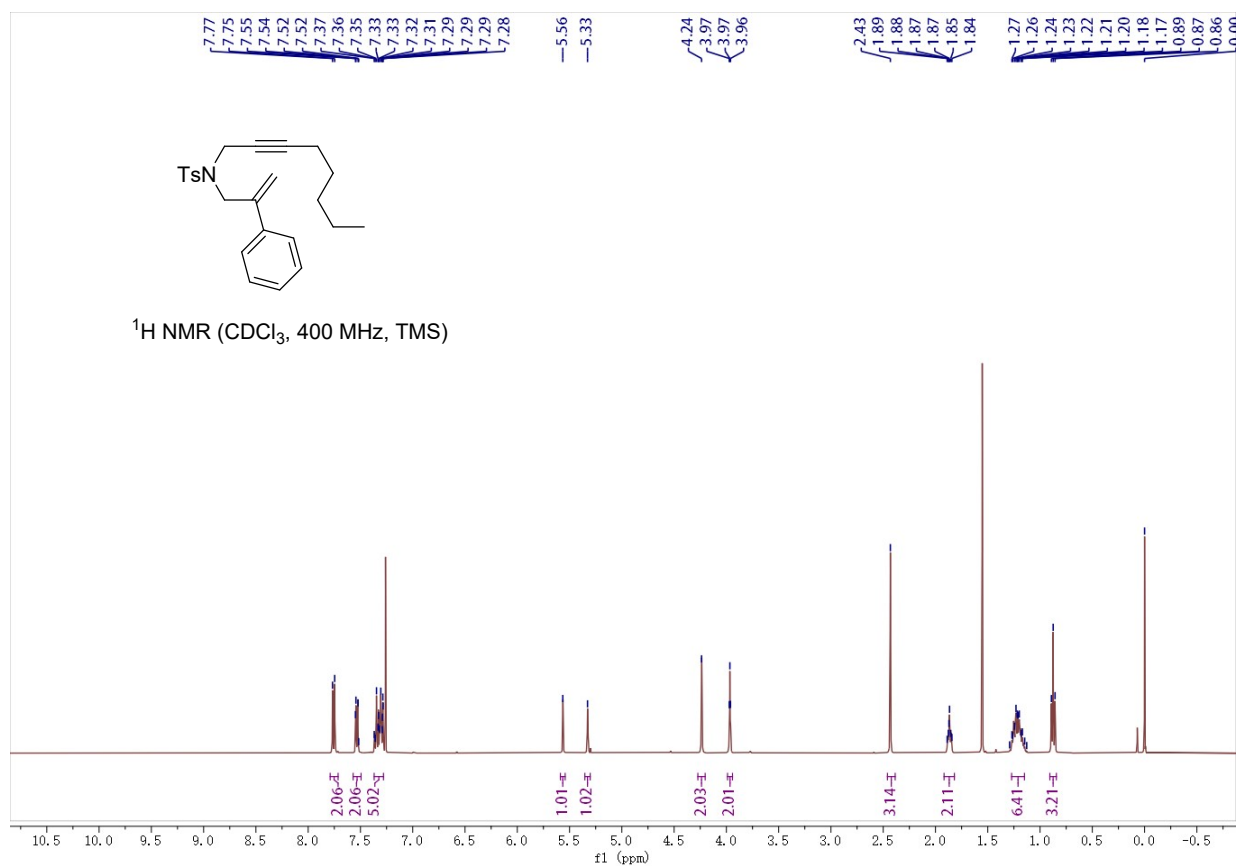


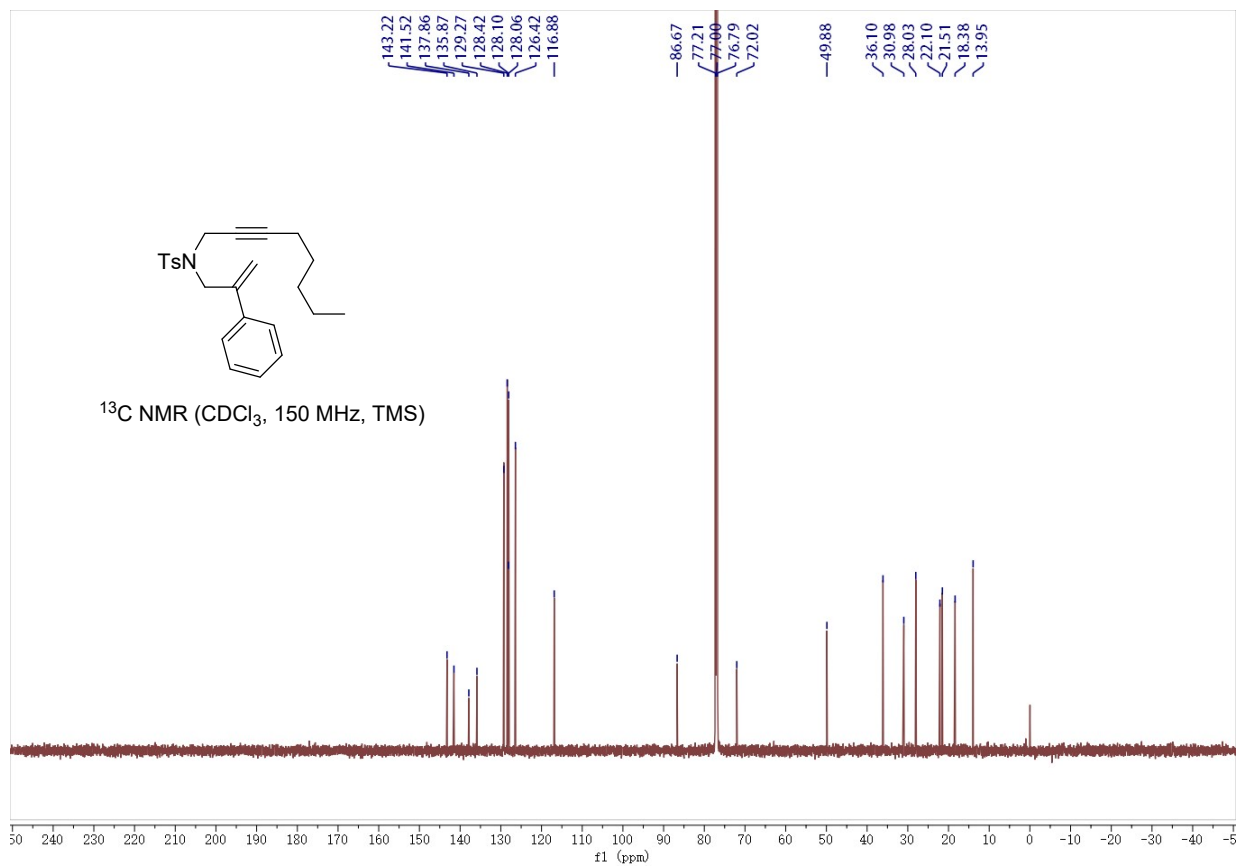


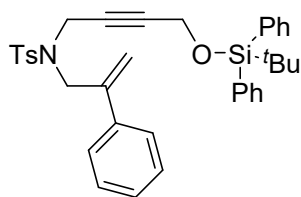


4-methyl-*N*-(oct-2-yn-1-yl)-*N*-(2-phenylallyl)benzenesulfonamide (**1f**)

A colorless oil, 62% yield, 282.0 mg. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.76 (d, $J = 8.3$ Hz, 2H), 7.57 – 7.49 (m, 2H), 7.37 – 7.28 (m, 5H), 5.56 (s, 1H), 5.33 (s, 1H), 4.24 (s, 2H), 3.97 (t, $J = 2.3$ Hz, 2H), 2.43 (s, 3H), 1.92 – 1.82 (m, 2H), 1.27 – 1.15 (m, 6H), 0.87 (t, $J = 7.0$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 143.2, 141.5, 137.9, 135.9, 129.3, 128.4, 128.10, 128.06, 126.4, 116.9, 72.0, 49.9, 36.1, 31.0, 28.0, 22.1, 21.5, 18.4, 14.0. IR (Acetone) ν 711, 1087, 1197, 1381, 1498, 2306, 2977 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{24}\text{H}_{30}\text{O}_2\text{NS}$ ($\text{M}+\text{H}$): 396.1992, Found: 396.1979.

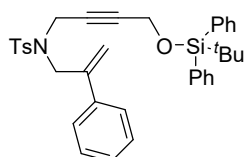




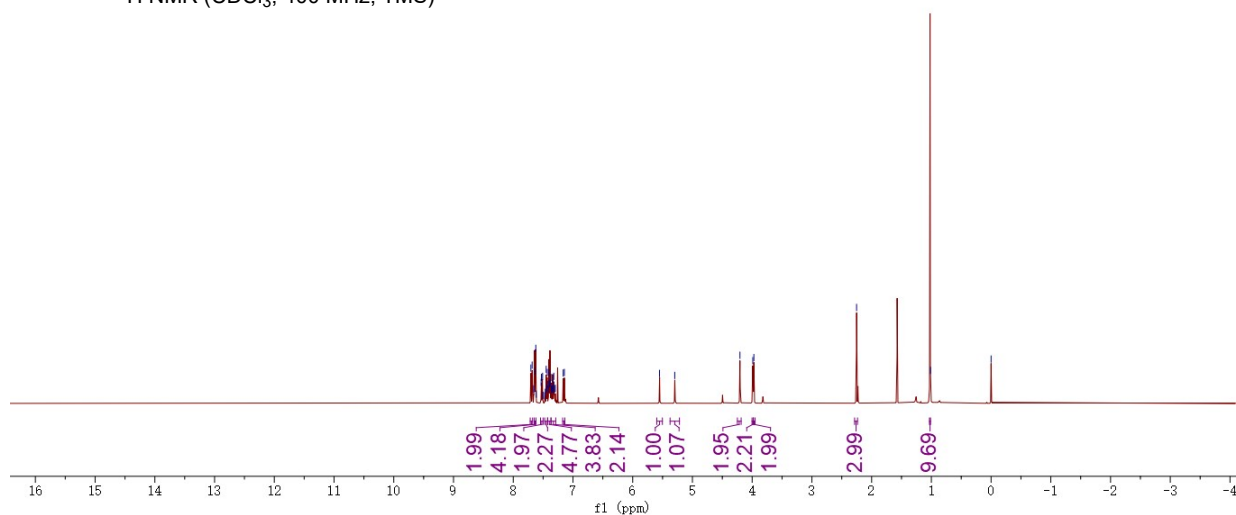


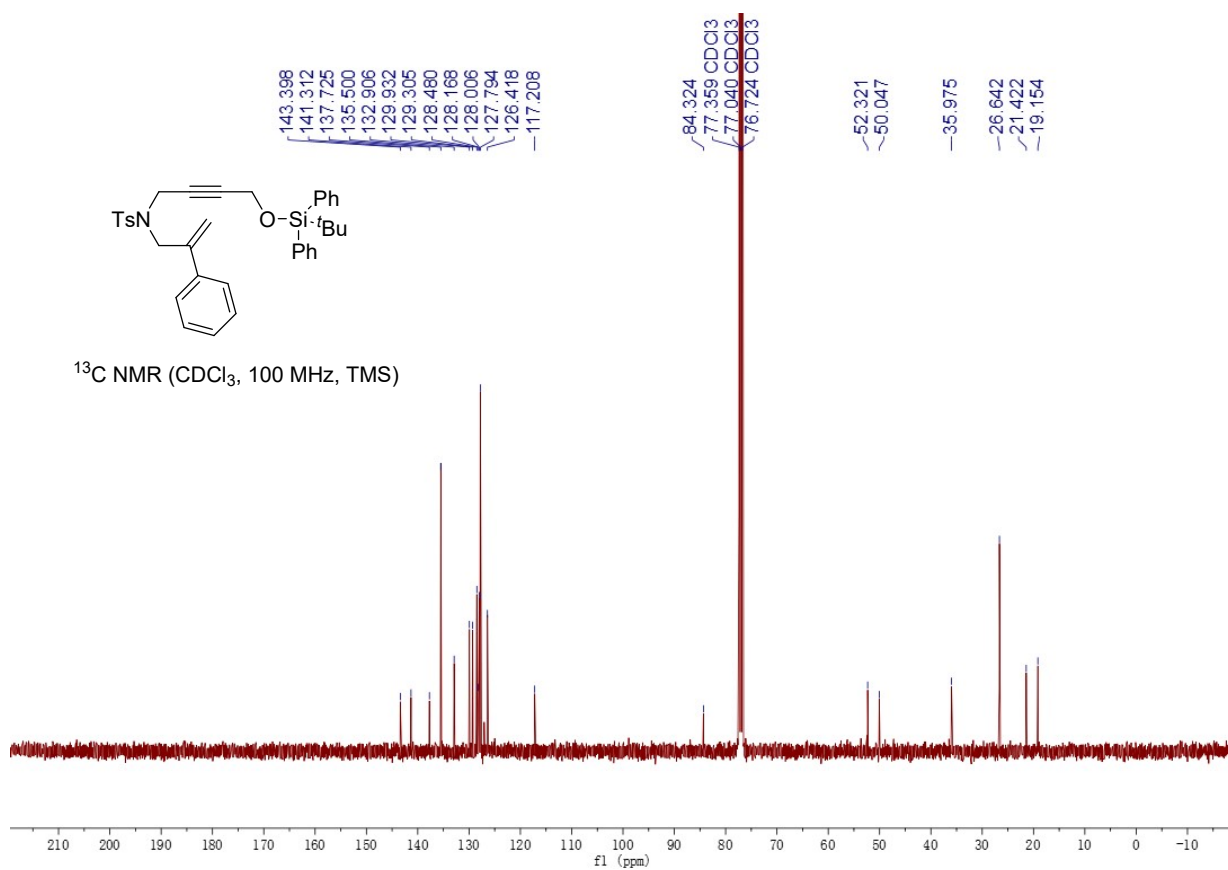
***N*-(4-((*tert*-butyldiphenylsilyloxy)but-2-yn-1-yl)-4-methyl-*N*-(2-phenylallyl)benzenesulfonamide (1g)**

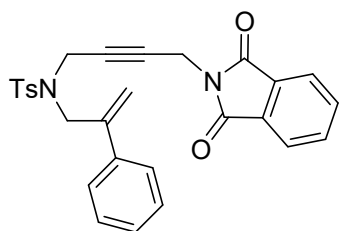
A colorless oil, 53% yield, 274.3 mg. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.69 (d, $J = 8.3$ Hz, 2H), 7.65 – 7.62 (m, 4H), 7.54 – 7.50 (m, 2H), 7.47 – 7.43 (m, 2H), 7.42 – 7.37 (m, 4H), 7.37 – 7.29 (m, 3H), 7.15 (d, $J = 8.0$ Hz, 2H), 5.55 (s, 1H), 5.30 (s, 1H), 4.20 (s, 2H), 3.99 (s, 2H), 3.97 (s, 2H), 2.25 (s, 3H), 1.01 (s, 9H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 143.4, 141.3, 137.7, 135.5, 132.9, 129.9, 129.3, 128.5, 128.2, 128.0, 127.8, 126.4, 117.2, 84.3, 52.3, 50.0, 36.0, 26.6, 21.4, 19.2. IR (Acetone) ν 661, 701, 1112, 1162, 1350, 2863 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{36}\text{H}_{40}\text{O}_3\text{NSSi}$ ($\text{M}+\text{H}$): 594.2493, Found: 594.2488.



^1H NMR (CDCl_3 , 400 MHz, TMS)

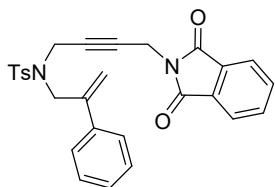




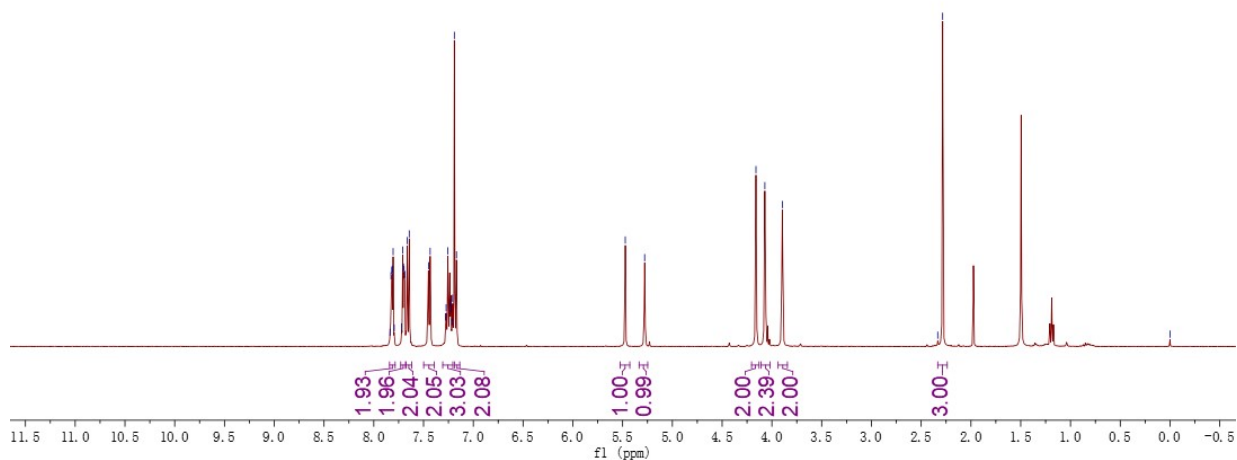


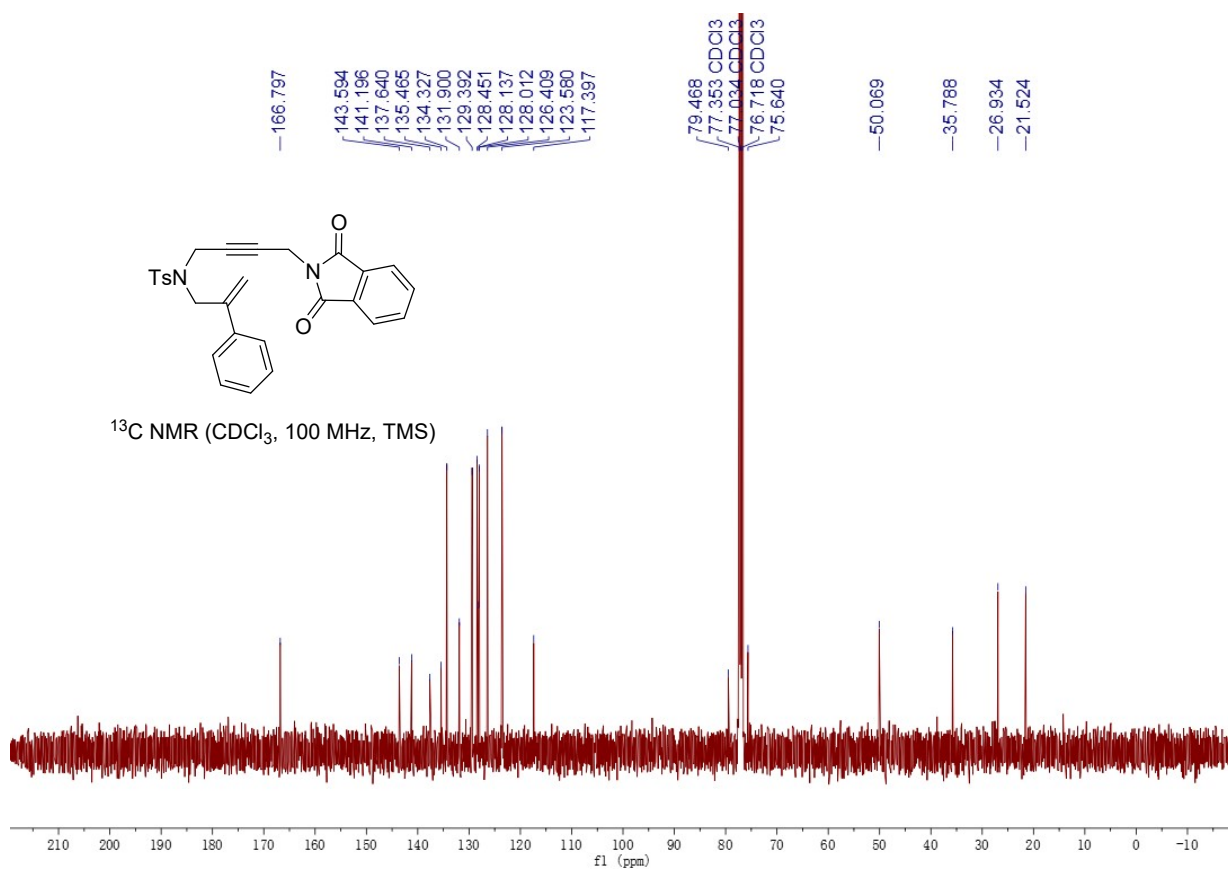
***N*-(4-(1,3-dioxoisindolin-2-yl)but-2-yn-1-yl)-4-methyl-*N*-(2-phenylallyl)benzenesulfonamide (1h)**

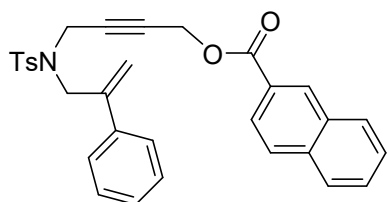
A colorless oil, 55% yield, 250.6 mg. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.84 – 7.79 (m, 2H), 7.73 – 7.68 (m, 2H), 7.65 (d, $J = 8.1$ Hz, 2H), 7.44 (d, $J = 6.7$ Hz, 2H), 7.31 – 7.21 (m, 3H), 7.19 – 7.14 (m, 2H), 5.47 (s, 1H), 5.28 (s, 1H), 4.16 (s, 2H), 4.07 (s, 2H), 3.89 (s, 2H), 2.28 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 166.8, 143.6, 141.2, 137.6, 135.5, 134.3, 131.9, 129.4, 128.5, 128.1, 128.0, 126.4, 123.6, 117.4, 79.5, 75.6, 50.1, 35.8, 26.9, 21.5. IR (Acetone) ν 729, 1107, 1161, 1229, 1345, 2287, 2984 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{28}\text{H}_{25}\text{O}_4\text{N}_2\text{S}$ ($\text{M}+\text{H}$): 485.1530, Found: 485.1514.



^1H NMR (CDCl_3 , 400 MHz, TMS)

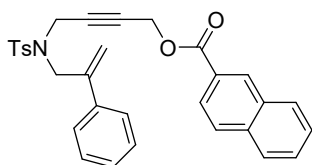




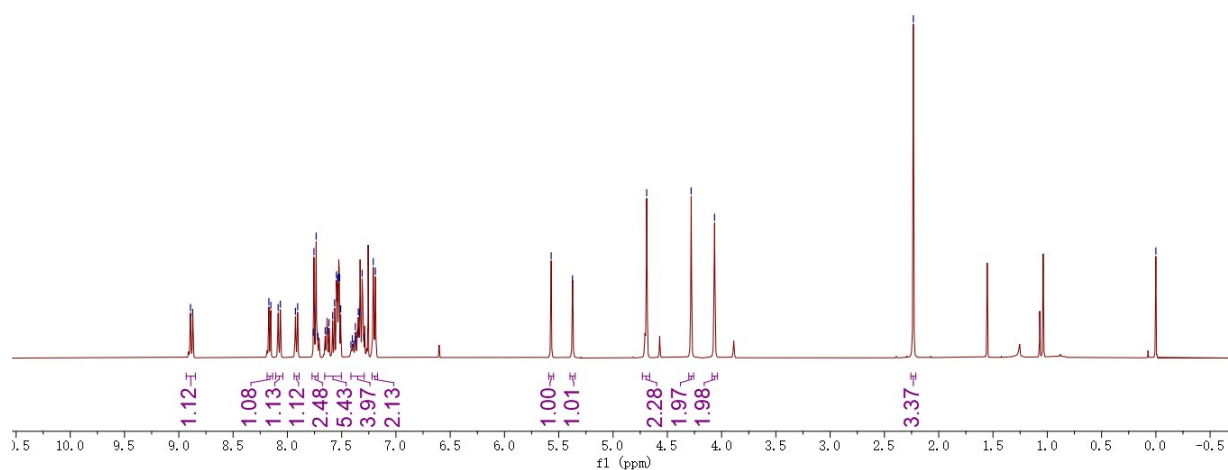


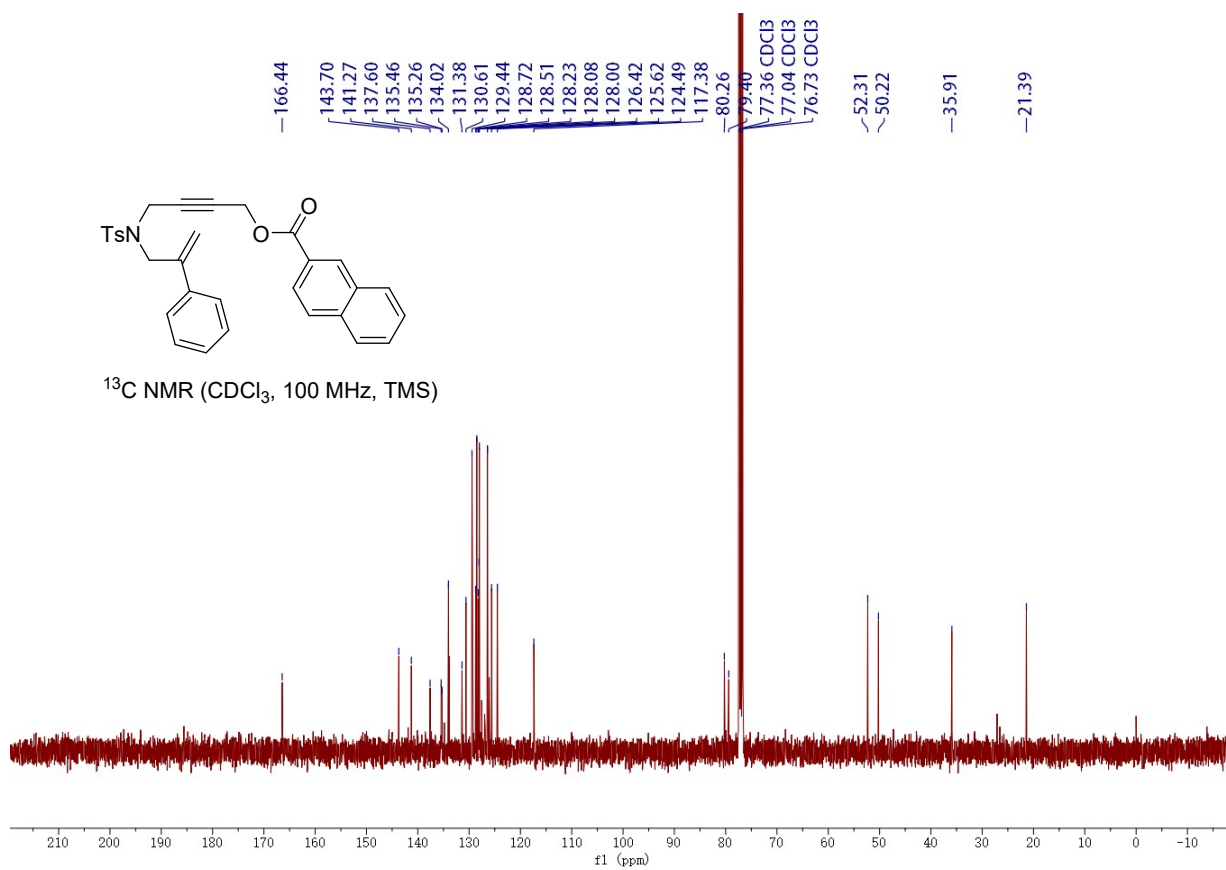
4-((4-methyl-N-(2-phenylallyl)phenyl)sulfonamido)but-2-yn-1-yl 2-naphthoate (**1i**)

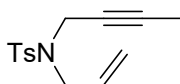
A colorless oil, 42% yield, 203.9 mg. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 8.88 (d, $J = 7.9$ Hz, 1H), 8.16 (d, $J = 7.3$ Hz, 1H), 8.07 (d, $J = 8.2$ Hz, 1H), 7.92 (d, $J = 8.2$ Hz, 1H), 7.77 – 7.72 (m, 2H), 7.66 – 7.50 (m, 5H), 7.41 – 7.29 (m, 4H), 7.20 (d, $J = 8.0$ Hz, 2H), 5.57 (s, 1H), 5.37 (s, 1H), 4.69 (s, 2H), 4.28 (s, 2H), 4.06 (s, 2H), 2.23 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 166.4, 143.7, 141.3, 137.6, 135.5, 135.3, 134.0, 131.4, 130.6, 129.4, 128.7, 128.5, 128.2, 128.1, 128.0, 126.4, 125.6, 124.5, 117.4, 80.3, 79.4, 52.3, 50.2, 35.9, 21.4. IR (Acetone) ν 661, 779, 1061, 1128, 1159, 1239, 1342, 3052 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{31}\text{H}_{28}\text{O}_4\text{NS}$ (M+H): 510.1734, Found: 510.1718.



^1H NMR (CDCl_3 , 400 MHz, TMS)

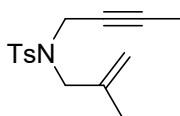






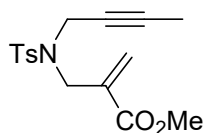
***N*-allyl-*N*-(but-2-yn-1-yl)-4-methylbenzenesulfonamide (1j)**

This is a known compound and its spectroscopic data are consistent with those reported in the previous literature,^[7] 80% yield, 238.0 mg. ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 8.2 Hz, 2H), 5.75 – 5.65 (m, 1H), 5.29 – 5.13 (m, 2H), 4.05 – 3.94 (m, 2H), 3.77 (q, *J* = 6.0 Hz, 2H), 2.39 (s, 3H), 1.50 (s, 3H).



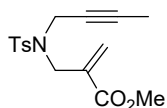
***N*-(but-2-yn-1-yl)-4-methyl-*N*-(2-methylallyl)benzenesulfonamide (1k)**

This is a known compound and its spectroscopic data are consistent with those reported in the previous literature,^[7] 89% yield, 348.0 mg. ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.75 – 7.73 (m, 2H), 7.30 – 7.28 (m, 2H), 4.94 (q, *J* = 1.0 Hz, 2H), 3.97 (q, *J* = 2.3 Hz, 2H), 3.69 (s, 2H), 2.42 (s, 3H), 1.75 (t, *J* = 1.1 Hz, 3H), 1.50 (t, *J* = 2.3 Hz, 3H).

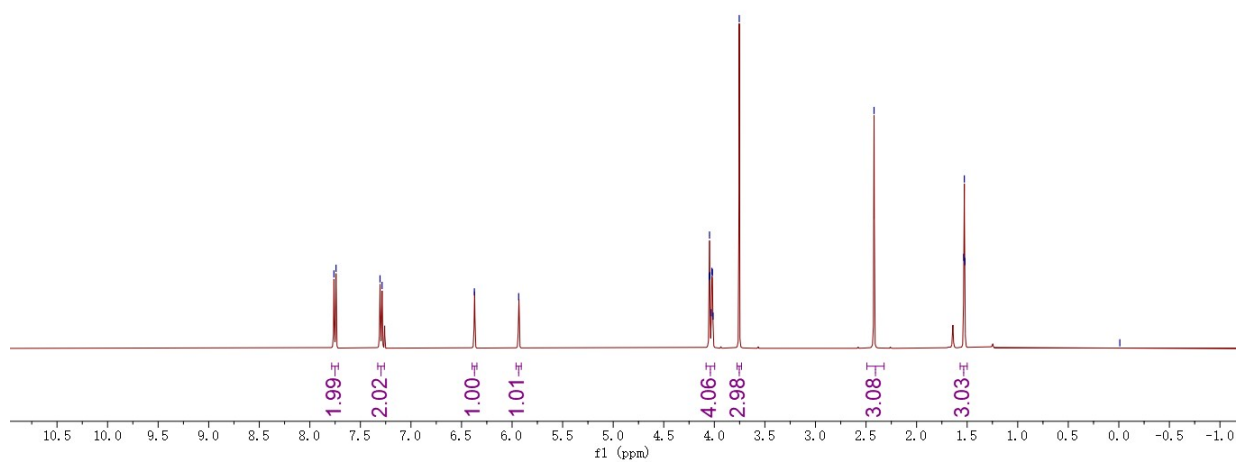


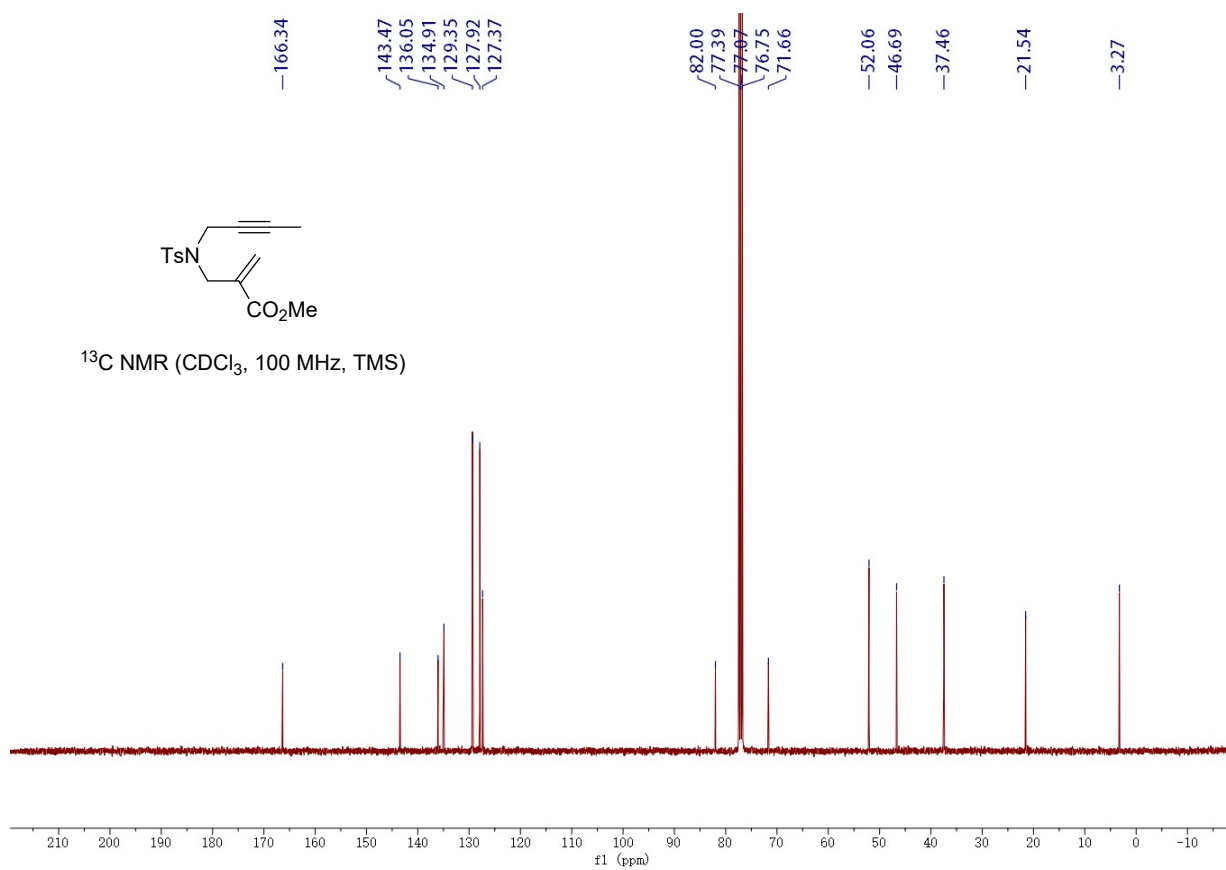
methyl 2-(((*N*-(but-2-yn-1-yl)-4-methylphenyl)sulfonamido)methyl)acrylate (11)

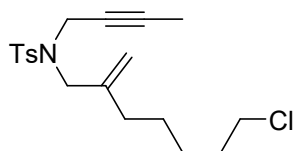
A colorless oil, 62% yield, 282.5 mg. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.75 (d, $J = 8.3$ Hz, 2H), 7.30 (d, $J = 8.0$ Hz, 2H), 6.37 (s, 1H), 5.93 (s, 1H), 4.08 – 4.00 (m, 4H), 3.75 (s, 3H), 2.42 (s, 3H), 1.53 (t, $J = 2.4$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 166.3, 143.4, 136.0, 134.8, 129.3, 127.8, 127.3, 81.9, 71.6, 52.0, 46.6, 37.4, 21.5, 3.2. IR (Acetone) ν 764, 1091, 1165, 1371, 2125, 2966 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{16}\text{H}_{19}\text{NO}_4\text{S}$ (M+H): 322.1133, Found: 322.1096.



^1H NMR (CDCl_3 , 400 MHz, TMS)

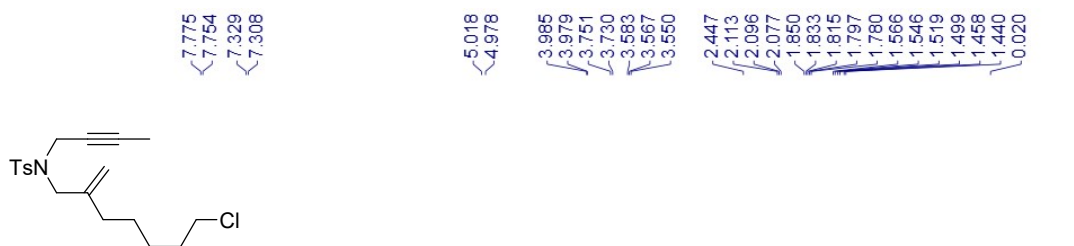




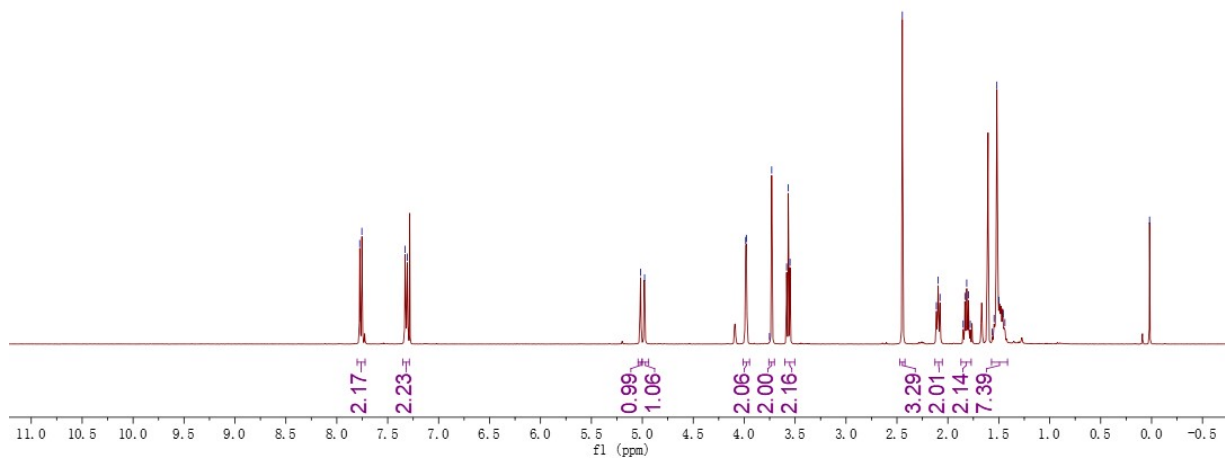


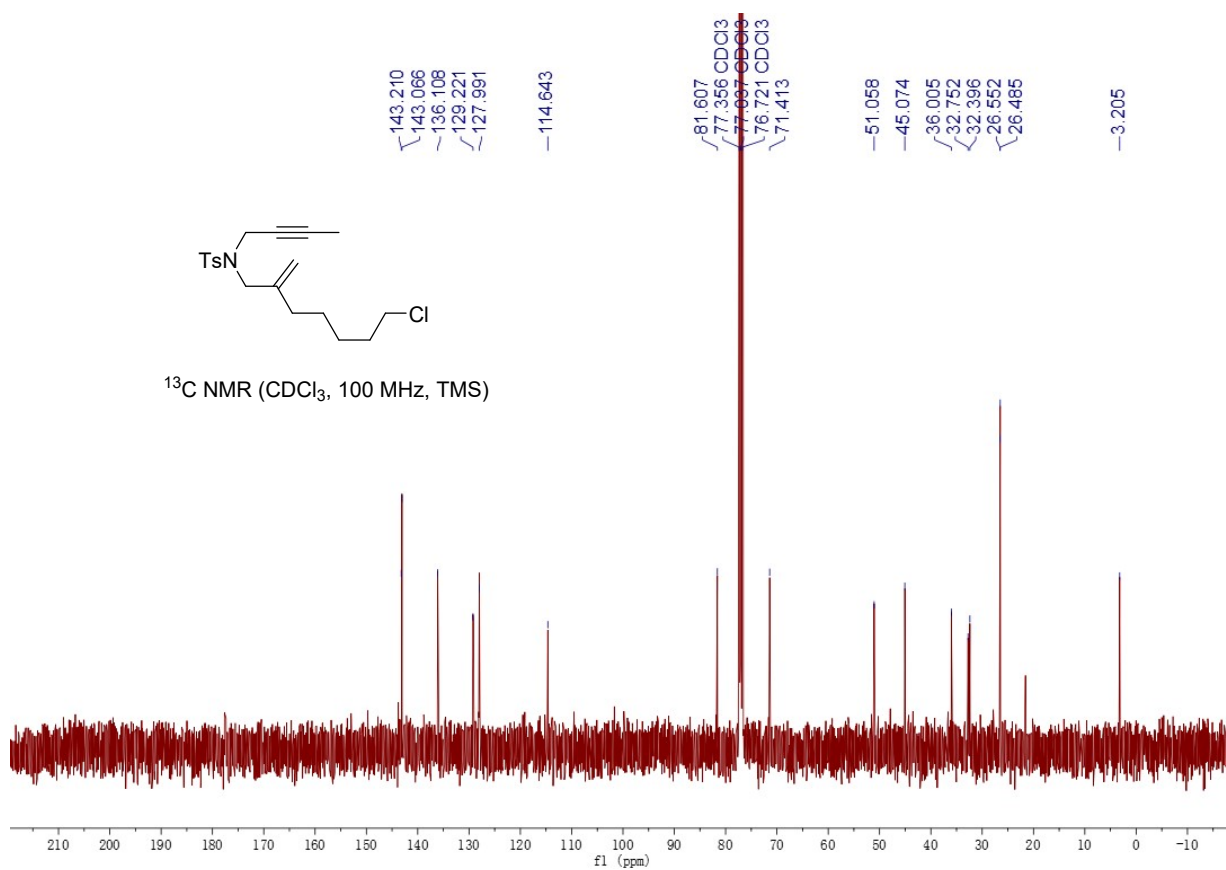
***N*-(but-2-yn-1-yl)-*N*-(7-chloro-2-methyleneheptyl)-4-methylbenzenesulfonamide (1m)**

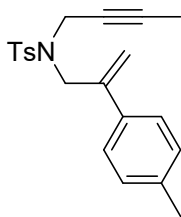
A colorless oil, 59%, 271.1 mg. ^1H NMR (CDCl_3 , TMS, 600 MHz) δ 7.76 (d, $J = 8.4$ Hz, 2H), 7.32 (d, $J = 8.1$ Hz, 2H), 5.02 (s, 1H), 4.98 (s, 1H), 3.98 (d, $J = 2.5$ Hz, 2H), 3.73 (s, 2H), 3.57 (t, $J = 6.7$ Hz, 2H), 2.45 (s, 3H), 2.10 (t, $J = 7.2$ Hz, 2H), 1.87 – 1.77 (m, 2H), 1.57 – 1.41 (m, 7H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 143.2, 143.1, 136.1, 129.2, 128.0, 114.6, 81.6, 71.4, 51.1, 45.1, 36.0, 32.8, 32.4, 26.6, 26.5, 3.2. IR (Acetone) ν 730, 987, 1258, 2983 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{19}\text{H}_{27}\text{O}_2\text{NCIS}$ ($\text{M}+\text{H}$): 368.1446, Found: 368.1434.



^1H NMR (CDCl_3 , 400 MHz, TMS)

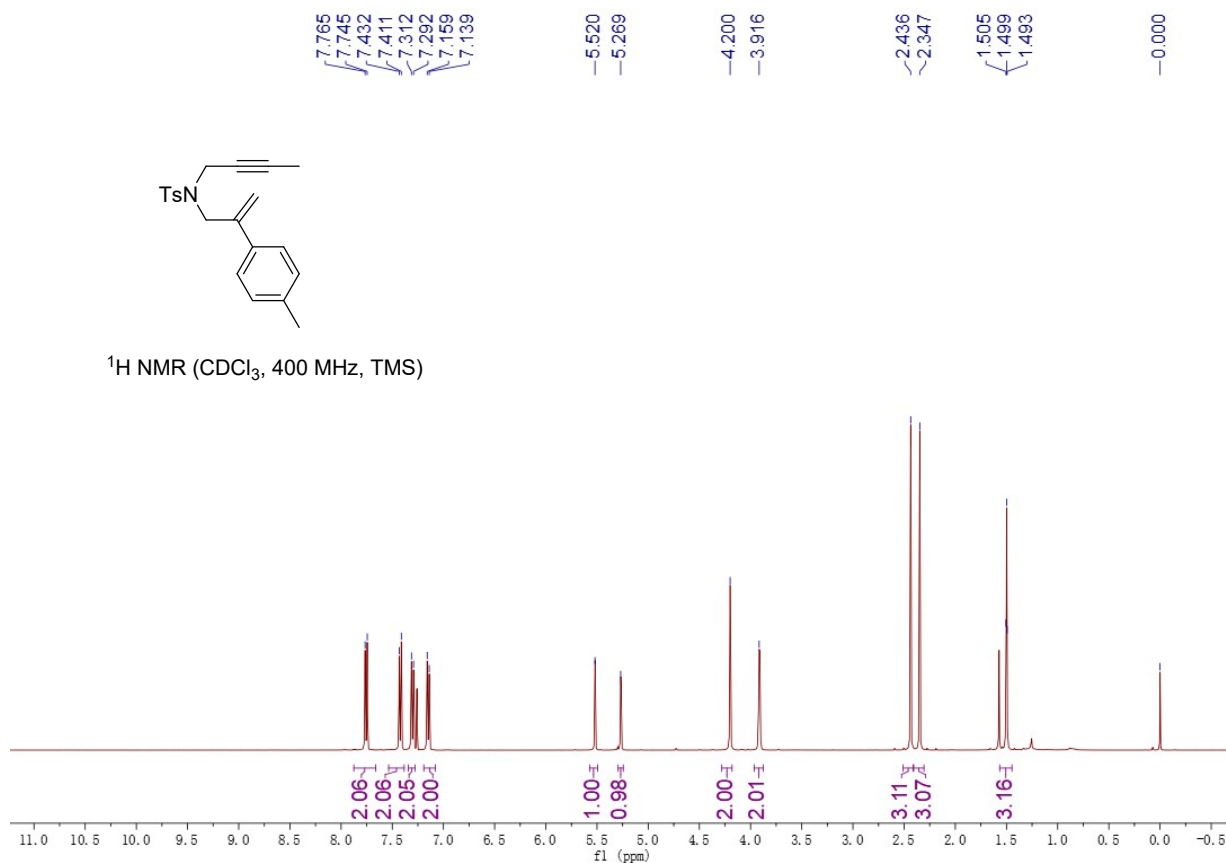


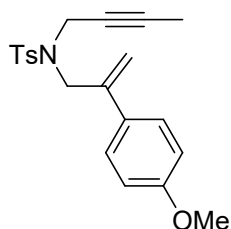
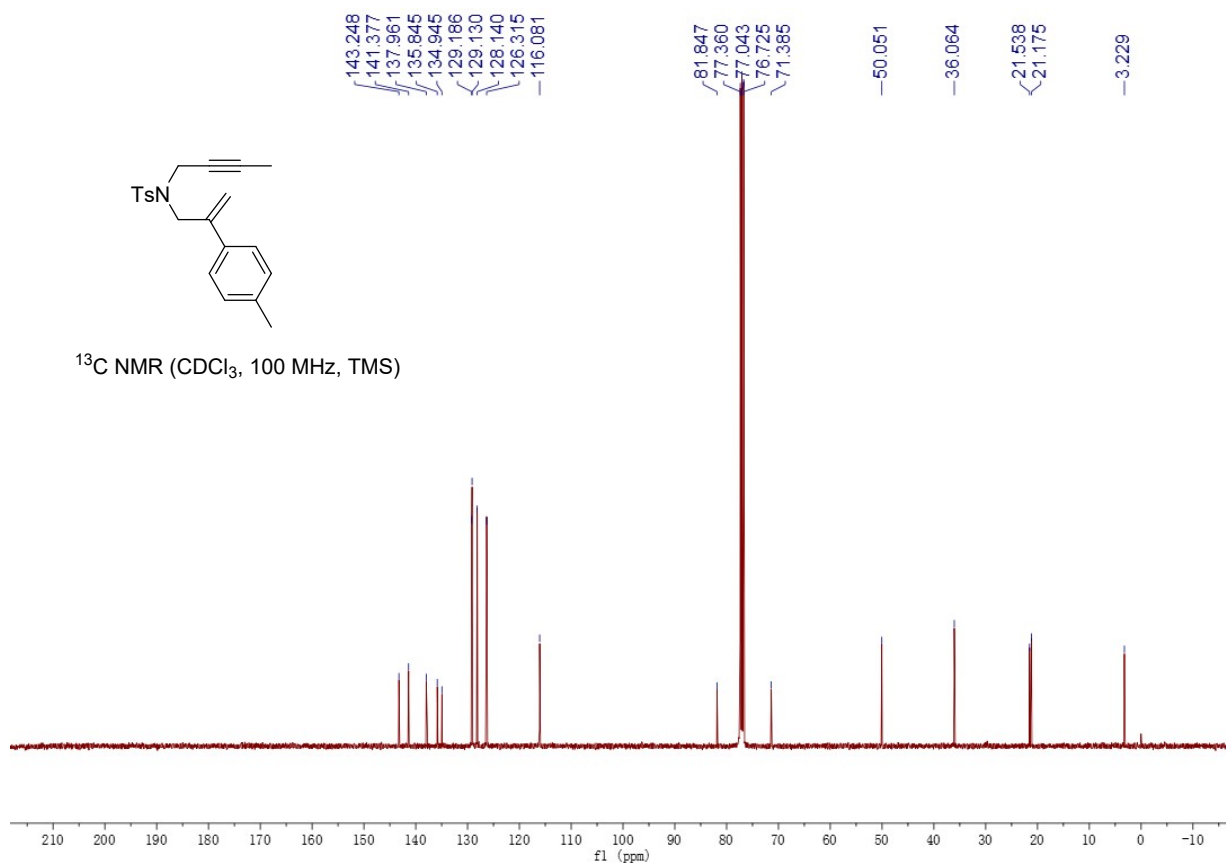




***N*-(but-2-yn-1-yl)-4-methyl-*N*-(2-(*p*-tolyl)allyl)benzenesulfonamide (1n)**

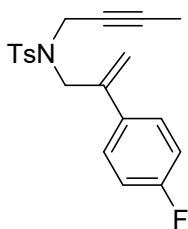
A colorless oil, 38% yield, 197.2 mg. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.75 (d, $J = 8.2$ Hz, 2H), 7.42 (d, $J = 8.2$ Hz, 2H), 7.30 (d, $J = 8.1$ Hz, 2H), 7.15 (d, $J = 8.0$ Hz, 2H), 5.52 (s, 1H), 5.27 (s, 1H), 4.20 (s, 2H), 3.92 (s, 2H), 2.44 (s, 3H), 2.35 (s, 3H), 1.50 (t, $J = 2.4$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 143.2, 141.4, 138.0, 135.8, 134.9, 129.2, 129.1, 128.1, 126.3, 116.1, 81.8, 71.4, 50.1, 36.1, 21.5, 21.2, 3.2. IR (Acetone) ν 719, 801, 1104, 1209, 1346, 1510, 2914 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{21}\text{H}_{24}\text{O}_2\text{NS}$ ($\text{M}+\text{H}$): 354.1522, Found: 354.1512.





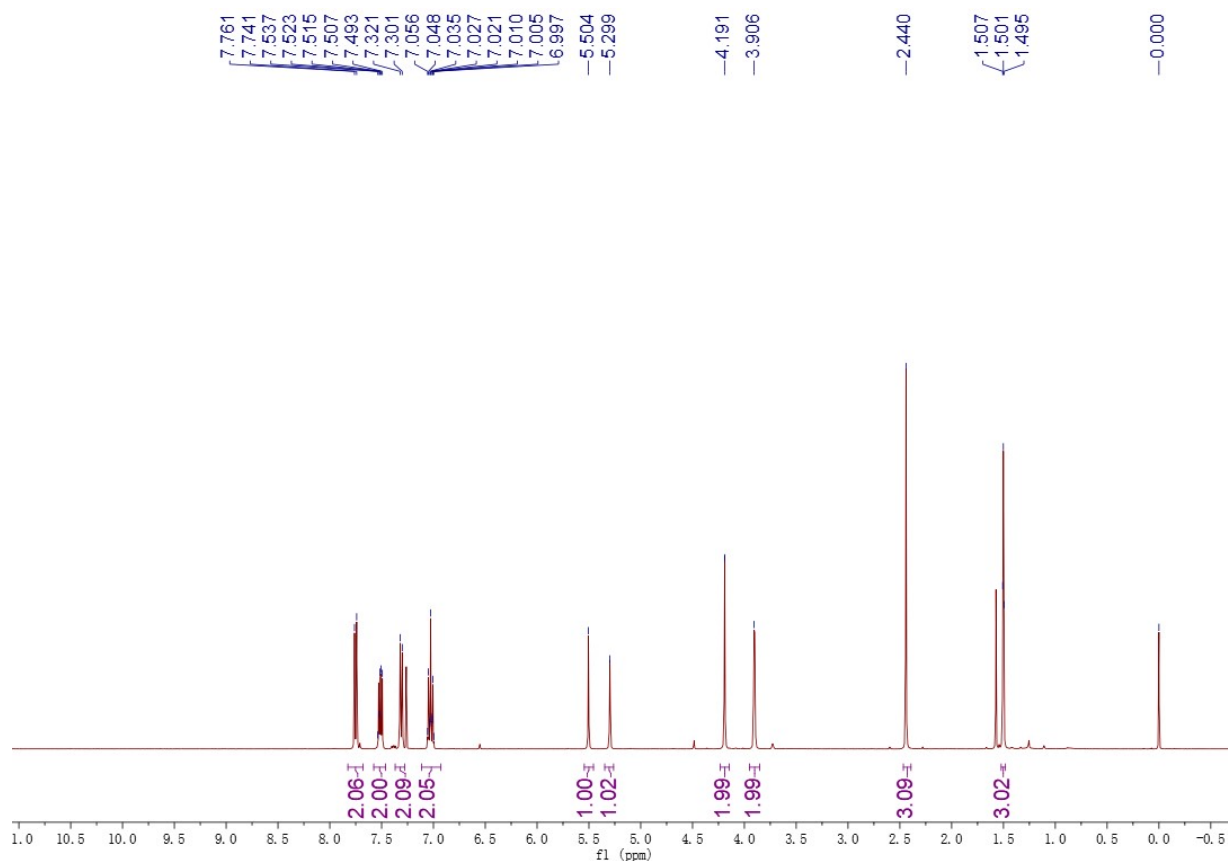
***N*-(but-2-yn-1-yl)-*N*-(2-(4-methoxyphenyl)allyl)-4-methylbenzenesulfonamide (1o)**

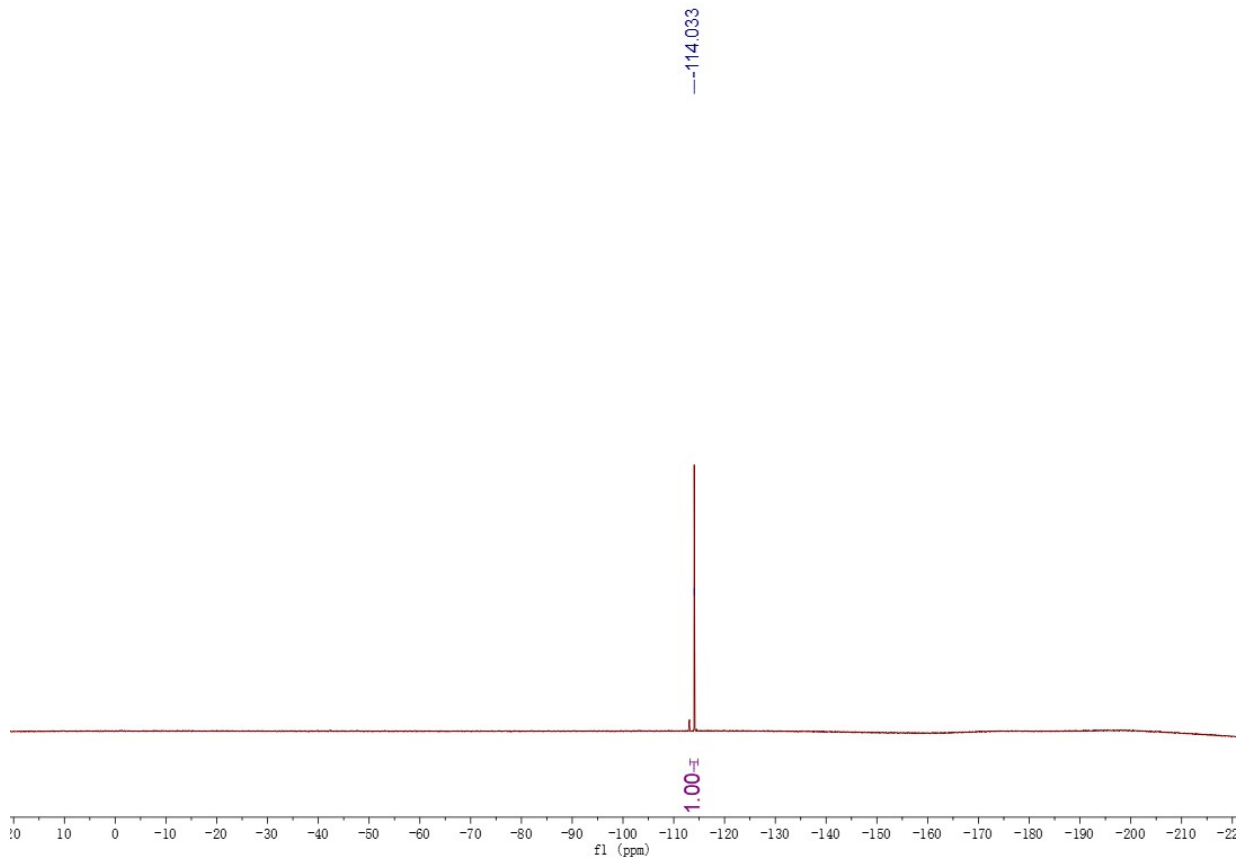
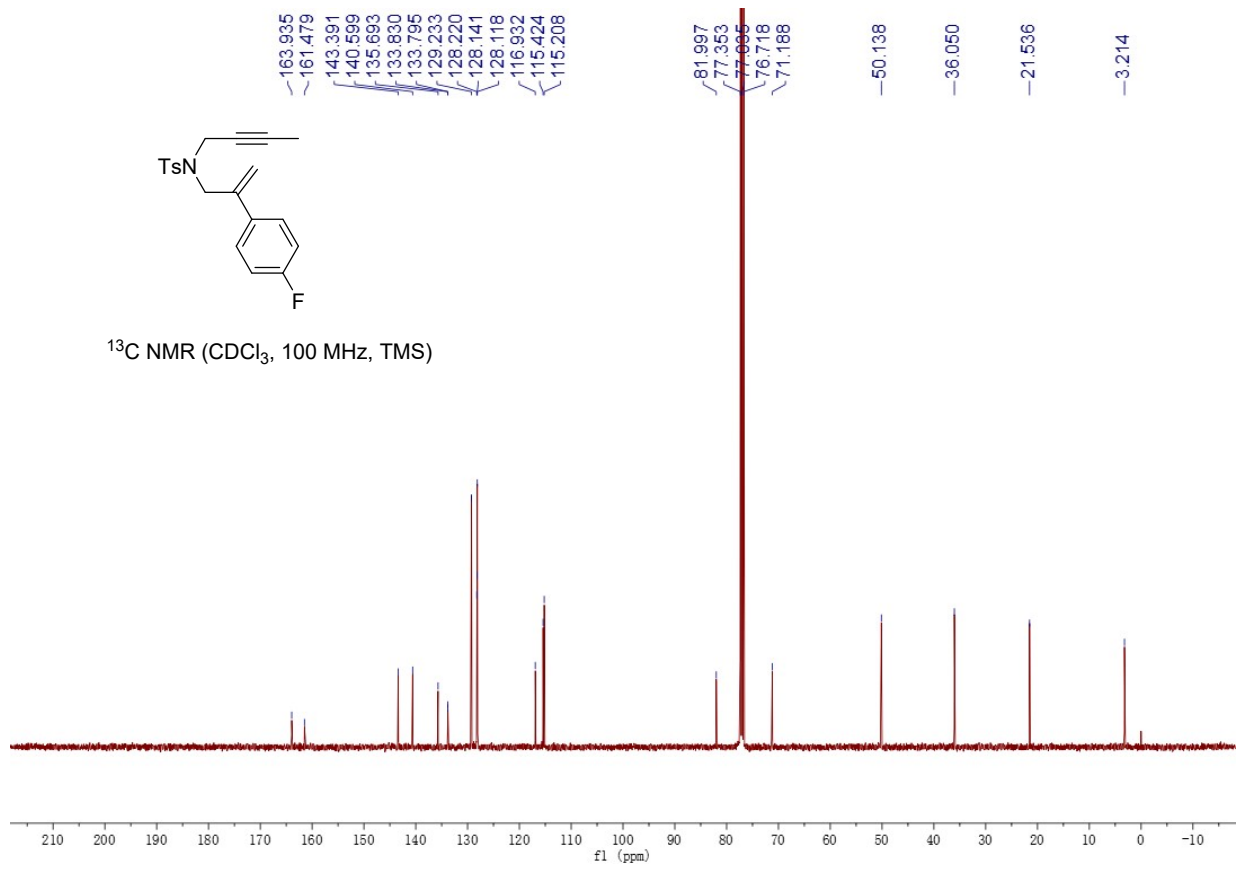
This is a known compound and its spectroscopic data are consistent with those reported in the previous literature,^[6] 62% yield, 218.0 mg. ¹H NMR (300 MHz, CDCl₃, TMS) δ 7.74 (d, *J* = 8.2 Hz, 2 H), 7.48 – 7.46 (m, 2 H), 7.29 (d, *J* = 8.2 Hz, 2 H), 6.86 (d, *J* = 8.9 Hz, 2 H), 5.46 (s, 1 H), 5.20 (s, 1 H), 4.17 (s, 2 H), 3.89 (q, *J* = 2.1 Hz, 2 H), 3.80 (s, 3 H), 2.42 (s, 3 H), 1.48 (t, *J* = 2.3 Hz, 3 H) ¹³C NMR (75.5 MHz, CDCl₃, TMS) δ 187.8, 142.8, 142.7, 139.2, 137.4, 129.4, 128.2, 127.7, 127.3, 126.5, 115.8, 108.0, 79.7, 50.6, 48.8, 38.2, 32.1, 26.3, 26.2, 21.4, 6.9.

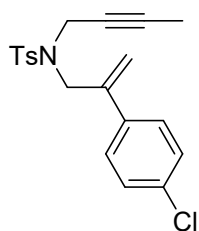


***N*-(but-2-yn-1-yl)-*N*-(2-(4-fluorophenyl)allyl)-4-methylbenzenesulfonamide (1p)**

A colorless oil, 41% yield, 193.4 mg. ^1H NMR (CDCl_3 , TMS, 600 MHz) δ 7.75 (d, $J = 8.3$ Hz, 2H), 7.58 – 7.46 (m, 2H), 7.31 (d, $J = 8.0$ Hz, 2H), 7.11 – 6.93 (m, 2H), 5.50 (s, 1H), 5.30 (s, 1H), 4.19 (s, 2H), 3.91 (s, 2H), 2.44 (s, 3H), 1.50 (t, $J = 2.4$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 162.7 (d, $J = 245.6$ Hz), 143.4, 140.6, 135.7, 133.8 (d, $J = 3.5$ Hz), 129.2, 128.2 (d, $J = 7.9$ Hz), 128.1, 116.9, 115.3 (d, $J = 21.6$ Hz), 82.0, 71.2, 50.1, 36.1, 21.5, 3.2. ^{19}F NMR (CDCl_3 , TMS, 376 MHz) δ -114.0 (s). IR (Acetone) ν 659, 842, 1095, 1160, 1347, 1511, 2198, 2914 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{20}\text{H}_{21}\text{O}_2\text{NFS}$ (M+H): 358.1272, Found: 358.1260.

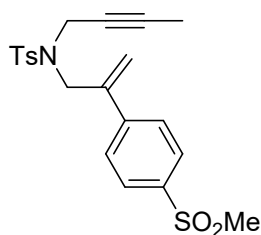






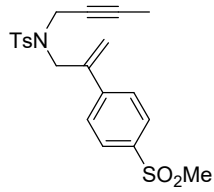
***N*-(but-2-yn-1-yl)-*N*-(2-(4-chlorophenyl)allyl)-4-methylbenzenesulfonamide (1q)**

This is a known compound and its spectroscopic data are consistent with those reported in the previous literature,^[8] 63% yield, 288.0 mg. ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.96 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.45 (dt, *J* = 7.5 Hz, *J* = 1.5 Hz, 1H), 7.31 (m, 1H), 7.10 – 7.24 (m, 5H), 5.46 (s, 1H), 5.37 (s, 1H), 4.25 (s, 2H), 3.92 (q, *J* = 2.4 Hz, 2H), 2.41 (s, 3H), 1.69 (t, *J* = 2.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃, TMS) δ 141.2, 138.5, 137.2, 136.7, 134.0, 133.0, 132.8, 130.4, 128.6, 127.8, 126.2, 118.3, 82.0, 72.2, 50.3, 35.8, 20.9, 3.9.

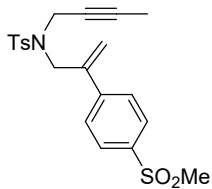
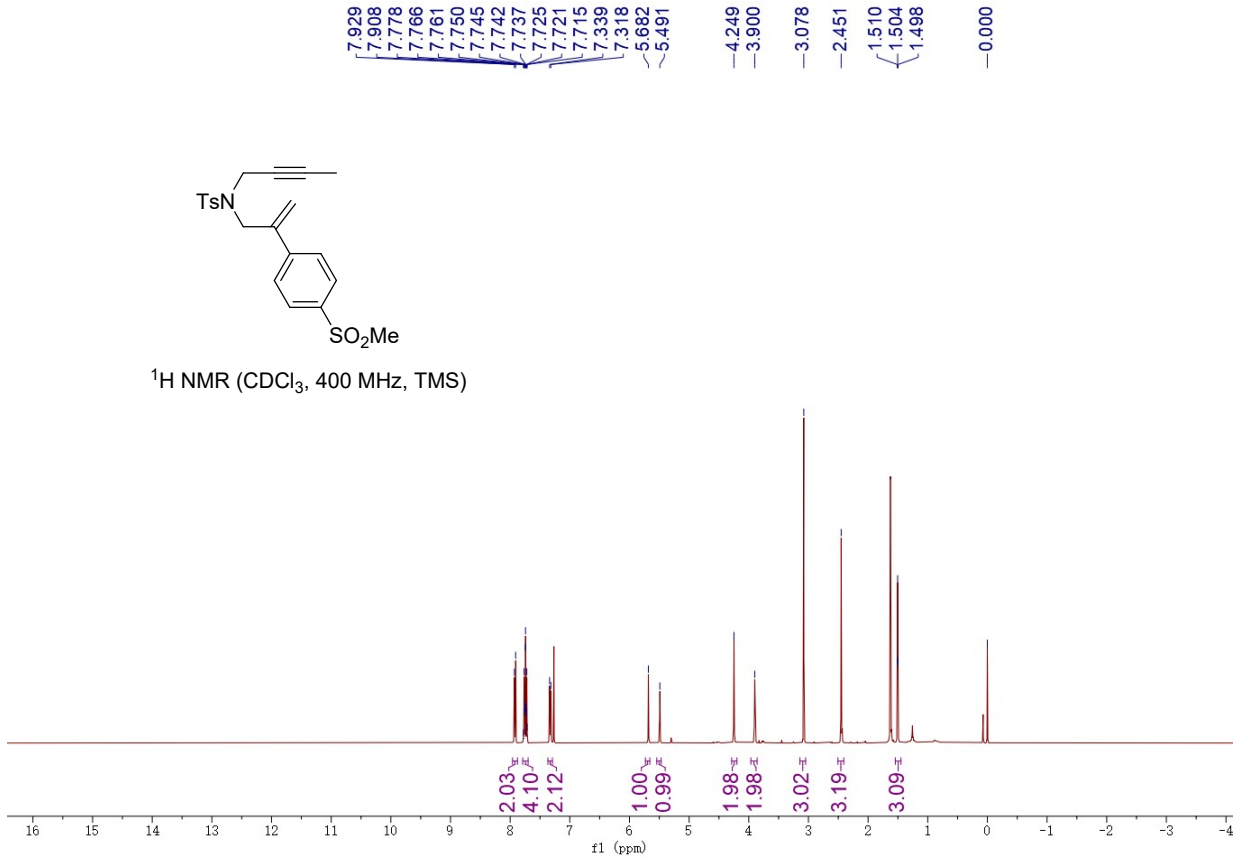


***N*-(but-2-yn-1-yl)-4-methyl-*N*-(2-(4-(methylsulfonyl)phenyl)allyl)benzenesulfonamide (1r)**

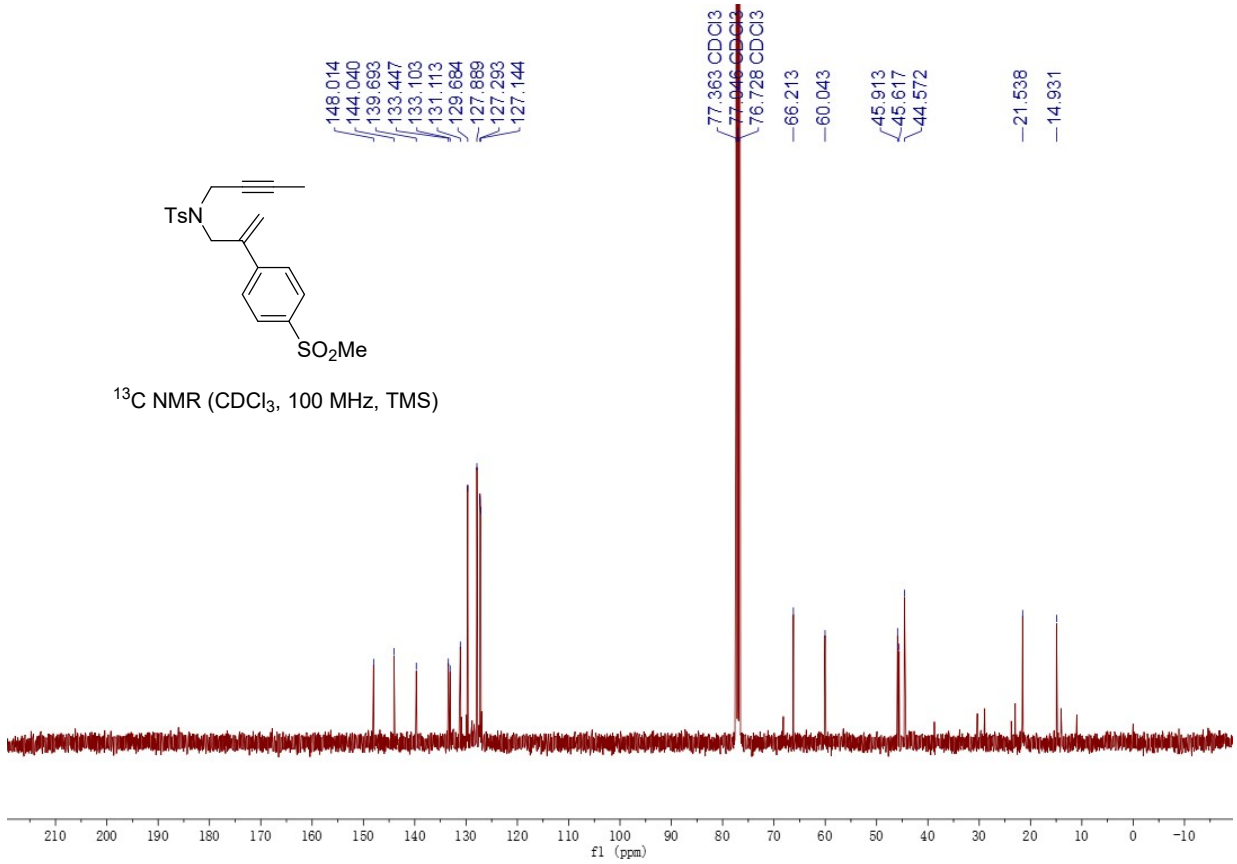
A colorless oil, 68% yield, 197.2 mg. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.92 (d, *J* = 8.4 Hz, 2H), 7.79 – 7.70 (m, 4H), 7.33 (d, *J* = 8.1 Hz, 2H), 5.68 (s, 1H), 5.49 (s, 1H), 4.25 (s, 2H), 3.90 (s, 2H), 3.08 (s, 3H), 2.45 (s, 3H), 1.50 (t, *J* = 2.4 Hz, 3H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 148.0, 144.0, 139.7, 133.4, 133.1, 131.1, 129.7, 127.9, 127.3, 127.1, 66.2, 60.0, 45.9, 45.6, 44.6, 21.5, 14.9. IR (Acetone) ν 660, 1092, 1161, 1349, 1491, 2988 cm⁻¹. HRMS (ESI) calcd. for C₂₁H₂₄O₄NS₂ (M+H): 418.1141, Found: 418.1125.

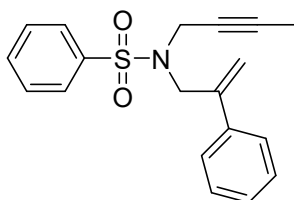


¹H NMR (CDCl₃, 400 MHz, TMS)



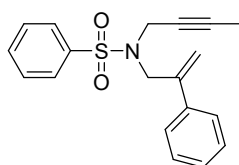
¹³C NMR (CDCl₃, 100 MHz, TMS)



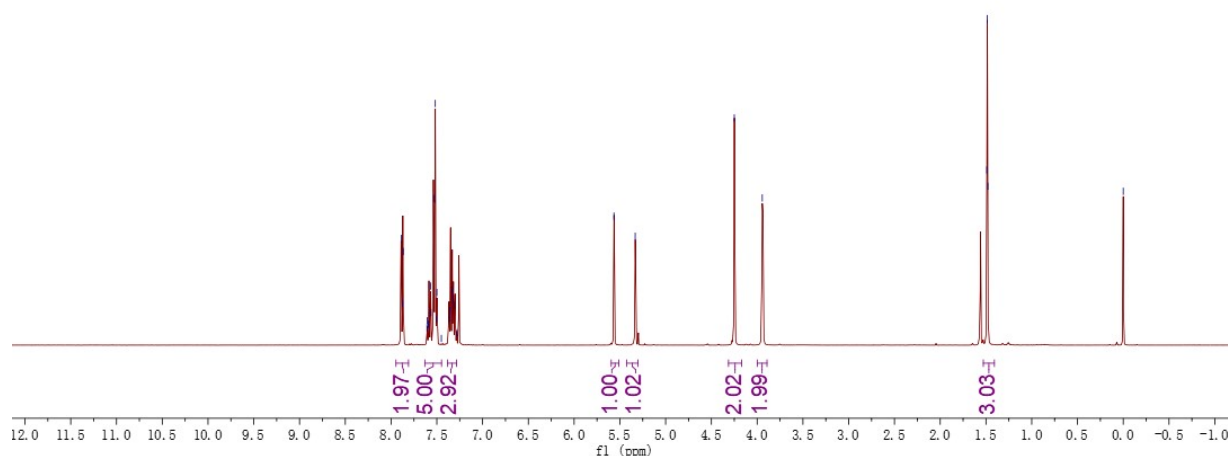


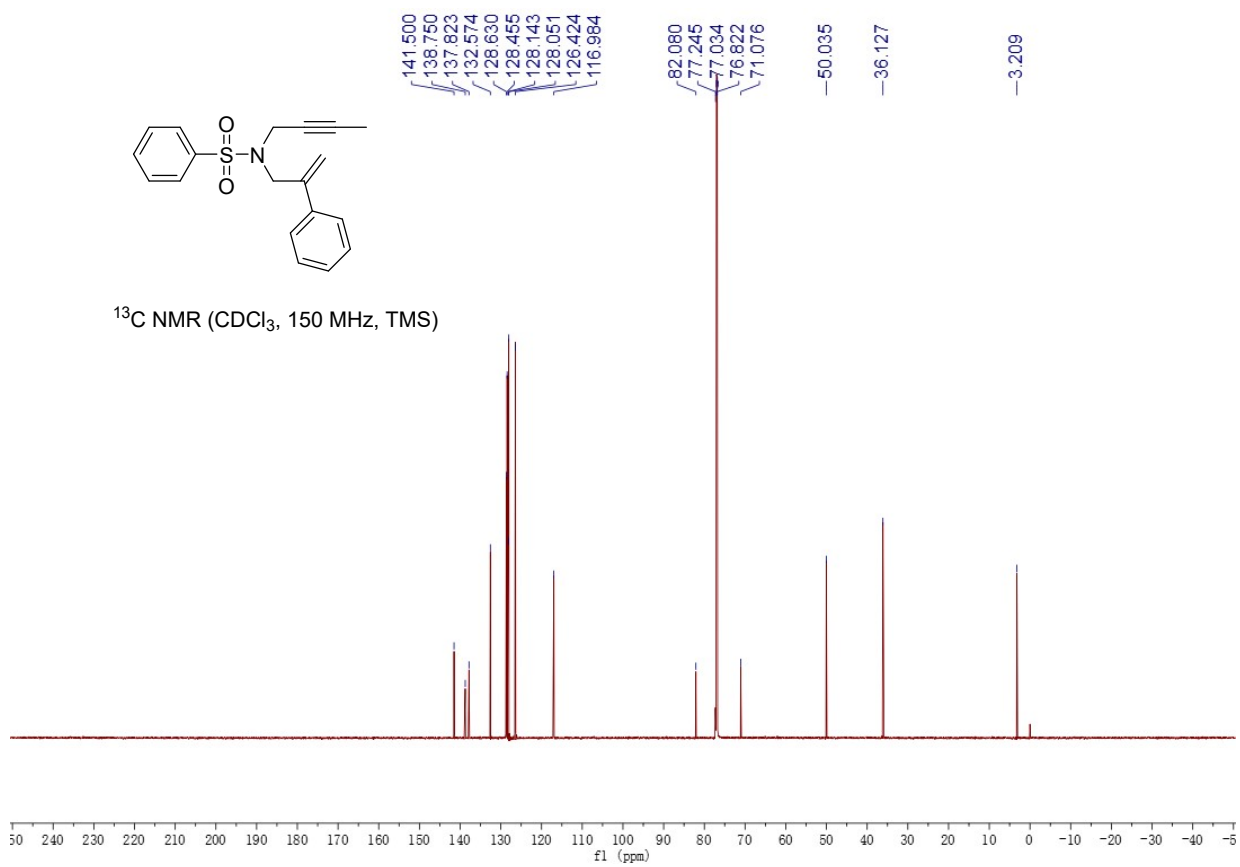
***N*-(but-2-yn-1-yl)-*N*-(2-phenylallyl)benzenesulfonamide (1s)**

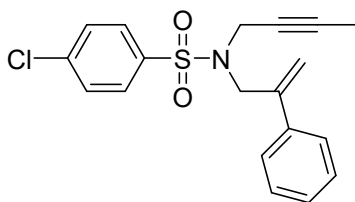
A colorless oil, 44.1 mg, 78% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.95 – 7.81 (m, 2H), 7.63 – 7.45 (m, 5H), 7.38 – 7.28 (m, 3H), 5.56 (s, 1H), 5.33 (s, 1H), 4.25 (s, 2H), 3.94 (s, 2H), 1.49 (t, *J* = 2.4 Hz, 3H). ¹³C NMR (CDCl₃, TMS, 150 MHz) δ 141.5, 138.7, 137.8, 132.6, 128.6, 128.5, 128.1, 128.1, 126.4, 117.0, 82.1, 77.2, 77.0, 76.8, 71.1, 50.0, 36.1, 3.2. IR (Acetone) ν 879, 1068, 1139, 1170, 1320, 2980 cm⁻¹. HRMS (ESI) calcd. for C₁₉H₂₀O₂NS (M+H): 326.1209, Found: 326.1201.



¹H NMR (CDCl₃, 400 MHz, TMS)

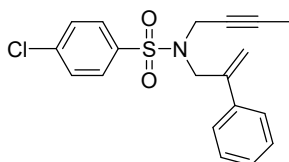




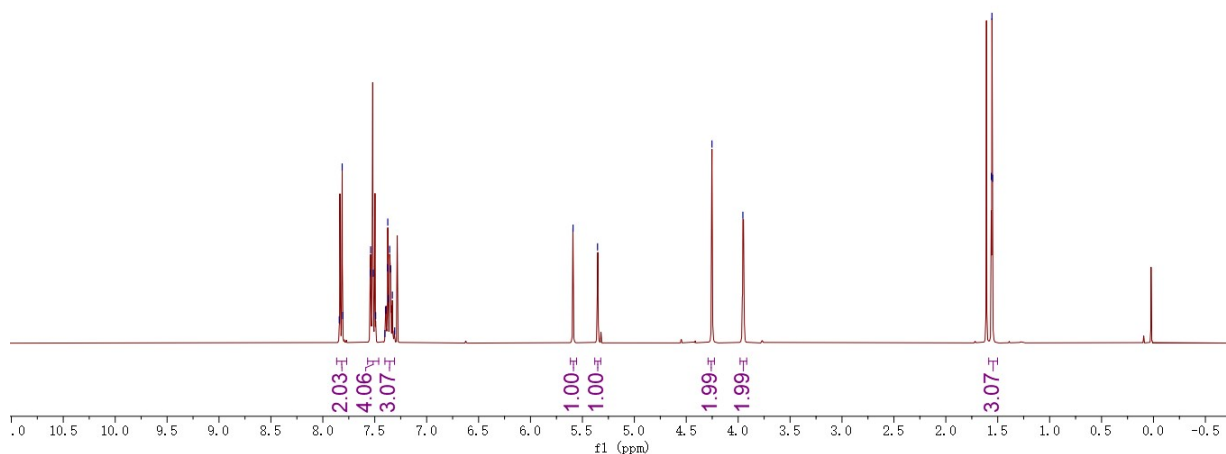


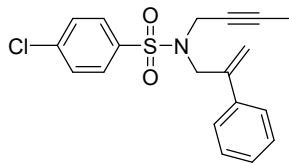
***N*-(but-2-yn-1-yl)-4-chloro-*N*-(2-phenylallyl)benzenesulfonamide (1t)**

A colorless oil, 41.7 mg, 70% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.87 – 7.77 (m, 2H), 7.57 – 7.46 (m, 4H), 7.40 – 7.31 (m, 3H), 5.59 (s, 1H), 5.35 (s, 1H), 4.25 (s, 2H), 3.95 (s, 2H), 1.56 (t, J = 2.4 Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 141.3, 139.1, 137.7, 137.3, 129.5, 128.9, 128.5, 128.2, 126.4, 117.2, 82.3, 71.1, 50.1, 36.1, 3.2. IR (Acetone) ν 917, 1058, 1140, 1158, 1339, 2278, 2902 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{19}\text{H}_{19}\text{O}_2\text{NCIS}$ ($\text{M}+\text{H}$): 360.0820, Found: 360.0808.

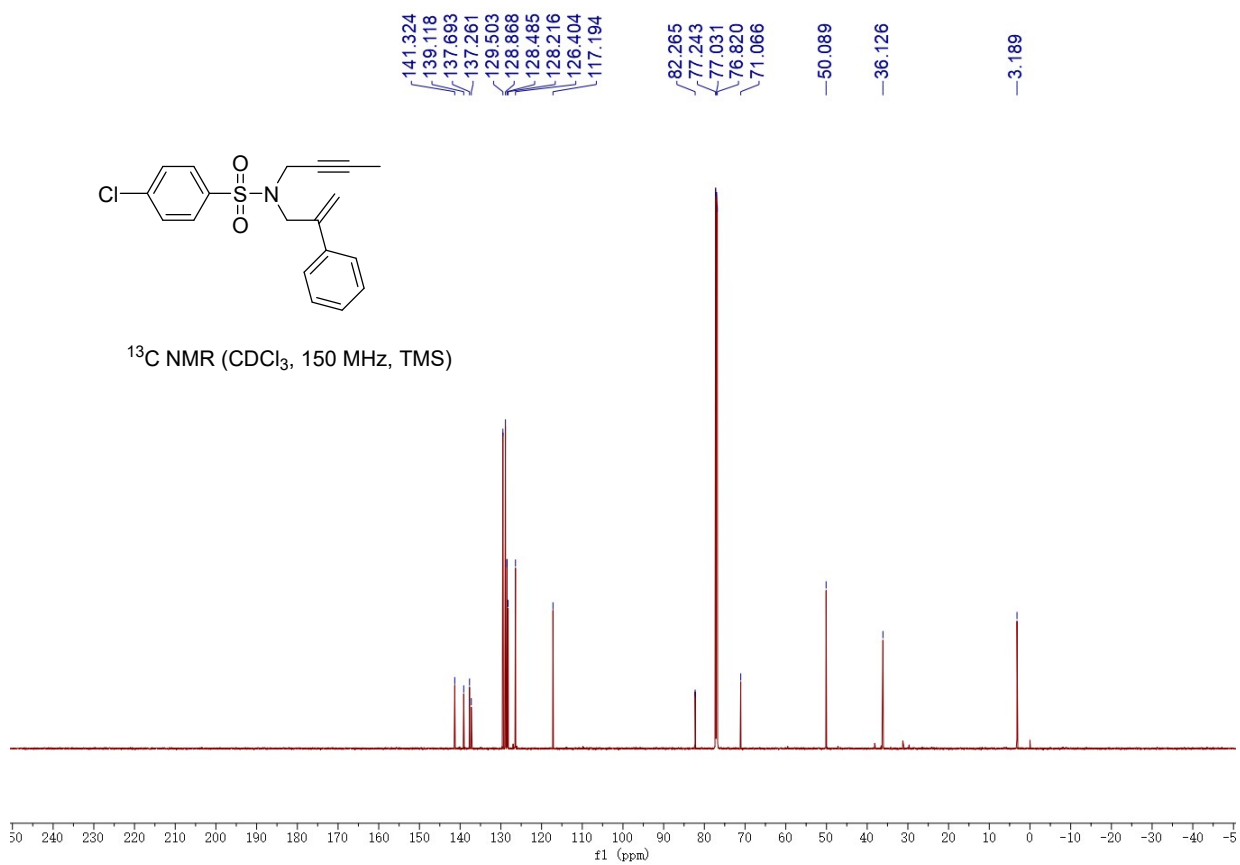


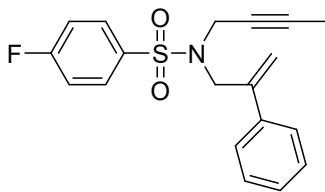
^1H NMR (CDCl_3 , 400 MHz, TMS)





^{13}C NMR (CDCl_3 , 150 MHz, TMS)

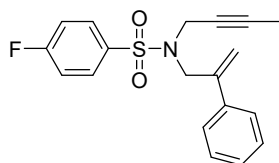




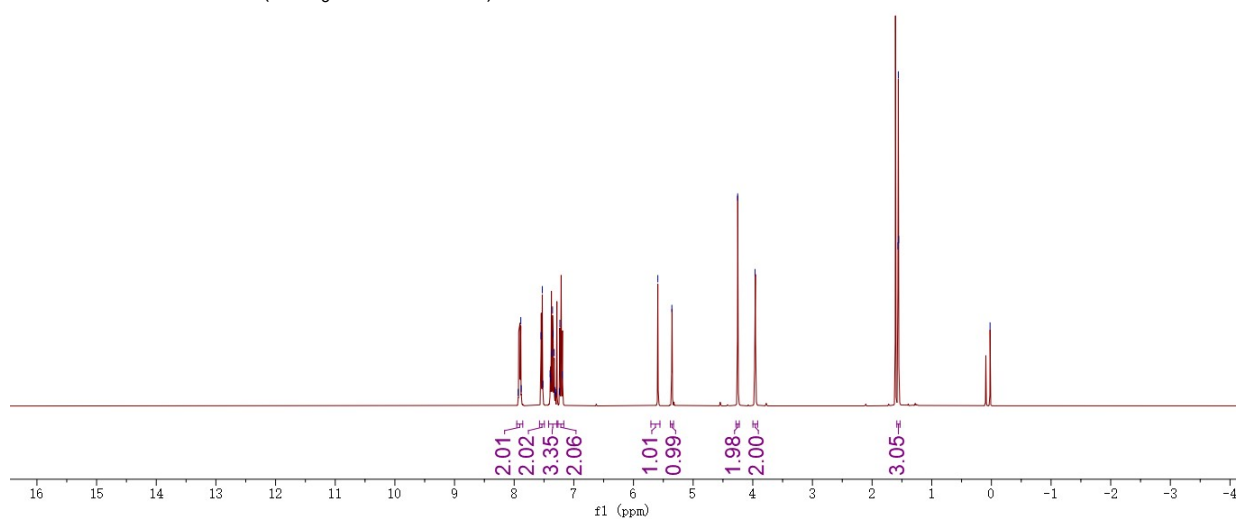
***N*-(but-2-yn-1-yl)-4-fluoro-*N*-(2-phenylallyl)benzenesulfonamide (1u)**

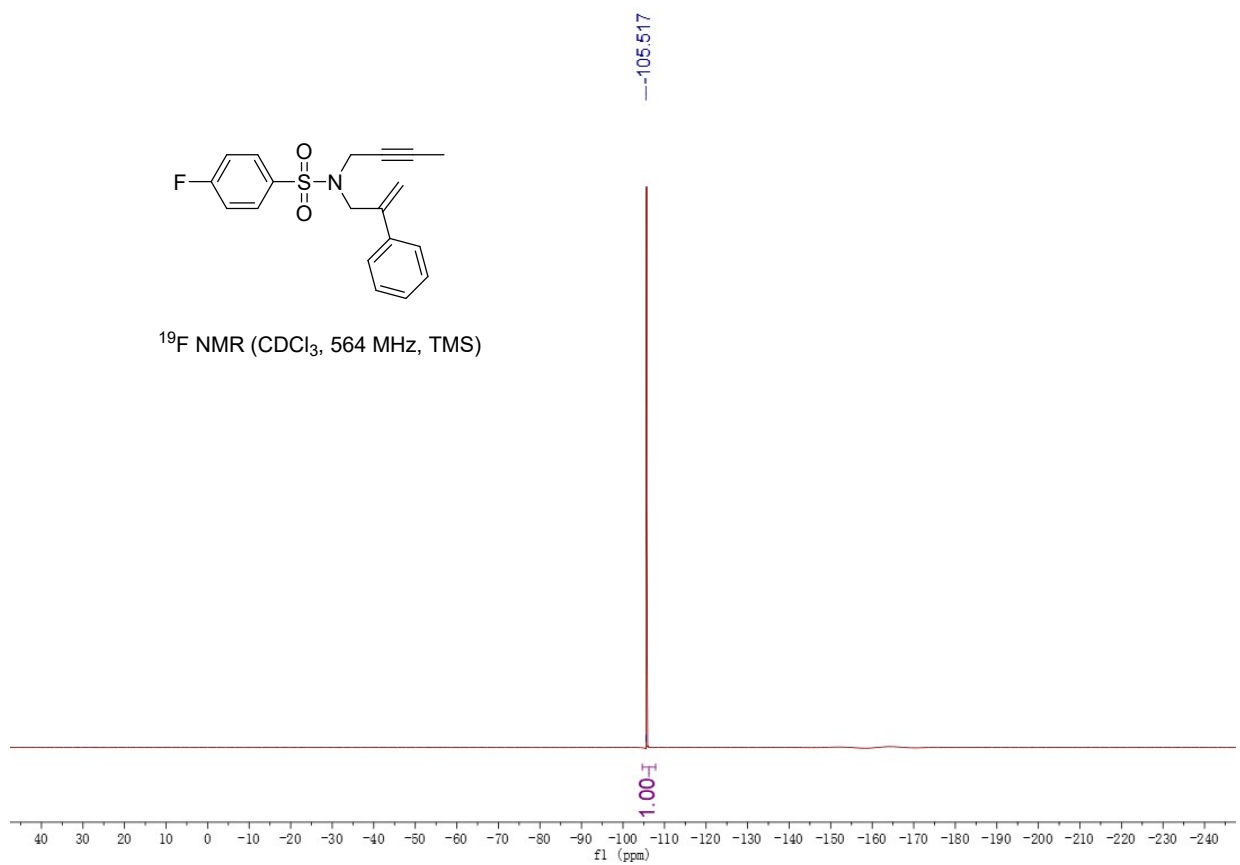
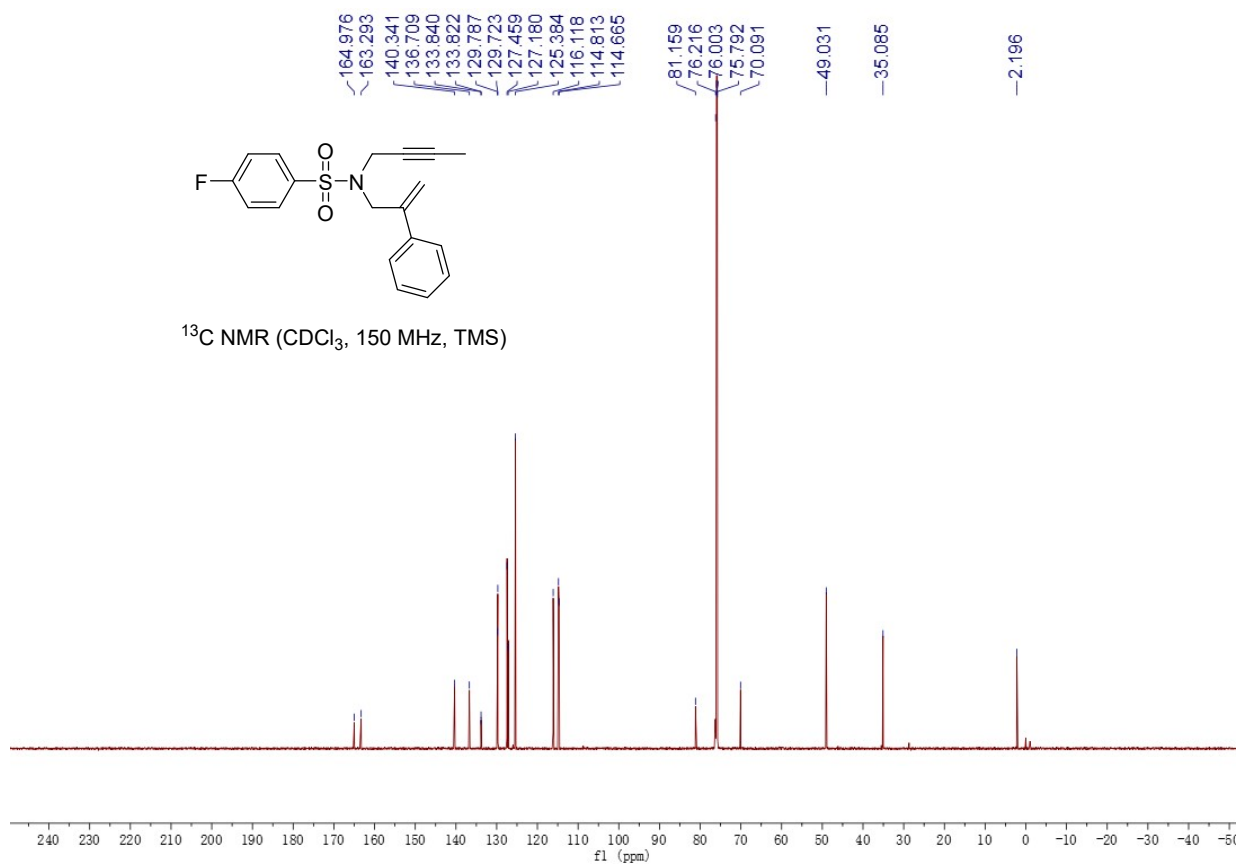
A colorless oil, 37.3 mg, 60% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.96 – 7.86 (m, 2H), 7.54 (d, $J = 8.5$ Hz, 2H), 7.42 – 7.28 (m, 3H), 7.21 (d, $J = 15.4$ Hz, 2H), 5.59 (s, 1H), 5.36 (s, 1H), 4.25 (s, 2H), 3.96 (s, 2H), 1.56 (t, $J = 2.4$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 164.1 (d, $J = 254.1$ Hz), 140.3, 136.7, 133.8 (d, $J = 2.7$ Hz), 129.8 (d, $J = 9.7$ Hz), 127.5, 127.2, 125.4, 116.1, 114.7 (d, $J = 22.2$ Hz), 81.2, 70.1, 49.0, 35.1, 2.2. ^{19}F NMR (CDCl_3 , TMS, 564 MHz) δ -105.5 (s). IR (Acetone) ν 815, 1033, 1187, 1199, 1281, 2230, 2970 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{19}\text{H}_{19}\text{O}_2\text{NFS}$ (M+H): 344.1115, Found: 344.1103.

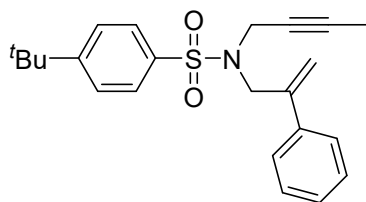
7.932
7.889
7.881
7.550
7.529
7.519
7.398
7.388
7.370
7.357
7.347
7.329
7.314
7.308
7.241
7.233
7.195
5.592
5.356
4.253
3.963
1.566
1.560
1.554
0.023



^1H NMR (CDCl_3 , 400 MHz, TMS)

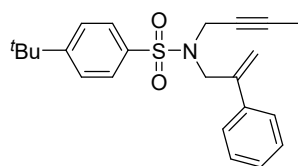




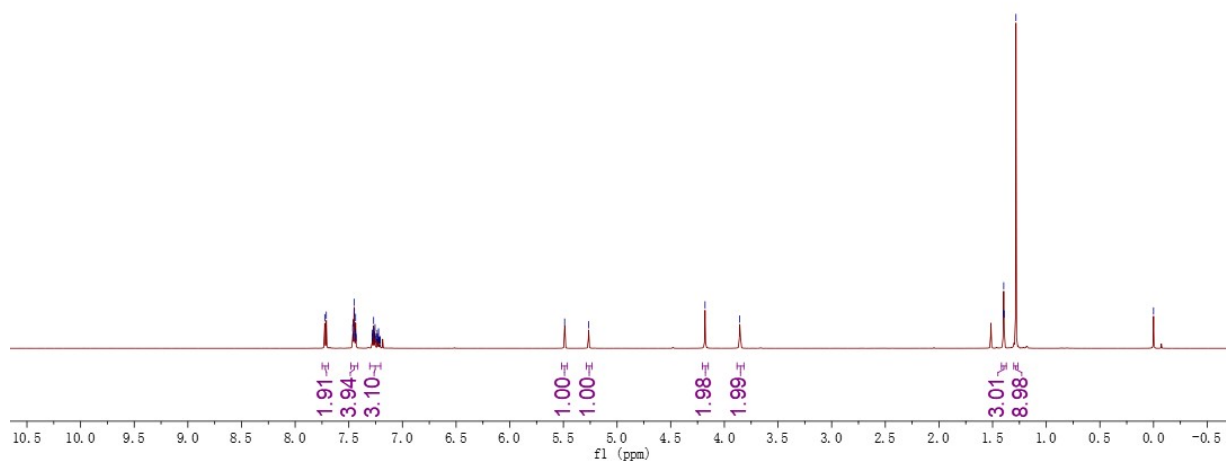


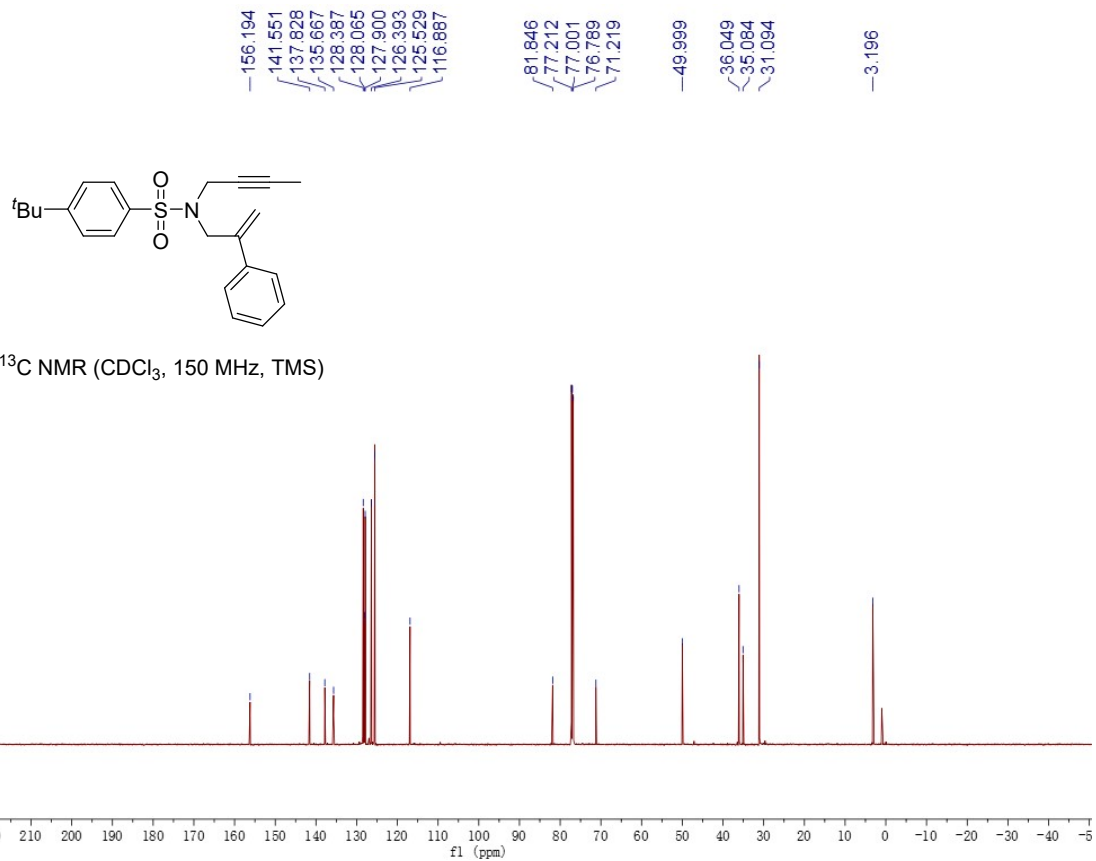
***N*-(but-2-yn-1-yl)-4-fluoro-*N*-(2-phenylallyl)benzenesulfonamide (1v)**

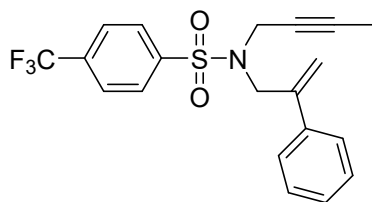
A colorless oil, 41.4 mg, 71% yield. ^1H NMR (CDCl_3 , TMS, 600 MHz) δ 7.72 (d, $J = 8.5$ Hz, 2H), 7.48 – 7.42 (m, 4H), 7.30 – 7.20 (m, 3H), 5.49 (s, 1H), 5.27 (s, 1H), 4.18 (s, 2H), 3.86 (s, 2H), 1.40 (t, $J = 2.4$ Hz, 3H), 1.28 (s, 9H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 156.2, 141.6, 137.8, 135.7, 128.4, 128.1, 127.9, 126.4, 125.5, 116.9, 81.8, 71.2, 50.0, 36.0, 35.1, 31.1, 3.2. IR (Acetone) ν 857, 1053, 1156, 1298, 2238, 2909 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{23}\text{H}_{28}\text{O}_2\text{NS}$ ($\text{M}+\text{H}$): 382.1835, Found: 382.1825.



^1H NMR (CDCl_3 , 600 MHz, TMS)

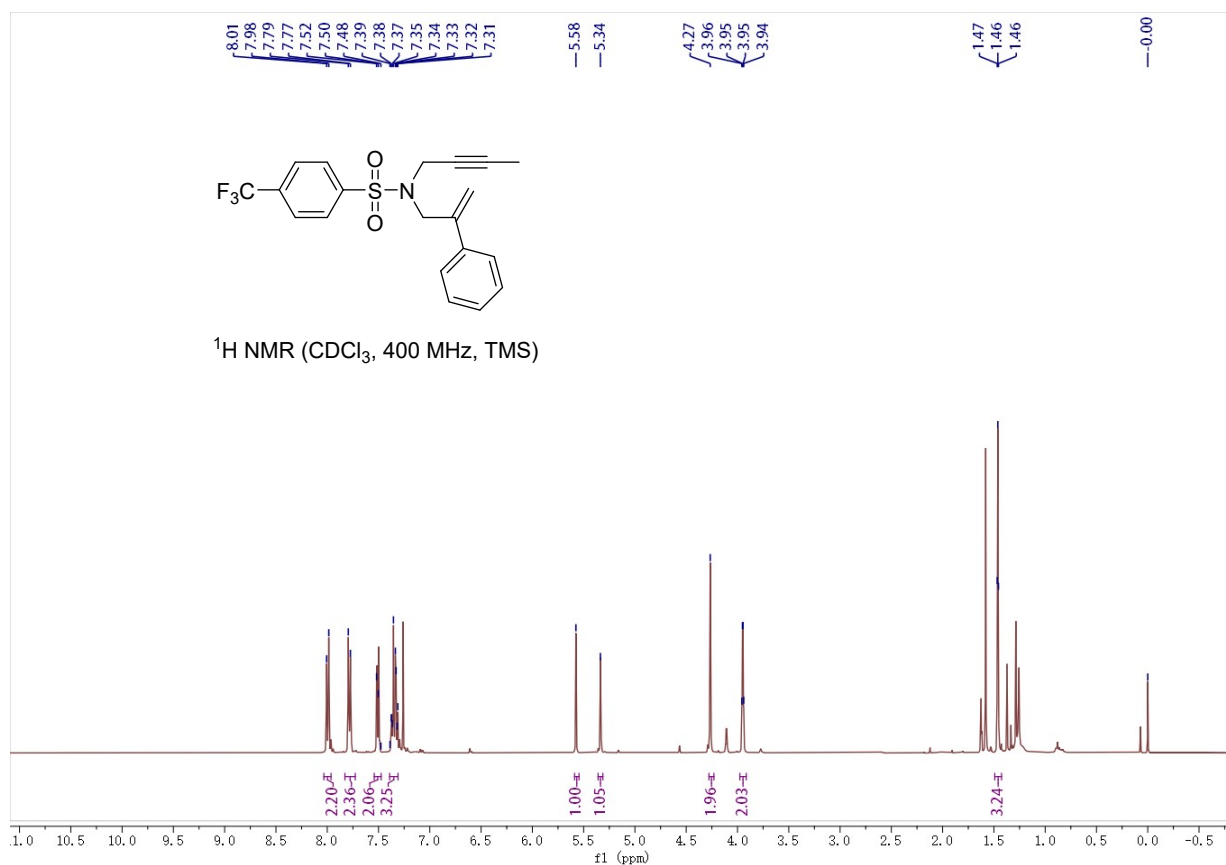


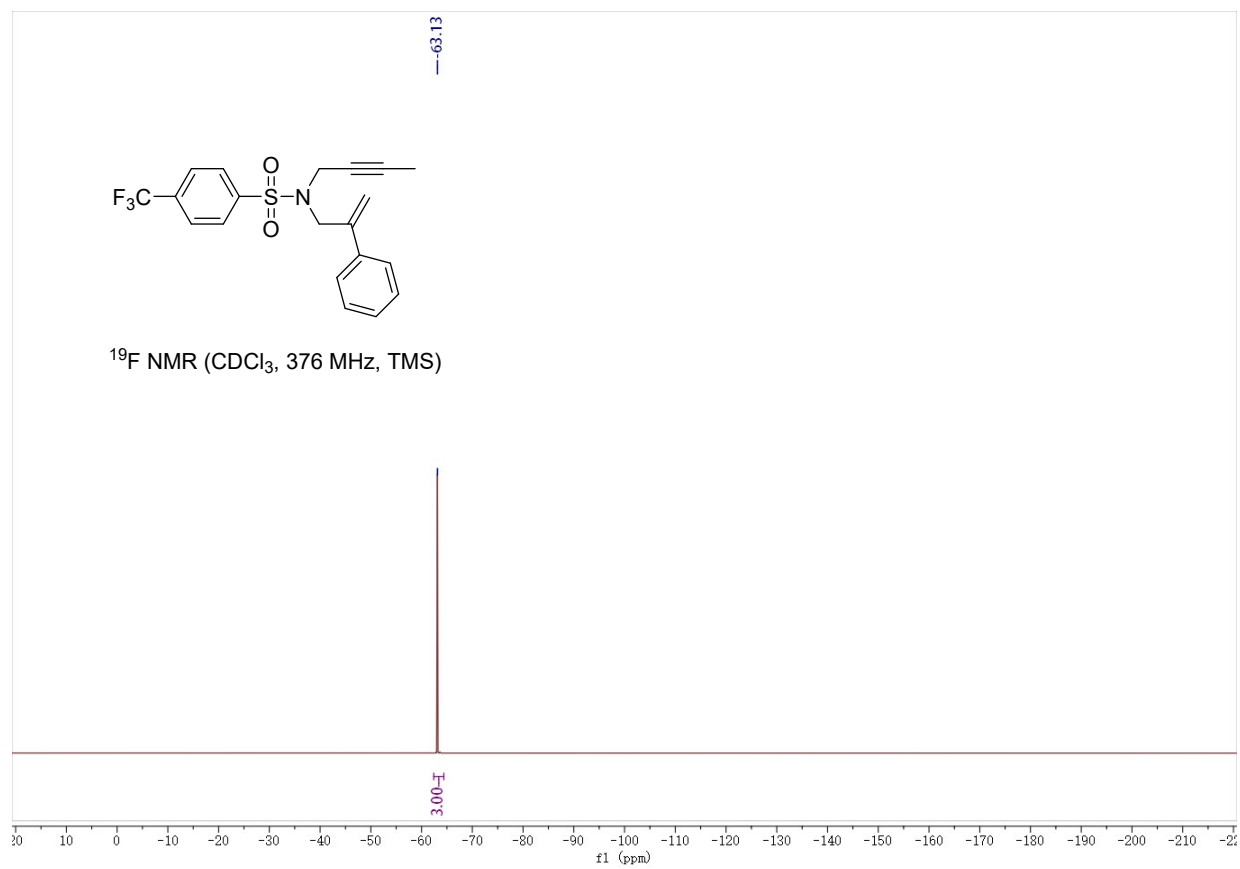
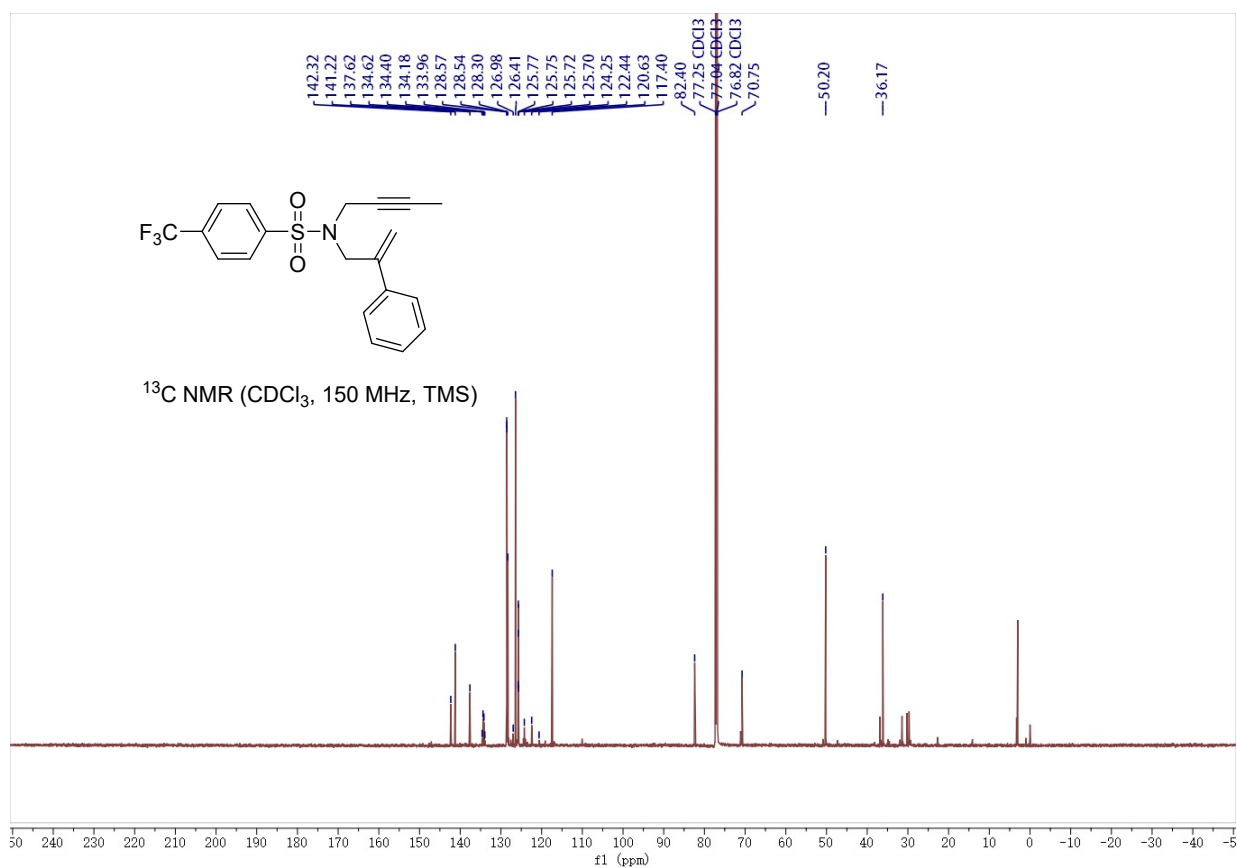


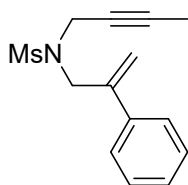


***N*-(but-2-yn-1-yl)-*N*-(2-phenylallyl)-4-(trifluoromethyl)benzenesulfonamide (1w)**

A colorless oil, 48.0 mg, 80% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 8.00 (d, $J = 8.2$ Hz, 2H), 7.78 (d, $J = 8.2$ Hz, 2H), 7.54 – 7.47 (m, 2H), 7.39 – 7.31 (m, 3H), 5.58 (s, 1H), 5.34 (s, 1H), 4.27 (s, 2H), 3.95 (q, $J = 2.4$ Hz, 2H), 1.46 (t, $J = 2.4$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 142.3, 141.2, 137.6, 134.6 (q, $J = 33.0$ Hz), 128.6, 128.5, 128.3, 126.4, 125.7 (q, $J = 3.0$ Hz), 123.3 (q, $J = 271.5$ Hz), 117.4, 82.4, 70.7, 50.2, 36.2. ^{19}F NMR (CDCl_3 , TMS, 376 MHz) δ -63.1 (s). IR (Acetone) ν 678, 962, 1031, 1186, 1311, 2160, 2990 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{20}\text{H}_{19}\text{O}_2\text{NF}_3\text{S}$ (M+H): 394.1083, Found: 394.1072.

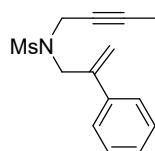




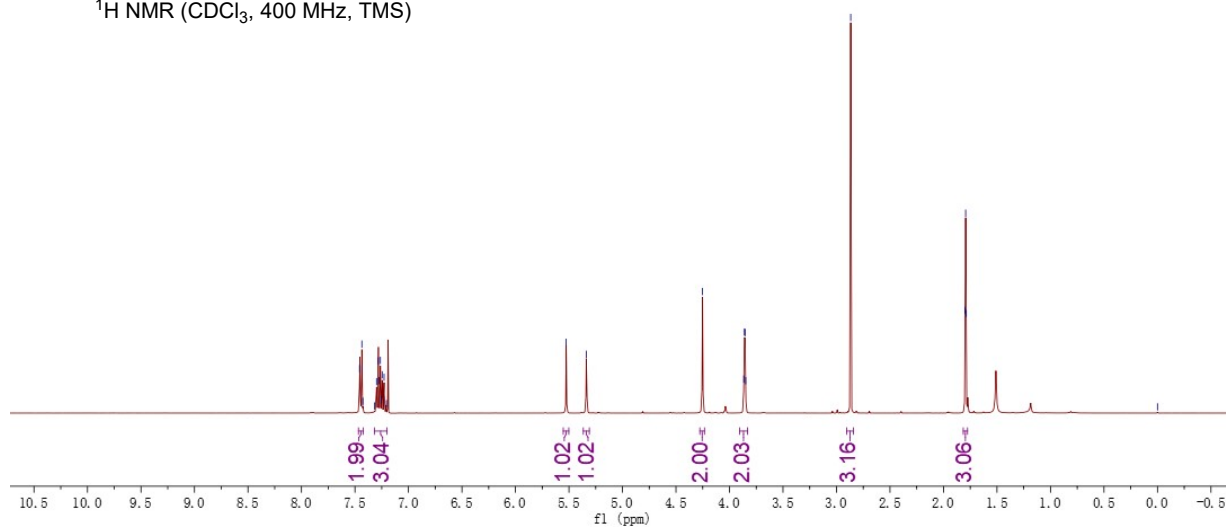


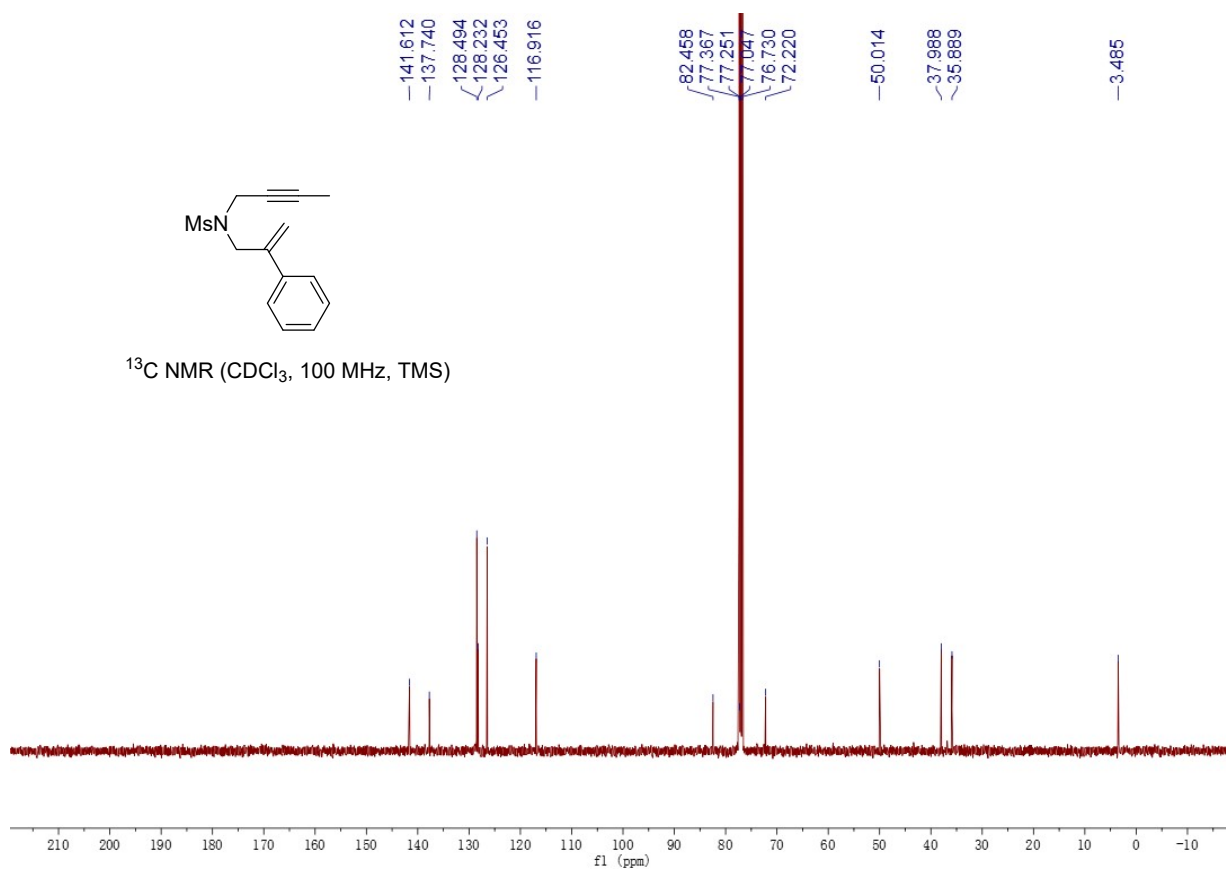
***N*-(but-2-yn-1-yl)-*N*-(2-phenylallyl)methanesulfonamide (1x)**

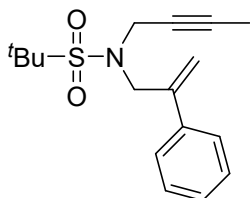
A colorless oil, 41% yield, 149.9 mg. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.47 – 7.42 (m, 2H), 7.32 – 7.20 (m, 3H), 5.53 (s, 1H), 5.34 (s, 1H), 4.25 (s, 2H), 3.86 (q, $J = 2.4$ Hz, 2H), 2.87 (s, 3H), 1.79 (t, $J = 2.4$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 141.6, 137.7, 128.5, 128.2, 126.5, 116.9, 82.5, 72.2, 50.0, 38.0, 35.9, 3.5. IR (Acetone) ν 909, 1062, 1131, 1166, 1321, 2917 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{14}\text{H}_{18}\text{O}_2\text{NS}$ ($\text{M}+\text{H}$): 264.1053, Found: 264.1043.



^1H NMR (CDCl_3 , 400 MHz, TMS)

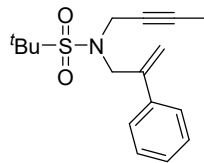




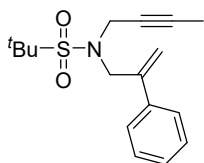
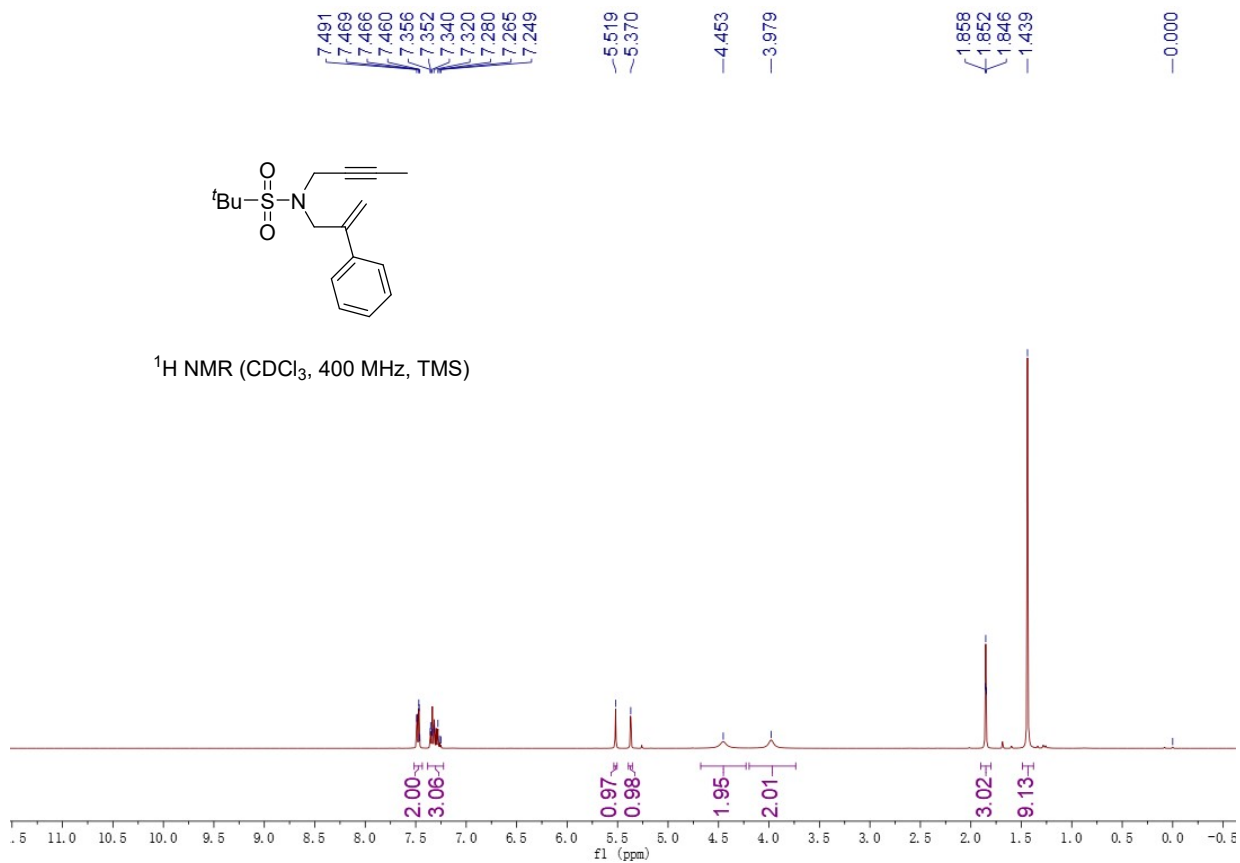


***N*-(but-2-yn-1-yl)-2-methyl-*N*-(2-phenylallyl)propane-2-sulfonamide (1y)**

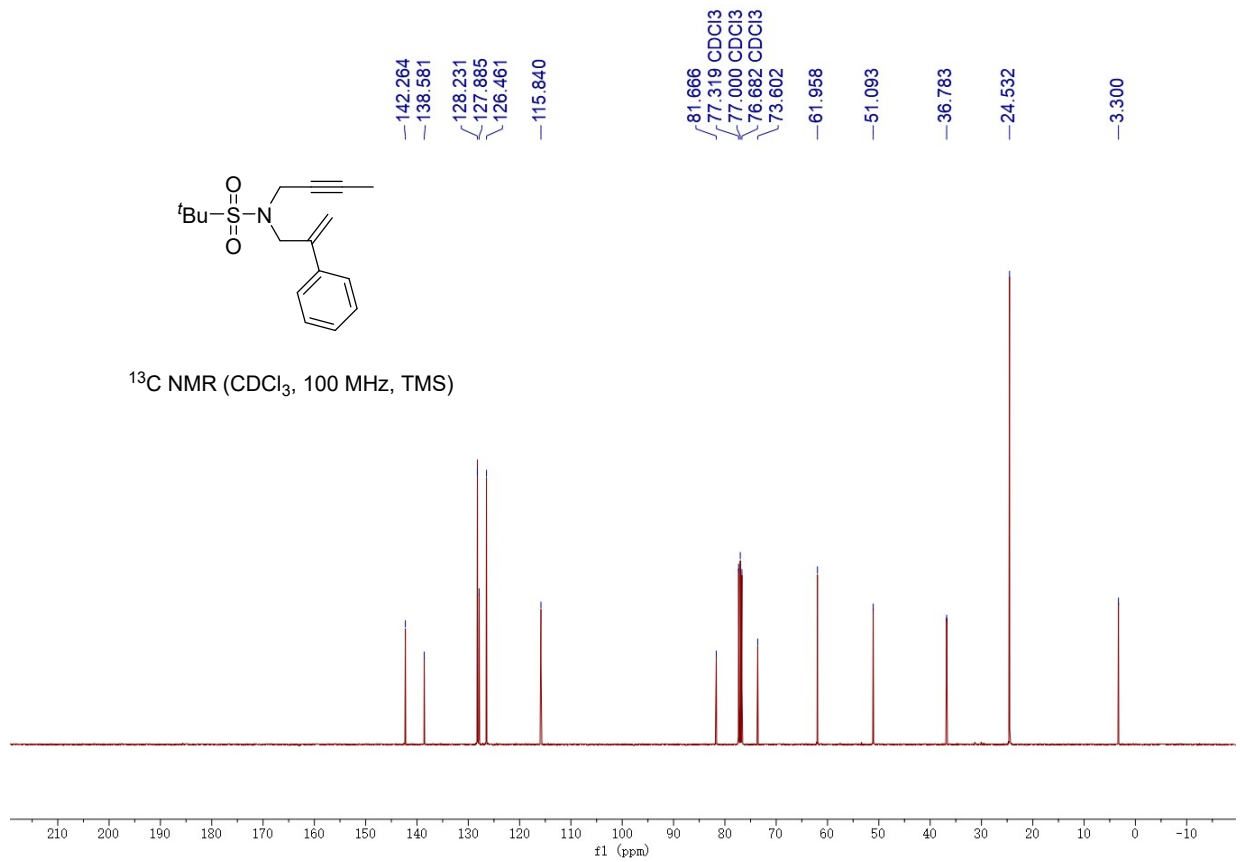
A colorless oil, 36.5 mg, 63% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.52 – 7.43 (m, 2H), 7.38 – 7.22 (m, 3H), 5.52 (s, 1H), 5.37 (s, 1H), 4.45 (s, 2H), 3.98 (s, 2H), 1.85 (t, $J = 2.4$ Hz, 3H), 1.44 (s, 9H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 142.3, 138.6, 128.2, 127.9, 126.5, 115.8, 81.7, 73.6, 62.0, 51.1, 36.8, 24.5, 3.3. IR (Acetone) ν 798, 905, 1181, 1308, 1742, 2909 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{17}\text{H}_{24}\text{O}_2\text{NS}$ ($\text{M}+\text{H}$): 306.1522, Found: 306.1512.

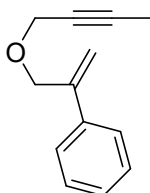


¹H NMR (CDCl₃, 400 MHz, TMS)



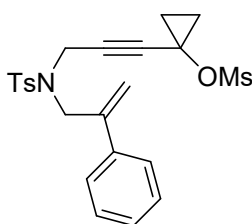
¹³C NMR (CDCl₃, 100 MHz, TMS)





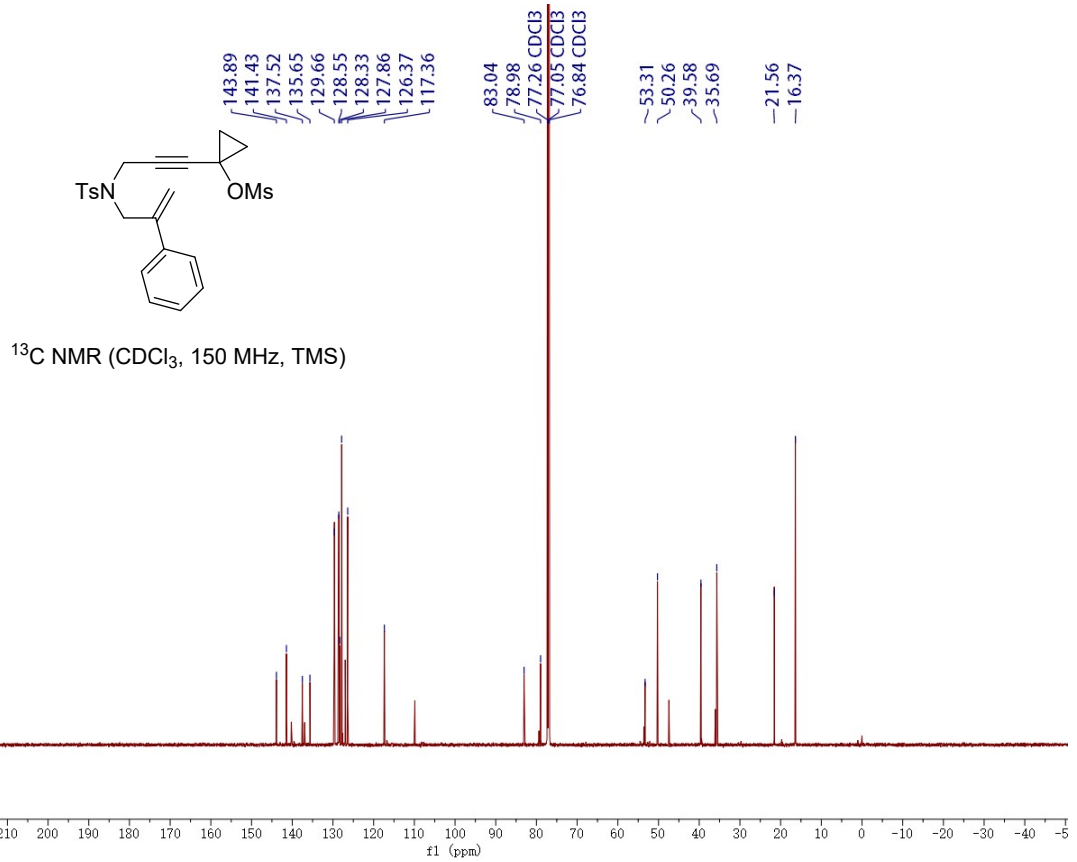
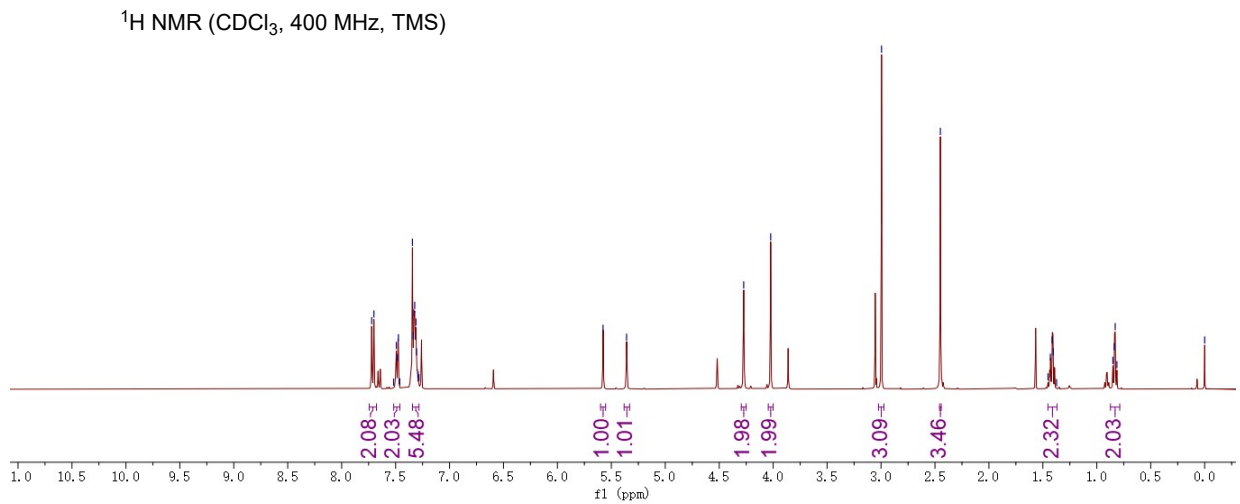
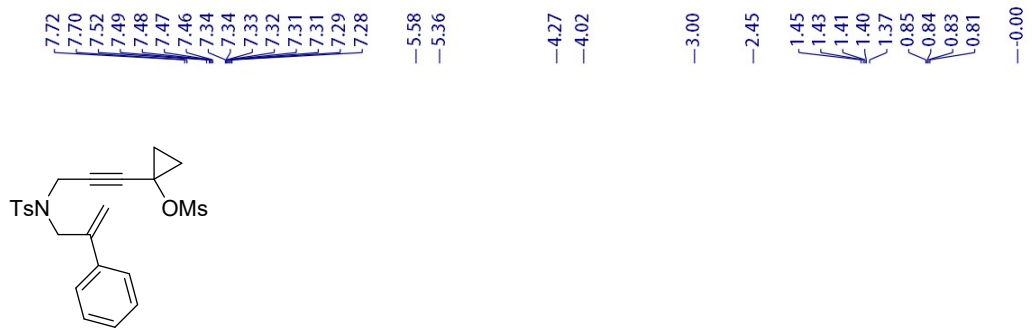
(3-(but-2-yn-1-yloxy)prop-1-en-2-yl)benzene (1z)

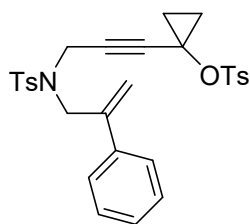
This is a known compound and its spectroscopic data are consistent with those reported in the previous literature,^[8] 102.5 mg, 55% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.24 – 7.49 (m, 5H), 5.55 (s, 1H), 5.36 (s, 1H), 4.45 (s, 2H), 4.15 (q, *J* = 2.4 Hz, 2H), 1.87 (t, *J* = 2.4 Hz, 3H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 143.5, 138.5, 128.2, 127.7, 125.9, 114.9, 82.6, 75.0, 71.2, 57.6, 3.8.



1-(3-(((4-methyl-*N*-(2-phenylallyl)phenyl)sulfonamido)prop-1-yn-1-yl)cyclopropyl methanesulfonate (1ab)

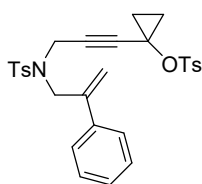
A colorless oil, 36.6 mg, 57% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.71 (d, *J* = 8.3 Hz, 2H), 7.52 – 7.46 (m, 2H), 7.34 – 7.28 (m, 5H), 5.58 (s, 1H), 5.36 (s, 1H), 4.27 (s, 2H), 4.02 (s, 2H), 3.00 (s, 3H), 2.45 (s, 3H), 1.45 – 1.37 (m, 2H), 0.87 – 0.79 (m, 2H). ¹³C NMR (CDCl₃, TMS, 150 MHz) δ 143.9, 141.4, 137.5, 135.7, 129.7, 128.6, 128.3, 127.9, 126.4, 117.4, 83.0, 79.0, 53.3, 50.3, 39.6, 35.7, 21.6, 16.4. IR (Acetone) ν 704, 778, 895, 1150, 1326, 2925 cm⁻¹. HRMS (ESI) calcd. for C₂₃H₂₆O₅NS₂ (M+H): 460.1247, Found: 460.1235.



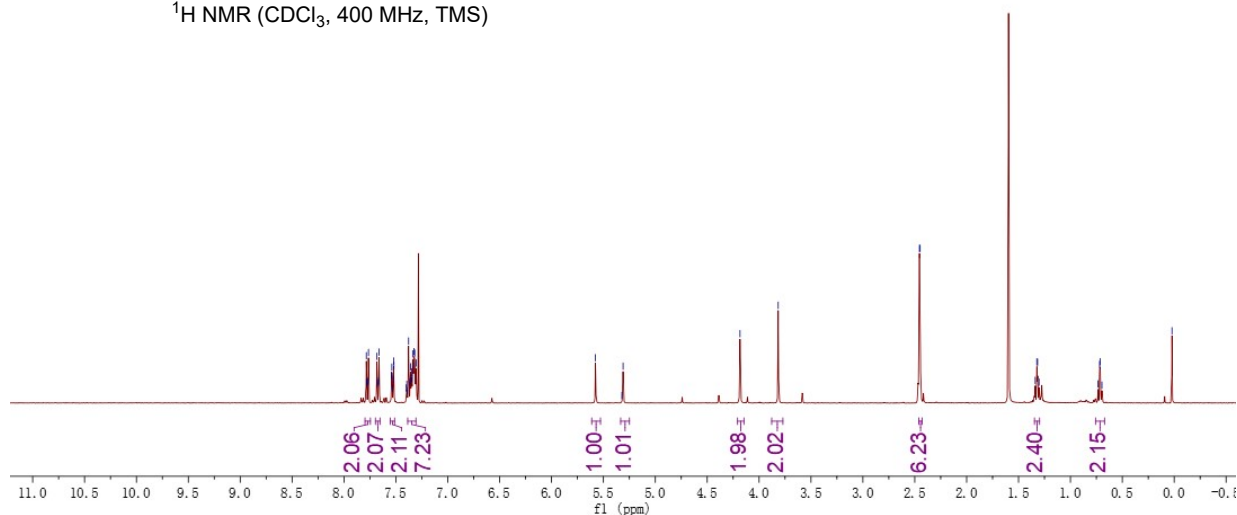


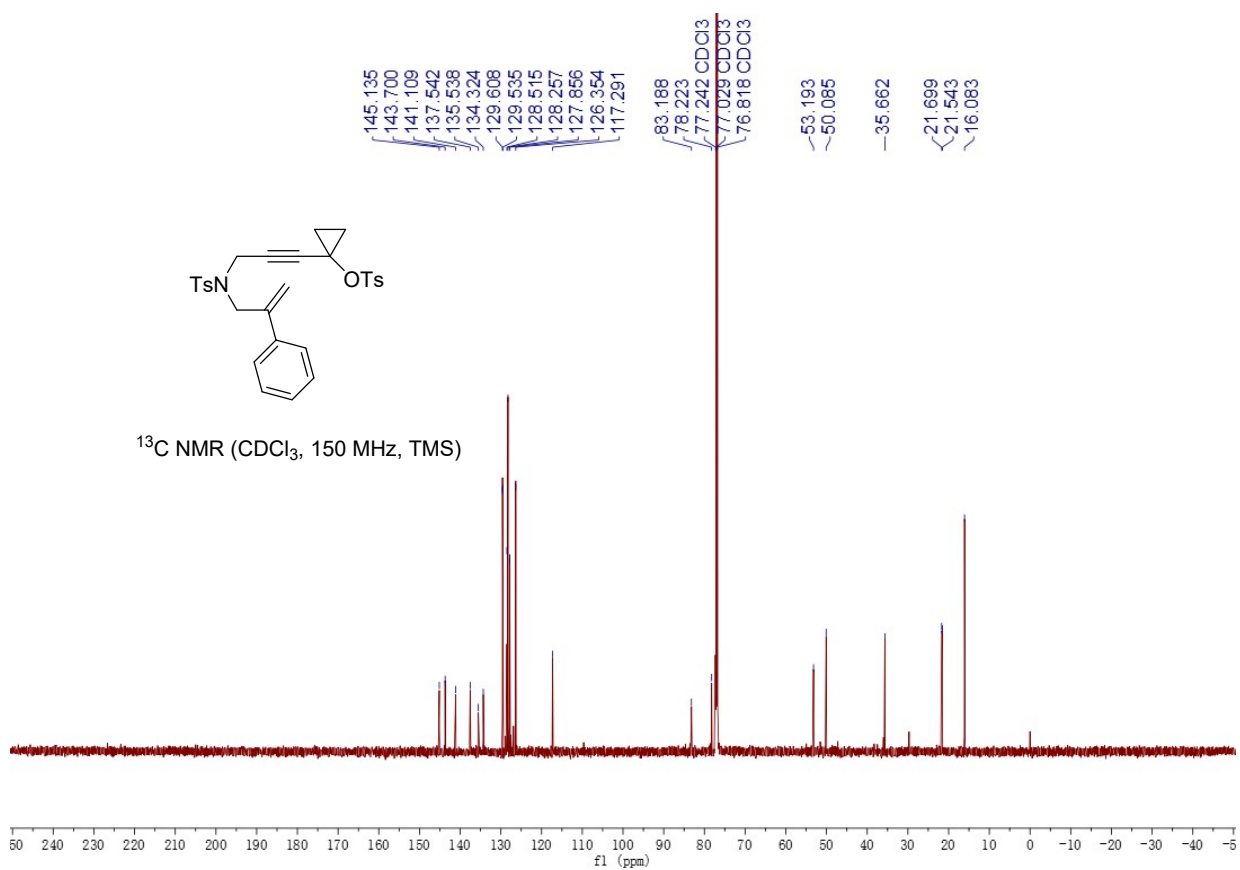
1-(3-((4-methyl-N-(2-phenylallyl)phenyl)sulfonamido)prop-1-yn-1-yl)cyclopropyl-4-methylbenzenesulfonate (1ac)

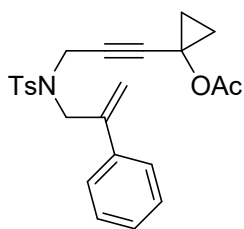
A colorless oil, 35.3 mg, 61% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.80 – 7.75 (m, 2H), 7.70 – 7.65 (m, 2H), 7.55 – 7.51 (m, 2H), 7.39 – 7.31 (m, 7H), 5.58 (s, 1H), 5.31 (s, 1H), 4.18 (s, 2H), 3.82 (s, 2H), 2.46 – 2.43 (m, 6H), 1.35 – 1.30 (m, 2H), 0.76 – 0.67 (m, 2H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 145.1, 143.7, 141.1, 137.5, 135.5, 134.3, 129.6, 129.5, 128.5, 128.3, 127.9, 126.4, 117.3, 83.2, 78.2, 53.2, 50.1, 35.7, 21.7, 21.5, 16.1. IR (Acetone) ν 1089, 1162, 1174, 1348, 1368, 2990 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{29}\text{H}_{30}\text{O}_5\text{NS}_2$ (M+H): 536.1560, Found: 536.1548.



^1H NMR (CDCl_3 , 400 MHz, TMS)

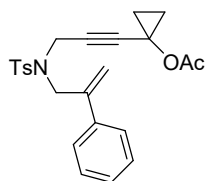




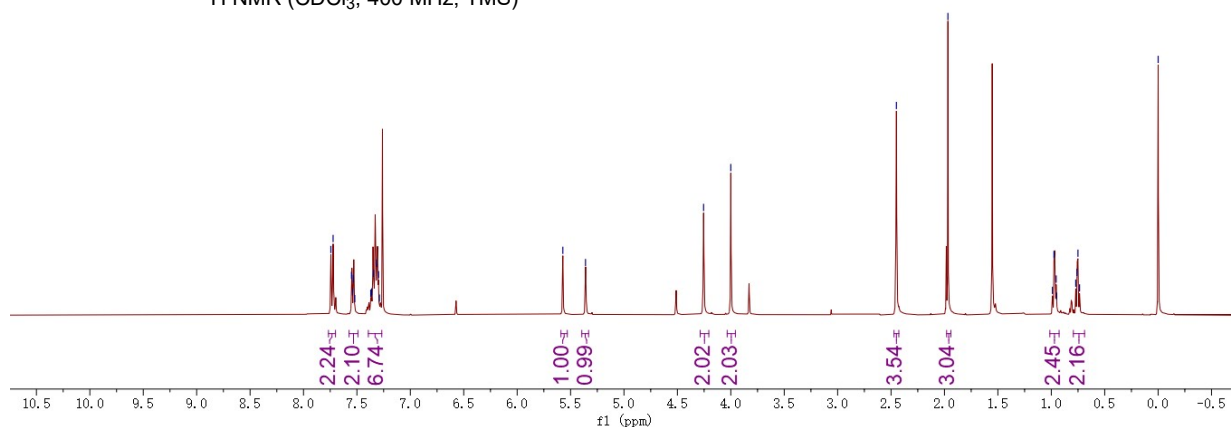


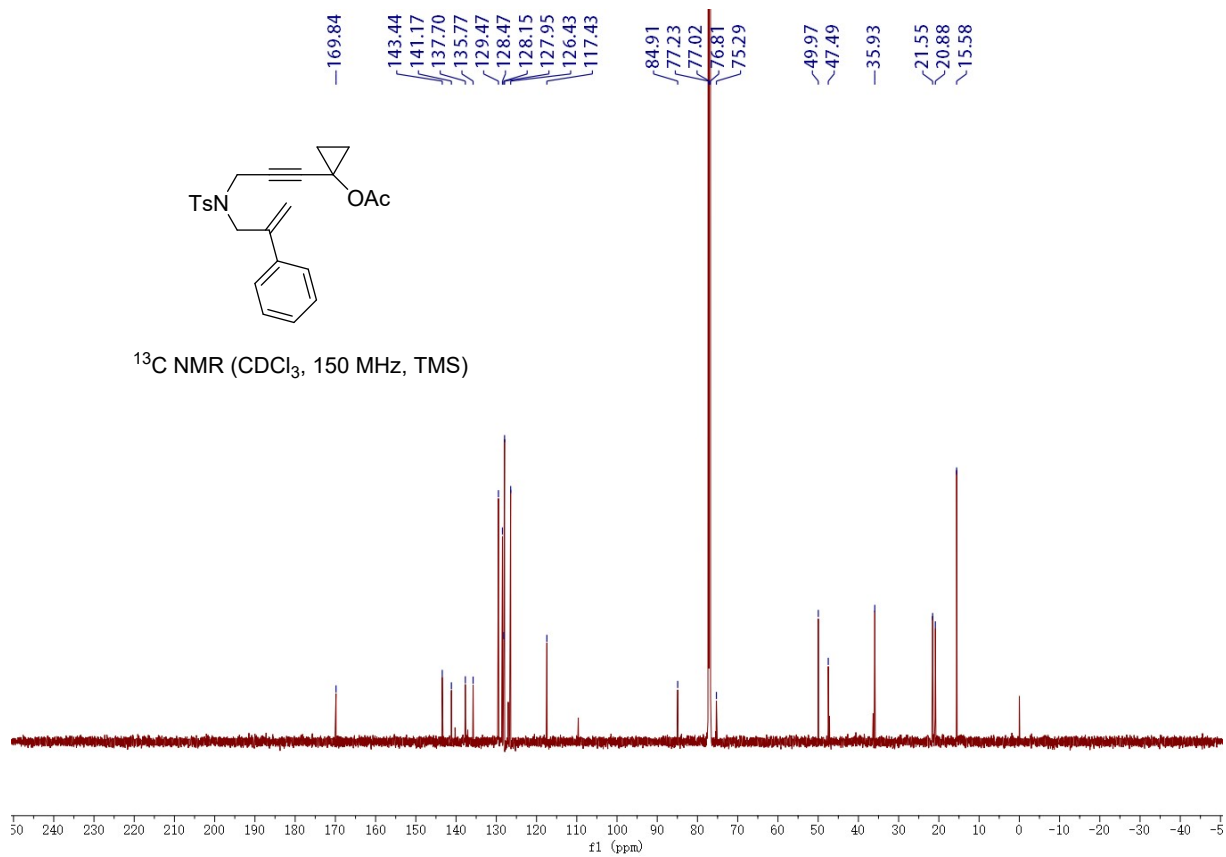
1-(3-((4-methyl-N-(2-phenylallyl)phenyl)sulfonamido)prop-1-yn-1-yl)cyclopropyl acetate (1ad)

A colorless oil, 35.3 mg, 61% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.73 (d, $J = 8.3$ Hz, 2H), 7.57 – 7.49 (m, 2H), 7.39 – 7.27 (m, 5H), 5.57 (s, 1H), 5.36 (s, 1H), 4.25 (s, 2H), 4.00 (s, 2H), 2.45 (s, 3H), 1.97 (s, 3H), 1.01 – 0.93 (m, 2H), 0.79 – 0.69 (m, 2H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 169.8, 143.4, 141.2, 137.7, 135.8, 129.5, 128.5, 128.1, 128.0, 126.4, 117.4, 84.9, 75.3, 50.0, 47.5, 35.9, 21.6, 20.9, 15.6. IR (Acetone) ν 1010, 1285, 1370, 2239, 3008 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{24}\text{H}_{26}\text{O}_4\text{NS}$ (M+H): 424.1577, Found: 424.1564.

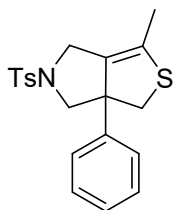


^1H NMR (CDCl_3 , 400 MHz, TMS)



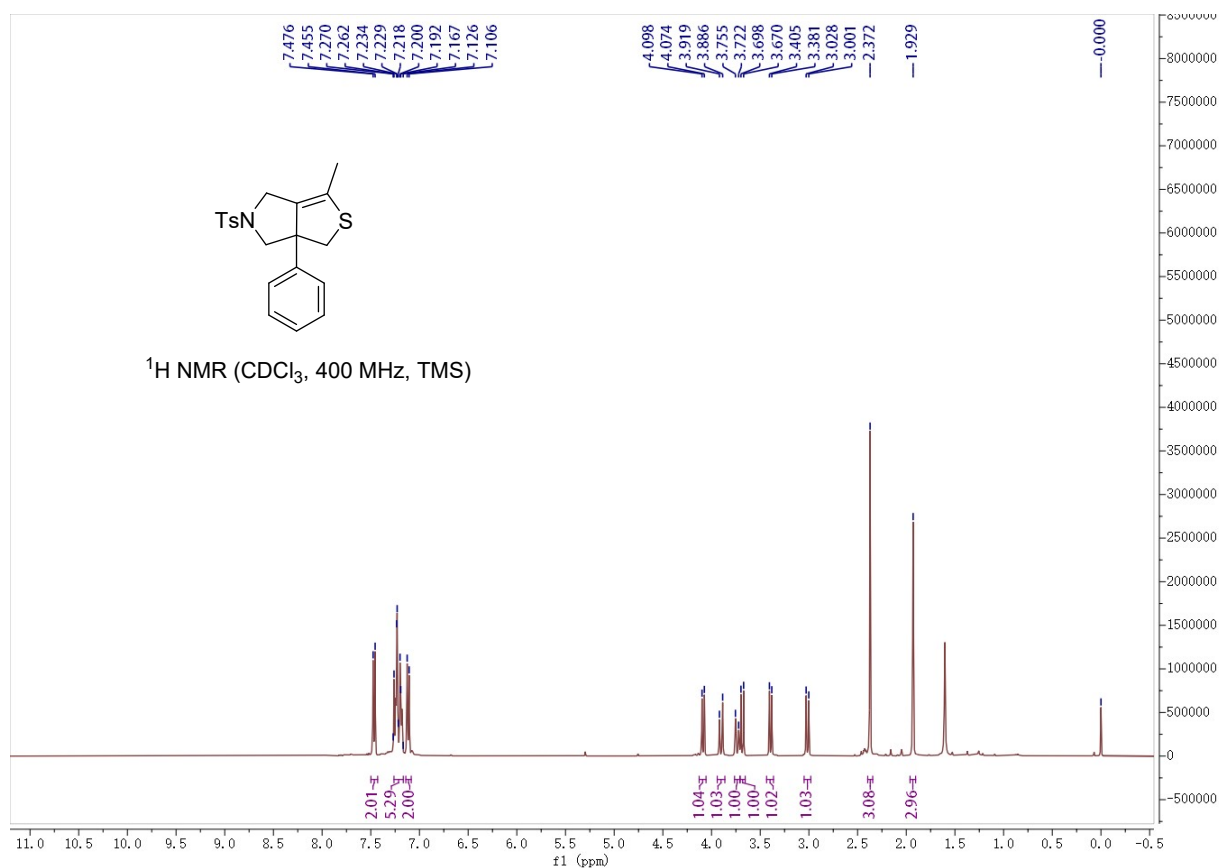


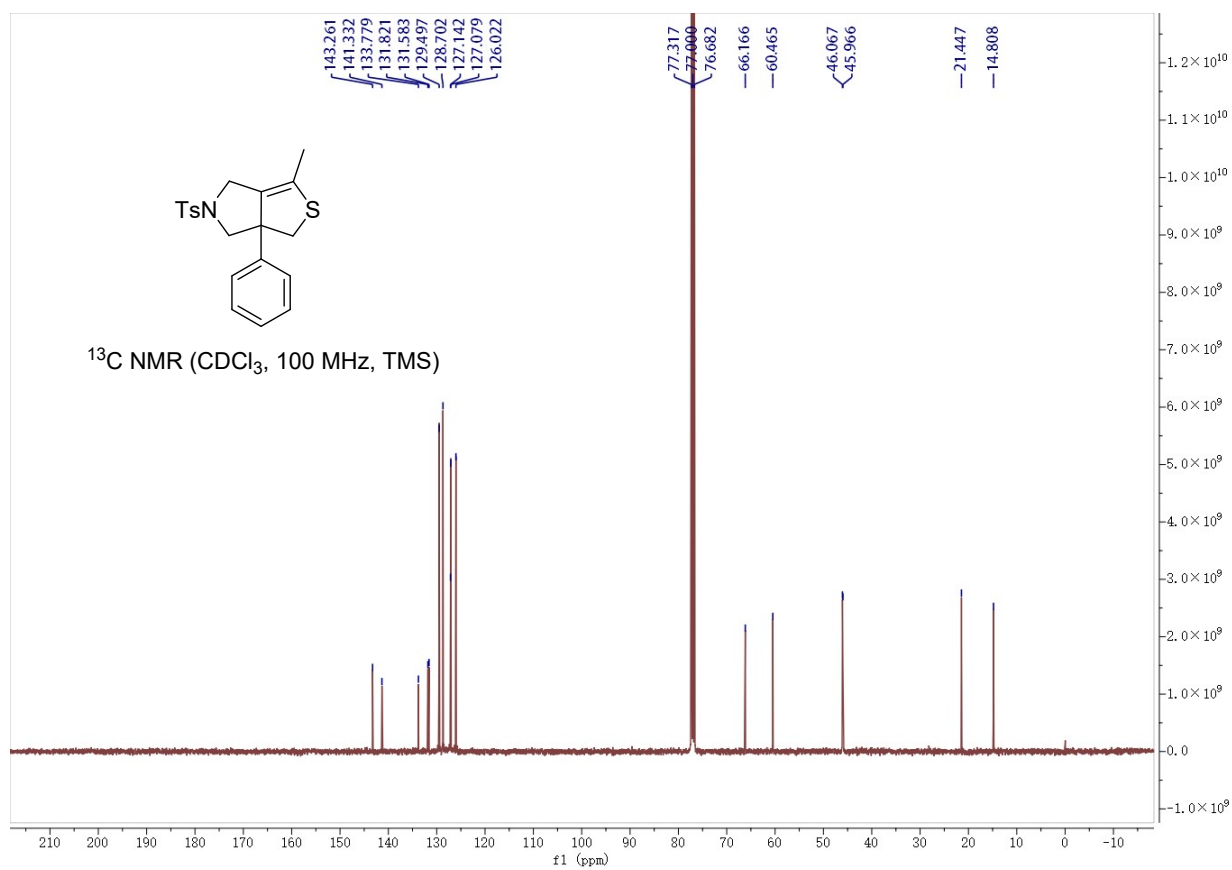
9. Spectroscopic data of products 3, 4, 5

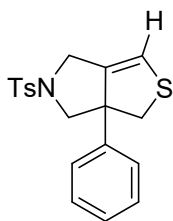


3-methyl-6a-phenyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3a)

A colorless oil, 34.5 mg, 95% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.47 (d, $J = 8.2$ Hz, 2H), 7.26 – 7.17 (m, 5H), 7.12 (d, $J = 8.0$ Hz, 2H), 4.09 (d, $J = 9.6$ Hz, 1H), 3.90 (d, $J = 13.3$ Hz, 1H), 3.74 (d, $J = 13.2$ Hz, 1H), 3.68 (d, $J = 11.0$ Hz, 1H), 3.39 (d, $J = 9.7$ Hz, 1H), 3.01 (d, $J = 10.9$ Hz, 1H), 2.37 (s, 3H), 1.93 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 143.3, 141.3, 133.8, 131.8, 131.6, 129.5, 128.7, 127.14, 127.08, 126.0, 66.2, 60.5, 46.1, 46.0, 21.4, 14.8. IR (Acetone) ν 615, 1052, 1134, 1388, 3006 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{20}\text{H}_{22}\text{O}_2\text{NS}_2$ (M+H): 372.1086, Found: 372.1075.

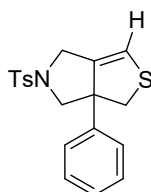




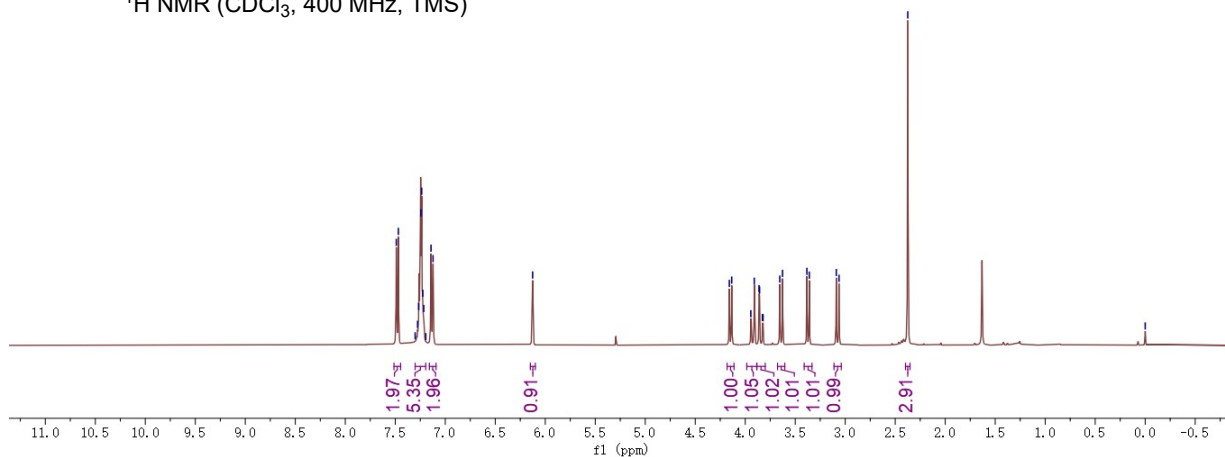


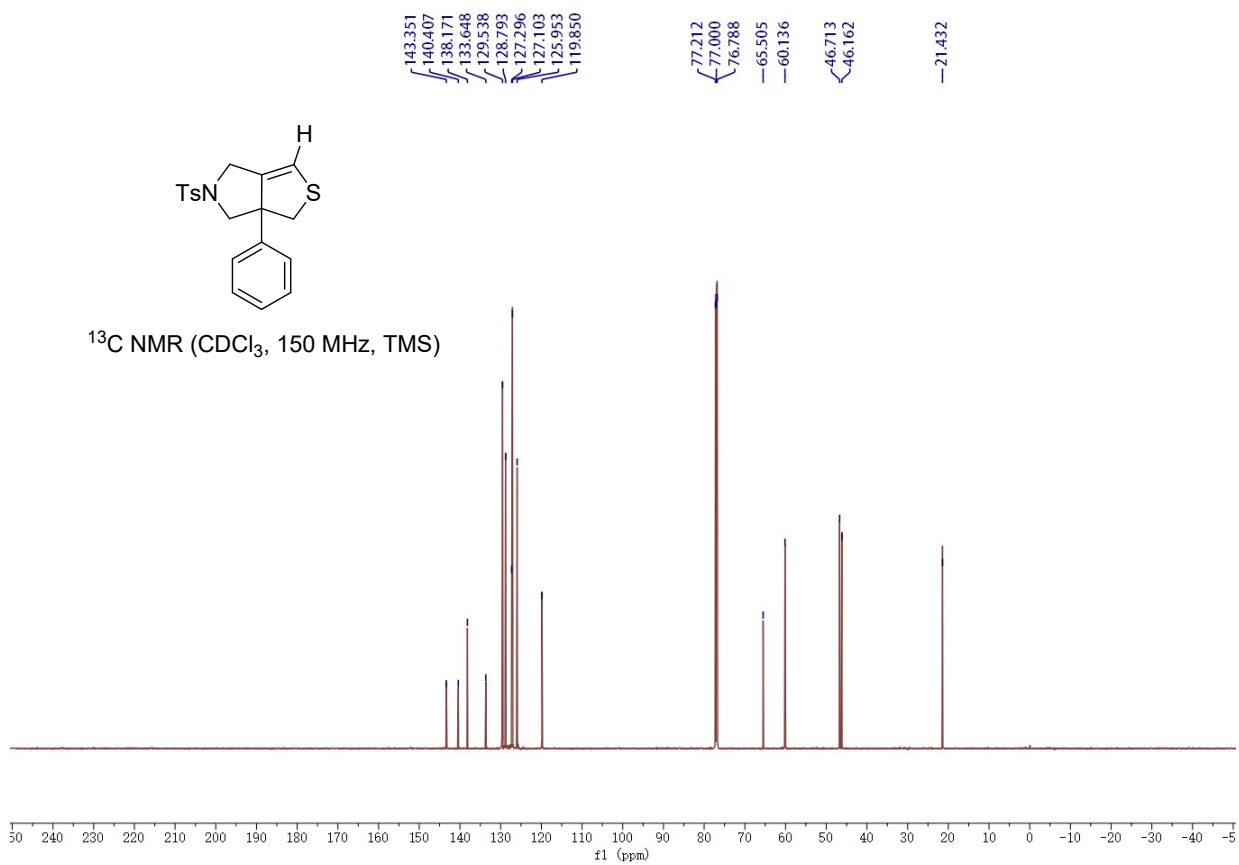
6a-phenyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3b)

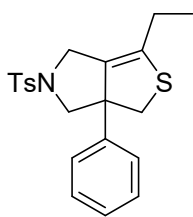
A colorless oil, 21.5 mg, 60% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.48 (d, $J = 8.2$ Hz, 2H), 7.30 – 7.20 (m, 5H), 7.13 (d, $J = 8.0$ Hz, 2H), 6.13 (s, 1H), 4.15 (d, $J = 9.6$ Hz, 1H), 3.93 (d, $J = 13.7$ Hz, 1H), 3.84 (dd, $J = 13.8, 2.2$ Hz, 1H), 3.64 (d, $J = 11.0$ Hz, 1H), 3.37 (d, $J = 9.6$ Hz, 1H), 3.08 (d, $J = 11.0$ Hz, 1H), 2.37 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 143.4, 140.4, 138.2, 133.6, 129.5, 128.8, 127.3, 127.1, 126.0, 119.9, 65.5, 60.1, 46.7, 46.2, 21.4. IR (Acetone) ν 665, 1161, 1344, 1710, 2979 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{19}\text{H}_{20}\text{O}_2\text{NS}_2$ (M+H): 358.0930, Found: 358.0916.



^1H NMR (CDCl_3 , 400 MHz, TMS)

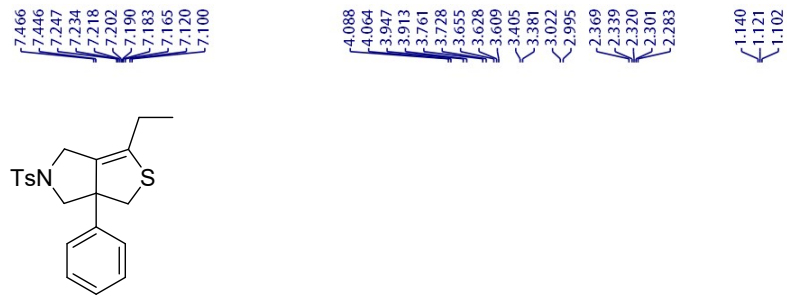




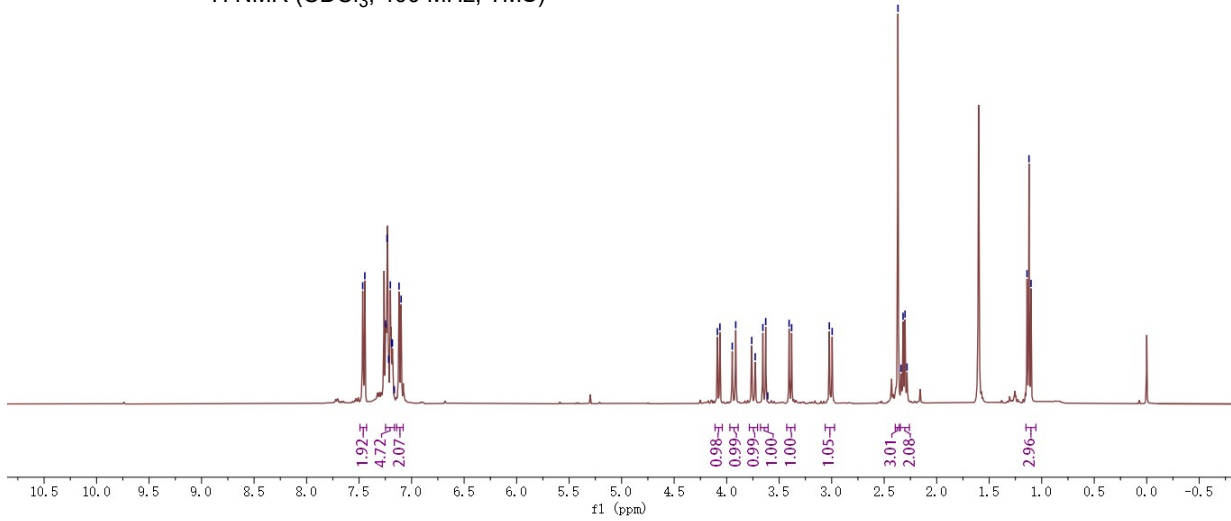


3-ethyl-6a-phenyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3c)

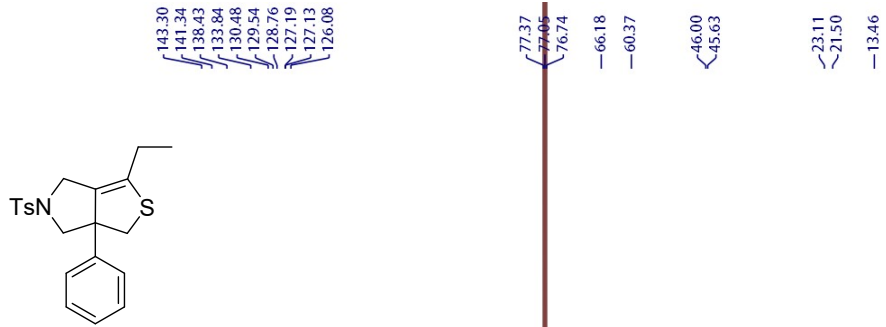
A colorless oil, 34.7 mg, 90% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.46 (d, $J = 8.0$ Hz, 2H), 7.25 – 7.16 (m, 5H), 7.11 (d, $J = 8.0$ Hz, 2H), 4.08 (d, $J = 9.6$ Hz, 1H), 3.93 (d, $J = 13.3$ Hz, 1H), 3.74 (d, $J = 13.2$ Hz, 1H), 3.64 (d, $J = 10.9$ Hz, 1H), 3.39 (d, $J = 9.6$ Hz, 1H), 3.01 (d, $J = 10.9$ Hz, 1H), 2.37 (s, 3H), 2.31 (q, $J = 7.5$ Hz, 2H), 1.12 (t, $J = 7.6$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 143.3, 141.3, 138.4, 133.8, 130.5, 129.5, 128.8, 127.2, 127.1, 126.1, 66.2, 60.4, 46.0, 45.6, 23.1, 21.5, 13.5. IR (Acetone) ν 678, 897, 1162, 1333, 1718, 2983 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{21}\text{H}_{24}\text{O}_2\text{NS}_2$ (M+H): 386.1243, Found: 386.1229.



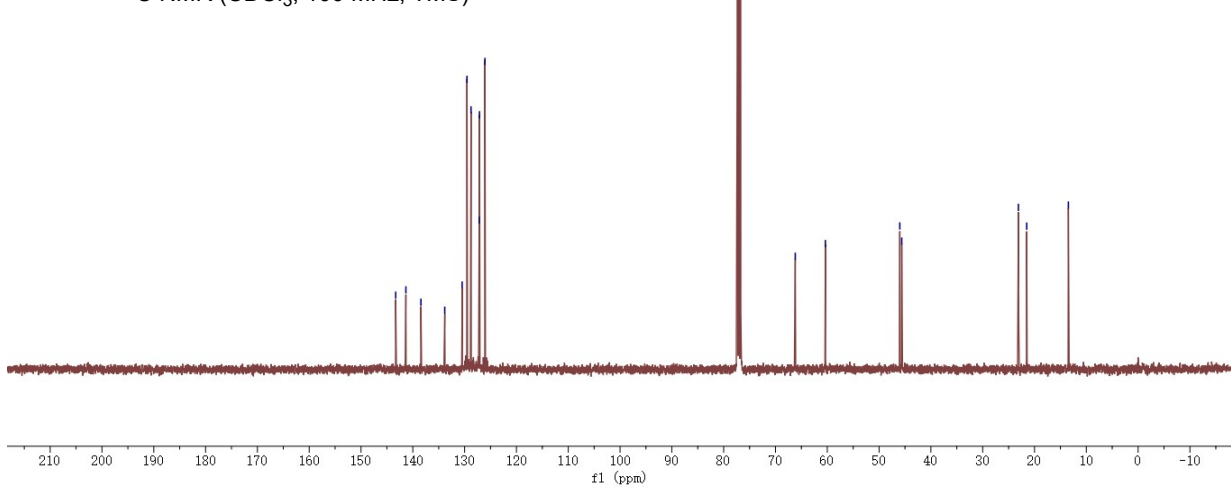
¹H NMR (CDCl₃, 400 MHz, TMS)

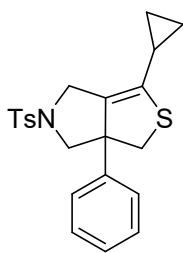


R1=Et. 2. 1. 1r



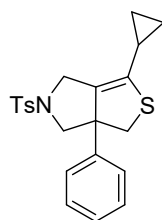
¹³C NMR (CDCl₃, 100 MHz, TMS)



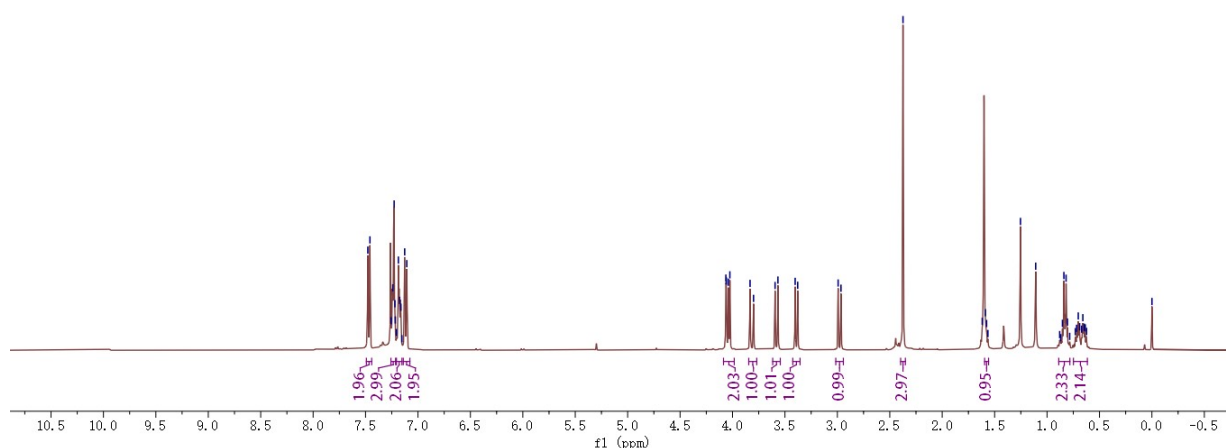


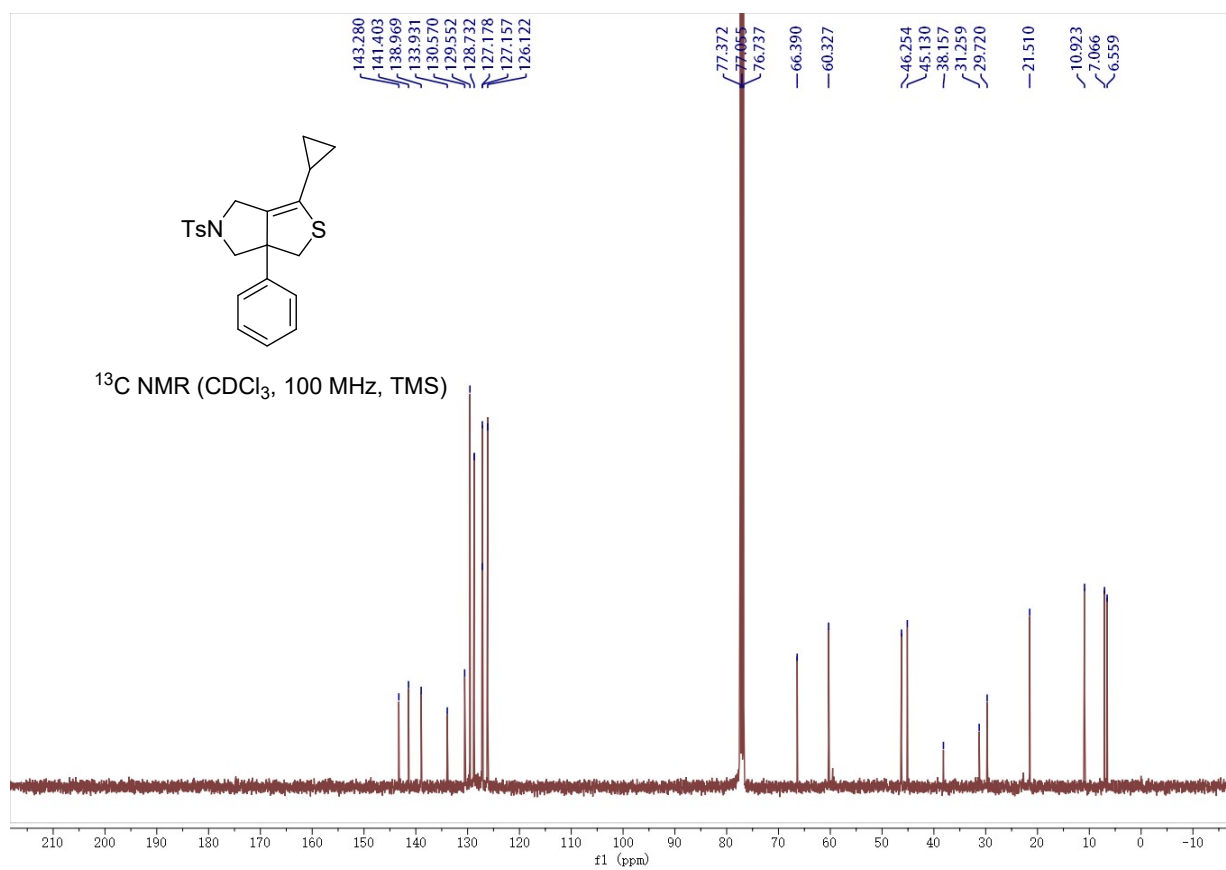
3-cyclopropyl-6a-phenyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3d)

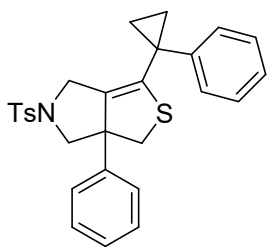
A colorless oil, 35.0 mg, 88% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.47 (d, $J = 8.0$ Hz, 2H), 7.26-7.21 (m, 3H), 7.21-7.15 (m, 2H), 7.12 (d, $J = 8.0$ Hz, 2H), 4.09 – 3.98 (m, 2H), 3.82 (d, $J = 13.3$ Hz, 1H), 3.58 (d, $J = 10.9$ Hz, 1H), 3.39 (d, $J = 9.6$ Hz, 1H), 2.98 (d, $J = 10.9$ Hz, 1H), 2.37 (s, 3H), 1.60 – 1.56 (m, 1H), 0.89 – 0.78 (m, 2H), 0.75 – 0.62 (m, 2H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 143.3, 141.4, 139.0, 133.9, 130.6, 129.6, 128.7, 127.18, 127.16, 126.1, 66.4, 60.3, 46.3, 45.1, 38.2, 31.3, 29.7, 21.5, 10.9, 7.1, 6.6. IR (Acetone) ν 679, 887, 1138, 1371, 1732, 2987 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{22}\text{H}_{24}\text{O}_2\text{NS}_2$ (M+H): 398.1243, Found: 398.1229.



^1H NMR (CDCl_3 , 400 MHz, TMS)

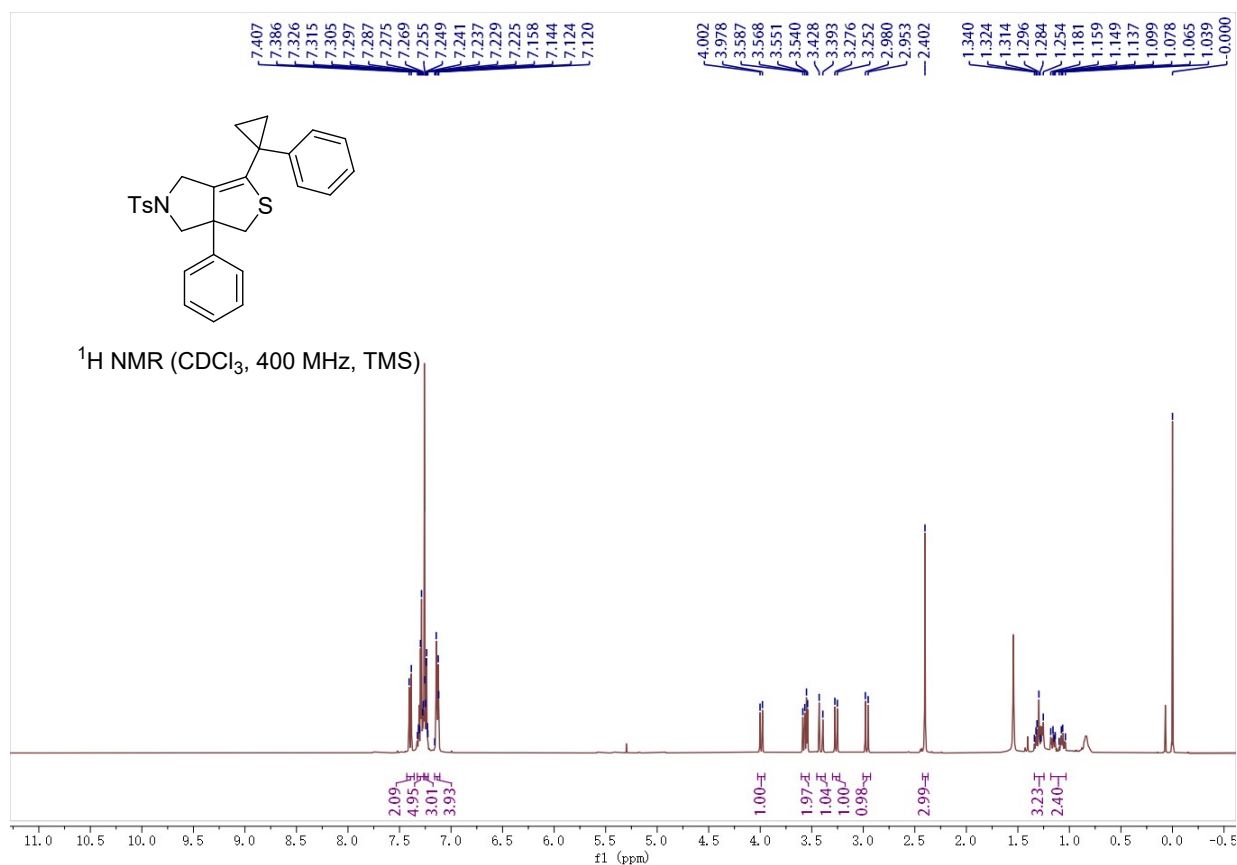


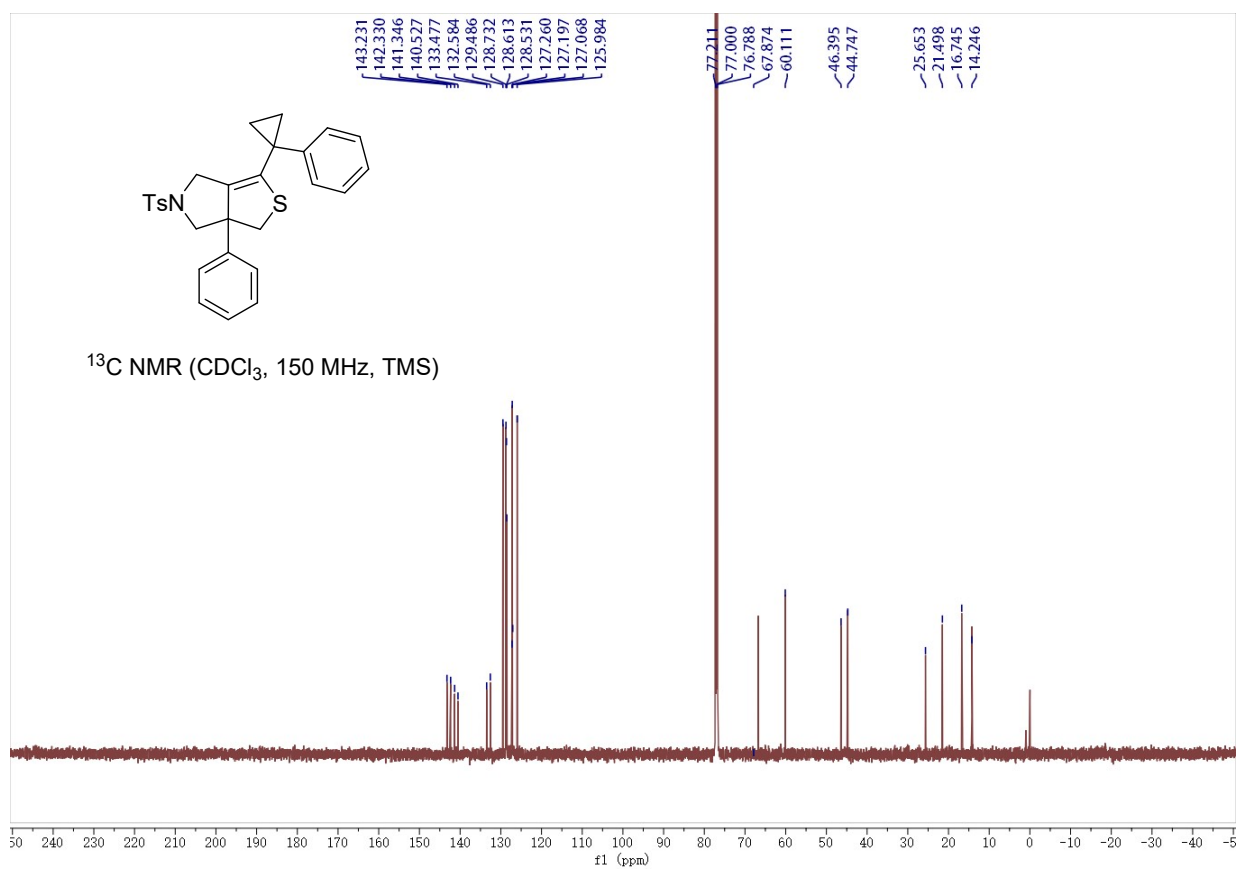


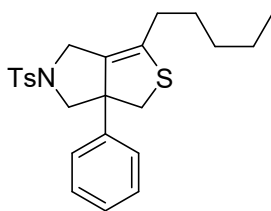


6a-phenyl-3-(1-phenylcyclopropyl)-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3e)

A colorless oil, 38.3 mg, 81% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.40 (d, $J = 8.3$ Hz, 2H), 7.33 – 7.27 (m, 5H), 7.26 – 7.22 (m, 3H), 7.16 – 7.11 (m, 4H), 3.99 (d, $J = 9.4$ Hz, 1H), 3.60 – 3.53 (m, 2H), 3.41 (d, $J = 14.3$ Hz, 1H), 3.26 (d, $J = 9.4$ Hz, 1H), 2.97 (d, $J = 10.9$ Hz, 1H), 2.40 (s, 3H), 1.34 – 1.25 (m, 2H), 1.18 – 1.03 (m, 2H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 143.2, 142.3, 141.3, 140.5, 133.5, 132.6, 129.5, 128.7, 128.6, 128.5, 127.3, 127.2, 127.1, 126.0, 67.9, 60.1, 46.4, 44.7, 25.7, 21.5, 16.7, 14.2. IR (Acetone) ν 636, 791, 901, 1361, 1779, 2921 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{28}\text{H}_{28}\text{O}_2\text{NS}_2$ (M+H): 474.1556, Found: 474.1544.

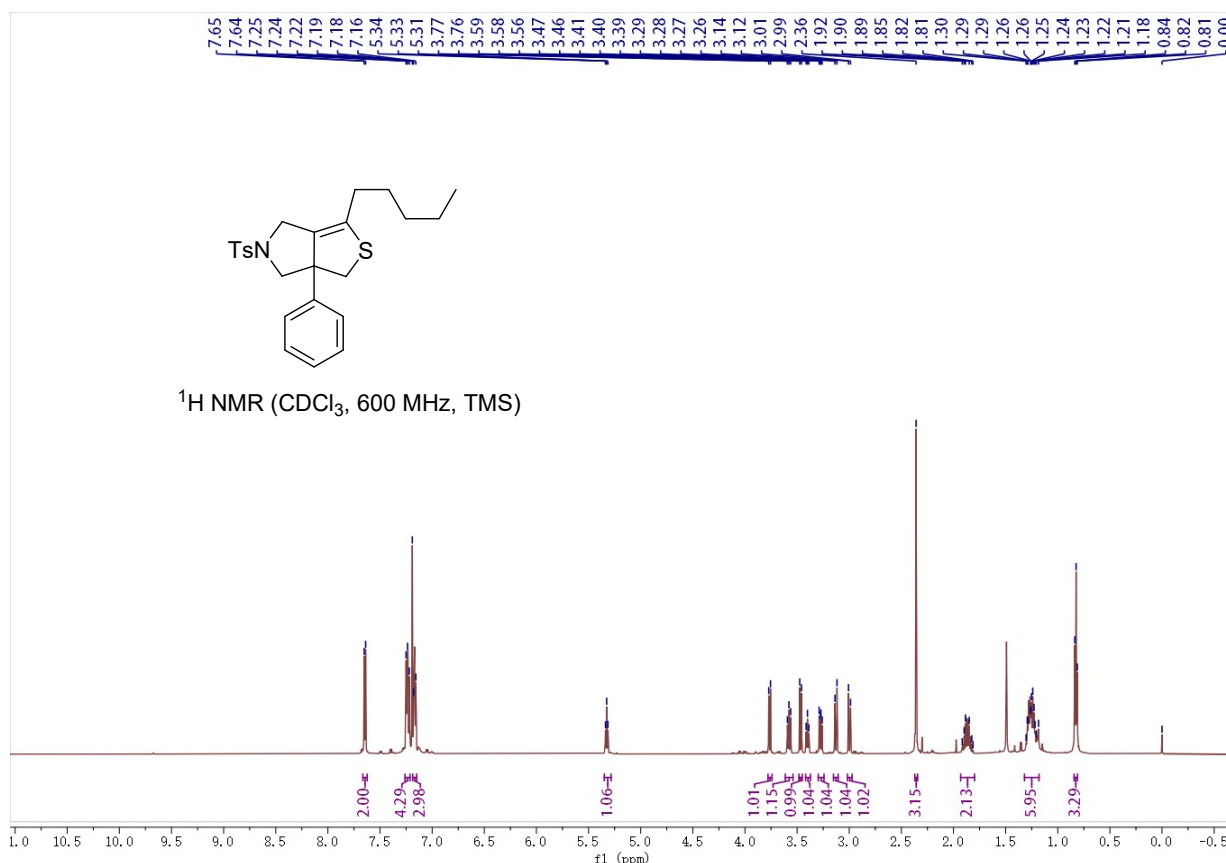


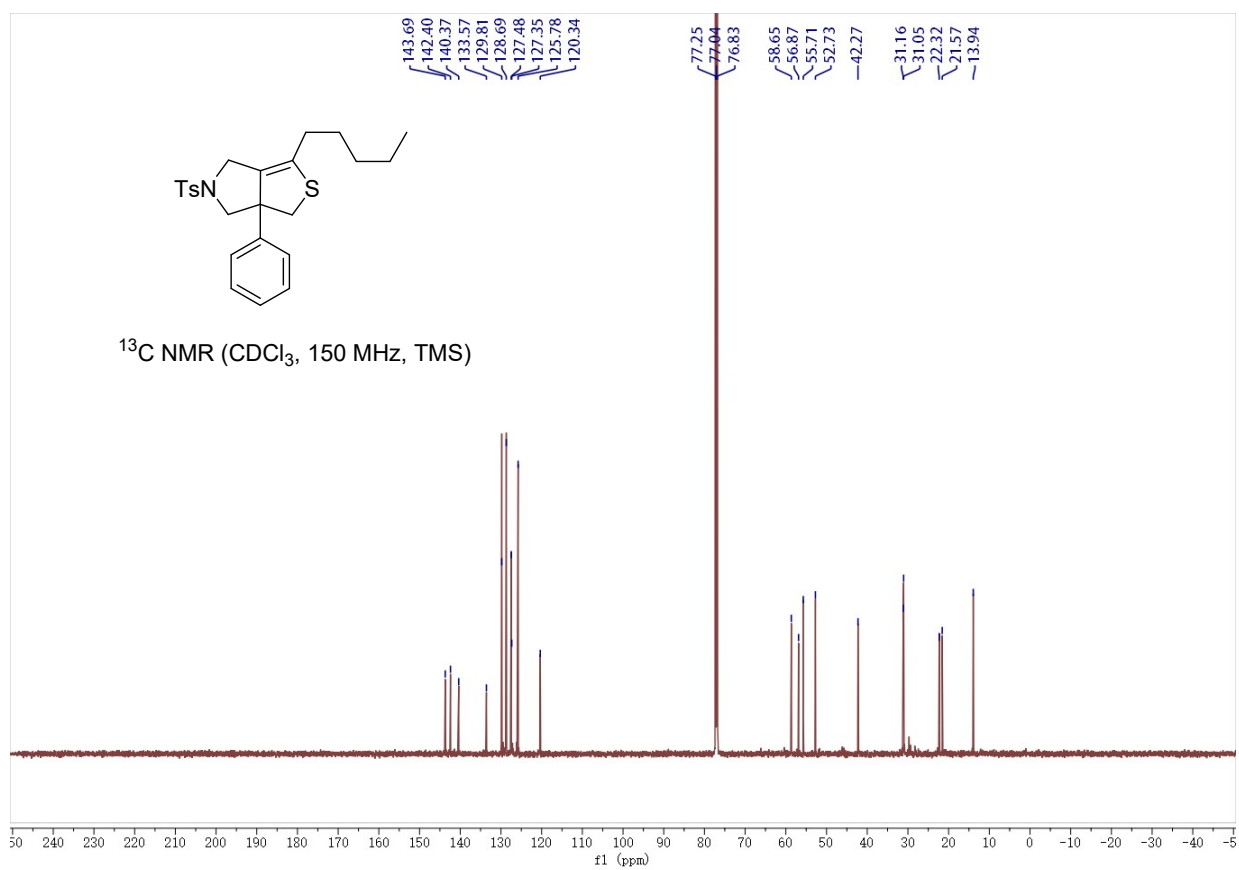


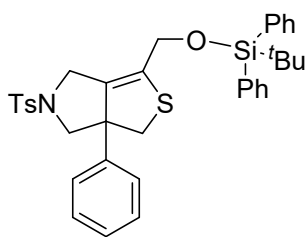


3-pentyl-6a-phenyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3f)

A colorless oil, 34.2 mg, 80% yield. ^1H NMR (CDCl_3 , TMS, 600 MHz) δ 7.65 (d, $J = 8.3$ Hz, 2H), 7.26 – 7.21 (m, 4H), 7.19 – 7.15 (m, 3H), 5.33 (t, $J = 7.0$ Hz, 1H), 3.76 (d, $J = 10.0$ Hz, 1H), 3.61 – 3.54 (m, 1H), 3.47 (d, $J = 10.0$ Hz, 1H), 3.40 (t, $J = 7.9$ Hz, 1H), 3.27 (dd, $J = 10.1, 7.2$ Hz, 1H), 3.13 (d, $J = 11.5$ Hz, 1H), 3.00 (d, $J = 11.4$ Hz, 1H), 2.36 (s, 3H), 1.93 – 1.80 (m, 2H), 1.32 – 1.18 (m, 4H), 0.82 (t, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 143.7, 142.4, 140.4, 133.6, 129.8, 128.7, 127.5, 127.4, 125.8, 120.3, 58.7, 56.9, 55.7, 52.7, 42.3, 31.2, 31.1, 22.3, 21.6, 13.9. IR (Acetone) ν 665, 1091, 1161, 1342, 1707, 2925 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{24}\text{H}_{30}\text{O}_2\text{NS}_2$ (M+H): 428.1712, Found: 428.1700.

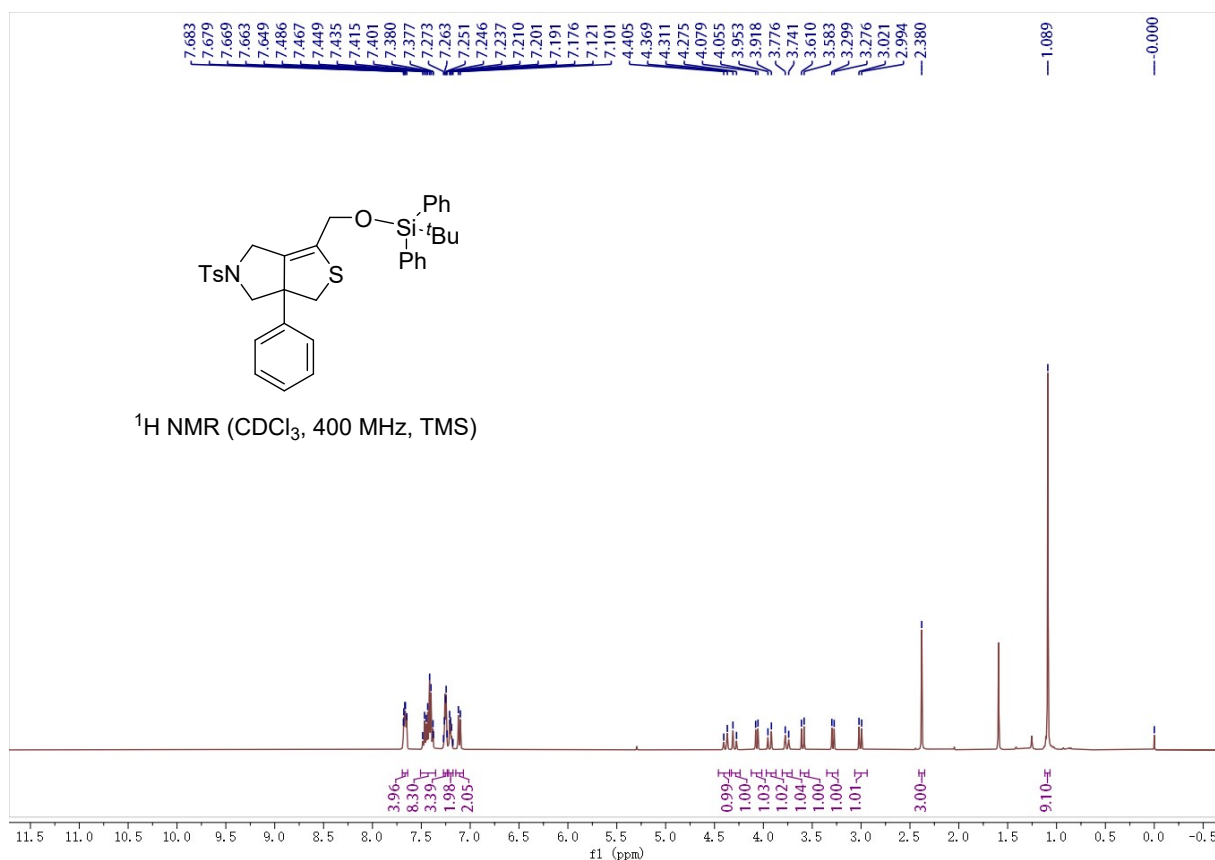


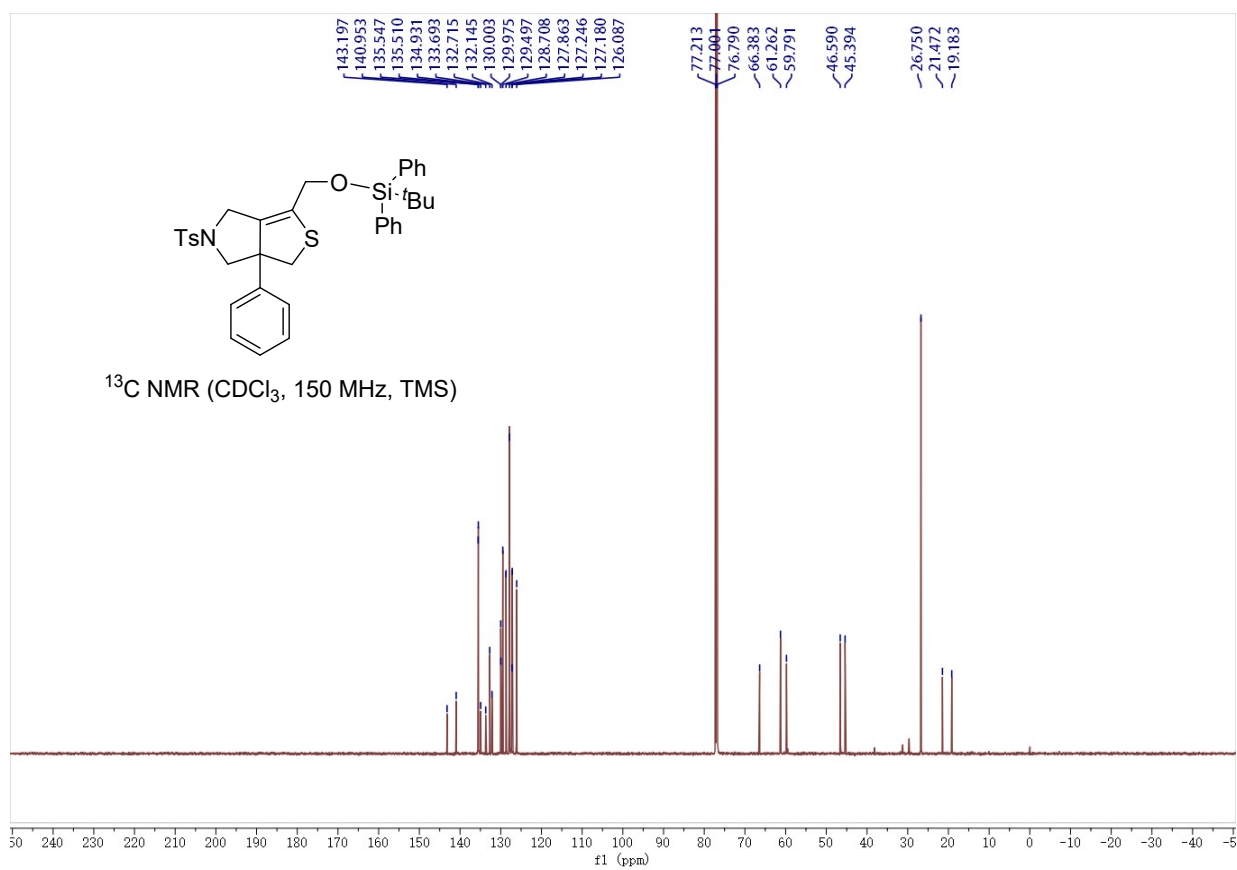


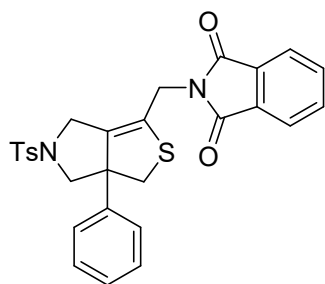


3-((*tert*-butyldiphenylsilyloxy)-6a-phenyl-5-tosyl-4,5,6,6a-tetrahydro-1*H*-thieno[3,4-*c*]pyrrole (3g)

A colorless oil, 46.9 mg, 75% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.69 – 7.64 (m, 4H), 7.51 – 7.35 (m, 8H), 7.27-7.24 (m, 3H), 7.22 – 7.18 (m, 2H), 7.11 (d, $J = 8.0$ Hz, 2H), 4.39 (d, $J = 14.6$ Hz, 1H), 4.29 (d, $J = 14.5$ Hz, 1H), 4.07 (d, $J = 9.5$ Hz, 1H), 3.94 (d, $J = 14.2$ Hz, 1H), 3.76 (d, $J = 14.2$ Hz, 1H), 3.60 (d, $J = 10.9$ Hz, 1H), 3.29 (d, $J = 9.5$ Hz, 1H), 3.01 (d, $J = 10.9$ Hz, 1H), 2.38 (s, 3H), 1.09 (s, 9H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 143.2, 141.0, 135.55, 135.51, 134.9, 133.7, 132.7, 132.1, 130.00, 129.98, 129.5, 128.7, 127.9, 127.25, 127.18, 126.1, 66.4, 61.3, 59.8, 46.6, 45.4, 26.8, 21.5, 19.2. IR (Acetone) ν 663, 821, 1092, 1112, 1161, 1347, 1710, 2848, 2916 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{36}\text{H}_{40}\text{O}_3\text{NS}_2\text{Si}$ ($\text{M}+\text{H}$): 626.2213, Found: 626.2192.

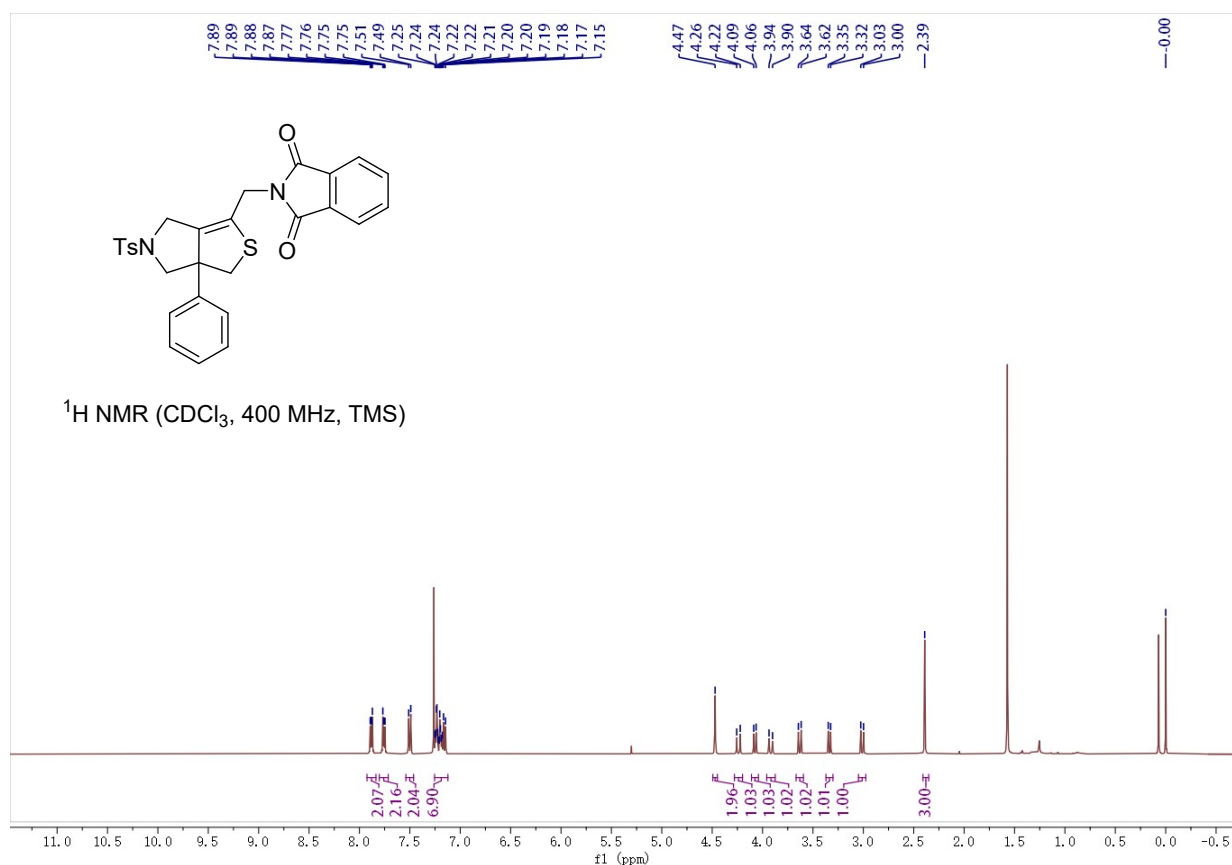


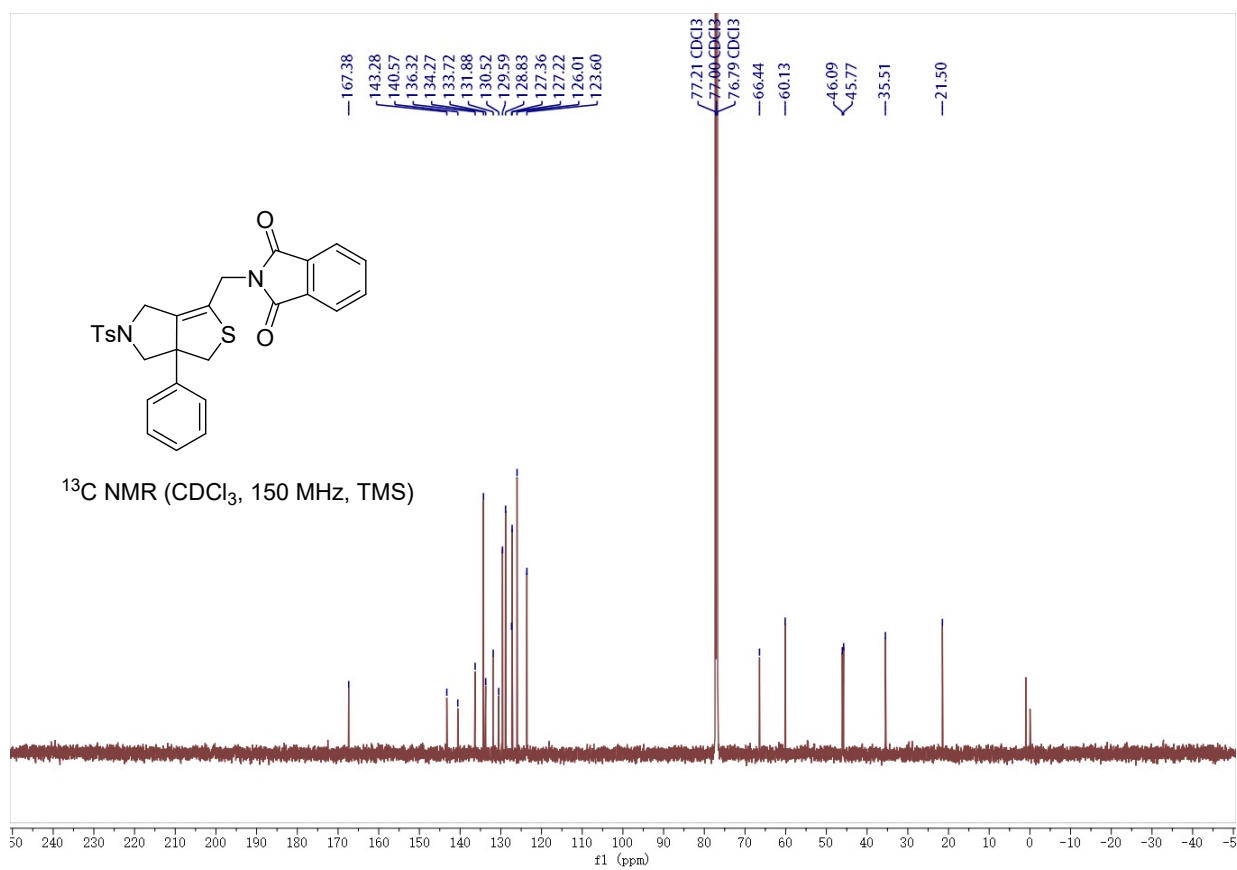


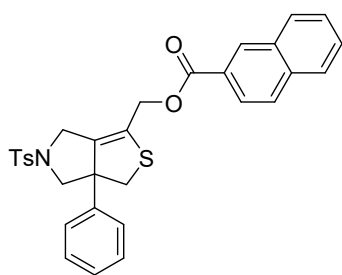


2-((6a-phenyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrol-3-yl)methyl)isoindoline-1,3-dione (3h)

A colorless oil, 53.4 mg, 78% yield. $^1\text{H NMR}$ (CDCl_3 , TMS, 600 MHz) δ 7.88 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.76 (dd, $J = 5.5, 3.1$ Hz, 2H), 7.50 (d, $J = 8.3$ Hz, 2H), 7.25 – 7.12 (m, 7H), 4.47 (s, 2H), 4.24 (d, $J = 14.0$ Hz, 1H), 4.08 (d, $J = 9.5$ Hz, 1H), 3.92 (d, $J = 14.1$ Hz, 1H), 3.63 (d, $J = 11.1$ Hz, 1H), 3.34 (d, $J = 9.6$ Hz, 1H), 3.01 (d, $J = 11.1$ Hz, 1H), 2.39 (s, 3H). $^{13}\text{C NMR}$ (CDCl_3 , TMS, 150 MHz) δ 167.4, 143.3, 140.6, 136.3, 134.3, 133.7, 131.9, 130.5, 129.6, 128.8, 127.4, 127.2, 126.0, 123.6, 66.4, 60.1, 46.1, 45.8, 35.5, 21.5. IR (Acetone) ν 729, 1108, 1161, 1229, 1345, 1716, 2985 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{28}\text{H}_{25}\text{O}_4\text{N}_2\text{S}_2$ (M+H): 517.1250, Found: 517.1239.

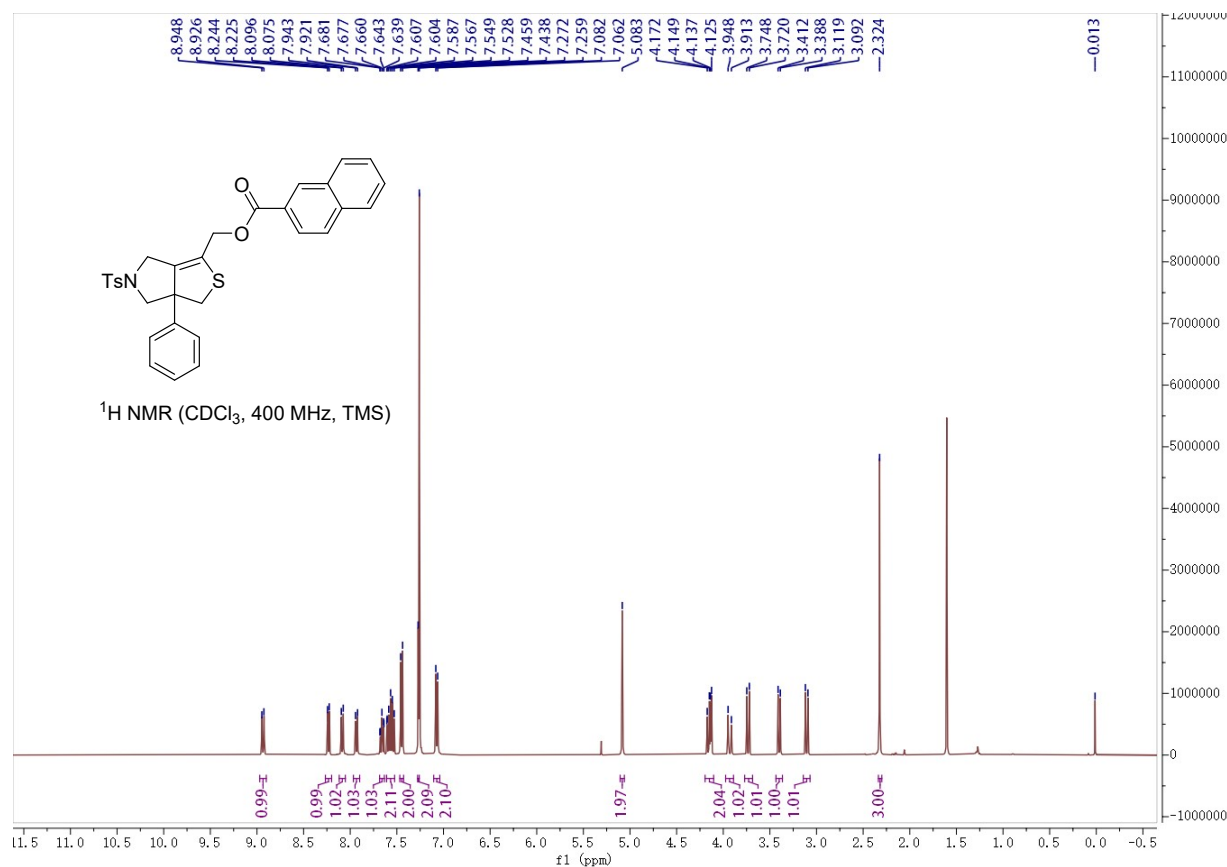


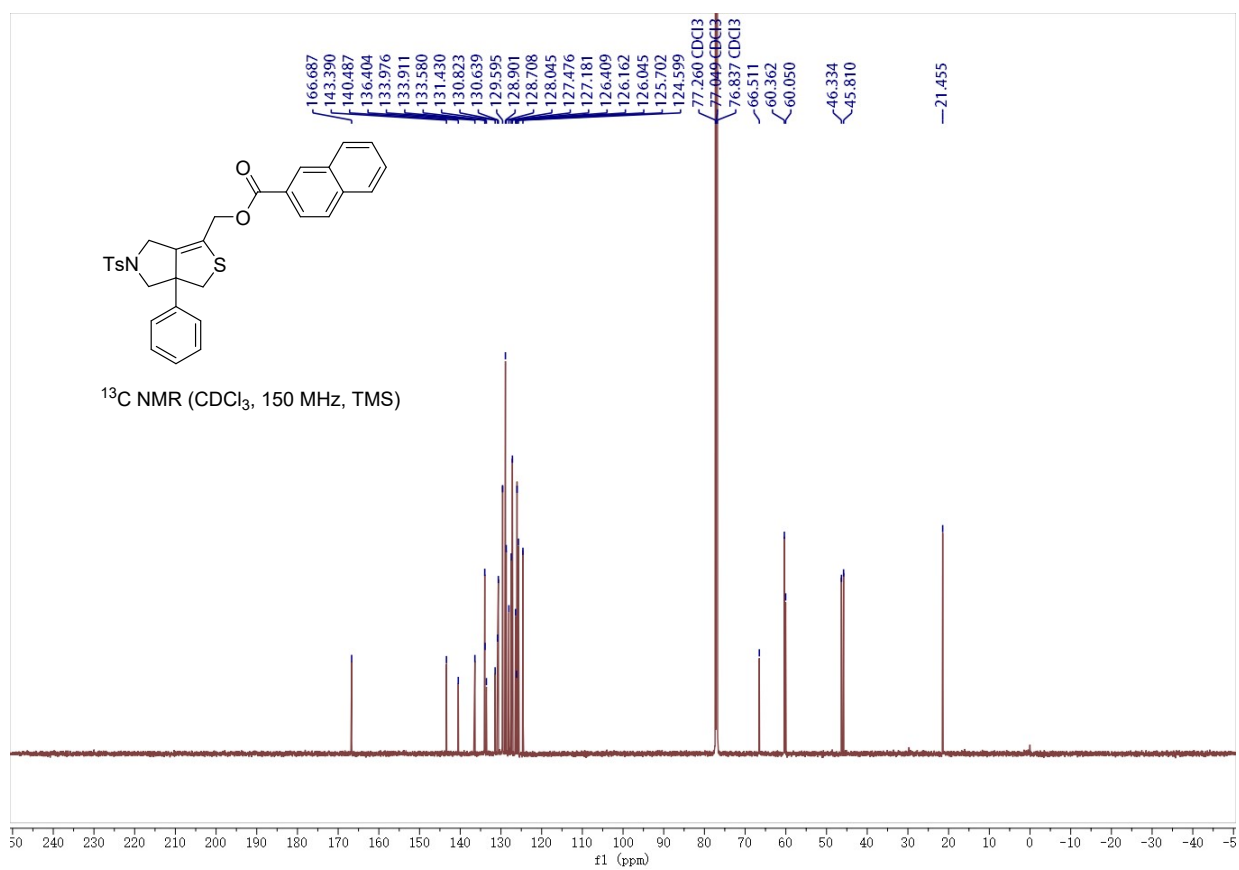


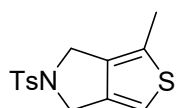


(6a-phenyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrol-3-yl)methyl 2-naphthoate (3i)

A colorless oil, 39.5 mg, 73% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 8.94 (d, $J = 8.8$ Hz, 1H), 8.23 (d, $J = 7.3$ Hz, 1H), 8.09 (d, $J = 8.2$ Hz, 1H), 7.93 (d, $J = 8.7$ Hz, 1H), 7.68 – 7.63 (m, 1H), 7.61 – 7.52 (m, 2H), 7.45 (d, $J = 8.3$ Hz, 2H), 7.28 – 7.26 (m, 2H), 7.07 (d, $J = 8.1$ Hz, 2H), 5.08 (s, 2H), 4.19 – 4.10 (m, 2H), 3.93 (d, $J = 14.3$ Hz, 1H), 3.73 (d, $J = 11.1$ Hz, 1H), 3.40 (d, $J = 9.6$ Hz, 1H), 3.11 (d, $J = 11.0$ Hz, 1H), 2.32 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 166.7, 143.4, 140.5, 136.4, 134.0, 133.9, 133.6, 131.4, 130.8, 130.6, 129.6, 128.9, 128.7, 128.0, 127.5, 127.2, 126.4, 126.2, 126.0, 125.7, 124.6, 66.5, 60.4, 60.1, 46.3, 45.8, 21.5. IR (Acetone) ν 661, 780, 1062, 1128, 1160, 1239, 1342, 1711, 3052 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{31}\text{H}_{28}\text{NO}_4\text{S}_2$ ($\text{M}+\text{H}$): 542.1437, Found: 542.1439.

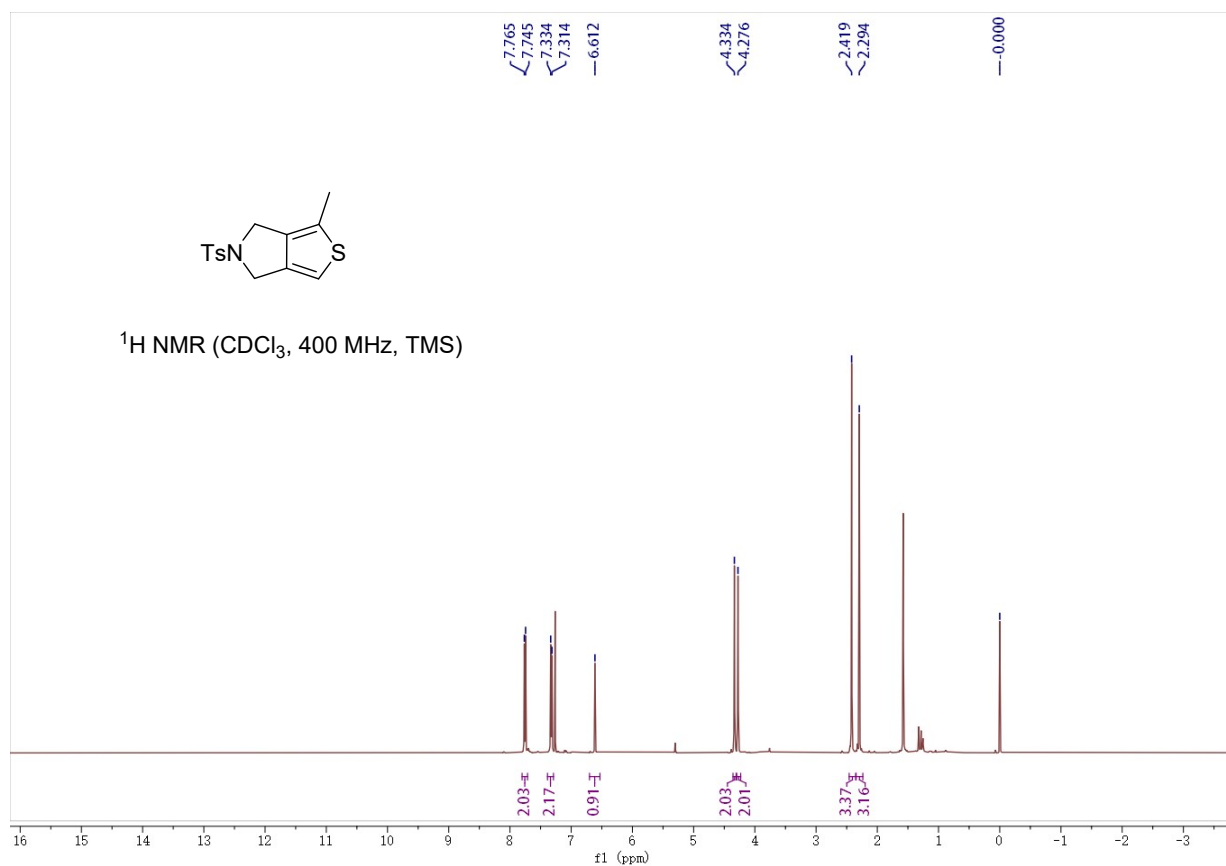


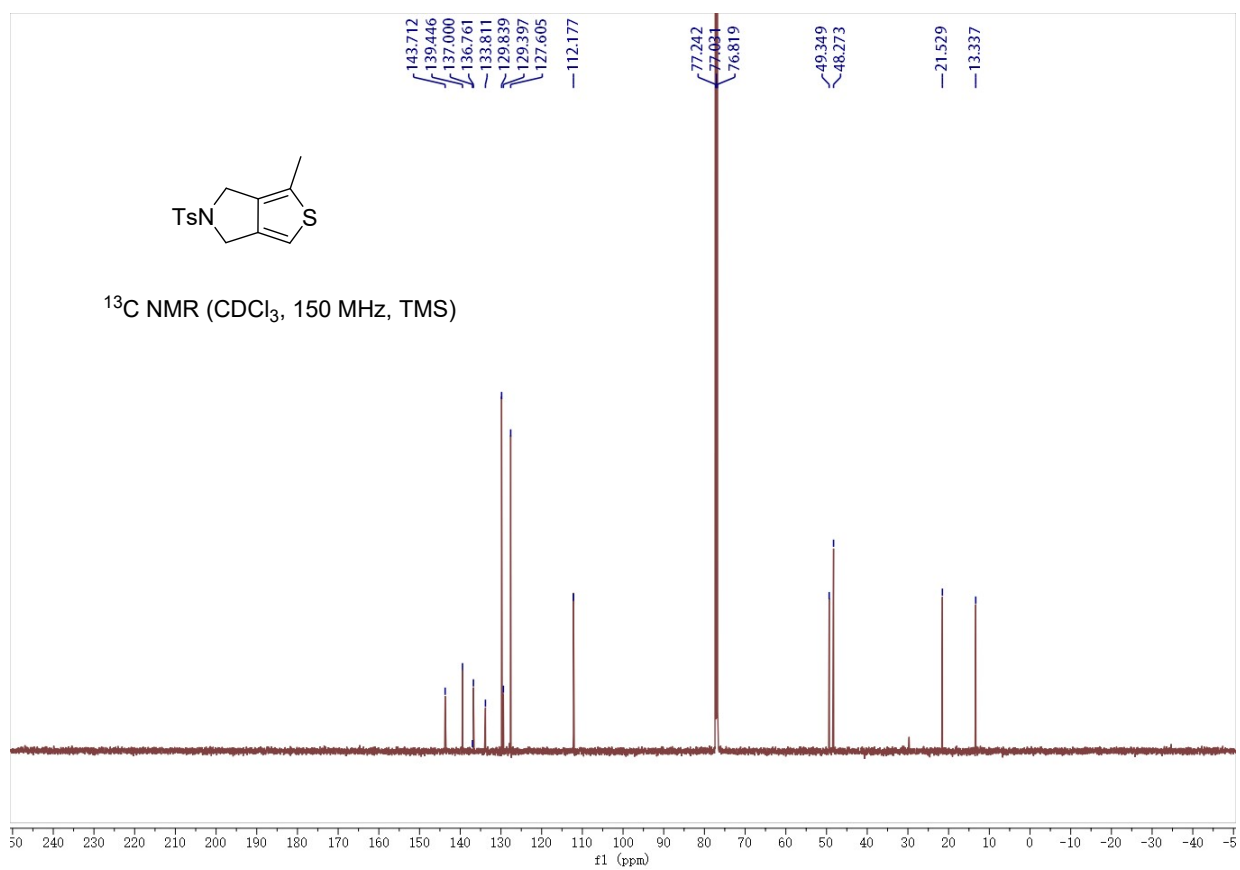


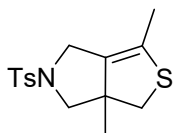


1-methyl-5-tosyl-5,6-dihydro-4H-thieno[3,4-c]pyrrole (3j)

A colorless oil, 15.6 mg, 53% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.76 (d, $J = 8.1$ Hz, 2H), 7.32 (d, $J = 8.1$ Hz, 2H), 6.61 (s, 1H), 4.33 (s, 2H), 4.28 (s, 2H), 2.42 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 143.7, 139.4, 137.0, 136.8, 133.8, 129.8, 129.4, 127.6, 112.2, 49.3, 48.3, 21.5, 13.3. IR (Acetone) ν 668, 813, 1044, 1095, 1158, 1344, 1601, 2971 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{14}\text{H}_{15}\text{NNaO}_2\text{S}_2(\text{M}+\text{Na})$: 316.0442, Found: 316.0522.

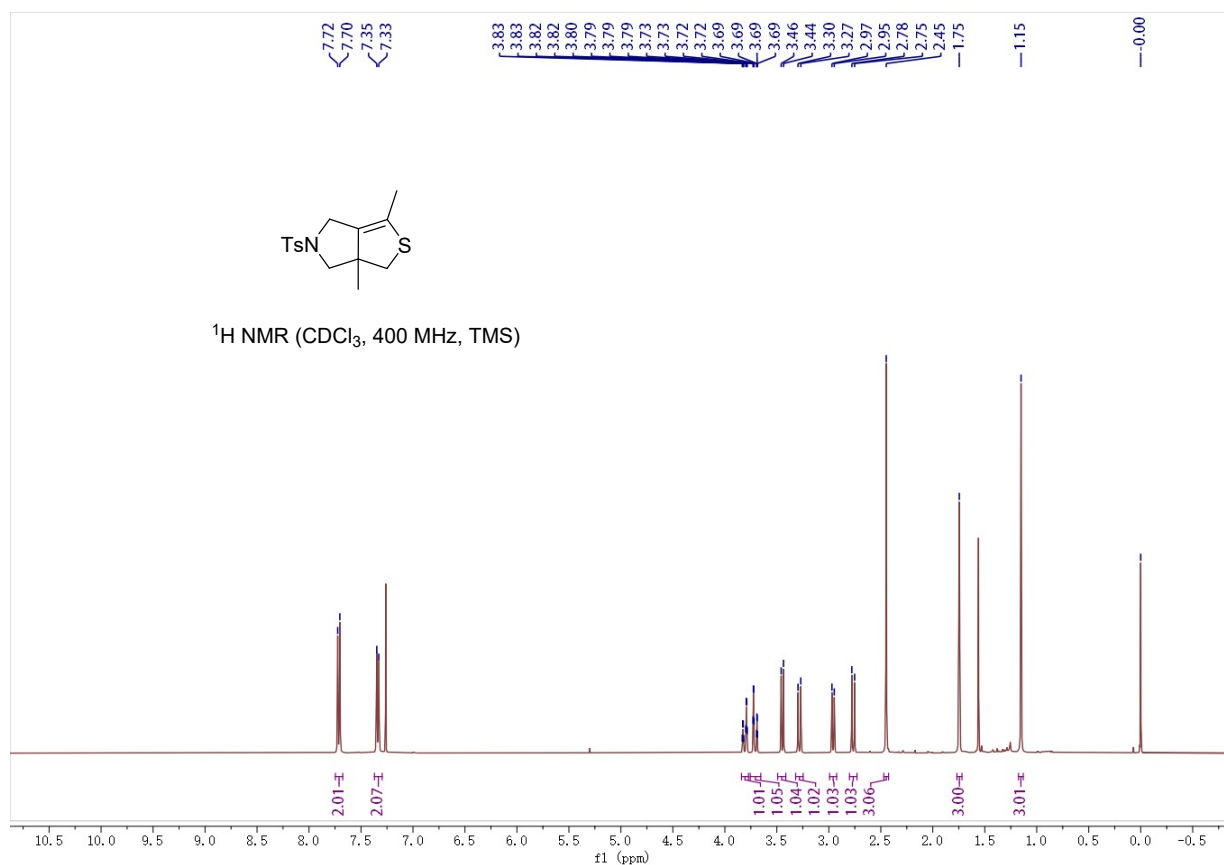


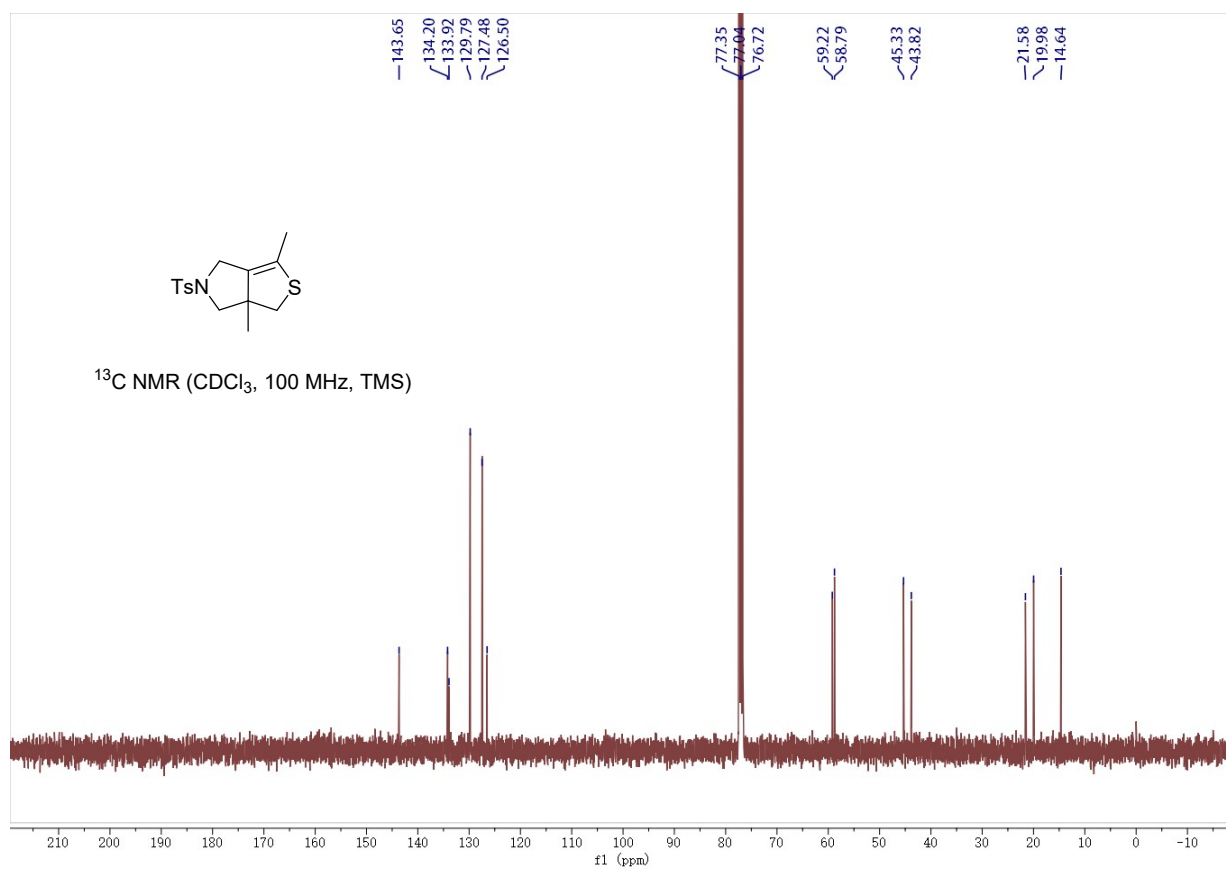


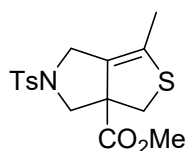


3,6a-dimethyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3k)

A colorless oil, 29.7 mg, 96% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.71 (d, $J = 8.3$ Hz, 2H), 7.34 (d, $J = 7.7$ Hz, 2H), 3.81 (dq, $J = 13.6, 1.8$ Hz, 1H), 3.71 (dq, $J = 13.5, 1.1$ Hz, 1H), 3.45 (d, $J = 9.0$ Hz, 1H), 3.28 (d, $J = 10.8$ Hz, 1H), 2.96 (d, $J = 9.0$ Hz, 1H), 2.77 (d, $J = 10.8$ Hz, 1H), 2.45 (s, 3H), 1.75 (s, 3H), 1.15 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 143.7, 134.2, 133.9, 129.8, 127.5, 126.5, 59.2, 58.8, 45.3, 43.8, 21.6, 20.0, 14.6. IR (Acetone) ν 668, 813, 1344, 1601, 2970 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{15}\text{H}_{20}\text{O}_2\text{NS}_2$ ($\text{M}+\text{H}$): 310.0930, Found: 310.0920.

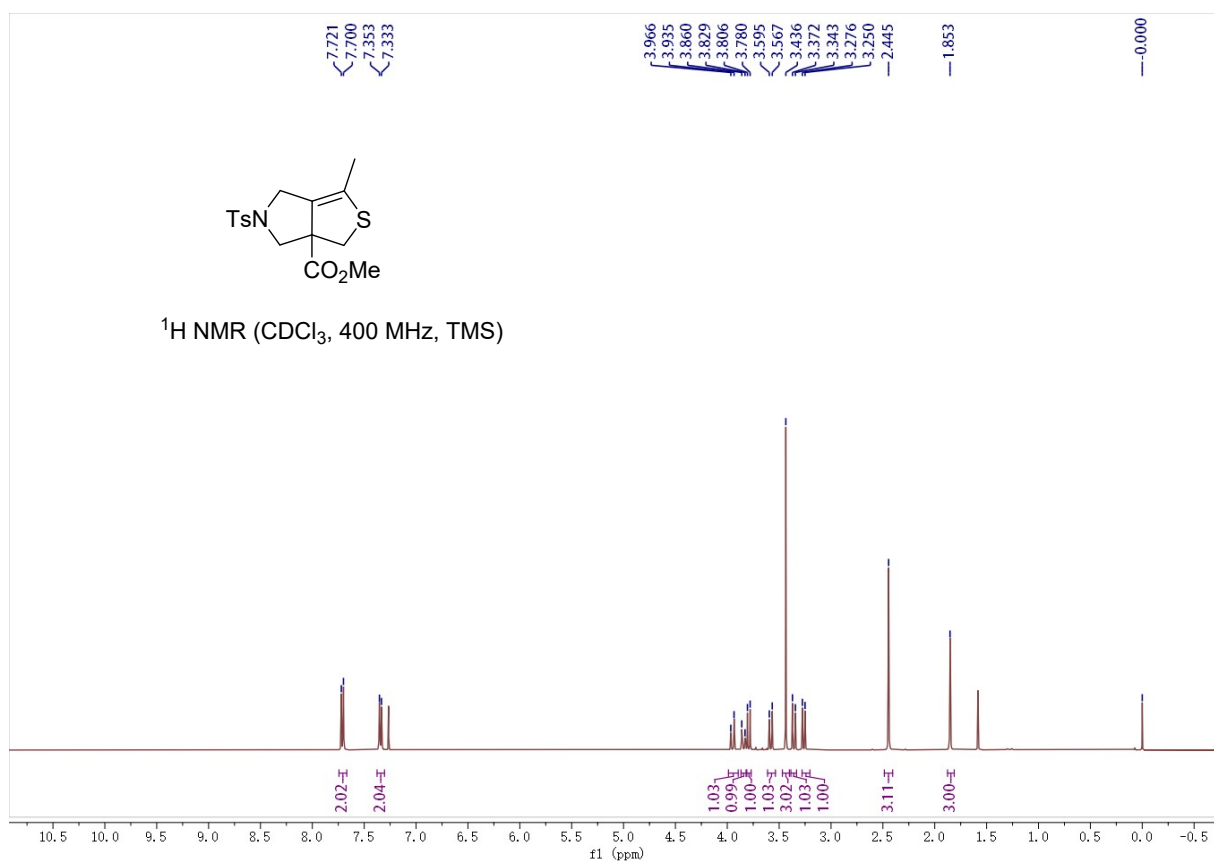


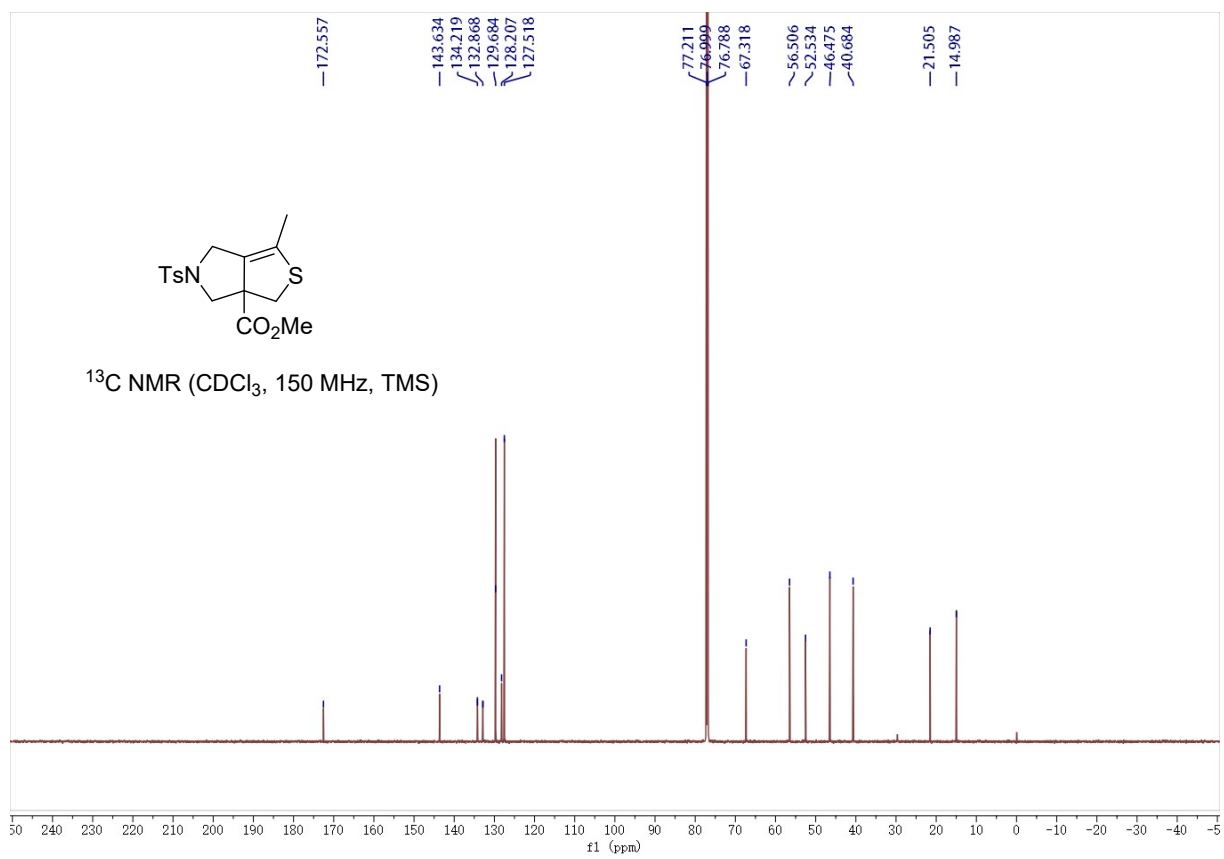


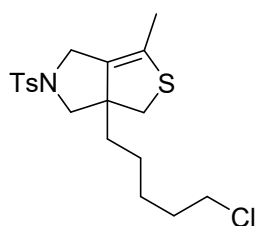


methyl 3-methyl-5-tosyl-5,6-dihydro-1*H*-thieno[3,4-*c*]pyrrole-6a(4*H*)-carboxylate (3I)

A colorless oil, 30.4 mg, 86% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.71 (d, $J = 8.3$ Hz, 2H), 7.34 (d, $J = 7.8$ Hz, 2H), 3.95 (d, $J = 12.5$ Hz, 1H), 3.84 (d, $J = 12.5$ Hz, 1H), 3.79 (d, $J = 10.3$ Hz, 1H), 3.58 (d, $J = 11.3$ Hz, 1H), 3.44 (s, 3H), 3.36 (d, $J = 11.4$ Hz, 1H), 3.26 (d, $J = 10.3$ Hz, 1H), 2.44 (s, 3H), 1.85 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 172.6, 143.6, 134.2, 132.9, 129.7, 128.2, 127.5, 67.3, 56.5, 52.5, 46.5, 40.7, 21.5, 15.0. IR (Acetone) ν 665, 1086, 1160, 1344, 1432, 1730, 2956 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{16}\text{H}_{20}\text{O}_4\text{NS}_2$ ($\text{M}+\text{H}$): 354.0828, Found: 354.0815.

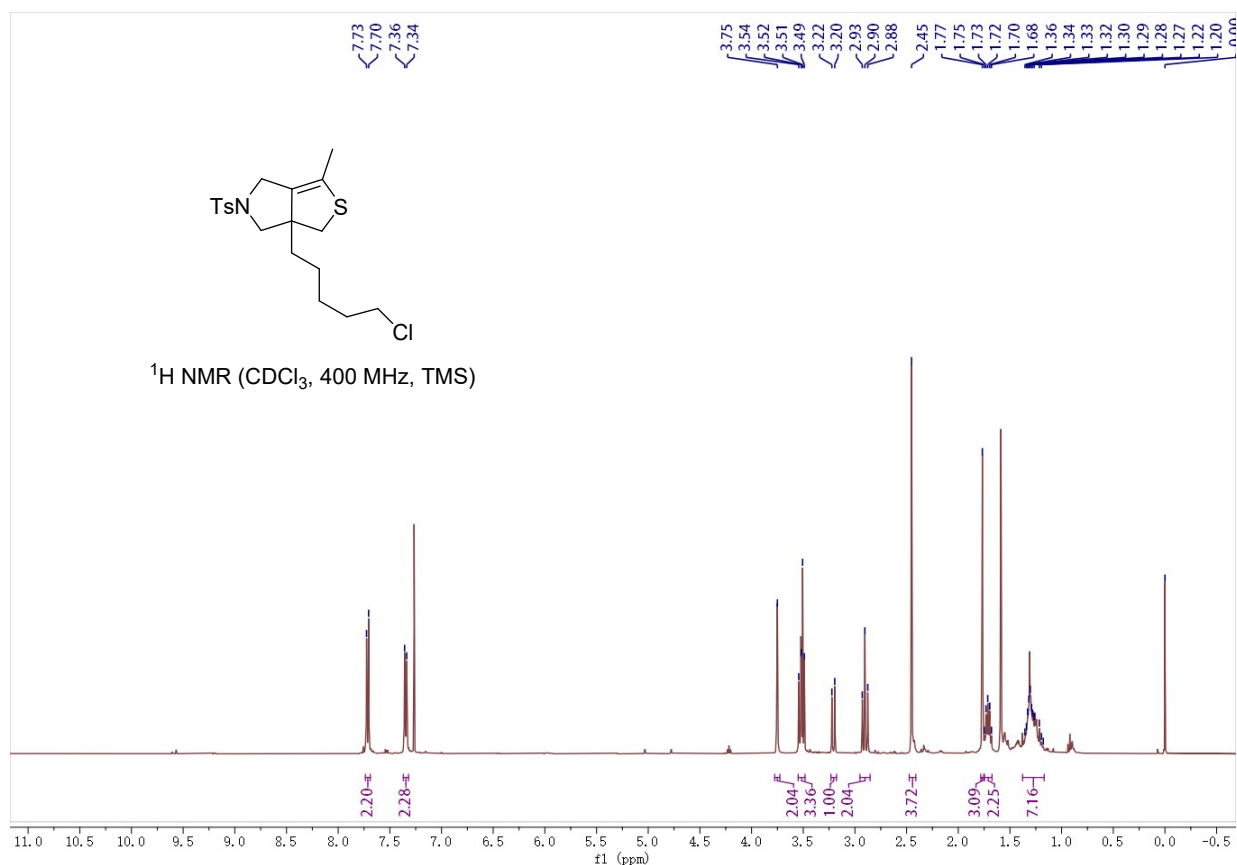


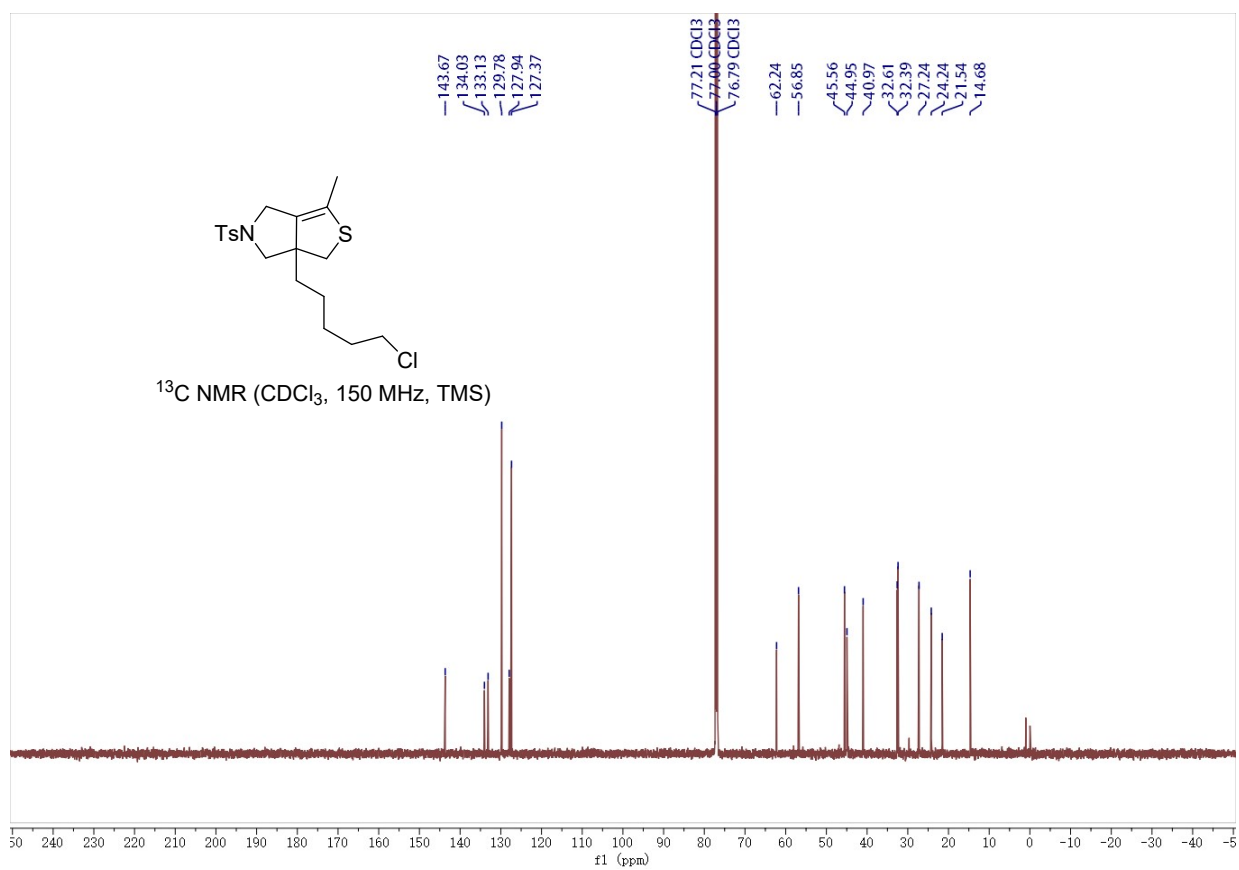


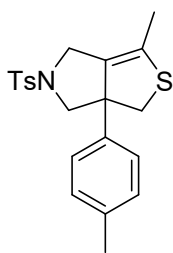


6a-(5-chloropentyl)-3-methyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3m)

A colorless oil, 20.4 mg, 51% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.72 (d, $J = 8.2$ Hz, 2H), 7.35 (d, $J = 8.0$ Hz, 2H), 3.75 (s, 2H), 3.55 – 3.48 (m, 3H), 3.21 (d, $J = 11.1$ Hz, 1H), 2.90 (t, $J = 10.6$ Hz, 2H), 2.45 (s, 3H), 1.77 (s, 3H), 1.75 – 1.67 (m, 2H), 1.38 – 1.17 (m, 6H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 143.7, 134.0, 133.1, 129.8, 127.9, 127.4, 62.2, 56.9, 45.6, 45.0, 41.0, 32.6, 32.4, 27.2, 24.2, 21.5, 14.7. IR (Acetone) ν 900, 1091, 1220, 1358, 1709, 3004 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{19}\text{H}_{27}\text{O}_2\text{NCIS}_2$ (M+H): 400.1166, Found: 400.1162.

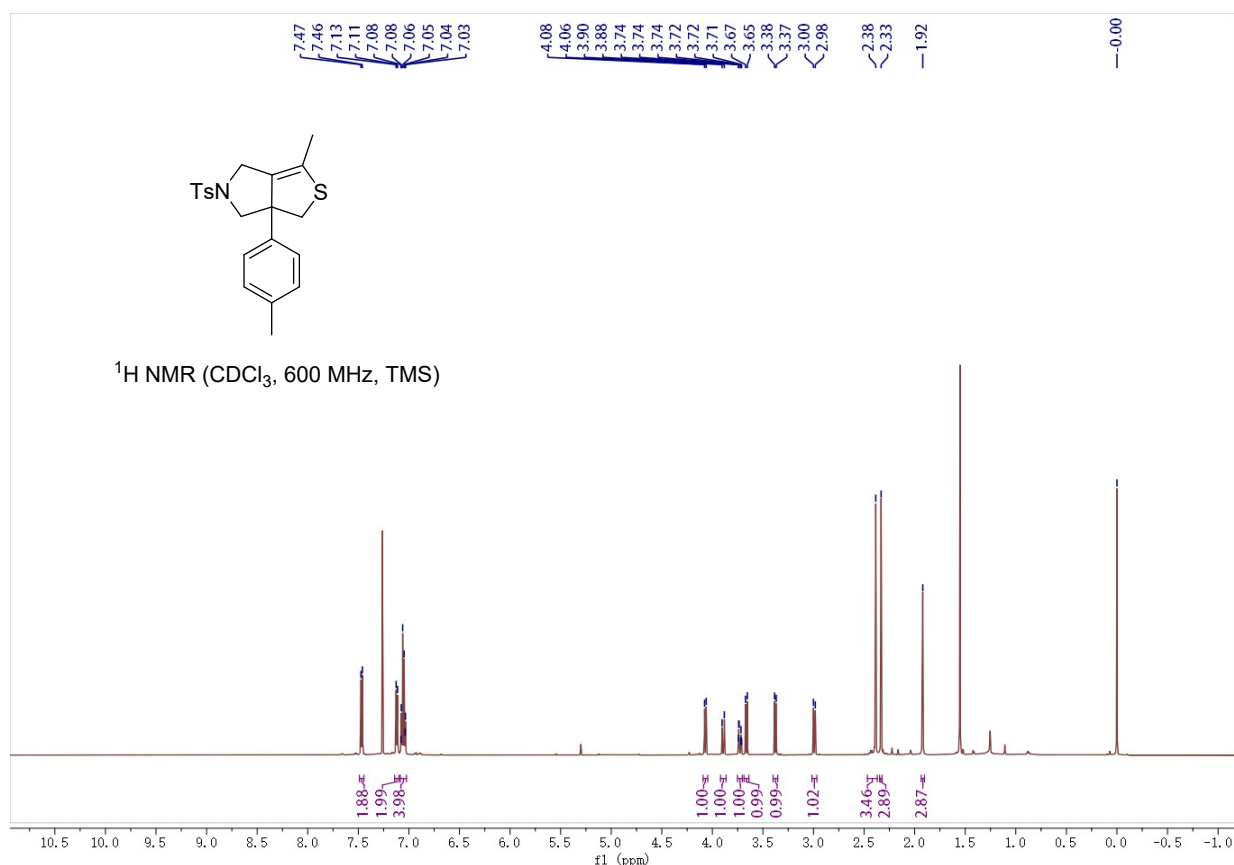


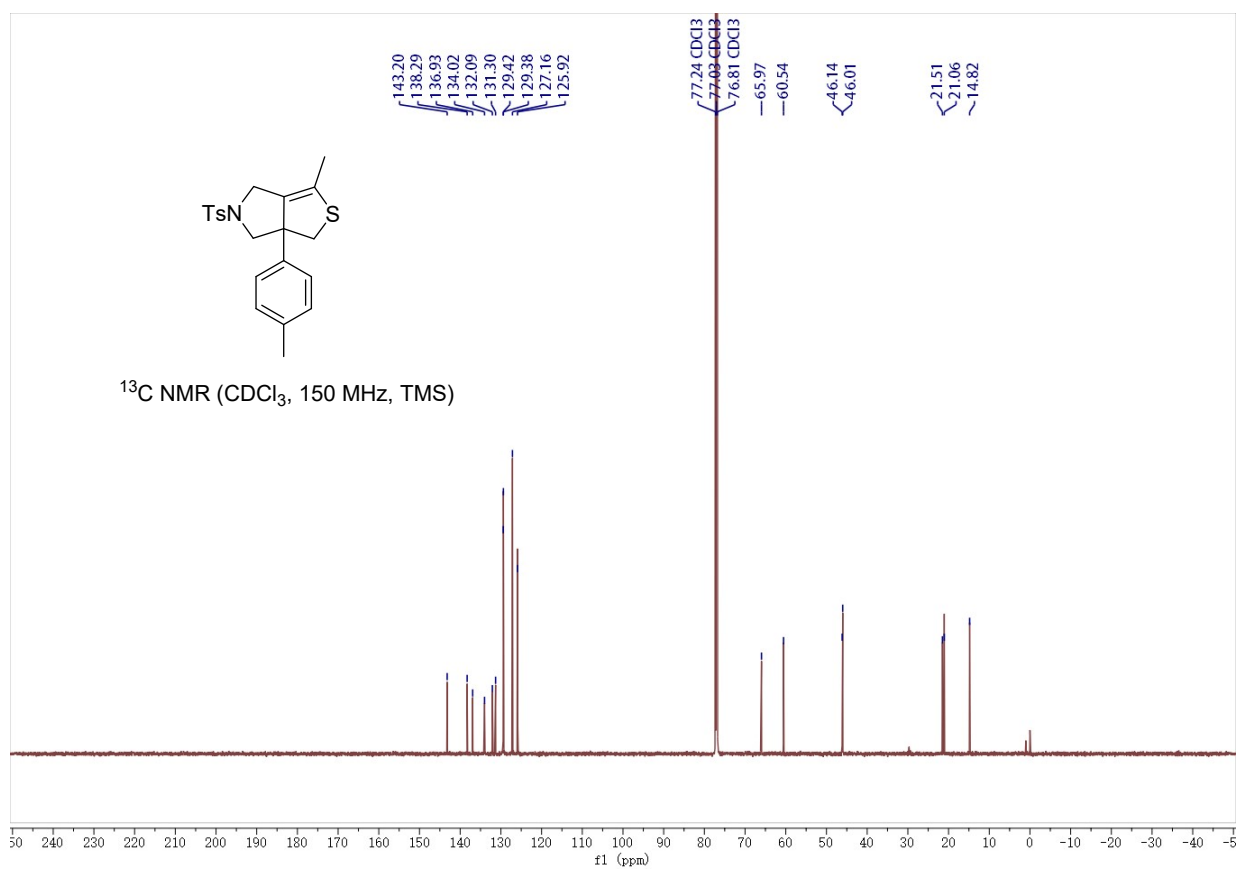


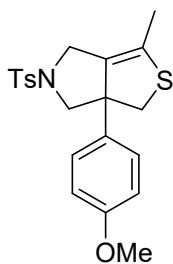


3-methyl-6a-(p-tolyl)-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3n)

A colorless oil, 32.8 mg, 85% yield. ^1H NMR (CDCl_3 , TMS, 600 MHz) δ 7.47 (d, $J = 8.3$ Hz, 2H), 7.12 (d, $J = 8.0$ Hz, 2H), 7.08 – 7.02 (m, 4H), 4.07 (d, $J = 9.6$ Hz, 1H), 3.89 (d, $J = 13.4$ Hz, 1H), 3.75 – 3.70 (m, 1H), 3.66 (d, $J = 11.0$ Hz, 1H), 3.38 (d, $J = 9.6$ Hz, 1H), 2.99 (d, $J = 10.9$ Hz, 1H), 2.38 (s, 3H), 2.33 (s, 3H), 1.92 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 143.2, 138.3, 136.9, 134.0, 132.1, 131.3, 129.42, 129.38, 127.2, 125.9, 66.0, 60.5, 46.1, 46.0, 21.5, 21.1, 14.8. IR (Acetone) ν 659, 841, 1094, 1159, 1346, 1510, 1598, 2914 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{21}\text{H}_{24}\text{O}_2\text{NS}_2$ (M+H): 386.1243, Found: 386.1228.

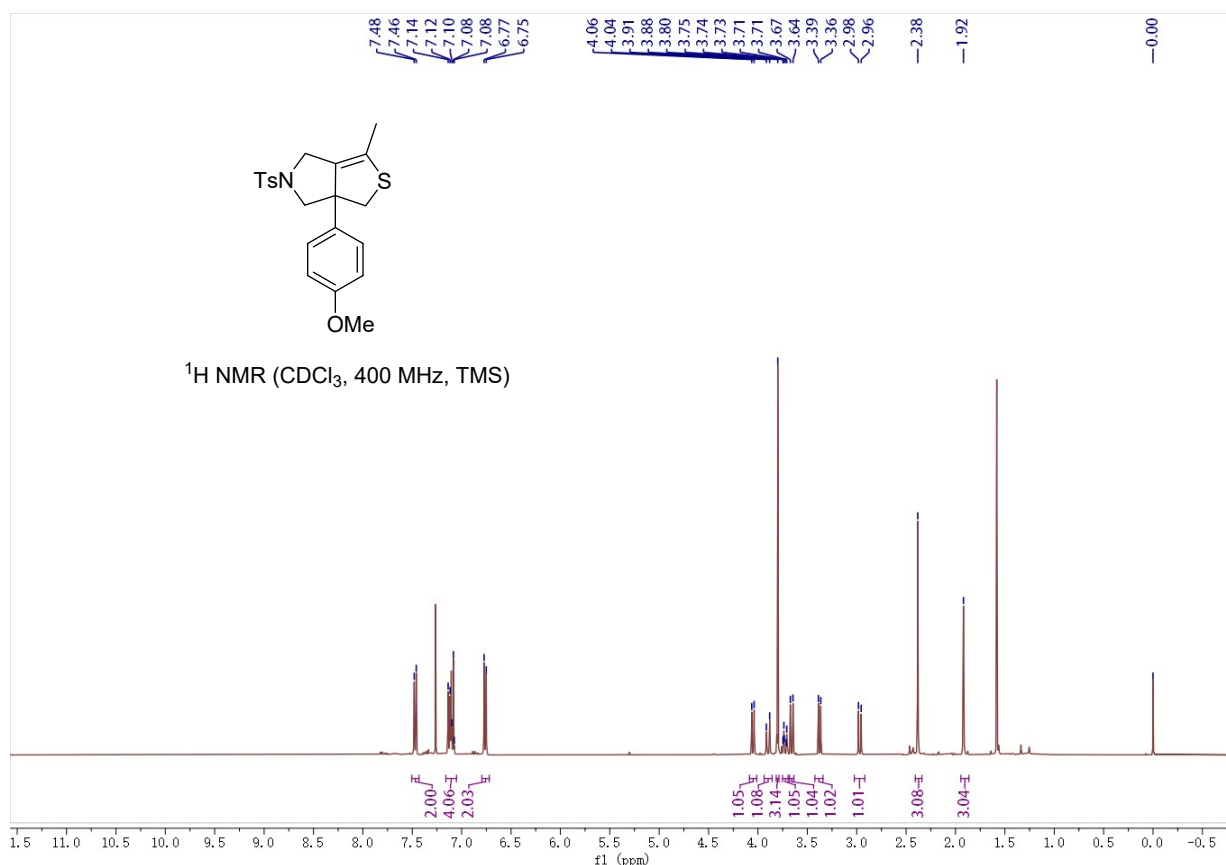


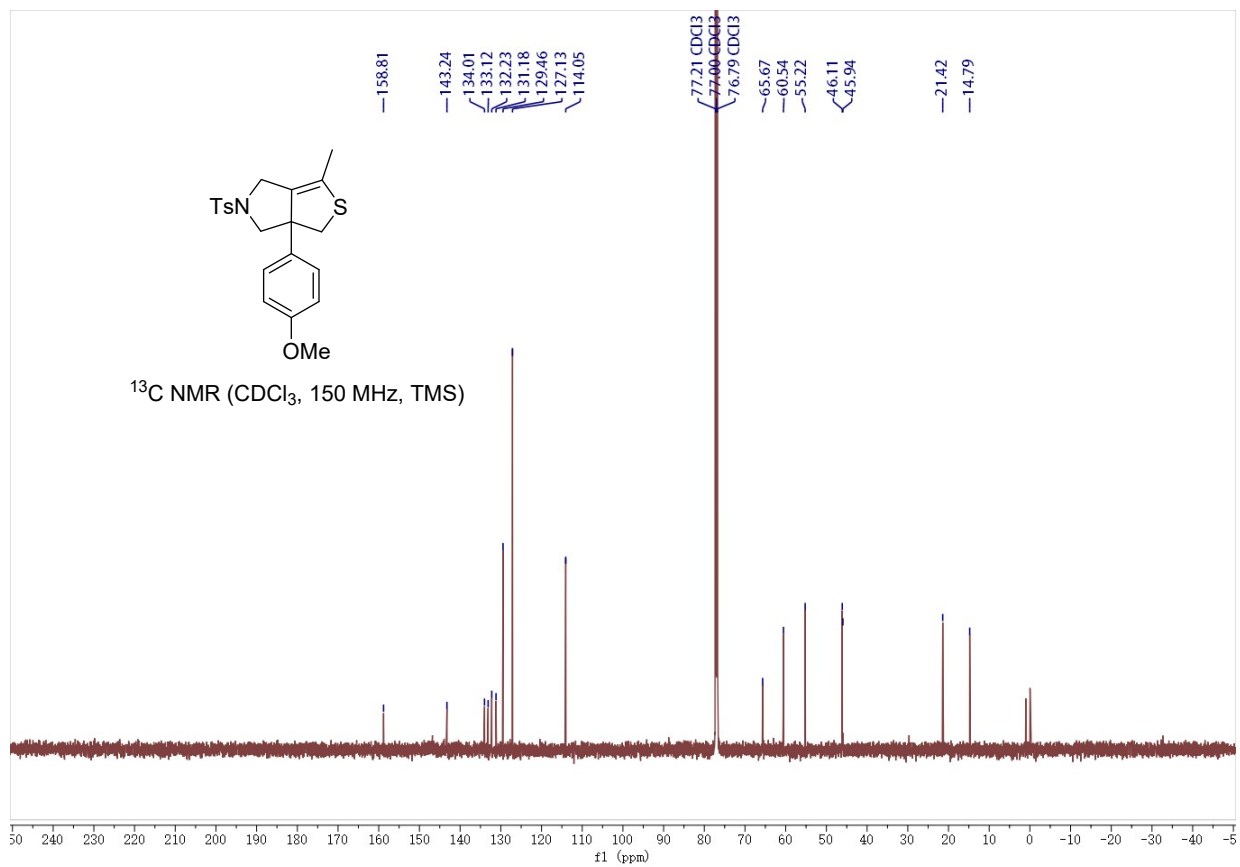


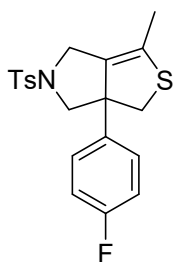


6a-(4-methoxyphenyl)-3-methyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3o)

A colorless oil, 32.5 mg, 82% yield. ^1H NMR (CDCl_3 , TMS, 600 MHz) δ 7.47 (d, $J = 8.2$ Hz, 2H), 7.16 – 7.05 (m, 4H), 6.76 (d, $J = 8.7$ Hz, 2H), 4.05 (d, $J = 9.6$ Hz, 1H), 3.90 (d, $J = 13.3$ Hz, 1H), 3.80 (s, 3H), 3.75 – 3.69 (m, 1H), 3.66 (d, $J = 10.9$ Hz, 1H), 3.38 (d, $J = 9.6$ Hz, 1H), 2.97 (d, $J = 10.8$ Hz, 1H), 2.38 (s, 3H), 1.92 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 158.8, 143.2, 134.0, 133.1, 132.2, 131.2, 129.5, 127.1, 114.1, 65.7, 60.5, 55.2, 46.1, 45.9, 21.4, 14.8. IR (Acetone) ν 890, 1120, 1209, 1533, 1700, 2903 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{21}\text{H}_{23}\text{O}_3\text{NNaS}_2$ ($\text{M}+\text{Na}$): 424.1012, Found: 424.1005.

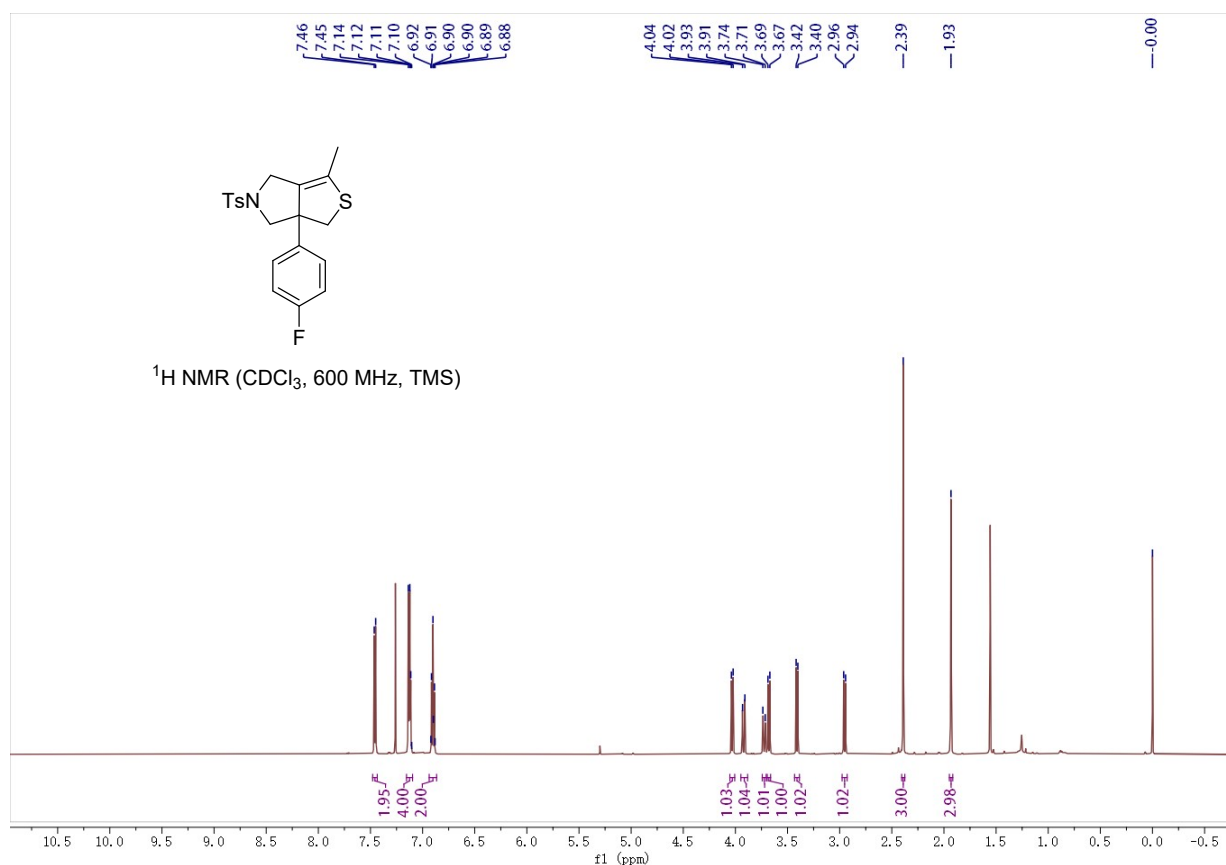


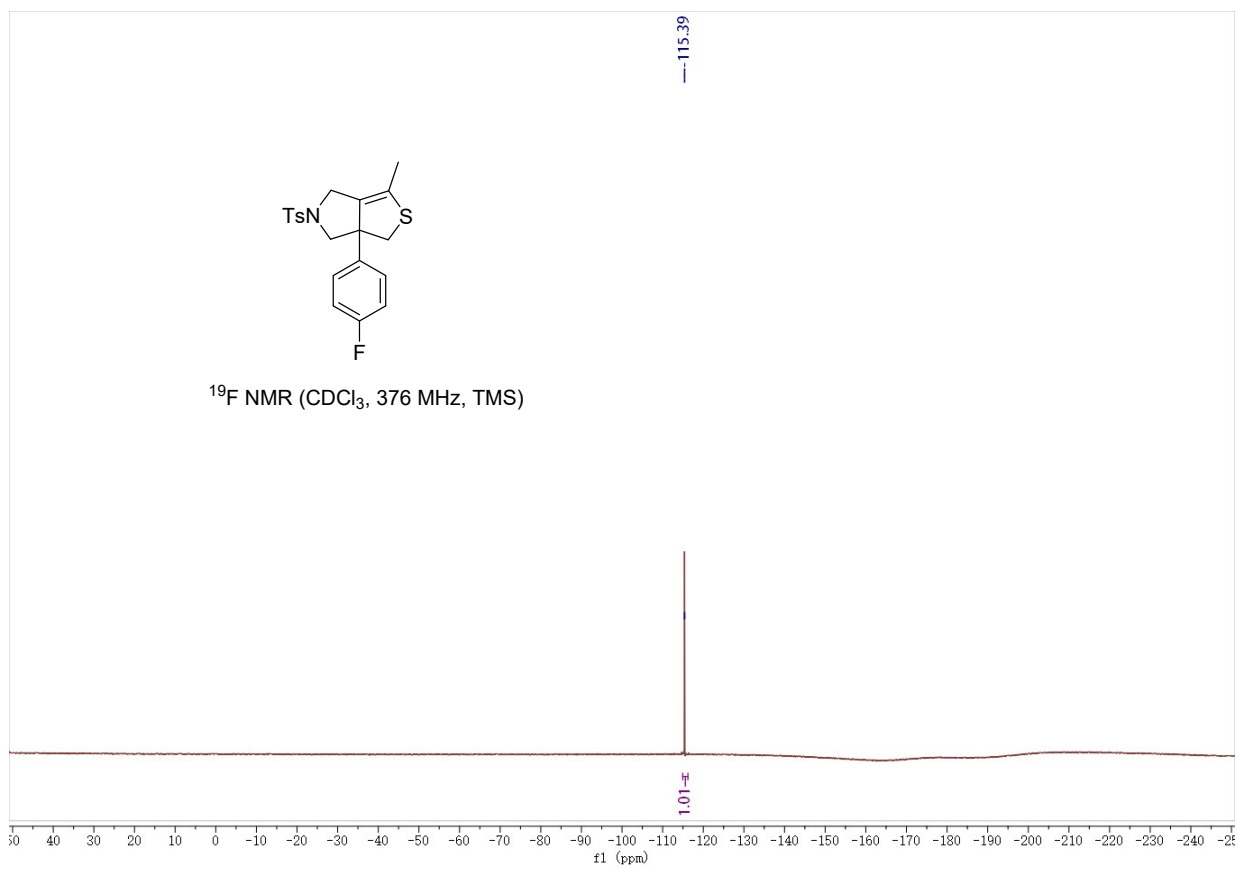
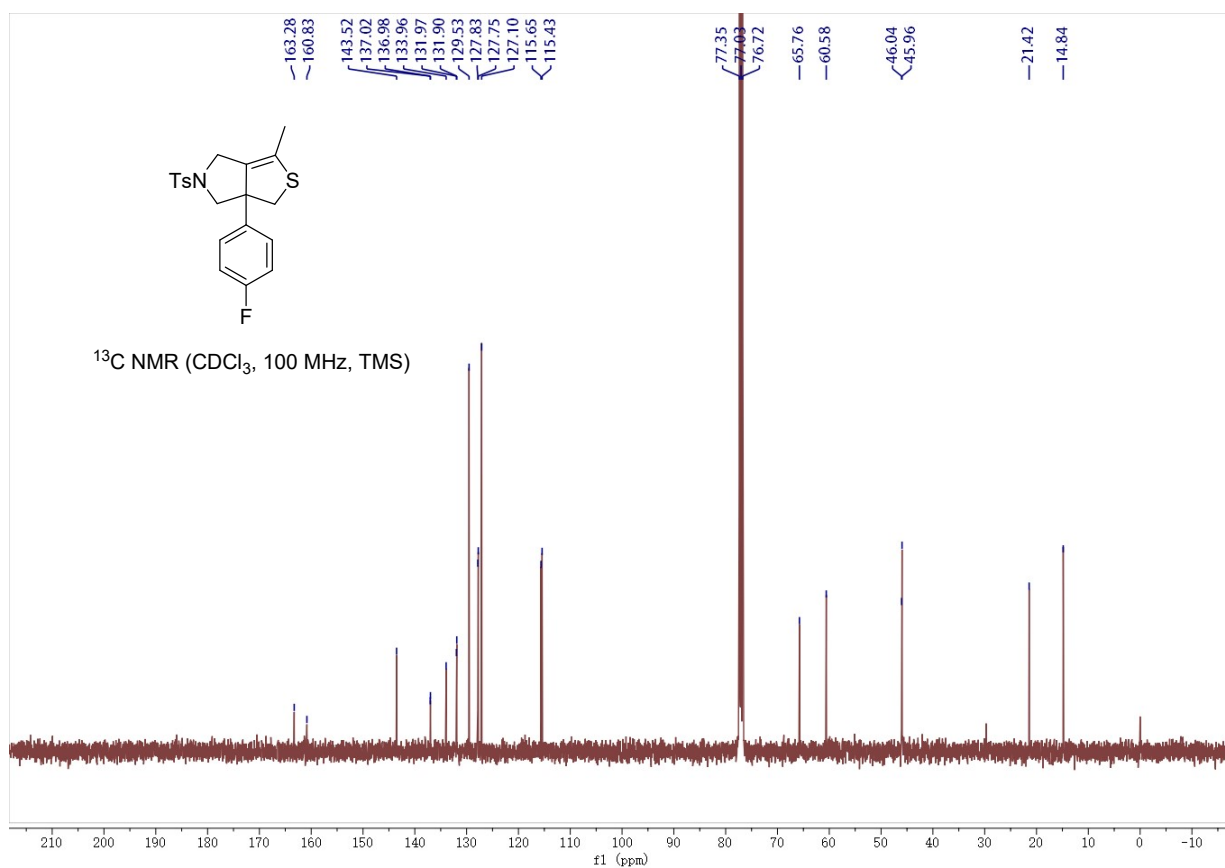


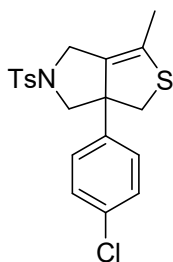


6a-(4-fluorophenyl)-3-methyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3p)

A colorless oil, 30.0 mg, 77% yield. ^1H NMR (CDCl_3 , TMS, 600 MHz) δ 7.46 (d, $J = 8.3$ Hz, 2H), 7.15 – 7.10 (m, 4H), 6.94 – 6.87 (m, 2H), 4.03 (d, $J = 9.9$ Hz, 1H), 3.92 (d, $J = 13.5$ Hz, 1H), 3.73 (d, $J = 13.4$ Hz, 1H), 3.68 (d, $J = 11.0$ Hz, 1H), 3.41 (d, $J = 9.9$ Hz, 1H), 2.95 (d, $J = 10.9$ Hz, 1H), 2.39 (s, 3H), 1.93 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 162.1 (d, $J = 245.0$ Hz), 143.5, 137.0 (d, $J = 4.0$ Hz), 134.0, 131.9 (d, $J = 7.0$ Hz), 129.5, 127.8, 127.7, 127.1, 115.5 (d, $J = 22.0$ Hz), 65.8, 60.6, 46.04, 45.96, 21.4, 14.8. ^{19}F NMR (CDCl_3 , TMS, 376 MHz) δ -115.4 (s). IR (Acetone) ν 611, 803, 1059, 1349, 1528, 2949 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{20}\text{H}_{21}\text{O}_2\text{NFS}_2$ (M+H): 390.0992, Found: 390.0980.

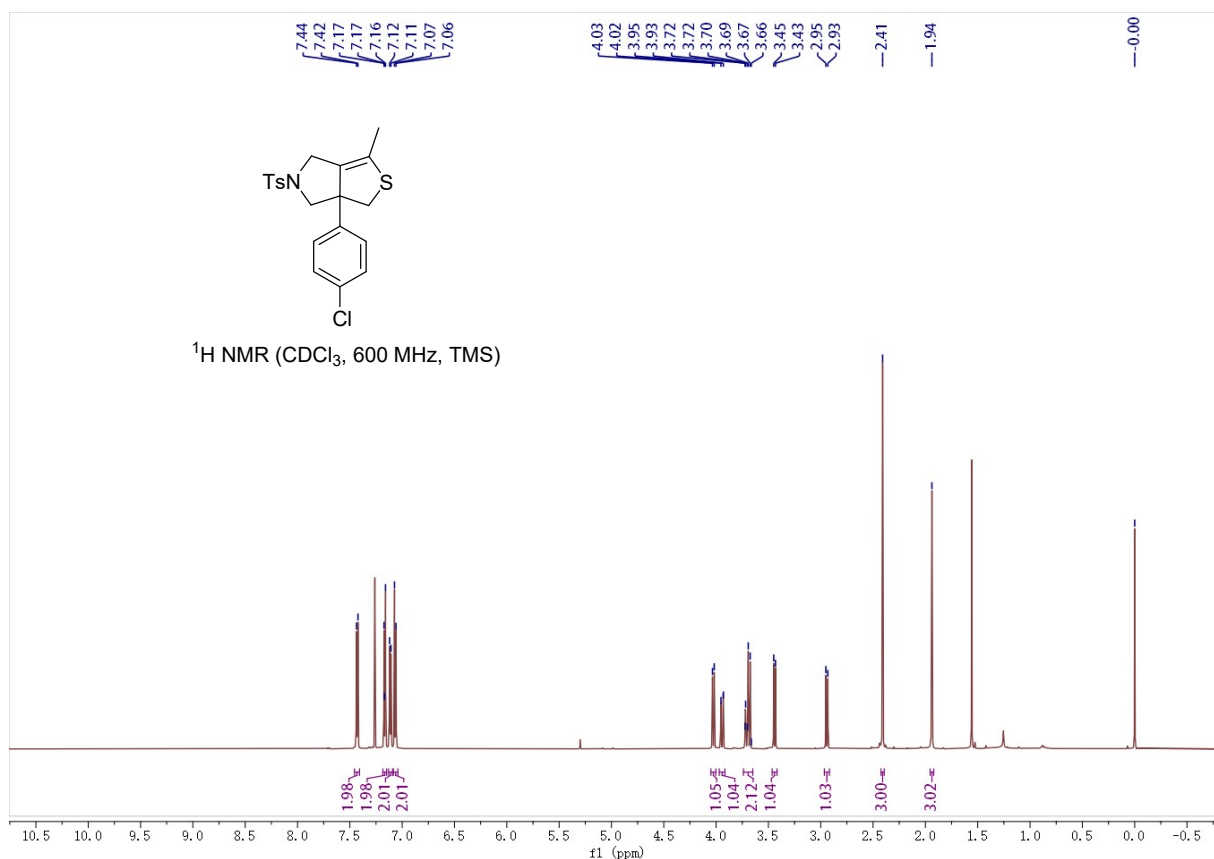


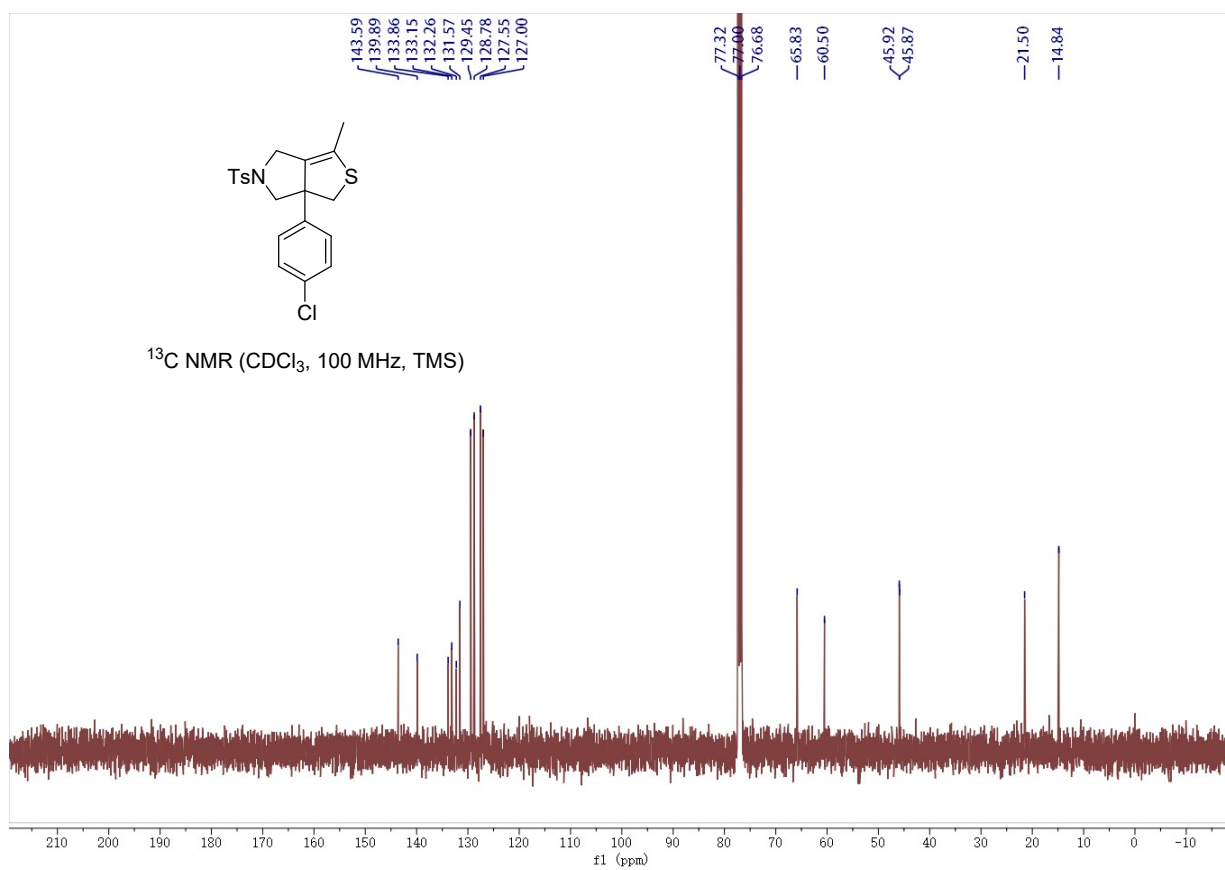


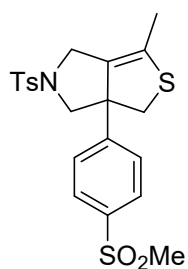


6a-(4-chlorophenyl)-3-methyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3q)

A colorless oil, 35.7 mg, 88% yield. ^1H NMR (CDCl_3 , TMS, 600 MHz) δ 7.43 (d, $J = 8.3$ Hz, 2H), 7.17 (d, $J = 8.5$ Hz, 2H), 7.11 (d, $J = 8.0$ Hz, 2H), 7.07 (d, $J = 8.5$ Hz, 2H), 4.03 (d, $J = 10.1$ Hz, 1H), 3.94 (d, $J = 13.6$ Hz, 1H), 3.74 – 3.65 (m, 2H), 3.44 (d, $J = 10.1$ Hz, 1H), 2.94 (d, $J = 11.0$ Hz, 1H), 2.41 (s, 3H), 1.94 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 143.6, 139.9, 133.9, 133.2, 132.3, 131.6, 129.4, 128.8, 127.6, 127.0, 65.8, 60.5, 45.92, 45.87, 21.5, 14.8. IR (Acetone) ν 863, 1125, 1396, 1600, 2908 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{20}\text{H}_{21}\text{O}_2\text{NCIS}_2$ (M+H): 406.0697, Found: 406.0684.

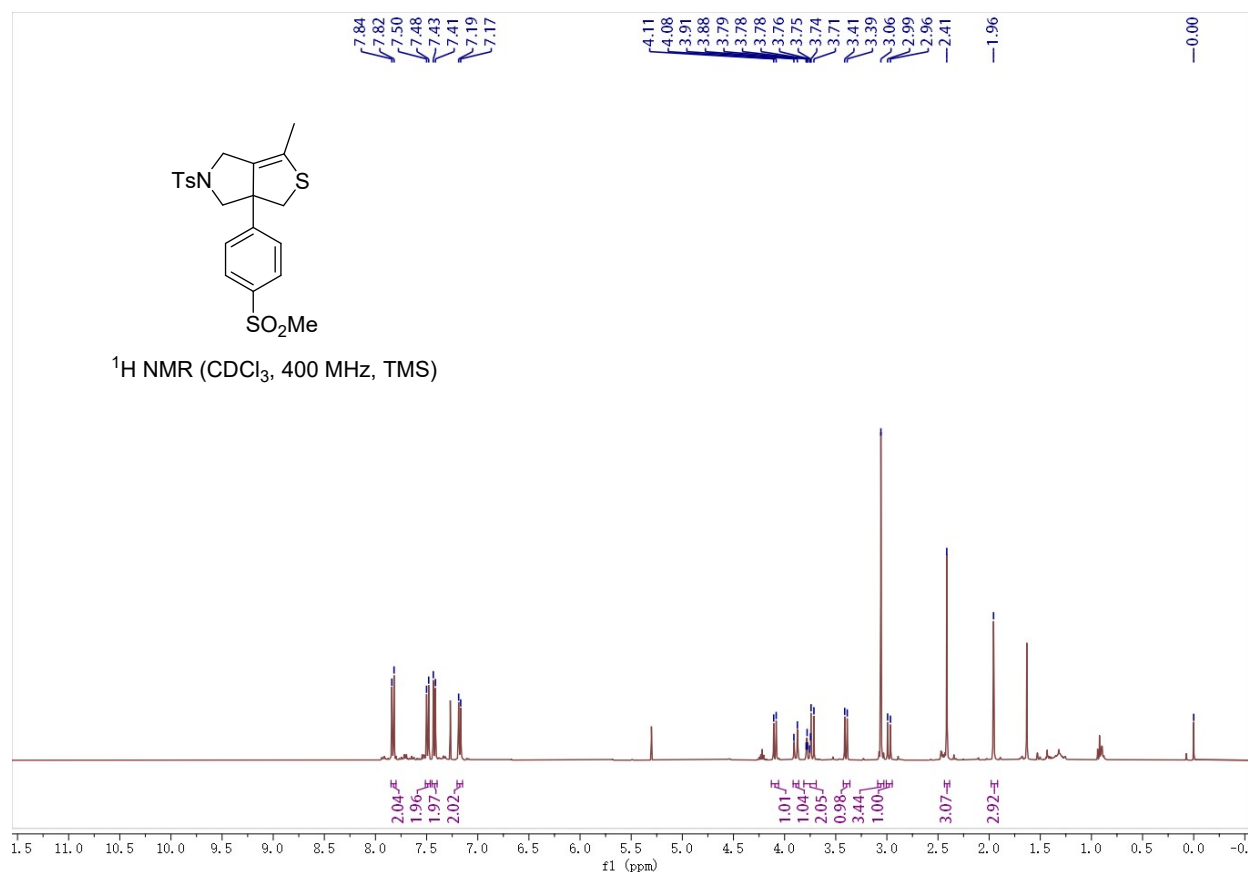


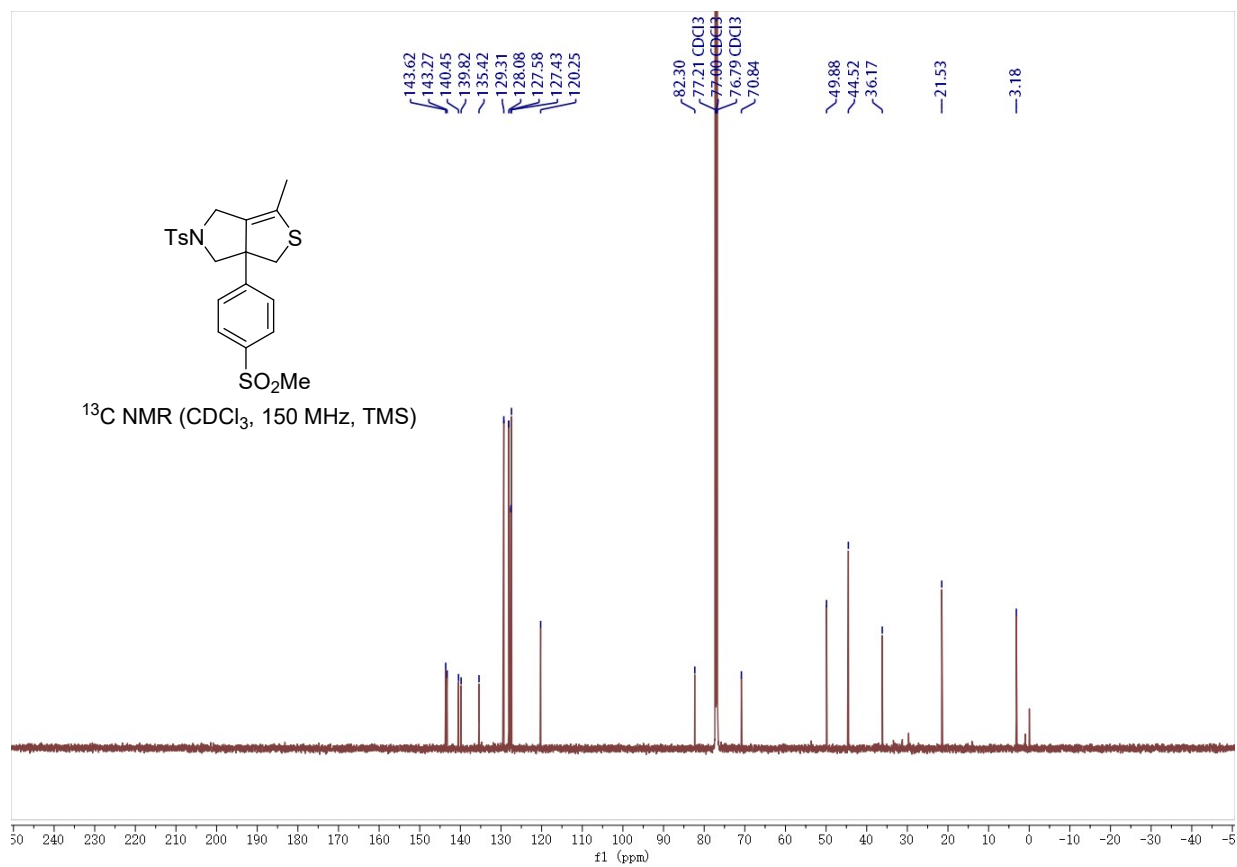


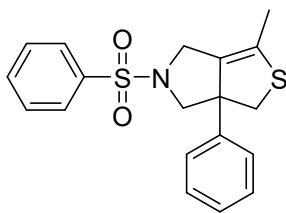


3-methyl-6a-(4-(methylsulfonyl)phenyl)-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3r)

A colorless oil, 36.0 mg, 80% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.83 (d, $J = 8.5$ Hz, 2H), 7.49 (d, $J = 8.3$ Hz, 2H), 7.42 (d, $J = 8.5$ Hz, 2H), 7.18 (d, $J = 7.9$ Hz, 2H), 4.09 (d, $J = 9.8$ Hz, 1H), 3.89 (d, $J = 13.6$ Hz, 1H), 3.81 – 3.69 (m, 2H), 3.40 (d, $J = 9.9$ Hz, 1H), 3.06 (s, 3H), 2.98 (d, $J = 11.2$ Hz, 1H), 2.41 (s, 3H), 1.96 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 143.6, 143.3, 140.5, 139.8, 135.4, 129.3, 128.1, 127.6, 127.4, 120.3, 82.3, 70.8, 49.9, 44.5, 36.2, 21.5, 3.2. IR (Acetone) ν 1012, 1125, 1319, 1400, 1608, 2933 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{21}\text{H}_{24}\text{NO}_4\text{S}_3$ (M+H): 450.0867, Found: 450.0909.

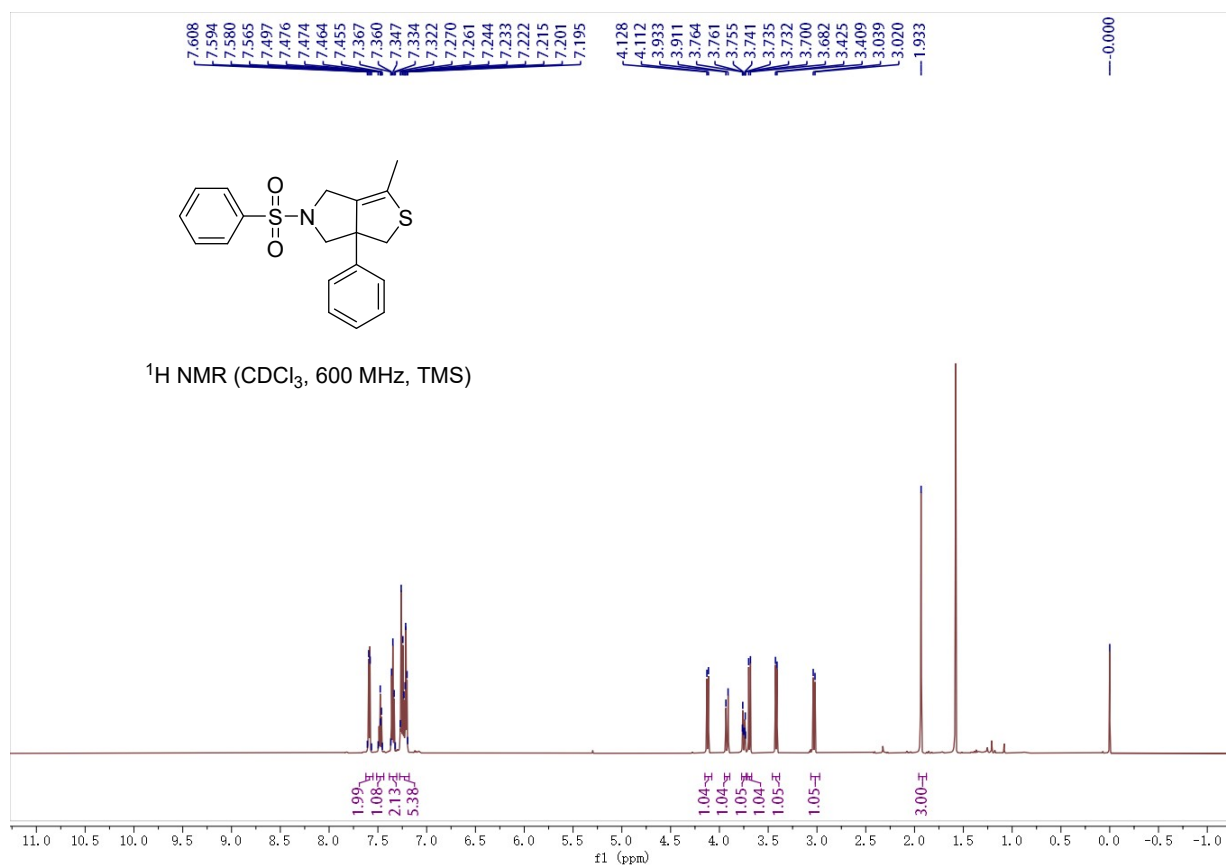


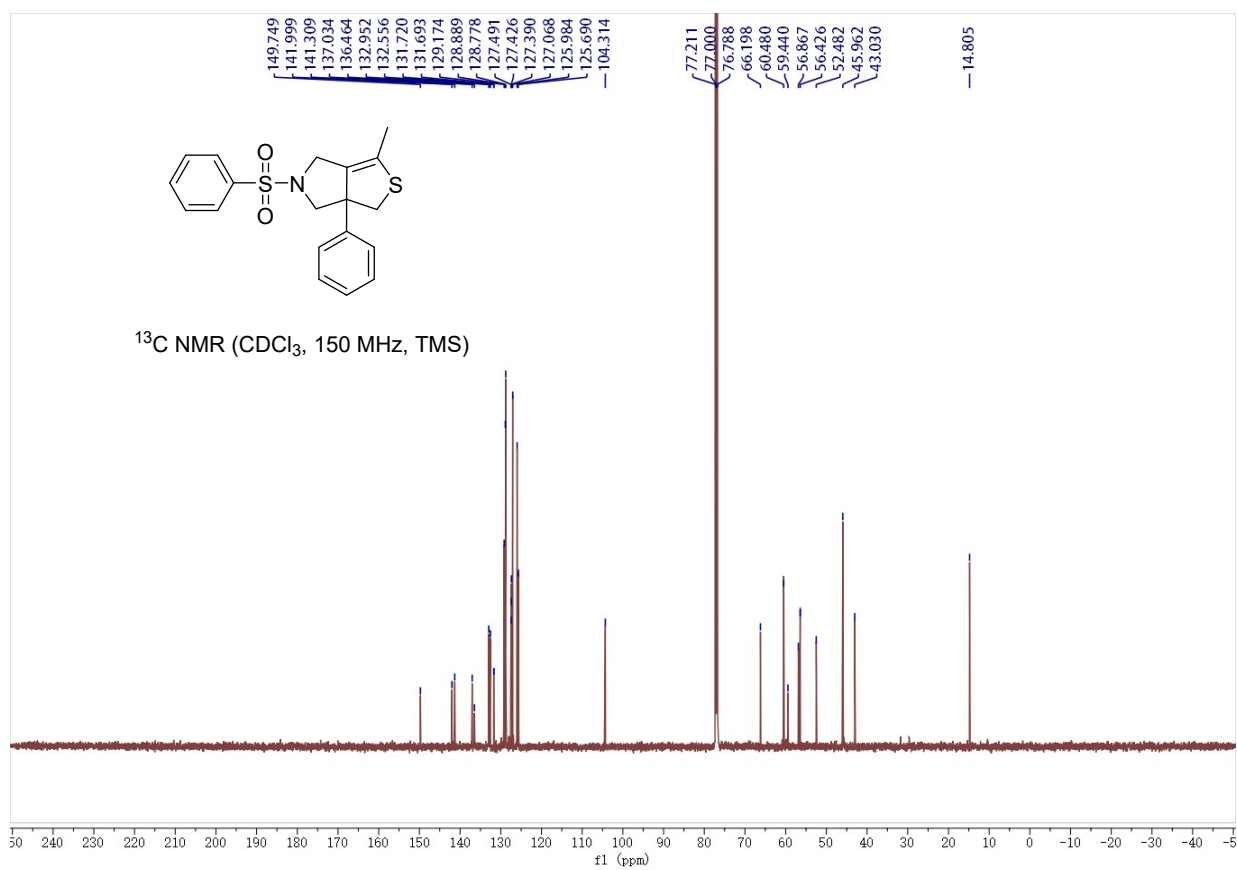


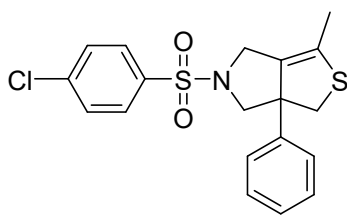


3-methyl-6a-phenyl-5-(phenylsulfonyl)-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3s)

A colorless oil, 30.0 mg, 84% yield. ^1H NMR (CDCl_3 , TMS, 600 MHz) δ 7.62 – 7.55 (m, 2H), 7.51 – 7.44 (m, 1H), 7.38 – 7.31 (m, 2H), 7.28 – 7.18 (m, 5H), 4.12 (d, $J = 9.6$ Hz, 1H), 3.92 (d, $J = 13.2$ Hz, 1H), 3.77 – 3.73 (m, 1H), 3.69 (d, $J = 11.0$ Hz, 1H), 3.42 (d, $J = 9.6$ Hz, 1H), 3.03 (d, $J = 11.0$ Hz, 1H), 1.93 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 149.7, 142.0, 141.3, 137.0, 136.5, 133.0, 132.6, 131.72, 131.69, 129.2, 128.9, 128.8, 127.5, 127.42, 127.39, 127.1, 126.0, 125.7, 104.3, 66.2, 60.5, 59.4, 56.9, 56.4, 52.5, 46.0, 43.0, 14.8. IR (Acetone) ν 719, 1042, 1129, 1301, 2980 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{19}\text{H}_{19}\text{O}_2\text{NNaS}$ ($\text{M}+\text{Na}$): 380.0749, Found: 380.0742.

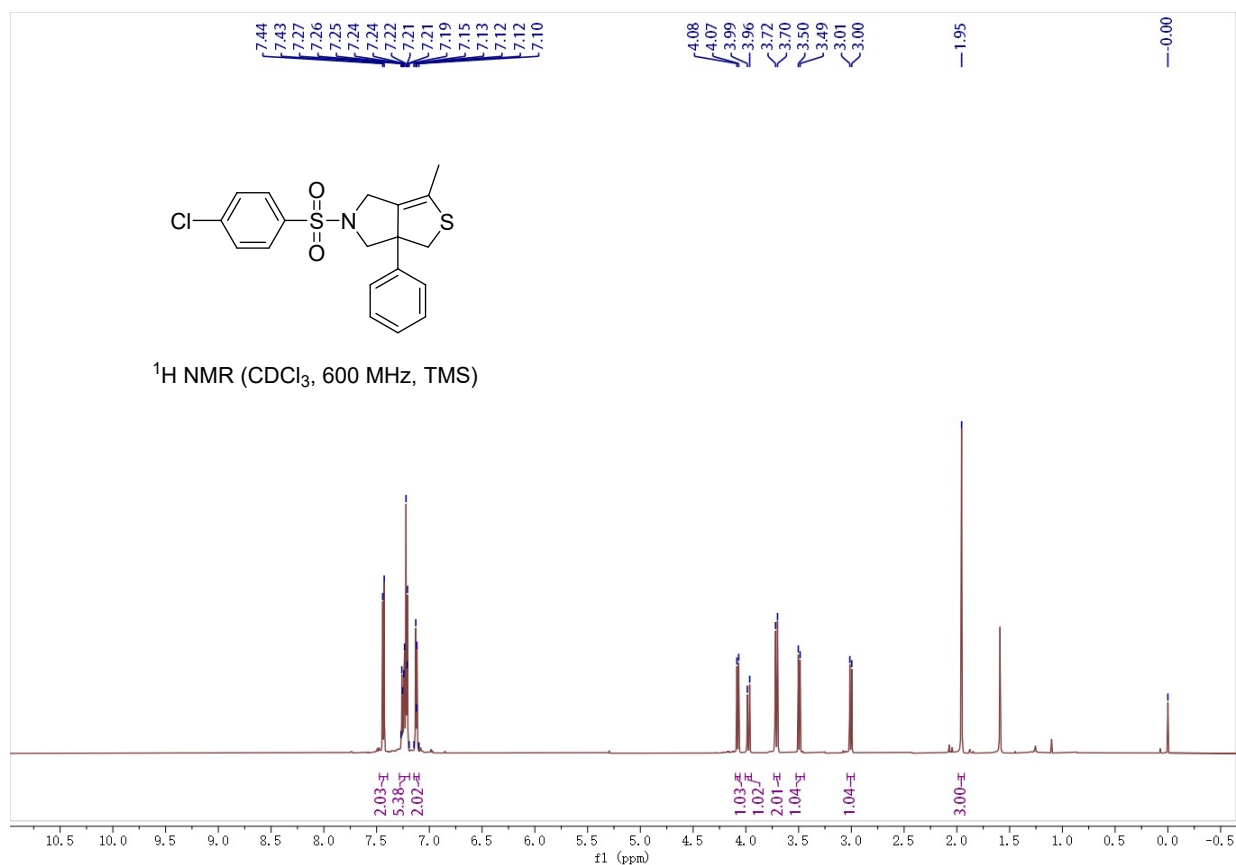


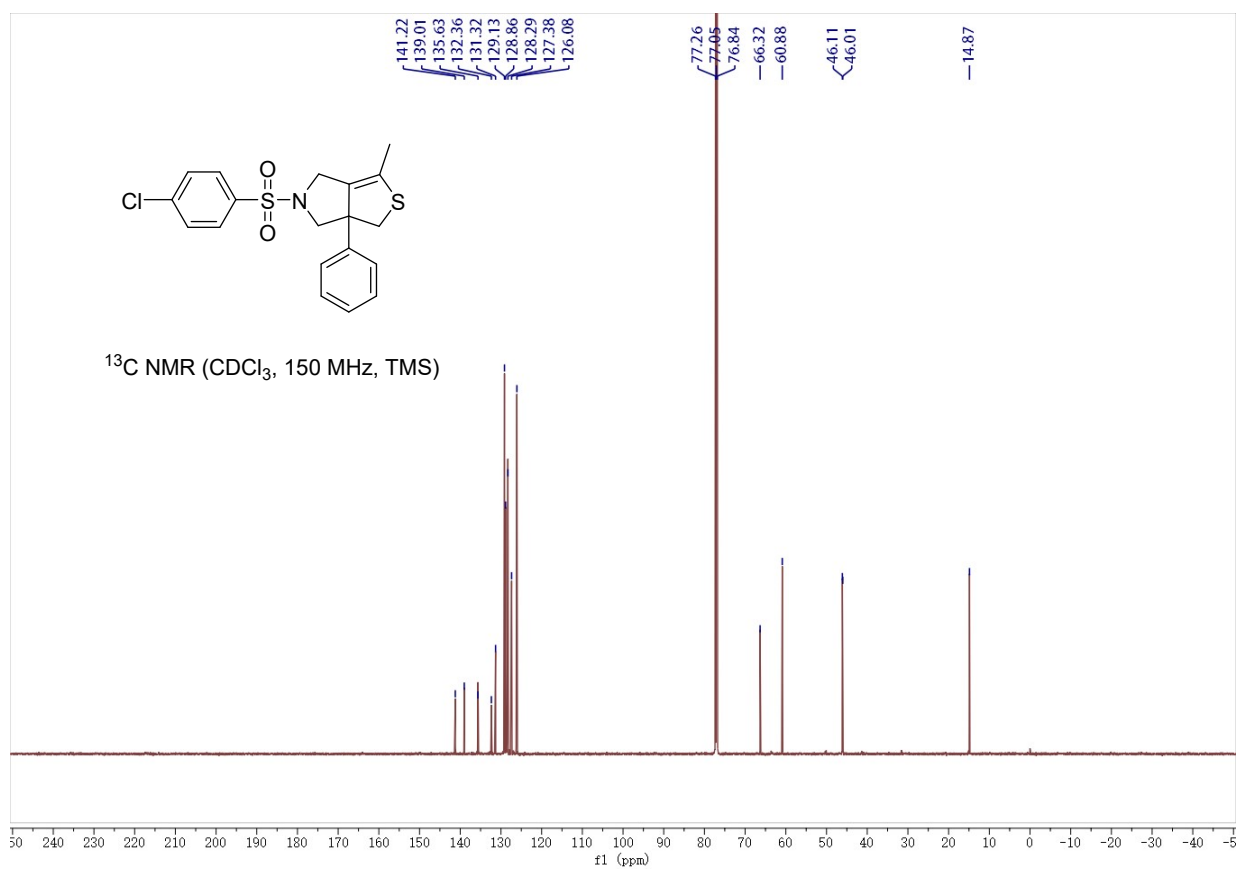


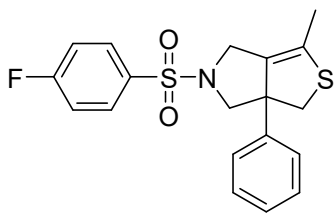


5-((4-chlorophenyl)sulfonyl)-3-methyl-6a-phenyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3t)

A colorless oil, 31.4 mg, 80% yield. ^1H NMR (CDCl_3 , TMS, 600 MHz) δ 7.44 (d, $J = 8.5$ Hz, 2H), 7.28 – 7.19 (m, 5H), 7.12 (d, $J = 6.6$ Hz, 2H), 4.08 (d, $J = 10.0$ Hz, 1H), 3.97 (d, $J = 13.3$ Hz, 1H), 3.71 (d, $J = 11.2$ Hz, 2H), 3.49 (d, $J = 10.0$ Hz, 1H), 3.01 (d, $J = 11.0$ Hz, 1H), 1.95 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 141.2, 139.0, 135.6, 132.4, 131.3, 129.1, 128.9, 128.3, 127.4, 126.1, 66.3, 60.9, 46.1, 46.0, 14.9. IR (Acetone) ν 685, 1078, 1371, 2944 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{19}\text{H}_{19}\text{O}_2\text{NCIS}_2$ ($\text{M}+\text{H}$): 392.0540, Found: 392.0534.

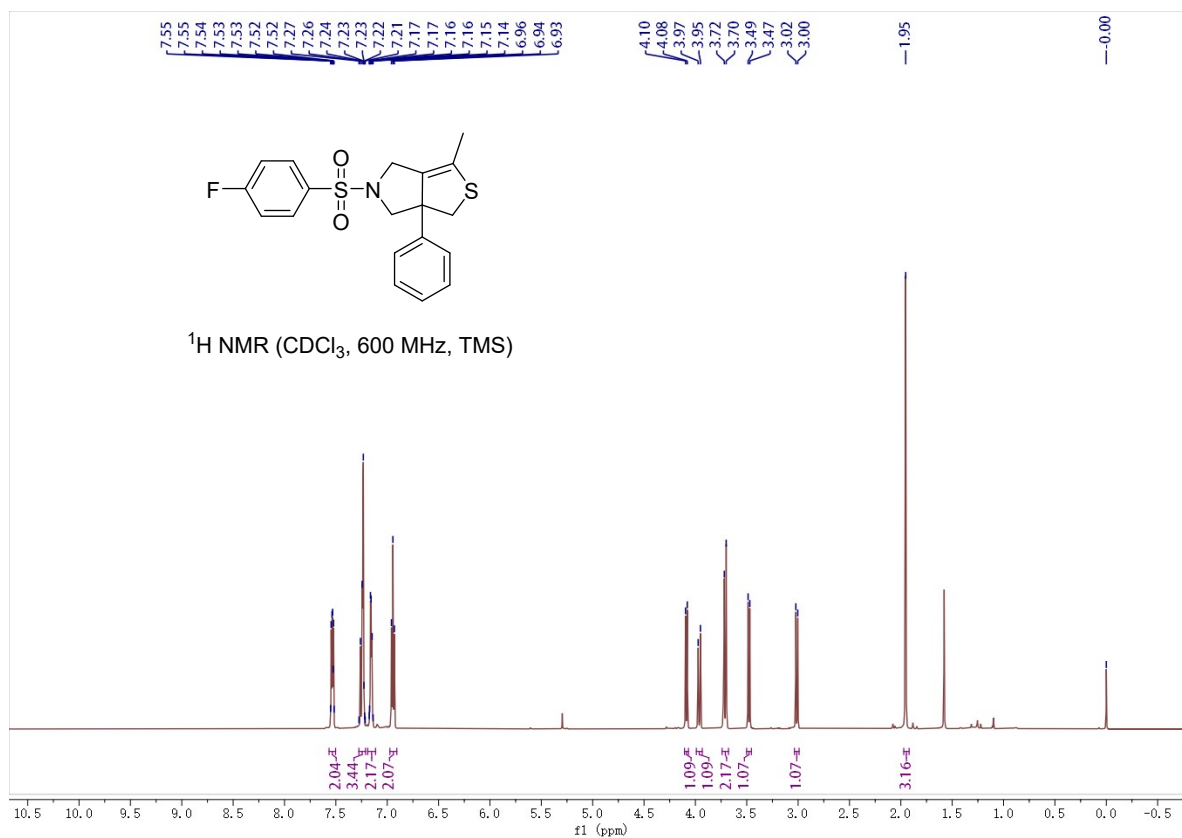


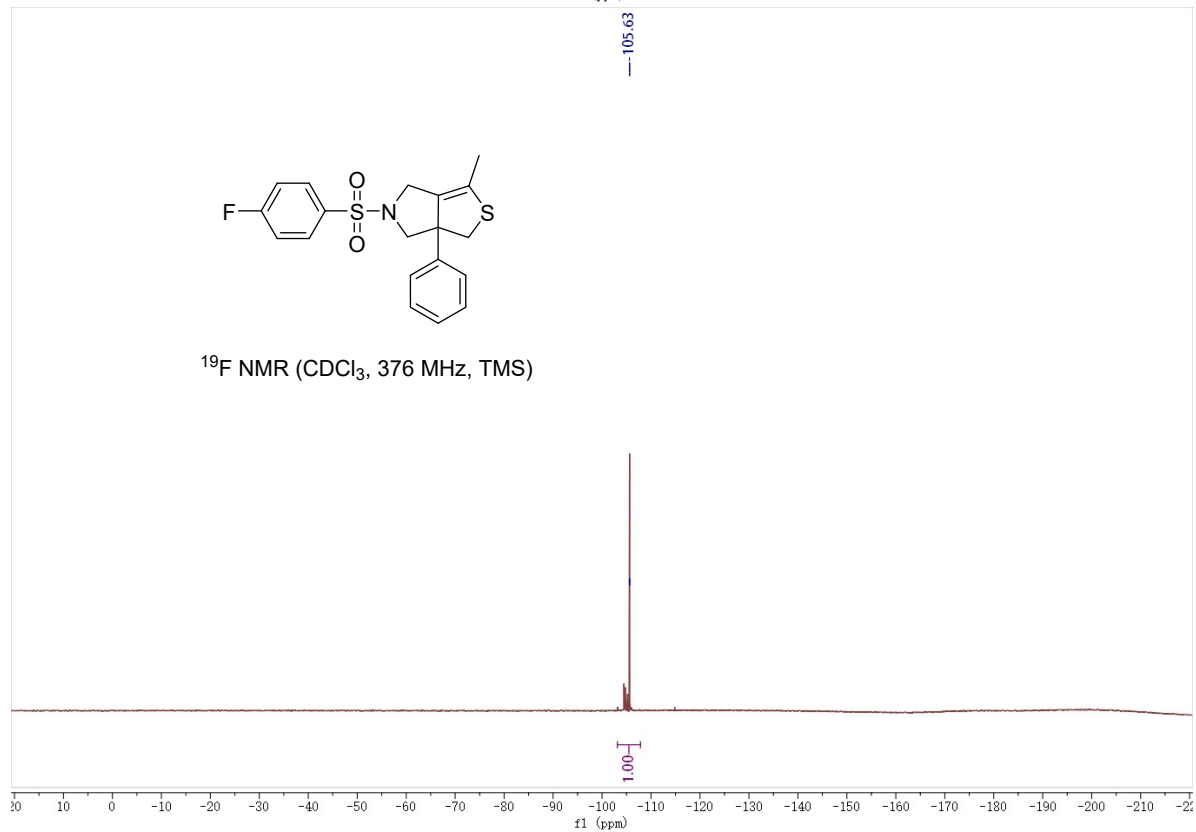
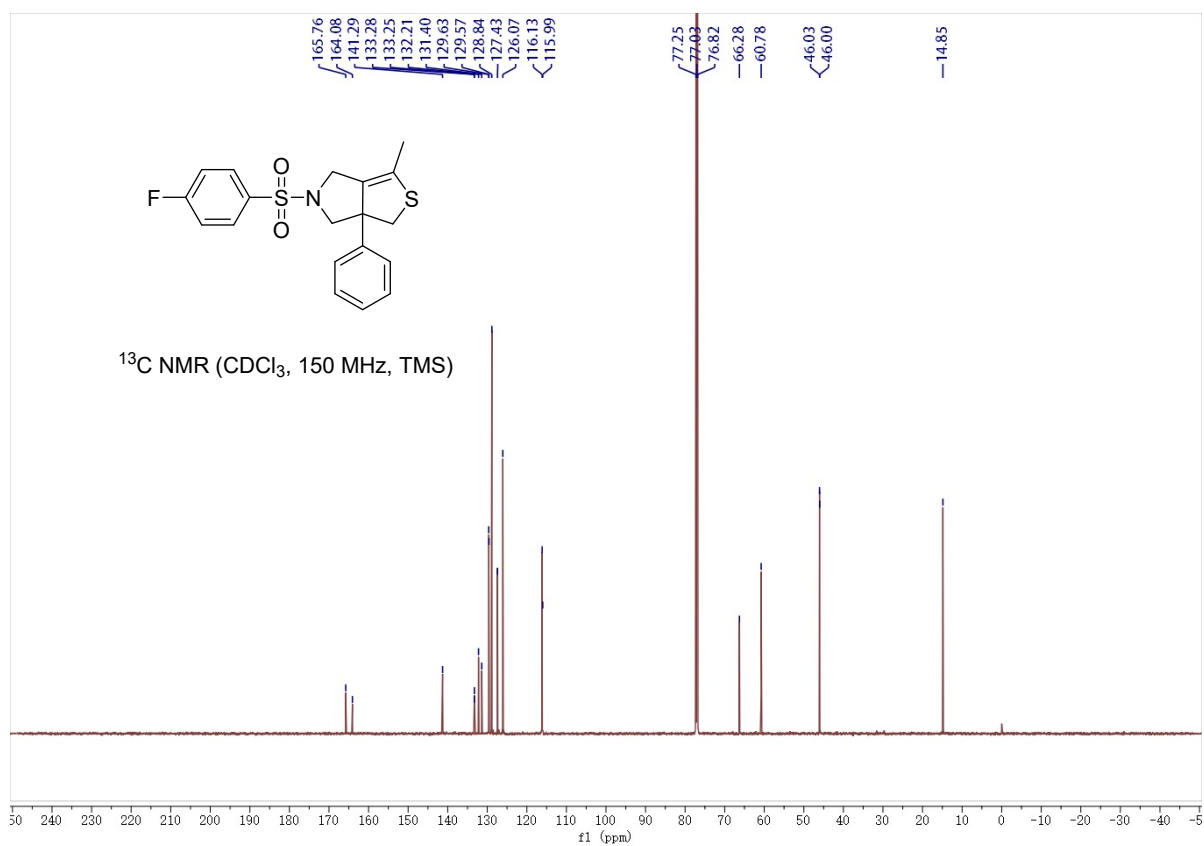


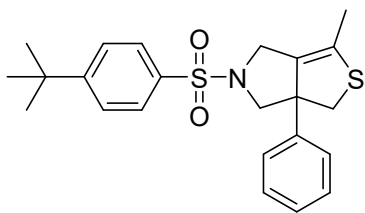


5-ethyl-3a-(4-methoxyphenyl)-6a-phenyl-6-(phenylthio)-2-tosyl-1,2,3,3a,4,6a-hexahydrocyclopenta[c]pyrrole (3u)

A colorless oil, 29.3 mg, 78% yield. ^1H NMR (CDCl_3 , TMS, 600 MHz) δ 7.57 – 7.50 (m, 2H), 7.28 – 7.21 (m, 3H), 7.19 – 7.11 (m, 2H), 6.94 (t, $J = 8.5$ Hz, 2H), 4.09 (d, $J = 9.9$ Hz, 1H), 3.96 (d, $J = 13.3$ Hz, 1H), 3.71 (d, $J = 10.9$ Hz, 2H), 3.48 (d, $J = 9.9$ Hz, 1H), 3.01 (d, $J = 11.0$ Hz, 1H), 1.95 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 164.9 (d, $J = 252.0$ Hz), 141.3, 133.3 (d, $J = 4.5$ Hz), 132.2, 131.4, 129.6 (d, $J = 9.0$ Hz), 128.8, 127.4, 126.1, 116.1 (d, $J = 21.0$ Hz), 116.0, 66.3, 60.8, 46.03, 46.00, 14.8. ^{19}F NMR (CDCl_3 , TMS, 376 MHz) δ -105.6 (s). IR (Acetone) ν 752, 1218, 1531, 3009 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{19}\text{H}_{19}\text{O}_2\text{NFS}_2$ (M+H): 376.0836, Found: 376.0826.

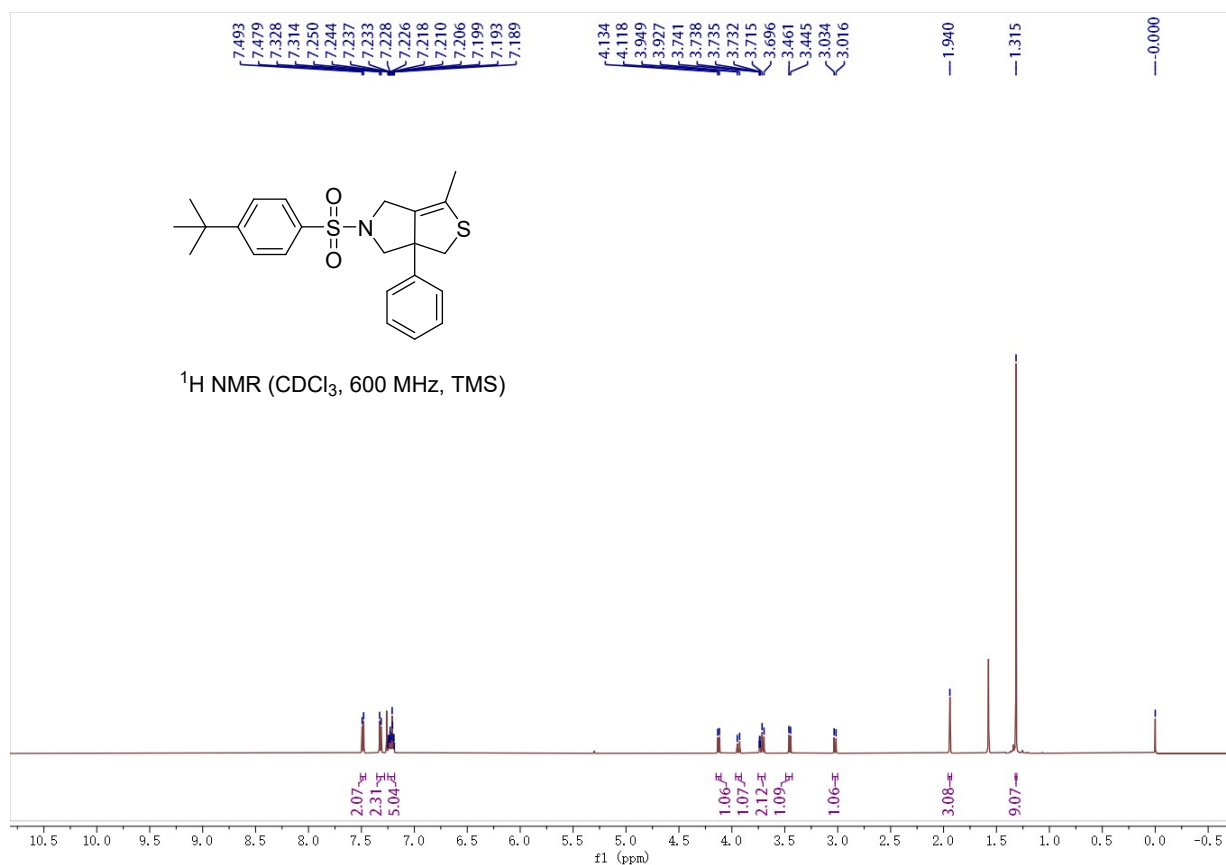


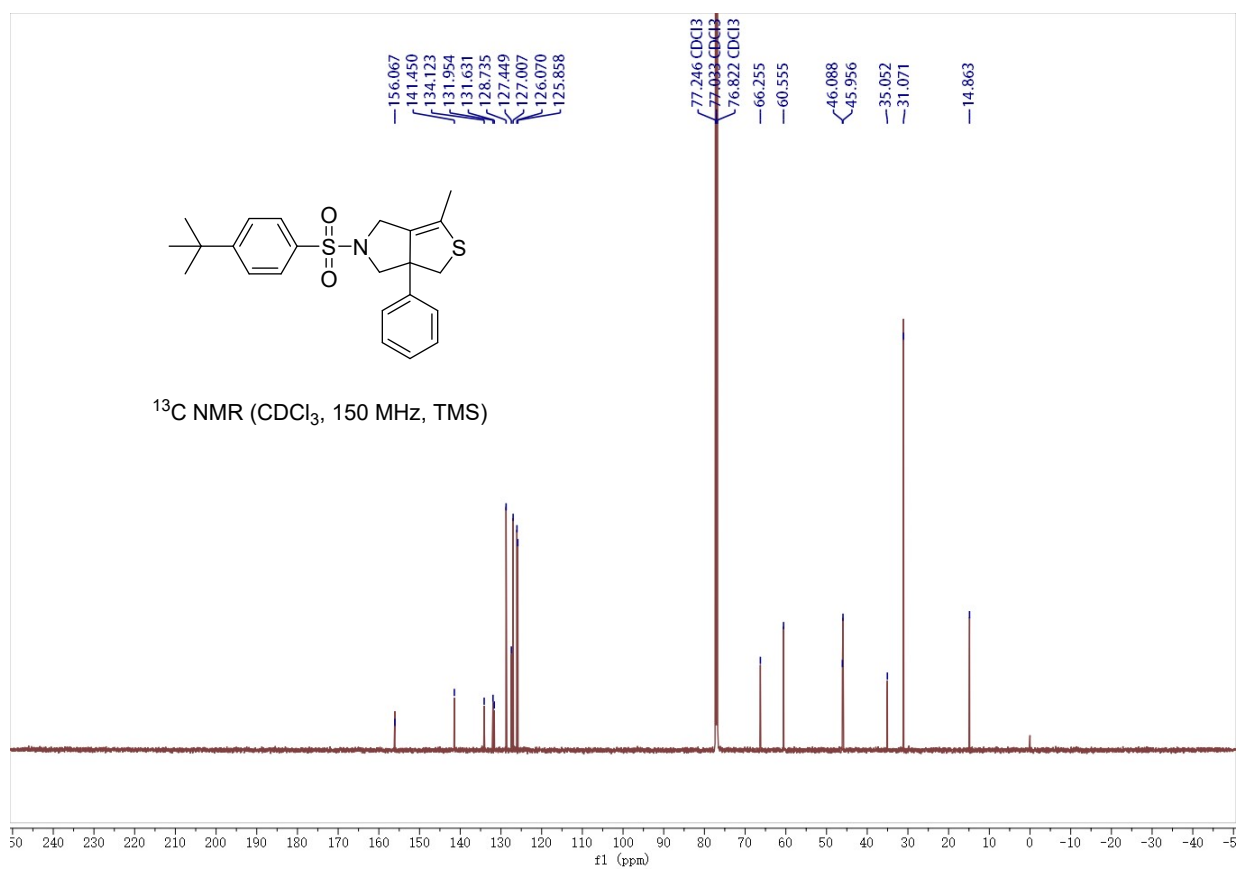


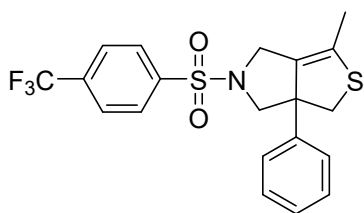


5-((4-(*tert*-butyl)phenyl)sulfonyl)-3-methyl-6a-phenyl-4,5,6,6a-tetrahydro-1*H*-thieno[3,4-*c*]pyrrole (3v)

A colorless oil, 25.6 mg, 62% yield. ^1H NMR (CDCl_3 , TMS, 600 MHz) δ 7.49 (d, $J = 8.5$ Hz, 2H), 7.32 (d, $J = 8.5$ Hz, 2H), 7.25 – 7.19 (m, 5H), 4.13 (d, $J = 9.7$ Hz, 1H), 3.94 (d, $J = 13.3$ Hz, 1H), 3.75 – 3.69 (m, 2H), 3.45 (d, $J = 9.8$ Hz, 1H), 3.02 (d, $J = 11.0$ Hz, 1H), 1.94 (s, 3H), 1.32 (s, 9H). ^{13}C NMR CDCl_3 , TMS, 150 MHz) δ 156.1, 141.5, 134.1, 132.0, 131.6, 128.7, 127.4, 127.0, 126.1, 125.9, 66.3, 60.6, 46.1, 46.0, 35.1, 31.1, 14.9. IR (Acetone) ν 1005, 1248, 1339, 1559, 2993 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{24}\text{H}_{26}\text{O}_4\text{NS}_2$ (M+H): 456.1298, Found: 456.1285.

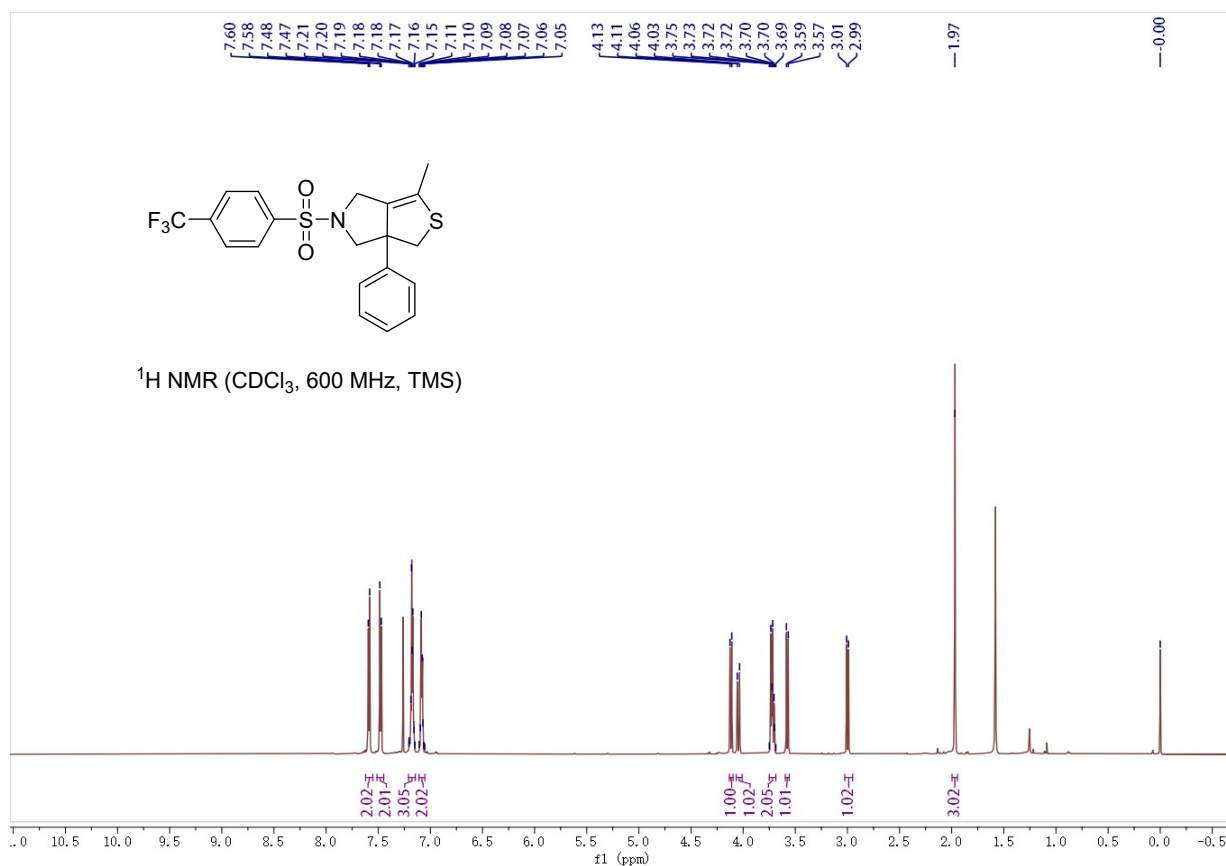


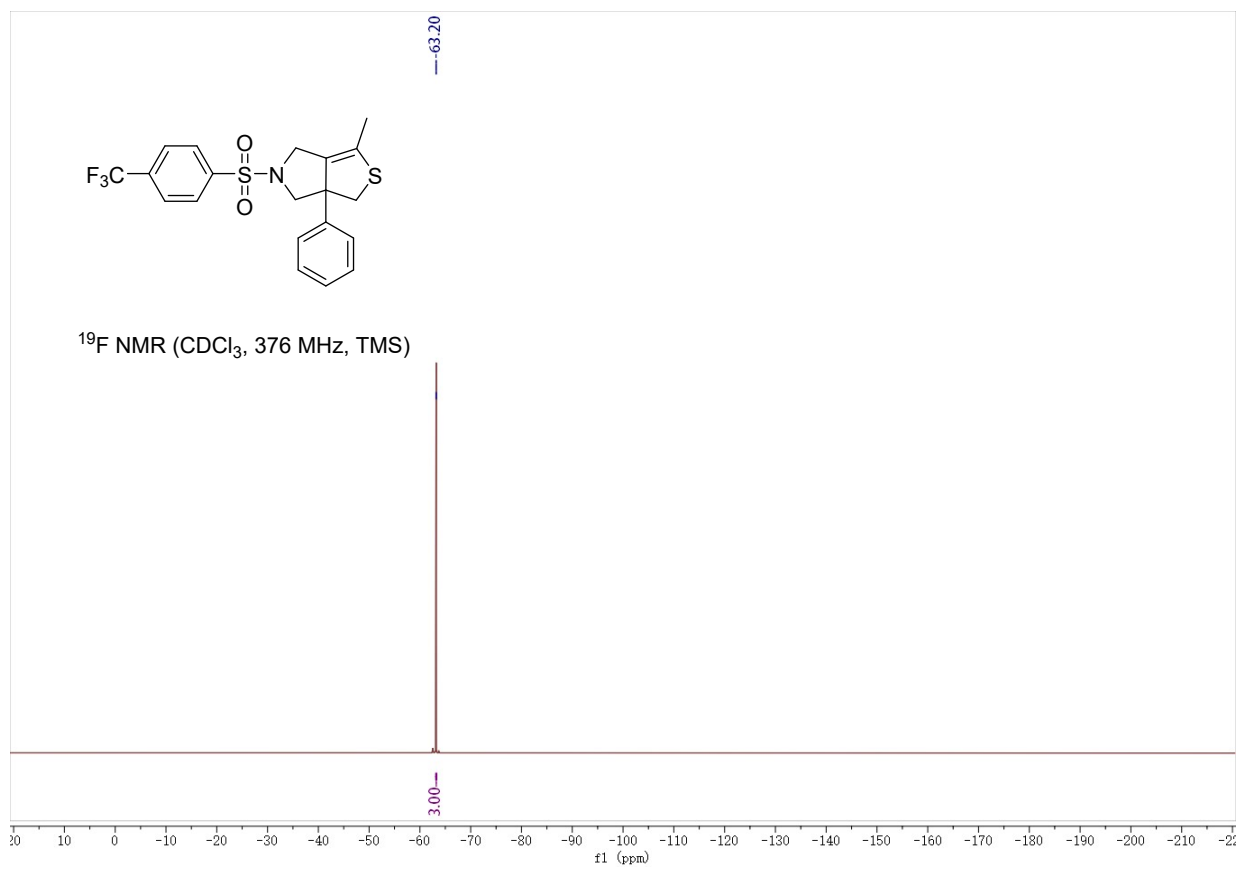
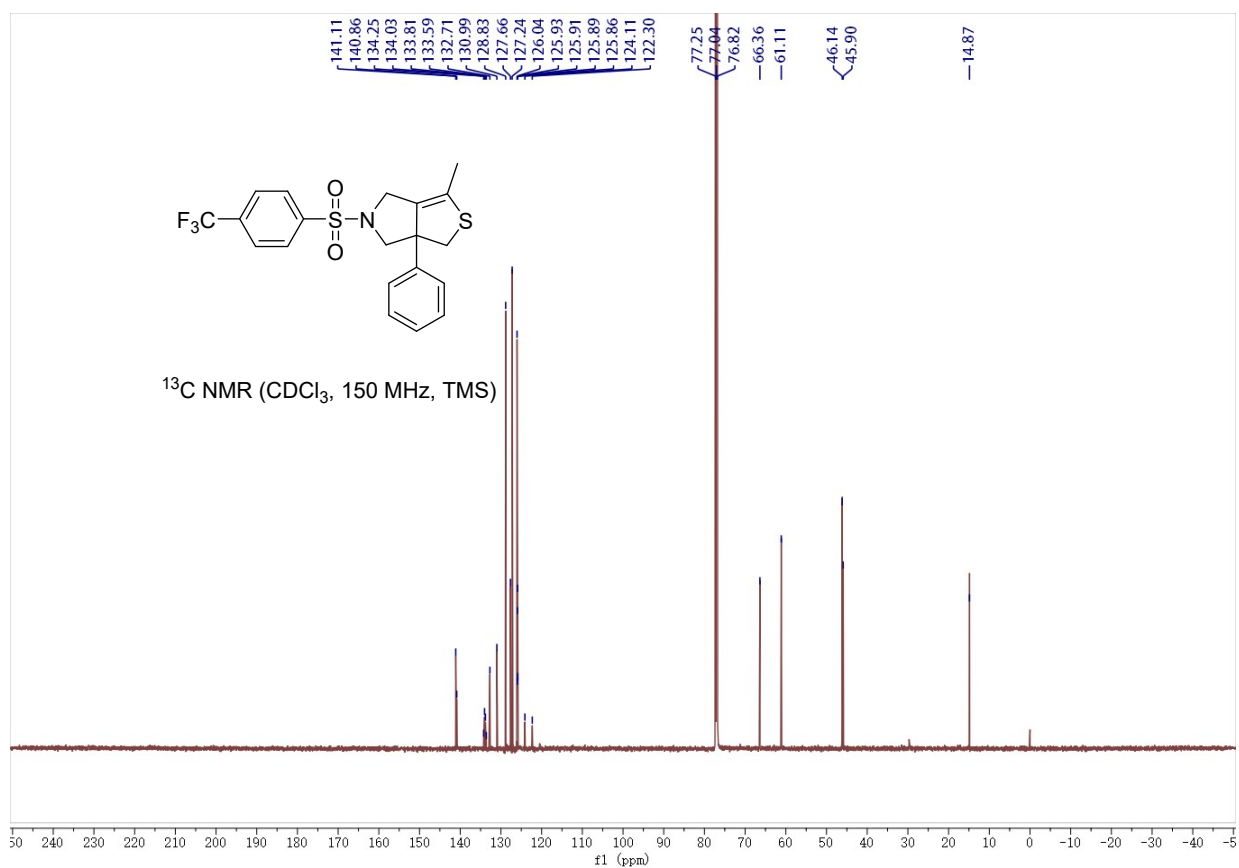


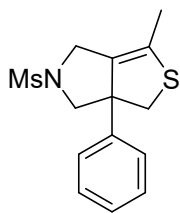


3-methyl-6a-phenyl-5-((4-(trifluoromethyl)phenyl)sulfonyl)-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3w)

A colorless oil, 34.0 mg, 80% yield. ^1H NMR (CDCl_3 , TMS, 600 MHz) δ 7.59 (d, $J = 8.1$ Hz, 2H), 7.48 (d, $J = 8.2$ Hz, 2H), 7.18 (dd, $J = 7.2, 3.8$ Hz, 3H), 7.08 (d, $J = 5.7$ Hz, 2H), 4.12 (d, $J = 10.2$ Hz, 1H), 4.05 (d, $J = 13.3$ Hz, 1H), 3.75 - 3.69 (m, 2H), 3.58 (d, $J = 10.3$ Hz, 1H), 3.00 (d, $J = 11.0$ Hz, 1H), 1.97 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 141.1, 140.9, 133.9 (q, $J = 33.0$ Hz), 132.7, 131.0, 128.8, 127.7, 127.2, 126.0, 125.9 (q, $J = 3.0$ Hz), 123.2 (q, $J = 271.5$ Hz), 66.4, 61.1, 46.1, 45.9, 14.9. ^{19}F NMR (CDCl_3 , TMS, 376 MHz) δ -63.2 (s). IR (Acetone) ν 901, 1035, 1208, 1339, 3012 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{20}\text{H}_{19}\text{O}_2\text{NF}_3\text{S}_2$ (M+H): 426.0804, Found: 426.0800.

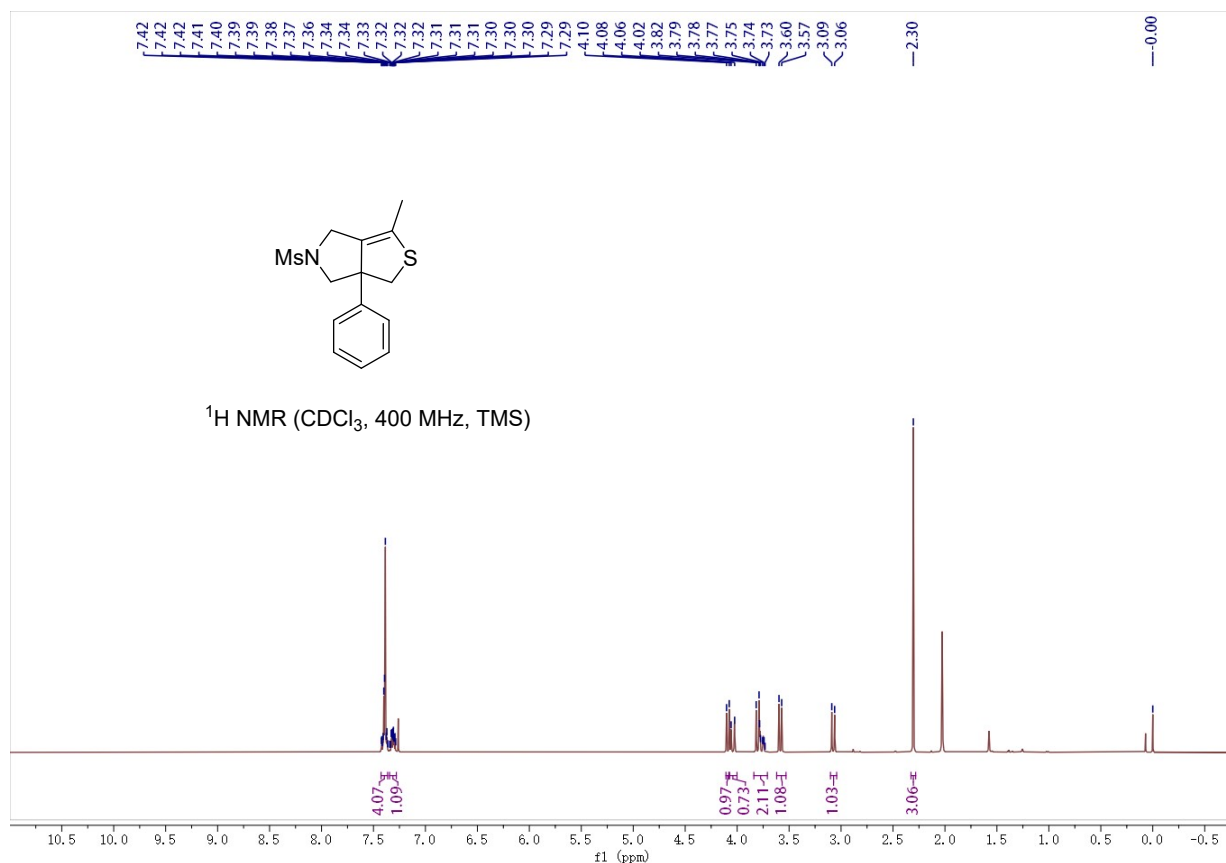


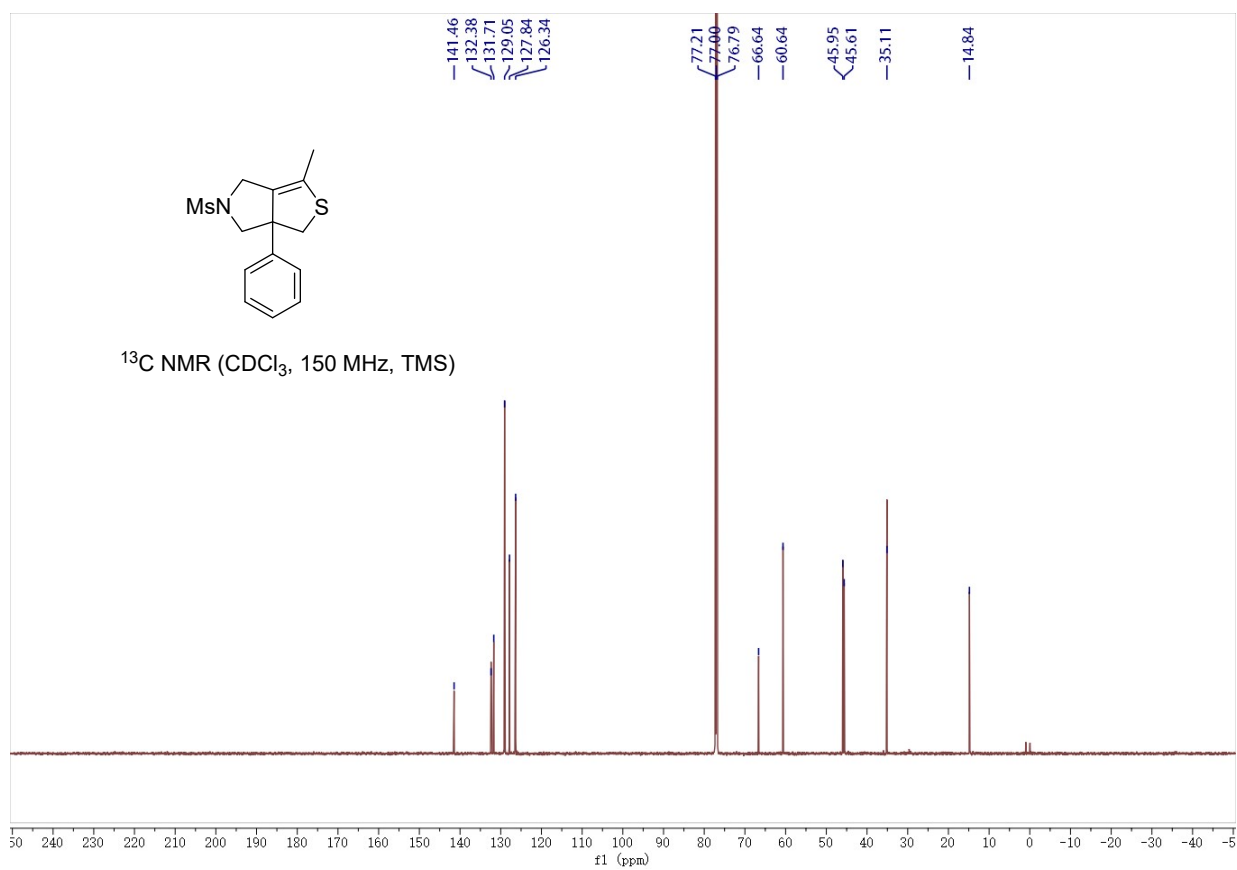


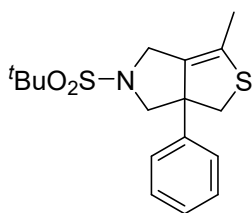


3-methyl-5-(methylsulfonyl)-6a-phenyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrole (3x)

A colorless oil, 20.7 mg, 91% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.43 – 7.36 (m, 4H), 7.35 – 7.28 (m, 1H), 4.09 (d, $J = 10.3$ Hz, 1H), 4.04 (d, $J = 13.7$ Hz, 1H), 3.84 – 3.71 (m, 2H), 3.58 (d, $J = 10.3$ Hz, 1H), 3.08 (d, $J = 11.0$ Hz, 1H), 2.30 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 141.5, 132.4, 131.7, 129.1, 127.8, 126.3, 66.6, 60.6, 46.0, 45.6, 35.1, 14.8. IR (Acetone) ν 702, 906, 1055, 1148, 1331, 2920 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{14}\text{H}_{18}\text{O}_2\text{NS}_2$ (M+H): 296.0773, Found: 296.0761.

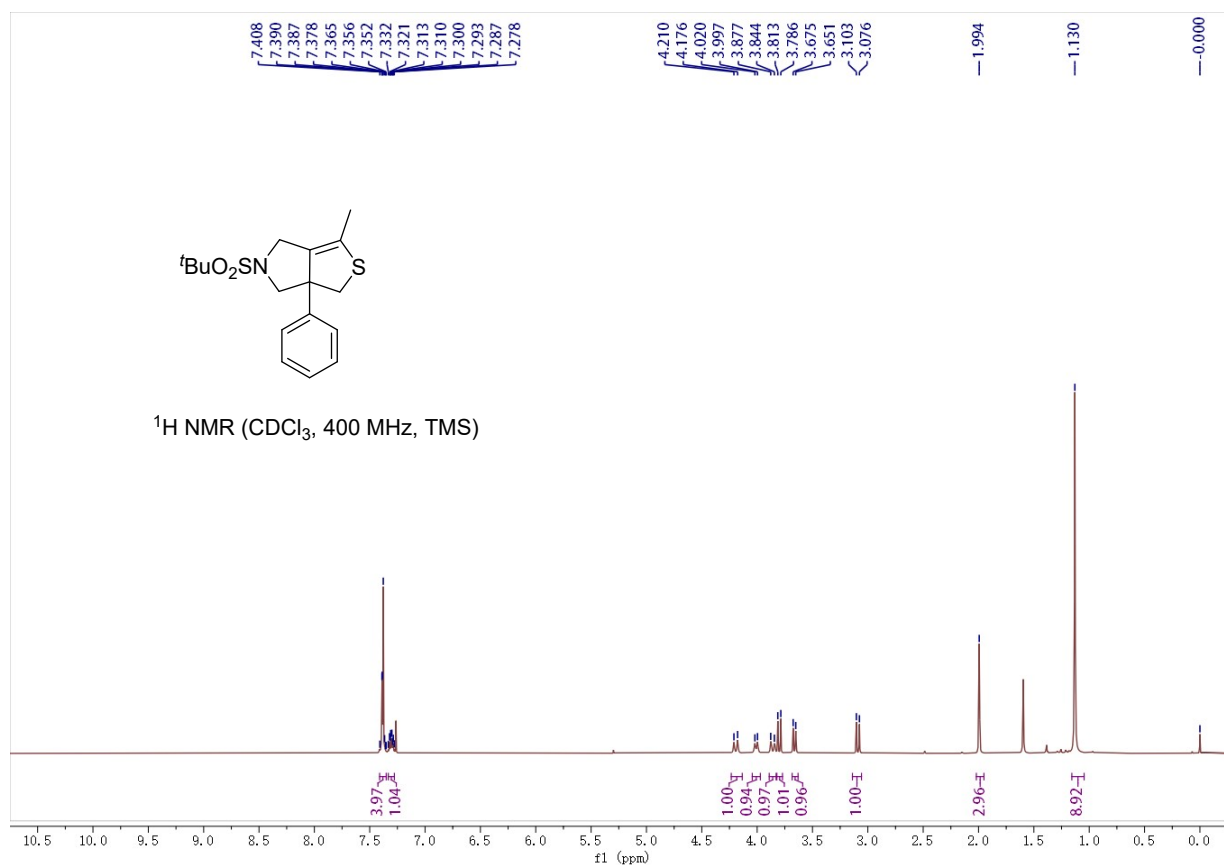


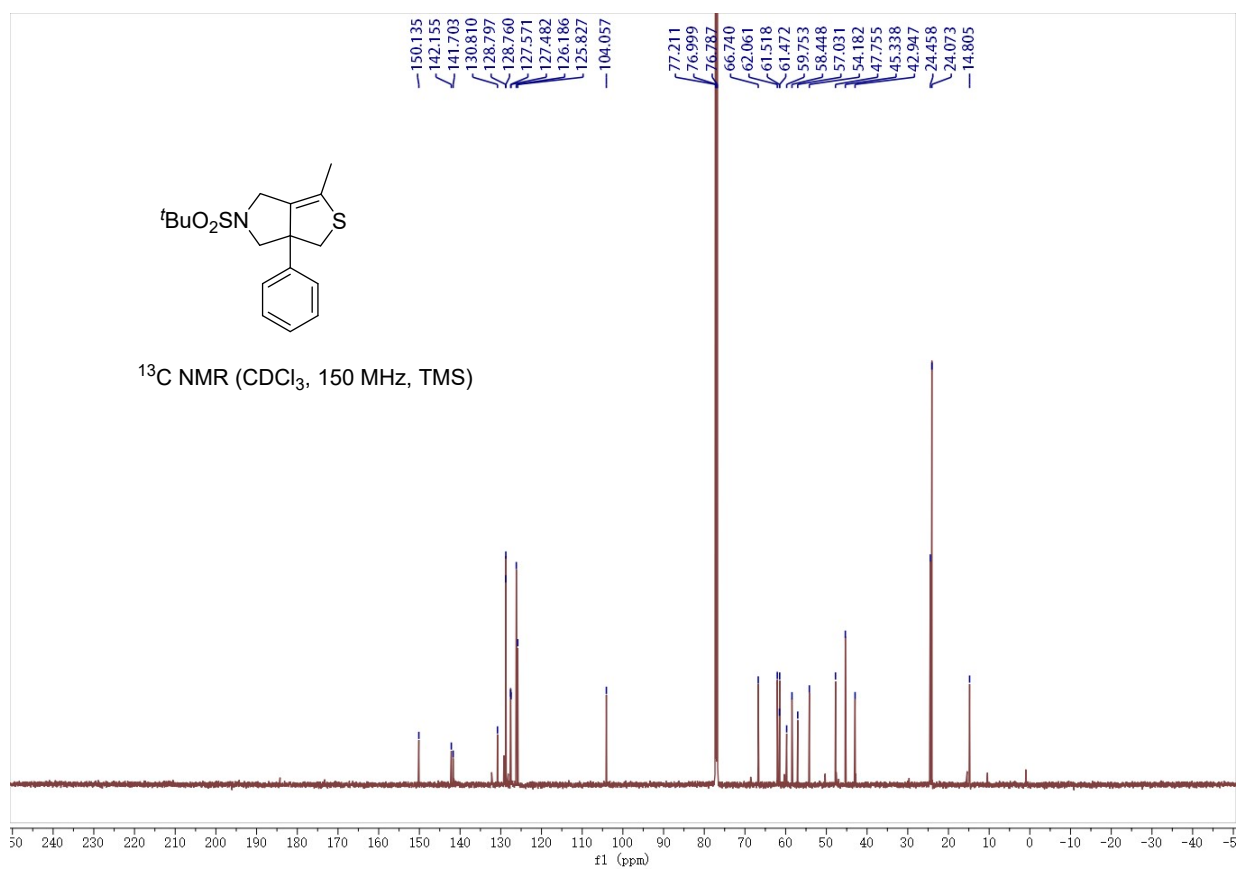


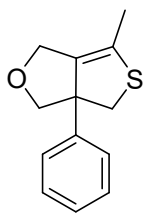


5-(*tert*-butylsulfonyl)-3-methyl-6a-phenyl-4,5,6,6a-tetrahydro-1*H*-thieno[3,4-*c*]pyrrole (3y)

A colorless oil, 30.4 mg, 90% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.38 (d, $J = 4.8$ Hz, 4H), 7.30 (ddd, $J = 8.6, 5.1, 3.4$ Hz, 1H), 4.19 (d, $J = 13.3$ Hz, 1H), 4.01 (d, $J = 9.4$ Hz, 1H), 3.86 (d, $J = 13.3$ Hz, 1H), 3.80 (d, $J = 10.9$ Hz, 1H), 3.66 (d, $J = 9.4$ Hz, 1H), 3.09 (d, $J = 10.9$ Hz, 1H), 1.99 (s, 3H), 1.13 (s, 9H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 150.1, 142.2, 141.7, 130.8, 128.8, 128.8, 127.6, 127.5, 126.2, 125.8, 104.1, 66.7, 62.1, 61.5, 61.5, 59.8, 58.4, 57.0, 54.2, 47.8, 45.3, 42.9, 24.5, 24.1, 14.8. IR (Acetone) ν 732, 1006, 1107, 1291, 3020 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{17}\text{H}_{23}\text{O}_2\text{NNaS}_2$ ($\text{M}+\text{Na}$): 360.1062, Found: 360.1054.

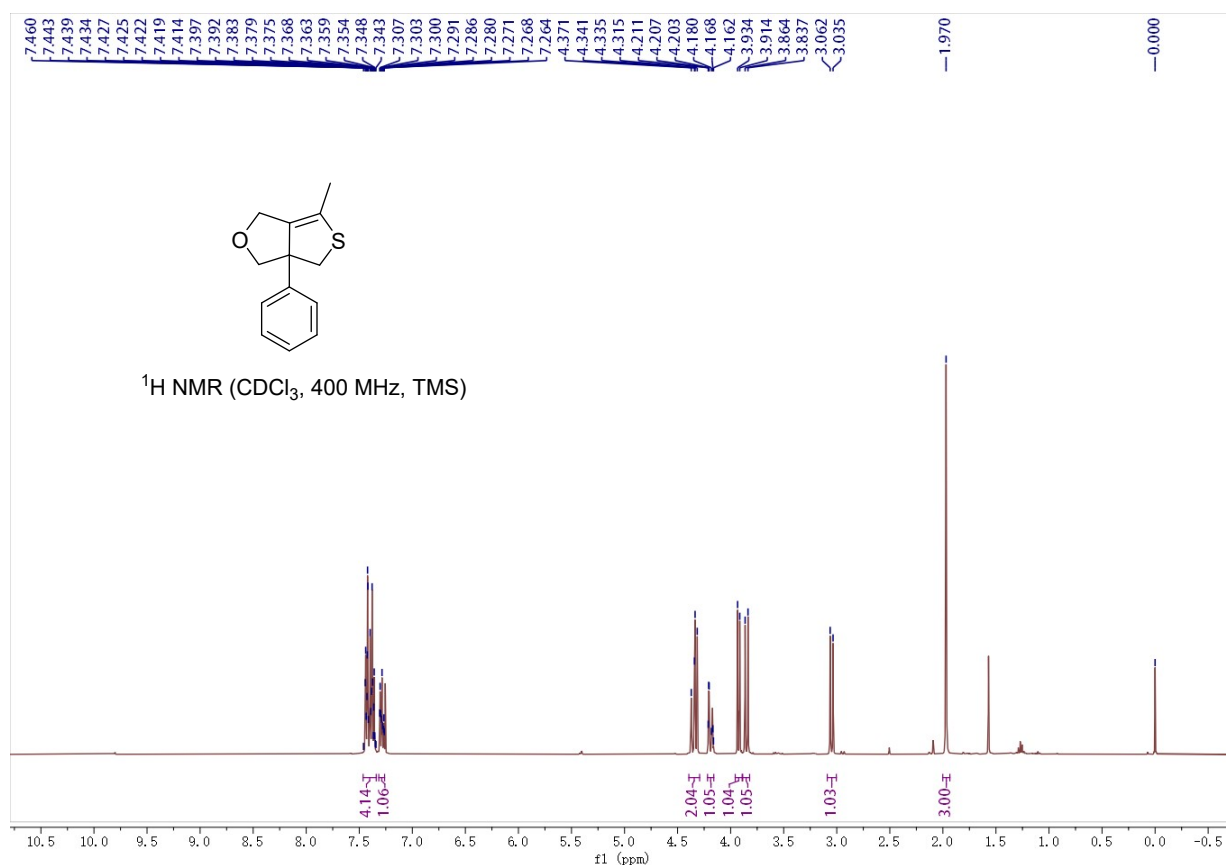


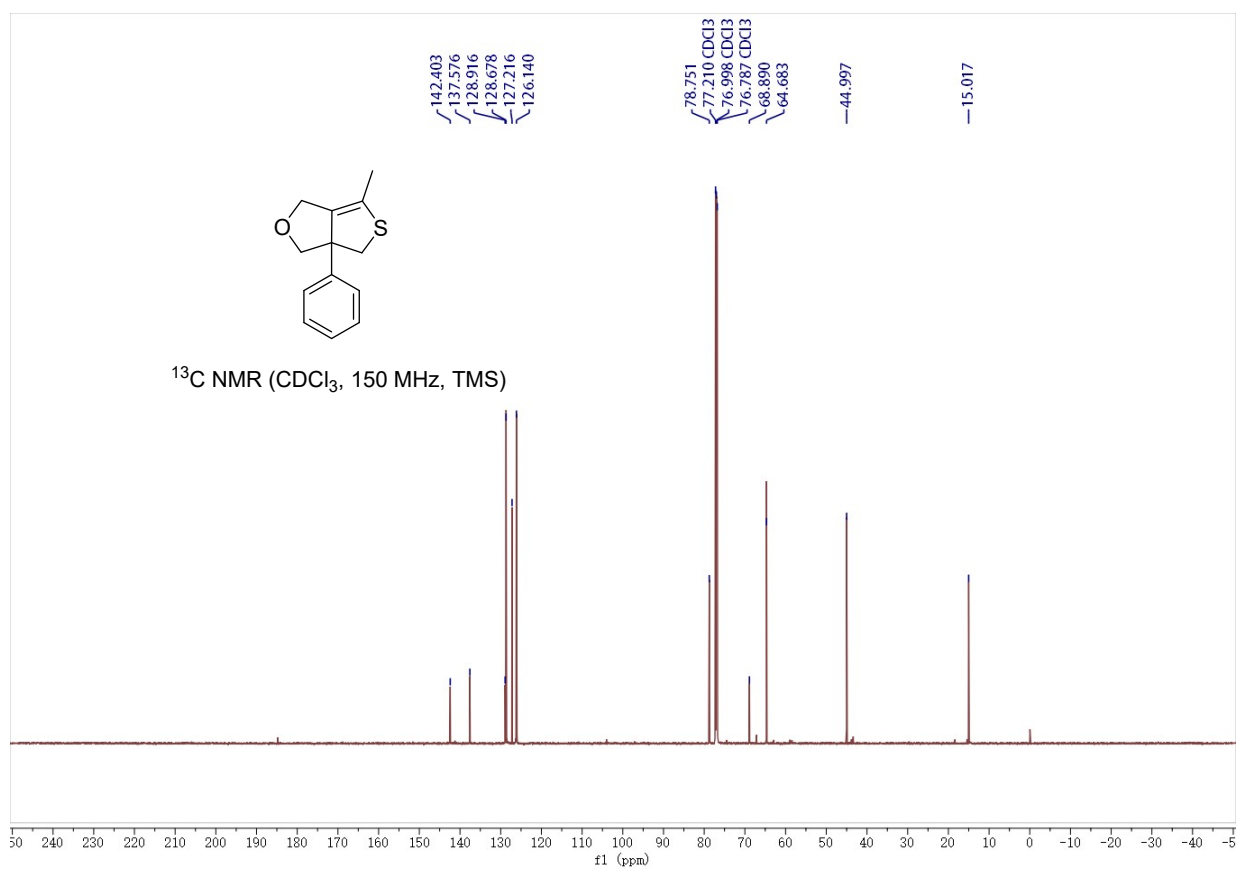


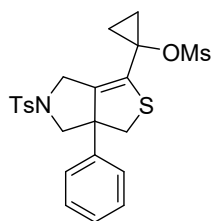


6-methyl-3a-phenyl-3a,4-dihydro-1H,3H-thieno[3,4-c]furan (**3z**)

A colorless oil, 18.8 mg, 43% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.46 – 7.34 (m, 4H), 7.32 – 7.26 (m, 1H), 4.39 – 4.29 (m, 2H), 4.22 – 4.16 (m, 1H), 3.92 (d, $J = 8.0$ Hz, 1H), 3.85 (d, $J = 10.9$ Hz, 1H), 3.05 (d, $J = 10.9$ Hz, 1H), 1.97 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 142.4, 137.6, 128.9, 128.7, 127.2, 126.1, 78.8, 68.9, 64.7, 45.0, 15.0. IR (Acetone) ν 699, 723, 896, 1034, 1446, 2849 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{13}\text{H}_{15}\text{OS}$ (M-H): 219.0838, Found: 219.0834.

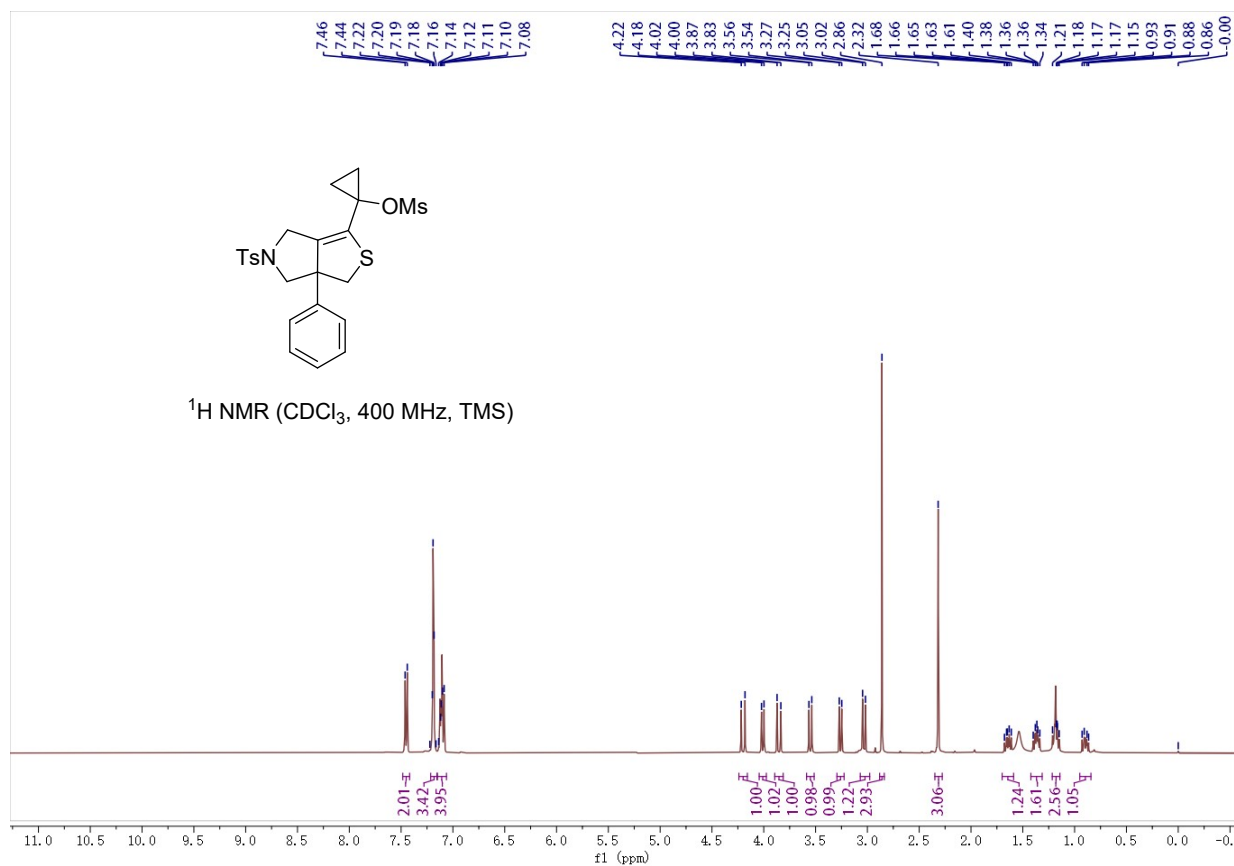


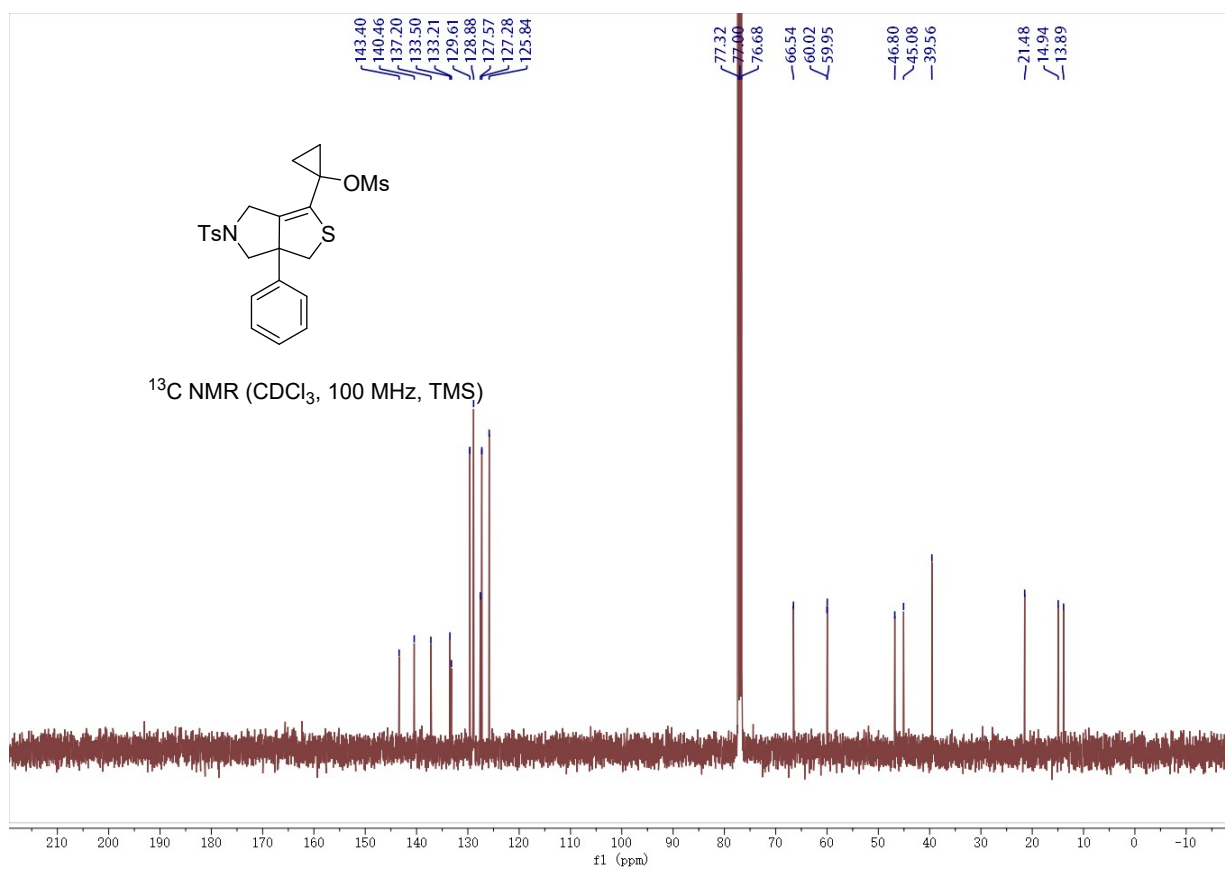


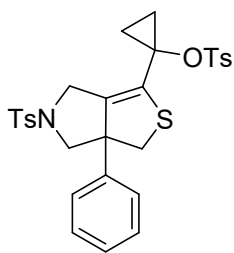


1-(6a-phenyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrol-3-yl)cyclopropyl methanesulfonate (3ab)

A colorless oil, 41.8 mg, 85% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.45 (d, $J = 8.2$ Hz, 2H), 7.21 – 7.15 (m, 3H), 7.15 – 7.06 (m, 4H), 4.20 (d, $J = 14.6$ Hz, 1H), 4.01 (d, $J = 9.6$ Hz, 1H), 3.85 (d, $J = 14.6$ Hz, 1H), 3.55 (d, $J = 11.1$ Hz, 1H), 3.26 (d, $J = 9.6$ Hz, 1H), 3.03 (d, $J = 11.1$ Hz, 1H), 2.86 (s, 3H), 2.32 (s, 3H), 1.70 – 1.59 (m, 1H), 1.42 – 1.31 (m, 2H), 1.22 – 1.14 (m, 3H), 0.95 – 0.84 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 143.4, 140.5, 137.2, 133.5, 133.2, 129.6, 128.9, 127.6, 127.3, 125.8, 66.5, 60.02, 59.95, 46.8, 45.1, 39.6, 21.5, 14.9, 13.9. IR (Acetone) ν 661, 1083, 1203, 1349, 1753, 3033 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{23}\text{H}_{26}\text{O}_5\text{NS}_3$ (M+H): 492.0968, Found: 492.0955.

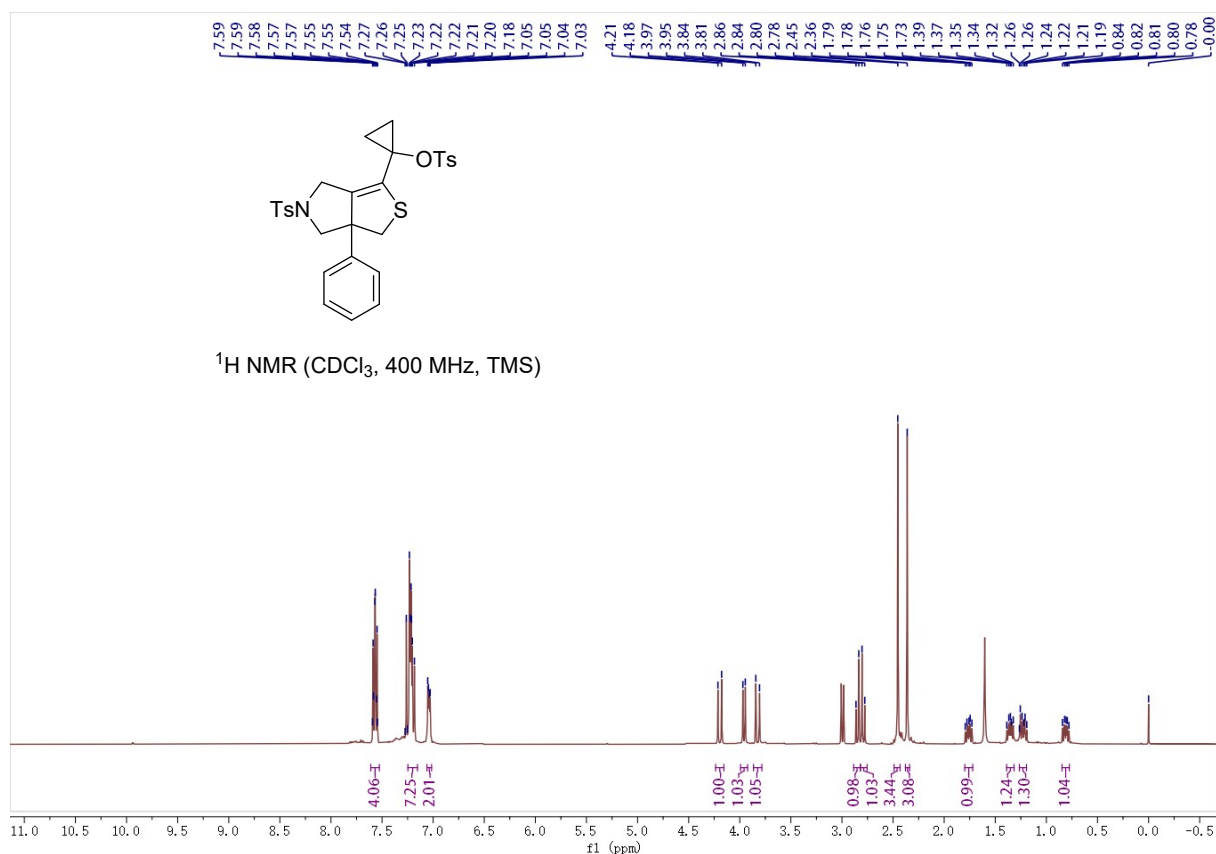


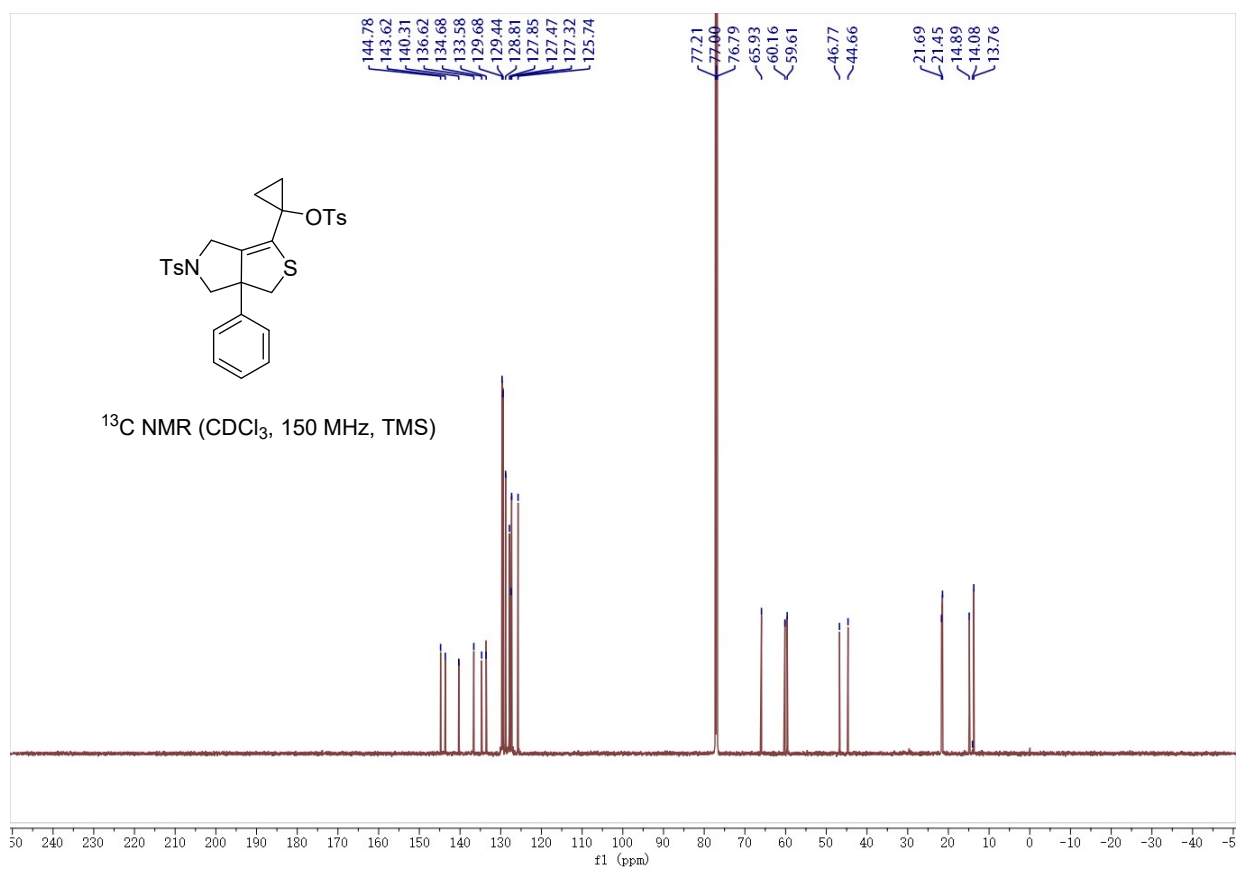


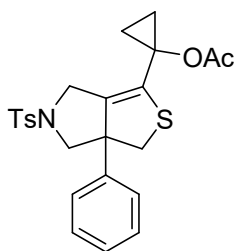


1-(6a-phenyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrol-3-yl)cyclopropyl methylbenzenesulfonate (3ac) 4-

A colorless oil, 48.2 mg, 90% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.61 – 7.53 (m, 4H), 7.25 – 7.15 (m, 7H), 7.06 – 7.02 (m, 2H), 4.20 (d, $J = 14.6$ Hz, 1H), 3.96 (d, $J = 9.4$ Hz, 1H), 3.82 (d, $J = 14.5$ Hz, 1H), 2.85 (d, $J = 10.9$ Hz, 1H), 2.79 (d, $J = 10.9$ Hz, 1H), 2.45 (s, 3H), 2.36 (s, 3H), 1.80 – 1.72 (m, 1H), 1.39 – 1.32 (m, 1H), 1.26 – 1.19 (m, 1H), 0.85 – 0.78 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 144.8, 143.6, 140.3, 136.6, 134.7, 133.6, 129.7, 129.4, 128.8, 127.9, 127.5, 127.3, 125.7, 65.9, 60.2, 59.6, 46.8, 44.7, 21.7, 21.4, 14.9, 14.1, 13.8. IR (Acetone) ν 1043, 1253, 1369, 1755, 3021 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{29}\text{H}_{30}\text{O}_5\text{NS}_3$ (M+H): 568.1281, Found: 568.1269.

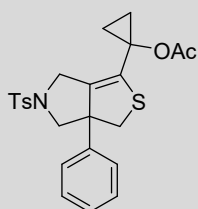




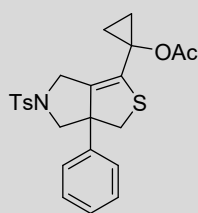


1-(6a-phenyl-5-tosyl-4,5,6,6a-tetrahydro-1H-thieno[3,4-c]pyrrol-3-yl)cyclopropyl acetate (3ad)

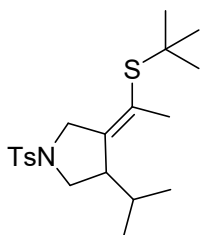
A colorless oil, 37.8 mg, 83% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.47 (d, $J = 8.3$ Hz, 2H), 7.27 – 7.23 (m, 3H), 7.19 – 7.10 (m, 4H), 4.21 (d, $J = 14.1$ Hz, 1H), 4.05 (d, $J = 9.6$ Hz, 1H), 3.78 (d, $J = 14.1$ Hz, 1H), 3.59 (d, $J = 10.9$ Hz, 1H), 3.35 (d, $J = 9.6$ Hz, 1H), 2.96 (d, $J = 10.8$ Hz, 1H), 2.38 (s, 3H), 2.06 (s, 3H), 1.26 – 1.00 (m, 4H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 170.2, 143.3, 140.7, 134.9, 133.9, 133.1, 129.6, 128.8, 127.3, 127.2, 126.1, 67.1, 59.9, 55.6, 46.6, 45.1, 21.5, 20.9, 15.1, 13.7. IR (Acetone) ν 1055, 1269, 1380, 1650, 3021 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{24}\text{H}_{25}\text{O}_4\text{NNaS}_2$ ($\text{M}+\text{Na}$): 478.1117, Found: 478.1108.



^1H NMR (CDCl_3 , 400 MHz, TMS)

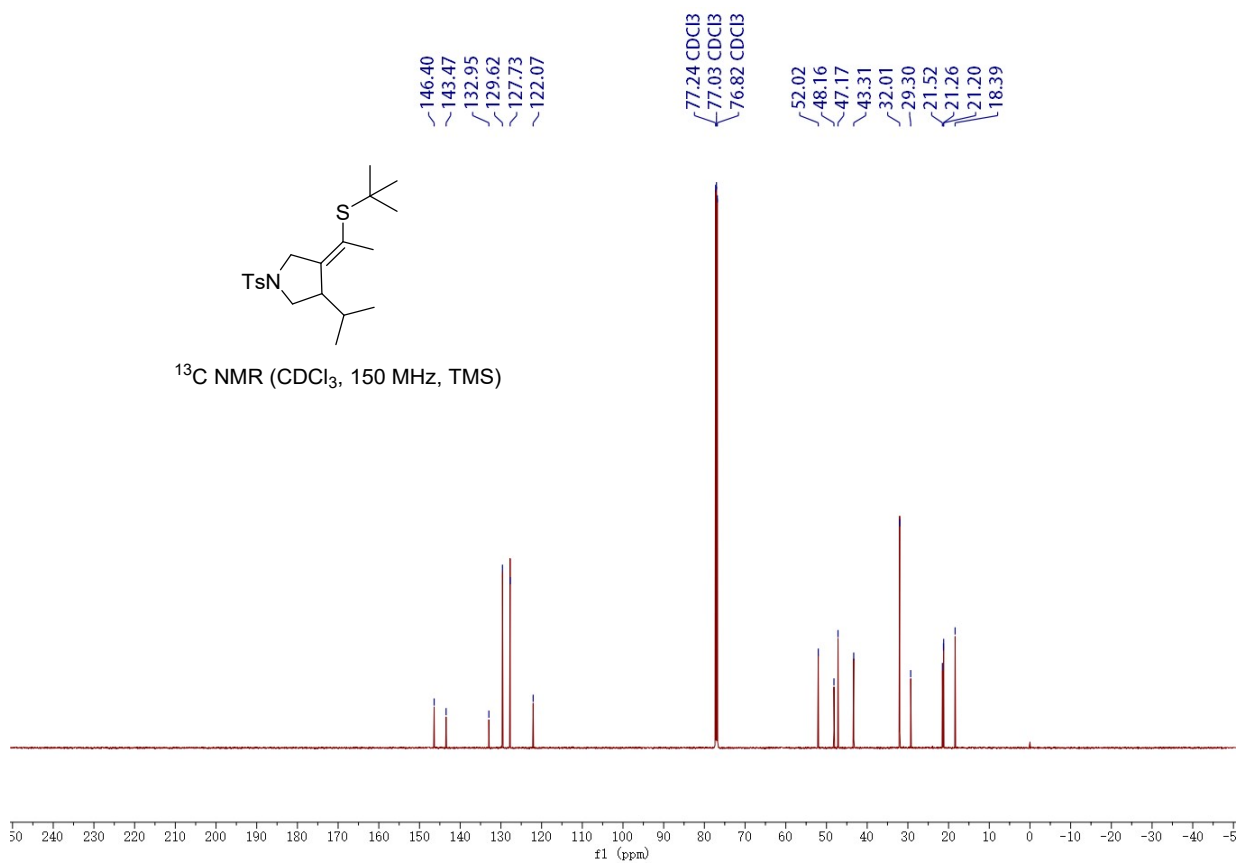
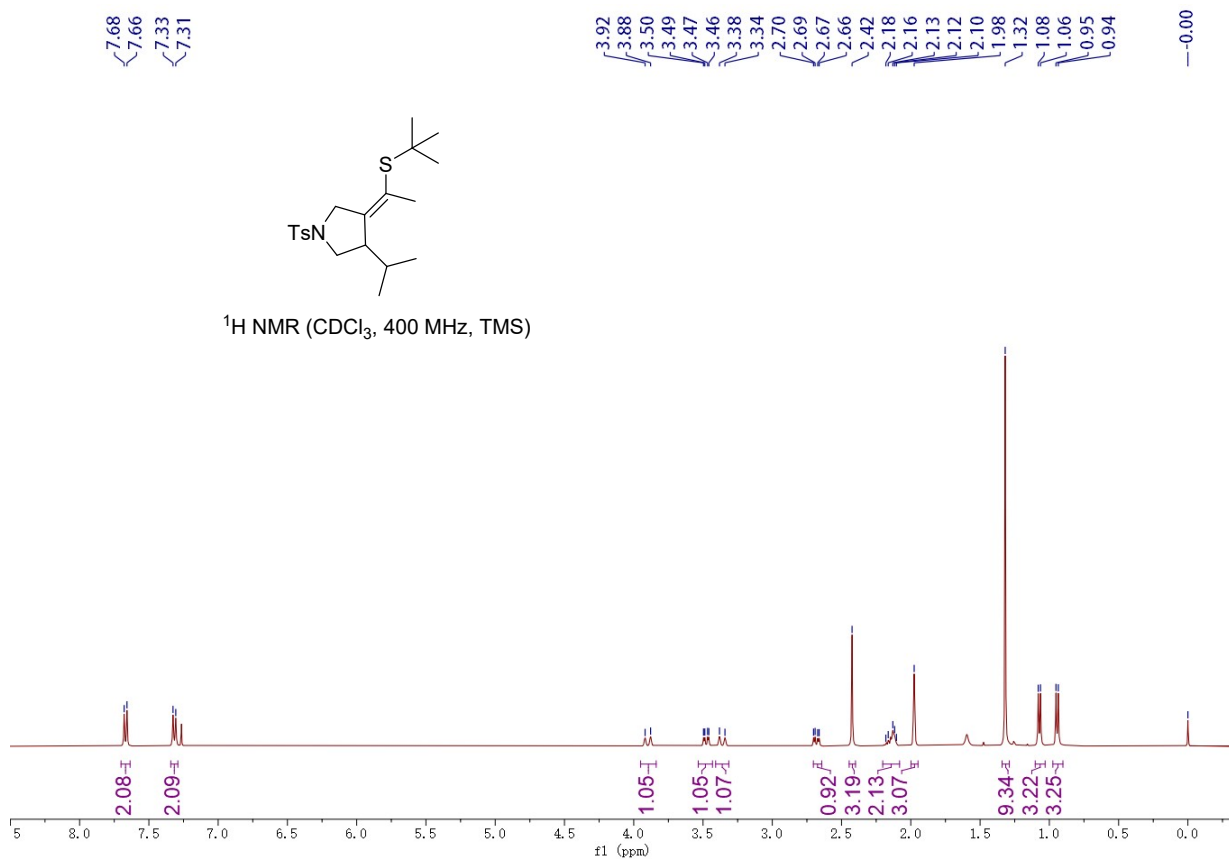


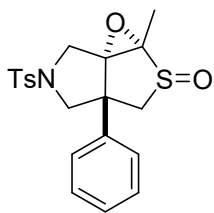
^{13}C NMR (CDCl_3 , 150 MHz, TMS)



(Z)-3-(1-(*tert*-butylthio)ethylidene)-4-isopropyl-1-tosylpyrrolidine (3ae)

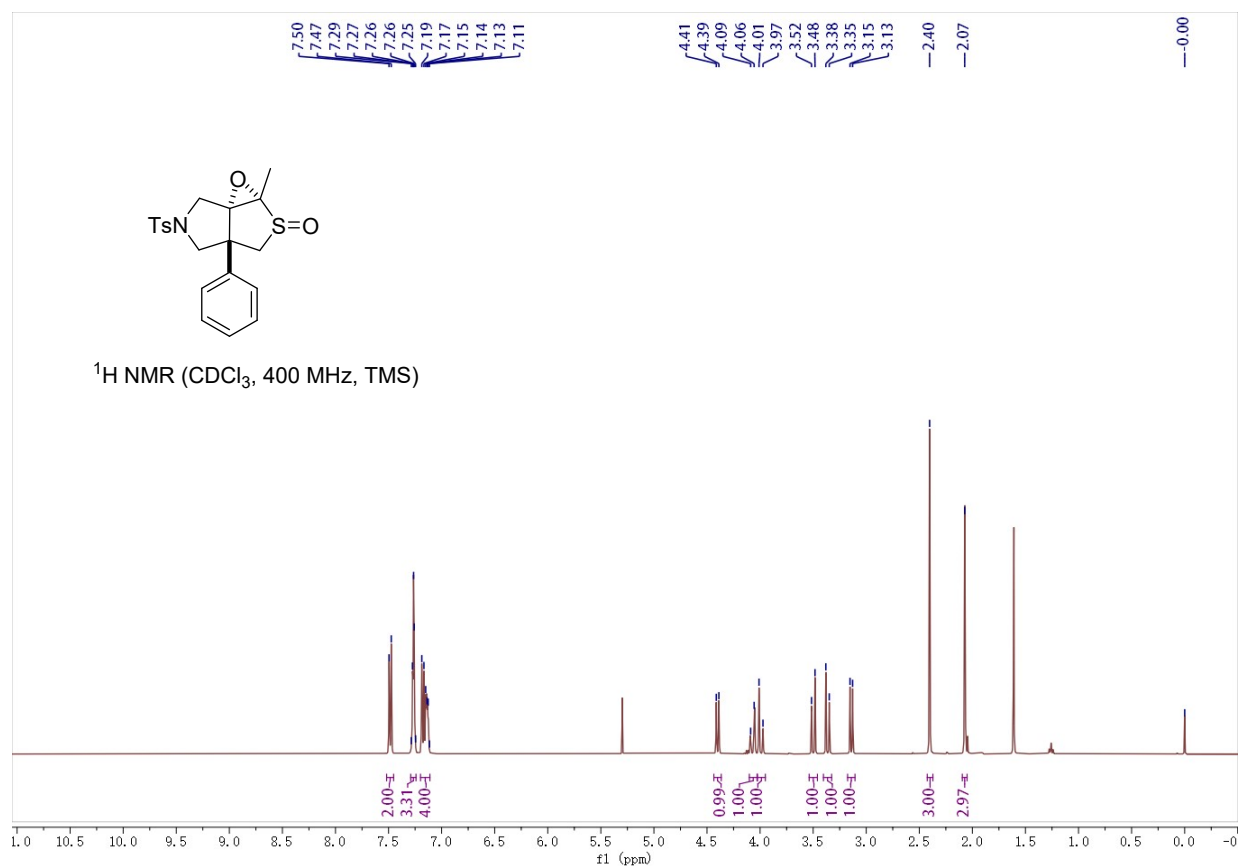
A colorless oil, 37.8 mg, 80% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.67 (d, $J = 8.2$ Hz, 2H), 7.32 (d, $J = 8.0$ Hz, 2H), 3.90 (d, $J = 15.9$ Hz, 1H), 3.48 (dd, $J = 11.8, 3.7$ Hz, 1H), 3.36 (d, $J = 15.8$ Hz, 1H), 2.68 (dd, $J = 11.8, 4.4$ Hz, 1H), 2.42 (s, 3H), 2.20 – 2.08 (m, 2H), 1.98 (s, 3H), 1.32 (s, 9H), 1.07 (d, $J = 6.6$ Hz, 3H), 0.94 (d, $J = 6.7$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 146.4, 143.5, 133.0, 129.6, 127.7, 122.1, 52.0, 48.2, 47.2, 43.3, 32.0, 29.3, 21.5, 21.3, 21.2, 18.4. IR (Acetone) ν 911, 1245, 1330, 1810, 2941 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{20}\text{H}_{32}\text{O}_2\text{NS}_2$ ($\text{M}+\text{H}$): 382.1869, Found: 382.1872.

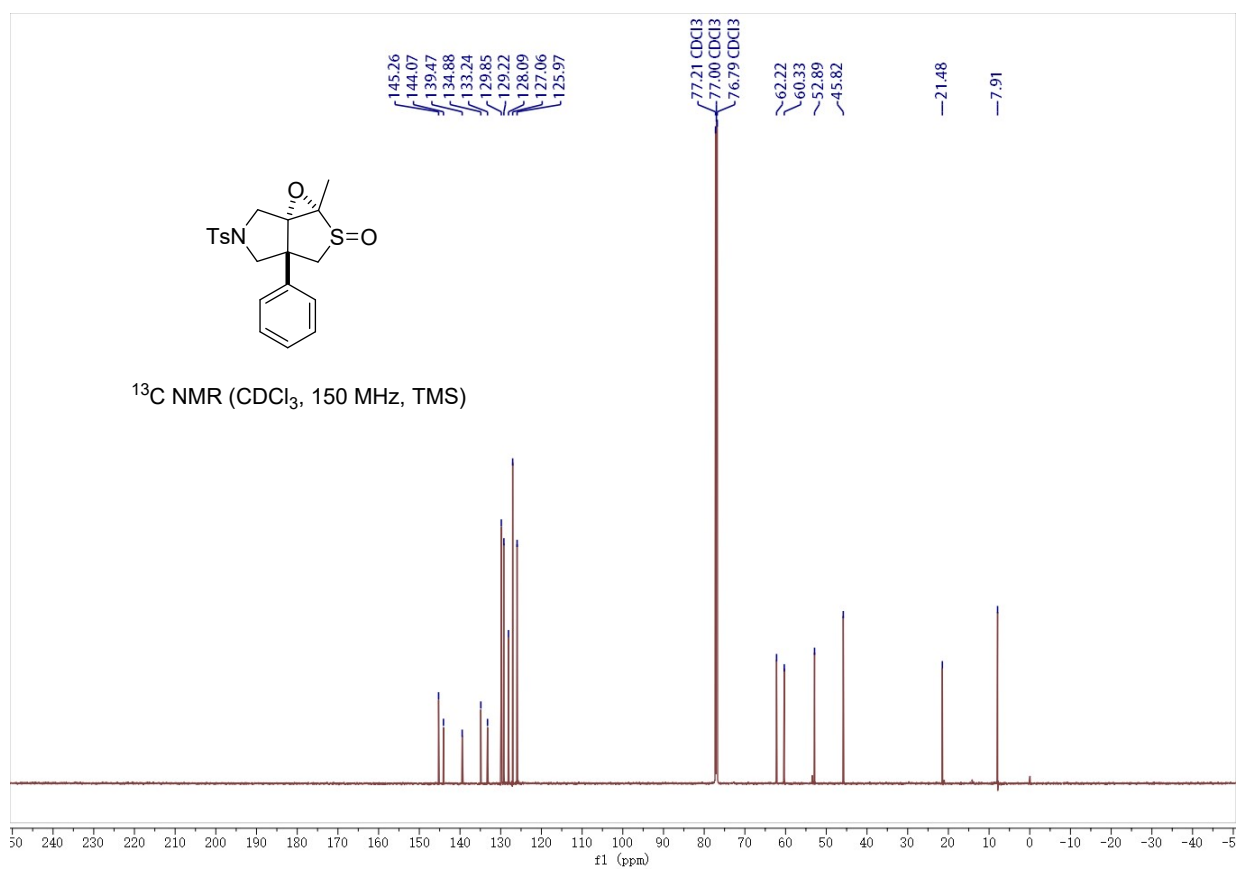


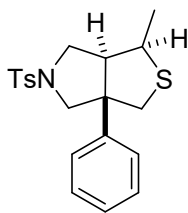


1a-methyl-3a-phenyl-5-tosyltetrahydro-1aH,3H-oxireno[2',3':2,3]thieno[3,4-c]pyrrole 2-oxide (4)

A colorless oil, 37.5 mg, 93% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.49 (d, $J = 8.4$ Hz, 2H), 7.29 – 7.24 (m, 3H), 7.20 – 7.11 (m, 4H), 4.40 (d, $J = 9.8$ Hz, 1H), 4.07 (d, $J = 13.2$ Hz, 1H), 3.99 (d, $J = 15.0$ Hz, 1H), 3.50 (d, $J = 13.1$ Hz, 1H), 3.36 (d, $J = 12.8$ Hz, 1H), 3.14 (d, $J = 9.8$ Hz, 1H), 2.40 (s, 3H), 2.07 (s, 3H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 145.3, 144.1, 139.5, 134.9, 133.2, 129.9, 129.2, 128.1, 127.1, 126.0, 62.2, 60.3, 52.9, 45.8, 21.5, 7.9. IR (Acetone) ν 689, 1013, 1137, 1229, 1340, 1703, 3001 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{20}\text{H}_{22}\text{O}_4\text{NS}_2$ (M+H): 404.0985, Found: 404.0973.

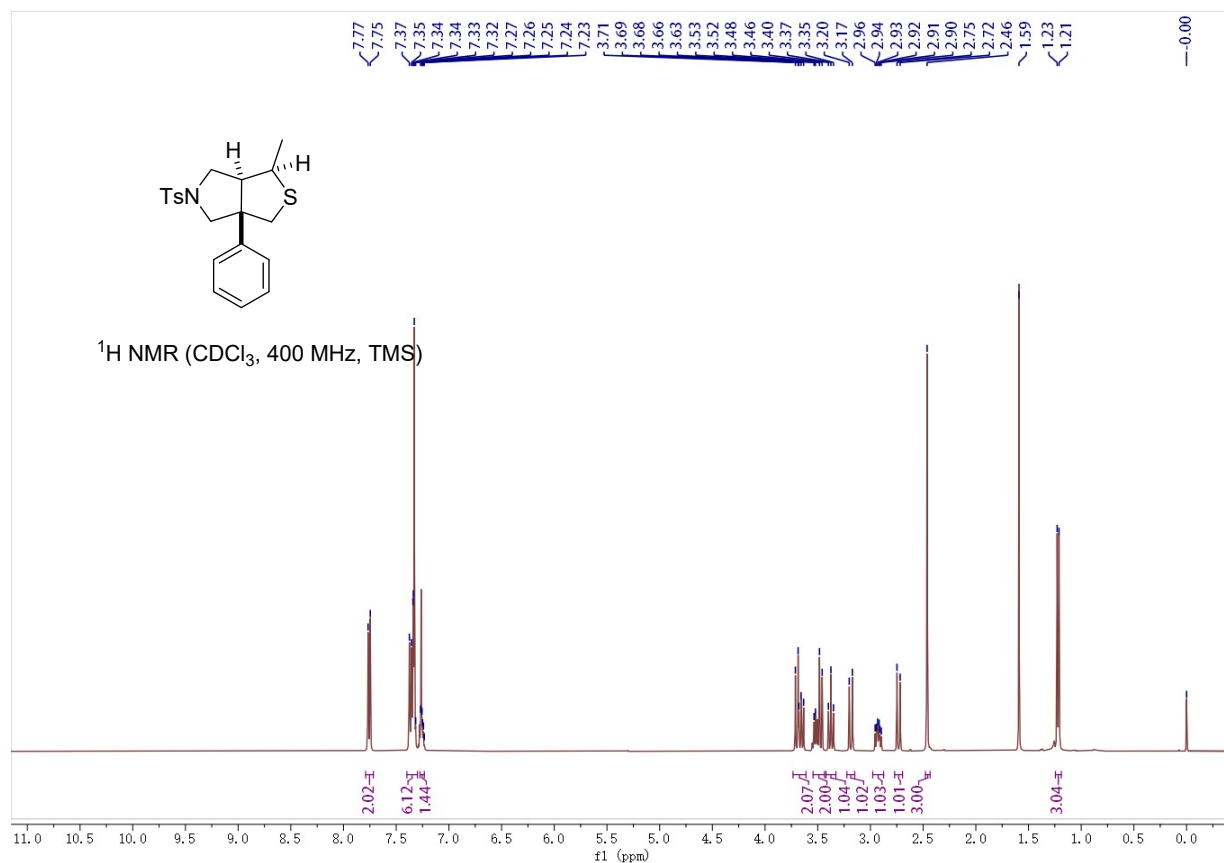


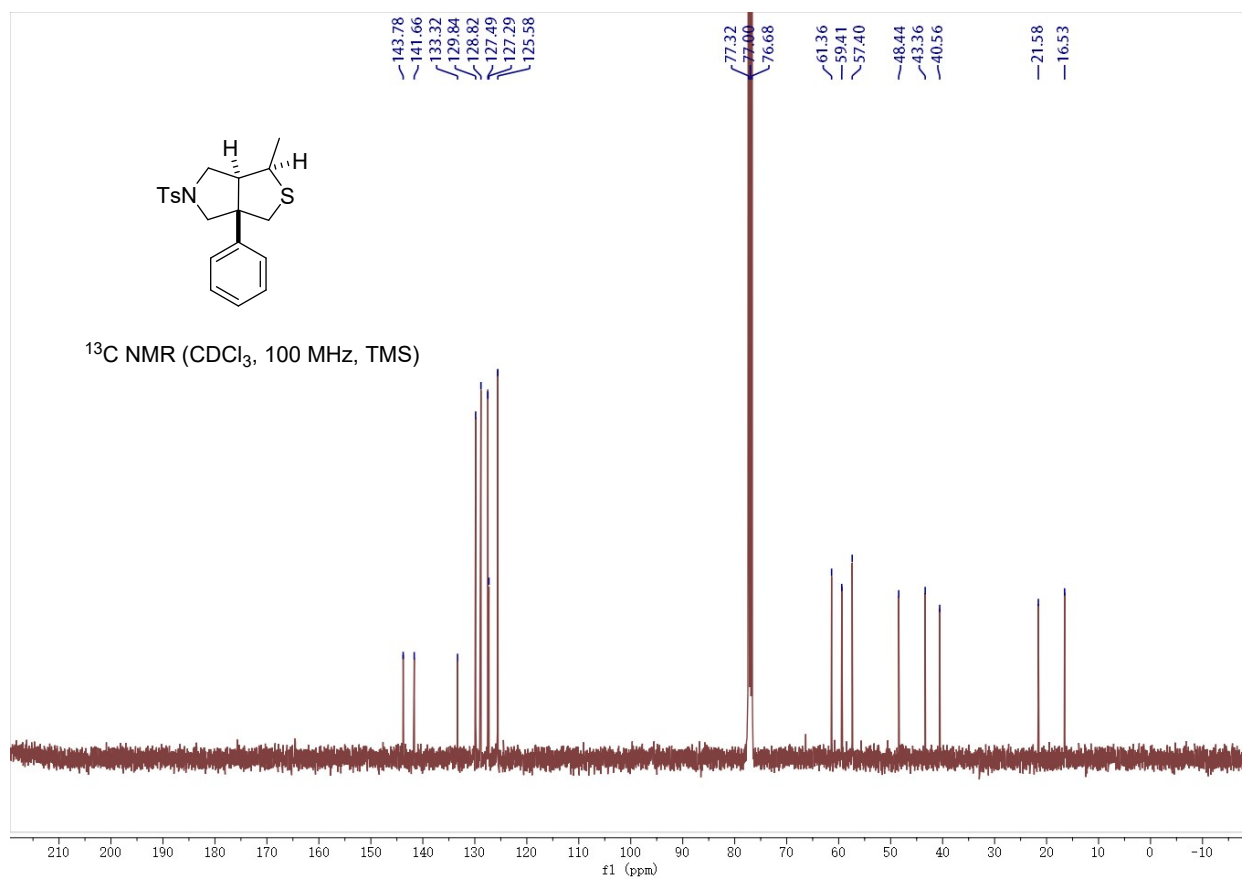




1-methyl-3a-phenyl-5-tosylhexahydro-1*H*-thieno[3,4-*c*]pyrrole (5)

A colorless oil, 26.1 mg, 70% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.76 (d, $J = 8.3$ Hz, 2H), 7.40 – 7.30 (m, 6H), 7.27 – 7.23 (m, 1H), 3.73 – 3.61 (m, 2H), 3.54 – 3.44 (m, 2H), 3.37 (t, $J = 9.7$ Hz, 1H), 3.19 (d, $J = 11.8$ Hz, 1H), 2.98 – 2.87 (m, 1H), 2.73 (d, $J = 11.9$ Hz, 1H), 2.46 (s, 3H), 1.22 (d, $J = 6.9$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 143.8, 141.7, 133.3, 129.8, 128.8, 127.5, 127.3, 125.6, 61.4, 59.4, 57.4, 48.4, 43.4, 40.6, 21.6, 16.5. IR (Acetone) ν 711, 1127, 1249, 1309, 1613, 2981 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{20}\text{H}_{24}\text{O}_2\text{NS}_2$ ($\text{M}+\text{H}$): 374.1243, Found: 374.1233.





10. Computational studies

All quantum mechanical calculations have been performed with Gaussian 16. The geometries of all species have been optimized at B3LYP/6-31G(d) level. The subsequent frequency calculations on the stationary points were carried out at the same level of theory to ascertain the nature of the stationary points as minima on the respective potential energy surfaces. The conformational space of flexible systems has first been searched manually and checked by xtb 6.0 program. Thermochemical corrections to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at this same level. The thermochemical corrections have been combined with single-point energies calculated at the SMD/B3LYP/6-311+G(d,p)// B3LYP/6-31G(d) level to yield free energy G_{298} at 298.15 K. The solvent effect was estimated by the IEFPCM method with radii and nonelectrostatic terms for SMD solvation model in DiChloroEthane: ($\epsilon = 10.13$).

Table S6. The total energies, enthalpies and free energies of all species in dichloromethane shown in Schemes 3E.

	E_{tot}	H_{298}	G_{298}
INT1	-556.085219	-555.955359	-555.993458
TS1'	-1742.616143	-1742.152088	-1742.24626
INT2'	-1742.630428	-1742.165063	-1742.257893
TS2'	-1742.618378	-1742.154848	-1742.244952
INT3'	-1742.658304	-1742.193524	-1742.284091
TS3'	-1742.64096	-1742.175945	-1742.264673
INT4	-1742.675333	-1742.209911	-1742.310505
1k	-1186.544676	-1186.211191	-1186.286879
TS1	-1742.625787	-1742.161629	-1742.258778
INT2	-1742.634759	-1742.170373	-1742.266615
TS2	-1742.617553	-1742.153582	-1742.245509
INT3	-1742.654178	-1742.188446	-1742.27581
TS3	-1742.643258	-1742.178092	-1742.265442

Archive entries

INT1

Opt @ B3LYP/6-311+G(d,p) in dichloroethane (SMD model)
SCF Done: E(RB3LYP) = -556.085219a.u.
Zero-point correction = 0.122166Hartree/Particle
Sum of electronic and thermal Free Energies = -555.993458a.u.

C 0.31161200,0.00008400,0.00679400
C 0.86075600,1.26951800,0.67817600
C 0.86050700,-1.26196600,0.69226700
S -1.53721100,0.00049000,0.07263200
C 0.67143200,-0.00842500,-1.49480800
H 0.47914900,2.17113600,0.18999800
H 1.95754400,1.27960800,0.61934900
H 0.58183200,1.31143900,1.73652100
H 0.47855100,-2.16886500,0.21426700
H 1.95728300,-1.27295500,0.63338200
H 0.58175800,-1.29190200,1.75106500
H 0.28423100,0.87802300,-2.00752900
H 1.76482900,-0.00890900,-1.59627900
H 0.28435300,-0.90068400,-1.99745400

TS1'

Opt @ B3LYP/6-311+G(d,p) in dichloroethane (SMD model)
SCF Done: E(RB3LYP) = -1742.616143a.u.
Zero-point correction = 0.434510Hartree/Particle
Sum of electronic and thermal Free Energies = -1742.24626a.u.

C -4.21035200,1.82940900,0.25249700
C -3.02718300,2.58309700,-0.37186000
C -5.29186700,1.56777400,-0.80546600
S -3.63815000,0.23247100,1.03752300
C -4.79986000,2.64935700,1.41673500
H -2.24408300,2.77241300,0.36932900
H -3.36309300,3.54988900,-0.77170500
H -2.59148200,2.01433500,-1.19987500
H -6.14021900,1.02343000,-0.37847300
H -5.66389500,2.51995500,-1.20802300
H -4.89312500,0.98731000,-1.64418600
H -4.04944400,2.84287000,2.19029500
H -5.15568300,3.61732000,1.03803600

H -5.64723800,2.13389900,1.88032700
C -0.54962700,-0.34885400,-1.15810400
C -1.90086200,-0.89954800,-1.06603500
C -3.07596400,-1.17106500,-0.76411600
C -4.26690700,-2.02604100,-0.96832500
C 0.32843300,-1.19355600,1.01364600
C 0.74811100,-2.46763800,1.71516200
C 0.21434500,-3.76136400,1.16037300
C 1.48187000,-2.39941700,2.83012800
N 0.43249400,-1.21180300,-0.46607700
C 2.84744900,0.22837600,-0.56263900
C 3.57950100,0.16839400,0.62587500
C 4.22409000,1.31603100,1.08434400
C 4.15082700,2.52378800,0.37604800
C 3.41950200,2.55192400,-0.82043000
C 2.76724100,1.41593500,-1.29459000
C 4.83108400,3.76779300,0.89541800
S 1.99120400,-1.23687700,-1.15139800
O 2.67550500,-2.39853900,-0.58671500
O 1.79627300,-1.08739500,-2.59799700
H -0.54368600,0.67542300,-0.74561600
H -0.24891600,-0.28496300,-2.20745500
H -4.52324200,-2.55056400,-0.04271000
H -5.13687300,-1.42757600,-1.25345500
H -4.06740800,-2.76349700,-1.75366100
H 0.85924200,-0.32746300,1.43581000
H -0.73877500,-1.03110500,1.20868100
H 0.64104000,-3.95806500,0.17182100
H 0.45742500,-4.60161800,1.81752800
H -0.87641000,-3.71802500,1.03973000
H 1.72944000,-3.28850000,3.40371100
H 1.85599400,-1.45348200,3.21521900
H 3.65596200,-0.77012200,1.16495100
H 4.80244500,1.26962800,2.00387200
H 3.36983000,3.47343300,-1.39539100
H 2.22954900,1.43608500,-2.23671300
H 5.71826500,3.52198300,1.48777600
H 5.13880500,4.42771600,0.07784000
H 4.15604500,4.34351200,1.54258400

INT2'

Opt @ B3LYP/6-311+G(d,p) in dichloroethane (SMD model)

SCF Done: E(RB3LYP) = -1742.630428a.u.

Zero-point correction = 0.436148Hartree/Particle

Sum of electronic and thermal Free Energies = -1742.257893a.u.

C -4.32801800,1.55000100,0.00541500
C -3.38221200,1.98025700,-1.12129900
C -5.59589700,0.90913800,-0.57229400
S -3.45479700,0.37721600,1.19781300
C -4.69241500,2.75276100,0.89111800
H -2.48369600,2.46324100,-0.72389300
H -3.89068100,2.69522900,-1.78186900
H -3.07681600,1.12429900,-1.73156700
H -6.26782300,0.56739300,0.22118200
H -6.13508100,1.64381700,-1.18525300
H -5.35560700,0.05753000,-1.21668500
H -3.80057100,3.21153200,1.33155700
H -5.19889600,3.51305400,0.28341200
H -5.36771700,2.46260900,1.70292700
C -0.69388200,-0.44430800,-0.69291800
C -1.92630100,-1.20487900,-0.40796100
C -3.08017500,-1.12822700,0.22228200
C -4.08463300,-2.25539700,0.29510600
C 0.74172100,-1.62325600,0.96574400
C 1.47384700,-2.92485000,1.21413500
C 1.01203500,-4.12755300,0.43530000
C 2.41670800,-2.98508200,2.15946700
N 0.51223400,-1.27263200,-0.45573700
C 2.62805700,0.57334600,-0.60881100
C 3.60947600,0.38576500,0.36771700
C 4.17521700,1.50024500,0.98480400
C 3.77777500,2.80069300,0.64362000
C 2.79970100,2.96016100,-0.34886100
C 2.22157200,1.85876900,-0.97621300
C 4.37760200,4.00028900,1.33744100
S 1.87061800,-0.85603900,-1.39132700
O 2.81515700,-1.96629100,-1.27604100
O 1.34822500,-0.42507200,-2.69259300
H -0.67750900,0.47419600,-0.07683900
H -0.67613300,-0.14670300,-1.74421500
H -4.24856600,-2.54695700,1.33943200
H -5.05635200,-1.95273700,-0.10941500
H -3.72762900,-3.12684800,-0.26258800
H 1.22674400,-0.79724100,1.50722700
H -0.26914700,-1.72173600,1.38071700
H 1.24036300,-4.00377100,-0.62780200
H 1.49990300,-5.03938700,0.79249000
H -0.07536700,-4.25864700,0.51903600

H 2.90239200,-3.92159800,2.41990500
H 2.73579100,-2.10307000,2.71023500
H 3.93513200,-0.61851100,0.61805200
H 4.94636600,1.35705700,1.73785800
H 2.49452900,3.96152900,-0.64287100
H 1.48799200,1.98941700,-1.76477300
H 5.39980300,3.79933900,1.67386800
H 4.40096900,4.87450800,0.67873700
H 3.79069600,4.27570600,2.22382700

TS2'

Opt @ B3LYP/6-311+G(d,p) in dichloroethane (SMD model)

SCF Done: E(RB3LYP) = -1742.618378a.u.

Zero-point correction = 0.435046Hartree/Particle

Sum of electronic and thermal Free Energies = -1742.244952a.u.

C 4.30962600,-1.58807900,0.48784400
C 5.27343700,-2.52077000,-0.26382700
C 2.95648100,-2.27556500,0.70434600
S 4.12667000,-0.11742700,-0.68177600
C 4.91871800,-1.17076700,1.83240000
C 0.88095700,0.24868200,-1.08734000
C 1.73603200,1.06677100,-0.19100100
C 3.01293000,1.06853900,0.15576500
C 3.66869400,2.08178100,1.06391800
C -0.80129500,1.89847700,-0.51384300
C 0.08007400,2.46479600,0.59668900
C 0.61789900,3.85688800,0.33645200
C -0.05074500,1.98473100,1.87239300
N -0.52959300,0.46269500,-0.67291500
C -3.03698600,-0.53118300,-0.47674700
C -4.22195700,0.15580800,-0.73125500
C -5.29505900,0.00766200,0.14969800
C -5.20013700,-0.82011900,1.27400400
C -3.99451100,-1.50596500,1.50103600
C -2.91573100,-1.37154000,0.63447400
C -6.36683100,-0.99306600,2.21689900
S -1.66477100,-0.38364000,-1.62126900
O -2.11752900,0.43117100,-2.75939900
O -1.08190800,-1.71085400,-1.84434700
H 6.24756000,-2.04611800,-0.42346200
H 5.43266800,-3.43295000,0.32514500
H 4.86856200,-2.81378500,-1.23828400
H 2.23317400,-1.59119800,1.15996100

H 3.07784900,-3.13364900,1.37947700
H 2.54096700,-2.64312800,-0.23915600
H 5.12420700,-2.06455200,2.43712500
H 5.85930500,-0.62813500,1.69503100
H 4.23201800,-0.53973500,2.40517400
H 1.10433800,-0.81766400,-1.02270100
H 1.03553000,0.56200000,-2.13365900
H 2.92099700,2.70690200,1.55851400
H 4.27722500,1.59597000,1.83255600
H 4.34245100,2.72998000,0.48965300
H -1.85698600,2.02837300,-0.25346800
H -0.62451400,2.43946900,-1.45514900
H 1.21551300,4.22335100,1.17591700
H -0.21665200,4.55842000,0.19576100
H 1.23090800,3.89469500,-0.56930700
H -0.57911600,1.05721600,2.07020300
H 0.45096500,2.46216000,2.70902200
H -4.29800600,0.78740300,-1.60997000
H -6.22118700,0.54265100,-0.04465100
H -3.90504300,-2.15722400,2.36731500
H -1.99116400,-1.91224000,0.80784300
H -6.06033400,-0.85599800,3.26040300
H -7.16612500,-0.27757100,2.00195400
H -6.79241700,-2.00144900,2.13641400

INT3'

Opt @ B3LYP/6-311+G(d,p) in dichloroethane (SMD model)

SCF Done: E(RB3LYP) = -1742.658304a.u.

Zero-point correction = 0.436015Hartree/Particle

Sum of electronic and thermal Free Energies = -1742.28409a.u.

C 4.52732800,-1.48775400,0.42741400
C 4.82398600,-2.67453800,-0.50613900
C 3.48489800,-1.88702300,1.47694400
S 3.83558300,-0.17545100,-0.74602200
C 5.83473600,-1.01846000,1.08432600
C 0.79125500,0.18676000,-1.04689800
C 1.54164400,1.09882700,-0.09675000
C 2.84291600,0.96828800,0.22691200
C 3.56828000,1.82613700,1.23498700
C -0.76188400,1.80866100,-0.32243700
C 0.55582000,2.16978000,0.44598000
C 0.96091700,3.61247600,0.07934700
C 0.35290900,2.01844900,1.92439300

N -0.61168400,0.37570200,-0.60496400
C -3.16471400,-0.48681400,-0.46146000
C -4.29040400,0.31707600,-0.62790000
C -5.36574800,0.16938500,0.25001800
C -5.33185200,-0.77249700,1.28471400
C -4.18539800,-1.57286500,1.42462200
C -3.10512200,-1.44023900,0.55934400
C -6.50451700,-0.94595500,2.22025900
S -1.78974100,-0.33292100,-1.60089900
O -2.20054700,0.58722200,-2.67346800
O -1.27996900,-1.66890300,-1.92580300
H 5.52025300,-2.39246400,-1.30415500
H 5.28712000,-3.48646800,0.06902200
H 3.90964200,-3.05732700,-0.96944400
H 3.21610900,-1.04986500,2.12876200
H 3.89011600,-2.68734900,2.11032900
H 2.56924100,-2.25773300,1.00538900
H 6.27427600,-1.84192400,1.66370600
H 6.56352800,-0.70657700,0.32967500
H 5.67817900,-0.18005100,1.76837700
H 1.08180200,-0.85948400,-0.96567700
H 0.93060600,0.49452900,-2.09652700
H 2.87588300,2.43181300,1.82465100
H 4.13109200,1.20522700,1.93915300
H 4.29422900,2.48448900,0.74220300
H -1.65813800,1.99386900,0.27567700
H -0.83168500,2.39323400,-1.25228100
H 1.86245500,3.93105700,0.60873800
H 0.15431200,4.30745500,0.34446000
H 1.14864700,3.70560100,-0.99507000
H 0.10012800,1.04837300,2.33939900
H 0.32080900,2.88592500,2.57710500
H -4.32014200,1.03775500,-1.43812100
H -6.24599300,0.79480500,0.12403600
H -4.14372200,-2.31231700,2.22093400
H -2.22652100,-2.06812600,0.66410800
H -7.22466500,-0.12867500,2.11707800
H -7.03607300,-1.88424500,2.01573900
H -6.17934400,-0.98222200,3.26633500

TS3'

Opt @ B3LYP/6-311+G(d,p) in dichloroethane (SMD model)

SCF Done: E(RB3LYP) = -1742.64096a.u.

Zero-point correction = 0.437086Hartree/Particle

Sum of electronic and thermal Free Energies = -1742.264673a.u.

C -5.19016600,-1.34425800,-0.34568400
C -4.99057900,-2.69989300,0.32579500
C -5.07201100,-1.41622500,-1.86363500
S -3.80168600,-0.04878300,0.39708200
C -6.50208800,-0.69577800,0.08685100
C 0.02953800,2.03206800,0.51761900
C -1.28710300,1.27696100,0.58957000
C -2.52563600,1.70852100,0.72757500
C -3.18378300,3.01153100,0.97310000
C 0.22313300,-0.14143200,-0.55787600
C -1.04116000,-0.20883200,0.32528000
C -2.28044300,-0.76439200,-0.38800900
C -0.75019500,-0.96941800,1.63598600
N 0.97571400,0.97280400,0.06250600
C 3.54922400,0.22200400,-0.29137600
C 3.97539500,-0.68360100,-1.26055800
C 4.90754700,-1.66289100,-0.91212700
C 5.42182300,-1.74389000,0.38693400
C 4.97832300,-0.81313200,1.34173100
C 4.05023200,0.16848800,1.01283900
C 6.44492200,-2.79099700,0.75756700
S 2.37100600,1.50145500,-0.72710600
O 2.19819300,1.46120100,-2.18760700
O 2.75051100,2.75098600,-0.05848100
H -5.03693400,-2.61597800,1.41621500
H -5.78319700,-3.39437300,0.00641700
H -4.03384200,-3.16134000,0.05788800
H -5.15284900,-0.42279000,-2.31743000
H -5.88167900,-2.03939300,-2.27246400
H -4.12639200,-1.86546900,-2.18523800
H -7.35050300,-1.32311400,-0.22054500
H -6.55119500,-0.57837700,1.17535100
H -6.62994200,0.29134300,-0.37026300
H 0.37023800,2.42768300,1.47936100
H -0.03223500,2.87217900,-0.18594600
H -2.45476400,3.83245200,1.02862900
H -3.90165200,3.24605700,0.17722900
H -3.74496800,2.99955300,1.91687700
H 0.82645400,-1.05445500,-0.52682900
H -0.03239600,0.07928500,-1.60374200
H -2.32745200,-1.85431600,-0.31983000
H -2.27258300,-0.47724600,-1.44440800
H 0.11655100,-0.54059700,2.14824300

H -0.53364000,-2.02555000,1.42961100
H 3.58697800,-0.61071200,-2.27075800
H 5.24252800,-2.37141400,-1.66558300
H 5.37087200,-0.85830400,2.35490400
H 3.72017500,0.89243900,1.75060300
H 7.43119400,-2.33808400,0.92113800
H 6.17056000,-3.30691800,1.68498900
H 6.55252800,-3.54340300,-0.02952700
H -1.61244100,-0.91803000,2.30717000

INT4

Opt @ B3LYP/6-311+G(d,p) in dichloroethane (SMD model)

SCF Done: E(RB3LYP) = -1742.675333a.u.

Zero-point correction = 0.435536Hartree/Particle

Sum of electronic and thermal Free Energies = -1742.310505a.u.

C 4.80911900,-2.88123900,0.18270400
C 4.53690400,-3.15161300,-1.26622200
C 4.33200500,-3.87339900,1.19972200
S 3.74013700,1.56064900,-0.04179300
C 5.95263900,-1.97989900,0.53842800
C -0.24133200,2.42336800,-0.53322800
C 1.19063200,1.96284300,-0.45920500
C 2.35297000,2.62300300,-0.47021200
C 2.60822900,4.07004400,-0.76129200
C -0.04260500,0.30326100,0.67501100
C 1.25422100,0.47632200,-0.14323400
C 2.57459500,0.27684700,0.62553400
C 1.21495400,-0.37287500,-1.43142000
N -0.97230600,1.21780700,-0.03147700
C -3.36831900,-0.01239700,0.23276600
C -3.64719900,-0.95959200,1.21589400
C -4.35001600,-2.11416700,0.86667700
C -4.78209700,-2.32983800,-0.44701000
C -4.49197100,-1.35425600,-1.41572900
C -3.79234500,-0.19865200,-1.08637100
C -5.56234100,-3.56836000,-0.81811500
S -2.48486800,1.48606000,0.66710500
O -2.38503600,1.52732200,2.13389000
O -3.06180300,2.61431700,-0.07239200
H 4.63907500,-2.24506300,-1.87550200
H 5.24329300,-3.89273800,-1.68661800
H 3.53044400,-3.55980700,-1.42382100
H 4.30563700,-3.44294300,2.20869100

H 4.99446800,-4.75828200,1.25555100
H 3.32992600,-4.25241800,0.96189600
H 6.92794000,-2.49358600,0.43916000
H 5.99715100,-1.10042500,-0.11626500
H 5.89020100,-1.63125100,1.57679500
H -0.59409700,2.65424700,-1.54426700
H -0.41840200,3.31061200,0.08775100
H 1.66963100,4.60196300,-0.94678500
H 3.12568000,4.55670300,0.07410800
H 3.24246100,4.18993100,-1.64908900
H -0.44450900,-0.71491800,0.65288200
H 0.10289500,0.60562200,1.72104000
H 3.01897800,-0.71272700,0.48439800
H 2.44803000,0.46434200,1.69682100
H 0.29945000,-0.17703400,-1.99812200
H 1.24419900,-1.44231100,-1.18874900
H -3.32535300,-0.78445400,2.23688400
H -4.56923300,-2.85568400,1.63086100
H -4.82409100,-1.50309900,-2.44049200
H -3.58218900,0.55759600,-1.83557600
H -6.61938000,-3.33004400,-0.99337300
H -5.17813200,-4.02197900,-1.73886800
H -5.52054300,-4.32164900,-0.02560500
H 2.07474600,-0.14210200,-2.06853400

1k

Opt @ B3LYP/6-311+G(d,p) in dichloroethane (SMD model)

SCF Done: E(RB3LYP) = -1186.544676a.u.

Zero-point correction = 0.311474Hartree/Particle

Sum of electronic and thermal Free Energies = -1186.286879a.u.

C -1.51017200,-1.52176600,0.11475800
C -2.87990100,-1.71334500,-0.36297000
C -4.00363600,-1.89431900,-0.77165000
C -5.36846700,-2.11513800,-1.24279900
C -1.20607900,0.71875200,-0.92900700
C -1.53209200,2.18770700,-0.76290200
C -2.71334200,2.53025000,0.10522600
C -0.84115900,3.10229600,-1.45024800
N -1.19475600,-0.08485400,0.31584500
C 1.60411800,-0.10456100,0.58239800
C 2.24152600,0.92997300,-0.10723500
C 3.43219600,0.66407600,-0.78149500

C 3.99868500,-0.61839800,-0.77948600
C 3.34434300,-1.63518300,-0.06880500
C 2.15311300,-1.38935500,0.61061900
C 5.27503500,-0.90211400,-1.53495700
S 0.05398700,0.21806300,1.43263300
O 0.01023800,1.64874500,1.73128200
O -0.09279400,-0.79140400,2.48628900
H -0.80232700,-1.98461600,-0.59430000
H -1.38110700,-2.01575700,1.08030100
H -5.39073300,-2.36147400,-2.31113700
H -5.84476000,-2.93996000,-0.69935100
H -5.98542900,-1.22105000,-1.09325600
H -0.27068100,0.59212300,-1.49515700
H -2.00554000,0.26388500,-1.52679600
H -2.50125400,2.28597700,1.15066900
H -2.95567500,3.59511700,0.03845900
H -3.59916700,1.95089100,-0.18760600
H -1.10387200,4.15621900,-1.41839700
H 0.00992600,2.83277700,-2.07171300
H 1.81784900,1.92876100,-0.09186900
H 3.93550800,1.47001100,-1.31010400
H 3.77995100,-2.63093200,-0.03672700
H 1.66858200,-2.17198100,1.18491600
H 5.90437700,-0.00941500,-1.60853100
H 5.85928000,-1.69248900,-1.05257200
H 5.06000200,-1.23510300,-2.55911700

TS1

Opt @ B3LYP/6-311+G(d,p) in dichloroethane (SMD model)

SCF Done: E(RB3LYP) = -1742.625787a.u.

Zero-point correction = 0.434160Hartree/Particle

Sum of electronic and thermal Free Energies = -1742.258778a.u.

C -1.22489600,2.30524200,-1.03095400
C -0.18546500,3.20887100,-1.52267400
C 0.67454500,3.94268200,-1.95216800
C 1.70802500,4.83894200,-2.46389800
C 0.38010400,0.78584600,0.15464600
C 1.25017300,0.80731200,1.38589400
C 1.49654200,2.12961300,2.04512000
C 1.94230400,-0.33090000,1.74578400
N -0.82052400,1.64391900,0.23464000
C -2.73977400,-0.40128800,0.38633800

C -2.23608200,-1.65593700,0.73869200
C -2.71426000,-2.79002100,0.08400400
C -3.69216600,-2.69402400,-0.91556100
C -4.18646000,-1.42312000,-1.24478800
C -3.72130700,-0.27859600,-0.60153100
C -4.22866800,-3.93056600,-1.59606900
S -2.09944100,1.07173100,1.19230800
O -1.49626600,0.64647100,2.45670000
O -3.14400700,2.09780500,1.13554600
H -1.46534100,1.55912900,-1.80719900
H -2.13789500,2.86644000,-0.81670000
H 1.59979400,5.84922200,-2.05195900
H 2.70858800,4.47547200,-2.20142300
H 1.65886600,4.91532000,-3.55669200
H 0.12316400,-0.24602500,-0.12782700
H 0.97037500,1.19809000,-0.67420200
H 0.58493200,2.48210500,2.54109100
H 2.29464500,2.06000800,2.78977800
H 1.76908800,2.89418100,1.30495700
H 2.50815600,-0.34519900,2.67027400
H 1.60715800,-1.30014900,1.38759500
H -1.50036900,-1.73706100,1.53179800
H -2.32609900,-3.76736300,0.36016500
H -4.95332700,-1.32929000,-2.00987900
H -4.13053000,0.69731700,-0.84079100
H -5.13106200,-4.29673300,-1.08892000
H -4.50112200,-3.72906800,-2.63729800
H -3.49619600,-4.74391400,-1.58601100
S 3.92075700,-0.32722600,0.37027200
C 3.96759900,-2.02622900,-0.40099600
C 2.76572500,-2.24413800,-1.33327900
C 5.27047600,-2.05153700,-1.22498700
C 4.01904200,-3.11744800,0.67977900
H 2.84011900,-3.22363800,-1.82630900
H 1.81838700,-2.22455500,-0.78286900
H 2.72425200,-1.47168100,-2.10747000
H 5.37751200,-3.03022100,-1.71322700
H 6.14728100,-1.89184900,-0.58910300
H 5.26493100,-1.28154700,-2.00333500
H 3.11227500,-3.12133200,1.29446300
H 4.10870900,-4.10936100,0.21484600
H 4.87573800,-2.97021200,1.34442100

INT2

Opt @ B3LYP/6-311+G(d,p) in dichloroethane (SMD model)

SCF Done: E(RB3LYP) = -1742.634759a.u.
Zero-point correction = 0.434863Hartree/Particle
Sum of electronic and thermal Free Energies = -1742.266615a.u.

C -2.07726400,2.16289900,-0.47964500
C -1.53330200,3.41218200,-1.01225800
C -1.09683400,4.43980800,-1.47714100
C -0.57336000,5.68791600,-2.02619800
C 0.17406600,1.02532500,-0.27273900
C 1.37676900,1.23652600,0.59618100
C 1.69329200,2.60696400,1.10519300
C 2.33655800,0.12503100,0.80935600
N -1.09736800,1.45447100,0.37714500
C -2.46693700,-0.98497000,0.56293200
C -1.69327500,-2.11979600,0.30627900
C -2.23466300,-3.15899500,-0.44857800
C -3.54001100,-3.08681600,-0.95403900
C -4.30216400,-1.94482900,-0.66779300
C -3.77760300,-0.89646500,0.08489000
C -4.10828600,-4.20488000,-1.79487300
S -1.76729900,0.38186900,1.50103500
O -0.64452100,-0.15412400,2.27394400
O -2.88291900,1.08816800,2.13661800
H -2.41484300,1.52227700,-1.31177200
H -2.94794100,2.37802200,0.14603600
H -1.06686500,6.55808900,-1.57723700
H 0.50228900,5.78003100,-1.83430300
H -0.72293300,5.73994100,-3.11127500
H 0.11180100,-0.01640100,-0.61723100
H 0.24219800,1.64847500,-1.17514800
H 0.87156200,3.30360600,0.91669300
H 1.88256600,2.59544300,2.18828200
H 2.60366800,3.01201000,0.63341100
H 2.94229200,0.29842500,1.70358500
H -1.06686500,6.55808900,-1.57723700
H 0.50228900,5.78003100,-1.83430300
H -0.72293300,5.73994100,-3.11127500
H 0.11180100,-0.01640100,-0.61723100
H 0.24219800,1.64847500,-1.17514800
H 0.87156200,3.30360600,0.91669300
H 1.88256600,2.59544300,2.18828200
H 2.60366800,3.01201000,0.63341100
H 2.94229200,0.29842500,1.70358500
H 1.81366300,-0.83019800,0.91691200
H -0.69477400,-2.19687400,0.72236300

H -1.63554300,-4.04604600,-0.63926100
H -5.32565900,-1.88041500,-1.02919700
H -4.38566200,-0.03205800,0.32997000
H -3.65234500,-5.16771700,-1.54299700
H -5.19139700,-4.29538200,-1.66272700
H -3.92432400,-4.02597200,-2.86262300
S 3.49059000,-0.00175900,-0.66819900
C 4.58259700,-1.47585100,-0.28260900
C 3.74960400,-2.76183200,-0.18139000
C 5.53906400,-1.56216500,-1.48366200
C 5.37950200,-1.24131100,1.00863200
H 4.40991400,-3.62442700,-0.01819100
H 3.04675300,-2.72677500,0.65801500
H 3.17993200,-2.93528600,-1.09992700
H 6.22523300,-2.40824400,-1.34917300
H 6.13894000,-0.65107800,-1.58151000
H 4.99133700,-1.71545000,-2.41981200
H 4.72505200,-1.16593800,1.88354700
H 6.06427500,-2.08218000,1.18389600
H 5.97272600,-0.32374000,0.94456900

TS2

Opt @ B3LYP/6-311+G(d,p) in dichloroethane (SMD model)

SCF Done: E(RB3LYP) = -1742.617553a.u.

Zero-point correction = 0.435031Hartree/Particle

Sum of electronic and thermal Free Energies = -1742.245509a.u.

C 0.15555500,-0.32816100,-1.01077900
C -1.28879600,-0.64065400,-0.69281800
C -0.73722900,-1.61201600,1.25953800
C 0.72847200,-1.52491200,1.02945900
C -2.14864200,0.57608700,-0.46322200
C -1.64330200,-1.99861500,2.00628300
C -2.83660500,-2.38807200,2.74606800
S -3.71318100,0.23923500,0.46698700
C -4.92288500,1.47606900,-0.24871100
C -6.18457600,1.30310500,0.61390600
C -4.38777800,2.90911900,-0.11167200
C -5.24742600,1.15004200,-1.71402300
C -1.88957600,-1.79390700,-1.45182800
N 0.99550000,-1.37911800,-0.41003800
C 3.44906900,-0.03445300,-0.28623400
C 4.05005900,-0.06860500,0.97482400
C 4.67663100,1.07657800,1.46283400
C 4.71282200,2.26068700,0.71291100

C 4.11301700,2.26488600,-0.55460700
C 3.48188000,1.12946100,-1.05879500
C 5.37011200,3.50438200,1.26201900
S 2.60185400,-1.49308200,-0.90868500
O 3.16063000,-2.65347900,-0.21109400
O 2.57965700,-1.39622900,-2.36971900
H 0.34315300,-0.33680000,-2.09105100
H 0.43168900,0.66593600,-0.62001500
H 1.22413300,-2.43234500,1.37988700
H 1.13530400,-0.66813300,1.59588200
H -2.44435200,0.99970400,-1.43598300
H -1.58259400,1.34756200,0.06856700

INT3

Opt @ B3LYP/6-311+G(d,p) in dichloroethane (SMD model)

SCF Done: E(RB3LYP) = -1742.654178a.u.

Zero-point correction = 0.438220Hartree/Particle

Sum of electronic and thermal Free Energies = -1742.27581a.u.

C 0.06289700,0.62705300,1.06110000
C -1.28010700,0.95478800,0.35884200
C -0.81188200,1.25544700,-1.07929600
C 0.68837600,1.58064700,-1.05582300
C -2.21408200,-0.26737200,0.45774000
C -1.56676800,1.23047200,-2.15169400
C -1.53062900,1.44090700,-3.60640000
S -3.81863400,-0.04075200,-0.42008500
C -4.92306900,-1.32265100,0.39139900
C -6.22173700,-1.26406700,-0.42995300
C -4.30341600,-2.72395300,0.29557000
C -5.21432100,-0.95143600,1.85276900
C -1.90173300,2.21526700,0.99514100
N 1.01078700,1.52050300,0.38019700
C 3.34951400,-0.00005800,0.35913600
C 3.95376600,-0.10989400,-0.89469500
C 4.48516000,-1.33750600,-1.29110600
C 4.42415100,-2.45923600,-0.45491900
C 3.81942400,-2.32011600,0.80436400
C 3.28383200,-1.10330500,1.21689100
C 5.00408200,-3.78616500,-0.88359800
S 2.61618500,1.56212900,0.86120200
O 3.24598900,2.61603900,0.06288700
O 2.59981400,1.58732300,2.32532800
H 0.05238400,0.84499400,2.13049600
H 0.32661800,-0.43394200,0.91405500

H 0.92789100,2.57295700,-1.44571100
H 1.25312100,0.83485500,-1.63854000
H -2.42297800,-0.45874200,1.51640600
H -1.70429700,-1.14443000,0.04599100
H -2.20728300,2.25033300,-3.90898800
H -0.51935300,1.70676200,-3.95875100
H -1.84315500,0.53846000,-4.14704100
H -6.95172100,-1.97193700,-0.01781500
H -6.66773300,-0.26386400,-0.40001000
H -6.04311300,-1.52950700,-1.47723700
H -4.99888600,-3.46857500,0.70554100
H -3.37147800,-2.79817600,0.86620500
H -4.09035000,-2.99088800,-0.74455500
H -5.67384700,0.03914300,1.92305500
H -5.90404700,-1.68362600,2.29409000
H -4.30704200,-0.95066600,2.46661100
H -2.21813400,2.00979200,2.02572400
H -1.16944800,3.02817100,1.01843300
H -2.77514000,2.54584300,0.42841900
H 4.03107900,0.76341100,-1.53360500
H 4.96363700,-1.42133400,-2.26371600
H 3.77705400,-3.17543300,1.47486100
H 2.84521700,-0.99352100,2.20310400
H 5.43427500,-3.73026600,-1.88795400
H 5.79488900,-4.11366300,-0.19770000
H 4.23835200,-4.57154600,-0.88915000

TS3

Opt @ B3LYP/6-311+G(d,p) in dichloroethane (SMD model)

SCF Done: E(RB3LYP) = -1742.643258a.u.

Zero-point correction = 0.437378Hartree/Particle

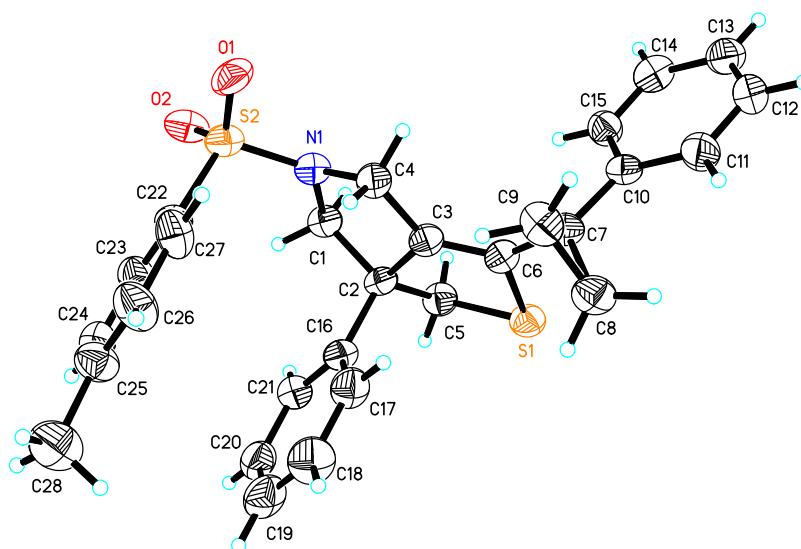
Sum of electronic and thermal Free Energies = -1742.265442a.u.

C 0.15013800,-1.04075600,-1.07765700
C -1.23828900,-1.16980700,-0.41122500
C -0.88937100,-0.89588400,1.05263200
C 0.54823500,-1.31425200,1.31517000
C -2.25156500,-0.10672400,-0.85453000
C -1.76919500,-0.28541500,1.82194300
C -1.83338300,0.15699600,3.23302700
S -3.47294500,0.17736300,0.51251300
C -4.92353300,1.14375900,-0.54348600
C -5.87556700,1.60276200,0.55738700
C -4.31898200,2.32550100,-1.29295200
C -5.59204300,0.13588200,-1.47392500

C -1.79277500,-2.59826600,-0.59297900
N 1.03726200,-1.62042700,-0.04941700
C 3.35153900,-0.08330400,-0.22645200
C 3.82825900,0.39872800,0.99536000
C 4.31101000,1.70414900,1.07240800
C 4.32530700,2.54118900,-0.05193400
C 3.85422800,2.02889600,-1.26955400
C 3.36822400,0.72666600,-1.36556000
C 4.82474200,3.96292400,0.04711400
S 2.68004300,-1.74757800,-0.32705700
O 3.22254200,-2.50358500,0.80418700
O 2.82571400,-2.19409600,-1.71447200
H 0.25219100,-1.60631600,-2.00571700
H 0.38892700,0.01733900,-1.27298100
H 0.64754800,-2.20509400,1.94294100
H 1.11579200,-0.49960100,1.78915600
H -2.79228600,-0.41938100,-1.75140900
H -1.74408500,0.84108100,-1.06222300
H -2.63872800,-0.35918900,3.77214500
H -0.89355800,-0.04365900,3.76717200
H -2.04194100,1.23210400,3.30031300
H -6.74264500,2.11308200,0.11519900
H -6.25015600,0.75497100,1.14208500
H -5.38648700,2.30269800,1.24343500
H -5.11582800,2.90258700,-1.78585600
H -3.62125900,2.00741400,-2.07492400
H -3.78923100,3.00053400,-0.61232000
H -5.98145600,-0.72306200,-0.91839000
H -6.43700600,0.61298900,-1.99433200
H -4.90964100,-0.23616600,-2.24582000
H -2.00131500,-2.79883000,-1.65152800
H -1.06927800,-3.34206500,-0.24554200
H -2.72064500,-2.72268600,-0.02705700
H 3.84964000,-0.25603400,1.86003400
H 4.69385000,2.07516200,2.02012700
H 3.87940500,2.65487600,-2.15837600
H 3.03605000,0.32558200,-2.31732000
H 4.00246800,4.65398500,0.27600200
H 5.57116200,4.07144600,0.84057100
H 5.27618500,4.29584200,-0.89321600

X-Ray structures

Compound 3e



The crystal data of **3e** have been deposited in CCDC with number 2222581. Empirical Formula: $C_{28}H_{27}NO_2S_2$; Formula Weight: 473.62; Crystal Color, Habit: colorless, Crystal Dimensions: 0.200 x 0.140 x 0.080 mm³; Crystal System: Orthorhombic; Lattice Parameters: $a = 12.067(2)$ Å, $b = 10.6363(17)$ Å, $c = 37.466(5)$ Å, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 4808.6(14)$ Å³; Space group: Pbc_2a ; $Z = 8$; $D_{calc} = 1.308$ g/cm³; $F_{000} = 2000$; Final R indices [$I > 2\sigma(I)$] $R1 = 0.0797$, $wR2 = 0.2101$.

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