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Supporting Information

Palladium/Et_3N·HI-Catalyzed Highly Selective 7-Endo Alkyl-Heck-Type Reaction of Epoxides and DFT Study on the Mechanism

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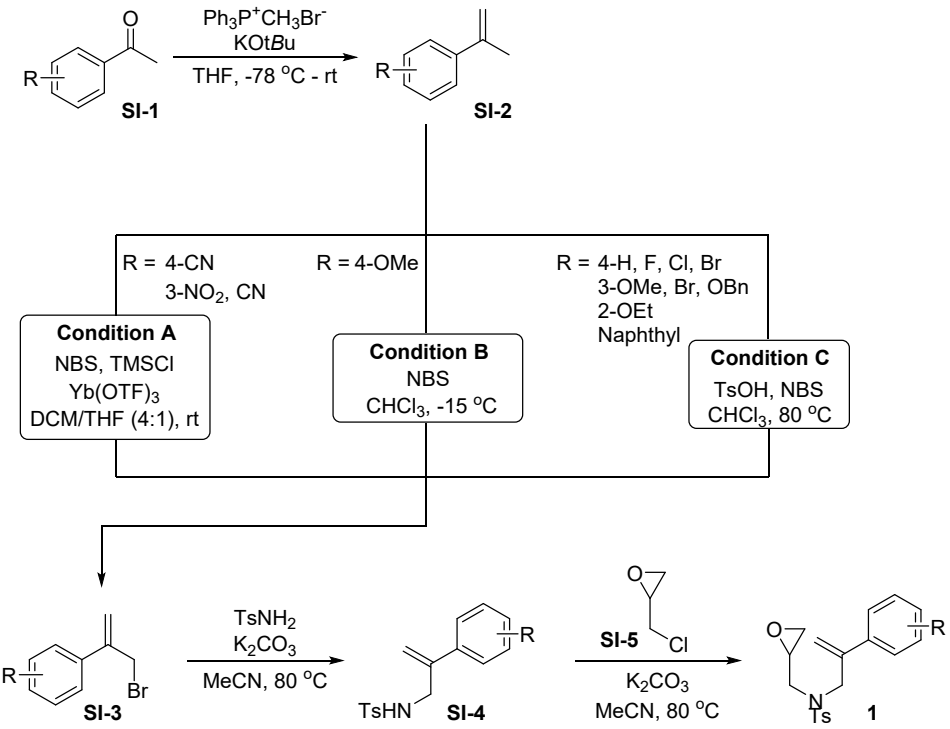
1. General Information

Organic solvents (Aldrich) were used without further purification. Purifications of reactions products were carried out by flash chromatography using Merck silica gel (40-63 μm). ^{1}H NMR (400 MHz), ^{13}C NMR (100 MHz) were measured on a Brucker Avance 400 MHz spectrometer. Chemical shifts are reported in parts per million (ppm, δ) downfield from residual solvents peaks and coupling constants are reported as Hertz (Hz). Splitting patterns are designated as singlet (s), doublet (d), triplet (t), …. Splitting patterns that could not be interpreted or easily visualized are designated as multiplet (m). Electrospray mass spectra were obtained using an ESI/TOF Mariner Mass Spectrometer. Unless otherwise noted, all other commercially available reagents and solvents were used without further purification.

2. Preparation of Starting Material

General Procedure I:



Scheme S1 General Procedure I: schematic diagram for preparation of epoxides **1a-1n**

Preparation of styrene SI-2 (R = 4-Cl): Potassium *tert*-butoxide (0.93 g, 8.3 mmol) was added to the suspension of methyltriphenylphosphonium bromide (2.96 g, 8.3 mmol) in dry THF (30 mL) at -78°C condition. After 1 h stirring at -78°C condition, a solution of 4-chloroacetophenone (1.00 g, 6.4 mmol) in THF (5 ml) was added dropwise. Then the reaction mixture was stirred at room temperature for 1 h. The reaction mixture was diluted with petroleum ether and filtered, filtrate was concentrated. The compound **SI-2 (R = 4-Cl)** was obtained as colorless liquid by column chromatographic purification of the crude product using hexanes as eluent. Yield (0.82 g, 85%)

Preparation of bromide SI-3 (R = 3-NO_2), Condition A: The styrene **SI-2 (R = 3-NO_2)** (1.75 g, 10.7 mmol) was dissolved in a mixture solution of DCM (20 mL) and THF (5 mL) at rt. Then *N*-bromosuccinimide (2.09 g, 11.8 mmol), $Yb(OTf)_3$ (Ytterbium(III) trifluoromethanesulfonate hydrate, 0.34 g, 0.54 mmol), and TMSCl (58.7 mg, 0.54 mmol) was added successively. The reaction mixture was stirred at rt for 1 h, and then it was diluted with water (30 mL) and the mixture was extracted with DCM (3×20 mL). The combined organic layers were washed with brine, dried, filtered and evaporated to afford crude product under reduced pressure. Purification on silica gel (hexanes/EtOAc = 15:1) afforded the bromide **SI-3 (R = 3-NO_2)**. Yield (1.44 g, 56%)

Preparation of bromide SI-3 (R = 4-OMe), Condition B: The styrene **SI-2 (R = 4-OMe)** (2.0 g, 13.5 mmol) was dissolved in 30 mL $CHCl_3$ at -15°C. Then *N*-bromosuccinimide (2.4 g, 13.5 mmol)

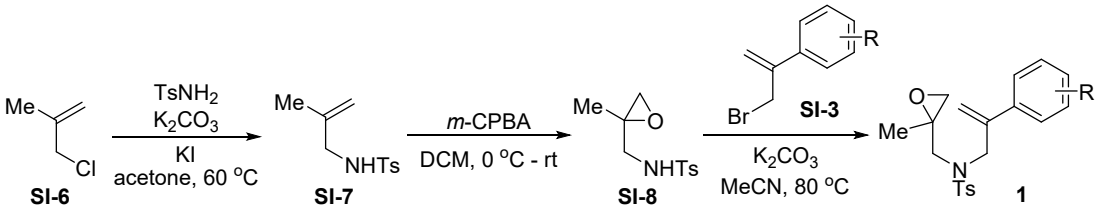
was added in batches during 2 min. The mixture was stirred at -15°C for 1.5 h. As reaction completed, the solvent was evaporated quickly *in vacuo*, and the compound **SI-3 (R = 4-OMe)** was obtained as a pale yellow oil by column chromatographic purification (hexanes/EtOAc = 20:1). Yield (0.98 g, 33%)

Preparation of bromide SI-3 (R = 4-Cl), Condition C: To a solution of **SI-2 (R = 4-Cl)** (0.82 g, 5.4 mmol) in 6 mL $CHCl_3$ was added *N*-bromosuccinimide (1.15 g, 6.5 mmol) and *p*-toluenesulfonic acid (0.09 g, 0.5 mmol). The mixture was stirred and heated to 80 °C under reflux for 3 h. After the concentration of the reaction liquid *in vacuo*, petroleum ether was added. The formed precipitate was filtered off and then the filtrate was dried over Na_2SO_4 and evaporated. The compound **SI-3 (R = 4-Cl)** was obtained as pale yellow liquid by column chromatographic purification of the crude product using hexanes as eluent. Yield (0.97 g, 77%)

Preparation of amine SI-4 (R = 4-Cl): The bromide **SI-3 (R = 4-Cl)** (0.97 g, 4.2 mmol) was dissolved in 25 mL acetonitrile, and then *p*-toluenesulfonamide (1.80 g, 10.5 mmol), K_2CO_3 (1.45 g, 10.5 mmol) was added successively. The resulting mixture was stirred and refluxed at 80 °C for 3.5 h. After successive filtration and purification by column chromatography (hexanes/EtOAc = 5:1), alcohol **SI-4 (R = 4-Cl)** was obtained as a white solid. Yield (0.99 g, 75%)

Preparation of epoxide 1d (R = 4-Cl): The amine **SI-4 (R = 4-Cl)** (0.99 g, 3.1 mmol), (±)-epichlorohydrin **SI-5** (0.86 g, 9.3 mmol), and K_2CO_3 (1.08 g, 7.8 mmol) was added successively to 15 mL acetonitrile. The resulting mixture was stirred and refluxed at 80 °C for 9 h. The precipitate was removed by filtration, and the filtrate was concentrated *in vacuo*. The epoxide **1d** was obtained as a white solid by column chromatographic purification (hexanes/EtOAc = 10:1 to 5:1) of the crude product. Yield (0.96 g, 82%)

General Procedure II:



Scheme S2 General Procedure II: schematic diagram for preparation of epoxides **1o-1t**

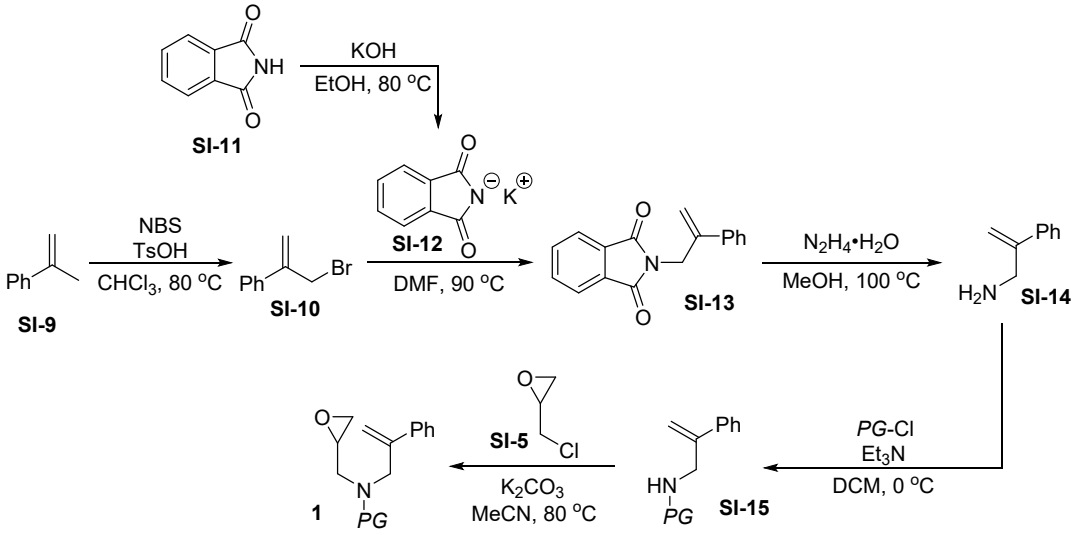
Preparation of alkene SI-7: Dropwise adding 3-chloro-2-methylpropene **SI-6** (0.91 g, 10 mmol) to the mixture of *p*-toluenesulfonamide (5.14 g, 30 mmol), K_2CO_3 (3.46 g, 25 mmol), KI (0.83 g, 5 mmol) and acetone (50 mL). The mixture was stirred and reflux at 60°C for 5 h. The precipitate that had formed was filtered off and then organic layer was dried over anhydrous Na_2SO_4 and evaporated. The crude product was purified by column chromatography (hexanes/EtOAc = 15:1) to give the **SI-7** as a white solid. Yield (1.53 g, 68%)

Preparation of epoxide SI-8: The alkene **SI-7** (1.0 g, 4.4 mmol) was dissolved in DCM (30 mL) at 0°C under N_2. Then the *m*-CPBA 85% (1.08 g, 5.3 mmol) was added and the resulting mixture was stirred for 2 h at 0°C. The reaction was quenched with saturated aqueous sodium thiosulfate solution (10 mL). It was extracted with DCM (3×10 mL) and the combined extract was washed with saturated sodium bicarbonate solution (20 mL) and brine (20 mL) and finally dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure and the residue obtained was purified by column chromatography (hexanes/EtOAc = 5:1) to yield epoxide **SI-8**. Yield (0.92 g, 87%)

Preparation of bromide SI-3: See Procedure I, Preparation of bromide **SI-3**.

Preparation of epoxide 1o: The epoxide **SI-8** (0.51 g, 2.1 mmol), bromide **SI-3 (R = H)** (0.63 g, 3.2 mmol), and K_2CO_3 (0.58 g, 4.2 mmol) was added successively to 10 mL acetonitrile. The resulting mixture was stirred and refluxed at 80 °C for 4 h. The precipitate was removed by filtration, and the filtrate was concentrated *in vacuo*. Epoxide **1o** was obtained as a white solid by column chromatographic purification (hexanes/EtOAc = 8:1 to 5:1) of the crude product. Yield (0.62 g, 83%)

General Procedure III:



Scheme S3 General Procedure III: schematic diagram for preparation of epoxides **1u-1w**

Preparation of bromide SI-10: See Procedure I, Preparation of bromide **SI-3**, Condition C.

Preparation of imide SI-12: To a solution of KOH 84% (9.5 g, 169.7 mmol) in absolute ethanol (100 mL), phthalimide **SI-11** (17.5 g, 119 mmol) was added and the resulting mixture was refluxed at 80°C for 1 h. The reaction mixture was then cooled to ambient temperature and filtered under vacuum. After filtration, washings with absolute EtOH and drying, potassium phthalimide **SI-12** was obtained as a white solid and used in the next step without further purification. Yield (21.2 g, 96%)

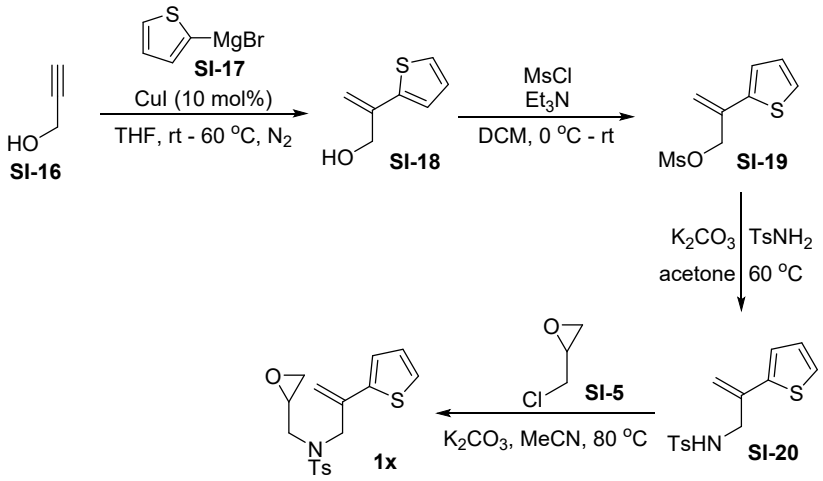
Preparation of imide SI-13: To a solution of bromide **SI-10** (3.0 g, 15.0 mmol) in 40 mL DMF, potassium phthalimide **SI-12** (2.78 g, 15 mmol) was added and the resulting mixture was stirred at 90°C for 2 h. As reaction completed, the reaction mixture was then cooled to ambient temperature and diluted with EtOAc (100 mL). Washings with water (4×25 mL), brine (30 mL), drying, and concentration *in vacuo* afforded the crude product, which purified by column chromatography (hexanes/EtOAc = 10:1 to 8:1) to give the imide **SI-13** as a white solid. Yield (2.5 g, 63%)

Preparation of amine SI-14: Compound **SI-13** (2.5 g, 9.5 mmol) was dissolved in MeOH (35 mL). Hydrazine hydrate 85% (1.4 mL, 23.7 mmol) was added and the reaction mixture was heated to reflux. While a white precipitate was formed (after ± 1 h), 20 mL of water was added and stirring was continued. After 4 hours, the mixture was concentrated *in vacuo* to remove most of the MeOH. The residue was dissolved in 30 mL H_2O, and transferred to a separation funnel. The water layer was extracted with CH_2Cl_2 (4×20 mL). The combined organic phases were washed with saturated $NaHCO_3$ solution (50 mL), brine (50 mL), dried over anhydrous Na_2SO_4, and concentrated under slightly reduced pressure at 35°C, yielding amine **SI-14** as a colorless oil. Yield (0.97 g, 77%)

Preparation of amine SI-15 (*PG* = Ms): To a solution of amine **SI-14** (0.97 g, 7.2 mmol) in DCM (10 mL.) was added triethylamine (1.0 mL, 7.2 mmol) and methanesulfonyl chloride (0.6 mL, 7.9 mmol) at 0 °C. The reaction mixture was allowed to stir at 0 °C for 1 hour and then gradually warmed up to room temperature over 1 hour. The resulting mixture was diluted with DCM (30 mL) and washed with saturated aqueous sodium bicarbonate solution (25 mL). The aqueous layer was extacted with DCM (3×10 mL) and the combined organic layers weredried over sodium sulfate, filtered and concentrated under reduced pressure. The amine **SI-15 (*PG* = Ms)** was obtained as a colorless oil and used in the next step without further purification. Yield (0.94 g, 62%)

Preparation of epoxide 1u (*PG* = Ms): The amine **SI-15 (*PG* = Ms)** (0.5 g, 2.4 mmol), (±)-epichlorohydrin **SI-5** (0.56 mL, 7.2 mmol), and K_2CO_3 (0.66 g, 4.8 mmol) was added successively to 10 mL acetonitrile. The resulting mixture was stirred and refluxed at 80 ^oC for 4 h. The precipitate was removed by filtration, and the filtrate was concentrated *in vacuo*. The epoxide **1u** was obtained as a white solid by column chromatographic purification (hexanes/EtOAc = 5:1 to 3:1) of the crude product. Yield (0.57 g, 89%)

General Procedure IV:



Scheme S4 General Procedure IV: schematic diagram for preparation of epoxide **1x**

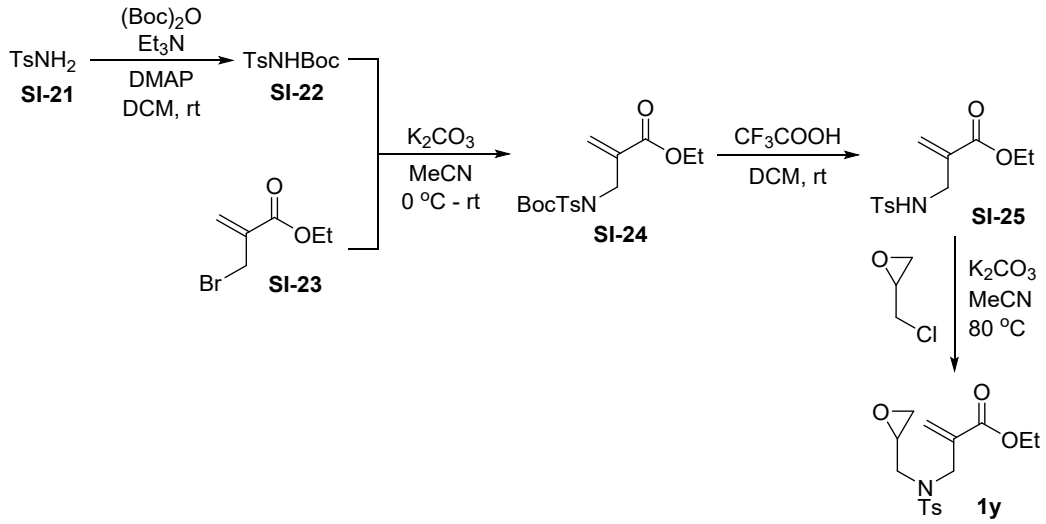
Preparation of alcohol SI-18: All of the following operations were carried out under a nitrogen atmosphere. In a 250 mL oven-dried three-necked round bottom flask, Mg (1.08 g, 44.5 mmol) and dry THF (5 mL) was added under nitrogen atmosphere. Then 0.2 mL of 2-bromothiophene was added by a syringe. The mixture was heated at 70°C until the colorless solution turned to light taupe, then the hot plate was removed. A solution of 2-bromothiophene (4.4 mL, 44.5 mmol) in dry THF (60 mL) was added dropwise. The resulting mixture was stirred at room temperature for 2 h, until the Mg was completely consumed, to give the solution of Grignard reagent of 2-bromothiophene **SI-17**. Then CuI (342.8 mg, 1.8 mmol) was added to the Grignard reagent, and the suspension was stirred for 30 min at ambient temperature. A solution of propargyl alcohol **SI-16** (1.1 mL, 17.8 mmol) in dry THF (40 mL) was added dropwise to the mixture by a constant pressure dropping funnel over 20 min. As the dropping was completed, the resulting mixture was heated to 70 °C and refluxed for 5 h. Then the mixture was cooled to ambient temperature and quenched slowly with NH_4Cl (80 mL, saturated aq.). The reaction mixture was transferred to a separating funnel, and EtOAc (80 mL) was added. The aqueous layer was extracted with EtOAc (3×50 mL). The combined organic layers were washed with brine (60 mL), dried with Na_2SO_4, and concentrated *in vacuo*. Purification by column chromatography (hexanes/EtOAc = 5:1) afforded the alcohol **SI-18** as a pale yellow liquid. Yield (0.77 g, 31%)

Preparation of alkene SI-19: The alcohol **SI-18** (0.49 g, 3.5 mmol) was dissolved in DCM (15 mL) at 0°C, then the methanesulfonyl chloride (0.33 mL, 4.2 mmol) and triethylamine (0.58 mL, 4.2 mmol) was added dropwise in sequence. The reaction mixture was gradually warmed to room temperature, and stirred for 2 hours. The reaction mixture was quenched with $NaHCO_3$ (saturated aq.), the organic phase was isolated, dried with Na_2SO_4, filtered, evaporated, purified by column chromatography (hexanes/EtOAc = 6:1) to afford alkene **SI-19** as a yellow oil. Yield (0.60 g, 79%) (Note: this compound should be used as soon as possible for it is easy to deteriorate)

Preparation of amine SI-20: The alkene **SI-19** (379.0 mg, 1.7 mmol) was dissolved in acetone (15 mL), and then *p*-toluenesulfonamide (582.1 mg, 3.4 mmol), K_2CO_3 (469.9 mg, 3.4 mmol) was added successively. The resulting mixture was stirred and refluxed at 60 ^oC for 4 h. After successive filtration, concentration, and purification by column chromatography (hexanes/EtOAc = 6:1), amine **SI-20** was obtained as a white solid. Yield (328.2 mg, 66%). **^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):** 7.75 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.18 (d, *J* = 5.2 Hz, 1H), 6.97-6.94 (m, 2H), 5.42 (s, 1H), 5.09 (s, 1H), 4.65 (t, *J* = 6.0 Hz, 1H), 3.96 (d, *J* = 6.4 Hz, 2H), 2.44 (s, 3H).

Preparation of epoxide 1x: SI-20 (328.2 mg, 1.1 mmol). (See Procedure I, Preparation of epoxide **1d**.) Yield of **1x** (268.2 mg, 70%)

General Procedure V:



Scheme S5 General Procedure V: schematic diagram for preparation of epoxides **1y**

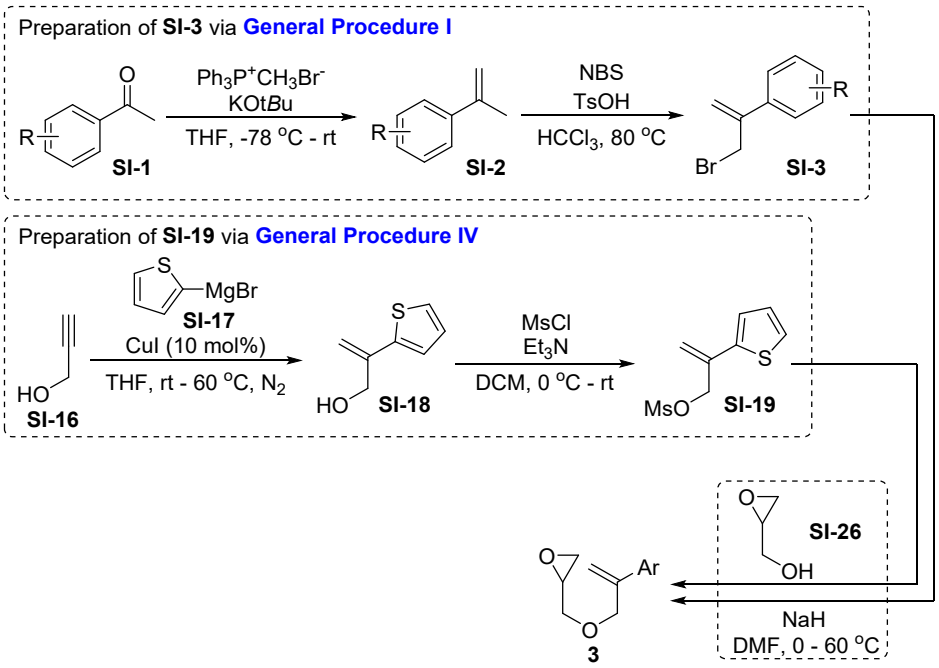
Preparation of amine SI-22: *p*-Toluenesulfonamide **SI-21** (17.1 g, 100 mmol) was dissolved in 100 mL CH_2Cl_2, and Et_3N (12.1 g, 120 mmol) and 4-dimethylaminopyridine (1.2 g, 10 mmol) were added under stirring successively. The mixture was stirred for 5 min, and then a solution of $(Boc)_2O$ (24.0 g, 110 mmol) in 20 mL CH_2Cl_2 was added dropwise via a constant pressure funnel. The resulting mixture was further stirred for 5 h at room temperature. The reaction mixture was quenched with NH_4Cl (50 mL saturated aq.) and 50 mL 1N hydrochloric acid, the organic phase was isolated, dried with Na_2SO_4, filtered, and evaporated. Purification by recrystallization (EtOAc and hexanes) afforded **SI-22** as a white acicular crystal. Yield (20.5 g, 77%)

Preparation of compound SI-24: Amine **SI-22** (1.69 g, 6.2 mmol) and K_2CO_3 (1.44 g, 10.4 mmol) were added into CH_3CN (20 mL), and the mixture was stirred for five minutes. Then the mixture was cooled to 0 °C, and bromide **SI-23** (0.71 mL, 5.2 mmol) was added. Until the reaction was completed, the crude product was purified by flash chromatography on silica gel (hexanes/EtOAc = 7:1) to give the desired product **SI-24** as a colorless oil. Yield (1.74 g, 92%)

Preparation of compound SI-25: A solution of compound **SI-24** (1.74 g, 4.5 mmol) in 15 mL CH_2Cl_2 was added CF_3COOH (1.68 mL, 22.7 mmol) at room temperature. The mixture was stirred for 3 h until the reaction was completed. After 10 mL water was added into the mixture, the K_2CO_3 was added slowly until no more bubbles released. The aqueous layer was extracted with CH_2Cl_2 (3×10 mL). The combined organic layers were washed with brine (20 mL), dried with Na_2SO_4, and concentrated *in vacuo*. Purification by column chromatography (hexanes/EtOAc = 4:1) afforded the alcohol **SI-25** as a pale yellow oil. Yield (0.93 g, 72%)

Preparation of epoxide 1y: SI-25 (283.5 mg, 1.0 mmol). (See Procedure I, Preparation of epoxide **1d**.) Yield of **1y** (231.3 mg, 68%)

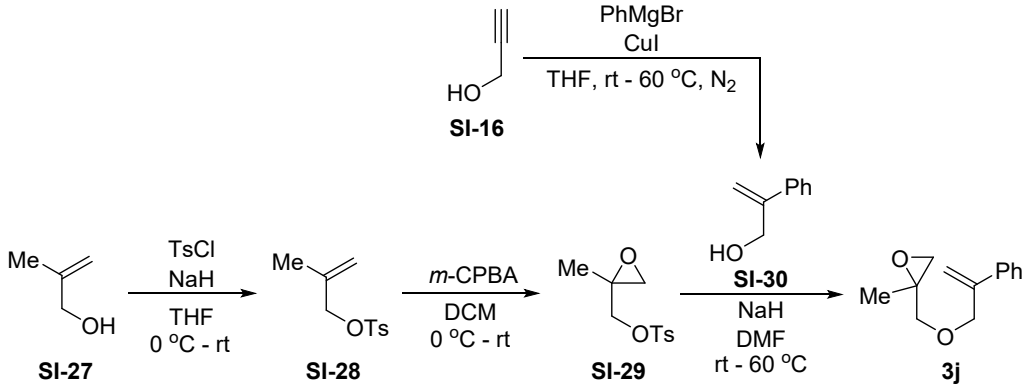
General Procedure VI:



Scheme S5 General Procedure VI: schematic diagram for preparation of epoxides **3a-3i**

Preparation of epoxide 3d (Ar = 4-F-C_6H_4): Under nitrogen atmosphere, to a suspension of NaH 60% (192.0 mg, 4.8 mmol) in dry *N,N*-dimethylformamide (10 mL) at 0 °C, the glycidol **SI-26** (0.26 mL, 4.0 mmol) was added and massive bubbles were released. The reaction mixture was keep stirring at 0°C for another 20 min after the bubble stopped forming. Then compound **SI-3 (R = 4-F)** (1.03 g, 4.8 mmol) was added, and the resulting mixture was warm to room temperature and stirred for 1 h. As reaction completed, the reaction mixture was diluted with EtOAc (50 mL). Washings with water (4×10 mL), brine (10 mL), drying, and concentration *in vacuo* afforded the crude product, which purified by column chromatography (hexanes/EtOAc = 15:1 to 10:1) to give the epoxide **3d** as a colorless oil. Yield (557.6 mg, 67%)

General Procedure VII:



Scheme S6 General Procedure VII: schematic diagram for preparation of epoxides **3j**

Preparation of alkene SI-28: To a solution Under nitrogen atmosphere, to a suspension of NaH 60% (0.717 g, 18 mmol) in dry THF (20 mL) at 0°C, the methallyl alcohol **SI-27** (1.2 mL, 14 mmol) was added slowly and massive bubbles were released. The reaction mixture was keep stirring at 0°C for another 20 min after the bubble stopped forming. The TsCl (2.67 g, 14 mmol) was dissolved in 10 mL THF and added dropwise, the resulting mixture was gradually warmed to rt and stirred for 2 h. As reaction completed, the reaction mixture was quenched with 40 mL water and extracted with EtOAc (3×30 mL). The combined organic layer was washed with brine (40 mL), drying, and concentrated *in vacuo* afforded the crude product, which was used without further purification. Yield (2.57 g, 82%)

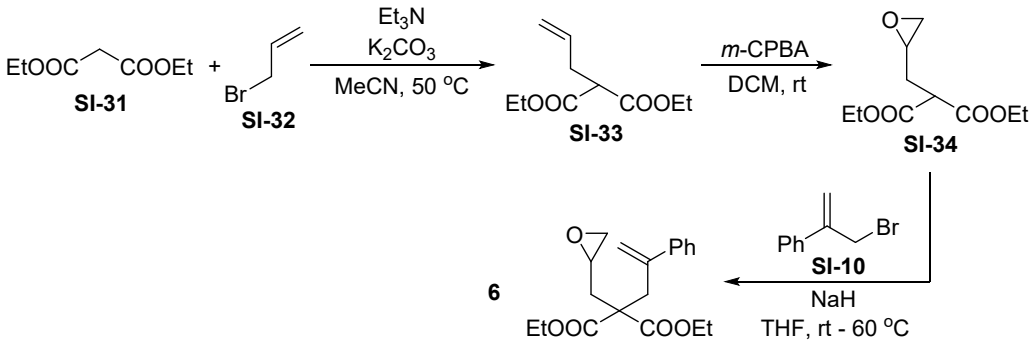
Preparation of epoxide SI-29: The alkene **SI-28** (1.22 g, 5.4 mmol) was dissolved in DCM (30 mL) at 0°C under N_2. Then the *m*-CPBA 85% (1.16 g, 6.75 mmol) was added and the resulting mixture was warmed to room temperature and stirred for 3 h. The reaction was quenched with saturated aqueous sodium thiosulfate solution (10 mL). Then the mixture was extracted with DCM (3×10 mL) and the combined extract was washed with saturated sodium bicarbonate solution (20 mL) and brine (20 mL) and finally dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure and the residue obtained was purified by column chromatography (hexanes/EtOAc = 10:1 to 5:1) to yield epoxide **SI-29**. Yield (0.98 g, 75%)

Preparation of alcohol SI-30: To a solution of propargyl alcohol **SI-16** (1.0 g, 18 mmol) in dry THF (40 mL) was vacuum purged three times, backfilling with N_2. CuI (0.343g, 1.8 mmol) was added under stirring and N_2 atmosphere. The suspension was cooled to –78°C. Then a solution of PhMgBr (8.2 g, 45 mmol) in 60 mL THF was added dropwise by constant pressure funnel under vigorous stirring. The resulting mixture held at –78°C for 1 h. Then it was warmed to room temperature and stirred for 18 h. The mixture was cooled to –78°C again and quenched slowly with H_2O (10 mL). After the suspension was warmed to room temperature, dilute HCl solution (1 N, 150 mL) was added and the aqueous layer was extracted with EtOAc (3×50 mL). The combined organic layers were washed brine (40 mL), dried with Na_2SO_4, and concentrated *in vacuo*. Purification by column chromatography (hexanes/EtOAc = 10:1 to 5:1) afforded the **SI-30**

as a light yellow liquid. Yield (2.33 g, 96%).

Preparation of epoxide 3j: Under nitrogen atmosphere, to a suspension of NaH 60% (57.6.0 mg, 2.4 mmol) in dry DMF (8 mL) at 0^{o}C, the alcohol **SI-30** (268.4 mg, 2.0 mmol) was added and massive bubbles were released. The reaction mixture was keep stirring at 0^{o}C for another 20 min after the bubble stopped forming. Then compound **SI-29** (581.5 mg, 2.4 mmol) was added, the resulting mixture was gradually heated to 60^{o}C and refluxed for 3 h. As reaction completed, the reaction mixture was diluted with EtOAc (40 mL). Washings with water (4×10 mL), brine (10 mL), drying, and concentration *in vacuo* afforded the crude product, which purified by column chromatography (hexanes/EtOAc = 20:1 to 10:1) to give the epoxide **3j** as a colorless oil. Yield (273.7 mg, 67%)

General Procedure VIII:



Scheme S7 General Procedure VIII: schematic diagram for preparation of epoxides **6**

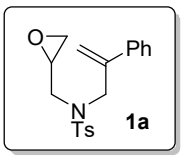
Preparation of olefin SI-33: The diethyl malonate **SI-31** (7.6 mL, 50 mmol), allyl bromide **SI-32** (8.6 mL, 100 mmol), Et_3N (6.9 mL, 50 mmol), and K_2CO_3 (17.3 g, 125 mmol) was added successively to 70 mL acetonitrile. The resulting mixture was stirred and refluxed at 50 °C overnight. The precipitate was removed by filtration, and the filtrate was concentrated *in vacuo*. The olefin **SI-33** was obtained as a colorless oil by column chromatographic purification (hexanes/EtOAc = 20:1 to 10:1) of the crude product. Yield (7.3 g, 73%)

Preparation of epoxide SI-34: The compound **SI-33** (3.1 g, 14.9 mmol) was dissolved in DCM (35 mL) at 0°C under N_2. Then the *m*-CPBA 85% (3.2 g, 18.6 mmol) was added and the resulting mixture was stirred for 2 h at 0°C. The reaction was quenched with saturated aqueous sodium thiosulfate solution (10 mL). It was extracted with DCM (3×10 mL) and the combined extract was washed with saturated sodium bicarbonate solution (20 mL) and brine (20 mL) and finally dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure and the residue obtained was purified by column chromatography (hexanes/EtOAc = 5:1) to yield **SI-34** as a colorless oil. Yield (2.35 g, 70%)

Preparation of epoxide 6: Under nitrogen atmosphere, to a suspension of NaH 60% (276.0 mg, 6.9 mmol) in dry THF (25 mL) at 0°C, the compound **SI-34** (1.5 g, 6.9 mmol) was added and massive bubbles were released. The reaction mixture was keep stirring at 0°C for another 20 min after the bubble stopped forming. Then bromine **SI-10** (2.0 g, 10.4 mmol) was added, the resulting mixture was gradually heated to 60°C and refluxed for 2 h. As reaction completed, the reaction mixture was diluted with EtOAc (50 mL). Washings with water (2×15 mL), brine (10 mL), drying, concentration *in vacuo*, and purification by column chromatography (hexanes/EtOAc = 10:1) gave the epoxide **6** as a colorless oil. Yield (1.71 g, 75%)

Analytical Data of Substrates:

4-methyl-*N*-(oxiran-2-ylmethyl)-*N*-(2-phenylallyl)benzenesulfonamide



$C_{19}H_{21}NO_3S$ **MW:** 343.44 g·mol^{-1}

The title compound was prepared according to **General Procedure I**.

Colorless Oil **Yield:** 82%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.67 (d, *J* = 8.0 Hz, 2H), 7.43 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.35-7.28 (m, 5H), 5.49 (s, 1H), 5.28 (s, 1H), 4.35-4.27 (m, 2H), 3.30 (dd, *J* = 15.2, 4.8 Hz, 1H), 3.09 (dd, *J* = 15.2, 5.6 Hz, 1H), 2.93-2.89 (m, 1H), 2.63 (t, *J* = 4.4 Hz, 1H), 2.43 (s, 3H), 2.40 (dd, 4.8, 2.4 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.5, 142.6, 138.1, 136.0, 129.7, 128.4, 128.0, 127.3, 126.4, 116.5, 52.4, 50.0, 49.6, 45.9, 21.5.

MS (EI) m/z 343 (M+)

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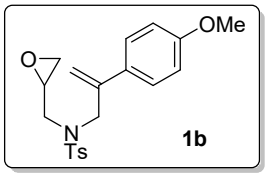
***N*-(2-(4-methoxyphenyl)allyl)-4-methyl-*N*-(oxiran-2-ylmethyl)benzenesulfonamide**



$C_{20}H_{23}NO_4S$ **MW:** 373.47 g·mol^{-1}

The title compound was prepared according to **General Procedure I**.

Colorless Oil **Yield:** 74%

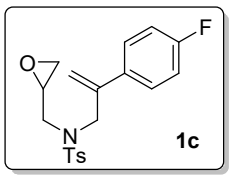
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.69 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 5.42 (s, 1H), 5.17 (s, 1H), 4.26 (s, 2H), 3.82 (s, 3H), 3.23 (dd, *J* = 15.2, 4.8 Hz, 1H), 3.11 (dd, *J* = 15.2, 5.2 Hz, 1H), 2.94-2.84 (m, 1H), 2.62 (t, *J* = 4.4 Hz, 1H), 2.44 (s, 3H), 2.41-2.38 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 159.5, 143.6, 141.9, 136.0, 130.4, 129.7, 127.7, 127.3, 115.1, 113.8, 55.3, 52.8, 50.0, 49.5, 46.2, 21.5.

MS (EI) m/z 373 (M+)

……

***N*-(2-(4-fluorophenyl)allyl)-4-methyl-*N*-(oxiran-2-ylmethyl)benzenesulfonamide**



$C_{19}H_{20}FNO_3S$ **MW:** 361.43 g·mol^{-1}

The title compound was prepared according to **General Procedure I**.

Colorless Oil **Yield:** 81%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.67 (d, *J* = 7.6 Hz, 2H), 7.44-7.40 (m, 2H), 7.30 (d, *J* = 7.6 Hz, 2H), 7.01 (t, *J* = 8.4 Hz, 2H), 5.44 (s, 1H), 5.26 (s, 1H), 4.27 (s, 2H), 3.33 (dd, *J* = 15.2, 4.8 Hz, 1H), 3.03 (dd, *J* = 15.2, 5.6 Hz, 1H), 2.91-2.86 (m, 1H), 2.64 (t, *J* = 4.4 Hz, 1H), 2.44 (s, 3H), 2.42-2.38 (m, 1H).

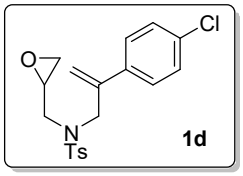
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 162.6 (d, *J* = 245.8 Hz), 143.7, 141.7, 135.9, 134.1 (d, *J* = 3.3 Hz), 129.8, 128.2 (d, *J* = 8.0 Hz), 127.3, 116.6, 115.3 (d, *J* = 21.3 Hz), 52.6, 50.0, 49.6, 45.8, 21.5.

^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): –113.9.

MS (EI) m/z 361 (M+)

……

***N*-(2-(4-chlorophenyl)allyl)-4-methyl-*N*-(oxiran-2-ylmethyl)benzenesulfonamide**

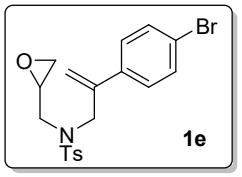


$C_{19}H_{20}ClNO_3S$ **MW:** 377.88 g·mol^{-1}
The title compound was prepared according to **General Procedure I**.
Colorless Oil **Yield:** 82%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.57 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.21-7.16 (m, 4H), 5.38 (s, 1H), 5.21 (s, 1H), 4.18 (s, 2H), 3.25 (dd, *J* = 15.2, 4.4 Hz, 1H), 2.93 (dd, *J* = 15.2, 5.6 Hz, 1H), 2.80-2.76 (m, 1H), 2.53 (t, *J* = 4.4 Hz, 1H), 2.33 (s, 3H), 2.30 (dd, *J* = 4.8, 2.8 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.6, 141.5, 136.4, 135.8, 133.7, 129.7, 128.4, 127.7, 127.1, 117.1, 52.4, 49.9, 49.5, 45.6, 21.4.
MS (EI) m/z 377 (M+)

……

***N*-(2-(4-bromophenyl)allyl)-4-methyl-*N*-(oxiran-2-ylmethyl)benzenesulfonamide**

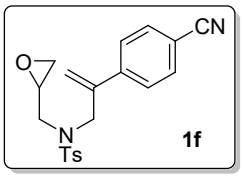


$C_{19}H_{20}BrNO_3S$ **MW:** 422.34 g·mol^{-1}
The title compound was prepared according to **General Procedure I**.
White Solid **Yield:** 60%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.66 (d, *J* = 8.0 Hz, 2H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.4 Hz, 4H), 5.48 (s, 1H), 5.30 (s, 1H), 4.27 (s, 2H), 3.35 (dd, *J* = 15.2, 4.0 Hz, 1H), 3.01 (dd, *J* = 15.2, 5.6 Hz, 1H), 2.92-2.86 (m, 1H), 2.64 (t, *J* = 4.4 Hz, 1H), 2.44 (s, 3H), 2.42-2.38 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.7, 141.7, 137.0, 136.0, 131.5, 129.8, 128.1, 127.2, 122.1, 117.3, 52.4, 50.0, 49.6, 45.7, 21.5.
MS (EI) m/z 421,423 (M+)

……

***N*-(2-(4-cyanophenyl)allyl)-4-methyl-*N*-(oxiran-2-ylmethyl)benzenesulfonamide**

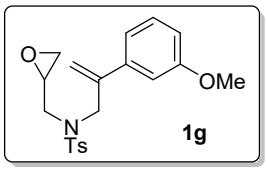


$C_{20}H_{20}N_2O_3S$ **MW:** 368.45 g·mol^{-1}
The title compound was prepared according to **General Procedure I**.
Colorless Oil **Yield:** 65%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.67 (d, *J* = 7.6 Hz, 2H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 5.60 (s, 1H), 5.45 (s, 1H), 4.31 (s, 2H), 3.47 (dd, *J* = 14.8, 2.8 Hz, 1H), 2.94-2.83 (m, 2H), 2.64 (t, *J* = 4.4 Hz, 1H), 2.45 (s, 3H), 2.41-2.37 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.9, 142.7, 141.5, 135.8, 132.2, 129.8, 127.2, 119.4, 118.7, 111.5, 52.2, 50.0, 49.8, 45.4, 21.5.
MS (EI) m/z 368 (M+)

……

***N*-(2-(3-methoxyphenyl)allyl)-4-methyl-*N*-(oxiran-2-ylmethyl)benzenesulfonamide**



$C_{20}H_{23}NO_4S$ **MW:** 373.47 g·mol^{-1}

The title compound was prepared according to **General Procedure I**.

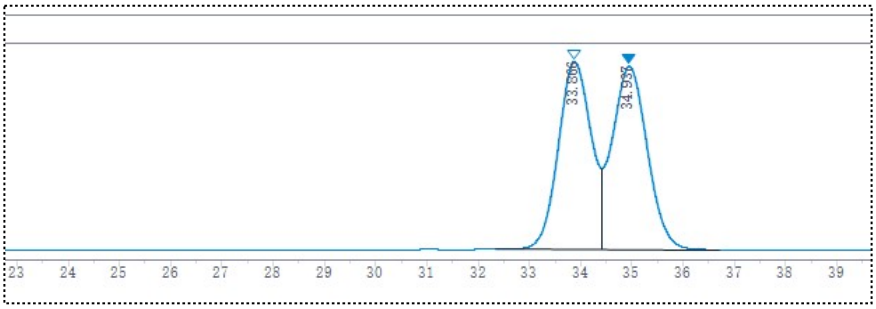
Colorless Oil **Yield:** 81%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.58 (d, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.16-7.12 (m, 1H), 6.94-6.93 (m, 2H), 6.75 (dd, *J* = 8.4, 2.0 Hz, 1H), 5.41 (s, 1H), 5.19 (s, 1H), 4.23 (d, *J* = 15.2 Hz, 1H), 4.18 (d, *J* = 15.2 Hz, 1H), 3.72 (s, 3H), 3.20 (dd, *J* = 15.2, 4.8 Hz, 1H), 3.00 (dd, *J* = 15.2, 6.0 Hz, 1H), 2.84-2.78 (m, 1H), 2.53 (t, *J* = 4.4 Hz, 1H), 2.32-2.30 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 159.6, 143.7, 142.6, 139.6, 136.1, 129.8, 129.4, 127.3, 118.9, 116.8, 113.9, 112.0, 55.3, 52.6, 50.0, 49.7, 46.0, 21.6.

MS (EI) m/z 373 (M+)

HPLC analysis CHIRALCEL AD-H column, 1.0 mL/min (5% *i*-PrOH in hexane), 254 nm UV detector, t_S = 33.9 min (peak area = 49.11%), t_R = 34.9 min (peak area = 50.89%).



Peak#	RT (min)	Area (mAU·s)	Area (%)	Starting (min)	Ending (min)
1	33.866	6126.979	49.11	32.331	34.404
2	34.937	6349.240	50.89	34.404	36.714

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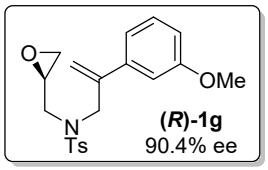
(*R*)-*N*-(2-(3-methoxyphenyl)allyl)-4-methyl-*N*-(oxiran-2-ylmethyl)benzenesulfonamide



$C_{20}H_{23}NO_4S$ **MW:** 373.47 g·mol^{-1}

The title compound was prepared according to **General Procedure I** (epichlorohydrin was instead by **(*S*)-(+)-epichlorohydrin**).

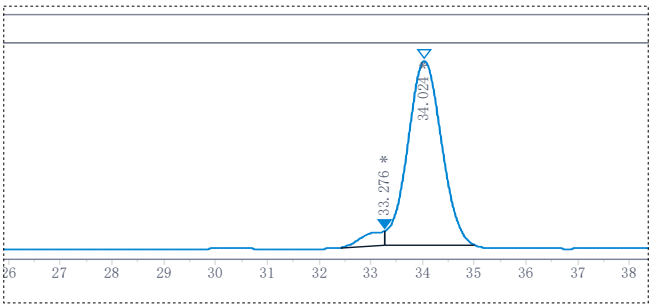
Colorless Oil **Yield:** 73%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.67 (d, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 7.6 Hz, 2H), 7.25-7.21 (m, 1H), 7.03-7.01 (m, 2H), 6.85 (d, *J* = 8.4 Hz, 1H), 5.50 (s, 1H), 5.28 (s, 1H), 4.34-4.25 (m, 2H), 3.83 (s, 3H), 3.30 (dd, *J* = 15.2, 4.4 Hz, 1H), 3.09 (dd, *J* = 15.6, 5.6 Hz, 1H), 2.95-2.88 (m, 1H), 2.67-2.62 (m, 1H), 2.43 (s, 3H), 2.42-2.39 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 159.6, 143.6, 142.6, 139.6, 136.1, 129.7, 129.4, 127.3, 118.9, 116.7, 113.9, 112.0, 55.3, 52.6, 50.0, 49.7, 46.0, 21.5.

MS (EI) m/z 373 (M+)

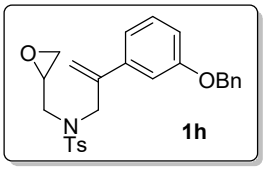
HPLC analysis CHIRALCEL AD-H column, 1.0 mL/min (5% *i*-PrOH in hexane), 254 nm UV detector, t_S = 33.2 min (peak area = 4.81%), t_R = 34.0 min (peak area = 95.19%).



Peak#	RT (min)	Area (mAU·s)	Area (%)	Starting (min)	Ending (min)
1	33.276	513.741	4.81	32.416	33.276
2	34.024	10165.683	95.19	33.276	34.992

……

***N*-(2-(3-(benzyloxy)phenyl)allyl)-4-methyl-*N*-(oxiran-2-ylmethyl)benzenesulfonamide**



$C_{26}H_{27}NO_4S$ **MW:** 449.57 g·mol^{-1}

The title compound was prepared according to **General Procedure I**.

Colorless Oil **Yield:** 69%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.67 (d, *J* = 7.6 Hz, 2H), 7.44 (d, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.2 Hz, 2H), 7.33-7.21 (m, 4H), 7.09 (s, 1H), 7.03 (d, *J* = 7.6 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 1H), 5.48 (s, 1H), 5.27 (s, 1H), 5.08 (s, 2H), 4.33-4.24 (m, 2H), 3.29 (dd, *J* = 15.2, 4.8 Hz, 1H), 3.08 (dd, *J* = 14.8, 5.6 Hz, 1H), 2.93-2.87 (m, 1H), 2.61 (t, *J* = 4.0 Hz, 1H), 2.40-2.37 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 158.7, 143.5, 142.4, 139.6, 136.9, 136.0, 129.7, 129.4, 128.5, 127.9, 127.5, 127.2, 119.1, 116.6, 114.6, 112.9, 69.9, 52.5, 49.9, 49.6, 45.9, 21.5.

MS (EI) m/z 449 (M+)

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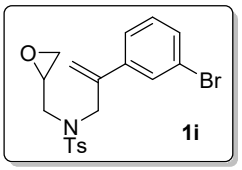
***N*-(2-(3-bromophenyl)allyl)-4-methyl-*N*-(oxiran-2-ylmethyl)benzenesulfonamide**



$C_{19}H_{20}BrNO_3S$ **MW:** 422.34 g·mol^{-1}

The title compound was prepared according to **General Procedure I**.

White Solid **Yield:** 73%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.66 (d, *J* = 8.0 Hz, 2H), 7.51 (s, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.19 (t, *J* = 7.6 Hz, 1H), 5.48 (s, 1H), 5.34 (s, 1H), 4.33-4.24 (m, 2H), 3.42 (dd, *J* = 15.2, 4.0 Hz, 1H), 3.01 (dd, *J* = 15.2, 6.0 Hz, 1H), 2.96-2.90 (m, 1H), 2.67 (t, *J* = 4.4 Hz, 1H), 2.43-2.39 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.7, 141.6, 140.5, 136.1, 131.0, 129.9, 129.8, 129.5, 127.2, 125.2, 122.5, 117.7, 52.2, 50.1, 49.7, 45.6, 21.5.

MS (EI) m/z 421, 423 (M+)

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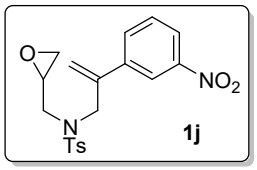
4-methyl-*N*-(2-(3-nitrophenyl)allyl)-*N*-(oxiran-2-ylmethyl)benzenesulfonamide

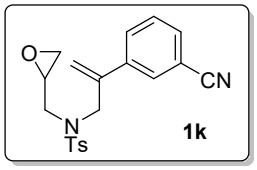


$C_{19}H_{20}N_2O_5S$ **MW:** 388.44 g·mol^{-1}
The title compound was prepared according to **General Procedure I**.
Light Yellow Solid **Yield:** 69%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.25 (s, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 7.6 Hz, 2H), 7.52 (t, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 7.6 Hz, 2H), 5.61 (s, 1H), 5.48 (s, 1H), 4.35 (s, 2H), 3.55 (d, *J* = 13.2 Hz, 1H), 2.96-2.87 (m, 2H), 2.67 (t, *J* = 3.6 Hz, 1H), 2.43-2.40 (m, 4H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 148.2, 143.9, 141.0, 140.0, 135.9, 132.6, 129.8, 129.4, 127.2, 122.7, 121.4, 119.1, 52.2, 50.0, 49.9, 45.2, 21.5.
MS (EI) m/z 388 (M+)

……

***N*-(2-(3-cyanophenyl)allyl)-4-methyl-*N*-(oxiran-2-ylmethyl)benzenesulfonamide**



$C_{20}H_{20}N_2O_3S$ **MW:** 368.45 g·mol^{-1}
The title compound was prepared according to **General Procedure I**.
Pale Yellow Oil **Yield:** 71%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.72-7.64 (m, 4H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.47-7.43 (m, 1H), 7.32 (d, *J* = 7.6 Hz, 2H), 5.53 (s, 1H), 5.43 (s, 1H), 4.30 (s, 2H), 3.53 (dd, *J* = 17.2, 6.0 Hz, 1H), 2.94-2.88 (m, 2H), 2.67 (t, *J* = 4.0 Hz, 1H), 2.45 (s, 3H), 2.43-2.39 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.9, 141.1, 139.6, 135.9, 131.4, 131.0, 130.1, 129.9, 129.3, 127.2, 118.7, 118.6, 112.6, 52.1, 50.0, 49.9, 45.3, 21.5.
MS (EI) m/z 368 (M+)

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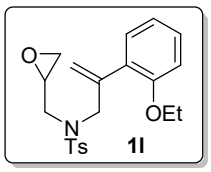
***N*-(2-(2-ethoxyphenyl)allyl)-4-methyl-*N*-(oxiran-2-ylmethyl)benzenesulfonamide**



$C_{21}H_{25}NO_4S$ **MW:** 387.49 g·mol^{-1}
The title compound was prepared according to **General Procedure I**.
Colorless Oil **Yield:** 80%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.55 (d, *J* = 8.0 Hz, 2H), 7.25-7.19 (m, 3H), 7.05 (d, *J* = 7.6 Hz, 1H), 6.86 (t, *J* = 7.2 Hz, 1H), 6.77 (d, *J* = 8.4 Hz, 1H), 5.36 (s, 1H), 5.22 (s, 1H), 4.35 (s, 2H), 3.97 (q, *J* = 6.8 Hz, 2H), 3.30 (dd, *J* = 15.2, 4.8 Hz, 1H), 3.23 (dd, *J* = 15.2, 5.2 Hz, 1H), 3.12-3.05 (m, 1H), 2.72 (t, *J* = 4.4 Hz, 1H), 2.51-2.48 (m, 1H), 2.39 (s, 3H), 1.40 (t, *J* = 6.8 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 155.9, 143.2, 143.1, 136.7, 130.3, 129.4, 129.0, 128.9, 127.1, 120.4, 117.7, 111.2, 63.5, 52.5, 50.2, 49.7, 46.0, 21.4, 14.7.
MS (EI) m/z 387 (M+)

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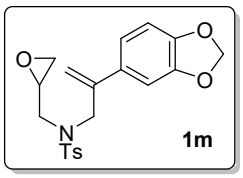
***N*-(2-(benzo[*d*][1,3]dioxol-5-yl)allyl)-4-methyl-*N*-(oxiran-2-ylmethyl)benzenesulfonamide**

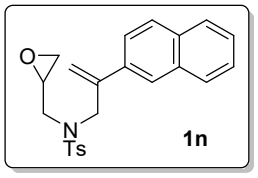


$C_{20}H_{21}ClNO_5S$ **MW:** 387.45 g·mol^{-1}
The title compound was prepared according to **General Procedure I**.
Colorless Oil **Yield:** 77%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.58 (d, *J* = 8.0 Hz, 2H), 7.18 (d, *J* = 8.4 Hz, 2H), 6.84-6.80 (m, 2H), 6.63 (d, *J* = 8.0 Hz, 1H), 5.82 (s, 2H), 5.28 (s, 1H), 5.09 (s, 1H), 4.17-4.08 (m, 2H), 3.20 (dd, *J* = 15.2, 4.4 Hz, 1H), 2.98 (dd, *J* = 15.2, 5.6 Hz, 1H), 2.84-2.77 (m, 1H), 2.53 (t, *J* = 4.4 Hz, 1H), 2.32-2.29 (m, 4H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 147.7, 147.5, 143.7, 142.1, 136.0, 132.3, 129.8, 127.3, 120.2, 115.7, 108.1, 107.0, 101.2, 52.7, 50.1, 49.6, 46.0, 21.5.
MS (EI) m/z 387 (M+)

……

4-methyl-*N*-(2-(naphthalen-2-yl)allyl)-*N*-(oxiran-2-ylmethyl)benzenesulfonamide

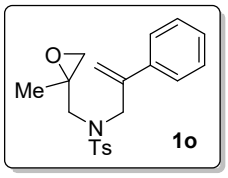


$C_{23}H_{23}NO_3S$ **MW:** 393.50 g·mol^{-1}
The title compound was prepared according to **General Procedure I**.
Colorless Viscous Oil **Yield:** 69%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.86 (s, 1H), 7.81-7.76 (m, 3H), 7.65 (d, *J* = 7.6 Hz, 2H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.47-7.45 (m, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 5.62 (s, 1H), 5.37 (s, 1H), 4.47-4.38 (m, 2H), 3.34 (dd, *J* = 15.2, 4.8 Hz, 1H), 3.12 (dd, *J* = 15.2, 5.6 Hz, 1H), 2.96-2.89 (m, 1H), 2.61 (t, *J* = 4.0 Hz, 1H), 2.43-2.39 (m, 1H), 2.37 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.5, 142.4, 136.0, 135.3, 133.1, 132.9, 129.6, 128.3, 127.9, 127.4, 127.2, 126.1, 126.1, 125.5, 124.4, 117.1, 52.5, 50.1, 49.5, 45.8, 21.4.
MS (EI) m/z 393 (M+)

……

4-methyl-*N*-((2-methyloxiran-2-yl)methyl)-*N*-(2-phenylallyl)benzenesulfonamide



$C_{20}H_{23}NO_3S$ **MW:** 357.47 g·mol^{-1}
The title compound was prepared according to **General Procedure II**.
Colorless Oil **Yield:** 83%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.64 (d, *J* = 8.0 Hz, 2H), 7.38-7.36 (m, 2H), 7.32-7.26 (m, 5H), 5.40 (s, 1H), 5.13 (s, 1H), 4.37 (d, *J* = 15.6 Hz, 1H), 4.21 (d, *J* = 15.6 Hz, 1H), 3.29 (d, *J* = 15.2 Hz, 1H), 3.12 (d, *J* = 14.8 Hz, 1H), 2.60 (d, *J* = 4.4 Hz, 1H), 2.52 (d, *J* = 4.4 Hz, 1H), 2.43 (s, 3H), 1.13 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.4, 142.6, 138.4, 136.2, 129.6, 128.3, 127.9, 127.3, 126.5, 116.4, 55.9, 53.3, 52.9, 52.7, 21.5, 18.8.
MS (EI) m/z 357 (M+)

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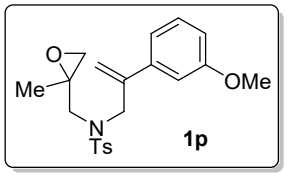
***N*-(2-(3-methoxyphenyl)allyl)-4-methyl-*N*-((2-methyloxiran-2-yl)methyl)benzenesulfonamide**



$C_{21}H_{25}NO_4S$ **MW:** 387.49 g·mol^{-1}
The title compound was prepared according to **General Procedure II**.
White Solid **Yield:** 80%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.54 (d, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 8.4 Hz, 2H), 7.13-7.09 (m, 1H), 6.88-6.86 (m, 2H), 6.75-6.72 (m, 1H), 5.32 (s, 1H), 5.06 (s, 1H), 4.28 (d, *J* = 15.6 Hz, 1H), 4.11 (d, *J* = 15.6 Hz, 1H), 3.72 (s, 3H), 3.20 (d, *J* = 14.8 Hz, 1H), 3.05 (d, *J* = 14.8 Hz, 1H), 2.50 (d, *J* = 4.4 Hz, 1H), 2.43 (d, *J* = 4.8 Hz, 1H), 2.32 (s, 3H), 1.06 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 159.4, 143.3, 142.4, 139.8, 136.1, 129.5, 129.2, 127.1, 118.9, 116.5, 113.6, 112.0, 55.8, 55.1, 53.1, 52.9, 52.8, 21.4, 18.8.
MS (EI) m/z 387 (M+)

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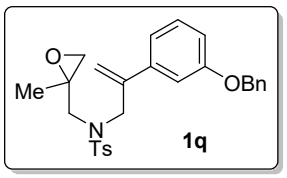
***N*-(2-(3-(benzyloxy)phenyl)allyl)-4-methyl-*N*-((2-methyloxiran-2-yl)methyl)benzenesulfonamide**



$C_{27}H_{29}NO_4S$ **MW:** 463.59 g·mol^{-1}
The title compound was prepared according to **General Procedure II**.
Colorless Viscous Oil **Yield:** 66%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.63 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.2 Hz, 2H), 7.33-7.30 (m, 1H), 7.25-7.17 (m, 3H), 7.01 (s, 1H), 6.97 (d, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 8.0 Hz, 1H), 5.39 (s, 1H), 5.13 (s, 1H), 5.07 (s, 2H), 4.36 (d, *J* = 15.6 Hz, 1H), 4.18 (d, *J* = 16.0 Hz, 1H), 3.28 (d, *J* = 14.8 Hz, 1H), 3.12 (d, *J* = 14.8 Hz, 1H), 2.58 (d, *J* = 4.4 Hz, 1H), 2.50 (d, *J* = 4.8 Hz, 1H), 2.39 (s, 3H), 1.14 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 158.6, 143.4, 142.4, 139.9, 136.9, 136.2, 129.6, 129.3, 128.5, 127.9, 127.5, 127.2, 119.2, 116.5, 114.5, 113.0, 69.9, 55.9, 53.2, 52.8, 21.4, 18.8.
MS (EI) m/z 463 (M+)

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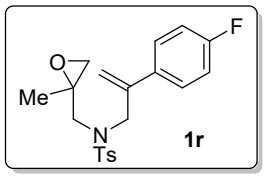
***N*-(2-(4-fluorophenyl)allyl)-4-methyl-*N*-((2-methyloxiran-2-yl)methyl)benzenesulfonamide**



$C_{20}H_{22}FNO_3S$ **MW:** 375.46 g·mol^{-1}
The title compound was prepared according to **General Procedure II**.
White Solid **Yield:** 81%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.63 (d, *J* = 7.6 Hz, 2H), 7.37-7.33 (m, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 6.97 (t, *J* = 8.4 Hz, 2H), 5.36 (s, 1H), 5.14 (s, 1H), 4.32 (d, *J* = 15.6 Hz, 1H), 4.18 (d, *J* = 15.2 Hz, 1H), 3.23 (d, *J* = 14.8 Hz, 1H), 3.16 (d, *J* = 15.2 Hz, 1H), 2.59 (d, *J* = 4.4 Hz, 1H), 2.53 (d, *J* = 4.4 Hz, 1H), 2.43 (s, 3H), 1.13 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 162.5 (d, *J* = 245.6 Hz), 143.5, 141.7, 136.1, 134.5 (d, *J* = 3.3 Hz), 129.6, 128.3 (d, *J* = 7.9 Hz), 127.3, 116.6, 115.2 (d, *J* = 21.3 Hz), 56.0, 53.1, 52.8, 21.5, 18.9.
^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): –114.1.

MS (EI) m/z 375 (M+)

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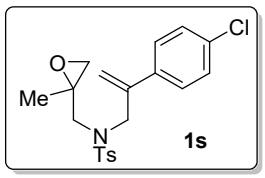
***N*-(2-(4-chlorophenyl)allyl)-4-methyl-*N*-((2-methyloxiran-2-yl)methyl)benzenesulfonamide**



$C_{20}H_{22}ClNO_3S$ **MW:** 391.91 g·mol^{-1}

The title compound was prepared according to **General Procedure II**.

White Solid **Yield:** 70%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.61 (d, *J* = 7.6 Hz, 2H), 7.30-7.23 (m, 6H), 5.39 (s, 1H), 5.18 (s, 1H), 4.32 (d, *J* = 16.4 Hz, 1H), 4.19 (d, *J* = 15.6 Hz, 1H), 3.21 (s, 2H), 2.59 (d, *J* = 4.4 Hz, 1H), 2.53 (d, *J* = 4.4 Hz, 1H), 2.43 (s, 3H), 1.15 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.5, 141.6, 136.9, 136.1, 133.8, 129.6, 128.4, 127.9, 127.2, 117.3, 56.0, 52.9, 52.9, 52.7, 21.5, 18.9.

MS (EI) m/z 391 (M+)

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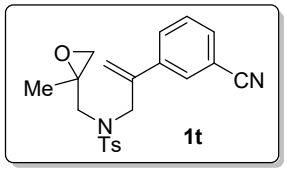
***N*-(2-(3-cyanophenyl)allyl)-4-methyl-*N*-((2-methyloxiran-2-yl)methyl)benzenesulfonamide**



$C_{21}H_{22}N_2O_3S$ **MW:** 382.48 g·mol^{-1}

The title compound was prepared according to **General Procedure II**.

White Solid **Yield:** 71%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.66-7.61 (m, 3H), 7.56-7.53 (m, 2H), 7.43-7.39 (m, 1H), 7.28 (d, *J* = 7.6 Hz, 2H), 5.43 (s, 1H), 5.31 (s, 1H), 4.33 (d, *J* = 16.0 Hz, 1H), 4.23 (d, *J* = 15.6 Hz, 1H), 3.40 (d, *J* = 15.2 Hz, 1H), 3.08 (d, *J* = 15.2 Hz, 1H), 2.58 (d, *J* = 4.4 Hz, 1H), 2.55 (d, *J* = 4.4 Hz, 1H), 2.44 (s, 3H), 1.17 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.7, 141.0, 139.9, 136.0, 131.1, 131.0, 130.2, 129.6, 129.0, 127.1, 118.7, 118.5, 112.3, 55.8, 52.9, 52.5, 52.1, 21.4, 18.7.

MS (EI) m/z 382 (M+)

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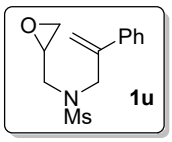
***N*-(oxiran-2-ylmethyl)-*N*-(2-phenylallyl)methanesulfonamide**



$C_{13}H_{17}NO_3S$ **MW:** 267.34 g·mol^{-1}

The title compound was prepared according to **General Procedure III**.

Colorless Oil **Yield:** 89%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.46 (d, *J* = 7.2 Hz, 2H), 7.38-7.30 (m, 3H), 5.51 (s, 1H), 5.37 (s, 1H), 4.46 (s, 2H), 3.47 (dd, *J* = 17.6, 6.0 Hz, 1H), 3.17-3.11 (m, 2H), 2.78 (t, *J* = 4.0 Hz, 1H), 2.72 (s, 3H), 2.54 (dd, *J* = 4.8, 2.4 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 142.9, 138.4, 128.5, 128.3, 126.6, 116.9, 51.8, 50.2, 48.7, 45.4, 39.2.

MS (EI) m/z 267 (M+)

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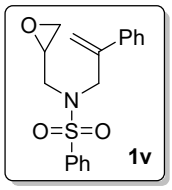
***N*-(oxiran-2-ylmethyl)-*N*-(2-phenylallyl)benzenesulfonamide**



$C_{18}H_{19}NO_3S$ **MW:** 329.41 g·mol^{-1}

The title compound was prepared according to **General Procedure III**.

Colorless Oil **Yield:** 75%

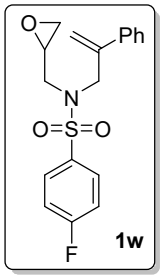
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.79 (d, *J* = 8.0 Hz, 2H), 7.60-7.57 (m, 1H), 7.52-7.48 (m, 2H), 7.42 (d, *J* = 7.2 Hz, 2H), 7.36-7.28 (m, 3H), 5.48 (s, 1H), 5.27 (s, 1H), 4.38-4.30 (m, 2H), 3.33 (dd, *J* = 15.2, 4.8 Hz, 1H), 3.10 (dd, *J* = 15.2, 6.0 Hz, 1H), 2.95-2.87 (m, 1H), 2.63 (t, *J* = 4.0 Hz, 1H), 2.43-2.38 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 142.5, 139.1, 138.1, 132.7, 129.1, 128.4, 128.1, 127.2, 126.4, 116.5, 52.4, 50.0, 49.6, 45.8.

MS (EI) m/z 329 (M+)

……

4-fluoro-*N*-(oxiran-2-ylmethyl)-*N*-(2-phenylallyl)benzenesulfonamide



$C_{18}H_{18}FNO_3S$ **MW:** 347.40 g·mol^{-1}

The title compound was prepared according to **General Procedure III**.

White Solid **Yield:** 80%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.78-7.75 (m, 2H), 7.40-7.38 (m, 2H), 7.35-7.27 (m, 3H), 7.14 (t, *J* = 8.0 Hz, 2H), 5.47 (s, 1H), 5.27 (s, 1H), 4.39-4.30 (m, 2H), 3.35 (dd, *J* = 15.2, 4.4 Hz, 1H), 3.09 (dd, *J* = 15.2, 6.0 Hz, 1H), 2.98-2.92 (m, 1H), 2.65 (t, *J* = 4.0 Hz, 1H), 2.44-2.41 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 165.0 (d, *J* = 253.4 Hz), 142.4, 138.1, 135.3 (d, *J* = 3.3 Hz), 129.9 (d, *J* = 9.3 Hz), 128.4, 128.1, 126.4, 116.8, 116.2 (d, *J* = 22.4 Hz), 52.3, 50.0, 49.4, 45.7.

^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): –105.0.

MS (EI) m/z 347 (M+)

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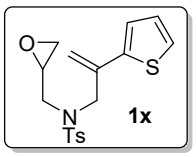
4-methyl-*N*-(oxiran-2-ylmethyl)-*N*-(2-(thiophen-2-yl)allyl)benzenesulfonamide



$C_{17}H_{19}NO_3S_2$ **MW:** 349.46 g·mol^{-1}

The title compound was prepared according to **General Procedure IV**.

Colorless Oil **Yield:** 70%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.73 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 3.6 Hz, 1H), 7.19 (d, *J* = 5.2 Hz, 1H), 6.99 (t, *J* = 4.4 Hz, 1H), 5.55 (s, 1H), 5.14 (s, 1H), 4.28 (d, *J* = 14.8 Hz, 1H), 4.20 (d, *J* = 14.8 Hz, 1H), 3.30 (dd, *J* = 14.8, 4.8 Hz, 1H), 3.16 (dd, *J* = 15.2, 5.6 Hz, 1H), 2.96-2.92 (m, 1H), 2.63 (t, *J* = 4.4 Hz, 1H), 2.44 (s, 3H), 2.41 (dd, *J* = 4.8, 2.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.8, 141.6, 136.2, 136.0, 129.9, 127.7, 127.3, 125.1, 124.9, 115.0, 52.8, 50.1, 49.9, 46.1, 21.6.

MS (EI) m/z 349 (M+)

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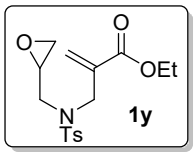
ethyl 2-(((4-methyl-*N*-(oxiran-2-ylmethyl)phenyl)sulfonamido)methyl)acrylate



$C_{16}H_{21}NO_5S$ **MW:** 339.41 g·mol^{-1}

The title compound was prepared according to **General Procedure V**.

Colorless Oil **Yield:** 68%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.71 (d, *J* = 7.6 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 6.36 (s, 1H), 5.93 (s, 1H), 4.18 (q, *J* = 7.2 Hz, 2H), 4.13 (s, 2H), 3.57 (d, *J* = 13.2 Hz, 1H), 3.07-2.98 (m, 2H), 2.71 (t, *J* = 4.0 Hz, 1H), 2.46-2.45 (m, 1H), 2.43 (s, 3H), 1.28 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 165.8, 143.6, 136.4, 135.7, 129.8, 127.2, 127.2, 61.0, 51.4, 50.2, 49.1, 45.3, 21.5, 14.1.

MS (EI) m/z 339 (M+)

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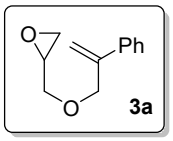
2-(((2-phenylallyl)oxy)methyl)oxirane



$C_{12}H_{14}O_2$ **MW:** 190.24 g·mol^{-1}

The title compound was prepared according to **General Procedure VI**.

Colorless Oil **Yield:** 66%

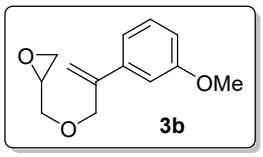
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.46 (d, *J* = 7.6 Hz, 2H), 7.35-7.26 (m, 3H), 5.54 (s, 1H), 5.35 (s, 1H), 4.47 (d, *J* = 12.8 Hz, 1H), 4.41 (d, *J* = 12.8 Hz, 1H), 3.77 (dd, *J* = 11.6, 2.8 Hz, 1H), 3.44 (dd, *J* = 11.6, 5.6 Hz, 1H), 3.17-3.12 (m, 1H), 2.77 (t, *J* = 4.4 Hz, 1H), 2.58 (dd, *J* = 5.2, 2.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.8, 138.5, 128.3, 127.8, 126.0, 114.6, 73.1, 70.5, 50.8, 44.3.

MS (EI) m/z 190 (M+)

……

2-(((2-(3-methoxyphenyl)allyl)oxy)methyl)oxirane



$C_{13}H_{16}O_3$ **MW:** 220.27 g·mol^{-1}

The title compound was prepared according to **General Procedure VI**.

Colorless Oil **Yield:** 58%

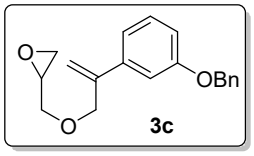
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.25 (t, *J* = 7.6 Hz, 1H), 7.06-7.02 (m, 2H), 6.84 (d, *J* = 8.0 Hz, 1H), 5.54 (s, 1H), 5.35 (s, 1H), 4.45 (d, *J* = 12.8 Hz, 1H), 4.39 (d, *J* = 12.8 Hz, 1H), 3.81 (s, 3H), 3.78 (d, *J* = 11.6 Hz, 1H), 3.45 (dd, *J* = 11.6, 6.0 Hz, 1H), 3.19-3.13 (m, 1H), 2.78 (t, *J* = 4.4 Hz, 1H), 2.61-2.58 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 159.5, 143.7, 140.1, 129.3, 118.5, 114.8, 113.0, 111.9, 73.1, 70.5, 55.1, 50.7, 44.2.

MS (EI) m/z 220 (M+)

……

2-(((2-(3-(benzyloxy)phenyl)allyl)oxy)methyl)oxirane

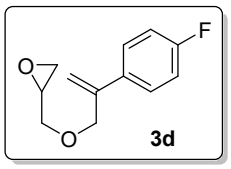


$C_{19}H_{20}O_3$ **MW:** 296.37 g·mol^{-1}
The title compound was prepared according to **General Procedure VI**.
Pale Yellow Oil **Yield:** 55%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.44-7.29 (m, 5H), 7.26-7.22 (m, 1H), 7.10-7.05 (m, 2H), 6.90 (d, *J* = 8.0 Hz, 1H), 5.52 (s, 1H), 5.34 (s, 1H), 5.06 (s, 2H), 4.43 (d, *J* = 12.8 Hz, 1H), 4.37 (d, *J* = 12.8 Hz, 1H), 3.75 (dd, *J* = 11.6, 2.4 Hz, 1H), 3.43 (dd, *J* = 11.2, 5.6 Hz, 1H), 3.17-3.11 (m, 1H), 2.76 (t, *J* = 4.8 Hz, 1H), 2.60-2.56 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 158.7, 143.6, 140.1, 136.9, 129.3, 128.5, 127.9, 127.4, 118.7, 114.9, 113.9, 112.8, 73.0, 70.5, 69.9, 50.7, 44.2.
MS (EI) m/z 296 (M+)

……

2-(((2-(4-fluorophenyl)allyl)oxy)methyl)oxirane



$C_{12}H_{13}FO_2$ **MW:** 208.23 g·mol^{-1}
The title compound was prepared according to **General Procedure VI**.
Colorless Oil **Yield:** 67%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.46-7.43 (m, 2H), 7.02 (t, *J* = 8.0 Hz, 2H), 5.48 (s, 1H), 5.32 (s, 1H), 4.44 (d, *J* = 12.8 Hz, 1H), 4.37 (d, *J* = 12.4 Hz, 1H), 3.77 (d, *J* = 11.2 Hz, 1H), 3.42 (dd, *J* = 11.6, 6.0 Hz, 1H), 3.17-3.12 (m, 1H), 2.77 (t, *J* = 4.4 Hz, 1H), 2.60-2.56 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 162.4 (d, *J* = 245.2 Hz), 142.8, 134.5 (d, *J* = 3.3 Hz), 127.6 (d, *J* = 7.9 Hz), 115.1 (d, *J* = 21.2 Hz), 114.6 (d, *J* = 4.4 Hz), 73.1, 70.4, 50.7, 44.1.
^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): –114.4.
MS (EI) m/z 208 (M+)

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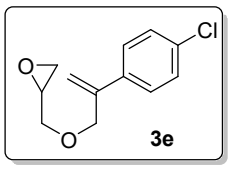
2-(((2-(4-chlorophenyl)allyl)oxy)methyl)oxirane

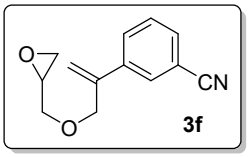


$C_{12}H_{13}ClO_2$ **MW:** 224.68 g·mol^{-1}
The title compound was prepared according to **General Procedure VI**.
Colorless Oil **Yield:** 70%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.41 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 7.6 Hz, 2H), 5.53 (s, 1H), 5.36 (s, 1H), 4.44 (d, *J* = 12.4 Hz, 1H), 4.38 (d, *J* = 12.8 Hz, 1H), 3.77 (d, *J* = 11.6 Hz, 1H), 3.42 (dd, *J* = 11.6, 6.0 Hz, 1H), 3.19-3.11 (m, 1H), 2.78 (t, *J* = 4.4 Hz, 1H), 2.59-2.58 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 142.8, 136.9, 133.6, 128.5, 127.4, 115.3, 73.0, 70.5, 50.8, 44.2.
MS (EI) m/z 224 (M+)

……

3-(3-(oxiran-2-ylmethoxy)prop-1-en-2-yl)benzonitrile



$C_{13}H_{13}NO_2$ **MW:** 215.25 g·mol^{-1}

The title compound was prepared according to **General Procedure VI**.

Pale Yellow Oil **Yield:** 61%

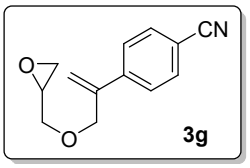
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.76 (s, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.48-7.44 (m, 1H), 5.61 (s, 1H), 5.47 (s, 1H), 4.47 (d, *J* = 12.8 Hz, 1H), 4.40 (d, *J* = 12.8 Hz, 1H), 3.81 (d, *J* = 11.2 Hz, 1H), 3.42 (dd, *J* = 11.2, 5.6 Hz, 1H), 3.19-3.13 (m, 1H), 2.80 (t, *J* = 4.4 Hz, 1H), 2.62-2.57 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 142.1, 139.7, 131.1, 130.4, 129.7, 129.2, 118.7, 117.1, 112.5, 72.8, 70.6, 50.7, 44.0.

MS (EI) m/z 215 (M+)

……

4-(3-(oxiran-2-ylmethoxy)prop-1-en-2-yl)benzonitrile



$C_{13}H_{13}NO_2$ **MW:** 215.25 g·mol^{-1}

The title compound was prepared according to **General Procedure VI**.

Colorless Oil **Yield:** 51%

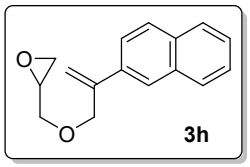
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.60 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 8.0 Hz, 2H), 5.63 (s, 1H), 5.48 (s, 1H), 4.45 (d, *J* = 12.8 Hz, 1H), 4.39 (d, *J* = 12.4 Hz, 1H), 3.79 (d, *J* = 11.6 Hz, 1H), 3.38 (dd, *J* = 11.2, 6.0 Hz, 1H), 3.16-3.10 (m, 1H), 2.77 (t, *J* = 4.8 Hz, 1H), 2.59-2.54 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 142.9, 142.4, 132.1, 126.6, 118.7, 117.8, 111.1, 72.6, 70.6, 50.6, 44.0.

MS (EI) m/z 215 (M+)

……

2-(((2-(naphthalen-2-yl)allyl)oxy)methyl)oxirane



$C_{16}H_{16}O_2$ **MW:** 240.30 g·mol^{-1}

The title compound was prepared according to **General Procedure VI**.

Colorless Oil **Yield:** 60%

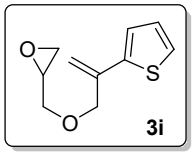
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.92 (s, 1H), 7.86-7.81 (m, 3H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.50-7.45 (m, 2H), 5.71 (s, 1H), 5.47 (s, 1H), 4.61 (d, *J* = 12.8 Hz, 1H), 4.54 (d, *J* = 12.8 Hz, 1H), 3.82 (d, *J* = 11.6 Hz, 1H), 3.50 (dd, *J* = 11.6, 5.6 Hz, 1H), 3.21-3.16 (m, 1H), 2.79 (t, *J* = 4.8 Hz, 1H), 2.63-2.61 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.6, 135.7, 133.3, 132.9, 128.2, 127.9, 127.5, 126.1, 126.0, 124.9, 124.2, 115.2, 73.2, 70.5, 50.8, 44.3.

MS (EI) m/z 240 (M+)

……

2-(((2-(thiophen-2-yl)allyl)oxy)methyl)oxirane



$C_{10}H_{12}O_2S$ **MW:** 196.26 g·mol^{-1}

The title compound was prepared according to **General Procedure VI**.

Pale Yellow Oil **Yield:** 56%

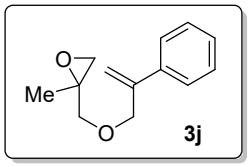
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.19 (d, *J* = 4.8 Hz, 1H), 7.15 (d, *J* = 3.2 Hz, 1H), 6.99 (t, *J* = 4.4 Hz, 1H), 5.56 (s, 1H), 5.24 (s, 1H), 4.42 (d, *J* = 12.4 Hz, 1H), 4.36 (d, *J* = 12.4 Hz, 1H), 3.79 (d, *J* = 11.2 Hz, 1H), 3.46 (dd, *J* = 11.6, 6.0 Hz, 1H), 3.21-3.15 (m, 1H), 2.80 (t, *J* = 4.8 Hz, 1H), 2.63-2.61 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 142.1, 137.7, 127.3, 124.5, 124.0, 113.2, 73.2, 70.5, 50.7, 44.2.

MS (EI) m/z 196 (M+)

……

2-methyl-2-(((2-phenylallyl)oxy)methyl)oxirane



$C_{13}H_{16}O_2$ **MW:** 204.27 g·mol^{-1}

The title compound was prepared according to **General Procedure VII**.

Colorless Oil **Yield:** 67%

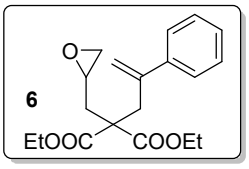
^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.46 (d, *J* = 7.6 Hz, 2H), 7.35-7.25 (m, 3H), 5.53 (s, 1H), 5.34 (s, 1H), 4.44 (d, *J* = 12.8 Hz, 1H), 4.40 (d, *J* = 12.8 Hz, 1H), 3.56 (d, *J* = 11.2 Hz, 1H), 3.45 (d, *J* = 10.8 Hz, 1H), 2.71 (d, *J* = 4.8 Hz, 1H), 2.60 (d, *J* = 4.8 Hz, 1H), 1.33 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.9, 138.5, 128.3, 127.7, 126.0, 114.5, 73.1, 73.0, 56.0, 51.5, 18.4.

MS (EI) m/z 204 (M+)

……

diethyl 2-(oxiran-2-ylmethyl)-2-(2-phenylallyl)malonate



$C_{19}H_{24}O_5$ **MW:** 332.40 g·mol^{-1}

The title compound was prepared according to **General Procedure VIII**.

Pale Yellow Oil **Yield:** 75%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.32-7.22 (m, 5H), 5.27 (s, 1H), 5.19 (s, 1H), 4.04-3.88 (m, 3H), 3.79-3.71 (m, 1H), 3.32 (d, *J* = 14.4 Hz, 1H), 3.26 (d, *J* = 14.4 Hz, 1H), 2.96-2.91 (m, 1H), 2.67 (t, *J* = 4.4 Hz, 1H), 2.34 (dd, *J* = 5.2, 2.8 Hz, 1H), 2.10 (dd, *J* = 14.8, 4.8 Hz, 1H), 1.91 (dd, *J* = 14.8, 7.2 Hz, 1H), 1.18 (t, *J* = 7.2 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):** 170.6, 170.5, 144.2, 141.5, 128.0, 127.5, 126.9, 118.9, 61.3, 61.2, 55.9, 48.5, 46.7, 38.5, 35.5, 13.8, 13.7.

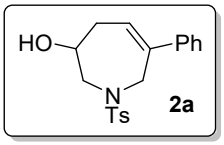
MS (EI) m/z 332 (M+)

3. General Procedure and Analytical Data of 7-Endo Heck Products

General procedures for synthesis of 2 and 4 (standard condition**).** $Pd(PPh_3)_4$ (10 mol%, 23.0 mg, 0.02 mmol), **L4** (20 mol%, 21.6 mg, 0.04 mmol) and $Et_3N{\cdot}HI$ (20 mol%, 9.2 mg, 0.40 mmol) were added to an oven-dried Schlenk tube. Then a solution of epoxide **1** or **3** (1.0 equiv, 0.20 mmol) in toluene (2 mL) was added. The resulting mixture was stirred at 130 °C for 12 h under nitrogen atmosphere (9 h for oxygen bridging substrates **3**). After cooling the reaction mixture at room temperature, it was quenched with a saturated aqueous solution of NH_4Cl (10 mL). The aqueous layer was extracted with EtOAc (3×8 mL). The combined organic phase was sequentially washed with saturated aqueous solution of NaCl and concentrated *in vacuo*. The resulting mixture was purified by silica gel column chromatography (hexanes/EtOAc = 2:1) to afford the 7-*endo* Heck product **2** or **4**.

Analytical Data:

6-phenyl-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{19}H_{21}NO_3S$ **MW:** 343.44 g·mol^{-1}
White Solid
Isolated Amount: 58.8 mg **Yield:** 86%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.69 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 7.2 Hz, 2H), 7.35-7.25 (m, 5H), 5.93 (t, *J* = 6.4 Hz, 1H), 4.42 (d, *J* = 16.0 Hz, 1H), 4.07-4.00 (m, 2H), 3.54-3.45 (m, 2H), 2.72-2.65 (m, 1H), 2.58-2.49 (m, 2H), 2.42 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.6, 141.0, 135.4, 129.8, 128.4, 127.5, 127.1, 126.1, 125.2, 67.7, 56.6, 51.7, 34.5, 21.5.
MS (EI) m/z 343 (M+); **HRMS (ESI)** Calcd for $C_{19}H_{21}NO_3S$−H 342.1164, Found 342.1162.

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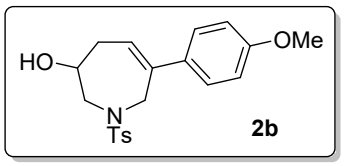
6-(4-methoxyphenyl)-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{20}H_{23}NO_4S$ **MW:** 373.47 g·mol^{-1}
Light Yellow Oil
Isolated Amount: 26.0 mg **Yield:** 35%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.70 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 5.86 (t, *J* = 6.8 Hz, 1H), 4.40 (d, *J* = 16.0 Hz, 1H), 4.03-3.97 (m, 2H), 3.81 (s, 3H), 3.52 (dd, *J* = 13.6, 5.2 Hz, 1H), 3.44 (dd, *J* = 13.6, 3.6 Hz, 1H), 2.70-2.63 (m, 1H), 2.52 (ddd, *J* = 14.8, 6.8, 2.8 Hz, 1H), 2.44-2.42 (m, 4H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 159.1, 143.6, 140.6, 135.5, 133.5, 129.8, 127.3, 127.1, 123.6, 113.8, 67.6, 56.8, 55.3, 51.7, 34.4, 21.5.
MS (EI) m/z 373 (M+); **HRMS (ESI)** Calcd for $C_{20}H_{23}NO_4S$−H 372.1270, Found 372.1275.

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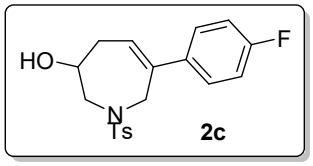
6-(4-fluorophenyl)-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{19}H_{20}FNO_3S$ **MW:** 361.43 g·mol^{-1}
White Solid
Isolated Amount: 59.2 mg **Yield:** 82%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.69 (d, *J* = 7.6 Hz, 2H), 7.42-7.39 (m, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.01 (t, *J* = 8.4 Hz, 2H), 5.89 (t, *J* = 6.4 Hz, 1H), 4.37 (d, *J* = 16.0 Hz, 1H), 4.08-4.01 (m, 1H), 3.99 (d, *J* = 16.0 Hz, 1H), 3.52 (dd, *J* = 13.6, 5.2 Hz, 1H), 3.46 (dd, *J* = 13.2, 3.2 Hz, 1H), 2.72-2.64 (m, 1H), 2.54 (dd, *J* = 14.4, 6.0 Hz, 1H), 2.49-2.41 (m, 4H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 162.3 (d, *J* = 245.3 Hz), 143.7, 140.4, 137.1 (d, *J* = 3.2 Hz), 135.4, 129.8, 127.9 (d, *J* = 7.9 Hz), 127.1, 125.3, 115.3 (d, *J* = 21.3 Hz), 67.5, 56.8, 51.7, 34.5, 21.5.
^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): –114.8.
MS (EI) m/z 361 (M+); **HRMS (ESI)** Calcd for $C_{19}H_{20}FNO_3S$−H 360.1070, Found 360.1077.

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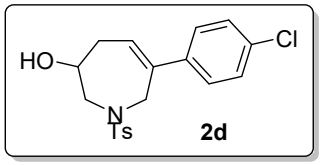
6-(4-chlorophenyl)-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{19}H_{20}ClNO_3S$ **MW:** 377.88 g·mol^{-1}
White Solid
Isolated Amount: 59.8 mg **Yield:** 79%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.58 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.8 Hz, 2H), 7.32-7.26 (m, 4H), 5.93 (t, *J* = 6.8 Hz, 1H), 4.34 (d, *J* = 16.0 Hz, 1H), 4.07-3.98 (m, 2H), 3.53-3.44 (m, 2H), 2.71-2.64 (m, 1H), 2.57-2.46 (m, 2H), 2.42 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.7, 140.3, 139.4, 135.4, 133.4, 129.8, 128.6, 127.5, 127.1, 126.0, 67.4, 56.8, 51.4, 34.6, 21.5.
MS (EI) m/z 377 (M+); **HRMS (ESI)** Calcd for $C_{19}H_{20}ClNO_3S$−H 376.0774, Found 376.0777.

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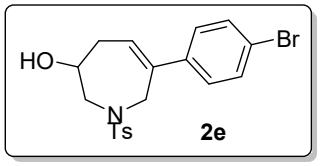
6-(4-bromophenyl)-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{19}H_{20}BrNO_3S$ **MW:** 422.34 g·mol^{-1}
Off-White Solid
Isolated Amount: 55.0 mg **Yield:** 65%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.69 (d, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.32-7.29 (m, 4H), 5.94 (t, *J* = 6.8 Hz, 1H), 4.37 (d, *J* = 15.6 Hz, 1H), 4.08-4.01 (m, 1H), 3.99 (d, *J* = 16.0 Hz, 1H), 3.53 (dd, *J* = 13.6, 4.8 Hz, 1H), 3.46 (dd, *J* = 13.6, 4.0 Hz, 1H), 2.72-2.65 (m, 1H), 2.54 (ddd, *J* = 15.2, 6.8, 2.8 Hz, 1H), 2.43 (s, 3H), 2.35 (d, *J* = 8.4 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.7, 140.4, 139.9, 135.4, 131.6, 129.9, 127.8, 127.1, 126.0, 121.6, 67.4, 56.8, 51.4, 34.6, 21.5.
MS (EI) m/z 421, 423 (M+); **HRMS (ESI)** Calcd for $C_{19}H_{20}BrNO_3S$−H 420.0269, Found 420.0273.

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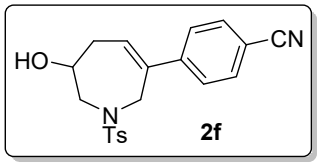
4-(6-hydroxy-1-tosyl-2,5,6,7-tetrahydro-1*H*-azepin-3-yl)benzonitrile



$C_{20}H_{20}N_2O_3S$ **MW:** 368.45 g·mol^{-1}
Light Yellow Oil
Isolated Amount: 52.1 mg **Yield:** 71%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.68 (d, *J* = 8.0 Hz, 2H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 6.08 (t, *J* = 6.4 Hz, 1H), 4.27 (d, *J* = 16.0 Hz, 1H), 4.09 (d, *J* = 16.0 Hz, 1H), 4.06-3.99 (m, 1H), 3.57 (dd, *J* = 13.6, 2.8 Hz, 1H), 3.44 (dd, *J* = 13.6, 6.0 Hz, 1H), 2.81 (d, *J* = 5.2 Hz, 1H), 2.72-2.64 (m, 1H), 2.59 (dd, *J* = 14.0, 6.4 Hz, 1H), 2.43 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 145.4, 143.8, 140.2, 135.1, 132.2, 129.8, 129.1, 127.0, 126.7, 118.7, 110.7, 66.8, 57.0, 50.6, 34.9, 21.4.
MS (EI) m/z 368 (M+); **HRMS (ESI)** Calcd for $C_{20}H_{20}N_2O_3S$−H 367.1116, Found 367.1115.

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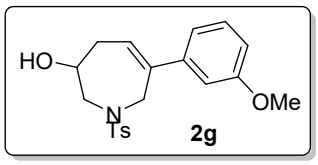
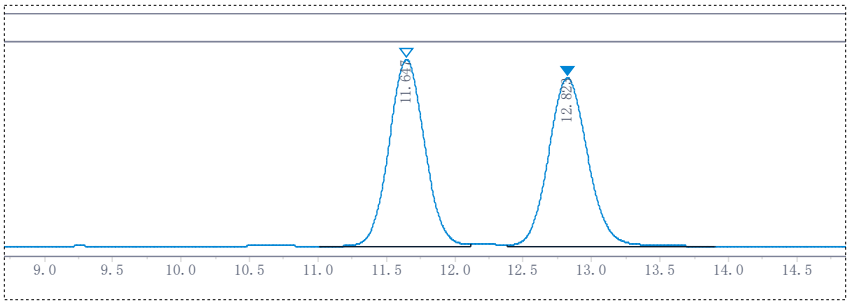
6-(3-methoxyphenyl)-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{20}H_{23}NO_4S$ **MW:** 373.47 g·mol^{-1}
Light Yellow Oil
Isolated Amount: 57.2 mg **Yield:** 77%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.69 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.24 (t, *J* = 8.0 Hz, 1H), 7.02-6.98 (m, 2H), 6.83 (dd, *J* = 8.0, 2.4 Hz, 1H), 5.95 (t, *J* = 6.8 Hz, 1H), 4.38 (d, *J* = 15.6 Hz, 1H), 4.06-3.99 (m, 2H), 3.83 (s, 3H), 3.53-3.44 (m, 2H), 2.71-2.63 (m, 1H), 2.57-2.51 (m, 2H), 2.42 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 159.6, 143.6, 142.5, 141.0, 135.3, 129.8, 129.4, 127.1, 125.4, 118.5, 113.3, 111.6, 67.5, 56.8, 55.3, 51.7, 34.5, 21.5.
MS (EI) m/z 373 (M+); **HRMS (ESI)** Calcd for $C_{20}H_{23}NO_4S$−H 372.1270, Found 372.1272.
HPLC analysis CHIRALCEL AD-H column, 1.0 mL/min (20% *i*-PrOH in hexane), 254 nm UV detector, t_S = 11.647 min (peak area = 50.17%), t_R = 12.823 min (peak area = 49.83%).



Peak#	RT (min)	Area (mAU·s)	Area (%)	Starting (min)	Ending (min)
1	11.647	6498.822	50.17	11.008	12.114
2	12.823	6455.586	49.83	12.380	13.897

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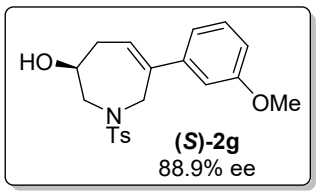
(*S*)-6-(3-methoxyphenyl)-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



(*S*)-2g (89% ee) was prepared from **(*R*)-1g (90% ee)**

$C_{20}H_{23}NO_4S$ **MW:** 373.47 g·mol^{-1}

Light Yellow Oil

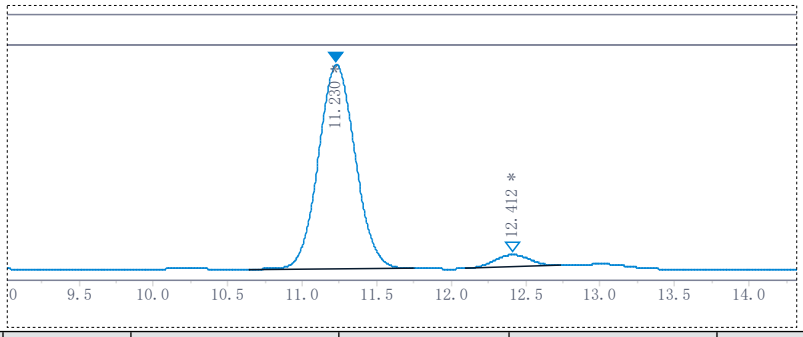
Isolated Amount: 53.8 mg **Yield:** 72%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.68 (d, *J* = 7.6 Hz, 2H), 7.28 (d, *J* = 7.6 Hz, 2H), 7.22 (t, *J* = 8.0 Hz, 1H), 7.02 (s, 1H), 6.98 (d, *J* = 7.6 Hz, 1H), 6.81 (d, *J* = 8.0 Hz, 1H), 5.94 (t, *J* = 6.4 Hz, 1H), 4.30 (d, *J* = 15.6 Hz, 1H), 4.04 (d, *J* = 16.4 Hz, 1H), 4.02-3.95 (m, 1H), 3.81 (s, 3H), 3.53-3.50 (m, 1H), 3.43 (dd, *J* = 13.2, 5.2 Hz, 1H), 2.77 (d, *J* = 4.8 Hz, 1H), 2.67-2.59 (m, 1H), 2.52 (dd, *J* = 14.8, 6.8 Hz, 1H), 2.40 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 159.5, 143.5, 142.5, 140.9, 135.3, 129.7, 129.3, 127.0, 125.5, 118.4, 113.1, 111.5, 67.3, 56.8, 55.2, 51.4, 34.6, 21.4.

MS (EI) m/z 373 (M+); **HRMS (ESI)** Calcd for $C_{20}H_{23}NO_4S$−H 372.1270, Found 372.1270.

HPLC analysis CHIRALCEL AD-H column, 1.0 mL/min (20% *i*-PrOH in hexane), 254 nm UV detector, t_S = 11.230 min (peak area = 94.46%), t_R = 12.412 min (peak area = 5.54%).



Peak#	RT (min)	Area (mAU·s)	Area (%)	Starting (min)	Ending (min)
1	11.230	7634.955	94.46	10.645	11.751
2	12.412	345.419	5.54	12.091	12.730

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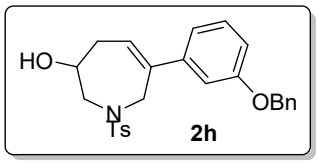
6-(3-(benzyloxy)phenyl)-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{26}H_{27}NO_4S$ **MW:** 449.57 g·mol^{-1}

Light Yellow Oil

Isolated Amount: 62.1 mg **Yield:** 69%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.67 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.35 (t, *J* = 6.8 Hz, 2H), 7.32-7.21 (m, 4H), 7.10 (s, 1H), 7.01 (d, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 8.4 Hz, 1H), 5.94 (t, *J* = 6.4 Hz, 1H), 5.08 (s, 2H), 4.34 (d, *J* = 15.6 Hz, 1H), 4.06-3.96 (m, 2H), 3.51-3.43 (m, 2H), 2.75-2.58 (m, 2H), 2.55-2.49 (m, 1H), 2.40 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 158.7, 143.6, 142.5, 140.9, 136.8, 135.3, 129.8, 129.4, 128.5, 127.9, 127.5, 127.1, 125.5, 118.8, 114.0, 112.5, 69.8, 67.5, 56.7, 51.5, 34.5, 21.4.

MS (EI) m/z 449 (M+); **HRMS (ESI)** Calcd for $C_{26}H_{27}NO_4S$−H 448.1583, Found 448.1585.

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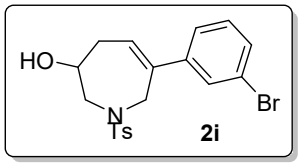
6-(3-bromophenyl)-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{19}H_{20}BrNO_3S$ **MW:** 422.34 g·mol^{-1}
Off-White Solid
Isolated Amount: 58.9 mg **Yield:** 70%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.69 (d, *J* = 8.4 Hz, 2H),7.50-7.49 (m, 1H), 7.40-7.36 (m, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.20 (t, *J* = 7.6 Hz, 1H), 5.94 (t, *J* = 6.8 Hz, 1H), 4.34 (d, *J* = 16.0 Hz, 1H), 4.07-3.99 (m, 2H), 3.54-3.46 (m, 2H), 2.72-2.64 (m, 1H), 2.55 (ddd, *J* = 15.2, 6.8, 3.2 Hz, 1H), 2.43-2.41 (m, 4H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.7, 143.1, 139.9, 135.4, 130.4, 130.0, 129.8, 129.2, 127.1, 126.7, 124.7, 122.5, 67.5, 56.6, 51.3, 34.5, 21.5.
MS (EI) m/z 421, 423 (M+); **HRMS (ESI)** Calcd for $C_{19}H_{20}BrNO_3S$−H 420.0269, Found 420.0269.

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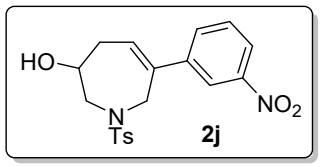
6-(3-nitrophenyl)-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{19}H_{20}N_2O_5S$ **MW:** 388.44 g·mol^{-1}
Off-White Solid
Isolated Amount: 51.1 mg **Yield:** 66%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 8.23-8.21 (m, 1H), 8.14 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 2H), 7.53 (t, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 2H), 6.10 (t, *J* = 6.8 Hz, 1H), 4.42 (d, *J* = 16.0 Hz, 1H), 4.13-4.05 (m, 2H), 3.56 (dd, *J* = 13.6, 4.8 Hz, 1H), 3.51 (dd, *J* = 13.6, 3.6 Hz, 1H), 2.80-2.72 (m, 1H), 2.61 (ddd, *J* = 15.2, 6.8, 2.8 Hz, 1H), 2.43 (s, 3H), 2.28 (d, *J* = 8.0 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 148.3, 143.9, 142.6, 139.8, 135.4, 132.2, 129.9, 129.6, 128.4, 127.1, 122.3, 121.1, 67.3, 56.9, 51.2, 34.7, 21.5.
MS (EI) m/z 388 (M+); **HRMS (ESI)** Calcd for $C_{19}H_{20}N_2O_5S$−H 387.1015, Found 387.1014.

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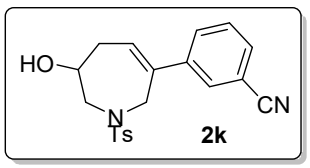
3-(6-hydroxy-1-tosyl-2,5,6,7-tetrahydro-1*H*-azepin-3-yl)benzonitrile



$C_{20}H_{20}N_2O_3S$ **MW:** 368.45 g·mol^{-1}
Light Yellow Oil
Isolated Amount: 55.9 mg **Yield:** 76%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.73 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.64 (s, 1H), 7.54 (d, *J* = 7.6 Hz, 1H), 7.46-7.43 (m, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 6.01 (t, *J* = 6.4 Hz, 1H), 4.27 (d, *J* = 16.0 Hz, 1H), 4.08 (d, *J* = 16.0 Hz, 1H), 4.08-4.01 (m, 1H), 3.58 (dd, *J* = 13.6, 3.6 Hz, 1H), 3.45 (dd, *J* = 13.6, 5.6 Hz, 1H), 2.81 (d, *J* = 5.2 Hz, 1H), 2.72-2.65 (m, 1H), 2.59 (dd, *J* = 14.0, 6.4 Hz, 1H), 2.43 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.8, 142.2, 139.6, 135.3, 130.8, 130.5, 129.8, 129.6, 129.3, 128.2, 127.0, 118.6, 112.4, 67.1, 56.8, 50.8, 34.8, 21.4.
MS (EI) m/z 368 (M+); **HRMS (ESI)** Calcd for $C_{20}H_{20}N_2O_3S$−H 367.1116, Found 367.1112.

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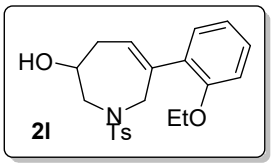
6-(2-ethoxyphenyl)-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{21}H_{25}NO_4S$ **MW:** 387.49 g·mol^{-1}
White Solid
Isolated Amount: 54.3 mg **Yield:** 70%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.65 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.24-7.20 (m, 1H), 7.09 (dd, *J* = 7.6, 1.6 Hz, 1H), 6.89 (t, *J* = 7.6 Hz, 1H), 6.80 (d, *J* = 8.0 Hz, 1H), 5.66 (t, *J* = 6.8 Hz, 1H), 4.39 (d, *J* = 16.0 Hz, 1H), 4.13-4.05 (m, 1H), 4.01-3.95 (m, 3H), 3.60 (dd, *J* = 14.0, 4.0 Hz, 1H), 3.53 (dd, *J* = 14.0, 4.0 Hz, 1H), 2.72-2.53 (m, 3H), 2.41 (s, 3H), 1.28 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 155.5, 143.3, 139.8, 135.8, 131.0, 129.8, 129.6, 128.8, 127.0, 125.9, 120.6, 111.2, 68.7, 63.4, 55.2, 52.0, 33.7, 21.5, 14.7.
MS (EI) m/z 387 (M+); **HRMS (ESI)** Calcd for $C_{21}H_{25}NO_4S$−H 386.1426, Found 386.1422.

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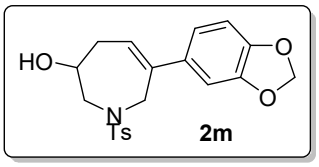
6-(benzo[*d*][1,3]dioxol-5-yl)-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{20}H_{21}NO_5S$ **MW:** 387.45 g·mol^{-1}
White Solid
Isolated Amount: 52.5 mg **Yield:** 68%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.70 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 6.96-6.89 (m, 2H), 6.77 (d, *J* = 8.0 Hz, 1H), 5.96 (s, 2H), 5.85 (t, *J* = 6.8 Hz, 1H), 4.38 (d, *J* = 15.6 Hz, 1H), 4.07-3.99 (m, 1H), 3.95 (d, *J* = 16.0 Hz, 1H), 3.53 (dd, *J* = 13.6, 5.2 Hz, 1H), 3.42 (dd, *J* = 14.0, 4.0 Hz, 1H), 2.71-2.63 (m, 1H), 2.52 (ddd, *J* = 14.8, 6.8, 2.8 Hz, 1H), 2.43 (s, 3H), 2.39-2.24 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 147.5, 147.2, 143.4, 141.9, 135.8, 132.0, 129.5, 127.0, 120.0, 115.4, 107.9, 106.7, 100.9, 52.4, 49.8, 49.4, 45.7, 21.3.
MS (EI) m/z 387 (M+); **HRMS (ESI)** Calcd for $C_{20}H_{21}NO_5S$−H 386.1062, Found 386.1062.

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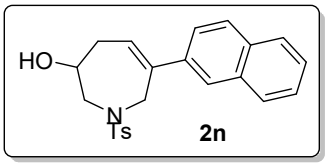
6-(naphthalen-2-yl)-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{23}H_{23}NO_3S$ **MW:** 393.50 g·mol^{-1}
Light Yellow Oil
Isolated Amount: 61.9 mg **Yield:** 79%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.84-7.78 (m, 4H), 7.71 (d, *J* = 8.4 Hz, 2H), 7.54 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.49-7.43 (m, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 6.07 (t, *J* = 6.8 Hz, 1H), 4.52 (d, *J* = 16.0 Hz, 1H), 4.14 (d, *J* = 15.2 Hz, 1H), 4.09-4.03 (m, 1H), 3.58-3.49 (m, 2H), 2.77-2.69 (m, 1H), 2.62-2.50 (m, 2H), 2.40 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.6, 140.9, 138.2, 135.5, 133.2, 132.6, 129.8, 128.1, 128.1, 127.5, 127.1, 126.2, 126.0, 125.8, 124.8, 124.5, 67.7, 56.7, 51.6, 34.6, 21.5.
MS (EI) m/z 393 (M+); **HRMS (ESI)** Calcd for $C_{23}H_{23}NO_3S$−H 392.1320, Found 392.1325.

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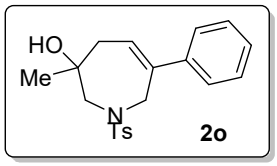
3-methyl-6-phenyl-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{20}H_{23}NO_3S$ **MW:** 357.47 g·mol^{-1}
White Solid
Isolated Amount: 49.2 mg **Yield:** 69%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.71 (d, *J* = 8.0 Hz, 2H), 7.41 (d, *J* = 7.6 Hz, 2H), 7.35-7.28 (m, 5H), 5.97 (t, *J* = 6.8 Hz, 1H), 4.63 (d, *J* = 15.6 Hz, 1H), 3.82 (d, *J* = 15.6 Hz, 1H), 3.54 (d, *J* = 13.6 Hz, 1H), 3.05 (d, *J* = 13.6 Hz, 1H), 2.83 (s, 1H), 2.74 (dd, *J* = 14.4, 7.2 Hz, 1H), 2.43-2.37 (m, 4H), 1.29 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.7, 140.8, 140.2, 135.1, 129.9, 128.5, 127.6, 127.1, 126.1, 125.9, 71.4, 61.2, 52.2, 40.0, 26.3, 21.5.
MS (EI) m/z 357 (M+); **HRMS (ESI)** Calcd for $C_{20}H_{23}NO_3S$−H 356.1320, Found 356.1319.

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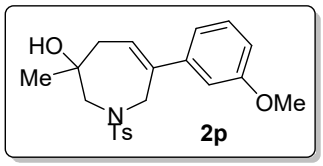
6-(3-methoxyphenyl)-3-methyl-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{21}H_{25}NO_4S$ **MW:** 387.49 g·mol^{-1}
White Solid
Isolated Amount: 42.7 mg **Yield:** 55%

^{1}H NMR (600 MHz, $CDCl_3$, δ ppm): 7.70 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.24 (t, *J* = 8.4 Hz, 1H), 7.02-7.01 (m, 1H), 6.98 (d, *J* = 8.4 Hz, 1H), 6.83 (dd, *J* = 8.4, 2.4 Hz, 1H), 5.97 (t, *J* = 6.6 Hz, 1H), 4.59 (d, *J* = 15.6 Hz, 1H), 3.83 (s, 3H), 3.81 (d, *J* = 15.6 Hz, 1H), 3.53 (d, *J* = 13.8 Hz, 1H), 3.04 (d, *J* = 13.2 Hz, 1H), 2.81 (s, 1H), 2.71 (dd, *J* = 14.4, 7.2 Hz, 1H), 2.42 (s, 3H), 2.39 (dd, *J* = 14.4, 6.6 Hz, 1H), 1.28 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 159.6, 143.7, 142.3, 140.3, 135.1, 129.9, 129.5, 127.1, 126.1, 118.5, 113.3, 111.7, 71.2, 61.4, 55.3, 52.2, 40.0, 26.4, 21.5.
MS (EI) m/z 387 (M+); **HRMS (ESI)** Calcd for $C_{21}H_{25}NO_4S$−H 386.1426, Found 386.1424.

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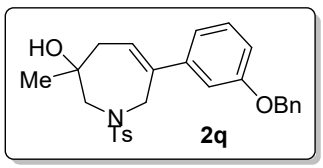
6-(3-(benzyloxy)phenyl)-3-methyl-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{27}H_{29}NO_4S$ **MW:** 463.59 g·mol^{-1}
Light Yellow Oil
Isolated Amount: 52.7 mg **Yield:** 57%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.69 (d, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 7.2 Hz, 2H), 7.35-7.31 (m, 3H), 7.26-7.22 (m, 1H), 7.09 (s, 1H), 7.00 (d, *J* = 8.0 Hz, 1H), 6.90 (d, *J* = 8.0 Hz, 1H), 5.97 (t, *J* = 6.4 Hz, 1H), 5.09 (s, 2H), 4.61 (d, *J* = 15.6 Hz, 1H), 3.78 (d, *J* = 16.0 Hz, 1H), 3.54 (d, *J* = 13.6 Hz, 1H), 3.03 (d, *J* = 13.6 Hz, 1H), 2.82 (s, 1H), 2.73 (dd, *J* = 14.4, 6.8 Hz, 1H), 2.43-2.36 (m, 4H), 1.28 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 158.8, 143.7, 142.3, 140.2, 136.9, 135.1, 129.9, 129.5, 128.5, 127.9, 127.6, 127.1, 126.1, 118.8, 114.1, 112.7, 71.3, 69.9, 61.3, 52.2, 40.0, 26.4, 21.5.
MS (EI) m/z 463 (M+); **HRMS (ESI)** Calcd for $C_{27}H_{29}NO_4S$−H 462.1739, Found 462.1742.

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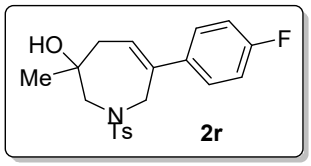
6-(4-fluorophenyl)-3-methyl-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{20}H_{22}FNO_3S$ **MW:** 375.46 g·mol^{-1}
White Solid
Isolated Amount: 50.8 mg **Yield:** 68%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.70 (d, *J* = 8.0 Hz, 2H), 7.42-7.38 (m, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.02 (t, *J* = 8.8 Hz, 2H), 5.92 (t, *J* = 6.8 Hz, 1H), 4.57 (d, *J* = 16.0 Hz, 1H), 3.79 (d, *J* = 16.0 Hz, 1H), 3.54 (d, *J* = 13.6 Hz, 1H), 3.04 (d, *J* = 13.6 Hz, 1H), 2.77 (s, 1H), 2.70 (dd, *J* = 14.8, 7.2 Hz, 1H), 2.43-2.37 (m, 4H), 1.29 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 162.3 (d, *J* = 245.4 Hz), 143.8, 139.7, 136.9 (d, *J* = 3.2 Hz), 135.2, 129.9, 127.9 (d, *J* = 7.9 Hz), 127.1, 126.0, 115.3 (d, *J* = 21.4 Hz), 71.0, 61.5, 52.1, 40.1, 26.5, 21.5.
^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): –114.6.
MS (EI) m/z 375 (M+); **HRMS (ESI)** Calcd for $C_{20}H_{22}FNO_3S$−H 374.1226, Found 374.1227.

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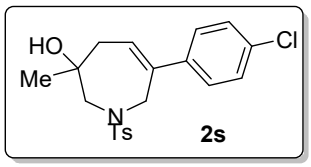
6-(4-chlorophenyl)-3-methyl-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{20}H_{22}ClNO_3S$ **MW:** 391.91 g·mol^{-1}
White Solid
Isolated Amount: 49.1 mg **Yield:** 63%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.70 (d, *J* = 8.0 Hz, 2H), 7.37-7.29 (m, 6H), 5.96 (t, *J* = 6.8 Hz, 1H), 4.56 (d, *J* = 15.6 Hz, 1H), 3.79 (d, *J* = 16.0 Hz, 1H), 3.54 (d, *J* = 14.0 Hz, 1H), 3.04 (d, *J* = 13.6 Hz, 1H), 2.74-2.68 (m, 2H), 2.43-2.37 (m, 4H), 1.29 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.8, 139.6, 139.2, 135.2, 133.5, 129.9, 128.6, 127.5, 127.1, 126.6, 71.0, 61.4, 51.9, 40.1, 26.5, 21.5.
MS (EI) m/z 391 (M+); **HRMS (ESI)** Calcd for $C_{20}H_{22}ClNO_3S$−H 390.0931, Found 390.0935.

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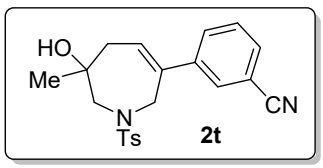
3-(6-hydroxy-6-methyl-1-tosyl-2,5,6,7-tetrahydro-1*H*-azepin-3-yl)benzonitrile



$C_{21}H_{22}N_2O_3S$ **MW:** 382.48 g·mol^{-1}
Light Yellow Oil
Isolated Amount: 35.8 mg **Yield:** 47%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.74 (d, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 7.6 Hz, 2H), 7.65 (s, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.48-7.44 (m, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 6.03 (t, *J* = 6.8 Hz, 1H), 4.51 (d, *J* = 15.6 Hz, 1H), 3.85 (d, *J* = 16.0 Hz, 1H), 3.54 (d, *J* = 13.6 Hz, 1H), 3.10 (d, *J* = 14.0 Hz, 1H), 2.79 (s, 1H), 2.73 (dd, *J* = 14.4, 7.2 Hz, 1H), 2.47-2.42 (m, 4H), 1.30 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.9, 142.0, 139.0, 135.0, 131.0, 130.6, 130.0, 129.7, 129.4, 128.3, 127.1, 118.6, 112.6, 70.8, 61.5, 51.5, 40.2, 26.6, 21.5.
MS (EI) m/z 382 (M+); **HRMS (ESI)** Calcd for $C_{21}H_{22}N_2O_3S$−H 381.1273, Found 381.1273.

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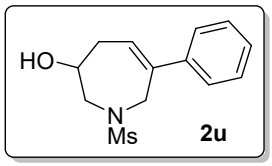
1-(methylsulfonyl)-6-phenyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{13}H_{17}NO_3S$ **MW:** 267.34 g·mol^{-1}
White Solid
Isolated Amount: 42.2 mg **Yield:** 79%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.44 (d, *J* = 7.2 Hz, 2H), 7.36-7.26 (m, 3H), 6.05 (t, *J* = 6.8 Hz, 1H), 4.52 (d, *J* = 16.4 Hz, 1H), 4.21 (d, *J* = 16.4 Hz, 1H), 4.12-4.04 (m, 1H), 3.75-3.65 (m, 2H), 2.91 (s, 3H), 2.79-2.71 (m, 1H), 2.66 (ddd, *J* = 15.2, 6.8, 3.2 Hz, 1H), 2.36 (d, *J* = 6.4 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 141.7, 140.6, 128.6, 127.7, 126.0, 125.4, 67.4, 56.6, 50.7, 38.6, 34.7.
MS (EI) m/z 267 (M+); **HRMS (ESI)** Calcd for $C_{13}H_{17}NO_3S$−H 266.0851, Found 266.0851.

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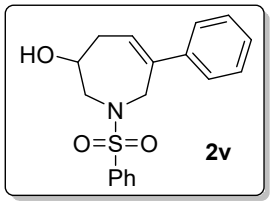
6-phenyl-1-(phenylsulfonyl)-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{18}H_{19}NO_3S$ **MW:** 329.41 g·mol^{-1}
White Solid
Isolated Amount: 52.9 mg **Yield:** 80%

^{1}H NMR (600 MHz, $CDCl_3$, δ ppm): 7.83-7.81 (m, 2H), 7.60-7.58 (m, 1H), 7.53-7.50 (m, 2H), 7.42-7.40 (m, 2H), 7.35-7.32 (m, 2H), 7.29-7.27 (m, 1H), 5.94 (t, *J* = 6.6 Hz, 1H), 4.46 (d, *J* = 15.6 Hz, 1H), 4.07-4.04 (m, 2H), 3.55 (dd, *J* = 13.8, 4.8 Hz, 1H), 3.50 (dd, *J* = 13.8, 4.2 Hz, 1H), 2.72-2.67 (m, 1H), 2.56 (ddd, *J* = 15.0, 6.6, 3.0 Hz, 1H), 2.40 (d, *J* = 8.4 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 141.0, 141.0, 138.6, 132.8, 129.2, 128.5, 127.6, 127.1, 126.2, 125.2, 67.8, 56.6, 51.7, 34.5.
MS (EI) m/z 329 (M+); **HRMS (ESI)** Calcd for $C_{13}H_{17}NO_3S$−H 328.1007, Found 328.1005.

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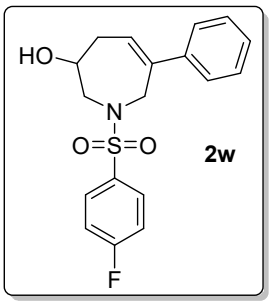
1-((4-fluorophenyl)sulfonyl)-6-phenyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{18}H_{18}FNO_3S$ **MW:** 347.40 g·mol^{-1}
White Solid
Isolated Amount: 52.2mg **Yield:** 75%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.83-7.80 (m, 2H), 7.39 (d, *J* = 7.6 Hz, 2H), 7.35-7.26 (m, 3H), 7.17 (t, *J* = 8.0 Hz, 2H), 5.93 (t, *J* = 6.4 Hz, 1H), 4.39 (d, *J* = 16.0 Hz, 1H), 4.09 (d, *J* = 16.0 Hz, 1H), 4.07-3.99 (m, 1H), 3.57-3.47 (m, 2H), 2.69-2.62 (m, 1H), 2.58-2.51 (m, 2H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 165.0 (d, *J* = 253.3 Hz), 140.9, 140.8, 134.7 (d, *J* = 3.4 Hz), 129.7 (d, *J* = 9.3 Hz), 128.5, 127.6, 126.0, 125.3, 116.4 (d, *J* = 22.5 Hz), 67.6, 56.6, 51.4, 34.5.

^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): –104.9.

MS (EI) m/z 347 (M+); **HRMS (ESI)** Calcd for $C_{18}H_{18}FNO_3S$−H 346.0913, Found 346.0916.

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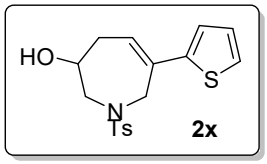
6-(thiophen-2-yl)-1-tosyl-2,3,4,7-tetrahydro-1*H*-azepin-3-ol



$C_{17}H_{19}NO_3S_2$ **MW:** 349.46 g·mol^{-1}

White Solid

Isolated Amount: 56.5 mg **Yield:** 81%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.71 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 5.2 Hz, 1H), 7.13 (d, *J* = 3.6 Hz, 1H), 7.00-6.98 (m, 1H), 6.10 (t, *J* = 6.8 Hz, 1H), 4.50 (d, *J* = 16.0 Hz, 1H), 4.06 (d, *J* = 16.0 Hz, 1H), 4.03-3.97 (m, 1H), 3.55 (dd, *J* = 14.0, 4.8 Hz, 1H), 3.45 (dd, *J* = 14.0, 3.6 Hz, 1H), 2.73-2.66 (m, 1H), 2.54 (ddd, *J* = 14.8, 7.2, 3.2 Hz, 1H), 2.43 (s, 3H), 2.29 (d, *J* = 8.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 143.7, 143.6, 135.8, 134.7, 129.9, 127.6, 127.1, 124.4, 123.5, 123.4, 67.8, 56.5, 51.1, 34.2, 21.5.

MS (EI) m/z 349 (M+); **HRMS (ESI)** Calcd for $C_{17}H_{19}NO_3S_2$−H 348.0728, Found 348.0715.

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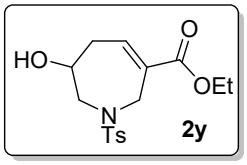
ethyl 6-hydroxy-1-tosyl-2,5,6,7-tetrahydro-1*H*-azepine-3-carboxylate



$C_{16}H_{21}NO_5S$ **MW:** 339.41 g·mol^{-1}

Light Yellow Oil

Isolated Amount: 23.6 mg **Yield:** 35%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.70 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.01 (t, *J* = 6.8 Hz, 1H), 4.35 (d, *J* = 16.8 Hz, 1H), 4.19 (q, *J* = 7.2 Hz, 2H), 4.11-4.04 (m, 1H), 4.01 (d, *J* = 16.8 Hz, 1H), 3.47 (d, *J* = 4.4 Hz, 2H), 2.78-2.70 (m, 1H), 2.64-2.58 (m, 1H), 2.56-2.45 (m, 1H), 2.43 (s, 3H), 1.29 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 165.5, 143.7, 138.9, 135.6, 132.4, 129.8, 127.1, 67.9, 61.1, 55.7, 47.9, 34.1, 21.5, 14.2.

MS (EI) m/z 339 (M+); **HRMS (ESI)** Calcd for $C_{16}H_{21}NO_5S$−H 338.1062, Found 338.1061.

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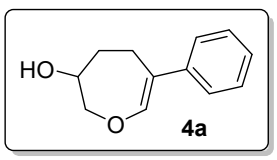
6-phenyl-2,3,4,5-tetrahydrooxepin-3-ol



$C_{12}H_{14}O_2$ **MW:** 190.24 g·mol^{-1}

Off-White Solid

Isolated Amount: 26.3 mg **Yield:** 69%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.32-7.20 (m, 5H), 6.69 (s, 1H), 4.15-4.09 (m, 2H), 3.98 (dd, *J* = 11.6, 4.0 Hz, 1H), 2.74 (dd, *J* = 16.8, 9.6 Hz, 1H), 2.52 (dd, *J* = 16.4, 10.0 Hz, 1H), 2.18-2.10 (m, 2H), 1.99-1.91 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 147.5, 140.7, 128.3, 126.6, 126.2, 126.1, 76.3, 70.8, 33.4, 25.4.

MS (EI) m/z 190 (M+); **HRMS (ESI)** Calcd for $C_{12}H_{14}O_2$−H 189.0916, Found 189.0919.

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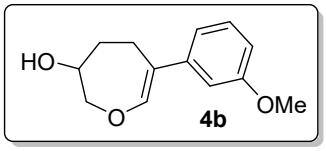
6-(3-methoxyphenyl)-2,3,4,5-tetrahydrooxepin-3-ol



$C_{13}H_{16}O_3$ **MW:** 220.27 g·mol^{-1}
Off-White Solid
Isolated Amount: 27.2 mg **Yield:** 62%

^{1}H NMR (600 MHz, $CDCl_3$, δ ppm): 7.22 (t, *J* = 7.8 Hz, 1H), 6.85 (d, *J* = 7.8 Hz, 1H), 6.79-6.77 (m, 2H), 6.70 (s, 1H), 4.14-4.07 (m, 2H), 3.98 (dd, *J* = 12.0, 4.2 Hz, 1H), 3.81 (s, 3H), 2.72 (dd, *J* = 16.2, 9.0 Hz, 1H), 2.51 (dd, *J* = 16.2, 9.6 Hz, 1H), 2.17-2.12 (m, 1H), 1.98-1.92 (m, 2H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 159.5, 147.6, 142.3, 129.3, 126.0, 118.7, 112.1, 111.8, 76.3, 70.9, 55.2, 33.4, 25.5.
MS (EI) m/z 220 (M+); **HRMS (ESI)** Calcd for $C_{13}H_{16}O_3$−H 219.1021, Found 219.1021.

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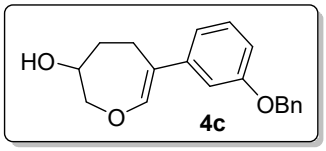
6-(3-(benzyloxy)phenyl)-2,3,4,5-tetrahydrooxepin-3-ol



$C_{19}H_{20}O_3$ **MW:** 296.37 g·mol^{-1}
Light Yellow Oil
Isolated Amount: 31.3 mg **Yield:** 53%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.45-7.33 (m, 5H), 7.21 (t, *J* = 8.0 Hz, 1H), 6.88-6.83 (m, 3H), 6.70 (s, 1H), 5.06 (s, 2H), 4.14-4.06 (m, 2H), 3.98 (dd, *J* = 11.6, 4.0 Hz, 1H), 2.71 (dd, *J* = 16.4, 9.2 Hz, 1H), 2.49 (dd, *J* = 16.4, 9.6 Hz, 1H), 2.17-2.09 (m, 1H), 1.98-1.90 (m, 2H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 158.7, 147.6, 142.3, 136.9, 129.3, 128.6, 128.0, 127.5, 126.0, 118.9, 113.1, 112.6, 76.3, 70.8, 70.0, 33.4, 25.4.
MS (EI) m/z 296 (M+); **HRMS (ESI)** Calcd for $C_{19}H_{20}O_3$−H 295.1334, Found 295.1336.

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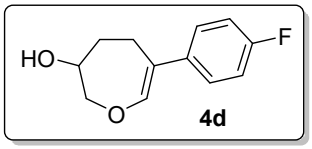
6-(4-fluorophenyl)-2,3,4,5-tetrahydrooxepin-3-ol



$C_{12}H_{13}FO_2$ **MW:** 208.23 g·mol^{-1}
White Solid
Isolated Amount: 28.2 mg **Yield:** 68%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.23-7.19 (m, 2H), 7.01-6.96 (m, 2H), 6.63 (s, 1H), 4.14-4.07 (m, 2H), 3.98 (dd, *J* = 12.4, 4.8 Hz, 1H), 2.70 (dd, *J* = 16.4, 9.2 Hz, 1H), 2.48 (dd, *J* = 15.6, 9.6 Hz, 1H), 2.18-2.10 (m, 1H), 1.99-1.91 (m, 2H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 161.8 (d, *J* = 243.8 Hz), 147.4, 136.7 (d, *J* = 3.3 Hz), 127.7 (d, *J* = 7.8 Hz), 125.3, 115.1 (d, *J* = 21.2 Hz), 76.3, 70.8, 33.4, 25.7.
^{19}F NMR (376 MHz, $CDCl_3$, δ ppm): –116.4.
MS (EI) m/z 208 (M+); **HRMS (ESI)** Calcd for $C_{12}H_{13}FO_2$−H 207.0821, Found 207.0825.

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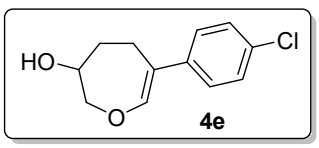
6-(4-chlorophenyl)-2,3,4,5-tetrahydrooxepin-3-ol



$C_{12}H_{13}ClO_2$ **MW:** 224.68 g·mol^{-1}
Light Yellow Oil
Isolated Amount: 29.3 mg **Yield:** 65%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.26 (d, *J* = 8.4 Hz, 2H), 7.18 (d, *J* = 8.4 Hz, 2H), 6.66 (s, 1H), 4.15-4.06 (m, 2H), 3.99 (dd, *J* = 12.0, 4.4 Hz, 1H), 2.69 (dd, *J* = 16.4, 9.2 Hz, 1H), 2.48 (dd,

J = 16.0, 9.6 Hz, 1H), 2.19-2.11 (m, 1H), 2.02-1.90 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 147.8, 139.2, 132.3, 128.4, 127.4, 124.9, 76.3, 70.8, 33.3, 25.4.

MS (EI) m/z 224 (M+); **HRMS (ESI)** Calcd for $C_{12}H_{13}ClO_2$−H 223.0526, Found 223.0527.

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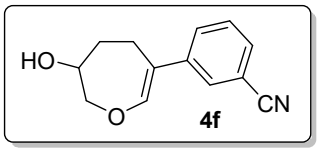
3-(6-hydroxy-4,5,6,7-tetrahydrooxepin-3-yl)benzonitrile



$C_{13}H_{13}NO_2$ **MW:** 215.25 g·mol^{-1}

Light Yellow Solid

Isolated Amount: 25.4 mg **Yield:** 59%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.53 (s, 1H), 7.51-7.48 (m, 2H), 7.41-7.38 (m, 1H), 6.70 (s, 1H), 4.20-4.11 (m, 2H), 4.02 (dd, *J* = 11.6, 4.0 Hz, 1H), 2.70 (dd, *J* = 16.4, 9.2 Hz, 1H), 2.51 (dd, *J* = 16.4, 10.0 Hz, 1H), 2.23-1.94 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 148.9, 142.1, 130.4, 129.9, 129.6, 129.1, 123.6, 118.8, 112.4, 76.4, 70.5, 33.3, 25.3.

MS (EI) m/z 215 (M+); **HRMS (ESI)** Calcd for $C_{13}H_{13}NO_2$−H 214.0868, Found 214.0867.

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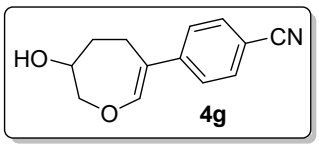
4-(6-hydroxy-4,5,6,7-tetrahydrooxepin-3-yl)benzonitrile



$C_{13}H_{13}NO_2$ **MW:** 215.25 g·mol^{-1}

Light Yellow Oil

Isolated Amount: 22.3 mg **Yield:** 52%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.57 (d, *J* = 7.6 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 6.77 (s, 1H), 4.22-4.11 (m, 2H), 4.03 (dd, *J* = 12.0, 4.4 Hz, 1H), 2.71 (dd, *J* = 16.4, 9.2 Hz, 1H), 2.52 (dd, *J* = 16.4, 10.0 Hz, 1H), 2.24-1.94 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 149.6, 145.7, 132.1, 126.3, 123.8, 119.0, 109.7, 76.4, 70.5, 33.3, 25.0.

MS (EI) m/z 215 (M+); **HRMS (ESI)** Calcd for $C_{13}H_{13}NO_2$−H 214.0868, Found 214.0868.

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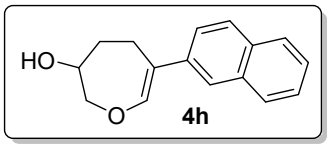
6-(naphthalen-2-yl)-2,3,4,5-tetrahydrooxepin-3-ol



$C_{16}H_{16}O_2$ **MW:** 240.3 g·mol^{-1}

Off-White Solid

Isolated Amount: 24.2 mg **Yield:** 50%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.81-7.76 (m, 3H), 7.69 (s, 1H), 7.49-7.41 (m, 3H), 6.83 (s, 1H), 4.20-4.10 (m, 2H), 4.04 (dd, *J* = 11.6, 4.0 Hz, 1H), 2.85 (dd, *J* = 16.4, 9.2 Hz, 1H), 2.63 (dd, *J* = 16.4, 10.0 Hz, 1H), 2.26-2.16 (m, 1H), 2.06-1.98 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 148.0, 138.0, 133.4, 132.2, 127.9, 127.7, 127.5, 126.2, 126.0, 125.5, 124.7, 124.3, 76.4, 70.9, 33.4, 25.4.

MS (EI) m/z 240 (M+); **HRMS (ESI)** Calcd for $C_{16}H_{16}O_2$−H 239.1072, Found 239.1077.

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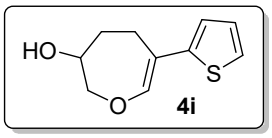
6-(thiophen-2-yl)-2,3,4,5-tetrahydrooxepin-3-ol

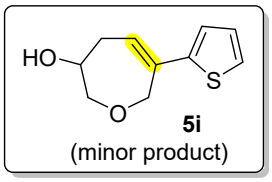


$C_{10}H_{12}O_2S$ **MW:** 196.26 g·mol^{-1}
Light Yellow Oil
Isolated Amount: 21.1 mg **Yield:** 54%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.08 (d, *J* = 5.2 Hz, 1H), 6.96-6.94 (m, 2H), 6.90 (d, *J* = 3.6 Hz, 1H), 4.15 (dd, *J* = 12.4, 3.2 Hz, 1H), 4.13-4.07 (m, 1H), 4.02 (dd, *J* = 12.0, 4.0 Hz, 1H), 2.75 (dd, *J* = 16.8, 9.2 Hz, 1H), 2.54 (dd, *J* = 16.4, 10.0 Hz, 1H), 2.23-2.15 (m, 1H), 2.02-1.94 (m, 1H), 1.90 (d, *J* = 5.6 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 146.8, 143.6, 127.2, 122.6, 122.0, 119.5, 76.8, 70.6, 33.1, 25.8.
MS (EI) m/z 196 (M+); **HRMS (ESI)** Calcd for $C_{10}H_{12}O_2S$−H 195.0480, Found 195.0477.

……

6-(thiophen-2-yl)-2,3,4,7-tetrahydrooxepin-3-ol

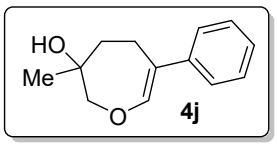


$C_{10}H_{12}O_2S$ **MW:** 196.26 g·mol^{-1}
Light Yellow Oil
Isolated Amount: < 3.8 mg **Yield:** < 10%

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.15 (d, *J* = 4.8 Hz, 1H), 6.98-6.96 (m, 1H), 6.93 (d, *J* = 3.6 Hz, 1H), 6.15 (t, *J* = 6.4 Hz, 1H), 4.68 (d, *J* = 15.2 Hz, 1H), 4.50 (d, *J* = 15.2 Hz, 1H), 4.03-3.97 (m, 1H), 3.94-3.93 (m, 2H), 2.78-2.71 (m, 1H), 2.64 (ddd, *J* = 15.6, 6.0, 2.0 Hz, 1H), 2.18 (d, *J* = 8.0 Hz, 1H).
MS (EI) m/z 196 (M+).

……

3-methyl-6-phenyl-2,3,4,5-tetrahydrooxepin-3-ol

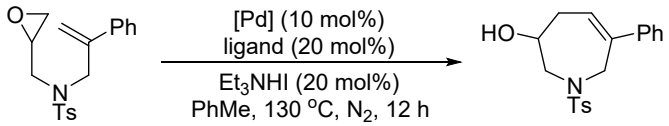


$C_{13}H_{16}O_2$ **MW:** 204.27 g·mol^{-1}
Light Yellow Oil
Isolated Amount: 22.3 mg **Yield:** 55 %

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.32-7.20 (m, 5H), 6.69 (s, 1H), 3.91 (d, *J* = 12.0 Hz, 1H), 3.80 (d, *J* = 12.0 Hz, 1H), 2.75 (dd, *J* = 16.4, 10.4 Hz, 1H), 2.47 (ddd, *J* = 16.4, 8.4, 1.6 Hz, 1H), 2.26 (s, 1H), 2.03-1.97 (m, 1H), 1.91-1.84 (m, 1H), 1.26 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 147.3, 140.6, 128.3, 126.6, 126.5, 126.1, 80.1, 72.8, 39.2, 26.0, 25.3.
MS (EI) m/z 204 (M+); **HRMS (ESI)** Calcd for $C_{13}H_{16}O_2$−H 203.1072, Found 203.1072.

4. Table S1 for selected preliminary experimental conditions screening

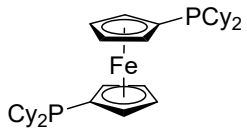
Table S1 Selected preliminary experimental conditions screening



1a **2a**

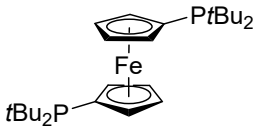
Entry	Cat. [Pd]	Ligand	Additive	Yield of **2a**
1	$Pd(PPh_3)_4$	-	-	13%
2	$Pd(dba)_2$	-	-	12%
3	$PdCl_2(PPh_3)_2$	-	-	trace
4	$PdCl_2$(dppf)	-	-	9%
5	$Pd(PPh_3)_4$	tris(2,6-dimethoxyphenyl)phosphine	-	ND
6	$Pd(PPh_3)_4$	tri(2-furyl)phosphine	-	11%
7	$Pd(PPh_3)_4$	RuPhos	-	ND
8	$Pd(PPh_3)_4$	4,4'-dimethoxy-2,2'-bipyridine	-	ND
9	$Pd(PPh_3)_4$	Xantphos	-	17%
10	$Pd(PPh_3)_4$	bis(2-diphenylphosphinophenyl)ether	-	ND
11	$Pd(PPh_3)_4$	BINAP	-	13%
12	$Pd(PPh_3)_4$	dppm	-	trace
13	$Pd(PPh_3)_4$	dppp	-	9%
14	*$Pd(PPh_3)_4$*	*dppf*	-	*41%*
15	$Pd(PPh_3)_4$	dppf	Et_3N (20 mol%)	28%
16	$Pd(PPh_3)_4$	dppf	Cy_2NMe (20 mol%)	25%
17	$Pd(PPh_3)_4$	dppf	$Cu(OAc)_2$ (10 mol%)	8%
18	$Pd(PPh_3)_4$	dppf	H_2O (1.0 equiv)	16%
19	$Pd(PPh_3)_4$	dppf	MeOH (1.0 equiv)	13%

5. CAS number of ligands L1-L6



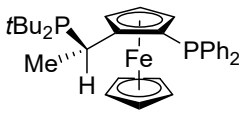
L1

CAS No. 146960-90-9
consumption of **1a**: 100%
yield of **2a**: 14%



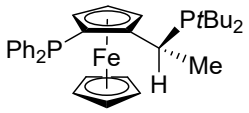
L2

CAS No. 84680-95-5
consumption of **1a**: 100%
yield of **2a**: 8%



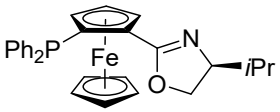
L3

CAS No. 277306-29-3
consumption of **1a**: 100%
yield of **2a**: 80%



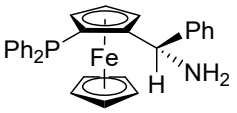
L4

CAS No. 155830-69-6
consumption of **1a**: 100%
yield of **2a**: 86%



L5

CAS No. 163169-29-7
consumption of **1a**: 20%
yield of **2a**: ND



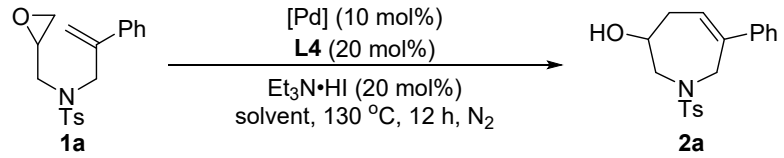
L6

CAS No. 498580-48-6
consumption of **1a**: 89%
yield of **2a**: ND

Figure S1 Details for reactions employing ligands **L1**-**L6**

6. Table S2 for Further Screening toward Palladium Catalysts and Solvents

Table S2 Further screening toward palladium catalysts and solvents under ligand-**L4** condition

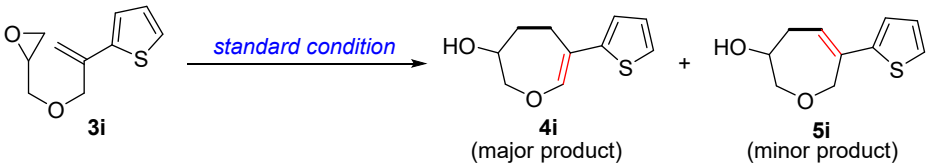


1a **2a**

Entry	Cat. [Pd]	Solvent	Yield of **2a**	Note
1	none	PhMe	ND	66% of **1a** was recovered
2	$PdCl_2$	PhMe	42%	15% of **1a** was recovered
3	$Pd(OAc)_2$	PhMe	trace	70% of **1a** was recovered
4	$PdCl_2(PPh_3)_2$	PhMe	trace	69% of **1a** was recovered
5	allylpalladium chloride dimer	PhMe	34%	messy reaction system
6	$Pd(dba)_2$	PhMe	75%	-
7	$Pd(PPh_3)_4$	$PhCF_3$	73%	-
8	$Pd(PPh_3)_4$	dioxane	trace	80% of **1a** was recovered
9	$Pd(PPh_3)_4$	MeCN	trace	21% of **1a** was recovered
10	$Pd(PPh_3)_4$	DMF	ND	**1a** was decomposed

7. Time Course Experiments of 3i

Table S3 Time Course Experiments of **3i**

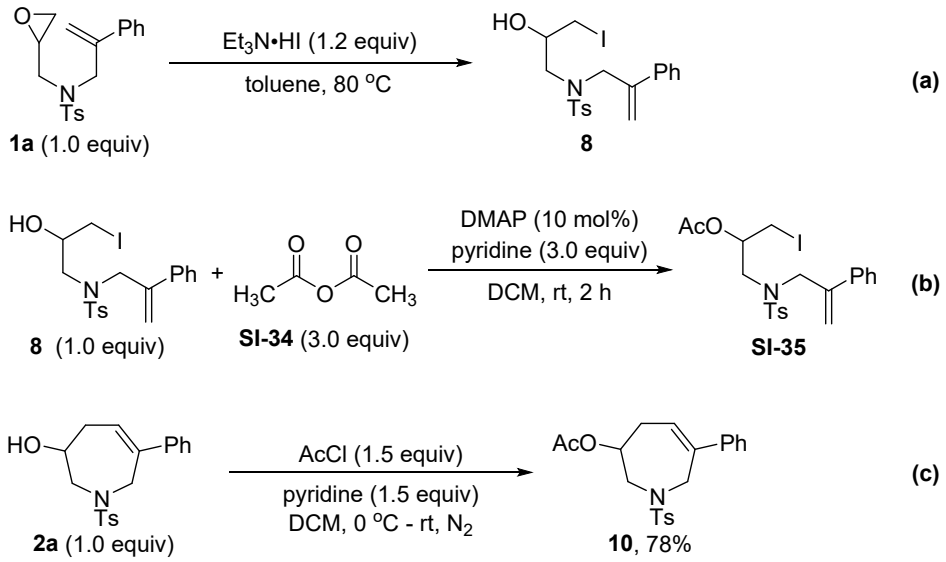


3i **4i** (major product) **5i** (minor product)

entry	reaction time	consumption of **3i**	**4i**:**5i**[a]
1	5 h	66%	6.0:1
2	9 h	100%	5.6:1
3	15 h	100%	5.7:1
4	20 h	100%	5.9:1

[a] detected by GC (rough proportion)

8. Verification Experiments



Scheme S1 Verification experiments of intermediate

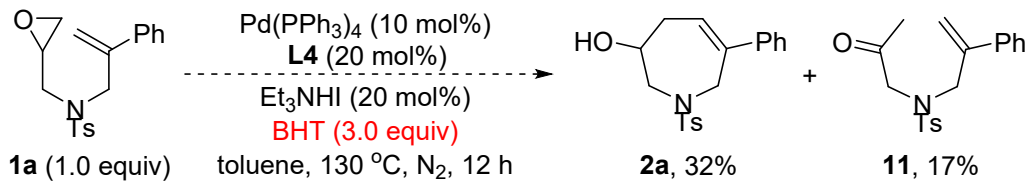
(Eq. a) Preparation of iodide 8: To a solution of the epoxide **1a** (0.58 g, 1.7 mmol) in toluene (10 mL) at rt was added $Et_3N{\cdot}HI$ (0.48 g, 2.1 mmol). The resulting mixture was heated to 80°C and stirred for 2 h. Upon completion, the reaction was quenched with 1N HCl solution (10 mL), extracted with EtOAc (3×8 mL), dried over Na_2SO_4, concentrated, and purified on silica gel packed flash chromatography (hexanes/EtOAc = 5:1), afforded the iodide **8** as a white solid. Yield (0.74 g, 92%). **^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):** 7.66 (d, *J* = 8.0 Hz, 2H), 7.46 (d, *J* = 7.2 Hz, 2H), 7.36-7.28 (m, 5H), 5.51 (s, 1H), 5.22 (s, 1H), 4.28-4.20 (m, 2H), 3.69-3.60 (m, 1H), 3.16 (dd, *J* = 15.2, 4.4 Hz, 1H), 3.10-3.01 (m, 3H), 2.91 (s, 1H), 2.43 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$, δ ppm):** 143.9, 142.2, 137.3, 134.5, 129.8, 128.5, 128.2, 127.4, 126.4, 117.5, 68.8, 54.2, 53.4, 21.5, 10.8.

(Eq. b) Preparation of iodide SI-35: To a solution of the iodide **8** (188.5 mg, 0.4 mmol), pyridine (97 µL, 1.2 mmol) and DMAP (4.9 mg, 0.04 mmol) in DCM (4 mL) was added acetic anhydride **SI-34**(113 µL, 1.2 mmol). The reaction was allowed to stir at room temperature for 4 h, then a 1N HCl solution (5 mL) was added to the reaction mixture and it was vigorously stirred for 10 minutes. The reaction mixture was transferred to a separatory funnel, and the organic layer was further washed with saturated aqueous $NaHCO_3$, dried, concentrated *in vacuo*, and purified by chromatography (hexanes/EtOAc = 5:1) to provide the product **SI-35** as a white solid. Yield (174.9 mg, 85%). **^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):** 7.67 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.35-7.28 (m, 5H), 5.54 (s, 1H), 5.25 (s, 1H), 4.92-4.86 (m, 1H), 4.42 (d, *J* = 14.8 Hz, 1H), 3.98 (d, *J* = 14.8 Hz, 1H), 3.28 (dd, *J* = 14.4, 6.4 Hz, 1H), 3.18-3.10 (m, 2H), 3.05 (dd, *J* = 10.8, 6.4 Hz, 1H), 2.44 (s, 3H), 1.93 (s, 3H).

Preparation of compound 10 from 9: The operation is the same as "Typical Procedure for 7-Endo Heck-Type Isomerization". Trace **10** was detected (the contrastive target product was obtained from the following reaction), and 50% of substrate **9** was recovered.

(Eq. c) Preparation of compound 10 from 2a: Under nitrogen atmosphere, to a solvent of **2a** (68.7 mg, 0.2 mmol) in DCM (4 mL) at 0°C, the pyridine (24 μL, 0.3 mmol) and acetyl chloride (21 μL, 0.3 mmol) was added slowly. The reaction mixture was keep stirring at 0°C for 10 min and then warmed to rt for another 50 min. As reaction completed, the reaction mixture was diluted with DCM (15 mL). Washings with 1N aqueous HCl (10 mL), brine (10 mL), drying, and concentration *in vacuo*, and purification by column chromatography (hexanes/EtOAc = 10:1) afforded the **10**. Yield (53.4 mg, 78%). **^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):** 7.69 (d, *J* = 8.4 Hz, 2H), 7.34-7.27 (m, 7H), 5.87-5.84 (m, 1H), 5.07-5.02 (m, 1H), 4.26 (s, 2H), 3.72 (dd, *J* = 14.0, 5.2 Hz, 1H), 3.45 (dd, *J* = 14.0, 6.0 Hz, 1H), 2.71-2.64 (m, 1H), 2.60-2.53 (m, 1H), 2.42 (s, 3H), 2.05 (s, 3H).

BHT Testing Experiment



Scheme S2 BHT testing experiment

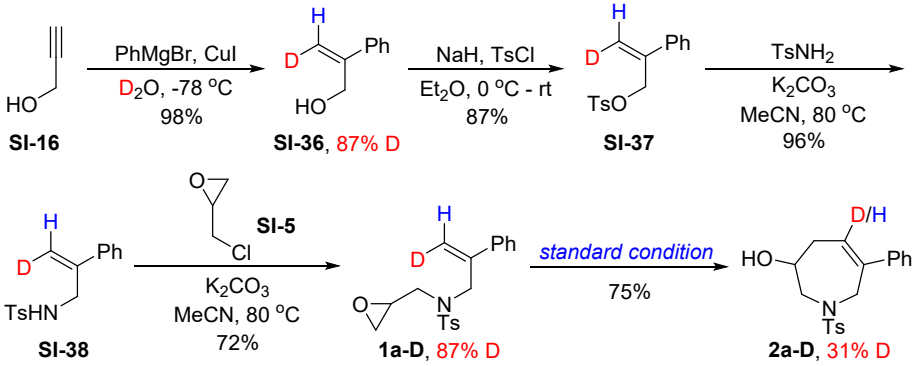
Analytical Data of ketone 11:

^{1}H NMR (400 MHz, $CDCl_3$, δ ppm): 7.55 (d, *J* = 7.6 Hz, 2H), 7.29-7.26 (m, 3H), 7.24-7.20 (m, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 5.35 (s, 1H), 5.16 (d, *J* = 4.4 Hz, 1H), 5.09 (s, 1H), 3.80 (q, *J* = 6.0 Hz, 1H), 2.87 (dd, *J* = 14.4, 6.4 Hz, 1H), 2.79 (dd, *J* = 14.4, 7.6 Hz, 1H), 2.38 (s, 3H), 2.04 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$, δ ppm): 206.6, 143.6, 142.7, 138.5, 136.1, 129.6, 128.6, 128.0, 127.1, 126.2, 117.2, 60.2, 38.5, 27.3, 21.5.

MS (EI) m/z 343 (M+)

9. The Synthetic Procedure and Analytical Data for Deuterium-Substrate



General Procedure:

Preparation of SI-36: To a solution of propargyl alcohol **SI-16** (1.0 g, 18 mmol) in dry THF (40 mL) was vacuum purged three times, backfilling with N_2. CuI (0.343g, 1.8 mmol) was added under stirring and N_2 atmosphere. The suspension was cooled to –78°C. Then a solution of PhMgBr (8.2 g, 45 mmol) in 60 mL THF was added dropwise by constant pressure funnel under vigorous stirring. The resulting mixture held at –78°C for 1 h. Then it was warmed to room temperature and stirred for 18 h. The mixture was cooled to –78°C again and quenched slowly with D_2O (3.6 g, 180 mmol). After the suspension was warmed to room temperature, dilute HCl solution (1 N, 150 mL) was added and the aqueous layer was extracted with EtOAc (3×50 mL). The combined organic layers were washed brine (30 mL), dried with Na_2SO_4, and concentrated *in vacuo*. Purification by column chromatography (hexanes/EtOAc = 10:1 to 5:1) afforded the **SI-36** as a pale yellow liquid. Yield (2.4g, 98%). **^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):** 7.43-7.41 (m, 2H), 7.35-7.26 (m, 3H), 5.43 (s, 1H), 5.32 (s, 0.13H), 4.49 (s, 2H), 2.40-2.14 (m, 1H).

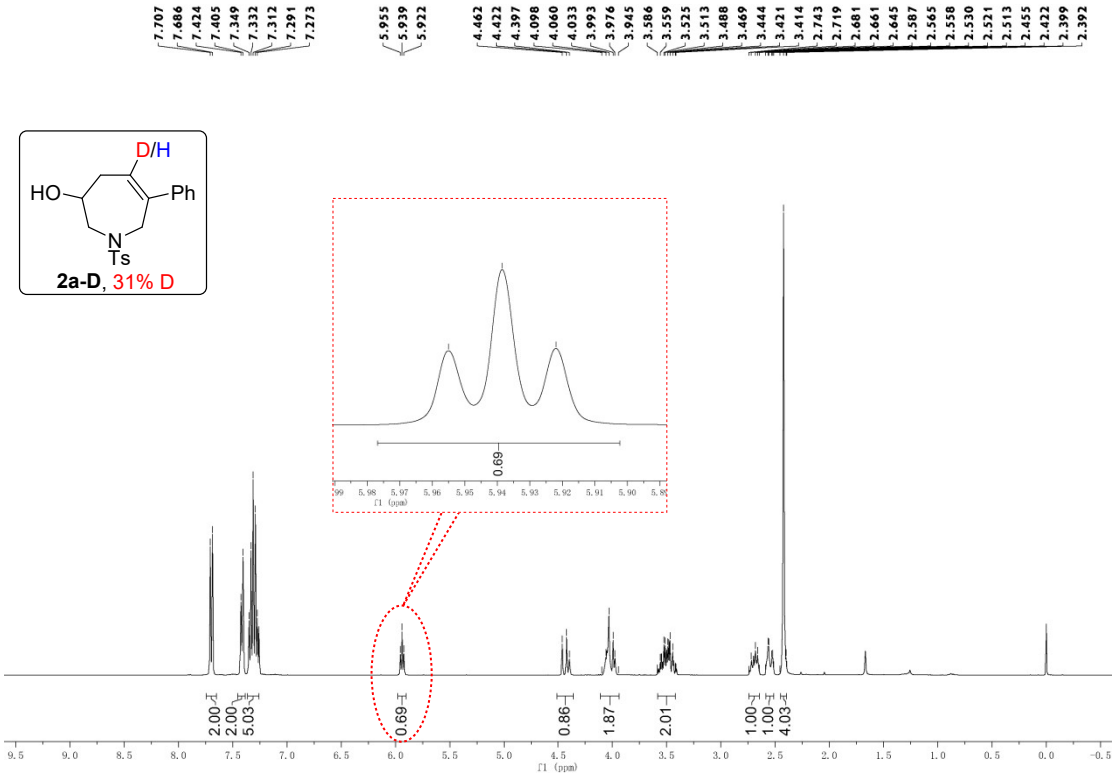
Preparation of SI-37: To a suspension of NaH 60% (0.72 g, 18.0 mmol) in Et_2O (15 mL) was added **SI-36** (2.03 g, 15.0 mmol) under N_2 atmosphere. The mixture was stirred for 30 min at room temperature and then cooled to 0 °C. A solution of TsCl (2.85 g, 15.0 mmol) in Et_2O (5 mL) was added dropwise. The resulting mixture was warmed to room temperature and stirred for 1 h. Then the solution was quenched with a saturated aqueous solution of NH_4Cl (30 mL). The aqueous layer was extracted with Et_2O (3×10 mL). The combined organic layers were washed with brine (40 mL), dried with Na_2SO_4, and concentrated *in vacuo* to afford the crude product **SI-37** as a light yellow solid, which was used without further purification. Yield (3.76 g, 87%)

Preparation of SI-38: The **SI-37** (3.26 g, 11.2 mmol) was dissolved in 35 mL acetonitrile, and then *p*-toluenesulfonamide (3.85 g, 22.5 mmol), K_2CO_3 (3.11 g, 22.5 mmol) was added successively. The resulting mixture was stirred and refluxed at 80 °C for 3.5 h. After successive filtration and purification by column chromatography (hexanes/EtOAc = 5:1), compound **SI-38** was obtained as a white solid. Yield (3.1 g, 96%)

Preparation of 1a-D: The **SI-38** (1.59 g, 5.5 mmol), (±)-epichlorohydrin **SI-5** (1.3 mL, 16.5

mmol), and K_2CO_3 (1.08 g, 7.8 mmol) was added successively to 15 mL acetonitrile. The resulting mixture was stirred and refluxed at 80 °C for 9 h. The precipitate was removed by filtration, and the filtrate was concentrated *in vacuo*. The **1a-D** was obtained as a white solid by column chromatographic purification (hexanes/EtOAc = 10:1 to 5:1) of the crude product. Yield (1.35 g, 72%, 87% D). **^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):** 7.67 (d, *J* = 8.0 Hz, 2H), 7.43 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.35-7.28 (m, 5H), 5.49-5.45 (m, 1H), 5.28 (s, 0.13H), 4.31 (dd, *J* = 18.8, 15.2 Hz, 2H), 3.30 (dd, *J* = 15.2, 4.8 Hz, 1H), 3.09 (dd, *J* = 15.2, 6.0 Hz, 1H), 2.94-2.88 (m, 1H), 2.63 (t, 4.4 Hz, 1H), 2.43 (s, 3H), 2.40 (dd, *J* = 4.8, 2.4 Hz, 1H).

Preparation of 2a-D: Substrate **1a-D** (68.9 mg, 0.2 mmol). The operation is the same as "Typical Procedure for 7-Endo Heck-Type Isomerization". Yield (51.5 mg, 75%, 31% D). **^{1}H NMR (400 MHz, $CDCl_3$, δ ppm):** 7.70 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 7.6 Hz, 2H), 7.35-7.27 (m, 5H), 5.94 (t, *J* = 6.4 Hz, 0.69H), 4.46-4.40 (m, 1H), 4.10-3.95 (m, 2H), 3.59-3.41 (m, 2H), 2.74-2.65 (m, 1H), 2.59-2.51 (m, 1H), 2.46-2.39 (m, 4H).



10. Computational Details

Geometry optimizations were performed using the B3LYP[1] density functional with Grimme's empirical dispersion-correction (D3)[2] and Becke-Johnson (BJ)'s damping schemes[3] (denoted as B3LYP-D3BJ) implemented in Gaussian 09[4] with the SMD[5] solvent model and toluene as the solvent. The [Lanl2dz]/[6-31G(d,p)] basis sets[6] were used for [Pd, Fe, I]/[C, H, O, N, S, P] atoms, respectively. Frequency calculations were carried out at the same level with geometry optimization to provide thermal corrections to the energies and to confirm the obtained stationary points are either intermediates (with zero imaginary frequency) or transition states (with only one imaginary frequency). 3D geometry structures were drawn by CYLview software.[7]

References:

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Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., *Gaussian 09, Revision D.01*, Gaussian, Inc., Wallingford CT, **2009**.

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The dissociation of $Et_3N{\cdot}HI$ into $Et_3N{\cdot}H^+$ and I^- (see below) requires 36.8 kcal/mol free energy, which indicates that this is a highly unfavorable and almost impossible process under the utilized reaction condition.

$$Et_3N{\cdot}HI \quad = \quad Et_3N{\cdot}H^+ \quad + \quad I^- \qquad\qquad \Delta G/\Delta H = 36.8/43.8 \text{ kcal/mol}$$

11. Distortion Interaction Analysis on the Distal and Proximal *β*-Hydride Elimination Transition States (TS4 and TS4')

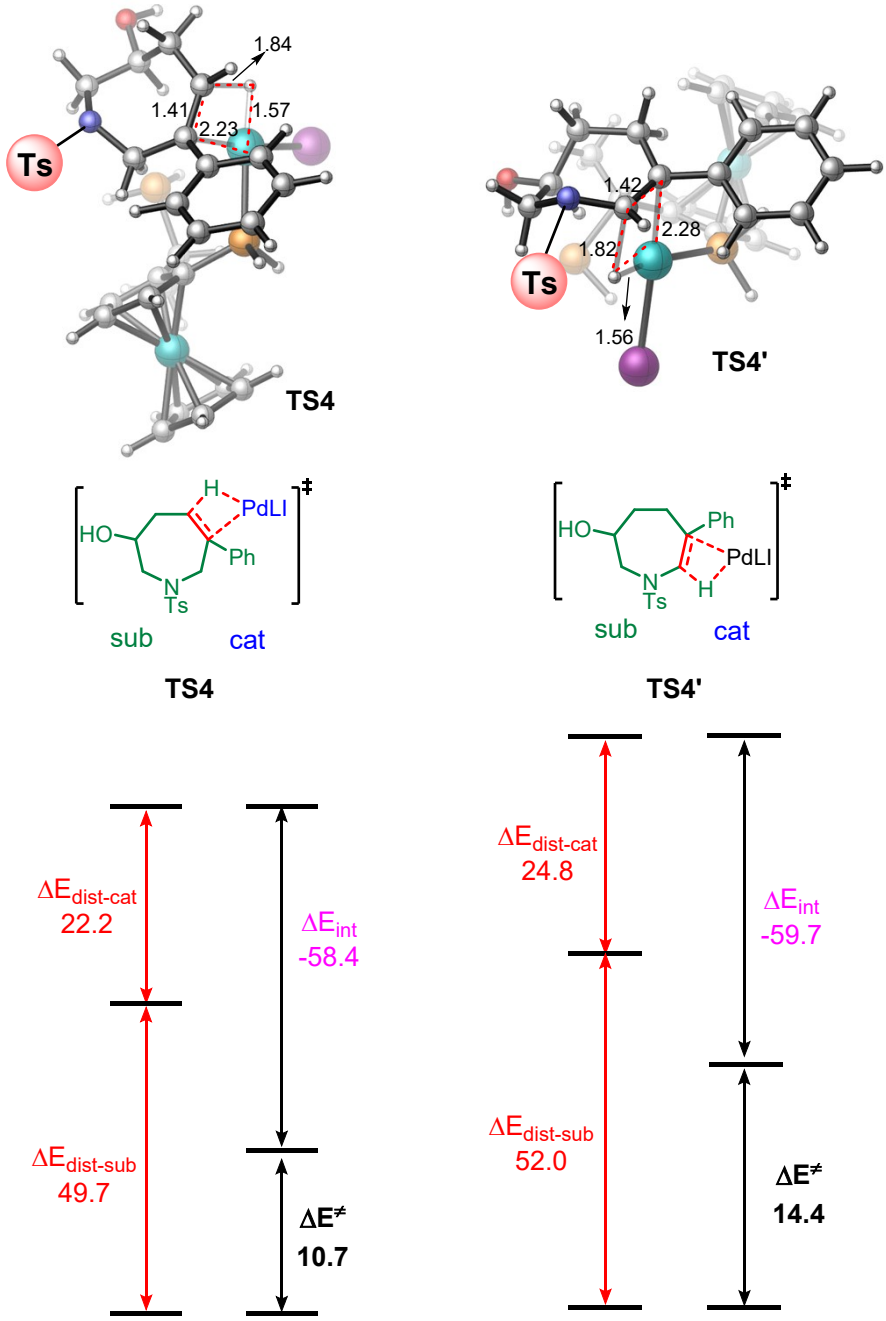

Figure S2. The distortion/interaction analysis on **TS4** and **TS4'**.

The transition state structures have been separated into two parts: the cat (catalyst, in blue) part and the sub (substrate, in green) part for the distortion/interaction analysis. As shown above (Figure S2), we can see that both the distortion of the catalyst and the substrate in **TS4'** (24.8 and 52.0 kcal/mol) are larger compared to those in **TS4** (22.2 and 49.7 kcal/mol), and this unfavorable distortion energy cannot be compensated by the slightly favorable interaction in the former (-59.7 kcal/mol) than the latter (-58.4 kcal/mol). Thus, the origin of the selectivity comes from the much

structure deformation in **TS4'**, which by close analyses is due to the steric repulsion between the "back" phosphine ligand and the substrate ring.

The different spin states of the ferrocene type ligand **L4**:

Spin state	singlet	Triplet	quintet
ΔG (kcal/mol)	0.0	11.7	3.7

12. Electronic Energies (E), Enthalpies (H), Gibbs Free Energies (G), and Coordinates for All the Calculated Species

Table S4. Energy Data for All Calculated Species

Structures	Electronic energy (E)	Enthalpy (H)	Gibbs free energy (G)	Imaginary Frequency	<S**2>
Et_3NHI	-304.516221	-304.28154	-304.333691		
IN1	-1704.481878	-1703.983578	-1704.079831		
TS1	-1704.462382	-1703.970673	-1704.063859	-83.89	
NEt_3	-292.46706	-292.250457	-292.294939		
IN2	-1411.983352	-1411.709625	-1411.780871		
1a	-1415.281459	-1414.892586	-1414.968808		
IN3	-2827.293481	-2826.626942	-2826.754194		
TS2	-2827.255851	-2826.590996	-2826.715192	-375.86	
IN4	-2827.307961	-2826.638069	-2826.763598		
IN4t	-2827.343975	-2826.673655	-2826.799783		2.0290
IN5	-1415.911007	-1415.508956	-1415.586913		0.7769
·Pd(I)LI	-1411.382884	-1411.117345	-1411.189352		0.7524
IN6	-2827.3386	-2826.667861	-2826.792736		
TS4	-2827.316983	-2826.651292	-2826.775721	-507.22	
TS4'	-2827.311335	-2826.645412	-2826.770244	-389.11	
2a	-1415.328706	-1414.937222	-1415.011731		
TS5	-2827.278479	-2826.614677	-2826.741349	-342.60	
TS2t	-2827.232039	-2826.569778	-2826.700800	-405.84	2.0641

Coordinates

Et_3NHI

N	-1.258326	-0.385175	-0.096331
C	-0.912654	0.449219	-1.302167
H	-1.404049	-0.031561	-2.146969
H	0.170409	0.375925	-1.440226
C	-1.380133	1.893888	-1.201543
H	-1.248680	2.361675	-2.181508
H	-2.442097	1.945105	-0.945281
H	-0.806810	2.478482	-0.478464
C	-0.781961	0.240008	1.189076
H	-1.262577	1.215819	1.241076
H	0.298043	0.386630	1.090158
C	-1.139085	-0.564450	2.430809
H	-0.918630	0.051153	3.307670
H	-2.206249	-0.803402	2.448609
H	-0.561316	-1.486743	2.523056
C	-0.805886	-1.814818	-0.240801
H	0.286673	-1.810716	-0.177446
H	-1.202942	-2.341805	0.625577
C	-1.305397	-2.487549	-1.511379
H	-0.813314	-2.116098	-2.413045
H	-1.091081	-3.557442	-1.435727
H	-2.387693	-2.368786	-1.615742
I	-4.680392	-0.466520	0.088418
H	-2.313890	-0.410019	-0.042507

IN1

P	-1.269640	-4.841964	-1.302597
C	-1.055036	-4.394601	-3.061482
C	-0.357146	-3.228421	-3.541361
C	-1.722533	-4.993243	-4.180346
C	-0.607427	-3.126827	-4.947338
H	-2.300089	-5.907224	-4.148733
C	-1.444451	-4.212272	-5.341918
H	-0.184690	-2.385432	-5.609755
H	-1.768213	-4.431296	-6.350150
C	0.457073	-2.282780	-2.701235
H	1.068920	-2.875654	-2.011040
Fe	0.306273	-4.933979	-4.516454
C	0.963166	-6.874129	-4.816730
C	1.284496	-6.068681	-5.951503
C	2.123615	-5.000736	-5.511234
C	1.603478	-6.303458	-3.675195
C	2.320582	-5.145705	-4.103866
H	0.923000	-6.217986	-6.959616
H	0.315619	-7.740069	-4.814746
H	1.517841	-6.656033	-2.656631
H	2.882190	-4.475386	-3.467883
H	2.511426	-4.202008	-6.128305
C	1.370279	-1.371783	-3.520501
H	1.986026	-0.751606	-2.863127
H	0.791170	-0.699265	-4.162148
H	2.038661	-1.958817	-4.160867
P	-0.699658	-1.337636	-1.528377
Pd	-1.972372	-2.858497	-0.344600
H	-1.200655	-0.407558	-2.484678
H	0.280934	-0.452346	-0.999854
H	-1.707943	-6.185498	-1.538478
H	0.056478	-5.224266	-0.967133
N	-5.399295	-3.381756	-1.396344
C	-4.944350	-4.741189	-1.861453
H	-3.951432	-4.595512	-2.281170
H	-5.625240	-5.040987	-2.663613
C	-4.881952	-5.769098	-0.742486
H	-4.388865	-6.664678	-1.131116
H	-4.288527	-5.394875	0.095874
H	-5.869203	-6.065557	-0.381859
C	-6.743370	-3.457142	-0.707449
H	-6.574857	-4.038766	0.197808
H	-7.400250	-4.020917	-1.376183
C	-7.341918	-2.107089	-0.344368
H	-8.223889	-2.291122	0.276122
H	-6.641931	-1.510054	0.245059
H	-7.665449	-1.536740	-1.217898
C	-5.382651	-2.358885	-2.505678
H	-6.226727	-2.594590	-3.160511
H	-5.573186	-1.400702	-2.023781
C	-4.065542	-2.301922	-3.262174
H	-3.918018	-3.147103	-3.936244
H	-4.052514	-1.387896	-3.862594
H	-3.223950	-2.262565	-2.560722
I	-3.929047	-2.356654	1.690485
H	-4.713161	-3.065435	-0.672077

TS1

P	-2.222850	-4.072401	-2.853333
C	-0.965459	-3.891228	-4.145701
C	0.176953	-3.010933	-4.100066
C	-0.999155	-4.504267	-5.441820
C	0.828190	-3.101224	-5.369161
H	-1.728072	-5.230749	-5.773136
C	0.109313	-4.018747	-6.189814
H	1.741571	-2.594149	-5.643227
H	0.382413	-4.323422	-7.190411
C	0.580856	-2.134619	-2.943495
H	0.563211	-2.733661	-2.024954
Fe	0.754429	-4.966041	-4.459121
C	0.854533	-7.024125	-4.257773
C	1.967873	-6.550390	-5.016334
C	2.698339	-5.633019	-4.202702
C	0.897873	-6.397732	-2.975498
C	2.037192	-5.538590	-2.940321
H	2.193630	-6.808378	-6.041704
H	0.092728	-7.707806	-4.605756
H	0.168728	-6.517445	-2.185491
H	2.330300	-4.904657	-2.114755
H	3.576799	-5.078677	-4.502500
C	1.968810	-1.515661	-3.103969
H	2.238974	-0.940667	-2.214346
H	2.006922	-0.839025	-3.963286
H	2.725134	-2.295018	-3.249974
P	-0.799742	-0.884905	-2.671073
Pd	-2.951226	-2.084782	-2.029445
H	-0.602883	-0.061001	-3.808133
H	-0.185141	-0.030945	-1.724358
H	-3.086086	-4.982690	-3.496309
H	-1.637157	-4.980388	-1.942139
N	-5.788011	-3.637765	-1.218184
C	-5.788009	-4.893844	-1.986872
H	-5.437426	-4.652560	-2.992838
H	-6.819820	-5.272840	-2.088658
C	-4.901759	-5.994134	-1.405382
H	-4.750322	-6.772985	-2.159436
H	-3.920708	-5.608831	-1.112338
H	-5.346423	-6.472230	-0.528941
C	-6.016516	-3.869619	0.220557
H	-5.242464	-4.557855	0.564977
H	-6.987496	-4.378780	0.360820
C	-5.954573	-2.616365	1.085978
H	-5.994593	-2.914403	2.139007
H	-5.026559	-2.067361	0.913779
H	-6.787539	-1.932773	0.906585
C	-6.735402	-2.654208	-1.778407
H	-7.769587	-3.002870	-1.608314
H	-6.597591	-1.726884	-1.222495
C	-6.519561	-2.351251	-3.257870
H	-6.794277	-3.184142	-3.911736
H	-7.140473	-1.494327	-3.536008
H	-5.476283	-2.079068	-3.444654
I	-4.141517	0.204882	-1.022375
H	-4.270012	-2.901645	-1.529524

NEt_3

N	-1.029410	-0.381462	-0.107699
C	-0.679298	0.537126	-1.196244
H	-0.776684	-0.005125	-2.141248
H	0.380058	0.852454	-1.130599
C	-1.590841	1.761086	-1.249051
H	-1.324511	2.400972	-2.097537
H	-2.634080	1.449607	-1.360606
H	-1.518398	2.370899	-0.342833
C	-0.545581	0.099004	1.190909
H	-0.619874	1.190277	1.197669
H	0.526808	-0.136777	1.332373
C	-1.363319	-0.444405	2.360649
H	-0.996965	-0.033894	3.308100
H	-2.416152	-0.168785	2.244957
H	-1.308896	-1.535446	2.433301
C	-0.584117	-1.751009	-0.385193
H	0.456175	-1.765483	-0.763556
H	-0.571479	-2.301769	0.559728
C	-1.508045	-2.483601	-1.355567
H	-1.548776	-1.997015	-2.335390
H	-1.162082	-3.511139	-1.513160
H	-2.526258	-2.515788	-0.955479

IN2

P	-2.502070	-4.060503	-2.915751
C	-1.213797	-3.796942	-4.151517
C	0.015506	-3.071229	-3.934857
C	-1.299740	-4.118371	-5.546657
C	0.666428	-2.962625	-5.201683

H	-2.099380	-4.675192	-6.014616
C	-0.137977	-3.606462	-6.186948
H	1.632271	-2.511655	-5.374552
H	0.113022	-3.723916	-7.231718
C	0.495011	-2.510119	-2.621007
H	0.432779	-3.294796	-1.857276
Fe	0.385576	-4.957276	-4.695459
C	0.286563	-7.011048	-4.950216
C	1.449879	-6.490836	-5.593992
C	2.252608	-5.848209	-4.604158
C	0.371131	-6.688196	-3.562395
C	1.585615	-5.969614	-3.347200
H	1.663855	-6.536309	-6.652747
H	-0.531349	-7.526042	-5.434474
H	-0.373026	-6.918098	-2.812192
H	1.927274	-5.564595	-2.404619
H	3.182695	-5.326349	-4.781767
C	1.925758	-1.974687	-2.669180
H	2.243602	-1.632758	-1.680731
H	2.014289	-1.131706	-3.361303
H	2.616033	-2.759424	-2.996620
P	-0.760561	-1.246194	-2.032959
Pd	-2.980896	-2.172057	-1.735260
H	-0.555877	-0.193680	-2.952425
H	-0.107716	-0.688331	-0.913453
H	-3.502297	-4.691721	-3.676590
H	-2.071340	-5.156098	-2.138887
H	-4.392799	-2.802440	-1.523915
I	-3.901681	-0.076996	-0.273541

1a

N	1.096058	-1.046466	0.352204
C	1.303430	-0.036228	1.384658
H	1.999229	-0.447953	2.119562
H	1.820951	0.810578	0.916955
C	0.822906	-0.614878	-1.020002
H	1.076715	-1.433824	-1.694739
H	1.483327	0.225926	-1.264737
C	0.056449	0.469783	2.094495
C	0.243743	1.693770	2.914224
C	-0.780233	2.652490	3.008418
C	1.448038	1.942173	3.595177
C	-0.616161	3.805392	3.771905
H	-1.701982	2.496341	2.456992
C	1.612338	3.097212	4.359369
H	2.258496	1.222082	3.549092
C	0.581962	4.032986	4.452611
H	-1.420149	4.533754	3.825590
H	2.548299	3.263496	4.884637
H	0.713043	4.934308	5.043774
C	-1.128849	-0.143535	1.997063
H	-1.993083	0.203534	2.553676
H	-1.263076	-1.019290	1.376658
C	-0.613473	-0.190439	-1.238038
C	-1.024949	1.205966	-1.096166
O	-0.833056	0.624670	-2.398091
H	-1.360946	-0.969039	-1.078228
H	-0.289846	1.956527	-0.805605
H	-2.055786	1.439803	-0.832916
S	1.452018	-2.652299	0.669864
O	1.887915	-3.260573	-0.592896
O	2.309789	-2.677276	1.860842
C	-0.102878	-3.409061	1.111908
C	-0.462934	-3.506192	2.454729
C	-0.970362	-3.826181	0.099486
C	-1.713542	-4.025710	2.783375
H	0.226015	-3.178516	3.224289
C	-2.217209	-4.336507	0.446414
H	-0.664678	-3.764361	-0.939030
C	-2.608956	-4.442815	1.790314
H	-1.999260	-4.105142	3.828204
H	-2.896072	-4.665275	-0.335549
C	-3.952888	-5.020847	2.149759
H	-3.948681	-6.112336	2.041487
H	-4.224260	-4.792163	3.183753
H	-4.740481	-4.635022	1.494652

IN3

P	-10.383916	-1.800442	-1.818675
C	-9.727616	-2.845998	-3.133805
C	-10.489529	-3.741420	-3.970322
C	-8.335894	-3.043452	-3.420693
C	-9.551801	-4.474504	-4.761426
H	-7.522356	-2.517908	-2.941499
C	-8.234115	-4.044991	-4.425055
H	-9.802293	-5.197282	-5.524015
H	-7.318529	-4.391084	-4.883735
C	-11.987547	-3.905270	-3.968962

H	-12.453270	-2.916264	-4.052569
Fe	-9.357768	-2.434872	-5.105756
C	-8.482999	-0.680919	-5.770487
C	-8.411163	-1.682903	-6.785450
C	-9.743166	-2.081645	-7.107925
C	-9.860143	-0.461135	-5.466627
C	-10.639949	-1.326751	-6.291474
H	-7.504989	-2.100128	-7.202150
H	-7.641865	-0.204521	-5.286511
H	-10.242941	0.214264	-4.713584
H	-11.717603	-1.416337	-6.279008
H	-10.021713	-2.847073	-7.818886
C	-12.506715	-4.799927	-5.094742
H	-13.599056	-4.840559	-5.083773
H	-12.130819	-5.823116	-4.996399
H	-12.190176	-4.413113	-6.069009
P	-12.513138	-4.480792	-2.261887
Pd	-11.974906	-2.841602	-0.560763
H	-12.022096	-5.805045	-2.257682
H	-13.879245	-4.767591	-2.475360
H	-9.201117	-1.359632	-1.207852
H	-10.807306	-0.613286	-2.447507
H	-11.723809	-1.664716	0.416005
I	-13.820158	-3.605447	1.288976
N	-7.221753	-1.794385	2.084449
C	-6.307310	-1.768924	3.228896
H	-5.724148	-2.690603	3.206814
H	-5.584215	-0.948187	3.119450
C	-7.848117	-0.514855	1.700968
H	-7.384587	-0.114736	0.794229
H	-7.661233	0.187823	2.514618
C	-7.010889	-1.638267	4.567330
C	-6.116096	-1.415644	5.733272
C	-6.534690	-0.618021	6.812834
C	-4.828511	-1.976702	5.785428
C	-5.707753	-0.408597	7.913290
H	-7.508985	-0.141566	6.773400
C	-3.999790	-1.765322	6.886970
H	-4.471321	-2.600834	4.972993
C	-4.435256	-0.982465	7.956115
H	-6.052402	0.214595	8.733361
H	-3.012143	-2.216463	6.908463
H	-3.787566	-0.814475	8.811302
C	-8.342447	-1.707710	4.699984
H	-8.814466	-1.658032	5.675322
H	-8.996892	-1.831365	3.846933
C	-9.335150	-0.682343	1.470962
C	-10.353087	0.075320	2.203771
O	-9.988215	0.434618	0.855535
H	-9.636355	-1.647829	1.069815
H	-10.042386	0.786144	2.968881
H	-11.352812	-0.341547	2.318365
S	-6.870597	-2.849731	0.818650
O	-6.927246	-2.096437	-0.449414
O	-5.642115	-3.580886	1.161379
C	-8.232870	-4.002628	0.784899
C	-8.993650	-4.278781	1.921654
C	-8.468182	-4.670521	-0.417632
C	-10.022313	-5.212233	1.834486
H	-8.794220	-3.760320	2.851241
C	-9.488974	-5.614754	-0.479341
H	-7.869203	-4.454285	-1.292758
C	-10.286458	-5.895006	0.637518
H	-10.636609	-5.411469	2.706959
H	-9.669215	-6.138418	-1.413124
C	-11.421647	-6.877525	0.556747
H	-11.372760	-7.475504	-0.357451
H	-11.417017	-7.560691	1.412237
H	-12.380691	-6.346234	0.575239

TS2

P	-10.192773	-1.273479	-1.936992
C	-9.847472	-2.543079	-3.191345
C	-10.832050	-3.418269	-3.777274
C	-8.552566	-2.994999	-3.610040
C	-10.125672	-4.398441	-4.544161
H	-7.611849	-2.523126	-3.361913
C	-8.727269	-4.137307	-4.442951
H	-10.578368	-5.172739	-5.146272
H	-7.940655	-4.680829	-4.947250
C	-12.321642	-3.321036	-3.583206
H	-12.610547	-2.265941	-3.661875
Fe	-9.701403	-2.492087	-5.241481
C	-8.703483	-1.017752	-6.302845
C	-8.933494	-2.153174	-7.137464
C	-10.342497	-2.372272	-7.206556
C	-9.970819	-0.535467	-5.856037
C	-10.984321	-1.371902	-6.414054

H	-8.171956	-2.764515	-7.601323
H	-7.737780	-0.617886	-6.026566
H	-10.132035	0.290081	-5.176491
H	-12.047791	-1.284116	-6.239495
H	-10.834415	-3.177254	-7.734650
C	-13.121402	-4.132979	-4.601317
H	-14.194645	-3.977941	-4.461635
H	-12.924400	-5.204757	-4.497922
H	-12.862356	-3.838127	-5.624340
P	-12.719000	-3.743585	-1.784788
Pd	-11.419678	-2.263308	-0.317186
H	-12.618172	-5.157660	-1.885663
H	-14.135525	-3.700304	-1.876124
H	-8.895734	-0.700567	-1.873884
H	-10.774410	-0.233760	-2.705754
H	-10.414721	-0.826967	0.768215
I	-12.190564	-3.057719	2.277125
N	-6.420978	-2.163350	1.938044
C	-5.956994	-1.904636	3.292888
H	-5.129103	-2.588186	3.498831
H	-5.544467	-0.888750	3.324371
C	-7.259836	-1.171051	1.273093
H	-7.134053	-1.249303	0.191452
H	-6.936678	-0.166916	1.570969
C	-7.012817	-2.050485	4.384617
C	-6.762165	-1.309629	5.641469
C	-7.829042	-0.869328	6.446371
C	-5.450227	-1.022476	6.058587
C	-7.591559	-0.180360	7.631823
H	-8.851209	-1.052858	6.131340
C	-5.214468	-0.337802	7.249730
H	-4.604345	-1.356472	5.467216
C	-6.282562	0.086942	8.040008
H	-8.430015	0.155796	8.234257
H	-4.193307	-0.138228	7.559922
H	-6.098150	0.625776	8.964311
C	-8.105693	-2.825603	4.217376
H	-8.812061	-2.991222	5.022630
H	-8.259062	-3.404871	3.316251
C	-8.711397	-1.395157	1.641190
C	-9.209650	-0.951153	2.928356
O	-9.609868	-0.325487	1.239624
H	-9.099816	-2.358053	1.306795
H	-8.752007	-0.104617	3.426762
H	-10.145542	-1.364544	3.292147
S	-5.838487	-3.454862	1.029319
O	-5.421155	-2.932096	-0.278036
O	-4.892238	-4.161615	1.899806
C	-7.273749	-4.471497	0.761077
C	-7.671050	-5.375328	1.749268
C	-8.034185	-4.285422	-0.393952
C	-8.862475	-6.074116	1.579417
H	-7.056029	-5.528132	2.629081
C	-9.221450	-4.996254	-0.547048
H	-7.700003	-3.602449	-1.163863
C	-9.662646	-5.885680	0.442655
H	-9.183477	-6.773854	2.345110
H	-9.811062	-4.849081	-1.444355
C	-10.986493	-6.584316	0.312758
H	-11.218486	-6.814925	-0.730874
H	-11.008161	-7.514587	0.887331
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P	-9.905810	-1.846885	-1.788720
C	-9.706843	-2.899962	-3.254937
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C	-8.470587	-3.365020	-3.813164
C	-10.187583	-4.459016	-4.896817
H	-7.486422	-3.018002	-3.529581
C	-8.769842	-4.322211	-4.824476
H	-10.725549	-5.077863	-5.600129
H	-8.050324	-4.823556	-5.456740
C	-12.248040	-3.418519	-3.643704
H	-12.467121	-2.348107	-3.552837
Fe	-9.642987	-2.494087	-5.269524
C	-8.592692	-0.905402	-6.081814
C	-8.903930	-1.860850	-7.096611
C	-10.324238	-1.993677	-7.157620
C	-9.821050	-0.448180	-5.516139
C	-10.891481	-1.120445	-6.179558
H	-8.188244	-2.418777	-7.684288
H	-7.601079	-0.610152	-5.768277
H	-9.920378	0.250988	-4.697016
H	-11.944034	-1.013452	-5.955828
H	-10.871864	-2.665834	-7.803530
C	-13.155724	-4.026721	-4.712590
H	-14.207128	-3.833115	-4.483399

H	-13.022415	-5.111166	-4.778733
H	-12.936215	-3.597573	-5.696525
P	-12.586261	-4.078398	-1.910784
Pd	-11.300442	-2.957340	-0.304013
H	-12.458072	-5.467675	-2.175667
H	-14.004381	-4.037602	-1.924523
H	-8.549497	-1.496894	-1.595369
H	-10.324595	-0.614634	-2.346449
H	-10.481216	-0.478226	0.748699
I	-12.131514	-3.230884	2.314779
N	-6.625621	-2.057273	1.942312
C	-6.069286	-1.843932	3.266123
H	-5.435607	-2.705889	3.509480
H	-5.399348	-0.973264	3.241546
C	-7.415039	-0.986542	1.327217
H	-7.274136	-1.013797	0.246452
H	-7.025785	-0.023399	1.680887
C	-7.108718	-1.661987	4.341490
C	-6.719747	-1.134565	5.602102
C	-7.680304	-0.819057	6.610185
C	-5.345215	-0.903757	5.918315
C	-7.290173	-0.314325	7.838654
H	-8.735484	-0.954858	6.409775
C	-4.968046	-0.408464	7.154117
H	-4.575047	-1.135249	5.192849
C	-5.934507	-0.107968	8.122903
H	-8.042826	-0.076223	8.583503
H	-3.916021	-0.252834	7.371546
H	-5.633552	0.284835	9.088888
C	-8.509597	-2.034257	4.025130
H	-9.091805	-2.195604	4.931782
H	-8.522433	-2.977397	3.464602
C	-8.900235	-1.120143	1.655756
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O	-9.589502	-0.122705	0.903086
H	-9.227593	-2.117335	1.330997
H	-8.966682	0.046038	3.469648
H	-10.294200	-1.116749	3.275699
S	-6.080287	-3.324082	0.988077
O	-5.758499	-2.795741	-0.344639
O	-5.057716	-4.015192	1.787104
C	-7.486318	-4.402580	0.803380
C	-7.984945	-5.081985	1.918804
C	-8.075722	-4.549047	-0.448502
C	-9.109480	-5.884191	1.771571
H	-7.497288	-4.989031	2.882910
C	-9.198637	-5.365946	-0.580391
H	-7.659137	-4.035243	-1.304178
C	-9.737903	-6.033948	0.524929
H	-9.515138	-6.399204	2.636781
H	-9.656625	-5.479740	-1.556966
C	-10.995643	-6.847664	0.400667
H	-11.171003	-7.162673	-0.631622
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P	-9.653810	-1.687306	-1.695230
C	-9.486309	-2.726305	-3.168347
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H	-7.268775	-2.934241	-3.415036
C	-8.590639	-4.156075	-4.751046
H	-10.565699	-4.812108	-5.566730
H	-7.884928	-4.676725	-5.383012
C	-12.041906	-3.111963	-3.605408
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Fe	-9.378442	-2.280296	-5.168990
C	-8.237711	-0.739489	-5.956841
C	-8.604621	-1.658057	-6.986497
C	-10.030034	-1.707297	-7.047491
C	-9.437005	-0.222303	-5.381059
C	-10.545249	-0.820170	-6.053500
H	-7.922798	-2.246262	-7.584723
H	-7.229988	-0.506446	-5.642199
H	-9.494882	0.468213	-4.550601
H	-11.590016	-0.654157	-5.828811
H	-10.616012	-2.336093	-7.703292
C	-12.965426	-3.690258	-4.677608
H	-14.009133	-3.444982	-4.464253
H	-12.880628	-4.780038	-4.731135
H	-12.713007	-3.280992	-5.661638
P	-12.431286	-3.730548	-1.879207
Pd	-11.171344	-2.717392	-0.163987
H	-12.377170	-5.128385	-2.072605
H	-13.834927	-3.579106	-1.843771
H	-8.292332	-1.398695	-1.448732

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N	-7.091533	-2.803142	2.334925
C	-6.175795	-2.305159	3.376497
H	-5.528519	-3.142960	3.661734
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C	-8.134702	-1.875323	1.877875
H	-8.287000	-1.997850	0.806178
H	-7.819149	-0.838456	2.042490
C	-6.963704	-1.793706	4.553738
C	-6.481329	-0.701511	5.337997
C	-7.292031	-0.094143	6.341931
C	-5.171102	-0.164300	5.168788
C	-6.829103	0.967938	7.104420
H	-8.301209	-0.452875	6.506129
C	-4.716914	0.894753	5.941516
H	-4.497730	-0.599004	4.439010
C	-5.538278	1.474912	6.914880
H	-7.480311	1.409288	7.853661
H	-3.709505	1.271441	5.788371
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C	-8.285059	-2.452619	4.840651
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H	-8.224247	-3.514724	4.576966
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H	-9.656566	-3.245388	2.470202
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S	-6.415008	-3.758960	1.126692
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C	-7.810583	-4.782289	0.699735
C	-8.454962	-5.530142	1.689420
C	-8.234417	-4.826580	-0.624380
C	-9.553930	-6.303649	1.338580
H	-8.110622	-5.490517	2.716599
C	-9.335506	-5.613556	-0.961372
H	-7.710181	-4.251600	-1.375213
C	-10.016488	-6.351926	0.012675
H	-10.074898	-6.870562	2.103803
H	-9.667639	-5.640191	-1.994441
C	-11.248345	-7.144596	-0.325648
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C	-0.583399	-0.478454	-0.312877
C	0.891315	-0.243279	-0.119622
C	1.313869	1.077149	0.471896
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H	2.320101	0.985868	0.885925
H	0.418261	1.044929	2.455797
H	-2.303673	0.832791	2.319609
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H	0.929125	2.627976	1.884703
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H	-0.965664	2.406068	0.108128
N	-1.419842	-0.416811	0.903642
S	-1.079055	-1.505732	2.142403
O	0.308842	-1.423985	2.630146
O	-2.168391	-1.353703	3.118901
C	-1.242227	-3.054278	1.273256
C	-2.419502	-3.332345	0.572932
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C	-2.537822	-4.548243	-0.089524
H	-3.216369	-2.597357	0.536169
C	-0.341812	-5.196517	0.669346
H	0.706588	-3.729799	1.868421
C	-1.503263	-5.498939	-0.050445
H	-3.444347	-4.768788	-0.646320
H	0.469986	-5.917146	0.703350
C	-1.656440	-6.819380	-0.759127
H	-2.347218	-7.475229	-0.215404
H	-2.065017	-6.685974	-1.766121
H	-0.700141	-7.342039	-0.843696
O	-1.560621	3.075104	1.979365
H	-1.046059	3.882715	1.848524
C	1.856402	-1.174951	-0.622222
C	1.494465	-2.461126	-1.123935
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C	2.443966	-3.358073	-1.589636

H	0.460051	-2.776018	-1.121928
C	4.190463	-1.766545	-1.125302
H	3.591943	0.103197	-0.307127
C	3.802930	-3.025115	-1.597593
H	2.120545	-4.331907	-1.946831
H	5.239974	-1.485607	-1.129398
H	4.542894	-3.729778	-1.964064
H	1.393778	1.816381	-0.345669

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P	-2.340601	-4.019150	-2.499339
C	-1.279649	-3.877507	-3.958733
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C	-1.584347	-4.327567	-5.284609
C	0.372869	-3.111071	-5.381893
H	-2.431474	-4.940046	-5.560031
C	-0.563278	-3.856635	-6.156271
H	1.281004	-2.660923	-5.755283
H	-0.486418	-4.065714	-7.214043
C	0.612652	-2.433401	-2.854882
H	0.664895	-3.135970	-2.014416
Fe	0.249453	-5.053610	-4.666236
C	1.182653	-6.652369	-5.595709
C	2.130932	-5.895676	-4.843587
C	1.715256	-5.900812	-3.477243
C	0.180477	-7.125141	-4.695488
C	0.510396	-6.660353	-3.386777
H	2.991053	-5.377368	-5.244072
H	1.197124	-6.803637	-6.666057
H	-0.692666	-7.703869	-4.963061
H	-0.068223	-6.829444	-2.488660
H	2.209642	-5.393202	-2.660165
C	2.018336	-1.918829	-3.165728
H	2.477343	-1.482055	-2.274968
H	2.000332	-1.151921	-3.946019
H	2.655329	-2.740526	-3.510288
P	-0.542350	-1.093755	-2.232577
Pd	-2.635683	-1.901329	-1.528430
H	-0.483913	-0.158826	-3.290399
H	0.269381	-0.417724	-1.295456
H	-3.395470	-4.799442	-3.022130
H	-1.719990	-5.018471	-1.716277
I	-3.598297	0.310908	-0.255105

IN6

C	-0.434263	-0.145471	-0.479381
C	1.066478	0.180205	-0.430646
C	1.507677	1.224012	0.578502
C	0.657021	1.531224	1.825135
C	-1.730547	0.746564	1.468104
C	-0.788034	1.953865	1.542767
H	-0.967590	0.704643	-0.909172
H	2.526389	1.023205	0.905624
H	0.681926	0.666809	2.496265
H	-1.987107	0.452626	2.485907
H	-0.626751	-0.973012	-1.159016
H	1.151916	2.355997	2.349484
H	-2.655587	1.022063	0.948739
H	-0.814737	2.502520	0.588360
N	-1.114880	-0.396329	0.794641
S	-0.830886	-1.814786	1.620290
O	0.608971	-2.049597	1.809922
O	-1.710935	-1.799529	2.797255
C	-1.410681	-3.029488	0.442881
C	-2.634276	-2.838684	-0.199706
C	-0.639504	-4.166089	0.199527
C	-3.078767	-3.794998	-1.108343
H	-3.216360	-1.943526	-0.009264
C	-1.098924	-5.112933	-0.712956
H	0.314813	-4.283334	0.699008
C	-2.320530	-4.943318	-1.380345
H	-4.026558	-3.646482	-1.617422
H	-0.498565	-5.996048	-0.913028
C	-2.816140	-5.984753	-2.349574
H	-3.300895	-6.811640	-1.816115
H	-3.550710	-5.569312	-3.045023
H	-1.994668	-6.413428	-2.931605
O	-1.327610	2.767374	2.581504
H	-0.911560	3.637711	2.521574
C	2.042903	-0.898191	-0.775914
C	1.631395	-2.146445	-1.278779
C	3.432672	-0.662891	-0.713261
C	2.553273	-3.111840	-1.681151
H	0.582259	-2.390999	-1.347816
C	4.353071	-1.622226	-1.122691
H	3.807842	0.294611	-0.370466
C	3.921935	-2.859140	-1.608310
H	2.191621	-4.068900	-2.046844

H	5.414397	-1.399883	-1.063416
H	4.640829	-3.609336	-1.922553
H	1.599851	2.238531	0.056377
P	1.028015	0.403771	-3.696217
C	-0.626052	-0.265456	-3.925156
C	-1.801418	0.531120	-4.165755
C	-1.021790	-1.643781	-3.848276
C	-2.905037	-0.371294	-4.254892
H	-0.359996	-2.483959	-3.696983
C	-2.428492	-1.701149	-4.058590
H	-3.924468	-0.093185	-4.481036
H	-3.022318	-2.602429	-4.106628
C	-1.845779	2.031447	-4.223488
H	-0.852881	2.408536	-4.491862
Fe	-1.472362	-0.843446	-5.689274
C	-2.050147	-1.871577	-7.395655
C	-2.257762	-0.469954	-7.569125
C	-0.997577	0.185257	-7.422160
C	-0.661598	-2.083735	-7.140416
C	-0.012229	-0.813068	-7.156192
H	-3.208940	0.013018	-7.743589
H	-2.816684	-2.633842	-7.414026
H	-0.191146	-3.034546	-6.931337
H	1.036272	-0.632791	-6.962625
H	-0.822655	1.250906	-7.469290
C	-2.872482	2.582108	-5.214054
H	-2.844235	3.674839	-5.229265
H	-3.889384	2.278180	-4.946758
H	-2.665924	2.216500	-6.224591
P	-2.100129	2.659792	-2.452875
Pd	1.319998	1.715377	-1.871479
H	-3.520441	2.530999	-2.443479
H	-2.109380	4.048355	-2.745721
H	1.819977	-0.757354	-3.785605
H	1.315925	1.028069	-4.924241
I	1.694729	4.153592	-3.126987

TS4

C	-0.451366	-0.311291	-0.521191
C	1.055370	-0.038308	-0.368984
C	1.502909	0.889675	0.600213
C	0.656929	1.509813	1.692884
C	-1.761080	0.828303	1.288092
C	-0.744492	1.974139	1.282807
H	-0.923482	0.494500	-1.085447
H	2.550967	0.811015	0.871265
H	0.589791	0.772594	2.504570
H	-2.058786	0.632022	2.318559
H	-0.613193	-1.208138	-1.114190
H	1.197064	2.371190	2.096560
H	-2.653749	1.124080	0.726371
H	-0.679767	2.405891	0.274272
N	-1.222064	-0.408180	0.717295
S	-0.988648	-1.754506	1.675315
O	0.441566	-1.999144	1.926103
O	-1.900408	-1.621978	2.819585
C	-1.549230	-3.048464	0.575492
C	-2.744211	-2.890052	-0.130532
C	-0.786762	-4.208139	0.449243
C	-3.162497	-3.902438	-0.986673
H	-3.321030	-1.977702	-0.025690
C	-1.223013	-5.214983	-0.411502
H	0.141929	-4.303138	0.999653
C	-2.407661	-5.076260	-1.145165
H	-4.087214	-3.782195	-1.544048
H	-0.630815	-6.119209	-0.518012
C	-2.857916	-6.146693	-2.104719
H	-3.928074	-6.351136	-1.998474
H	-2.690495	-5.835802	-3.143554
H	-2.314141	-7.081697	-1.947529
O	-1.271641	2.934605	2.192967
H	-0.838427	3.779107	2.009802
C	2.028442	-1.042946	-0.912992
C	1.624854	-2.334674	-1.281601
C	3.386280	-0.710321	-1.093054
C	2.534272	-3.255854	-1.806741
H	0.602448	-2.654463	-1.144178
C	4.290790	-1.625326	-1.619802
H	3.729961	0.291737	-0.857302
C	3.870772	-2.908467	-1.984014
H	2.186026	-4.250842	-2.069249
H	5.327318	-1.331411	-1.755682
H	4.576897	-3.621223	-2.398606
H	1.793787	2.522463	-0.186228
P	1.064871	0.680844	-3.622825
C	-0.525560	-0.130597	-3.890761
C	-1.768603	0.560128	-4.111237
C	-0.795771	-1.538124	-3.837728

C	-2.790177	-0.435094	-4.208114
H	-0.055955	-2.313944	-3.704457
C	-2.194163	-1.719988	-4.038812
H	-3.832561	-0.246025	-4.421456
H	-2.705609	-2.670101	-4.099597
C	-1.940996	2.052278	-4.136766
H	-0.988238	2.513175	-4.421392
Fe	-1.335294	-0.749879	-5.659801
C	-1.825608	-1.789412	-7.386696
C	-2.157165	-0.408358	-7.530394
C	-0.959091	0.352291	-7.369851
C	-0.422893	-1.883062	-7.137658
C	0.111495	-0.560046	-7.126280
H	-3.147968	-0.007691	-7.692721
H	-2.521673	-2.616158	-7.419952
H	0.129995	-2.792634	-6.948034
H	1.139837	-0.292045	-6.926335
H	-0.878814	1.429956	-7.394055
C	-3.032831	2.537426	-5.091560
H	-3.097620	3.628766	-5.079963
H	-4.013898	2.143369	-4.808547
H	-2.822102	2.214104	-6.115887
P	-2.200465	2.607962	-2.343632
Pd	1.427239	1.820982	-1.542015
H	-3.610582	2.402056	-2.315259
H	-2.294905	4.004035	-2.586500
H	1.952440	-0.374414	-3.916552
H	1.217440	1.453656	-4.791456
I	1.746406	4.264995	-2.677255

TS4'

C	0.014572	-0.297542	-0.436788
C	1.329551	0.216222	-0.339829
C	1.795047	1.054286	0.842162
C	0.766375	1.722356	1.778912
C	-1.552924	1.120510	0.980580
C	-0.506243	2.234742	1.106665
H	-1.028425	0.570207	-1.648145
H	2.412721	0.394319	1.462086
H	0.500420	1.032901	2.585206
H	-2.040005	0.985757	1.946402
H	-0.117061	-1.201888	-1.022681
H	1.256411	2.577478	2.252008
H	-2.315069	1.395037	0.242631
H	-0.262783	2.584057	0.094187
N	-0.976936	-0.173029	0.589324
S	-0.916123	-1.441780	1.713110
O	0.449039	-1.609446	2.237327
O	-2.030462	-1.222264	2.641063
C	-1.256836	-2.828624	0.647276
C	-2.510330	-2.918234	0.034584
C	-0.264147	-3.777008	0.413800
C	-2.761144	-3.979392	-0.825884
H	-3.267545	-2.165225	0.224400
C	-0.535904	-4.835723	-0.452747
H	0.701032	-3.676543	0.896264
C	-1.779954	-4.952762	-1.083361
H	-3.730313	-4.057018	-1.310263
H	0.233049	-5.578090	-0.644864
C	-2.075393	-6.099559	-2.013873
H	-2.810310	-6.781877	-1.570423
H	-2.497342	-5.743235	-2.959484
H	-1.174757	-6.677078	-2.237072
O	-1.058286	3.315103	1.852086
H	-1.368252	3.975575	1.211093
C	2.398865	-0.444572	-1.151404
C	2.104270	-1.144446	-2.340819
C	3.745733	-0.372386	-0.757790
C	3.109604	-1.741730	-3.093205
H	1.084724	-1.190291	-2.707014
C	4.753940	-0.974438	-1.514542
H	4.024271	0.146285	0.150099
C	4.444499	-1.660088	-2.686503
H	2.848722	-2.265580	-4.007838
H	5.783882	-0.903162	-1.177616
H	5.228580	-2.122818	-3.277579
H	2.471435	1.819306	0.448736
P	2.198826	2.580193	-2.778005
C	2.779038	4.268873	-2.450036
C	2.388570	5.133426	-1.363002
C	3.743850	4.972268	-3.248213
C	3.122865	6.348379	-1.506656
H	4.242065	4.579579	-4.123566
C	3.951763	6.250896	-2.662614
H	3.086144	7.185947	-0.825039
H	4.650555	7.000251	-3.007752
C	1.379680	4.817785	-0.306814
H	1.362544	3.734318	-0.181031

Fe	4.427557	4.742318	-1.319437
C	6.372840	5.084703	-0.688590
C	5.501947	4.979036	0.436930
C	4.891577	3.688640	0.403721
C	6.301627	3.859442	-1.418569
C	5.386260	2.998325	-0.744617
H	5.309930	5.754875	1.164945
H	6.950258	5.956253	-0.964162
H	6.817146	3.639481	-2.343092
H	5.091538	2.010237	-1.067942
H	4.167130	3.309877	1.110570
C	1.658712	5.459735	1.057280
H	0.912606	5.132093	1.786210
H	1.623538	6.552674	1.003254
H	2.649850	5.174749	1.420046
P	-0.386510	5.262428	-0.817914
Pd	0.242553	1.435186	-1.925152
H	-0.336245	4.887406	-2.181143
H	-0.161755	6.646994	-1.044885
H	2.090958	2.611321	-4.182745
H	3.381464	1.818358	-2.675261
I	-1.416602	2.396156	-3.850135

2a

C	-0.622654	-0.232248	-0.233219
C	0.830739	0.173735	-0.001209
C	1.186919	1.190009	0.800855
C	0.295564	2.087862	1.616011
C	-2.069619	1.140867	1.282426
C	-1.116198	2.321849	1.063492
H	-1.100643	0.394555	-0.994038
H	2.251352	1.382413	0.916433
H	0.226241	1.693653	2.639358
H	-2.372151	1.133149	2.331570
H	-0.651667	-1.250593	-0.621564
H	0.782073	3.068542	1.699428
H	-2.976572	1.295362	0.687139
H	-1.034050	2.528550	-0.015150
N	-1.498475	-0.167684	0.941954
S	-1.164641	-1.196420	2.244590
O	0.086815	-0.872423	2.951087
O	-2.406193	-1.244453	3.030678
C	-0.914083	-2.731081	1.375540
C	-2.011634	-3.381438	0.807406
C	0.380090	-3.225268	1.226012
C	-1.796093	-4.541196	0.071125
H	-3.009826	-2.977711	0.936204
C	0.577128	-4.384975	0.479714
H	1.214270	-2.696690	1.669403
C	-0.501778	-5.057087	-0.107756
H	-2.641652	-5.054862	-0.377731
H	1.585838	-4.762134	0.340678
C	-0.285206	-6.321430	-0.897353
H	-0.460200	-7.205119	-0.271109
H	-0.972467	-6.385516	-1.746510
H	0.738252	-6.384897	-1.276896
O	-1.759962	3.413093	1.717546
H	-1.273002	4.218560	1.497931
C	1.850168	-0.691408	-0.645641
C	1.638677	-1.232727	-1.925234
C	3.025181	-1.051204	0.037630
C	2.569437	-2.095036	-2.503202
H	0.742993	-0.970819	-2.480661
C	3.956746	-1.911261	-0.540011
H	3.184468	-0.680203	1.045031
C	3.732284	-2.440108	-1.813007
H	2.385424	-2.497138	-3.495336
H	4.851799	-2.182679	0.012488
H	4.453711	-3.117786	-2.259682

TS5

C	0.106685	-0.364788	-0.550251
C	1.289205	0.363518	0.066079
C	1.132889	1.468392	0.847153
C	-0.159367	2.060646	1.344828
C	-2.027605	0.698618	0.245714
C	-1.316446	2.052695	0.337058
H	-0.193321	0.123481	-1.486560
H	2.022469	1.852245	1.337532
H	-0.464420	1.546728	2.266708
H	-2.704910	0.605304	1.095469
H	0.393670	-1.377662	-0.836268
H	0.028689	3.103983	1.614921
H	-2.635405	0.660568	-0.665964
H	-0.887870	2.304035	-0.653557
N	-1.114541	-0.448500	0.252304
S	-1.073302	-1.446177	1.603803
O	0.041473	-1.142570	2.514685

O	-2.441929	-1.459346	2.138807
C	-0.705023	-3.013965	0.829547
C	-1.587216	-3.529256	-0.123550
C	0.444611	-3.707715	1.198450
C	-1.299060	-4.752210	-0.717314
H	-2.475799	-2.971810	-0.399689
C	0.717670	-4.934877	0.592737
H	1.112232	-3.283397	1.939296
C	-0.144661	-5.473990	-0.369178
H	-1.977687	-5.158145	-1.462359
H	1.614719	-5.479247	0.872972
C	0.139270	-6.808599	-1.007603
H	-0.516181	-7.584314	-0.593336
H	-0.039230	-6.779772	-2.087385
H	1.172410	-7.123521	-0.838980
O	-2.326868	2.983595	0.670233
H	-1.969465	3.869999	0.489517
C	2.641529	-0.096166	-0.306375
C	2.935099	-1.452458	-0.557250
C	3.702873	0.828640	-0.417861
C	4.228279	-1.863896	-0.875822
H	2.161660	-2.205886	-0.457697
C	4.994123	0.414174	-0.734244
H	3.496611	1.882633	-0.268814
C	5.267660	-0.936049	-0.964936
H	4.425642	-2.918413	-1.045741
H	5.790434	1.150482	-0.803517
H	6.273050	-1.259511	-1.215510
H	1.496302	2.907891	-0.507296
P	1.249661	1.845703	-3.385597
C	2.384729	2.326462	-4.705575
C	3.576674	3.117389	-4.520660
C	2.213318	2.105610	-6.111285
C	4.120214	3.370855	-5.817831
H	1.421408	1.525518	-6.563643
C	3.286151	2.746757	-6.791124
H	5.037712	3.902337	-6.023323
H	3.462716	2.727133	-7.857381
C	4.111270	3.596698	-3.197476
H	4.115981	2.755304	-2.495745
Fe	4.011534	1.329285	-5.456637
C	4.960447	-0.155825	-6.544548
C	5.902173	0.529235	-5.719173
C	5.487430	0.380000	-4.360940
C	3.962982	-0.725978	-5.695792
C	4.289001	-0.393645	-4.345897
H	6.755987	1.095530	-6.064664
H	4.975579	-0.198065	-7.624854
H	3.093933	-1.280714	-6.021611
H	3.717986	-0.649675	-3.464491
H	5.967769	0.809696	-3.494272
C	5.516179	4.194862	-3.276348
H	5.879376	4.462321	-2.280482
H	5.536976	5.096440	-3.896131
H	6.211154	3.467631	-3.709441
P	2.857174	4.776342	-2.460735
Pd	0.832963	3.669451	-1.890307
H	2.933066	5.873018	-3.351257
H	3.549673	5.322583	-1.360945
H	0.266942	1.147211	-4.124544
H	1.878357	0.744986	-2.770646
I	-0.429734	5.848023	-0.699929

TS2t

P	-10.003338	-1.716370	-1.843040
C	-9.860874	-2.890316	-3.223046
C	-10.973643	-3.592238	-3.838859
C	-8.663661	-3.440608	-3.757971
C	-10.439125	-4.603648	-4.679673
H	-7.655209	-3.143315	-3.504195
C	-9.030310	-4.461117	-4.695588
H	-11.013980	-5.262787	-5.314725
H	-8.338189	-5.051735	-5.281323
C	-12.429749	-3.348196	-3.542696
H	-12.593941	-2.265454	-3.491596
Fe	-9.754211	-2.444848	-5.334169
C	-9.084095	-0.288571	-5.930795
C	-8.542725	-1.274892	-6.792851
C	-9.624970	-1.950438	-7.455956
C	-10.492738	-0.438023	-5.951559
C	-10.834486	-1.433031	-6.933659
H	-7.490167	-1.459801	-6.964675
H	-8.521589	0.359307	-5.271986
H	-11.201393	0.133878	-5.366289
H	-11.837302	-1.722096	-7.217256
H	-9.522254	-2.717719	-8.211360
C	-13.375333	-3.948689	-4.582393
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H	-13.306312	-5.040979	-4.601802	H	-5.999403	1.112676	8.757199
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P	-12.783463	-3.917442	-1.773102	H	-8.743528	-2.882108	5.206104
Pd	-11.364947	-2.600612	-0.269803	H	-8.203359	-3.438202	3.533343
H	-12.819938	-5.316834	-2.028674	C	-8.711553	-1.575597	1.700644
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H	-8.622274	-1.429116	-1.691074	O	-9.632921	-0.559820	1.222072
H	-10.329309	-0.502661	-2.501850	H	-9.071454	-2.570276	1.433967
H	-10.417524	-1.113759	0.771688	H	-8.791183	-0.167376	3.395084
I	-12.208750	-3.232658	2.341444	H	-10.153697	-1.465150	3.340665
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C	-5.915522	-1.946554	3.351703	O	-5.310056	-3.125465	-0.124401
H	-5.097041	-2.629848	3.593591	O	-4.915129	-4.315819	2.099962
H	-5.486088	-0.938667	3.299354	C	-7.250622	-4.598710	0.851900
C	-7.264210	-1.347732	1.320494	C	-7.753407	-5.421243	1.864343
H	-7.141053	-1.475041	0.242830	C	-7.907497	-4.479846	-0.372423
H	-6.950638	-0.327016	1.567807	C	-8.943003	-6.106427	1.643790
C	-6.955592	-1.993424	4.467482	H	-7.216862	-5.525139	2.800963
C	-6.693803	-1.138420	5.646291	C	-9.098020	-5.175833	-0.575326
C	-7.752989	-0.630329	6.420919	H	-7.491623	-3.858007	-1.155034
C	-5.378492	-0.803955	6.015102	C	-9.638929	-5.987324	0.430464
C	-7.504735	0.171248	7.530998	H	-9.344818	-6.743256	2.426130
H	-8.777800	-0.849222	6.138463	H	-9.607346	-5.082403	-1.527924
C	-5.131743	-0.006552	7.131441	C	-10.958086	-6.680627	0.241272
H	-4.538548	-1.189008	5.446638	H	-11.185839	-6.828566	-0.817357
C	-6.192335	0.485431	7.892335	H	-10.973786	-7.654081	0.740700
H	-8.337286	0.559012	8.110127	H	-11.756138	-6.068713	0.678260
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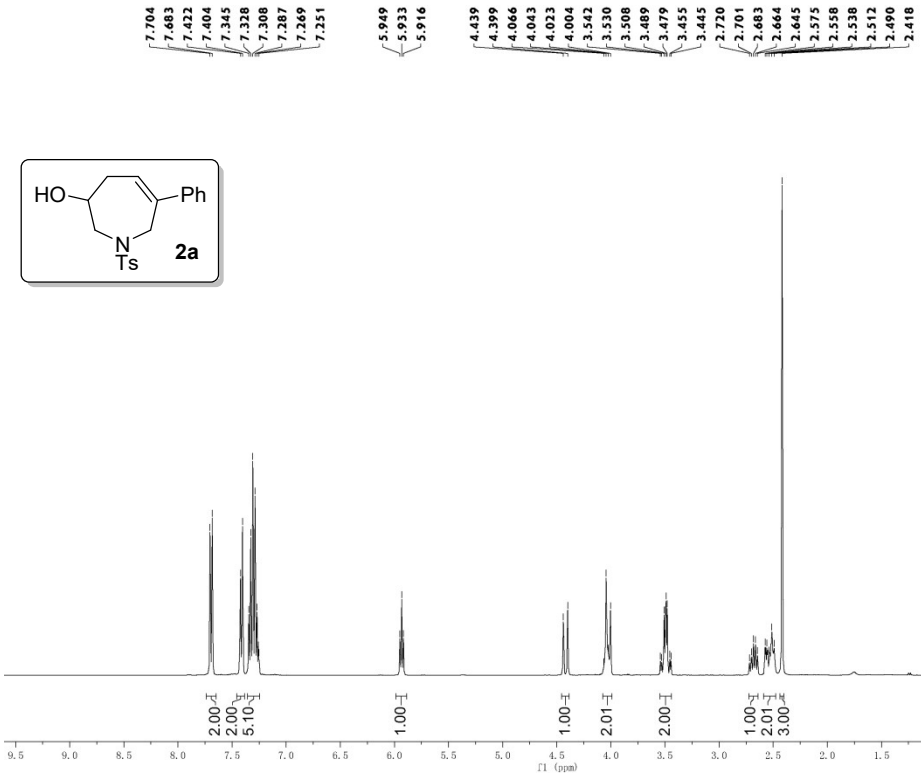
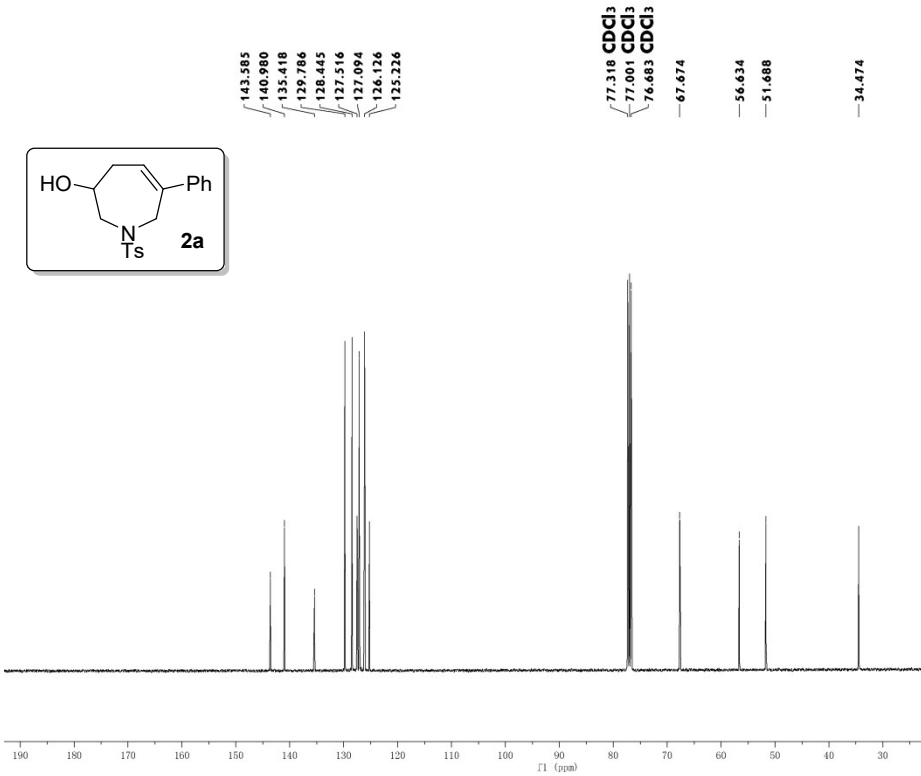
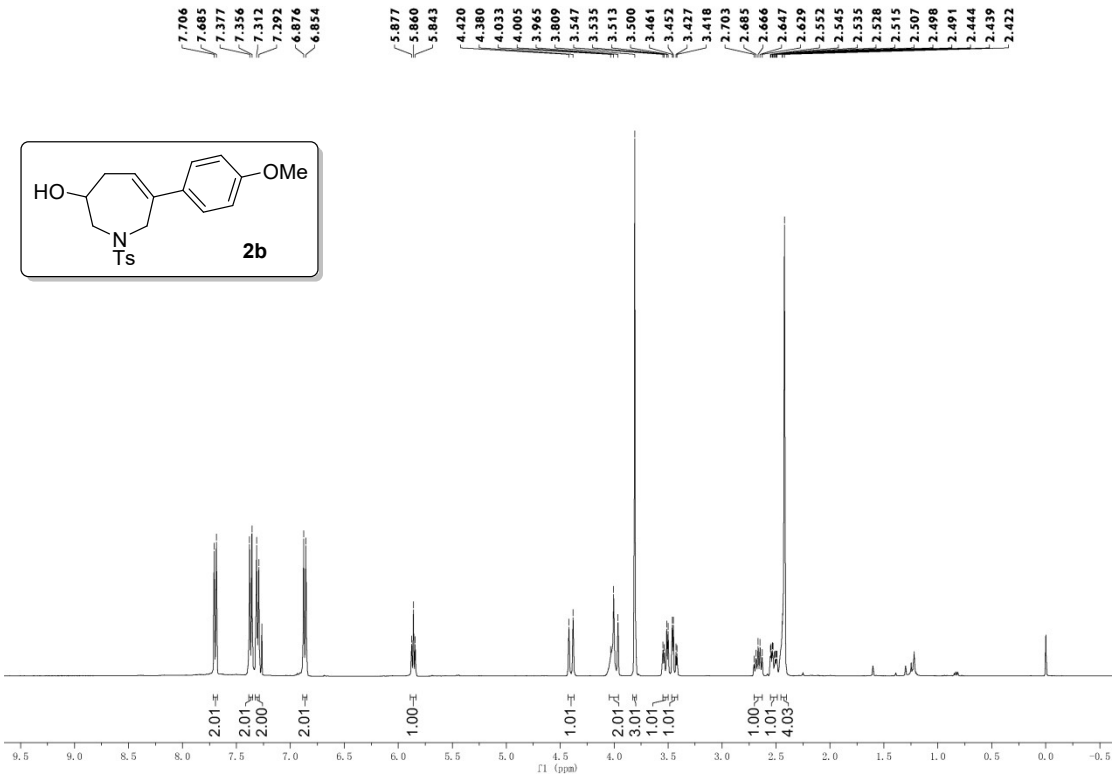
13. Copies of the NMR Spectra for 7-Endo Heck-Type Products



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3.547
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3.513
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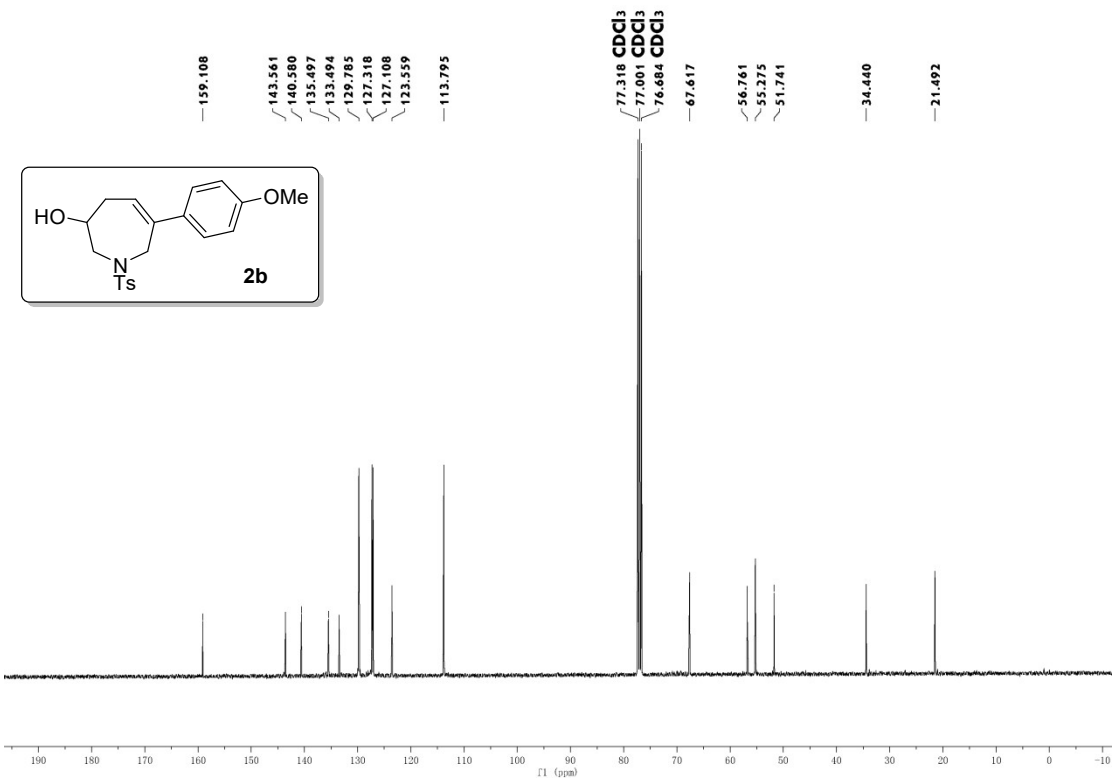
2.629
2.552
2.545
2.535
2.528
2.515
2.507
2.498
2.491
2.444
2.439
2.422
HO
OMe
N
Ts
2b
2.01
2.01
2.00
2.01
1.00
1.01
2.01
3.01
1.01
1.01
1.00
1.01
4.03
f1 (ppm)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127.108
123.559
113.795
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77.001 CDCl3
76.684 CDCl3
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55.275
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34.440
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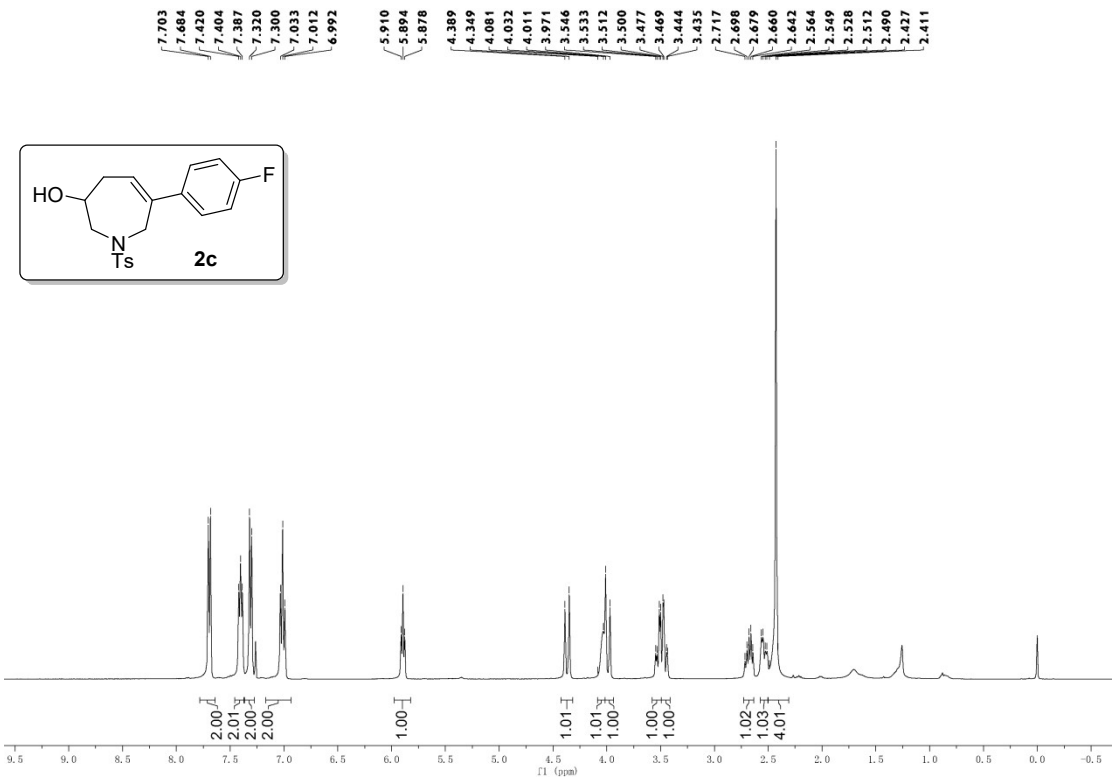
HO
OMe
N
Ts
2b
f1 (ppm)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4.389
4.349
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4.032
4.011
3.971
3.546
3.533
3.512
3.500
3.477
3.469
3.444
3.435
2.717
2.698
2.679
2.660
2.642
2.564
2.549
2.528
2.512
2.490
2.427
2.411
HO
F
N
Ts
2c
2.00
2.01
2.00
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1.01
1.00
1.00
1.00
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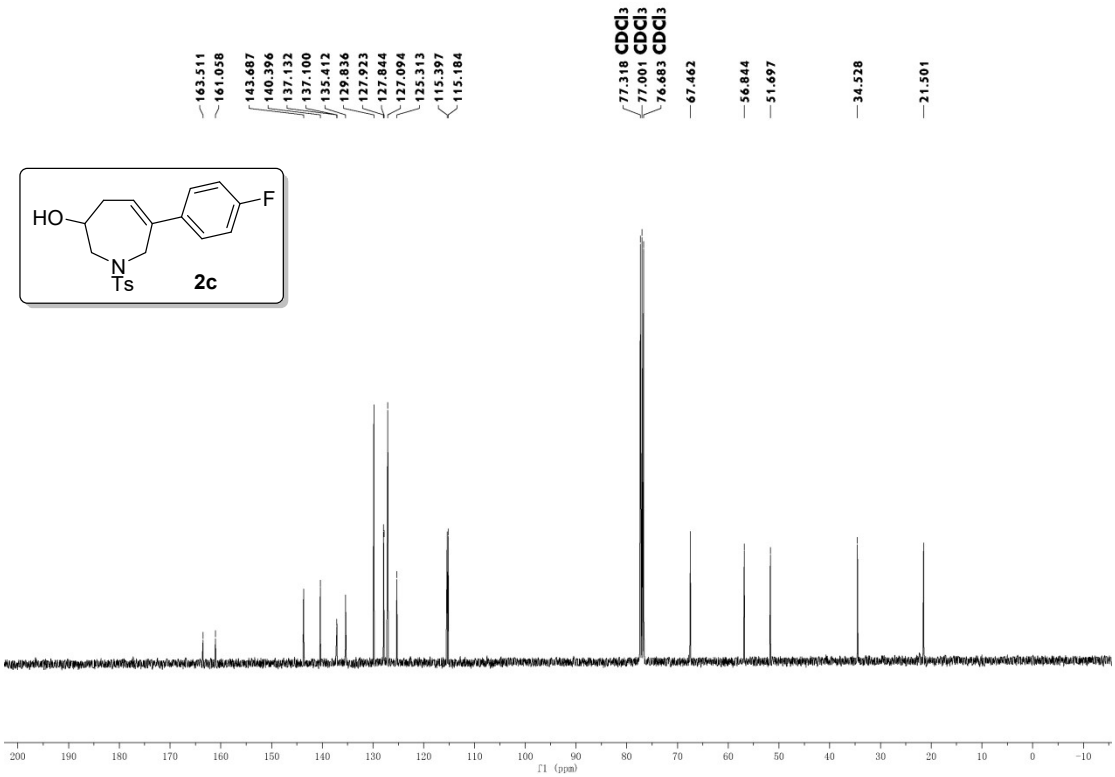
1.03
4.01
f1 (ppm)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143.687
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137.100
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129.836
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127.094
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115.397
115.184
77.318 CDCl3
77.001 CDCl3
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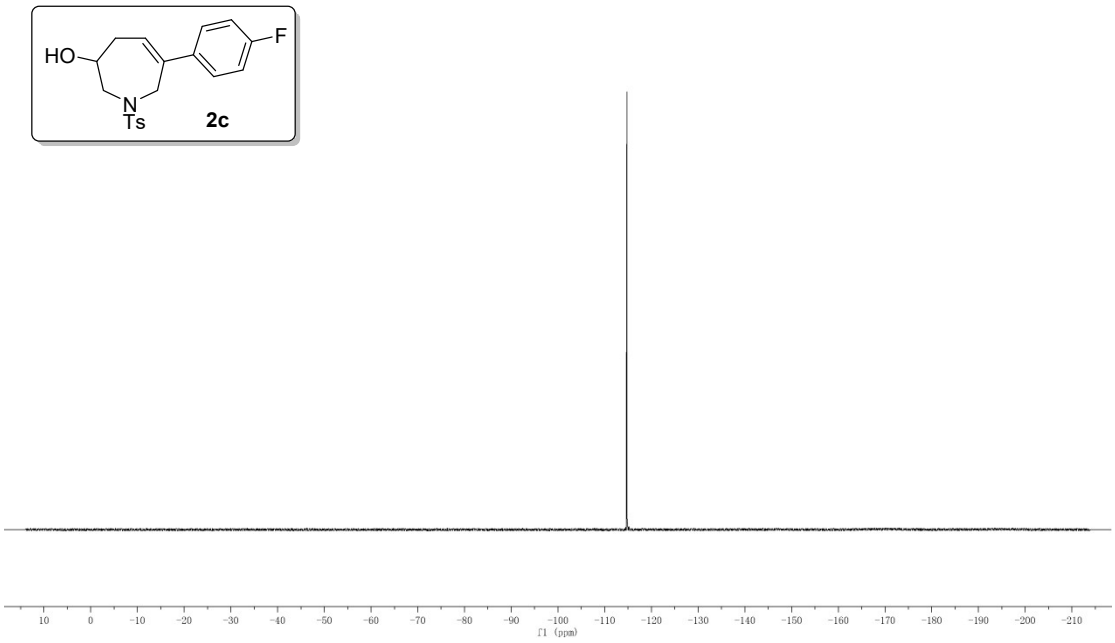
HO
F
N
Ts
2c
f1 (ppm)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F
N
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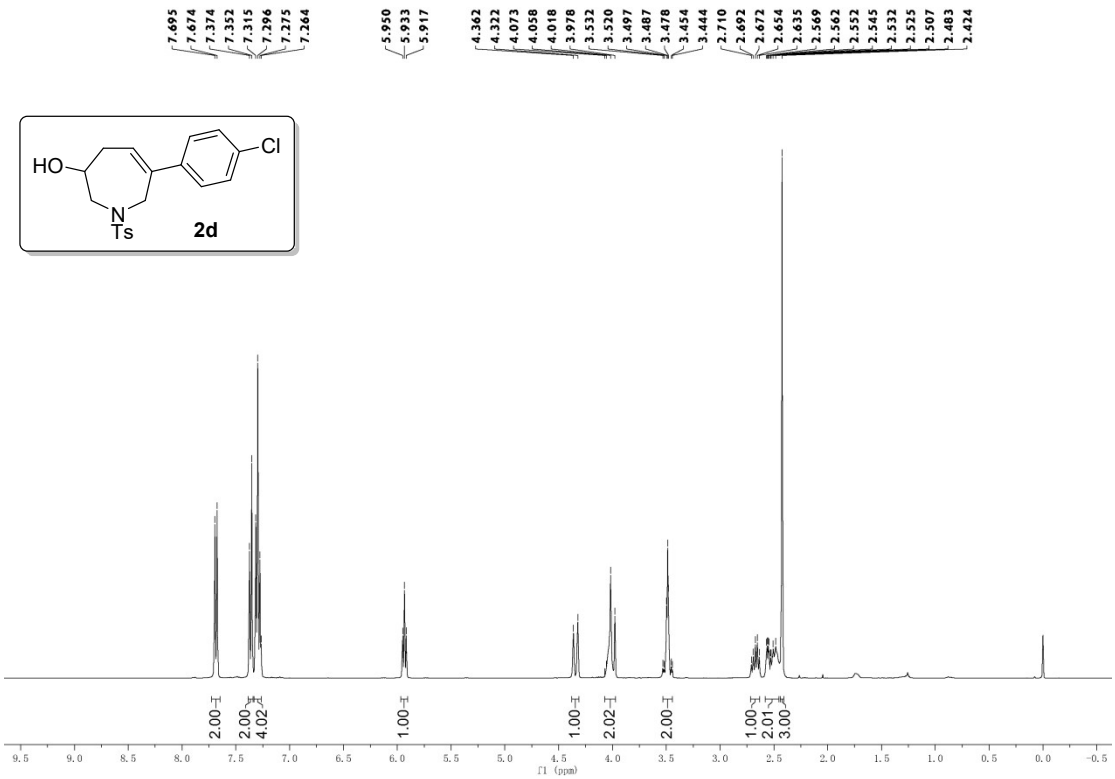
2c
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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3.478
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3.444
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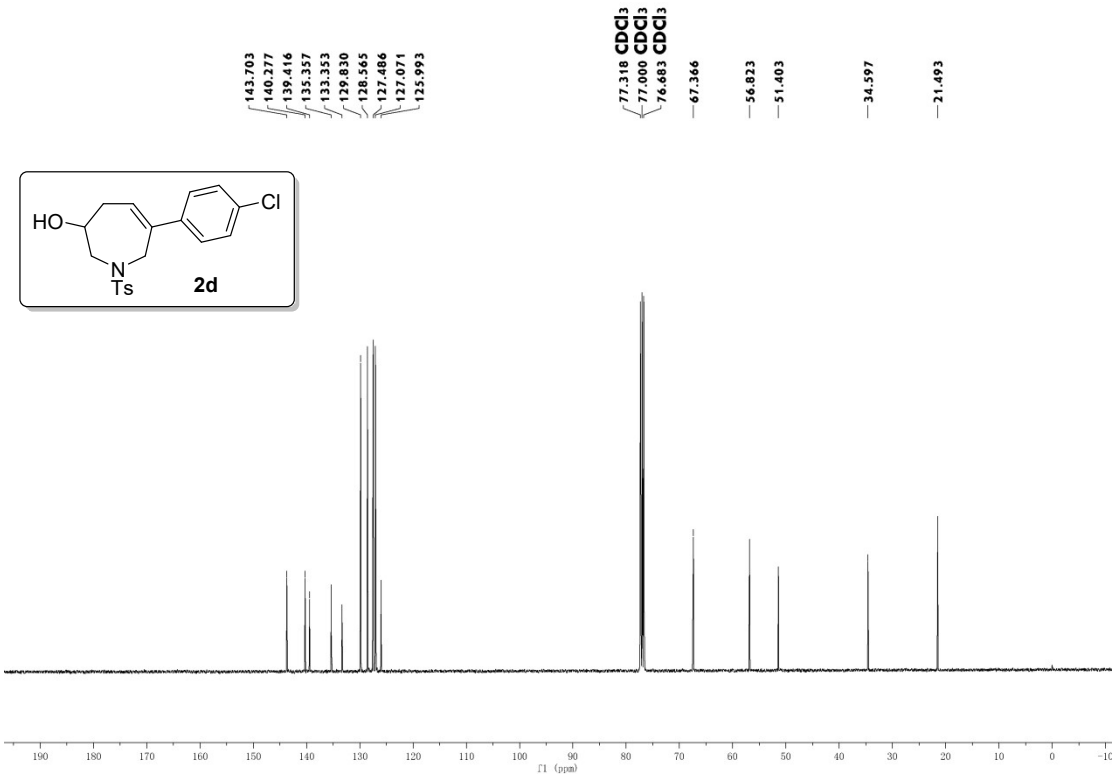
2.654
2.635
2.569
2.562
2.552
2.545
2.532
2.525
2.507
2.483
2.424
HO
Cl
N
Ts
2d
2.00
2.00
4.02
1.00
1.00
2.02
2.00
1.00
2.01
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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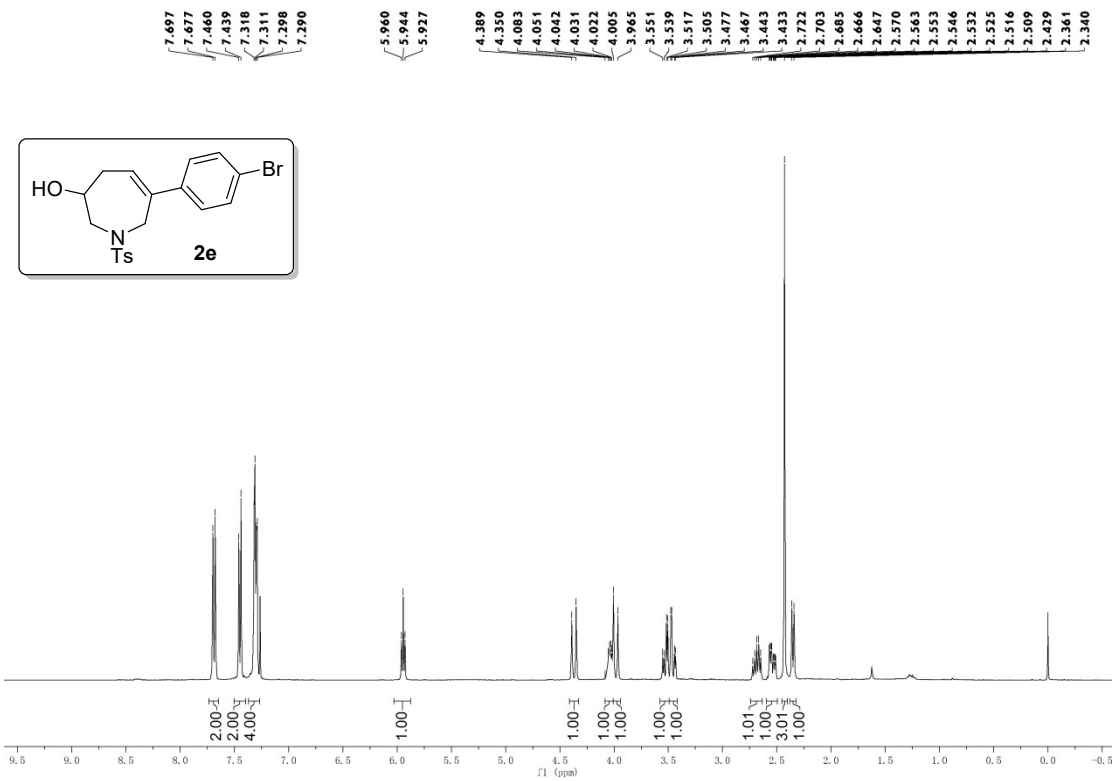
21.493
HO
Cl
N
Ts
2d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4.350
4.083
4.051
4.042
4.031
4.022
4.005
3.965
3.551
3.539
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3.477
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3.443
3.433
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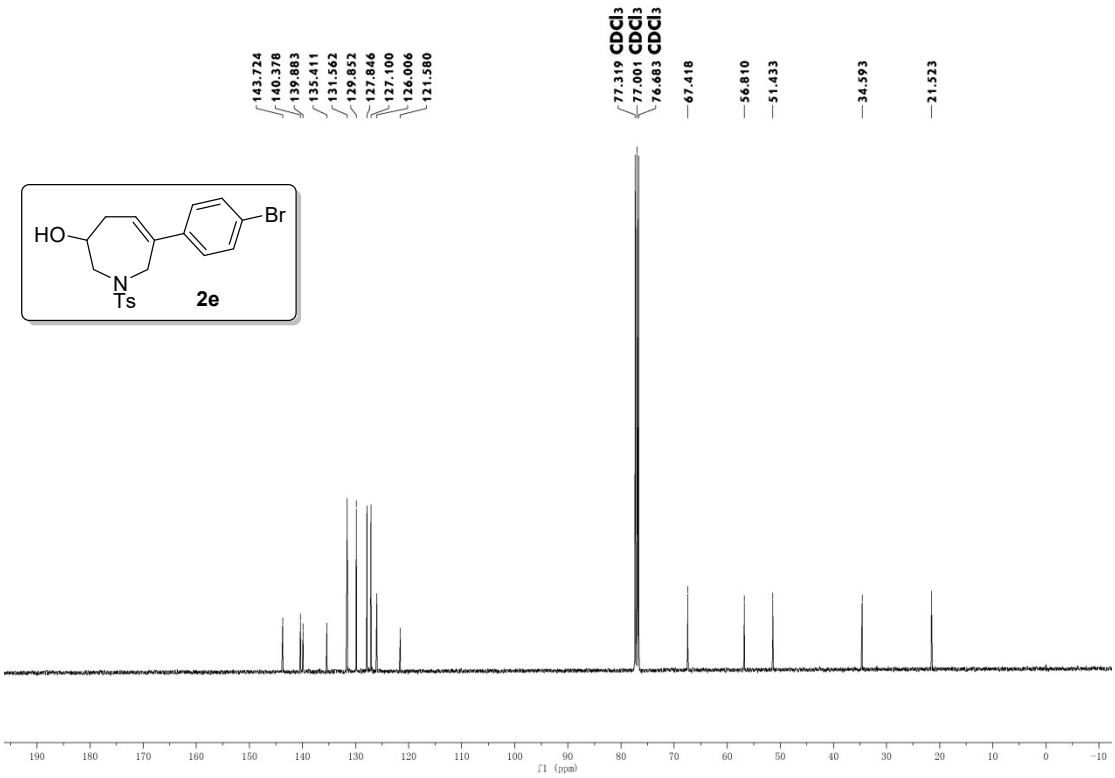
Br
N
Ts
2e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139.883
135.411
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127.100
126.006
121.580
77.319 CDCl3
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76.683 CDCl3
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56.810
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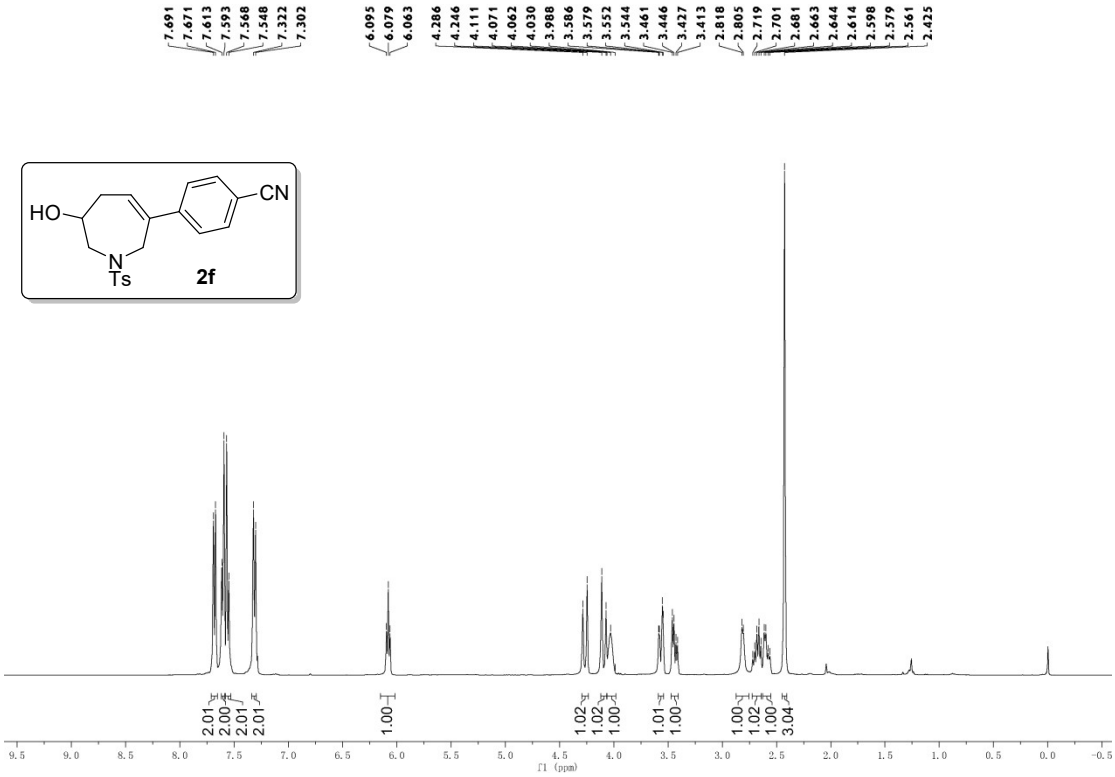
34.593
21.523
HO
Br
N
Ts
2e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6.079
6.063
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4.030
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3.544
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2.719
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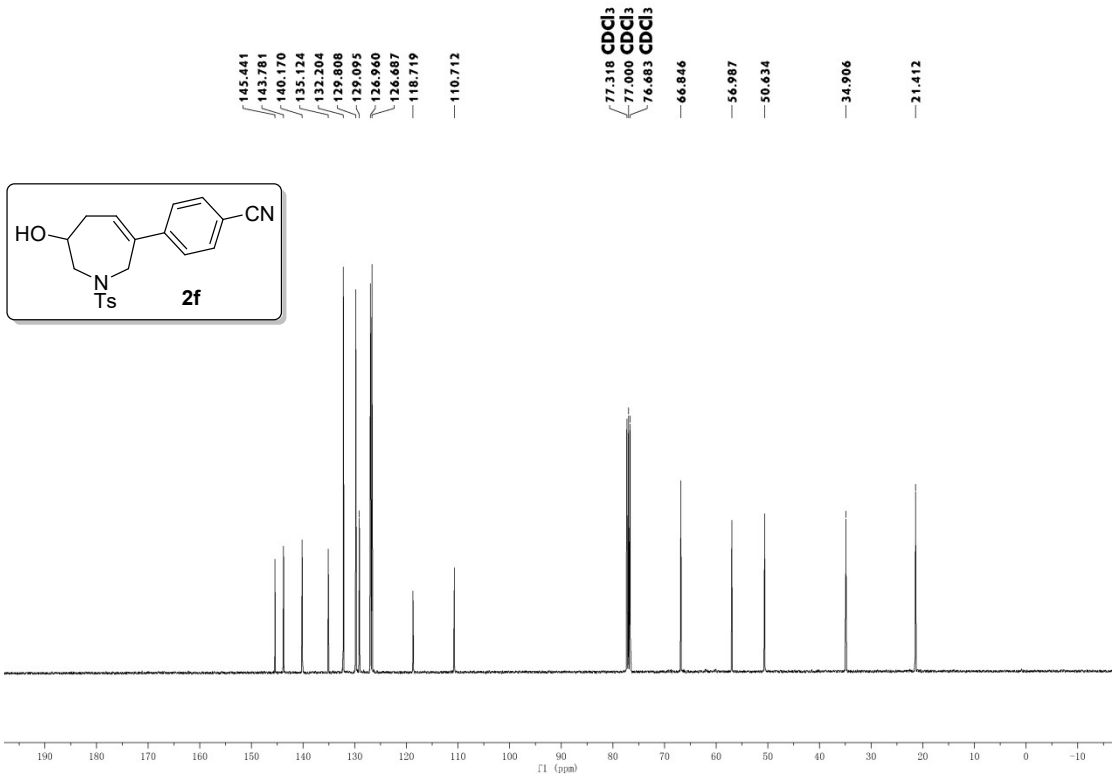
2.425
HO
CN
N
Ts
2f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110.712
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77.000 CDCl3
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56.987
50.634
34.906
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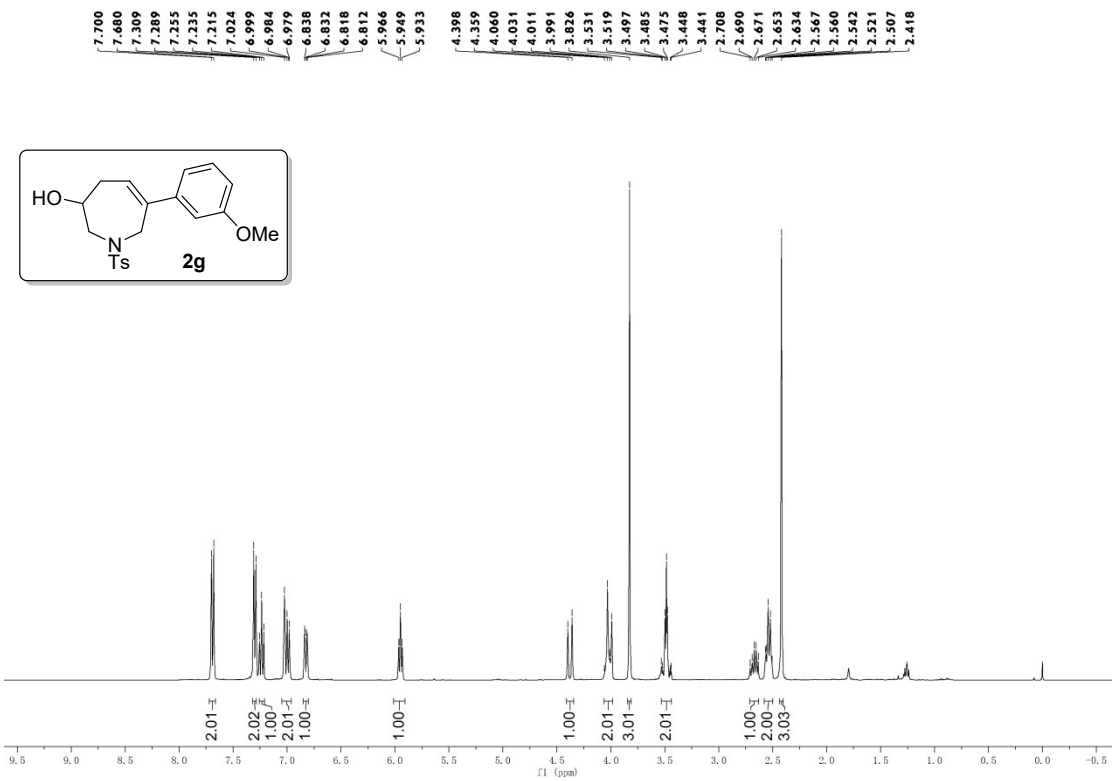
HO
CN
N
Ts
2f
f1 (ppm)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6.832
6.818
6.812
5.966
5.949
5.933
4.398
4.359
4.060
4.031
4.011
3.991
3.826
3.531
3.519
3.497
3.485
3.475
3.448
3.441
2.708
2.690
2.671
2.653
2.634
2.567
2.560
2.542
2.521
2.507
2.418
HO
OMe
N
Ts
2g
2.01
2.02
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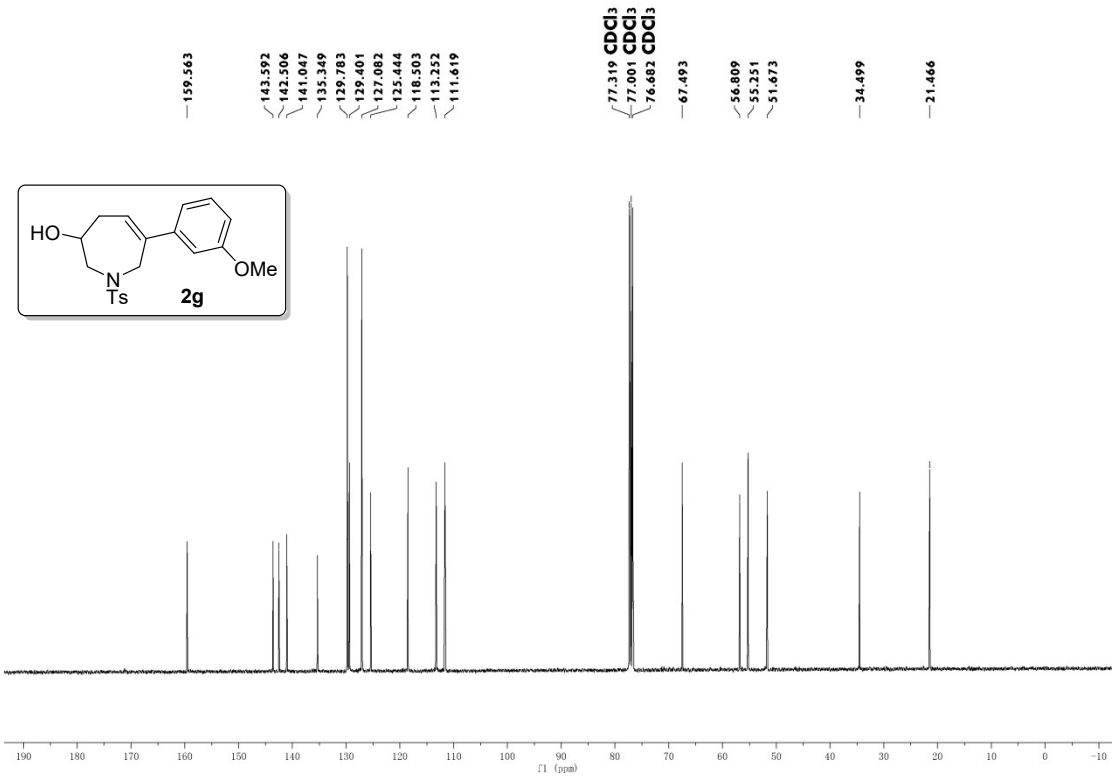
2.01
1.00
1.00
1.00
2.01
3.01
2.01
1.00
2.00
3.03
f1 (ppm)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113.252
111.619
77.319 CDCl3
77.001 CDCl3
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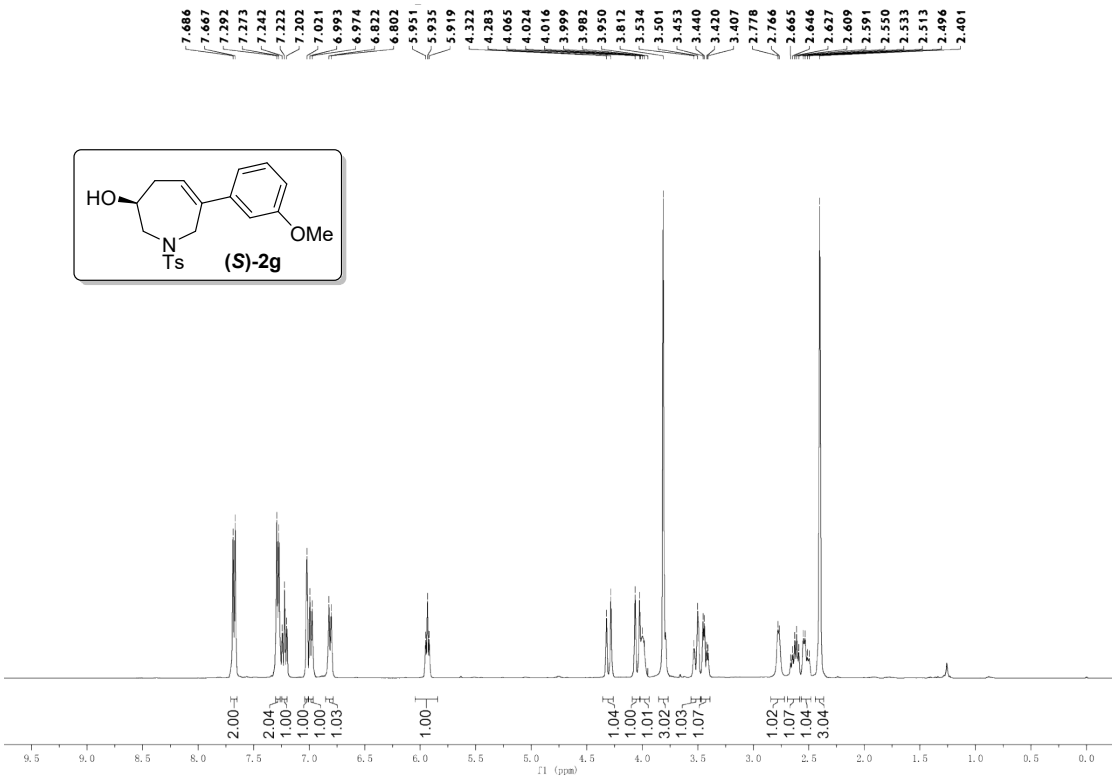
HO
N
Ts
OMe
2g
f1 (ppm)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5.935
5.919
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4.283
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4.024
4.016
3.999
3.982
3.950
3.812
3.534
3.501
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3.440
3.420
3.407
2.778
2.766
2.665
2.646
2.627
2.609
2.591
2.550
2.533
2.513
2.496
2.401
HO
N
Ts
OMe
(S)-2g
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2.04
1.00
1.00
1.03
1.00
1.04
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1.01
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1.07
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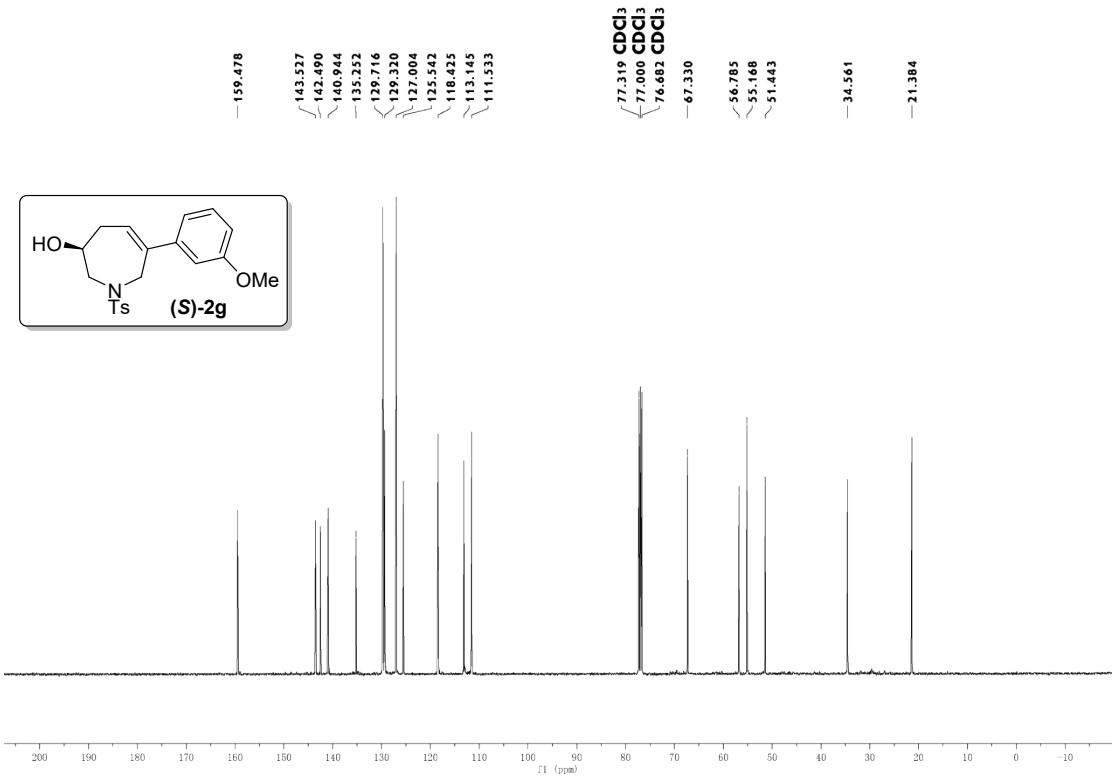
f1 (ppm)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77.000 CDCl3
76.682 CDCl3
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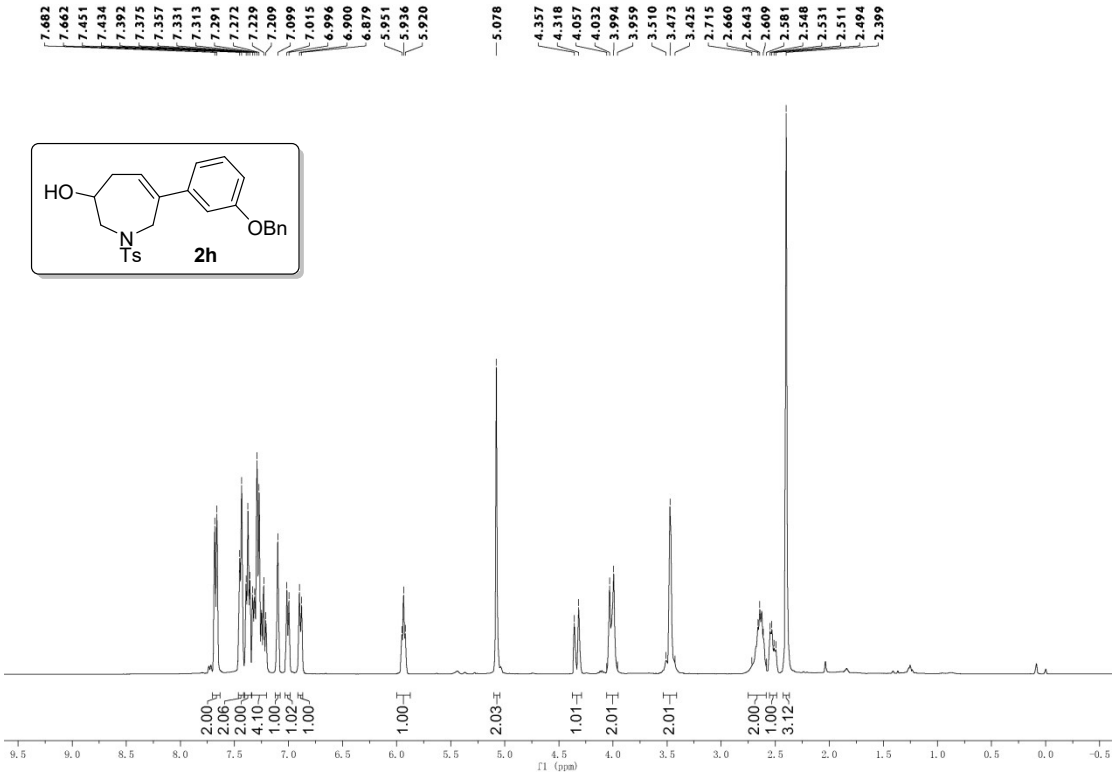
HO
OMe
N
Ts
(S)-2g
f1 (ppm)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2.399
HO
OBn
N
Ts
2h
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2.00
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2.00
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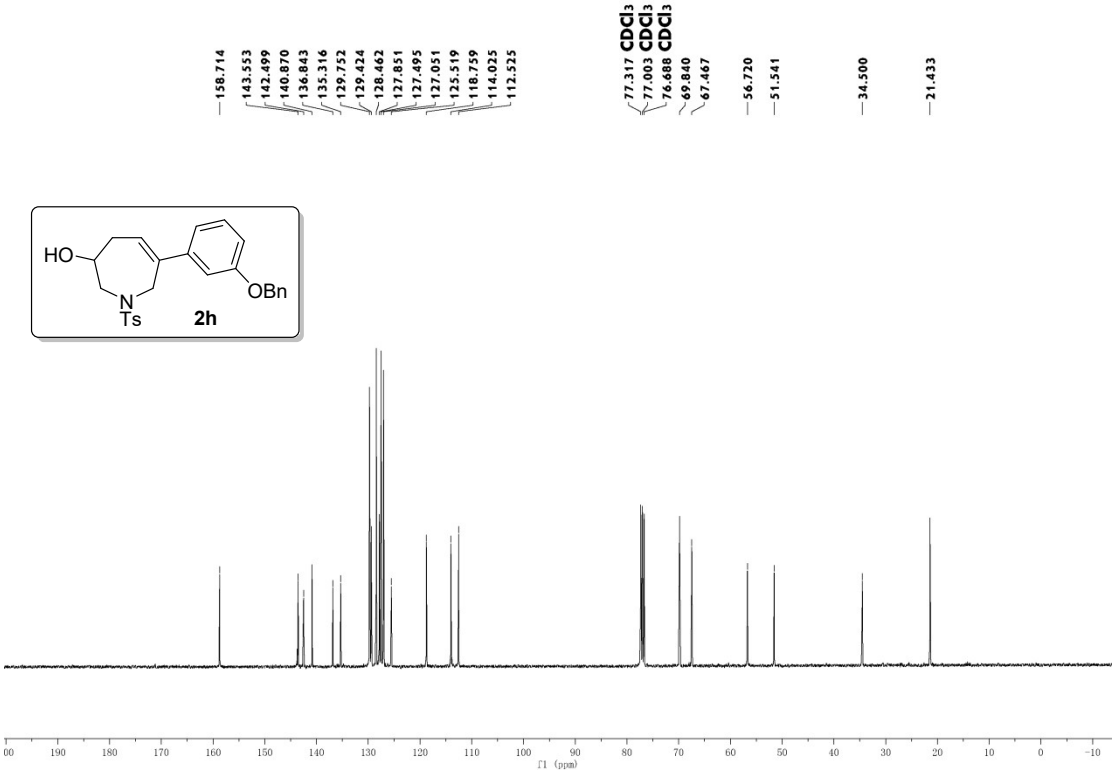
f1 (ppm)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125.519
118.759
114.025
112.525
77.317 CDCl3
77.003 CDCl3
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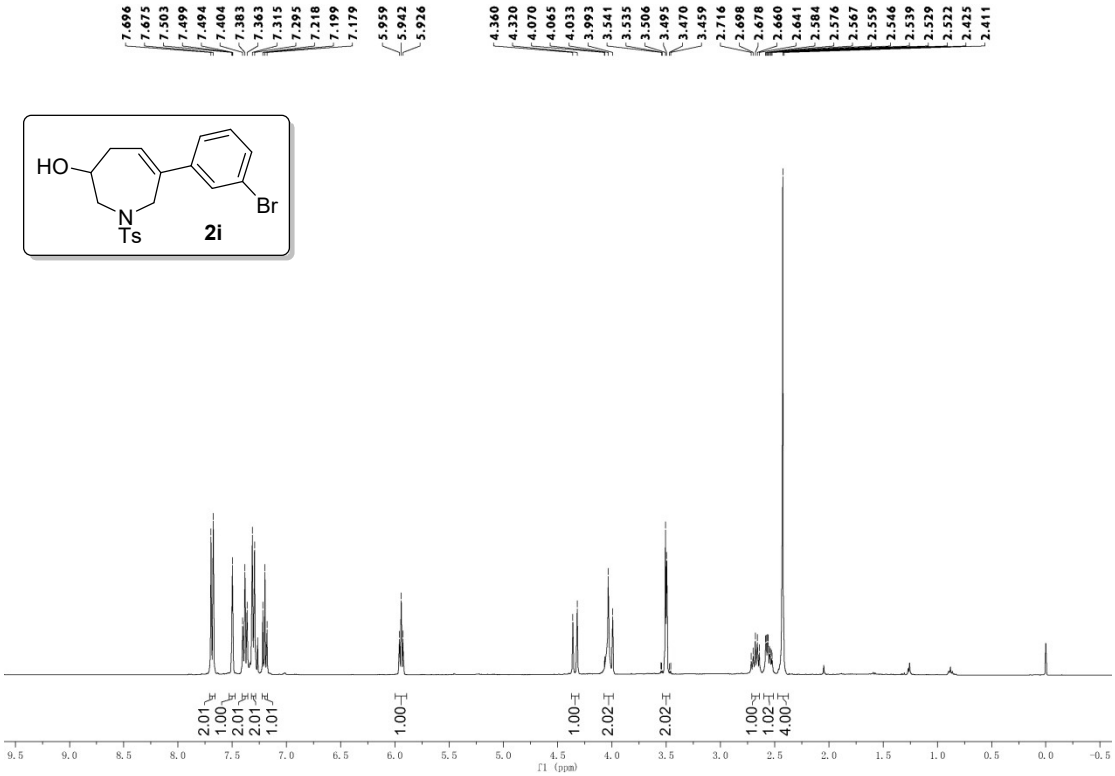
HO
N
Ts
OBn
2h
f1 (ppm)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HO
N
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Br
2i
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1.01
1.00
1.00
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1.00
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4.00
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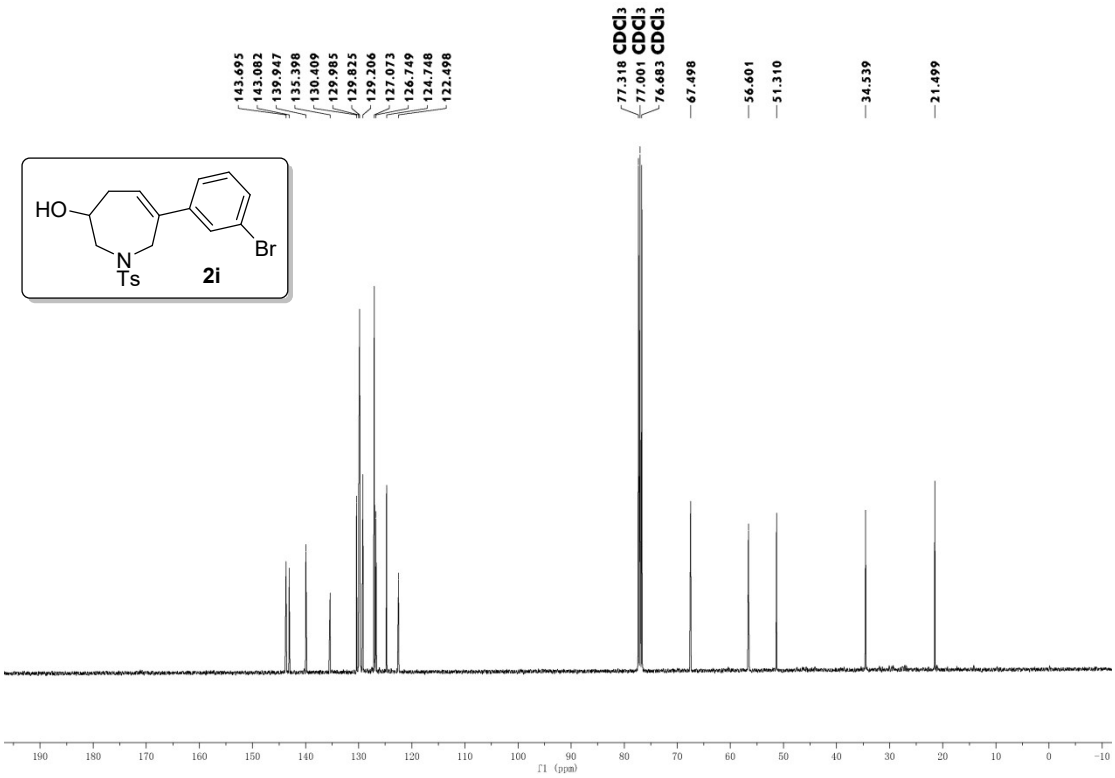
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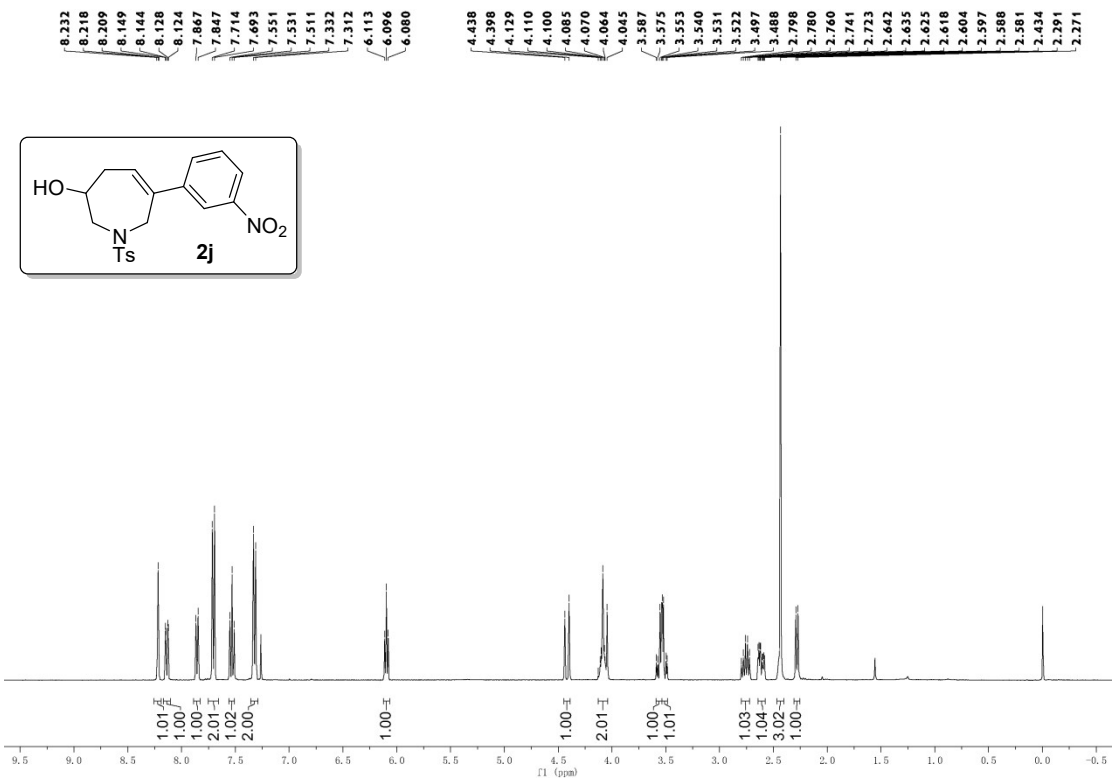
77.001 CDCl3
76.683 CDCl3
67.498
56.601
51.310
34.539
21.499
HO
N
Ts
Br
2i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7.332
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6.096
6.080
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4.398
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4.110
4.100
4.085
4.070
4.064
4.045
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3.575
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3.540
3.531
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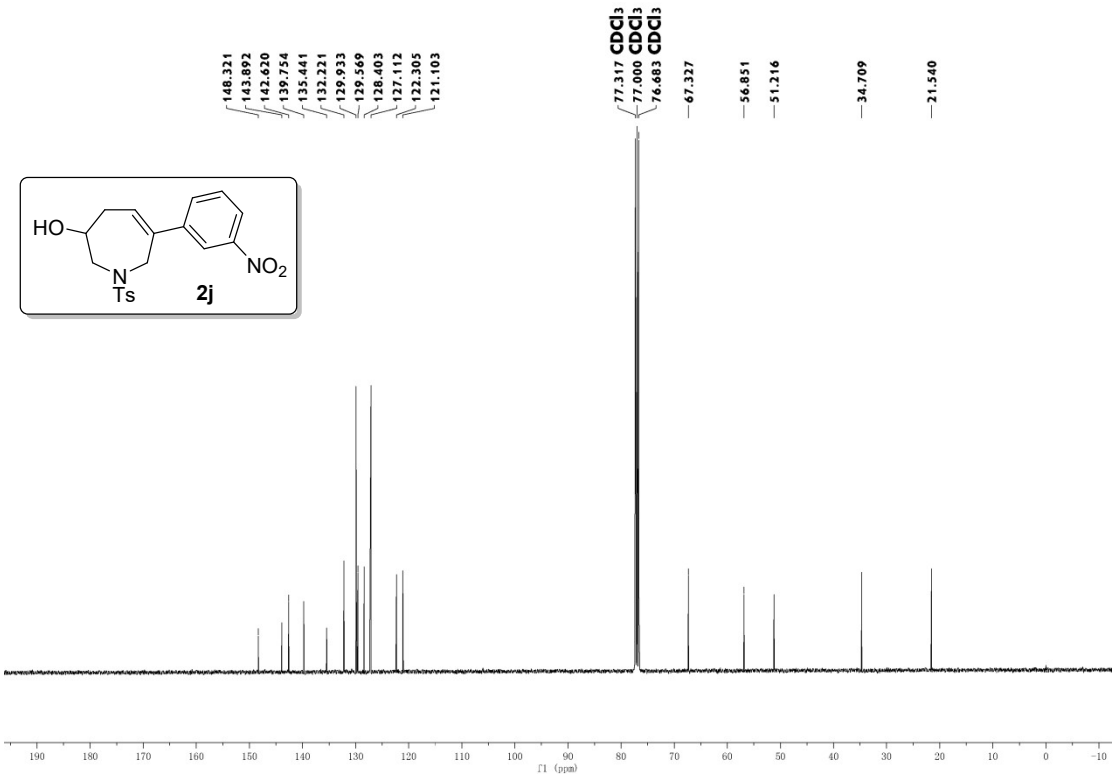
Ts
NO2
2j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121.103
77.317 CDCl3
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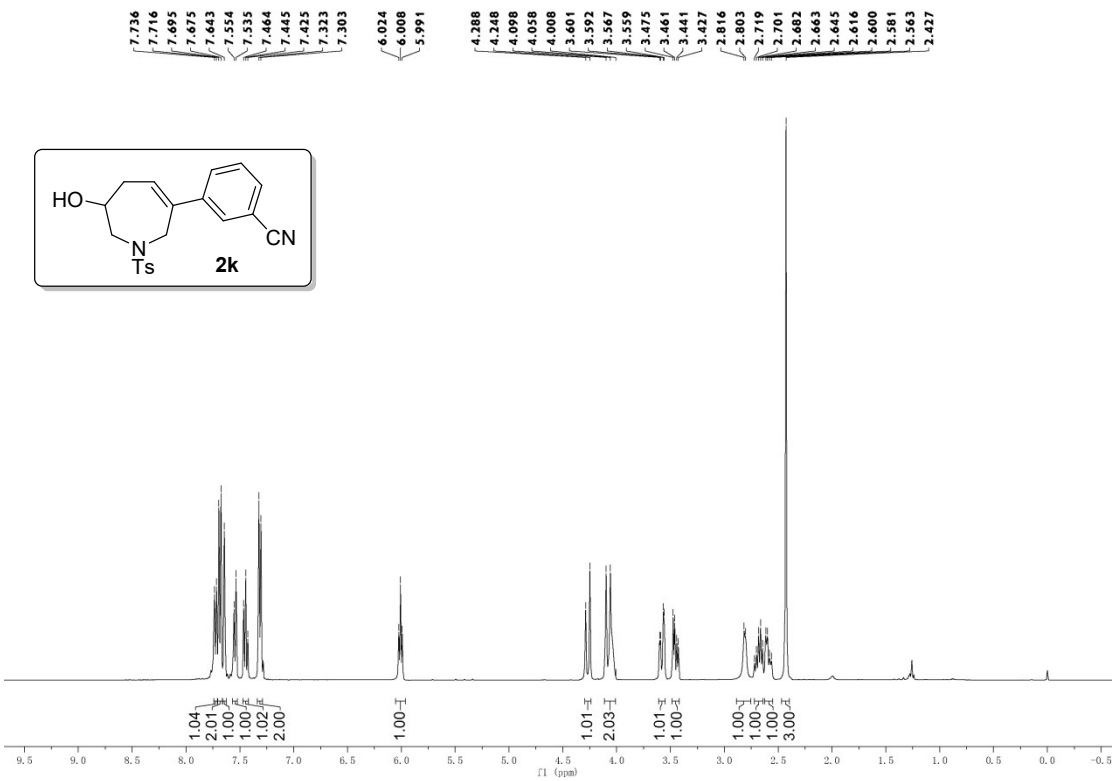
NO2
2j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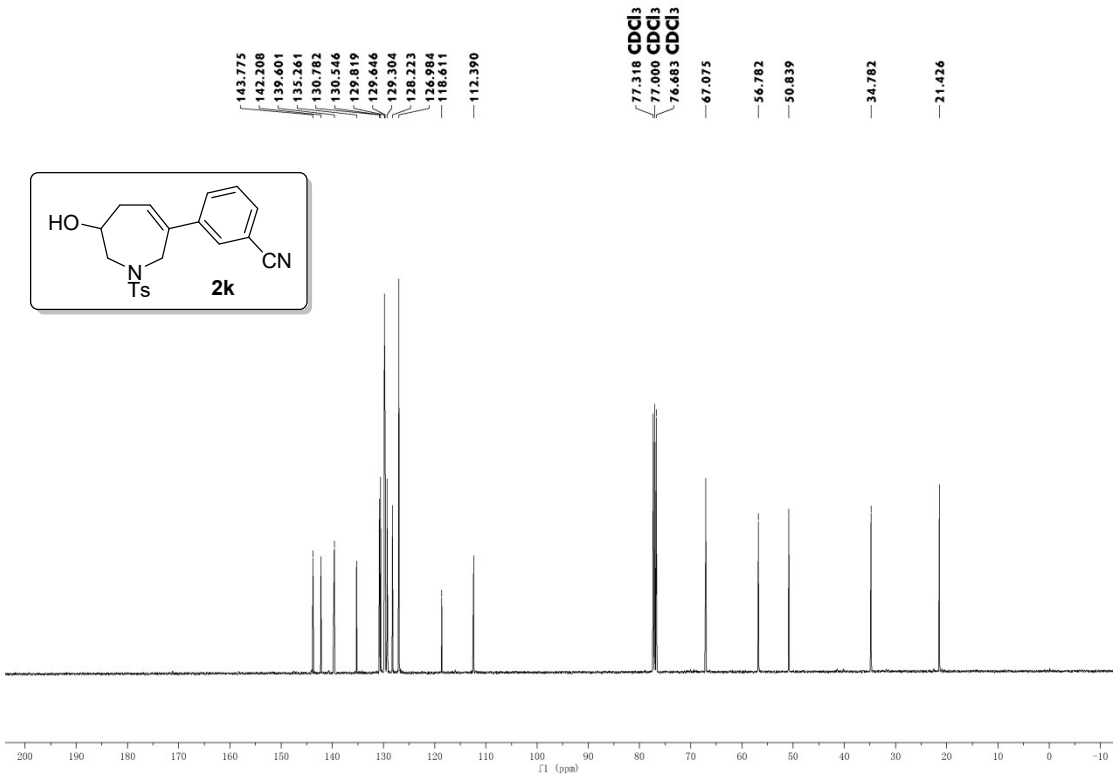
Ts
CN
2k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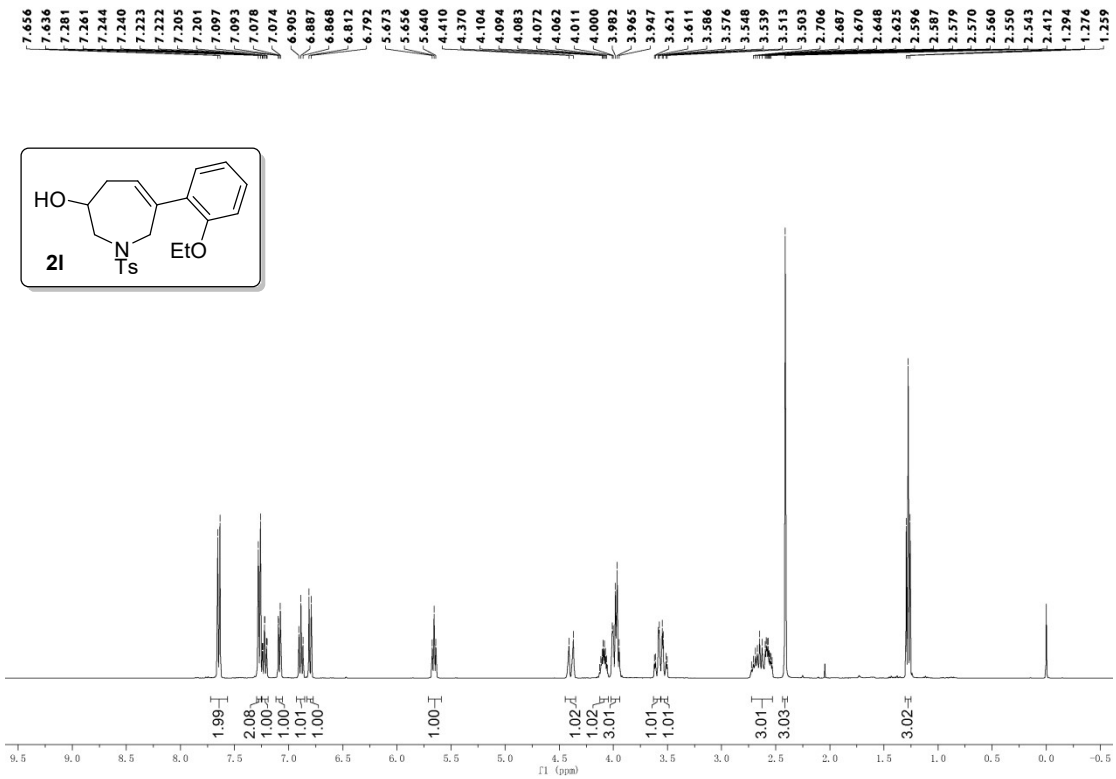
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5.673
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5.640
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4.104
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2.706
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2.596
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2.579
2.570
2.560
2.550
2.543
2.412
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1.276
1.259
HO
N
Ts
EtO
2l
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2.08
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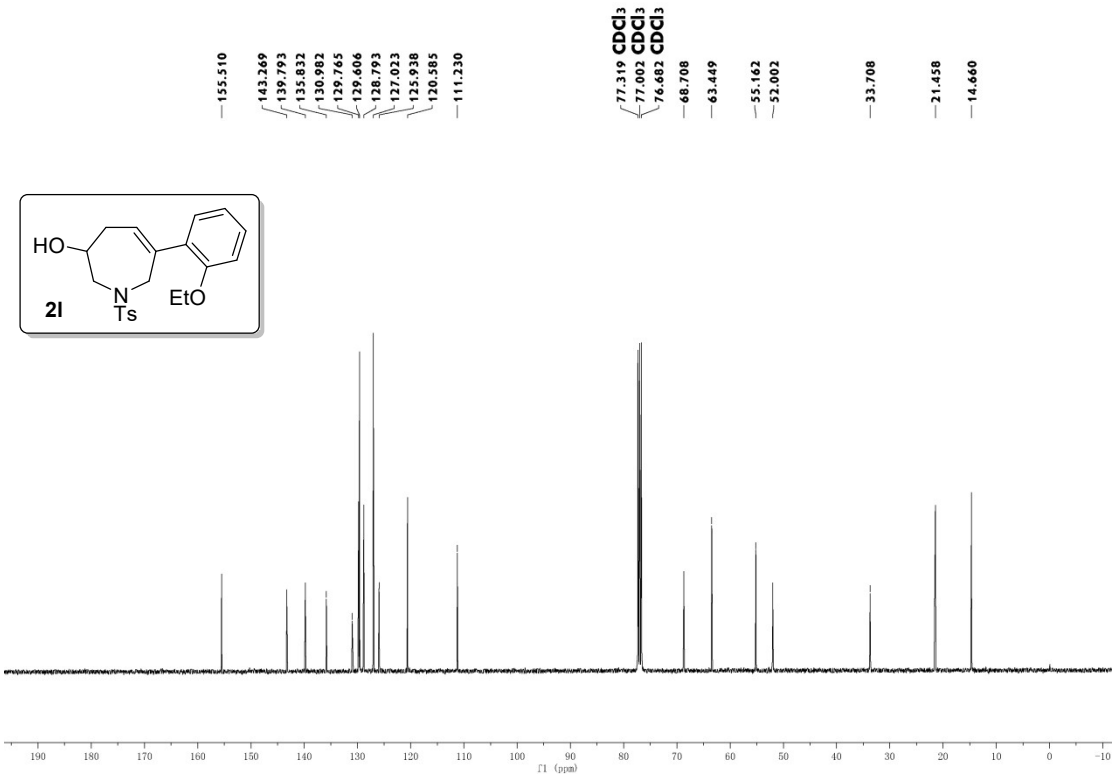
3.03
3.02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128.793
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111.230
77.319 CDCl3
77.002 CDCl3
76.682 CDCl3
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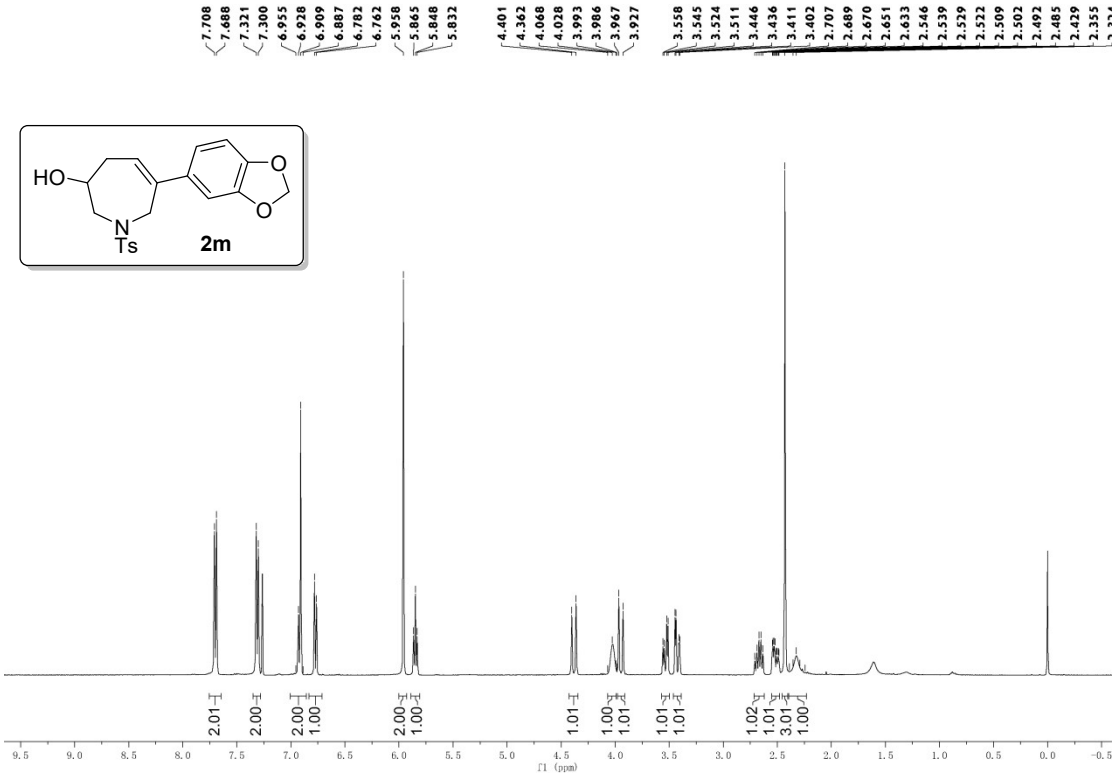
52.002
33.708
21.458
14.660
HO
N
Ts
EtO
2l
f1 (ppm)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6.887
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5.848
5.832
4.401
4.362
4.068
4.028
3.993
3.986
3.967
3.927
3.558
3.545
3.524
3.511
3.446
3.436
3.411
3.402
2.707
2.689
2.670
2.651
2.633
2.546
2.539
2.529
2.522
2.509
2.502
2.492
2.485
2.429
2.355
HO
N
Ts
O
O
2m
2.01
2.00
2.00
1.00
2.00
1.00
1.01
1.00
1.01
1.01
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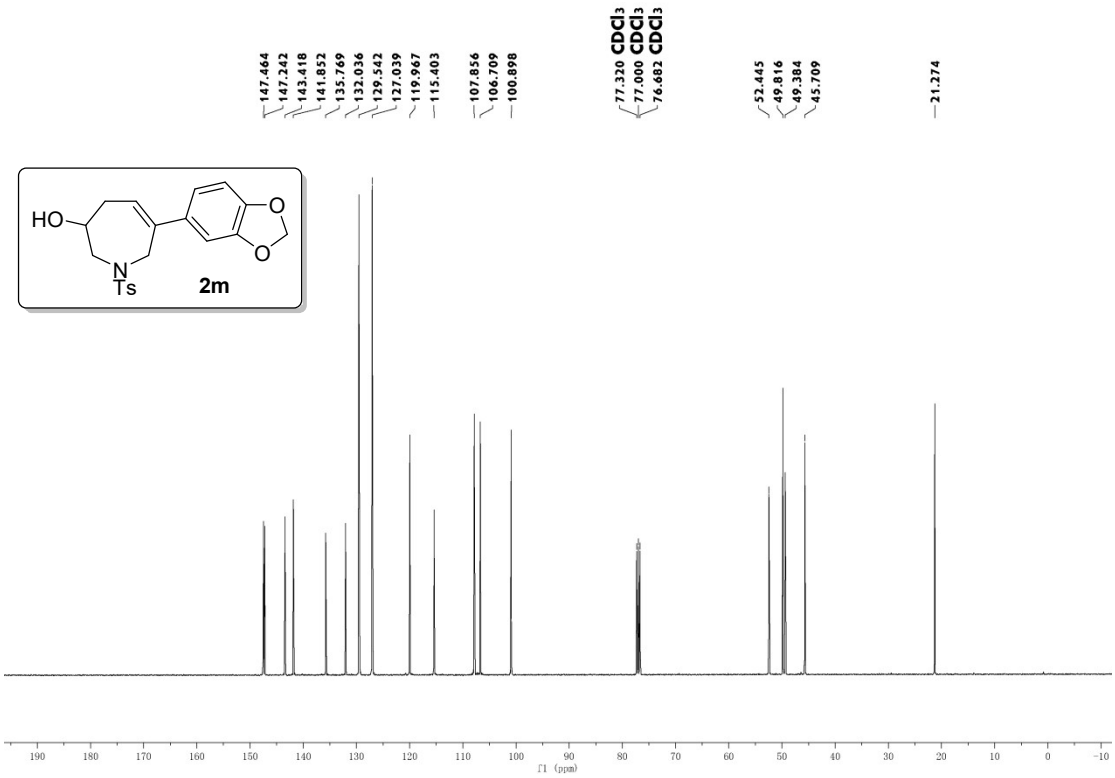
1.02
1.01
3.01
1.00
f1 (ppm)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106.709
100.898
77.320 CDCl3
77.000 CDCl3
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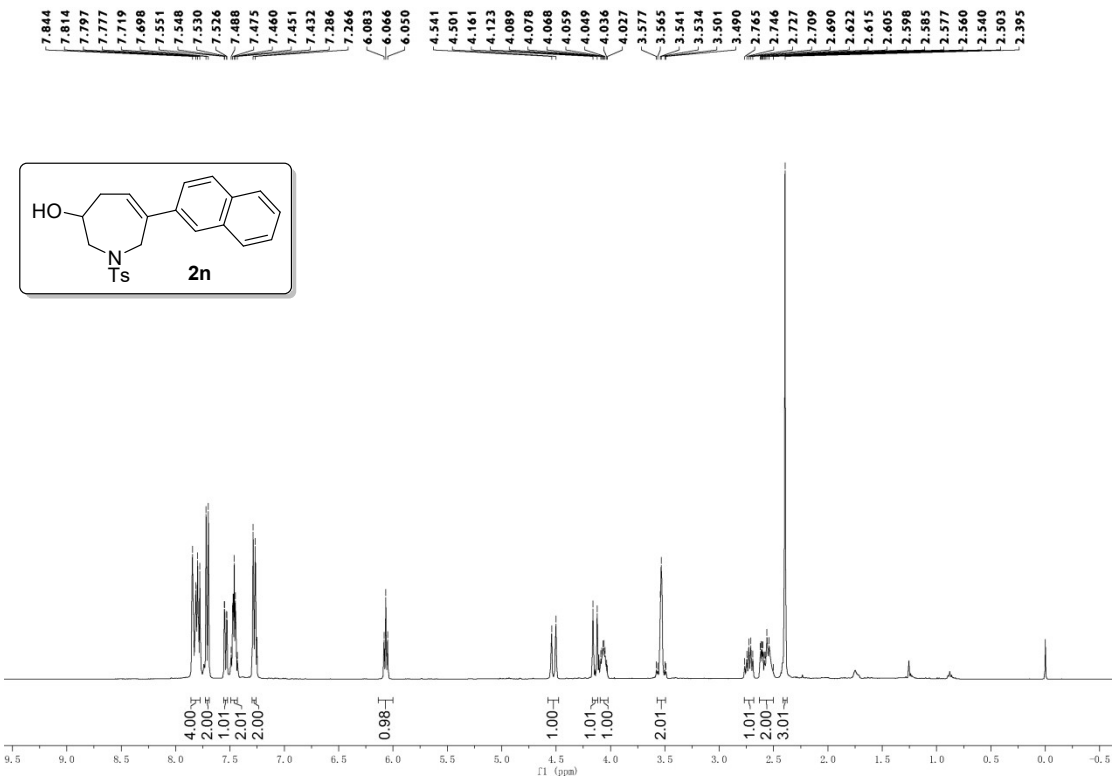
49.816
49.384
45.709
21.274
HO
N
Ts
O
O
2m
f1 (ppm)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7.451
7.432
7.286
7.266
6.083
6.066
6.050
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4.123
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4.078
4.068
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3.541
3.534
3.501
3.490
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2.709
2.690
2.622
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2.605
2.598
2.585
2.577
2.560
2.540
2.503
2.395
HO
N
Ts
2n
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2.00
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1.00
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1.01
2.00
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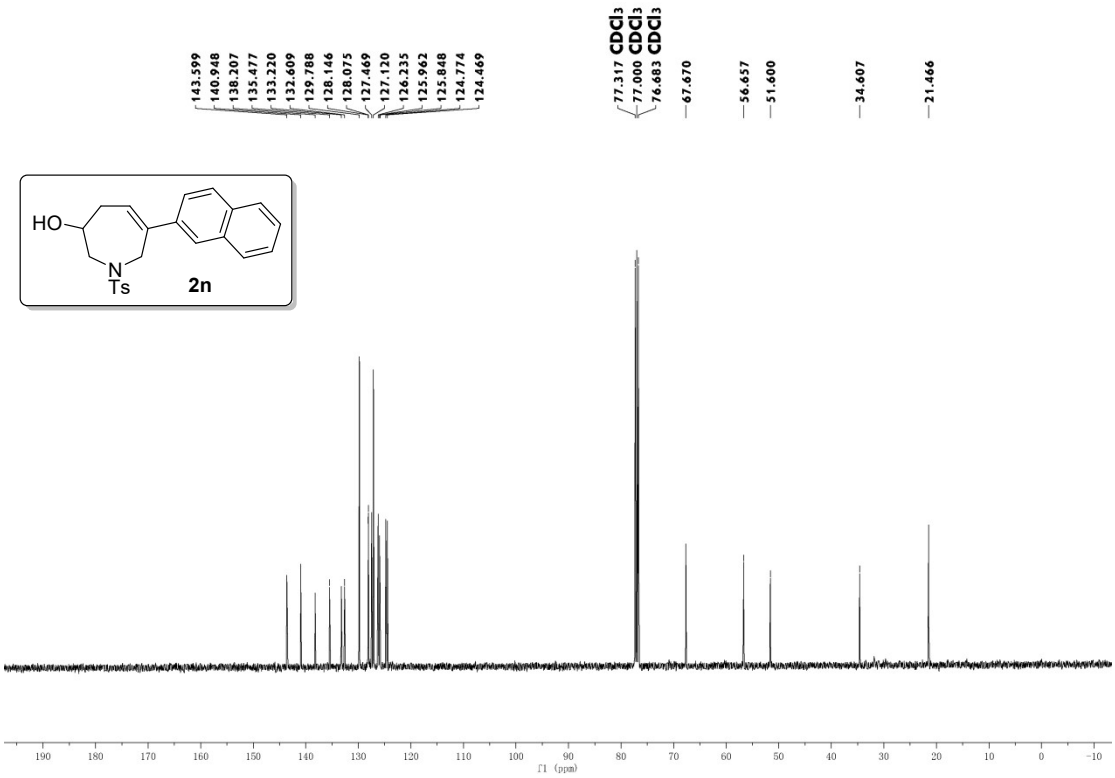
f1 (ppm)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124.774
124.469
77.317 CDCl3
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76.683 CDCl3
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21.466
HO
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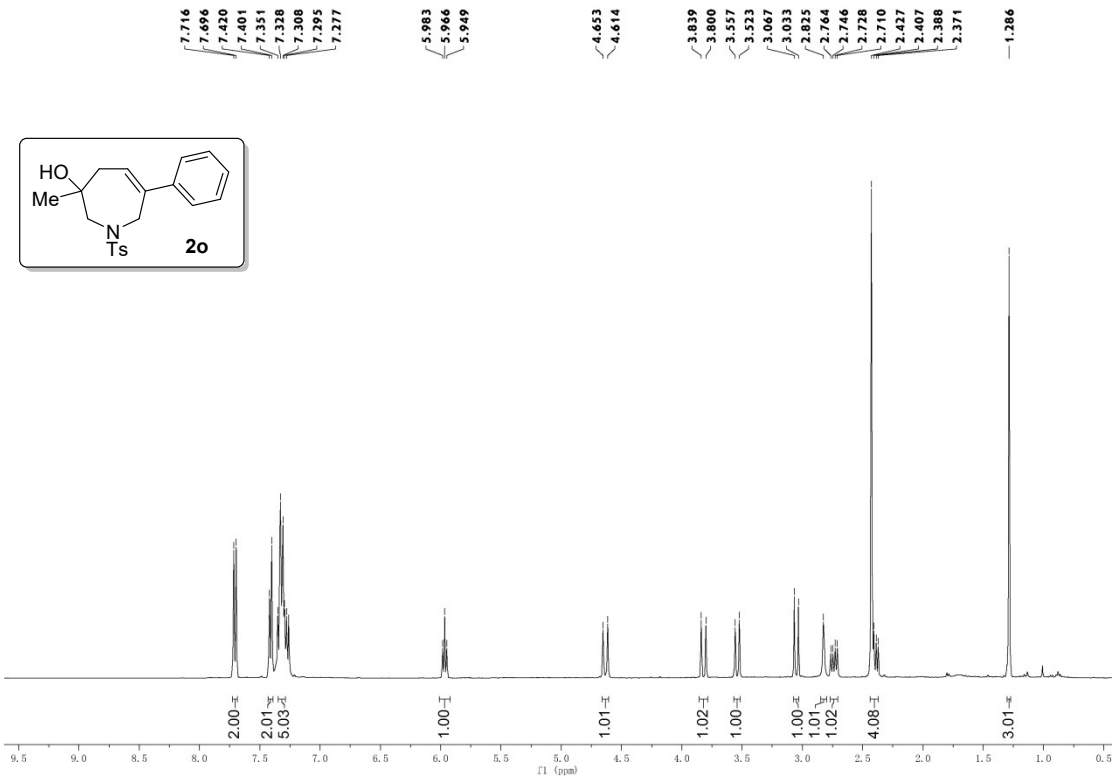
Ts
2n
f1 (ppm)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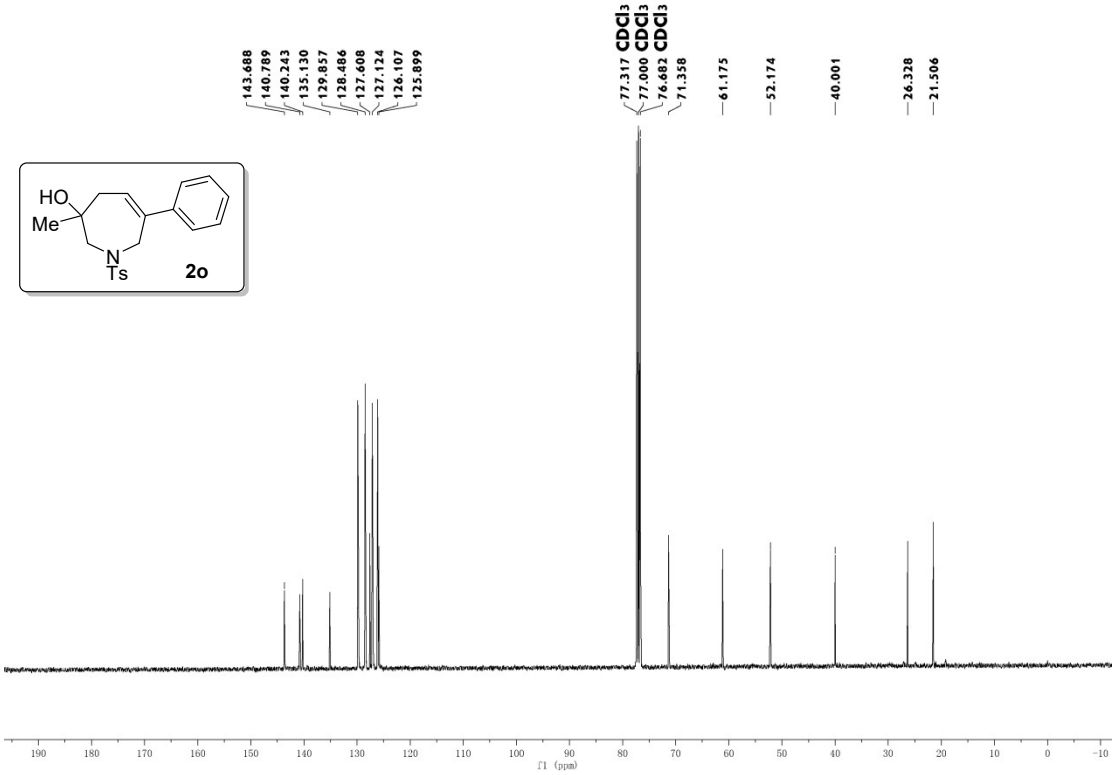
5.966
5.949
4.653
4.614
3.839
3.800
3.557
3.523
3.067
3.033
2.825
2.764
2.746
2.728
2.710
2.427
2.407
2.388
2.371
1.286
HO
Me
N
Ts
2o
2.00
2.01
5.03
1.00
1.01
1.02
1.00
1.00
1.01
1.02
4.08
3.01
f1 (ppm)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127.124
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125.899
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77.000 CDCl3
76.682 CDCl3
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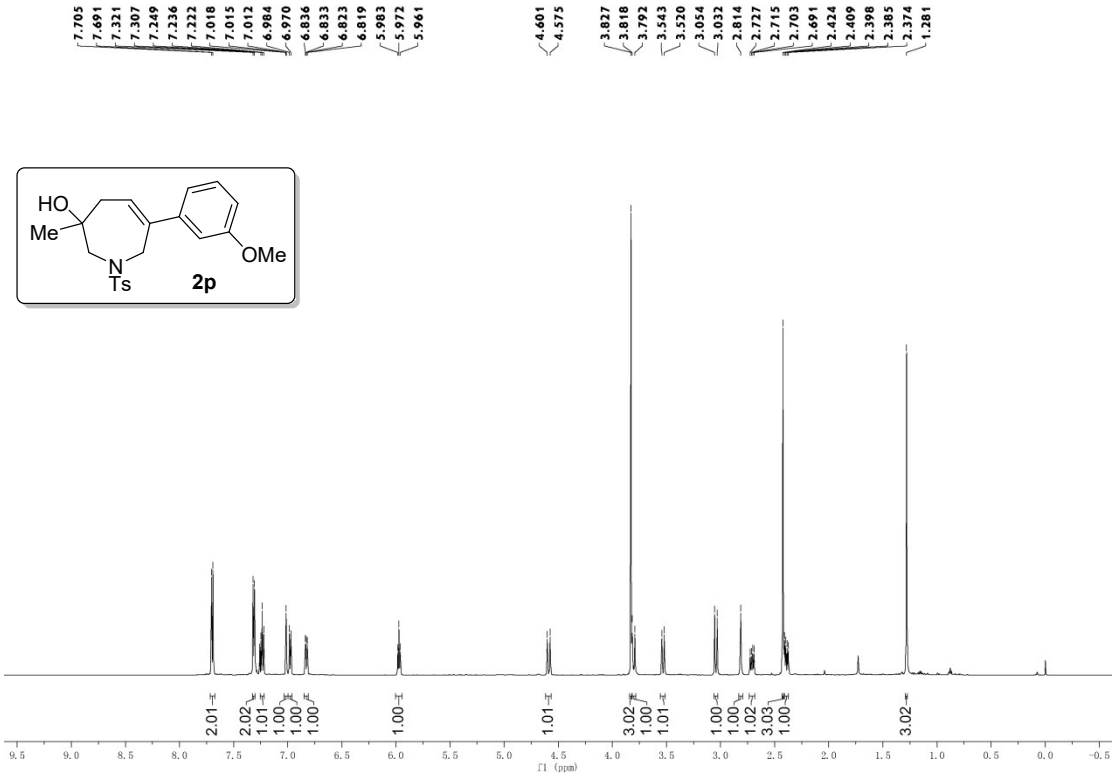
61.175
52.174
40.001
26.328
21.506
HO
Me
N
Ts
2o
f1 (ppm)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6.836
6.833
6.823
6.819
5.983
5.972
5.961
4.601
4.575
3.827
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3.032
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2.424
2.409
2.398
2.385
2.374
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HO
Me
N
Ts
OMe
2p
2.01
2.02
1.01
1.00
1.00
1.00
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1.01
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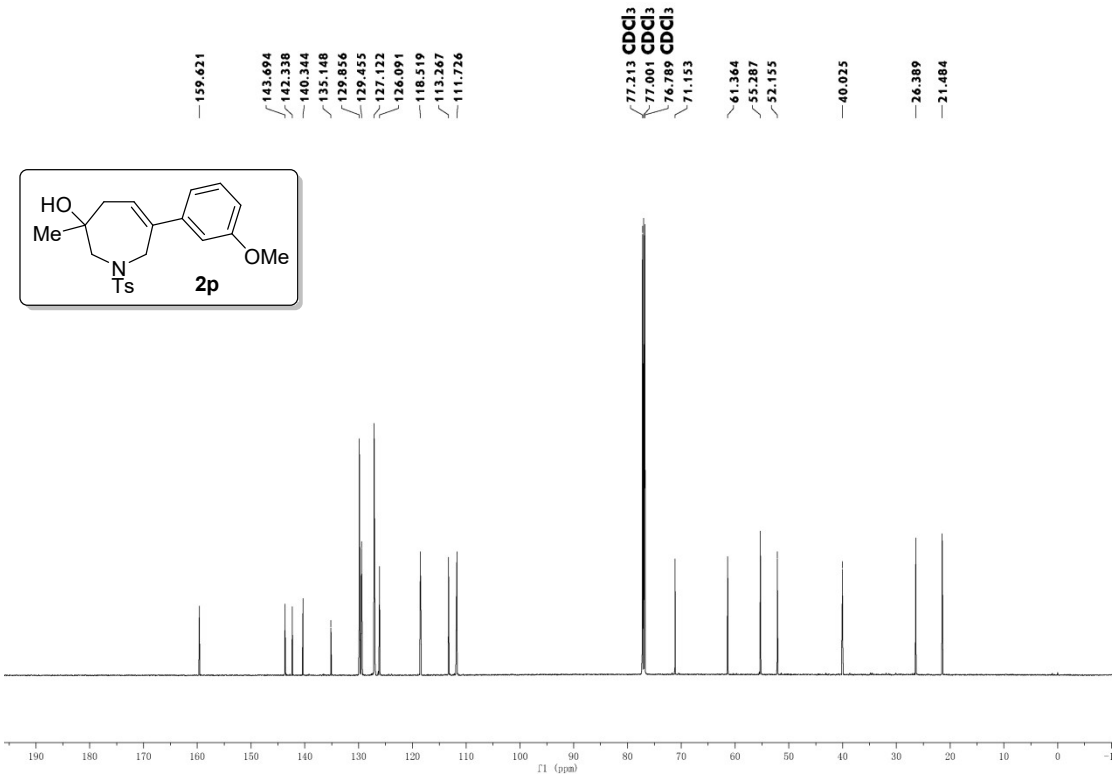
1.02
3.03
1.00
3.02
f1 (ppm)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111.726
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76.789 CDCl3
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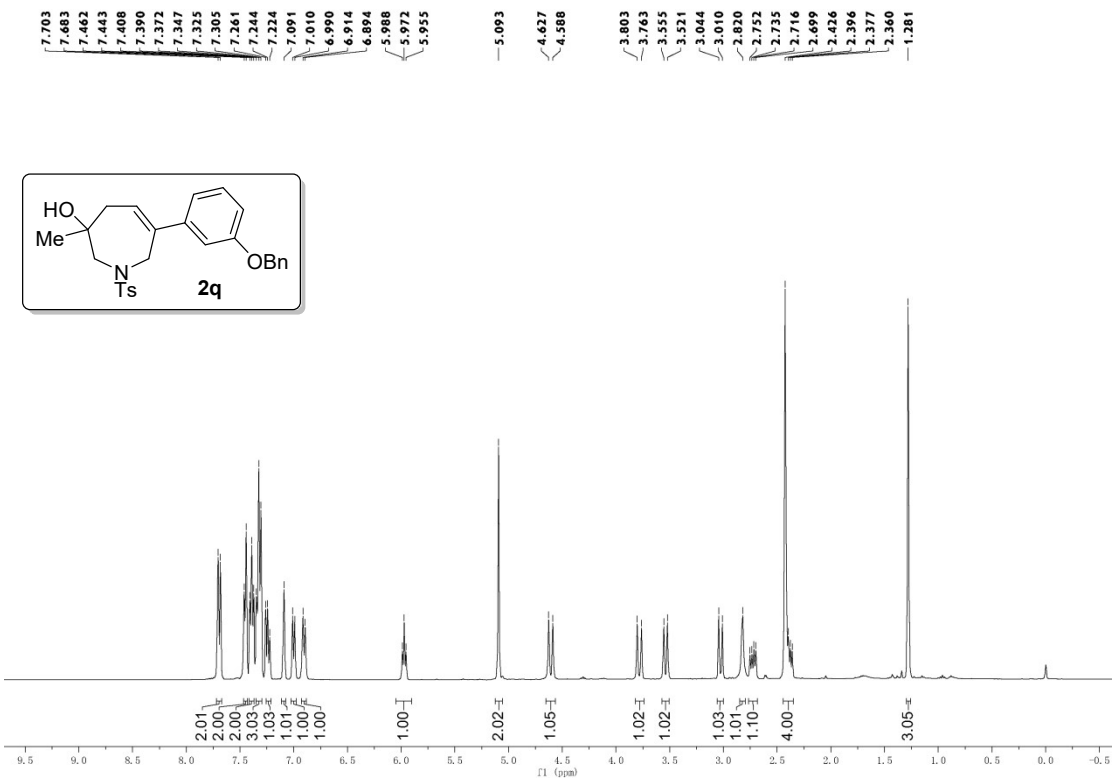
Me
N
Ts
OMe
2p
f1 (ppm)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2.360
1.281
HO
Me
N
Ts
OBn
2q
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2.00
2.00
3.03
1.03
1.01
1.00
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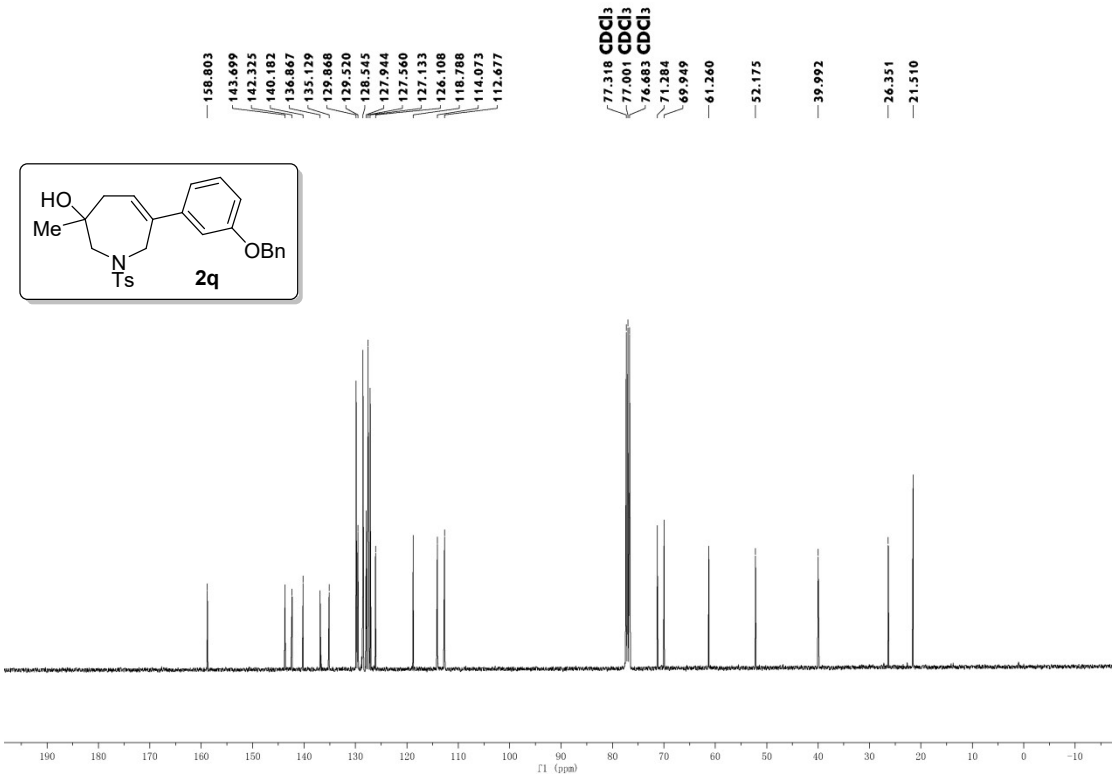
3.05
f1 (ppm)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77.001 CDCl3
76.683 CDCl3
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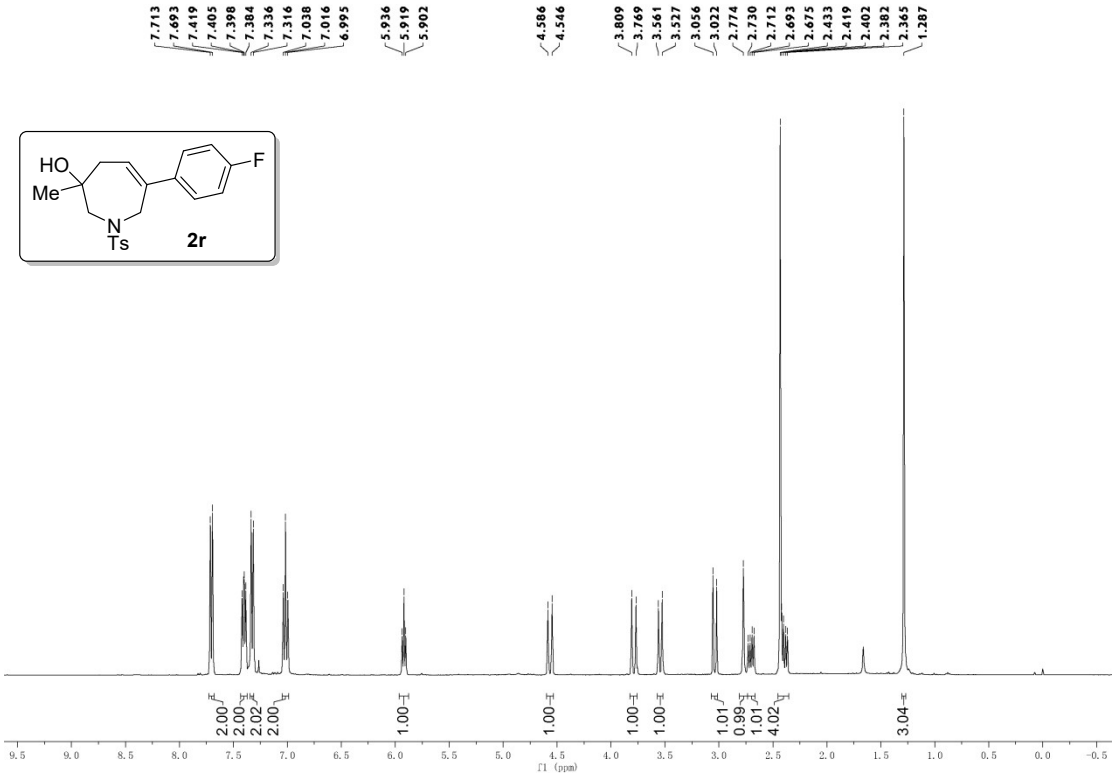
2q
f1 (ppm)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2.774
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1.287
HO
Me
N
Ts
F
2r
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2.00
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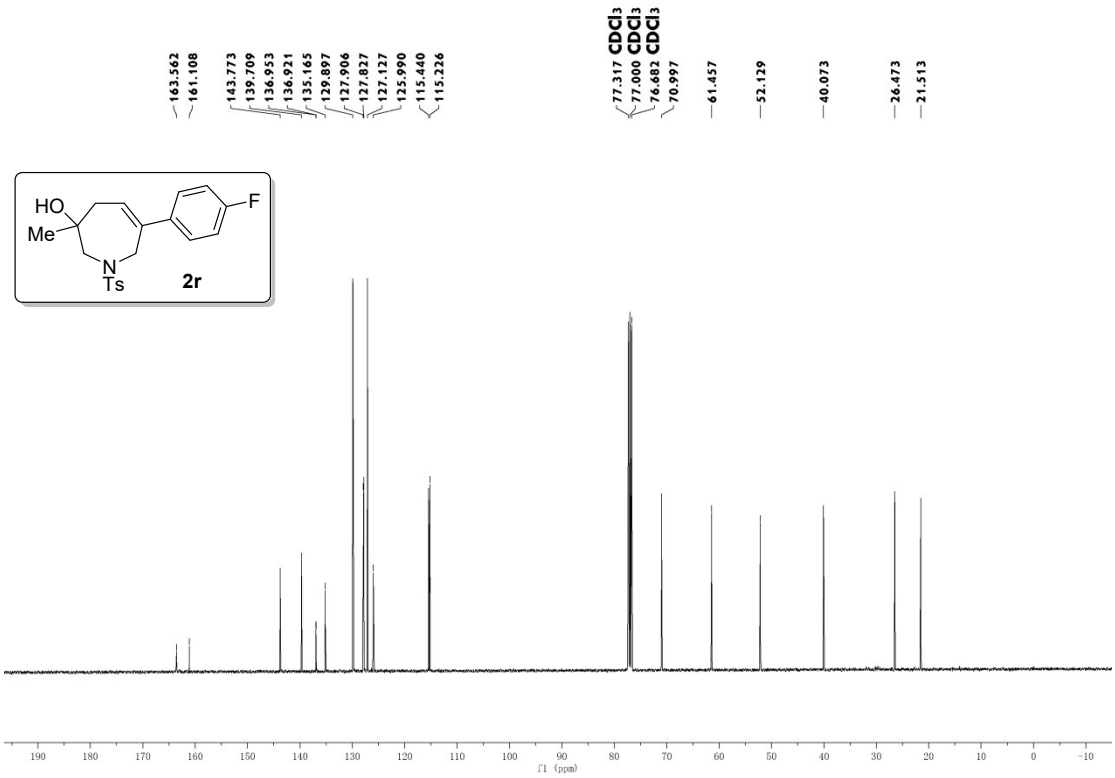
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115.226
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77.000 CDCl3
76.682 CDCl3
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21.513
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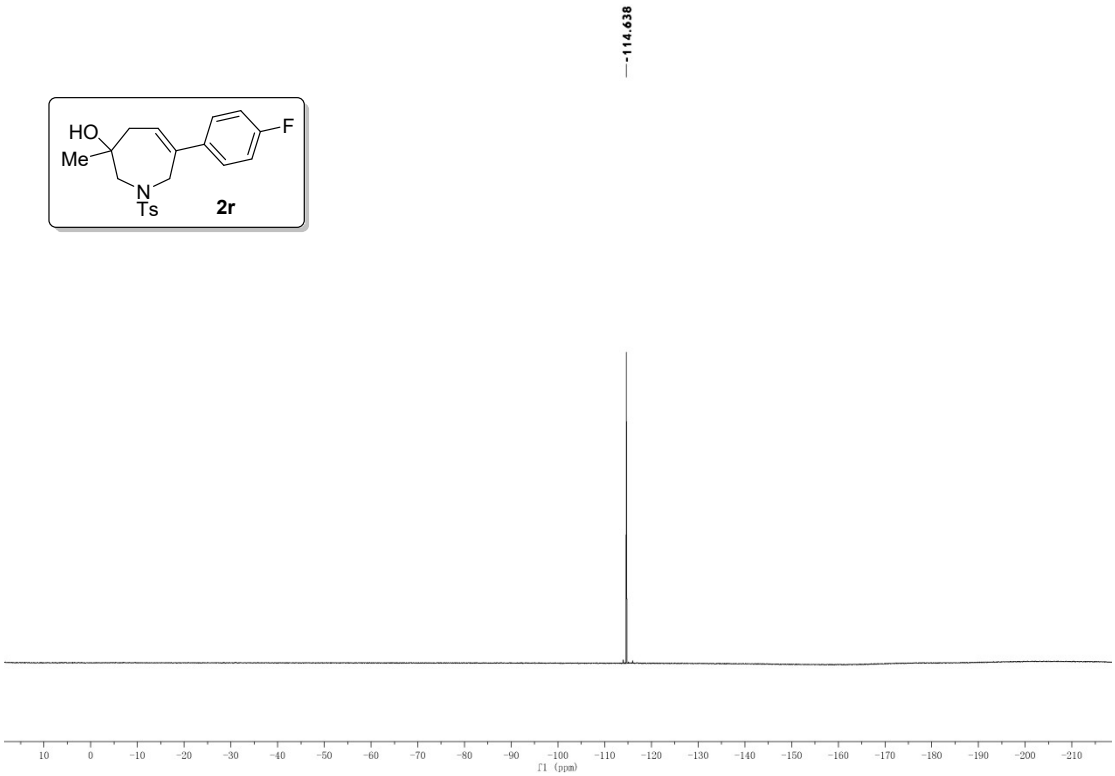
Me
N
Ts
F
2r
f1 (ppm)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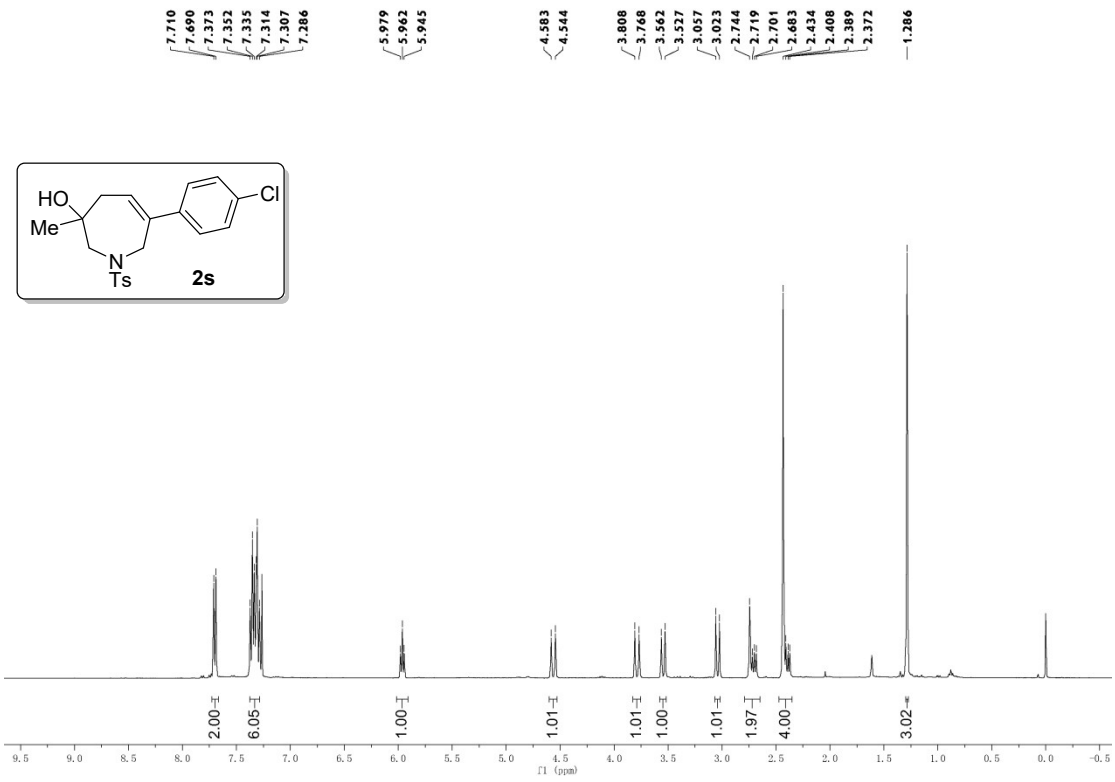
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2.683
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2.372
1.286
HO
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N
Ts
Cl
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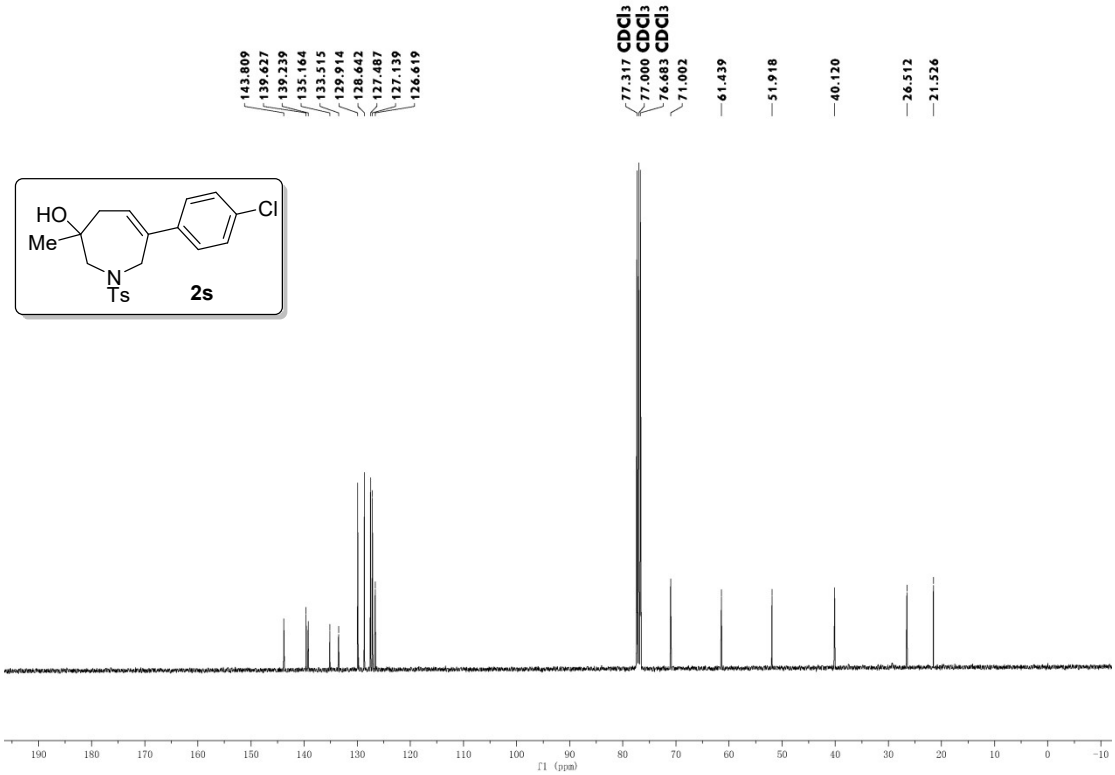
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126.619
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77.000 CDCl3
76.683 CDCl3
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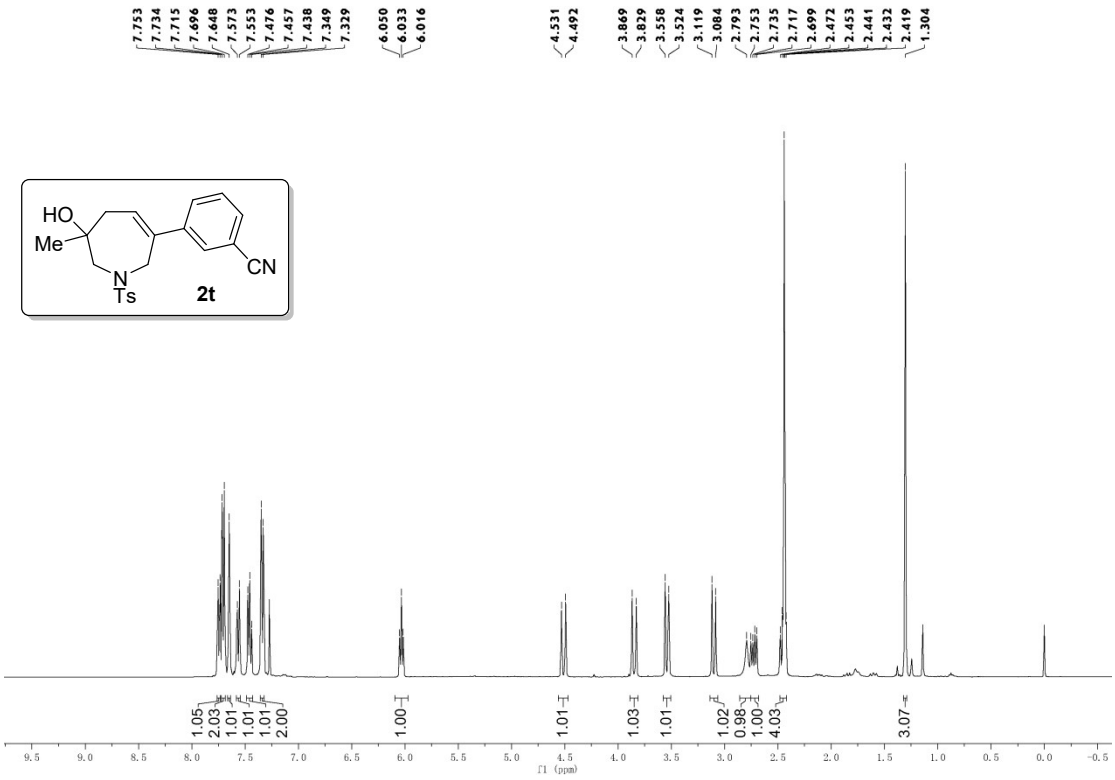
Cl
2s
f1 (ppm)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2.472
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2.441
2.432
2.419
1.304
HO
Me
N
Ts
CN
2t
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2.03
1.01
1.01
1.01
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1.03
1.01
1.02
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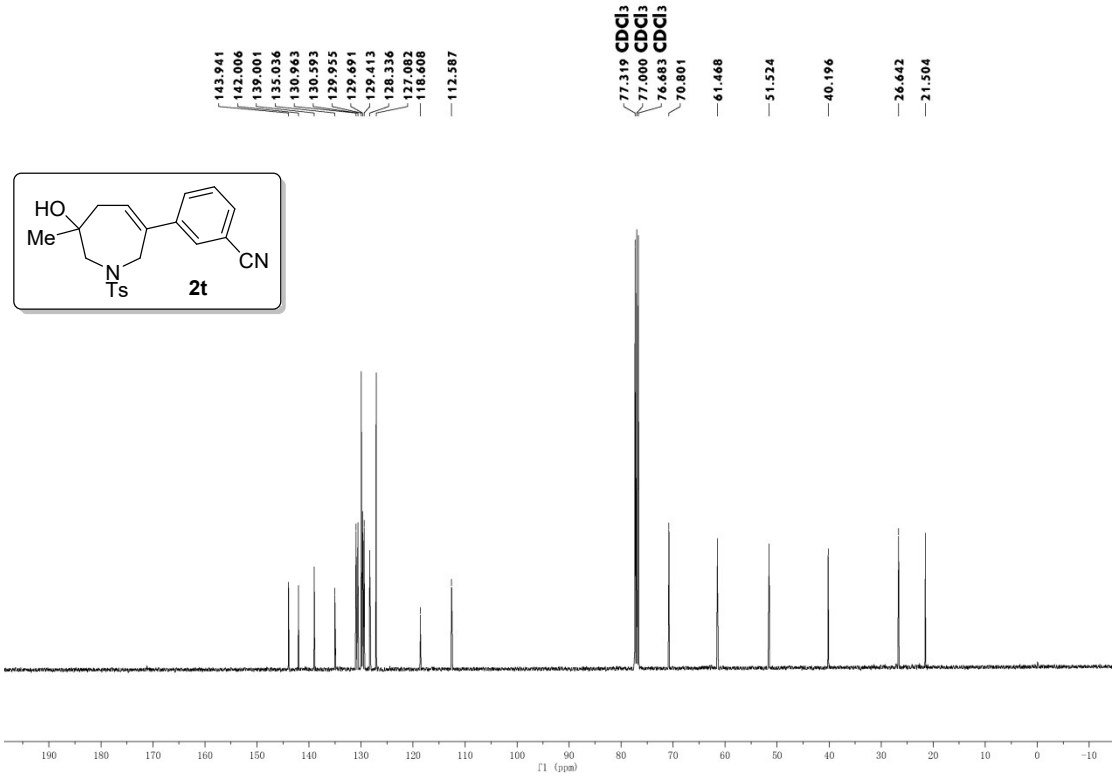
f1 (ppm)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112.587
77.319 CDCl3
77.000 CDCl3
76.683 CDCl3
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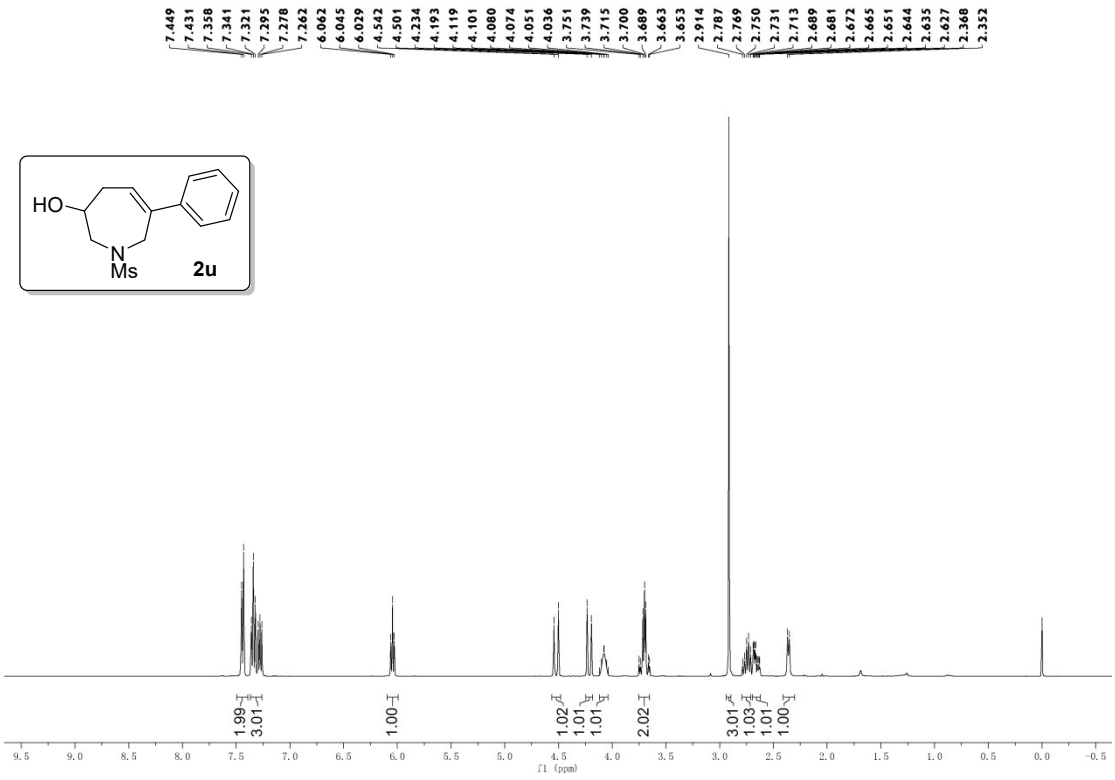
Me
N
Ts
CN
2t
f1 (ppm)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HO
N
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1.02
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1.01
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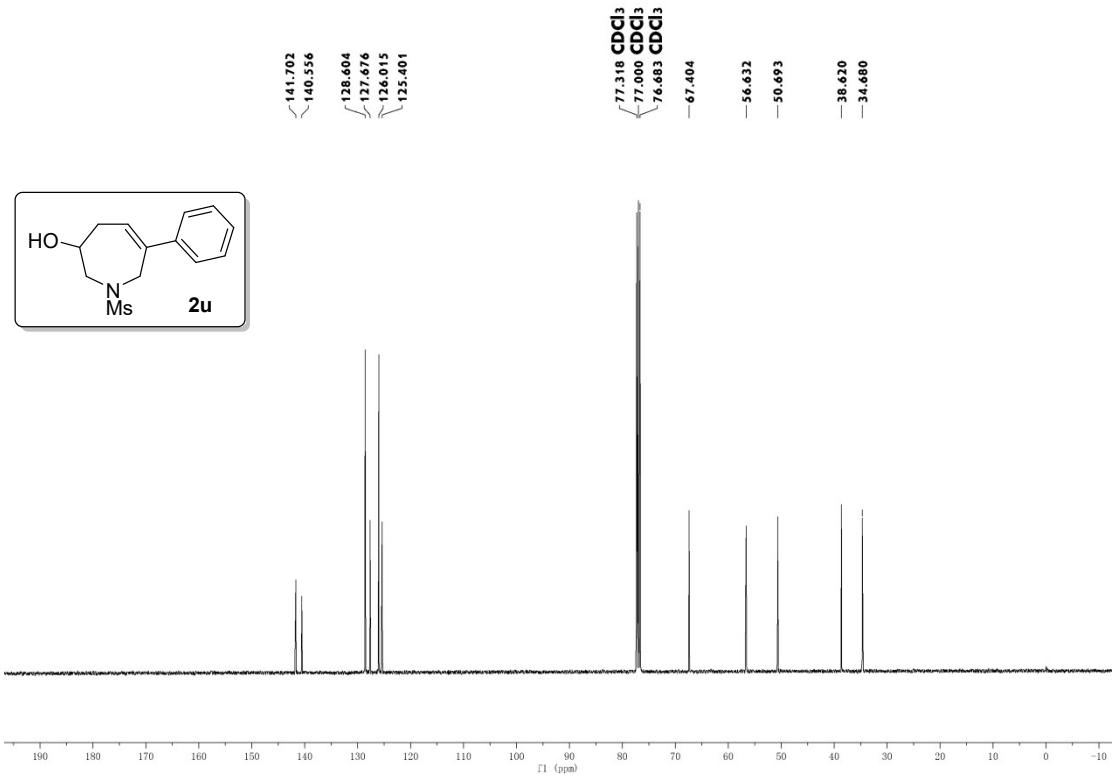
1.01
1.00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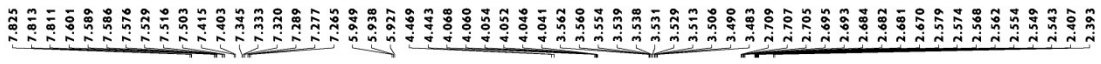
140.556
128.604
127.676
126.015
125.401
CDCl3
77.318
77.000
76.683
67.404
56.632
50.693
38.620
34.680
HO
N
Ms
2u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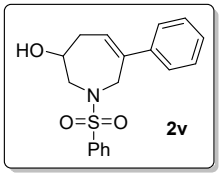
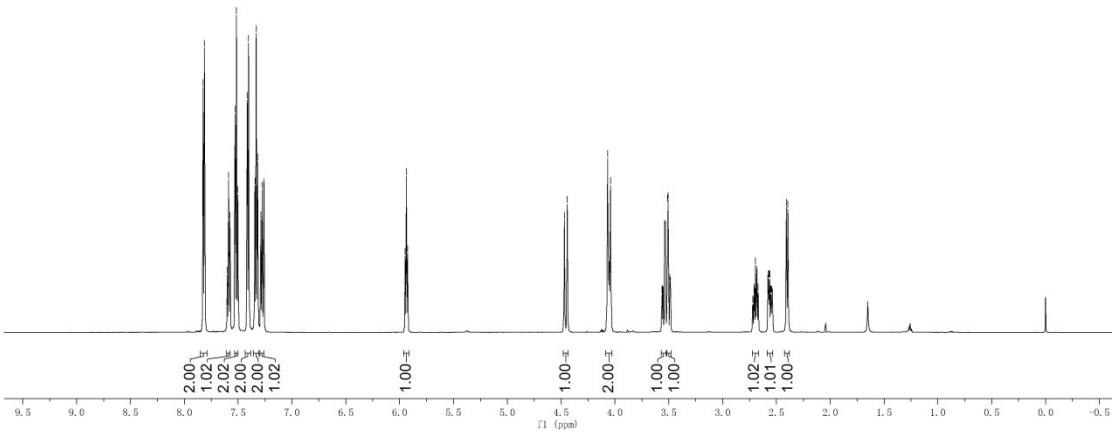
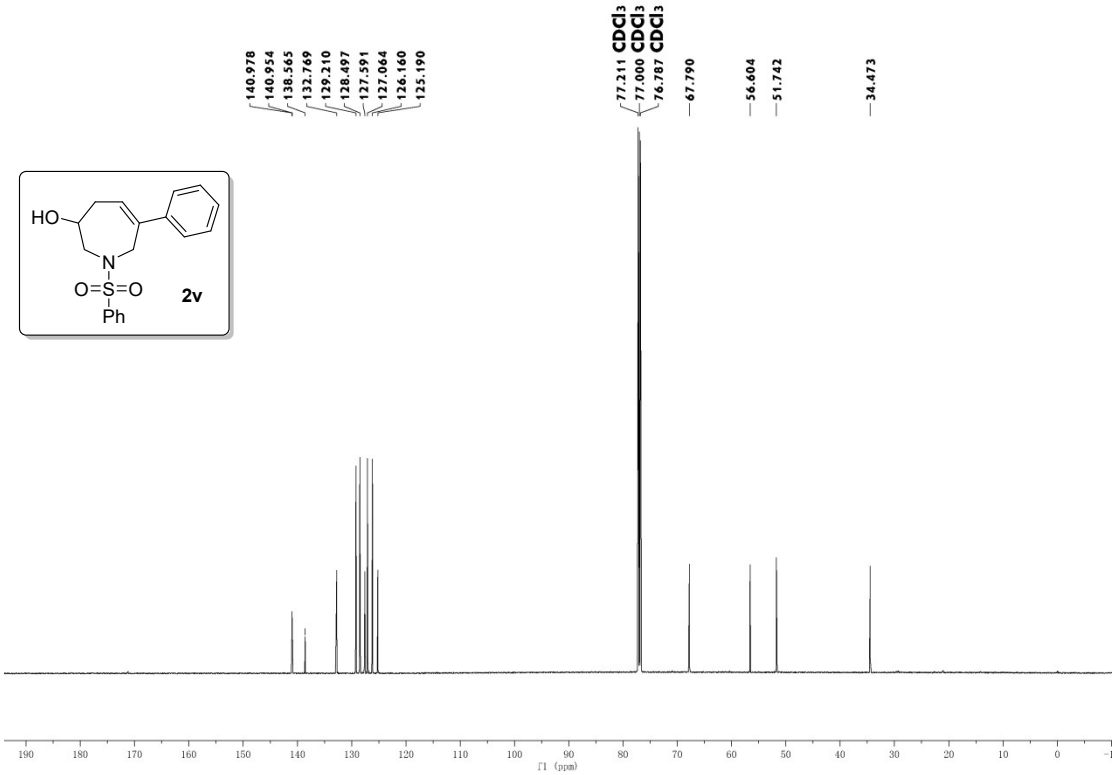
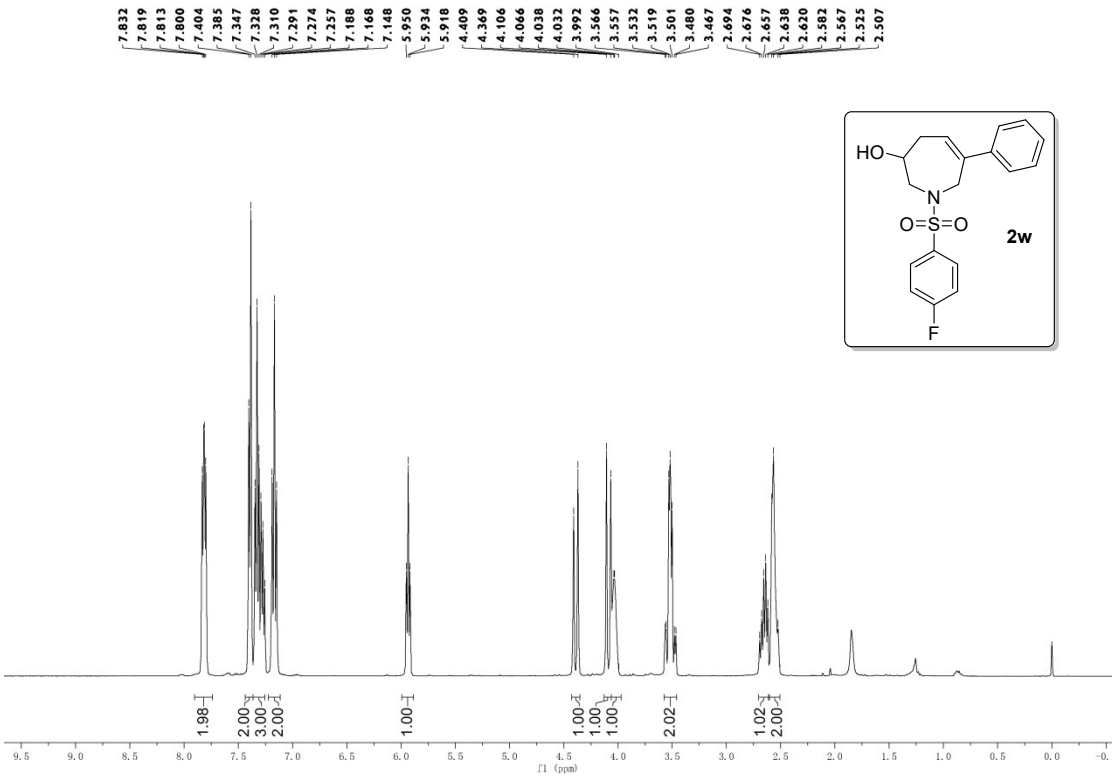
7.813
7.811
7.601
7.589
7.586
7.576
7.529
7.516
7.503
7.415
7.403
7.345
7.333
7.320
7.289
7.277
7.265
5.949
5.938
5.927
4.469
4.443
4.068
4.060
4.054
4.052
4.046
4.041
3.562
3.560
3.554
3.539
3.538
3.531
3.529
3.513
3.506
3.490
3.483
2.709
2.707
2.705
2.695
2.693
2.684
2.682
2.681
2.670
2.579
2.574
2.568
2.562
2.554
2.549
2.543
2.407
2.393

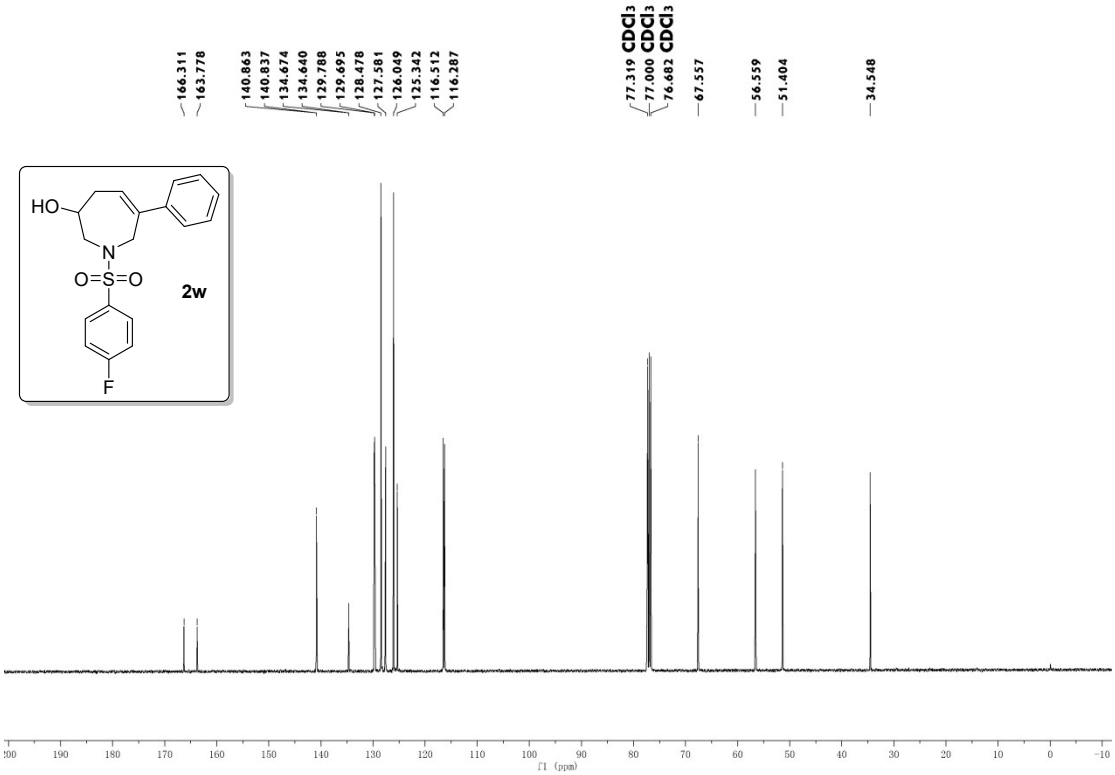

HO
N
O=S=O
Ph
2v

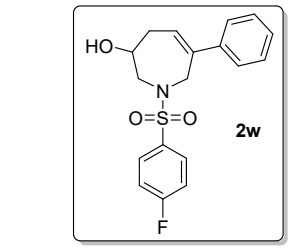

2.00
1.02
2.02
2.00
2.00
1.02
1.00
1.00
2.00
1.00
1.00
1.02
1.01
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


140.978
140.954
138.565
132.769
129.210
128.497
127.591
127.064
126.160
125.190
CDCl3
77.211
CDCl3
77.000
CDCl3
76.787
67.790
56.604
51.742
34.473
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

HO
N
O=S=O
Ph
2v

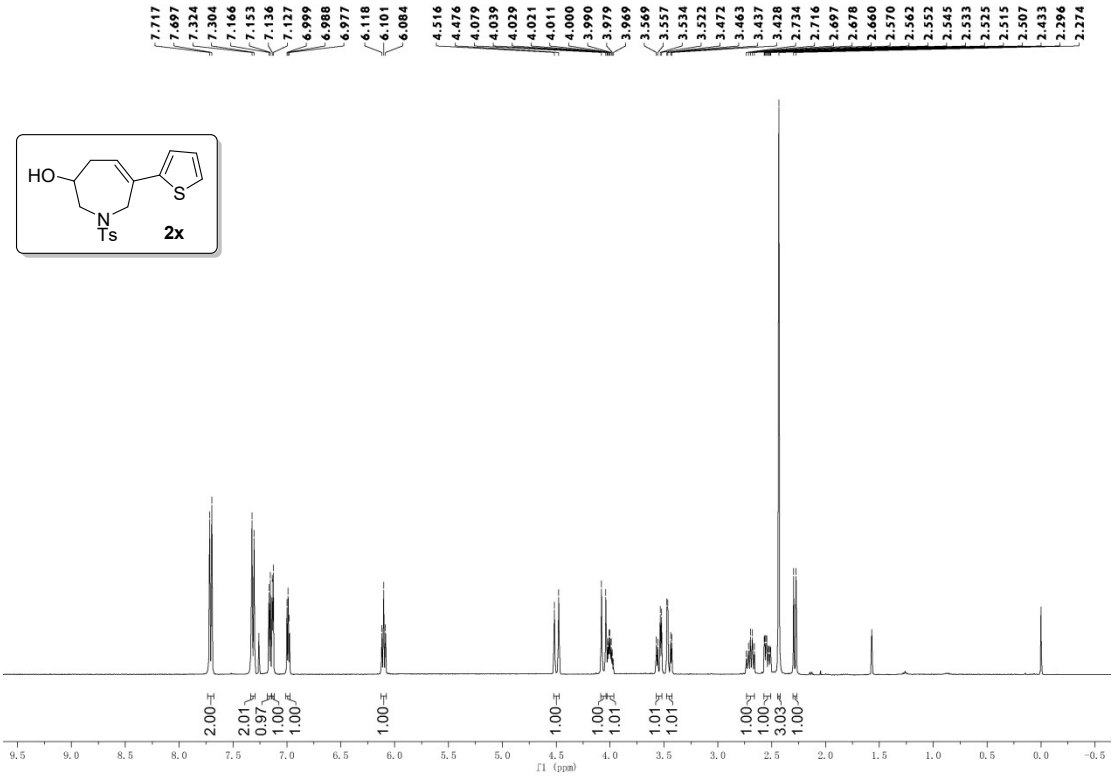

7.832
7.819
7.813
7.800
7.404
7.385
7.347
7.328
7.310
7.291
7.274
7.257
7.188
7.168
7.148
5.950
5.934
5.918
4.409
4.369
4.106
4.066
4.038
4.032
3.992
3.566
3.557
3.532
3.519
3.501
3.480
3.467
2.694
2.676
2.657
2.638
2.620
2.582
2.567
2.525
2.507
HO
N
O=S=O
F
2w
1.98
2.00
3.00
2.00
1.00
1.00
1.00
1.00
2.02
1.02
2.00
f1 (ppm)


166.311
163.778
140.863
140.837
134.674
134.640
129.788
129.695
128.478
127.581
126.049
125.342
116.512
116.287
77.319 CDCl3
77.000 CDCl3
76.682 CDCl3
67.557
56.559
51.404
34.548
HO
N
O=S=O
F
2w
f1 (ppm)

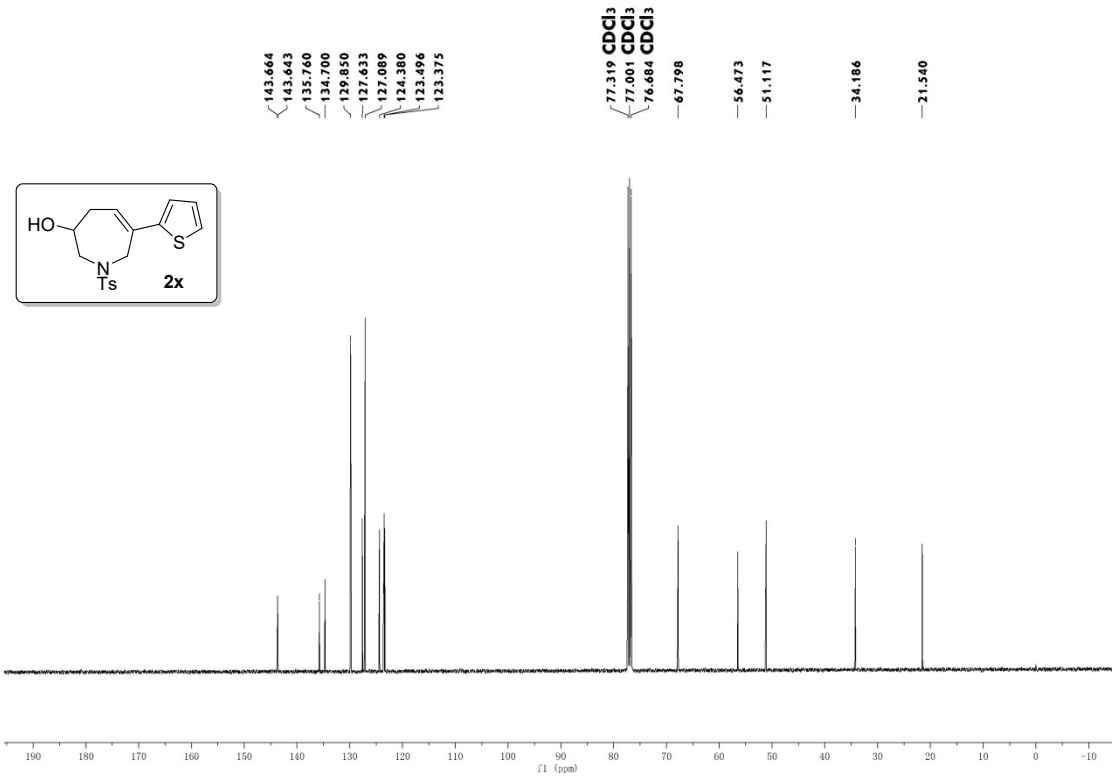

HO
N
O=S=O
F

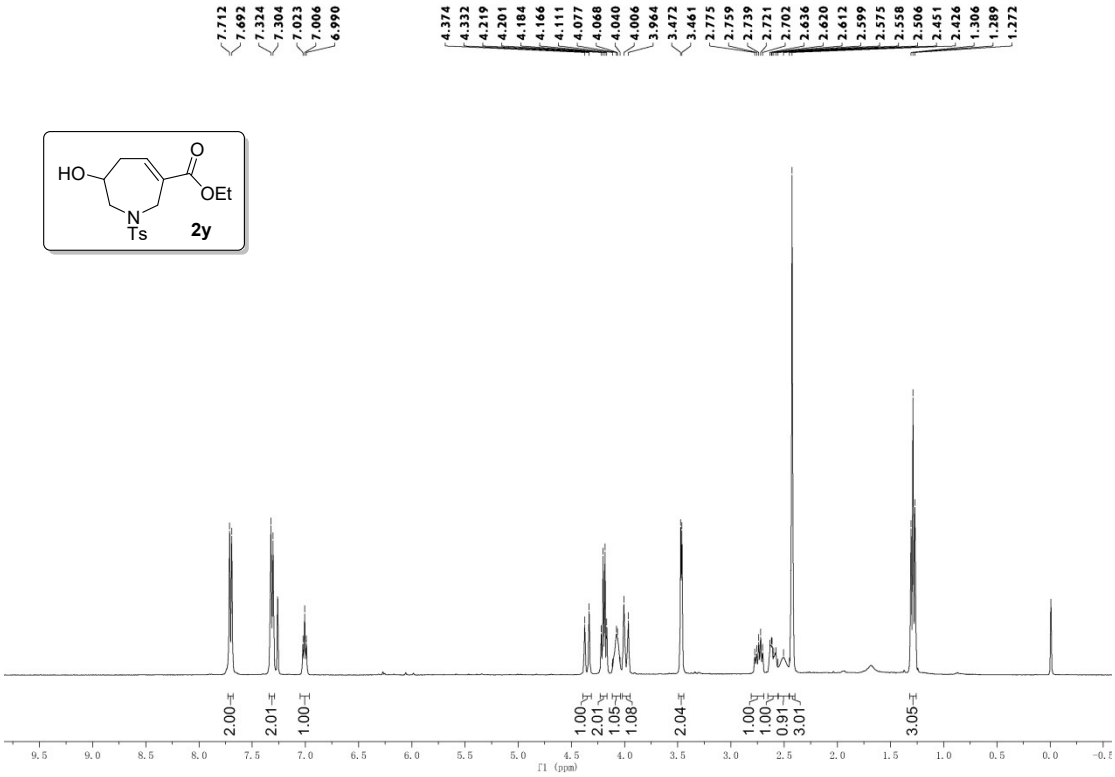
2w

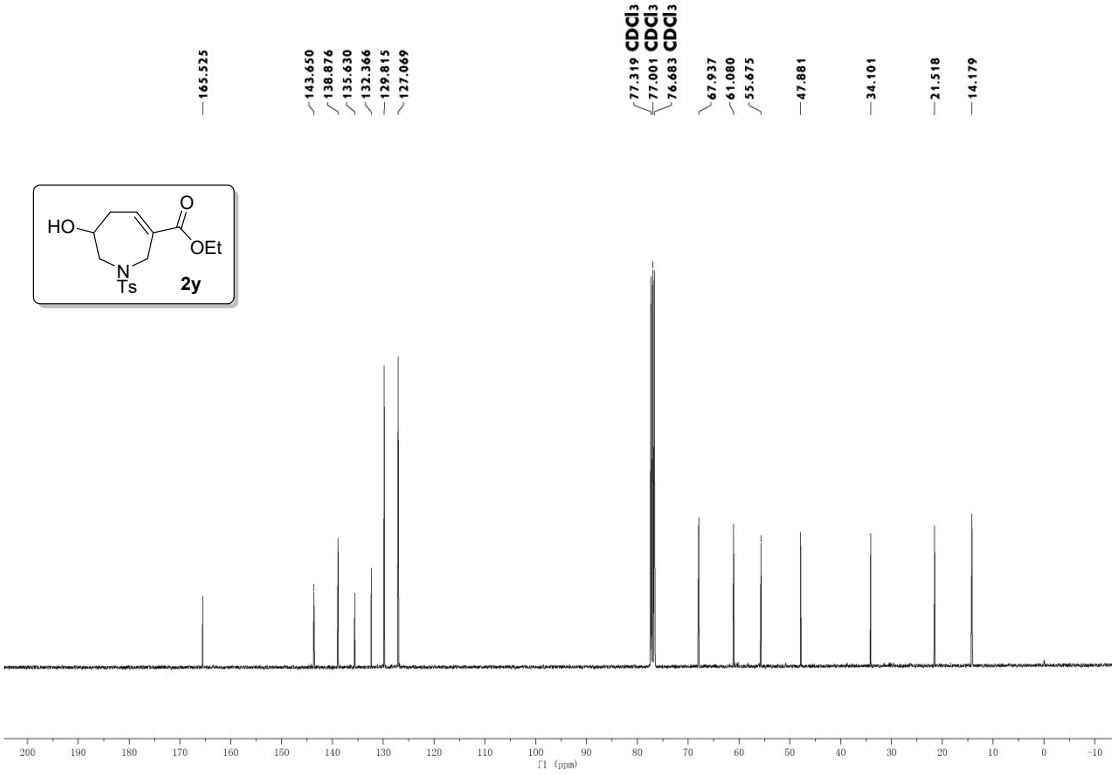
-104.914
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

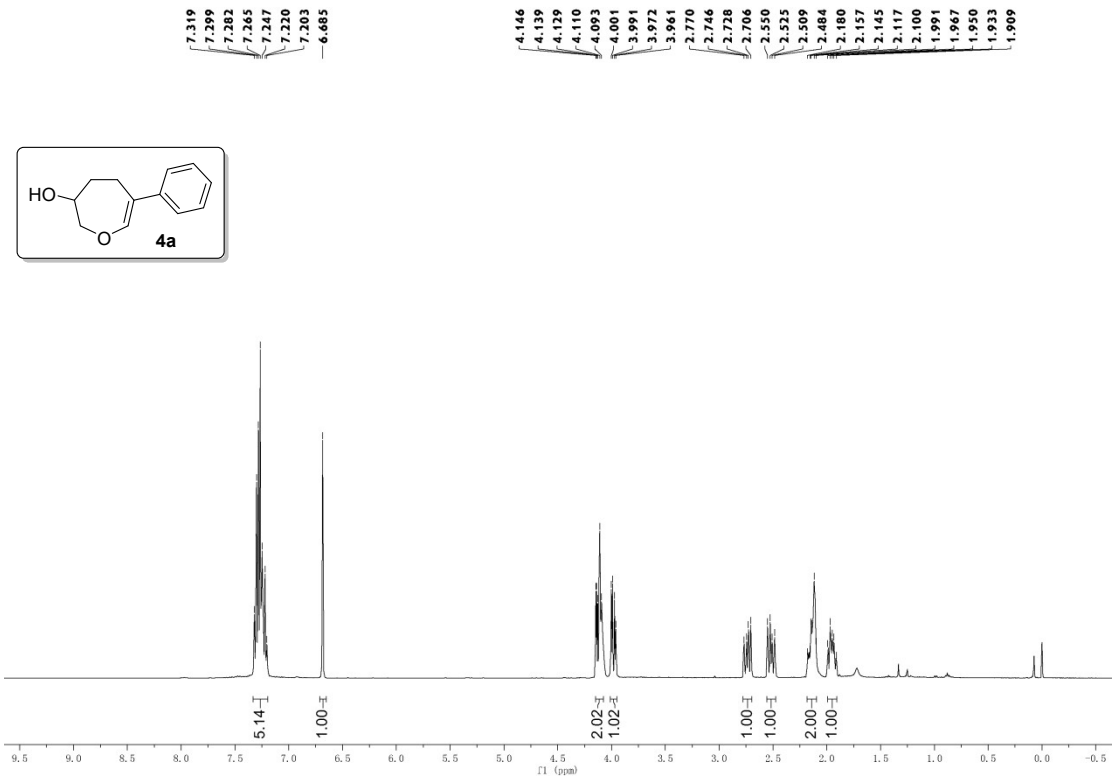

7.717
7.697
7.324
7.304
7.166
7.153
7.136
7.127
6.999
6.988
6.977
6.118
6.101
6.084
4.516
4.476
4.079
4.039
4.029
4.021
4.011
4.000
3.990
3.979
3.969
3.569
3.557
3.534
3.522
3.472
3.463
3.437
3.428
2.734
2.716
2.697
2.678
2.660
2.570
2.562
2.552
2.545
2.533
2.525
2.515
2.507
2.433
2.296
2.274
HO
S
N
Ts
2.00
2.01
0.97
1.00
1.00
1.00
1.00
1.00
1.01
1.01
1.01
1.00
1.00
3.03
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

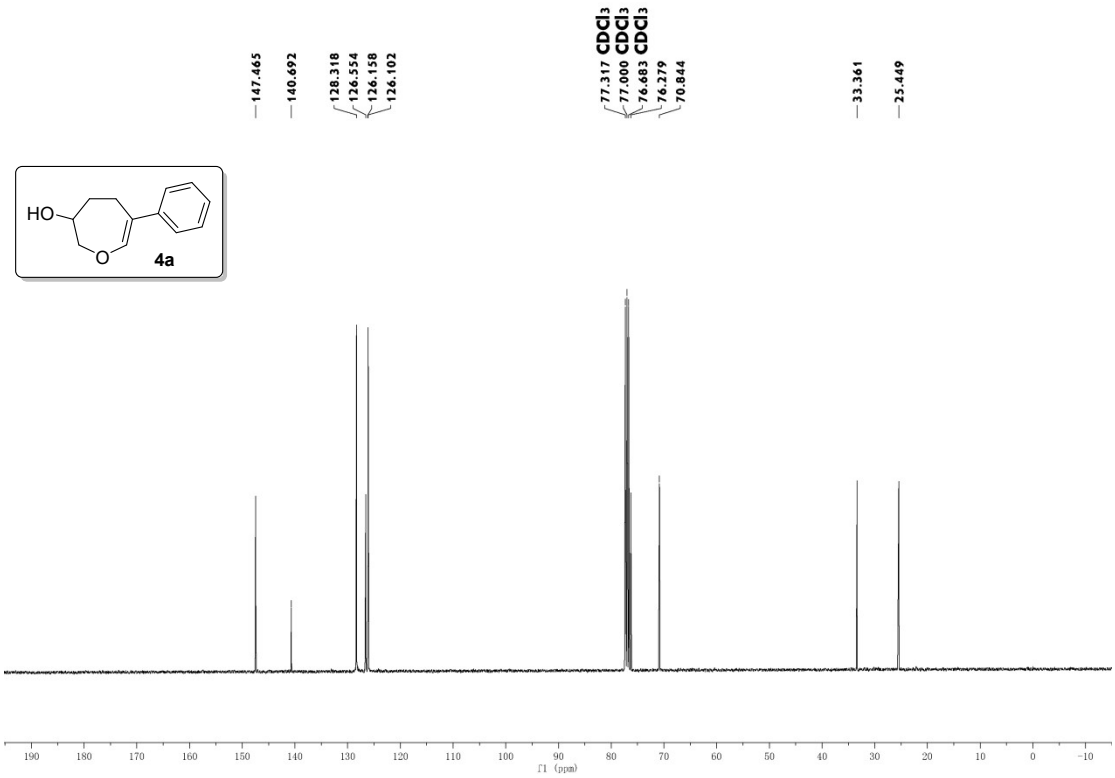
2x

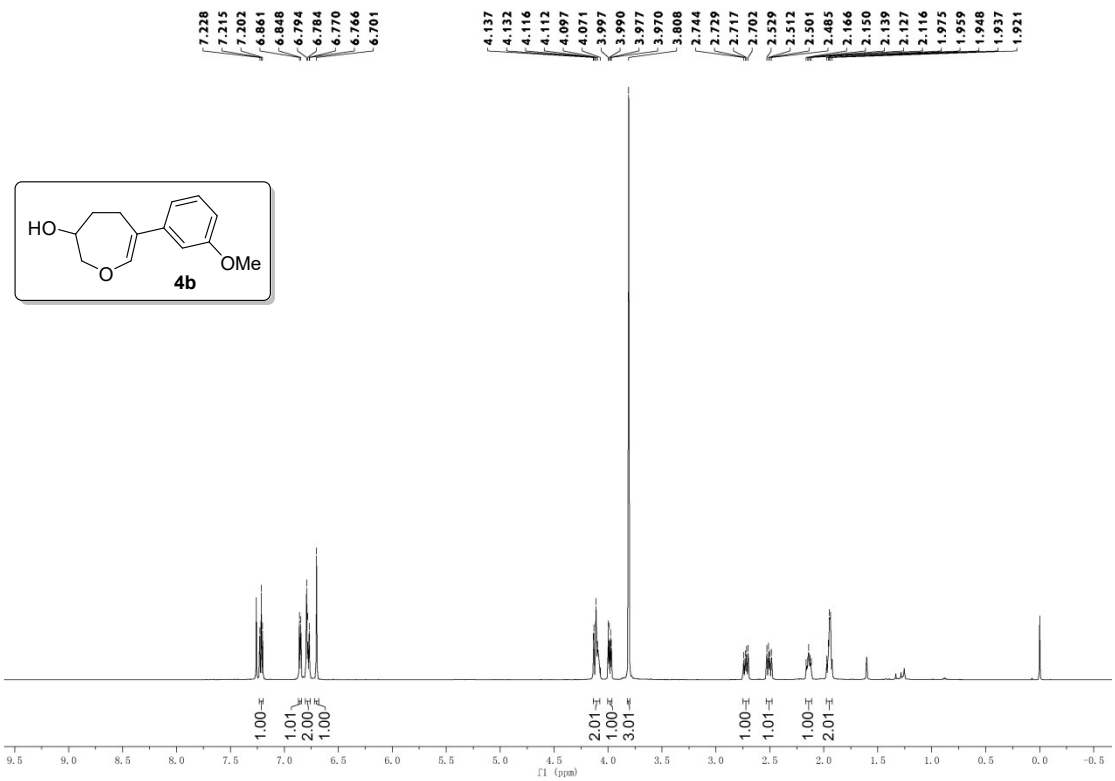

143.664
143.643
135.760
134.700
129.850
127.633
127.089
124.380
123.496
123.375
77.319 CDCl3
77.001 CDCl3
76.684 CDCl3
67.798
56.473
51.117
34.186
21.540
HO
S
N
Ts
2x
f1 (ppm)

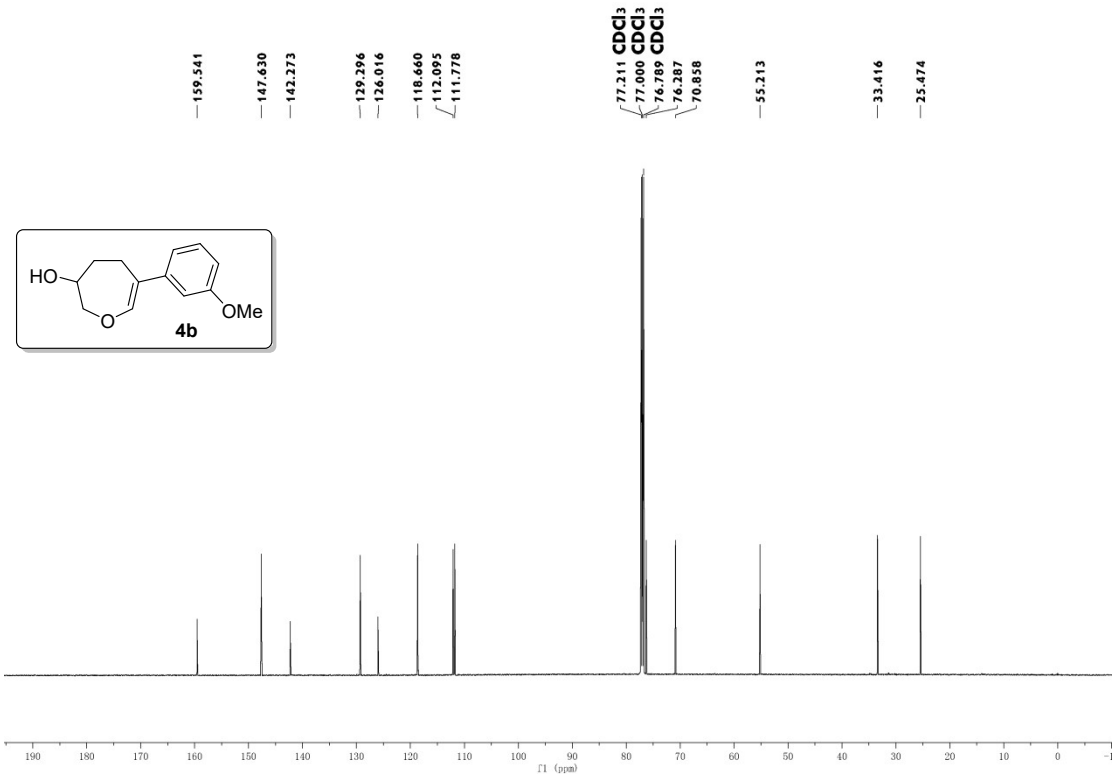

7.712
7.692
7.324
7.304
7.023
7.006
6.990
4.374
4.332
4.219
4.201
4.184
4.166
4.111
4.077
4.068
4.040
4.006
3.964
3.472
3.461
2.775
2.759
2.739
2.721
2.702
2.636
2.620
2.612
2.599
2.575
2.558
2.506
2.451
2.426
1.306
1.289
1.272
HO
O
OEt
N
Ts
2y
2.00
2.01
1.00
1.00
2.01
1.05
1.08
2.04
1.00
1.00
0.91
3.01
3.05
f1 (ppm)

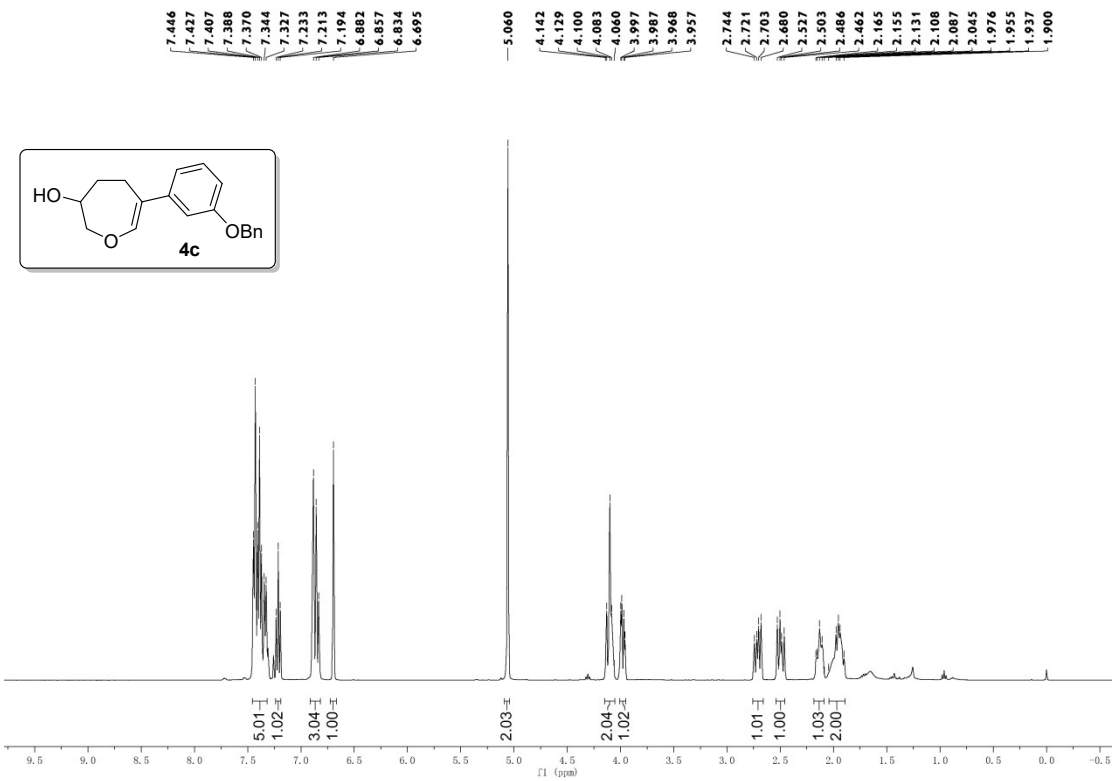

165.525
143.650
138.876
135.630
132.366
129.815
127.069
77.319 CDCl3
77.001 CDCl3
76.683 CDCl3
67.937
61.080
55.675
47.881
34.101
21.518
14.179
HO
O
OEt
N
Ts
2y
f1 (ppm)

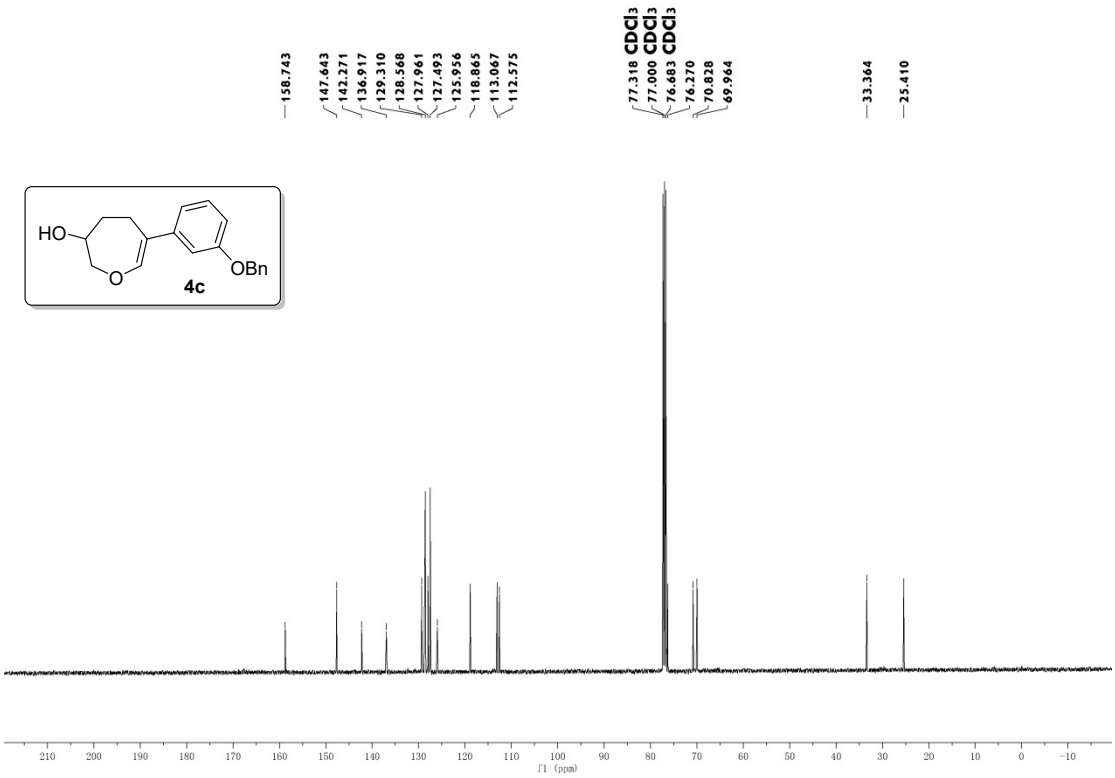

7.319
7.299
7.282
7.265
7.247
7.220
7.203
6.685
4.146
4.139
4.129
4.110
4.093
4.001
3.991
3.972
3.961
2.770
2.746
2.728
2.706
2.550
2.525
2.509
2.484
2.180
2.157
2.145
2.117
2.100
1.991
1.967
1.950
1.933
1.909
HO
O
4a
5.14
1.00
2.02
1.02
1.00
1.00
2.00
1.00
f1 (ppm)

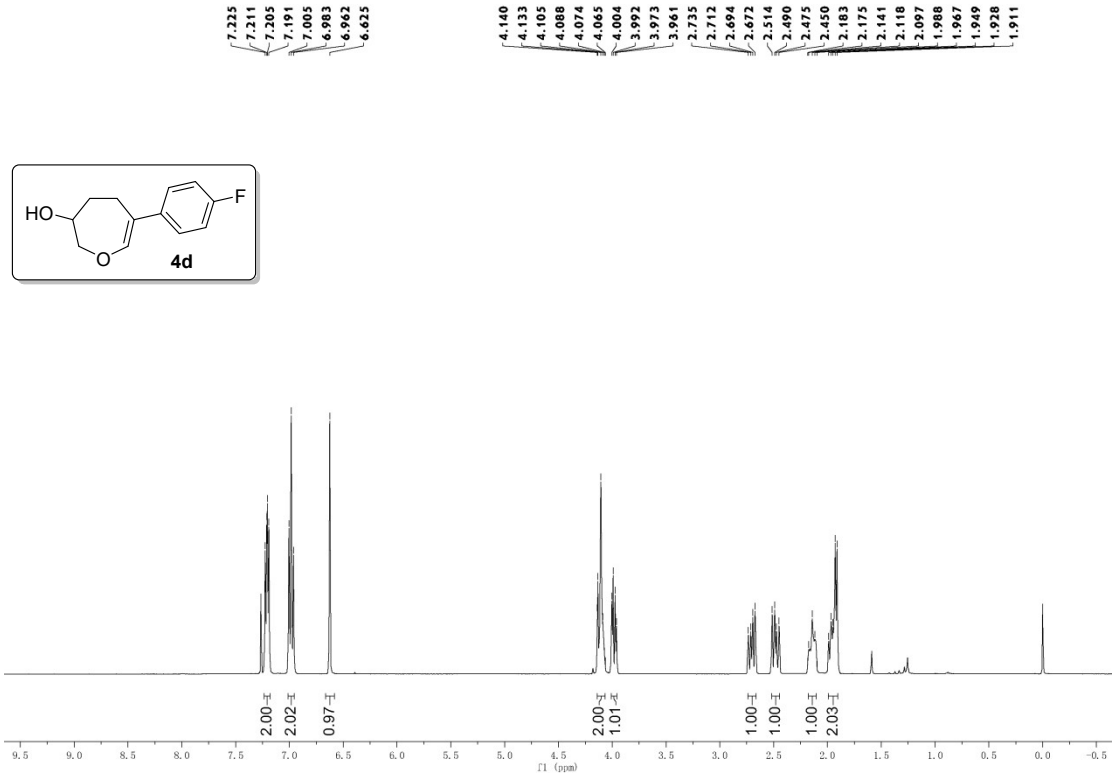

147.465
140.692
128.318
126.554
126.158
126.102
77.317 CDCl3
77.000 CDCl3
76.683 CDCl3
76.279
70.844
33.361
25.449
HO
O
4a
f1 (ppm)

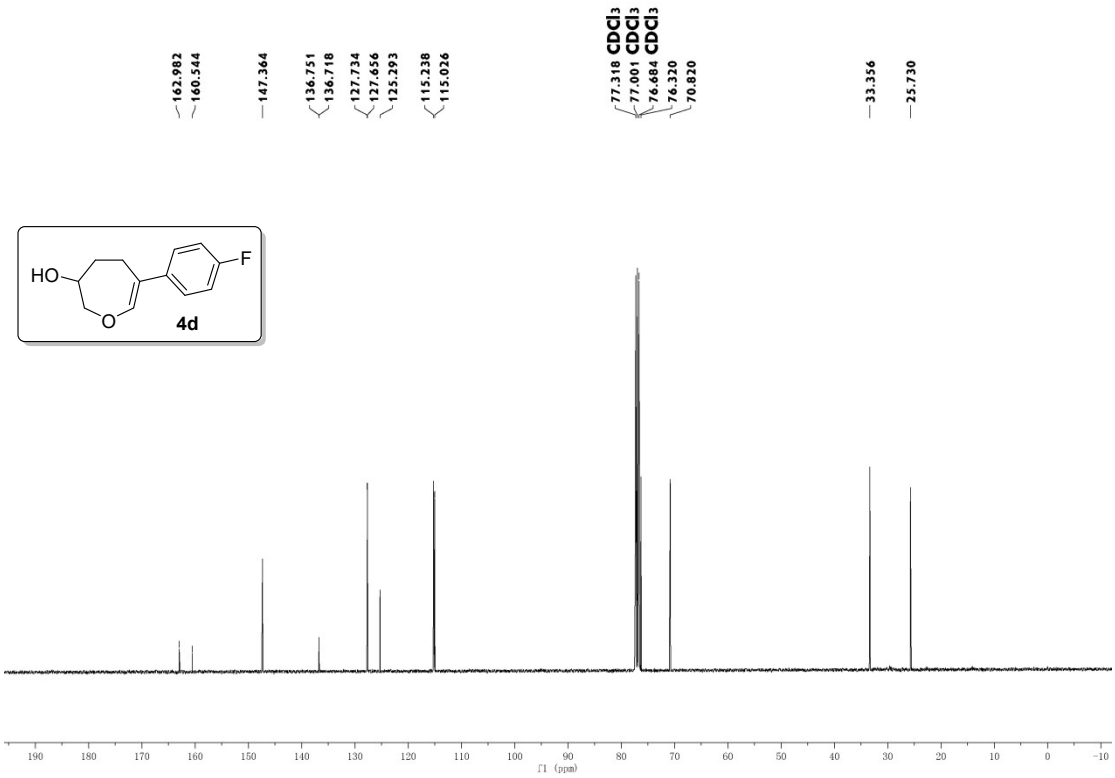

7.228
7.215
7.202
6.861
6.848
6.794
6.784
6.770
6.766
6.701
4.137
4.132
4.116
4.112
4.097
4.071
3.997
3.990
3.977
3.970
3.808
2.744
2.729
2.717
2.702
2.529
2.512
2.501
2.485
2.166
2.150
2.139
2.127
2.116
1.975
1.959
1.948
1.937
1.921
HO
O
OMe
4b
1.00
1.01
2.00
1.00
2.01
1.00
3.01
1.00
1.01
1.00
2.01
f1 (ppm)

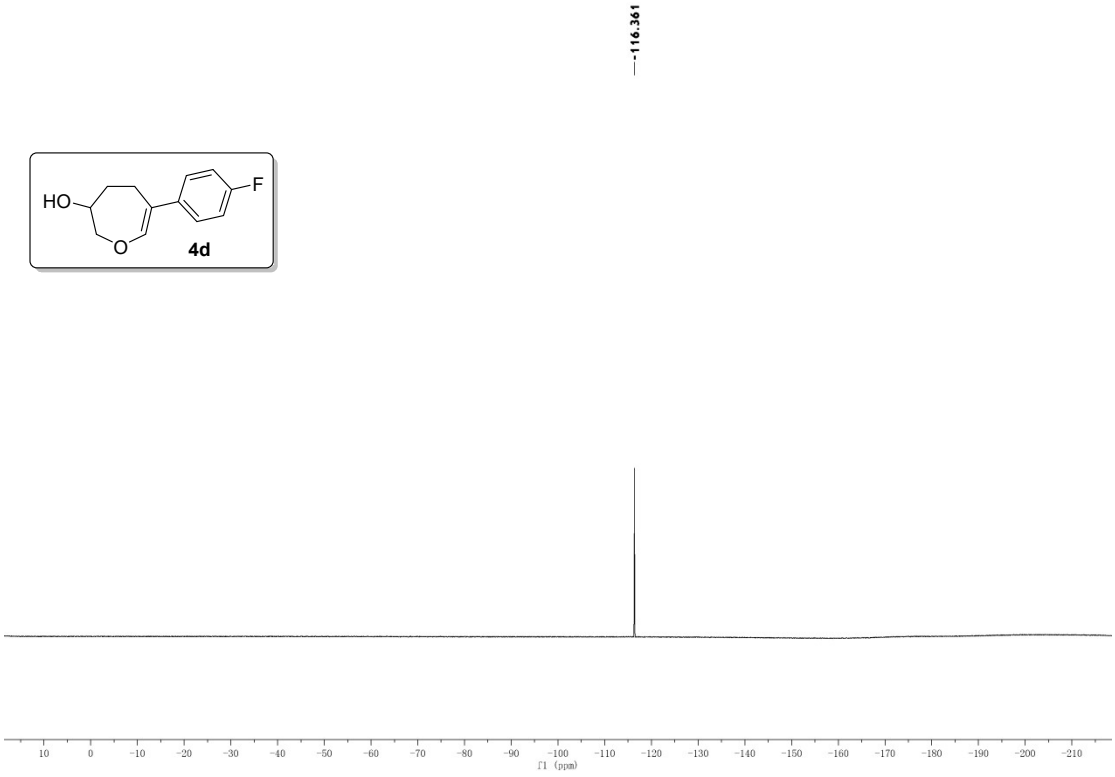

159.541
147.630
142.273
129.296
126.016
118.660
112.095
111.778
77.211 CDCl3
77.000 CDCl3
76.789 CDCl3
76.287
70.858
55.213
33.416
25.474
HO
O
OMe
4b
f1 (ppm)

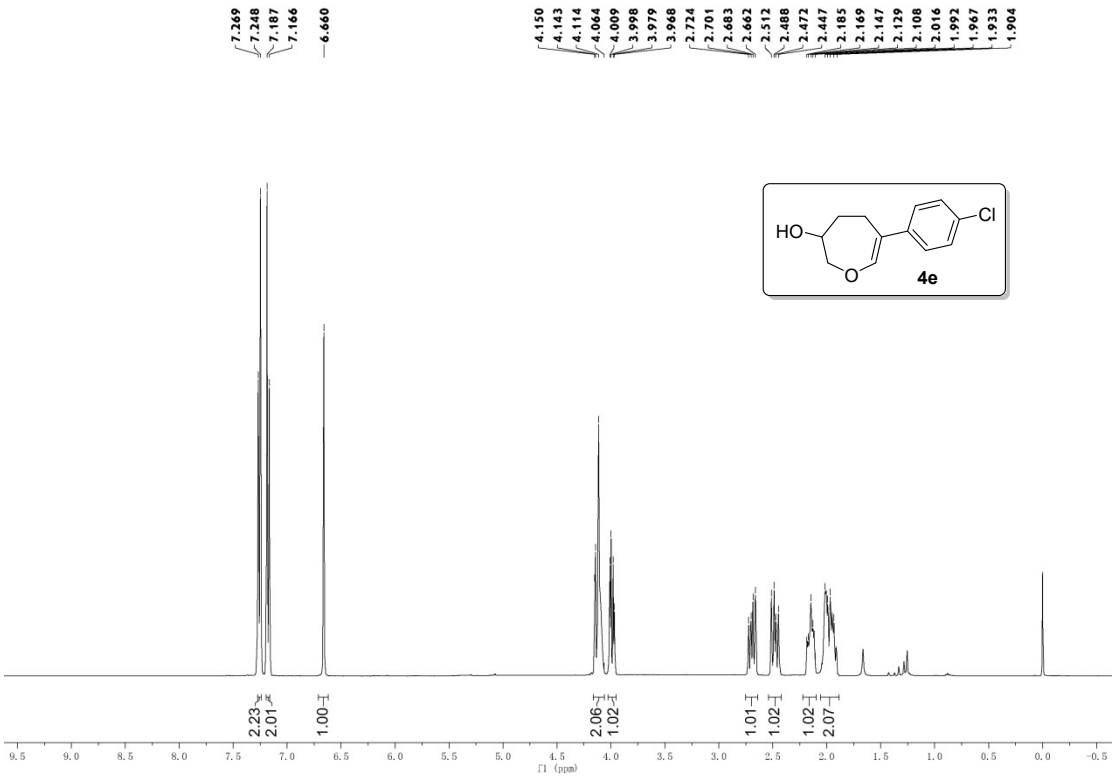

7.446
7.427
7.407
7.388
7.370
7.344
7.327
7.233
7.213
7.194
6.882
6.857
6.834
6.695
5.060
4.142
4.129
4.100
4.083
4.060
3.997
3.987
3.968
3.957
2.744
2.721
2.703
2.680
2.527
2.503
2.486
2.462
2.165
2.155
2.131
2.108
2.087
2.045
1.976
1.955
1.937
1.900
HO
O
OBn
4c
5.01
1.02
3.04
1.00
2.03
2.04
1.02
1.01
1.00
1.03
2.00
f1 (ppm)

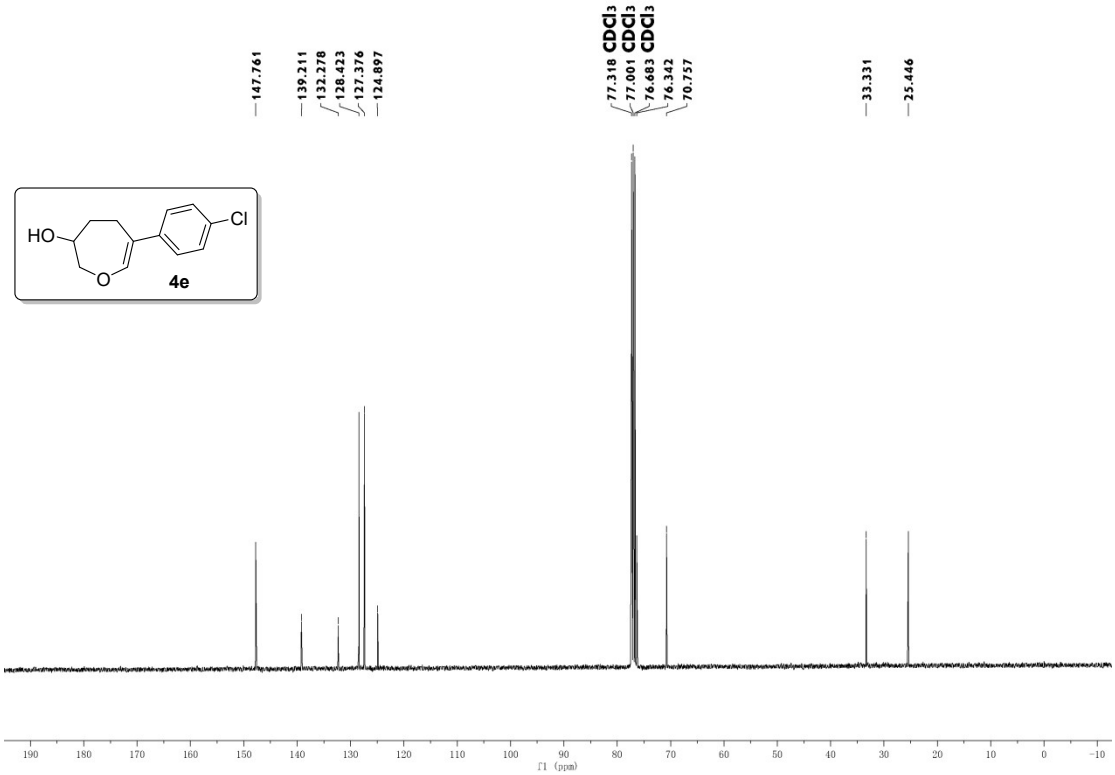

158.743
147.643
142.271
136.917
129.310
128.568
127.961
127.493
125.956
118.865
113.067
112.575
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
76.270
70.828
69.964
33.364
25.410
HO
O
OBn
4c
f1 (ppm)

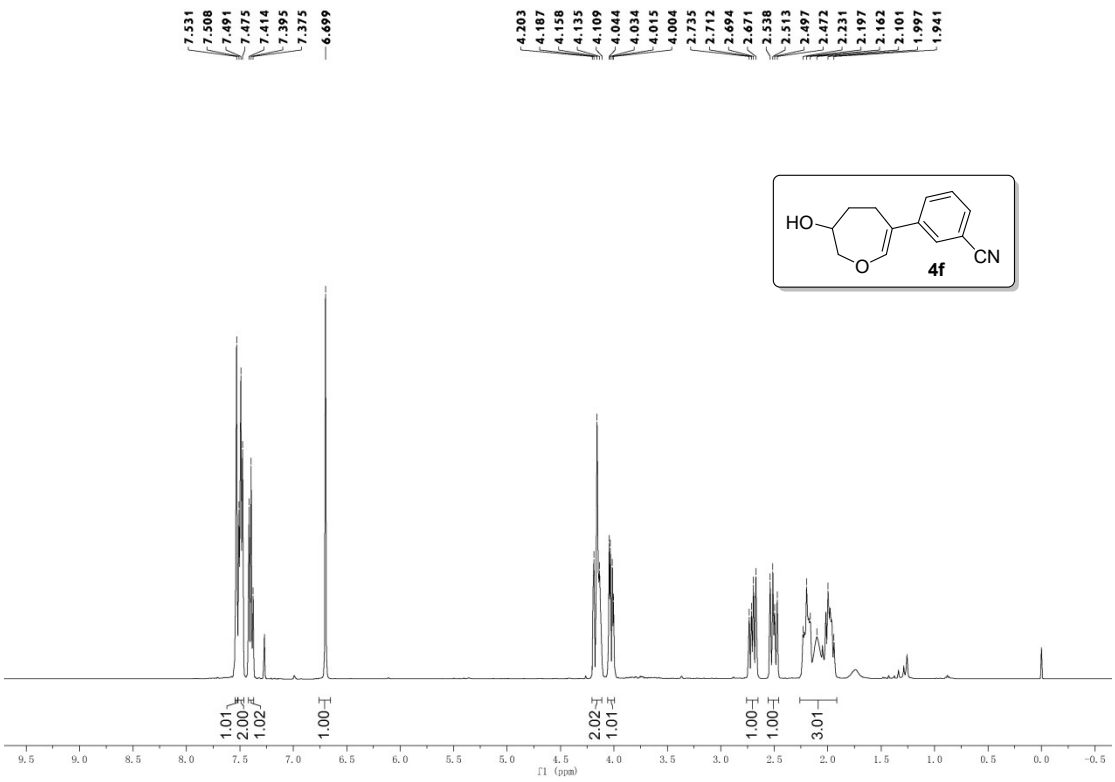

7.225
7.211
7.205
7.191
7.005
6.983
6.962
6.625
4.140
4.133
4.105
4.088
4.074
4.065
4.004
3.992
3.973
3.961
2.735
2.712
2.694
2.672
2.514
2.490
2.475
2.450
2.183
2.175
2.141
2.118
2.097
1.988
1.967
1.949
1.928
1.911
HO
O
F
4d
2.00
2.02
0.97
2.00
1.01
1.00
1.00
1.00
2.03
f1 (ppm)

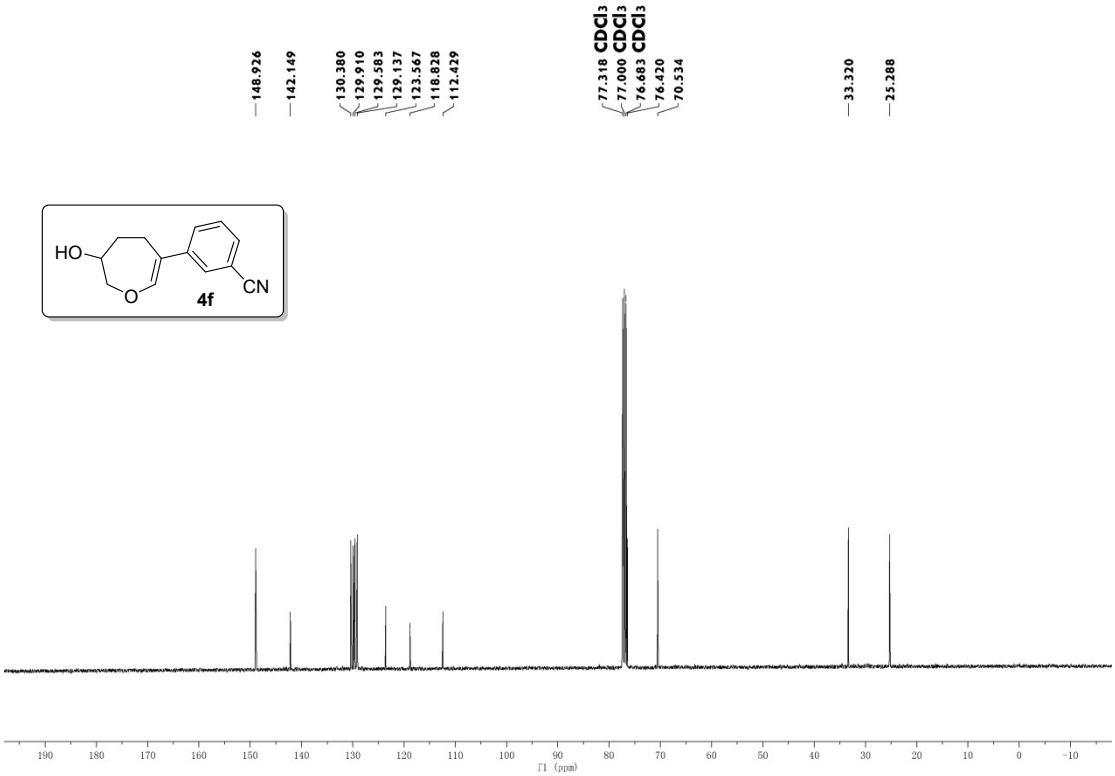

162.982
160.544
147.364
136.751
136.718
127.734
127.656
125.293
115.238
115.026
77.318 CDCl3
77.001 CDCl3
76.684 CDCl3
76.320
70.820
33.356
25.730
HO
F
O
4d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

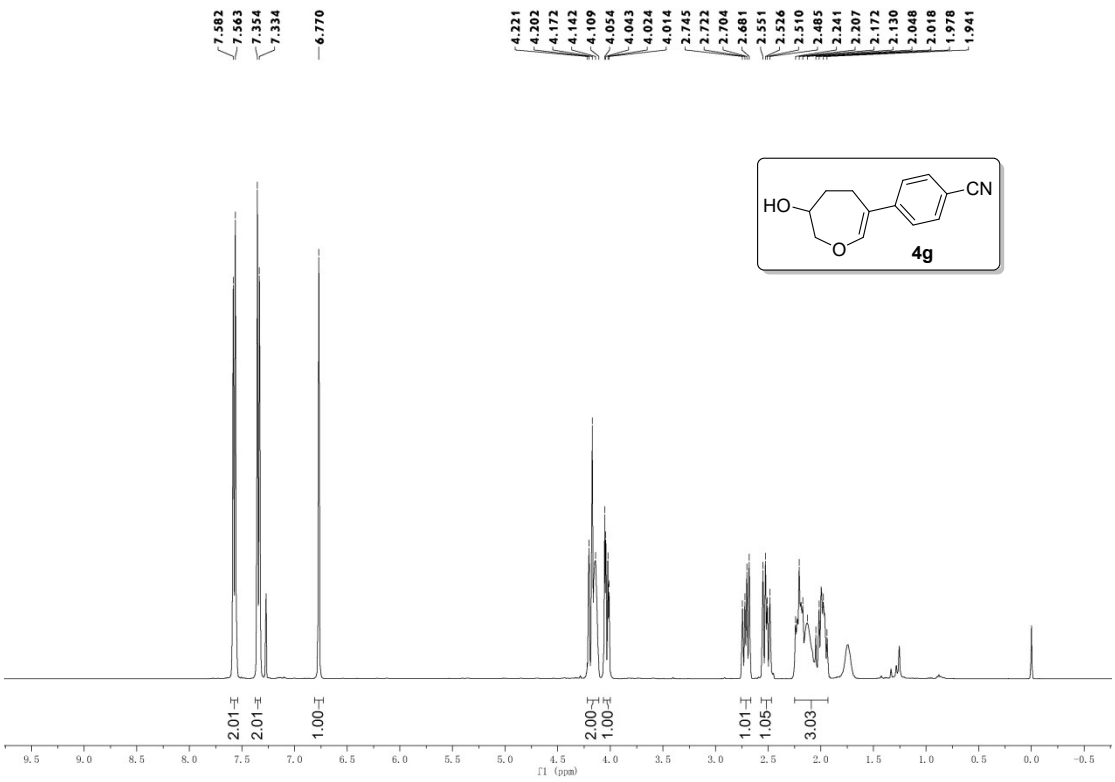

-116.361
HO
F
O
4d
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

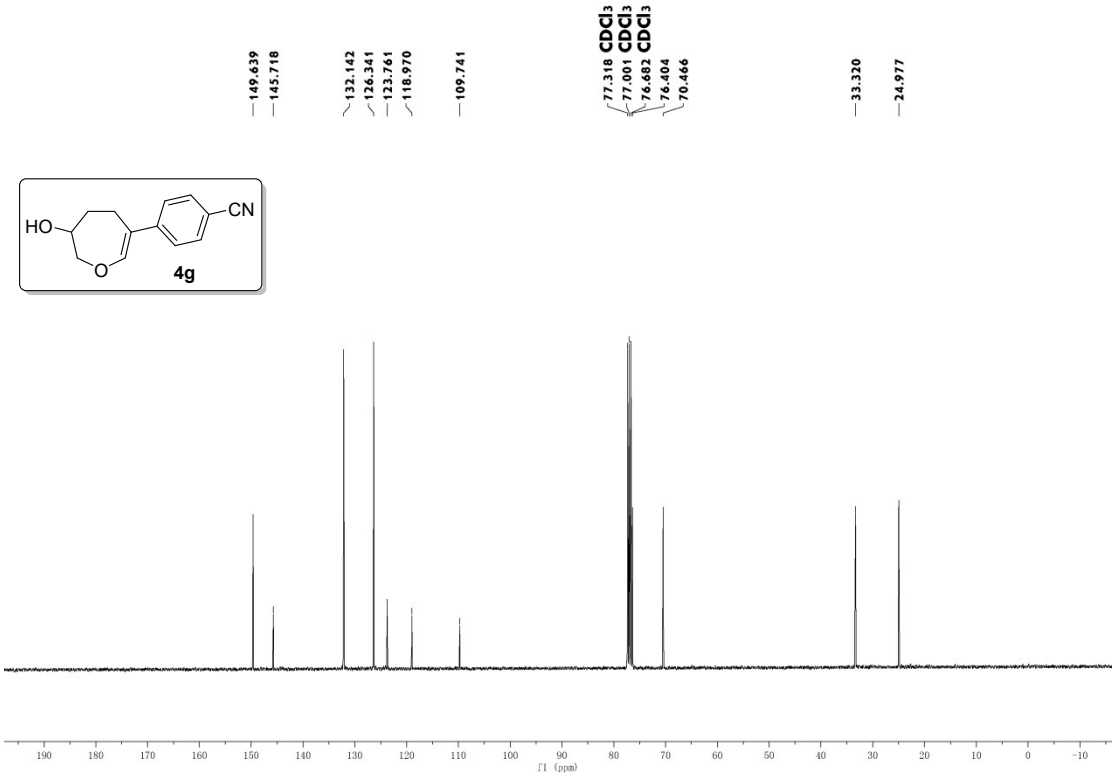

7.269
7.248
7.187
7.166
6.660
4.150
4.143
4.114
4.064
4.009
3.998
3.979
3.968
2.724
2.701
2.683
2.662
2.512
2.488
2.472
2.447
2.185
2.169
2.147
2.129
2.108
2.016
1.992
1.967
1.933
1.904
HO
Cl
O
4e
2.23
2.01
1.00
2.06
1.02
1.01
1.02
1.02
2.07
f1 (ppm)

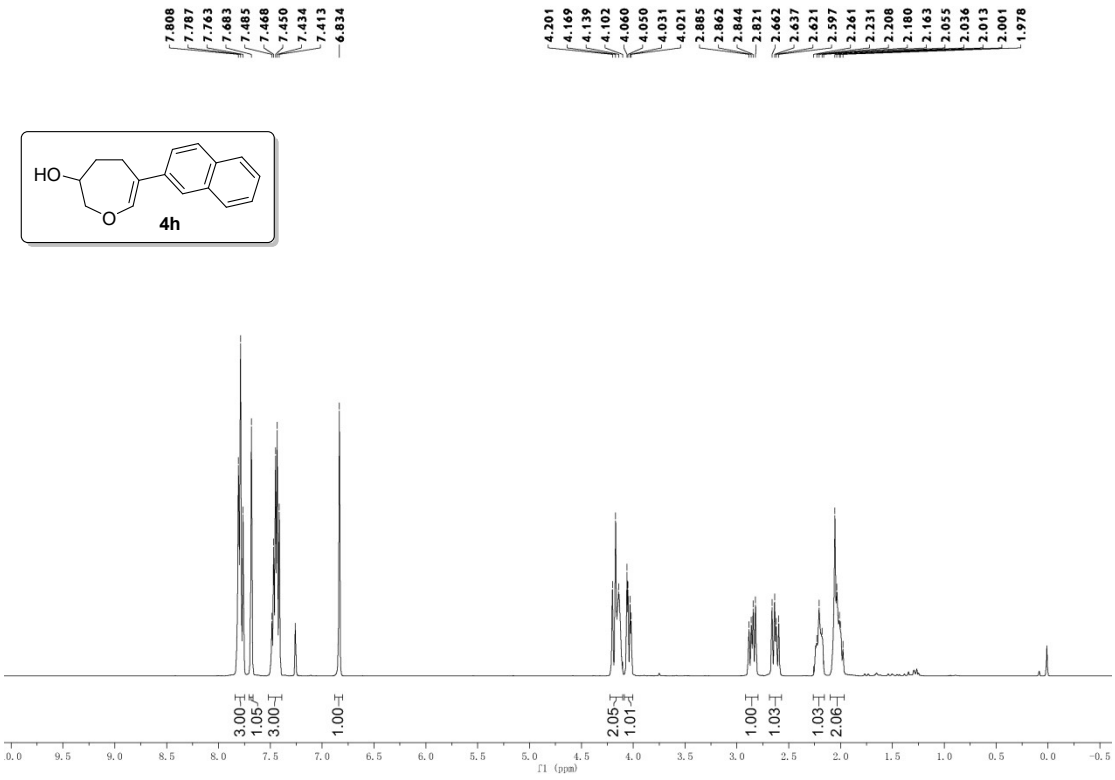

147.761
139.211
132.278
128.423
127.376
124.897
77.318 CDCl3
77.001 CDCl3
76.683 CDCl3
76.342
70.757
33.331
25.446
HO
Cl
O
4e
f1 (ppm)

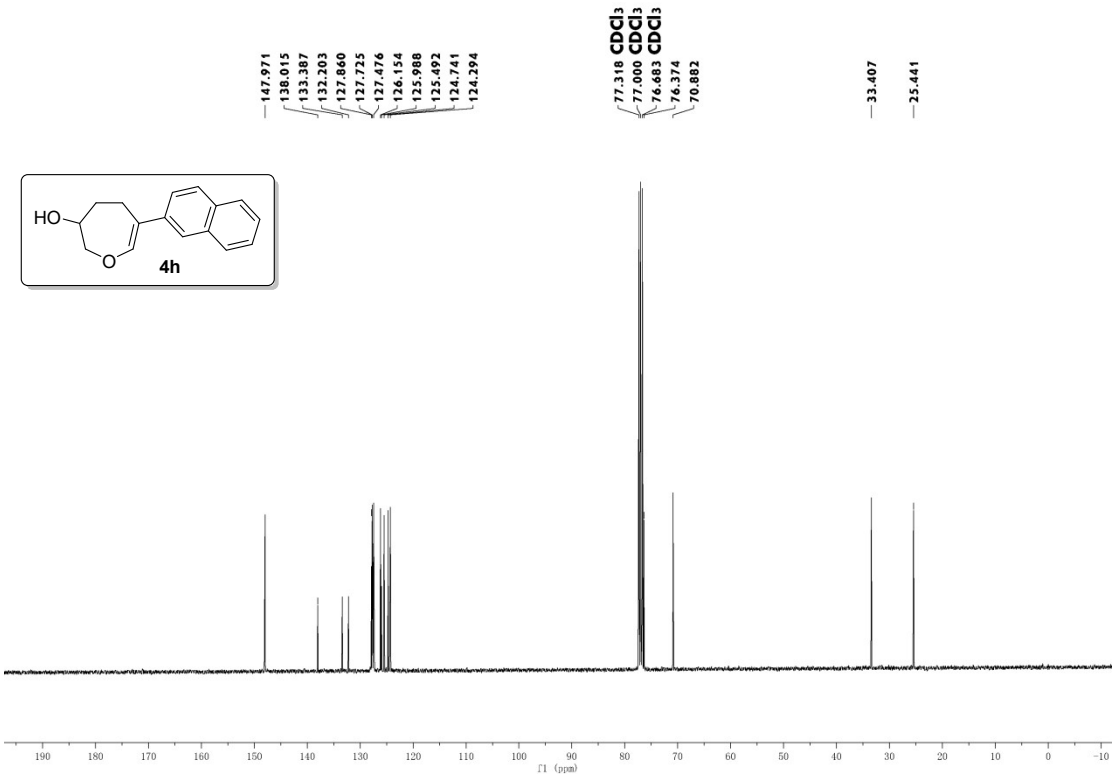

7.531
7.508
7.491
7.475
7.414
7.395
7.375
6.699
4.203
4.187
4.158
4.135
4.109
4.044
4.034
4.015
4.004
2.735
2.712
2.694
2.671
2.538
2.513
2.497
2.472
2.231
2.197
2.162
2.101
1.997
1.941
HO
O
CN
4f
1.01
2.00
1.02
1.00
2.02
1.01
1.00
1.00
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

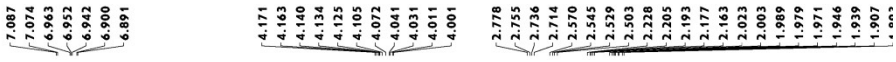

148.926
142.149
130.380
129.910
129.583
129.137
123.567
118.828
112.429
CDCl3
77.318
CDCl3
77.000
CDCl3
76.683
76.420
70.534
33.320
25.288
HO
O
CN
4f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

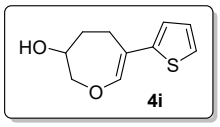

7.582
7.563
7.354
7.334
6.770
4.221
4.202
4.172
4.142
4.109
4.054
4.043
4.024
4.014
2.745
2.722
2.704
2.681
2.551
2.526
2.510
2.485
2.241
2.207
2.172
2.130
2.048
2.018
1.978
1.941
HO
CN
O
4g
2.01
2.01
1.00
2.00
1.00
1.01
1.05
3.03
f1 (ppm)

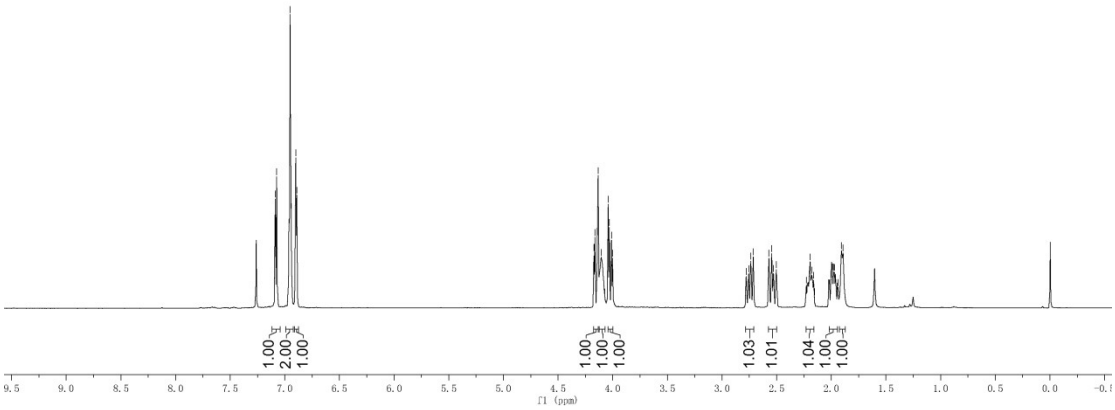

149.639
145.718
132.142
126.341
123.761
118.970
109.741
CDCl3
CDCl3
CDCl3
77.318
77.001
76.682
76.404
70.466
33.320
24.977
HO
CN
O
4g
f1 (ppm)

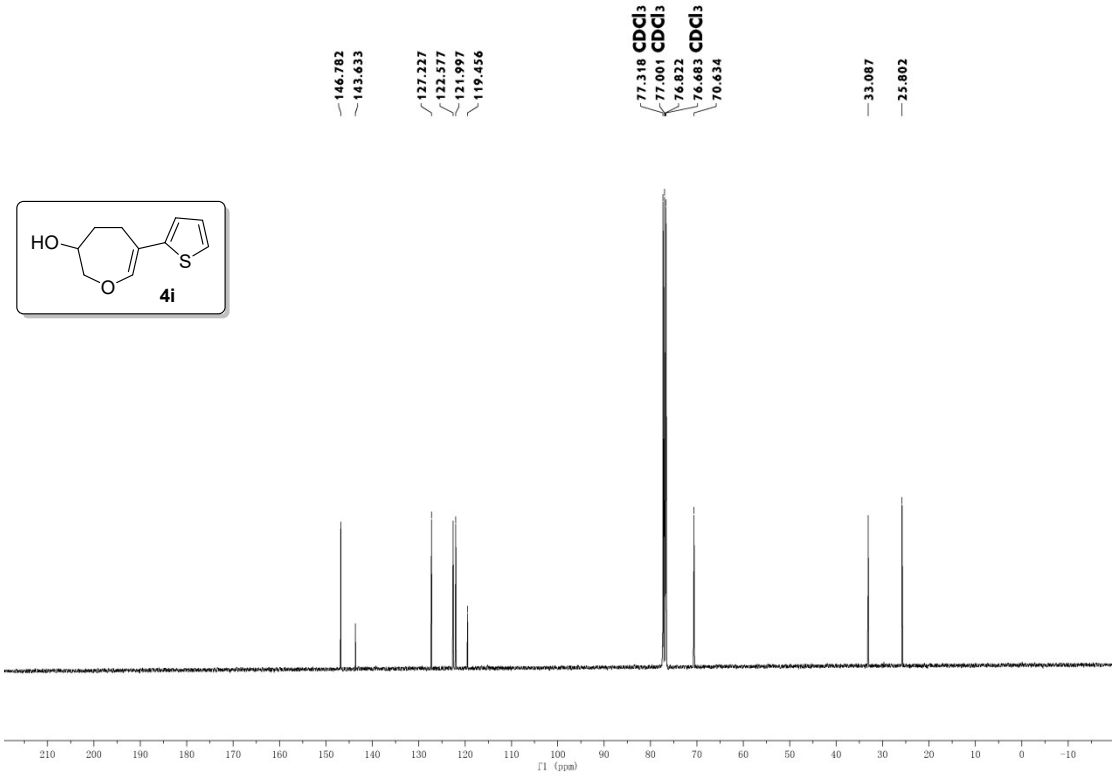

7.808
7.787
7.763
7.683
7.485
7.468
7.450
7.434
7.413
6.834
4.201
4.169
4.139
4.102
4.060
4.050
4.031
4.021
2.885
2.862
2.844
2.821
2.662
2.637
2.621
2.597
2.261
2.231
2.208
2.180
2.163
2.055
2.036
2.013
2.001
1.978
HO
O
4h
3.00
1.05
3.00
1.00
2.05
1.01
1.00
1.03
1.03
2.06
f1 (ppm)


147.971
138.015
133.387
132.203
127.860
127.725
127.476
126.154
125.988
125.492
124.741
124.294
CDCl3
CDCl3
CDCl3
77.318
77.000
76.683
76.374
70.882
33.407
25.441
HO
O
4h
f1 (ppm)

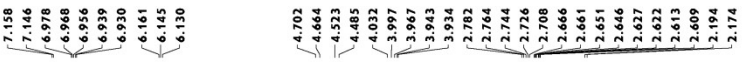

7.087
7.074
6.963
6.952
6.942
6.900
6.891
4.171
4.163
4.140
4.134
4.125
4.105
4.072
4.041
4.031
4.011
4.001
2.778
2.755
2.736
2.714
2.570
2.545
2.529
2.503
2.228
2.205
2.193
2.177
2.163
2.023
2.003
1.989
1.979
1.971
1.946
1.939
1.907

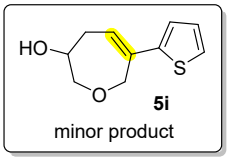

HO
S
O
4i


1.00
2.00
1.00
1.00
1.00
1.00
1.03
1.01
1.04
1.00
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

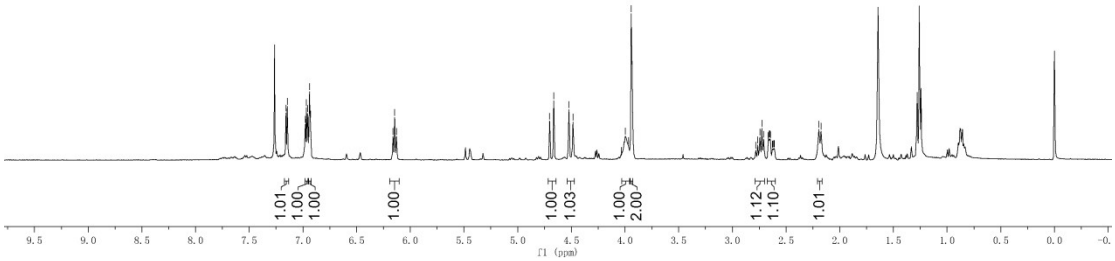

146.782
143.633
127.227
122.577
121.997
119.456
77.318 CDCl3
77.001 CDCl3
76.822
76.683 CDCl3
70.634
33.087
25.802
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

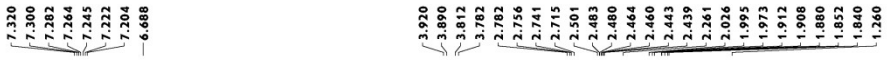
HO
S
O
4i

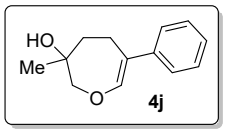




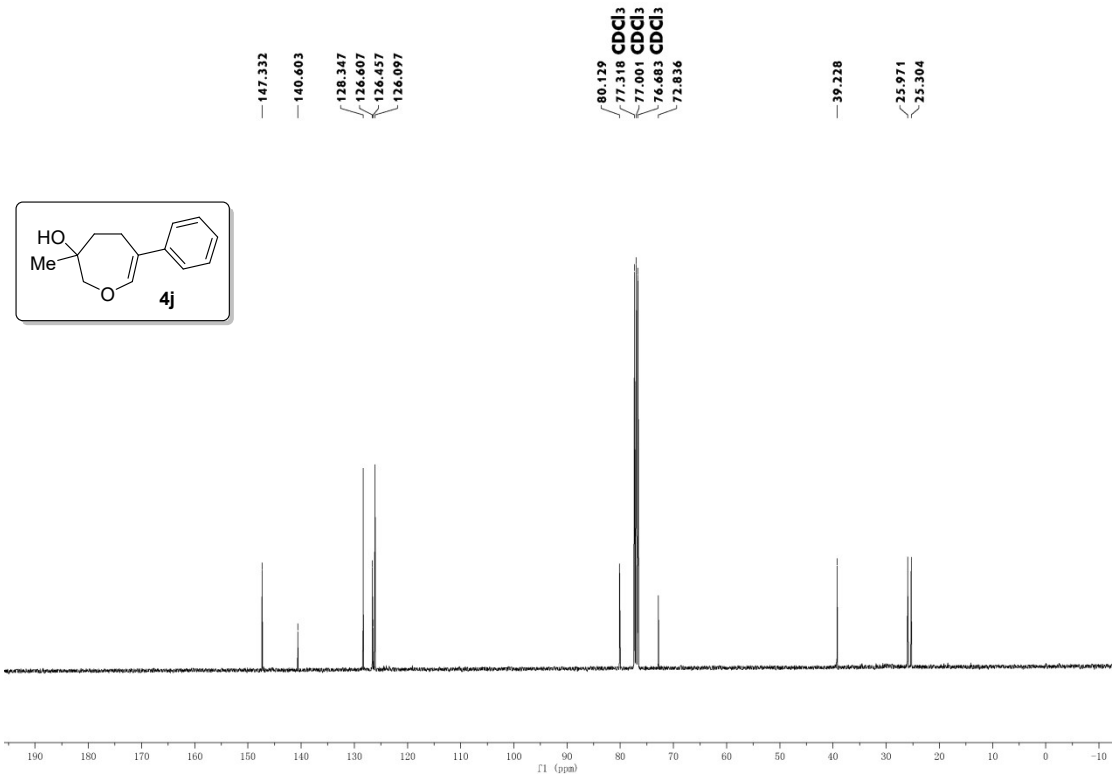
5i
minor product



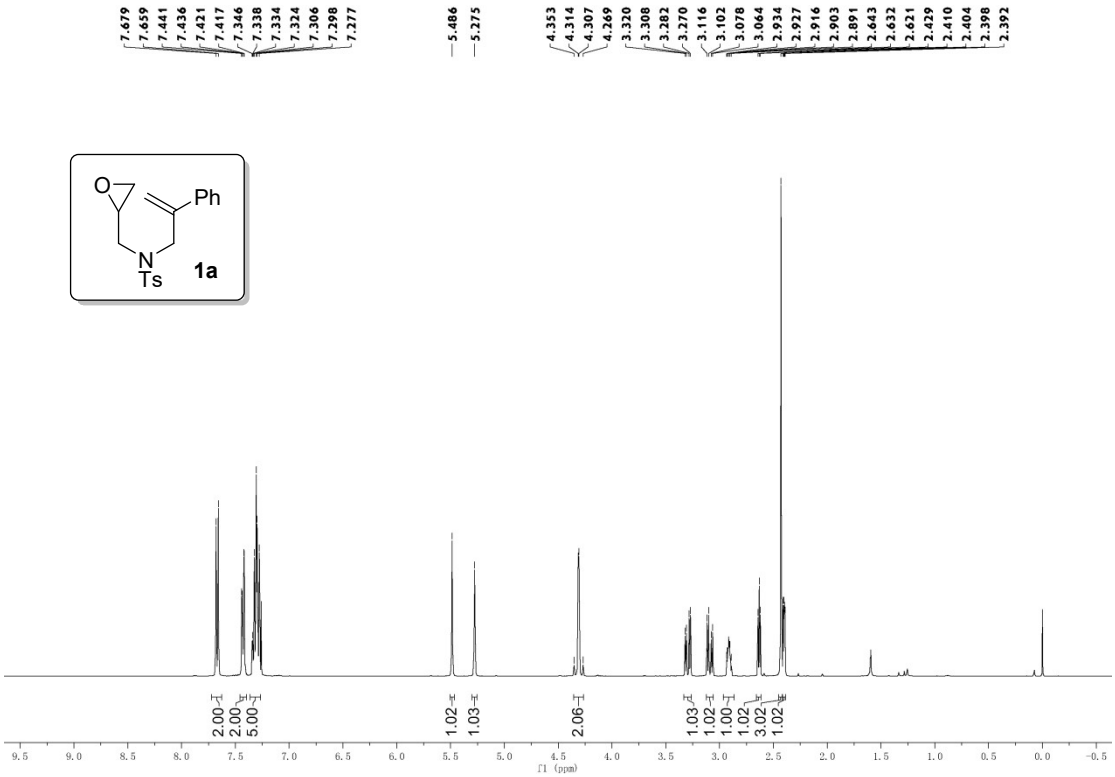


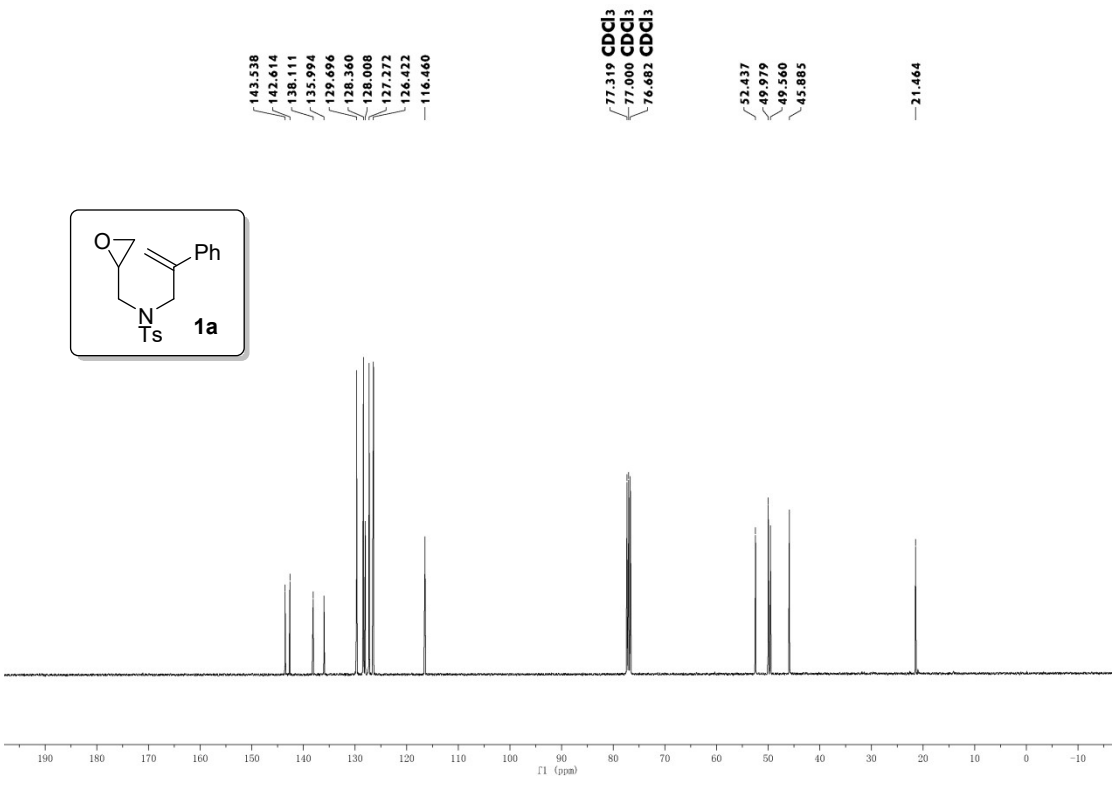


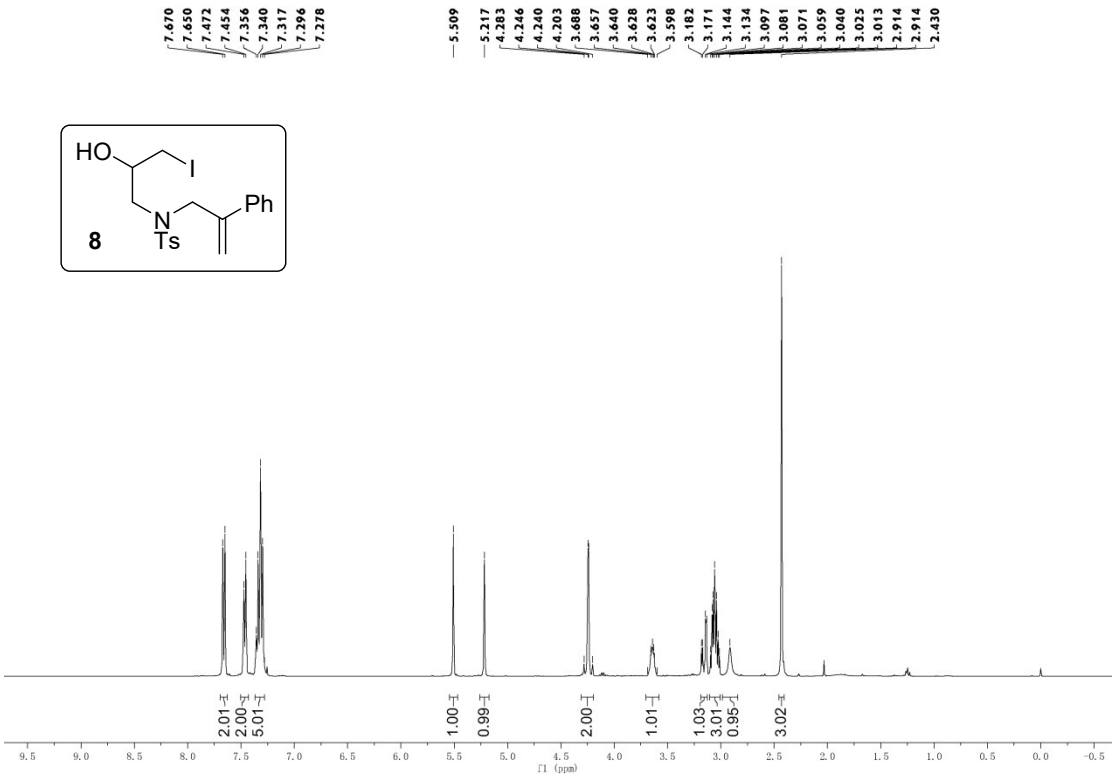
4j

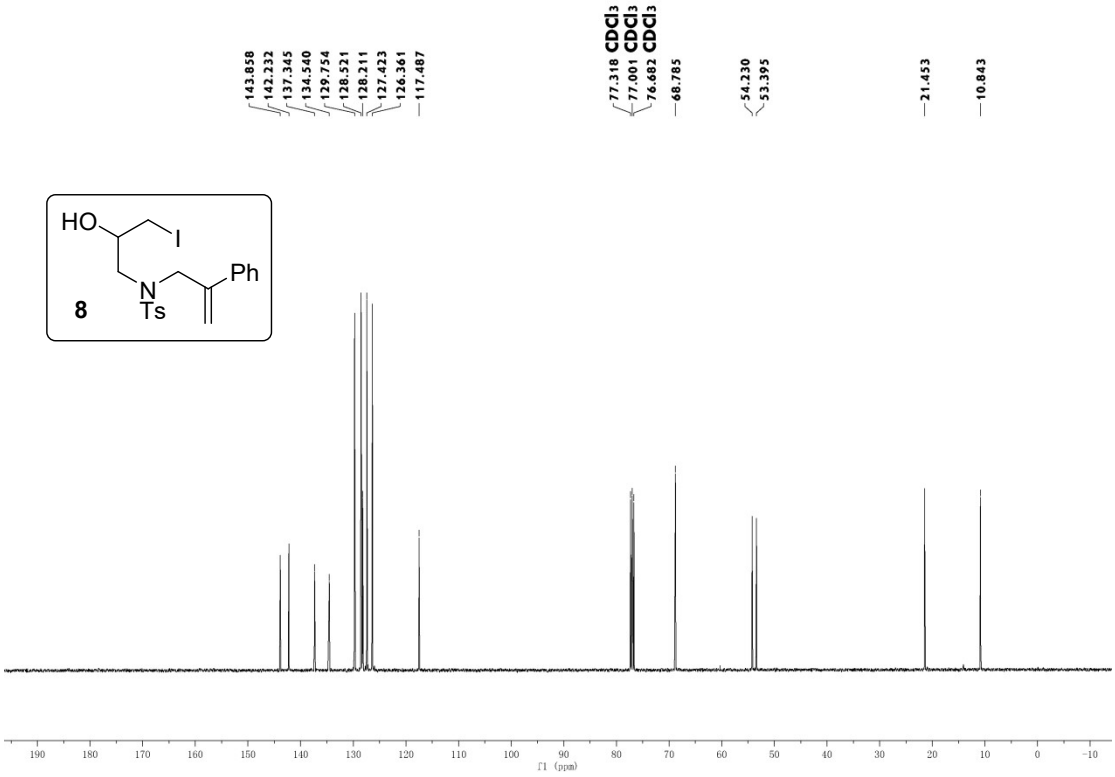

147.332
140.603
128.347
126.607
126.457
126.097
80.129
77.318 CDCl3
77.001 CDCl3
76.683 CDCl3
72.836
39.228
25.971
25.304
HO
Me
O
4j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

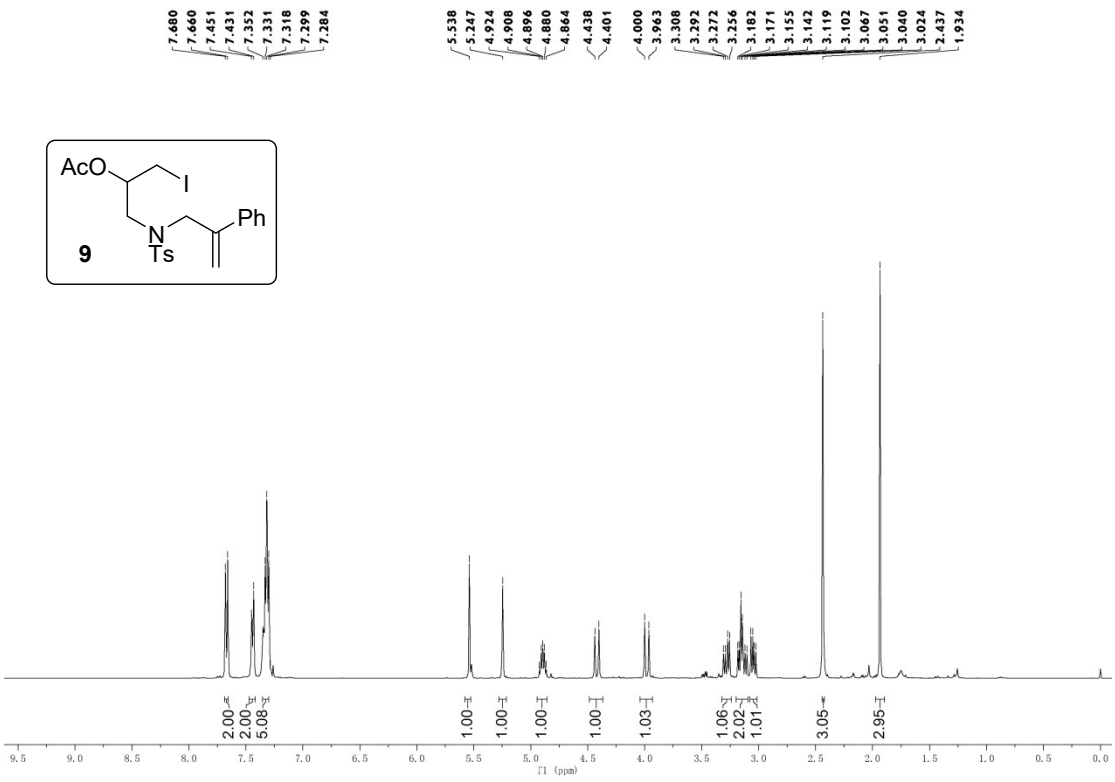
14. Copies of the NMR Spectra for Partial Materials

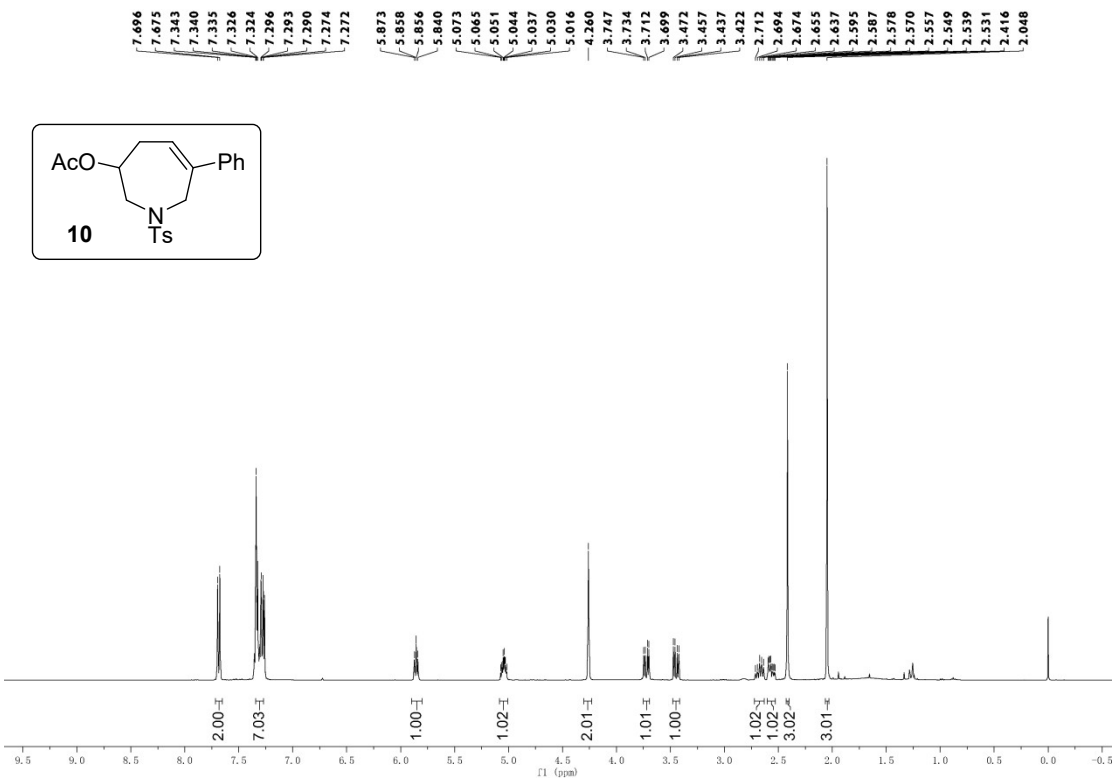


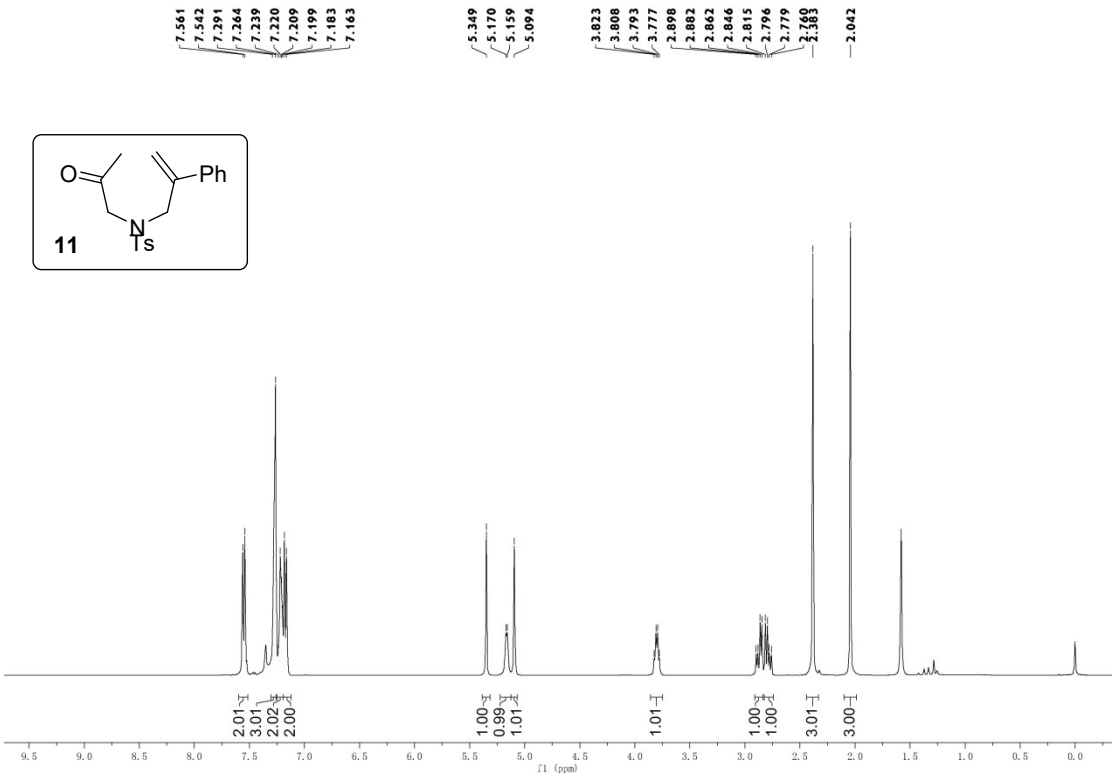


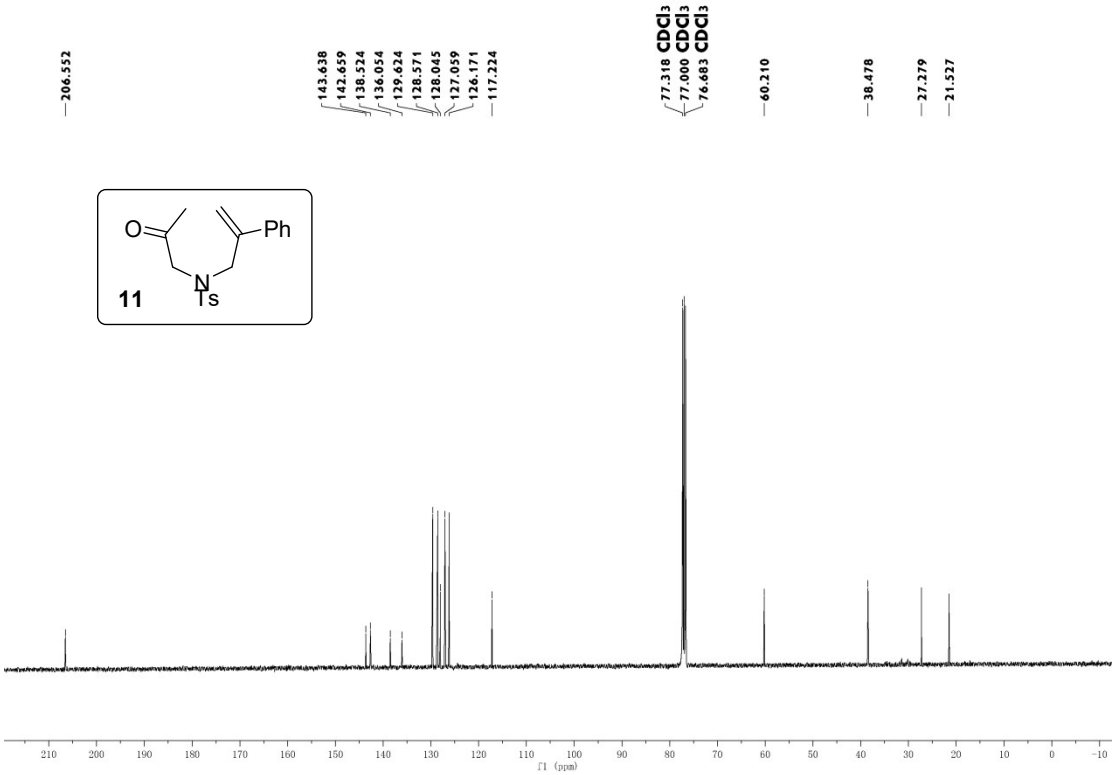

7.670
7.650
7.472
7.454
7.356
7.340
7.317
7.296
7.278
5.509
5.217
4.283
4.246
4.240
4.203
3.688
3.657
3.640
3.628
3.623
3.598
3.182
3.171
3.144
3.134
3.097
3.081
3.071
3.059
3.040
3.025
3.013
2.914
2.914
2.430
HO
I
Ph
N
Ts
8
2.01
2.00
5.01
1.00
0.99
2.00
1.01
1.03
3.01
0.95
3.02
f1 (ppm)

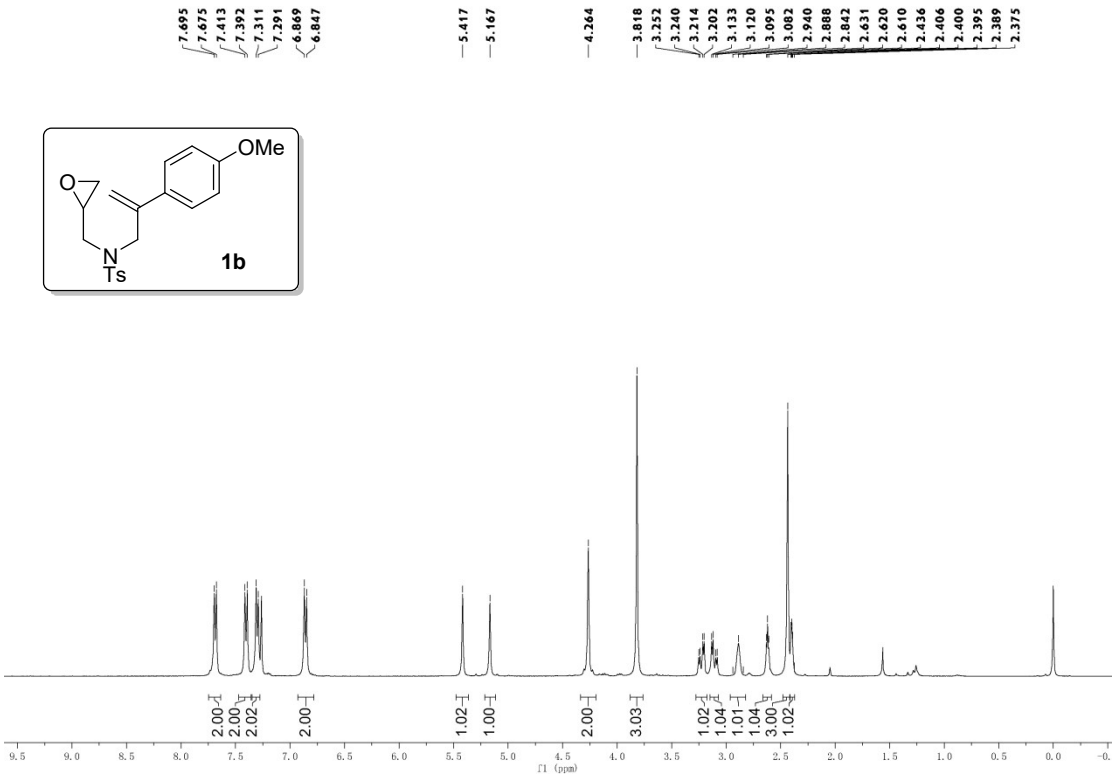

143.858
142.232
137.345
134.540
129.754
128.521
128.211
127.423
126.361
117.487
77.318 CDCl3
77.001 CDCl3
76.682 CDCl3
68.785
54.230
53.395
21.453
10.843
HO
I
Ph
N
Ts
8
f1 (ppm)

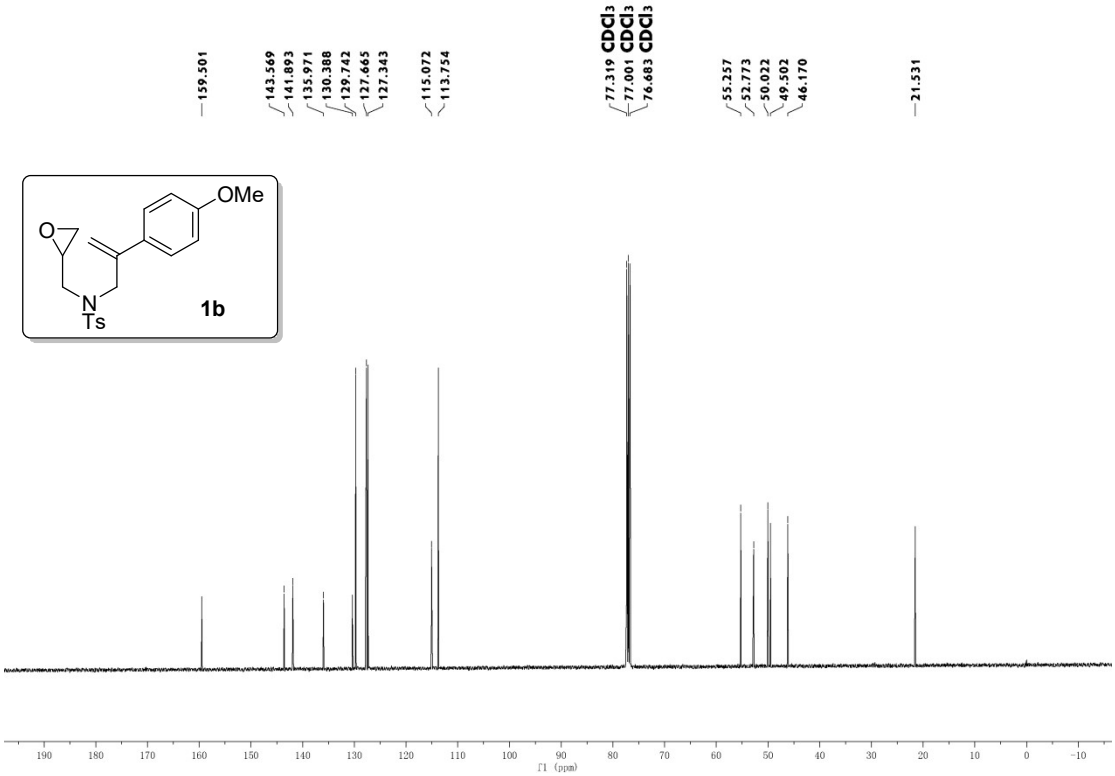

7.680
7.660
7.451
7.431
7.352
7.331
7.318
7.299
7.284
5.538
5.247
4.924
4.908
4.896
4.880
4.864
4.438
4.401
4.000
3.963
3.308
3.292
3.272
3.256
3.182
3.171
3.155
3.142
3.119
3.102
3.067
3.051
3.040
3.024
2.437
1.934
AcO
I
Ph
N
Ts
9
2.00
2.00
5.08
1.00
1.00
1.00
1.00
1.03
1.06
2.02
1.01
3.05
2.95
f1 (ppm)

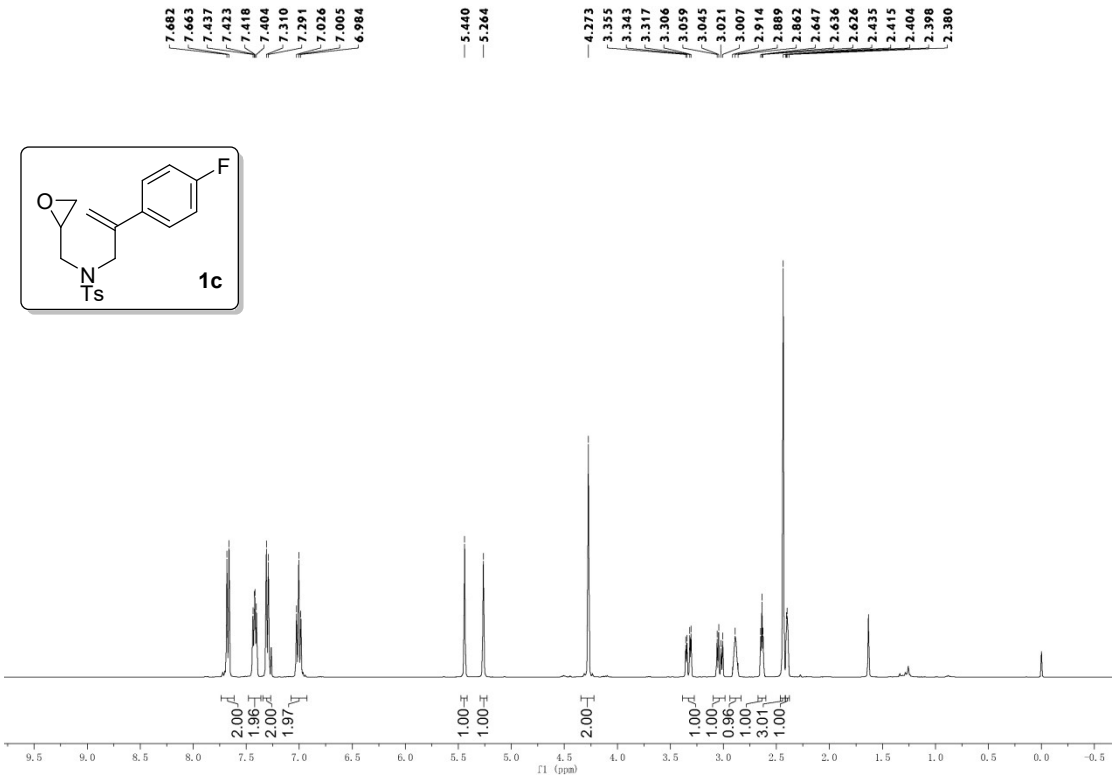

7.696
7.675
7.343
7.340
7.335
7.326
7.324
7.296
7.293
7.290
7.274
7.272
5.873
5.858
5.856
5.840
5.073
5.065
5.051
5.044
5.037
5.030
5.016
4.260
3.747
3.734
3.712
3.699
3.472
3.457
3.437
3.422
2.712
2.694
2.674
2.655
2.637
2.595
2.587
2.578
2.570
2.557
2.549
2.539
2.531
2.416
2.048
AcO
Ph
N
Ts
10
2.00
7.03
1.00
1.02
2.01
1.01
1.00
1.02
1.02
3.02
3.01
f1 (ppm)

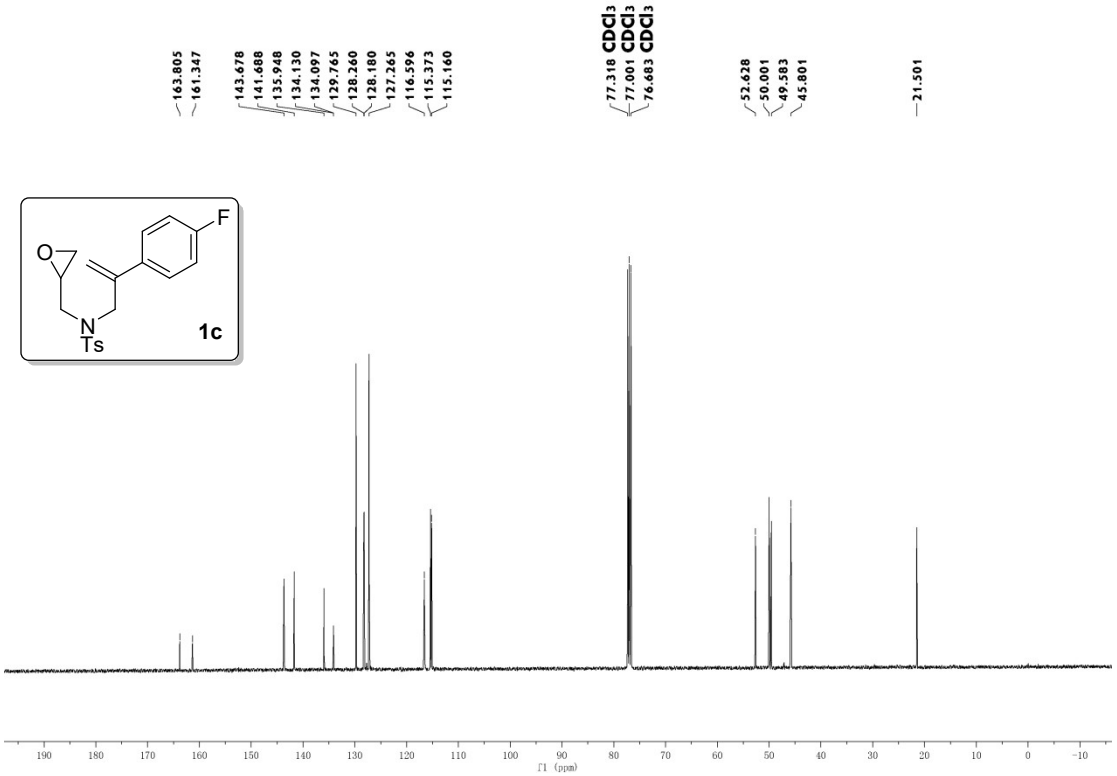

7.561
7.542
7.291
7.264
7.239
7.220
7.209
7.199
7.183
7.163
5.349
5.170
5.159
5.094
3.823
3.808
3.793
3.777
2.898
2.882
2.862
2.846
2.815
2.796
2.779
2.760
2.383
2.042
O
Ph
N
Ts
11
2.01
3.01
2.02
2.00
1.00
0.99
1.01
1.01
1.00
1.00
3.01
3.00
f1 (ppm)


206.552
143.638
142.659
138.524
136.054
129.624
128.571
128.045
127.059
126.171
117.224
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
60.210
38.478
27.279
21.527
O
Ph
N
Ts
11
f1 (ppm)


7.695
7.675
7.413
7.392
7.311
7.291
6.869
6.847
5.417
5.167
4.264
3.818
3.252
3.240
3.214
3.202
3.133
3.120
3.095
3.082
2.940
2.888
2.842
2.631
2.620
2.610
2.436
2.406
2.400
2.395
2.389
2.375
OMe
O
N
Ts
1b
2.00
2.00
2.02
2.00
1.02
1.00
2.00
3.03
1.02
1.04
1.01
1.04
3.00
1.02
f1 (ppm)


159.501
143.569
141.893
135.971
130.388
129.742
127.665
127.343
115.072
113.754
77.319 CDCl3
77.001 CDCl3
76.683 CDCl3
55.257
52.773
50.022
49.502
46.170
21.531
OMe
O
N
Ts
1b
f1 (ppm)


7.682
7.663
7.437
7.423
7.418
7.404
7.310
7.291
7.026
7.005
6.984
5.440
5.264
4.273
3.355
3.343
3.317
3.306
3.059
3.045
3.021
3.007
2.914
2.889
2.862
2.647
2.636
2.626
2.435
2.415
2.404
2.398
2.380
F
O
N
Ts
1c
2.00
1.96
2.00
1.97
1.00
1.00
2.00
1.00
1.00
0.96
1.00
3.01
1.00
f1 (ppm)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161.347
143.678
141.688
135.948
134.130
134.097
129.765
128.260
128.180
127.265
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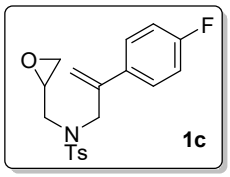
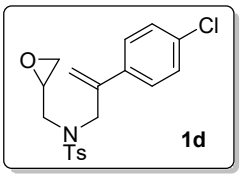
115.373
115.160
77.318 CDCl3
77.001 CDCl3
76.683 CDCl3
52.628
50.001
49.583
45.801
21.501
F
O
N
Ts
1c
f1 (ppm)


F
O
N
Ts

1c

-113.929
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


Cl
O
N
Ts

1d

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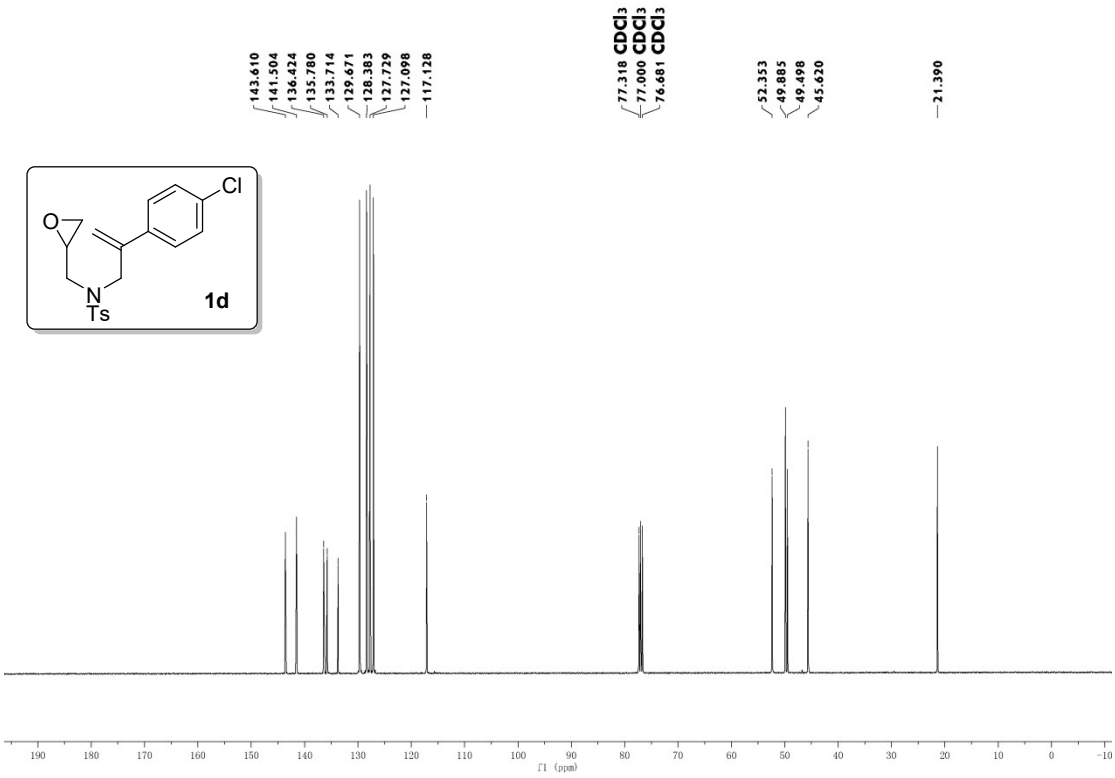
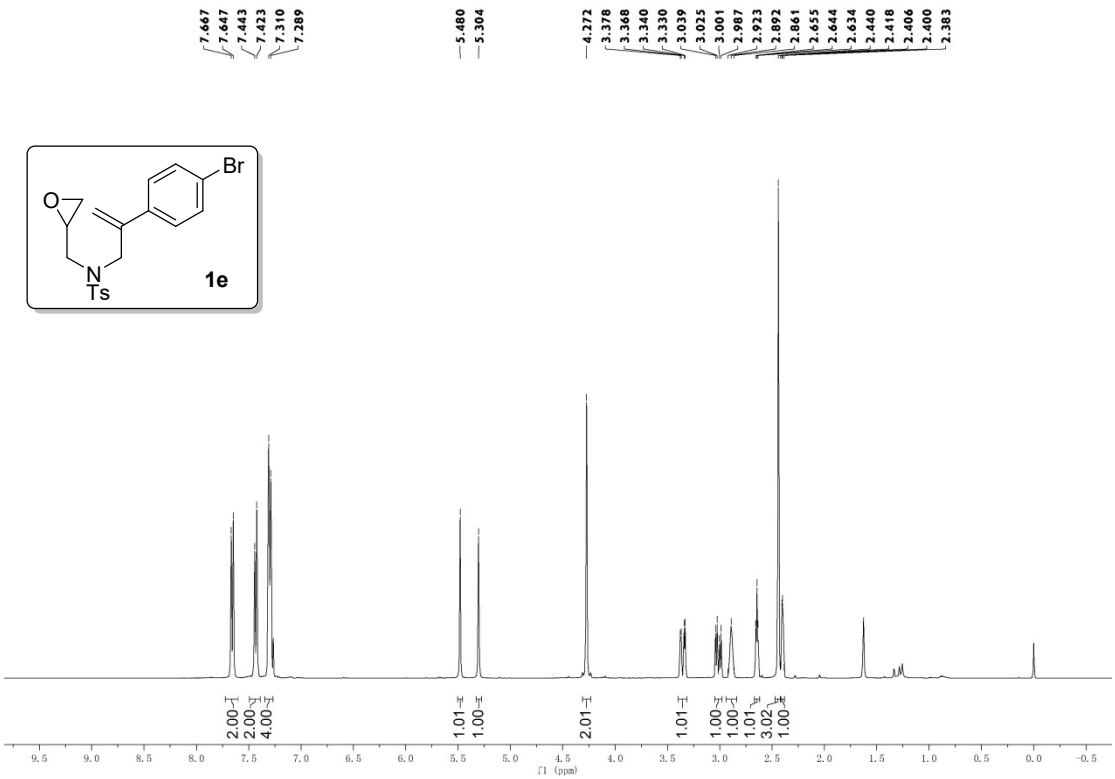
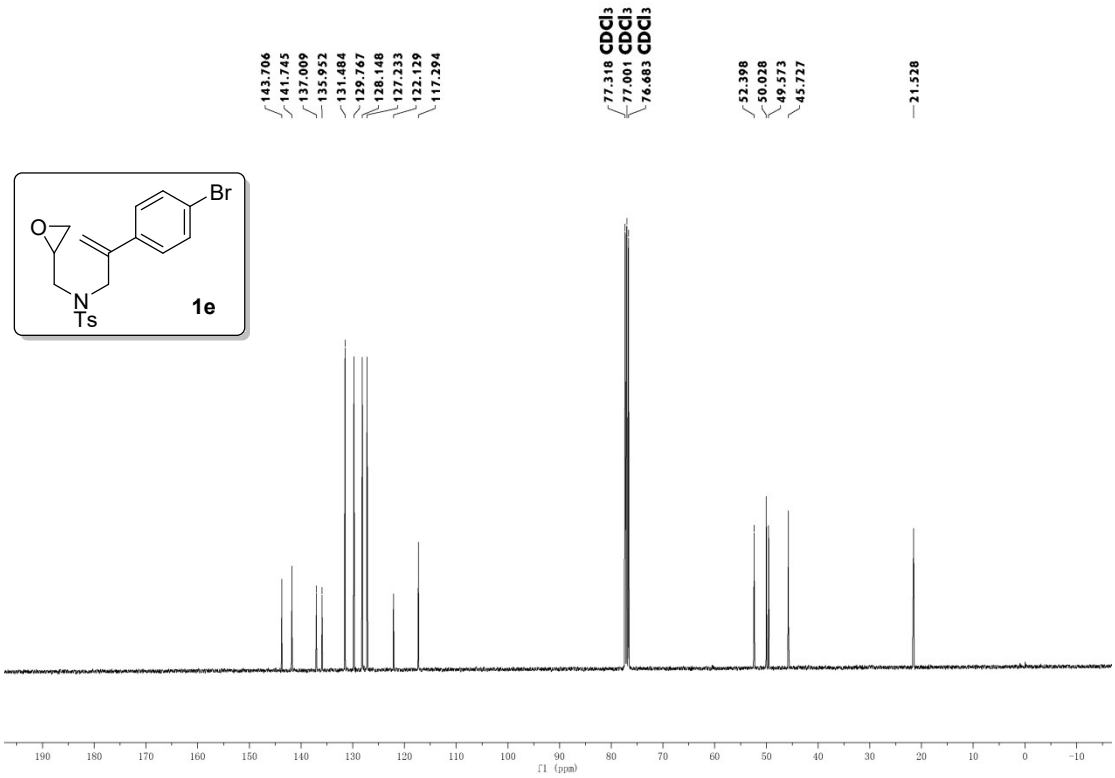
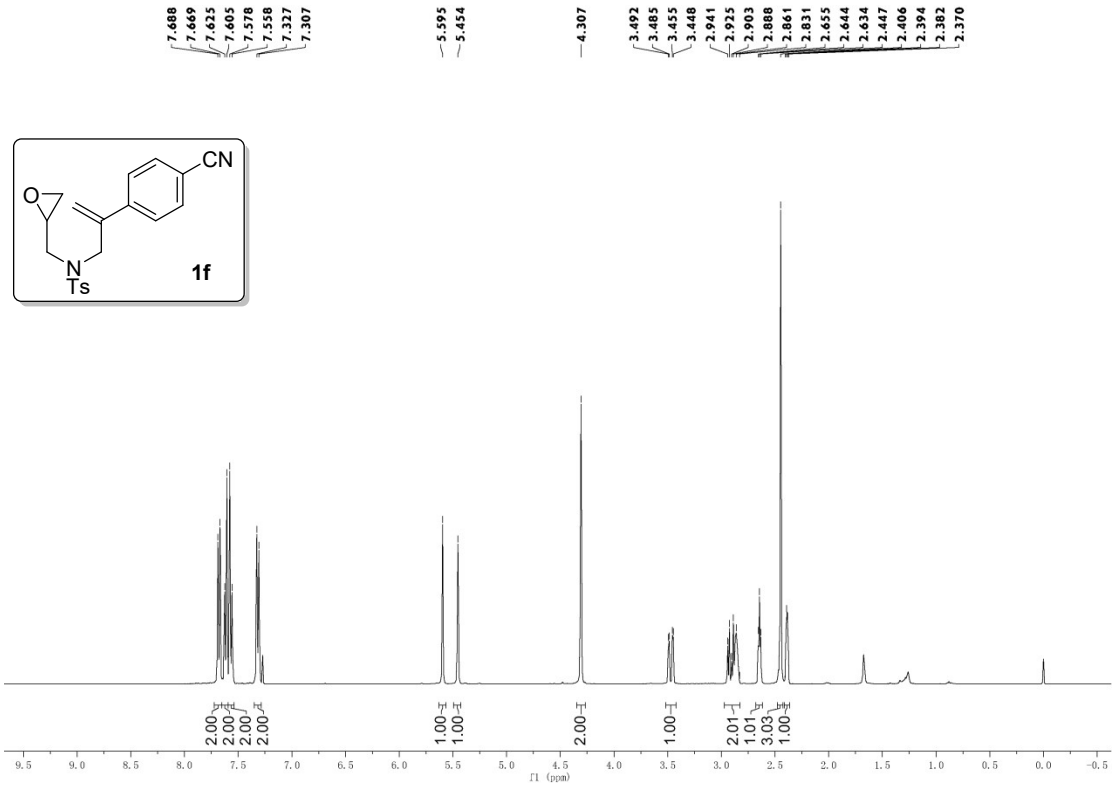
7.293
7.272
7.207
7.184
7.162
5.380
5.205
4.176
3.272
3.261
3.234
3.223
2.953
2.939
2.915
2.901
2.804
2.794
2.788
2.784
2.779
2.774
2.763
2.542
2.531
2.520
2.330
2.306
2.299
2.294
2.288
2.00
2.02
4.01
1.00
1.00
2.01
1.00
1.00
1.00
1.01
3.00
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


143.610
141.504
136.424
135.780
133.714
129.671
128.383
127.729
127.098
117.128
77.318 CDCl3
77.000 CDCl3
76.681 CDCl3
52.353
49.885
49.498
45.620
21.390
Cl
O
N
Ts
1d
f1 (ppm)


7.667
7.647
7.443
7.423
7.310
7.289
5.480
5.304
4.272
3.378
3.368
3.340
3.330
3.039
3.025
3.001
2.987
2.923
2.892
2.861
2.655
2.644
2.634
2.440
2.418
2.406
2.400
2.383
Br
O
N
Ts
1e
2.00
2.00
4.00
1.01
1.00
2.01
1.01
1.00
1.00
1.01
3.02
1.00
f1 (ppm)


143.706
141.745
137.009
135.952
131.484
129.767
128.148
127.233
122.129
117.294
77.318 CDCl3
77.001 CDCl3
76.683 CDCl3
52.398
50.028
49.573
45.727
21.528
Br
O
N
Ts
1e
f1 (ppm)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3.448
2.941
2.925
2.903
2.888
2.861
2.831
2.655
2.644
2.634
2.447
2.406
2.394
2.382
2.370
CN
O
N
Ts
1f
2.00
2.00
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1.00
2.00
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1.01
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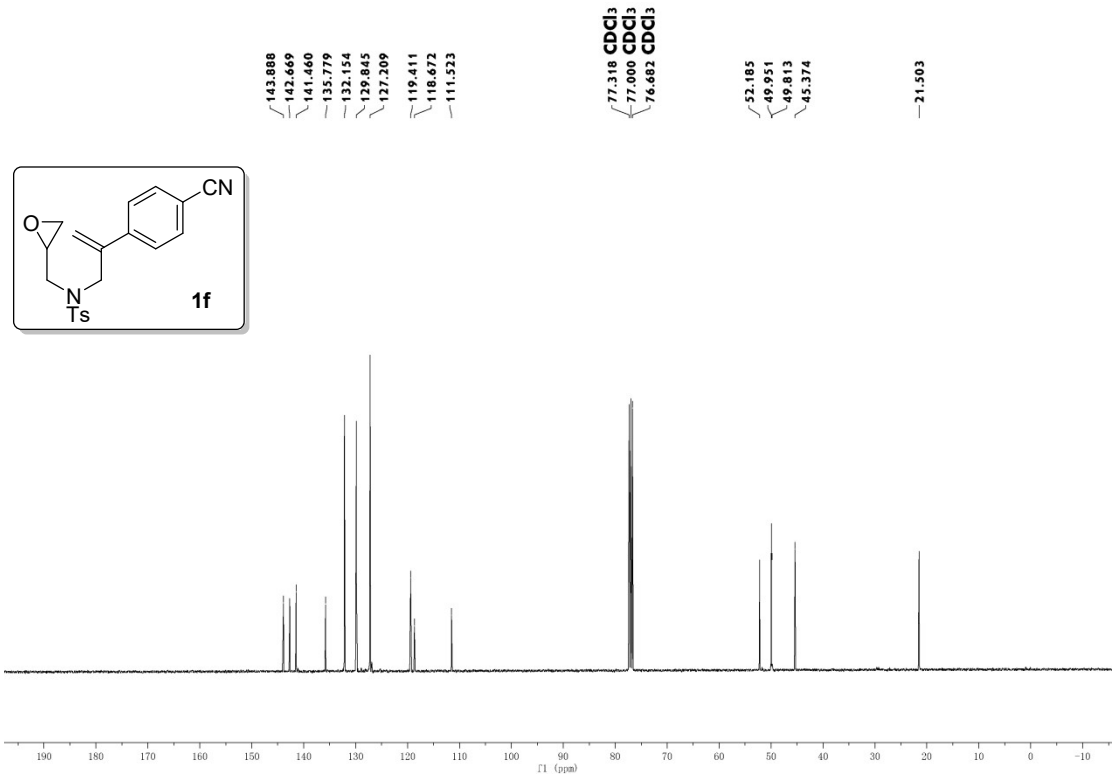
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77.000 CDCl3
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49.951
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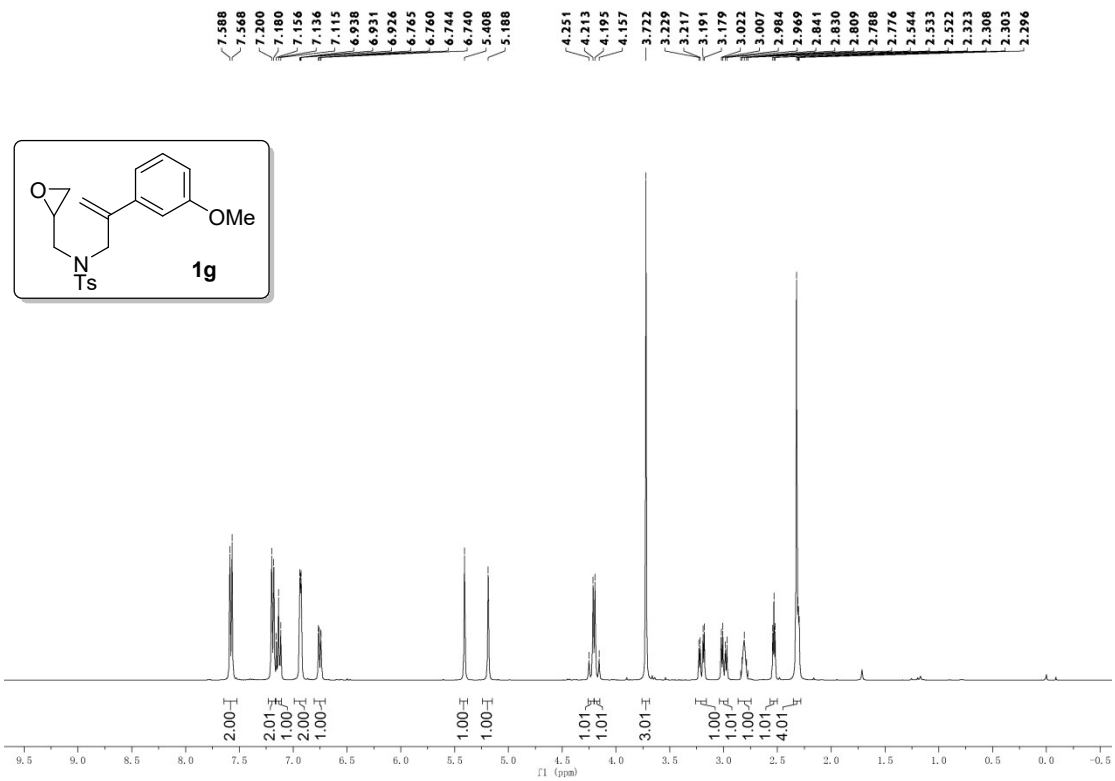
CN
O
N
Ts
1f
f1 (ppm)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6.740
5.408
5.188
4.251
4.213
4.195
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3.229
3.217
3.191
3.179
3.022
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2.522
2.323
2.308
2.303
2.296
OMe
O
N
Ts
1g
2.00
2.01
1.00
2.00
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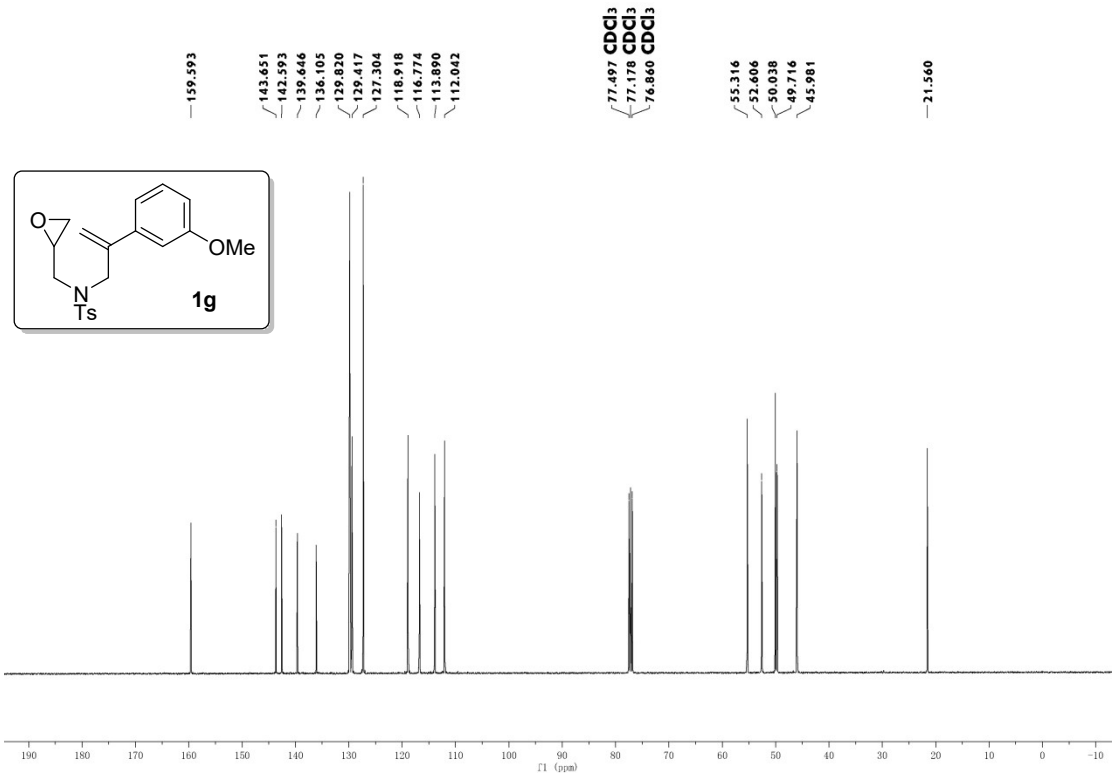
f1 (ppm)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127.304
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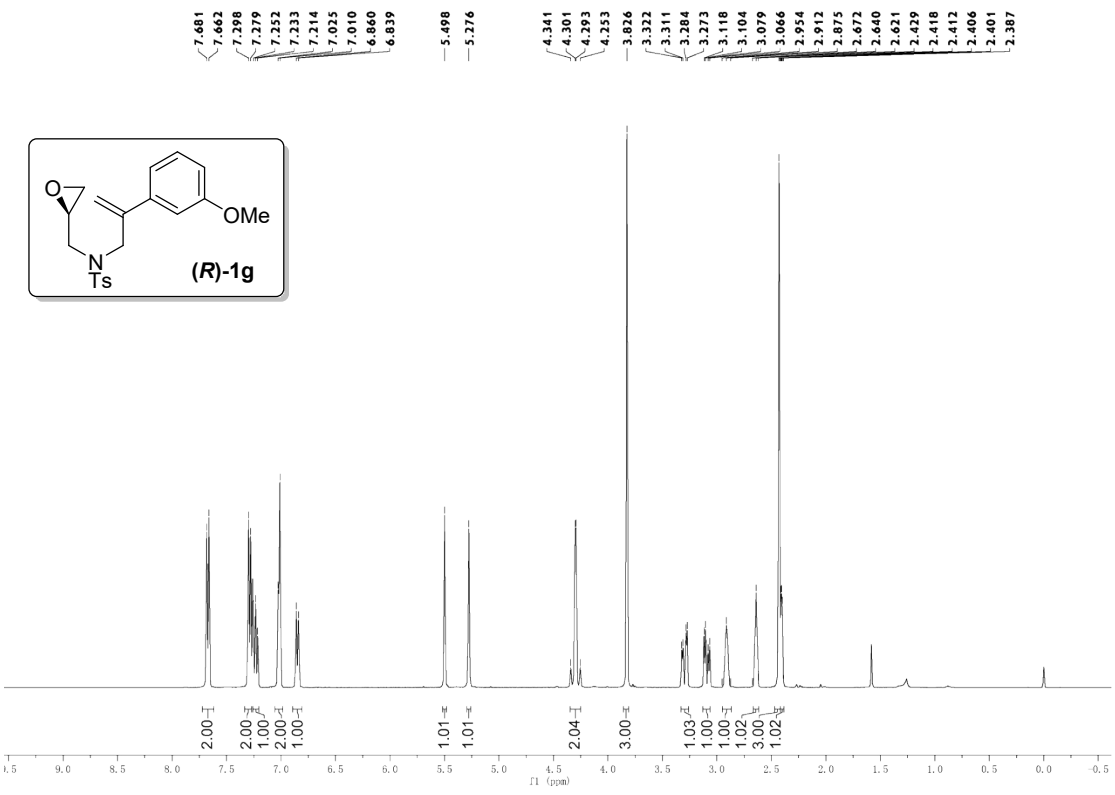
21.560
O
OMe
N
Ts
1g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5.276
4.341
4.301
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3.284
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3.079
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2.954
2.912
2.875
2.672
2.640
2.621
2.429
2.418
2.412
2.406
2.401
2.387
O
OMe
N
Ts
(R)-1g
2.00
2.00
1.00
2.00
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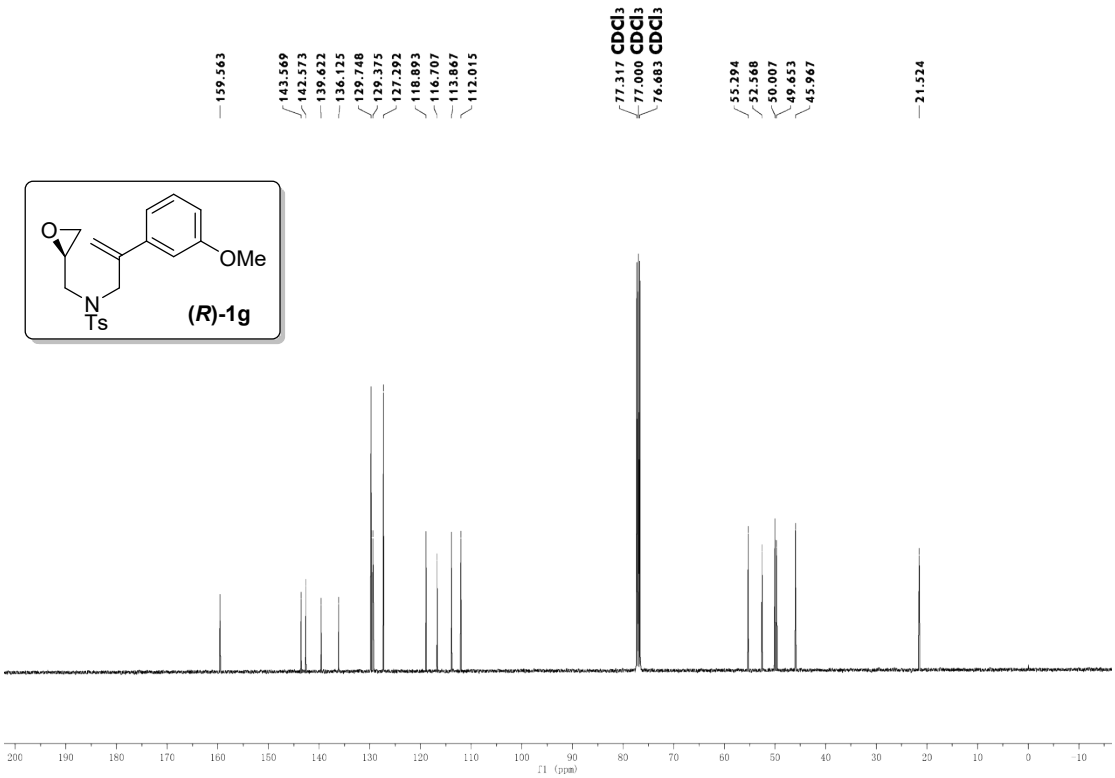
1.01
2.04
3.00
1.03
1.00
1.00
1.02
3.00
1.02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77.000 CDCl3
76.683 CDCl3
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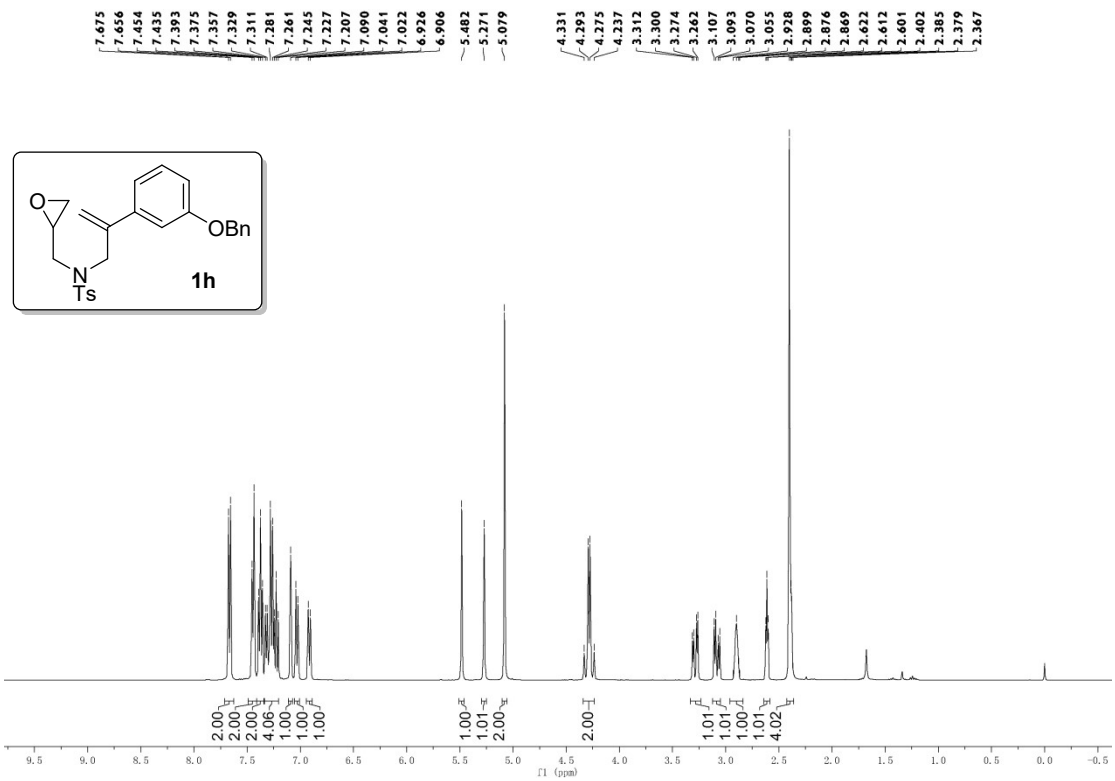
45.967
21.524
O
OMe
N
Ts
(R)-1g
f1 (ppm)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7.207
7.090
7.041
7.022
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6.906
5.482
5.271
5.079
4.331
4.293
4.275
4.237
3.312
3.300
3.274
3.262
3.107
3.093
3.070
3.055
2.928
2.899
2.876
2.869
2.622
2.612
2.601
2.402
2.385
2.379
2.367
O
OBn
N
Ts
1h
2.00
2.00
2.00
4.06
1.00
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1.01
2.00
2.00
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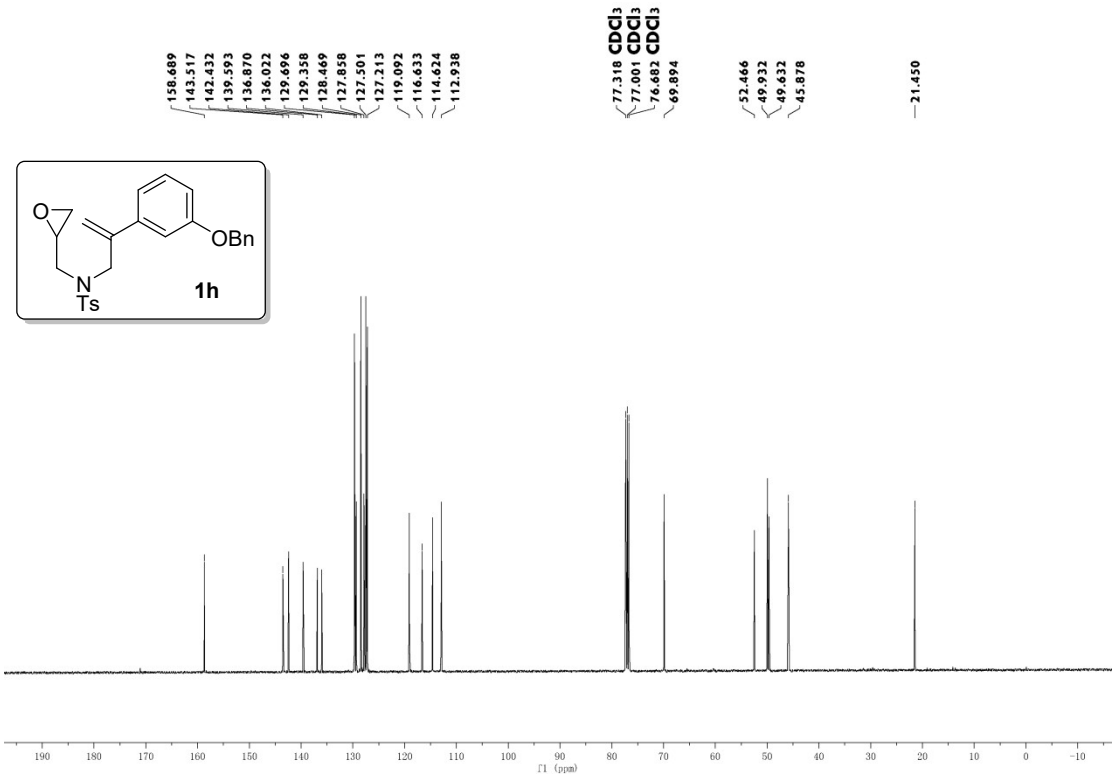
1.00
1.01
4.02
f1 (ppm)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112.938
77.318 CDCl3
77.001 CDCl3
76.682 CDCl3
69.894
52.466
49.932
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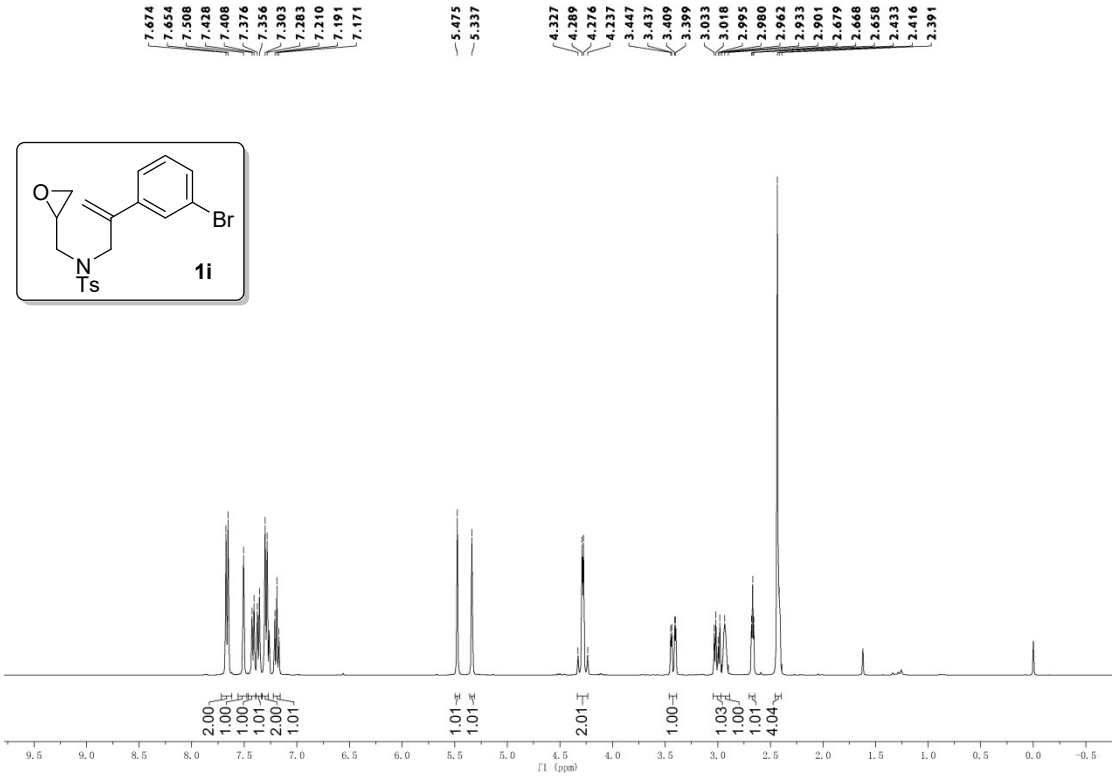
O
OBn
N
Ts
1h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.171
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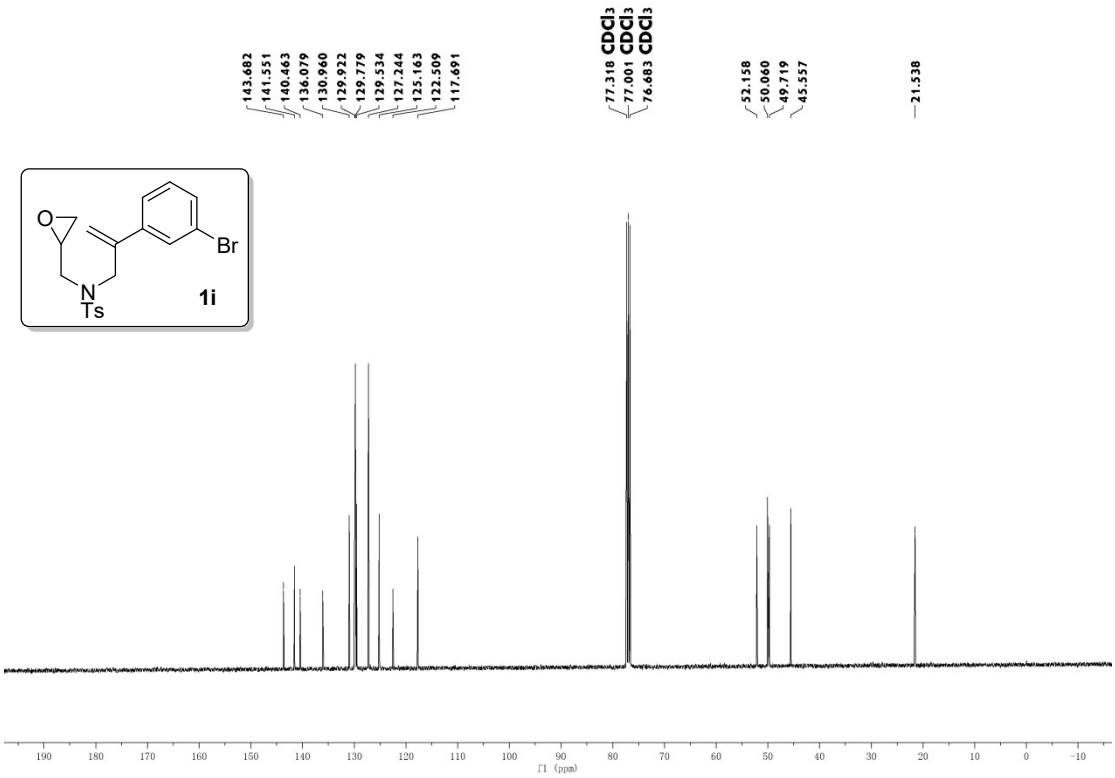
5.337
4.327
4.289
4.276
4.237
3.447
3.437
3.409
3.399
3.033
3.018
2.995
2.980
2.962
2.933
2.901
2.679
2.668
2.658
2.433
2.416
2.391
O
Br
N
Ts
1i
2.00
1.00
1.00
1.01
2.00
1.01
1.01
1.01
2.01
1.00
1.03
1.00
1.01
4.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.534
127.244
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122.509
117.691
77.318 CDCl3
77.001 CDCl3
76.683 CDCl3
52.158
50.060
49.719
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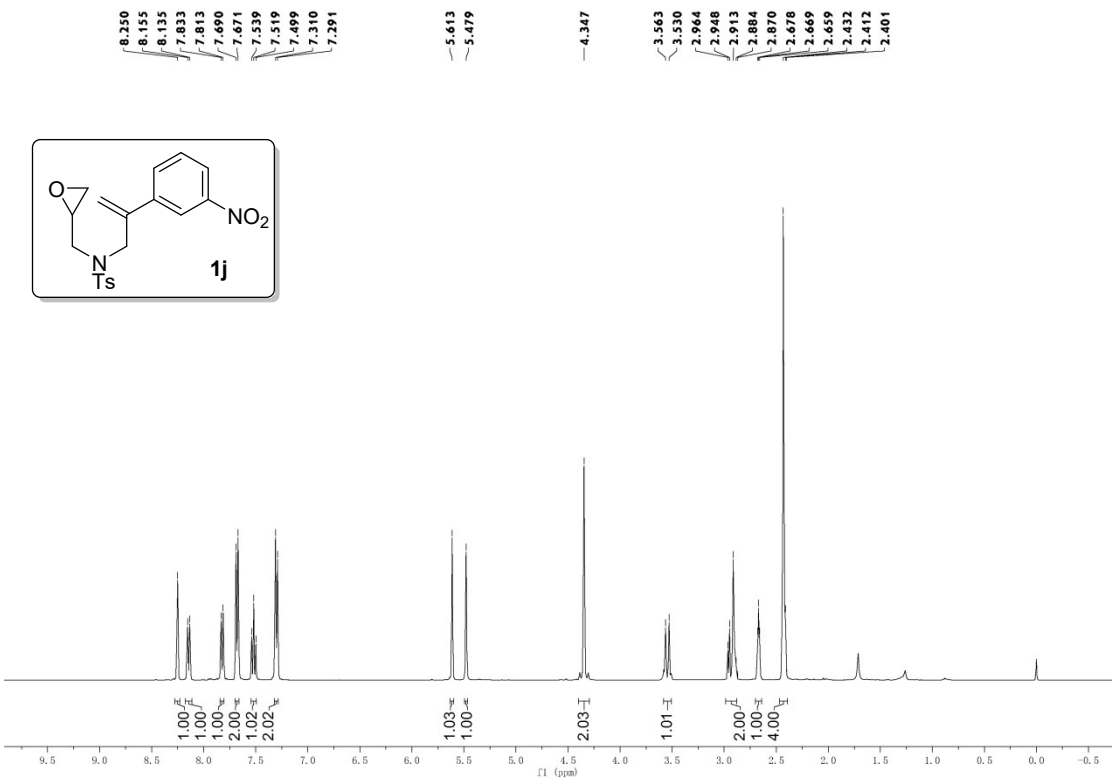
21.538
Br
N
Ts
1i
f1 (ppm)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5.479
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3.530
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2.870
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2.669
2.659
2.432
2.412
2.401
NO2
N
Ts
1j
1.00
1.00
1.00
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2.02
1.03
1.00
2.03
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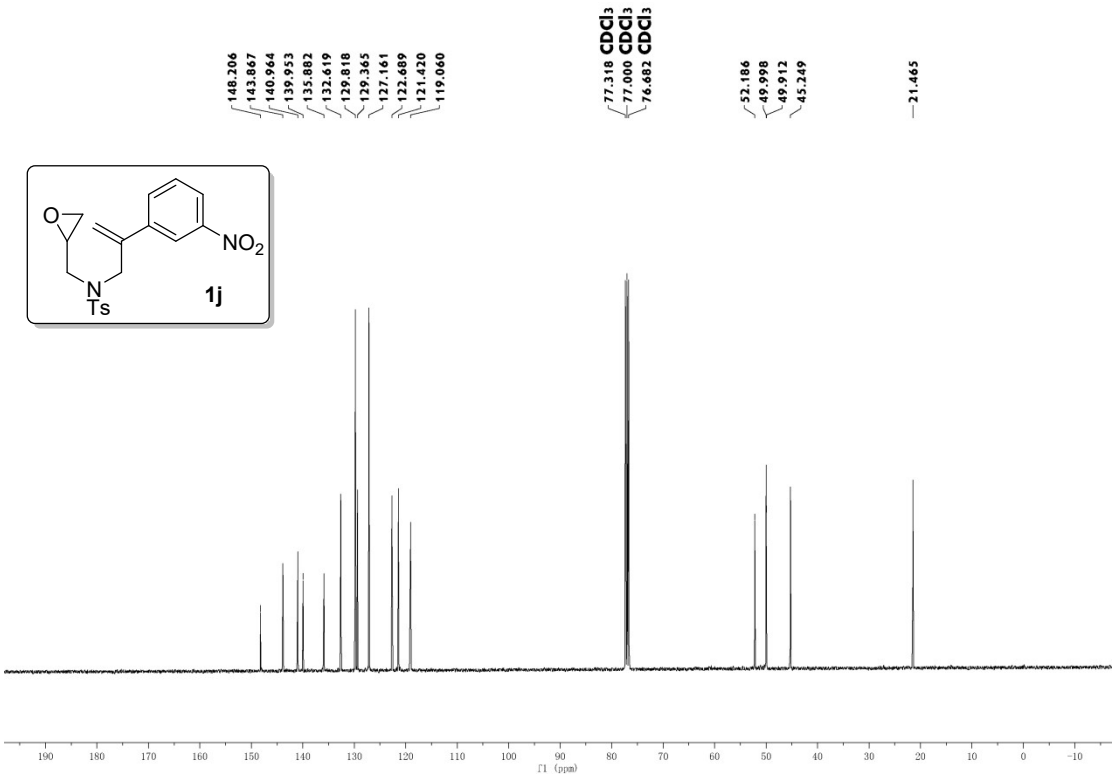
2.00
1.00
4.00
f1 (ppm)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119.060
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77.000 CDCl3
76.682 CDCl3
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49.912
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21.465
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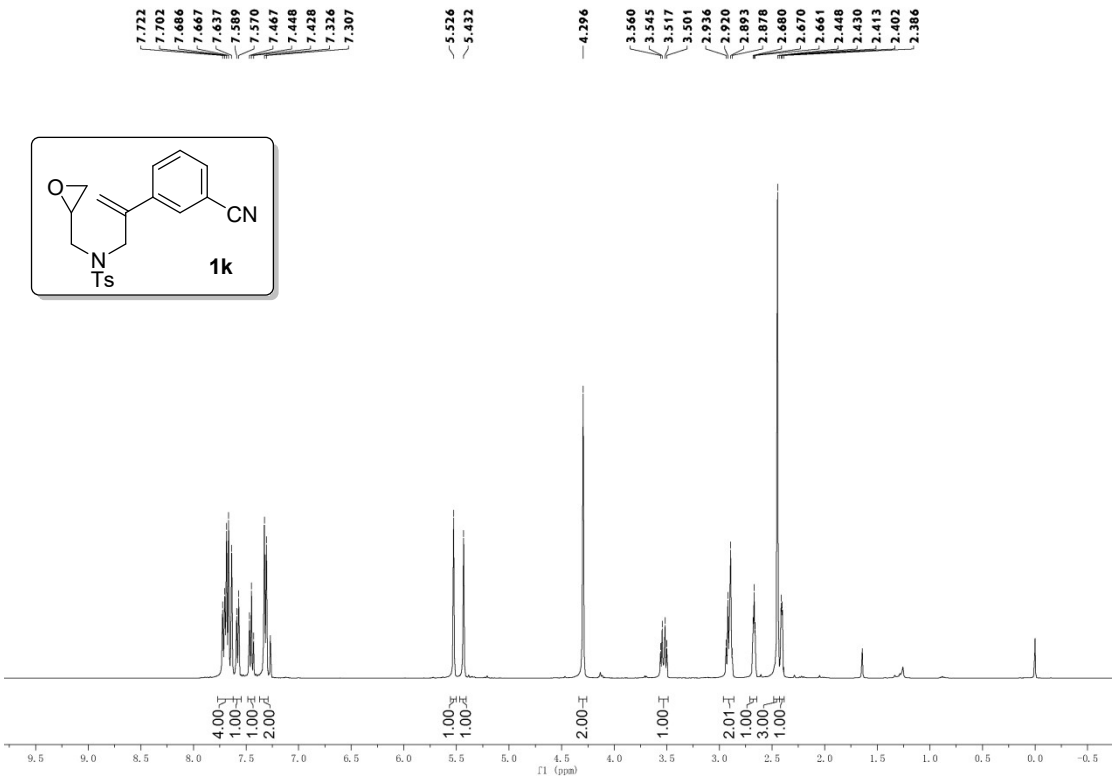
NO2
N
Ts
1j
f1 (ppm)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5.432
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3.545
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2.936
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O
CN
N
Ts
1k
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1.00
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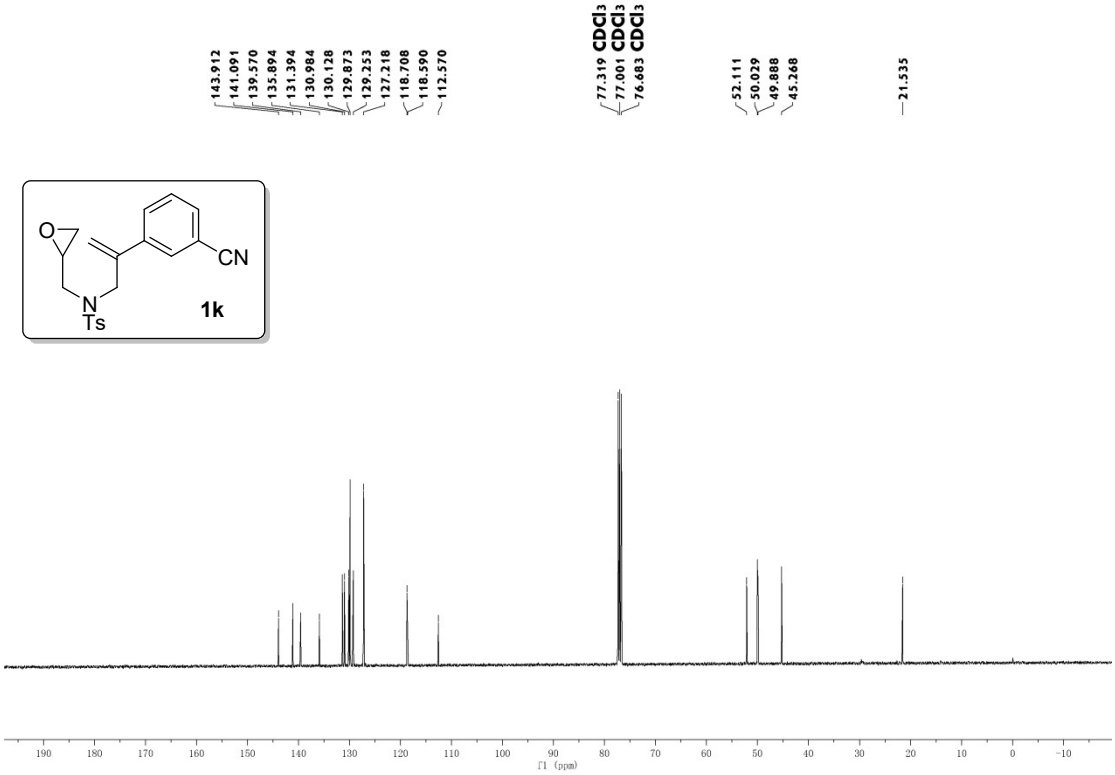
3.00
1.00
f1 (ppm)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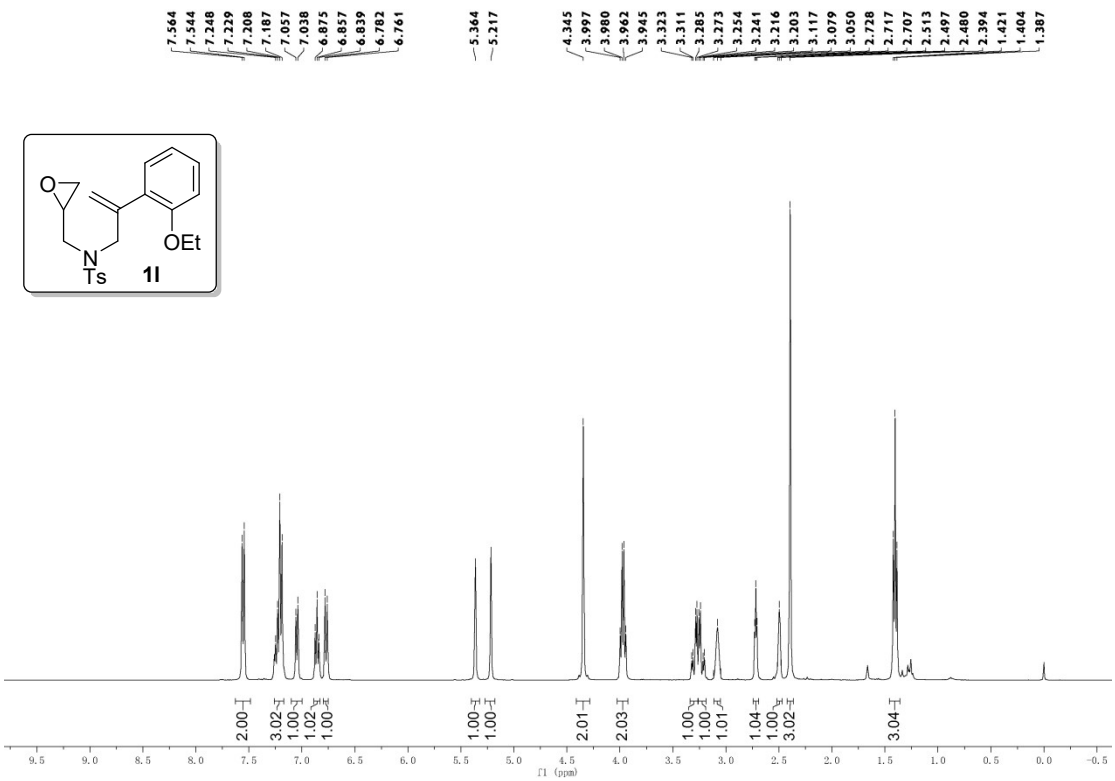
CN
1k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5.217
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3.050
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1.404
1.387
O
N
Ts
OEt
1l
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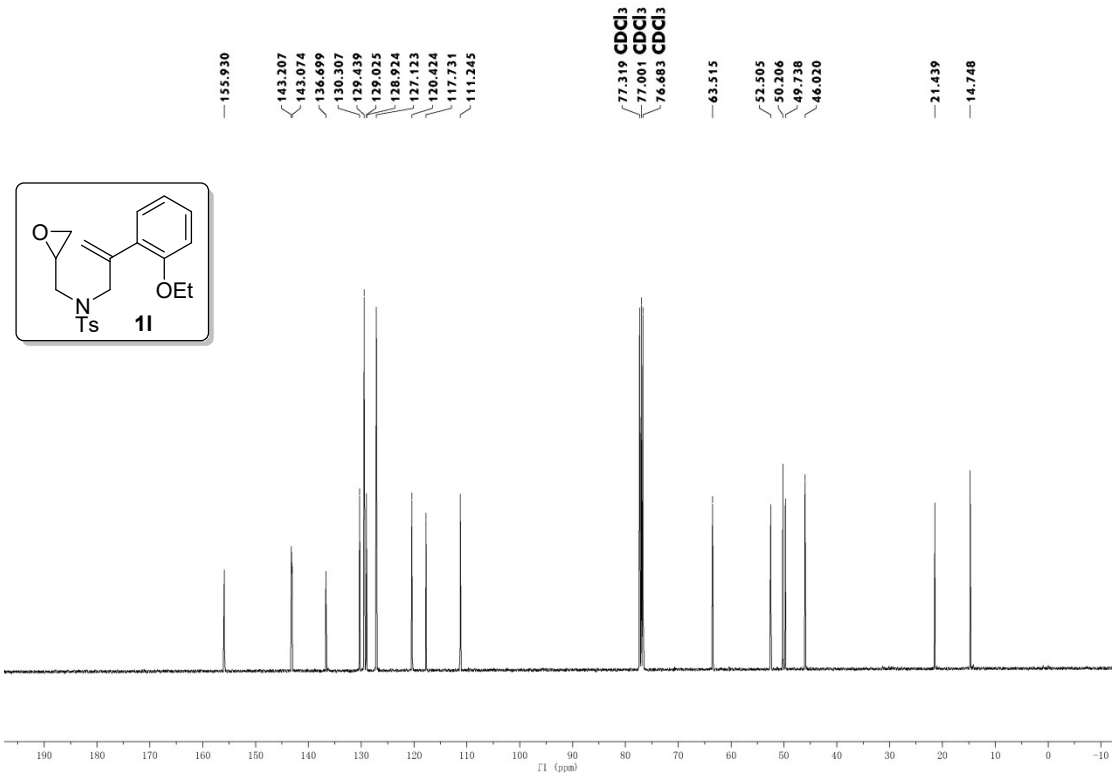
3.04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77.001 CDCl3
76.683 CDCl3
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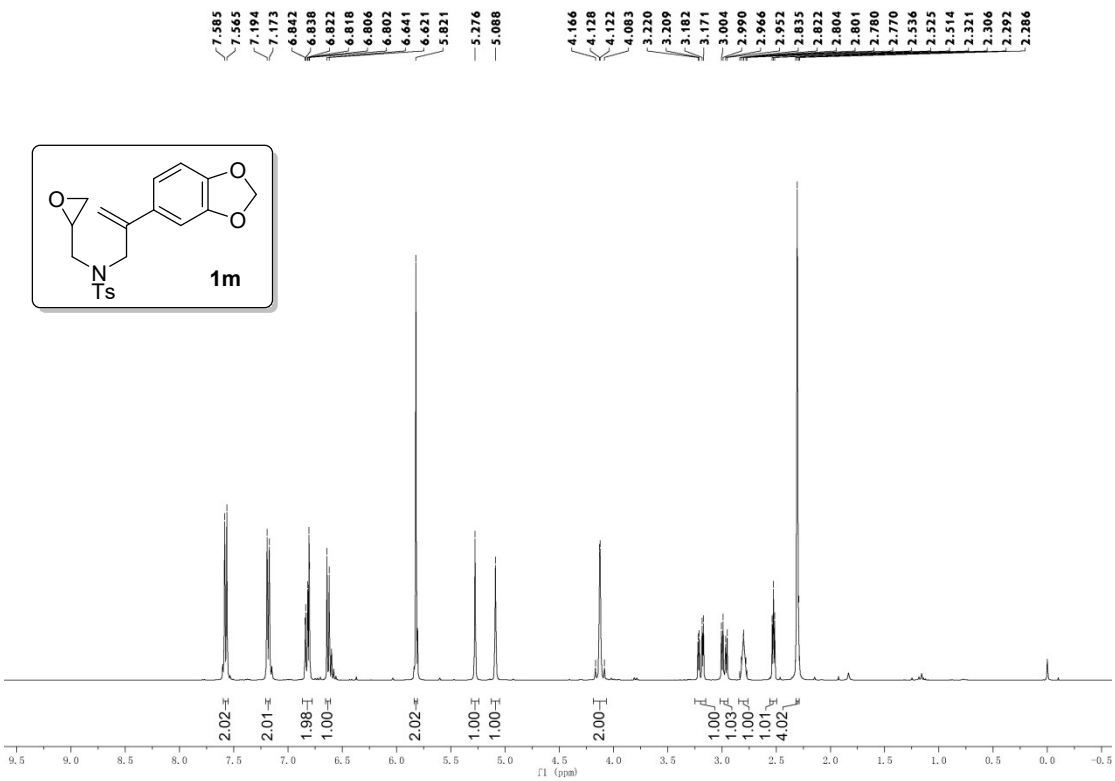
Ts
OEt
1l
f1 (ppm)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O
O
O
N
Ts
1m
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2.01
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1.00
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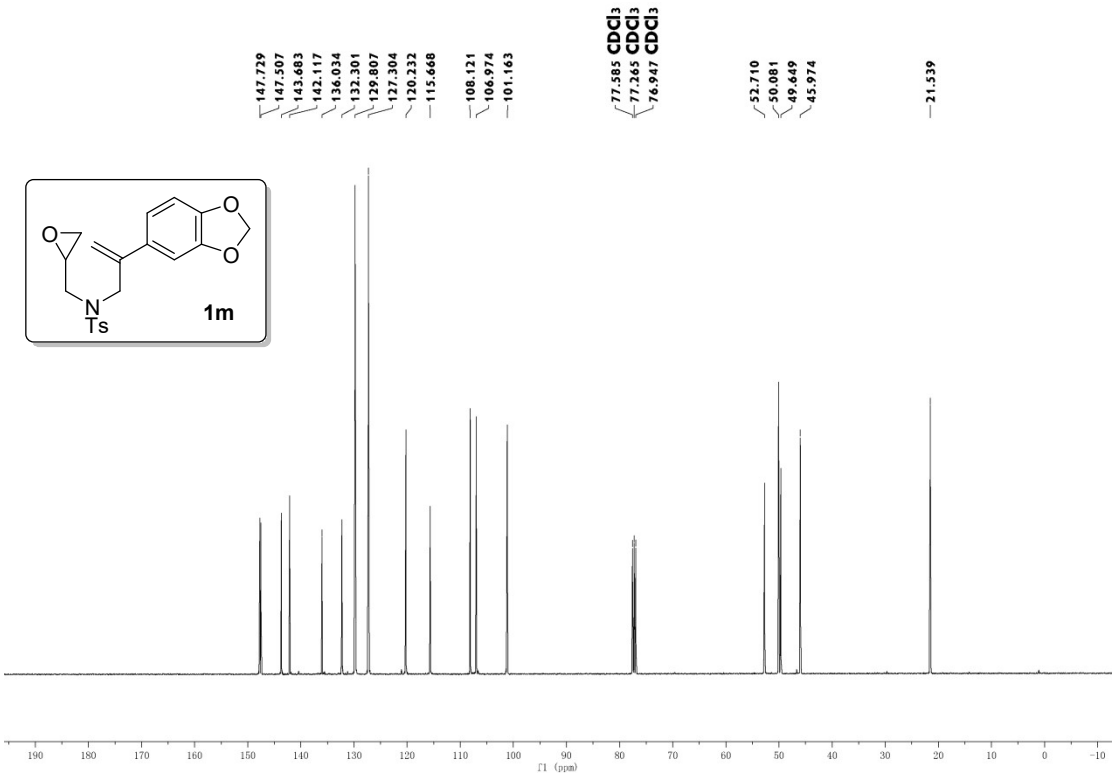
f1 (ppm)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77.585 CDCl3
77.265 CDCl3
76.947 CDCl3
52.710
50.081
49.649
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O
O
O
N
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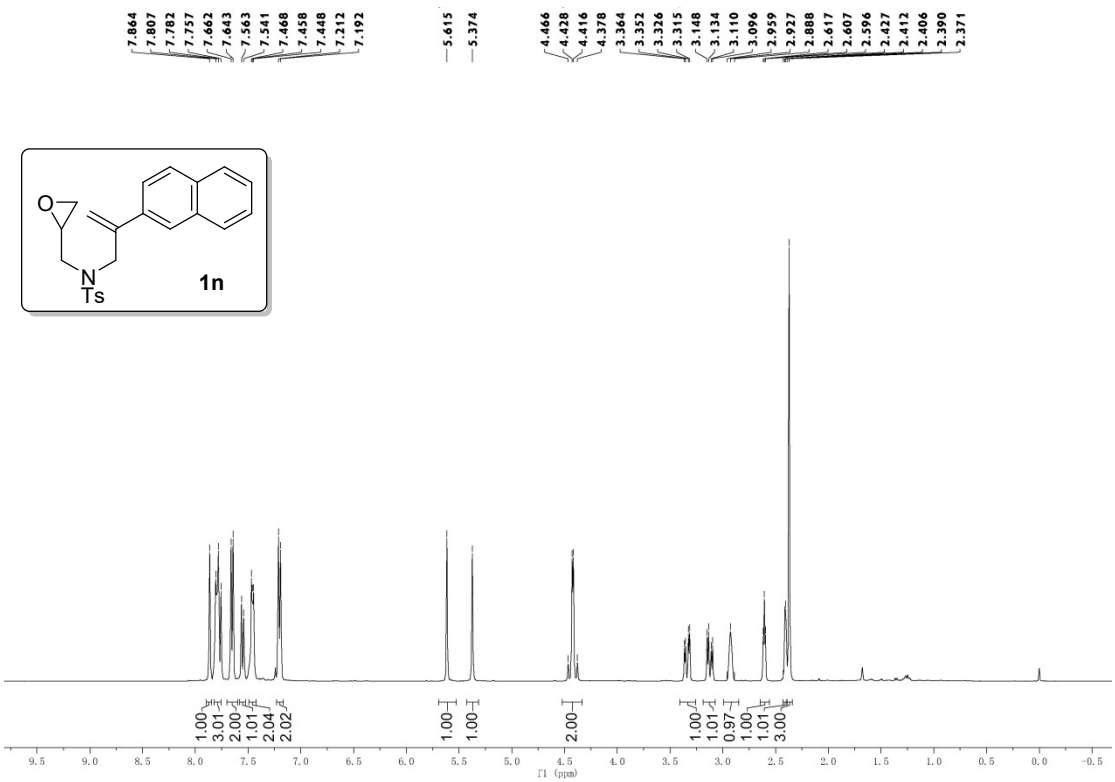
f1 (ppm)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4.466
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2.607
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O
N
Ts
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2.00
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2.04
2.02
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1.00
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1.01
3.00
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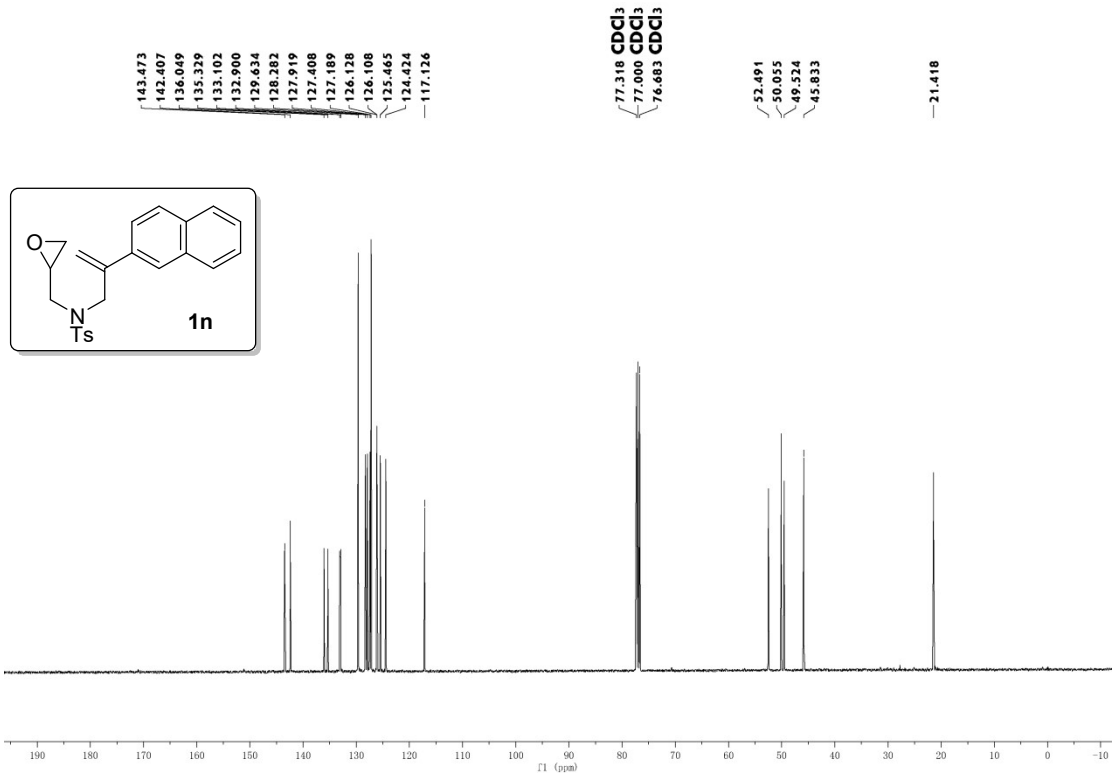
f1 (ppm)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125.465
124.424
117.126
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
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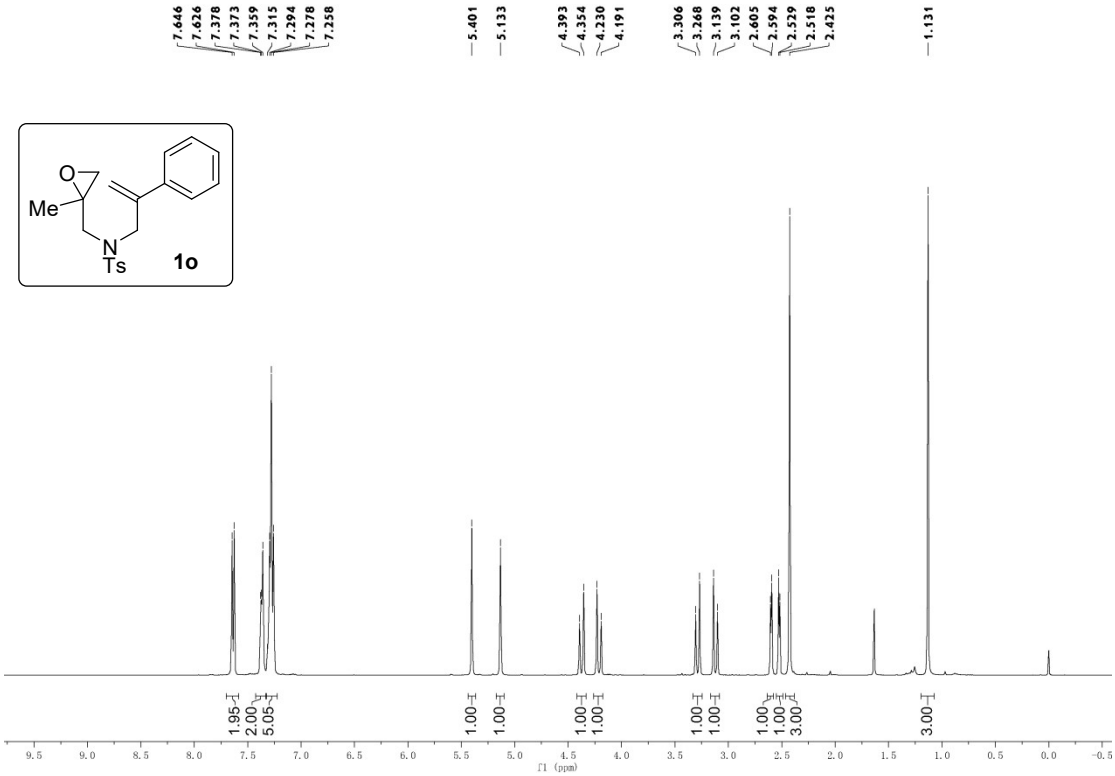
49.524
45.833
21.418
O
N
Ts
1n
f1 (ppm)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Me
N
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1o
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1.00
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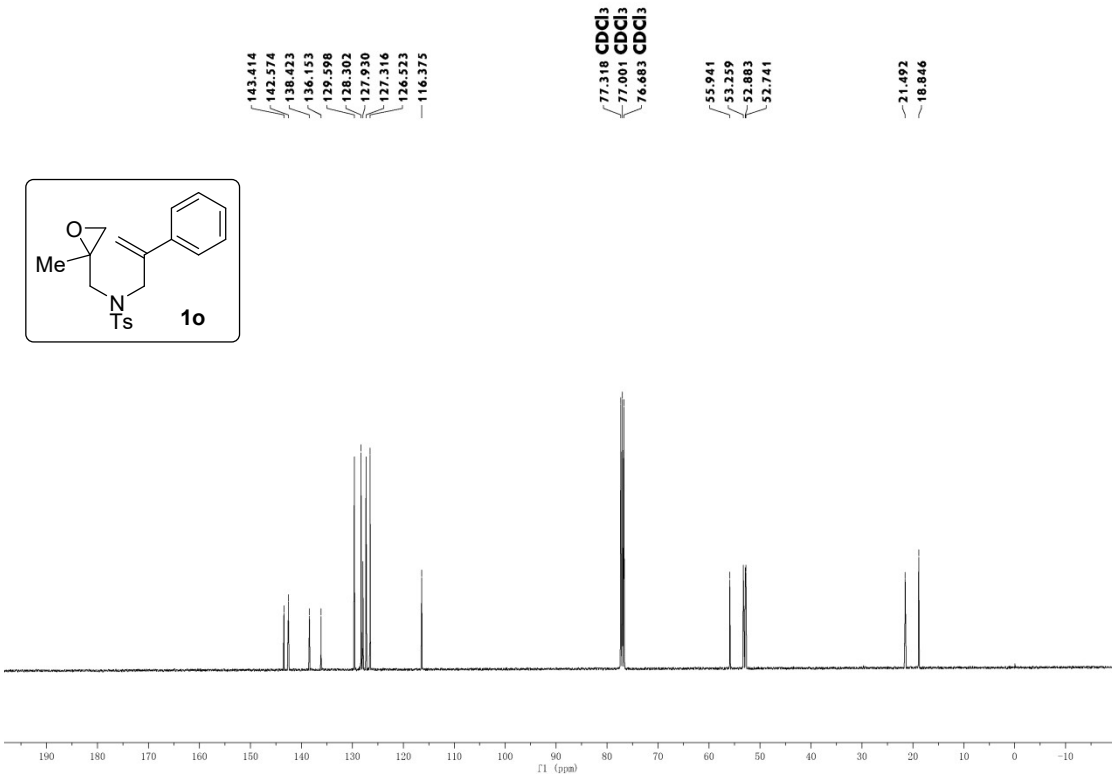
f1 (ppm)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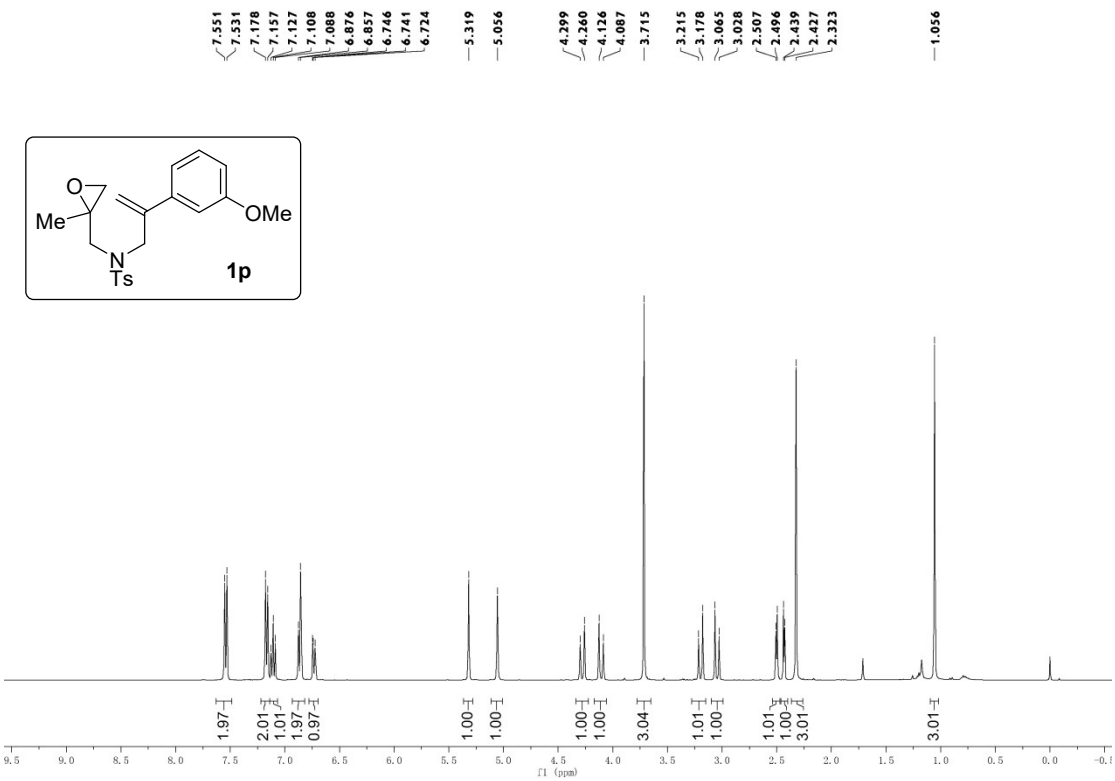
Ts
1o
f1 (ppm)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4.299
4.260
4.126
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3.715
3.215
3.178
3.065
3.028
2.507
2.496
2.439
2.427
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O
Me
OMe
N
Ts
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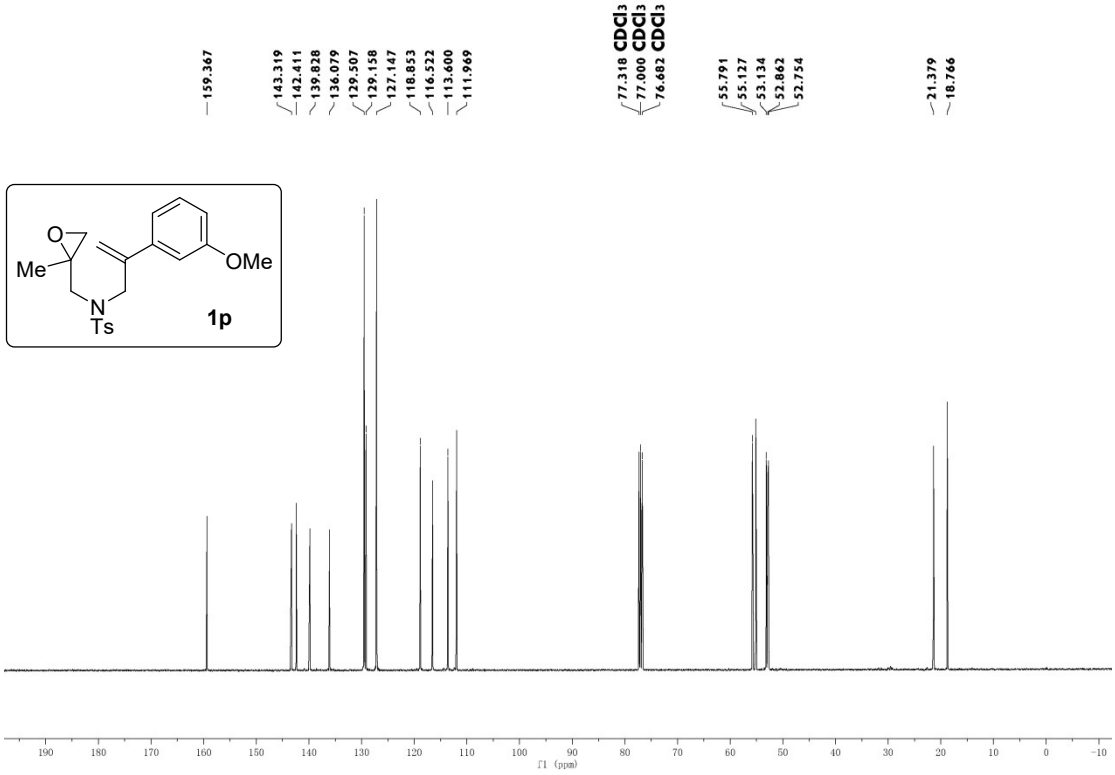
f1 (ppm)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77.318 CDCl3
77.000 CDCl3
76.682 CDCl3
55.791
55.127
53.134
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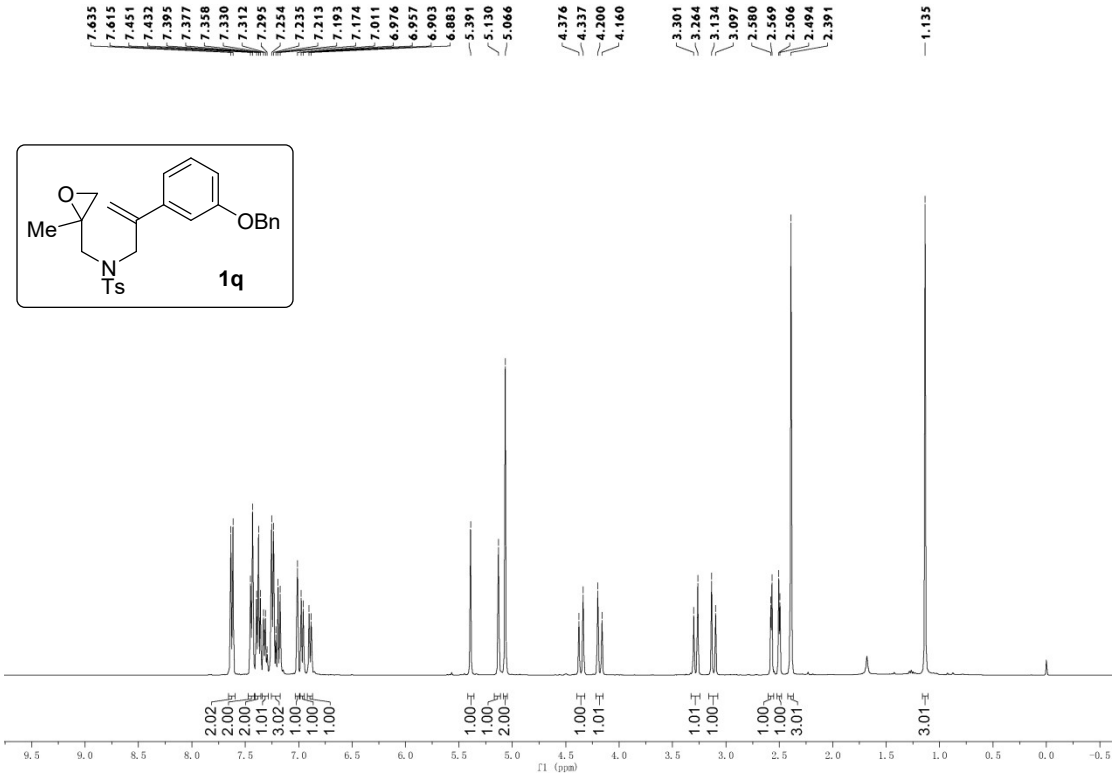
Me
OMe
N
Ts
1p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7.213
7.193
7.174
7.011
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6.957
6.903
6.883
5.391
5.130
5.066
4.376
4.337
4.200
4.160
3.301
3.264
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2.506
2.494
2.391
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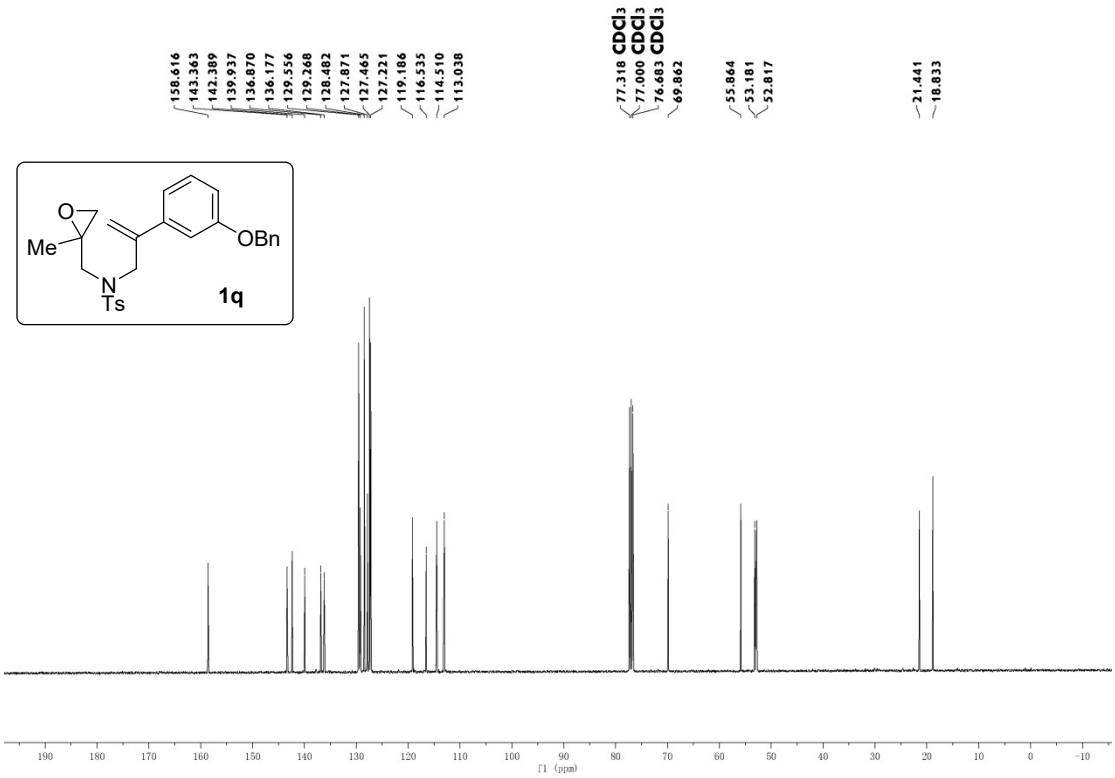
Me
OBn
N
Ts
1q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129.268
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127.871
127.465
127.221
119.186
116.535
114.510
113.038
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
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53.181
52.817
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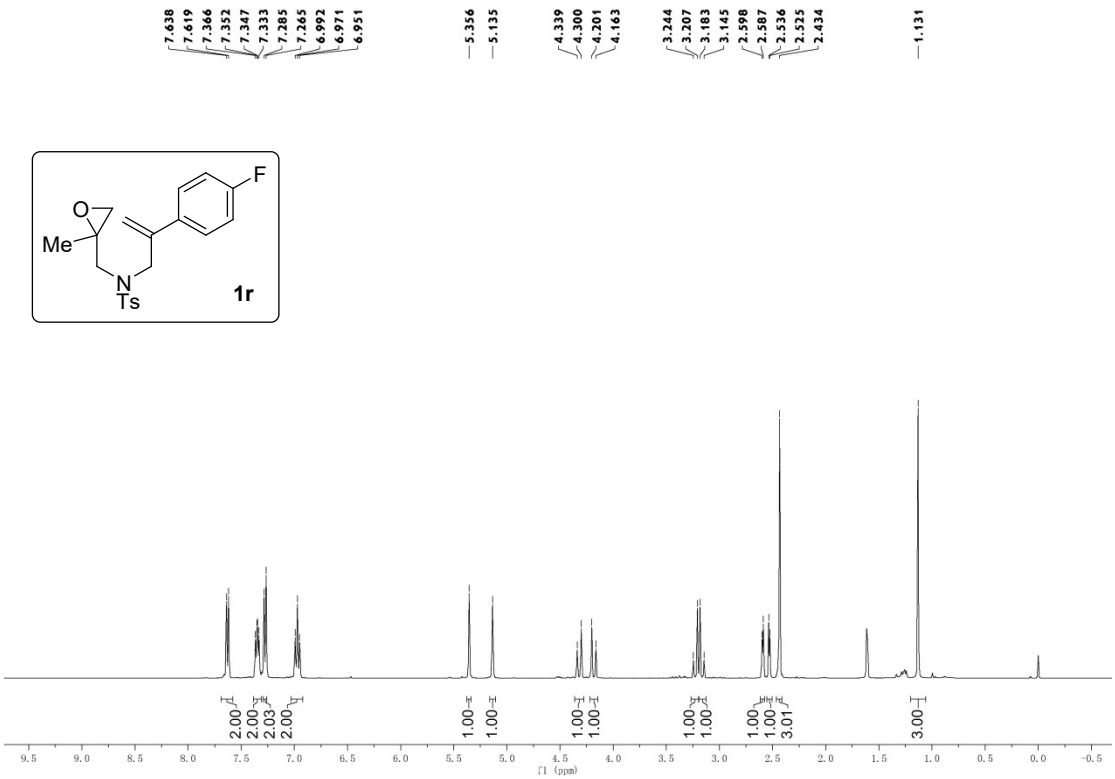
18.833
O
Me
N
Ts
OBn
1q
f1 (ppm)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7.265
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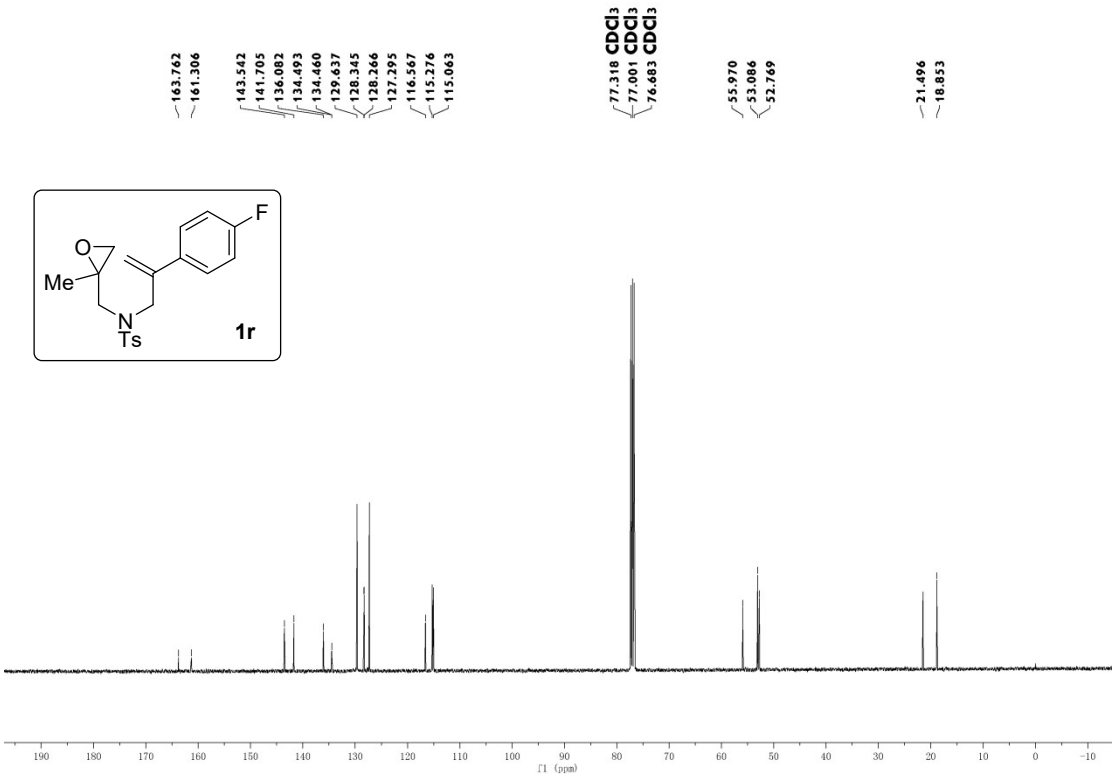
6.951
5.356
5.135
4.339
4.300
4.201
4.163
3.244
3.207
3.183
3.145
2.598
2.587
2.536
2.525
2.434
1.131
O
Me
N
Ts
F
1r
2.00
2.00
2.03
2.00
1.00
1.00
1.00
1.00
1.00
1.00
1.00
1.00
3.01
3.00
f1 (ppm)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141.705
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134.493
134.460
129.637
128.345
128.266
127.295
116.567
115.276
115.063
77.318 CDCl3
77.001 CDCl3
76.683 CDCl3
55.970
53.086
52.769
21.496
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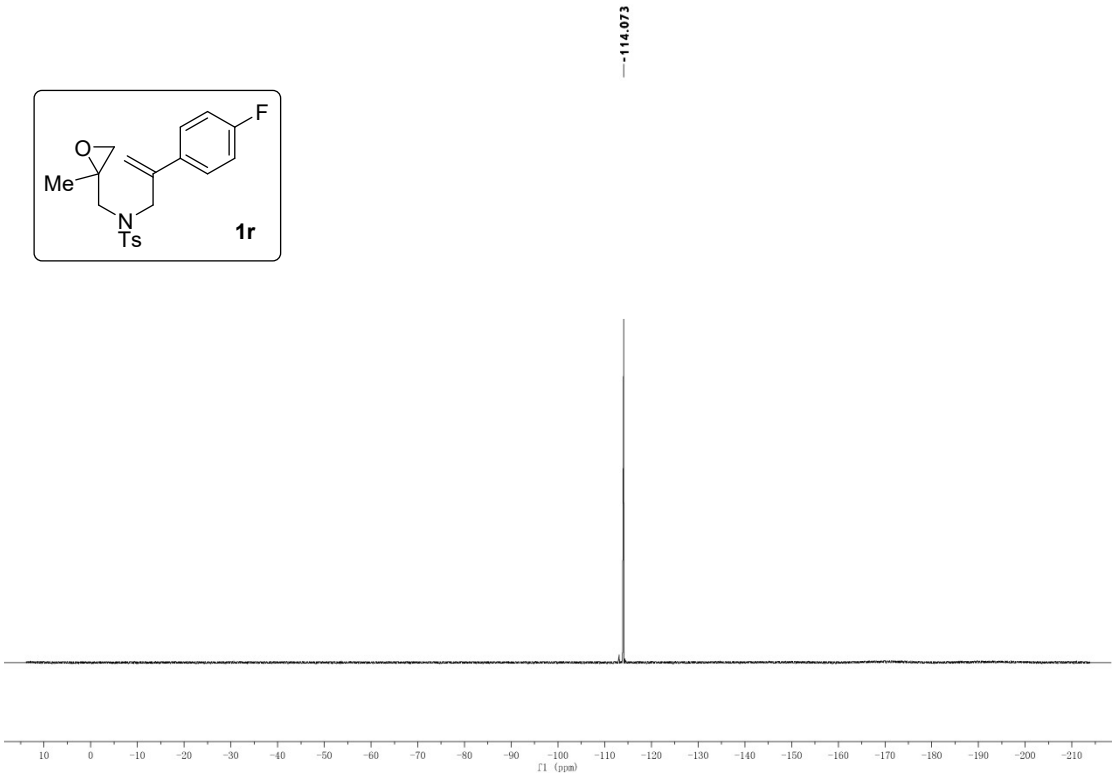
F
O
Me
N
Ts
1r
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-114.073
F
O
Me
N
Ts
1r
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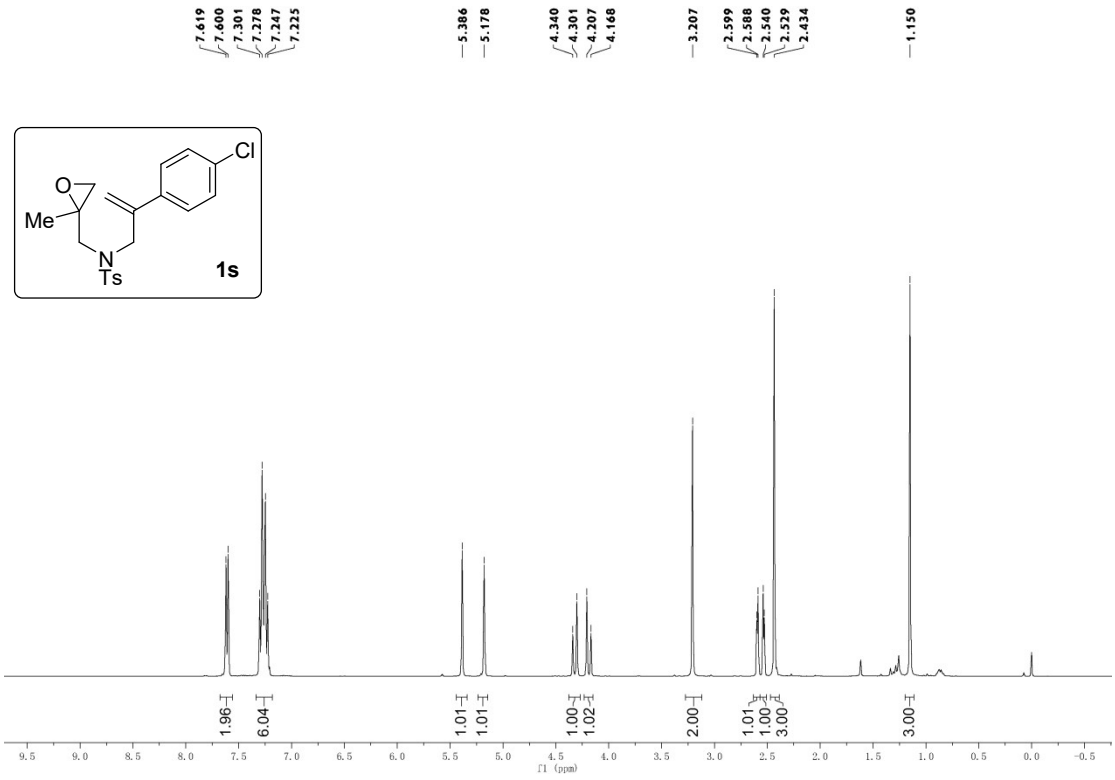
f1 (ppm)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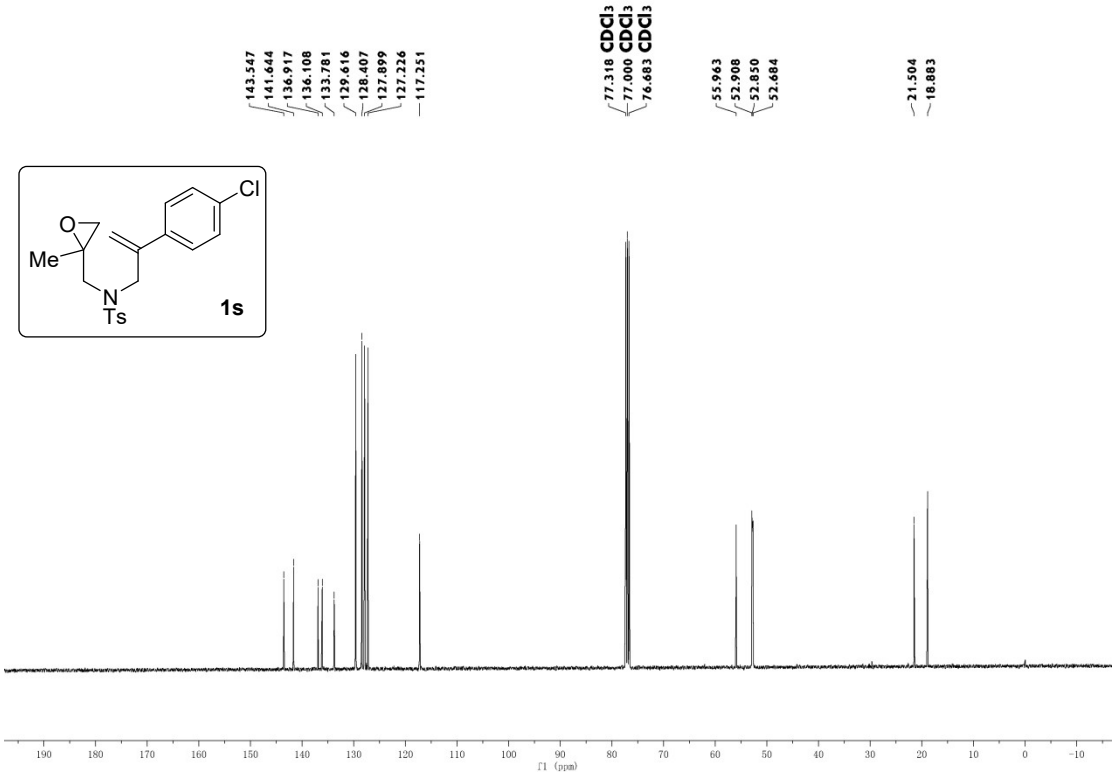
7.278
7.247
7.225
5.386
5.178
4.340
4.301
4.207
4.168
3.207
2.599
2.588
2.540
2.529
2.434
1.150
Cl
O
Me
N
Ts
1s
1.96
6.04
1.01
1.01
1.00
1.02
2.00
1.01
1.00
3.00
3.00
f1 (ppm)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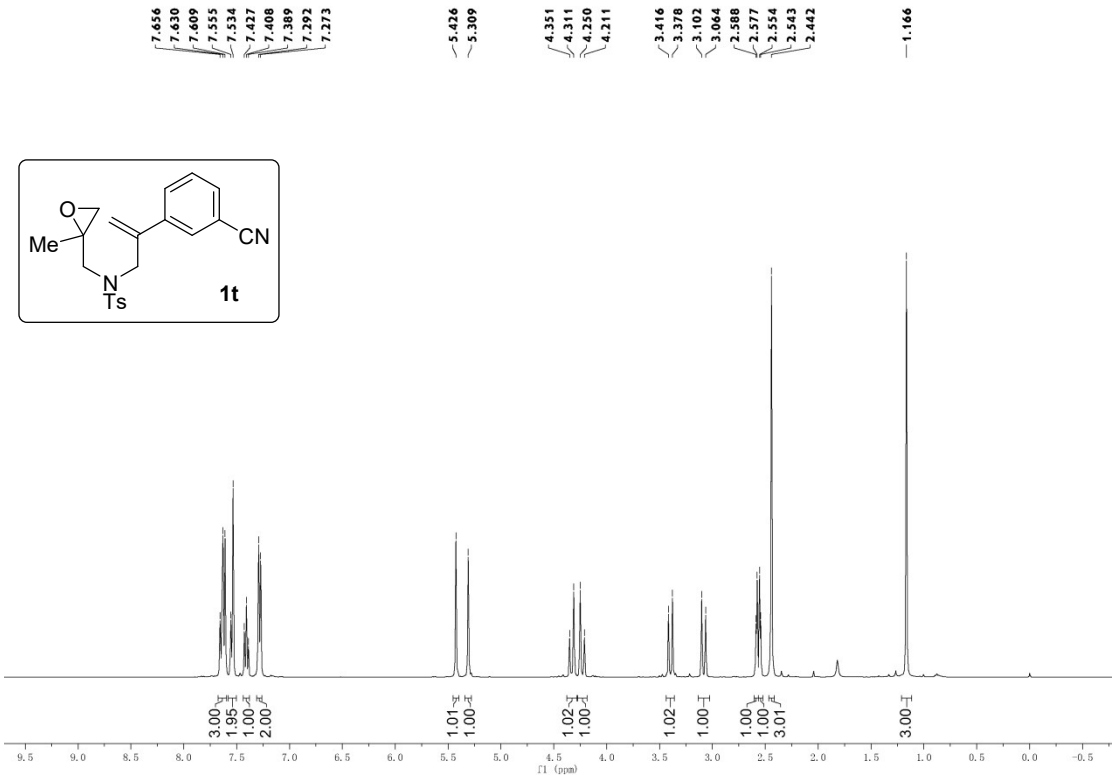
141.644
136.917
136.108
133.781
129.616
128.407
127.899
127.226
117.251
CDCl3
CDCl3
CDCl3
77.318
77.000
76.683
55.963
52.908
52.850
52.684
21.504
18.883
Cl
O
Me
N
Ts
1s
f1 (ppm)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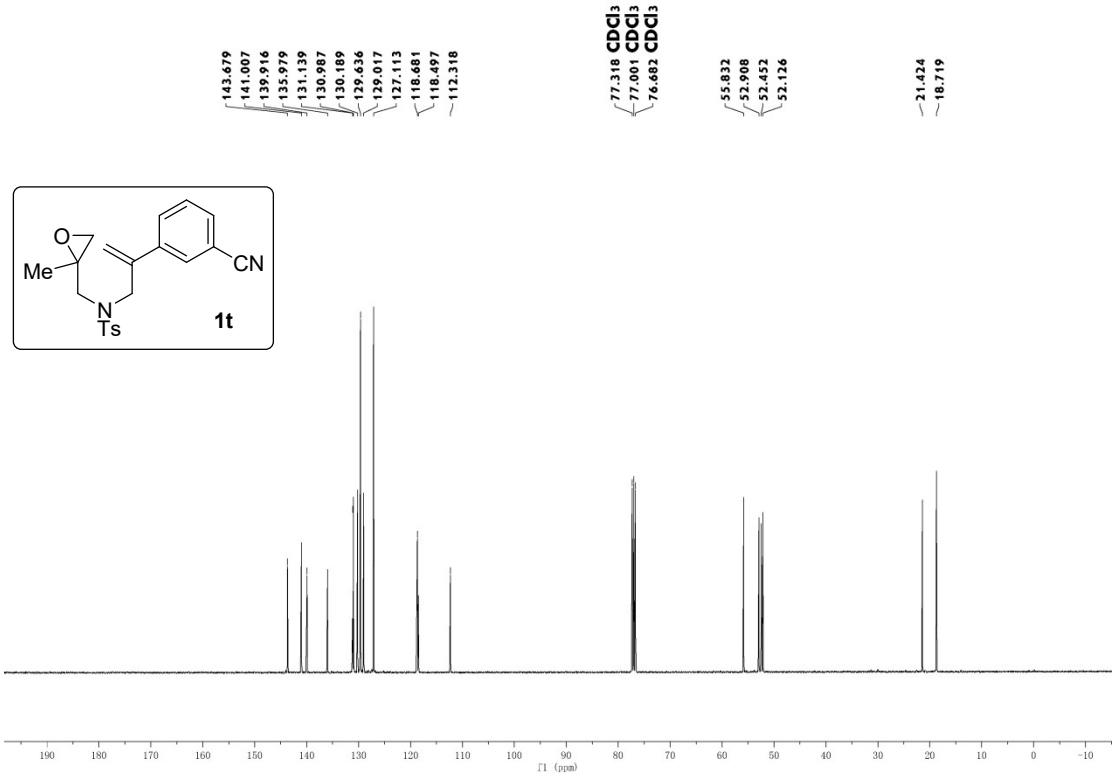
7.555
7.534
7.427
7.408
7.389
7.292
7.273
5.426
5.309
4.351
4.311
4.250
4.211
3.416
3.378
3.102
3.064
2.588
2.577
2.554
2.543
2.442
1.166
O
Me
CN
N
Ts
1t
3.00
1.95
1.00
2.00
1.01
1.00
1.02
1.00
1.02
1.00
1.00
1.00
3.01
3.00
f1 (ppm)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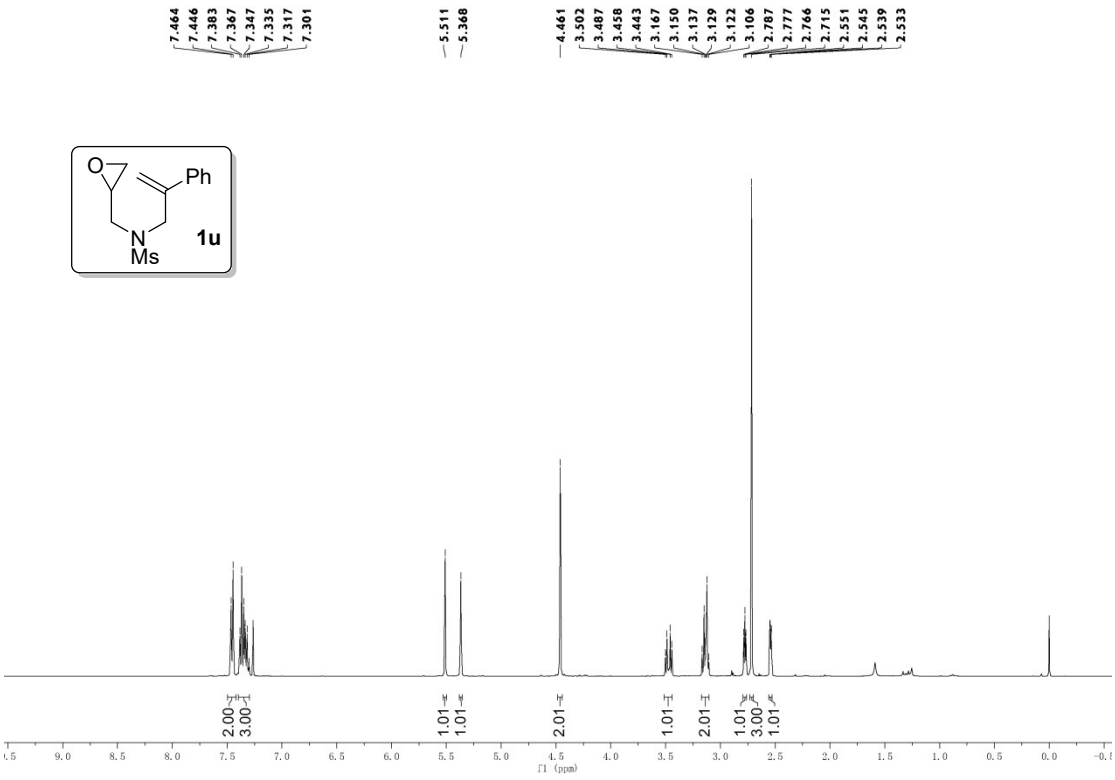
141.007
139.916
135.979
131.139
130.987
130.189
129.636
129.017
127.113
118.681
118.497
112.318
77.318 CDCl3
77.001 CDCl3
76.682 CDCl3
55.832
52.908
52.452
52.126
21.424
18.719
O
Me
CN
N
Ts
1t
f1 (ppm)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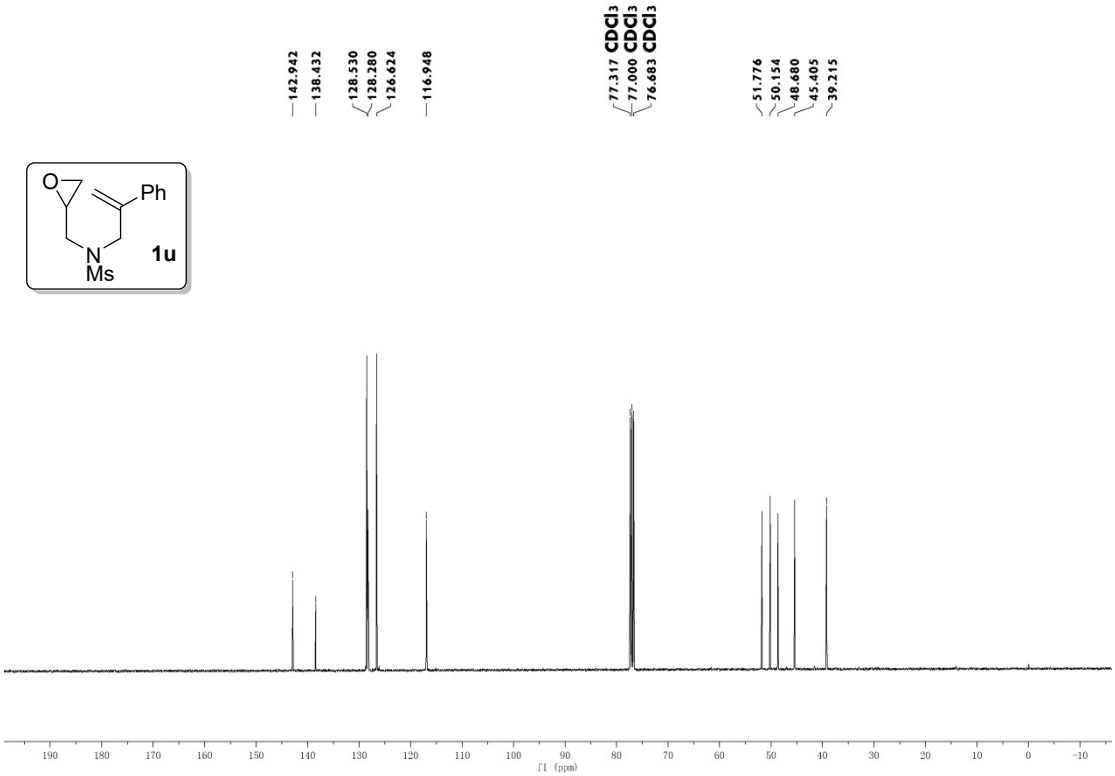
7.446
7.383
7.367
7.347
7.335
7.317
7.301
5.511
5.368
4.461
3.502
3.487
3.458
3.443
3.167
3.150
3.137
3.129
3.122
3.106
2.787
2.777
2.766
2.715
2.551
2.545
2.539
2.533
O
Ph
N
Ms
1u
2.00
3.00
1.01
1.01
2.01
1.01
2.01
1.01
3.00
1.01
f1 (ppm)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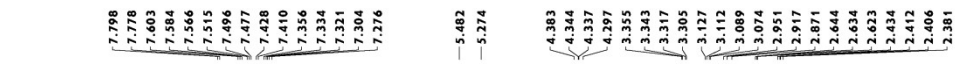
128.530
128.280
126.624
116.948
77.317 CDCl3
77.000 CDCl3
76.683 CDCl3
51.776
50.154
48.680
45.405
39.215
O
Ph
N
Ms
1u
f1 (ppm)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7.584
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7.515
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7.477
7.428
7.410
7.356
7.334
7.321
7.304
7.276
5.482
5.274
4.383
4.344
4.337
4.297
3.355
3.343
3.317
3.305
3.127
3.112
3.089
3.074
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2.917
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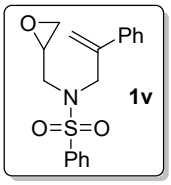
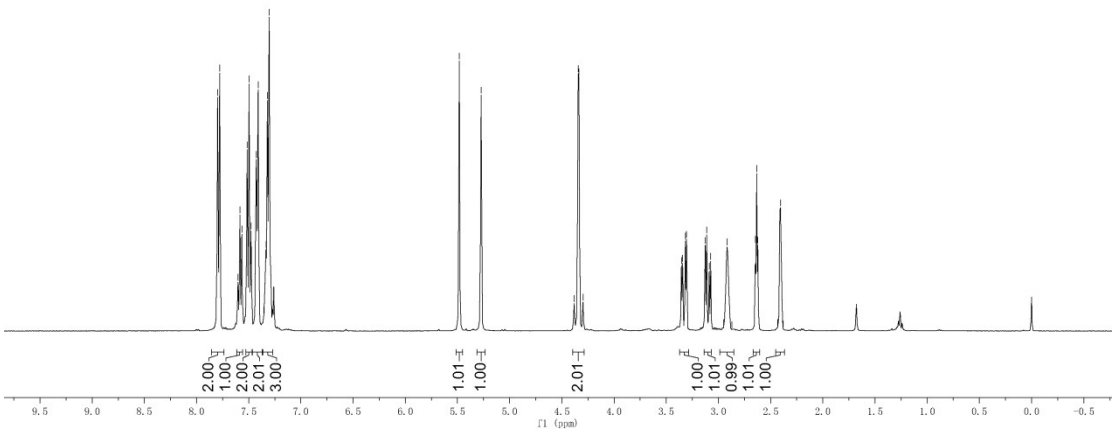
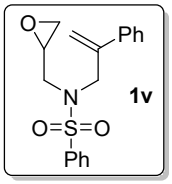
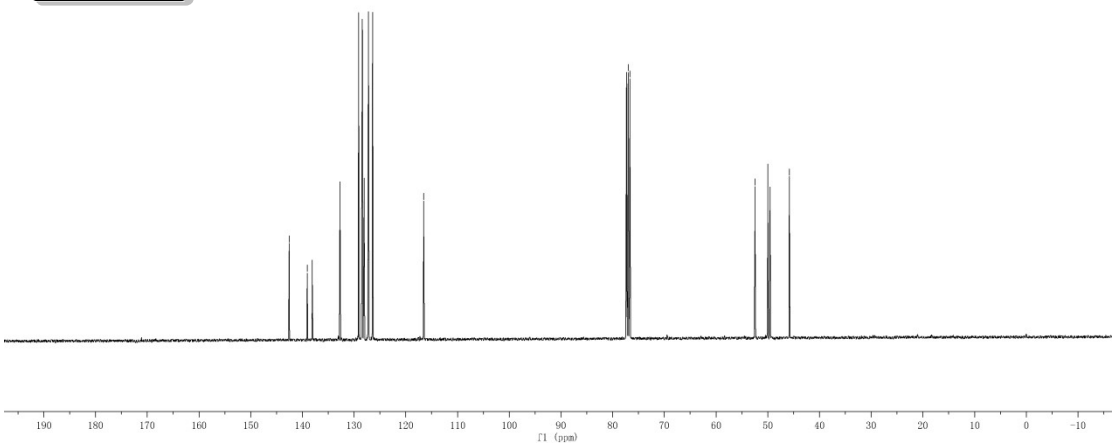
2.623
2.434
2.412
2.406
2.381

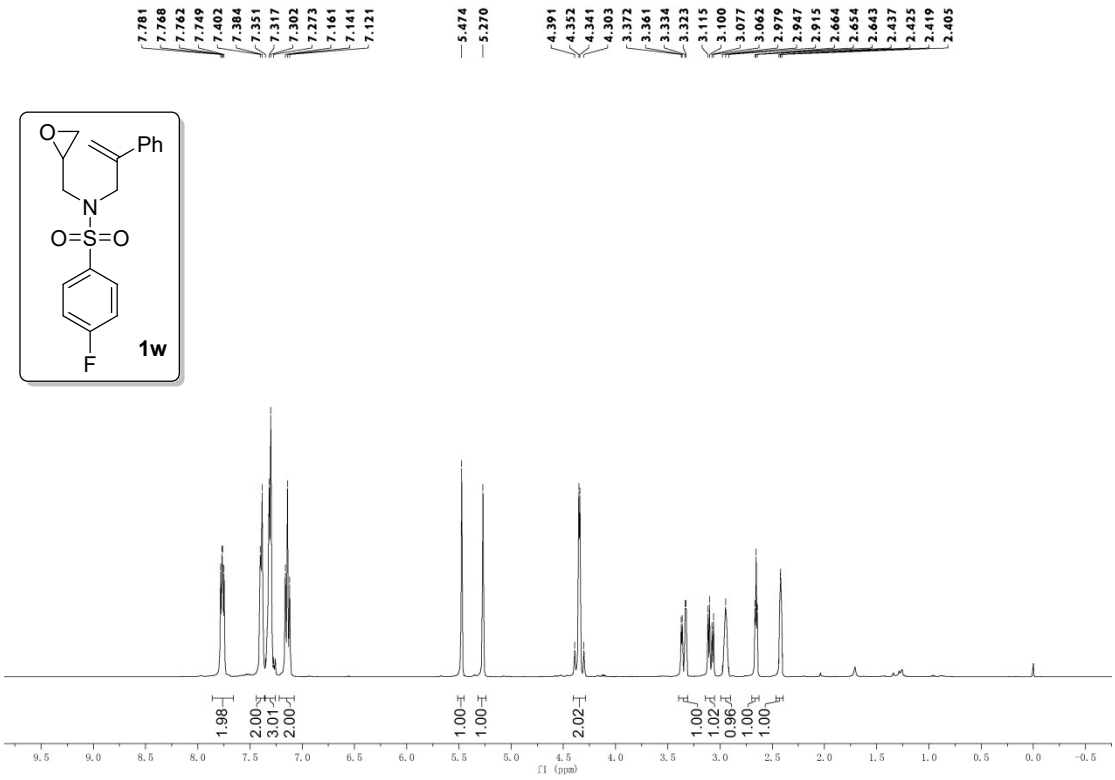

O
Ph
N
1v
O=S=O
Ph


2.00
1.00
2.00
2.01
3.00
1.01
1.00
2.01
1.00
1.01
0.99
1.01
1.00
f1 (ppm)


142.545
139.059
138.102
132.727
129.110
128.400
128.067
127.221
126.428
116.548
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
52.430
49.993
49.557
45.831


O
Ph
N
1v
O=S=O
Ph


f1 (ppm)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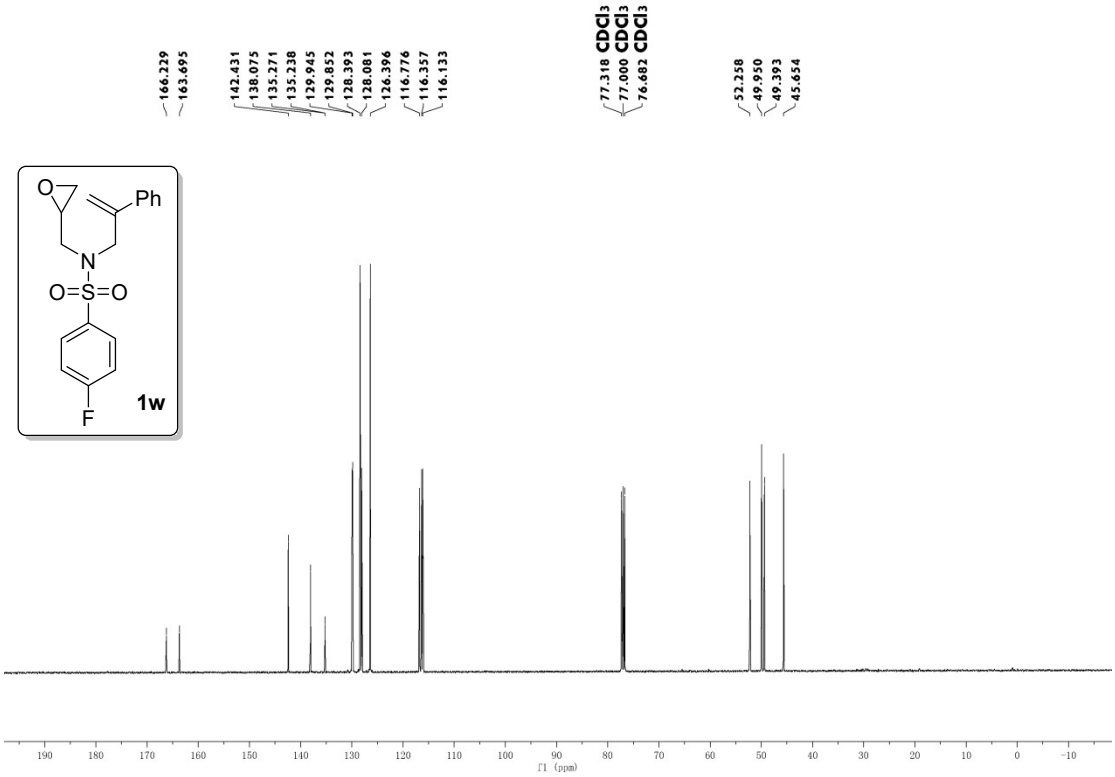
7.384
7.351
7.317
7.302
7.273
7.161
7.141
7.121
5.474
5.270
4.391
4.352
4.341
4.303
3.372
3.361
3.334
3.323
3.115
3.100
3.077
3.062
2.979
2.947
2.915
2.664
2.654
2.643
2.437
2.425
2.419
2.405
O
Ph
N
O=S=O
F
1w
1.98
2.00
3.01
2.00
1.00
1.00
2.02
1.00
1.02
0.96
1.00
1.00
f1 (ppm)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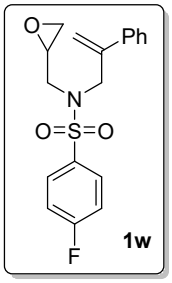
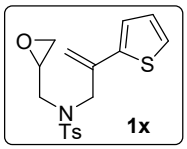
142.431
138.075
135.271
135.238
129.945
129.852
128.393
128.081
126.396
116.776
116.357
116.133
CDCl3
CDCl3
CDCl3
77.318
77.000
76.682
52.258
49.950
49.393
45.654
O
Ph
N
O=S=O
F
1w
f1 (ppm)


O
Ph
N
O=S=O
F
1w

-105.041
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


O
S
N
Ts
1x

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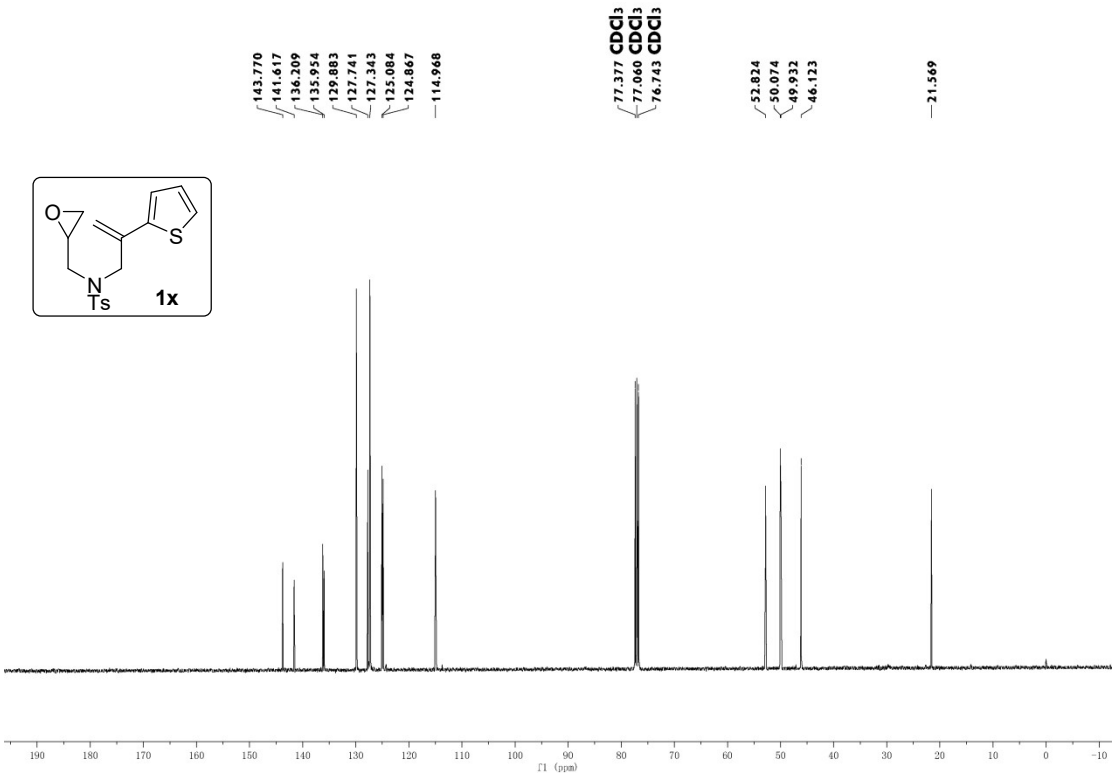
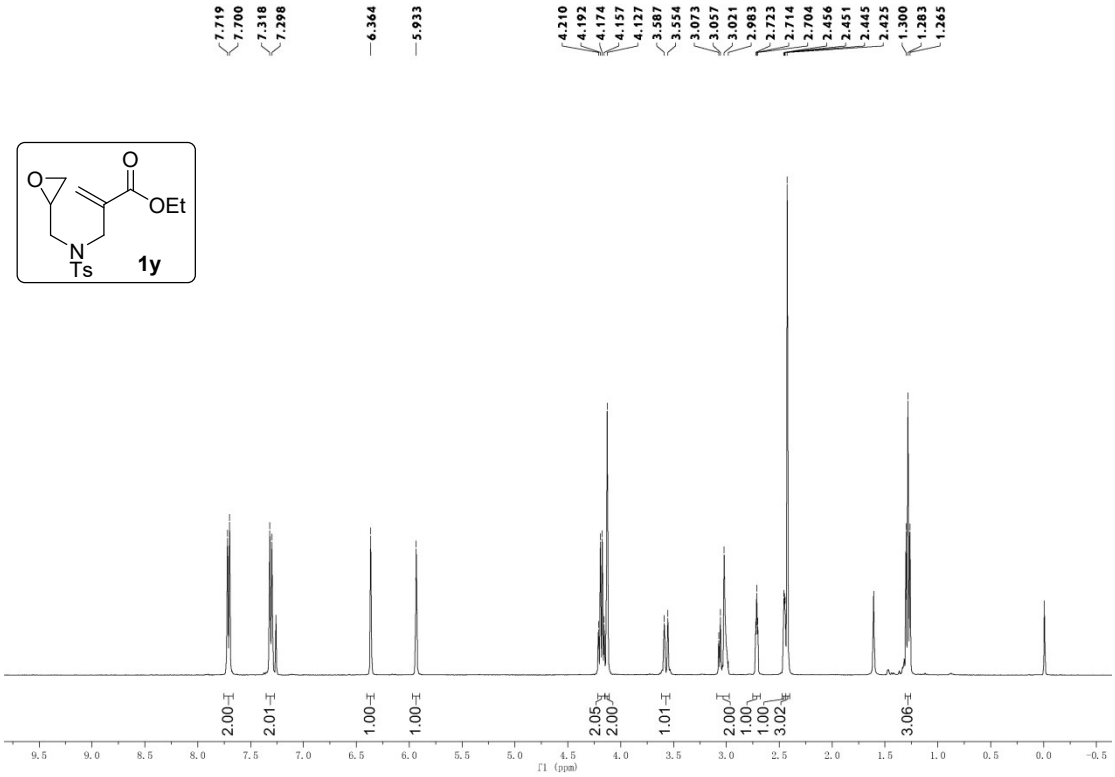
7.277
7.268
7.199
7.186
6.999
6.988
6.977
5.550
5.141
4.299
4.262
4.217
4.180
3.324
3.312
3.287
3.274
3.184
3.170
3.146
3.132
2.959
2.945
2.938
2.930
2.916
2.643
2.632
2.621
2.438
2.424
2.417
2.412
2.405
2.00
2.00
1.00
0.84
0.98
1.00
1.00
1.01
1.01
1.01
1.01
0.94
1.01
3.00
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


143.770
141.617
136.209
135.954
129.883
127.741
127.343
125.084
124.867
114.968
77.377 CDCl3
77.060 CDCl3
76.743 CDCl3
52.824
50.074
49.932
46.123
21.569
O
S
N
Ts
1x
f1 (ppm)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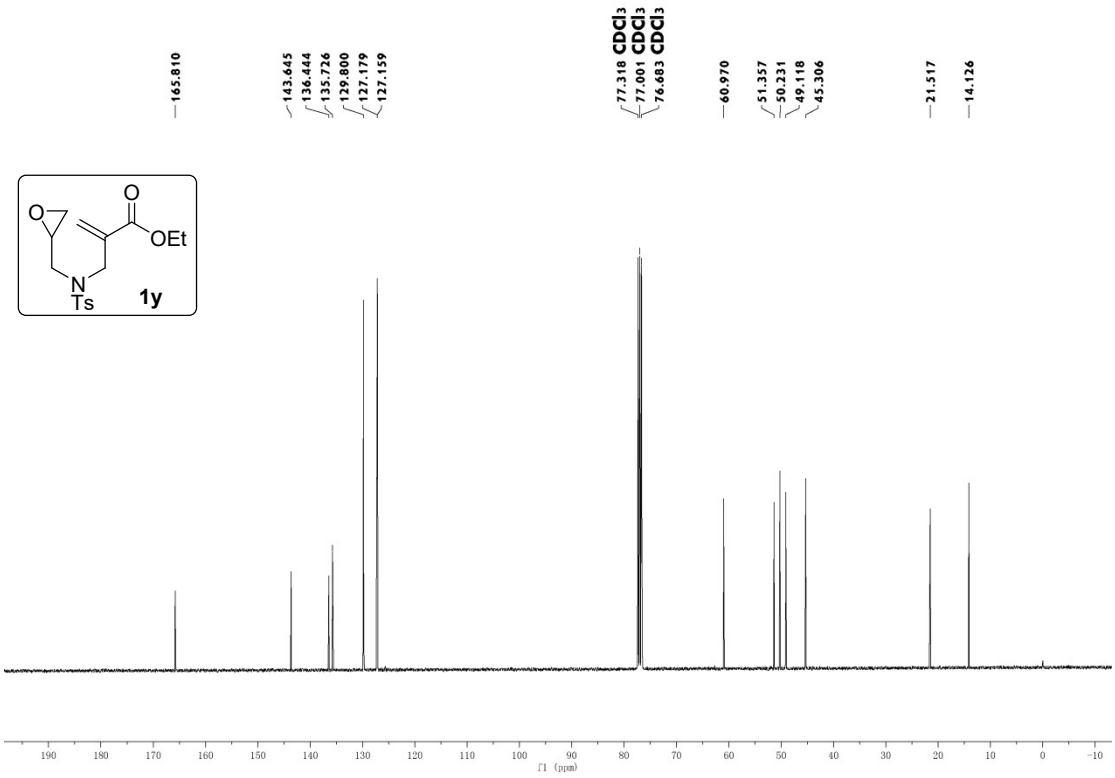
7.700
7.318
7.298
6.364
5.933
4.210
4.192
4.174
4.157
4.127
3.587
3.554
3.073
3.057
3.021
2.983
2.723
2.714
2.704
2.456
2.451
2.445
2.425
1.300
1.283
1.265
O
O
OEt
N
Ts
1y
2.00
2.01
1.00
1.00
2.05
2.00
1.01
2.00
1.00
1.00
3.02
3.06
f1 (ppm)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127.179
127.159
77.318 CDCl3
77.001 CDCl3
76.683 CDCl3
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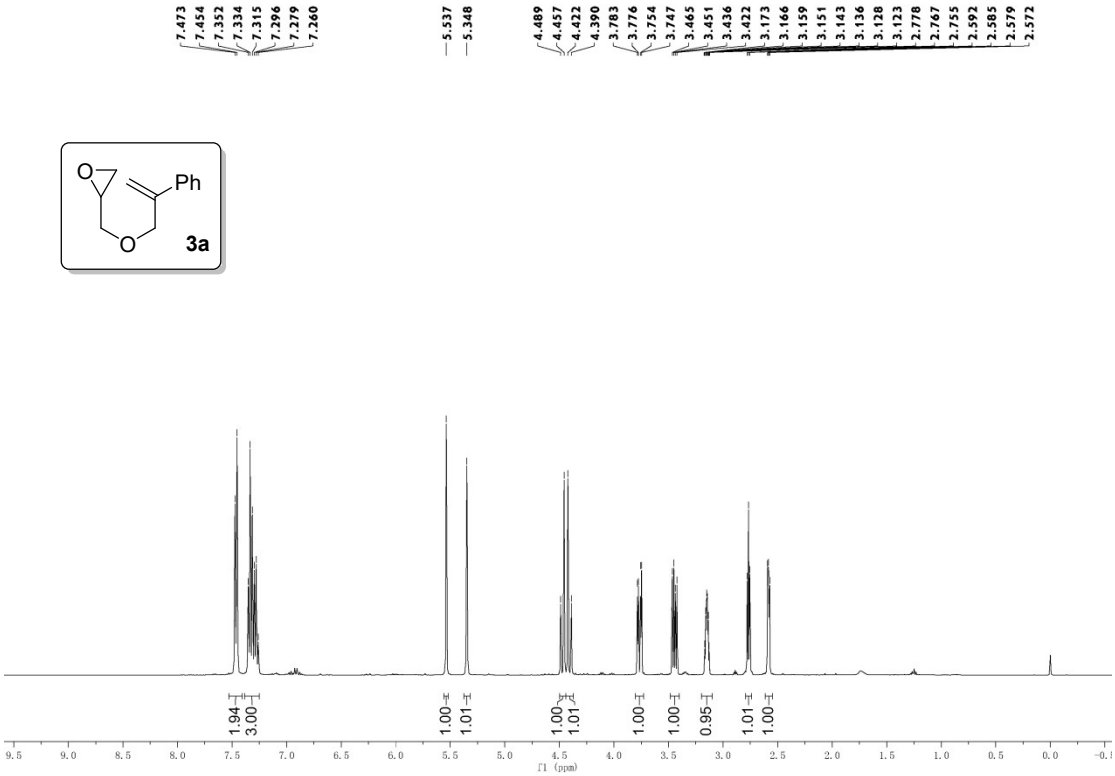
50.231
49.118
45.306
21.517
14.126
O
OEt
N
Ts
1y
f1 (ppm)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7.260
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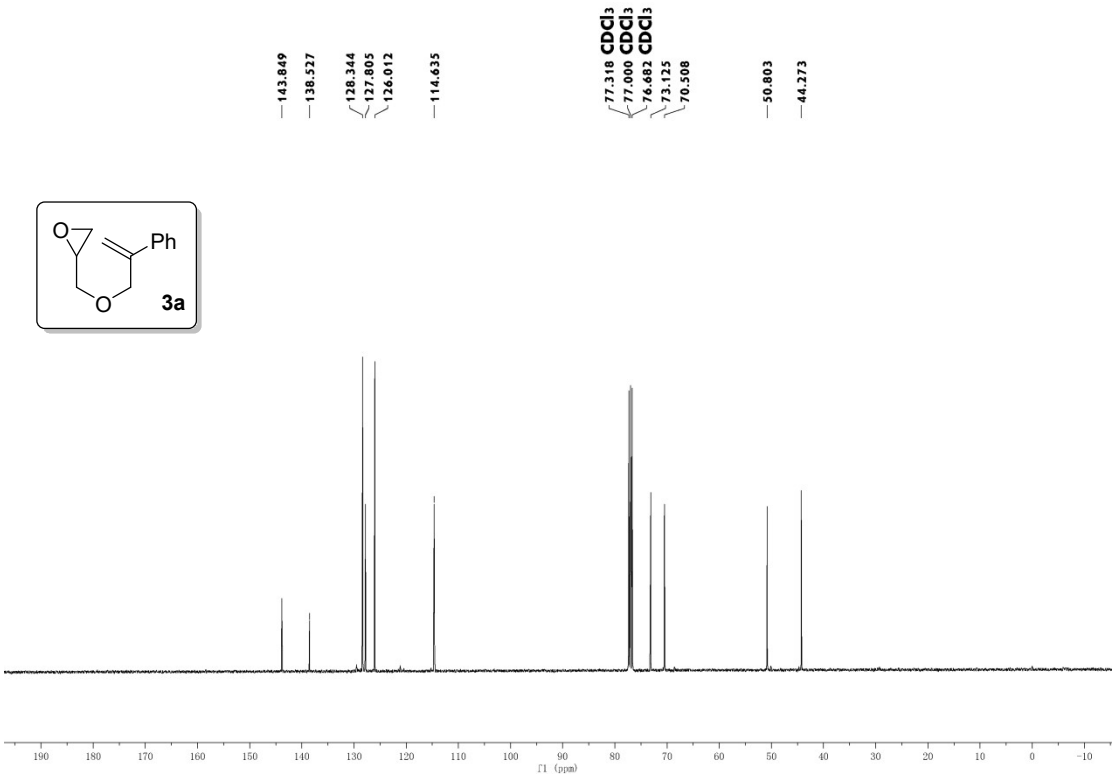
5.348
4.489
4.457
4.422
4.390
3.783
3.776
3.754
3.747
3.465
3.451
3.436
3.422
3.173
3.166
3.159
3.151
3.143
3.136
3.128
3.123
2.778
2.767
2.755
2.592
2.585
2.579
2.572
O
Ph
O
3a
1.94
3.00
1.00
1.01
1.00
1.01
1.00
1.00
0.95
1.01
1.00
f1 (ppm)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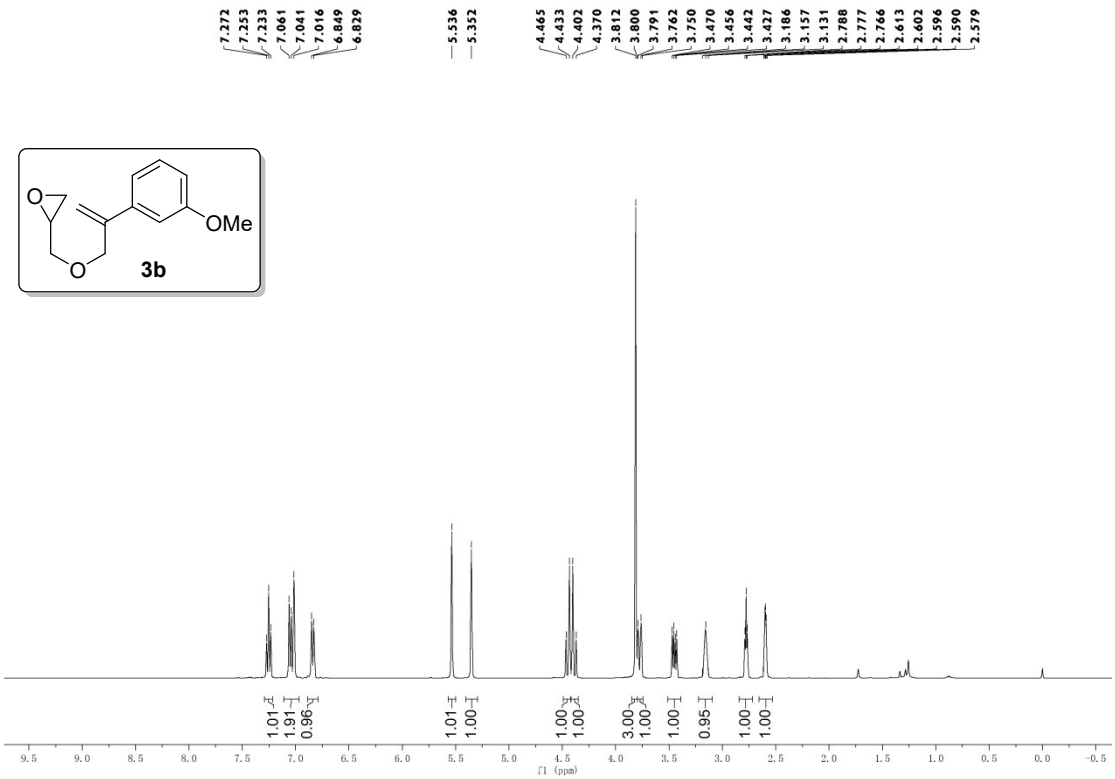
127.805
126.012
114.635
77.318 CDCl3
77.000 CDCl3
76.682 CDCl3
73.125
70.508
50.803
44.273
O
O
Ph
3a
f1 (ppm)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6.829
5.536
5.352
4.465
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4.402
4.370
3.812
3.800
3.791
3.762
3.750
3.470
3.456
3.442
3.427
3.186
3.157
3.131
2.788
2.777
2.766
2.613
2.602
2.596
2.590
2.579
O
O
OMe
3b
1.01
1.91
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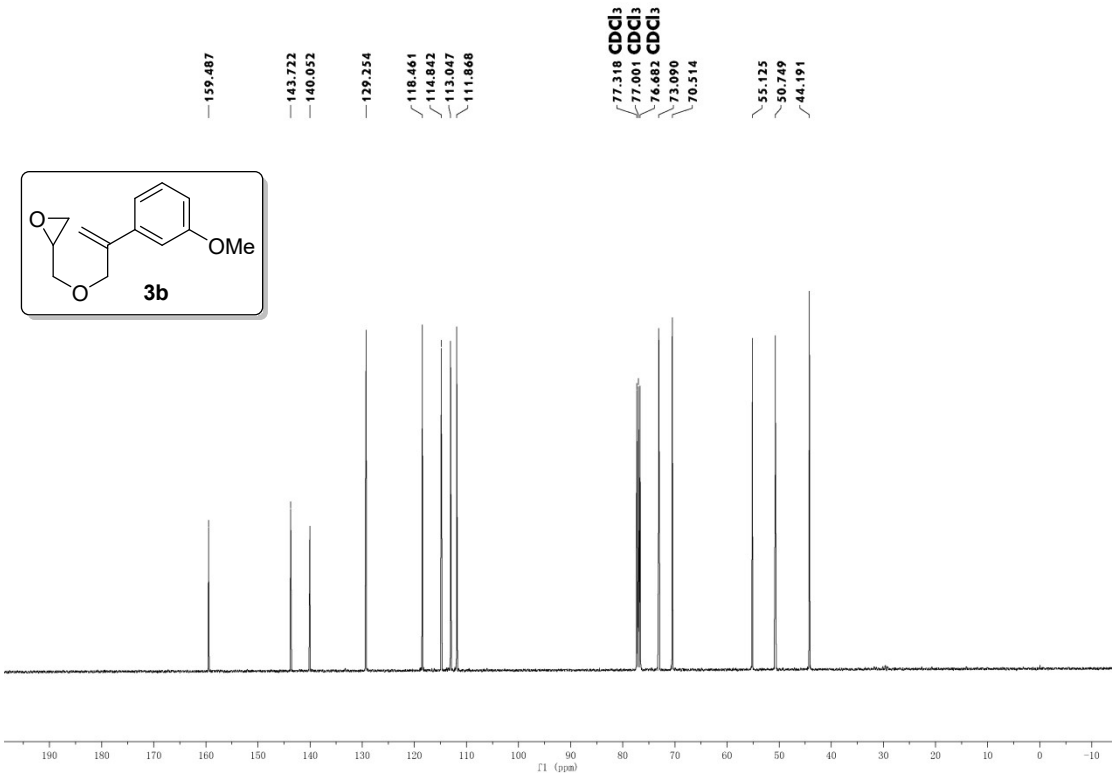
1.01
1.00
1.00
1.00
3.00
1.00
1.00
0.95
1.00
1.00
f1 (ppm)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129.254
118.461
114.842
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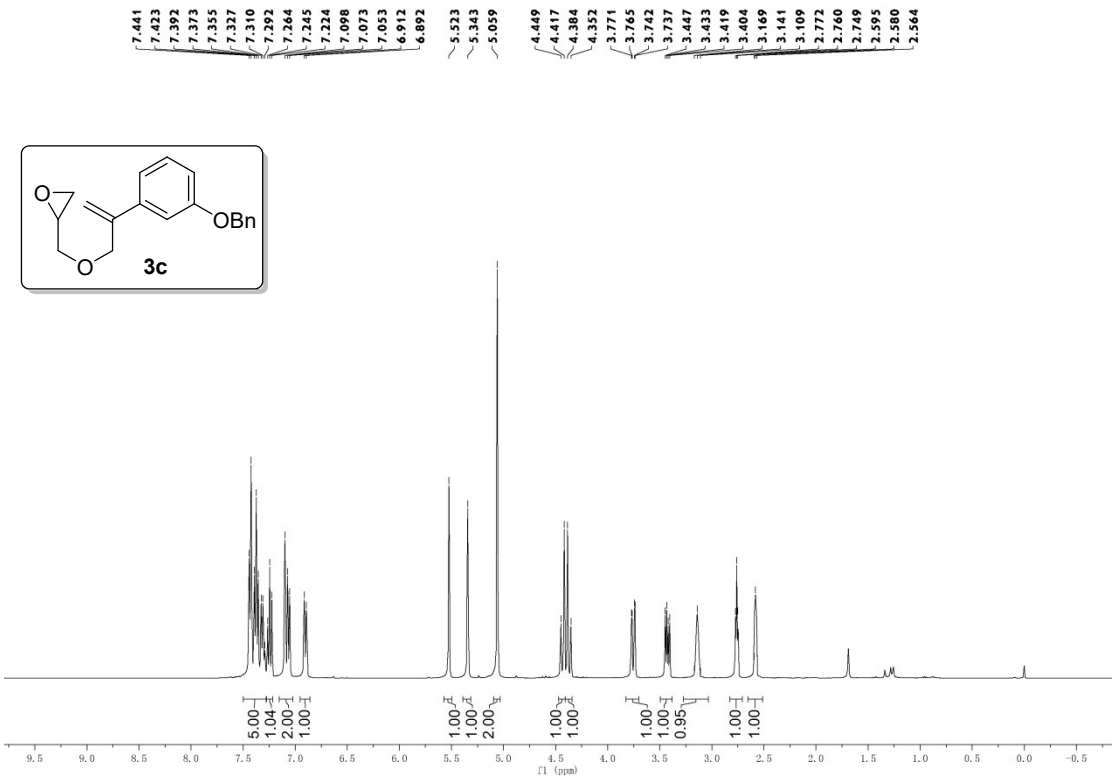
111.868
77.318 CDCl3
77.001 CDCl3
76.682 CDCl3
73.090
70.514
55.125
50.749
44.191
OMe
3b
f1 (ppm)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7.423
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7.292
7.284
7.245
7.224
7.098
7.073
7.053
6.912
6.892
5.523
5.343
5.059
4.449
4.417
4.384
4.352
3.771
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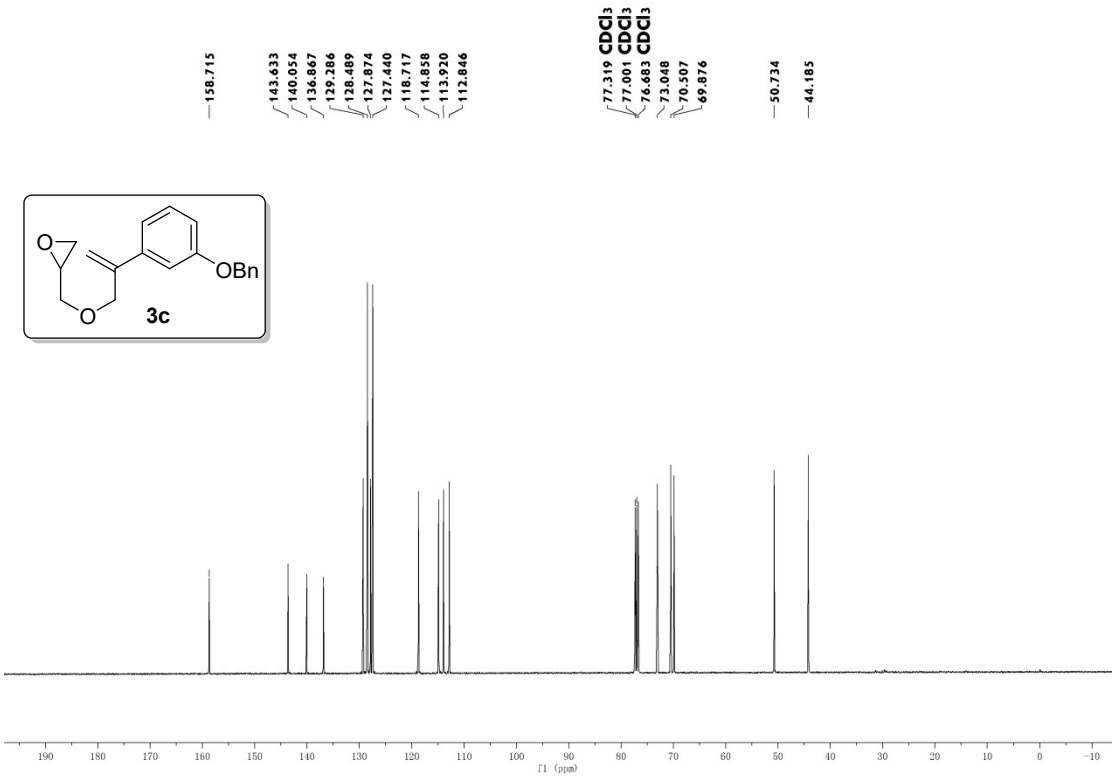
2.772
2.760
2.749
2.595
2.580
2.564
OBn
3c
5.00
1.04
2.00
1.00
1.00
1.00
2.00
1.00
1.00
1.00
1.00
0.95
1.00
1.00
f1 (ppm)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140.054
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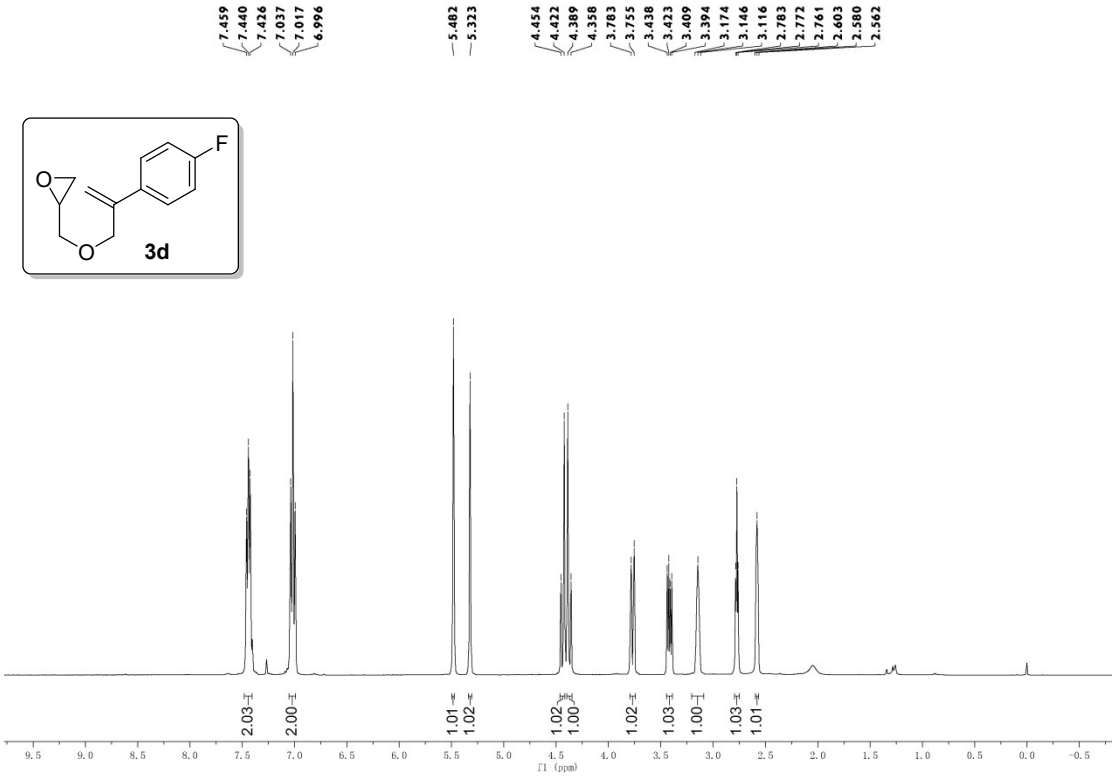
128.489
127.874
127.440
118.717
114.858
113.920
112.846
77.319 CDCl3
77.001 CDCl3
76.683 CDCl3
73.048
70.507
69.876
50.734
44.185
O
O
OBn
3c
f1 (ppm)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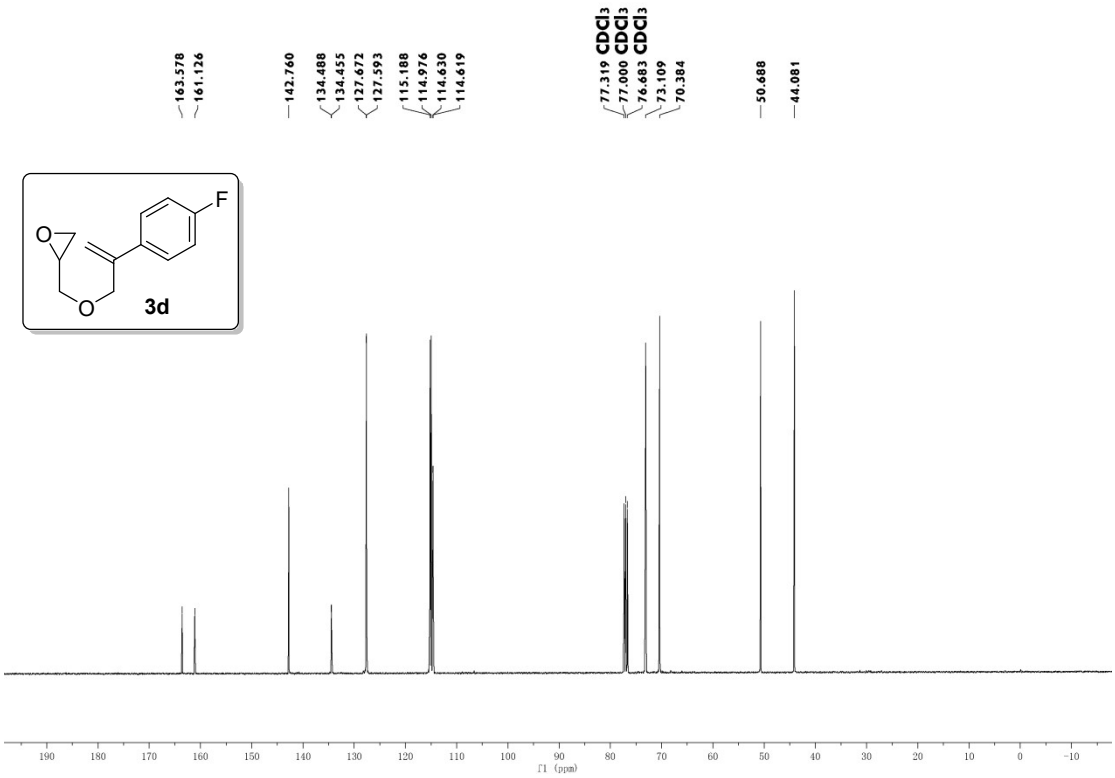
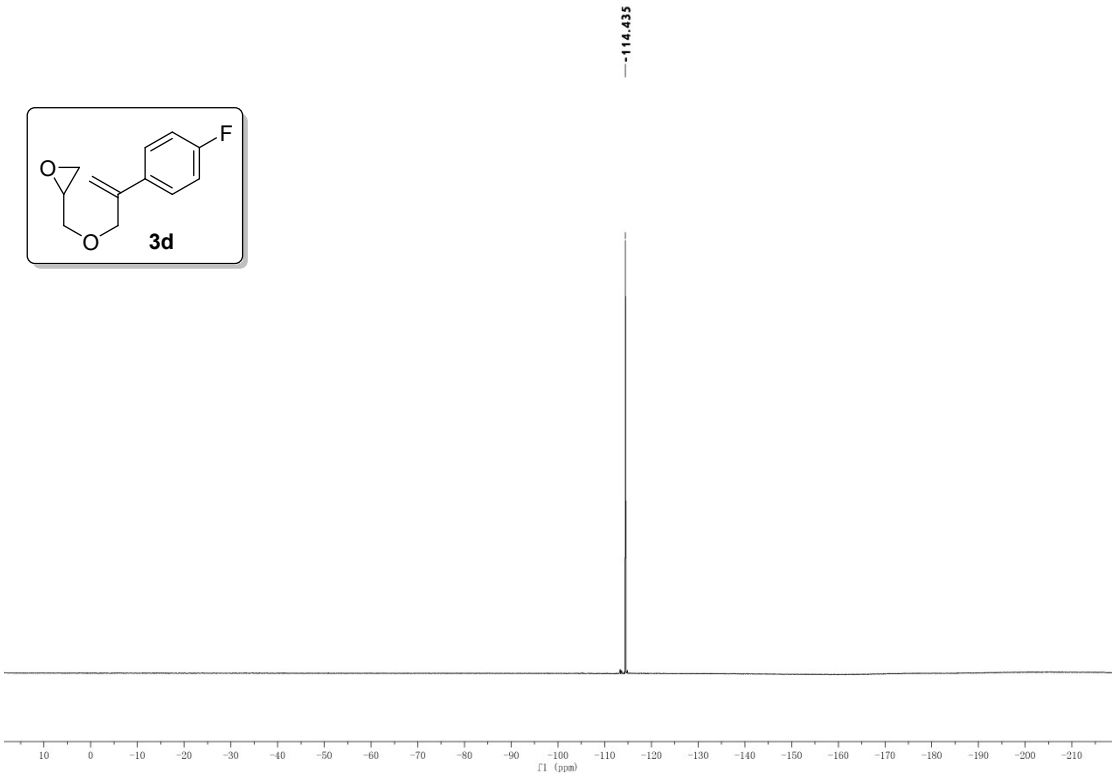
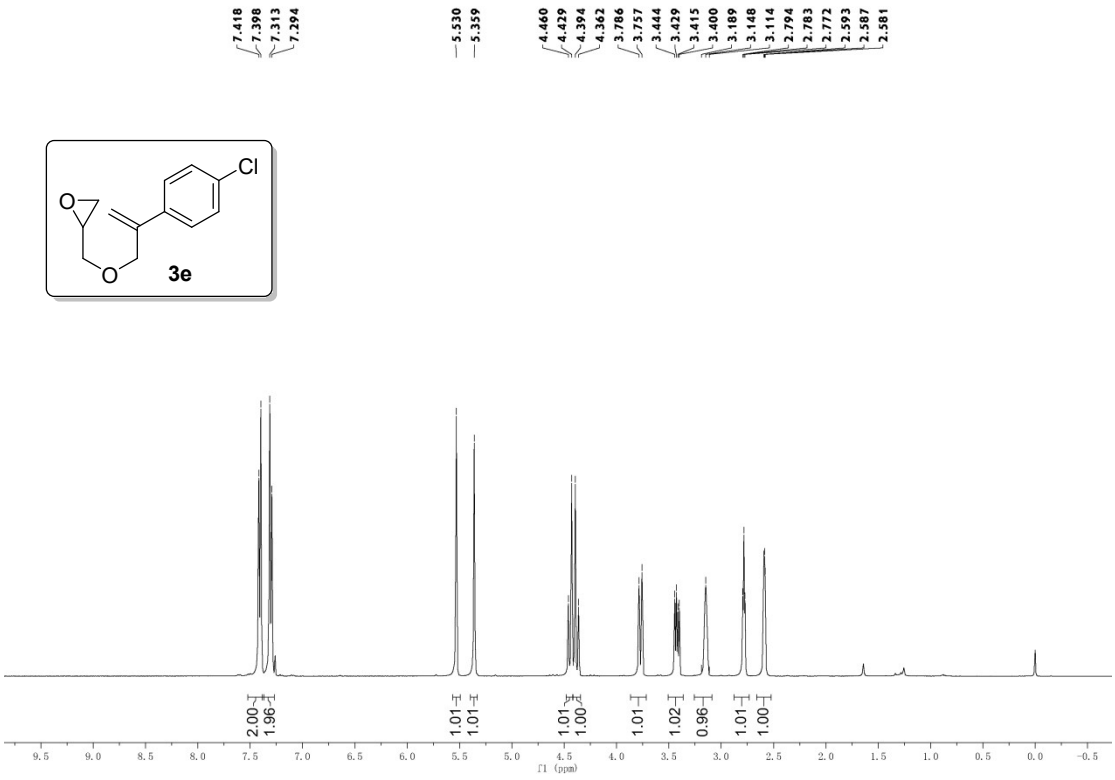
7.440
7.426
7.037
7.017
6.996
5.482
5.323
4.454
4.422
4.389
4.358
3.783
3.755
3.438
3.423
3.409
3.394
3.174
3.146
3.116
2.783
2.772
2.761
2.603
2.580
2.562
O
O
F
3d
2.03
2.00
1.01
1.02
1.02
1.00
1.02
1.03
1.00
1.03
1.01
f1 (ppm)


163.578
161.126
142.760
134.488
134.455
127.672
127.593
115.188
114.976
114.630
114.619
77.319 CDCl3
77.000 CDCl3
76.683 CDCl3
73.109
70.384
50.688
44.081
F
O
O
3d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-114.435
F
O
O
3d
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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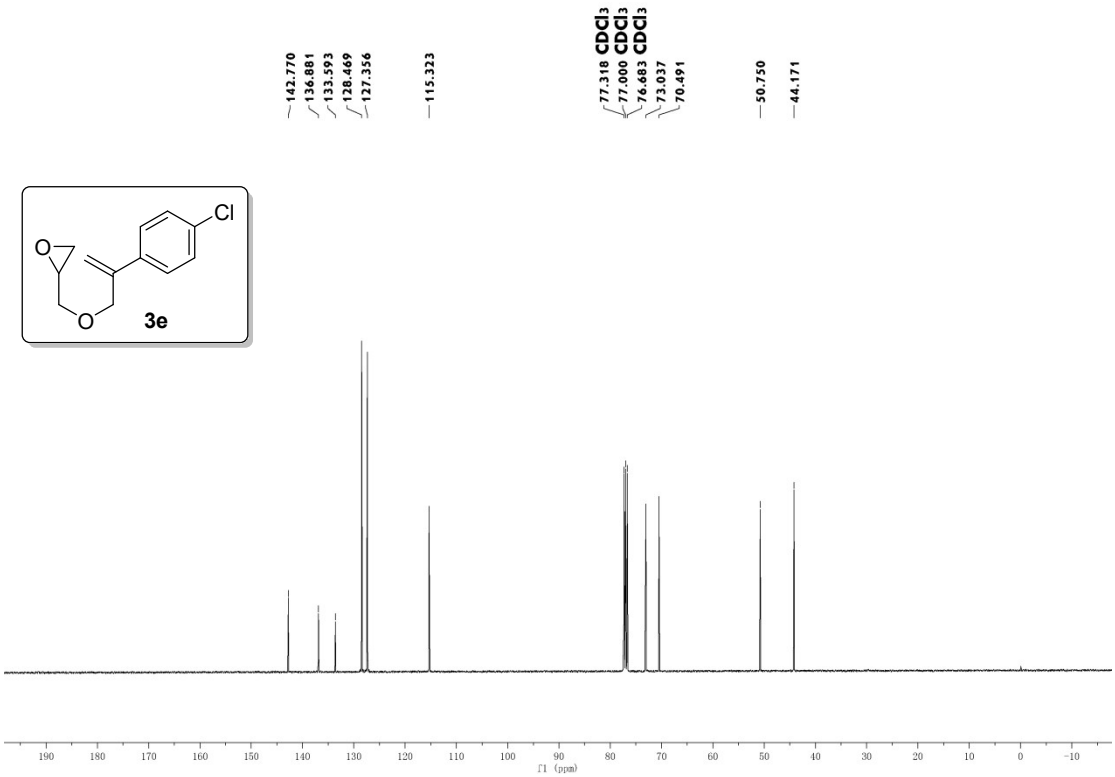
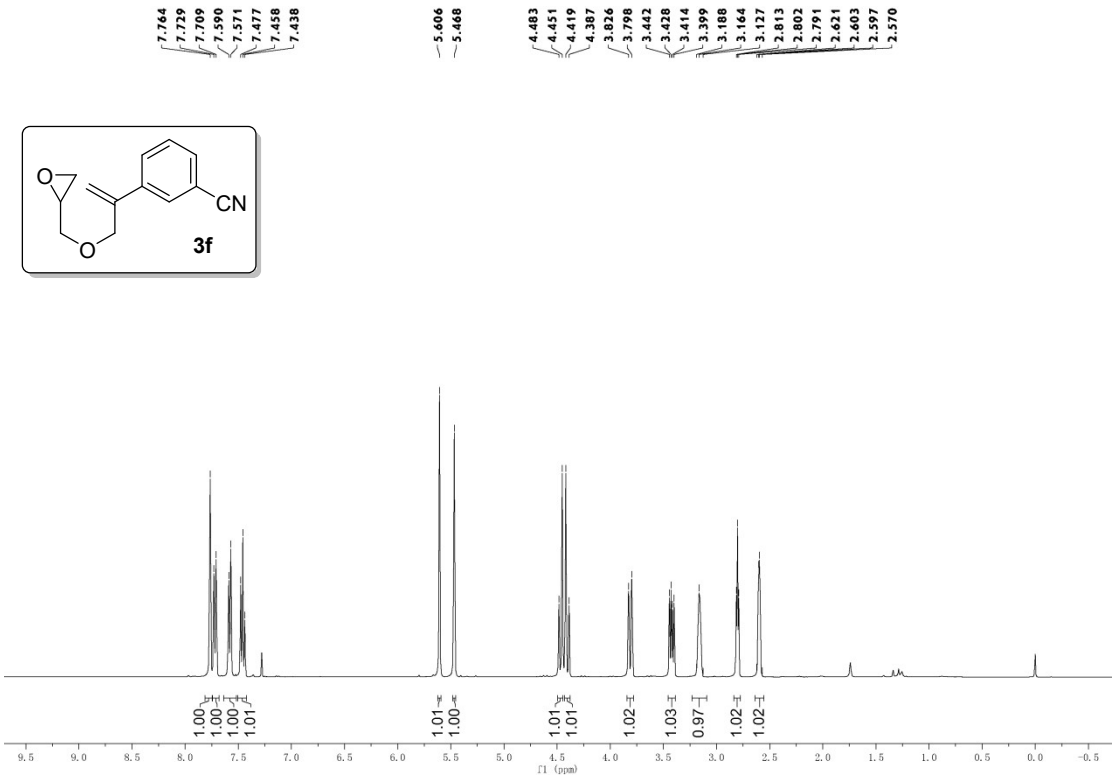
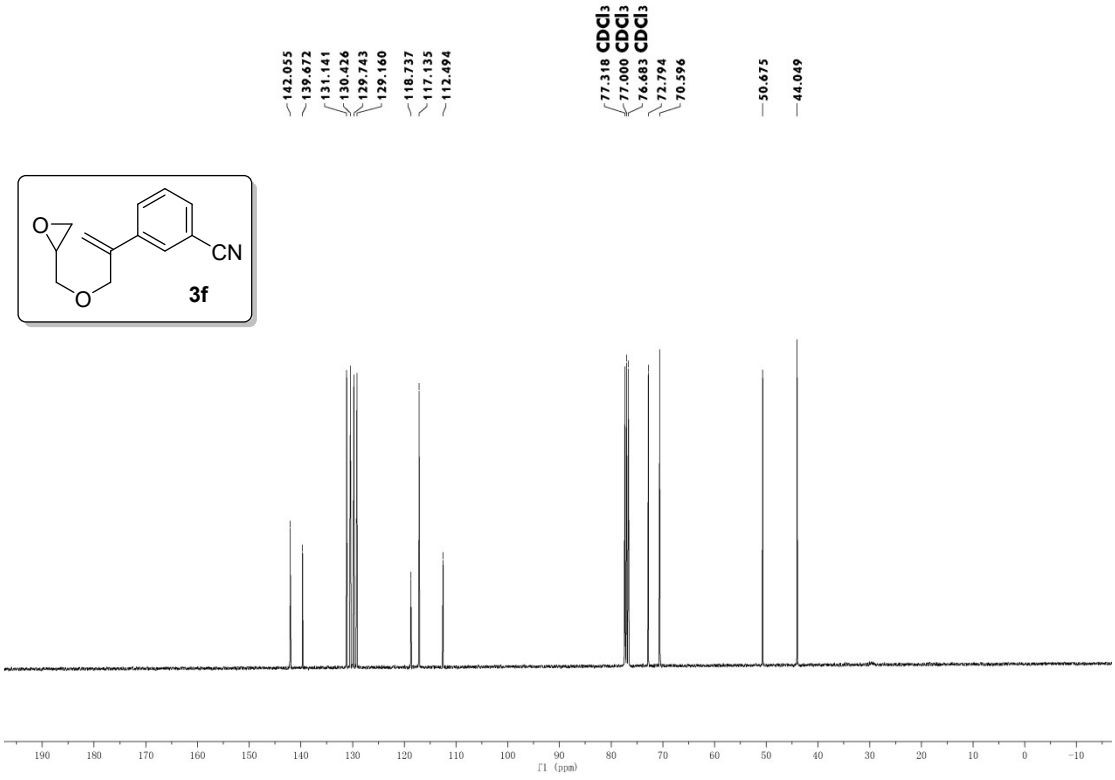
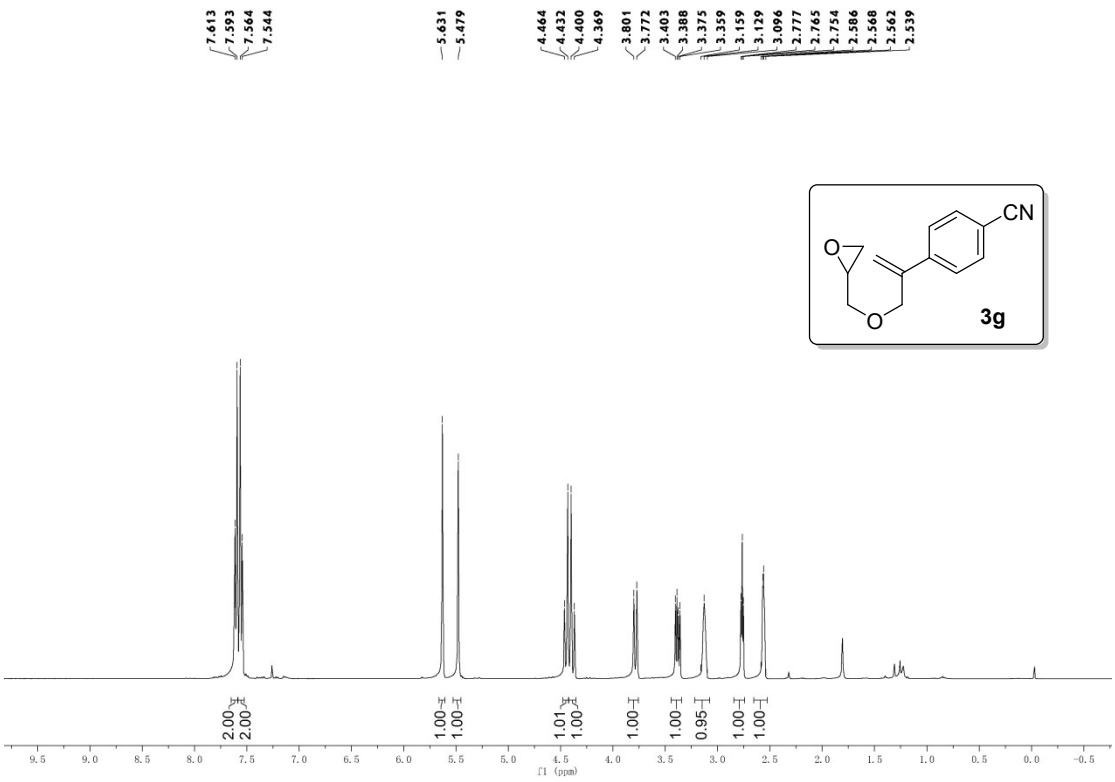
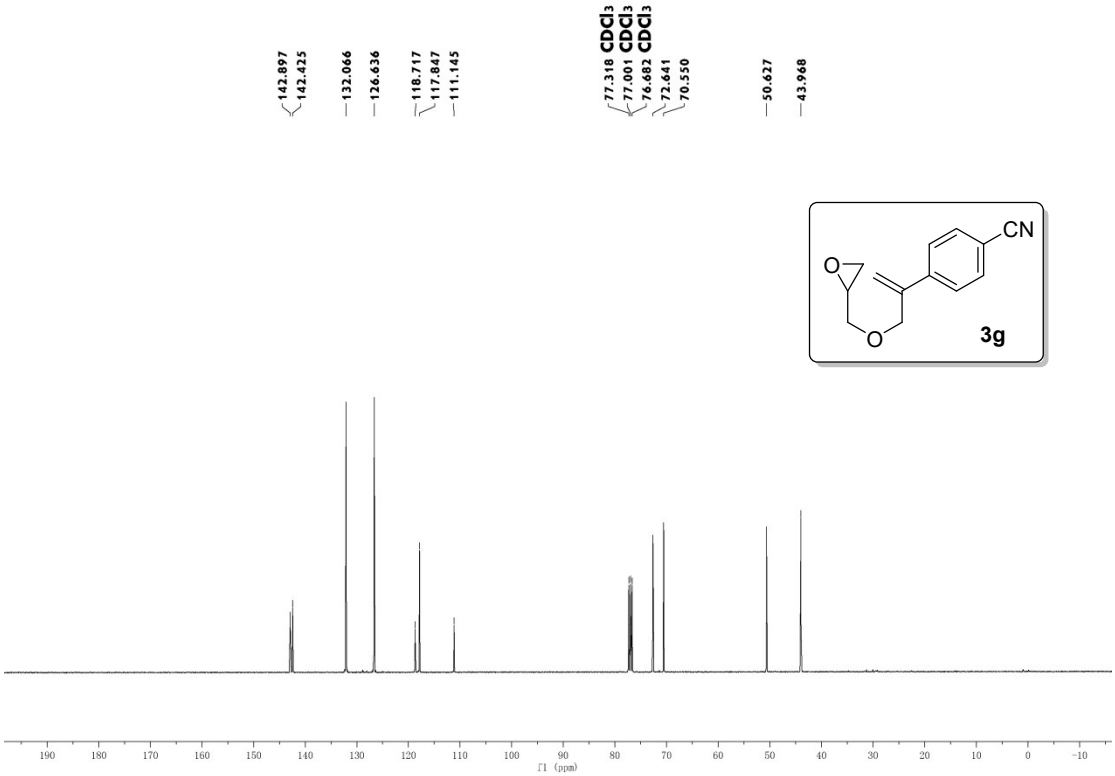
7.398
7.313
7.294
5.530
5.359
4.460
4.429
4.394
4.362
3.786
3.757
3.444
3.429
3.415
3.400
3.189
3.148
3.114
2.794
2.783
2.772
2.593
2.587
2.581
Cl
O
O
3e
2.00
1.96
1.01
1.01
1.01
1.00
1.01
1.02
0.96
1.01
1.00
f1 (ppm)

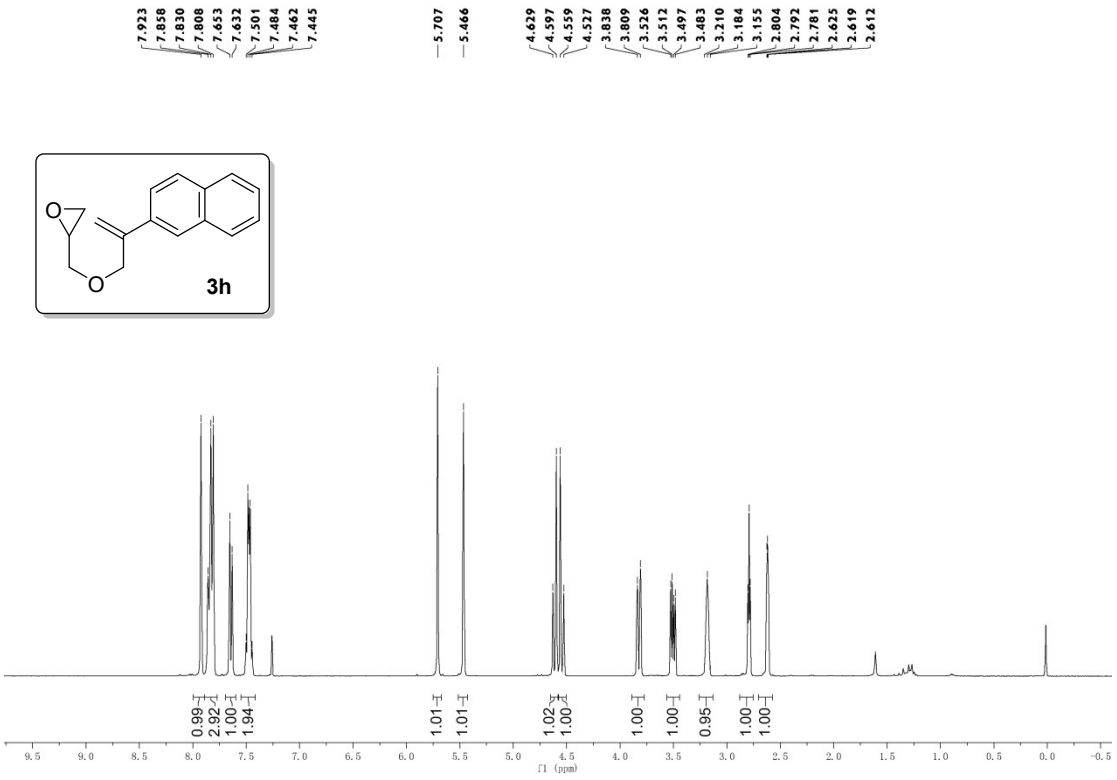

142.770
136.881
133.593
128.469
127.356
115.323
CDCl3
77.318
77.000
76.683
73.037
70.491
50.750
44.171
Cl
O
O
3e
f1 (ppm)


7.764
7.729
7.709
7.590
7.571
7.477
7.458
7.438
5.606
5.468
4.483
4.451
4.419
4.387
3.826
3.798
3.442
3.428
3.414
3.399
3.188
3.164
3.127
2.813
2.802
2.791
2.621
2.603
2.597
2.570
O
CN
O
3f
1.00
1.00
1.00
1.01
1.01
1.00
1.01
1.01
1.02
1.03
0.97
1.02
1.02
f1 (ppm)


142.055
139.672
131.141
130.426
129.743
129.160
118.737
117.135
112.494
CDCl3
CDCl3
CDCl3
77.318
77.000
76.683
72.794
70.596
50.675
44.049
O
CN
O
3f
f1 (ppm)


7.613
7.593
7.564
7.544
5.631
5.479
4.464
4.432
4.400
4.369
3.801
3.772
3.403
3.388
3.375
3.359
3.159
3.129
3.096
2.777
2.765
2.754
2.586
2.568
2.562
2.539
CN
O
O
3g
2.00
2.00
1.00
1.00
1.01
1.00
1.00
1.00
0.95
1.00
1.00
f1 (ppm)


142.897
142.425
132.066
126.636
118.717
117.847
111.145
CDCl3
CDCl3
CDCl3
77.318
77.001
76.682
72.641
70.550
50.627
43.968
CN
O
O
3g
f1 (ppm)


7.923
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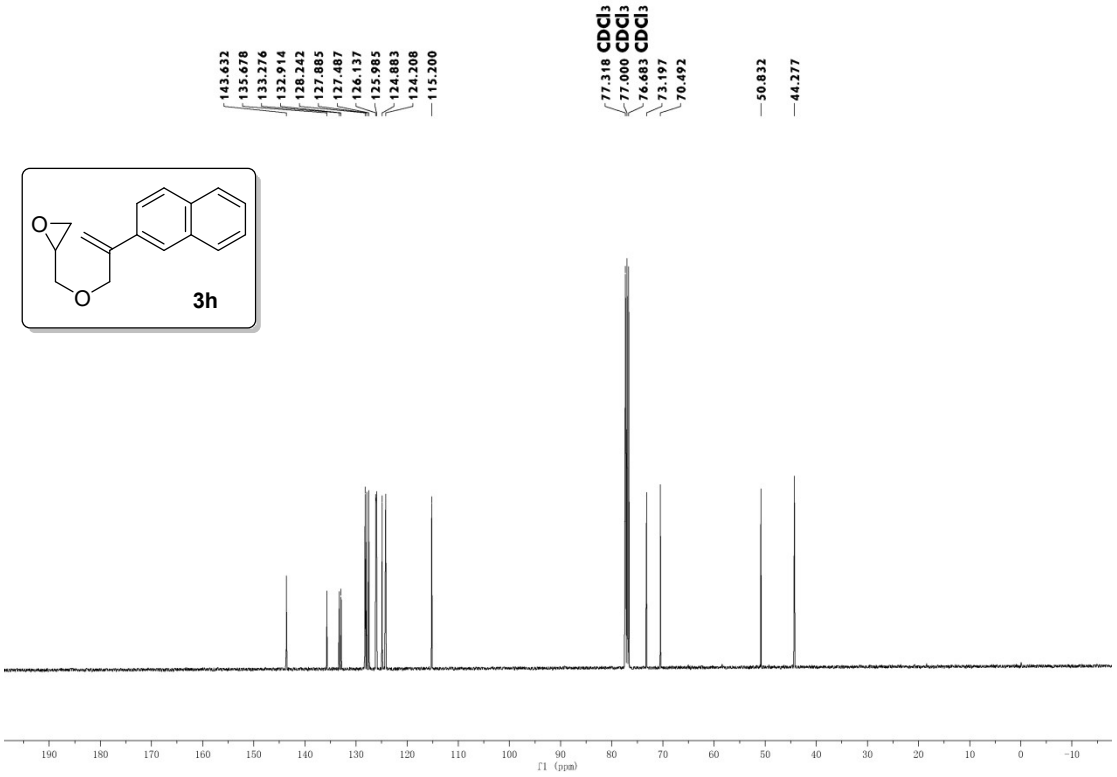
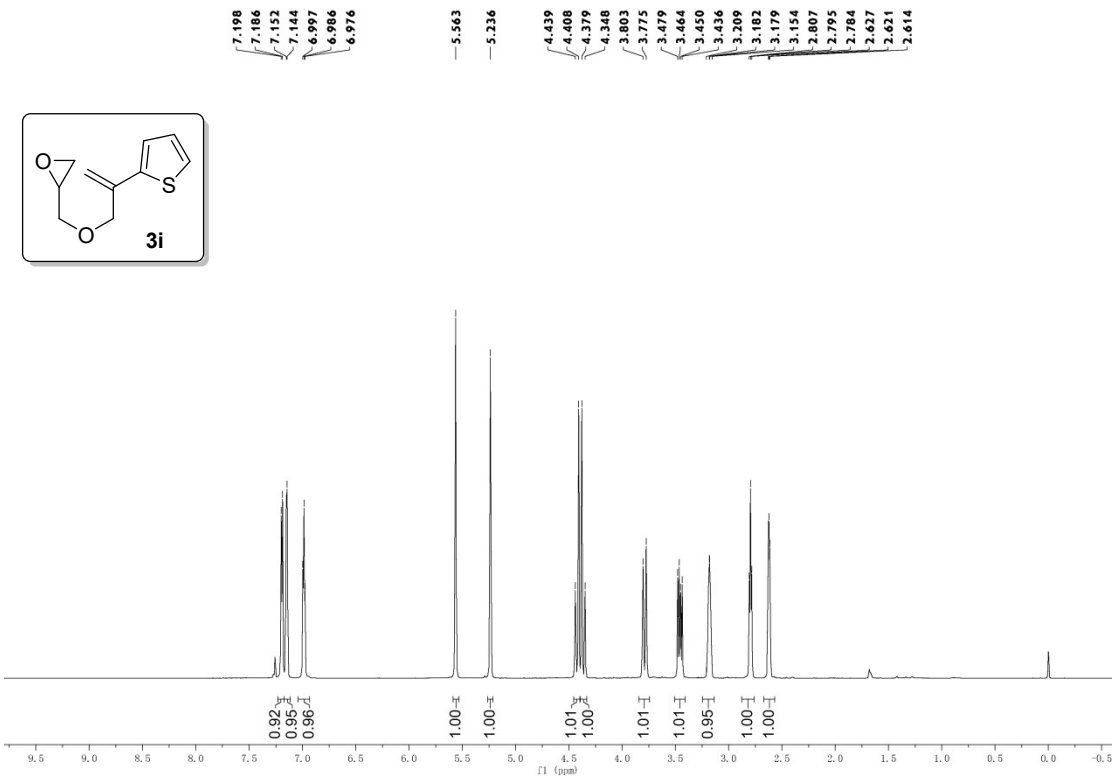
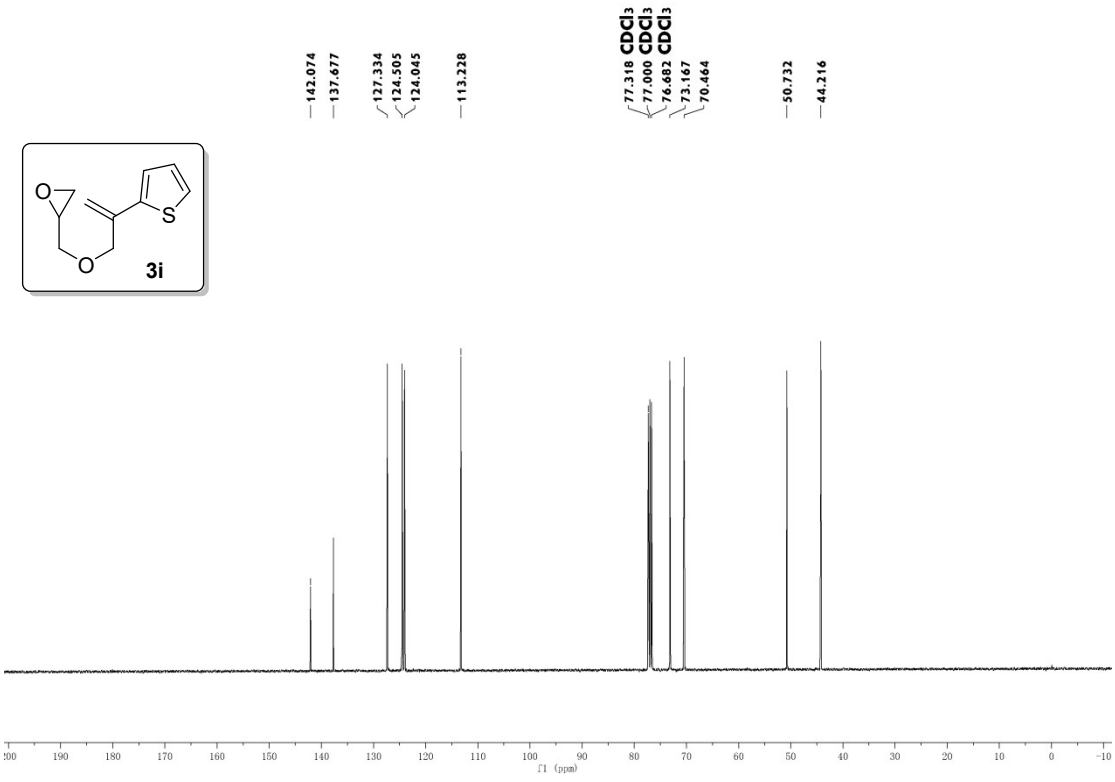
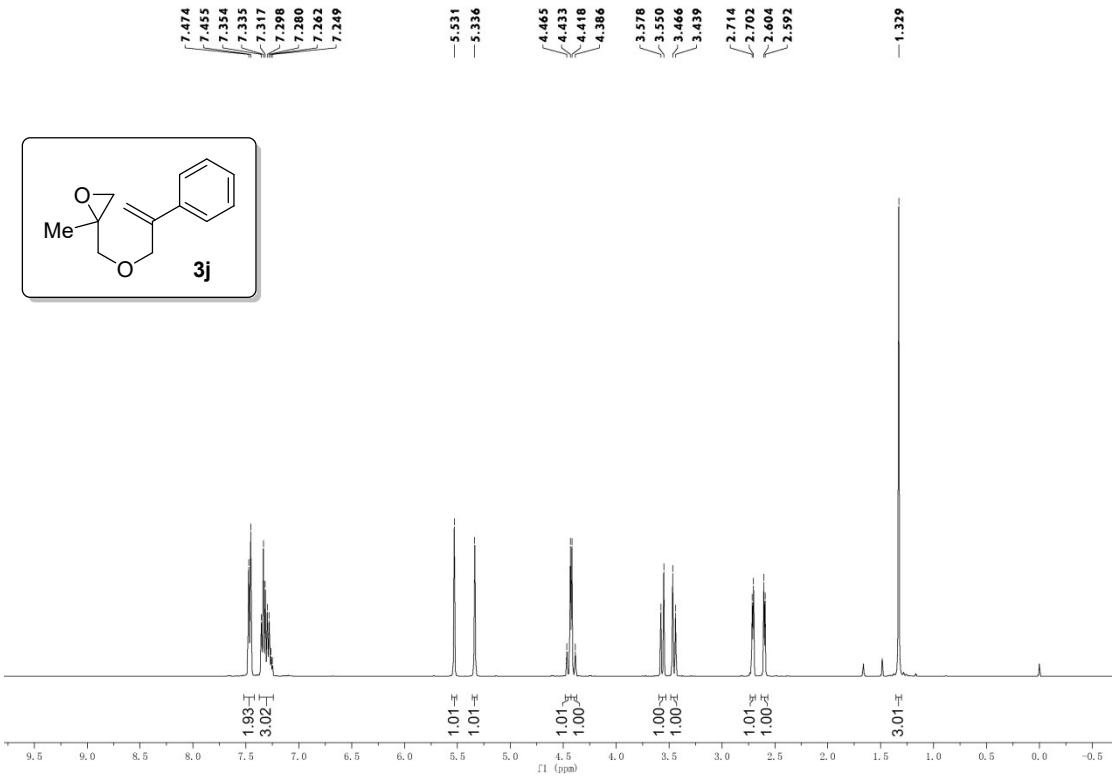
7.830
7.808
7.653
7.632
7.501
7.484
7.462
7.445
5.707
5.466
4.629
4.597
4.559
4.527
3.838
3.809
3.526
3.512
3.497
3.483
3.210
3.184
3.155
2.804
2.792
2.781
2.625
2.619
2.612
3h
0.99
2.92
1.00
1.94
1.01
1.01
1.02
1.00
1.00
1.00
0.95
1.00
1.00
f1 (ppm)


143.632
135.678
133.276
132.914
128.242
127.885
127.487
126.137
125.985
124.883
124.208
115.200
CDCl3
CDCl3
CDCl3
77.318
77.000
76.683
73.197
70.492
50.832
44.277
3h
f1 (ppm)


7.198
7.186
7.152
7.144
6.997
6.986
6.976
5.563
5.236
4.439
4.408
4.379
4.348
3.803
3.775
3.479
3.464
3.450
3.436
3.209
3.182
3.179
3.154
2.807
2.795
2.784
2.627
2.621
2.614
O
S
O
3i
0.92
0.95
0.96
1.00
1.00
1.01
1.00
1.01
1.01
0.95
1.00
1.00
f1 (ppm)


142.074
137.677
127.334
124.505
124.045
113.228
77.318 CDCl3
77.000 CDCl3
76.682 CDCl3
73.167
70.464
50.732
44.216
O
S
O
3i
f1 (ppm)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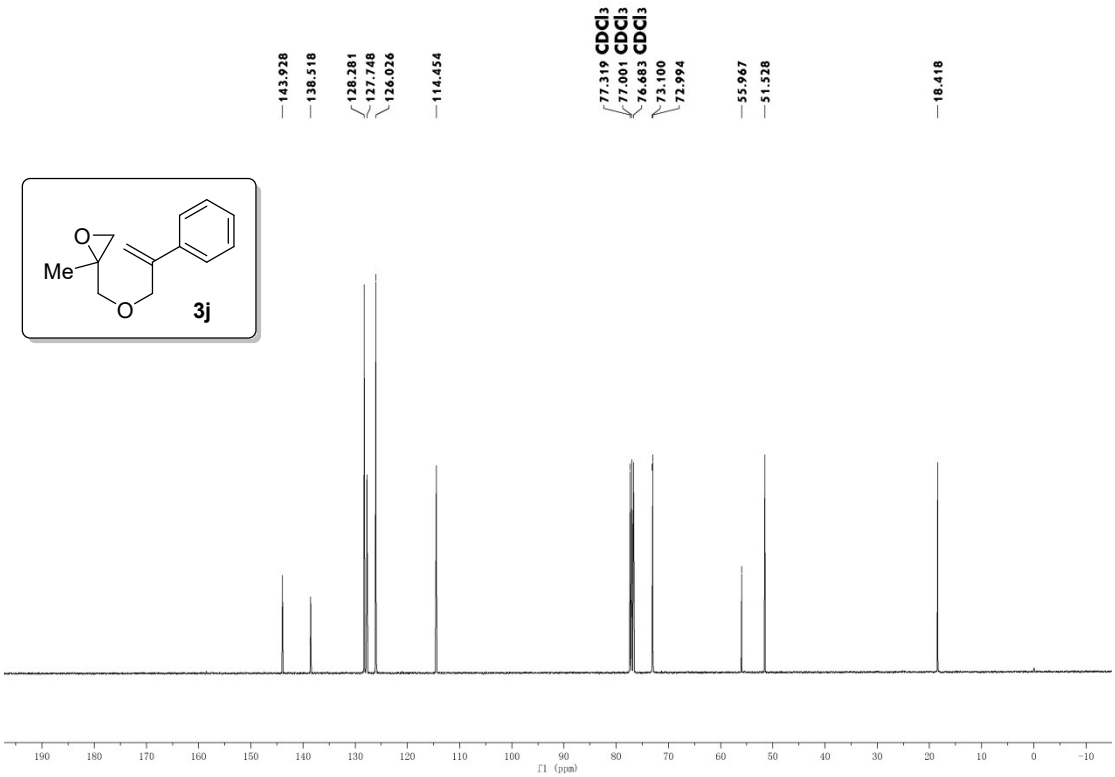
7.354
7.335
7.317
7.298
7.280
7.262
7.249
5.531
5.336
4.465
4.433
4.418
4.386
3.578
3.550
3.466
3.439
2.714
2.702
2.604
2.592
1.329
Me
O
O
3j
1.93
3.02
1.01
1.01
1.01
1.00
1.00
1.00
1.01
1.00
3.01
f1 (ppm)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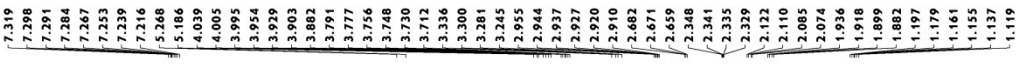
126.026
114.454
CDCl3
77.319
77.001
76.683
73.100
72.994
55.967
51.528
18.418
Me
O
O
3j
f1 (ppm)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7.267
7.253
7.239
7.216
5.268
5.186
4.039
4.005
3.995
3.954
3.929
3.903
3.882
3.791
3.777
3.756
3.748
3.730
3.712
3.336
3.300
3.281
3.245
2.955
2.944
2.937
2.927
2.920
2.910
2.682
2.671
2.659
2.348
2.341
2.335
2.329
2.122
2.110
2.085
2.074
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1.918
1.899
1.882
1.197
1.179
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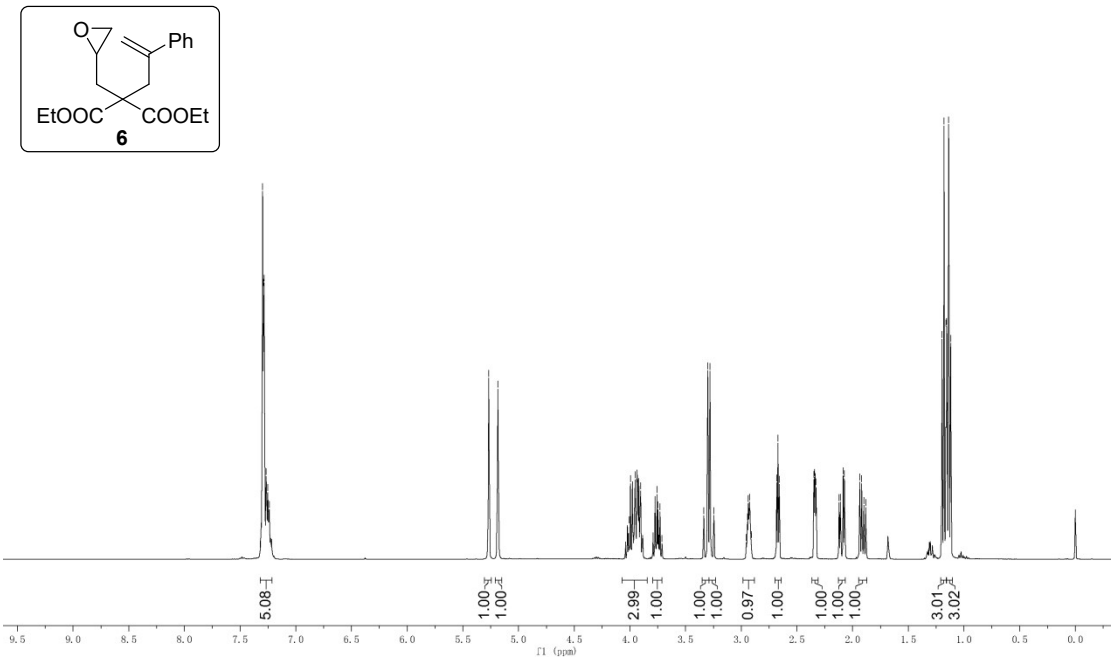
1.155
1.137
1.119


O
Ph
EtOOC
COOEt
6
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1.00
1.00
2.99
1.00
1.00
1.00
0.97
1.00
1.00
1.00
1.00
3.01
3.02
f1 (ppm)


170.621
170.512
144.235
141.490
127.979
127.507
126.858
118.943
77.318 CDCl3
77.000 CDCl3
76.683 CDCl3
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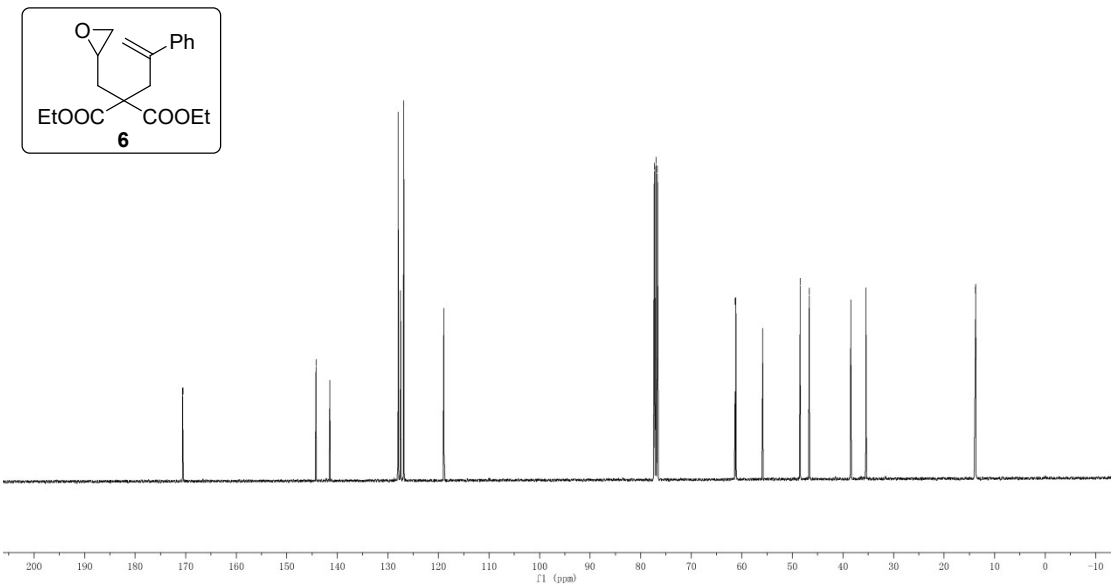
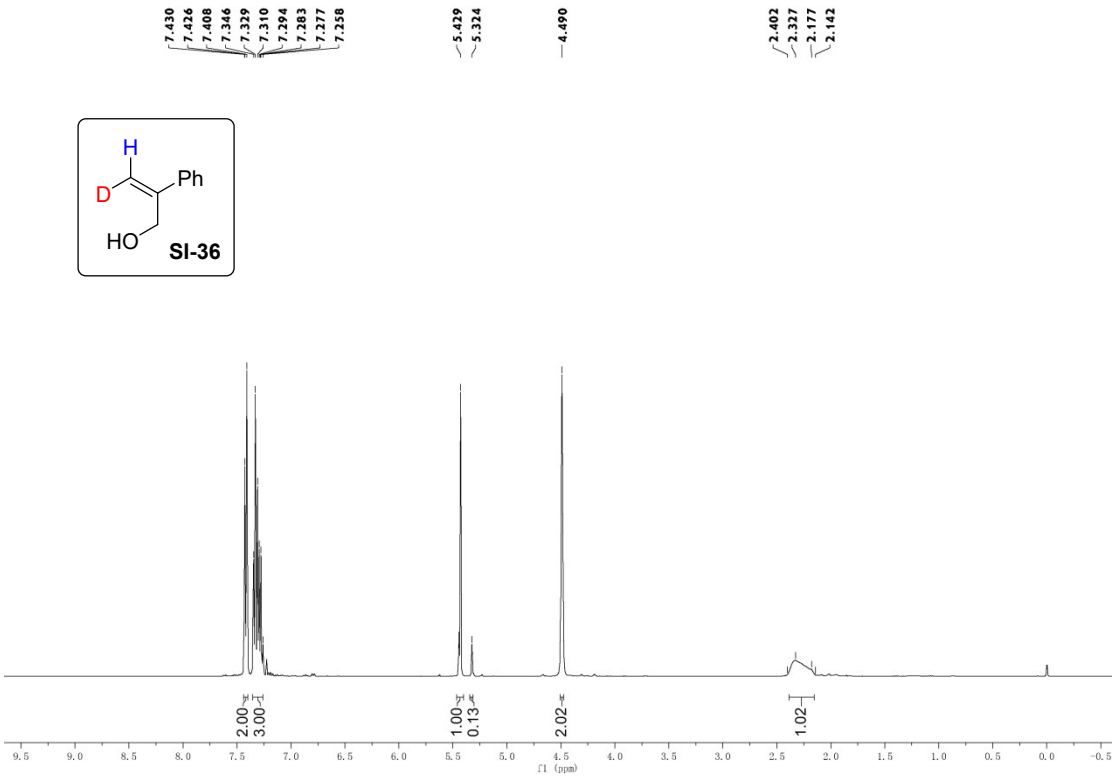
61.163
55.882
48.453
46.670
38.456
35.457
13.801
13.728


O
Ph
EtOOC
COOEt
6
f1 (ppm)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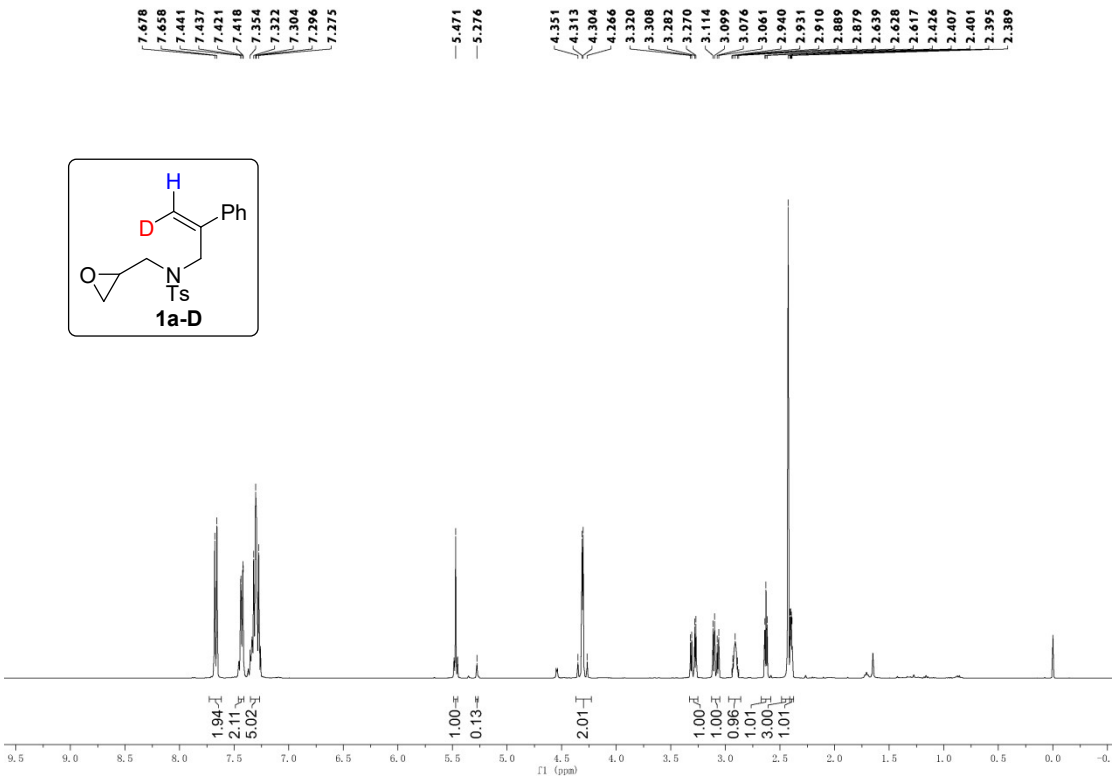
7.283
7.277
7.258
5.429
5.324
4.490
2.402
2.327
2.177
2.142
H
D
Ph
HO
SI-36
2.00
3.00
1.00
0.13
2.02
1.02
f1 (ppm)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7.322
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7.296
7.275
5.471
5.276
4.351
4.313
4.304
4.266
3.320
3.308
3.282
3.270
3.114
3.099
3.076
3.061
2.940
2.931
2.910
2.889
2.879
2.639
2.628
2.617
2.426
2.407
2.401
2.395
2.389
H
D
Ph
O
N
Ts
1a-D
1.94
2.11
5.02
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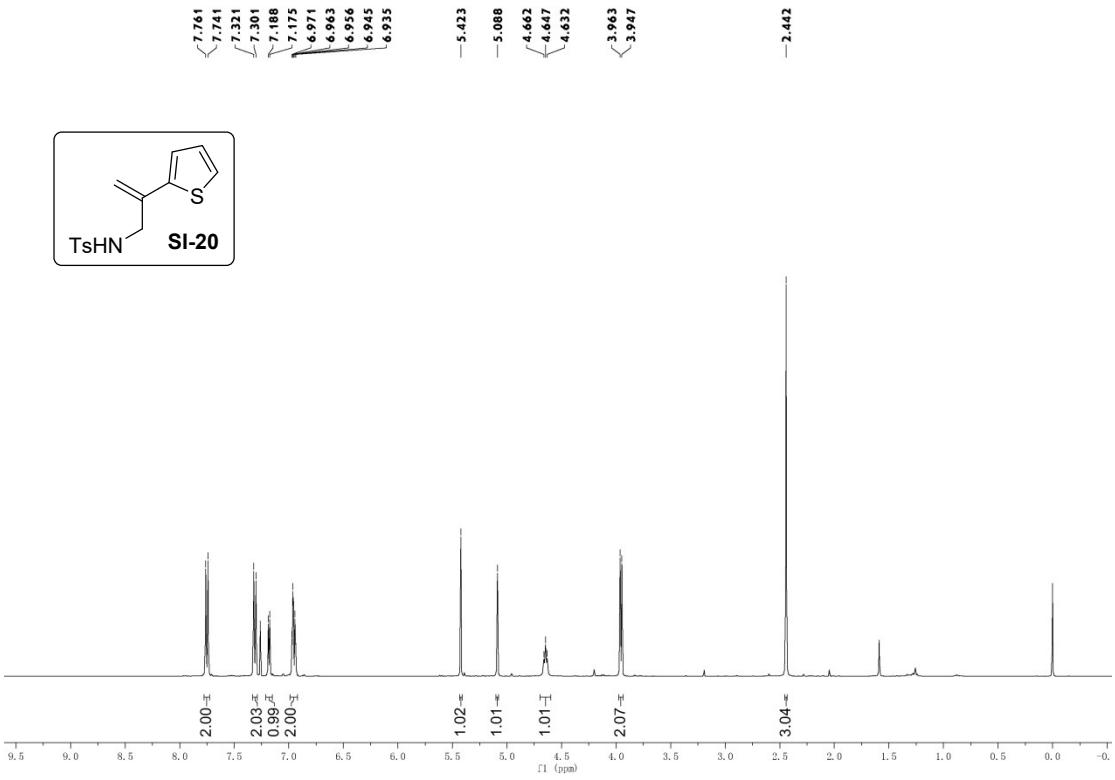
2.01
1.00
1.00
0.96
1.01
3.00
1.01
f1 (ppm)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7.741
7.321
7.301
7.188
7.175
6.971
6.963
6.956
6.945
6.935
5.423
5.088
4.662
4.647
4.632
3.963
3.947
2.442
TsHN
SI-20
2.00
2.03
0.99
2.00
1.02
1.01
1.01
2.07
3.04
f1 (ppm)