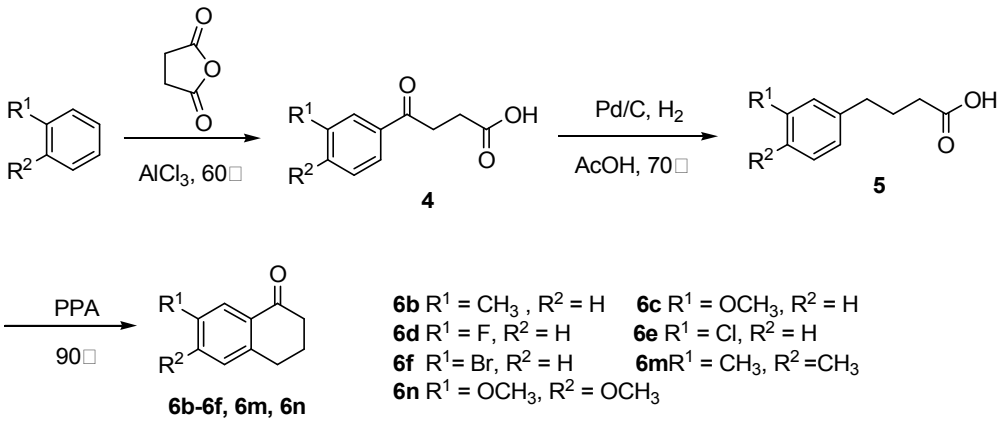
1. General remarks

Chemicals were purchased from commercial suppliers and used without further purification unless otherwise stated. Chiral phophoric acids **PA1-PA5** and racemic phophoric acid were purchased from commercial suppliers. Solvents were dried and purified according to the standard procedures before use. Reactions were monitored by TLC. Racemic products were obtained from corresponding substrates catalyzed by racemic phophoric acid at room temperature. Flash column chromatography was performed on silica gels (200-300 mesh). ^{1}H NMR and ^{13}C NMR (300 or 400 and 75 or 101 MHz, respectively) spectra were recorded on a Bruker 300 or 400 MHz NMR spectrometer in $CDCl_3$. ^{1}H NMR chemical shifts are reported in ppm (δ) relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard ($CDCl_3$, δ 7.26 ppm, DMSO-d_6 at 2.50 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, brs = broad singlet, d = doublet, t = triplet, td = triplet of doublets, q = quartet, m = multiplet), coupling constants (Hz) and integration. ^{13}C NMR chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard ($CDCl_3$, δ 77.0 ppm, DMSO-d_6 at 39.51 ppm). All enantiomeric ratios have been controlled by co-injections of the pure sample with the racemates. HRMS data were obtained on a Bruker Daltonics. Inc mass instrument (ESI). Chiralpak AD-H column was purchased from Daicel Chemical Industries (Hong Kong, China). Optical rotations were measured on a Perkin-Elmer 241 Polarimeter. Melting points were recorded on a Buchi Melting Point B-545.

2. Procedures and characterizations data of compounds.

2.1 Synthesis of Substituted Ketones 6

Method 1: [1,2]



To substituted benzene (10 mL), anhydrous aluminum chloride (4.8 g, 36 mmol) was added. Nitrobenzene (30 mL) was used as solvent. The mixture was stirred using a magnetic stirrer at room temperature for 30 min. To this mixture, succinic anhydride (3.0 g, 30 mmol) was added in five portions with continuous stirring. Vigorous reaction started with the evolution of HCl gas. Stirring was continued for overnight at 60℃. The mixture decomposed by adding ice-water . The reaction was extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with sat. $NaHCO_3$ (5 × 50 mL). The combined water layers were added 3 N HCl to adjust pH = 1−2 then produced white precipitate. It was filtered and the residue was washed with cold water and dried to give **4** in 50-80% yield.

To a three-necked flask was added compound **4** (10 mol), 30 mL AcOH and Pd/C (10%) and stirred under H_2 atmosphere in 70℃. The reaction was monitored by TLC. When the reaction was completed, The reaction mixture was filtered through a Celite pad which was washed with acetic acid, then concentrated in vacuo to give the crude **5**.

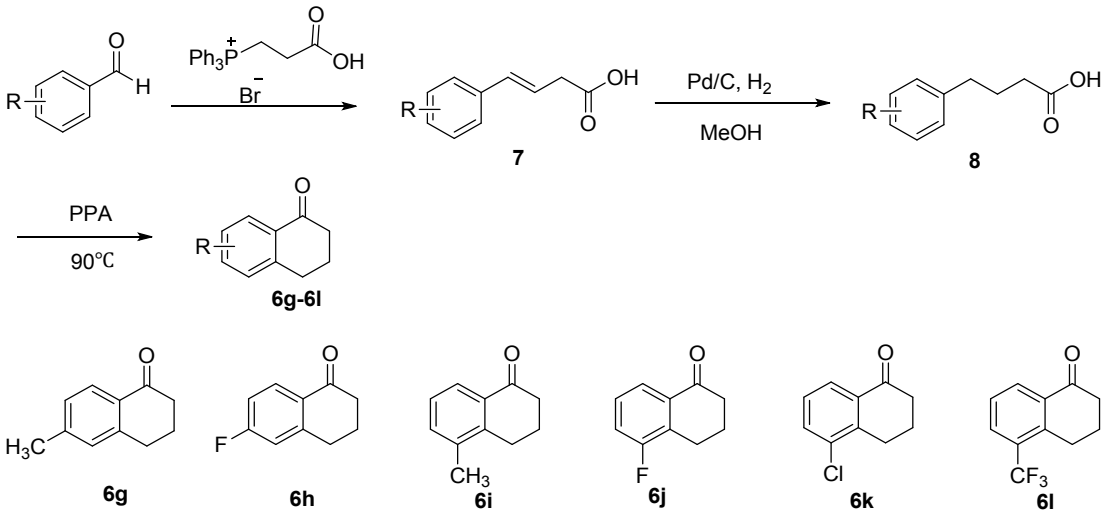
4-(4-chlorophenyl)butanoic acid and 4-(4-bromophenyl)butanoic acid were prepared according to a known procedure[2] with minor modification:

4-(4-chlorophenyl)-4-oxobutanoic acid or 4-(4-bromophenyl)-4-oxobutanoic acid 10 mmol) was dissolved in diethylene glycol (30 mL) and hydrazine hydrate (80% aqueous, 3 mL) was added. After stirring at RT for 30 min, potassium hydroxide (3.0 g) was added and the mixture was brought to reflux (~130 °C) for 1.5 h. The temperature was gradually increased to distill low boiling material until the bath temperature reached 190 °C and then the reaction was refluxed for 6 h. After cooling, the reaction mixture was poured into water, acidified with HC1

to pH 2 and extracted with diethyl ether (5 × 50 mL). The combined organic extracts were backwashed with water (2 × 30 mL) and brine (25 mL), dried over anhydrous Na_2SO_4 and the solvent evaporated to give the crude **5**.

The crude compound **5** was dissolved in polyphosphoric acid, and stirred at 90℃. The reaction was monitored by TLC. When the reaction was completed, the mixtures were poured into ice-water then extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and the solvent was removed in vacuo The residue was subjected to flash column chromatography (PE : EA = 50:1 to 30:1) to give the desired product **6**. Total yield of the two-step reaction was 60-80%.

Method 2 :



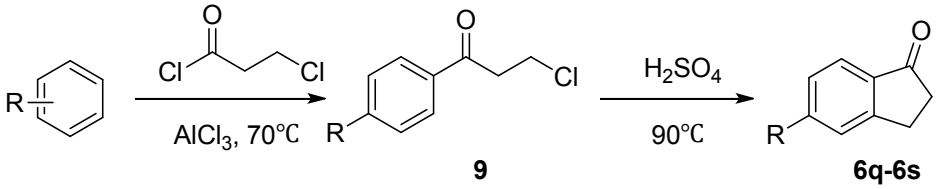
Compounds **7** were prepared according to a known procedure[3] with minor modification: A three-neck 100 mL round-bottom flask was charged with substituted benzaldehyde (10 mol) and (2-caroboxyethyl)triphenylphosphonium bromide (4.98 g, 12 mmol). Then dry THF (25 mL) was added to the mixture under N_2. The reaction mixture was cooled to 0℃, then LiHMDS (1mol /L in THF, 25 mL) was added slowly to the mixture. The solution was stirred at 0℃ for 15 min before the solution was stirred at room temperature for overnight. The resulting reaction mixture was concentrated in vacuo and the residue was treated with aqueous NaOH. The mixture was washed with CH_2Cl_2 for three times. 3N HCl was added to aqueous NaOH at 0℃ and the solution was stirred at 0℃. After 1 h, CH_2Cl_2 was added to the aqueous

solution, and the organic phase was washed with H_2O, dried over anhydride Na_2SO_4, and filtered. The filtrate was concentrated in vacuo to give the crude **7**.

To a three-necked flask was added the crude **7**, 20 mL of MeOH and Pd/C (10%) and stirred under H_2 atmosphere in rt. The reaction was monitored by TLC. When the reaction was completed, the mixtures were filtered through through a Celite pad then concentrated in vacuo to give the crude **8**.

Compounds **6g-6l** were prepared according to the procedure of **6a**.

Method 3[4] :

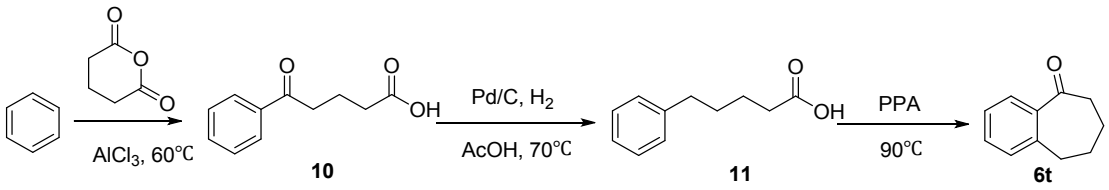


6q R = F
6r R = Cl
6s R = Br

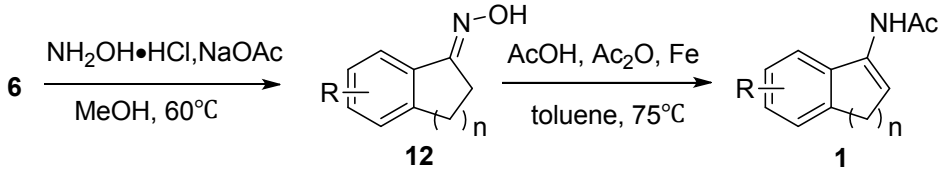
A solution of substituted benzene (3.1 mL, 20 mmol) and 3-chloro-propionyl chloride (1.9 ml, 20 mmol) in CH_2Cl_2 (25 mL) was added dropwise to a suspension of aluminum chloride (2.9 g, 22 mmol) in CH_2Cl_2 (30 mL) at 0° C. The reaction mixture was allowed to warm to ambient temperature, stirred for overnight, and quenched with water dropwise. The reaction mixture was washed with water, dried with anhydrous Na_2SO_4 and the filtrate was evaporated under reduced pressure to provide the compound **9** which were used without further purification in the next step.

The crude compound **9** was added to concd H_2SO_4. The mixture were stirred in 90℃. The reaction was monitored by TLC. When the reaction was completed, the mixture poured in to ice-water (200 mL), then extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO4 and the solvent was removed in vacuo The residue was subjected to flash column chromatography (PE : EA = 50:1 to 30:1) to give the desired product **6**. Total yield of the two-step reaction was 30-50%.

The compound **6t** were prepared as according to the the procedure of **6a**.

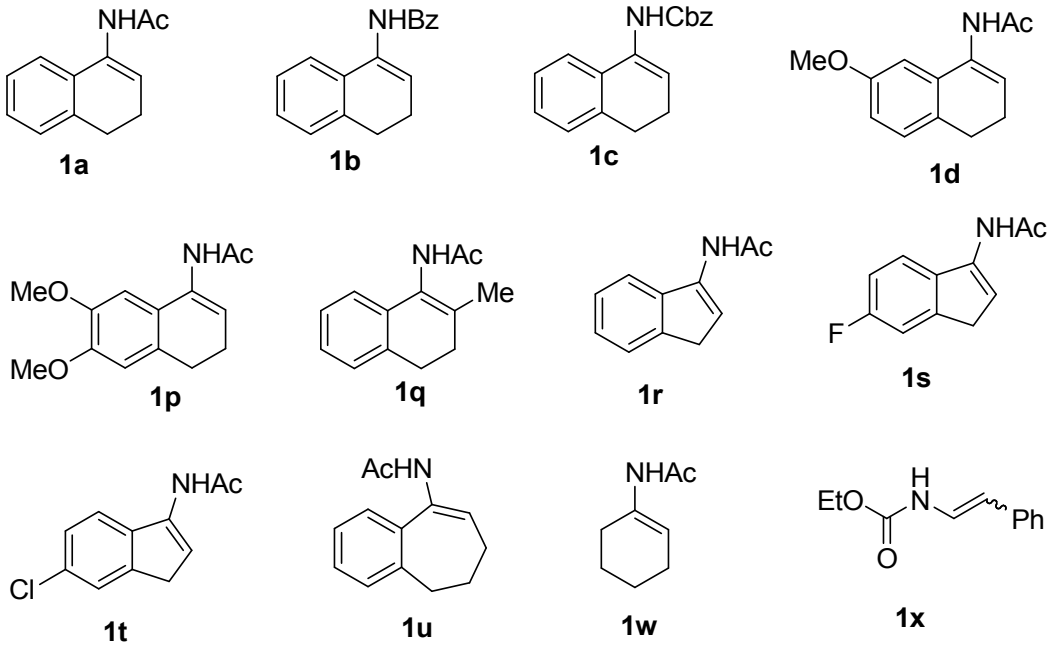


2.2 Synthesis of Enamides 1

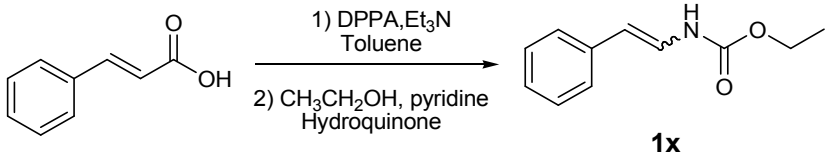


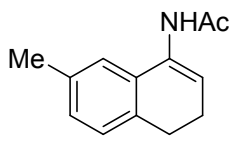
Compounds **12** were prepared according to a known procedure[5] with minor modification: The compound **6** (5 mmol), NaOAc (0.5 g, 6 mmol, 1.2 equiv) and hydroxylamine hydrochloride (0.42 g, 6 mmol, 1.2 equiv) in methanol (20 mL) was stirred for 2 h at 60ºC. The reaction mixture was allowed to be cooled to r.t., 30% NaOH (10 mL) was added before diluting with EA (50 mL). The mixtures were extracted with EtOAc (3 × 50 mL). The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered and concentrated to afford the crude ketoxime **12** which was used in next step directly.

Compounds **1** were prepared according to a known procedure[6]: Acetic anhydride (1.5 mL, 15 mmol) and acetic acid (0.9 mL, 15 mmol) was added to a solution of ketone oxime **7** (5 mmol) in toluene (20 mL). Fe powder (0.6 g, 10 mmol) was added and the mixture was heated to 75℃ for 5 h. After cooled to room temperature, the reaction mixture was filtered to remove the solid residues which were washed with EtOAc (2 × 20 mL). The combined filtrate was diluted with EtOAc (20 mL) and washed with 30% NaOH (2 × 20 mL). The organic phase was separated, dried over Na_2SO_4 and concentrated under reduced pressure. The obtained residue was chromatographed on a silica gel column eluted with PE:EA = 3:1 to afford the desired enamides **1**. Enamides **1a-1d**, **1p-1u**, **1w** are known compounds.[5-12]



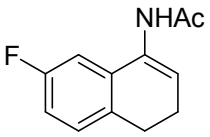
Enecarbamate **1x** was prepared according to a known procedure[13]: To a solution of the corresponding carboxylic acid (10 mmol) in toluene (70 mL), was added Et_3N (7 mL) and diphenylphosphoryl azide (DPPA, 8.6 mL). The mixture was stirred at RT overnight. Then the reaction was diluted in CH_2Cl_2 and washed with brine. The organic layer was dried over $NaSO_4$ and concentrated in vacuo. The crude acyl azide was purified by column chromatography on silica gel (PE/EA). Then, a solution of the acyl azide in toluene (50 mL) was added dropwise to a stirred mixture of hydroquinone (55 mg), pyridine (39.5mg), and benzyl alcohol (1.1 mL) at 100 °C. The mixture was then stirred for 30 min at 110 °C and the toluene was removed by rotary evaporation. The product was purified by column chromatography on silica gel(PE/EA) to afford the desired enecarbamate **1x**.



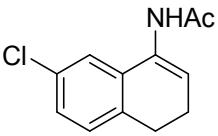


N-(7-methyl-3,4-dihydronaphthalen-1-yl)acetamide (1e): white solid, 50 % yield, ^{1}H NMR (300 MHz, DMSO) δ 9.07 (s, 1H), 7.09 – 7.01 (m, 2H), 6.97 (d, J = 7.6 Hz, 1H), 6.18 (t, J = 4.7 Hz, 1H), 2.63 (t, J = 7.9 Hz, 2H), 2.32 – 2.16 (m, 5H), 2.03 (s, 3H), ^{13}C NMR (75 MHz, DMSO) δ 168.9, 135.0, 133.1,

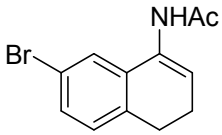
132.4, 131.6, 127.6, 127.3, 122.7, 118.8, 26.8, 23.4, 22.0, 21.0. HRMS (ESI) Calcd for $C_{13}H_{15}NONa^+$ $[M+Na]^+$ 224.1046; Found: 224.1048.



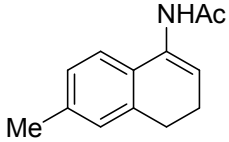
N-(7-fluoro-3,4-dihydronaphthalen-1-yl)acetamide (1f): yellow solid, 45 % yield, ^{1}H NMR (300 MHz, DMSO) δ 9.15 (s, 1H), 7.34 – 7.10 (m, 1H), 6.99 (m, 2H), 6.23 (t, J = 4.3 Hz, 1H), 2.66 (t, J = 7.8 Hz, 2H), 2.26 (dd, J = 12.4, 7.6 Hz, 2H), 2.03 (s, 3H), ^{13}C NMR (75 MHz, DMSO) δ 169.07, 161.1 ($J_{C\text{-}F}$ = 238.4 Hz), 133.9 ($J_{C\text{-}F}$ = 7.6 Hz), 131.9 ($J_{C\text{-}F}$ = 2.9 Hz), 131.9, 128.9 ($J_{C\text{-}F}$ = 7.8 Hz), 120.6, 113.3 ($J_{C\text{-}F}$ = 21 Hz), 109.3 ($J_{C\text{-}F}$ = 23.2 Hz), 26.3, 23.3, 21.9. HRMS (ESI) Calcd for $C_{12}H_{12}FNONa^+$ $[M+Na]^+$ 228.0795; Found: 228.0800.



N-(7-chloro-3,4-dihydronaphthalen-1-yl)acetamide (1g): yellow solid, 30 % yield, ^{1}H NMR (300 MHz, DMSO) δ 9.19 (s, 1H), 7.52 – 6.95 (m, 3H), 6.24 (t, J = 4.7 Hz, 1H), 2.67 (t, J = 7.9 Hz, 2H), 2.38 – 2.15 (m, 2H), 2.04 (s, 3H), ^{13}C NMR (75 MHz, DMSO) δ 169.0, 134.9, 133.7, 131.6, 130.9, 129.1, 126.7, 121.9, 120.7, 26.4, 23.3, 21.7. HRMS (ESI) Calcd for $C_{12}H_{12}ClNONa^+$ $[M+Na]^+$ 244.0500; Found: 244.0498.

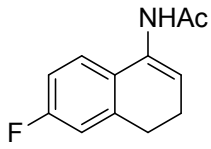


N-(7-bromo-3,4-dihydronaphthalen-1-yl)acetamide (1h): yellow solid, 32 % yield, ^{1}H NMR (300 MHz, DMSO) δ 9.15 (s, 1H), 7.54 – 7.16 (m, 2H), 7.08 (d, J = 8.5 Hz, 1H), 6.20 (t, J = 4.7 Hz, 1H), 2.61 (t, J = 7.9 Hz, 2H), 2.23 (dt, J = 12.5, 6.5 Hz, 2H), 2.00 (s, 3H), ^{13}C NMR (75 MHz, DMSO) δ 169.0, 135.3, 134.0, 131.4, 129.7, 129.5, 124.7, 26.5, 23.3, 21.6. HRMS (ESI) Calcd for $C_{12}H_{12}BrNONa^+$ $[M+Na]^+$ 287.9994; Found: 287.9998.

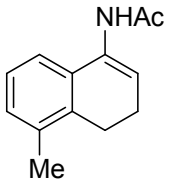


N-(6-methyl-3,4-dihydronaphthalen-1-yl)acetamide (1i): yellow solid, 43 % yield, ^{1}H NMR (300 MHz, DMSO) δ 9.06 (s, 1H), 7.12 (d, J = 7.6 Hz, 1H), 6.99 (d, J = 9.4 Hz, 2H), 6.14 (t, J = 4.3 Hz, 1H), 2.65 (t, J = 7.7 Hz, 2H), 2.27 (m,5H), 2.03 (s, 3H), ^{13}C NMR (75 MHz, DMSO) δ 168.8, 136.4, 136.1, 132.4,

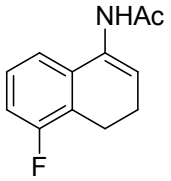
129.2, 126.5, 122.1, 117.6, 27.3, 23.4, 21.9, 20.8. HRMS (ESI) Calcd for $C_{13}H_{15}NONa^+$ $[M+Na]^+$ 224.1046; Found: 224.1052.



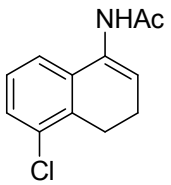
N-(6-fluoro-3,4-dihydronaphthalen-1-yl)acetamide (1j): yellow solid, 30 % yield, ^{1}H NMR (300 MHz, DMSO) δ 9.15 (s, 1H), 7.22 (dd, *J* = 8.1, 5.9 Hz, 1H), 7.00 (t, *J* = 9.9 Hz, 2H), 6.11 (t, *J* = 4.5 Hz, 1H), 2.70 (t, *J* = 7.9 Hz, 2H), 2.26 (dd, *J* = 12.4, 7.6 Hz, 2H), 2.00 (d, *J* = 11.3 Hz, 3H), ^{13}C NMR (75 MHz, DMSO) δ 168.9,161.2 ($J_{C\text{-}F}$ = 242.7 Hz), 139.1 ($J_{C\text{-}F}$ = 7.8 Hz), 131.9,128.3 ($J_{C\text{-}F}$ = 2.8 Hz), 124.2 ($J_{C\text{-}F}$ = 8.4 Hz), 118.5, 114.4 ($J_{C\text{-}F}$ = 21.5 Hz), 112.4 ($J_{C\text{-}F}$ = 21.1 Hz), 27.2, 23.3, 22.4, 21.5. HRMS (ESI) Calcd for $C_{12}H_{12}FNONa^+$ $[M+Na]^+$ 228.0795; Found: 228.0797.



N-(5-methyl-3,4-dihydronaphthalen-1-yl)acetamide (1k): yellow solid, 37 % yield, ^{1}H NMR (300 MHz, DMSO) δ 9.08 (s, 1H), 7.22- 6.92 (m, 3H), 6.15 (t, *J* = 4.6 Hz, 1H), 2.64 (t, *J* = 8.0 Hz, 2H), 2.27 (m, 5H), 2.02 (s, 3H), ^{13}C NMR (75 MHz, DMSO) δ 168.9, 134.4, 134.4, 132.6, 131.7, 129.2, 125.3, 120.2, 118.8, 23.3, 23.0, 21.5, 19.2. HRMS (ESI) Calcd for $C_{13}H_{15}NONa^+$ $[M+Na]^+$ 224.1046; Found: 224.1052.

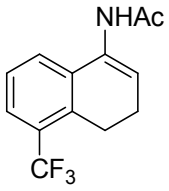


N-(5-fluoro-3,4-dihydronaphthalen-1-yl)acetamide (1l): yellow solid, 40 % yield, ^{1}H NMR (300 MHz, DMSO) δ 9.17 (s, 1H), 7.22 (m, 1H), 7.05 (m, 2H), 6.19 (t, *J* = 4.5 Hz, 1H), 2.70 (t, *J* = 8.0 Hz, 2H), 2.30 (m, 2H), 2.02 (s, 3H), ^{13}C NMR (75 MHz, DMSO) δ 168.9, 158.9 ($J_{C\text{-}F}$ = 239.0 Hz), 134.1 ($J_{C\text{-}F}$ = 5.4 Hz), 131.9 ($J_{C\text{-}F}$ = 4.2 Hz), 127.1 ($J_{C\text{-}F}$ = 8.7 Hz), 122.1 ($J_{C\text{-}F}$ = 17.9 Hz), 120.5, 118.4 ($J_{C\text{-}F}$ = 2.7 Hz), 114.3 ($J_{C\text{-}F}$ = 22.4 Hz), 23.2, 20.9, 18.57, 18.5 ($J_{C\text{-}F}$ = 3.2 Hz). HRMS (ESI) Calcd for $C_{12}H_{12}FNONa^+$ $[M+Na]^+$ 228.0795; Found: 228.0796.

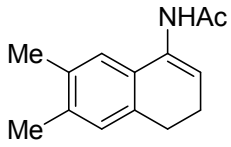


N-(5-chloro-3,4-dihydronaphthalen-1-yl)acetamide (1m): yellow solid, 45 % yield, ^{1}H NMR (300 MHz, DMSO) δ 9.21 (s, 1H), 7.29 (m, 1H), 7.25 – 7.10 (m, 2H), 6.18 (m, 1H), 2.80 (t, *J* = 7.9 Hz, 2H), 2.31 (m, 2H), 2.03 (s, 3H), ^{13}C NMR (75 MHz, DMSO) δ 169.0, 134.1, 133.3, 132.0 131.9, 127.9, 127.2, 121.3,

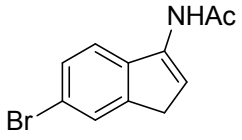
120.7, 23.6, 23.2, 21.1. HRMS (ESI) Calcd for $C_{12}H_{12}ClNONa^+$ $[M+Na]^+$ 224.0500; Found: 224.0511.



N-(5-(trifluoromethyl)-3,4-dihydronaphthalen-1-yl)acetamide (1n) : brown solid, 30 % yield, ^{1}H NMR (300 MHz, DMSO) δ 9.30 (s, 1H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.47 (d, *J* = 7.3 Hz, 1H), 7.39 (t, *J* = 7.7 Hz, 1H), 6.21 (t, *J* = 4.7 Hz, 1H), 2.82 (t, *J* = 7.7 Hz, 2H), 2.32 (m, 2H), 2.03 (s, 3H), ^{13}C NMR (75 MHz, DMSO) δ 169.0, 134.6, 133.7, 132.0, 129.9, 126.6, 126.4, 126.2, 125.8, 124.2 (J_{C-F} = 5.6 Hz), 122.7, 121.2, 23.5, 23.1, 21.1. HRMS (ESI) Calcd for $C_{13}H_{12}F_3NONa^+$ $[M+Na]^+$ 278.0763; Found: 278.0774.



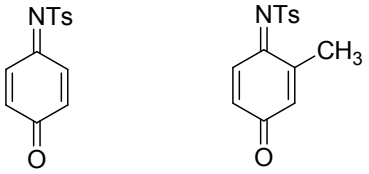
N-(6,7-dimethyl-3,4-dihydronaphthalen-1-yl)acetamide (1o): white solid, 50 % yield, ^{1}H NMR (300 MHz, DMSO) δ 8.99 (s, 1H), 6.97 (s, 1H), 6.88 (s, 1H), 6.11 (t, *J* = 4.4 Hz, 1H), 2.56 (t, *J* = 7.8 Hz, 2H), 2.25–2.05 (m, 8H), 2.00 (s, 3H), ^{13}C NMR (75 MHz, DMSO) δ 168.9, 134.9, 133.5, 133.4, 132.4, 129.3, 128.8, 123.3, 117.3, 26.8, 23.4, 22.0, 19.2, 19.1. HRMS (ESI) Calcd for $C_{14}H_{17}NONa^+$ $[M+Na]^+$ 238.1202; Found: 238.1209.



N-(6-bromo-1H-inden-3-yl)acetamide (1u) : brown solid, 38 % yield, ^{1}H NMR (300 MHz, DMSO) δ 9.80 (s, 1H), 7.72 (d, *J* = 8.2 Hz, 1H), 7.63 (s, 1H), 7.52 (dd, *J* = 8.2, 1.6 Hz, 1H), 6.76 (t, 1H), 3.41-3.37 (m, 2H), 2.12 (s, 3H), ^{13}C NMR (75 MHz, DMSO) δ 168.9, 145.0, 139.3, 136.1, 128.7, 126.9, 120.0, 118.5, 114.6, 36.0, 23.5. HRMS (ESI) Calcd for $C_{11}H_{10}BrNONa^+$ $[M+Na]^+$ 273.9838; Found: 273.9848.

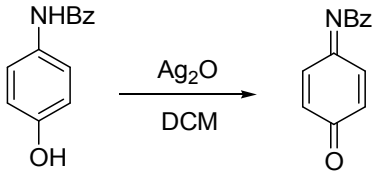
2.3 Synthesis and characterization of quinone monoimines

Quinone monoimines **2a** and **2b** were prepared according to the known procedure.[14]



2a **2b**

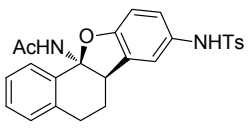
Quinone monoimine **2c** was prepared according to the known procedure[15]: N-(4-hydroxyphenyl)benzamide (2.0 mmol) was dissolved in dry CH_2Cl_2 (10 mL) andAg_2O (4.0 mmol) was added. The mixture was stirred at R.T. The reaction was monitored by TLC. When the reaction was completed, the solution was filtered through celatom. The organic layer was concentrated to yield the crude product. The product **2c** was purified by silica gel column using PE/ EA (10:1) as eluent 70 % yields.



2c

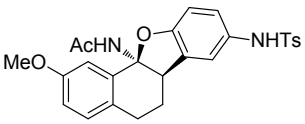
2.4 General procedure of enantioselective [3+2] coupling of N-Acetyl Enamines 1 with quinone monoimine 2:

N-Acetyl enamide **1** (0.10 mmol), quinone monoimine **2** (0.15 mmol) and chiral phosphoric acid (*R*)-**PA5** (0.005 mmol, 5 mol%) were placed in a flame-dried vial equipped with a magnetic stirring bar. The mixture was cooled to 0℃ then 1 mL of DCM was added to dissolve the mixture. The reaction mixture was stirred at 0℃ until no starting material was detected by TLC. The mixture was subjected to chromatography (silica gel, Petroleum ether/ EtOAc: 3/1 to 1/1) to afford the desired product **3**.

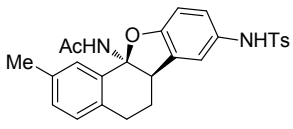


N-((6aR,11aS)-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3a): White solid, m.p.: 121.5-124.5℃, 88% yield, 99.6% ee, HPLC condition:

Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA) , 1.0 mL/min, t_{major} = 11.7 min, t_{minor} = 13.4 min). $[\alpha]_D^{20}$ = + 177.3 (c 1.51, CH_2Cl_2) ^{1}H NMR (300 MHz, DMSO) δ 9.77 (s, 1H), 8.94 (s, 1H), 7.53 (t, *J* = 9.2 Hz, 3H), 7.31 (d, *J* = 8.2 Hz, 2H), 7.28 – 7.17 (m, 2H), 7.11 (d, *J* = 6.7 Hz, 1H), 6.91 (s, 1H), 6.76 (dd, *J* = 8.4, 2.1 Hz, 1H), 6.62 (d, *J* = 8.5 Hz, 1H), 4.03 (t, *J* = 6.6 Hz, 1H), 2.71 (dd, *J* = 12.0, 8.6 Hz, 1H), 2.45-2.26 (m, 4H), 2.22-2.04 (m, 1H), 1.78 (s, 3H), 1.62-1.39 (m, 1H), ^{13}C NMR (75 MHz, DMSO) δ 169.2, 154.6, 143.0, 138.5, 136.6, 135.9, 131.5, 130.8, 129.5, 128.0, 127.6, 126.8, 126.7, 126.5, 122.5, 119.4, 109.2, 95.6, 46.0, 28.1, 26.4, 23.0, 21.0. HRMS (ESI) Calcd for $C_{25}H_{24}N_2O_4SNa^+$ $[M+Na]^+$ 471.1349; Found: 471.1345.

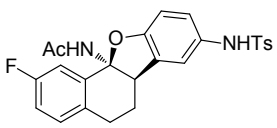


N-((6aR,11aS)-2-methoxy-8-(4-methylphenylsulfon- amido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl) acetamide (3d): White solid, m.p.: 205.3-208.9℃, 70% yield, 100% ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 13.5 min, t_{minor} = 19.5 min). $[\alpha]_D^{20}$ = + 269.2 (c 1, CH_2Cl_2). ^{1}H NMR (400 MHz, DMSO) δ 9.78 (s, 1H), 8.91 (s, 1H), 7.55 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.04 (d, *J* = 8.6 Hz, 2H), 6.91 (s, 1H), 6.83 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.80-6.71 (m, 1H), 6.63 (d, *J* = 8.5 Hz, 1H), 4.04 (t, *J* = 6.5 Hz, 1H), 3.74 (s, 3H), 2.71-2.57 (m, 1H), 2.33 (d, *J* = 12.4 Hz, 4H), 2.18-2.06 (m, 1H), 1.58-1.41 (m, 1H). ^{13}C NMR (101 MHz, DMSO) δ 169.8, 158.3, 155.0, 143.5, 137.3, 137.0, 132.0, 131.2, 130.9, 130.0, 129.1, 127.3, 123.0, 119.8, 114.5, 112.2, 109.6, 96.2, 55.5, 46.1, 28.5, 25.9, 23.5, 21.4. HRMS (ESI) Calcd for $C_{26}H_{26}N_2O_5SNa^+$ $[M+Na]^+$ 501.1455; Found: 501.1463.

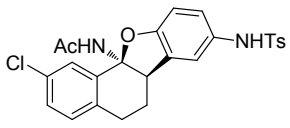


N-((6aR,11aS)-2-methyl-8-(4-methylphenylsulfonamido)-5,6,6a, 11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3e): White solid, m.p.: 125.7-127.2℃, 83% yield, 97.2% ee, HPLC condition: Chiralpak AD-H (n-hexane/2-propanol/ethanol: 85/5/10, 1.0 mL/min, t_{major} = 18.3 min, t_{minor} = 15.0 min). $[\alpha]_D^{20}$ = + 155.8 (c 1.49, CH_2Cl_2). ^{1}H NMR (400 MHz, DMSO) δ 9.77 (s, 1H), 8.88 (s, 1H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 3H), 7.07-7.02 (m, 1H), 6.99 (d, *J* = 7.8 Hz, 1H), 6.91 (d, *J* =

1.8 Hz, 1H), 6.76 (dd, *J* = 8.5, 2.2 Hz, 1H), 6.61 (d, *J* = 8.5 Hz, 1H), 4.10-4.01 (m, 1H), 2.74-2.59 (m, 1H), 2.42 – 2.35 (m, 1H), 2.34 (s, 3H), 2.29 (s, 3H), 2.19-2.05 (m, 1H), 1.79 (d, *J* = 6.6 Hz, 3H), 1.50 (ddd, *J* = 13.0, 8.4, 4.1 Hz, 1H). ^{13}C NMR (101 MHz, DMSO) δ 169.7, 155.1, 143.4, 137.0, 136.1, 135.8, 131.9, 131.1, 129.9, 129.3, 128.0, 127.5, 127.3, 123.0, 119.8, 109.6, 96.2, 46.2, 28.4, 26.4, 23.6, 21.4, 21.3. HRMS (ESI) Calcd for $C_{26}H_{26}N_2O_4SNa^+$ $[M+Na]^+$ 485.1505; Found: 485.1496.

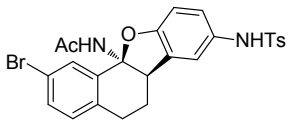


N-((6aR,11aS)-2-fluoro-8-(4-methylphenylsulfonamido)- 5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3f): White solid, m.p.: 118.5-121.5℃, 74% yield, 97.7% ee, HPLC condition: Chiralpak AD-H (n-hexane/2-propanol/ ethanol: 85/5/10, 1.0 mL/min, t_{major} = 25.7 min, t_{minor} = 22.7 min). $[\alpha]_D^{20}$ = + 188.0 (c 1.51, CH_2Cl_2). ^{1}H NMR (400 MHz, DMSO) δ 9.80 (s, 1H), 8.99 (s, 1H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.26 (dd, *J* = 9.9, 2.7 Hz, 1H), 7.18 (dd, *J* = 8.4, 5.9 Hz, 1H), 7.09 (td, *J* = 8.5, 2.7 Hz, 1H), 6.94 (d, *J* = 1.8 Hz, 1H), 6.78 (dd, *J* = 8.5, 2.2 Hz, 1H), 6.66 (d, *J* = 8.5 Hz, 1H), 4.06 – 3.96 (m, 1H), 2.75 – 2.62 (m, 1H), 2.47 – 2.37 (m, 1H), 2.35 (d, *J* = 8.5 Hz, 3H), 2.16 (dd, *J* = 8.0, 4.0 Hz, 1H), 1.80 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 169.9, 161.3 ($J_{C\text{-}F}$ = 242.1 Hz), 154.8, 143.5, 138.4 ($J_{C\text{-}F}$ = 6.9 Hz), 137.0, 135.1 ($J_{C\text{-}F}$ = 2.8 Hz), 131.8, 131.4, 130.0, 127.3, 123.0, 119.8, 115.6 ($J_{C\text{-}F}$ = 21.1 Hz), 113.3 ($J_{C\text{-}F}$ = 21.9 Hz), 109.8, 95.6, 46.3, 28. 7, 26.1, 23.4, 21.4. HRMS (ESI) Calcd for $C_{25}H_{23}FN_2O_4SNa^+$ $[M+Na]^+$ 489.1255; Found: 489.1247.



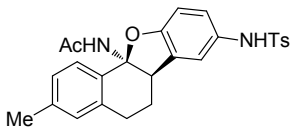
N-((6aR,11aS)-2-chloro-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl) acetamide (3g) : m.p.: 130.2-134.5℃, 51% yield, 97.5% ee, HPLC condition: Chiralpak AD-H(n-hexane/ethanol: 85/15 (0.1% TFA, 0.1% DEA), 1.0 mL/min, t_{major} = 17.0 min, t_{minor} = 15.3 min), $[\alpha]_D^{20}$ = + 175.0 (c 1.23, CH_2Cl_2). ^{1}H NMR (300 MHz, DMSO) δ 9.80 (s, 1H), 9.01 (s, 1H), 7.54 (t, *J* = 8.7 Hz, 2H), 7.49 (d, *J* = 2.2 Hz, 1H), 7.36 – 7.24 (m, 3H), 7.16 (d, *J* = 8.3 Hz, 1H), 6.94 (d, *J* = 1.7 Hz, 1H), 6.77 (dd, *J* = 8.5, 2.1 Hz, 1H),

6.66 (d, *J* = 8.5 Hz, 1H), 4.13 – 3.86 (m, 1H), 2.79 – 2.60 (m, 1H), 2.39 (m, 7.8, 4.4 Hz, 1H), 2.33 (s, 3H), 2.16 (m, 1H), 1.79 (s, 3H), 1.59 – 1.33 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.4, 154.3, 143.0, 138.0, 137.5, 136.6, 131.3, 131.0, 130.8, 129.6, 129.5, 128.0, 126.8, 126.3, 122.5, 119.4, 109.4, 95.0, 45.9, 28.0, 25.9, 23.0, 21.0. HRMS (ESI) Calcd for $C_{25}H_{23}ClN_2O_4SNa^+$ $[M+Na]^+$ 505.0959; Found: 505.0954.



N-((6aR,11aS)-2-bromo-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide

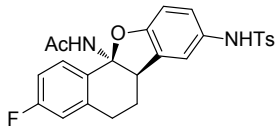
(3h): White solid, m.p.: 135.2-137.8℃, 72% yield, 97.9% ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 85/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 10.3 min, t_{minor} = 9.2 min), $[\alpha]_D^{20}$ = + 144.3 (c 1.30, CH_2Cl_2).^{1}H NMR (300 MHz, DMSO) δ 9.80 (s, 1H), 9.01 (s, 1H), 7.62 (d, *J* = 1.8 Hz, 1H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.41 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.2 Hz, 1H), 6.93 (s, 1H), 6.87 – 6.71 (m, 1H), 6.66 (d, *J* = 8.5 Hz, 1H), 4.16 – 3.89 (m, 1H), 2.79 – 2.57 (m, 1H), 2.36 (d, *J* = 19.8 Hz, 4H), 2.15 (s, 1H), 1.78 (s, 3H), 1.45 (d, *J* = 9.3 Hz, 1H), ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.5, 154.3, 143.0, 138.4, 137.9, 136.6, 131.3, 131.0, 130.9, 130.0, 129.5, 129.2, 126.8, 122.6, 119.4, 119.1, 109.4, 95.0, 45.9, 28.0, 25.9, 23.0, 21.0. HRMS (ESI) Calcd for $C_{25}H_{23}BrN_2O_4SNa^+$ $[M+Na]^+$ 549.0631; Found: 549.0632.



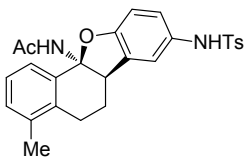
N-((6aR,11aS)-3-methyl-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide

(3i): White solid, m.p.: 119.5-120.3℃, 89% yield, 99.3% ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 6.0 min, t_{minor} = 7.4 min), $[\alpha]_D^{20}$ = + 171.0 (c 1.88, CH_2Cl_2)^{1}H NMR (400 MHz, DMSO) δ 9.77 (s, 1H), 8.89 (s, 1H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.41 (d, *J* = 7.9 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.07 (d, *J* = 7.1 Hz, 1H), 6.92 (s, 2H), 6.76 (dd, *J* = 8.5, 2.2 Hz, 1H), 6.62 (d, *J* = 8.5 Hz, 1H), 4.08 – 3.98 (m, 1H), 2.72 – 2.62 (m, 1H), 2.38 (dd, *J* = 8.0, 3.3 Hz, 1H), 2.34 (s, 3H), 2.26 (s, 3H), 2.17 – 2.06 (m, 1H), 1.78 (s, 3H), 1.56 – 1.44 (m, 1H), ^{13}C NMR (101 MHz, DMSO) δ 169.6, 155.2, 143.4, 138.7, 137.8, 137.1, 133.5, 132.0, 131.1, 130.0, 128.4, 127.6,

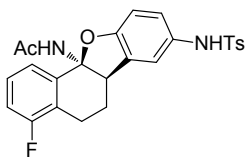
127.3, 127.1, 123.0, 119.8, 109.6, 96.2, 46.3, 28.4, 26.8, 23.5, 21.4, 21.1. HRMS (ESI) Calcd for $C_{26}H_{26}N_2O_4SNa^+$ $[M+Na]^+$ 485.1505; Found: 485.1499.



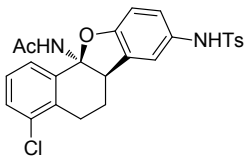
N-((6aR,11aS)-3-fluoro-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3j): White solid, m.p.: 104.7-106.5℃, 99% yield, 99.5% ee, HPLC condition: Chiralpak AD-H (n-hexane/2-propanol/ethanol: 85/5/10, 1.0 mL/min, t_{major} = 30.2 min, t_{minor} = 24.0 min), $[\alpha]_D^{20}$ = +199.9 (c 0.43, CH_2Cl_2).^{1}H NMR (400 MHz, DMSO) δ 9.79 (s, 1H), 8.98 (s, 1H), 7.55 (m, 3H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.09 (td, *J* = 8.7, 2.7 Hz, 1H), 6.98 (dd, *J* = 9.7, 2.6 Hz, 1H), 6.94 (d, *J* = 1.8 Hz, 1H), 6.78 (dd, *J* = 8.5, 2.1 Hz, 1H), 6.65 (d, *J* = 8.5 Hz, 1H), 4.01 (dd, *J* = 7.8, 6.0 Hz, 1H), 2.85 – 2.67 (m, 1H), 2.48 – 2.39 (m, 1H), 2.34 (s, 3H), 2.21 – 2.09 (m, 1H), 1.78 (s, 3H), 1.54 – 1.40 (m, 1H). ^{13}C NMR (101 MHz, DMSO) δ 169.7, 161.9 (J_{C-F} = 245.8 Hz), 154.9, 143.4, 141.8 (J_{C-F} = 8.1 Hz), 137.0, 132.7 (J_{C-F} = 2.8 Hz), 131.8, 131.3, 130.0, 129.4 (J_{C-F} = 8.8 Hz), 127.3, 123.0, 119.9, 114.2 (J_{C-F} = 21.0 Hz), 114.0 (J_{C-F} = 21.8 Hz), 109.7, 95.6, 46.5, 28.5, 27.0, 23.4, 21.4. HRMS (ESI) Calcd for $C_{25}H_{23}FN_2O_4SNa^+$ $[M+Na]^+$ 489.1255; Found: 489.1249.



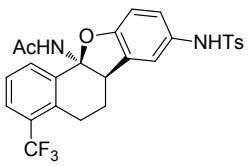
N-((6aR,11aS)-4-methyl-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3k) : White solid, m.p.: 210.1-213.5℃, 82% yield, 99.7% ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 10.5 min, t_{minor} = 12.5 min). $[\alpha]_D^{20}$ = + 151.8 (c 1.86, CH_2Cl_2)^{1}H NMR (300 MHz, DMSO) δ 9.74 (s, 1H), 8.86 (s, 1H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 7.2 Hz, 1H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.09 (q, *J* = 7.0 Hz, 2H), 6.87 (s, 1H), 6.70 (d, *J* = 8.5 Hz, 1H), 6.55 (d, *J* = 8.4 Hz, 1H), 4.03 (t, *J* = 6.2 Hz, 1H), 2.55 (m, 1H), 2.26 (m, 4H), 2.16 (s, 3H), 2.08 (m, 1H), 1.74 (s, 3H), 1.55 (m, 1H), ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.41, 154.7, 143.1, 136.8, 136.6, 135.9, 134.5, 131.5, 130.7, 129.6, 129.5, 126.9, 125.9, 124.7, 122.5, 119.3, 109.3, 96.2, 45.0, 26.8, 23.2, 22.4, 21.0, 19.4. HRMS (ESI) Calcd for $C_{26}H_{26}N_2O_4SNa^+$ $[M+Na]^+$ 485.1505; Found: 485.1503.



N-((6aR,11aS)-4-fluoro-8-(4-methylphenylsulfonamido)- 5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3l): White solid, m.p.: 92.5-95.0℃, 98% yield, 98.6% ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 9.6 min, t_{minor} = 11.5 min). $[\alpha]_D^{20}$ = + 101.5 (c 2.50, CH_2Cl_2)^{1}H NMR (300 MHz, DMSO) δ 9.68 (br, 1H), 9.03 (s, 1H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.41-7.22 (m, 4H), 7.10 (t, *J* = 8.7 Hz, 1H), 6.94 (d, *J* = 1.3 Hz, 1H), 6.78 (dd, *J* = 8.5, 1.9 Hz, 1H), 6.65 (d, *J* = 8.5 Hz, 1H), 4.02 (dd, *J* = 14.1, 6.9 Hz, 1H), 2.74- 2.57 (m, 1H), 2.48-2.37 (m, 1H), 2.33 (s, 3H), 2.15 (m, 1H), 1.76 (s, 3H), 1.50 (m, 1H), ^{13}C NMR (75 MHz, DMSO) δ 169.4, 158.5 (J_{C-F} = 240.3 Hz), 154.32, 143.06, 138.4 (J_{C-F} = 4.5 Hz), 136.62, 131.28, 131.09, 129.54, 127.5 (J_{C-F} = 8.6 Hz), 126.88, 125.8 (J_{C-F} = 18.5 Hz), 122.7 (J_{C-F} = 2.8 Hz), 122.62, 119.38, 114.52, 114.23, 109.49, 94.9 (J_{C-F} = 3.4 Hz), 45.72, 27.05, 22.97, 20.98, 18.4 (J_{C-F} = 3.0 Hz). HRMS (ESI) Calcd for $C_{25}H_{23}FN_2O_4SNa^+$ $[M+Na]^+$ 489.1255; Found: 489.1254.

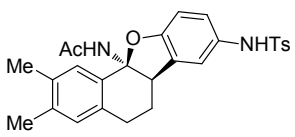


N-((6aR,11aS)-4-chloro-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3m): White solid, m.p.: 112.3-115.8℃, 81% yield, 97.0% ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 9.1 min, t_{minor} = 11.3 min). $[\alpha]_D^{20}$ = + 115.3 (c 1.95, CH_2Cl_2)^{1}H NMR (400 MHz, DMSO) δ 9.83 (s, 1H), 9.05 (s, 1H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.40 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.37-7.24 (m, 3H), 6.96 (d, *J* = 1.5 Hz, 1H), 6.79 (dd, *J* = 8.5, 2.1 Hz, 1H), 6.66 (d, *J* = 8.5 Hz, 1H), 4.05-4.00 (m, 1H), 2.75 (m, 1H), 2.65-2.51 (m, 1H), 2.34 (s, 3H), 2.18 (m, 1H), 1.78 (s, 3H), 1.61-1.41 (m, 1H). ^{13}C NMR (101 MHz, DMSO) δ 169.8, 154.6, 143.5, 139.0, 137.0, 136.4, 132.2, 131. 7, 131.5, 130.0, 129.1, 128.1, 127.3, 126.4, 123.0, 119.7, 110.0, 95.8, 45.9, 27.5, 24.0, 23.4, 21.4. HRMS (ESI) Calcd for $C_{25}H_{23}ClN_2O_4SNa^+$ $[M+Na]^+$ 505.0959; Found: 505.0951.

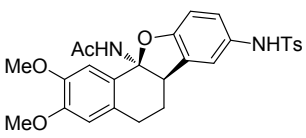


N-((6aR,11aS)-8-(4-methylphenylsulfonamido)-4-(trifluoromethyl) -5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide

(3n): White solid, m.p.: 104.3-106.2℃, 81% yield, 98.5% ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 6.0 min, t_{minor} = 7.4 min). $[\alpha]_D^{20}$ = + 165.8 (c 1.80, CH_2Cl_2)^{1}H NMR (400 MHz, DMSO) δ 9.84 (s, 1H), 9.12 (s, 1H), 7.84 (d, *J* = 7.8 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.31 (d, *J* = 8.1 Hz, 2H), 6.98 (d, *J* = 1.9 Hz, 1H), 6.81 (dd, *J* = 8.5, 2.2 Hz, 1H), 6.69 (d, *J* = 8.5 Hz, 1H), 4.01 (dd, *J* = 8.5, 5.8 Hz, 1H), 2.98-2.77 (m, 1H), 2.59 (m, 1H), 2.33 (s, 3H), 2.23 (m, 1H), 1.77 (s, 3H), 1.53-1.40 (m, 1H). ^{13}C NMR (101 MHz, DMSO) δ 169.8, 154.7, 143.4, 138.7, 137.6, 137.0, 131.7, 131.6, 130.0, 127.3, 127.2, 126.1 (q, J_{C-F} = 3.8 Hz), 123.0, 119.8, 109.9, 95.4, 46.2, 28.2, 23.3, 23.2, 21.4. HRMS (ESI) Calcd for $C_{26}H_{23}F_3N_2O_4SNa^+$ $[M+Na]^+$ 539.1223; Found: 539.1226.

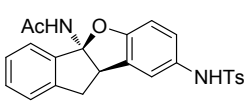


N-((6aR,11aS)-2,3-dimethyl-8-(4-methylphenylsulfon-amido) -5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl) acetamide (3o): White solid, m.p.: 137.2-140.5℃, 63% yield, 93.7% ee, HPLC condition: Chiralpak AD-H (n-hexane/2-propanol/ ethanol: 85/5/10, 1.0 mL/min, t_{major} = 20.4 min, t_{minor} = 18.1 min). $[\alpha]_D^{20}$ = + 183.8 (c 1.34, CH_2Cl_2).^{1}H NMR (400 MHz, DMSO) δ 9.77 (s, 1H), 8.84 (s, 1H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.27 (s, 1H), 6.90 (d, *J* = 1.1 Hz, 1H), 6.86 (s, 1H), 6.75 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.60 (d, *J* = 8.5 Hz, 1H), 4.05 (t, *J* = 6.5 Hz, 1H), 2.62 (m, 1H), 2.32 (m, 4H), 2.20 (s, 3H), 2.16 (s, 3H), 2.14-2.06 (m, 1H), 1.79 (s, 3H), 1.57-1.41 (m, 1H). ^{13}C NMR (101 MHz, DMSO) δ 169.7, 155.2, 143.4, 137.0, 136.7, 136.0, 134.6, 133.6, 131.9, 131.0, 129.9, 129.0, 128.1, 127.3, 123.0, 119.8, 109.6, 96.2, 46.0, 28.1, 26.2, 23.6, 21.4, 19.7, 19.5. HRMS (ESI) Calcd for $C_{27}H_{28}N_2O_4SNa^+$ $[M+Na]^+$499.1662; Found: 499.1656.

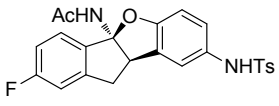


N-((6aR,11aS)-2,3-dimethoxy-8-(4-methylphenyl-sulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl) acetamide (3p): White solid, m.p.: 170.1-174.0℃, 89% yield, 99.2% ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 14.8 min, t_{minor} = 28.1 min). $[\alpha]_D^{20}$ = + 111.1 (c 0.44, CH_2Cl_2). ^{1}H NMR (300

MHz, DMSO) δ 9.75 (s, 1H), 8.79 (s, 1H), 7.55 (d, *J* = 7.9 Hz, 2H), 7.31 (d, *J* = 7.8 Hz, 2H), 7.03 (s, 1H), 6.89 (s, 1H), 6.72 (s, 1H), 6.66 (s, 1H), 6.59 (d, *J* = 8.4 Hz, 1H), 4.06 (m, 1H), 3.73 (m, 6H), 2.59 (m, 1H), 2.34 (m, 4H), 2.09 (m, 1H), 1.57 (m, 1H), ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.4, 154.7, 148.7, 147.4, 143.0, 136.6, 131.5, 131.0, 130.5, 129.5, 127.5, 126.9, 122.5, 119.3, 110.7, 110.2, 109.2, 95.9, 55.6, 55.5, 45.0, 27.4, 25.8, 23.2, 21.0. HRMS (ESI) Calcd for $C_{27}H_{28}N_2O_6SNa^+$ $[M+Na]^+$ 531.1560; Found: 531.1552.

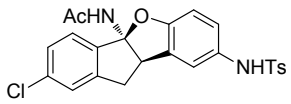


N-((4bS,9bR)-8-(4-methylphenylsulfonamido)-9b,10-dihydro-4bH-indeno[1,2-b]benzofuran-4b-yl)acetamide (3s): White solid, m.p.: 196.6-200.1℃, 52% yield, 99.5% ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 12.9 min, t_{minor} = 12.2 min). $[\alpha]_D^{20}$ = + 47.0 (c 0.56, CH_2Cl_2). ^{1}H NMR (400 MHz, DMSO) δ 9.76 (s, 1H), 8.94 (s, 1H), 7.54 (m, 3H), 7.39-7.22 (m, 5H), 6.91 (s, 1H), 6.68 (dd, *J* = 8.4, 2.2 Hz, 1H), 6.49 (dd, *J* = 8.5, 2.7 Hz, 1H), 4.44 (d, *J* = 8.1 Hz, 1H), 3.51 (dd, *J* = 16.6, 8.6 Hz, 1H), 2.84 (d, *J* = 16.7 Hz, 1H), 2.34 (s, 3H), 1.88 (s, 3H), ^{13}C NMR (101 MHz, DMSO) δ 170.5, 155.4, 143.4, 142.3, 141.1, 137.1, 132.6, 130.7, 130.3, 130.0, 127.6, 127.2, 125.5, 125.0, 123.0, 119.9, 109.3, 106.4, 48.4, 39.5, 39.3, 38.1, 23.6, 21.4. HRMS (ESI) Calcd for $C_{24}H_{22}N_2O_4SNa^+$ $[M+Na]^+$ 457.1192; Found: 457.1189.



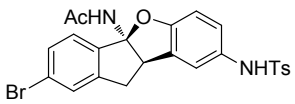
N-((4bS,9bR)-2-fluoro-8-(4-methylphenylsulfonamido)-9b,10-dihydro-4bH-indeno[1,2-b]benzofuran-4b-yl)acetamide (3t): White solid, m.p.: 228.2-230.8℃, 83% yield, 99.6% ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 26.6 min, t_{minor} = 22.7 min). $[\alpha]_D^{20}$ = + 60.4 (c 1.88, CH_2Cl_2), ^{1}H NMR (400 MHz, DMSO) δ 9.78 (s, 1H), 8.97 (s, 1H), 7.55 (m, 3H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.17-7.07 (m, 2H), 6.94 (s, 1H), 6.70 (dd, *J* = 8.5, 1.8 Hz, 1H), 6.50 (d, *J* = 8.5 Hz, 1H), 4.46 (d, *J* = 8.3 Hz, 1H), 3.51 (dd, *J* = 17.1, 8.6 Hz, 1H), 2.85 (d, *J* = 17.0 Hz, 1H), 2.34 (s, 3H), 1.88 (s, 3H), ^{13}C NMR (101 MHz, DMSO) δ 170.4, 163.7 (J_{C-F} = 246.0 Hz), 155.2, 145.3 (J_{C-F} = 9.0 Hz), 143.4, 137.4 (J_{C-F} = 2.1 Hz), 137.1, 132.3, 130.9, 130.0, 127.2, 126.9 (J_{C-F} = 9.7 Hz), 123.0, 119.8, 115.1 (J_{C-F} = 23.3 Hz), 112.1 (J_{C-F} =

22.4 Hz), 109.4, 105.6, 49.1, 39.3, 38.1, 23.6, 21.4. HRMS (ESI) Calcd for $C_{24}H_{21}FN_2O_4SNa^+$ $[M+Na]^+$ 475.1098; Found: 475.1098.



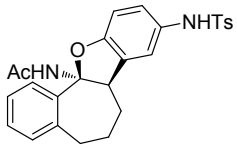
N-((4bS,9bR)-2-chloro-8-(4-methylphenylsulfonamido)-9b,10-dihydro-4bH-indeno[1,2-b]benzofuran-4b-yl)acetamide (3u):

White solid, m.p. 232.3-236.5℃, 64% yield, 99.9 % ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 15.1 min, t_{minor} = 13.6 min). $[\alpha]_D^{20}$ = + 100.6 (c 10.78, CH_2Cl_2). ^{1}H NMR (300 MHz, DMSO) δ 9.78 (s, 1H), 8.99 (s, 1H), 7.54 (m, 3H), 7.40-7.33 (m, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 6.93 (s, 1H), 6.69 (dd, *J* = 8.5, 1.8 Hz, 1H), 6.50 (m, 1H), 4.43 (d, *J* = 8.0 Hz, 1H), 3.51 (dd, *J* = 17.0, 8.5 Hz, 1H), 2.85 (d, *J* = 17.0 Hz, 1H), 2.33 (s, 3H), 1.87 (s, 3H), ^{13}C NMR (75 MHz, DMSO) δ 170.0, 154.7, 144.5, 143.0, 139.7, 136.6, 134.4, 131.8, 130.6, 129.5, 127.4, 126.8, 126.2, 125.0, 122.5, 119.3, 109.0, 105.3, 48.5, 37.5, 23.1, 21.0. HRMS (ESI) Calcd for $C_{24}H_{21}ClN_2O_4SNa^+$ $[M+Na]^+$ 491.0803; Found: 491.0804.



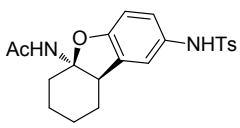
N-((4bS,9bR)-2-bromo-8-(4-methylphenylsulfonamido)-9b,10-dihydro-4bH-indeno[1,2-b]benzofuran-4b-yl)acetamide (3v):

White solid, m.p.: 230.3-231.4℃, 40 % yield, 99.0 % ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 16.2 min, t_{minor} = 14.5 min). $[\alpha]_D^{20}$ = + 91.8 (c 0.51, CH_2Cl_2). ^{1}H NMR (400 MHz, DMSO) δ 9.79 (s, 1H), 9.00 (s, 1H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.48 (m, 3H), 7.30 (d, *J* = 8.1 Hz, 2H), 6.94 (s, 1H), 6.69 (dd, *J* = 8.5, 1.7 Hz, 1H), 6.51 (d, *J* = 8.5 Hz, 1H), 4.42 (d, *J* = 8.3 Hz, 1H), 3.52 (dd, *J* = 17.0, 8.6 Hz, 1H), 2.86 (d, *J* = 16.9 Hz, 1H), 2.34 (s, 3H), 1.87 (s, 3H), ^{13}C NMR (101 MHz, DMSO) δ 170.4, 155.1, 145.3, 143.4, 140.5, 137.1, 132.2, 131.0, 130.7, 130.0, 128.5, 127.2, 127.0, 123.5, 122.9, 119.8, 109.4, 105.8, 48.8, 38.0, 23.6, 21.4. HRMS (ESI) Calcd for $C_{24}H_{21}BrN_2O_4SNa^+$ $[M+Na]^+$ 535.0298; Found: 535.0294.

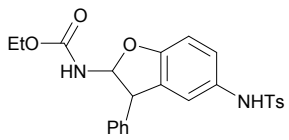


N-((7aR,12aS)-9-(4-methylphenylsulfonamido)-6,7,7a,12a-tetrahydro-5H-benzo[6,7]cyclohepta[1,2-b]benzofuran-12a-yl)

acetamide (3w): White solid, m.p.: 207.5-208.6℃, 30 % yield, 94.7% ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 9.6 min, t_{minor} = 10.4 min). $[\alpha]_D^{20}$ = + 50.5 (c 0.71, CH_2Cl_2). ^1H NMR (300 MHz, DMSO) δ 9.71 (s, 1H), 8.70 (s, 1H), 7.69-7.58 (m, 1H), 7.53 (m, 2H), 7.32-7.19 (m, 4H), 7.16 (d, *J* = 7.0 Hz, 1H), 6.78 (s, 1H), 6.74 (d, *J* = 8.6 Hz, 1H), 6.65 (d, *J* = 8.4 Hz, 1H), 3.83 (d, *J* = 11.7 Hz, 1H), 3.05-2.79 (m, 1H), 2.62 (dd, *J* = 13.4, 6.4 Hz, 1H), 2.30 (s, 3H), 1.77 (m, 4H), 1.62 (d, *J* = 12.6 Hz, 1H), 1.45 (m, 1H), 0.81 (m, 1H), ^{13}C NMR (75 MHz, DMSO) δ 169.6, 154.6, 142.9, 138.0, 136.7, 131.7, 130.0, 129.5, 129.3, 128.9, 126.8, 126.0, 125.9, 122.4, 118.9, 108.1, 99.5, 48.7, 30.2, 28.9, 23.8, 23.4, 21.0. HRMS (ESI) Calcd for $C_{26}H_{26}N_2O_4SNa^+$ $[M+Na]^+$ 485.1505; Found: 485.1502.



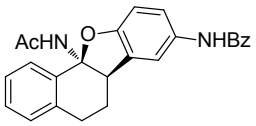
N-((4aR,9bR)-8-(4-methylphenylsulfonamido)-1,2,3,4,4a,9b-hexahydrodibenzo[b,d]furan-4a-yl)acetamide (3x): White solid, m.p.: 191.1-194.0℃, 70% yield, 11% ee, HPLC condition: Chiralpak AD-H (n-hexane/ethanol: 80/20 (0.2% TFA, 0.2% DEA), 1.0 mL/min, t_{major} = 10.4 min, t_{minor} = 9.5 min). $[\alpha]_D^{20}$ = + 2.8 (c 0.64, CH_2Cl_2). ^1H NMR (300 MHz, DMSO) δ 9.68 (s, 1H), 8.38 (s, 1H), 7.53 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.2 Hz, 2H), 6.75 (s, 1H), 6.73 – 6.68 (m, 1H), 6.55 (d, *J* = 8.3 Hz, 1H), 3.84 (m, 1H), 2.32 (s, 3H), 2.14 (m, 1H), 1.83 (s, 3H), 1.80 – 1.44 (m, 3H), 1.36 (s, 3H), 1.06 (m, 1H), ^{13}C NMR (75 MHz, DMSO) δ 170.3, 155.3, 143.0, 136.6, 131.9, 130.1, 129.5, 126.9, 122.4, 118.7, 109.3, 97.7, 42.9, 30.9, 24.9, 23.8, 21.0, 19.7, 19.4. HRMS (ESI) Calcd for $C_{21}H_{24}N_2O_4SNa^+$ $[M+Na]^+$ 423.1349; Found: 423.1347.



Ethyl (5-(4-methylphenylsulfonamido)-3-phenyl-2,3-dihydro- benzofuran-2-yl)carbamate (3y): **Racemate:** White solid, m.p.:63.4-68.0℃, ^1H NMR (300 MHz, DMSO) δ 9.73 (s, 1H), 8.69 (d, *J* = 9.2 Hz, 1H), 7.49 – 7.45 (m, 2.5H), 7.36-7.28 (m, 6.3H), 7.13 (dd, *J* = 7.1, 2.3 Hz, 0.4H),

7.06 (dd, *J* = 7.6, 1.6 Hz, 2H), 6.90 (dd, *J* = 8.5, 1.8 Hz, 1.2H), 6.75 (t, *J* = 9.5 Hz, 1.2H), 6.60 (s, 0.2H), 6.54 (d, *J* = 1.2 Hz, 1H), 6.41 – 6.27 (m, 0.2H), 5.75 (t, *J* = 8.5 Hz, 1H), 4.90 (d, *J* = 8.8 Hz, 0.2H), 4.48 (d, *J* = 7.5 Hz, 1H), 4.11 – 3.80 (m, 2H), 2.36 (s, 1H), 2.34 (s, 1H), 1.15 (t, *J* = 7.0 Hz, 1H), 1.03 (t, *J* = 6.9 Hz, 1H), 1.15 (t, *J* = 7.0 Hz, 1H), 1.03 (t, *J* = 6.9 Hz, 0.7H). ^{13}C NMR (75 MHz, DMSO) δ 155.7, 155.2, 143.0, 142.9, 140.0, 136.3, 130.7, 130.6, 129.7, 129.5, 129.0, 128.3, 127.9, 127.5, 127.3, 126.8, 123.4, 123.3, 119.7, 119.3, 109.5, 94.2, 88.7, 79.2, 60.6, 60.3, 52.0, 49.7, 21.0, 14.4, 14.4. HRMS (ESI) Calcd for $C_{24}H_{24}N_2O_5SNa^+$ $[M+Na]^+$ 475.1296; Found: 475.1292.

Optically active 3y: White solid, 99 % yield, Chiral HPLC showed 97%, 99.8% ee, dr = 34.5:65.5, HPLC condition: Chiralpak AD-H (n-hexane/2-propanol/ethanol: 70/10/20, 1.0 mL/min,t_{min} = 14.3, 15.7, 18.1, 32.6). $[\alpha]_D^{20}$ = - 97.2 (c 2.16, CH_2Cl_2).



N-((6aR,11aS)-11a-acetamido-5,6,6a,11a-tetrahydronaphtho[1,2-b] benzofuran-8-yl)benzamide (3z): White solid, m.p.: 224.2-226.8℃, 75% yield, 94.3 % ee, HPLC condition: Chiralpak AD-H (n-hexane/2-propanol: 70/30, 1.0 mL/min, t_{major} = 8.1 min, t_{minor} = 6.7 min). $[\alpha]_D^{20}$ = + 226.2 (c 0.38, CH_3OH : DMF = 1：1). ^{1}H NMR (300 MHz, DMSO) δ 10.14 (s, 1H), 9.01 (s, 1H), 7.94 (d, *J* = 6.9 Hz, 2H), 7.69 (s, 1H), 7.62 – 7.38 (m, 5H), 7.26 (dt, *J* = 14.7, 7.3 Hz, 2H), 7.14 (d, *J* = 7.1 Hz, 1H), 6.78 (d, *J* = 8.6 Hz, 1H), 4.21 – 4.06 (m, 1H), 2.78 (m, 1H), 2.58 (m, 1H), 2.26 (m, 1H), 1.80 (s, 3H), 1.63 (m, 1H). ^{13}C NMR (75 MHz, DMSO) δ 169.2, 165.1, 153.6, 138.6, 136.0, 135.0, 132.7, 131.4, 131.0, 128.3, 128.0, 127.5, 127.5, 126.6, 126.4, 121.0, 117.9, 108.8, 95.5, 46.3, 28.6, 26.7, 23.0. HRMS (ESI) Calcd for $C_{25}H_{22}N_2O_3Na^+$ $[M+Na]^+$ 421.1523; Found: 421.1508.

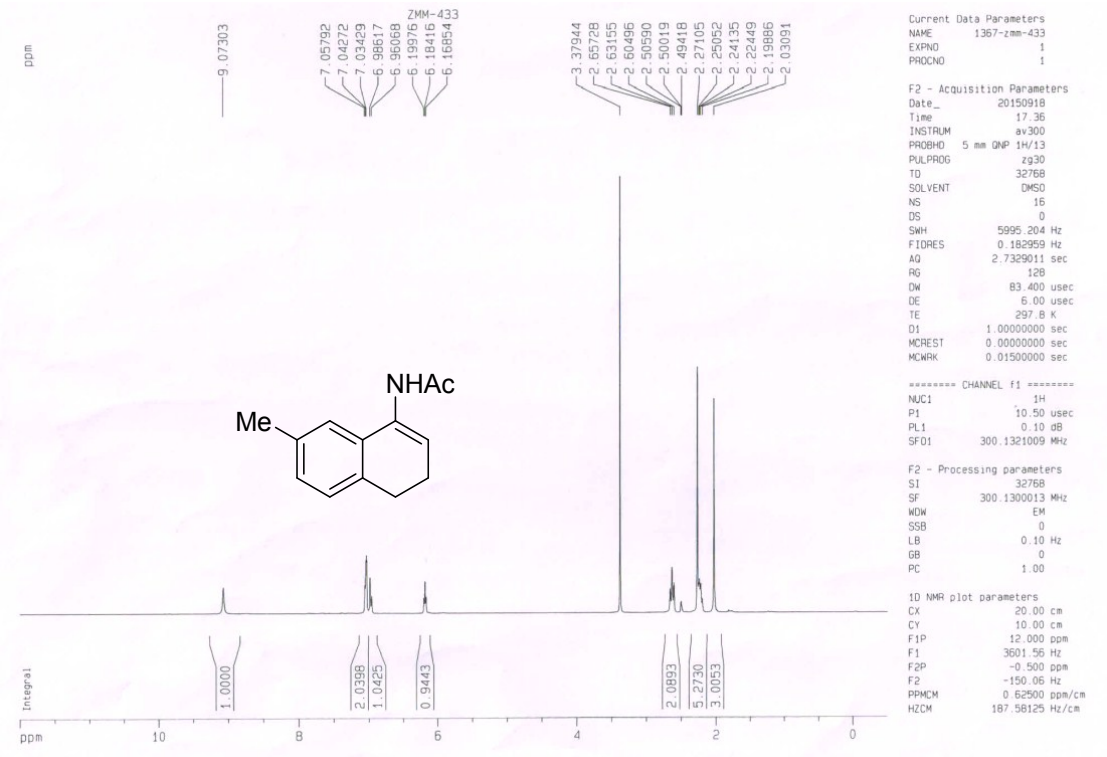
References:

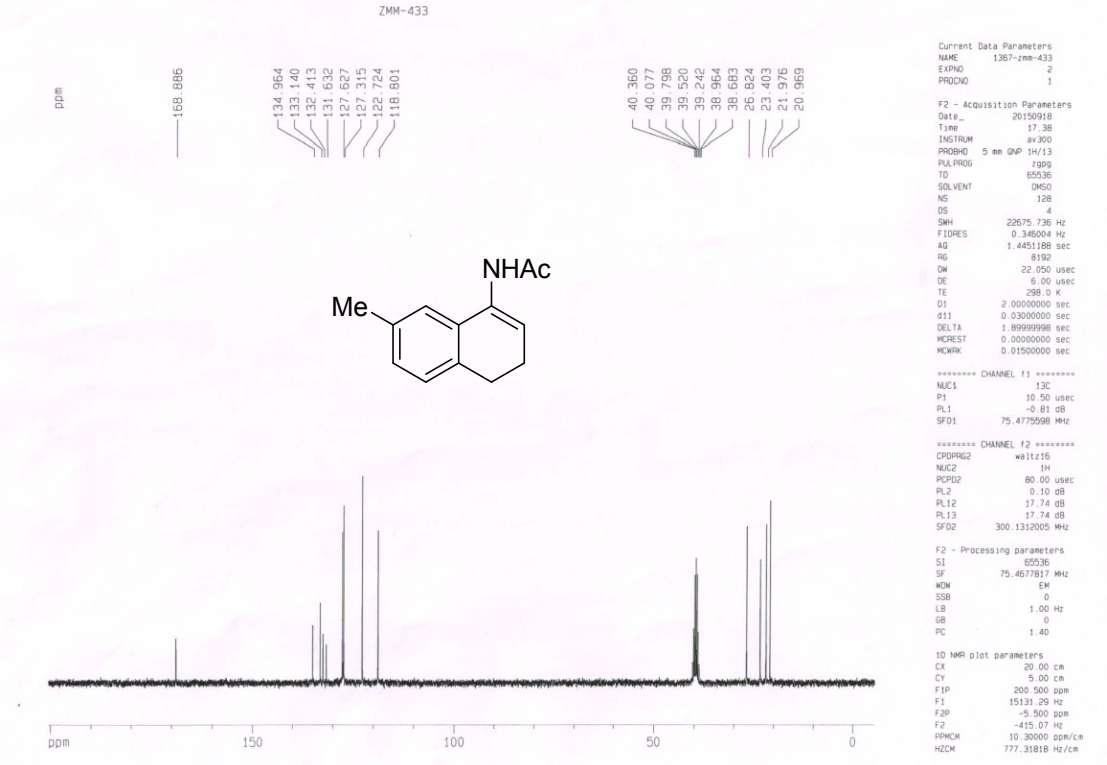
1. C. Wright and G. V. Ullas, *J. Label. Compd. Radiopharm.* 2002, **45**, 1265.
2. Z.-F. Zhang, R. Sangaiah, A. Gold and L. M. Ball, *Org. Biomol. Chem.* 2011, **9**, 5431.
3. Y. Yasu, Y. Arai, R. Tomita, T. Koike and M. Akita, *Org. Lett.* 2014, **16**, 780.
4. A. Gomtsyan, E. K. Bayburt, R. G. Schmidt, C. S. Surowy, P. Honore, K. C. Marsh, S. M. Hannick, H. A. McDonald, J. M. Wetter, J. P. Sullivan, M. F. Jarvis, C. R. Faltynek and C.-H. Lee, *J. Med. Chem.* 2008, **51**, 392.

5. H. Zhou, Y. H. Xu, W. J. Chung and T. P. Loh, *Angew. Chem. Int. Ed*. 2009, **48**, 5355.
6. Q.-S. Wang, J.-H. Xie, W. Li, S.-F. Zhu, L.-X. Wang and Q.-L. Zhou, *Org. Lett.* 2011, **13**, 3388.
7. W.-J. Tang, Y.-X. Chi and X.-M. Zhang, *Org. Lett*. 2002, **4**, 1695.
8. Z.-G. Zhang, G.-X. Zhu, Q.-Z. Jiang, D.-M. Xiao and X.-M. Zhang, *J. Org. Chem.* 1999, **64**, 1774.
9. K. Murugan, D.-W. Huang, Y.-T. Chien and S.-T. Liu, *Tetrahedron* 2013, **69**, 268.
10. Z.-H. Guan, Z.-Y. Zhang, Z.-H. Ren, Y.-Y. Wang and X.-M. Zhang, *J. Org. Chem.* 2011, **76**, 339.
11. J. T. Reeves, Z. L. Tan, Z. X. S. Han, G. S. Li, Y. D. Zhang, Y. B. Xu, D. C. Reeves, N. C. Gonnella, S. L. Ma, H. Lee, B. Z. Lu and C. H. Senanayake, *Angew. Chem. Int. Ed*. 2012, **51**, 1400.
12. C. X. Sun and S. M. Weinreb, *Synthesis* 2006, **21**, 3585.
13. A. Carboni, G. Dagousset, E. Magnier, and G. Masson, *Org. Lett.* 2014**, 16**, 1240.
14. L.-H. Liao, C. Shu, M.-M. Zhang, Y.-J. Liao, X.-Y. Hu, Y.-H. Zhang, Z.-J. Wu, W.-C. Yuan and X.-M. Zhang, *Angew. Chem. Int. Ed*. 2014, **53**, 10471.
15. J.-Z. Wang, J. Zhou, C. Xu, H.-B. Sun, L. Kürti and Q.-L. Xu, *J. Am. Chem. Soc*, 2016, **138**, 5202−5205.

^{1}H NMR and ^{13}C NMR spectra

N-(7-methyl-3,4-dihydronaphthalen-1-yl)acetamide (1e)





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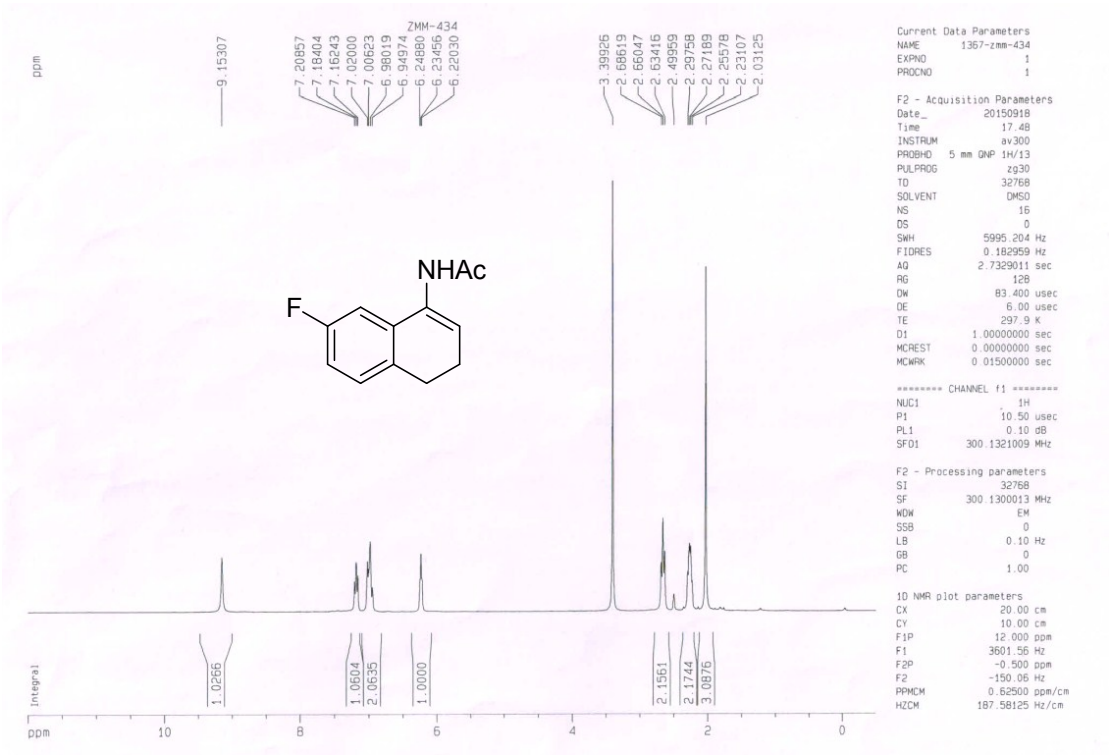

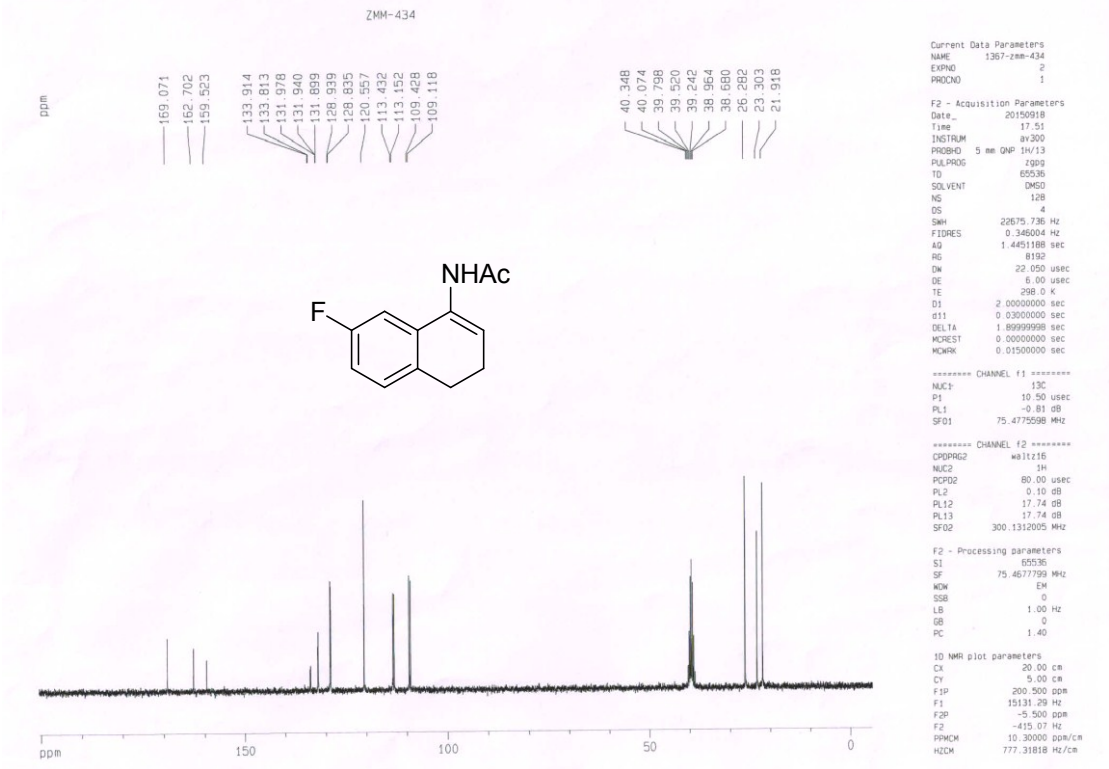

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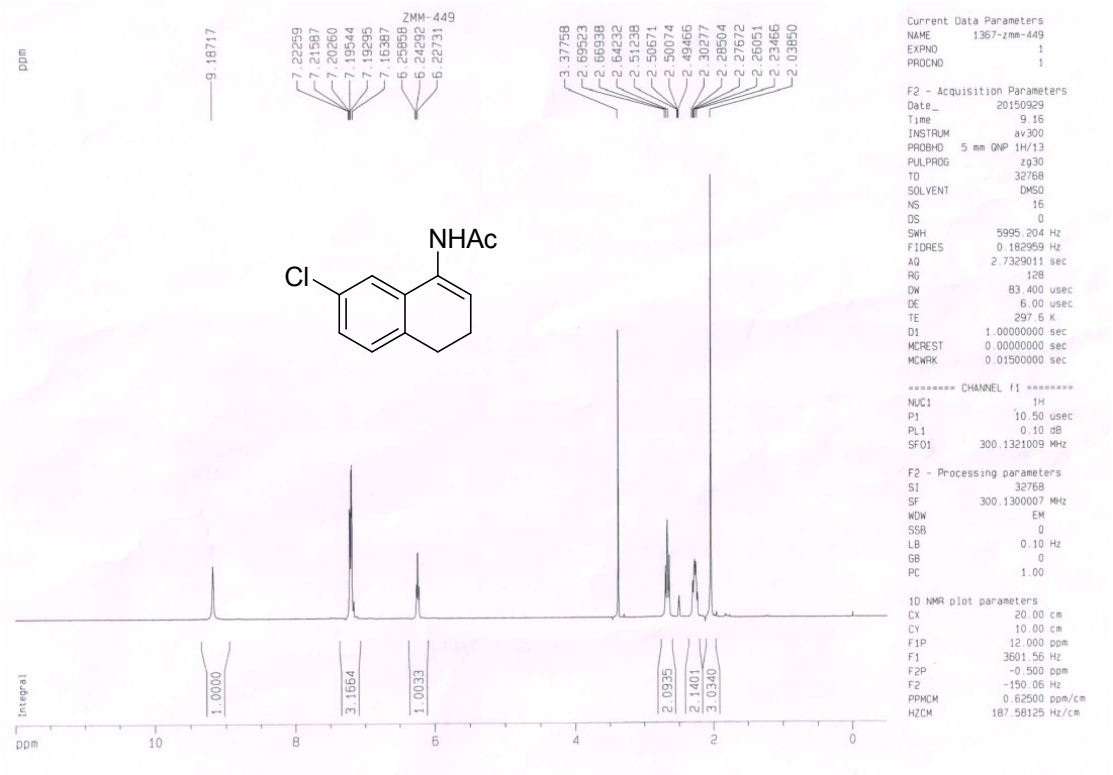

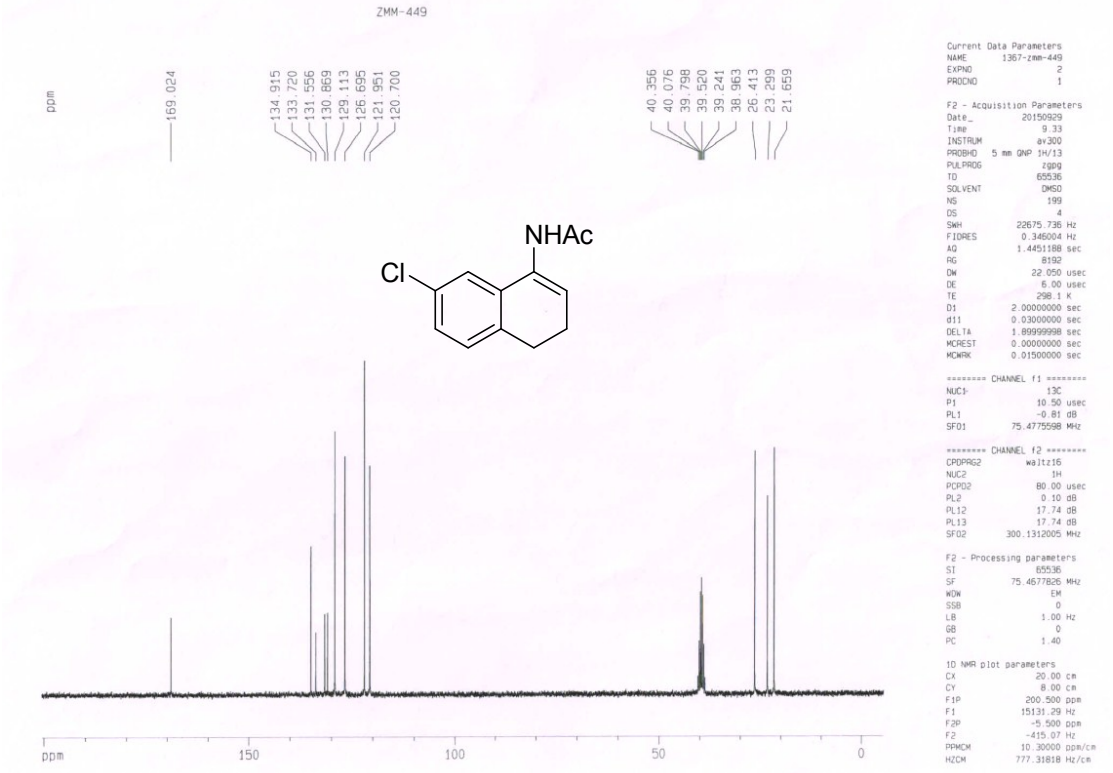

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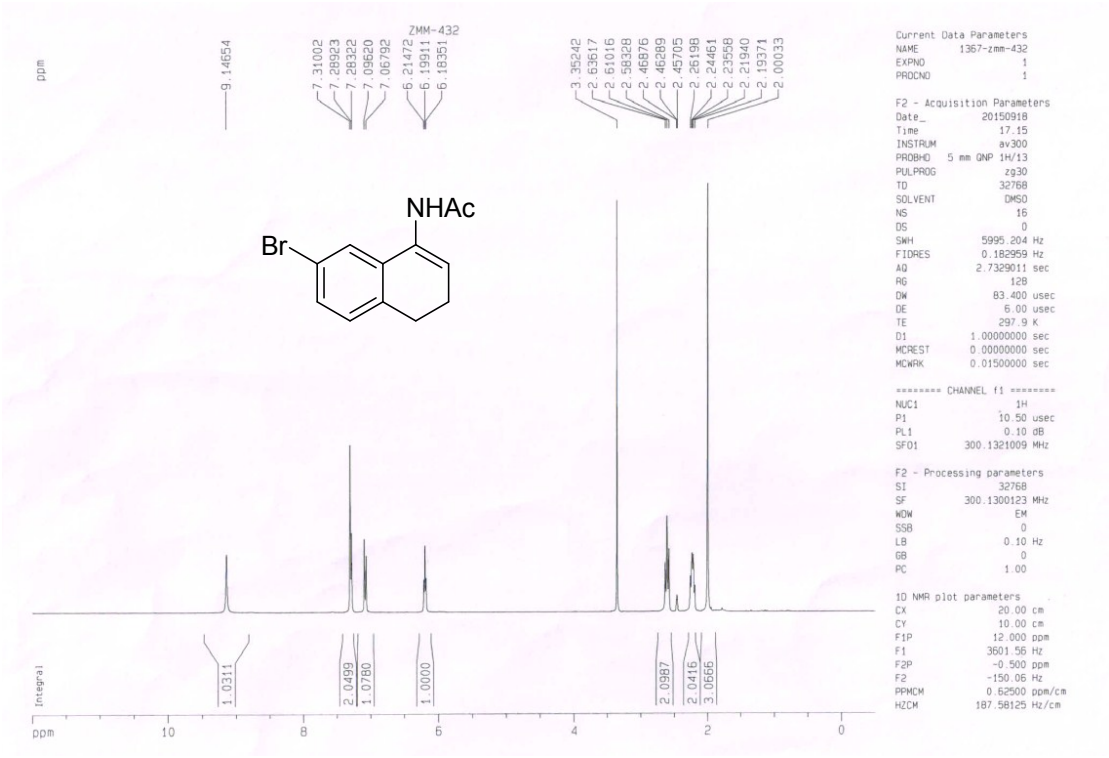
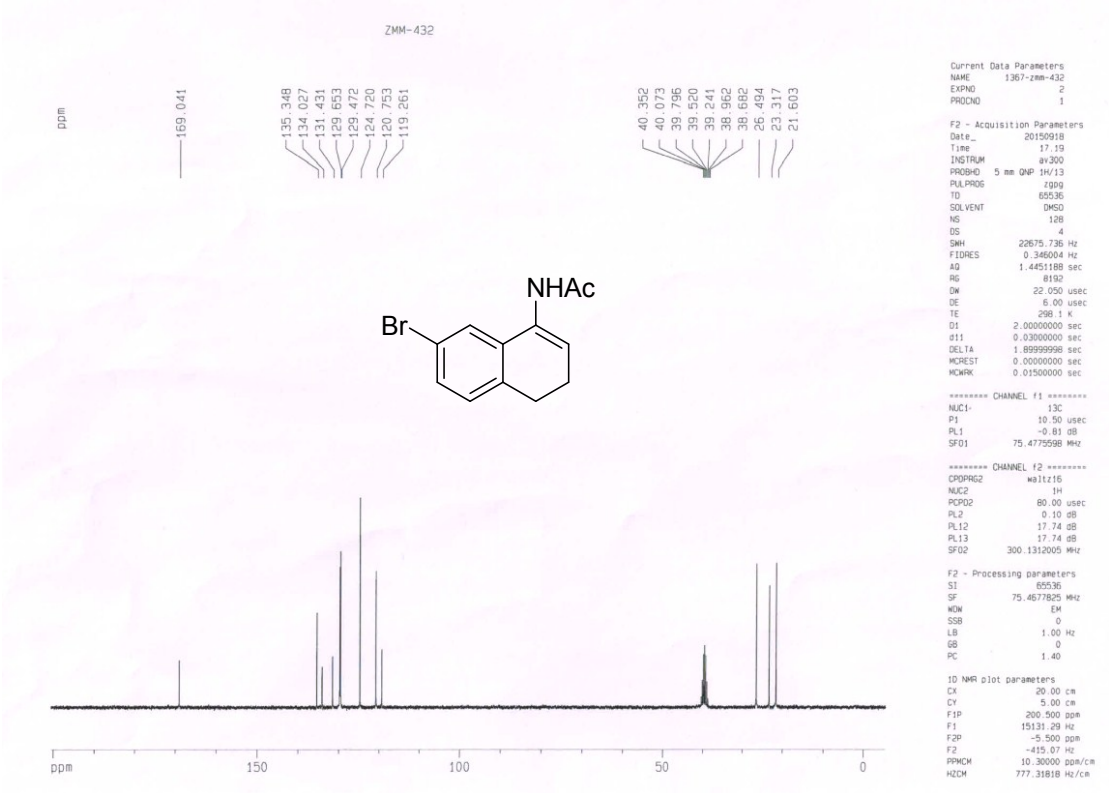
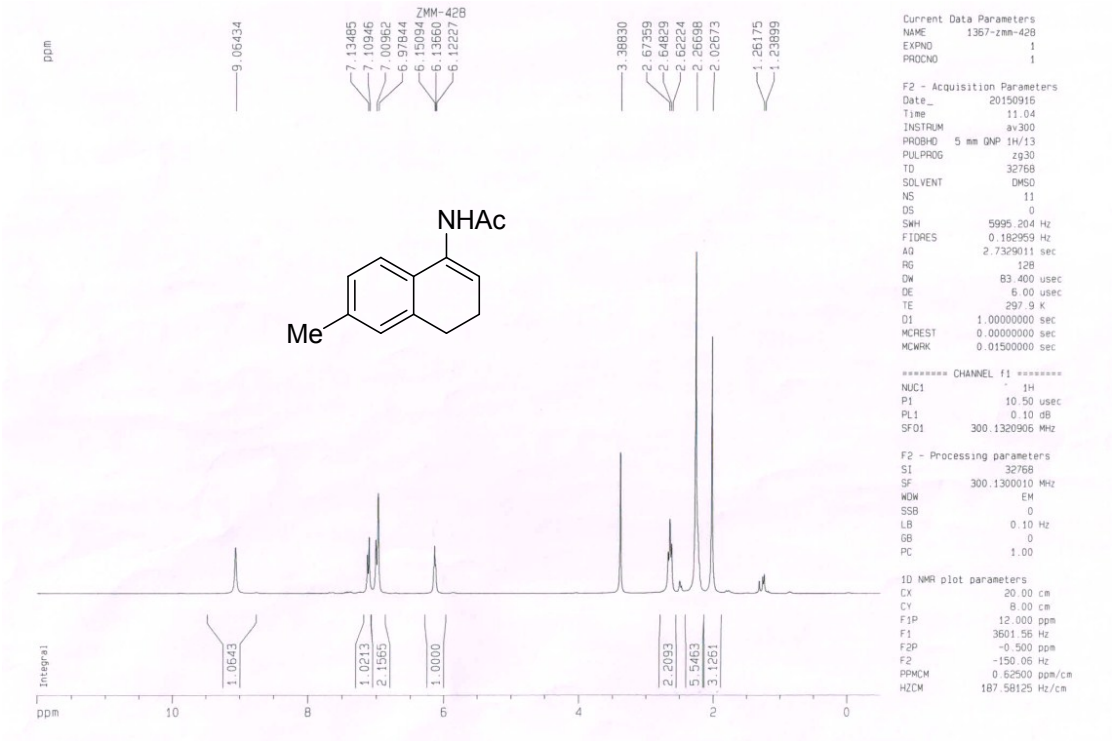
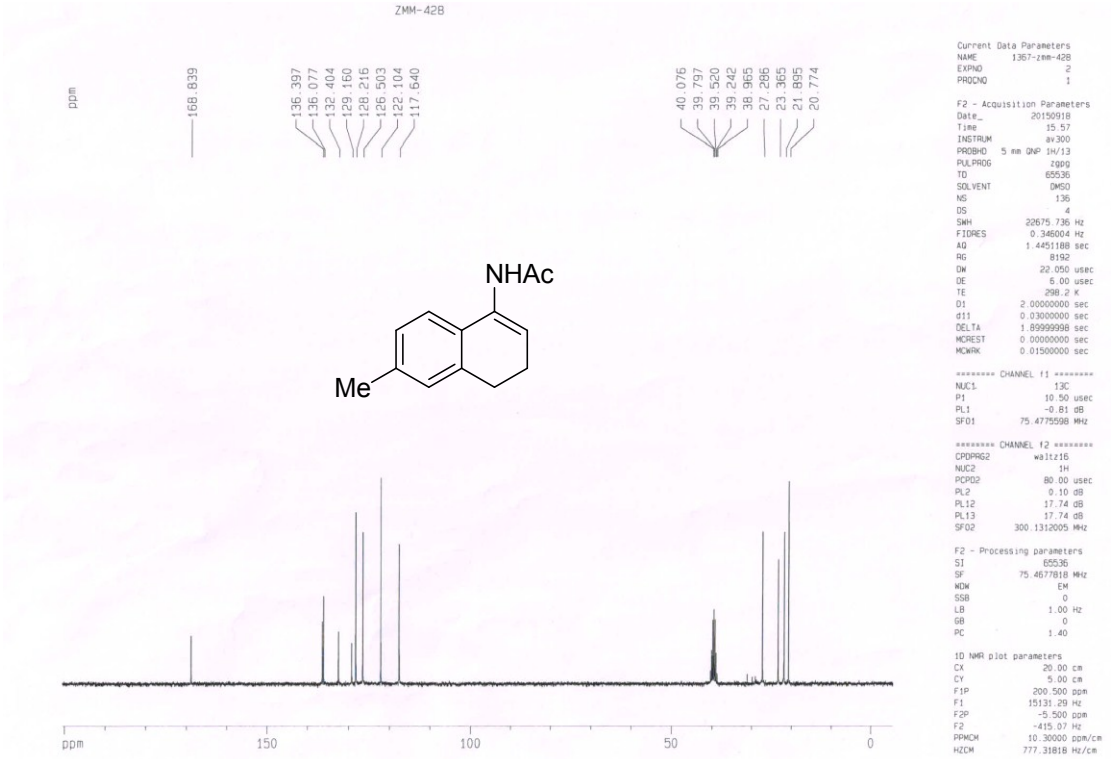




N-(6-methyl-3,4-dihydronaphthalen-1-yl)acetamide (1i)





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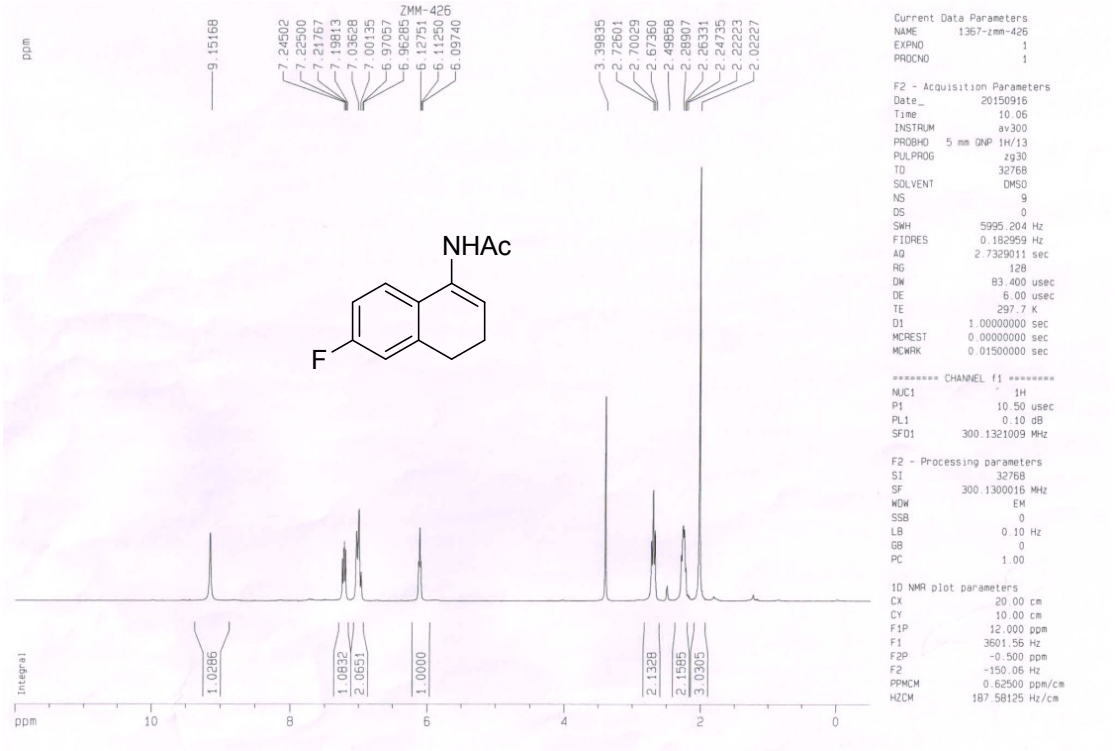

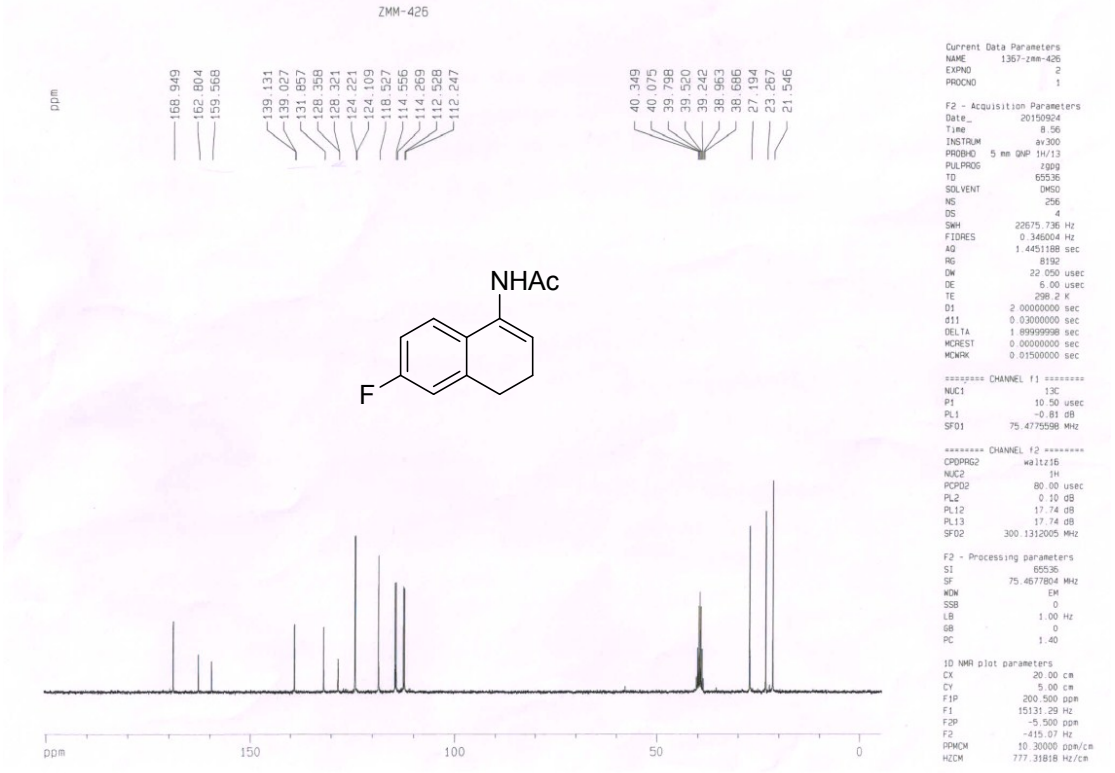

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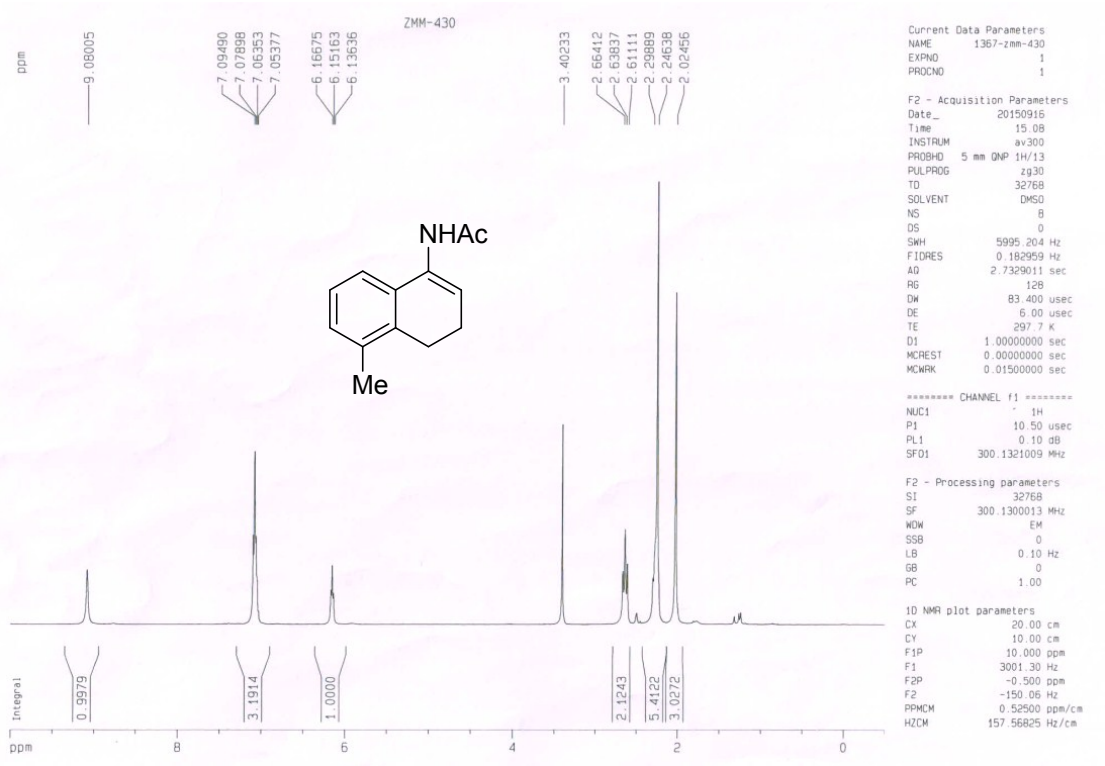
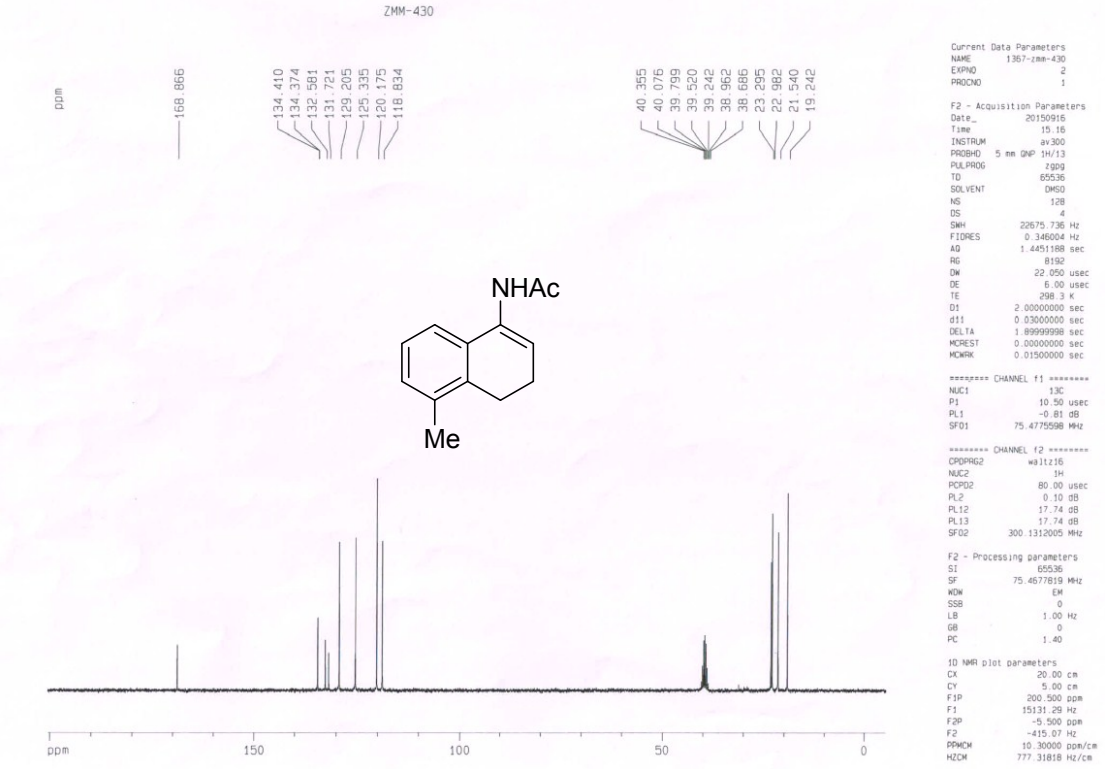
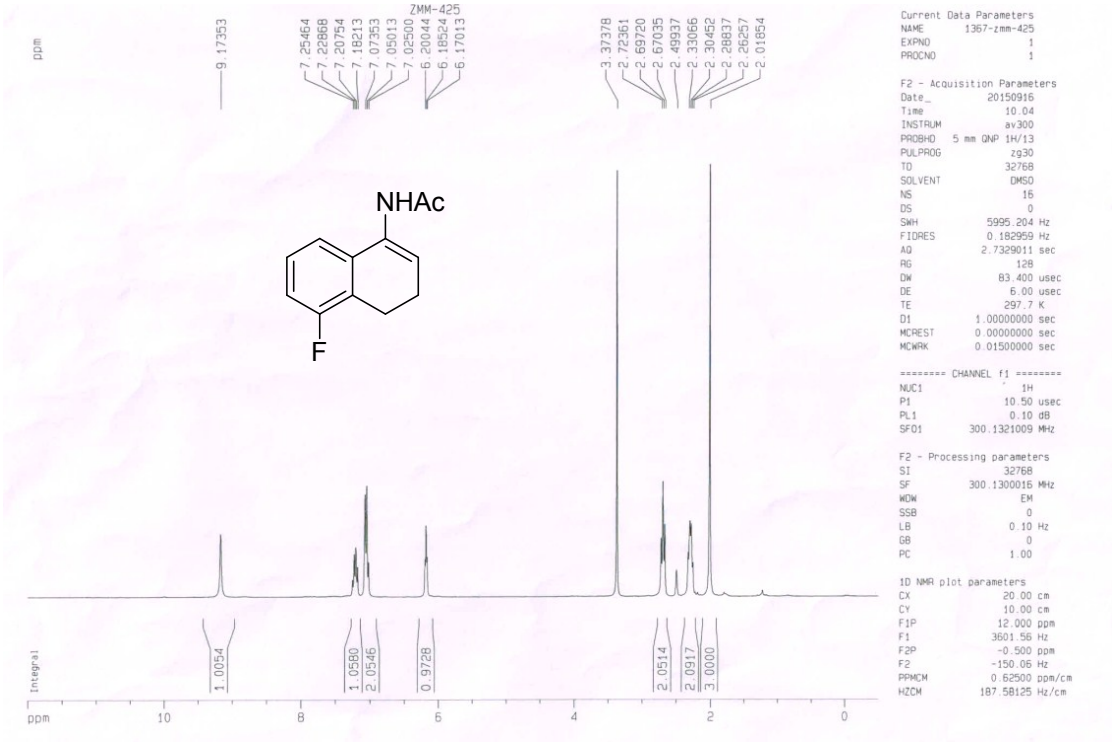
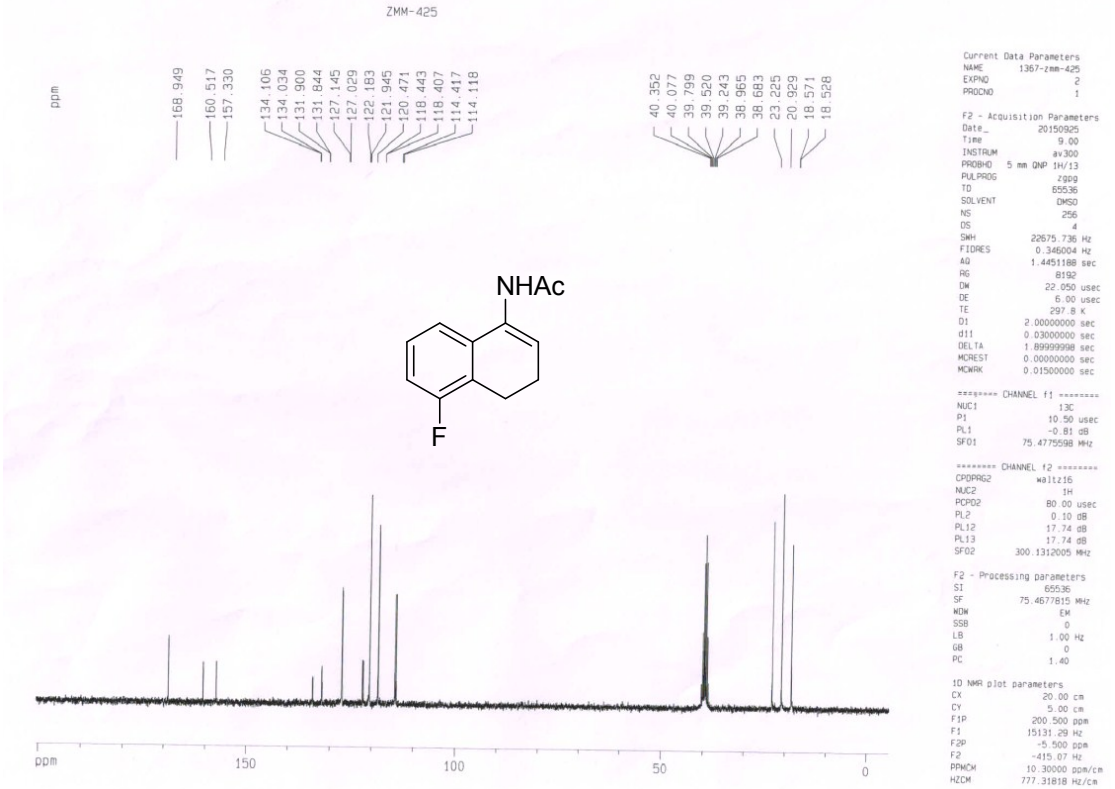


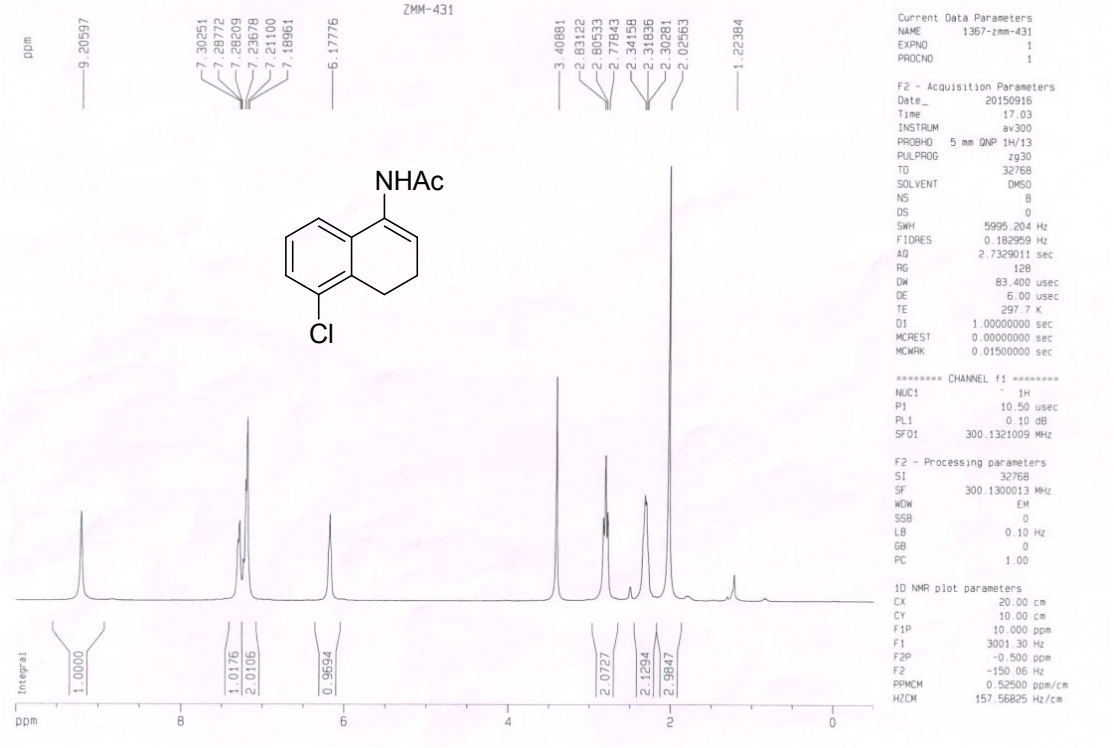


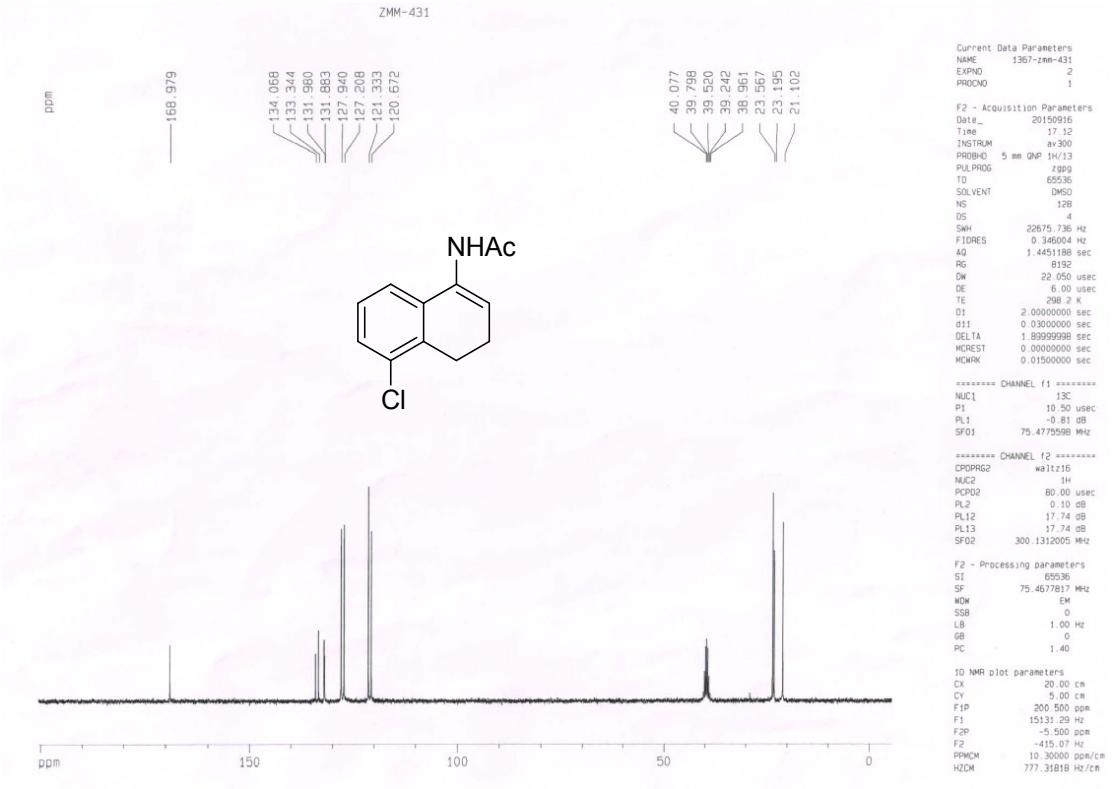
N-(5-fluoro-3,4-dihydronaphthalen-1-yl)acetamide (1l)



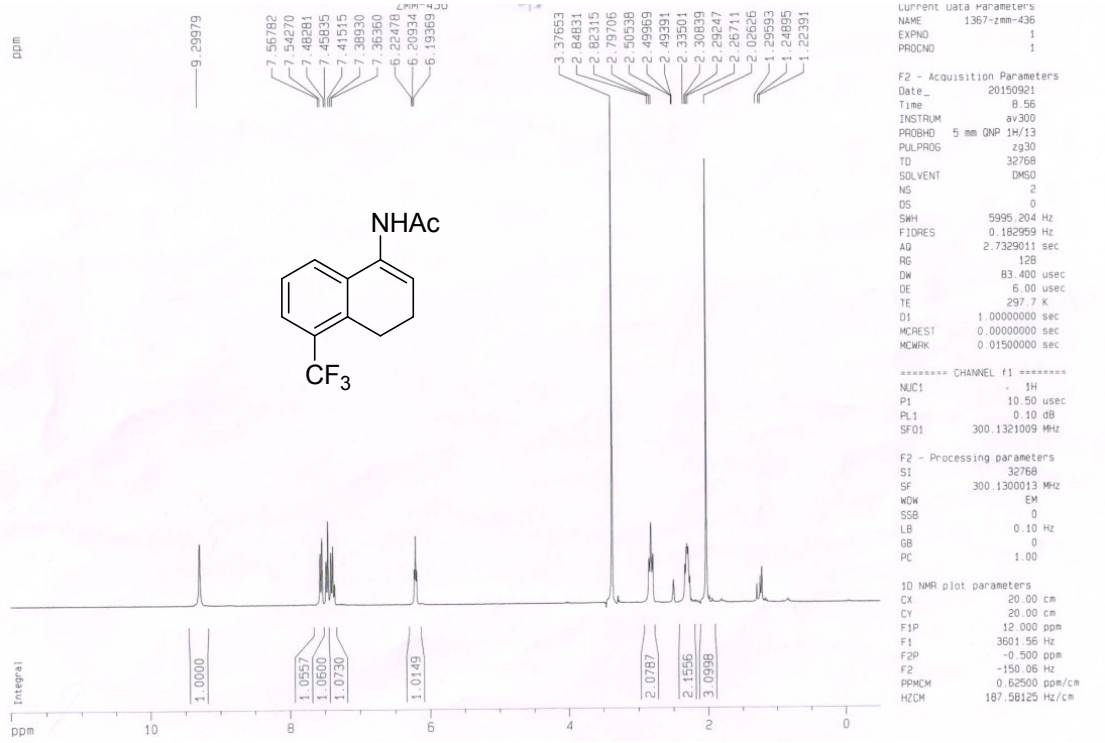


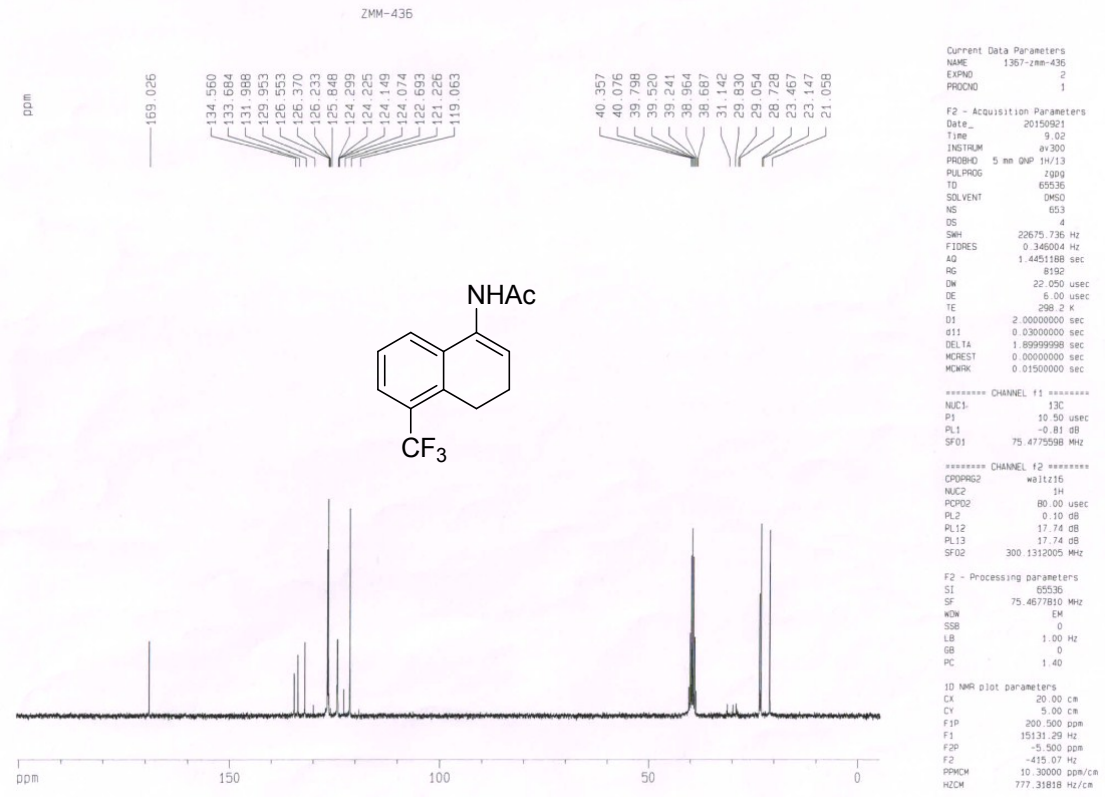
N-(5-chloro-3,4-dihydronaphthalen-1-yl)acetamide (1m)



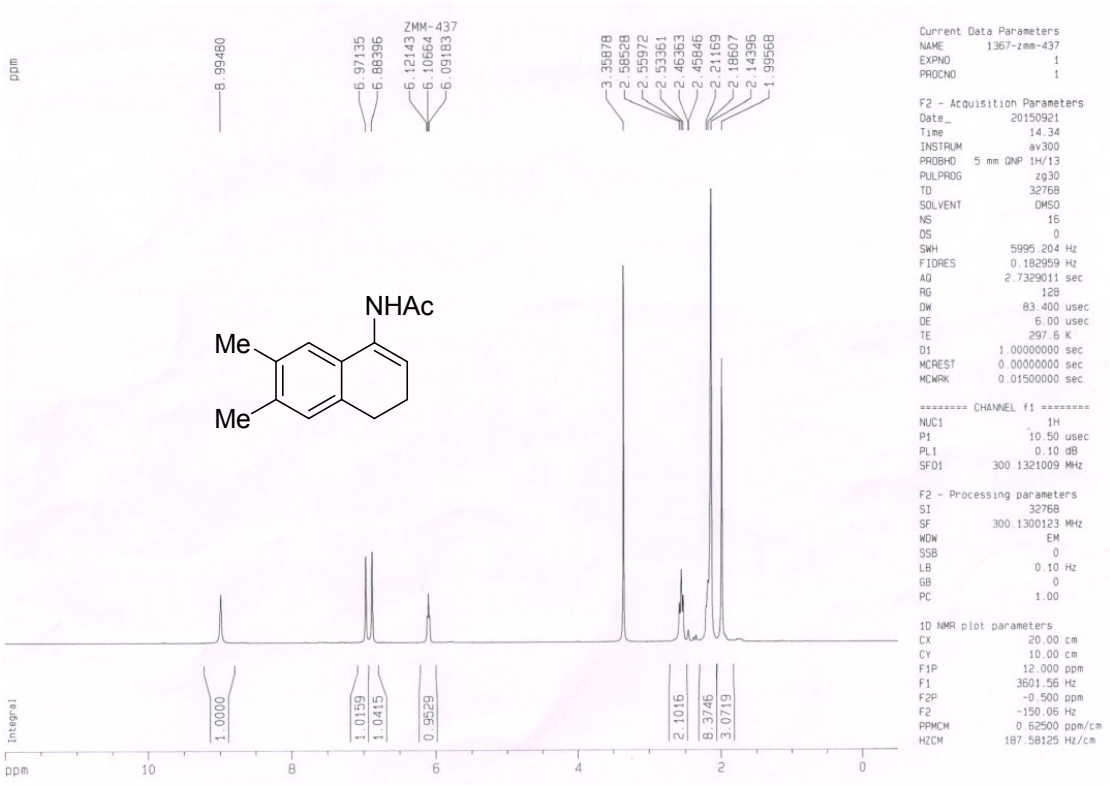


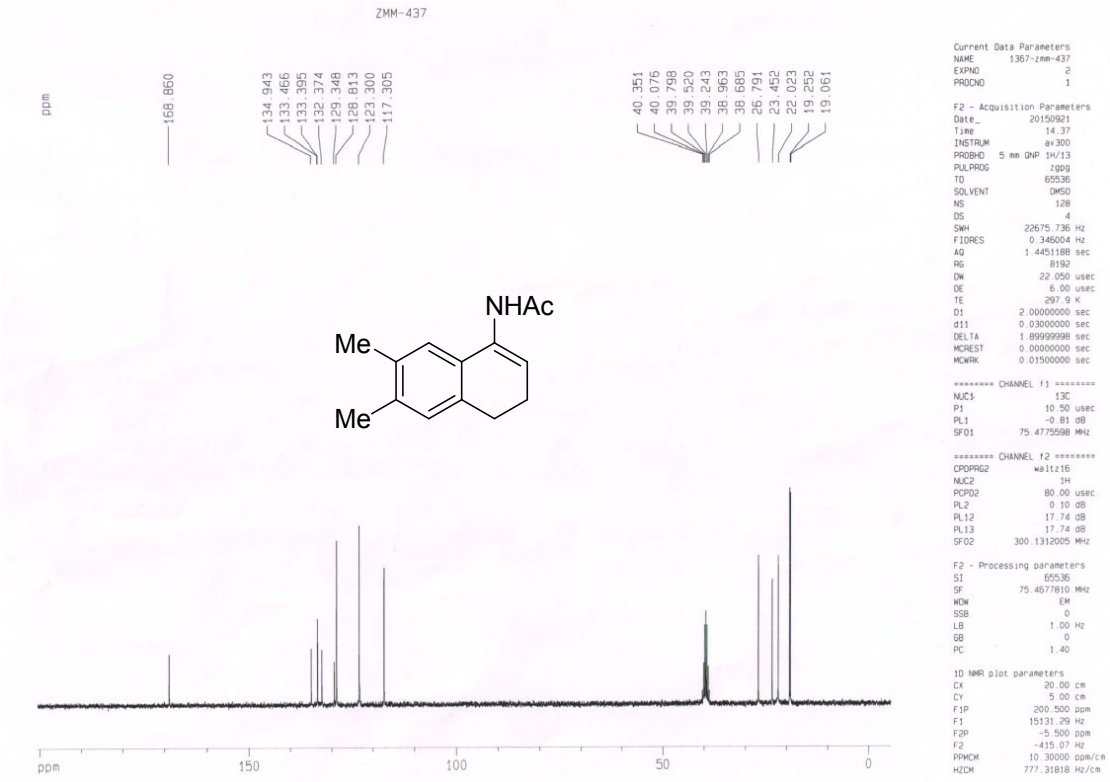
N-(5-(trifluoromethyl)-3,4-dihydronaphthalen-1-yl)acetamide (1n)



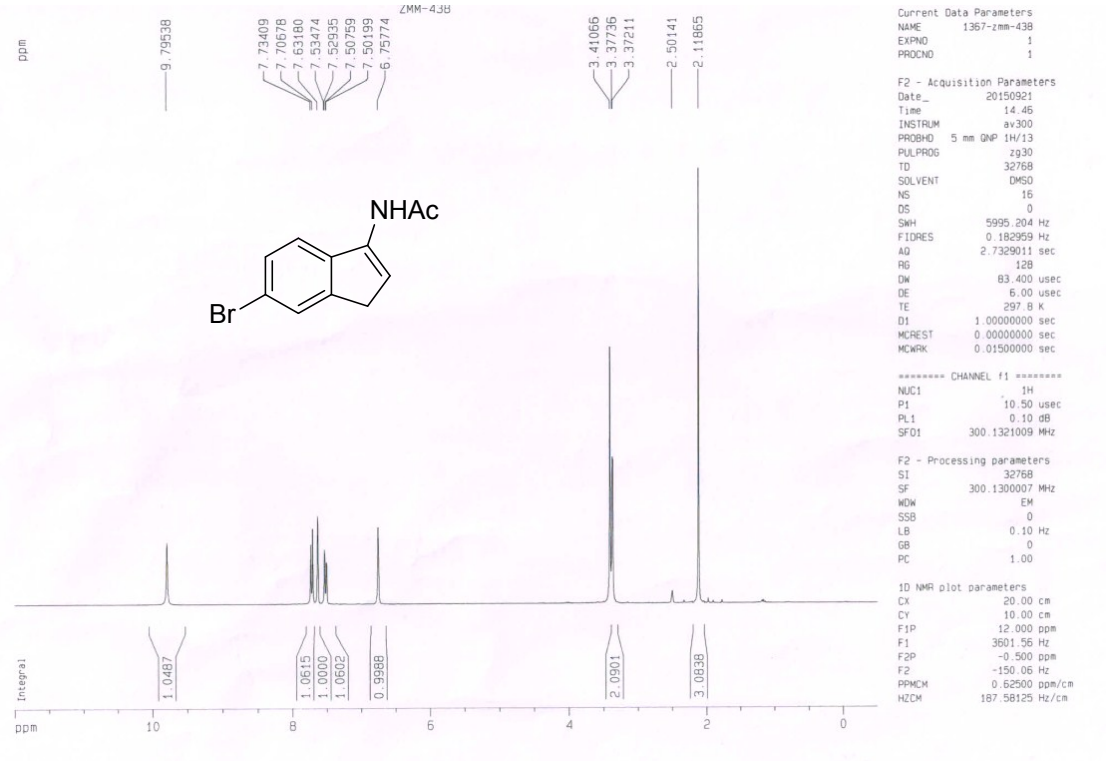


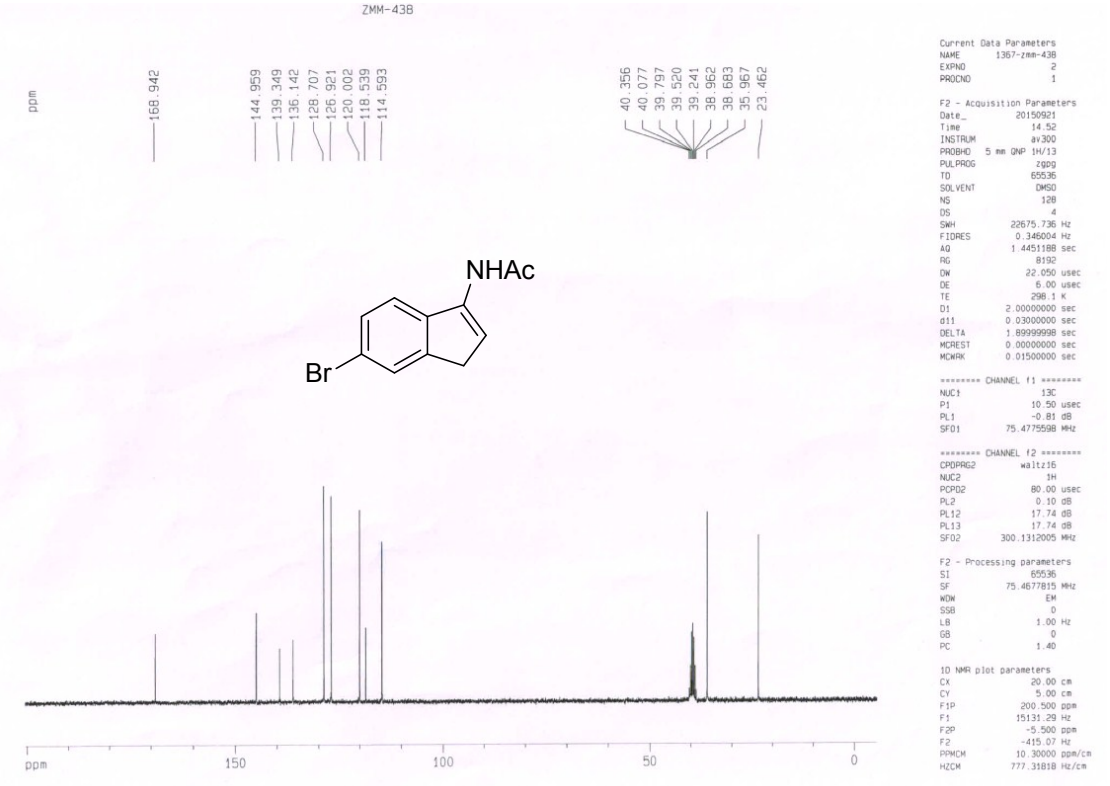
N-(6,7-dimethyl-3,4-dihydronaphthalen-1-yl)acetamide (1o)



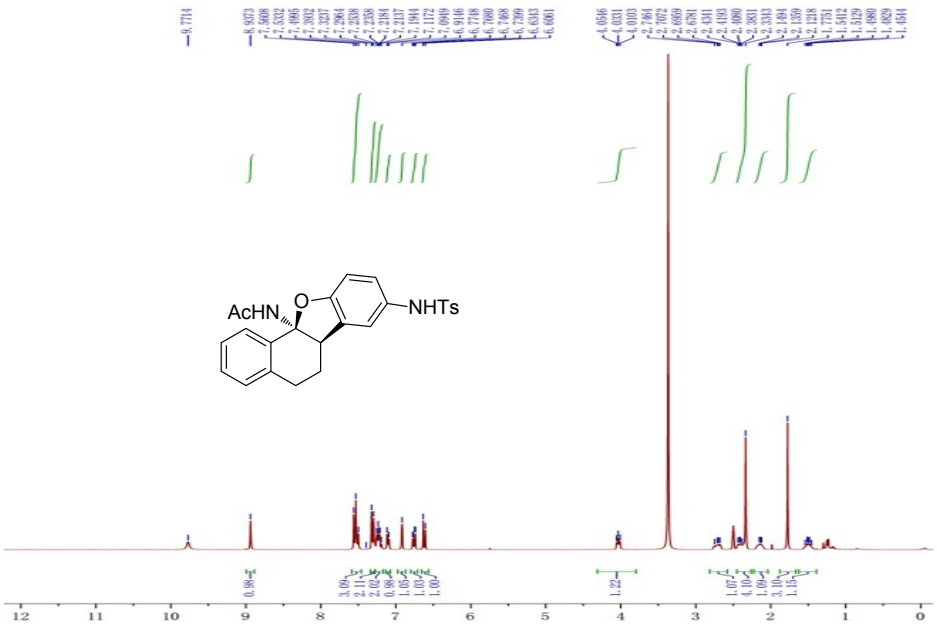


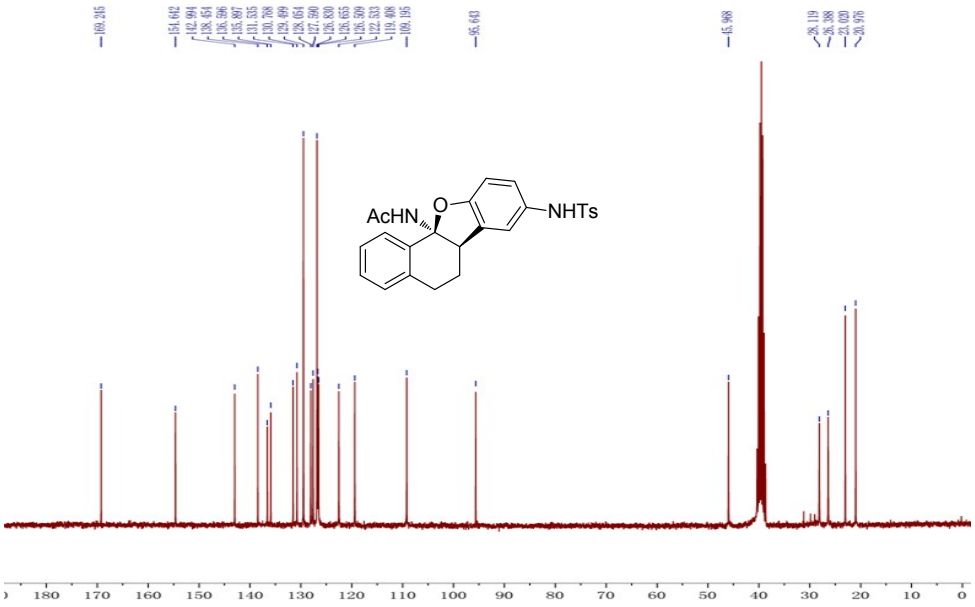
N-(6-bromo-1H-inden-3-yl)acetamide (1u)



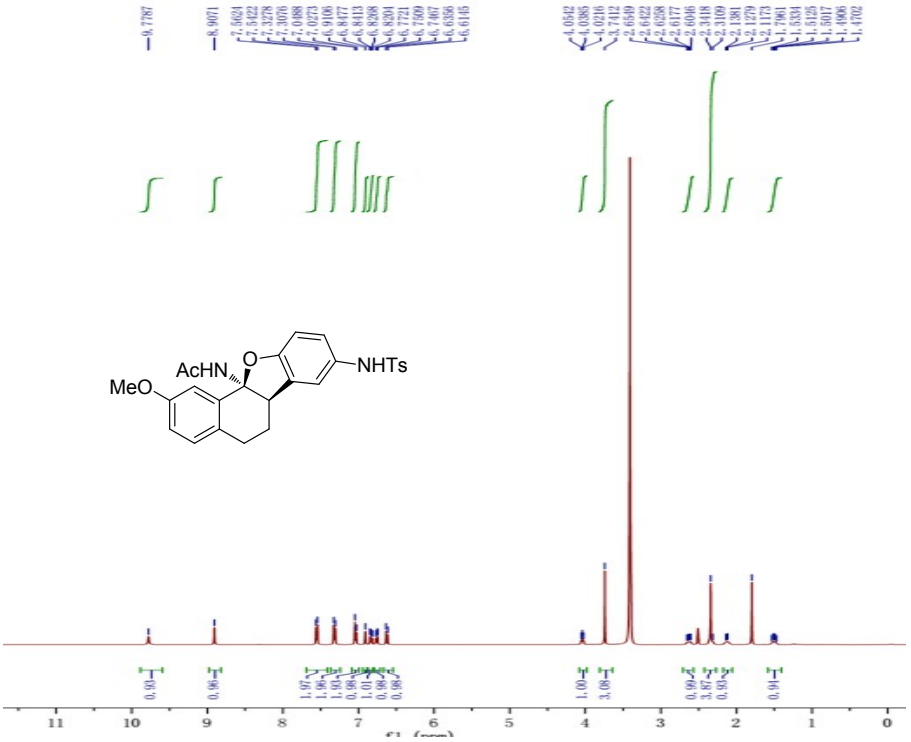


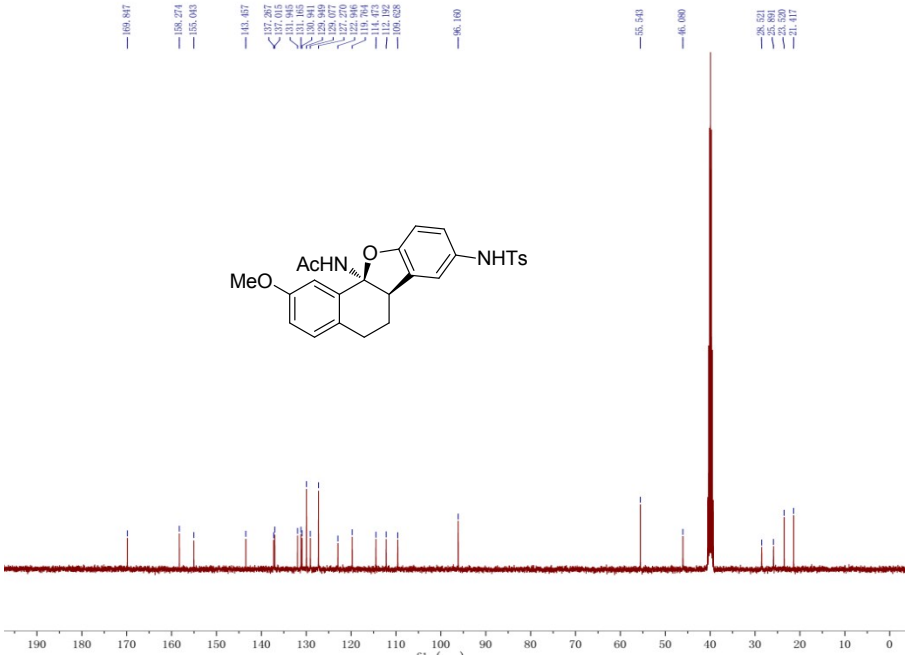
N-(8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b] benzofuran-11a-yl)acetamide (3a):



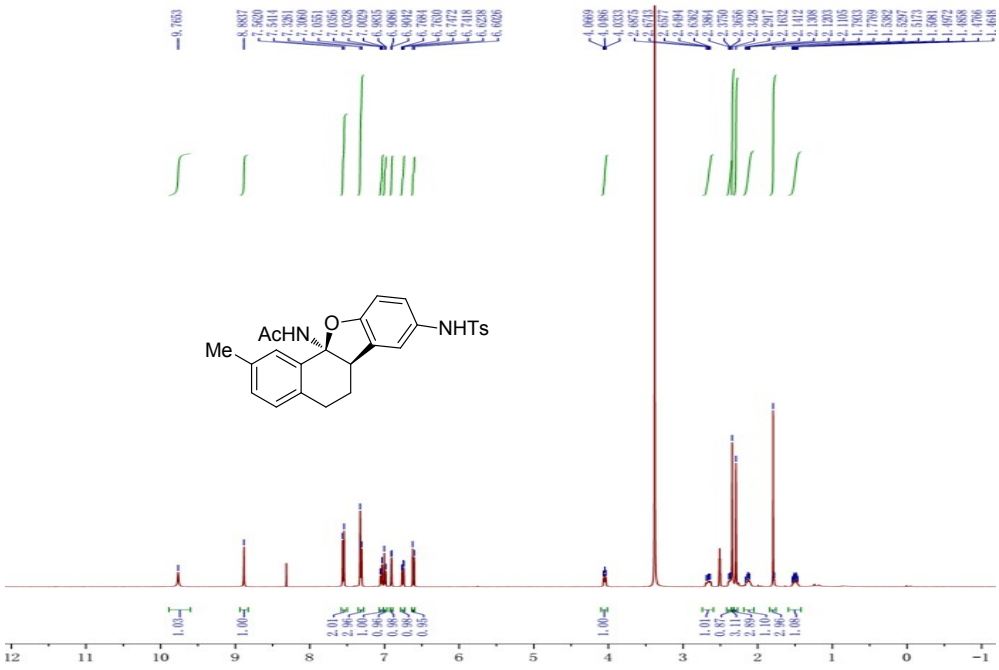


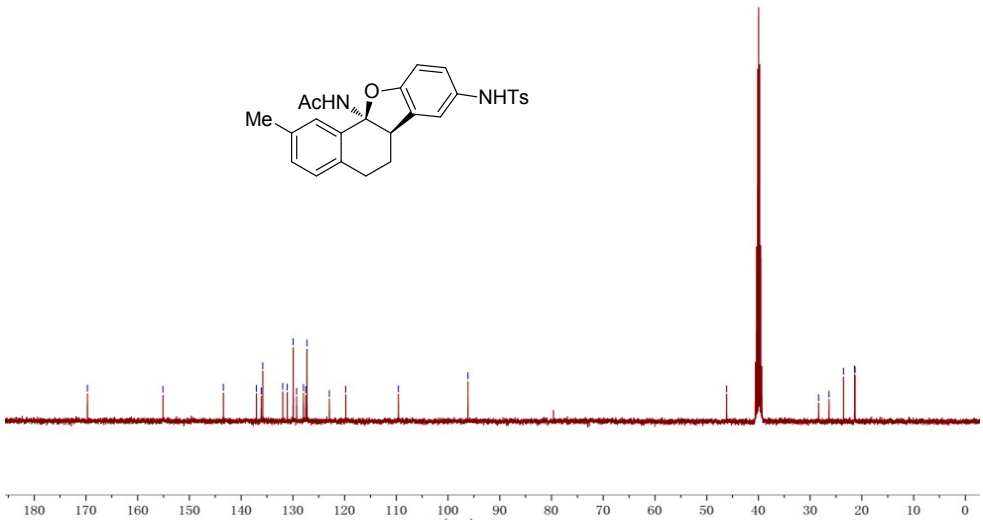
N-(2-methoxy-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3d):



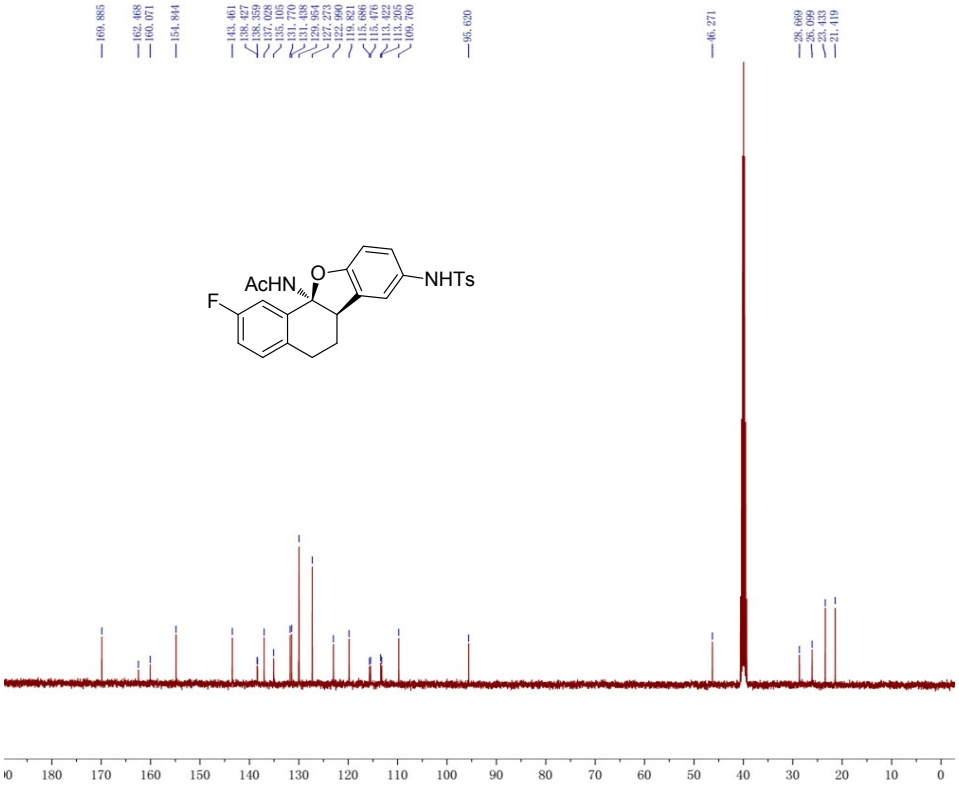


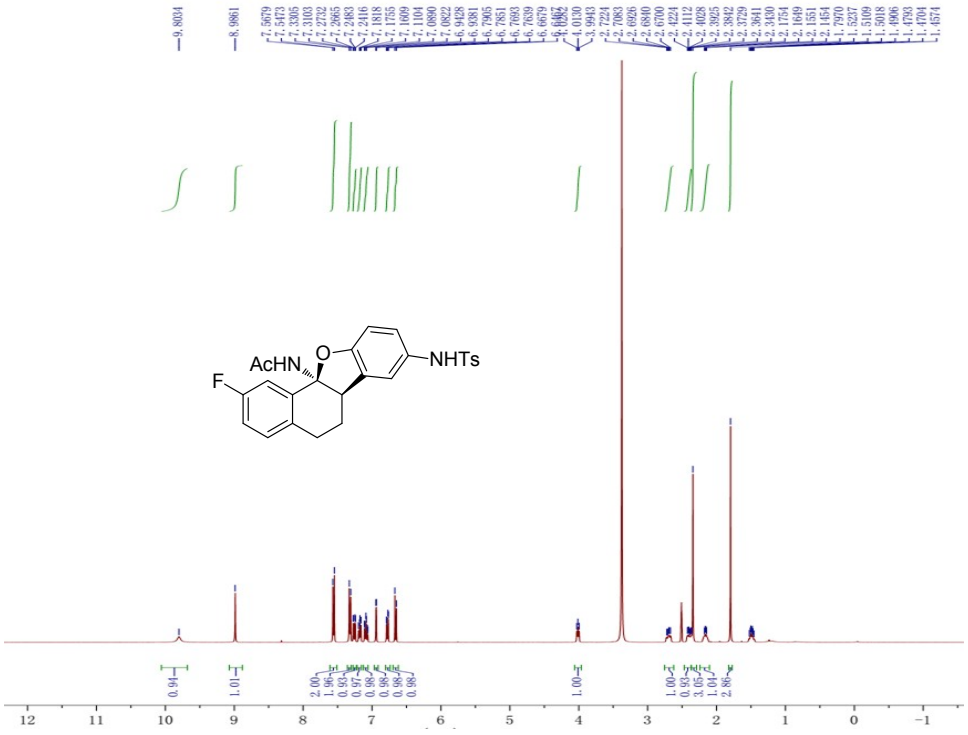
N-(2-methyl-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3e):



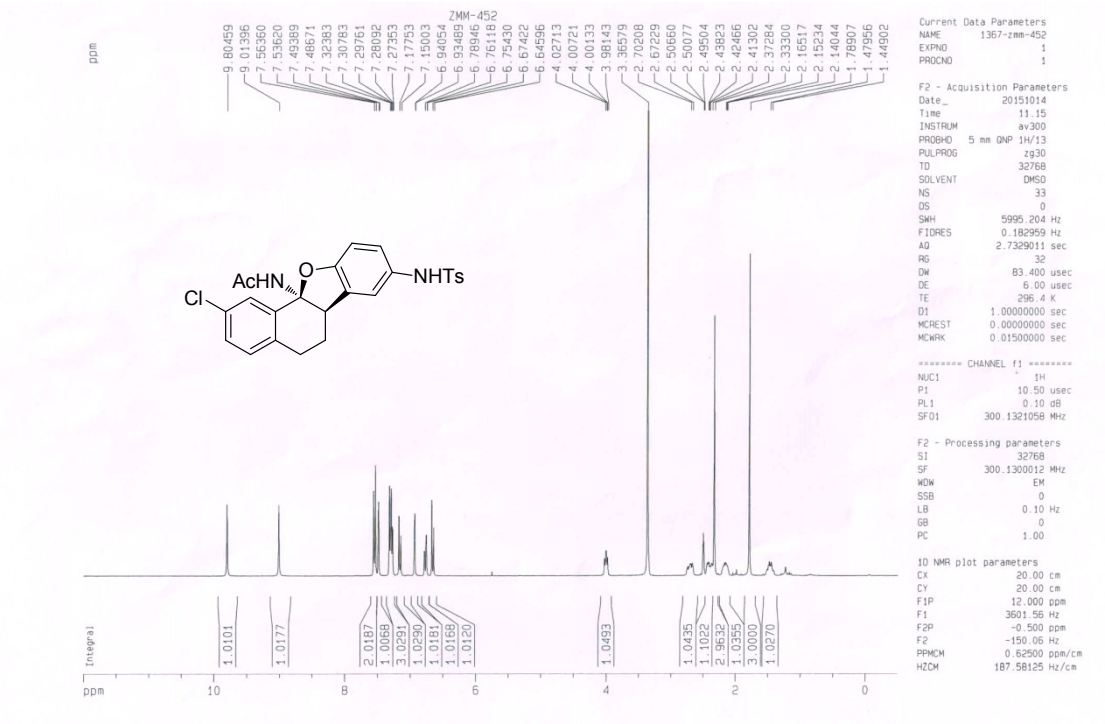


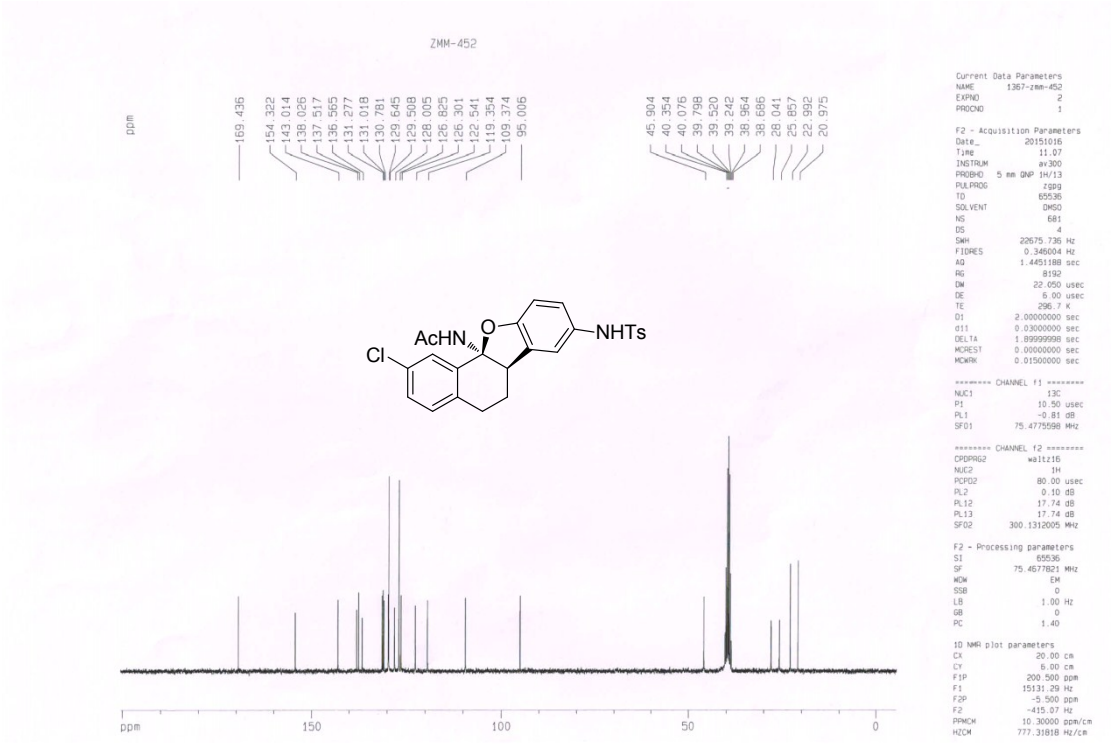
N-(2-fluoro-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3f)



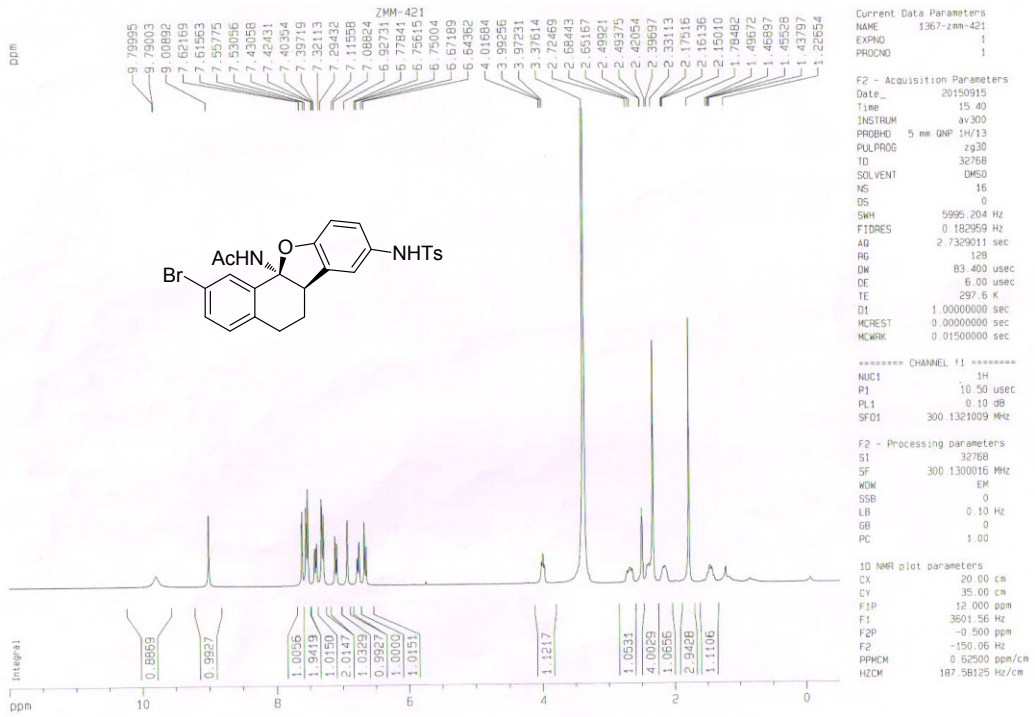


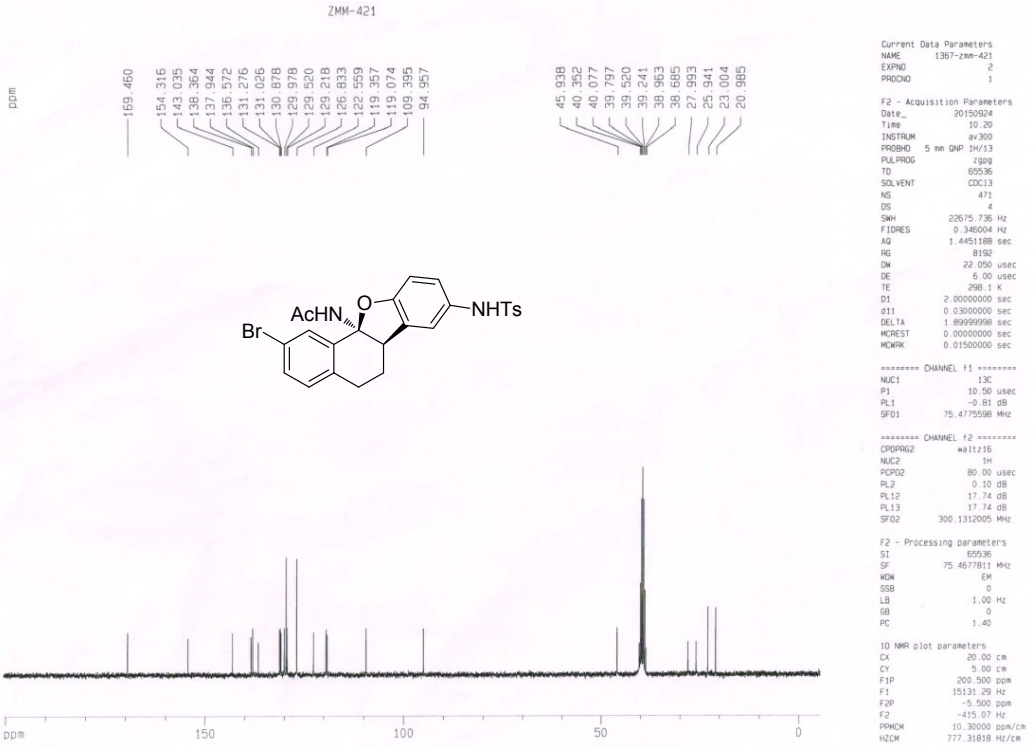
N-(2-chloro-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3g)



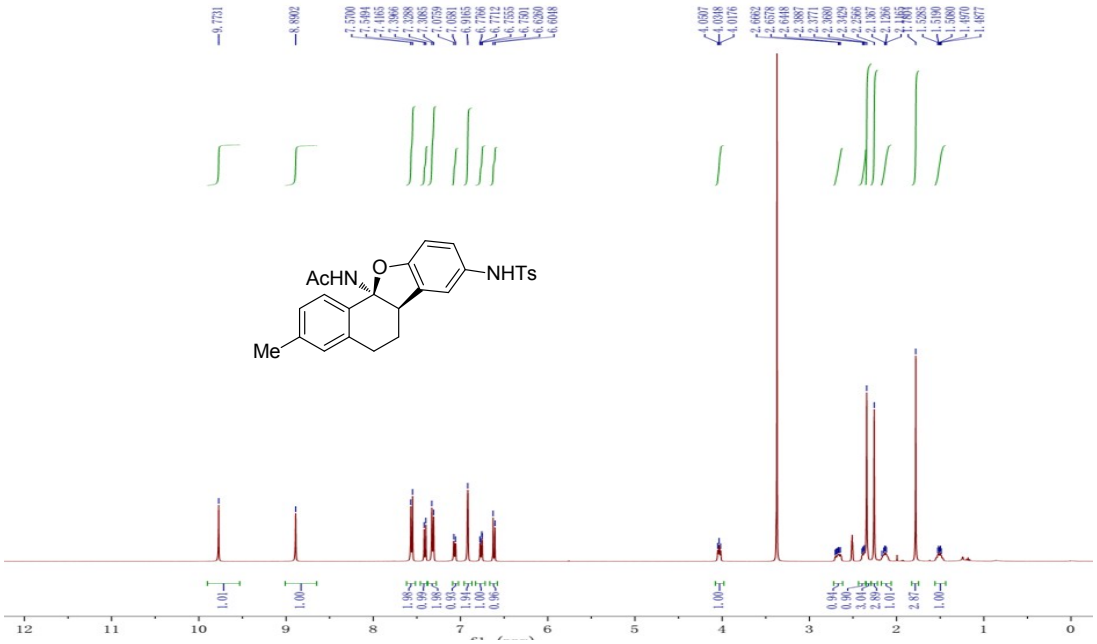


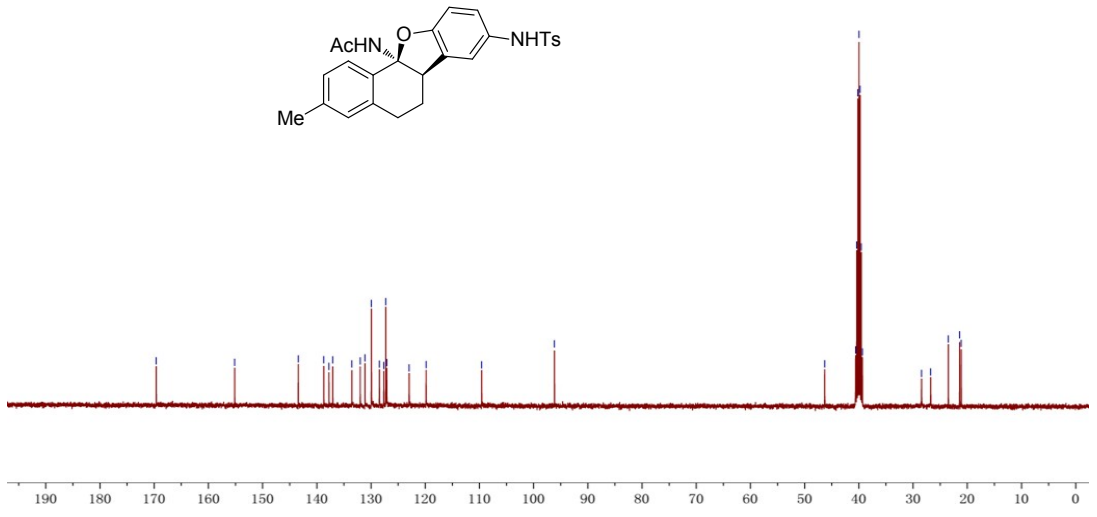
N-(2-bromo-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3h)



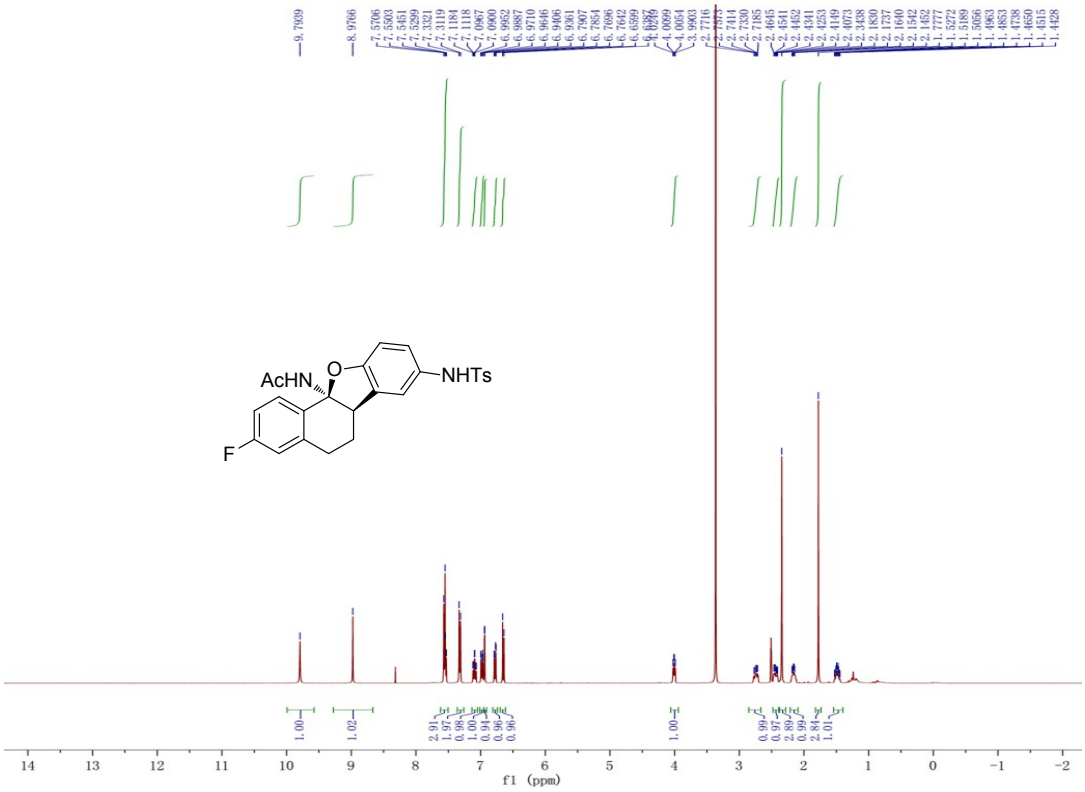


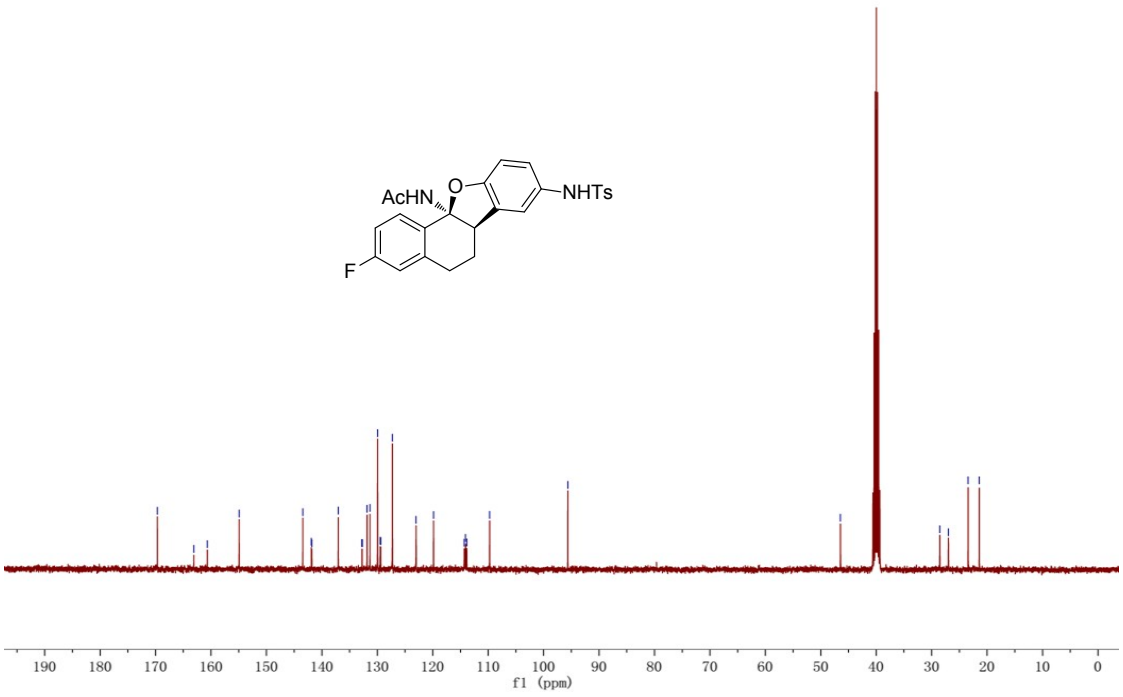
N-(3-methyl-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3i)



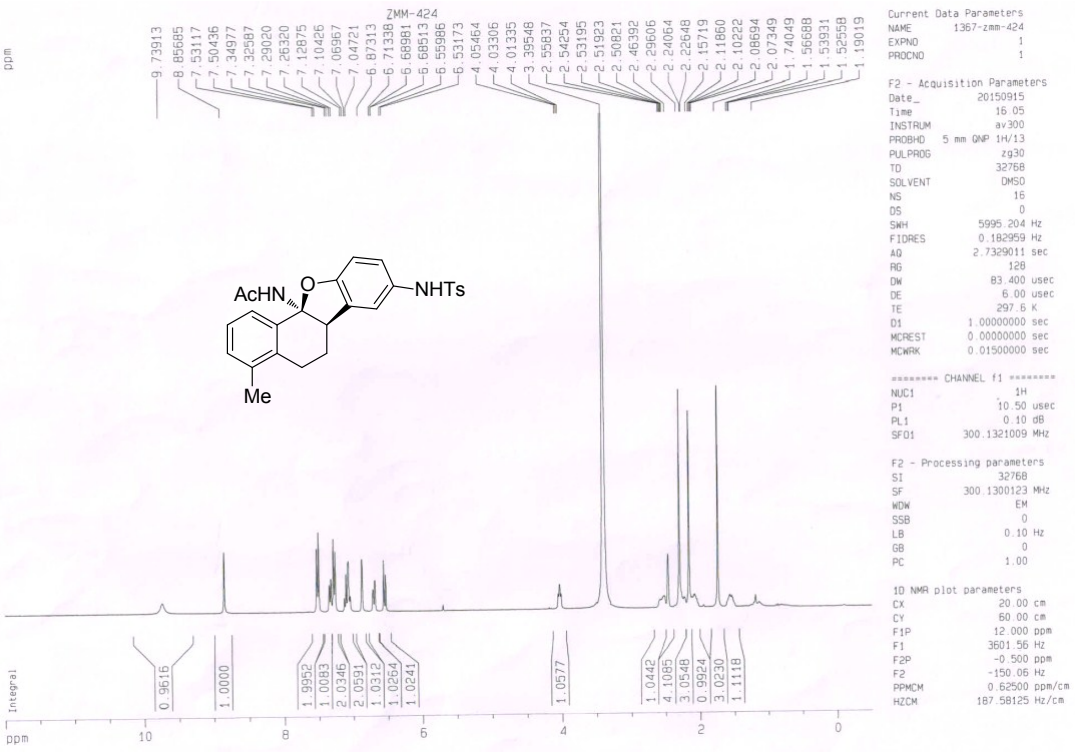


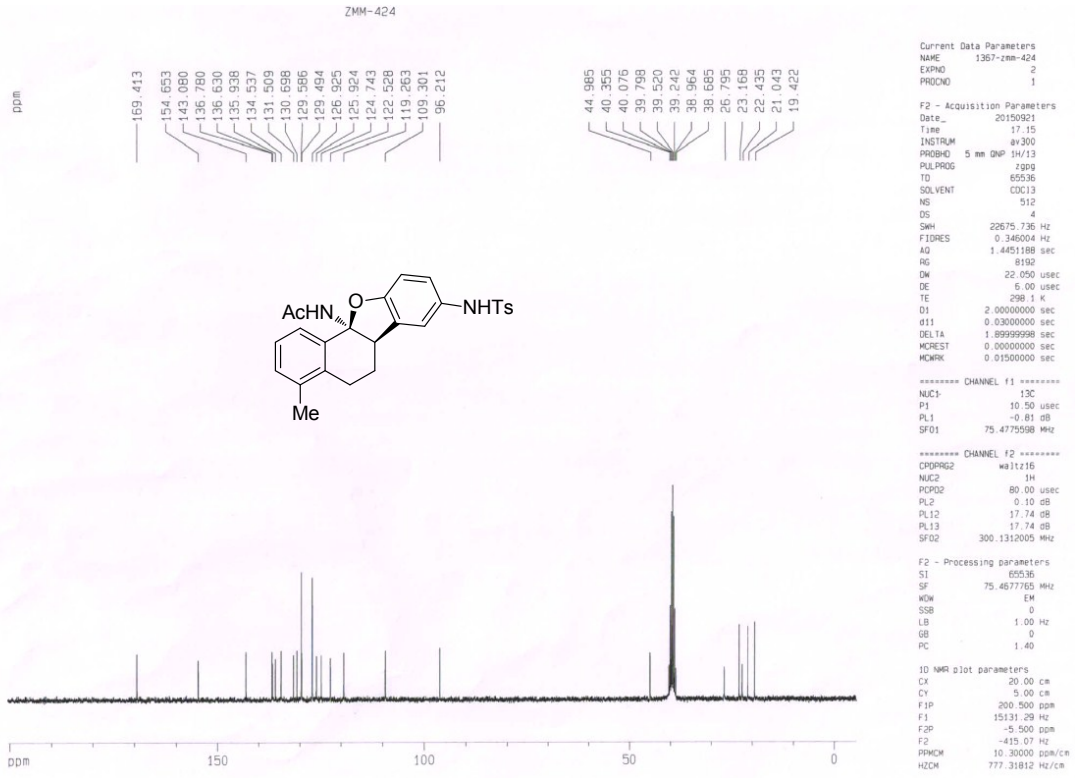
N-(3-fluoro-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3j) :



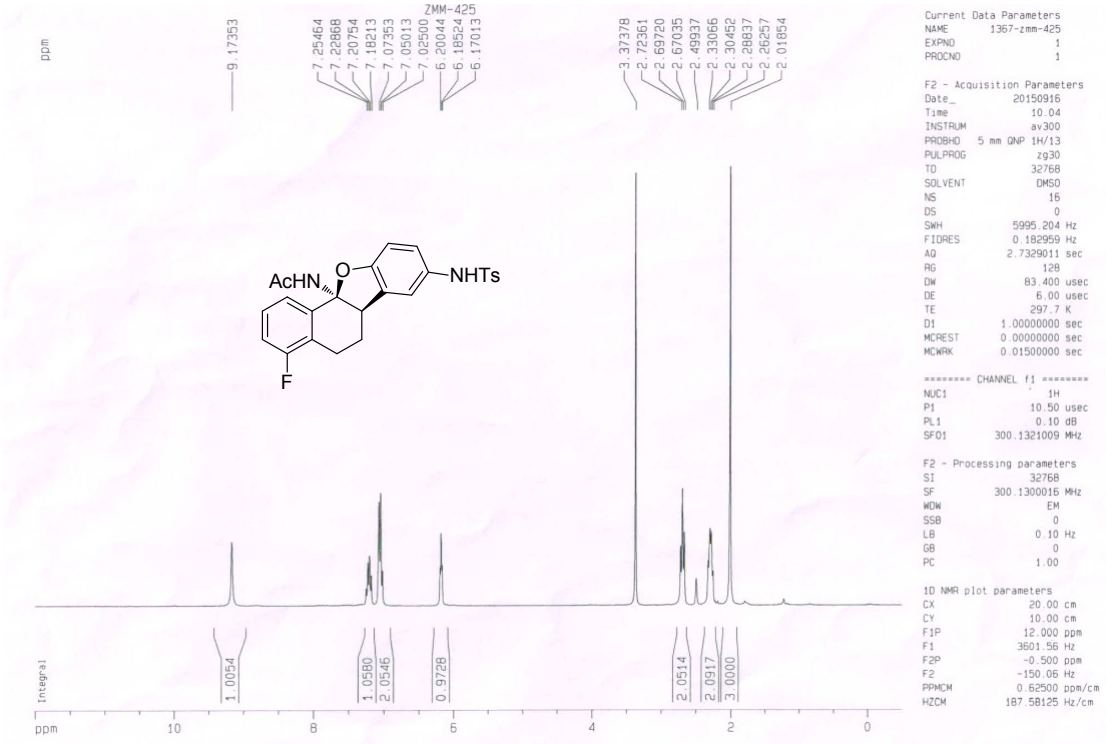


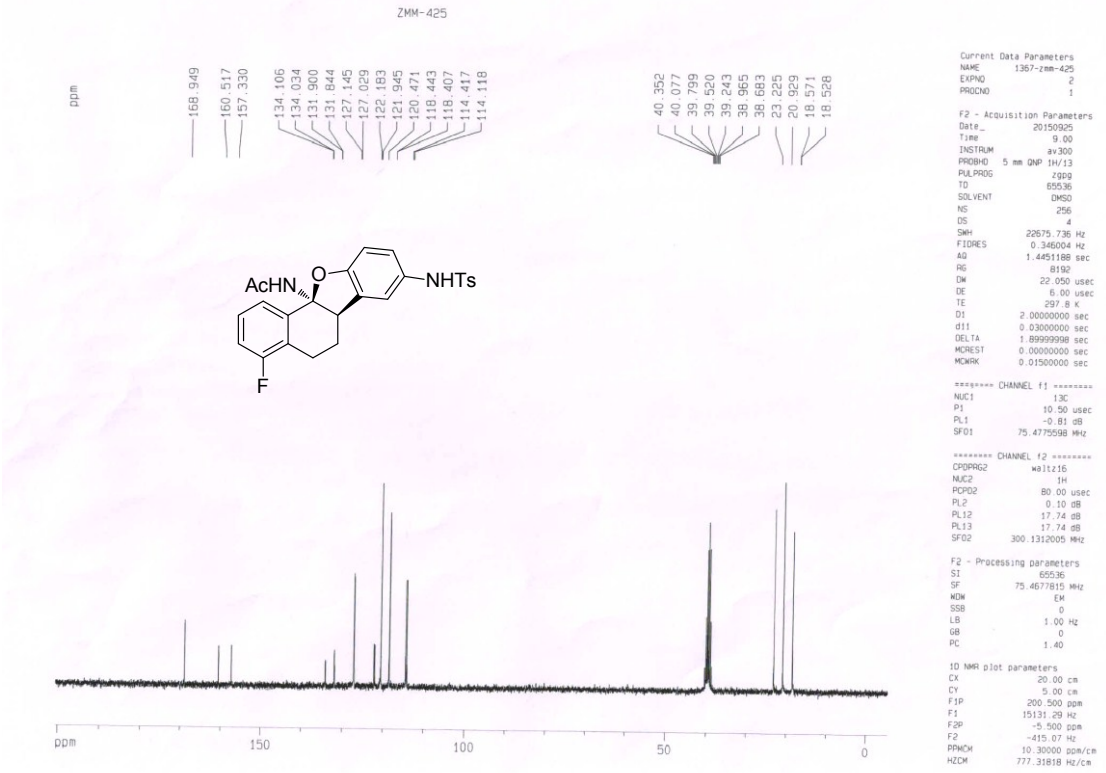
N-(4-methyl-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamid (3k)



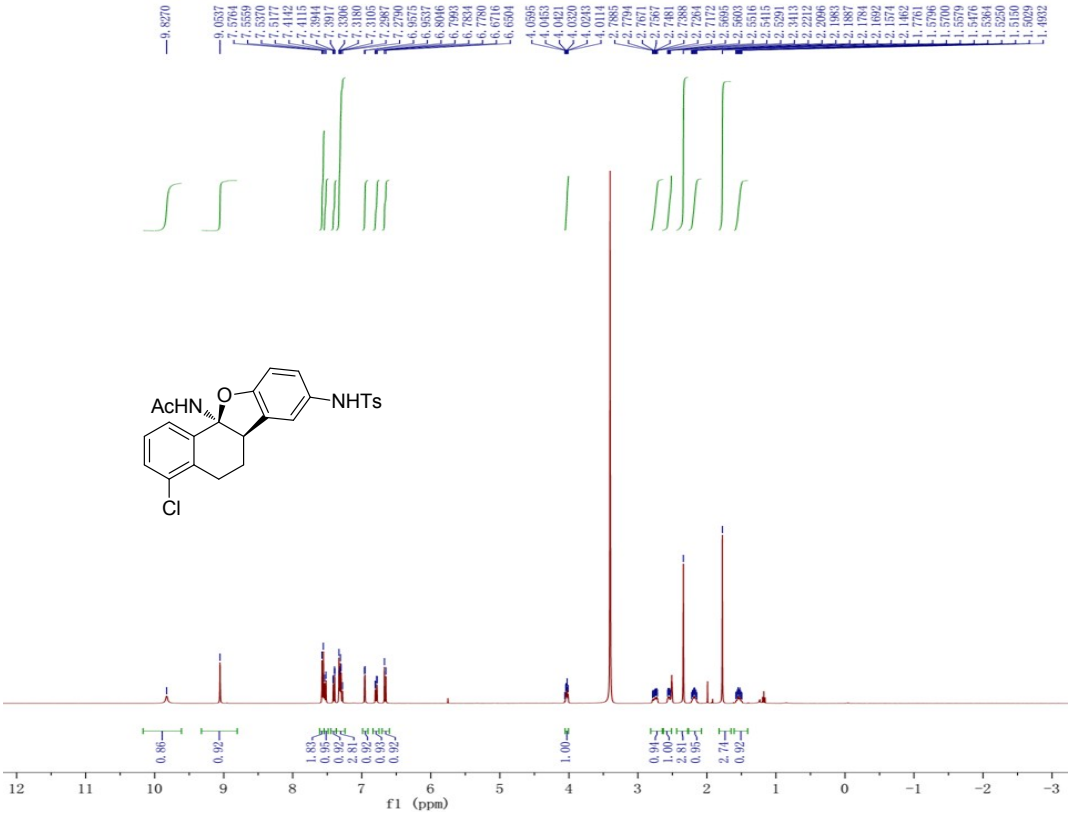


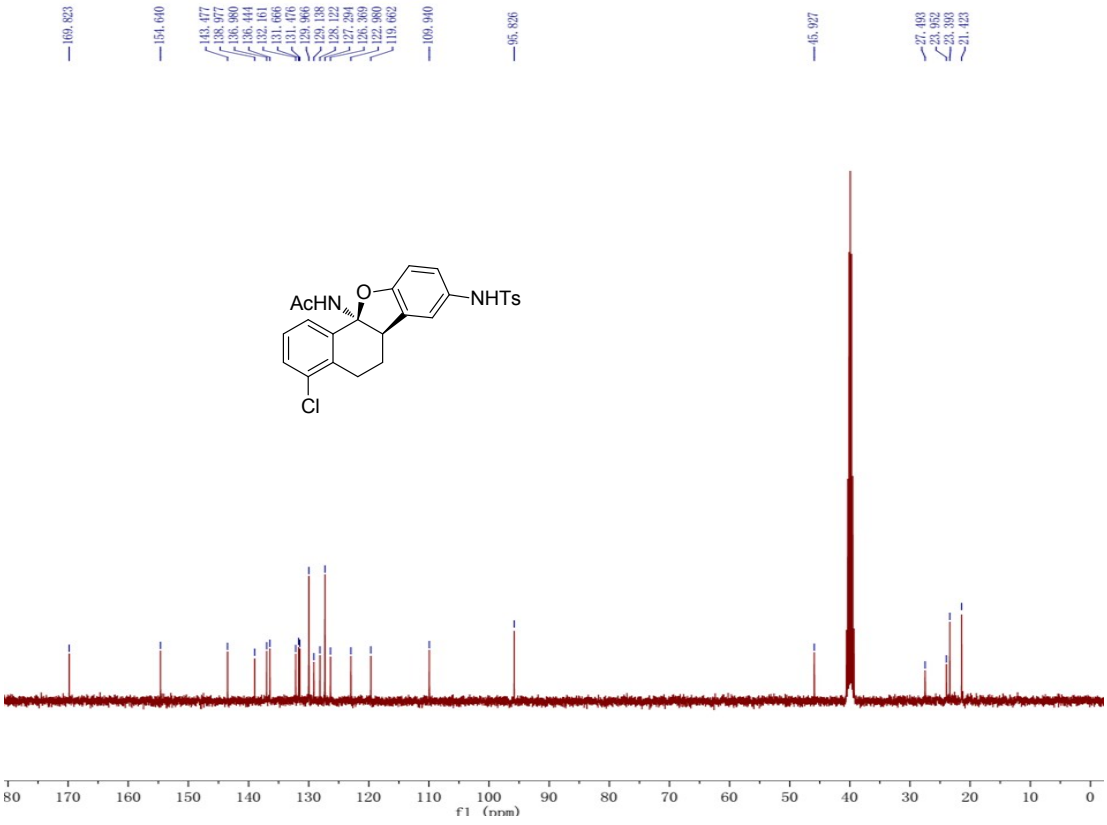
N-(4-fluoro-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3l)



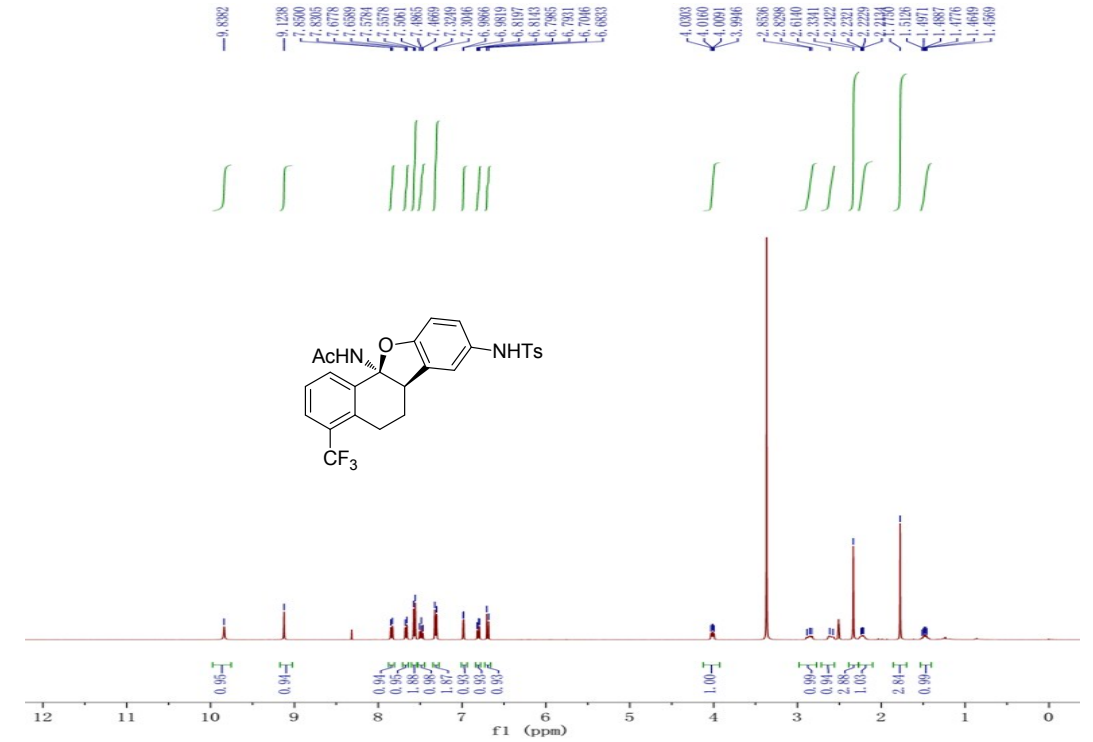


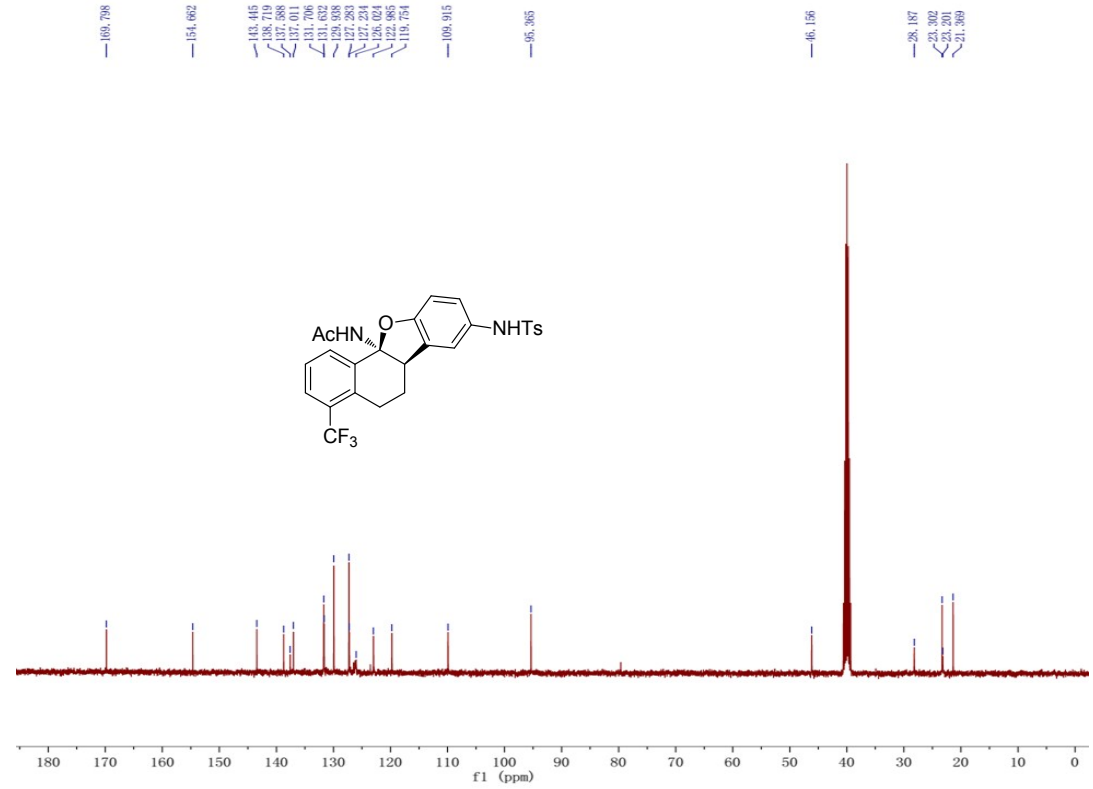
N-(4-chloro-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3m)



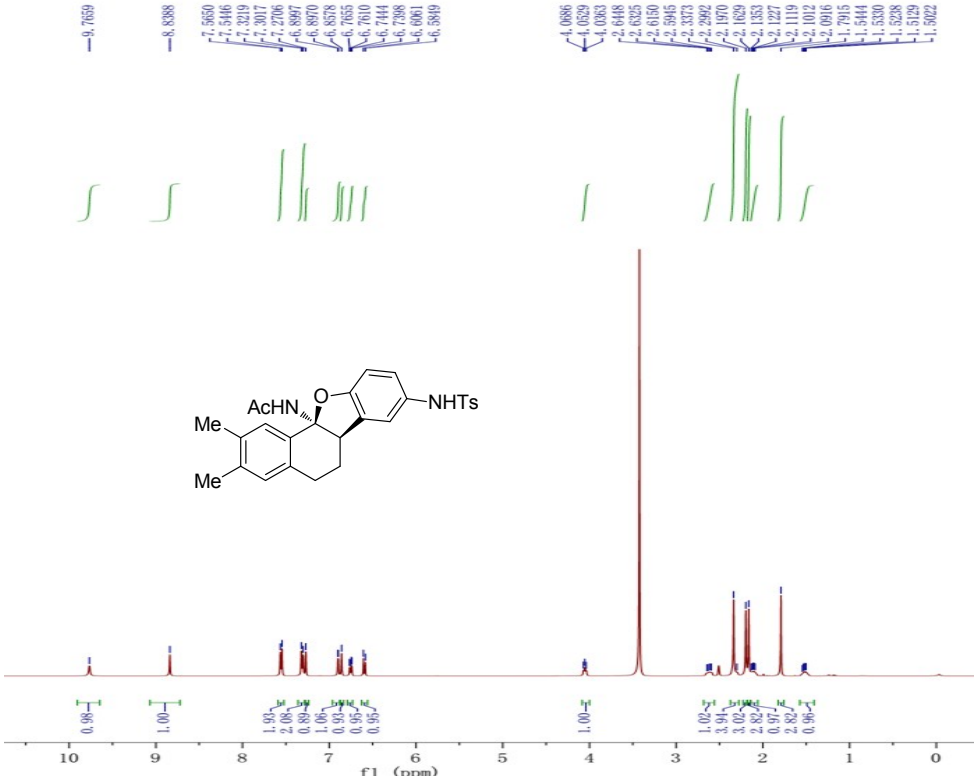


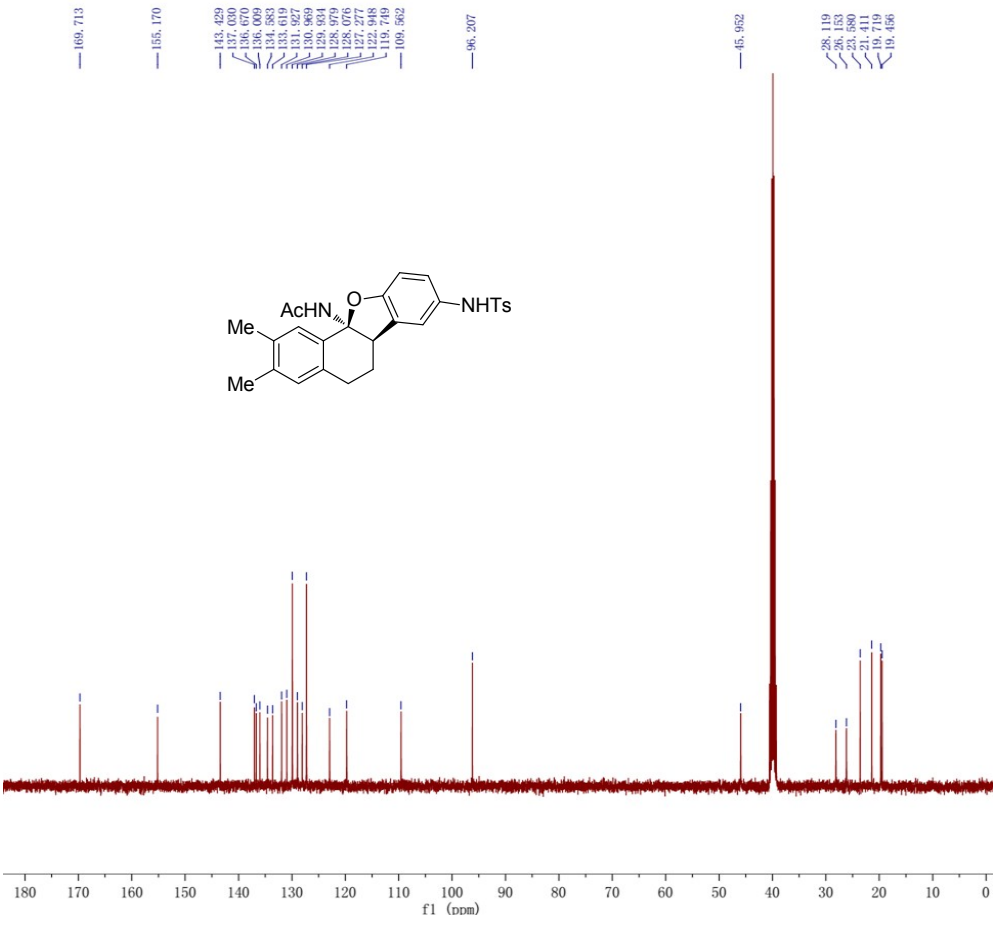
N-(8-(4-methylphenylsulfonamido)-4-(trifluoromethyl)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3n):



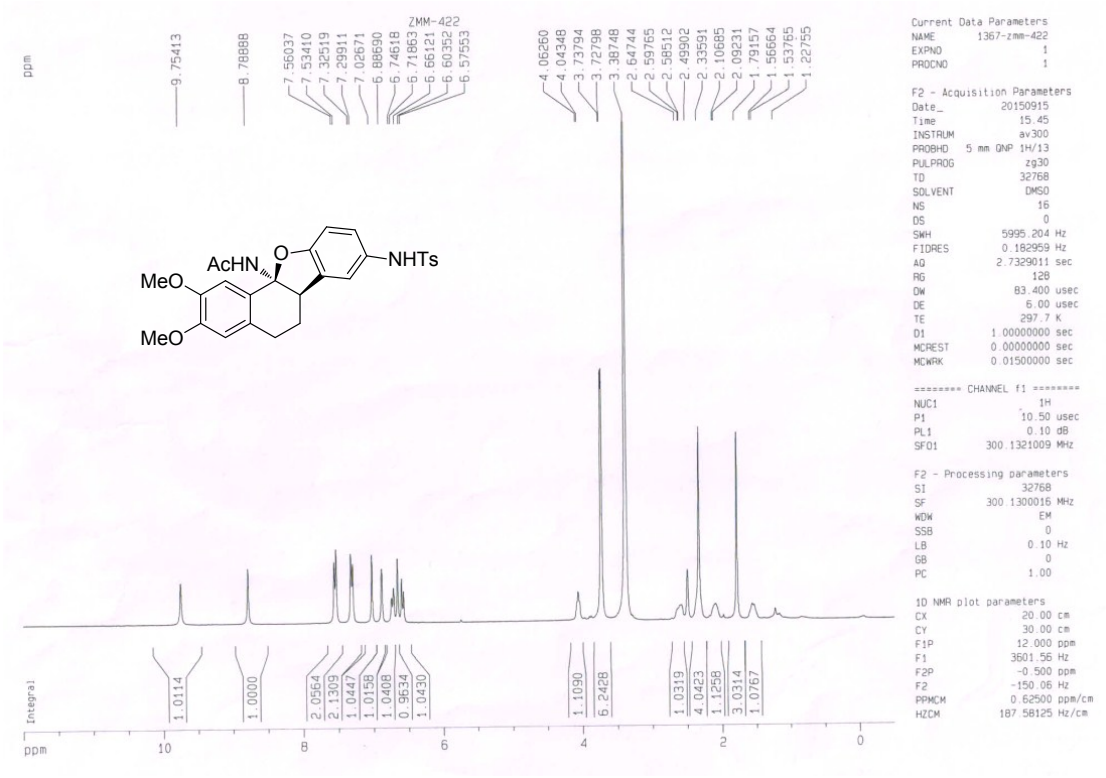


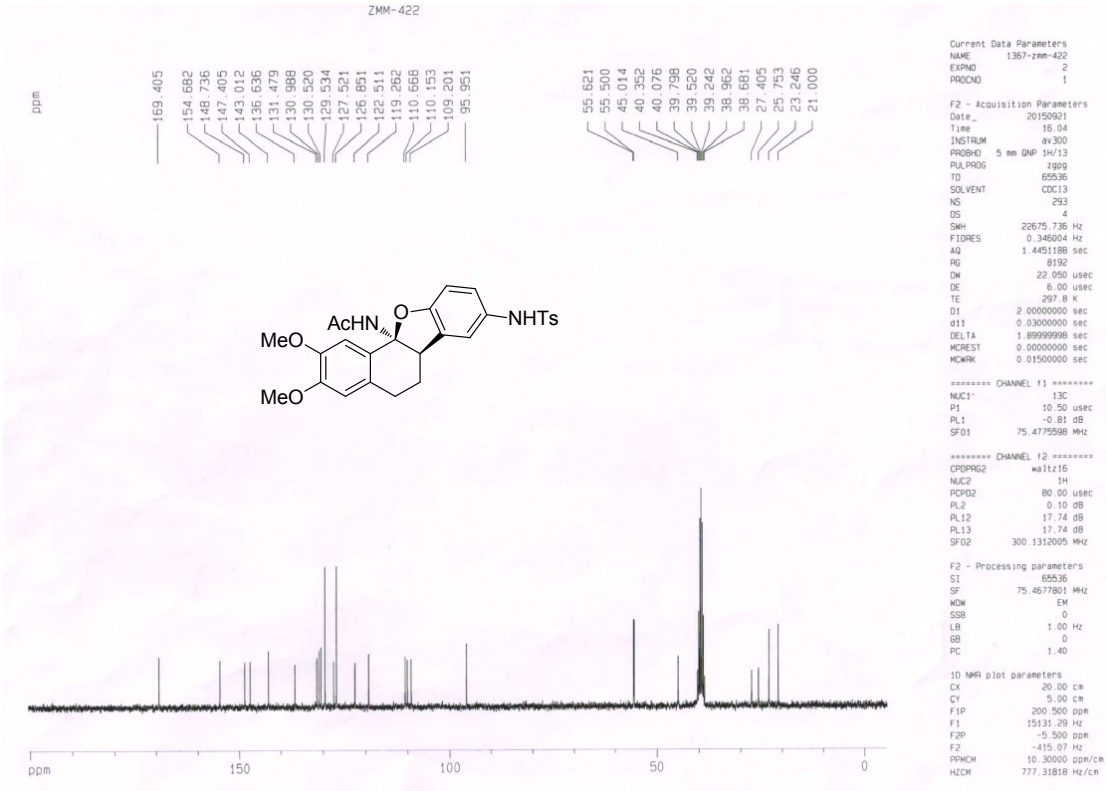
N-(2,3-dimethyl-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3o)



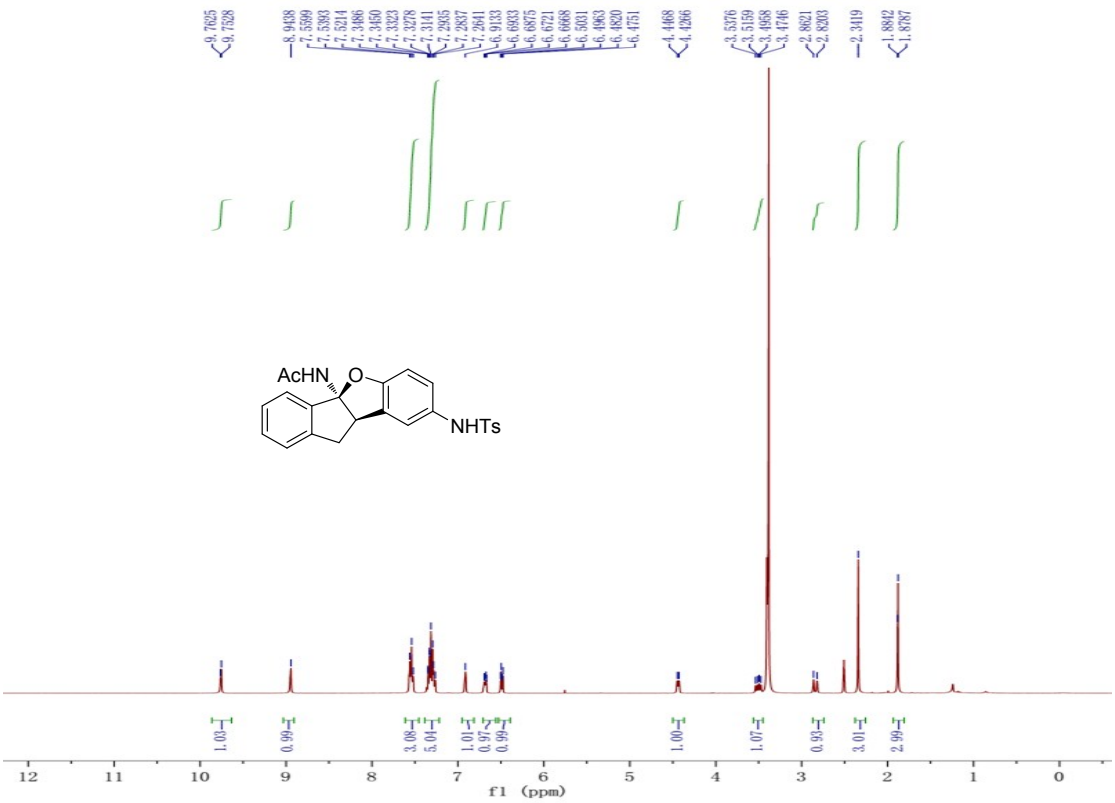


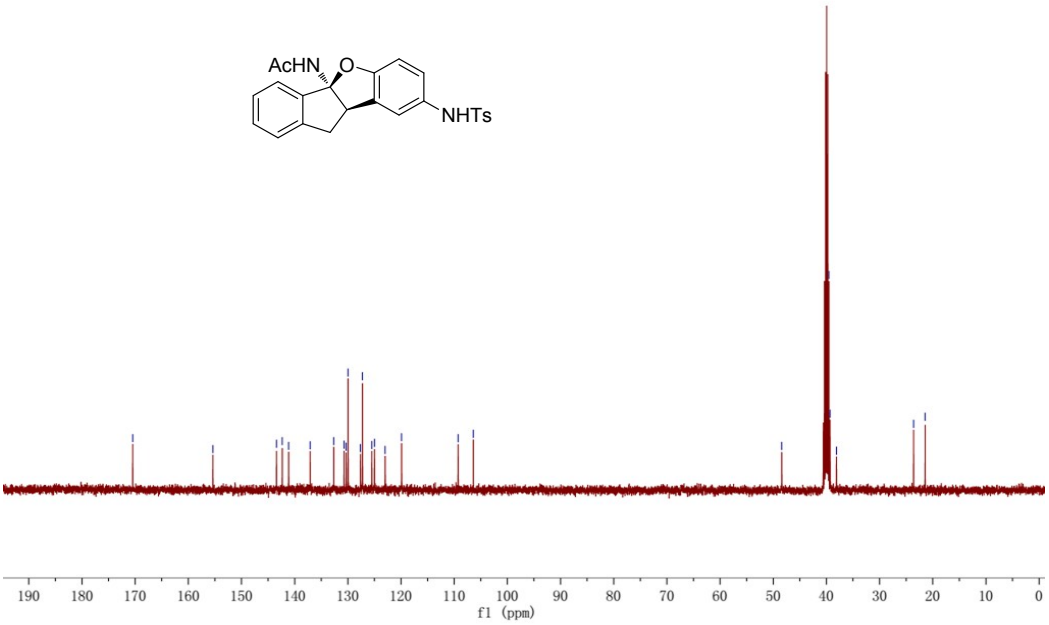
N-(2,3-dimethoxy-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3p)



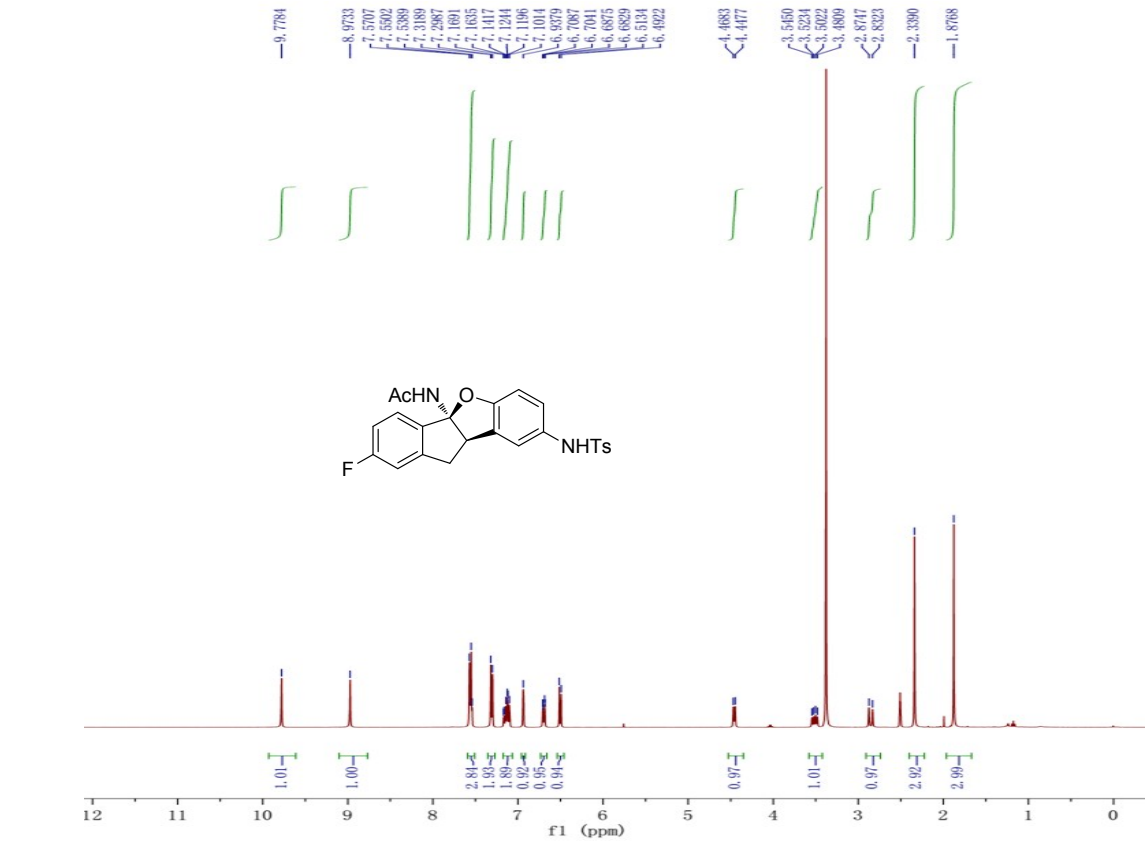


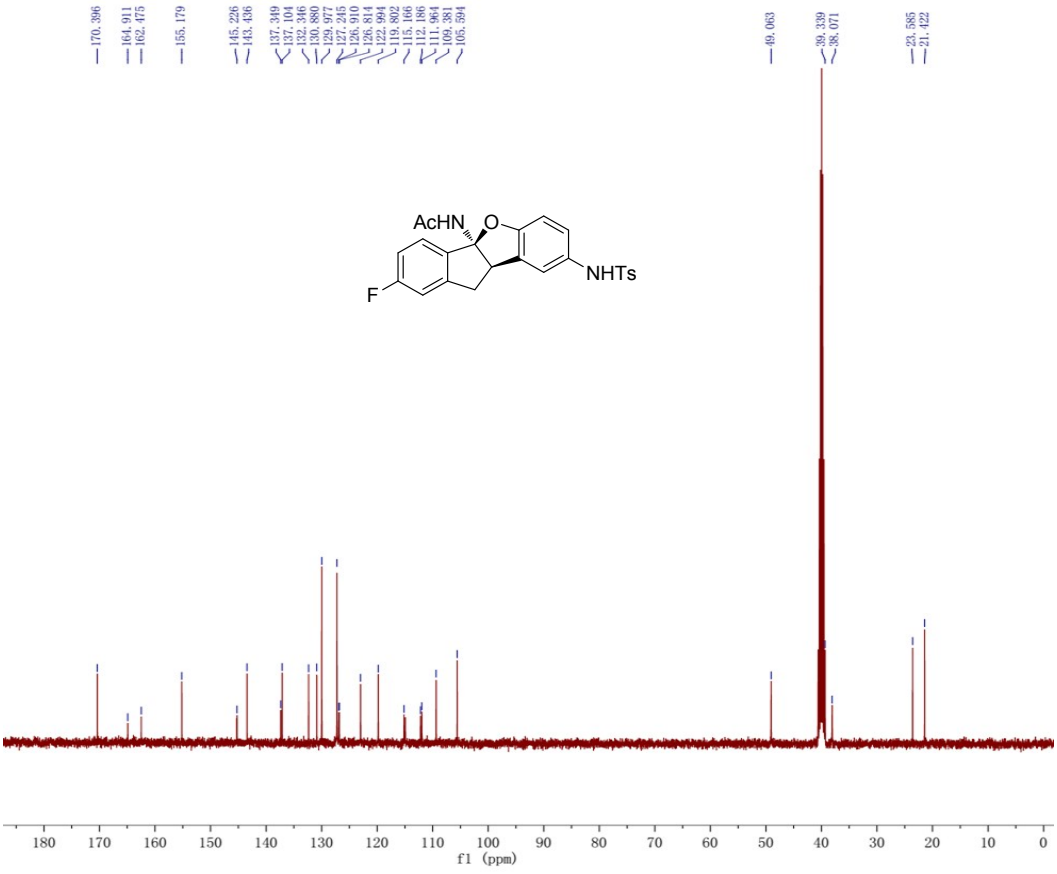
N-(8-(4-methylphenylsulfonamido)-9b,10-dihydro-4bH-indeno[1,2-b]benzofuran-4b-yl) acetamide (3s)



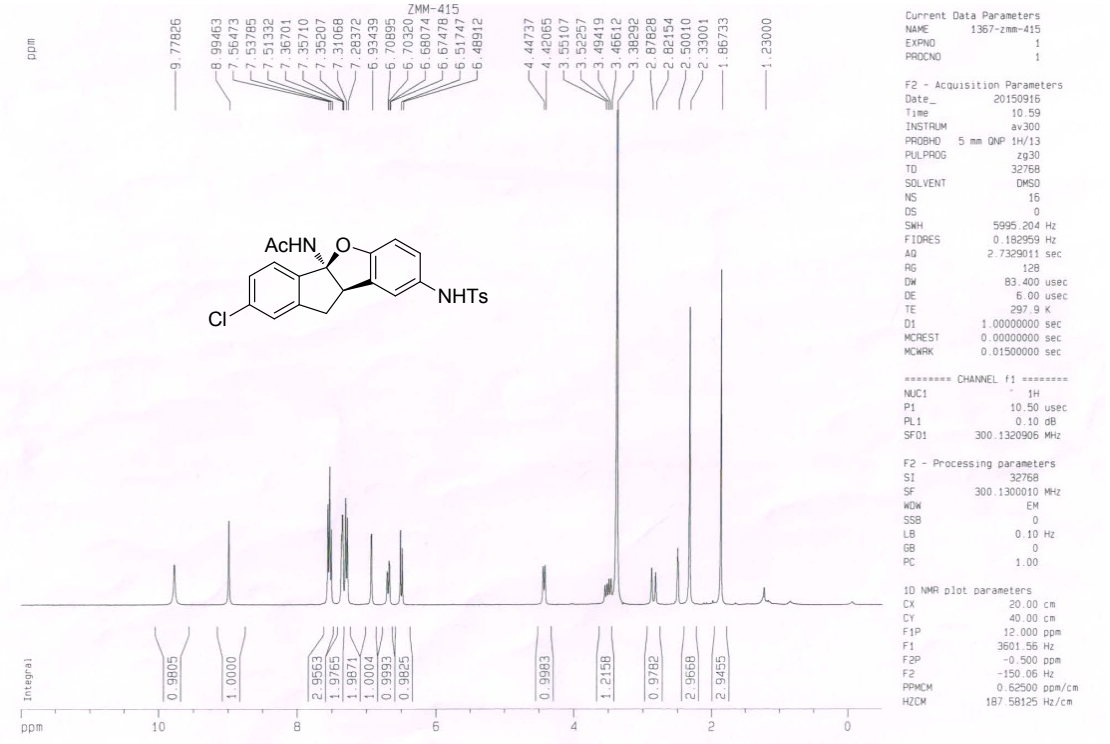


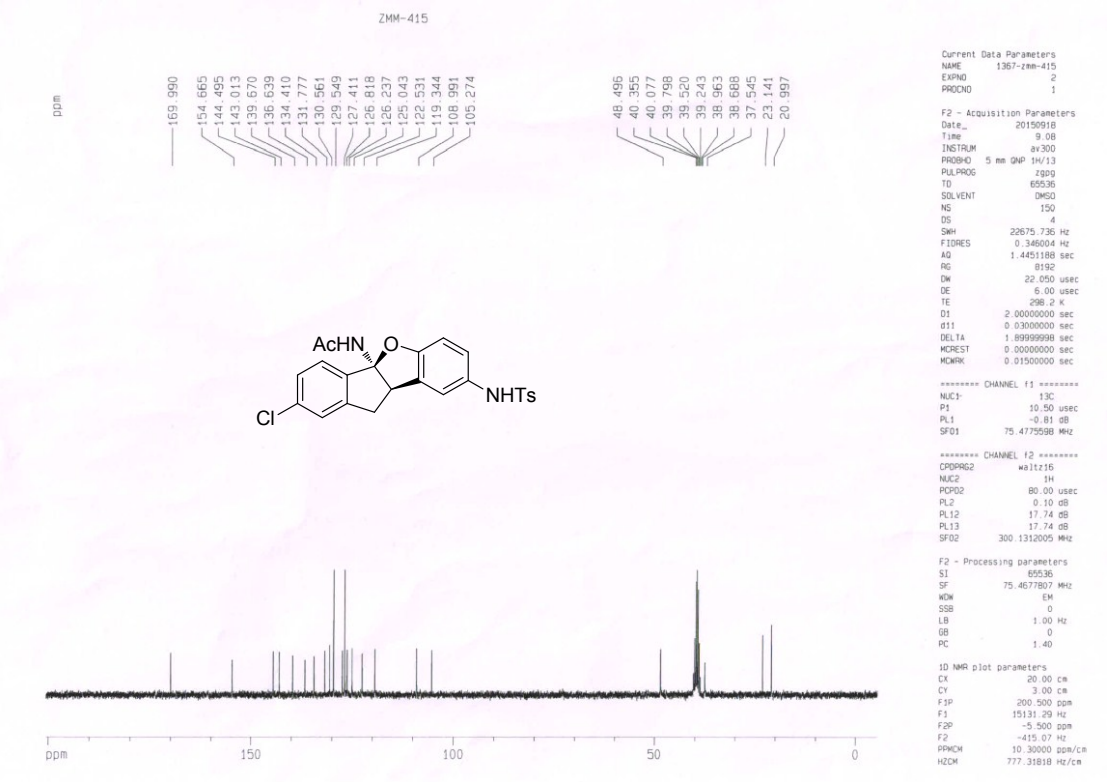
N-(2-fluoro-8-(4-methylphenylsulfonamido)-9b,10-dihydro-4bH-indeno[1,2-b] benzofuran-4b-yl)acetamide (3t)



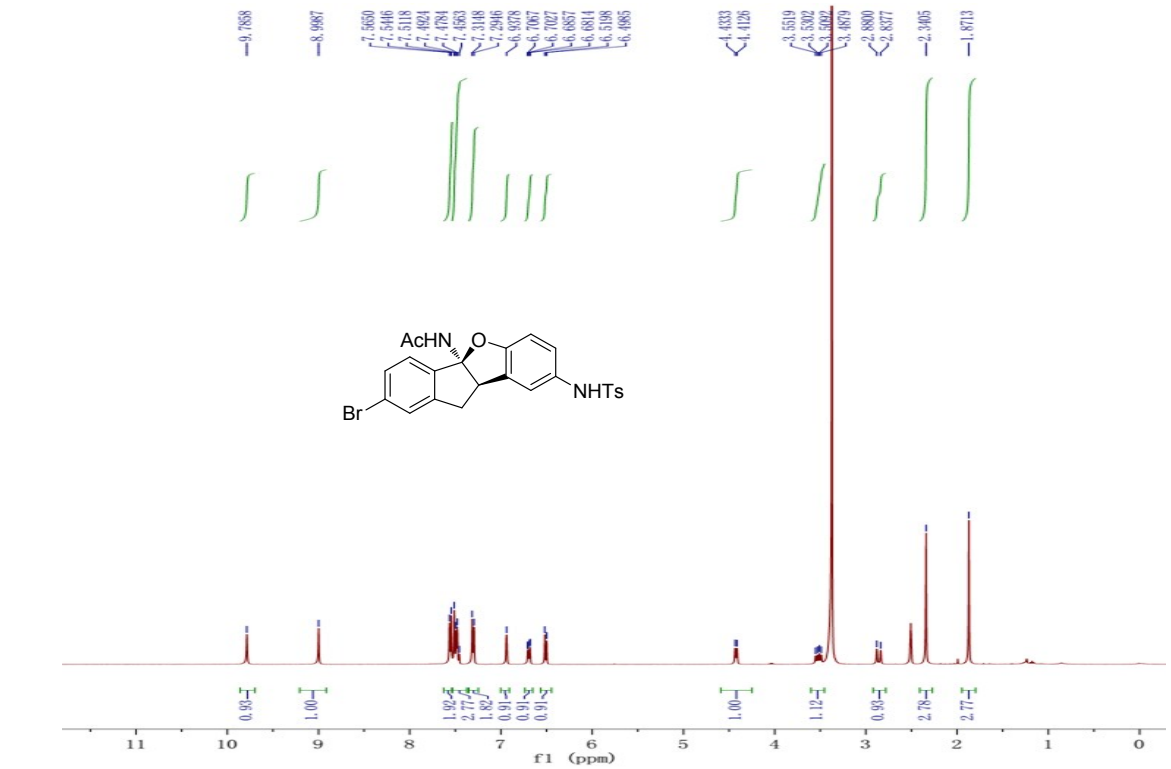


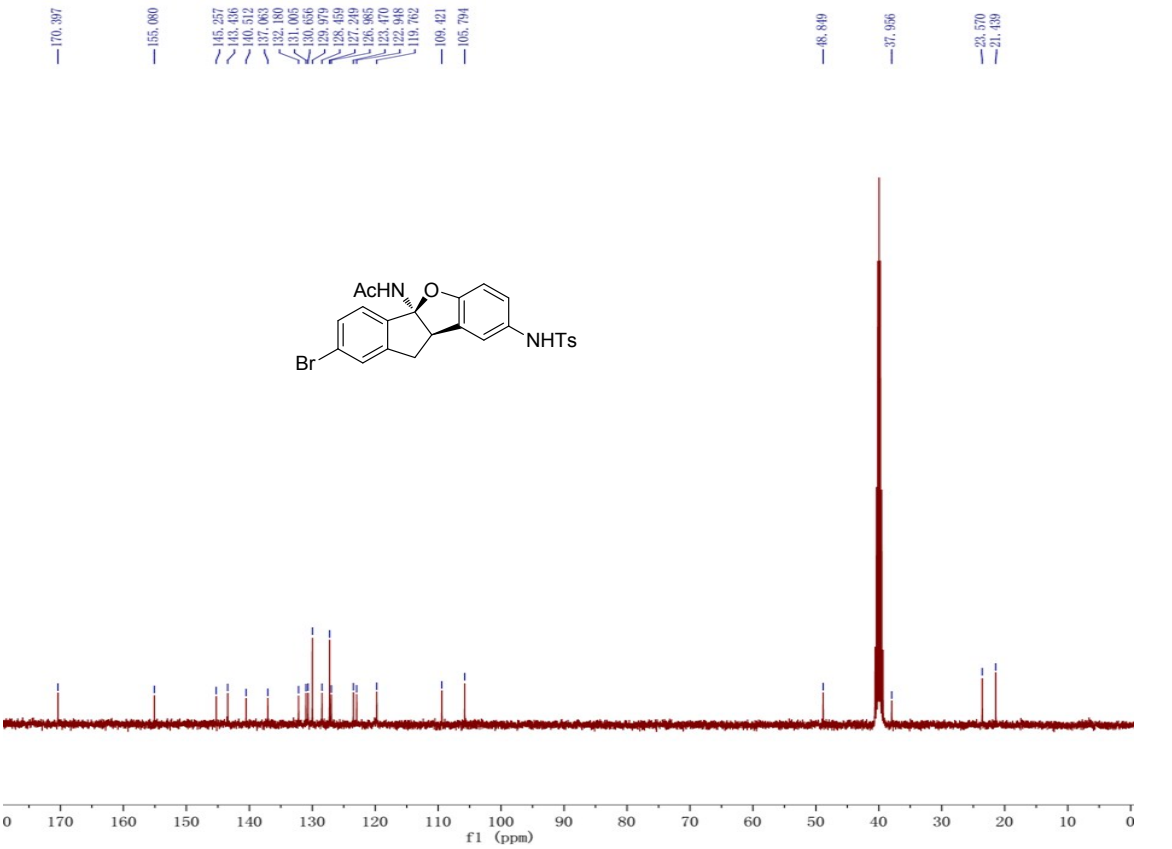
N-(2-chloro-8-(4-methylphenylsulfonamido)-9b,10-dihydro-4bH-indeno [1,2-b] benzofuran-4b-yl)acetamide (3u)



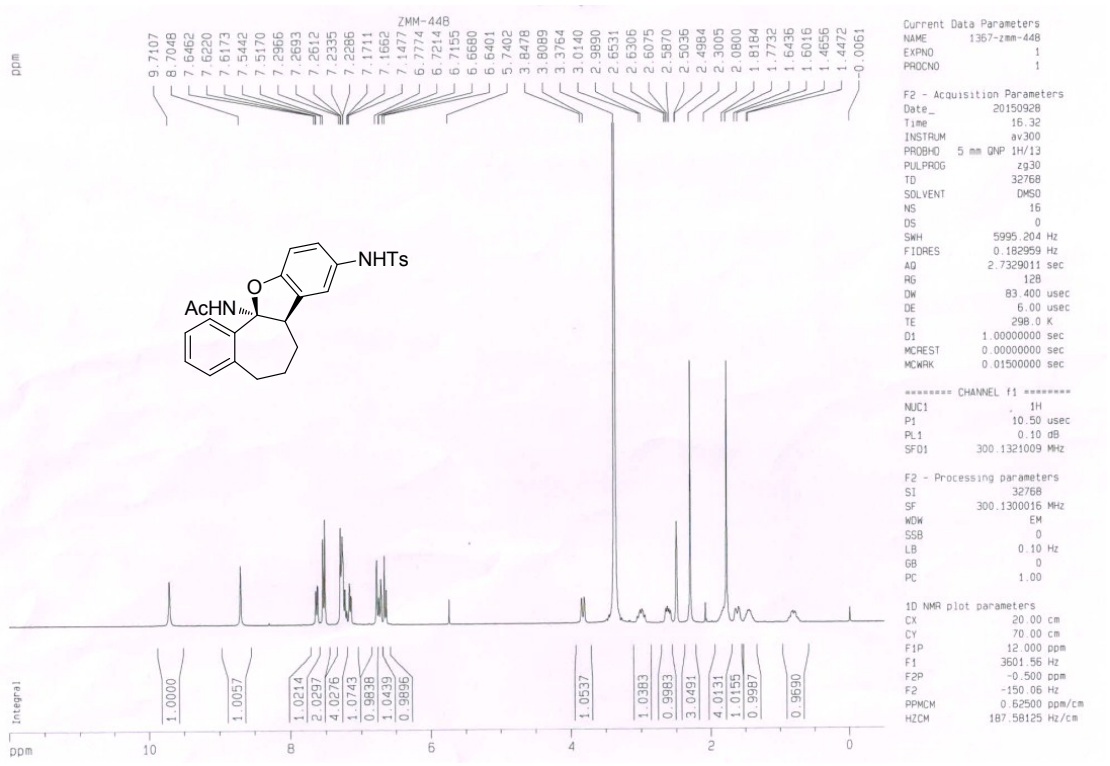


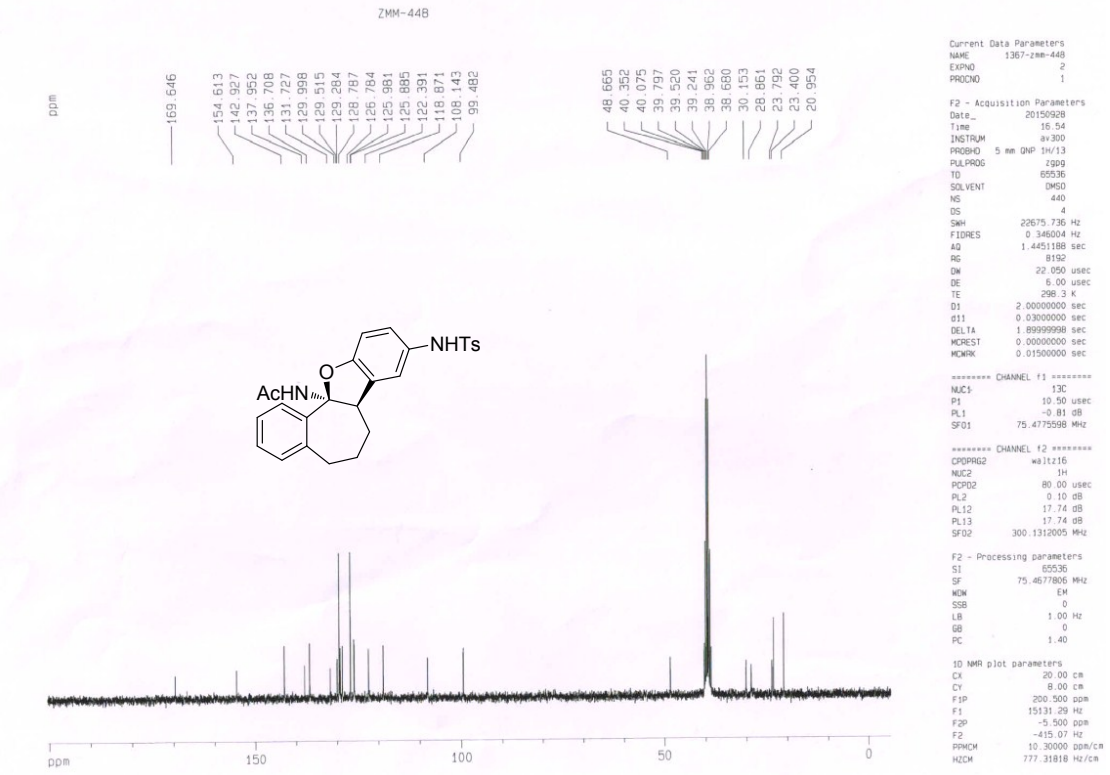
N-(2-bromo-8-(4-methylphenylsulfonamido)-9b,10-dihydro-4bH-indeno[1,2-b] benzofuran-4b-yl)acetamide (3v):



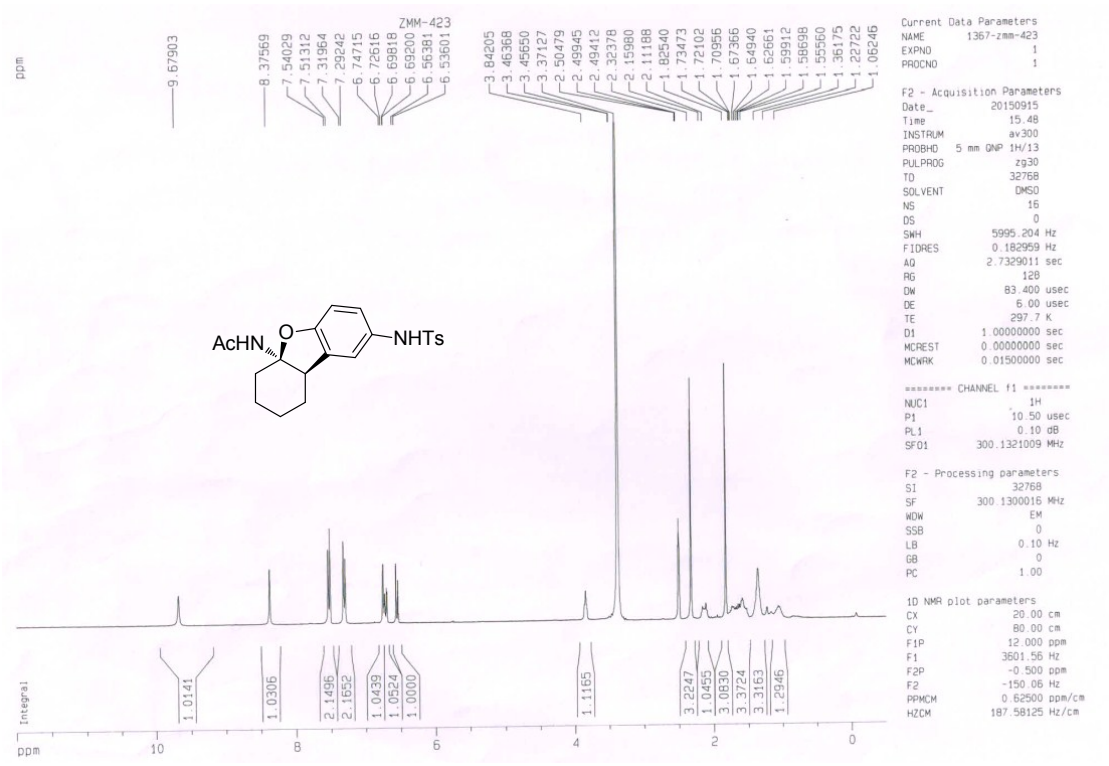


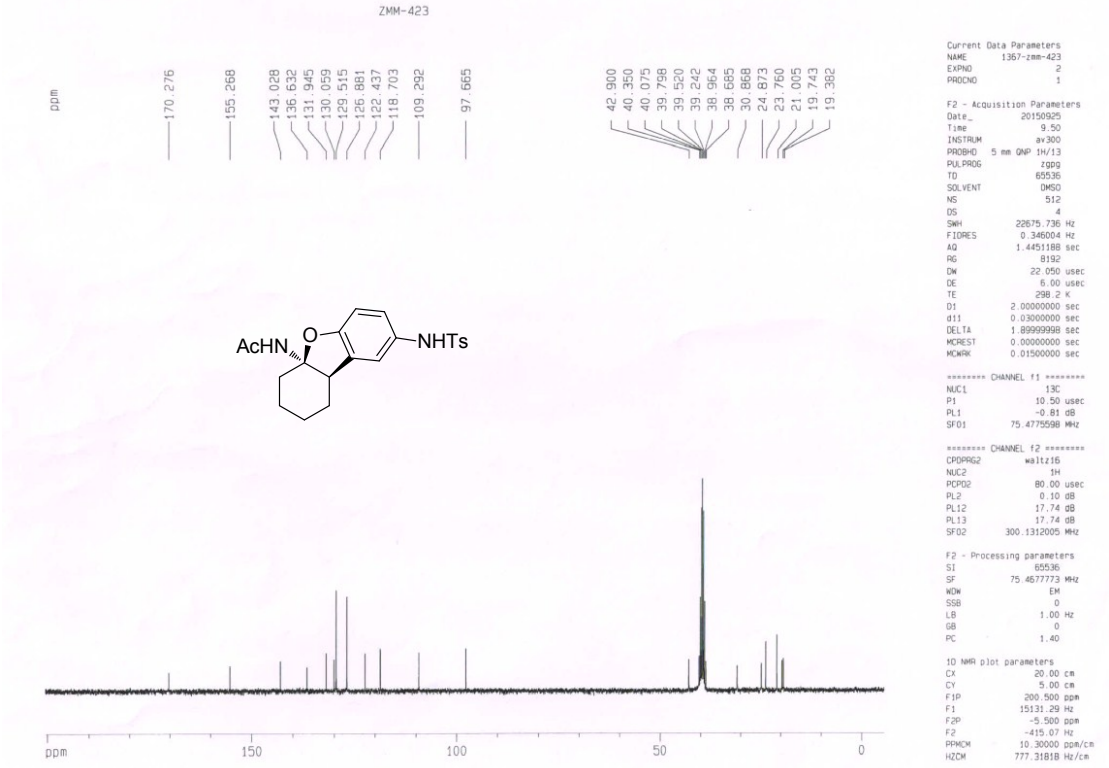
N-(9-(4-methylphenylsulfonamido)-6,7,7a,12a-tetrahydro-5H-benzo[6,7]cyclohepta [1,2-b]benzofuran-12a-yl)acetamide (3w)



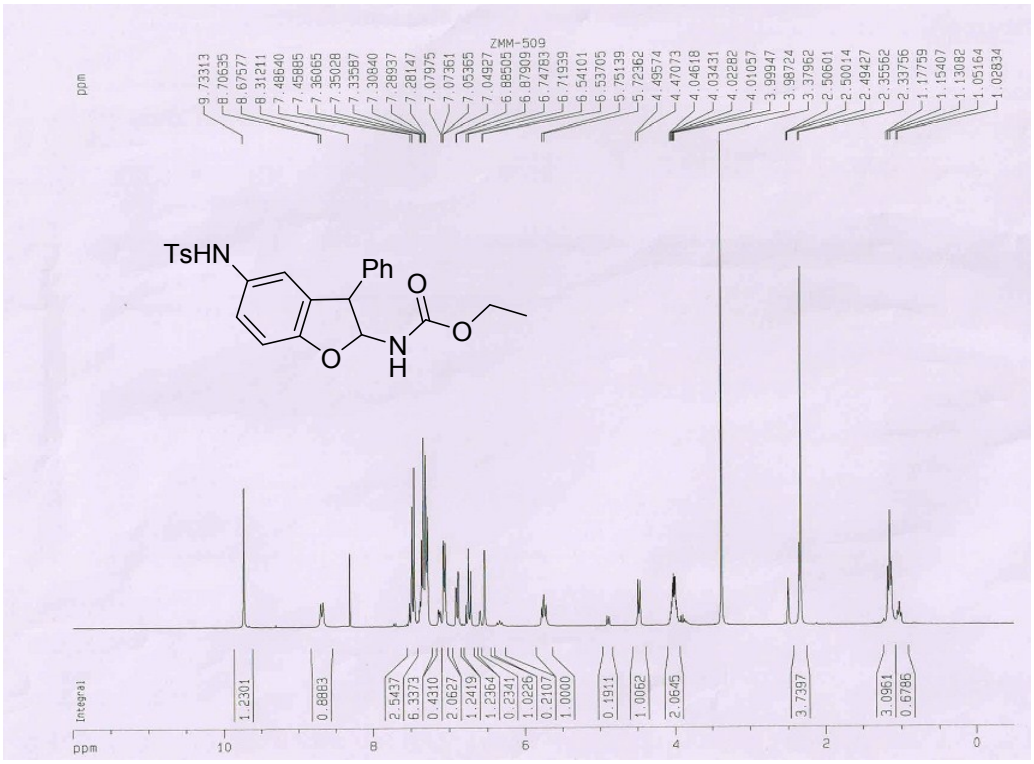


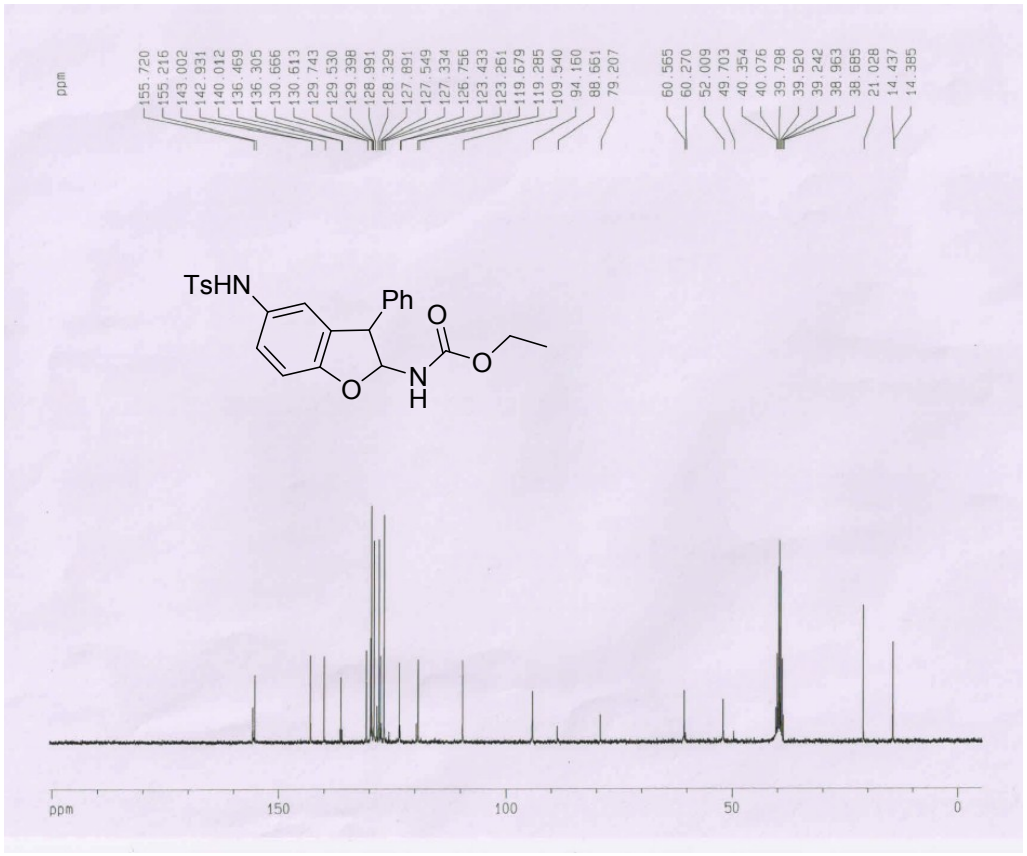
N-(8-(4-methylphenylsulfonamido)-1,2,3,4,4a,9b-hexahydrodibenzo[b,d]furan-4a-yl) acetamide (3x)



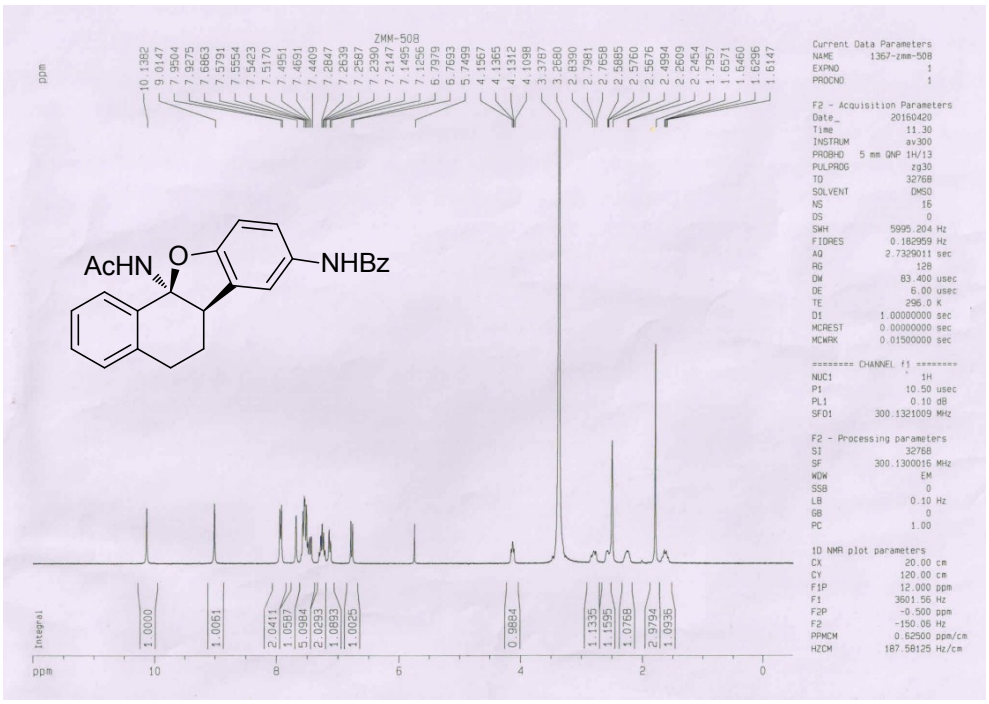


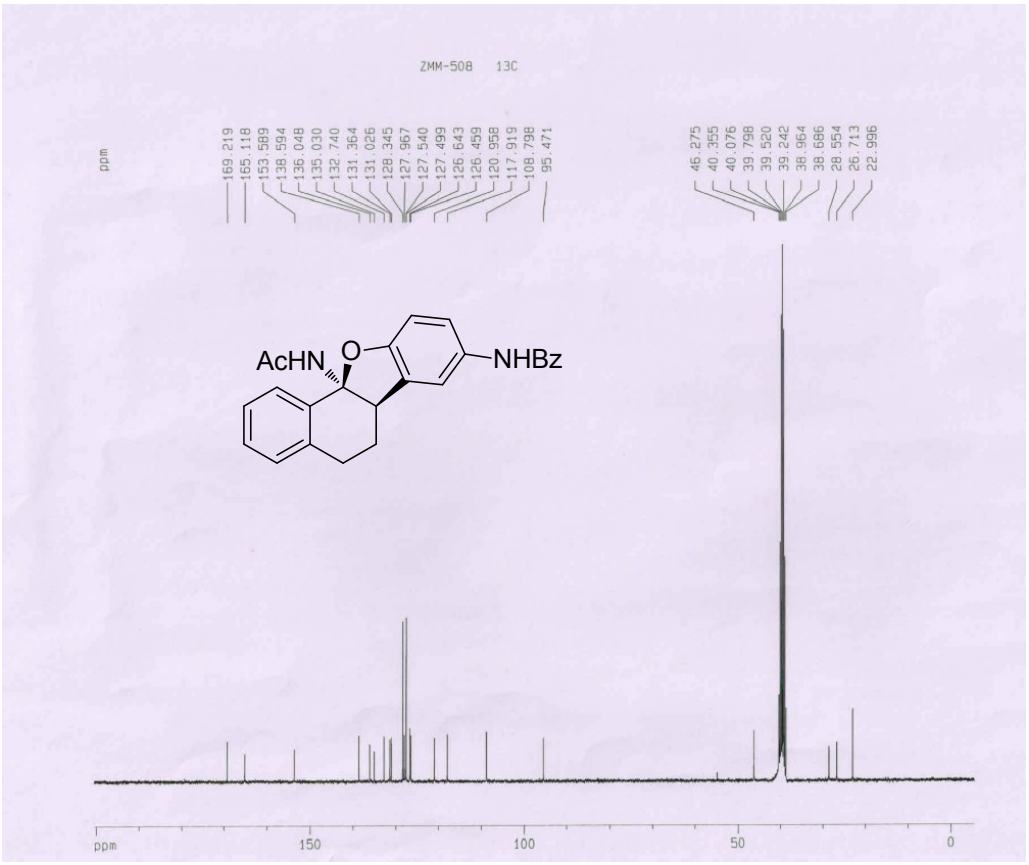
Ethyl (5-(4-methylphenylsulfonamido)-3-phenyl-2,3-dihydrobenzofuran-2-yl) carbamate (3y)





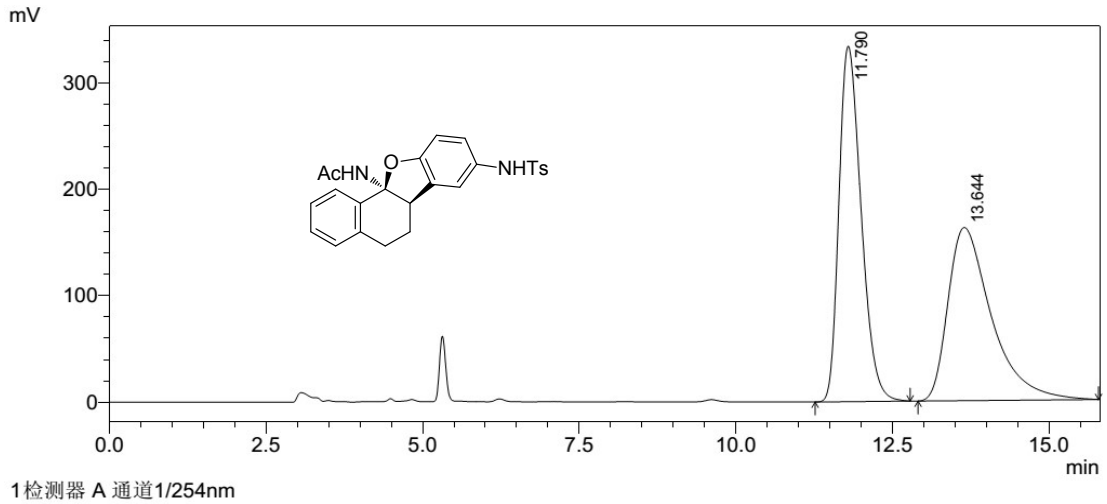
N-((6aR,11aS)-11a-acetamido-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-8-yl) benzamide (3z)





5. HPLC Charts of Products

N-((6aR,11aS)-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b] benzofuran-11a-yl)acetamide (3a)

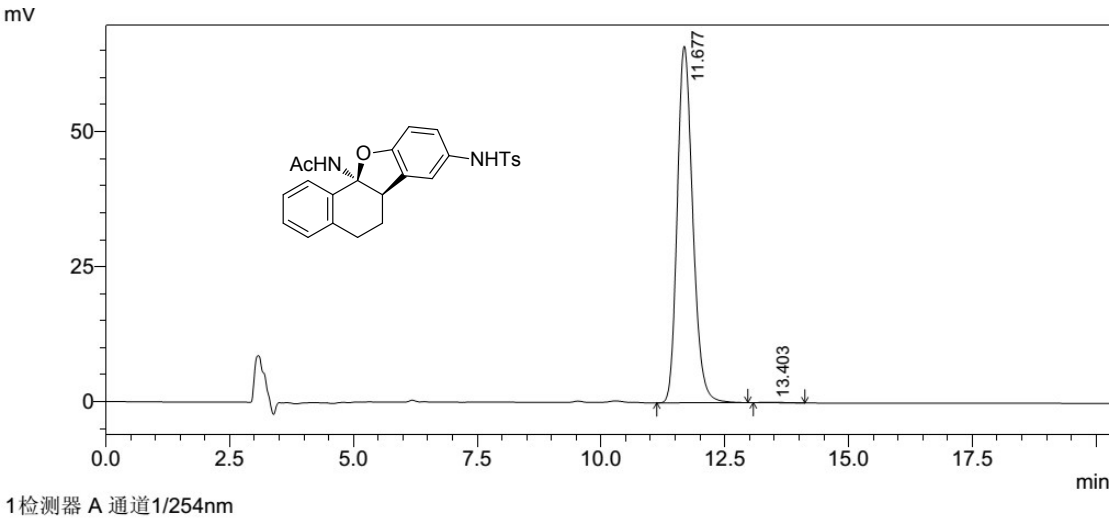


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	11.790	8234114	333956	51.187	5240.592	1.348	0.000
2	13.644	7852345	162687	48.813	2033.933	1.687	1.992
总计		16086460	496643	100.000			



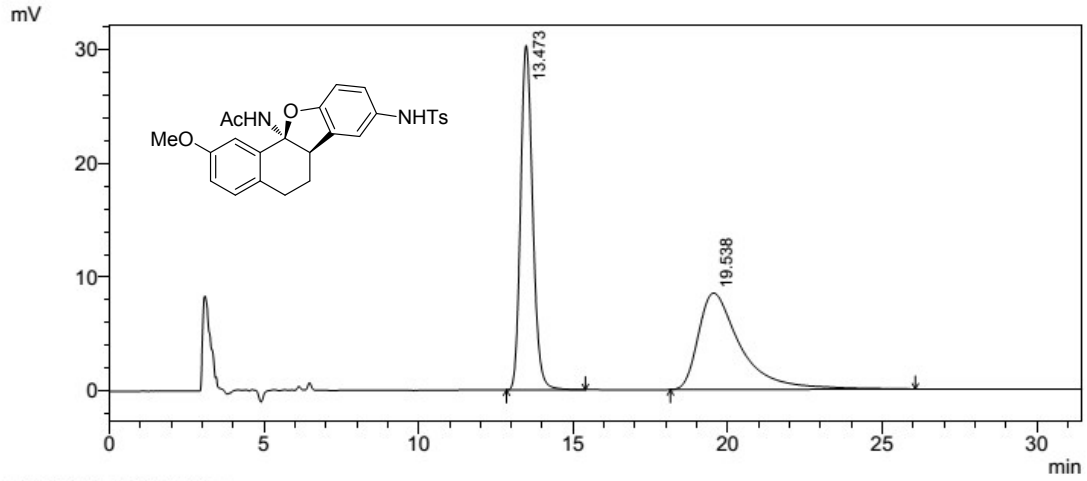
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	11.677	1443173	66064	99.817	6677.295	1.227	0.000
2	13.403	2649	80	0.183	4030.920	1.531	2.438
总计		1445822	66144	100.000			

N-((6aR,11aS)-2-methoxy-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3d)

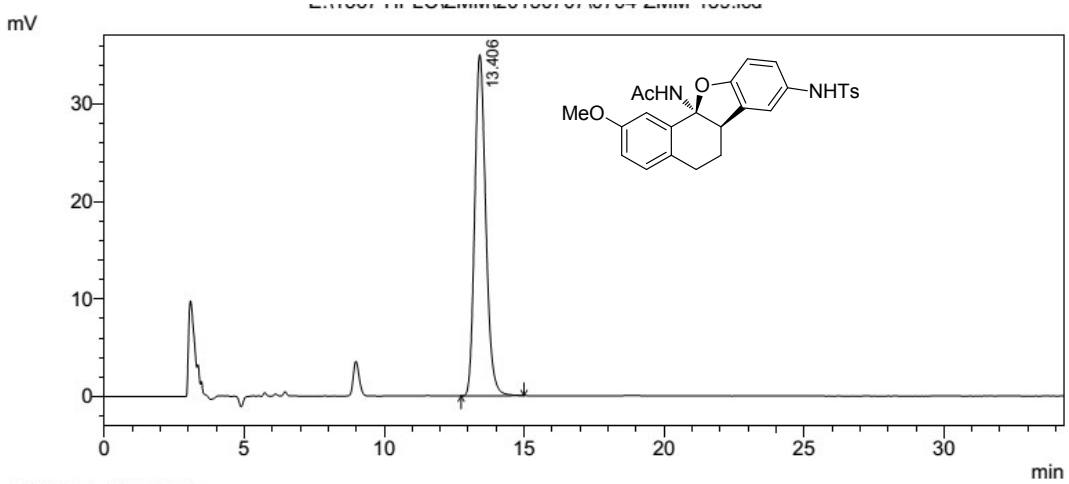


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	13.473	822608	30246	50.601	5754.922	1.193	0.000
2	19.538	803072	8466	49.399	1178.058	1.828	4.061
总计		1625681	38712	100.000			



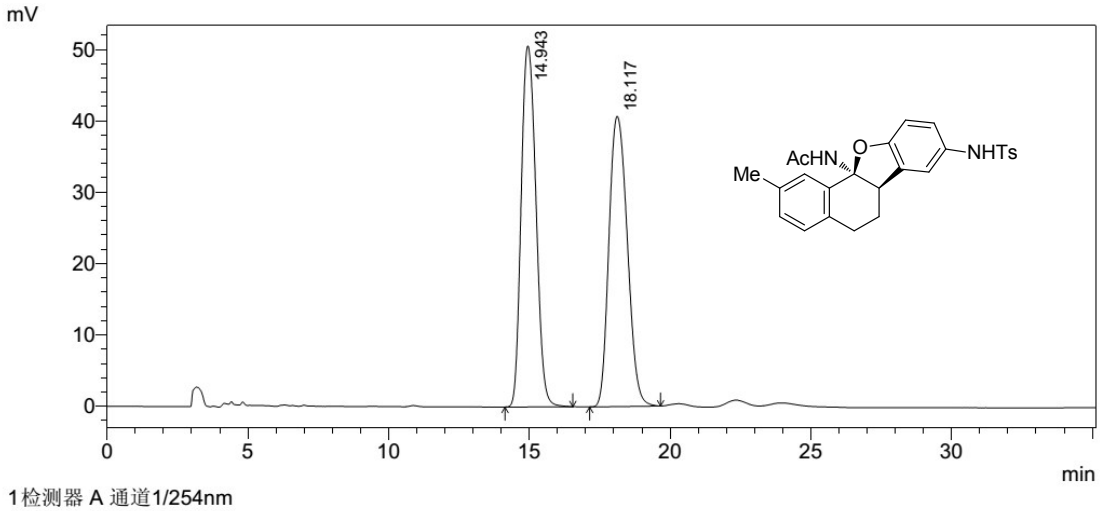
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	13.406	964337	35022	100.000	5584.526	1.216	0.000
总计		964337	35022	100.000			

N-((6aR,11aS)-2-methyl-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3e)

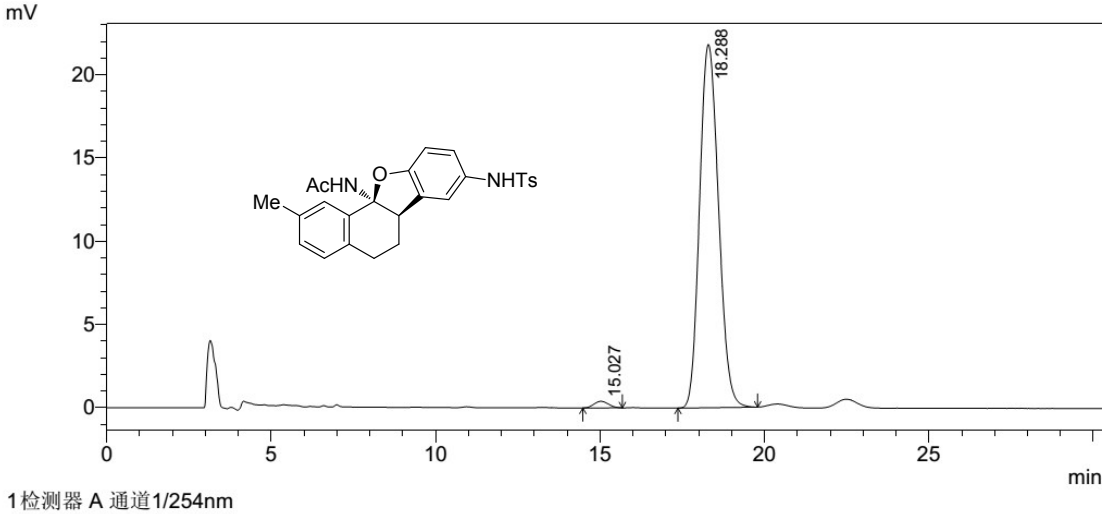


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	14.943	1847257	50591	49.999	3935.206	1.175	0.000
2	18.117	1847326	40684	50.001	3713.586	1.192	2.963
总计		3694583	91276	100.000			



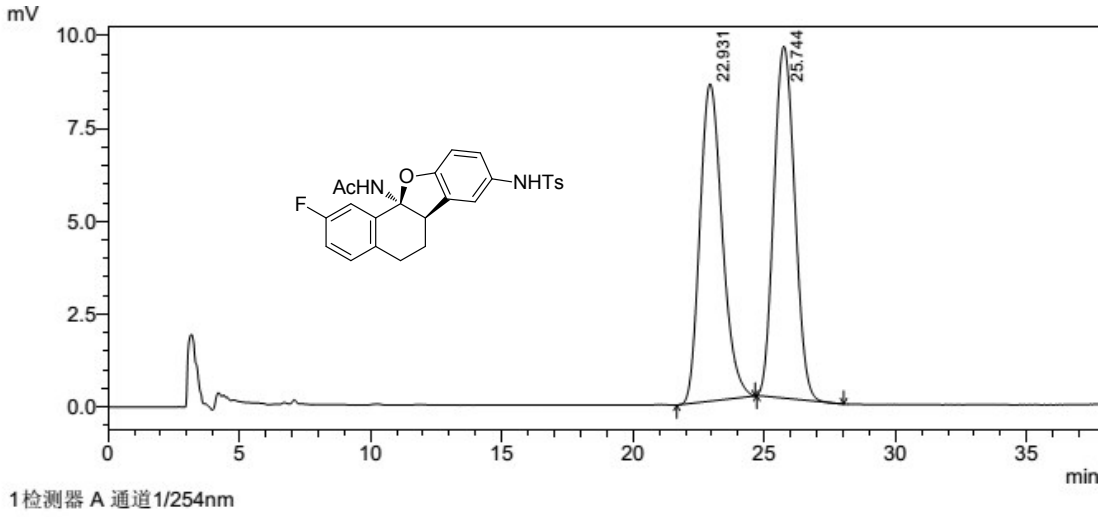
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	15.027	12216	396	1.377	5353.974	1.093	0.000
2	18.288	875067	21845	98.623	4768.737	1.155	3.468
总计		887283	22241	100.000			

N-((6aR,11aS)-2-fluoro-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3f)

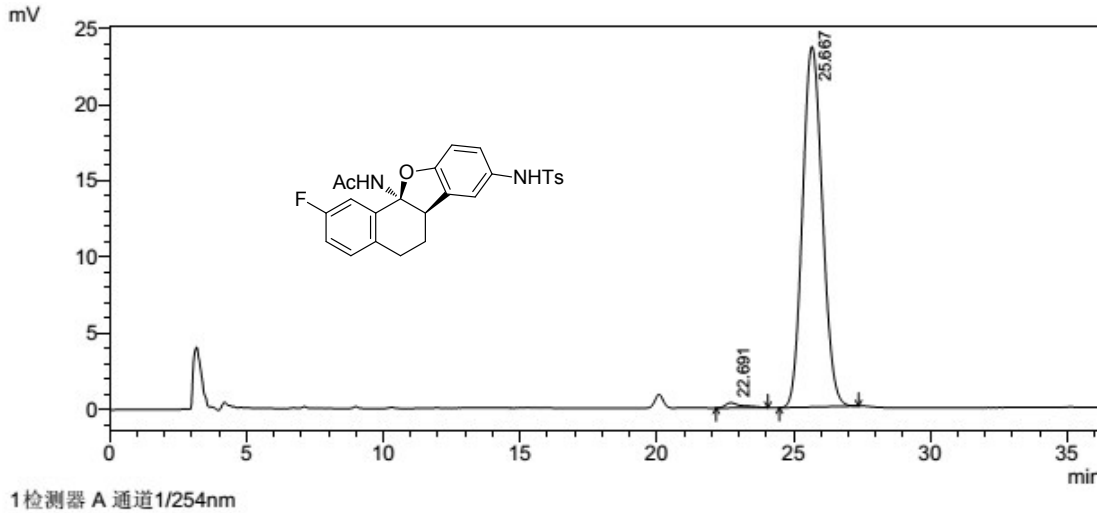


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	22.931	506434	8551	49.084	3504.937	1.239	0.000
2	25.744	525328	9477	50.916	4865.051	1.105	1.859
总计		1031762	18028	100.000			



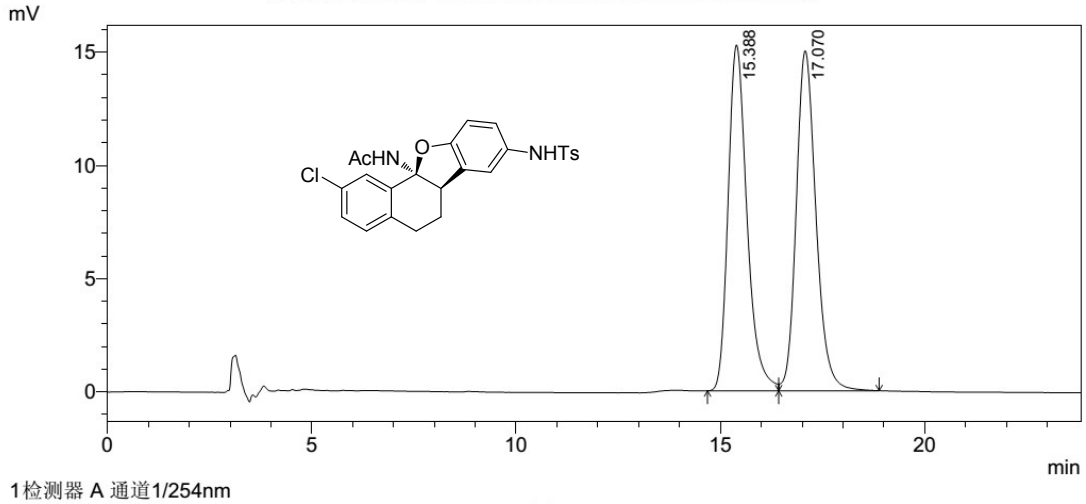
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	22.691	13809	331	1.144	11746.458	2.026	0.000
2	25.667	1193571	23629	98.856	5864.391	1.112	2.733
总计		1207380	23960	100.000			

N-((6aR,11aS)-2-chloro-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3g)

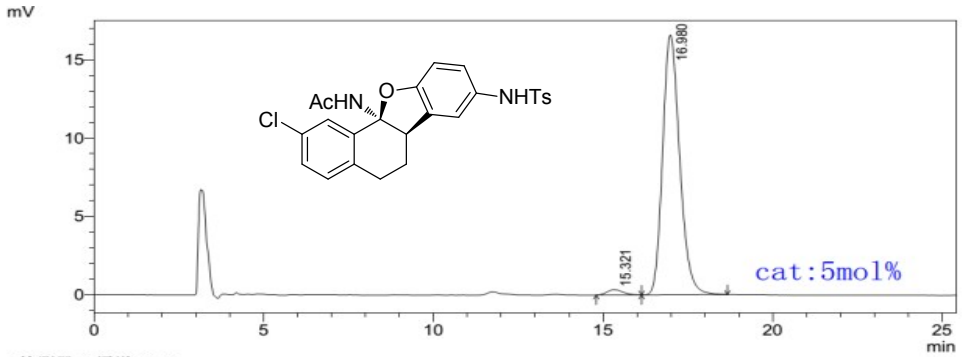


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	15.388	490823	15266	49.304	5585.415	1.324	0.000
2	17.070	504671	15005	50.696	6200.943	1.208	1.989
总计		995494	30271	100.000			

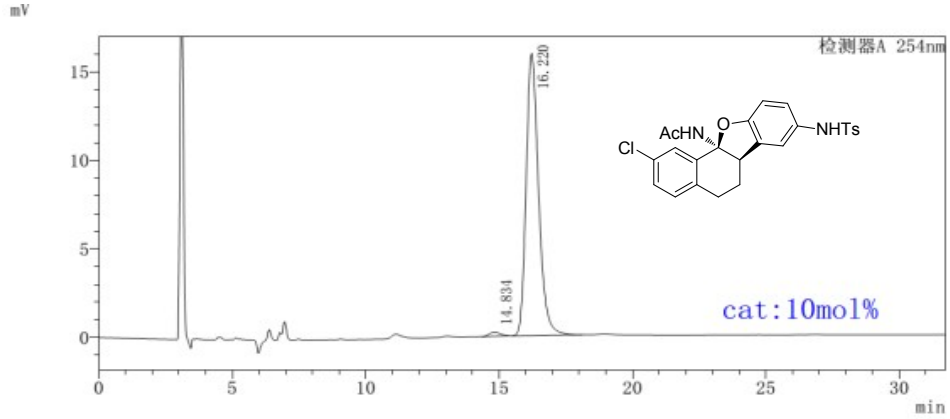


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	15.321	11213	344	1.893	4876.281	1.275	0.000
2	16.980	581149	16596	98.107	5549.854	1.228	1.855
总计		592362	16939	100.000			

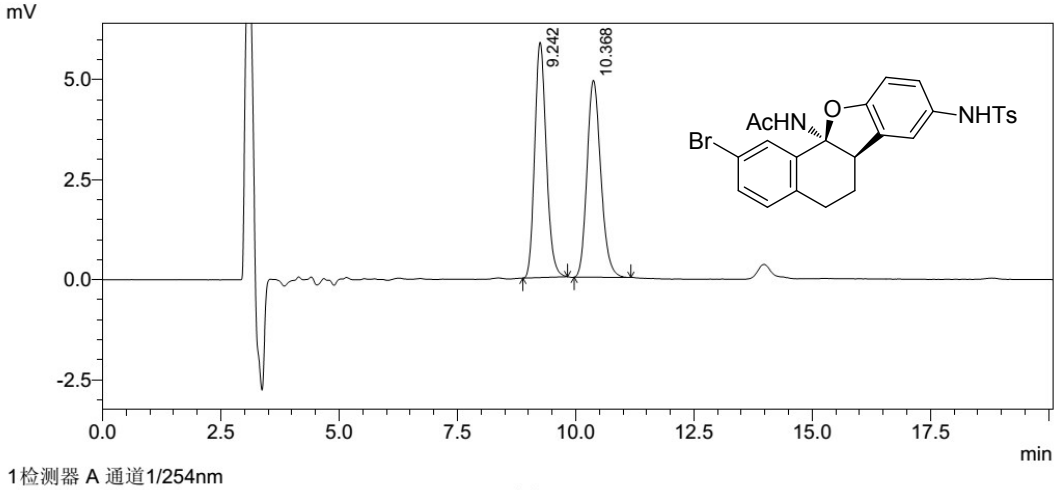


<峰表>

检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	14.834	6601	237	1.265		M	
2	16.220	515180	15907	98.735		M	
总计		521781	16144				

N-((6aR,11aS)-2-bromo-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3h)

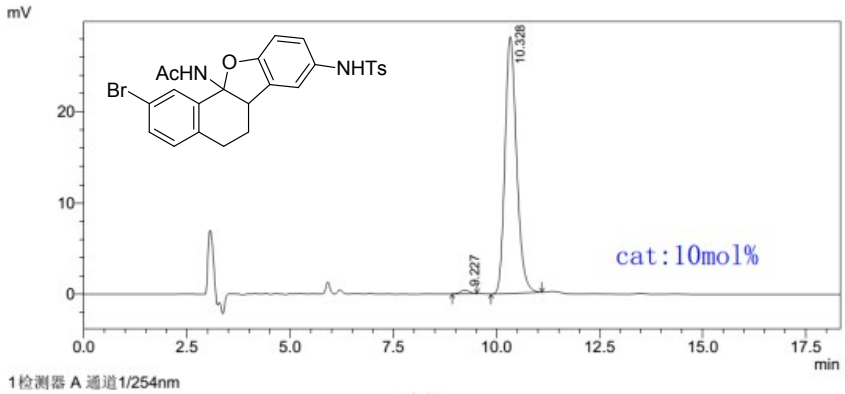


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	9.242	99997	5870	50.033	6751.684	1.197	0.000
2	10.368	99866	4917	49.967	6016.219	1.205	2.288
总计		199863	10788	100.000			

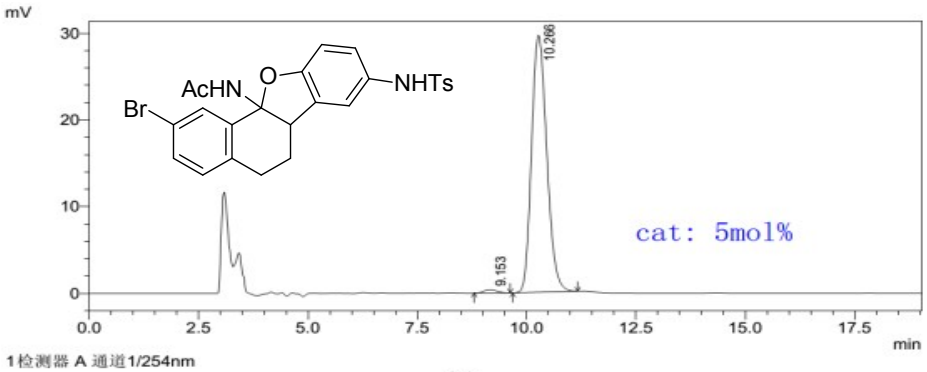


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	9.227	5854	391	1.051	8165.592	1.048	0.000
2	10.328	551197	28118	98.949	6464.287	1.234	2.387
总计		557051	28509	100.000			



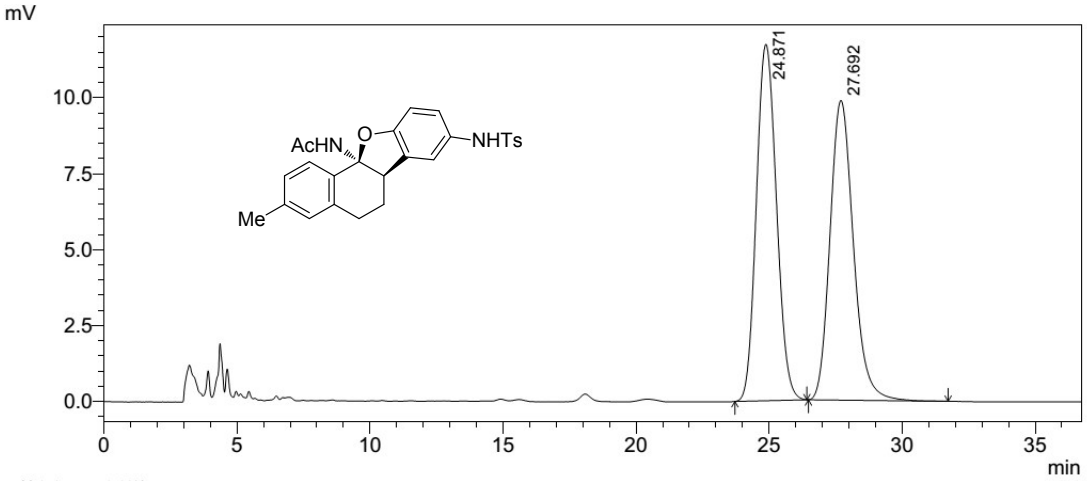
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	9.153	8010	382	1.104	4218.584	1.161	0.000
2	10.266	717845	29634	98.896	4129.398	1.216	1.851
总计		725856	30016	100.000			

N-((6aR,11aS)-3-methyl-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3i)

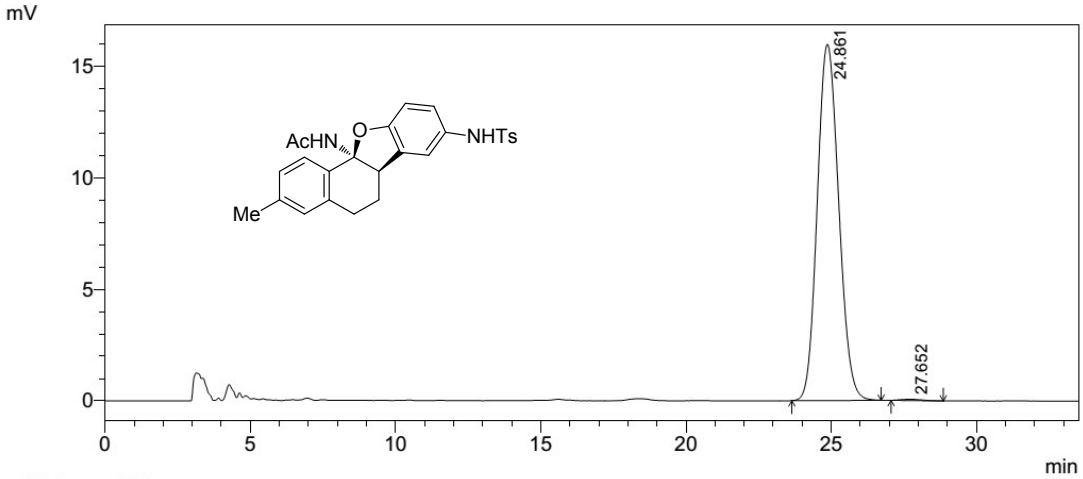


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	24.871	616854	11736	50.591	5119.460	1.120	0.000
2	27.692	602430	9869	49.409	4902.756	1.202	1.898
总计		1219285	21605	100.000			



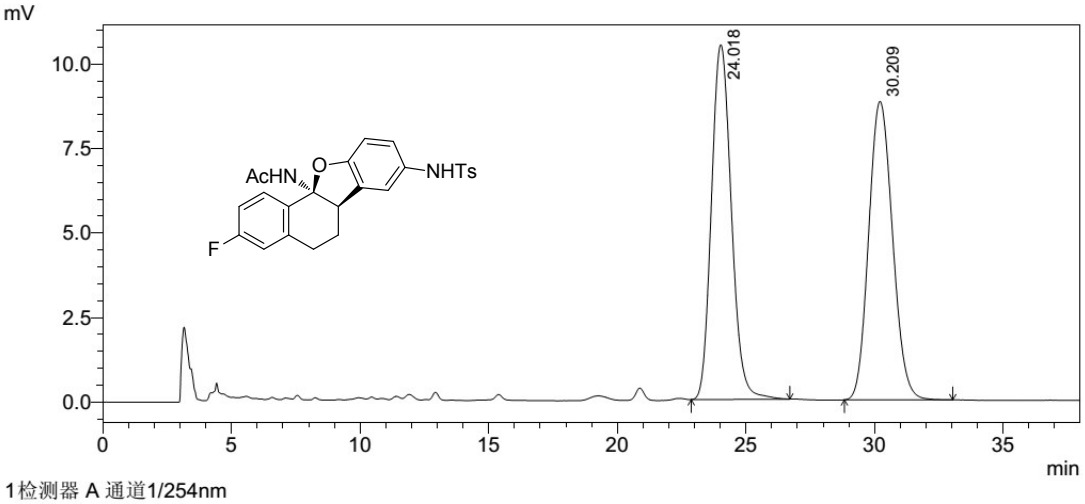
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	24.861	822036	15974	99.657	5349.057	1.126	0.000
2	27.652	2833	57	0.343	8628.230	1.324	2.189
总计		824869	16030	100.000			

N-((6aR,11aS)-3-fluoro-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3j)

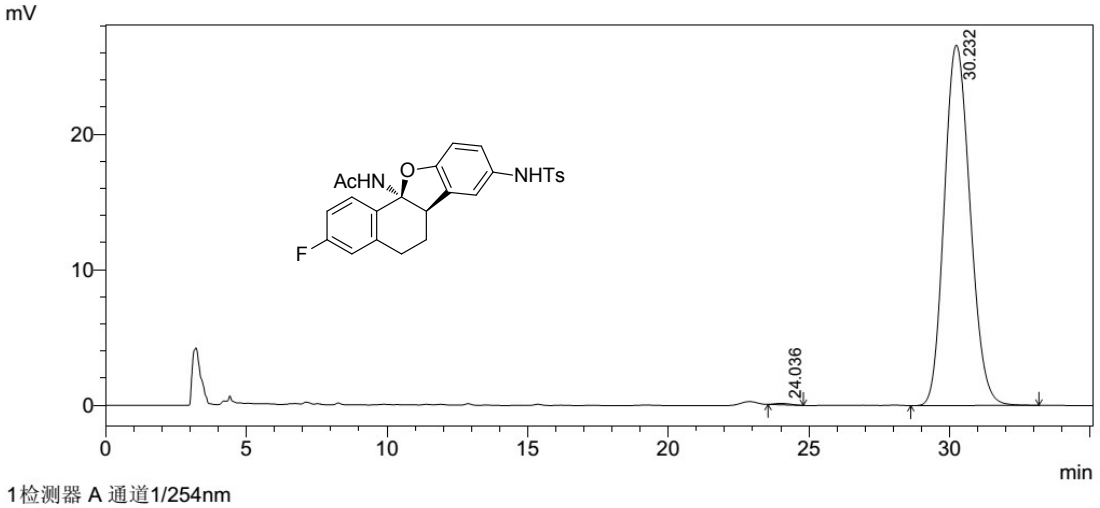


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	24.018	565495	10489	49.840	4698.930	1.159	0.000
2	30.209	569117	8826	50.160	5027.423	1.123	3.987
总计		1134612	19315	100.000			



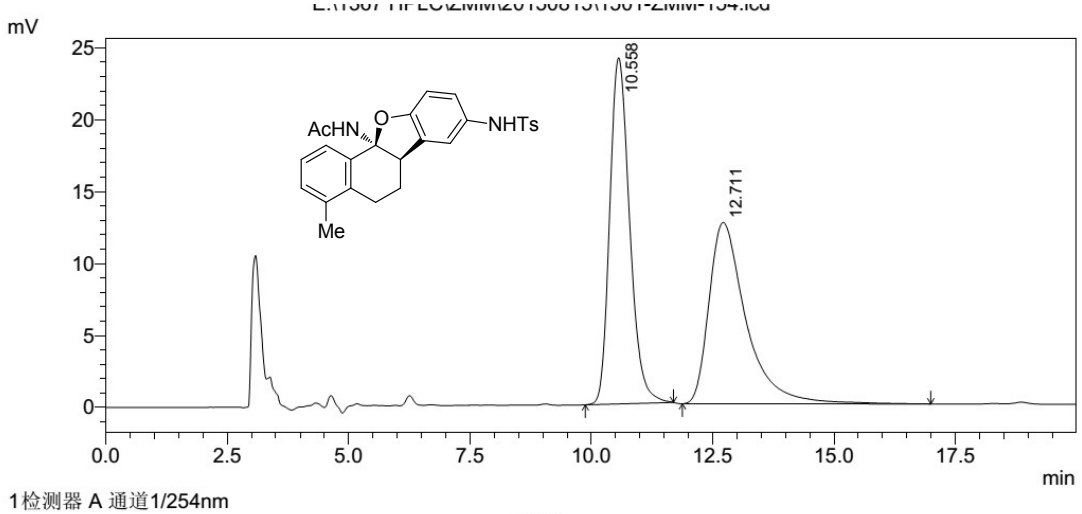
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	24.036	4023	104	0.236	9403.379	1.228	0.000
2	30.232	1702882	26605	99.764	5112.433	1.152	4.619
总计		1706904	26709	100.000			

N-((6aR,11aS)-4-methyl-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3k)

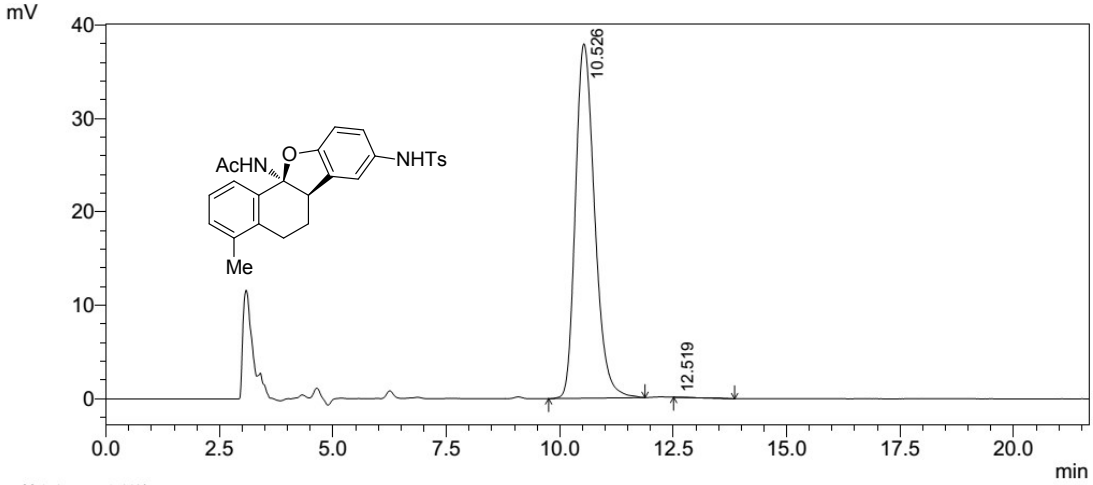


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	10.558	686118	24051	50.595	3232.934	1.259	0.000
2	12.711	669972	12604	49.405	1540.611	1.677	2.113
总计		1356090	36655	100.000			



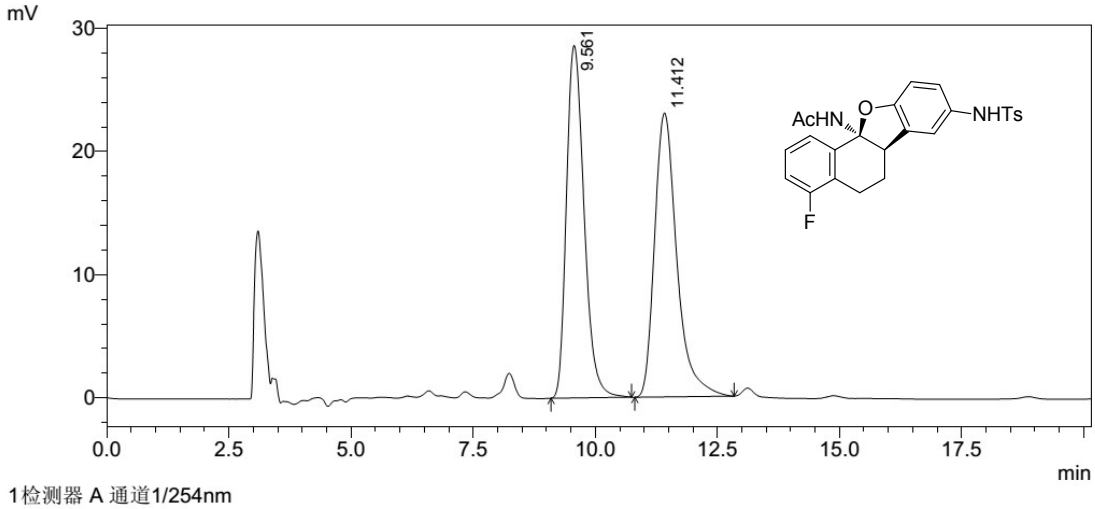
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	10.526	1119188	37943	99.860	3025.302	1.275	0.000
2	12.519	1567	1	0.140	12219.159	0.000	3.271
总计		1120755	37944	100.000			

N-((6aR,11aS)-4-fluoro-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3l)

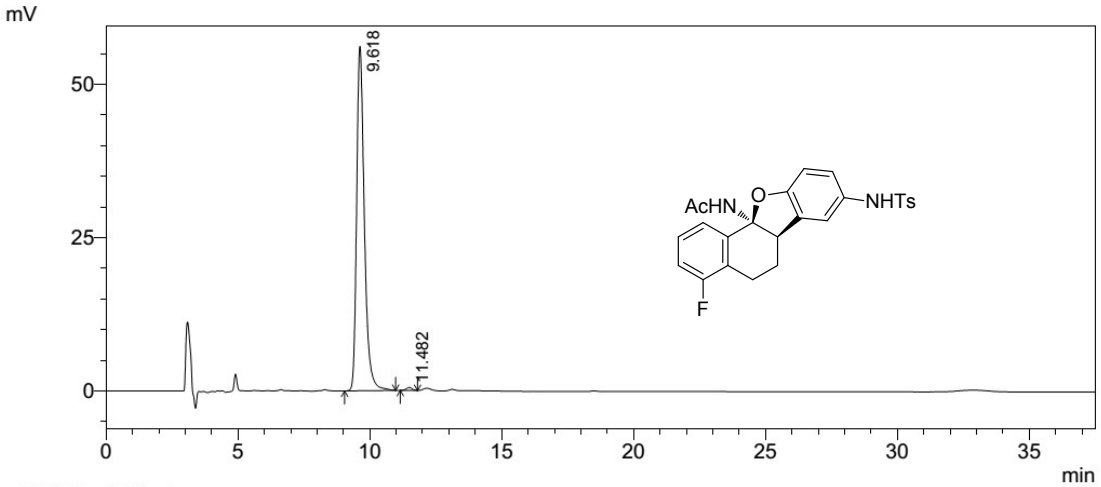


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	9.561	718461	28634	49.625	3442.286	1.315	0.000
2	11.412	729316	23057	50.375	3304.194	1.416	2.560
总计		1447776	51691	100.000			



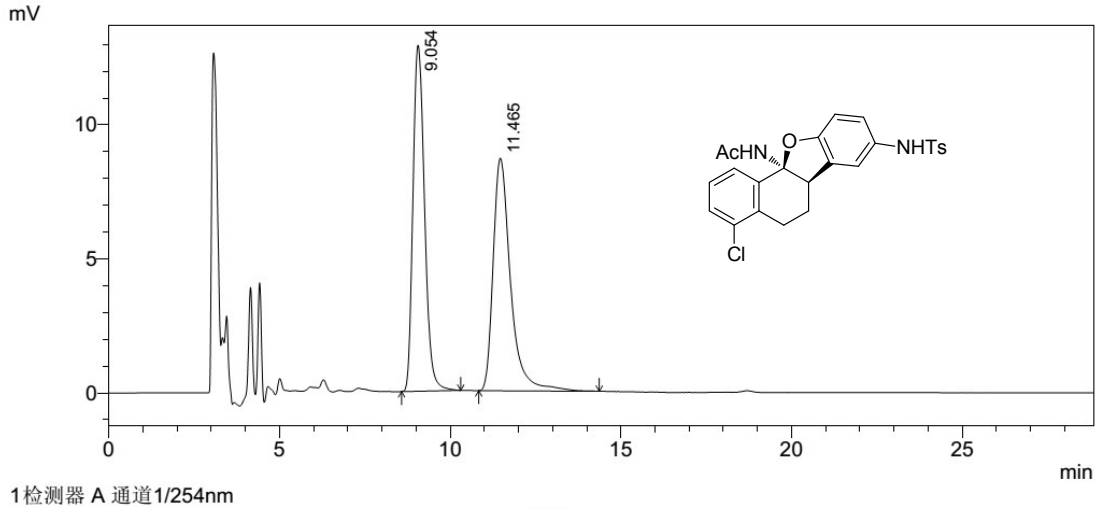
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	9.618	1140380	56194	99.327	5544.738	1.382	0.000
2	11.482	7722	496	0.673	12328.255	1.009	4.009
总计		1148102	56690	100.000			

N-((6aR,11aS)-4-chloro-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho [1,2-b]benzofuran-11a-yl)acetamide (3m)

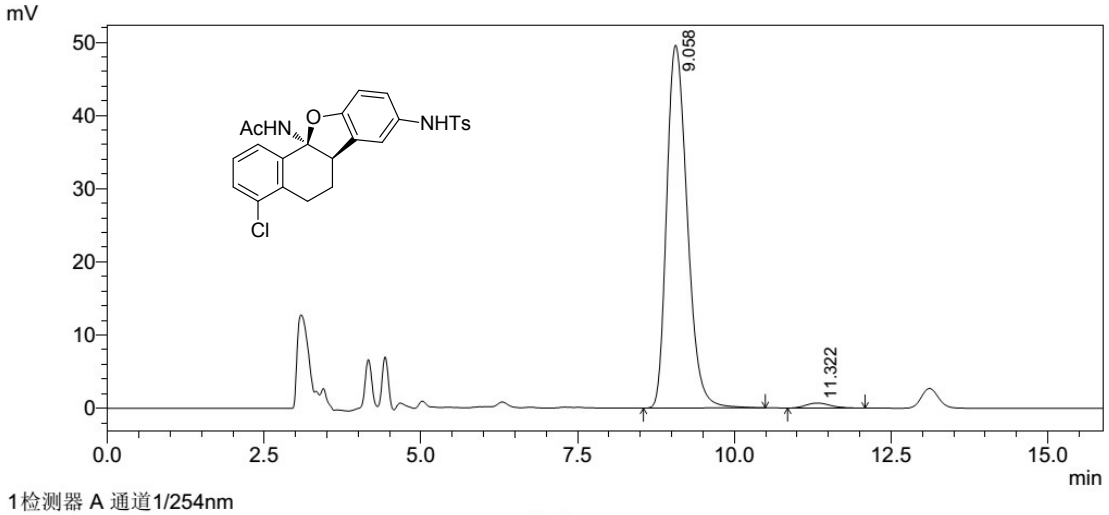


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	9.054	305361	12916	49.836	3469.683	1.276	0.000
2	11.465	307371	8682	50.164	2780.002	1.486	3.247
总计		612732	21598	100.000			



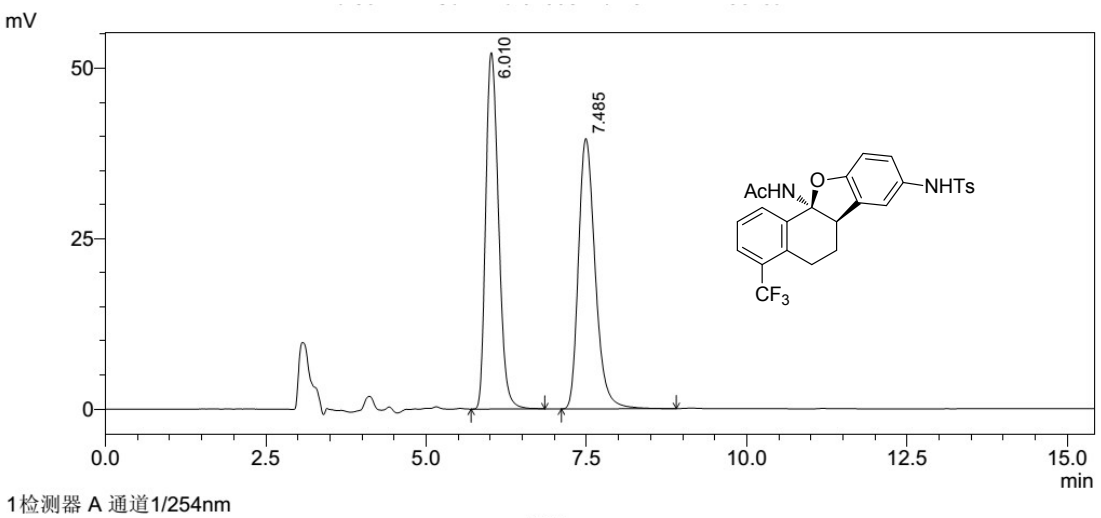
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	9.058	1130599	49545	98.409	3696.822	1.299	0.000
2	11.322	18275	674	1.591	4077.468	1.204	3.470
总计		1148874	50219	100.000			

N-((6aR,11aS)-8-(4-methylphenylsulfonamido)-4-(trifluoromethyl)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3n)

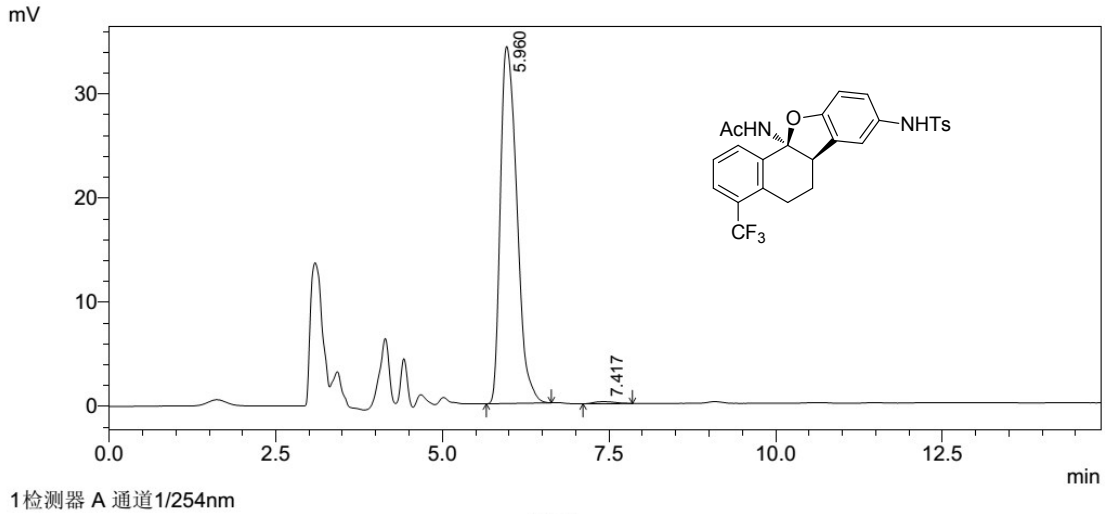


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	6.010	727038	52326	50.230	4254.362	1.295	0.000
2	7.485	720391	39666	49.770	4048.123	1.306	3.516
总计		1447430	91992	100.000			



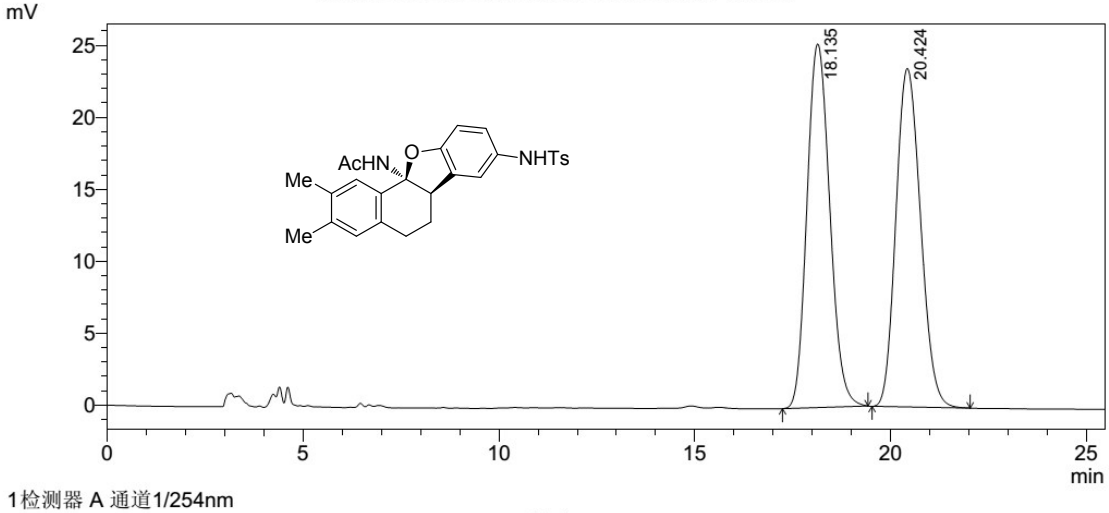
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	5.960	590899	34302	99.313	2809.295	1.494	0.000
2	7.417	4085	184	0.687	2929.929	1.261	2.920
总计		594984	34486	100.000			

N-((6aR,11aS)-2,3-dimethyl-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3o)

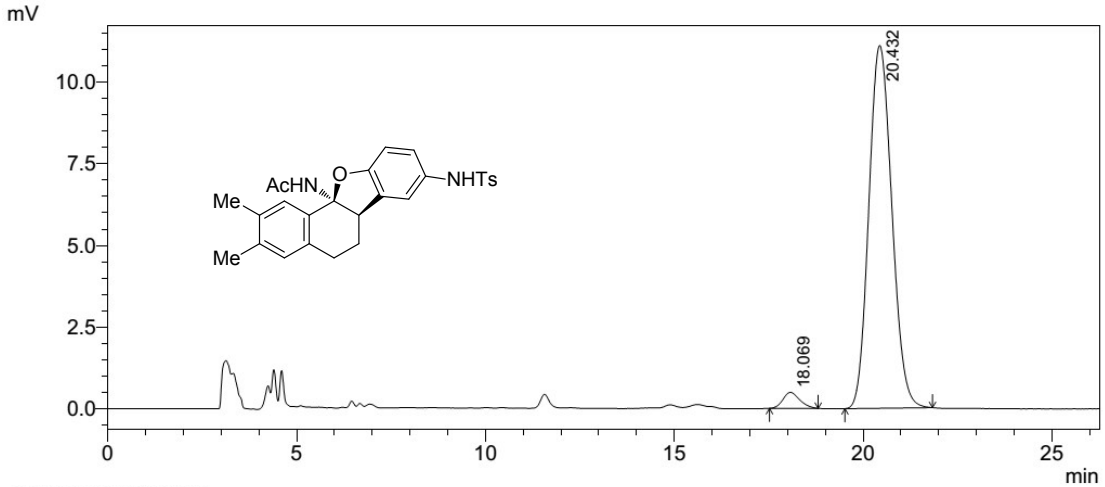


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	18.135	1024219	25268	49.881	4619.745	1.153	0.000
2	20.424	1029087	23517	50.119	4960.473	1.161	2.055
总计		2053306	48785	100.000			



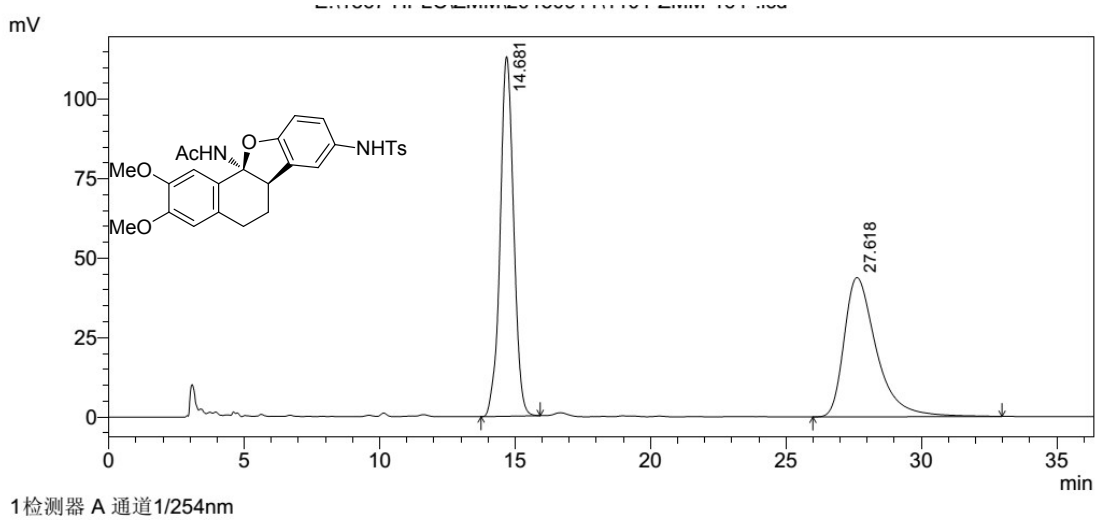
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	18.069	15208	489	3.129	7745.357	1.212	0.000
2	20.432	470828	11110	96.871	5313.541	1.134	2.433
总计		486035	11599	100.000			

N-((6aR,11aS)-2,3-dimethoxy-8-(4-methylphenylsulfonamido)-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3p)

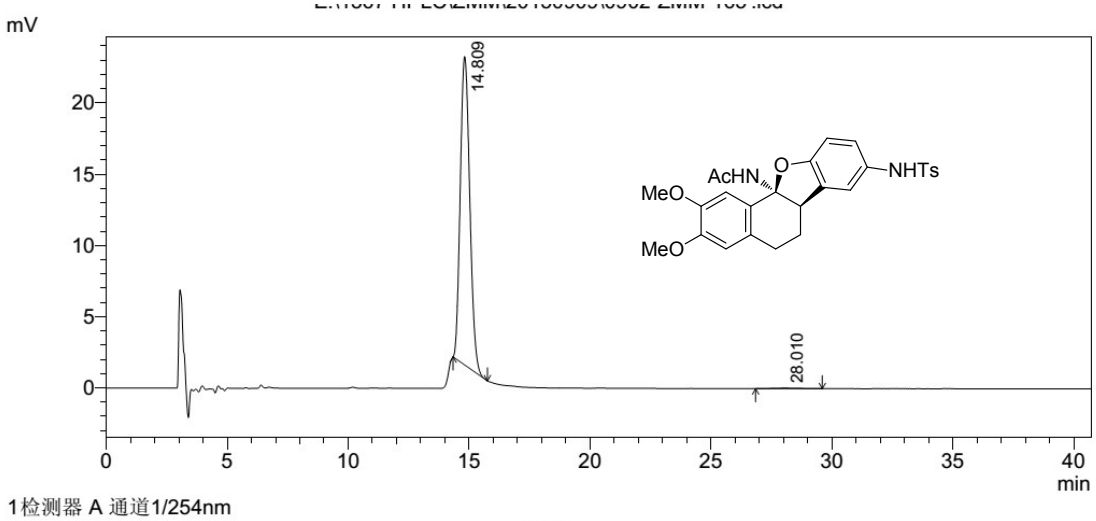


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	14.681	3928141	113267	51.892	4332.021	1.008	0.000
2	27.618	3641695	43866	48.108	2849.024	1.528	8.736
总计		7569836	157133	100.000			



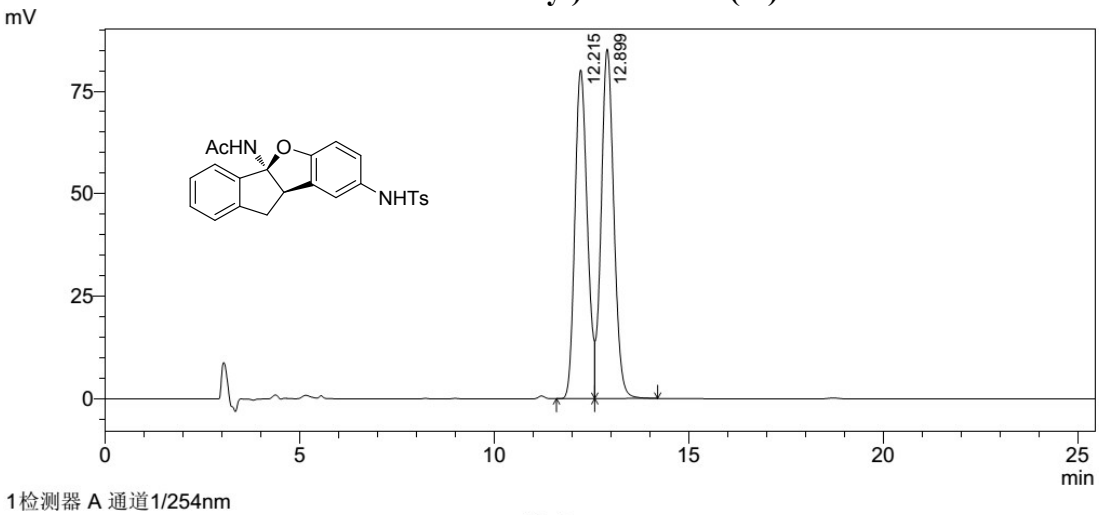
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	14.809	591282	21645	99.584	6577.005	1.183	0.000
2	28.010	2469	35	0.416	4955.244	1.116	11.370
总计		593751	21680	100.000			

N-((4bS,9bR)-8-(4-methylphenylsulfonamido)-9b,10-dihydro-4bH-indeno[1,2-b] benzofuran-4b-yl)acetamide (3s)

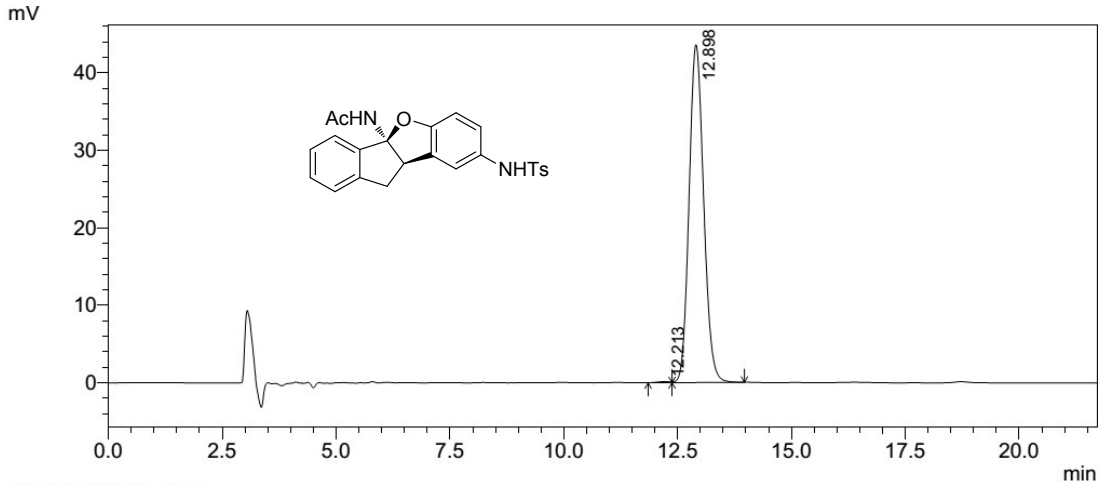


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	12.215	1776432	80193	47.912	6739.292	0.000	0.000
2	12.899	1931251	85292	52.088	7483.418	0.000	1.146
总计		3707683	165485	100.000			



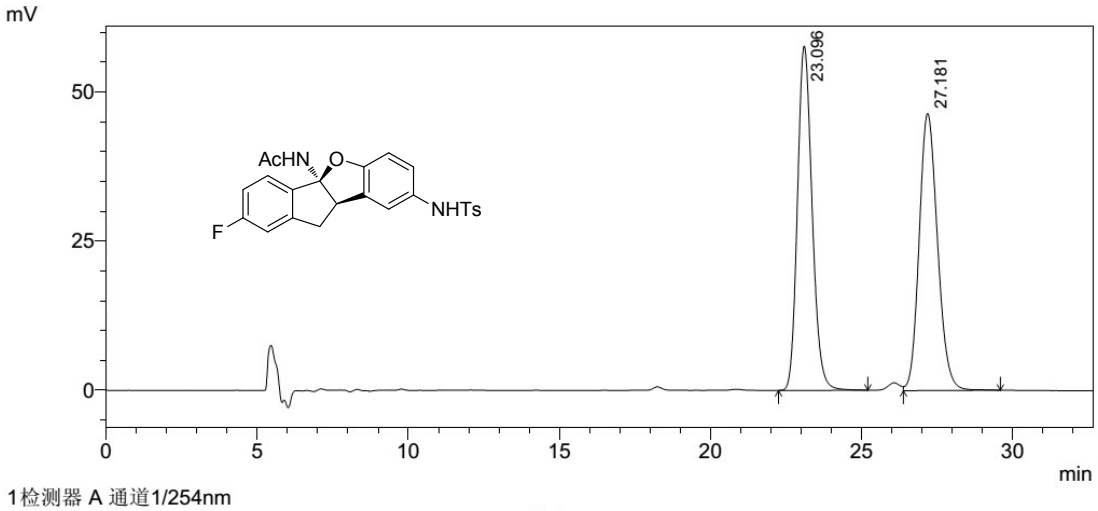
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	12.213	2558	136	0.263	6007.123	0.000	0.000
2	12.898	971140	43591	99.737	7682.446	1.140	1.123
总计		973698	43726	100.000			

N-((4bS,9bR)-2-fluoro-8-(4-methylphenylsulfonamido)-9b,10-dihydro-4bH-indeno [1,2-b]benzofuran-4b-yl)acetamide (3t)

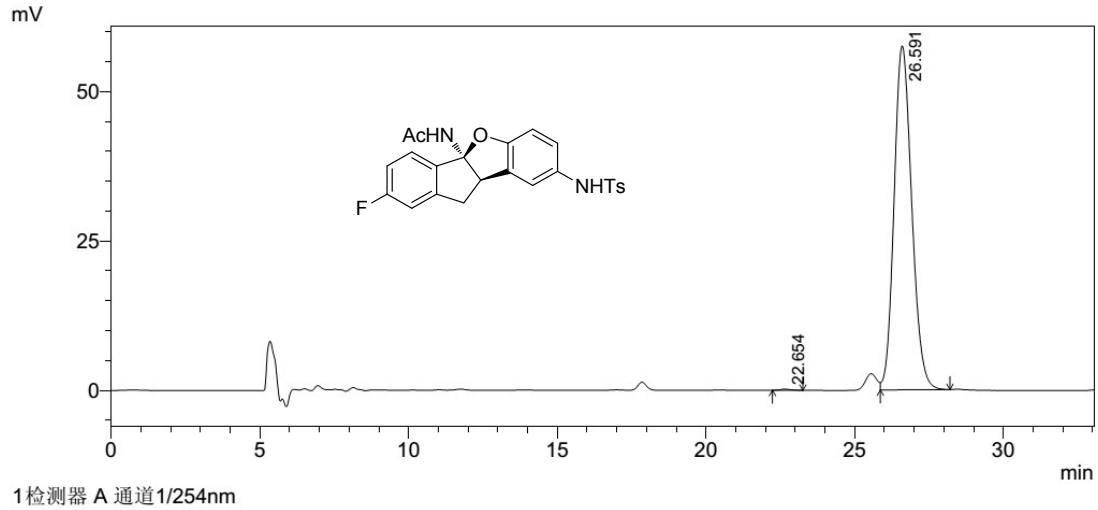


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	23.096	1950912	57742	49.864	10951.191	1.185	0.000
2	27.181	1961555	46456	50.136	9646.974	1.167	4.106
总计		3912467	104199	100.000			



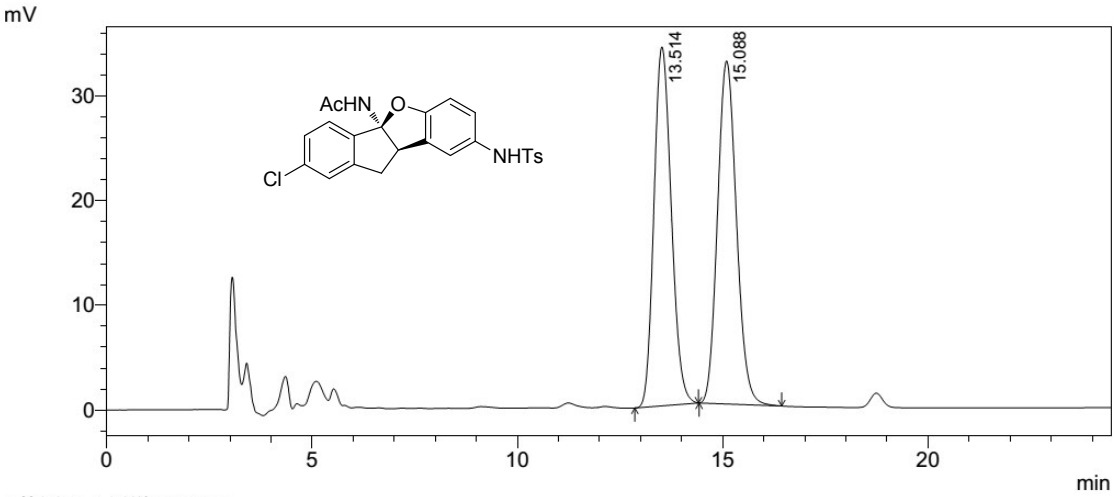
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	22.654	4573	160	0.192	13135.228	1.184	0.000
2	26.591	2378001	57567	99.808	9564.531	1.173	4.192
总计		2382573	57727	100.000			

N-((4bS,9bR)-2-chloro-8-(4-methylphenylsulfonamido)-9b,10-dihydro-4bH-indeno [1,2-b]benzofuran-4b-yl)acetamide (3u)

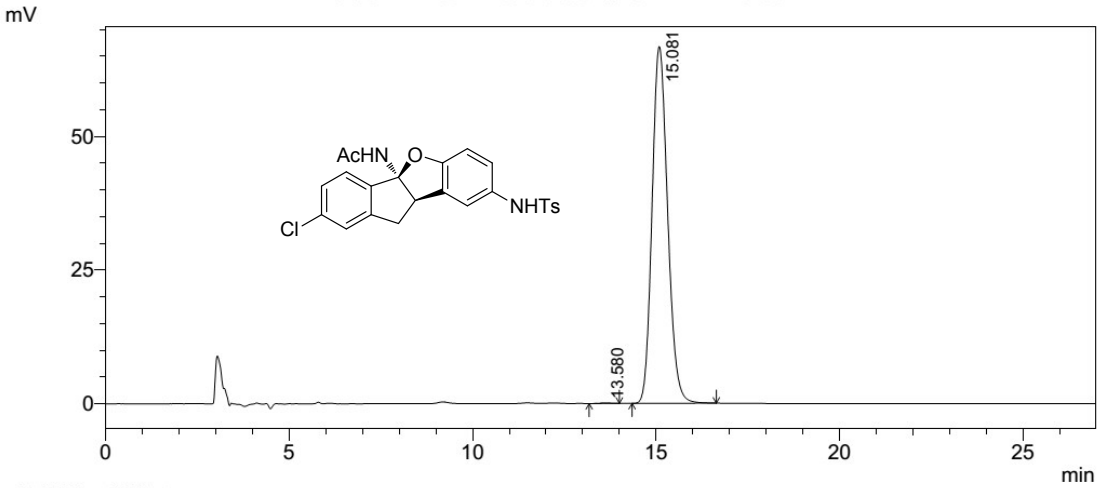


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	13.514	1007713	34352	48.908	4835.552	1.182	0.000
2	15.088	1052720	32822	51.092	5086.938	1.138	1.940
总计		2060432	67174	100.000			



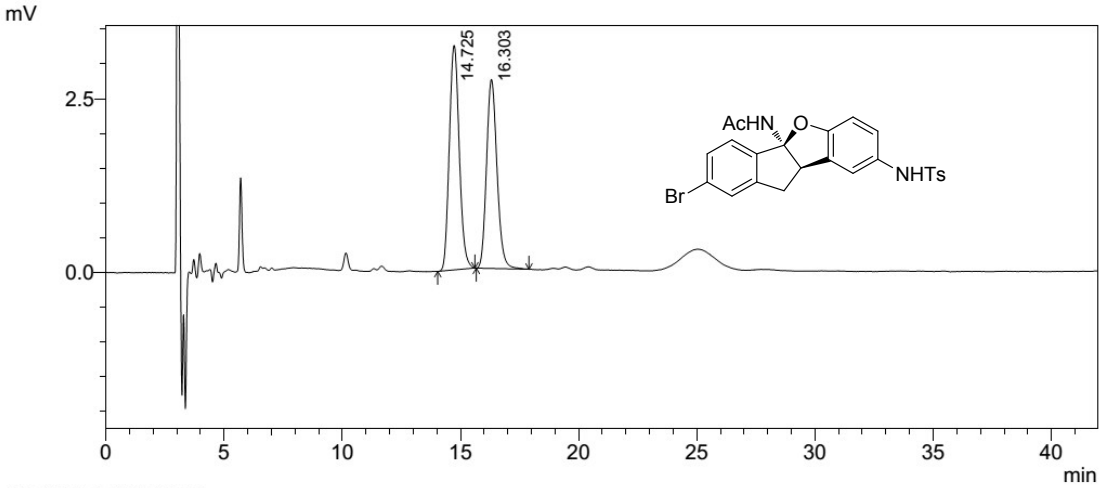
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	13.580	1265	62	0.064	9841.456	1.191	0.000
2	15.081	1971157	66757	99.936	6033.944	1.175	2.267
总计		1972422	66818	100.000			

N-((4bS,9bR)-2-bromo-8-(4-methylphenylsulfonamido)-9b,10-dihydro-4bH-indeno [1,2-b]benzofuran-4b-yl)acetamide (3v)

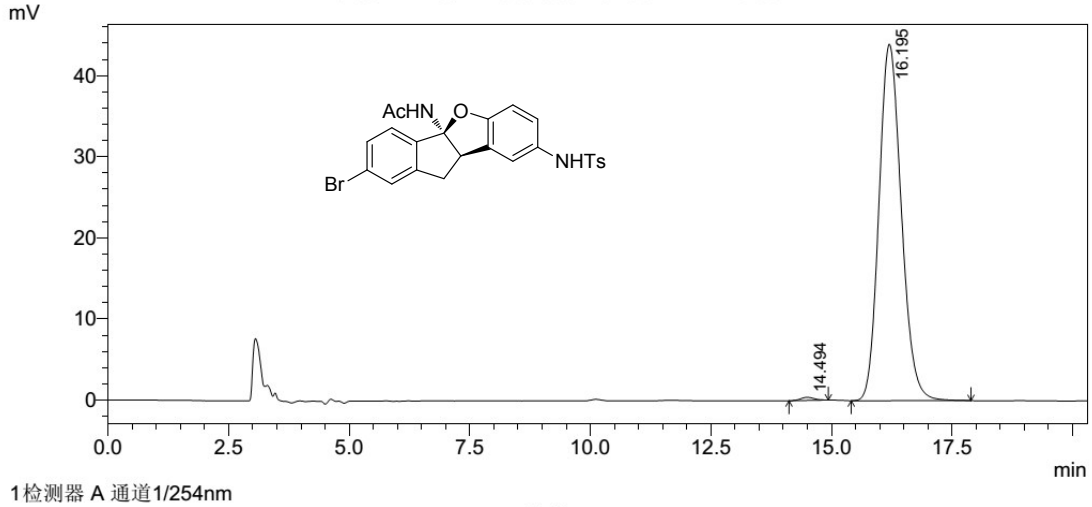


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	14.725	94310	3228	52.960	5877.084	1.143	0.000
2	16.303	83767	2718	47.040	6601.827	1.171	2.009
总计		178077	5946	100.000			



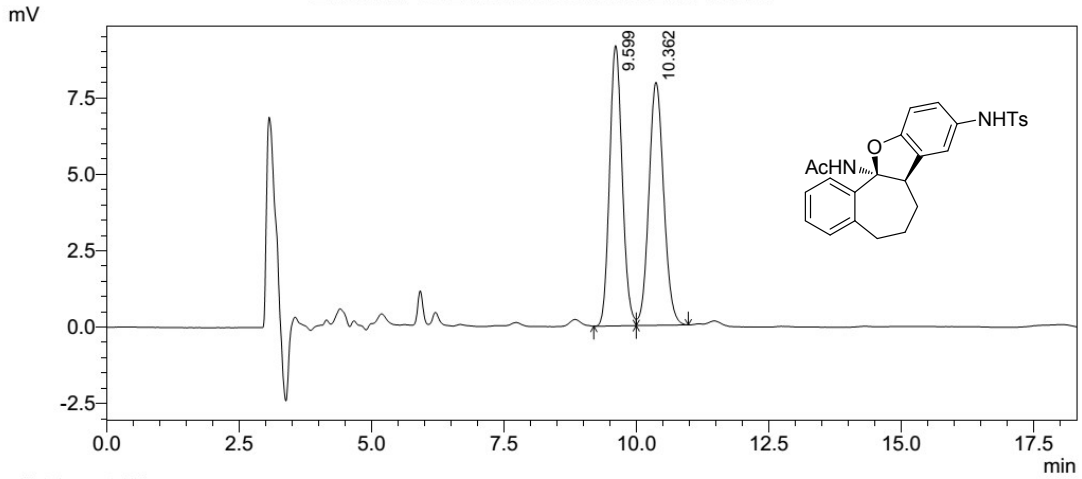
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	14.494	7671	393	0.538	12379.803	1.131	0.000
2	16.195	1419347	43949	99.462	5837.051	1.169	2.486
总计		1427018	44341	100.000			

N-((7aR,12aS)-9-(4-methylphenylsulfonamido)-6,7,7a,12a-tetrahydro-5H-benzo[6,7]cyclohepta[1,2-b]benzofuran-12a-yl)acetamide (3w)

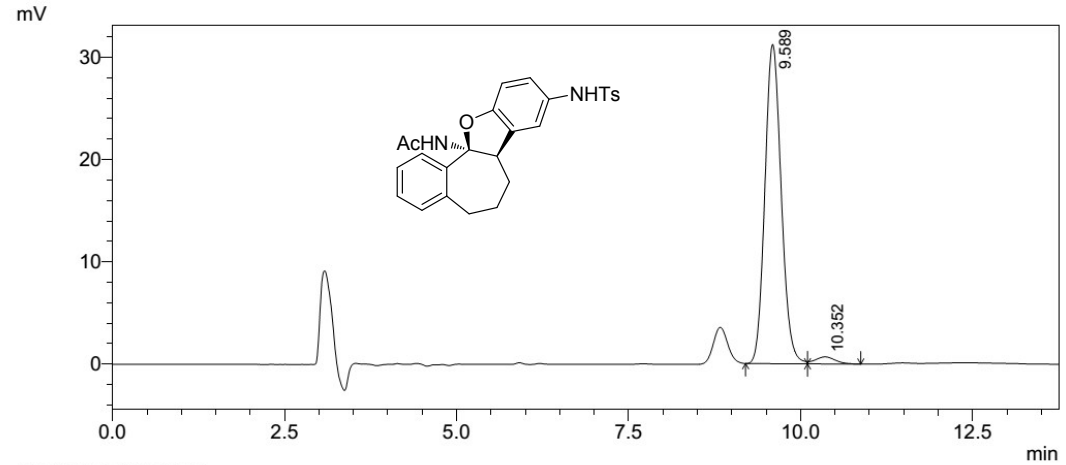


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	9.599	152241	9171	49.533	7533.557	1.136	0.000
2	10.362	155112	7958	50.467	6463.299	1.105	1.593
总计		307353	17128	100.000			



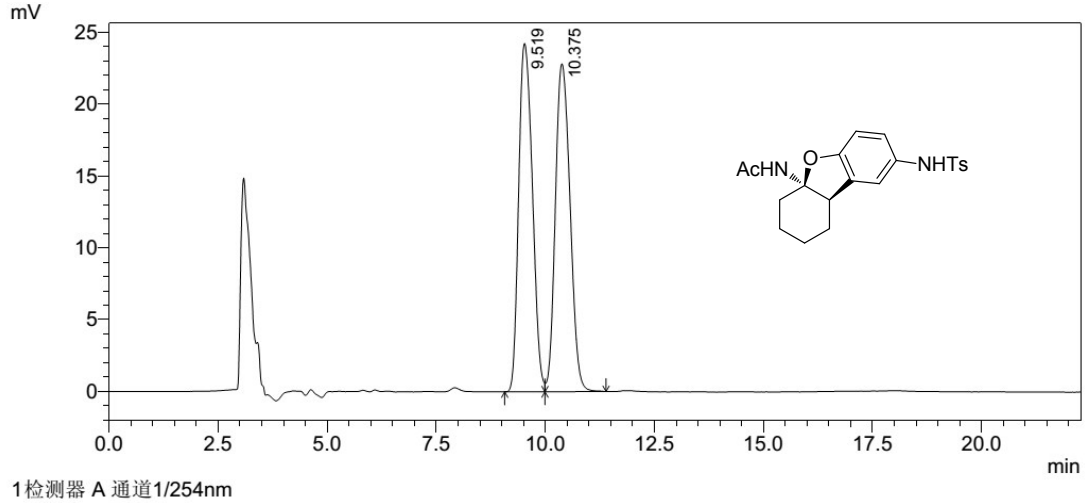
1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	9.589	515157	31230	97.373	7674.456	1.141	0.000
2	10.352	13899	687	2.627	5584.896	0.000	1.537
总计		529056	31917	100.000			

N-((4aR,9bR)-8-(4-methylphenylsulfonamido)-1,2,3,4,4a,9b-hexahydrodibenzo[b,d]furan-4a-yl)acetamide (3x)

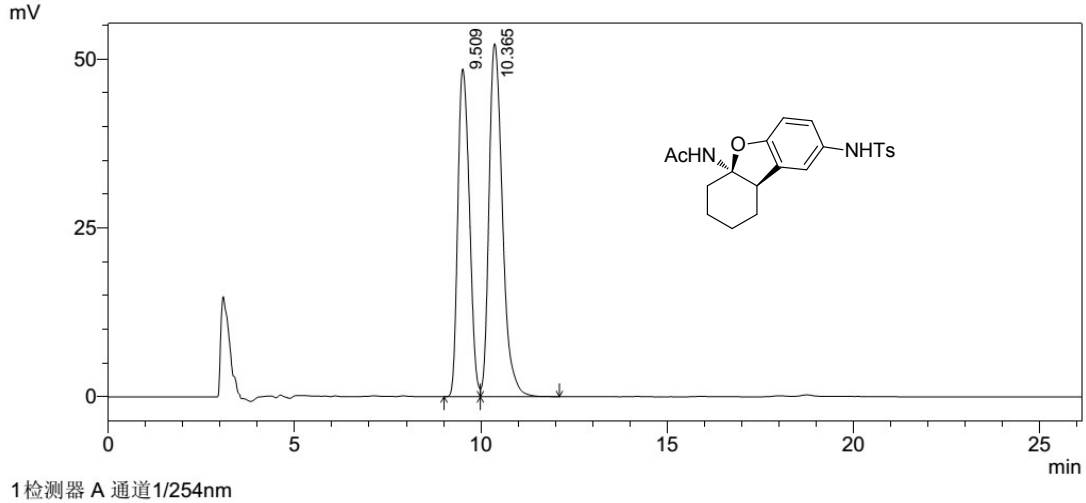


1检测器 A 通道1/254nm

峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	9.519	531487	24269	49.728	4235.532	1.227	0.000
2	10.375	537309	22828	50.272	4437.390	1.175	1.418
总计		1068796	47098	100.000			



1检测器 A 通道1/254nm

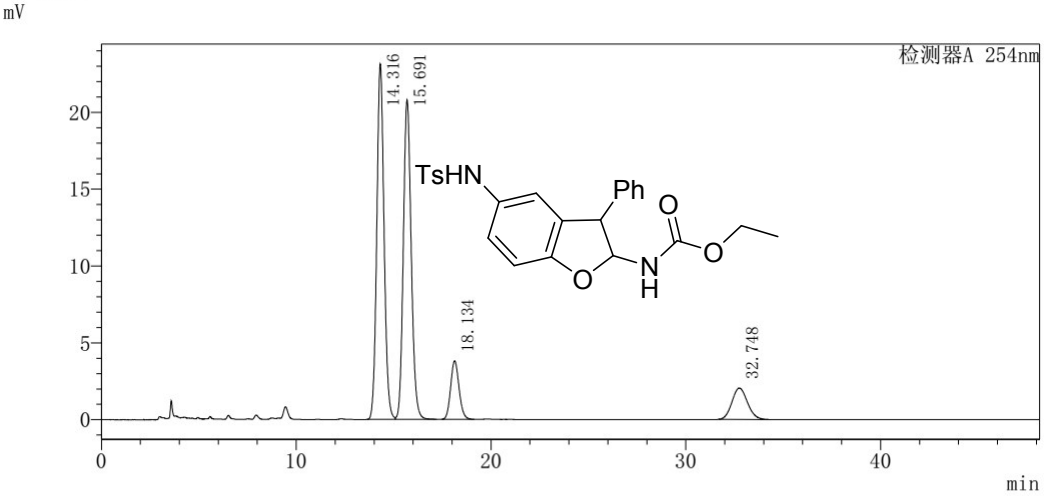
峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	理论塔板#	拖尾因子	分离度
1	9.509	1047700	48502	44.428	4353.482	1.230	0.000
2	10.365	1310498	52261	55.572	4182.764	1.407	1.406
总计		2358198	100763	100.000			

Ethyl (5-(4-methylphenylsulfonamido)-3-phenyl-2,3-dihydrobenzofuran-2-yl) carbamate

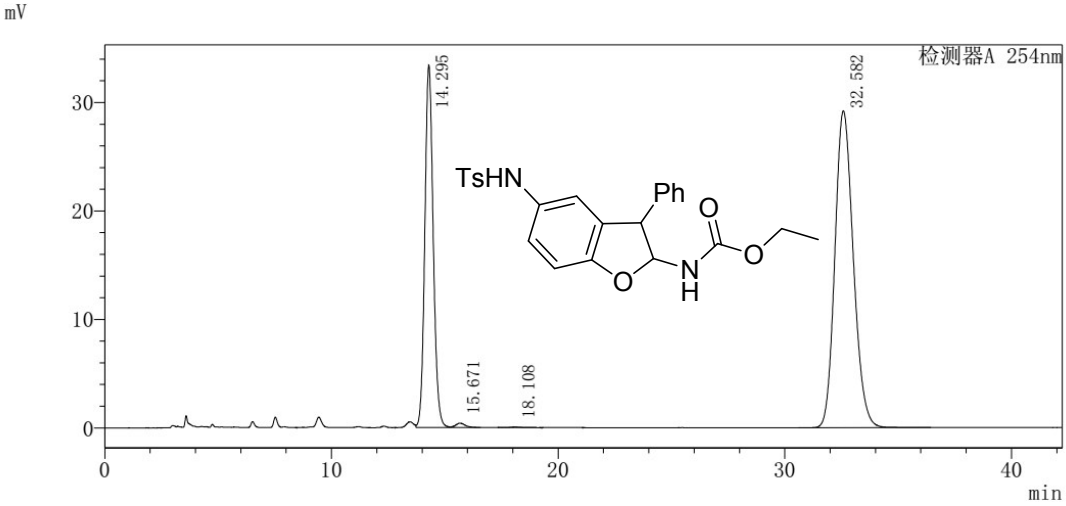
<色谱图>



<峰表>

检测器A 254nm

峰号	保留时间	面积	高度	面积%	理论塔板数(USP)	拖尾因子	分离度(USP)
1	14.316	598432	23129	42.386	7156	1.088	--
2	15.691	586270	20784	41.524	7201	1.143	1.940
3	18.134	114032	3807	8.077	8441	1.124	3.196
4	32.748	113138	2043	8.013	8047	1.110	12.992
总计		1411872	49763	100.000			



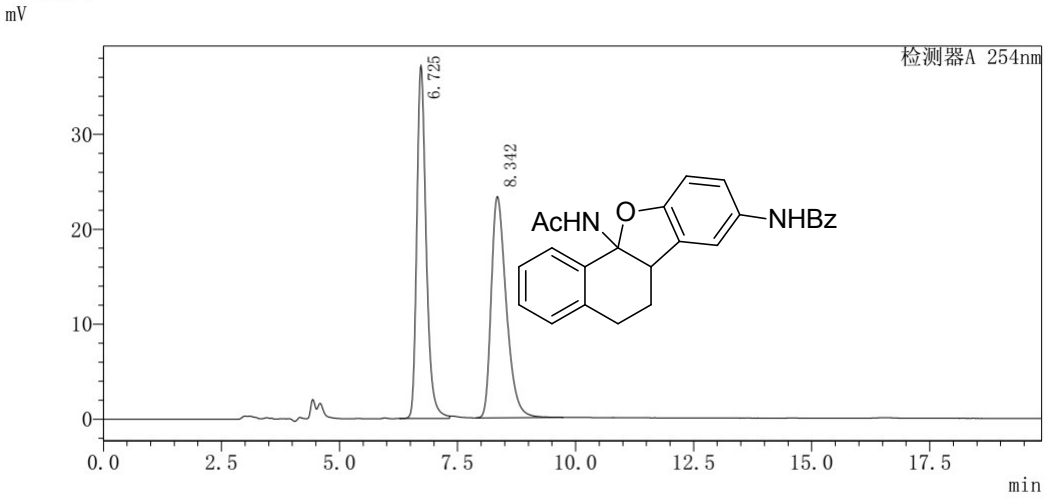
<峰表>

检测器A 254nm

峰号	保留时间	面积	高度	面积%	理论塔板数(USP)	拖尾因子	分离度(USP)
1	14.295	858426	33414	34.043	7242	1.115	--
2	15.671	11924	399	0.473	6823	--	1.924
3	18.108	1737	53	0.069	9841	1.146	3.272
4	32.582	1649506	29225	65.415	7710	1.169	13.073
总计		2521593	63091	100.000			

N-((6aR,11aS)-11a-acetamido-5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-8-yl) benzamide (3z)

〈色谱图〉

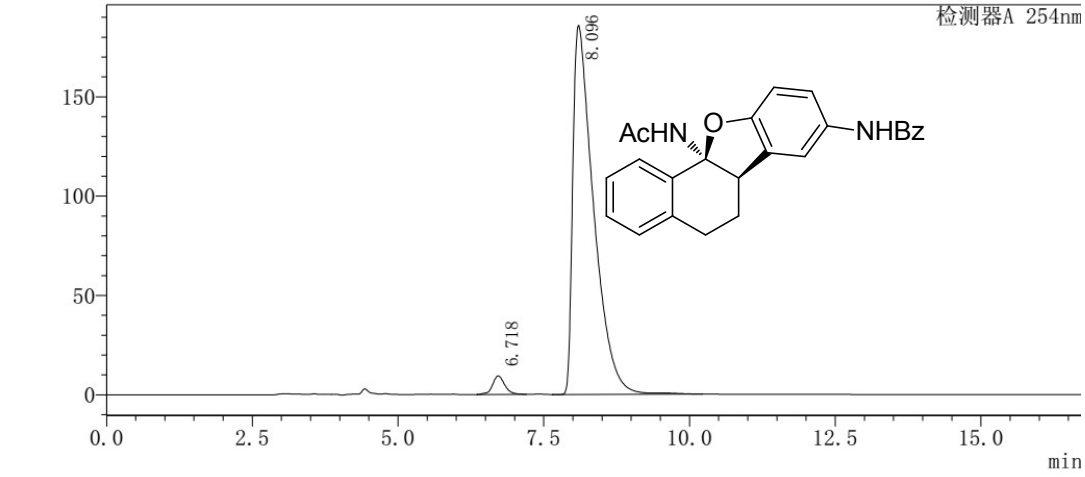


〈峰表〉

检测器A 254nm

峰号	保留时间	面积	高度	面积%	理论塔板数(USP)	拖尾因子	分离度(USP)
1	6.725	515126	37113	49.966	5590	1.300	--
2	8.342	515820	23278	50.034	3348	1.420	3.453
总计		1030945	60391	100.000			

〈色谱图〉

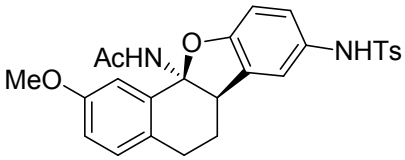


〈峰表〉

检测器A 254nm

峰号	保留时间	面积	高度	面积%	理论塔板数(USP)	拖尾因子	分离度(USP)
1	6.718	135045	9298	2.835	5158	1.038	--
2	8.096	4628298	185729	97.165	2488	2.332	2.694
总计		4763342	195026	100.000			

6. X-ray crystal structure of N-(2-methoxy-8-(4-methylphenylsulfonamido)- 5,6,6a,11a-tetrahydronaphtho[1,2-b]benzofuran-11a-yl)acetamide (3d):



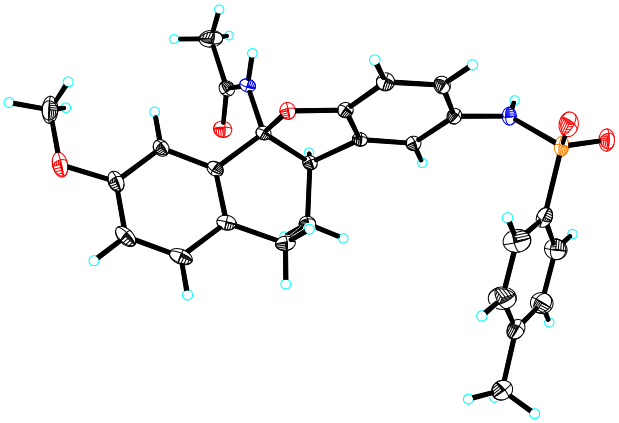


Table 1. Crystal data and structure refinement for wlx_zmm2.

Identification code	mo_wlx_zmm2_0m
Empirical formula	$C_{27}H_{30}N_2O_6S$
Formula weight	510.59
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P 21 21 21
Unit cell dimensions	a = 8.931(4) A alpha = 90 deg. b = 10.538(5) A beta = 90 deg. c = 28.633(13) A gamma = 90 deg.
Volume	2695(2) A^3

Z, Calculated density	4, 1.258 Mg/m^3
Absorption coefficient	0.163 mm^-1
F(000)	1080
Crystal size	1.10 x 0.72 x 0.20 mm
Theta range for data collection	1.42 to 29.99 deg.
Limiting indices	-12<=h<=12, -14<=k<=14, -39<=l<=40
Reflections collected / unique	28329 / 7553 [R(int) = 0.0522]
Completeness to theta = 29.99	98.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9682 and 0.8414
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7553 / 0 / 330
Goodness-of-fit on F^2	1.063
Final R indices [I>2sigma(I)]	R1 = 0.0416, wR2 = 0.1065
R indices (all data)	R1 = 0.0472, wR2 = 0.1094
Absolute structure parameter	0.07(6)
Largest diff. peak and hole	0.392 and -0.389 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for wlx_zmm2. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	6064(1)	5566(1)	1679(1)	32(1)
O(1)	-2665(2)	5259(2)	-1487(1)	56(1)
O(2)	7309(2)	5031(2)	1931(1)	44(1)
O(3)	2074(1)	5977(1)	-259(1)	24(1)
O(4)	1930(2)	2481(1)	-956(1)	33(1)
O(5)	5914(2)	6927(1)	1656(1)	44(1)
C(6)	563(4)	2327(2)	3900(1)	68(1)
N(1)	2625(1)	4518(1)	-831(1)	23(1)
O(6)	1458(2)	3263(1)	3676(1)	48(1)
C(1)	311(3)	3443(3)	2498(1)	65(1)
C(2)	1728(2)	3974(3)	2287(1)	48(1)
C(3)	1738(3)	5135(3)	2059(1)	60(1)
C(4)	3051(3)	5638(2)	1877(1)	54(1)
C(5)	4383(2)	4965(2)	1918(1)	35(1)
N(2)	6210(2)	5025(1)	1150(1)	26(1)
C(7)	5092(2)	5326(1)	802(1)	23(1)
C(8)	4220(2)	4334(1)	618(1)	22(1)
C(9)	3245(2)	4616(1)	256(1)	21(1)
C(10)	2170(2)	3777(1)	-13(1)	21(1)
C(11)	1689(2)	4699(1)	-417(1)	20(1)
C(12)	17(2)	4731(1)	-522(1)	23(1)
C(13)	-503(2)	4948(2)	-975(1)	29(1)
C(14)	-2047(2)	5053(2)	-1054(1)	37(1)
C(15)	-1658(3)	5348(3)	-1875(1)	62(1)
C(16)	3067(3)	3308(3)	2318(1)	56(1)
C(17)	4388(2)	3794(2)	2138(1)	50(1)
C(18)	4960(2)	6564(1)	633(1)	28(1)
C(19)	3944(2)	6852(1)	278(1)	28(1)
C(20)	3114(2)	5857(1)	95(1)	22(1)
C(21)	2645(2)	3430(2)	-1080(1)	27(1)
C(22)	3603(3)	3439(2)	-1514(1)	47(1)
C(23)	-970(2)	4624(1)	-146(1)	26(1)
C(24)	-353(2)	4355(2)	333(1)	31(1)
C(25)	845(2)	3317(1)	291(1)	28(1)
C(26)	-2511(2)	4733(2)	-237(1)	36(1)
C(27)	-3042(2)	4944(2)	-683(1)	40(1)

Table 3. Bond lengths [A] and angles [deg] for wlx_zmm2.

S(1)-O(2)	1.4394(15)
S(1)-O(5)	1.4424(15)
S(1)-N(2)	1.6241(15)
S(1)-C(5)	1.767(2)
O(1)-C(14)	1.374(2)
O(1)-C(15)	1.432(3)
O(3)-C(20)	1.3818(19)
O(3)-C(11)	1.4612(17)
O(4)-C(21)	1.238(2)
C(6)-O(6)	1.422(3)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
N(1)-C(21)	1.350(2)
N(1)-C(11)	1.4629(19)
N(1)-H(1)	0.8800
O(6)-H(6)	0.8400
C(1)-C(2)	1.510(3)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(3)	1.387(4)
C(2)-C(16)	1.390(4)
C(3)-C(4)	1.388(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.390(3)
C(4)-H(4)	0.9500
C(5)-C(17)	1.385(3)
N(2)-C(7)	1.447(2)
N(2)-H(2)	0.8800
C(7)-C(18)	1.397(2)
C(7)-C(8)	1.405(2)
C(8)-C(9)	1.386(2)
C(8)-H(8)	0.9500
C(9)-C(20)	1.3917(19)
C(9)-C(10)	1.515(2)
C(10)-C(25)	1.548(2)
C(10)-C(11)	1.570(2)
C(10)-H(10)	1.0000
C(11)-C(12)	1.523(2)
C(12)-C(23)	1.395(2)

C(12)-C(13)	1.397(2)
C(13)-C(14)	1.402(2)
C(13)-H(13)	0.9500
C(14)-C(27)	1.391(3)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(17)	1.385(3)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-C(19)	1.395(2)
C(18)-H(18)	0.9500
C(19)-C(20)	1.387(2)
C(19)-H(19)	0.9500
C(21)-C(22)	1.511(3)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(26)	1.405(2)
C(23)-C(24)	1.506(2)
C(24)-C(25)	1.534(2)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(27)	1.381(3)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500

O(2)-S(1)-O(5)	118.95(9)
O(2)-S(1)-N(2)	105.51(8)
O(5)-S(1)-N(2)	108.29(8)
O(2)-S(1)-C(5)	108.78(9)
O(5)-S(1)-C(5)	107.16(10)
N(2)-S(1)-C(5)	107.69(8)
C(14)-O(1)-C(15)	117.18(16)
C(20)-O(3)-C(11)	107.49(10)
O(6)-C(6)-H(6A)	109.5
O(6)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
O(6)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(21)-N(1)-C(11)	123.12(12)

C(21)-N(1)-H(1)	118.4
C(11)-N(1)-H(1)	118.4
C(6)-O(6)-H(6)	109.5
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(3)-C(2)-C(16)	118.0(2)
C(3)-C(2)-C(1)	121.4(2)
C(16)-C(2)-C(1)	120.6(2)
C(2)-C(3)-C(4)	121.3(2)
C(2)-C(3)-H(3)	119.4
C(4)-C(3)-H(3)	119.4
C(3)-C(4)-C(5)	119.7(2)
C(3)-C(4)-H(4)	120.1
C(5)-C(4)-H(4)	120.1
C(17)-C(5)-C(4)	119.7(2)
C(17)-C(5)-S(1)	119.50(15)
C(4)-C(5)-S(1)	120.73(16)
C(7)-N(2)-S(1)	120.73(11)
C(7)-N(2)-H(2)	119.6
S(1)-N(2)-H(2)	119.6
C(18)-C(7)-C(8)	121.22(14)
C(18)-C(7)-N(2)	120.10(13)
C(8)-C(7)-N(2)	118.54(13)
C(9)-C(8)-C(7)	117.96(13)
C(9)-C(8)-H(8)	121.0
C(7)-C(8)-H(8)	121.0
C(8)-C(9)-C(20)	120.08(13)
C(8)-C(9)-C(10)	130.79(12)
C(20)-C(9)-C(10)	109.09(13)
C(9)-C(10)-C(25)	112.41(13)
C(9)-C(10)-C(11)	100.77(11)
C(25)-C(10)-C(11)	113.50(12)
C(9)-C(10)-H(10)	109.9
C(25)-C(10)-H(10)	109.9
C(11)-C(10)-H(10)	109.9
O(3)-C(11)-N(1)	103.64(11)
O(3)-C(11)-C(12)	105.77(10)
N(1)-C(11)-C(12)	113.79(13)
O(3)-C(11)-C(10)	106.17(11)
N(1)-C(11)-C(10)	111.05(11)

C(12)-C(11)-C(10)	115.27(12)
C(23)-C(12)-C(13)	121.29(14)
C(23)-C(12)-C(11)	117.75(14)
C(13)-C(12)-C(11)	120.81(14)
C(12)-C(13)-C(14)	119.38(16)
C(12)-C(13)-H(13)	120.3
C(14)-C(13)-H(13)	120.3
O(1)-C(14)-C(27)	116.43(16)
O(1)-C(14)-C(13)	123.68(19)
C(27)-C(14)-C(13)	119.89(18)
O(1)-C(15)-H(15A)	109.5
O(1)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
O(1)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-C(2)	121.5(2)
C(17)-C(16)-H(16)	119.3
C(2)-C(16)-H(16)	119.3
C(16)-C(17)-C(5)	119.7(2)
C(16)-C(17)-H(17)	120.2
C(5)-C(17)-H(17)	120.2
C(19)-C(18)-C(7)	120.69(14)
C(19)-C(18)-H(18)	119.7
C(7)-C(18)-H(18)	119.7
C(20)-C(19)-C(18)	117.25(13)
C(20)-C(19)-H(19)	121.4
C(18)-C(19)-H(19)	121.4
O(3)-C(20)-C(19)	124.58(13)
O(3)-C(20)-C(9)	112.67(12)
C(19)-C(20)-C(9)	122.75(14)
O(4)-C(21)-N(1)	121.80(15)
O(4)-C(21)-C(22)	122.28(15)
N(1)-C(21)-C(22)	115.92(15)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(12)-C(23)-C(26)	118.03(16)
C(12)-C(23)-C(24)	119.12(14)
C(26)-C(23)-C(24)	122.82(15)
C(23)-C(24)-C(25)	108.53(13)

C(23)-C(24)-H(24A)	110.0
C(25)-C(24)-H(24A)	110.0
C(23)-C(24)-H(24B)	110.0
C(25)-C(24)-H(24B)	110.0
H(24A)-C(24)-H(24B)	108.4
C(24)-C(25)-C(10)	110.72(12)
C(24)-C(25)-H(25A)	109.5
C(10)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
C(10)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	108.1
C(27)-C(26)-C(23)	121.36(17)
C(27)-C(26)-H(26)	119.3
C(23)-C(26)-H(26)	119.3
C(26)-C(27)-C(14)	120.06(16)
C(26)-C(27)-H(27)	120.0
C(14)-C(27)-H(27)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for wlx_zmm2.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	38(1)	33(1)	25(1)	-6(1)	-7(1)	0(1)
O(1)	35(1)	83(1)	51(1)	6(1)	-19(1)	6(1)
O(2)	40(1)	58(1)	35(1)	-2(1)	-13(1)	1(1)
O(3)	27(1)	15(1)	28(1)	0(1)	-4(1)	0(1)
O(4)	38(1)	24(1)	37(1)	-7(1)	3(1)	-5(1)
O(5)	62(1)	32(1)	38(1)	-14(1)	-6(1)	-4(1)
C(6)	74(2)	42(1)	86(2)	-13(1)	14(2)	-13(1)
N(1)	21(1)	20(1)	27(1)	0(1)	3(1)	-2(1)
O(6)	59(1)	36(1)	50(1)	-7(1)	-11(1)	0(1)
C(1)	47(1)	108(2)	39(1)	10(1)	0(1)	-11(1)
C(2)	43(1)	74(2)	28(1)	4(1)	-2(1)	0(1)
C(3)	44(1)	70(2)	65(2)	10(1)	11(1)	19(1)
C(4)	51(1)	49(1)	62(1)	11(1)	9(1)	18(1)
C(5)	40(1)	40(1)	24(1)	-2(1)	-3(1)	6(1)
N(2)	28(1)	26(1)	26(1)	-5(1)	-5(1)	2(1)
C(7)	29(1)	20(1)	22(1)	-1(1)	-1(1)	-1(1)
C(8)	25(1)	18(1)	23(1)	-1(1)	1(1)	0(1)
C(9)	23(1)	17(1)	23(1)	-1(1)	1(1)	-1(1)
C(10)	23(1)	15(1)	25(1)	0(1)	-1(1)	-1(1)
C(11)	21(1)	16(1)	25(1)	-1(1)	1(1)	0(1)
C(12)	19(1)	19(1)	32(1)	0(1)	1(1)	2(1)
C(13)	22(1)	31(1)	33(1)	0(1)	-2(1)	1(1)
C(14)	27(1)	39(1)	44(1)	1(1)	-10(1)	2(1)
C(15)	53(1)	94(2)	40(1)	1(1)	-20(1)	8(1)
C(16)	49(1)	66(2)	55(1)	26(1)	-7(1)	-3(1)
C(17)	39(1)	54(1)	56(1)	18(1)	-4(1)	8(1)
C(18)	35(1)	20(1)	29(1)	-3(1)	-4(1)	-6(1)
C(19)	38(1)	16(1)	32(1)	1(1)	-3(1)	-3(1)
C(20)	26(1)	18(1)	23(1)	0(1)	0(1)	0(1)
C(21)	24(1)	28(1)	29(1)	-4(1)	1(1)	1(1)
C(22)	52(1)	48(1)	42(1)	-11(1)	21(1)	-5(1)
C(23)	25(1)	18(1)	35(1)	-1(1)	6(1)	0(1)
C(24)	33(1)	29(1)	30(1)	0(1)	9(1)	-2(1)
C(25)	30(1)	22(1)	32(1)	5(1)	-1(1)	-6(1)
C(26)	23(1)	30(1)	53(1)	-3(1)	11(1)	1(1)
C(27)	20(1)	39(1)	61(1)	-1(1)	-3(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for wlx_zmm2.

	x	y	z	U(eq)
H(6A)	1103	1986	4170	102
H(6B)	347	1639	3680	102
H(6C)	-378	2712	4004	102
H(1)	3202	5148	-922	27
H(6)	2207	2914	3553	73
H(1A)	234	3711	2825	97
H(1B)	335	2514	2482	97
H(1C)	-557	3759	2324	97
H(3)	829	5594	2026	72
H(4)	3039	6439	1725	65
H(2)	6978	4544	1074	32
H(8)	4296	3497	738	26
H(10)	2718	3032	-145	26
H(13)	183	5023	-1227	34
H(15A)	-960	6052	-1823	94
H(15B)	-2230	5500	-2161	94
H(15C)	-1096	4554	-1904	94
H(16)	3078	2501	2466	68
H(17)	5293	3326	2165	59
H(18)	5569	7217	760	34
H(19)	3824	7696	167	34
H(22A)	4342	2753	-1496	71
H(22B)	4122	4256	-1539	71
H(22C)	2968	3314	-1790	71
H(24A)	-1167	4069	543	37
H(24B)	93	5135	466	37
H(25A)	397	2549	149	34
H(25B)	1214	3089	606	34
H(26)	-3202	4661	14	43
H(27)	-4089	5015	-736	48

Table 6. Torsion angles [deg] for wlx_zmm2.

C(16)-C(2)-C(3)-C(4)	-1.8(4)
C(1)-C(2)-C(3)-C(4)	178.1(3)
C(2)-C(3)-C(4)-C(5)	0.8(4)
C(3)-C(4)-C(5)-C(17)	0.4(4)
C(3)-C(4)-C(5)-S(1)	178.6(2)
O(2)-S(1)-C(5)-C(17)	-26.55(19)
O(5)-S(1)-C(5)-C(17)	-156.35(17)
N(2)-S(1)-C(5)-C(17)	87.34(18)
O(2)-S(1)-C(5)-C(4)	155.20(18)
O(5)-S(1)-C(5)-C(4)	25.4(2)
N(2)-S(1)-C(5)-C(4)	-90.91(19)
O(2)-S(1)-N(2)-C(7)	177.10(12)
O(5)-S(1)-N(2)-C(7)	-54.53(14)
C(5)-S(1)-N(2)-C(7)	61.05(14)
S(1)-N(2)-C(7)-C(18)	68.93(19)
S(1)-N(2)-C(7)-C(8)	-115.18(14)
C(18)-C(7)-C(8)-C(9)	1.4(2)
N(2)-C(7)-C(8)-C(9)	-174.45(13)
C(7)-C(8)-C(9)-C(20)	-2.1(2)
C(7)-C(8)-C(9)-C(10)	-179.92(14)
C(8)-C(9)-C(10)-C(25)	68.5(2)
C(20)-C(9)-C(10)-C(25)	-109.52(14)
C(8)-C(9)-C(10)-C(11)	-170.37(15)
C(20)-C(9)-C(10)-C(11)	11.64(15)
C(20)-O(3)-C(11)-N(1)	-97.93(13)
C(20)-O(3)-C(11)-C(12)	142.09(12)
C(20)-O(3)-C(11)-C(10)	19.15(14)
C(21)-N(1)-C(11)-O(3)	178.11(13)
C(21)-N(1)-C(11)-C(12)	-67.53(18)
C(21)-N(1)-C(11)-C(10)	64.50(18)
C(9)-C(10)-C(11)-O(3)	-18.33(13)
C(25)-C(10)-C(11)-O(3)	102.06(13)
C(9)-C(10)-C(11)-N(1)	93.68(13)
C(25)-C(10)-C(11)-N(1)	-145.93(12)
C(9)-C(10)-C(11)-C(12)	-135.06(13)
C(25)-C(10)-C(11)-C(12)	-14.66(17)
O(3)-C(11)-C(12)-C(23)	-80.44(15)
N(1)-C(11)-C(12)-C(23)	166.47(12)
C(10)-C(11)-C(12)-C(23)	36.52(18)
O(3)-C(11)-C(12)-C(13)	95.20(16)
N(1)-C(11)-C(12)-C(13)	-17.90(19)

C(10)-C(11)-C(12)-C(13)	-147.84(14)
C(23)-C(12)-C(13)-C(14)	-0.4(2)
C(11)-C(12)-C(13)-C(14)	-175.87(15)
C(15)-O(1)-C(14)-C(27)	-178.8(2)
C(15)-O(1)-C(14)-C(13)	1.1(3)
C(12)-C(13)-C(14)-O(1)	-179.68(17)
C(12)-C(13)-C(14)-C(27)	0.2(3)
C(3)-C(2)-C(16)-C(17)	1.6(4)
C(1)-C(2)-C(16)-C(17)	-178.2(2)
C(2)-C(16)-C(17)-C(5)	-0.5(4)
C(4)-C(5)-C(17)-C(16)	-0.5(4)
S(1)-C(5)-C(17)-C(16)	-178.8(2)
C(8)-C(7)-C(18)-C(19)	0.6(3)
N(2)-C(7)-C(18)-C(19)	176.41(15)
C(7)-C(18)-C(19)-C(20)	-1.9(3)
C(11)-O(3)-C(20)-C(19)	168.26(15)
C(11)-O(3)-C(20)-C(9)	-12.18(16)
C(18)-C(19)-C(20)-O(3)	-179.34(15)
C(18)-C(19)-C(20)-C(9)	1.1(2)
C(8)-C(9)-C(20)-O(3)	-178.69(13)
C(10)-C(9)-C(20)-O(3)	-0.45(17)
C(8)-C(9)-C(20)-C(19)	0.9(2)
C(10)-C(9)-C(20)-C(19)	179.12(15)
C(11)-N(1)-C(21)-O(4)	-4.4(2)
C(11)-N(1)-C(21)-C(22)	176.23(16)
C(13)-C(12)-C(23)-C(26)	0.4(2)
C(11)-C(12)-C(23)-C(26)	176.02(13)
C(13)-C(12)-C(23)-C(24)	178.37(14)
C(11)-C(12)-C(23)-C(24)	-6.0(2)
C(12)-C(23)-C(24)-C(25)	-43.79(18)
C(26)-C(23)-C(24)-C(25)	134.08(15)
C(23)-C(24)-C(25)-C(10)	62.86(17)
C(9)-C(10)-C(25)-C(24)	80.08(16)
C(11)-C(10)-C(25)-C(24)	-33.48(17)
C(12)-C(23)-C(26)-C(27)	-0.2(2)
C(24)-C(23)-C(26)-C(27)	-178.11(15)
C(23)-C(26)-C(27)-C(14)	0.0(3)
O(1)-C(14)-C(27)-C(26)	179.87(18)
C(13)-C(14)-C(27)-C(26)	0.0(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for wlx_zmm2 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(6)#1	0.88	2.06	2.853(2)	150.1
O(6)-H(6)...O(5)#2	0.84	2.06	2.897(2)	171.7
O(6)-H(6)...S(1)#2	0.84	2.99	3.743(2)	149.9
N(2)-H(2)...O(4)#3	0.88	2.16	2.775(2)	126.3

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y+1,z-1/2 #2 -x+1,y-1/2,-z+1/2 #3 x+1/2,-y+1/2,-z