Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Highly Enantioselective Transfer Hydrogenation of Racemic α-Substituted β-keto Sulfonamides *via* Dynamic Kinetic Resolution

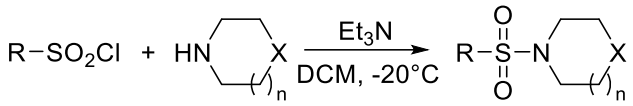
Zhichao Xionga, Chengfeng Peia, Peng Xue, Hui Lv and Xumu Zhang**

Table of contents

1. General Information

Unless otherwise noted, all reagents and solvents were purchased from commercial suppliers and used without further purification. NMR spectra were recorded on Bruker ADVANCE III (400 MHz) spectrometers for ^{1}H NMR and ^{13}C NMR. $CDCl_3$ was the solvent used for the NMR analysis, with tetramethylsilane as the internal standard. Chemical shifts were reported upfield to TMS (0.00 ppm) for ^{1}H NMR and relative to $CDCl_3$ (77.3 ppm) for ^{13}C NMR. Optical rotation was determined using a Perkin Elmer 343 polarimeter. HPLC analysis was conducted on an Agilent 1260 Series instrument. Column Chromatography was performed with silica gel Merck 60 (300-400 mesh). All new products were further characterized by HRMS. A positive ion mass spectrum of sample was acquired on a Thermo LTQ-FT mass spectrometer with an electrospray ionization source.

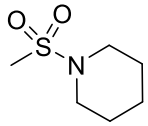
2. General procedure for the synthesis of α-Substituted β-keto Sulfonamides



I II III

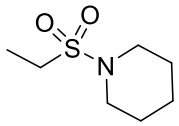
Preparation of III according to the literature [1]:

To a solution of amine (I, 10 mmol) dissolved in 20 mL of CH_2Cl_2 was added triethyl amine (1.01g, 10 mmol) at -20 °C. Then sulfonyl chloride (II, 15 mmol) was added slowly at -20 °C. After stirring for 6 h from -20 °C to room temperature, aqueous NH_4Cl solution (3 mL) was added to reaction mixture. The solution was extracted with CH_2Cl_2 (3×10 mL) and the combined organic phase was washed with H_2O (3×10 mL) and brine and dried over Na_2SO_4, filtered and concentrated under vacuum. The residue was purified by chromatography on silica gel using hexanes-ethyl acetate (10:1) as eluant to give the sulfonamide (III).



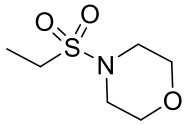
1-(methylsulfonyl) piperidine:

White solid, 2.6g, 75% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.28 – 3.11 (m, 4H), 2.77 (s, 3H), 1.74 – 1.66 (m, 4H), 1.63 – 1.52 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 46.77, 34.31, 25.35, 23.68; ESI-HRMS Calculated for $C_6H_{14}NO_2S^+$ ($[M+H]^+$): 164.0740, found: 164.0737.



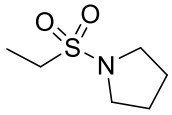
1-(ethylsulfonyl) piperidine:

Colorless oil, 7.6g, 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.18 (m, 4H), 2.94 – 2.82 (q, 2H), 1.65 – 1.45 (m, 6H), 1.36 – 1.24 (t, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 46.67, 43.65, 25.73, 23.82, 7.84; ESI-HRMS Calculated for $C_7H_{16}NO_2S^+$ ($[M+H]^+$): 178.0896, found: 178.0898.



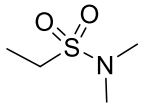
4-(ethylsulfonyl) morpholine

White solid, 1.4g, 70% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.86 – 3.68 (m, 4H), 3.29 (m, 4H), 2.97 (q, J = 7.4 Hz, 2H), 1.40 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 66.67, 45.88, 43.46, 7.73; ESI-HRMS Calculated for $C_6H_{14}NO_3S^+$ ($[M+H]^+$): 180.0689, found: 180.0692.



1-(ethylsulfonyl) pyrrolidine:

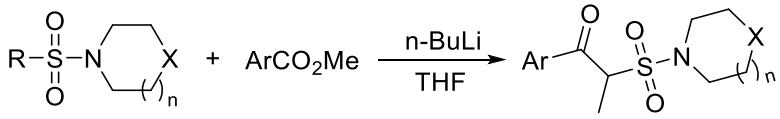
Colorless oil, 1.8g, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.37 (m, 4H), 3.02 (q, J = 7.4 Hz, 2H), 2.00 – 1.89 (m, 4H), 1.38 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 47.77, 44.04, 25.92, 8.00; ESI-HRMS Calculated for $C_6H_{14}NO_2S^+$ ($[M+H]^+$): 164.0740, found: 164.0735.



N, N-dimethylethanesulfonamide

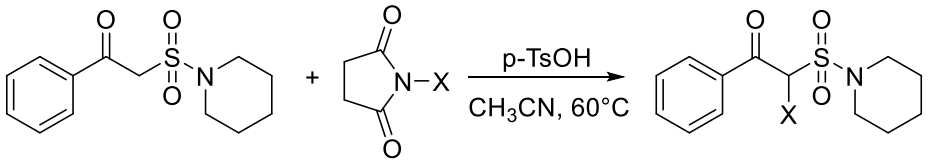
Colorless oil, 1.5g, 76% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.95 (q, J = 7.4 Hz, 2H), 2.87 (s, 6H), 1.34 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 42.84, 37.57, 7.82.

*Preparation of V (**1a-1o**):*



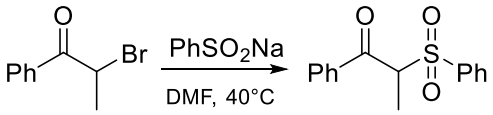
A solution of sulfamide (10 mmol) in 20 ml of dry tetrahydrofuran at -78 °C was treated dropwise with 11 mmol n-BuLi (2.5 M) in hexanes. The reaction mixture was stirred in an ice bath for 1 h and then cooled again to -78 °C. Then 12 mmol benzoate was added dropwise and stirred at room temperature for 16h. The mixture was concentrated and the residue was treated with 1N HCl (until pH~3), diluted with 10 ml water, and extracted with ethyl acetate. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated under vacuum. The residue was purified by

chromatography on silica gel using hexanes-ethyl acetate (8:1) as eluant to give the target compound.[2]



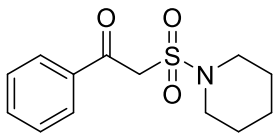
VI VII (X=Br, Cl) VIII

Intermediate VI (1 eq.), VII (1.1 eq.) and p-TsOH (0.1 eq.) were dissolved in anhydrate CH_3CN and stirred at 60 °C for 6 h. After the reaction was completed (monitored by TLC), 20 mL H_2O was added. The solution was extracted with ethyl acetate (3×10 mL) and the combined organic phase was washed with H_2O (3×10 mL) and brine and dried over Na_2SO_4, filtered and concentrated under vacuum. The residue was purified by chromatography on silica gel using hexanes-ethyl acetate (5:1) as eluant to give the product.

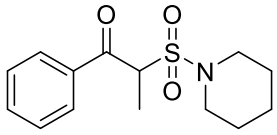


IX **2l**

2-bromo-1-phenylpropan-1-one (1 eq.) and $PhSO_2Na$ (1.2 eq.) were dissolved in DMF and heated at 40 °C. When TLC showed the reaction was completed, H_2O and ethyl acetate were added and the reaction mixture was washed with H_2O for three times and brine for one time. The organic layer was dried over Na_2SO_4, filtered and concentrated under vacuum. The residue was purified by chromatography on silica gel using hexanes-ethyl acetate (10:1) as eluant to give the product.[3]

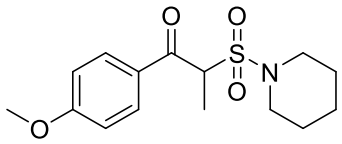


1-phenyl-2-(piperidin-1-ylsulfonyl) ethan-1-one:
White solid, 3.2g, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.00 (m, 2H), 7.68 – 7.60 (m, 1H), 7.51 (dd, J = 10.6, 4.8 Hz, 2H), 4.55 (s, 2H), 3.39 – 3.22 (m, 4H), 1.60 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.50, 135.87, 134.35, 129.49, 128.89, 57.36, 47.10, 25.66, 23.67; ESI-HRMS Calculated for $C_{13}H_{18}NO_3S^+$ ($[M+H]^+$): 268.1002, found: 268.1006.



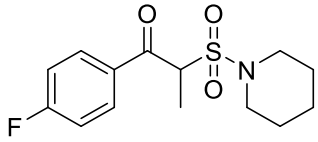
1-phenyl-2-(piperidin-1-ylsulfonyl) propan-1-one (1a)

White solid, 2.5g, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 – 7.99 (m, 2H), 7.68 – 7.57 (m, 1H), 7.55 – 7.46 (m, 2H), 5.13 (q, J = 6.9 Hz, 1H), 3.26 (m, J = 12.4 Hz, 4H), 1.65 (d, J = 6.9 Hz, 3H), 1.55 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.47, 136.21, 134.03, 129.17, 128.82, 62.82, 47.94, 26.12, 23.77, 13.42; ESI-HRMS Calculated for $C_{14}H_{20}NO_3S^+$ ($[M+H]^+$): 282.1158, found: 282.1153.



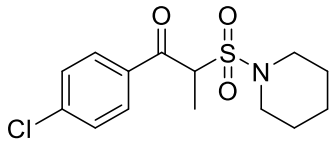
1-(4-methoxyphenyl)-2-(piperidin-1-ylsulfonyl) propan-1-one (1b)

White solid, 0.48g, 72% yield; ^{1}H NMR (400 MHz, CDCl3) δ 8.30 – 7.88 (m, 2H), 7.17 – 6.77 (m, 2H), 5.07 (q, *J* = 6.9 Hz, 1H), 3.89 (s, 3H), 3.28 (m, 4H), 1.63 (d, *J* = 6.9 Hz, 3H), 1.55 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.60, 164.30, 131.71, 129.20, 114.01, 62.74, 55.63, 47.97, 26.15, 23.81, 13.45. ESI-HRMS Calculated for $C_{15}H_{22}NO_4S^+$ ($[M+H]^+$): 312.1264, found: 312.1267.



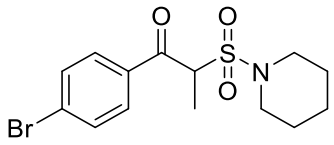
1-(4-fluorophenyl)-2-(piperidin-1-ylsulfonyl) propan-1-one (1c)

White solid, 0.41g, 71% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 – 8.03 (m, 2H), 7.18 (t, *J* = 8.6 Hz, 2H), 5.08 (q, *J* = 6.9 Hz, 1H), 3.28 (m, 4H), 1.64 (d, *J* = 6.9 Hz, 3H), 1.57 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.89, 167.55, 165.00, 132.65, 132.62, 132.11, 132.02, 116.10, 115.89, 63.05, 48.03, 26.14, 23.76, 13.32; ESI-HRMS Calculated for $C_{14}H_{19}FNO_3S^+$ ($[M+H]^+$): 300.1064, found: 300.1059.



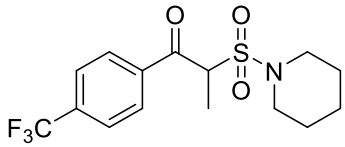
1-(4-chlorophenyl)-2-(piperidin-1-ylsulfonyl) propan-1-one (1d)

White solid, 0.45g, 75% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.6 Hz, 2H), 7.48 (d, *J* = 8.6 Hz, 2H), 5.06 (q, *J* = 6.9 Hz, 1H), 3.29 (m, 4H), 1.64 (d, *J* = 6.9 Hz, 3H), 1.57 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.35, 140.70, 140.43, 134.51, 130.66, 129.14, 63.13, 48.06, 26.14, 23.76, 13.28; ESI-HRMS Calculated for $C_{14}H_{19}ClNO_3S^+$ ($[M+H]^+$): 316.0769, found: 316.0766.



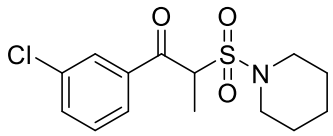
1-(4-bromophenyl)-2-(piperidin-1-ylsulfonyl) propan-1-one (1e)

White solid, 0.4g, 72% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.6 Hz, 2H), 7.48 (d, *J* = 8.6 Hz, 2H), 5.06 (q, *J* = 6.9 Hz, 1H), 3.29 (m, 4H), 1.64 (d, *J* = 6.9 Hz, 3H), 1.57 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.57, 134.92, 132.14, 130.71, 129.54, 63.12, 48.06, 26.14, 23.76, 13.27; ESI-HRMS Calculated for $C_{14}H_{19}BrNO_3S^+$ ($[M+H]^+$): 360.0264, found: 360.0259.



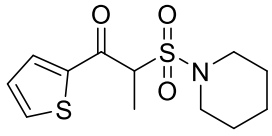
2-(piperidin-1-ylsulfonyl)-1-(4-(trifluoromethyl) phenyl) propan-1-one (1f)

White solid, 0.43g, 76% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (dd, *J* = 8.9, 5.3 Hz, 2H), 7.18 (t, *J* = 8.6 Hz, 2H), 5.07 (q, *J* = 6.9 Hz, 1H), 3.27 (m, 4H), 1.64 (d, *J* = 6.9 Hz, 3H), 1.57 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.89, 167.56, 165.00, 132.65, 132.62, 132.11, 132.02, 116.11, 115.89, 77.39, 77.07, 76.75, 63.07, 48.03, 26.14, 23.76, 13.32; ESI-HRMS Calculated for $C_{15}H_{19}F_3NO_3S^+$ ($[M+H]^+$): 350.1032, found: 350.1026.



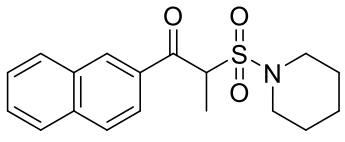
1-(3-chlorophenyl)-2-(piperidin-1-ylsulfonyl) propan-1-one (1g)

White solid, 0.4g, 72% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.56 (m, 1H), 7.47 – 7.40 (m, 2H), 7.37 (ddd, *J* = 7.6, 6.0, 2.7 Hz, 1H), 5.02 (q, *J* = 6.9 Hz, 1H), 3.33 (m, 4H), 1.68 (d, *J* = 6.9 Hz, 3H), 1.58 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.63, 138.82, 132.50, 130.76, 130.39, 130.31, 127.21, 66.49, 47.84, 26.12, 23.77; ESI-HRMS Calculated for $C_{14}H_{19}ClNO_3S^+$ ($[M+H]^+$): 316.0769, found: 316.0764.



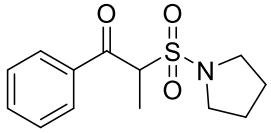
2-(piperidin-1-ylsulfonyl)-1-(thiophen-2-yl) propan-1-one (1h)

White solid, 0.38g, 70%yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 3.9, 1.0 Hz, 1H), 7.76 (dd, *J* = 4.9, 1.1 Hz, 1H), 7.19 (dd, *J* = 4.9, 3.9 Hz, 1H), 4.88 (q, *J* = 7.0 Hz, 1H), 3.30 (m, 4H), 1.66 (d, *J* = 7.0 Hz, 3H), 1.56 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 185.70, 143.55, 135.93, 134.49, 128.71, 64.86, 47.96, 26.12, 23.76, 13.31; ESI-HRMS Calculated for $C_{12}H_{18}NO_3S_2^+$ ($[M+H]^+$): 288.0723, found: 288.0717.



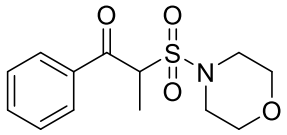
1-(naphthalen-2-yl)-2-(piperidin-1-ylsulfonyl) propan-1-one (1i)

White solid, 0.51g, 76% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (s, 1H), 8.11 – 7.97 (m, 2H), 7.91 (dd, *J* = 14.7, 8.4 Hz, 2H), 7.69 – 7.54 (m, 2H), 5.30 (q, *J* = 6.9 Hz, 1H), 3.29 (m, 4H), 1.71 (d, *J* = 6.9 Hz, 3H), 1.55 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.40, 193.38, 137.64, 135.94, 134.63, 133.51, 132.41, 131.66, 131.61, 130.01, 129.73, 129.19, 128.88, 128.76, 127.80, 127.07, 127.03, 124.20, 121.53, 63.09, 48.04, 26.16, 23.79, 13.57; ESI-HRMS Calculated for $C_{18}H_{22}NO_3S^+$ ($[M+H]^+$): 332.1315, found: 332.1308.



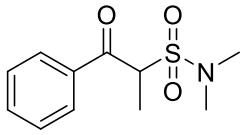
1-phenyl-2-(pyrrolidin-1-ylsulfonyl) propan-1-one (1j)

White solid, 0.48g, 74% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.01 (m, 2H), 7.67 – 7.60 (m, 1H), 7.55 – 7.48 (m, 2H), 5.17 (q, *J* = 6.9 Hz, 1H), 3.42 – 3.33 (m, 4H), 1.87 – 1.78 (m, 4H), 1.70 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.61, 136.29, 134.02, 129.07, 128.85, 63.02, 48.90, 47.77, 44.08, 25.93, 25.73, 13.52, 8.01; ESI-HRMS Calculated for $C_{13}H_{18}NO_3S^+$ ($[M+H]^+$): 268.1002, found: 268.1006.



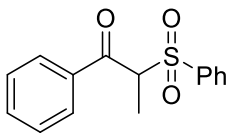
2-(morpholinosulfonyl)-1-phenylpropan-1-one (1k)

White solid, 0.48g, 744%yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.00 (m, 2H), 7.68 – 7.60 (m, 1H), 7.57 – 7.48 (m, 2H), 5.16 (q, *J* = 6.9 Hz, 1H), 3.73 – 3.61 (m, 4H), 3.44 – 3.27 (m, 4H), 1.67 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.28, 135.97, 134.29, 129.14, 128.95, 66.97, 62.90, 47.14, 13.52; ESI-HRMS Calculated for $C_{13}H_{18}NO_4S^+$ ($[M+H]^+$): 284.0951, found: 284.0956.



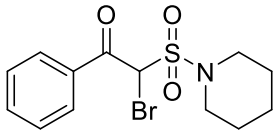
N, N-dimethyl-1-oxo-1-phenylpropane-2-sulfonamide (1l)

White solid, 0.45g, 87% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.01 (m, 2H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 2H), 5.17 (q, *J* = 7.0 Hz, 1H), 2.89 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.54, 136.13, 134.12, 129.13, 128.87, 62.92, 38.52, 13.62; ESI-HRMS Calculated for $C_{11}H_{16}NO_3S^+$ ($[M+H]^+$): 242.0845, found: 242.0847.



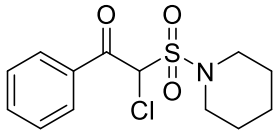
1-phenyl-2-(phenylsulfonyl) propan-1-one (1m)

White solid, 0.39g, 93% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.93 (m, 2H), 7.84 – 7.76 (m, 2H), 7.63 (dt, *J* = 16.1, 7.4 Hz, 2H), 7.50 (dt, *J* = 17.3, 7.8 Hz, 4H), 5.18 (q, *J* = 6.9 Hz, 1H), 1.58 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.50, 136.16, 135.97, 134.29, 134.16, 129.85, 129.19, 128.93, 128.81, 64.92, 13.23. ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.50, 136.16, 135.97, 134.29, 134.16, 129.85, 129.19, 128.93, 128.81, 64.92, 13.23.



2-bromo-1-phenyl-2-(piperidin-1-ylsulfonyl) ethan-1-one (1n)

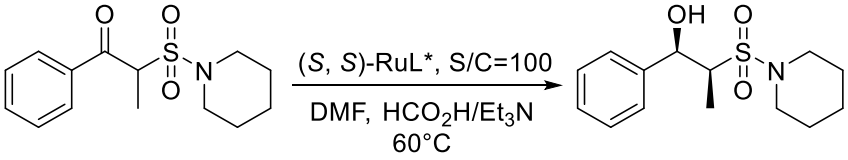
White solid, 0.54g, 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.6 Hz, 2H), 7.48 (d, *J* = 8.6 Hz, 2H), 5.06 (q, *J* = 6.9 Hz, 1H), 3.29 (m, 4H), 1.64 (d, *J* = 6.9 Hz, 3H), 1.57 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 187.66, 134.66, 134.23, 129.52, 129.02, 58.22, 48.99, 26.12, 23.66; ESI-HRMS Calculated for $C_{13}H_{17}BrNO_3S^+$ ($[M+H]^+$): 346.0107, found: 346.0103



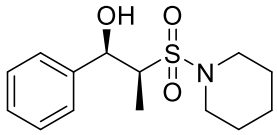
2-chloro-1-phenyl-2-(piperidin-1-ylsulfonyl) ethan-1-one (1o)

White solid, 0.3g, 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.6 Hz, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.7 Hz, 2H), 6.23 (s, 1H), 3.46 (m, 4H), 1.62 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 187.38, 134.72, 134.51, 129.62, 128.96, 70.34, 48.77, 26.07, 23.64; ESI-HRMS Calculated for $C_{13}H_{17}ClNO_3S^+$ ($[M+H]^+$): 302.0612, found: 302.0609.

General procedure of the asymmetric hydrogen transfer reduction

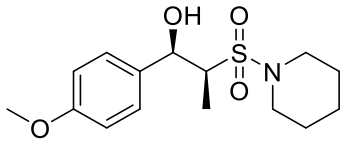


A suspension of β-keto sulfamide (0.16 mmol), (*S*, *S*)-RuL*(0.0016 mmol), 5:2 HCO_2H/Et_3N (0.2 mL) in anhydrous DMF (1 mL) were stirred under N_2 at 60 °C for 12 h until completion according to TLC detection. 5.0 mL water was added to the reaction, the mixture was then extracted with ethyl acetate (3×5mL) threetimes, dried over Na_2SO_4 and concentrated. The desired product was purified by silica gel chromatography (hexanes: ethyl acetate = 1:3). The enantioselectivity of the products was determined by HPLC analysis. The racemic samples of diastereomeric mixtures of 2a-2p for HPLC analysis were prepared following literature procedures.



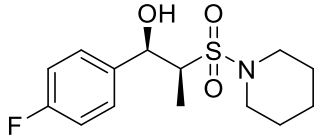
(1*R*, 2*S*)-1-phenyl-2-(piperidin-1-ylsulfonyl) propan-1-ol (2a)

White solid, 21.8mg, 96% yield, 99% ee, dr= 20:1; $[\alpha]_D^{20}$ = 11.6 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95: 5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 22.26 min (minor), 31.65 min (major), 33.04 min (minor), 37.21 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.33 (m, 4H), 7.28 (m, *J* = 3.0, 2.0 Hz, 1H), 5.46 (s, 1H), 3.38 – 3.33 (m, 4H), 3.31 (d, *J* = 1.8 Hz, 1H), 3.18 (qd, *J* = 7.1, 1.4 Hz, 1H), 1.67 – 1.61 (m, 6H), 1.19 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.22, 128.46, 127.68, 125.65, 70.65, 63.07, 47.06, 46.69, 43.70, 26.08, 25.75, 23.87, 23.85, 7.87, 6.81; ESI-HRMS Calculated for $C_{14}H_{22}NO_3S^+$ ($[M+H]^+$): 284.1315, found: 284.1311.



(1*R*, 2S)-1-(4-methoxyphenyl)-2-(piperidin-1-ylsulfonyl) propan-1-ol (2b)

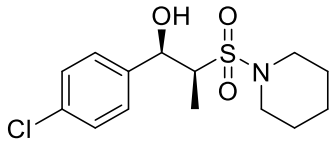
White solid, 23.8 mg, 95% yield, 98% ee, dr= 20:1; $[\alpha]_D^{20}$ = 6.8 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 21.31 min (minor), 27.08 min (major), 30.95 min (minor), 36.62 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (d, *J* = 8.6 Hz, 2H), 6.93 – 6.72 (m, 2H), 4.76 (d, *J* = 9.1 Hz, 1H), 4.37 (d, *J* = 1.0 Hz, 1H), 3.73 (s, 3H), 3.39 – 3.26 (m, 4H), 3.17 (tt, *J* = 9.0, 5.8 Hz, 1H), 1.69 – 1.46 (m, 6H), 0.85 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.62, 132.13, 128.28, 114.00, 73.67, 63.54, 55.32, 47.24, 26.09, 23.84, 12.82; ESI-HRMS Calculated for $C_{15}H_{24}NO_4S^+$ ($[M+H]^+$): 314.1421, found: 314.1425.



(1*R*, 2*S*)-1-(4-fluorophenyl)-2-(piperidin-1-ylsulfonyl) propan-1-ol (2c)

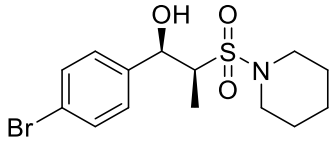
White solid, 23.1 mg, 95% yield, 99% ee, dr=20:1; $[\alpha]_D^{20}$ = 1.2 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 92: 8; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 17.07 min (minor), 20.75 min (major), 23.93 min (minor), 28.36 min (minor). ^{1}H NMR (400 MHz, CDCl3) δ 7.39 – 7.28 (m, 2H), 7.12 – 6.99 (m, 2H), 5.45 (s, 1H), 3.35 (m, J = 5.9, 4.2 Hz, 4H), 3.27 – 3.19 (m, 1H), 3.13 (qd, J = 7.1, 1.3 Hz, 1H), 1.67 – 1.61 (m, 6H), 1.17 (d, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, CDCl3) δ 162.34, 159.89, 134.85, 134.82, 126.32, 126.24, 114.41, 114.20, 69.14, 61.95, 46.03, 45.65, 42.68, 25.03, 24.71, 24.31,

22.80, 6.82, 5.70; ESI-HRMS Calculated for $C_{14}H_{21}FNO_3S^+$ ([M+H]$^+$): 302.1221, found: 302.1216.



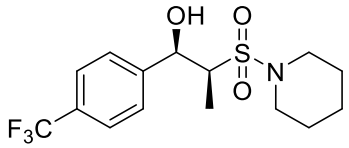
(1*R*, 2*S*)-1-(4-chlorophenyl)-2-(piperidin-1-ylsulfonyl) propan-1-ol (2d)

White solid, 24.2 mg, 95% yield, 98% ee, dr=20:1; $[\alpha]_D^{20}$ = 8.1 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 15.29 min (minor), 17.93 min (major), 21.69 min (minor), 27.00 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.21 (m, 4H), 5.38 (s, 1H), 3.35 – 3.28 (m, 4H), 3.28 (m, 1H), 3.06 (qd, *J* = 7.1, 1.3 Hz, 1H), 1.65 – 1.56 (m, 6H), 1.11 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.60, 132.38, 127.59, 126.04, 69.15, 61.82, 46.04, 25.03, 22.80, 5.73; ESI-HRMS Calculated for $C_{14}H_{21}ClNO_3S^+$ ([M+H]$^+$): 318.0925, found: 318.0919.



(1*R*, 2*S*)-1-(4-bromophenyl)-2-(piperidin-1-ylsulfonyl) propan-1-ol (2e)

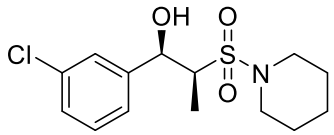
White solid, 27.2 mg, 94% yield, 99% ee, dr = 20:1; $[\alpha]_D^{20}$ = 9.5 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 16.54 min (minor), 19.40 min (major), 23.41 min (minor), 30.29 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 8.5 Hz, 2H), 7.17 (d, *J* = 8.3 Hz, 2H), 5.30 (d, *J* = 51.2 Hz, 1H), 3.29 (m, 4H), 3.28 (s, 1H), 3.06 (qd, *J* = 7.1, 1.3 Hz, 1H), 1.59 (dd, *J* = 9.8, 4.6 Hz, 6H), 1.10 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.23, 131.58, 127.44, 121.54, 70.24, 62.83, 47.09, 26.08, 25.37, 23.85, 6.79; ESI-HRMS Calculated for $C_{14}H_{21}BrNO_3S^+$ ([M+H]$^+$): 362.0420, found: 362.0414.



(1*R*, 2*S*)-2-(piperidin-1-ylsulfonyl)-1-(4-(trifluoromethyl) phenyl) propan-1-ol (2f)

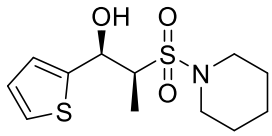
White solid, 27.2 mg, 96% yield, 99% ee, dr=20:1; $[\alpha]_D^{20}$ = 9.7 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95: 5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 23.43 min (minor), 26.43 min (major), 33.70 min (minor), 46.38 min (minor). ^{1}H NMR (400 MHz, CDCl3) δ 7.56 (d, J = 8.2 Hz, 2H), 7.42 (d, J = 8.5 Hz, 2H), 5.46 (s, 1H), 3.38 (d, J = 1.7 Hz, 1H), 3.34 – 3.25 (m, 4H), 3.11 (qd, J = 7.1, 1.3 Hz, 1H), 1.64 – 1.55 (m, 6H), 1.10 (d, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, CDCl3) δ 144.24, 130.08, 129.76, 126.11,

125.48, 125.45, 125.41, 125.37, 122.69, 77.38, 77.27, 77.07, 76.75, 70.34, 62.78, 47.12, 46.70, 26.07, 25.75, 25.35, 23.83, 6.84; ESI-HRMS Calculated for $C_{15}H_{21}F_3NO_3S^+$ ($[M+H]^+$): 352.1189, found: 352.1183.



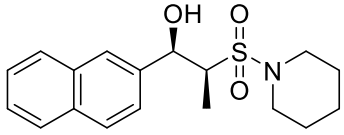
(1*R*, 2*S*)-1-(3-chlorophenyl)-2-(piperidin-1-ylsulfonyl) propan-1-ol (2g)

White solid, 24.2 mg, 95% yield, 99% ee, dr=20:1; $[\alpha]_D^{20}$ = 11.3 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak IB column, hexane: isopropanol = 97: 3; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 19.20 min (major), 23.29 min (minor), 26.76 min (minor), 32.71 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.22 (m, 4H), 5.38 (s, 1H), 3.33 – 3.28 (m, 4H), 3.28 (s, 1H), 3.06 (qd, *J* = 7.1, 1.3 Hz, 1H), 1.65 – 1.56 (m, 6H), 1.11 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.29, 134.51, 129.77, 127.88, 125.94, 123.84, 70.18, 62.82, 47.11, 26.08, 23.85, 6.84; ESI-HRMS Calculated for $C_{14}H_{21}ClNO_3S^+$ ($[M+H]^+$): 318.0925, found: 318.0921.



(1*S*, 2*S*)-2-(piperidin-1-ylsulfonyl)-1-(thiophen-2-yl) propan-1-ol (2h)

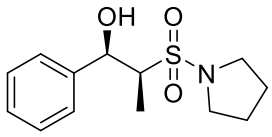
White solid, 21.5 mg, 93% yield, 99% ee, dr=20:1; $[\alpha]_D^{20}$ = 14.3 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak IB column, hexane: isopropanol = 95: 5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 14.82 min (major), 16.15 min (minor), 18.56 min (minor), 19.78 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (m, *J* = 1.2 Hz, 1H), 7.26 (d, *J* = 1.2 Hz, 1H), 7.05 – 6.93 (m, 2H), 5.71 (s, 1H), 3.38 (m, 4H), 3.35 (s, 1H), 3.28 (qd, *J* = 7.1, 1.4 Hz, 1H), 1.65 (m, 6H), 1.34 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.89, 126.88, 124.69, 123.43, 68.44, 63.17, 47.07, 26.06, 23.85, 7.46; ESI-HRMS Calculated for $C_{12}H_{20}NO_3S_2^+$ ($[M+H]^+$): 290.0879, found: 290.0873.



(1*R*, 2*S*)-1-(naphthalen-2-yl)-2-(piperidin-1-ylsulfonyl) propan-1-ol (2i)

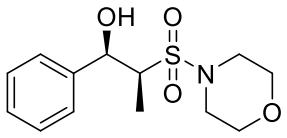
White solid, 25.1 mg, 94% yield, 99% ee, dr=20:1; $[\alpha]_D^{20}$ = 14.3 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak IB column, hexane: isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 14.20 min (major), 15.11 min (minor), 18.21 min (minor), 23.56 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.82 (m, 4H), 7.53 – 7.45 (m, 2H), 7.39 (dd, *J* = 8.5, 1.6 Hz, 1H), 5.65

(s, 1H), 3.43 (d, *J* = 1.7 Hz, 1H), 3.42 – 3.36 (m, 4H), 3.30 (tt, *J* = 7.1, 3.5 Hz, 1H), 1.74 – 1.64 (m, 6H), 1.22 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.50, 133.21, 132.86, 128.25, 128.07, 127.71, 126.39, 126.10, 124.69, 123.51, 70.80, 62.92, 47.13, 46.71, 26.11, 25.76, 23.89, 6.88; ESI-HRMS Calculated for $C_{18}H_{24}NO_3S^+$ ($[M+H]^+$): 334.1471, found: 334.1466.



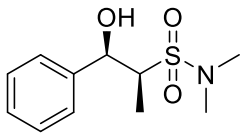
(1*R*, 2*S*)-1-phenyl-2-(pyrrolidin-1-ylsulfonyl) propan-1-ol (2j)

White solid, 20.6 mg, 95% yield, 99% ee, dr=20:1; $[\alpha]_D^{20}$ = 4.0 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak IB column, hexane: isopropanol = 95: 5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 16.08 min (major), 19.34 min (minor), 20.76 min (minor), 24.66 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 4.4 Hz, 4H), 7.33 – 7.26 (m, 1H), 5.50 (s, 1H), 3.53 – 3.43 (m, 4H), 3.39 (m, *J* = 1.2 Hz, 1H), 3.28 (qd, *J* = 7.1, 1.3 Hz, 1H), 2.01 – 1.96 (m, 4H), 1.24 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.21, 128.46, 127.68, 125.66, 70.63, 64.44, 63.14, 48.25, 26.08, 25.36, 6.72; ESI-HRMS Calculated for $C_{13}H_{20}NO_3S^+$ ($[M+H]^+$): 270.1158, found: 270.1163.



(1*R*, 2*S*)-2-(morpholinosulfonyl)-1-phenylpropan-1-ol (2k)

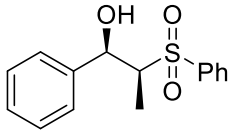
White solid, 19.9 mg, 96% yield, 99% ee, dr=20:1; $[\alpha]_D^{20}$ = 2.8 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak IB column, hexane: isopropanol = 95: 5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 27.81 min (major), 31.88 min (minor), 34.27 min (minor), 39.55 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.22 (m, 5H), 5.43 (s, 1H), 3.70 (t, *J* = 4.7 Hz, 4H), 3.35 (m, 4H), 3.15 (m, *J* = 7.0, 3.5 Hz, 1H), 3.05 (s, 1H), 1.14 (d, *J* = 6.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.03, 128.56, 127.88, 125.64, 70.68, 66.98, 63.57, 46.31, 25.37, 6.91; ESI-HRMS Calculated for $C_{13}H_{20}NO_4S^+$ ($[M+H]^+$): 286.1108, found: 286.1111.



(1*R*, 2*S*)-1-hydroxy-N, N-dimethyl-1-phenylpropane-2-sulfonamide (2l)

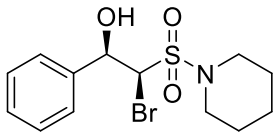
White solid, 19.0 mg, 97% yield, 99% ee, dr=20:1; $[\alpha]_D^{20}$ = 3.3 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak IB column, hexane: isopropanol = 95: 5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 17.18 min (major), 21.09 min (minor), 23.06 min (minor), 28.65 min (minor). ^{1}H NMR (400 MHz,

$CDCl_3$) δ 7.38 (d, *J* = 4.4 Hz, 4H), 7.30 (dd, *J* = 8.8, 4.5 Hz, 1H), 5.49 (s, 1H), 3.28 (qd, *J* = 7.1, 1.1 Hz, 1H), 3.24 (d, *J* = 1.7 Hz, 1H), 2.99 (d, *J* = 5.6 Hz, 6H), 1.21 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.06, 128.50, 127.76, 125.68, 70.69, 62.86, 37.82, 6.85; ESI-HRMS Calculated for $C_{11}H_{16}NO_3S^+$ ($[M+H]^+$): 242.0845, found: 242.0841.



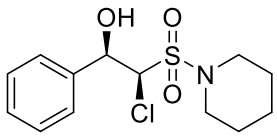
(1*R*, 2*S*)-1-phenyl-2-(phenylsulfonyl)propan-1-ol (2m)

White solid, 21.1 mg, 95% yield, 99% ee, dr=20:1; $[\alpha]_D^{20}$ = -11.5 (c = 1.00, acetone); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 18.19 min (minor), 25.32 min (major), 31.53 min (minor), 34.37 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 – 7.90 (m, 2H), 7.73 (t, *J* = 7.4 Hz, 1H), 7.64 (t, *J* = 7.6 Hz, 2H), 7.34 (dd, *J* = 10.4, 4.4 Hz, 2H), 7.28 (s, 3H), 5.54 (s, 1H), 3.31 (d, *J* = 1.9 Hz, 1H), 3.23 (qd, *J* = 7.1, 1.1 Hz, 1H), 1.22 (d, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 139.81, 137.29, 134.18, 129.45, 128.76, 128.49, 127.80, 125.57, 69.24, 65.66, 64.48, 25.38, 5.80.



(1*R*, 2*S*)-2-bromo-1-phenyl-2-(piperidin-1-ylsulfonyl) ethan-1-ol (2n)

White solid, 25.2 mg, 90% yield, 99% ee, dr=10:1; $[\alpha]_D^{20}$ = -28.2 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 90: 10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 23.11 min (major), 24.45 min (minor), 26.74 min (minor), 28.73 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.32 (m, 5H), 5.31 (m, 1H), 3.69 (s, 1H), 3.26 (m, 4H), 3.12 (dd, *J* = 14.0, 2.0 Hz, 1H), 1.65 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.09, 128.84, 128.46, 128.33, 126.11, 125.68, 68.80, 57.07, 46.63, 25.56, 23.69; ESI-HRMS Calculated for $C_{13}H_{19}BrNO_3S^+$ ($[M+H]^+$): 348.0264, found: 348.0267.

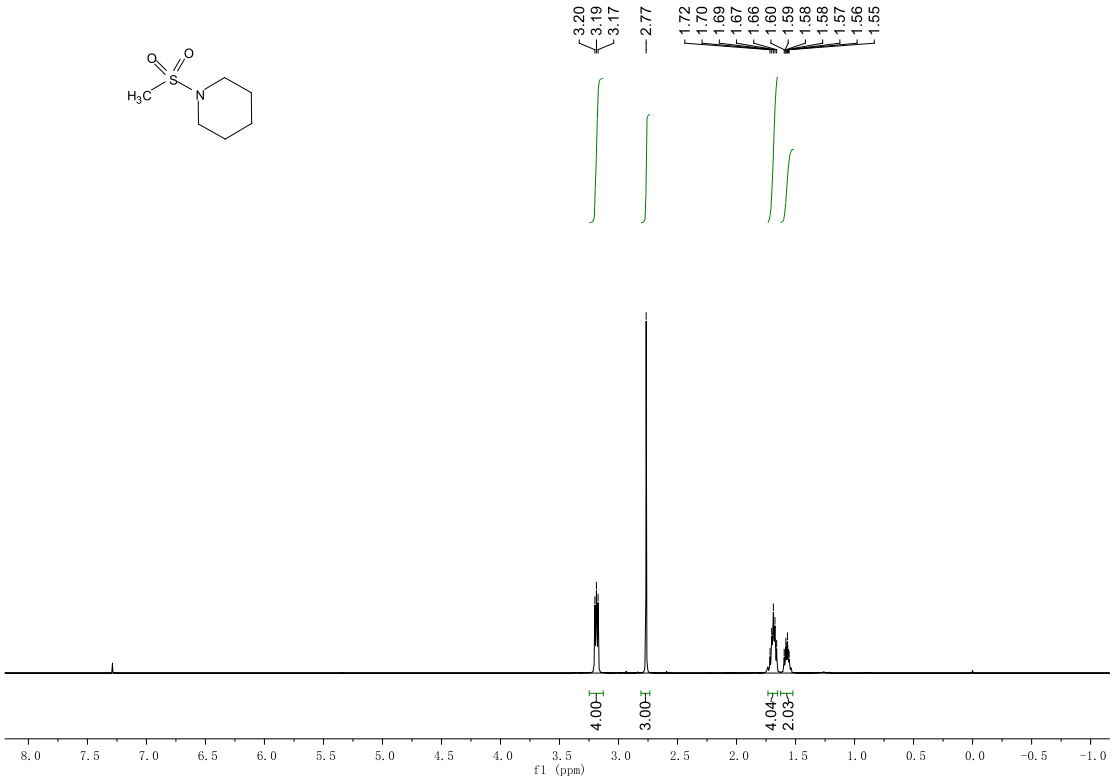


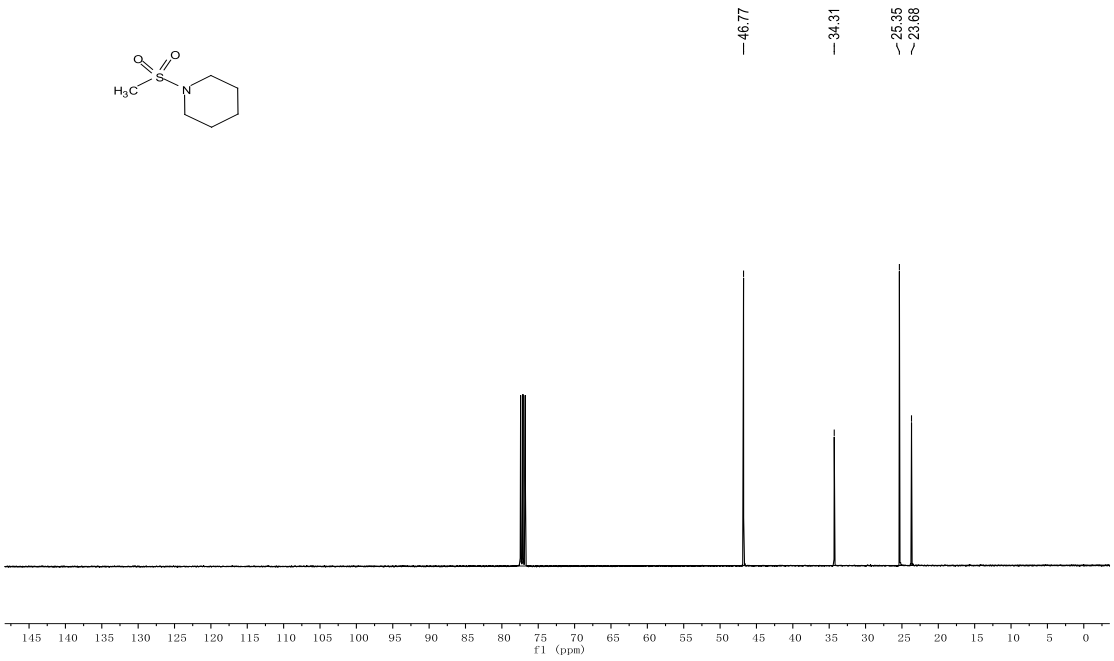
(1*R*, 2*S*)-2-chloro-1-phenyl-2-(piperidin-1-ylsulfonyl) ethan-1-ol (2o)

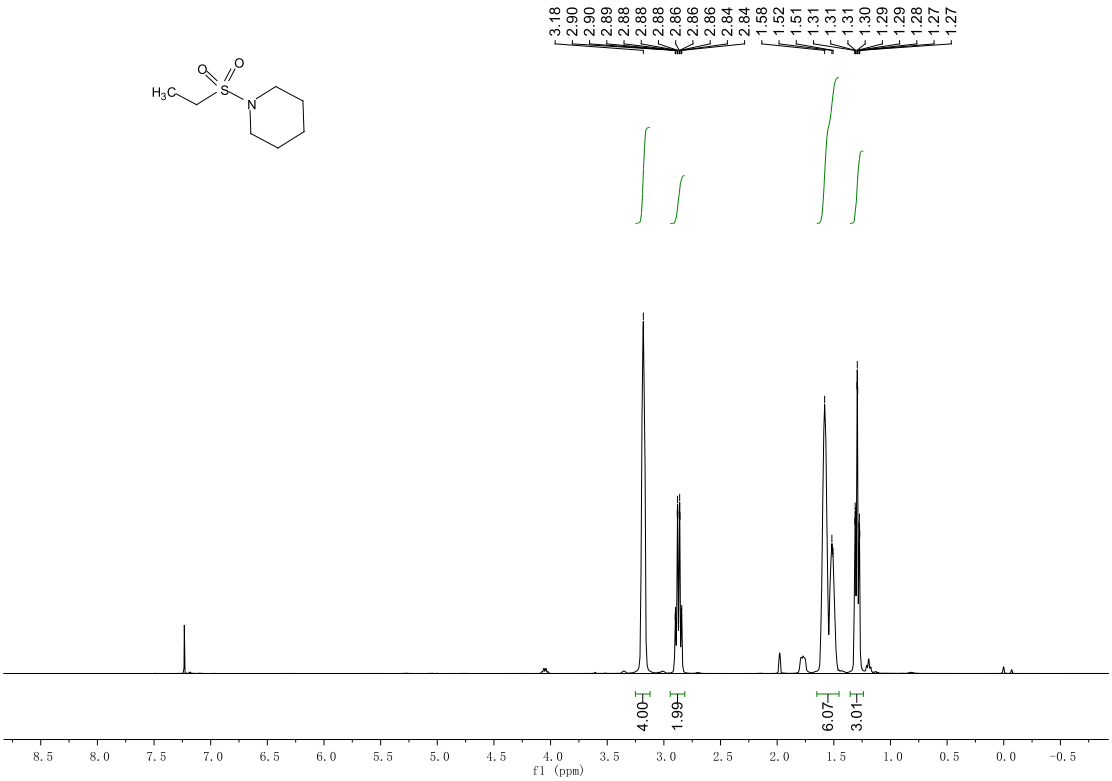
White solid, 22.3 mg, 92% yield, 99% ee, dr=20:1; $[\alpha]_D^{20}$ = 6.4 (c = 1.00, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak IA column, hexane: isopropanol = 95: 5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 24.88 min (minor), 30.27 min (major), 37.74 min (minor), 46.31 min (minor). ^{1}H NMR (400 MHz,

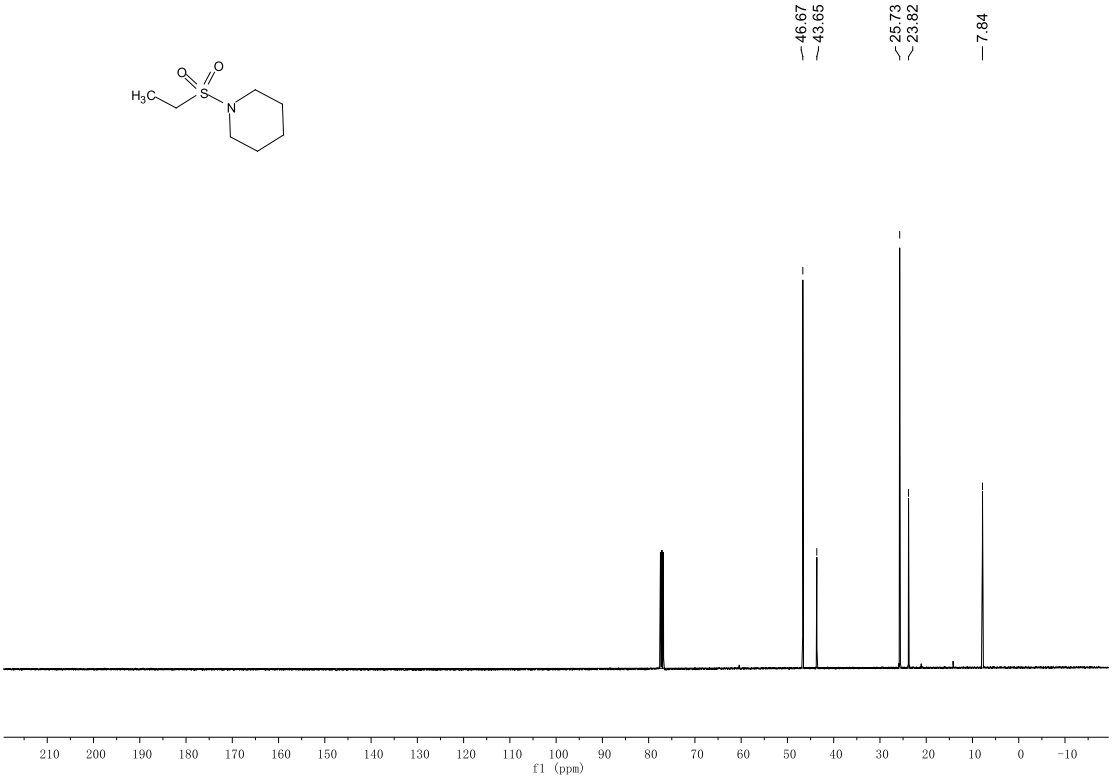
$CDCl_3$) δ 7.47 – 7.32 (m, 5H), 5.65 (s, 1H), 4.80 (d, J = 1.2 Hz, 1H), 3.56 – 3.41 (m, 4H), 3.39 (s, 1H), 1.71 – 1.60 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.29, 128.50, 126.26, 71.16, 47.88, 25.90, 23.67. ESI-HRMS Calculated for $C_{13}H_{19}ClNO_3S^+$ ($[M+H]^+$): 304.0769, found: 304.0772.

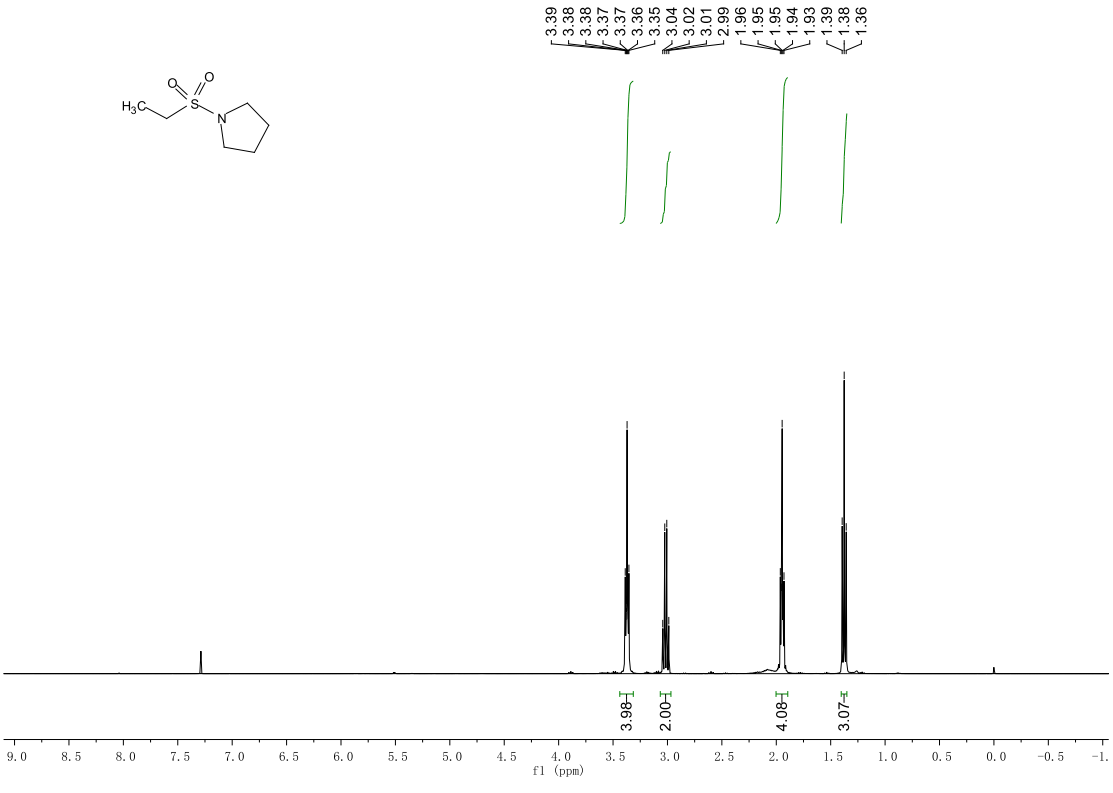
3. NMR spectra

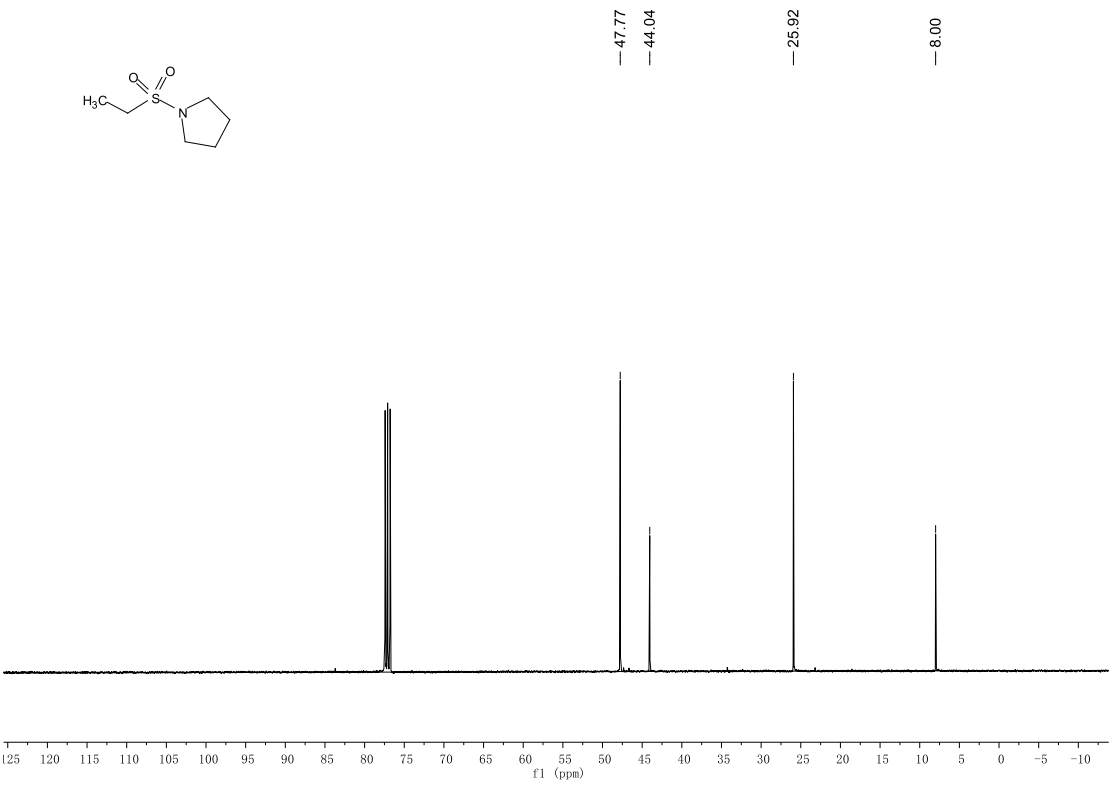


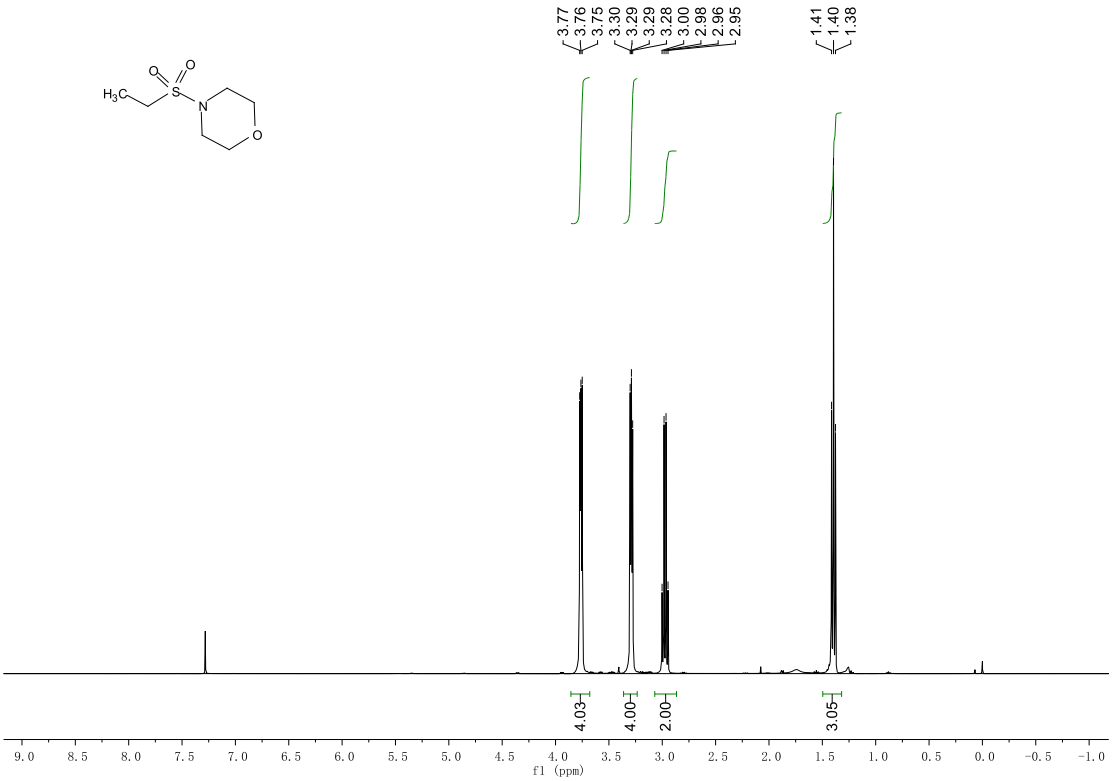


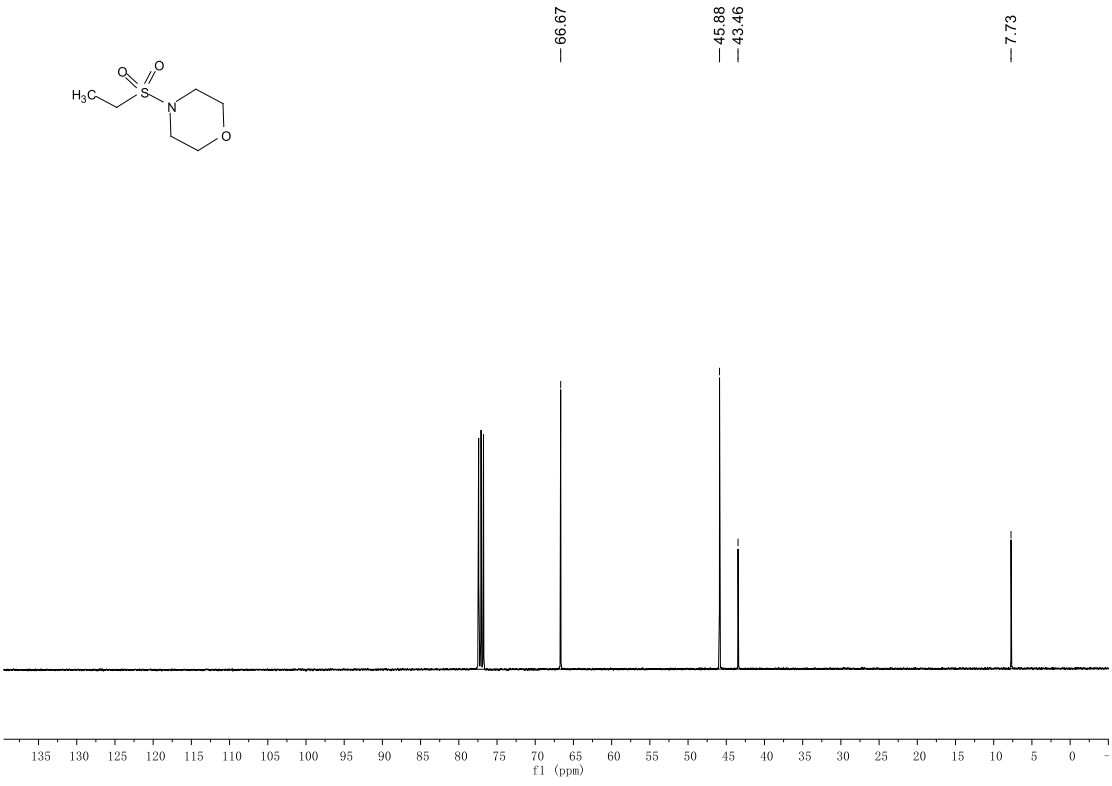

3.18
2.90
2.90
2.89
2.88
2.88
2.88
2.86
2.86
2.86
2.84
2.84
1.58
1.52
1.51
1.31
1.31
1.30
1.29
1.29
1.28
1.27
1.27
4.00
1.99
6.07
3.01
f1 (ppm)

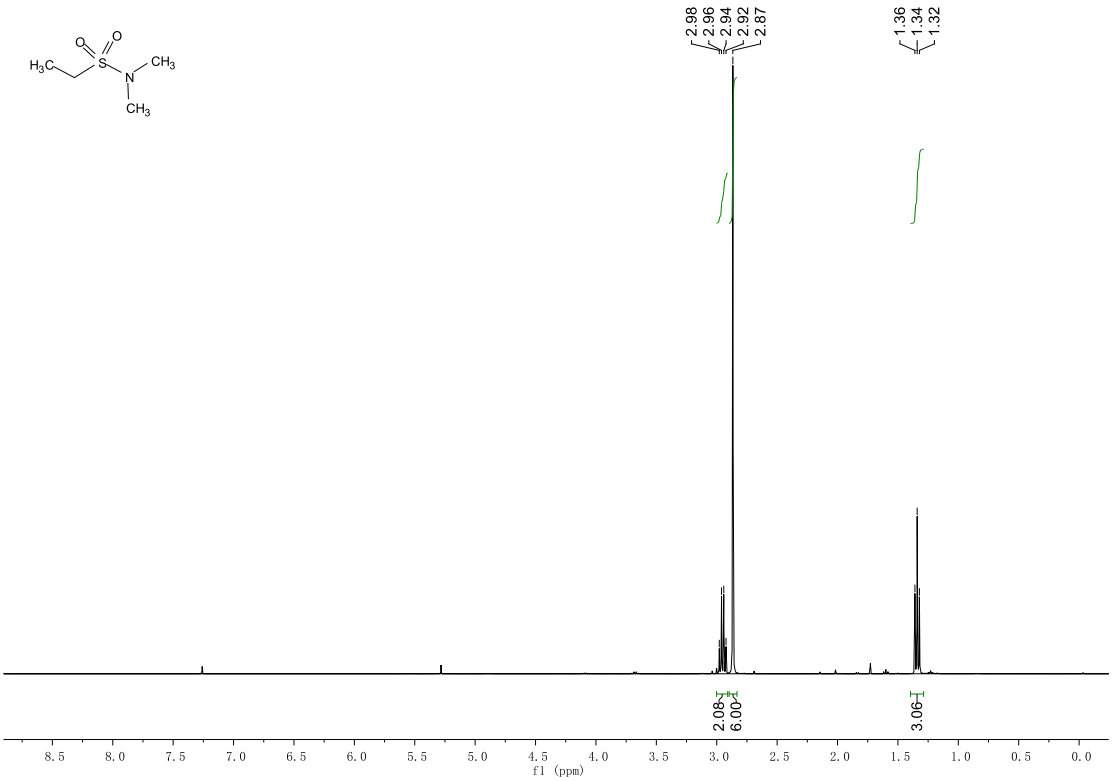

46.67
43.65
25.73
23.82
7.84
f1 (ppm)

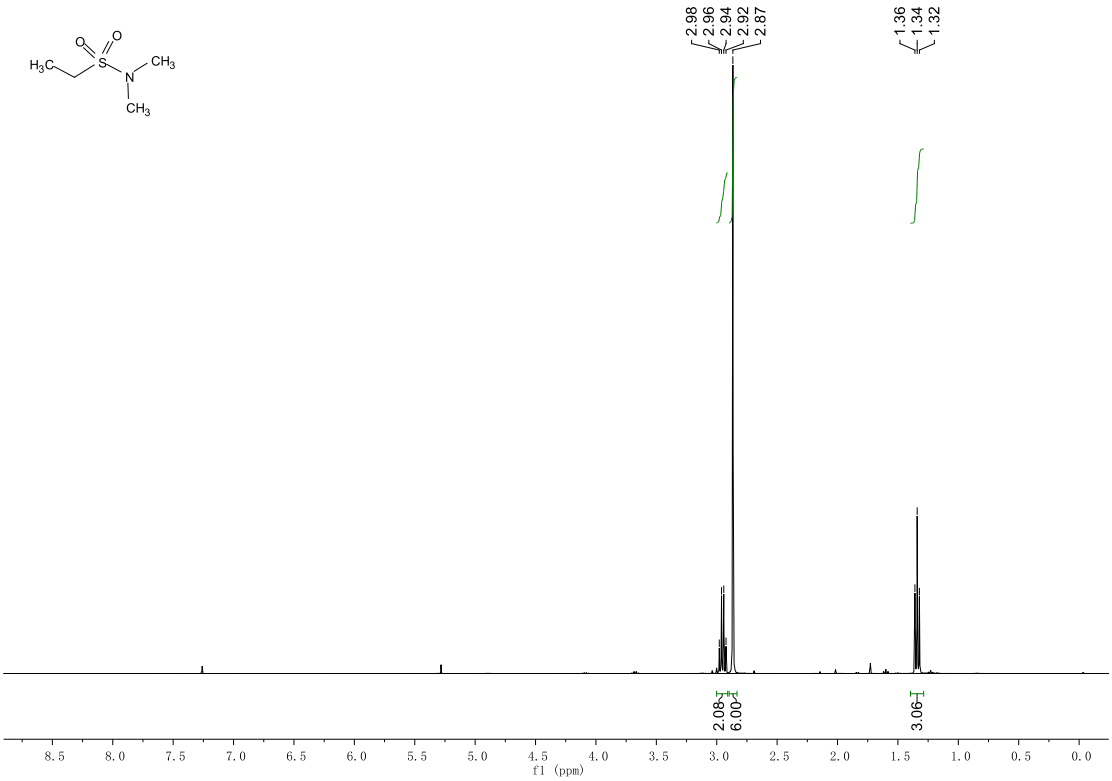

3.39
3.38
3.38
3.37
3.37
3.36
3.35
3.04
3.02
3.01
2.99
1.96
1.95
1.95
1.94
1.93
1.39
1.38
1.36
3.98
2.00
4.08
3.07
f1 (ppm)

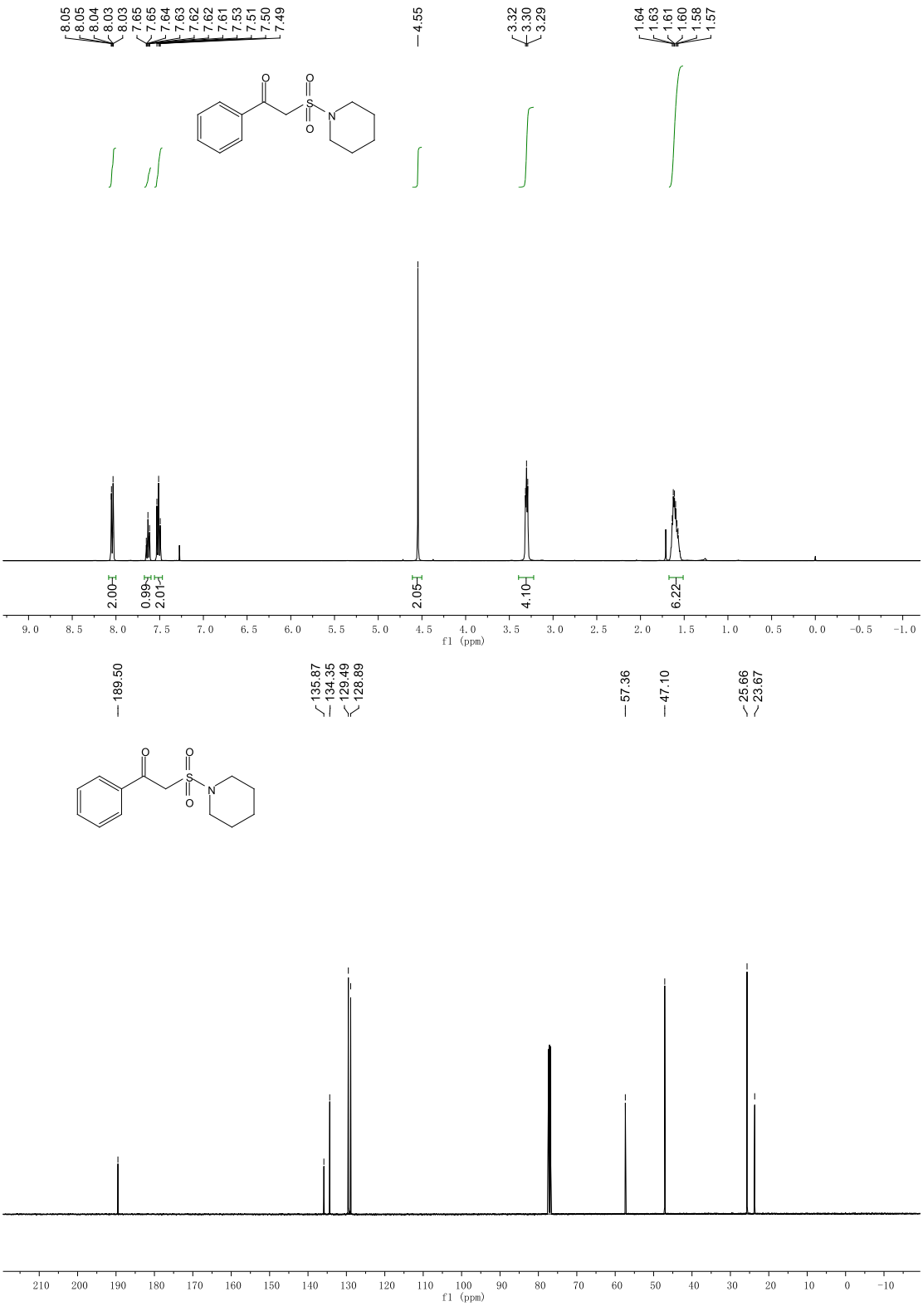

47.77
44.04
25.92
8.00
f1 (ppm)


3.77
3.76
3.75
3.30
3.29
3.29
3.28
3.00
2.98
2.96
2.95
1.41
1.40
1.38
4.03
4.00
2.00
3.05
f1 (ppm)

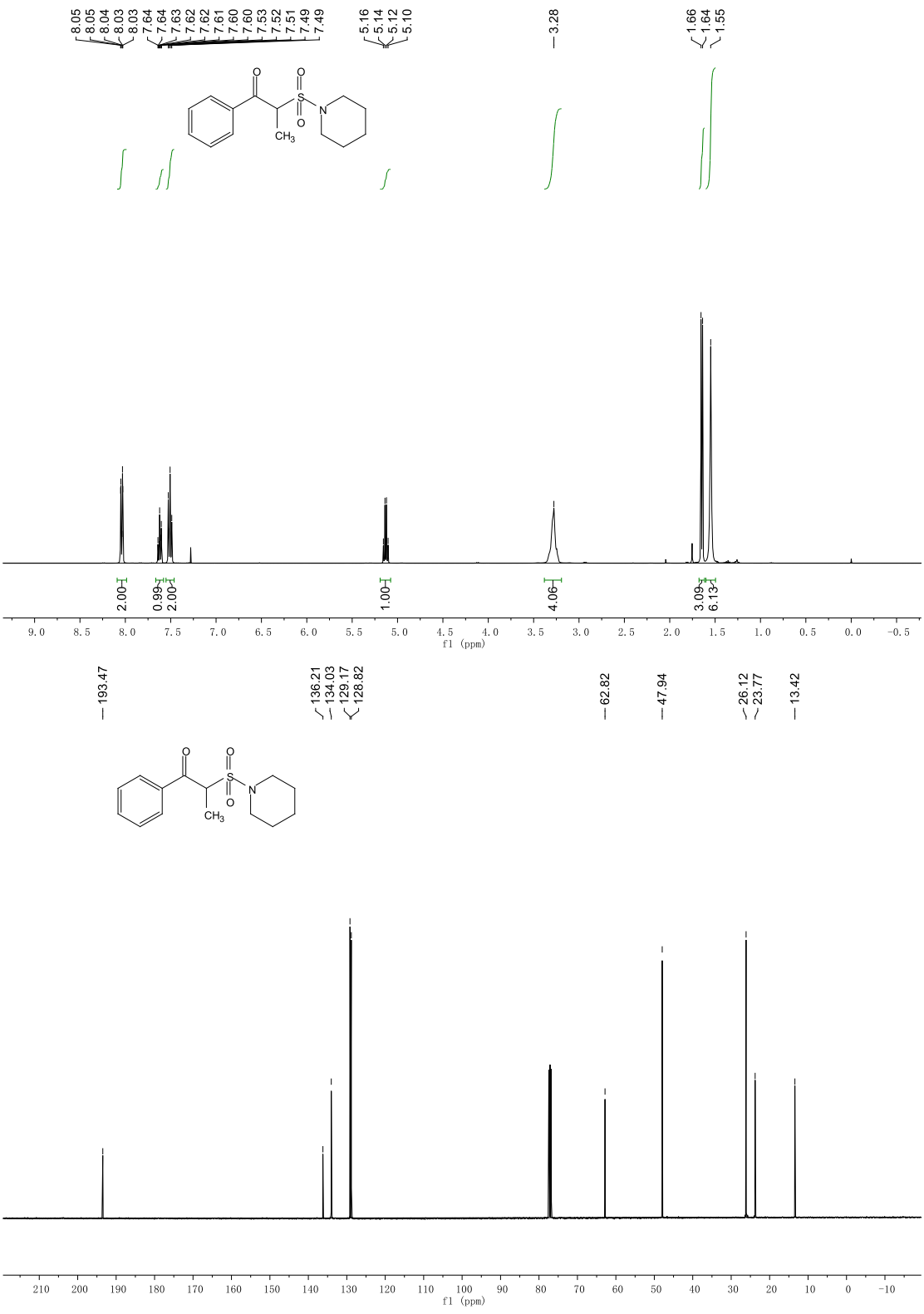

66.67
45.88
43.46
7.73
f1 (ppm)


2.98
2.96
2.94
2.92
2.87
1.36
1.34
1.32
2.08
6.00
3.06
f1 (ppm)

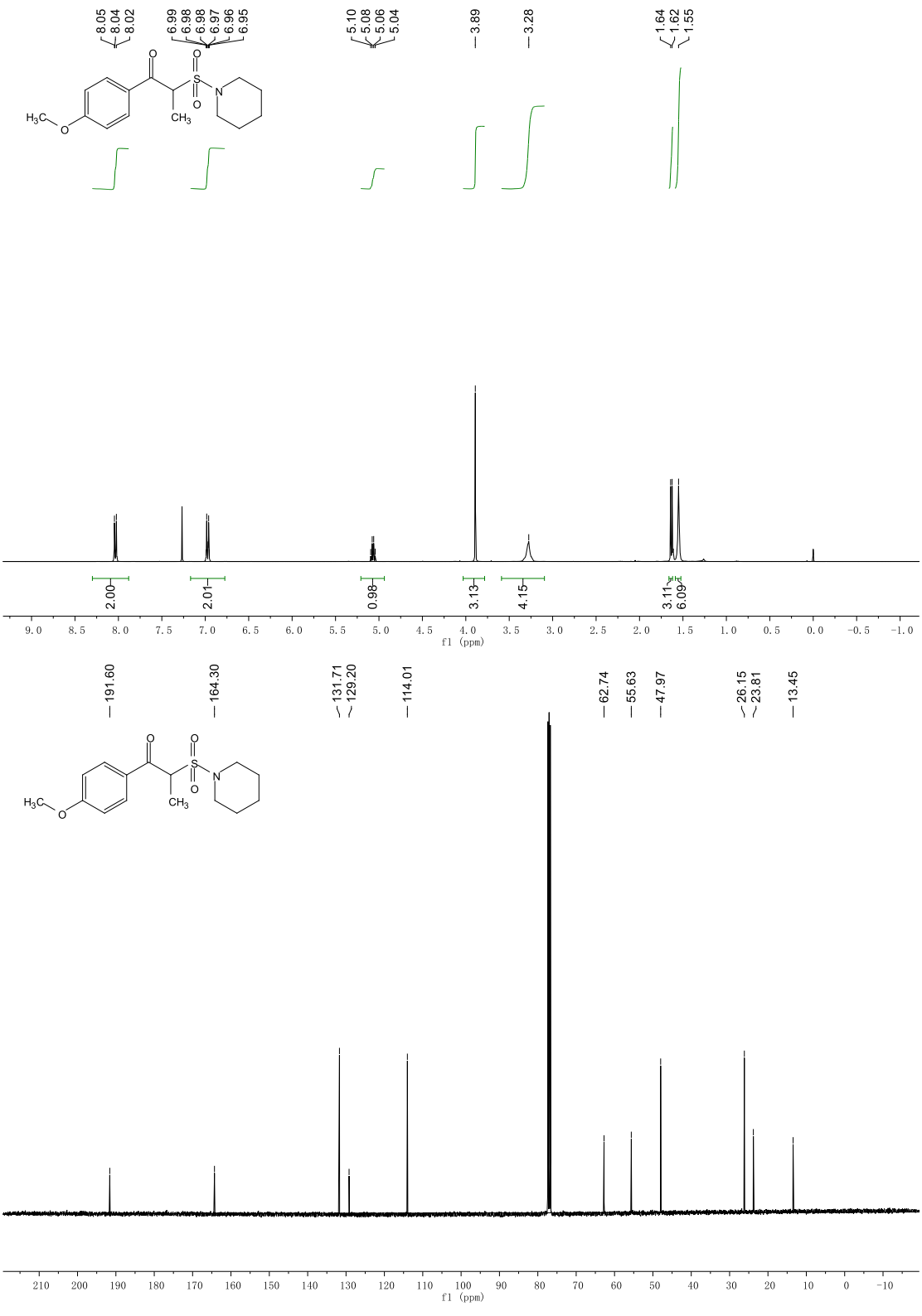

2.98
2.96
2.94
2.92
2.87
1.36
1.34
1.32
2.08
6.00
3.06
f1 (ppm)



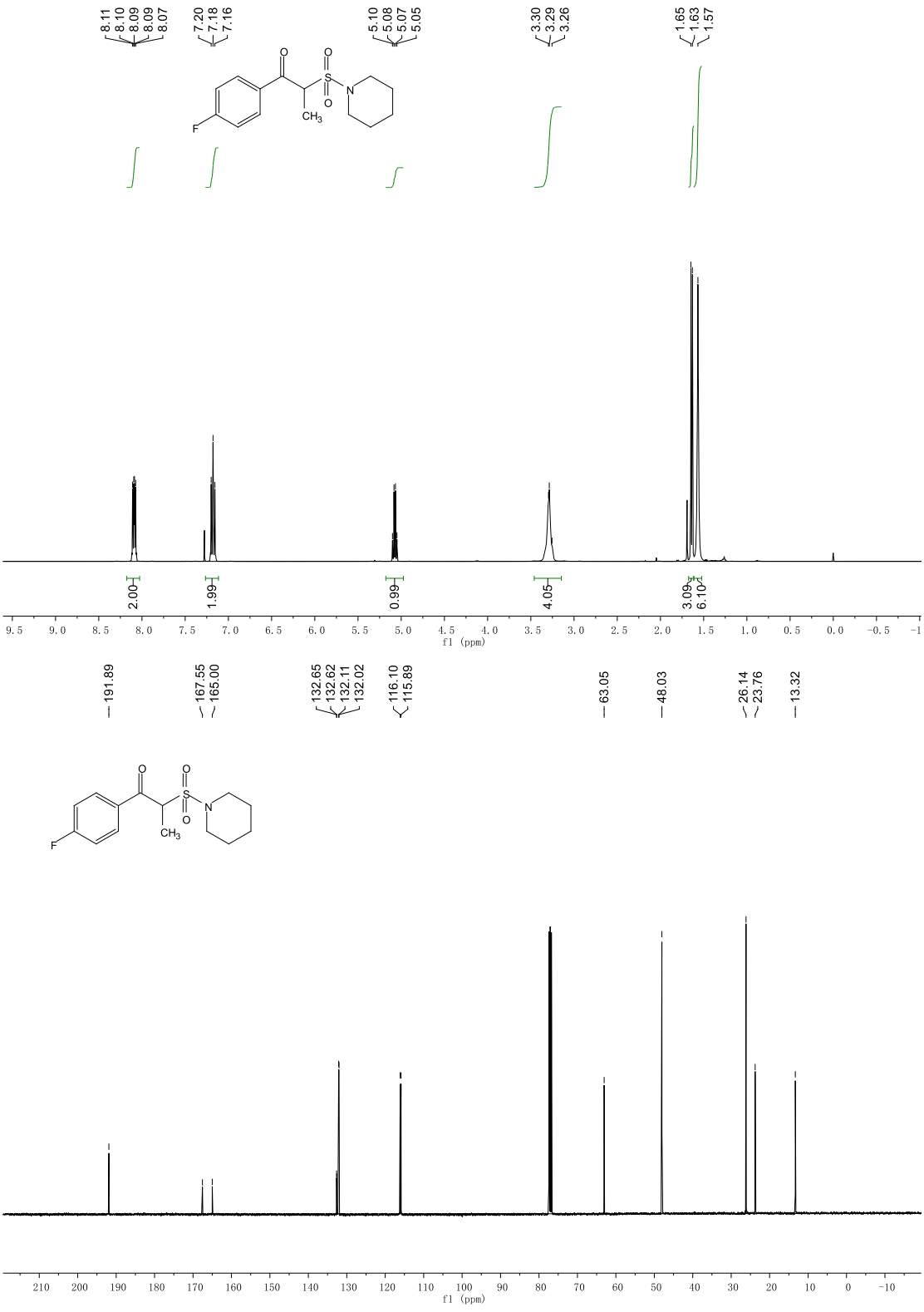
NMR spectra of **1a**



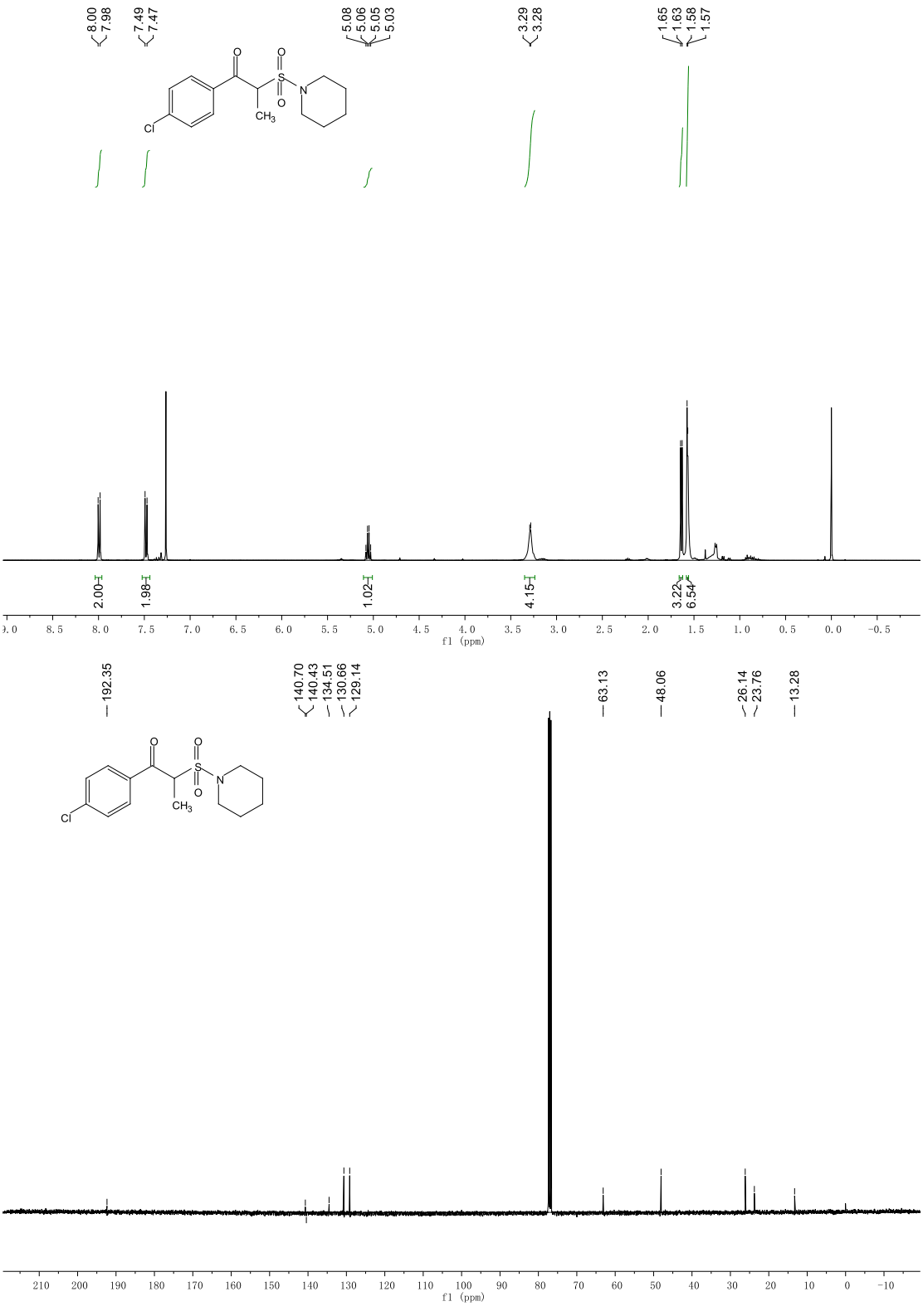
NMR spectra of **1b**



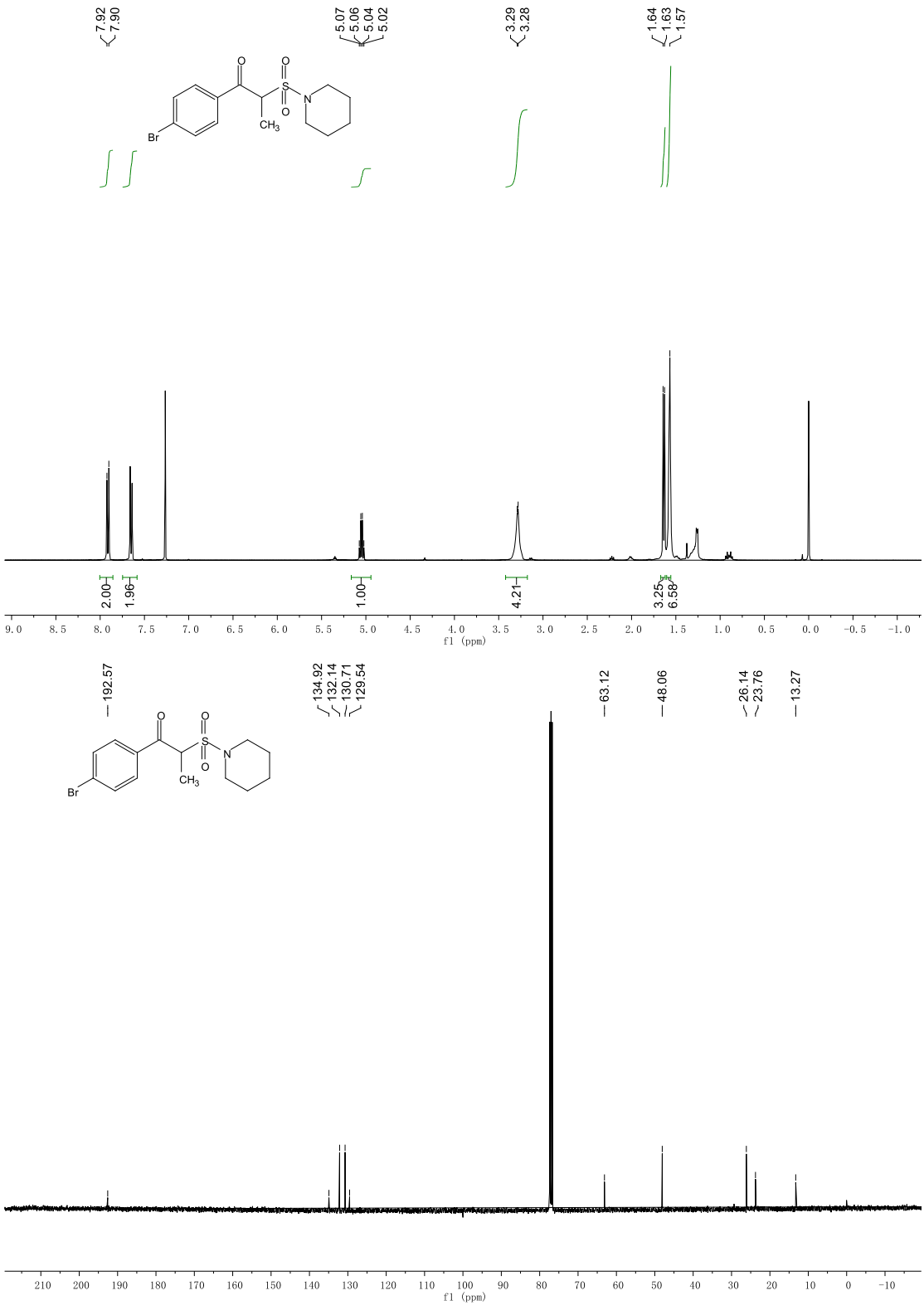
NMR spectra of **1c**



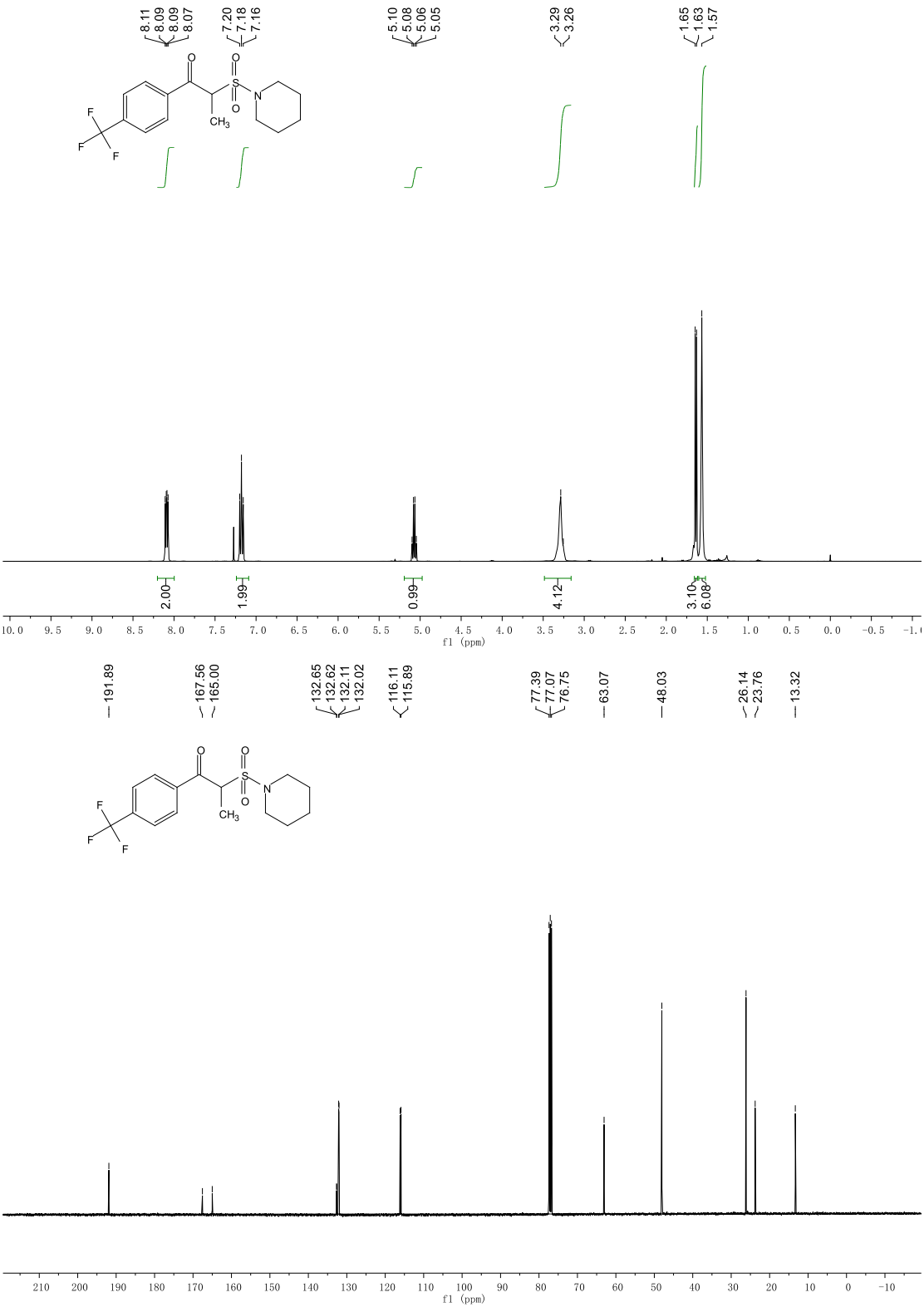
NMR spectra of **1d**



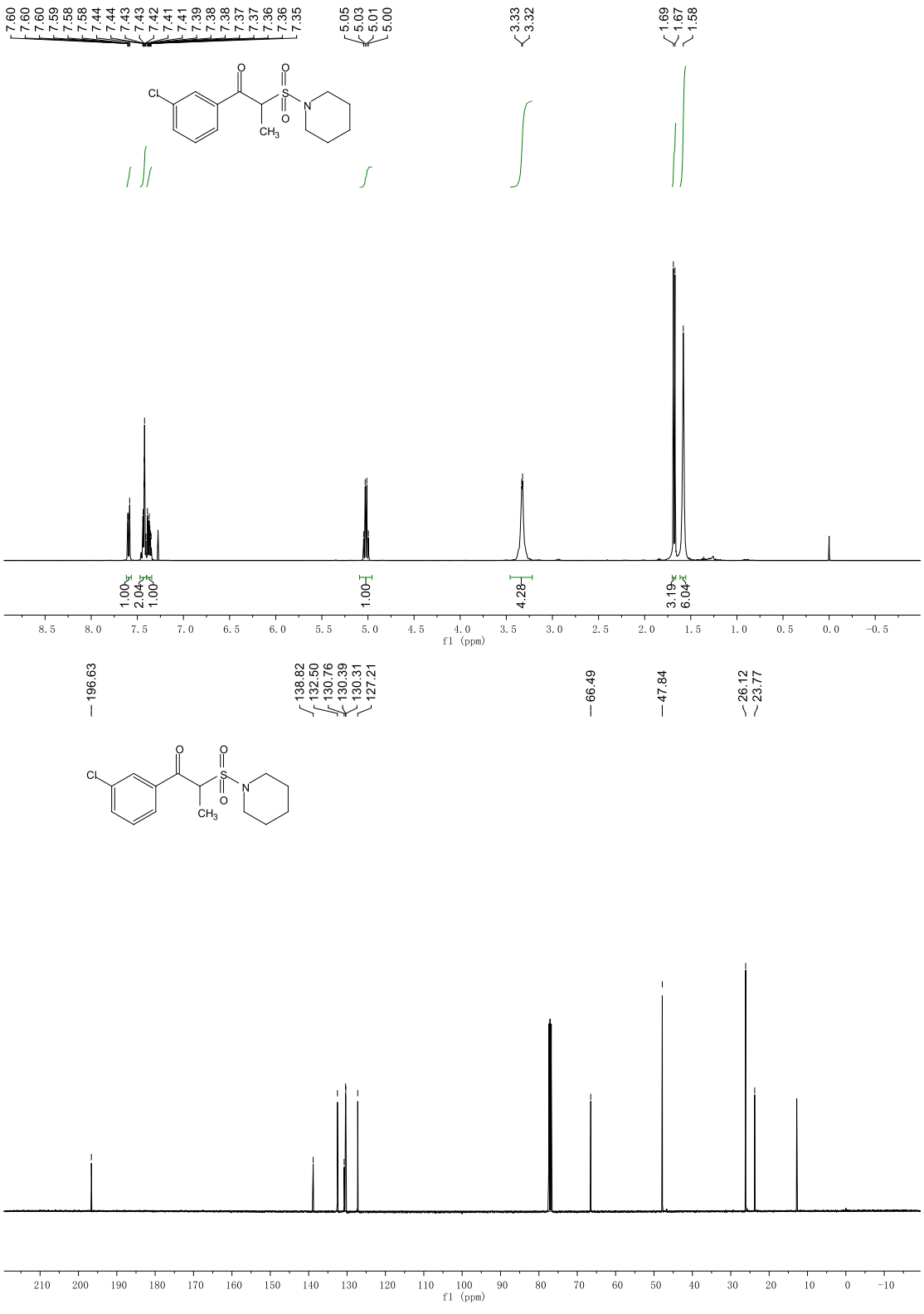
NMR spectra of **1e**



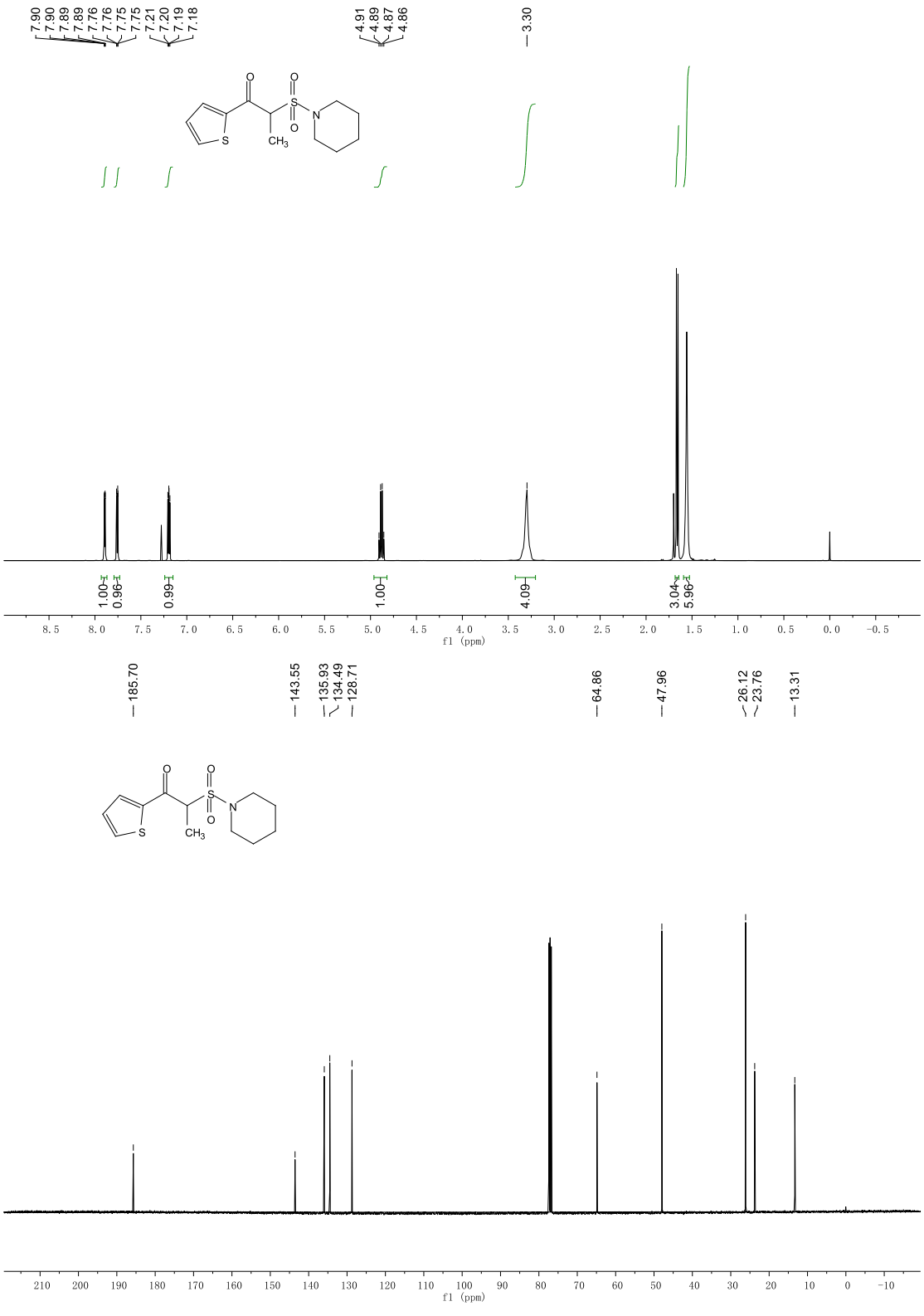
NMR spectra of **1f**



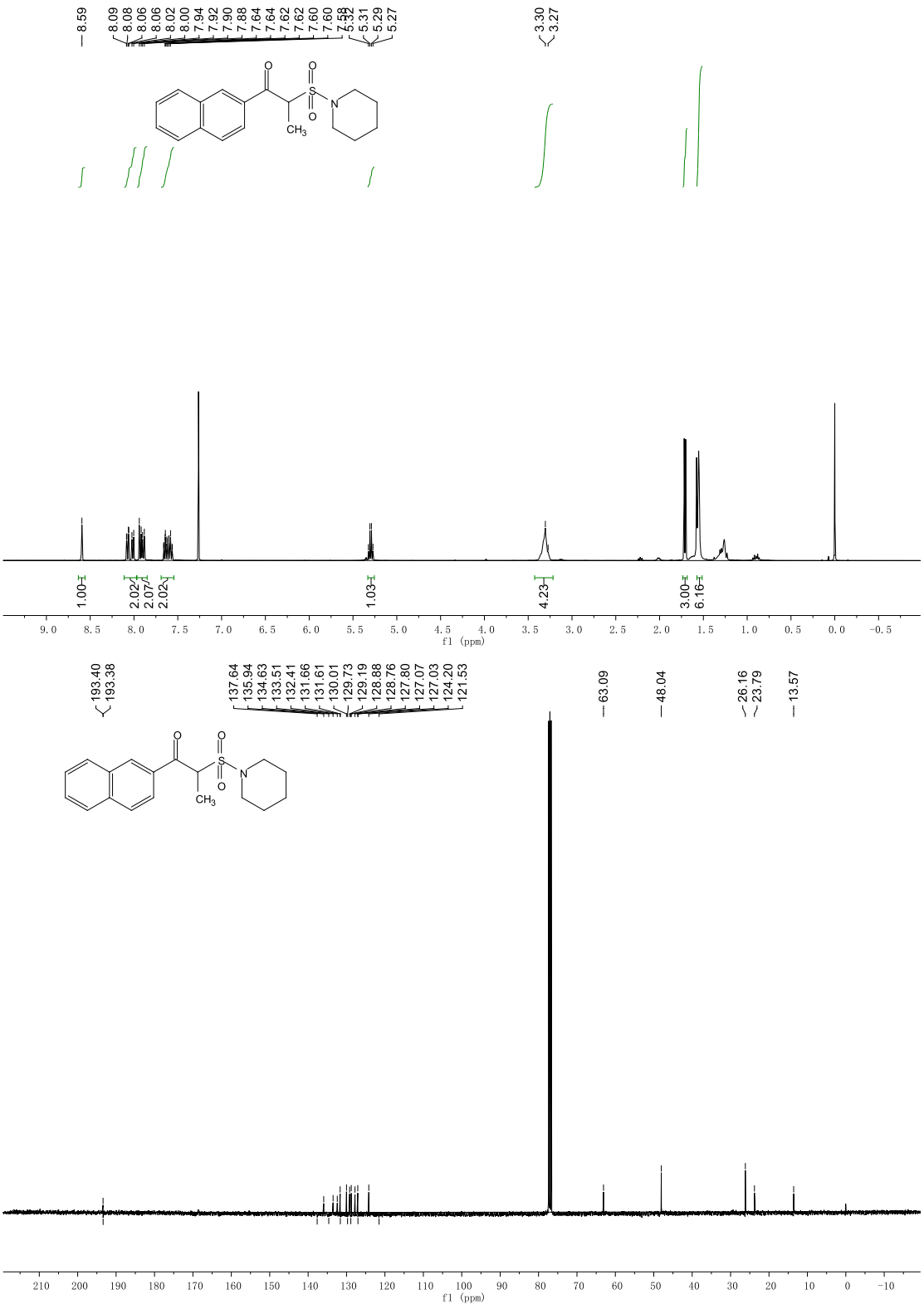
NMR spectra of **1g**



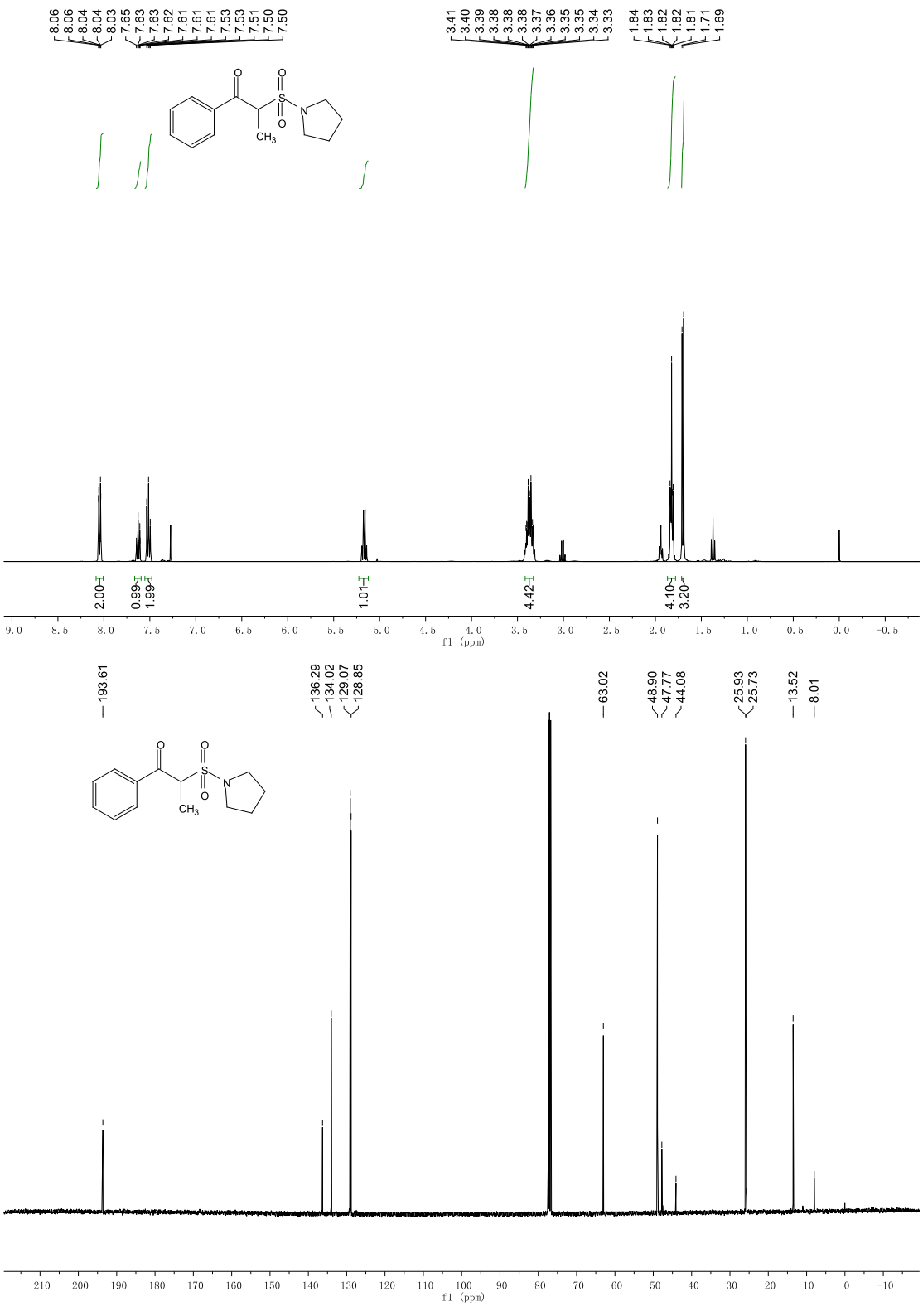
NMR spectra of **1h**



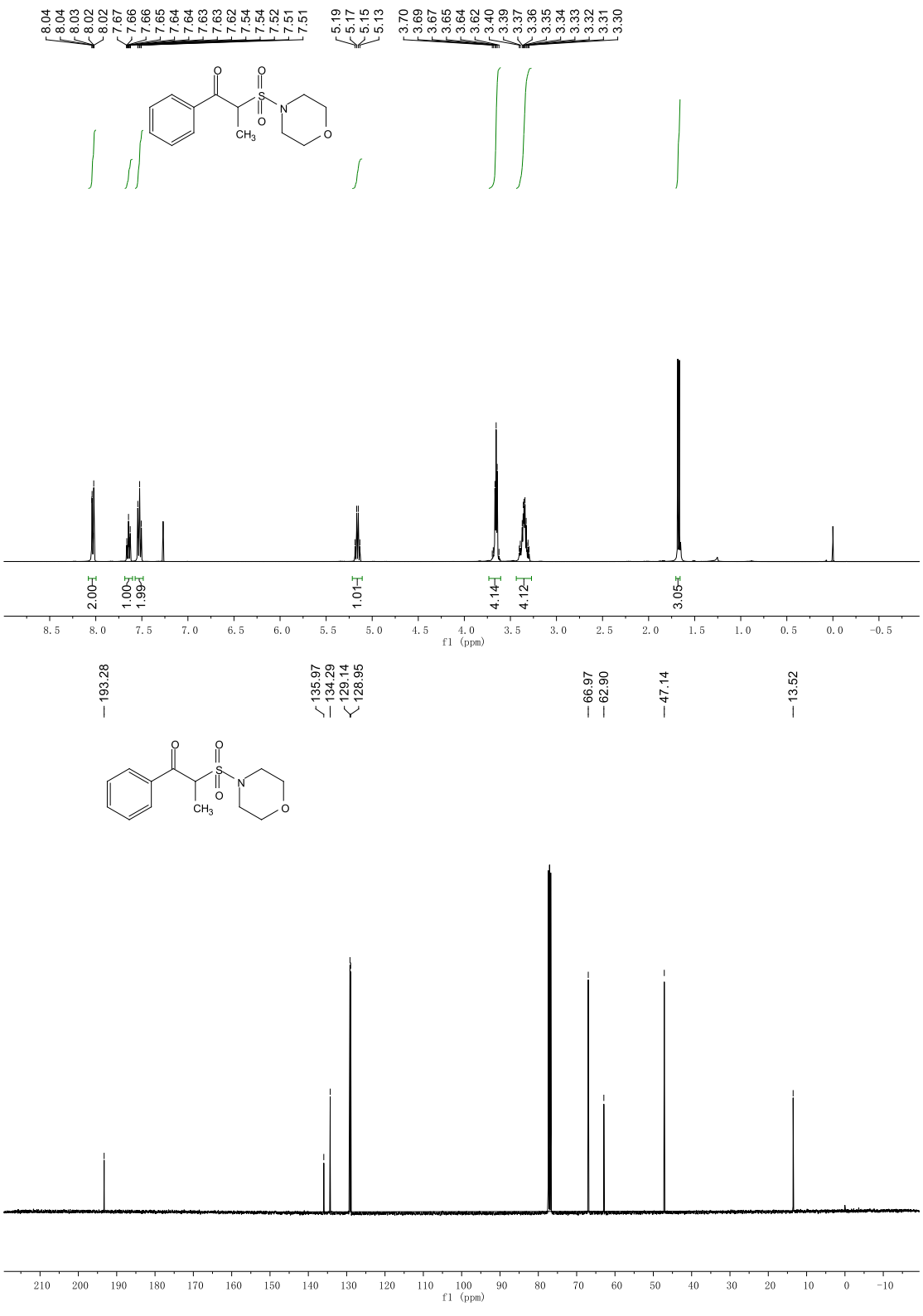
NMR spectra of **1i**



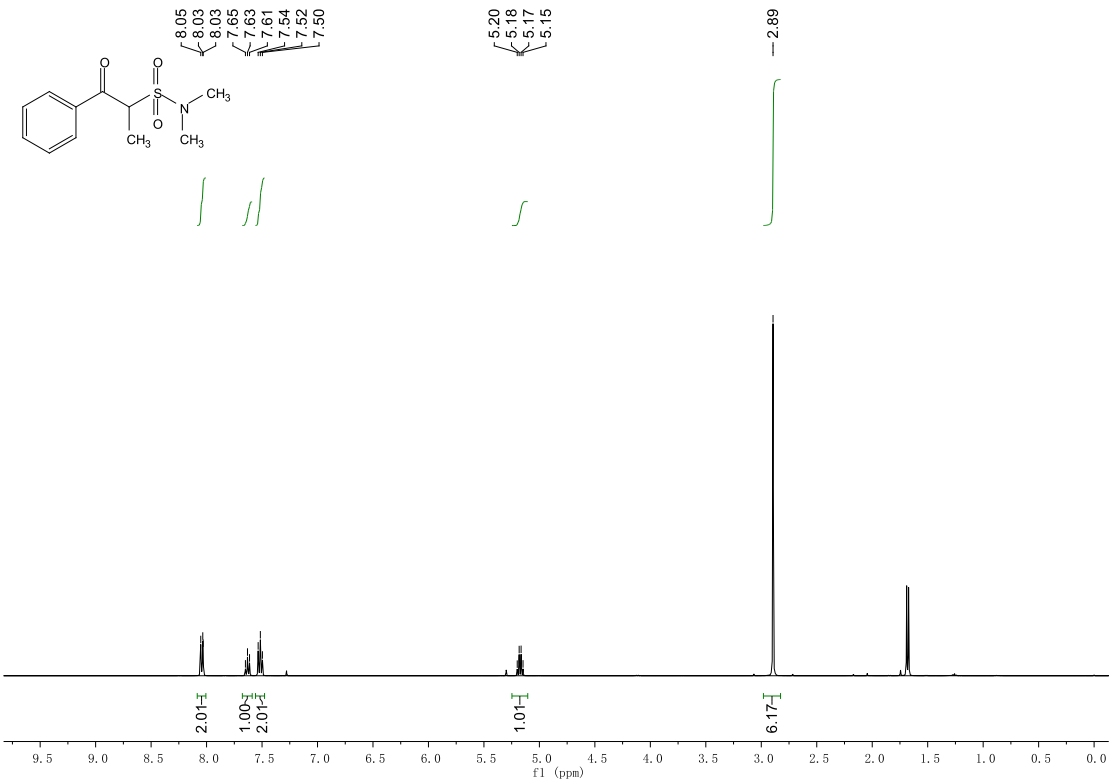
NMR spectra of **1j**

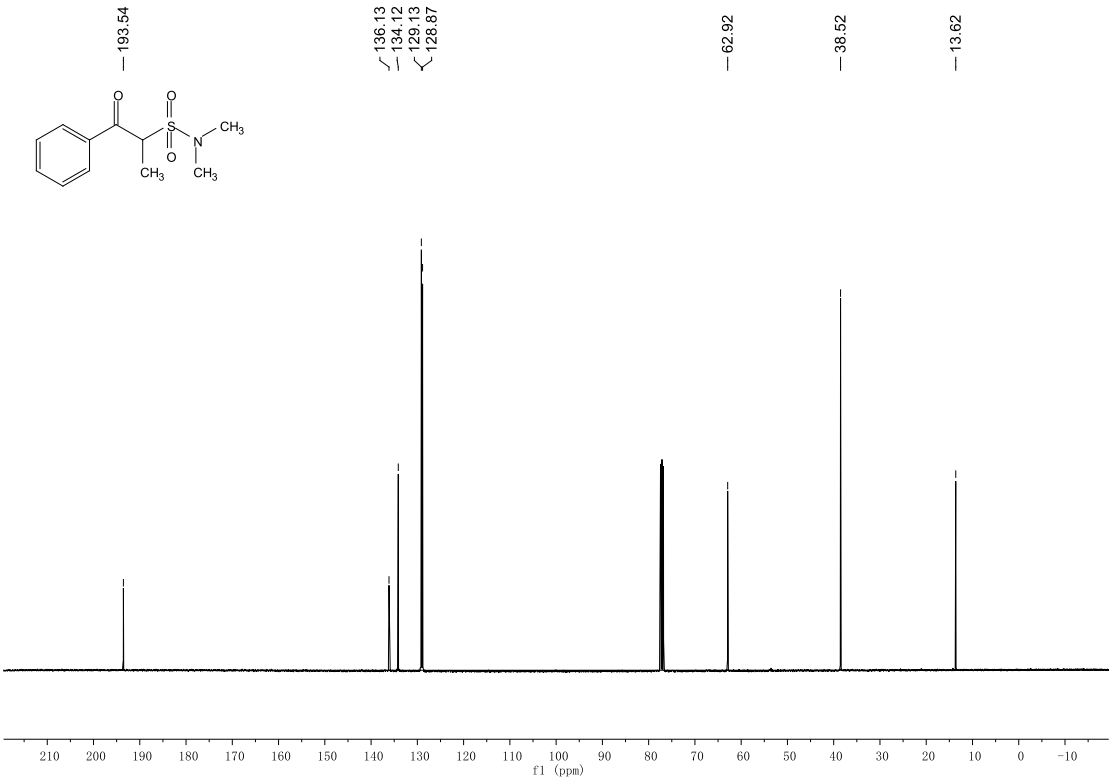


NMR spectra of **1k**

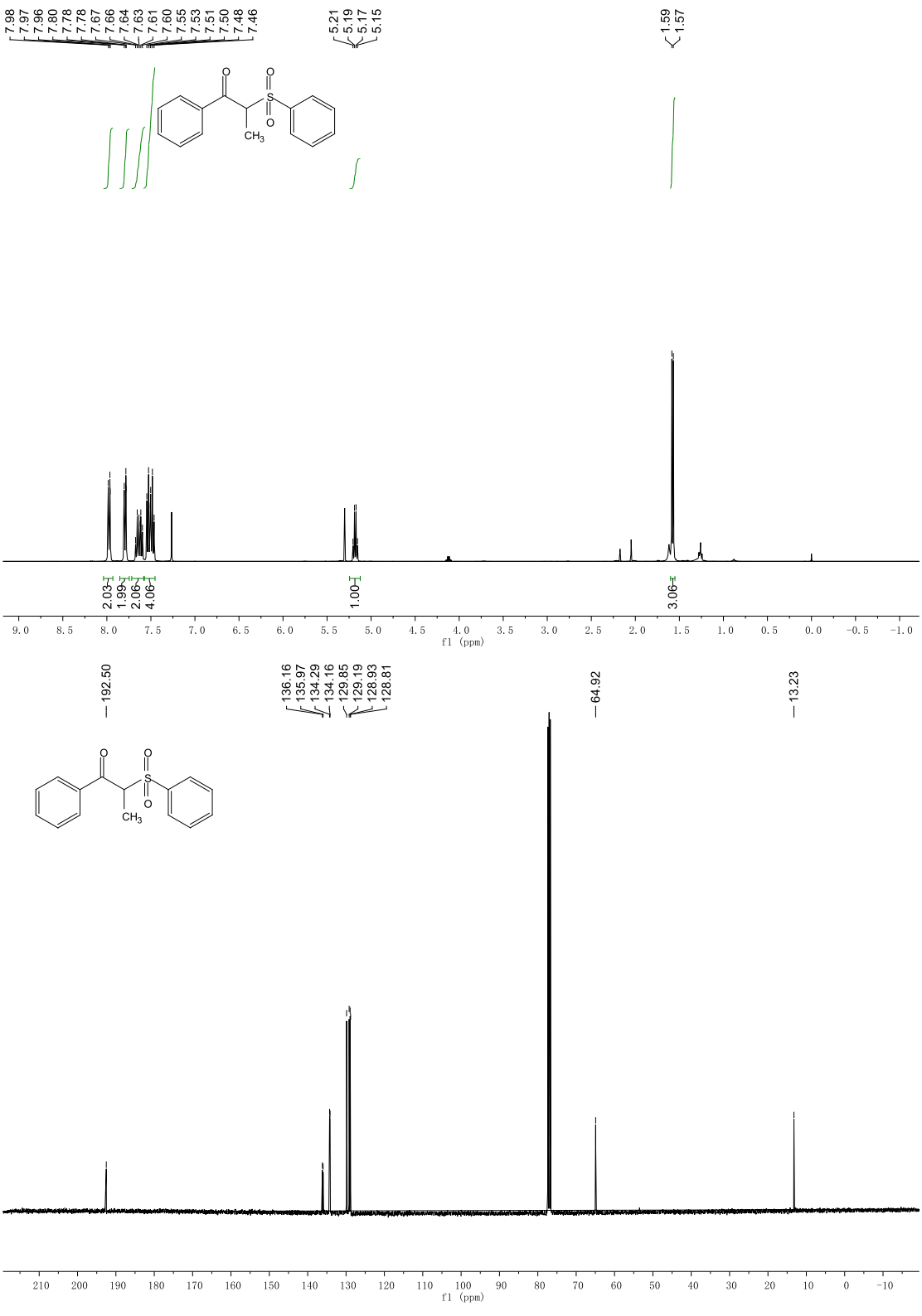


NMR spectra of **1l**

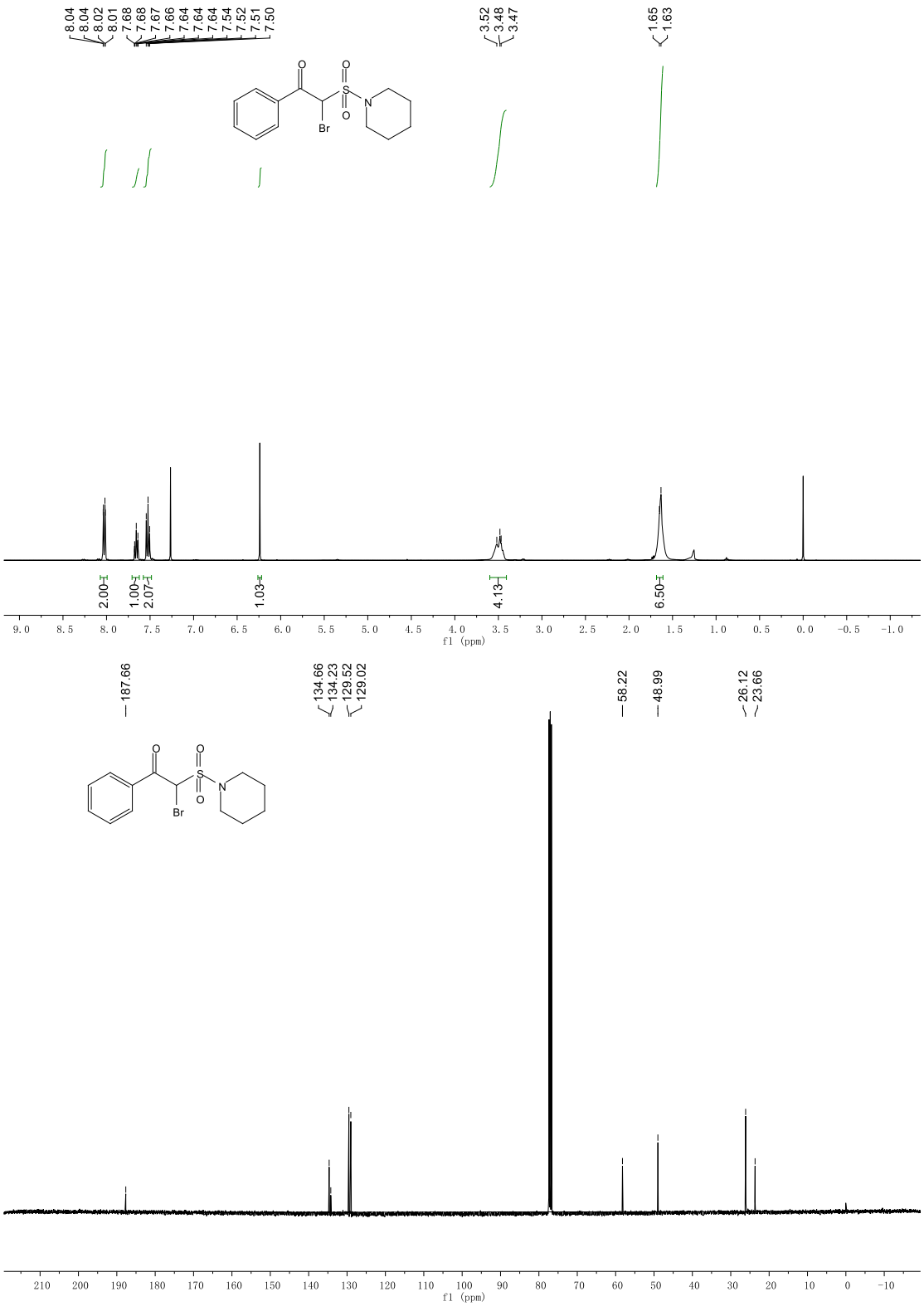




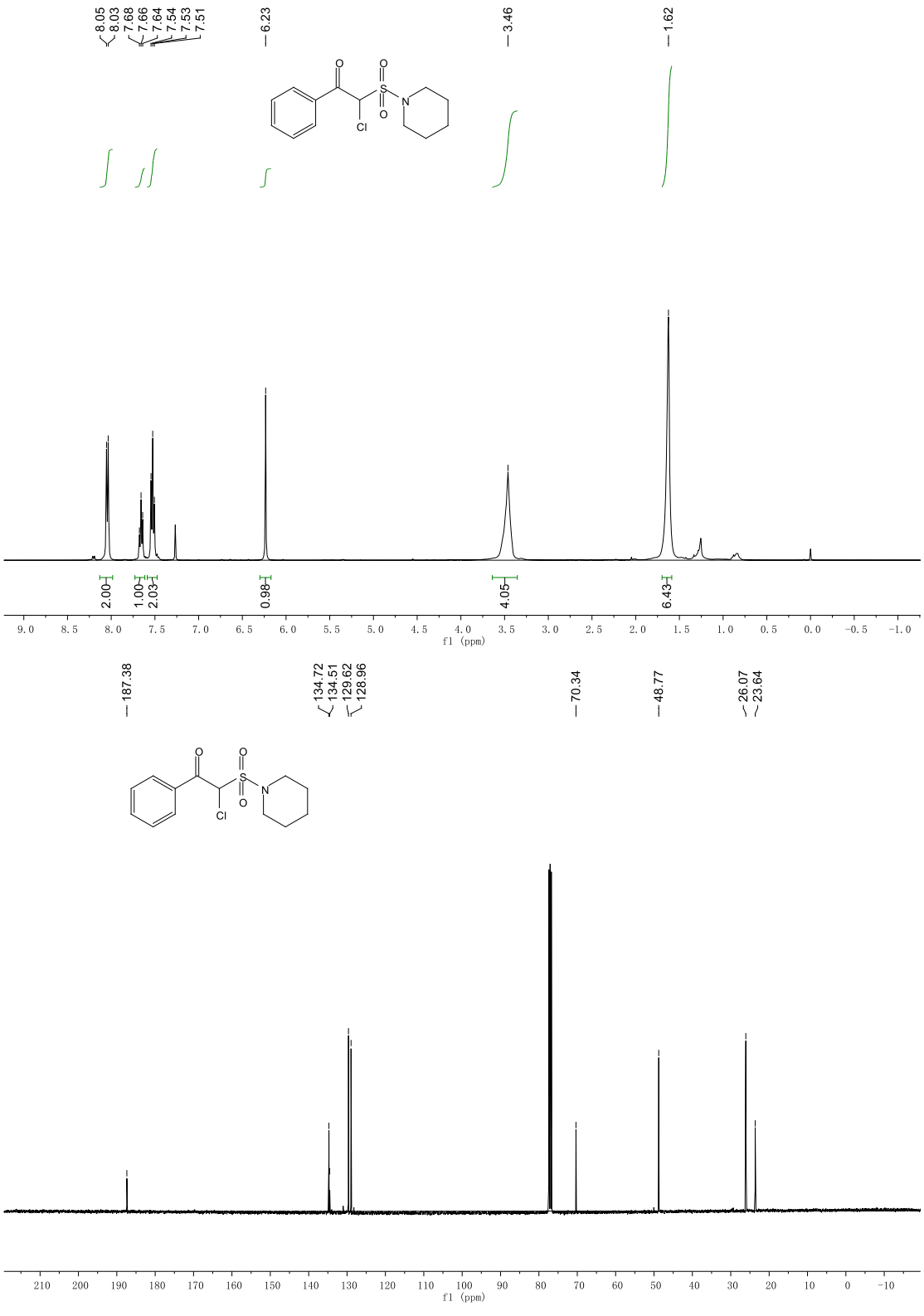
NMR spectra of **1m**



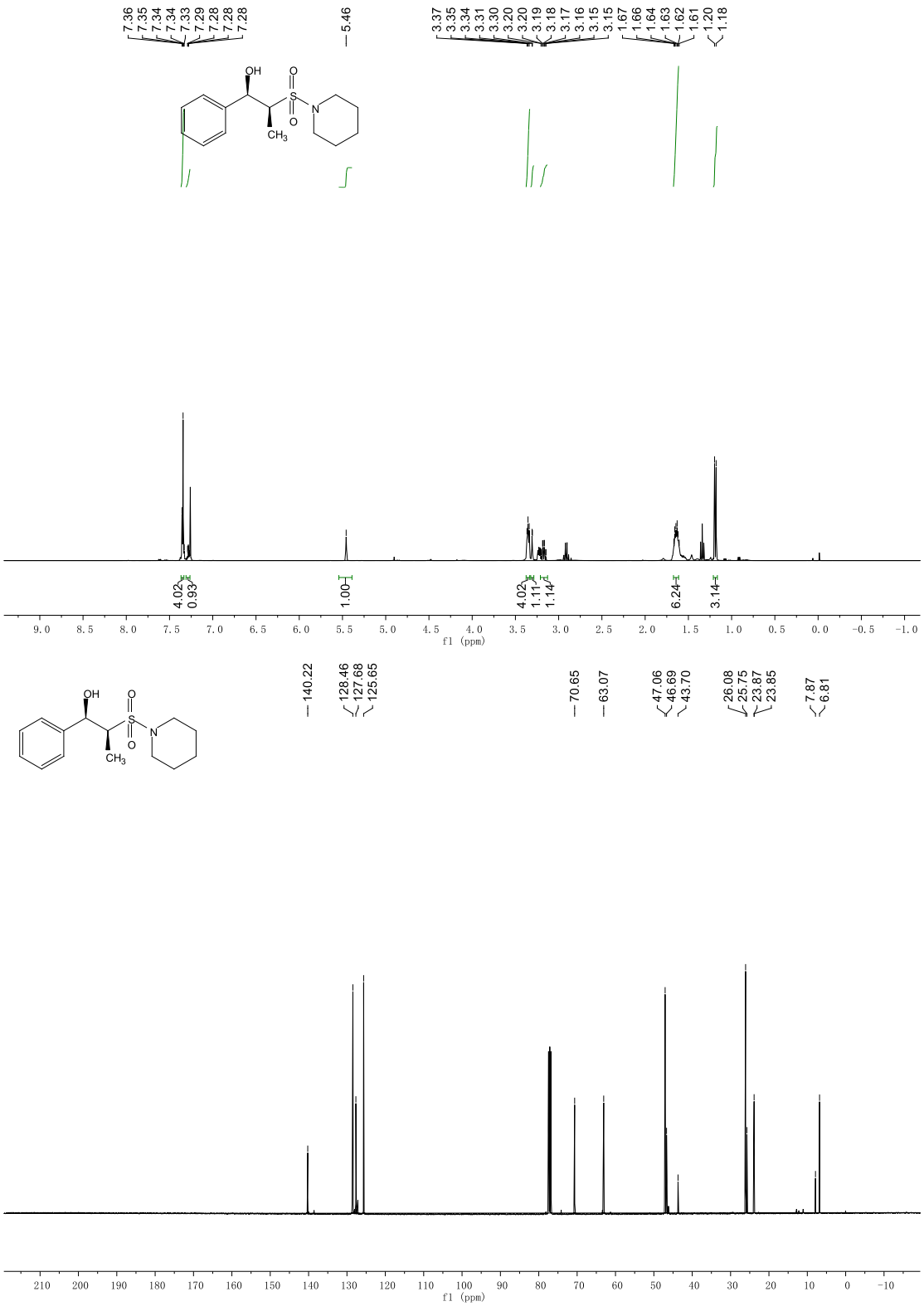
NMR spectra of **1n**



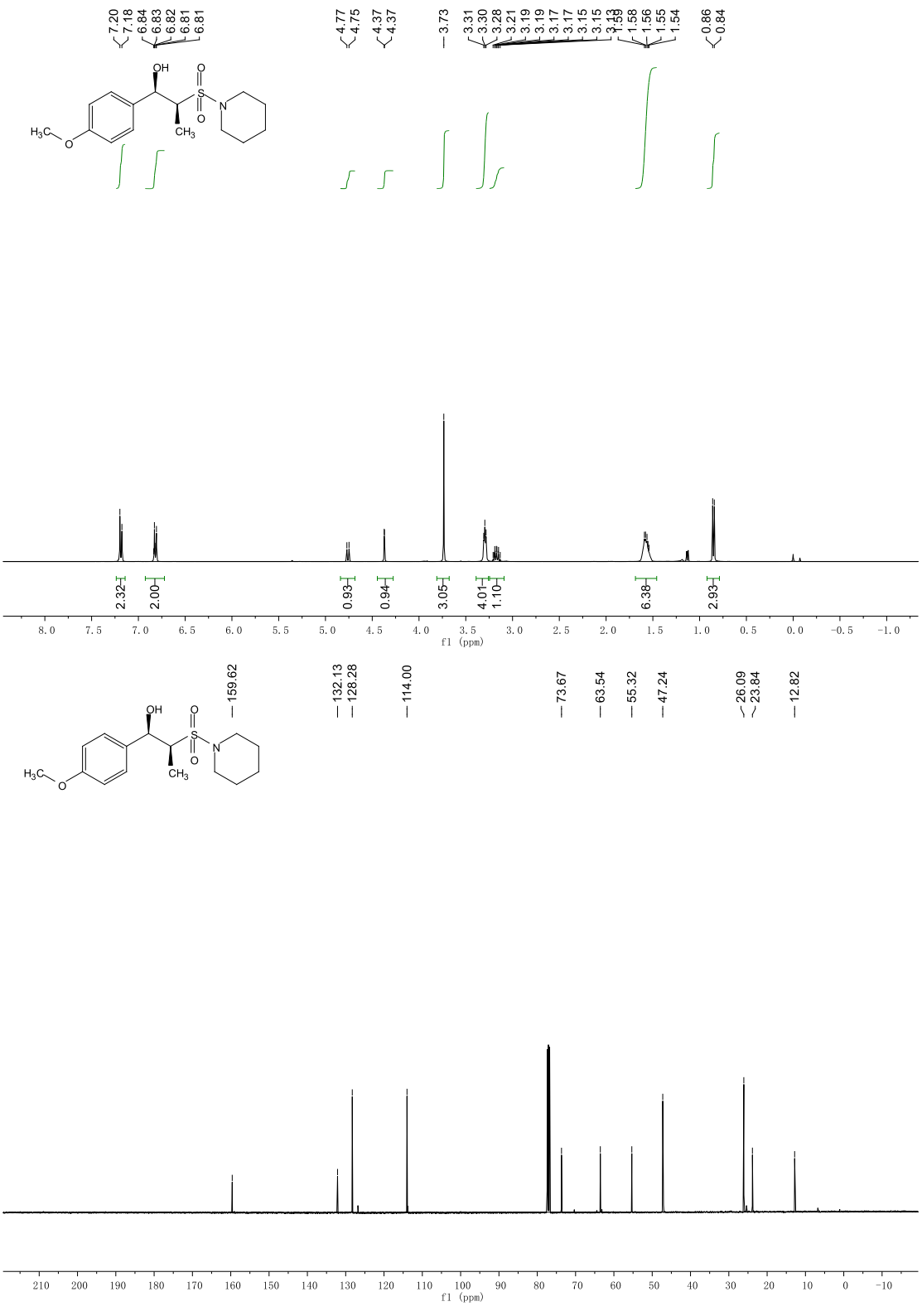
NMR spectra of **1o**



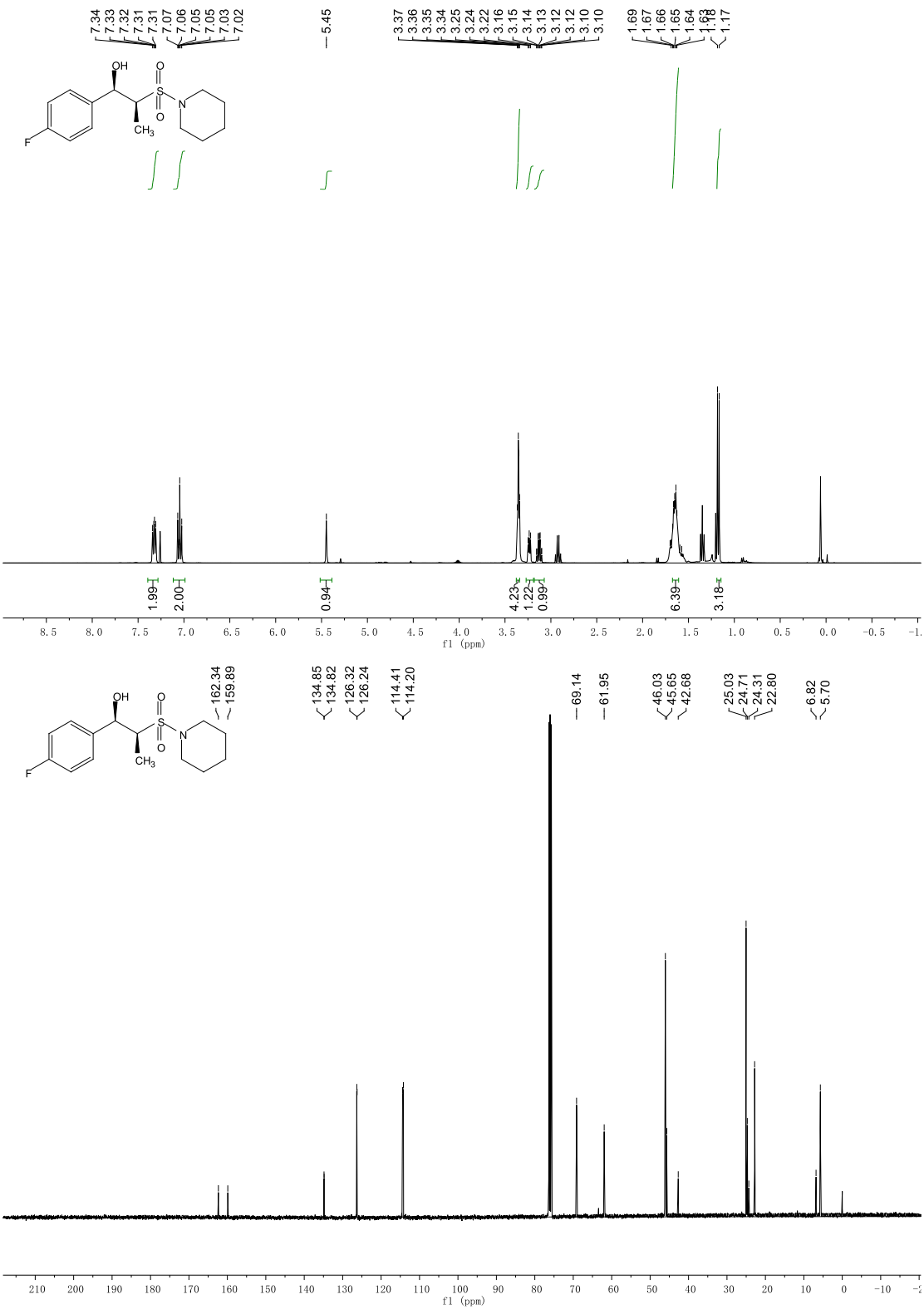
NMR spectra of **2a**



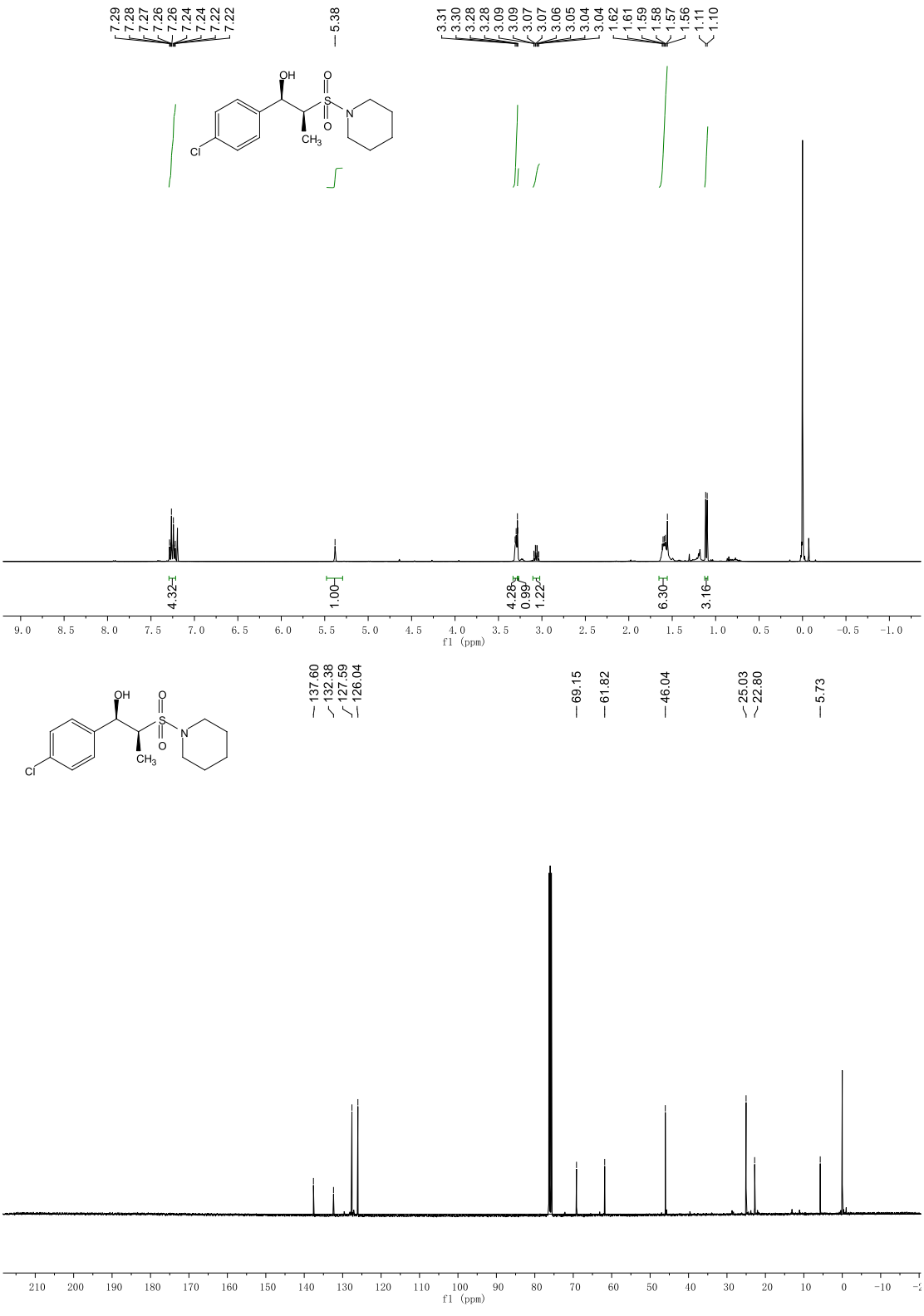
NMR spectra of **2b**



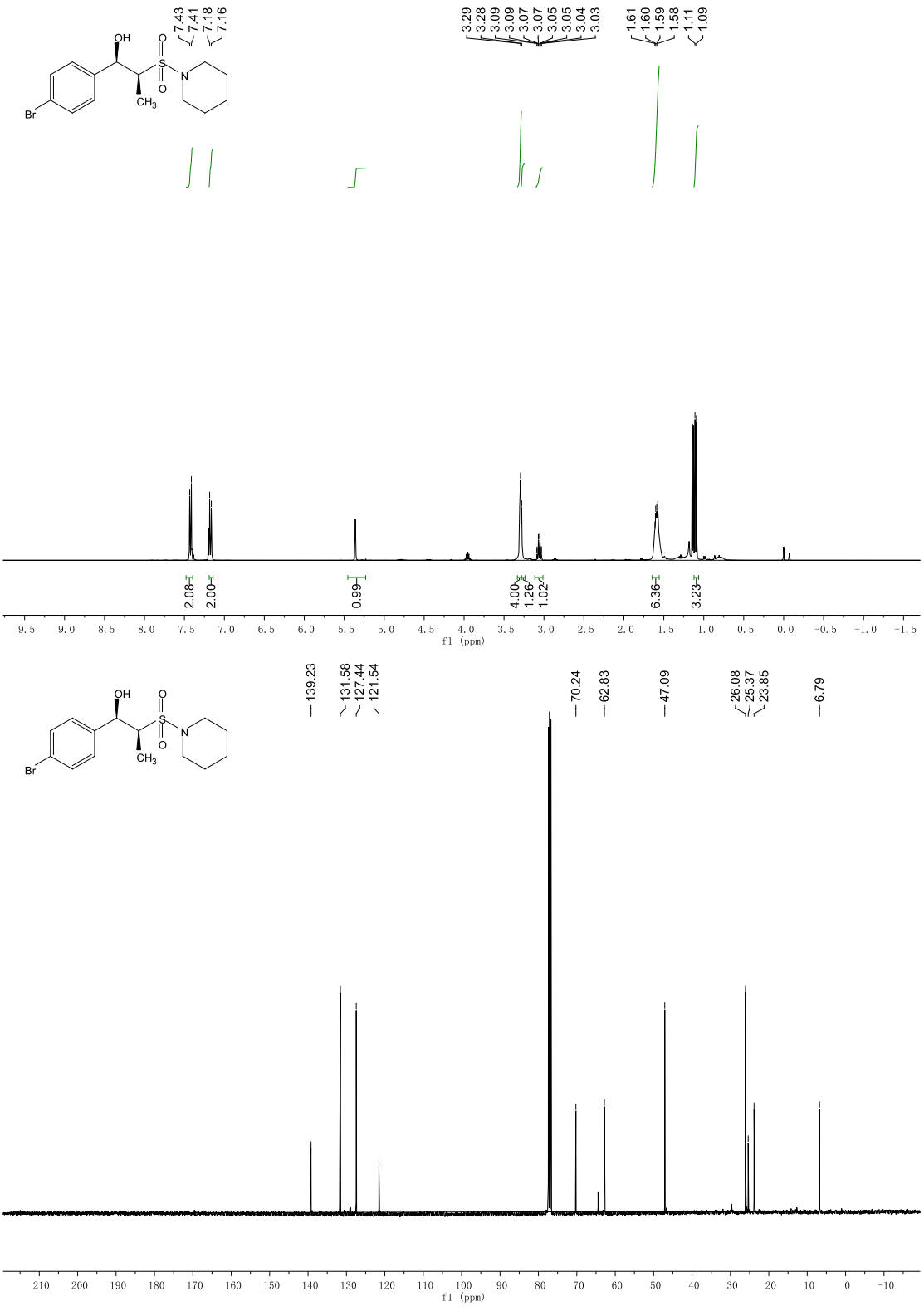
NMR spectra of **2c**



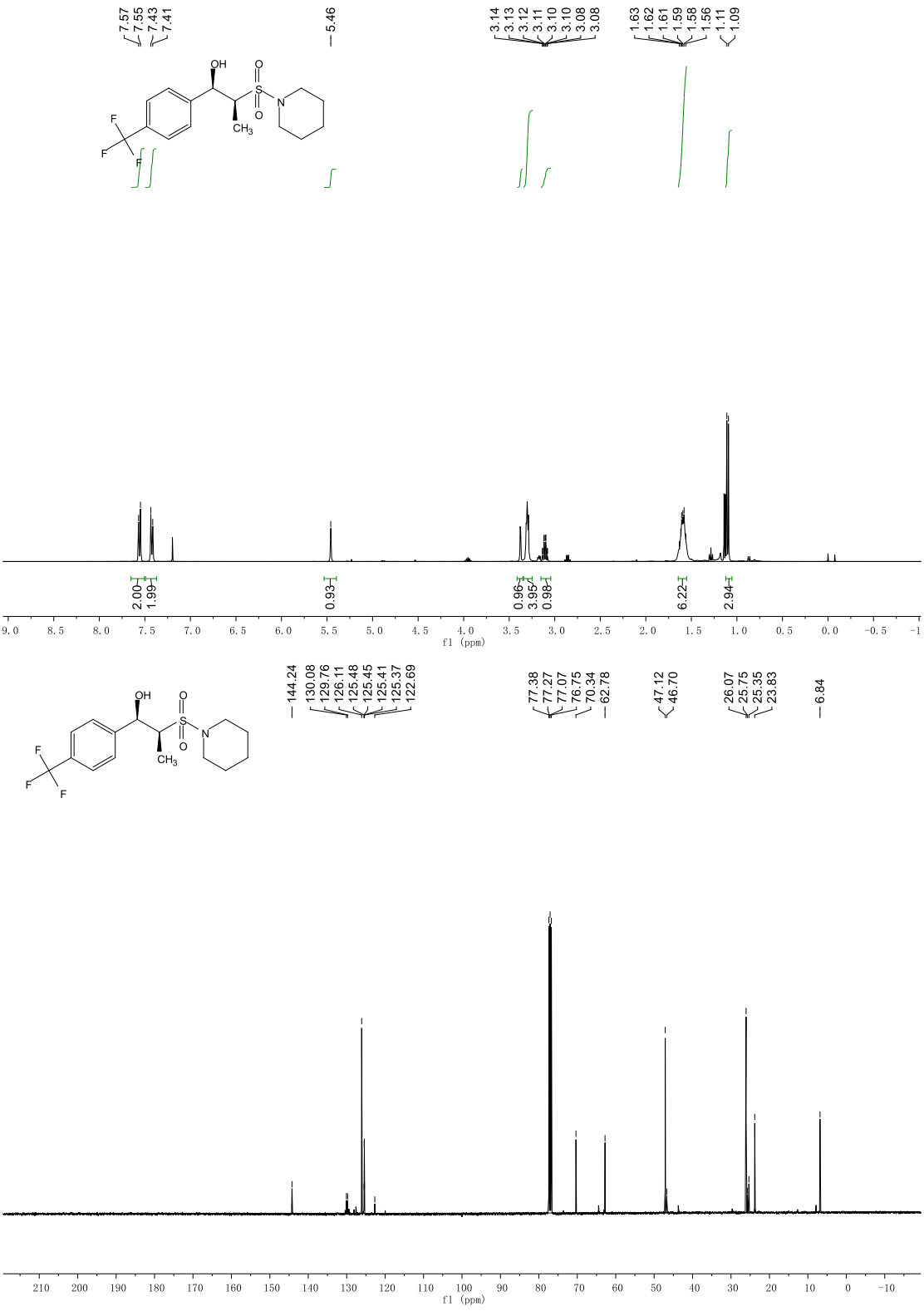
NMR spectra of **2d**



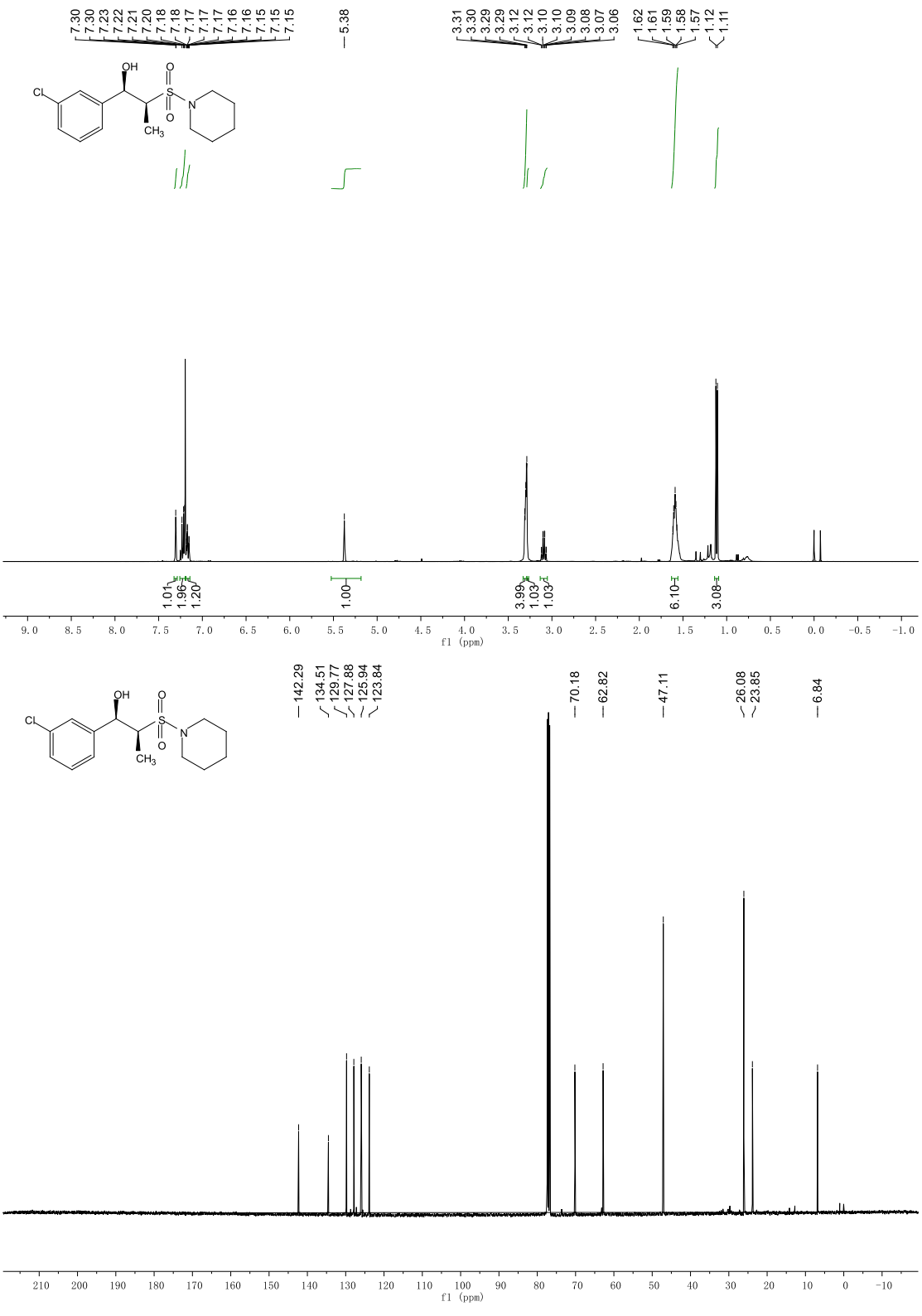
NMR spectra of **2e**



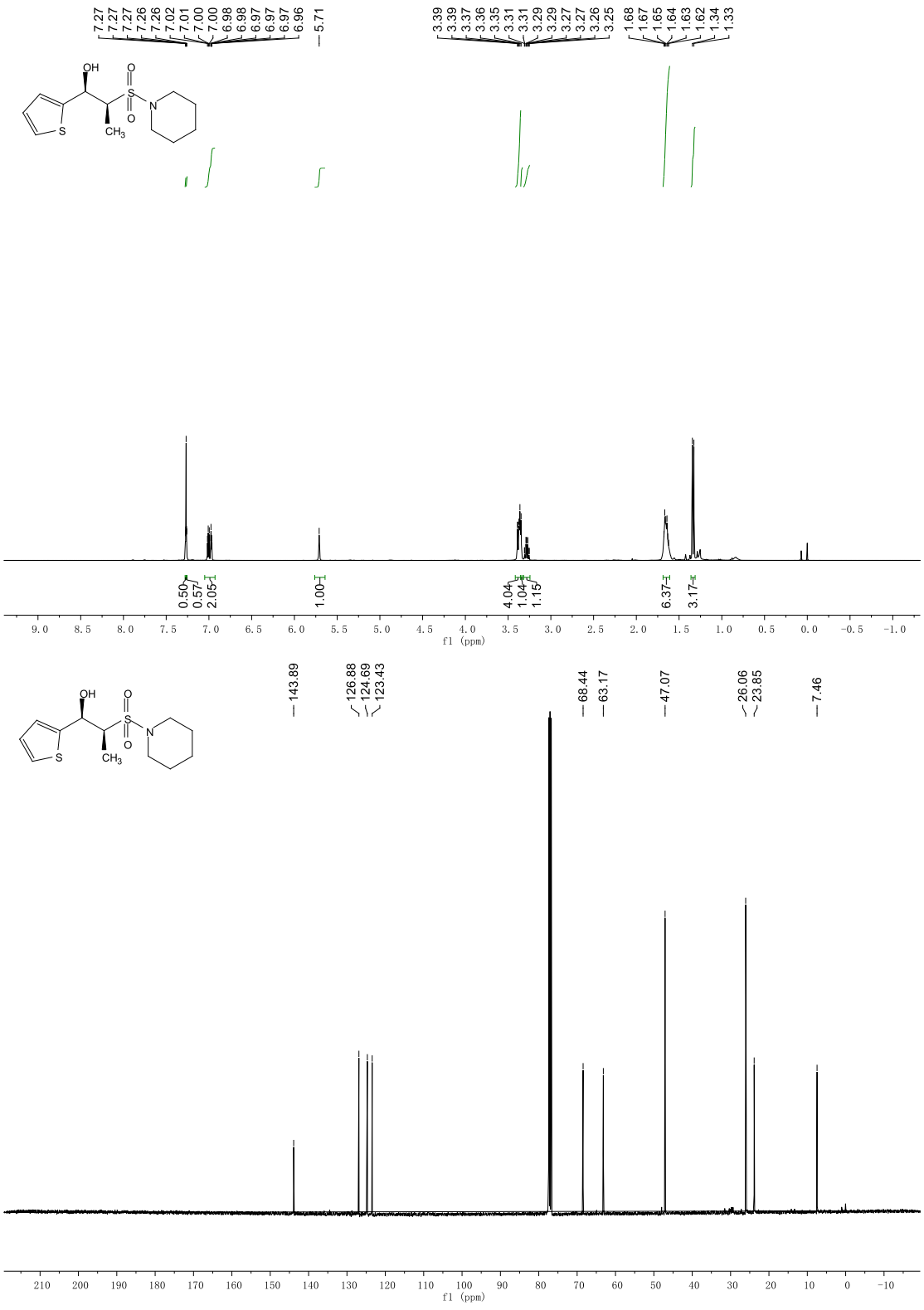
NMR spectra of **2f**



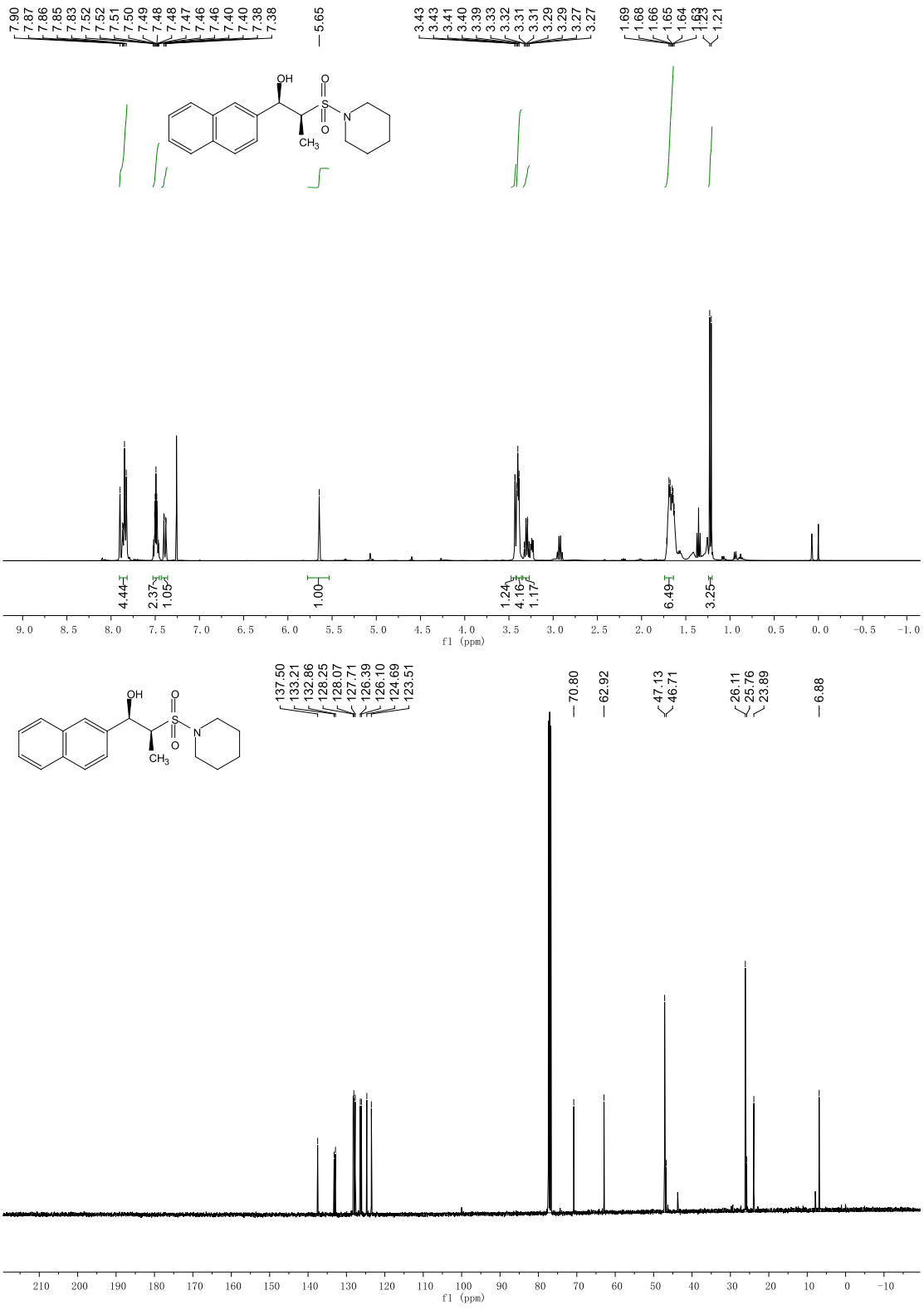
NMR spectra of **2g**



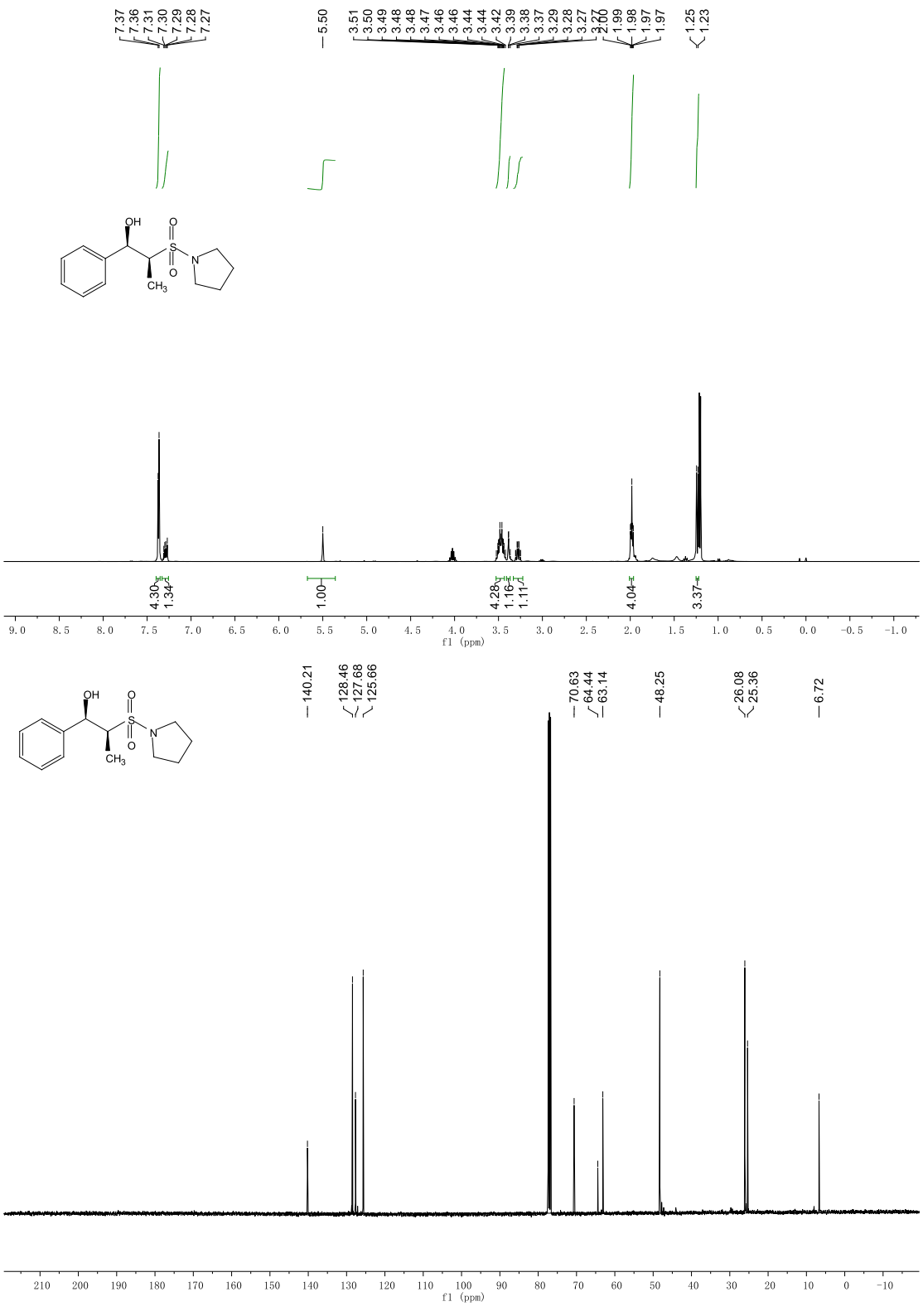
NMR spectra of **2h**



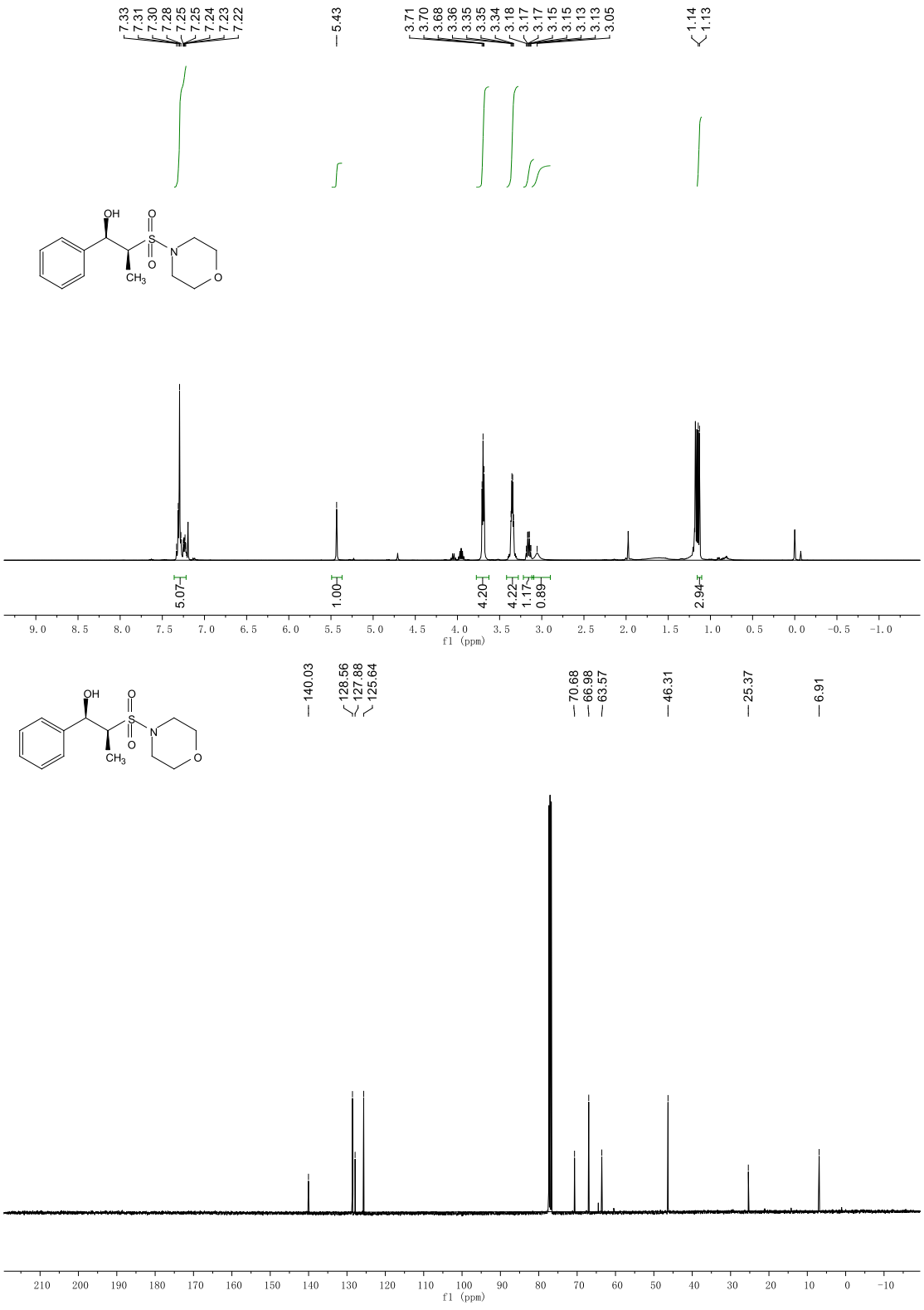
NMR spectra of **2i**



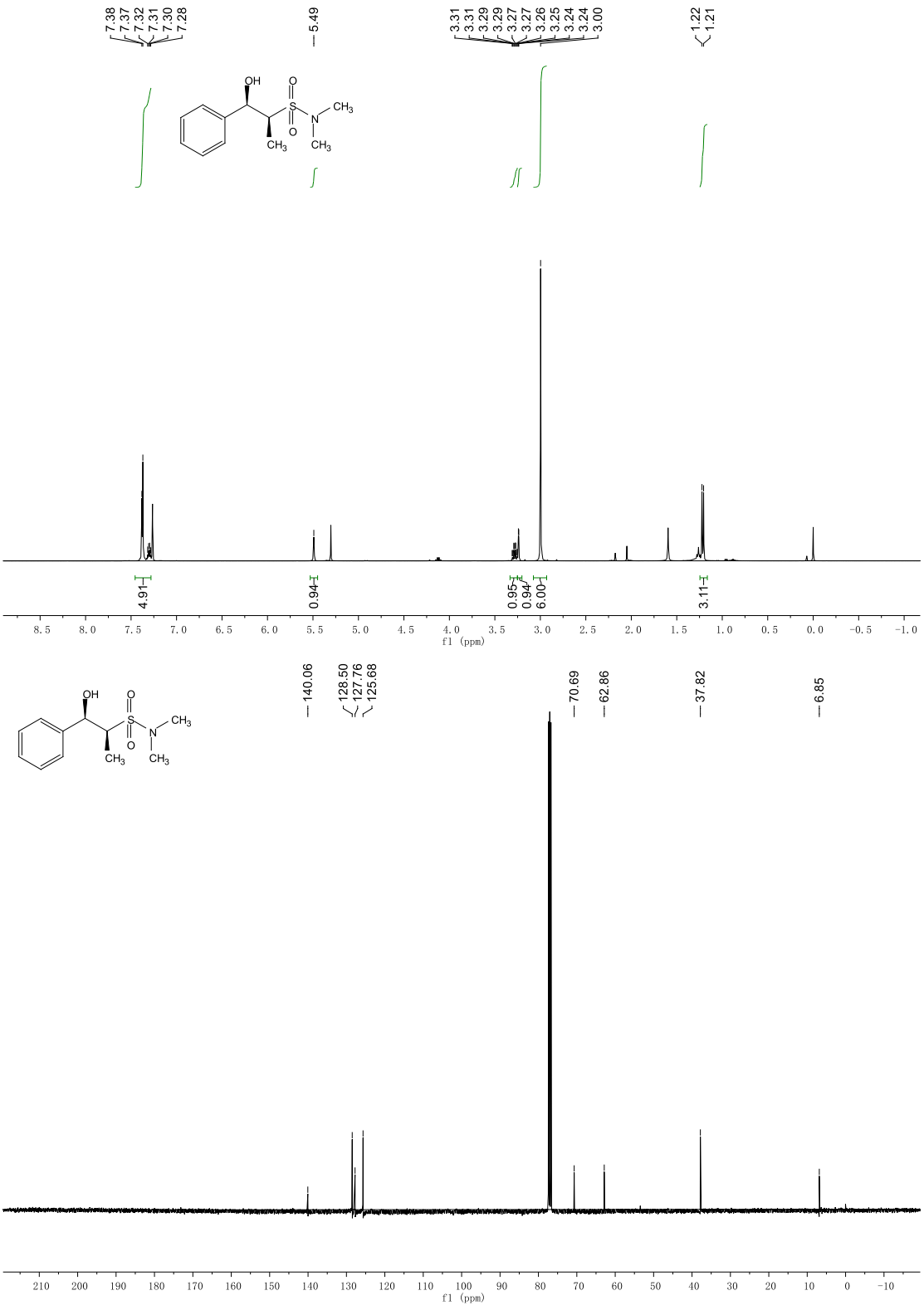
NMR spectra of **2j**



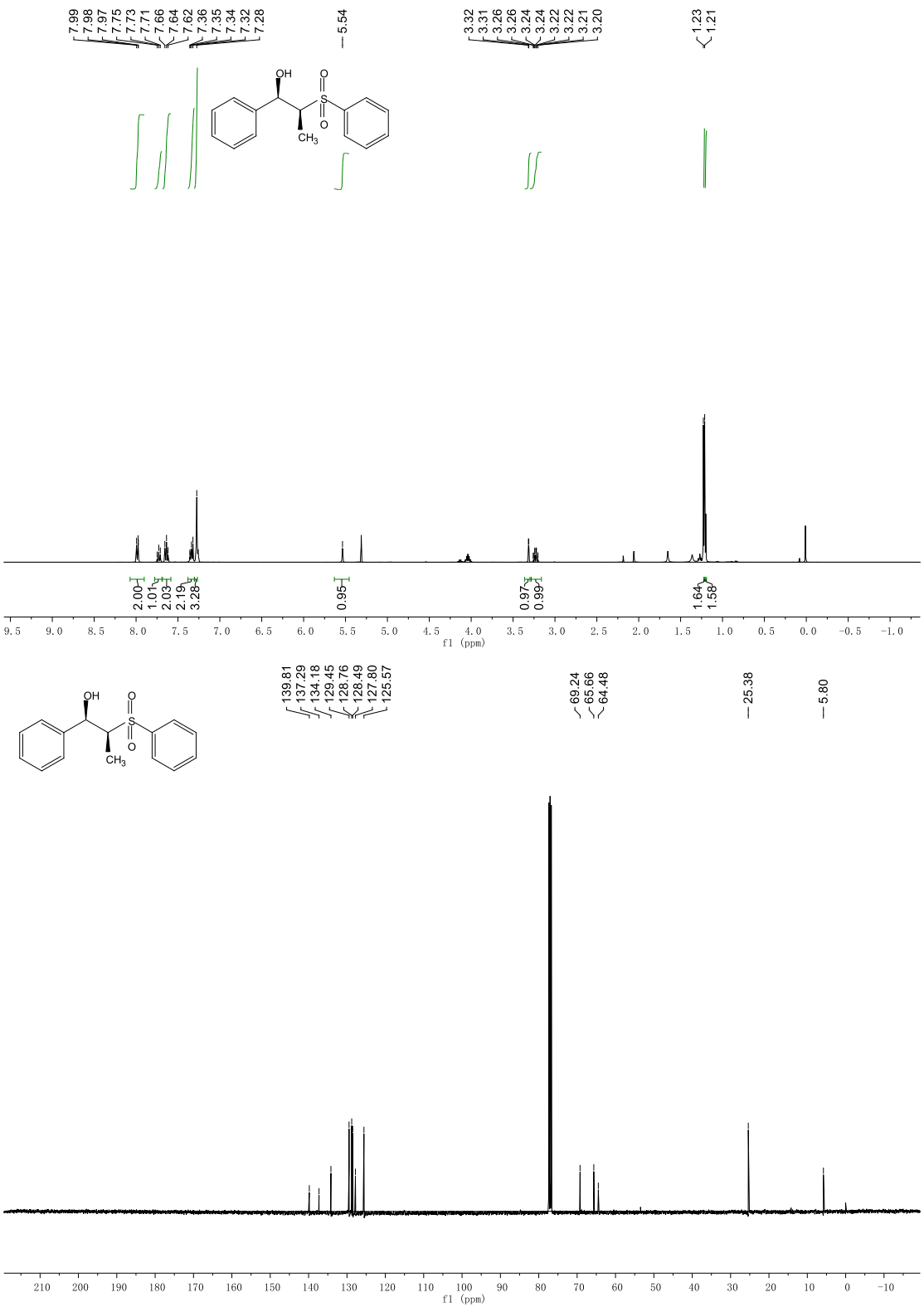
NMR spectra of **2k**



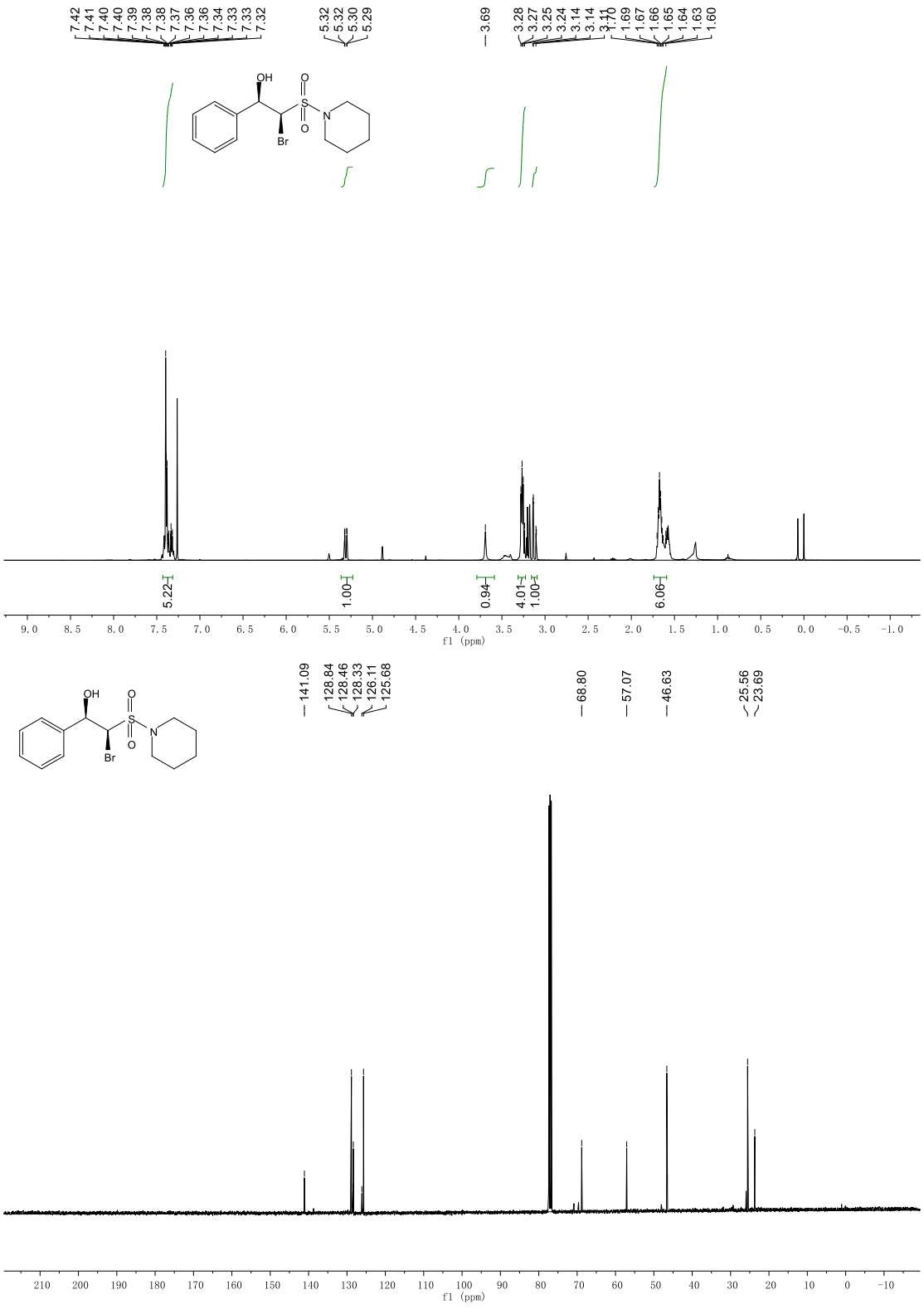
NMR spectra of **2l**



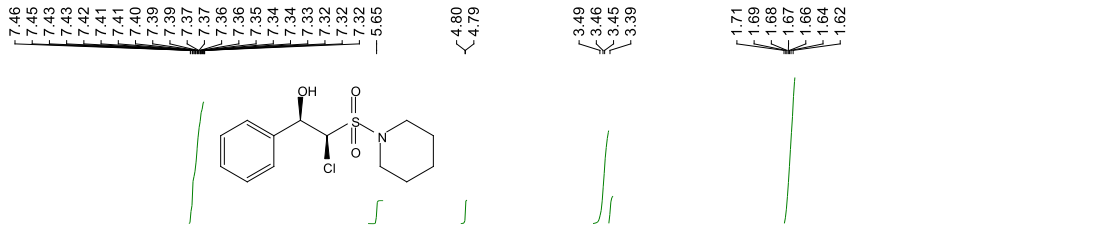
NMR spectra of **2m**

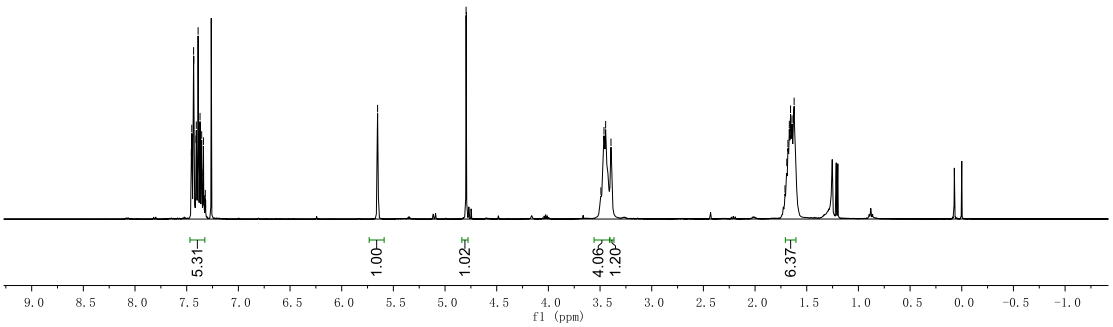


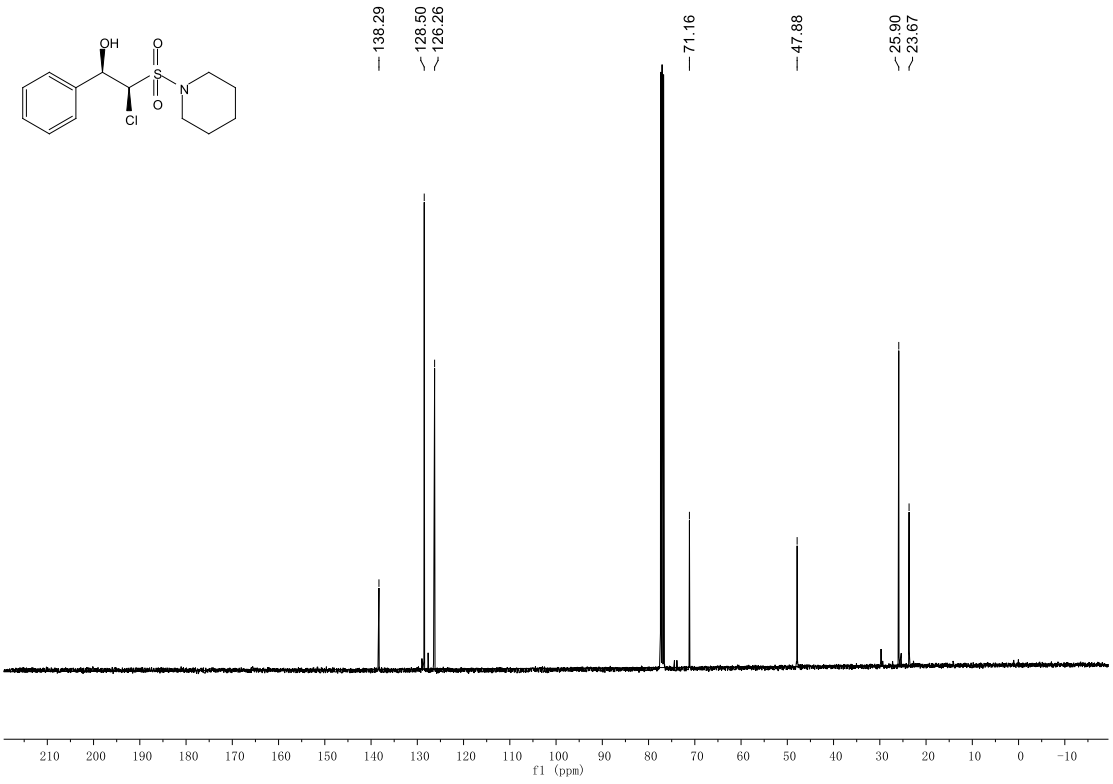
NMR spectra of **2n**



NMR spectra of **2o**


7.46
7.45
7.43
7.43
7.42
7.41
7.41
7.40
7.39
7.39
7.37
7.37
7.36
7.36
7.35
7.34
7.34
7.33
7.32
7.32
7.32
5.65
4.80
4.79
3.49
3.46
3.45
3.39
1.71
1.69
1.68
1.67
1.66
1.64
1.62
OH
O
S
O
N
Cl

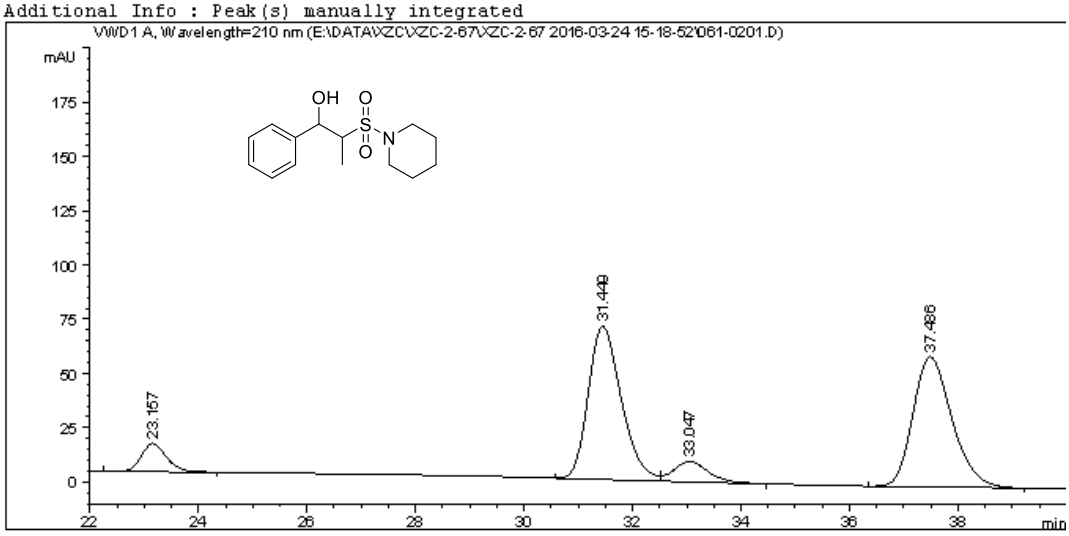

5.31
1.00
1.02
4.06
1.20
6.37
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


OH
O
S
O
N
Cl
138.29
128.50
126.26
71.16
47.88
25.90
23.67
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

4. HPLC spectra of 2

Data File E:\DATA\XZC\XZC-2-67\XZC-2-67 2016-03-24 15-18-52\061-0201.D
Sample Name: XZC-2-67-RAC

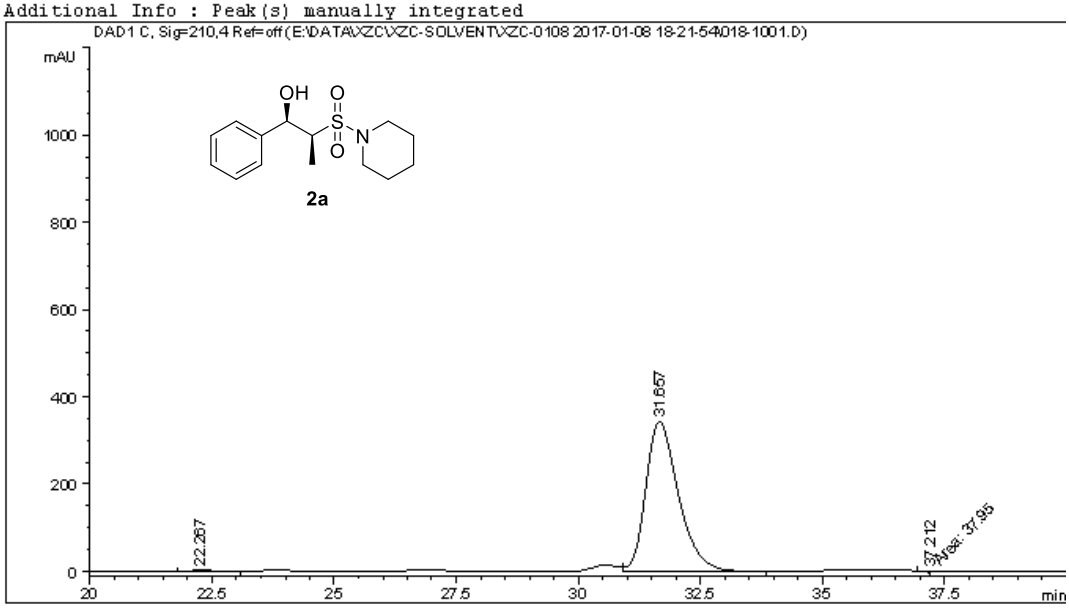
```
    ======================================================================
    Acq. Operator   : SYSTEM                       Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 61
    Injection Date  : 3/24/2016 3:32:09 PM               Inj :   1
                                                  Inj Volume : 2.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-2-67\XZC-2-67 2016-03-24 15-18-52\VWD-AD(1-6)-95-5-1ML-
                      2UL-210NM-40MIN.M
    Last changed    : 3/24/2016 3:18:53 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-2-67\XZC-2-67 2016-03-24 15-18-52\VWD-AD(1-6)-95-5-1ML-
                      2UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 1/31/2018 10:45:18 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  23.157 BB    0.4983  421.81094   12.97389   6.1793
       2  31.449 BV    0.6489 2989.59863   70.61687  43.7959
       3  33.047 VB    0.6679  422.25525    9.47600   6.1858
       4  37.486 BB    0.7661 2992.54688   59.97440  43.8391

    Totals :                  6826.21170  153.04116


    ======================================================================
                            *** End of Report ***

1260HPLC-VWD 1/31/2018 10:45:34 AM SYSTEM                    Page 1 of 1
```

Data File E:\DATA\XZC\XZC-SOLVENT\XZC-0108 2017-01-08 18-21-54\018-1001.D
Sample Name: XZC-8

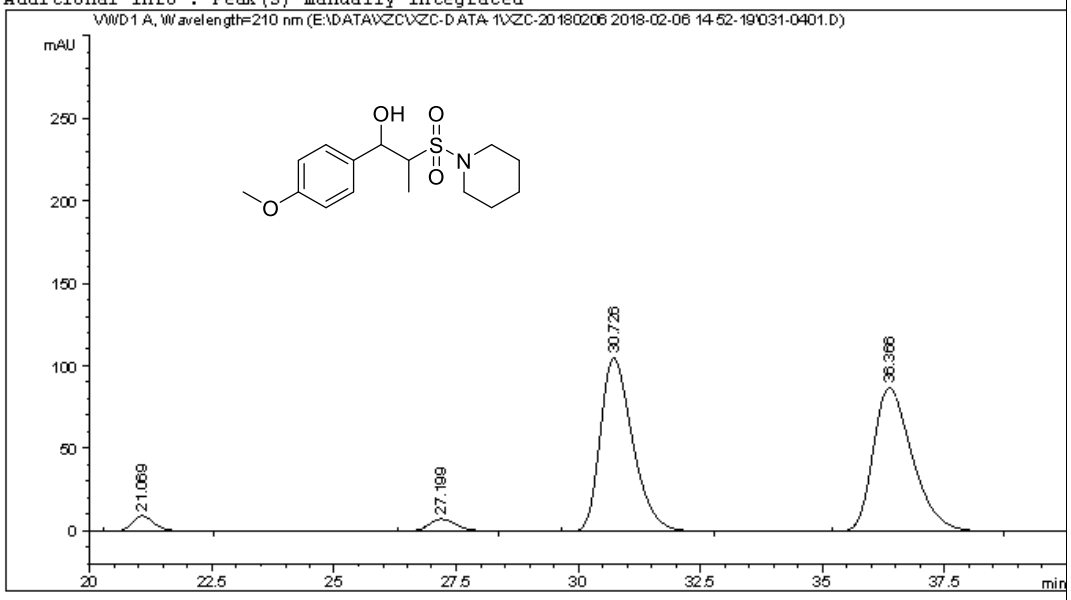
```
    ====================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :  10
    Acq. Instrument : 1260HPLC-DAD                     Location : Vial 18
    Injection Date  : 1/8/2017 11:31:08 PM                  Inj :  1
                                                    Inj Volume : 2.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-SOLVENT\XZC-0108 2017-01-08 18-21-54\DAD-AD(1-6)-95-5-
                      1ML-2UL-ALL-40MIN.M
    Last changed    : 1/8/2017 6:21:54 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-SOLVENT\XZC-0108 2017-01-08 18-21-54\DAD-AD(1-6)-95-5-
                      1ML-2UL-ALL-40MIN.M (Sequence Method)
    Last changed    : 1/31/2018 11:14:59 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ====================================================================
                            Area Percent Report
    ====================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 C, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1  22.267 BB    0.3636   73.06175    2.43803   0.4573
       2  31.657 VB    0.7057 1.58643e4   342.95178  99.3051
       3  37.212 MM    0.2184   37.95001    2.89608   0.2376

    Totals :                  1.59753e4   348.28589


    ====================================================================
```

Data File E:\DATA\XZC\XZC-DATA-1\XZC-20180206 2018-02-06 14-52-19\031-0401.D
Sample Name: XZC-pMeO-RAC

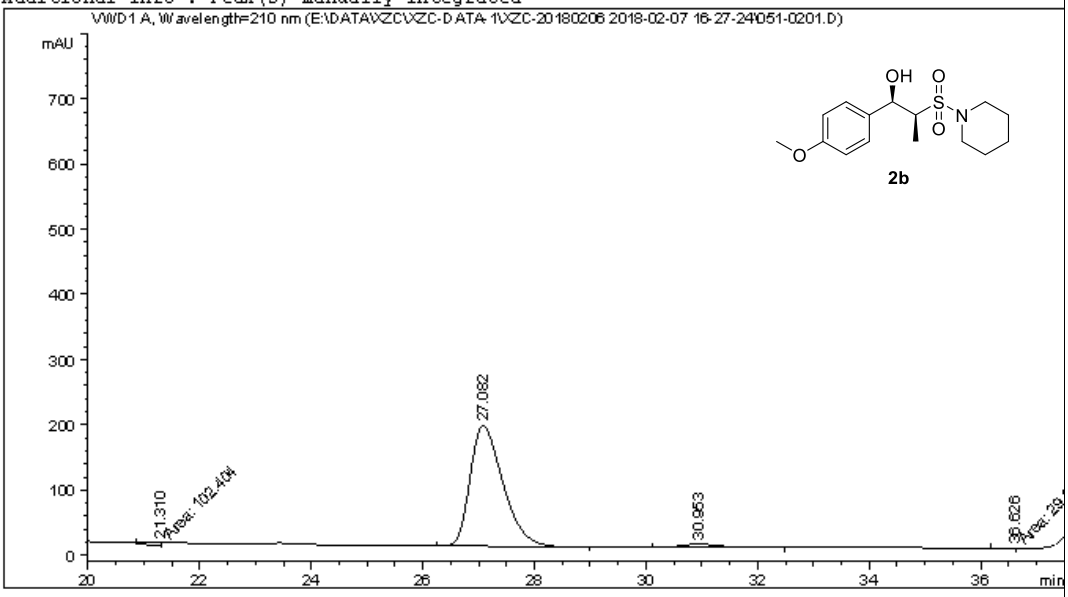
```
    ==================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   4
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 31
    Injection Date  : 2/6/2018 4:11:48 PM                 Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-DATA-1\XZC-20180206 2018-02-06 14-52-19\VWD-AD(1-2)-90-
                      10-1ML-3UL-210NM-60MIN.M
    Last changed    : 2/6/2018 2:52:19 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-DATA-1\XZC-20180206 2018-02-06 14-52-19\VWD-AD(1-2)-90-
                      10-1ML-3UL-210NM-60MIN.M (Sequence Method)
    Last changed    : 2/7/2018 5:31:16 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ==================================================================
                          Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  21.069 BB    0.4805  297.71381    9.40053   2.9016
       2  27.199 BB    0.5998  287.37119    7.29231   2.8008
       3  30.726 BB    0.7111 4836.73535  105.05968  47.1408
       4  36.366 BB    0.8573 4838.36865   86.93582  47.1567

    Totals :                  1.02602e4   208.68834
```

Data File E:\DATA\XZC\XZC-DATA-1\XZC-20180206 2018-02-07 16-27-24\051-0201.D
Sample Name: XZC-pMeO

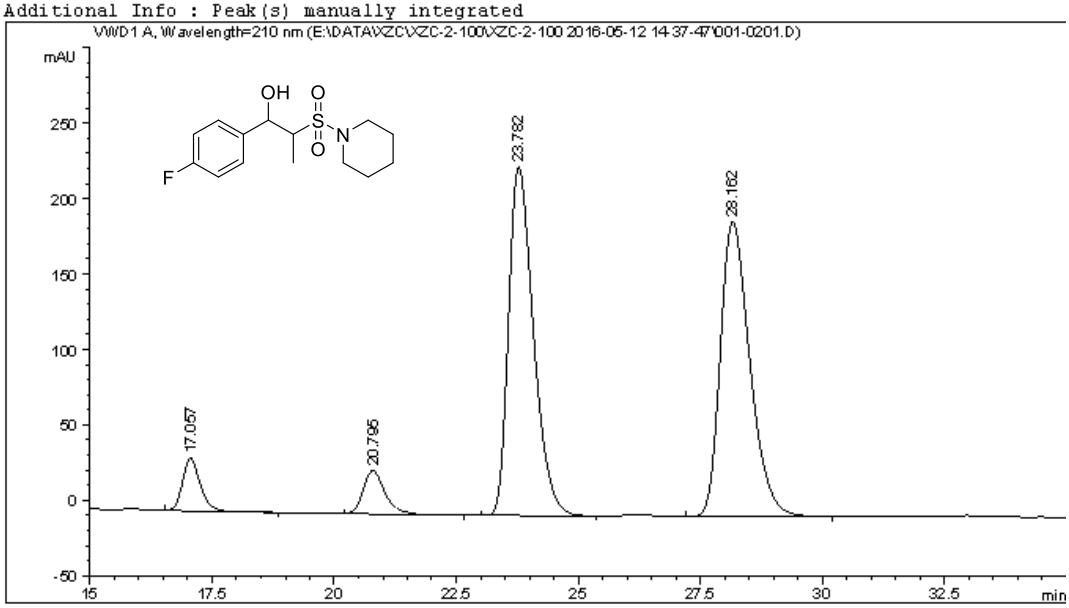
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 51
    Injection Date  : 2/7/2018 4:34:07 PM                  Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-DATA-1\XZC-20180206 2018-02-07 16-27-24\VWD-AD(1-2)-90-
                      10-1ML-3UL-210NM-55MIN.M
    Last changed    : 2/7/2018 5:01:54 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\XZC\XZC-DATA-1\XZC-20180206 2018-02-07 16-27-24\VWD-AD(1-2)-90-
                      10-1ML-3UL-210NM-55MIN.M (Sequence Method)
    Last changed    : 2/7/2018 5:20:57 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  21.310 MM    0.3104  102.40383    5.49849   1.2971
       2  27.082 BB    0.6249 7546.66797  184.60147  95.5934
       3  30.953 BB    0.6843  216.19571    4.72986   2.7385
       4  36.626 MM    0.4421   29.27939    1.10390   0.3709

    Totals :                  7894.54690  195.93371
```

Data File E:\DATA\XZC\XZC-2-100\XZC-2-100 2016-05-12 14-37-47\001-0201.D
Sample Name: XZC-pF-RAC

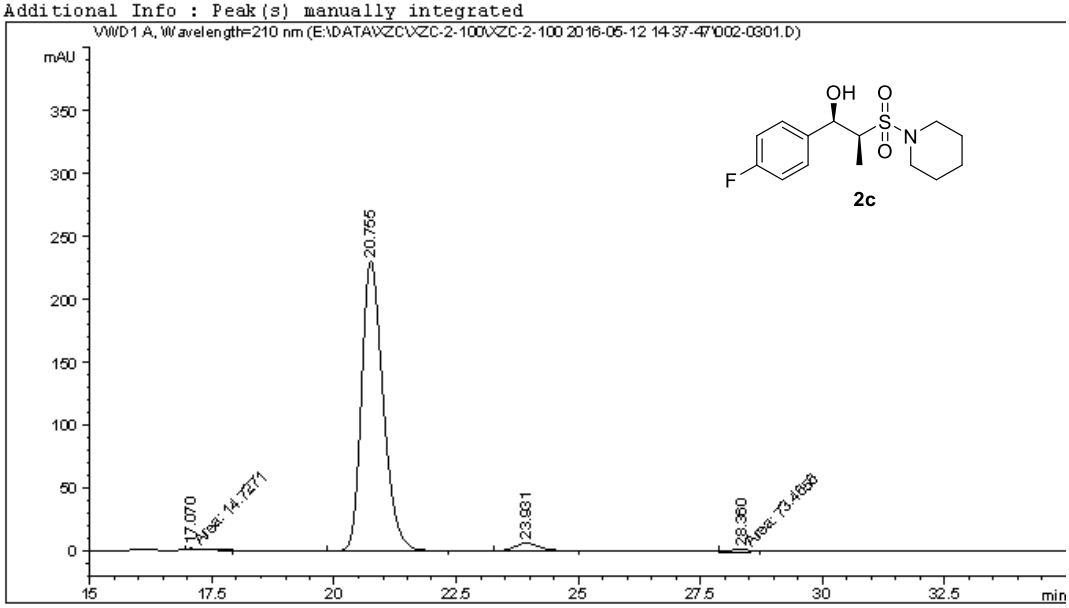
```
    ====================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 1
    Injection Date  : 5/12/2016 2:49:23 PM                 Inj :   1
                                                     Inj Volume : 4.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-2-100\XZC-2-100 2016-05-12 14-37-47\VWD-AD(1-6)-92-8-1ML
                      -4UL-210-40MIN.M
    Last changed    : 5/12/2016 2:37:47 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-2-100\XZC-2-100 2016-05-12 14-37-47\VWD-AD(1-6)-92-8-1ML
                      -4UL-210-40MIN.M (Sequence Method)
    Last changed    : 11/28/2017 4:23:15 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ====================================================================
                            Area Percent Report
    ====================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  17.057 VB    0.3898  899.51599   35.00694   4.9471
       2  20.795 BB    0.4714  889.47961   28.71784   4.8919
       3  23.782 BB    0.5454 8183.15869  230.95163  45.0055
       4  28.162 BB    0.6484 8210.42480  195.33456  45.1554

    Totals :                  1.81826e4   490.01097
```

Data File E:\DATA\XZC\XZC-2-100\XZC-2-100 2016-05-12 14-37-47\002-0301.D
Sample Name: XZC-pF

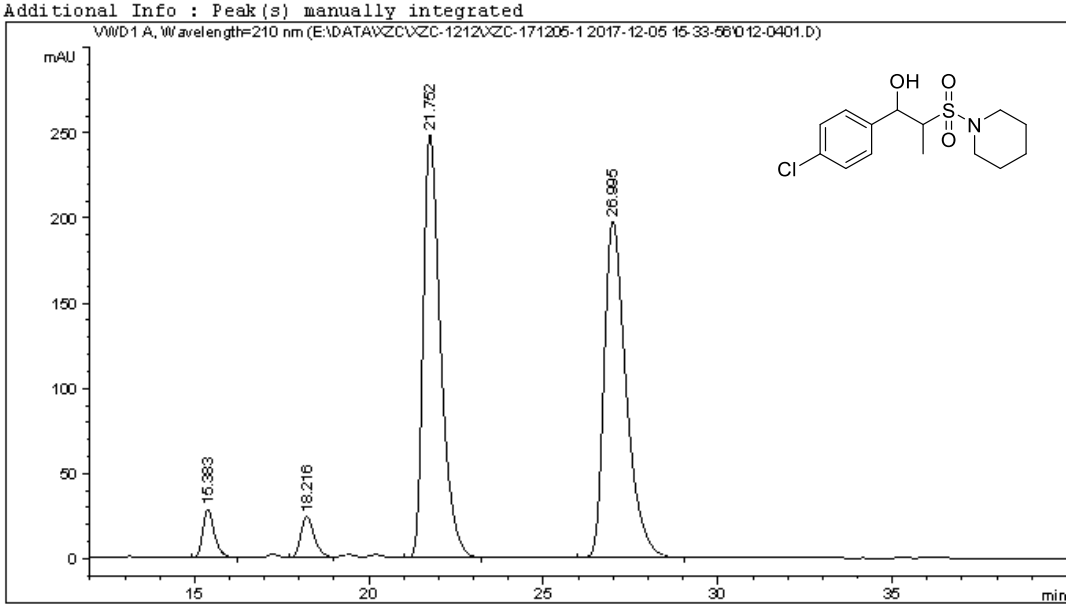
```
    ==================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   3
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 2
    Injection Date  : 5/12/2016 3:30:05 PM                 Inj :   1
                                                     Inj Volume : 4.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-2-100\XZC-2-100 2016-05-12 14-37-47\VWD-AD(1-6)-92-8-1ML
                      -4UL-210-40MIN.M
    Last changed    : 5/12/2016 2:37:47 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-2-100\XZC-2-100 2016-05-12 14-37-47\VWD-AD(1-6)-92-8-1ML
                      -4UL-210-40MIN.M (Sequence Method)
    Last changed    : 1/30/2018 9:47:38 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ==================================================================
                          Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1  17.070 MM    0.2400   14.72710    1.02256   0.2004
       2  20.755 BB    0.4715 7050.44043  230.05257  95.9543
       3  23.931 BB    0.5263  209.07404    5.94462   2.8454
       4  28.360 MM    0.5776   73.46560    1.59887   0.9998

    Totals :                  7347.70716  238.61861
```

Data File E:\DATA\XZC\XZC-1212\XZC-171205-1 2017-12-05 15-33-56\012-0401.D
Sample Name: XZC-pCl-RAC

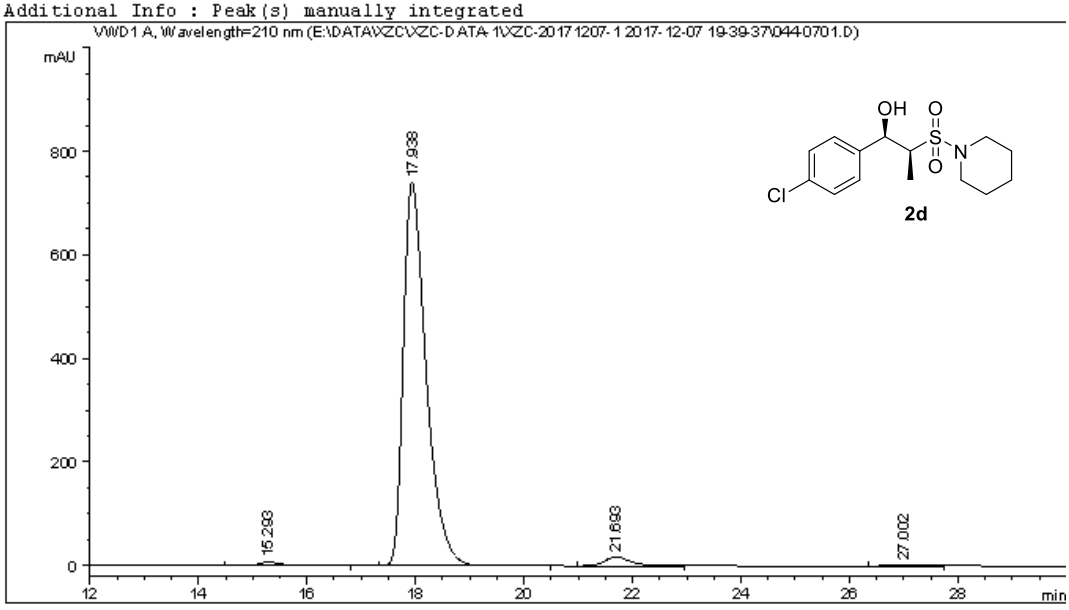
```
    ====================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   4
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 12
    Injection Date  : 12/5/2017 4:57:02 PM                  Inj :   1
                                                    Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-1212\XZC-171205-1 2017-12-05 15-33-56\VWD-AD(1-2)-90-10-
                      1ML-3UL-210NM-60MIN.M
    Last changed    : 12/5/2017 3:33:56 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-1212\XZC-171205-1 2017-12-05 15-33-56\VWD-AD(1-2)-90-10-
                      1ML-3UL-210NM-60MIN.M (Sequence Method)
    Last changed    : 12/5/2017 7:31:54 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ====================================================================
                            Area Percent Report
    ====================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1  15.383 BB    0.3529  664.29095   28.50526   3.5790
       2  18.216 BB    0.4116  643.54938   23.86432   3.4672
       3  21.752 BB    0.5257 8609.07129  248.15921  46.3830
       4  26.995 BB    0.6656 8643.92383  197.49571  46.5708

    Totals :                  1.85608e4   498.02450
```

Data File E:\DATA\XZC\XZC-DATA-1\XZC-20171207-1 2017-12-07 19-39-37\044-0701.D
Sample Name: XZC-pCl

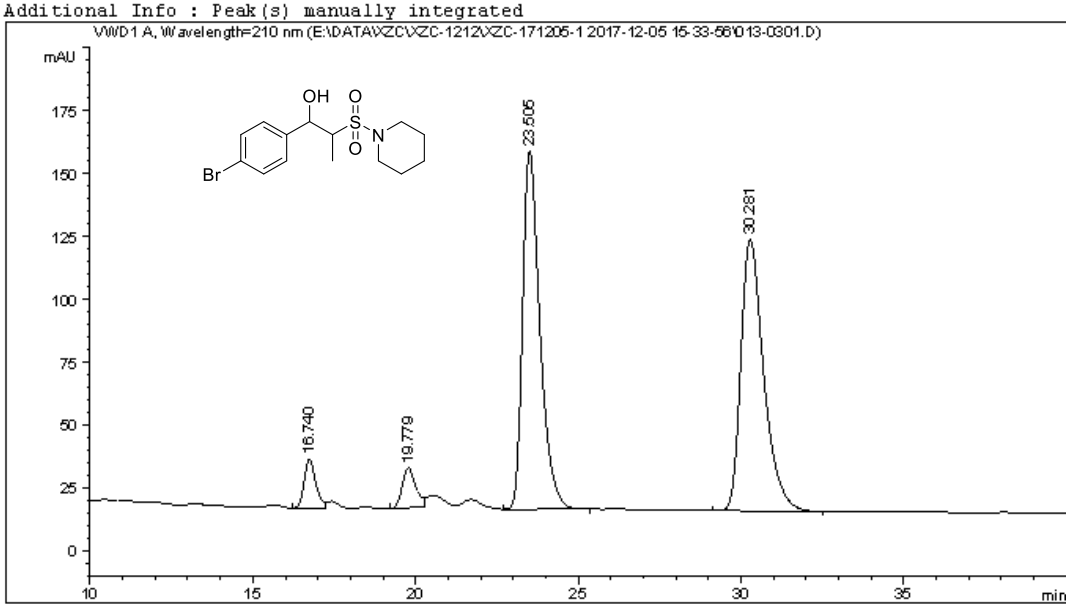
```
    ====================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   7
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 44
    Injection Date  : 12/7/2017 11:01:41 PM                 Inj :   1
                                                    Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-DATA-1\XZC-20171207-1 2017-12-07 19-39-37\VWD-AD(1-2)-90
                      -10-1ML-3UL-210NM-35MIN.M
    Last changed    : 12/7/2017 9:21:36 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-DATA-1\XZC-20171207-1 2017-12-07 19-39-37\VWD-AD(1-2)-90
                      -10-1ML-3UL-210NM-35MIN.M (Sequence Method)
    Last changed    : 12/8/2017 3:43:40 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ====================================================================
                            Area Percent Report
    ====================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  15.293 BB    0.4480  232.02040    7.39508   1.0296
       2  17.938 BB    0.4440 2.16397e4   740.34814  96.0304
       3  21.693 BB    0.5052  574.63031   17.26842   2.5500
       4  27.002 BB    0.5256   87.86292    2.47838   0.3899

    Totals :                  2.25342e4   767.49003
```

Data File E:\DATA\XZC\XZC-1212\XZC-171205-1 2017-12-05 15-33-56\013-0301.D
Sample Name: XZC-pBr-RAC

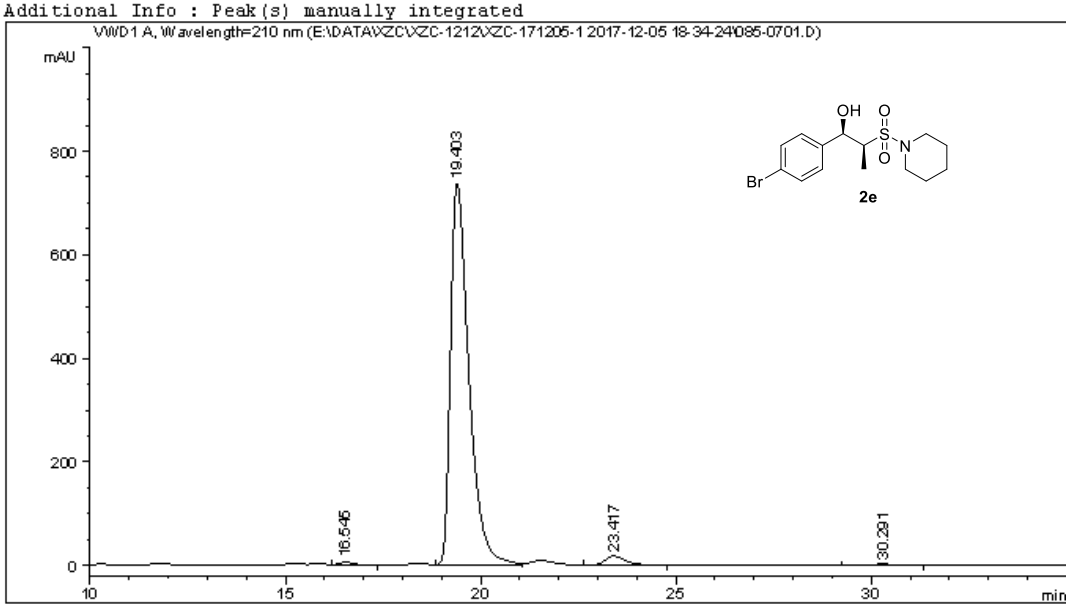
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   3
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 13
    Injection Date  : 12/5/2017 3:56:19 PM                  Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-1212\XZC-171205-1 2017-12-05 15-33-56\VWD-AD(1-2)-90-10-
                      1ML-3UL-210NM-60MIN.M
    Last changed    : 12/5/2017 3:33:56 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-1212\XZC-171205-1 2017-12-05 15-33-56\VWD-AD(1-2)-90-10-
                      1ML-3UL-210NM-60MIN.M (Sequence Method)
    Last changed    : 12/5/2017 7:33:52 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1  16.740 BV    0.3770  483.89499   19.53674   4.2205
       2  19.779 BV    0.4401  453.79520   15.75098   3.9580
       3  23.505 BB    0.5596 5252.73975  142.31259  45.8139
       4  30.281 BB    0.7396 5274.95996  108.05169  46.0077

    Totals :                  1.14654e4   285.65200
```

Data File E:\DATA\XZC\XZC-1212\XZC-171205-1 2017-12-05 18-34-24\085-0701.D
Sample Name: XZC-pBr

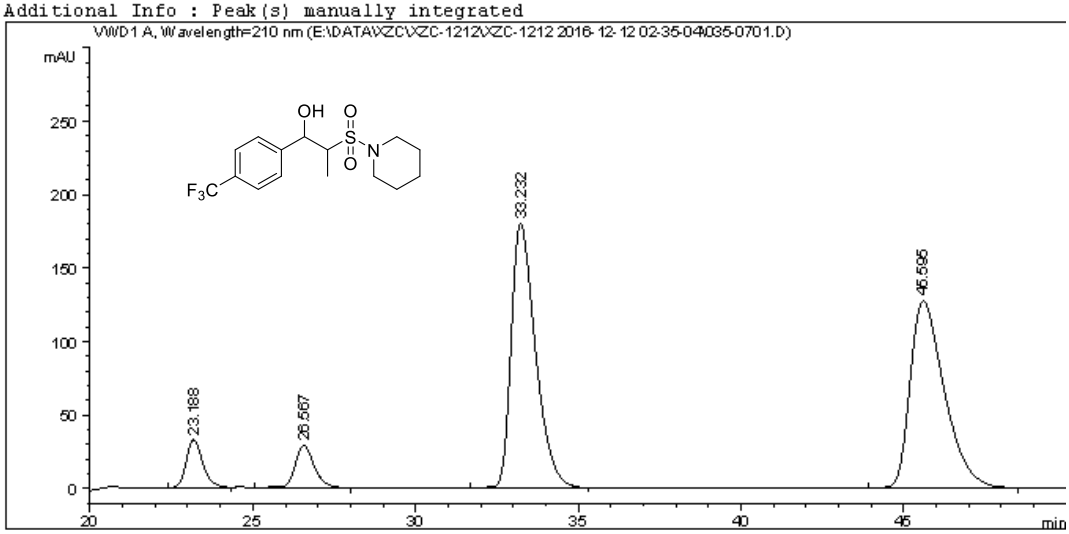
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   7
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 85
    Injection Date  : 12/5/2017 9:49:50 PM                  Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-1212\XZC-171205-1 2017-12-05 18-34-24\VWD-AD(1-2)-90-10-
                      1ML-3UL-210NM-35MIN.M
    Last changed    : 12/5/2017 7:44:47 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-1212\XZC-171205-1 2017-12-05 18-34-24\VWD-AD(1-2)-90-10-
                      1ML-3UL-210NM-35MIN.M (Sequence Method)
    Last changed    : 12/6/2017 9:45:16 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  16.545 VB    0.4059  166.05728    6.05576   0.6628
       2  19.403 VV    0.4950 2.41477e4   737.42615  96.3779
       3  23.417 BB    0.5564  647.40631   17.58978   2.5839
       4  30.291 BB    0.6023   94.07124    1.92788   0.3755

    Totals :                  2.50553e4   762.99957
```

Data File E:\DATA\XZC\XZC-1212\XZC-1212 2016-12-12 02-35-04\035-0701.D
Sample Name: xzc-CF3-rac

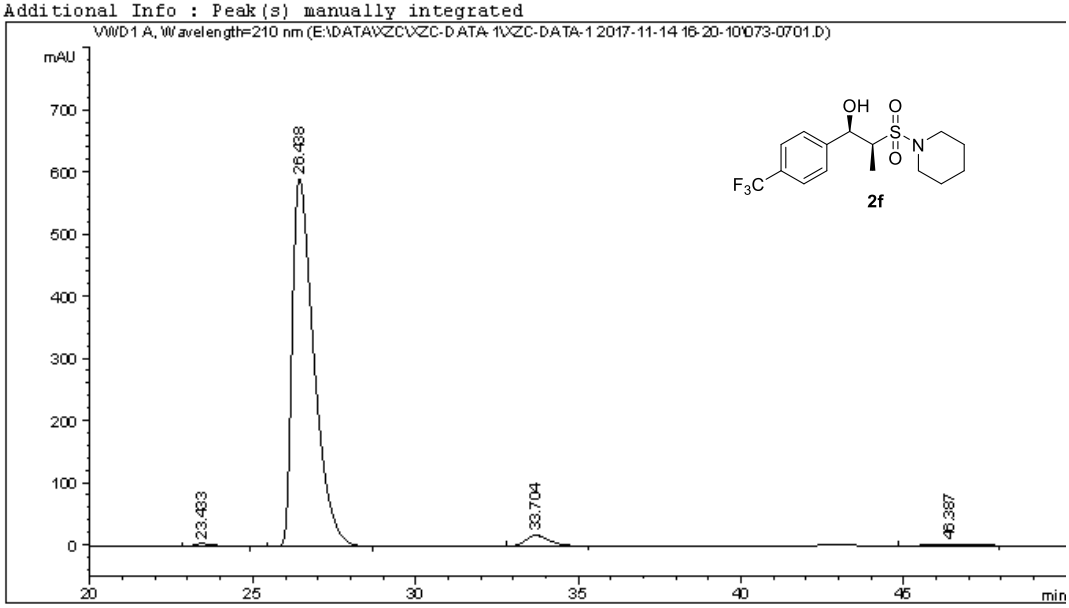
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   7
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 35
    Injection Date  : 12/12/2016 5:01:36 AM              Inj :   1
                                                   Inj Volume : 4.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-1212\XZC-1212 2016-12-12 02-35-04\VWD-AD(1-6)-95-5-1ML-
                      4UL-210NM-50MIN.M
    Last changed    : 12/12/2016 2:35:05 AM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-1212\XZC-1212 2016-12-12 02-35-04\VWD-AD(1-6)-95-5-1ML-
                      4UL-210NM-50MIN.M (Sequence Method)
    Last changed    : 11/28/2017 4:40:11 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  23.188 BB    0.5425 1149.04565   32.41593   5.4825
       2  26.567 BB    0.6273 1200.33289   29.03751   5.7272
       3  33.232 BB    0.7942 9298.99902  179.55937  44.3685
       4  45.595 BB    1.1117 9310.17188  127.37707  44.4218

    Totals :                  2.09585e4   368.38988


    ======================================================================
                            *** End of Report ***
```

Data File E:\DATA\XZC\XZC-DATA-1\XZC-DATA-1 2017-11-14 16-20-10\073-0701.D
Sample Name: XZC-pCF3

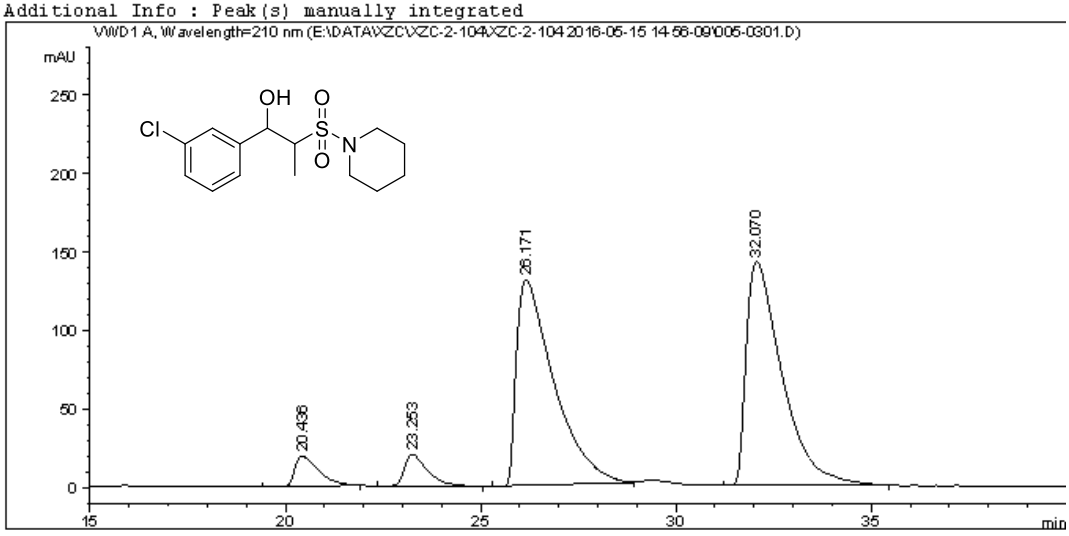
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   7
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 73
    Injection Date  : 11/14/2017 6:35:30 PM                 Inj :   1
                                                    Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-DATA-1\XZC-DATA-1 2017-11-14 16-20-10\VWD-AD(1-6)-95-5-
                      1ML-3UL-210NM-50MIN.M
    Last changed    : 11/14/2017 4:27:08 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-DATA-1\XZC-DATA-1 2017-11-14 16-20-10\VWD-AD(1-6)-95-5-
                      1ML-3UL-210NM-50MIN.M (Sequence Method)
    Last changed    : 11/28/2017 4:37:32 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  23.433 BB    0.6091  188.38914    4.53110   0.6593
       2  26.438 BB    0.7038 2.73050e4   592.32495  95.5608
       3  33.704 BB    0.7839  894.46082   17.36694   3.1304
       4  46.387 BB    0.9704  185.56932    2.43977   0.6494

    Totals :                  2.85734e4   616.66276
```

Data File E:\DATA\XZC\XZC-2-104\XZC-2-104 2016-05-15 14-56-09\005-0301.D
Sample Name: XZC-mCl-RAC

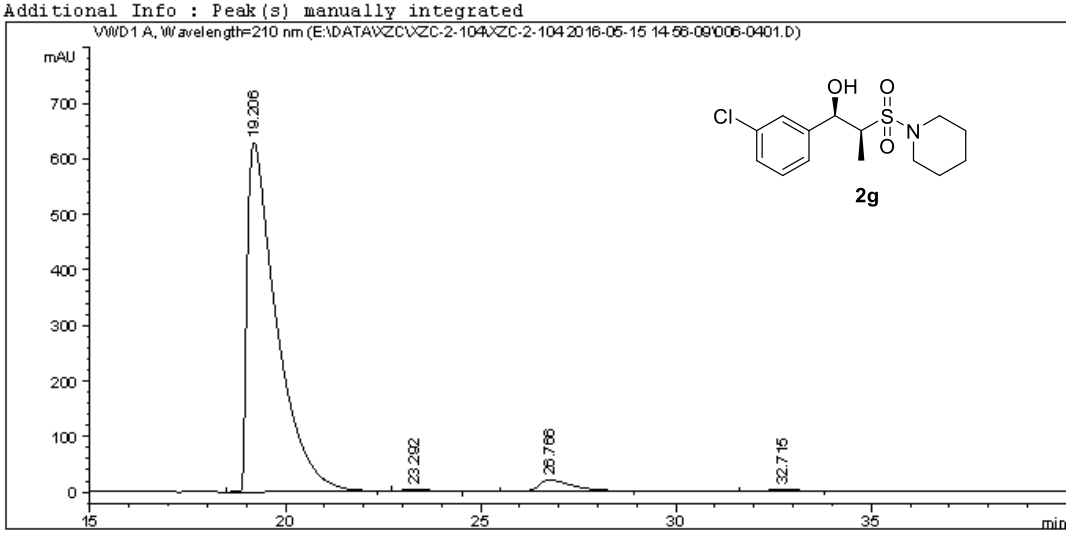
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   3
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 5
    Injection Date  : 5/15/2016 3:19:36 PM               Inj :   1
                                                   Inj Volume : 2.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-2-104\XZC-2-104 2016-05-15 14-56-09\VWD-IB(1-2)-97-3-1ML
                      -2UL-210NM-40MIN.M
    Last changed    : 5/15/2016 2:56:09 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-2-104\XZC-2-104 2016-05-15 14-56-09\VWD-IB(1-2)-97-3-1ML
                      -2UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 11/28/2017 4:26:54 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  20.436 BB    0.6218  802.07056   18.91135   4.1311
       2  23.253 BB    0.6063  833.85675   20.33982   4.2948
       3  26.171 BB    0.9635 8723.99121  130.73433  44.9332
       4  32.070 BB    0.9634 9055.54590  142.10783  46.6409

    Totals :                  1.94155e4   312.09334


    ======================================================================
                            *** End of Report ***
```

Data File E:\DATA\XZC\XZC-2-104\XZC-2-104 2016-05-15 14-56-09\006-0401.D
Sample Name: XZC-mCl

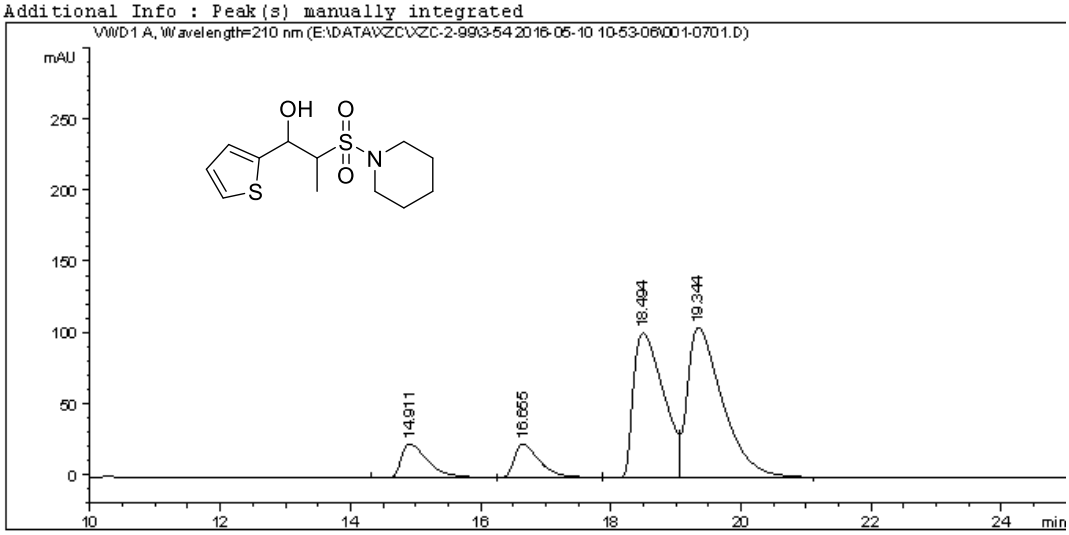
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   4
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 6
    Injection Date  : 5/15/2016 4:00:23 PM                 Inj :   1
                                                     Inj Volume : 4.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-2-104\XZC-2-104 2016-05-15 14-56-09\VWD-IB(1-2)-97-3-1ML
                      -4UL-210NM-40MIN.M
    Last changed    : 5/15/2016 2:56:09 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-2-104\XZC-2-104 2016-05-15 14-56-09\VWD-IB(1-2)-97-3-1ML
                      -4UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 11/28/2017 4:28:42 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  19.206 BB    0.7531 3.28460e4   629.11493  95.4122
       2  23.292 BB    0.6077  139.80862    3.42178   0.4061
       3  26.766 BB    0.8807 1271.44910   20.93083   3.6933
       4  32.715 BB    0.6438  168.11588    3.13922   0.4883

    Totals :                  3.44254e4   656.60676


    ======================================================================
                            *** End of Report ***
```

Data File E:\DATA\XZC\XZC-2-99\3-54 2016-05-10 10-53-06\001-0701.D
Sample Name: XZC-thio-RAC

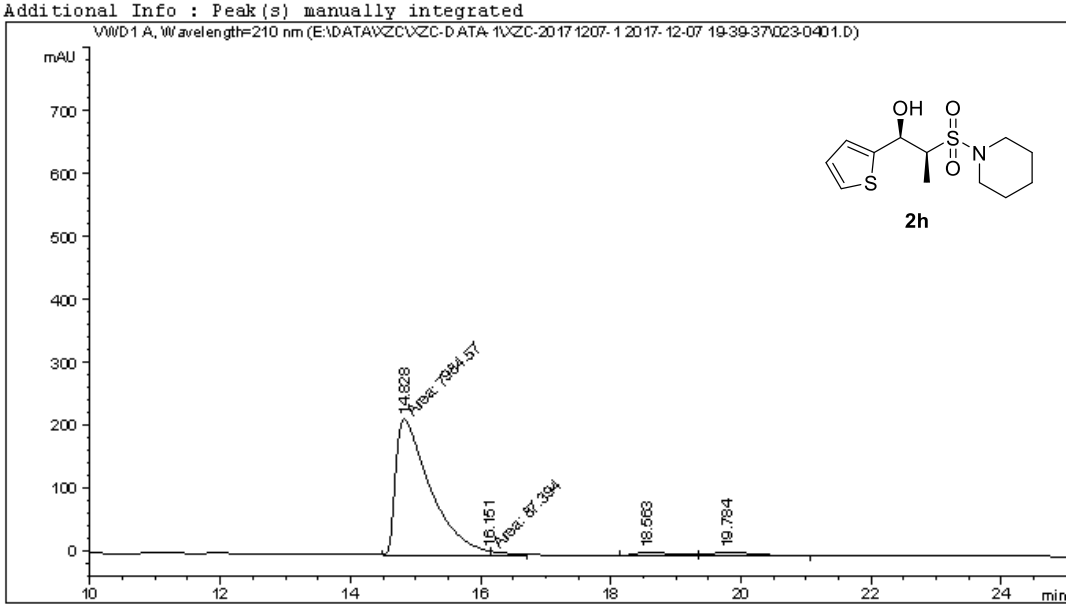
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   7
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 1
    Injection Date  : 5/10/2016 1:58:30 PM                  Inj :   1
                                                      Inj Volume : 4.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-2-99\3-54 2016-05-10 10-53-06\VWD-IB(1-2)-95-5-1ML-4UL-
                      210NM-40MIN.M
    Last changed    : 5/10/2016 2:28:03 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\XZC\XZC-2-99\3-54 2016-05-10 10-53-06\VWD-IB(1-2)-95-5-1ML-4UL-
                      210NM-40MIN.M (Sequence Method)
    Last changed    : 1/31/2018 11:30:28 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  14.911 BB    0.4353  671.86102   23.65860   7.9328
       2  16.655 BB    0.4026  629.86420   23.65797   7.4370
       3  18.494 BV    0.5004 3243.50854  101.34515  38.2969
       4  19.344 VB    0.5566 3924.13721  105.10754  46.3333

    Totals :                  8469.37097  253.76925


    ======================================================================
                              *** End of Report ***
```

Data File E:\DATA\XZC\XZC-DATA-1\XZC-20171207-1 2017-12-07 19-39-37\023-0401.D
Sample Name: XZC-thio

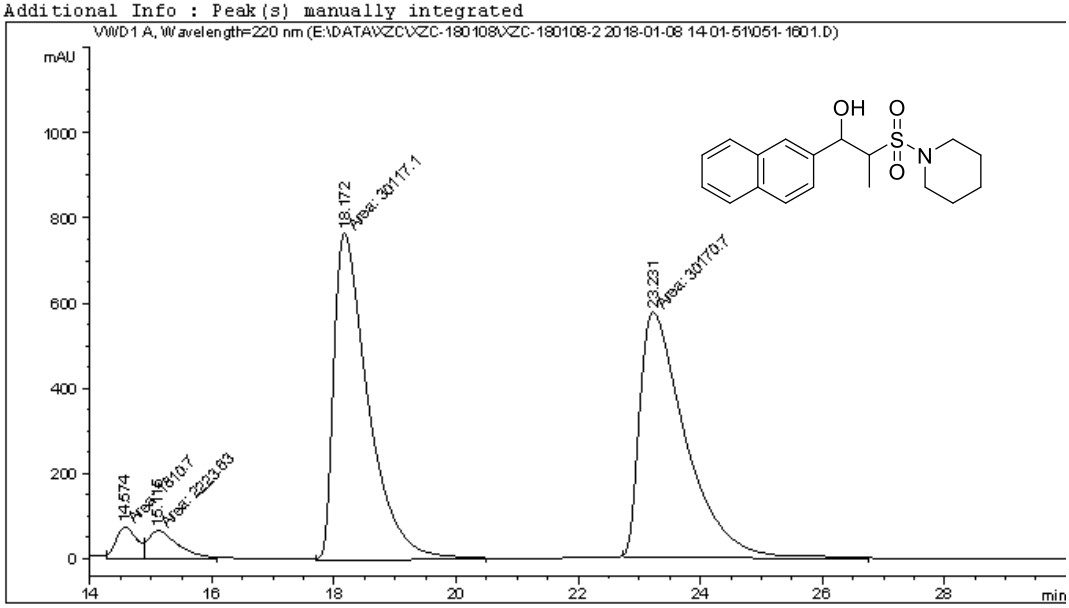
```
    ====================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   4
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 23
    Injection Date  : 12/7/2017 9:33:18 PM               Inj :   1
                                                   Inj Volume : 2.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-DATA-1\XZC-20171207-1 2017-12-07 19-39-37\VWD-IB(1-6)-95
                      -5-1ML-2UL-210NM-40MIN.M
    Last changed    : 12/7/2017 7:46:25 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-DATA-1\XZC-20171207-1 2017-12-07 19-39-37\VWD-IB(1-6)-95
                      -5-1ML-2UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 1/31/2018 11:32:04 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ====================================================================
                            Area Percent Report
    ====================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  14.828 MF    0.6176 7984.56689  215.48038  94.3728
       2  16.151 FM    0.2478   87.39399    5.87807   1.0329
       3  18.563 BV    0.5765  162.58961    4.02280   1.9217
       4  19.784 VB    0.5908  226.11237    5.55620   2.6725

    Totals :                  8460.66286  230.93745
```

Data File E:\DATA\XZC\XZC-180108\XZC-180108-2 2018-01-08 14-01-51\051-1601.D
Sample Name: XZC-naph-RAC

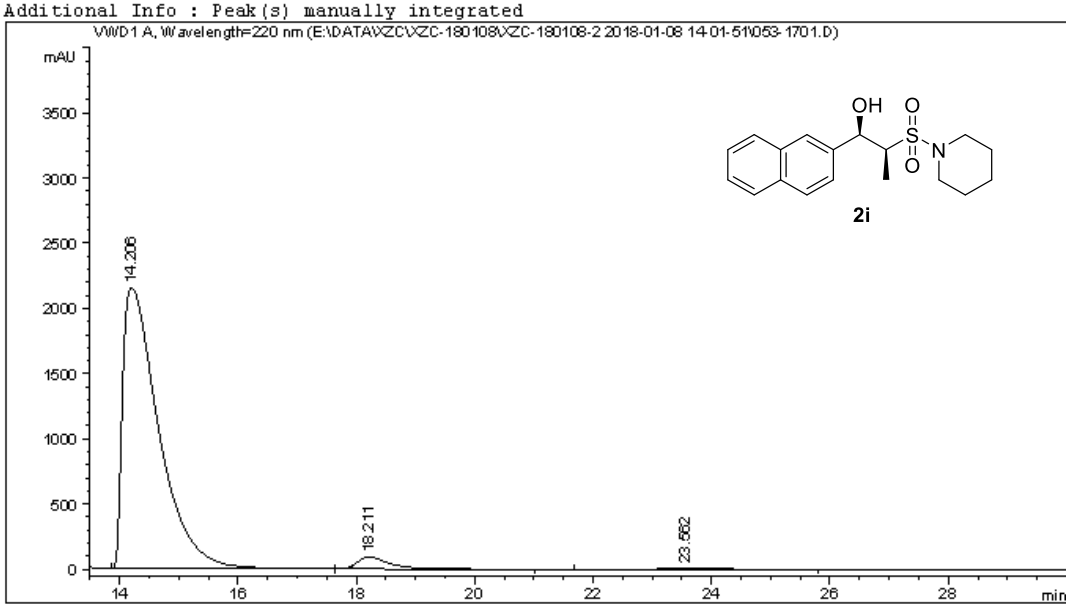
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :  16
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 51
    Injection Date  : 1/8/2018 10:39:31 PM                  Inj :  1
                                                     Inj Volume : 1.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-180108\XZC-180108-2 2018-01-08 14-01-51\VWD-IB(1-6)-90-
                      10-1ML-1UL-220NM-30MIN.M
    Last changed    : 1/8/2018 9:58:10 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-180108\XZC-180108-2 2018-01-08 14-01-51\VWD-IB(1-6)-90-
                      10-1ML-1UL-220NM-30MIN.M (Sequence Method)
    Last changed    : 1/31/2018 10:18:34 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=220 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1  14.574 MF    0.4078 1810.70276   74.00624   2.8151
       2  15.115 FM    0.5645 2223.62793   65.64807   3.4570
       3  18.172 MM    0.6538 3.0117le4   767.68579  46.8223
       4  23.231 MM    0.8742 3.01707e4   575.20032  46.9056

    Totals :                  6.43220e4  1482.54042
```

Data File E:\DATA\XZC\XZC-180108\XZC-180108-2 2018-01-08 14-01-51\053-1701.D
Sample Name: XZC-naph

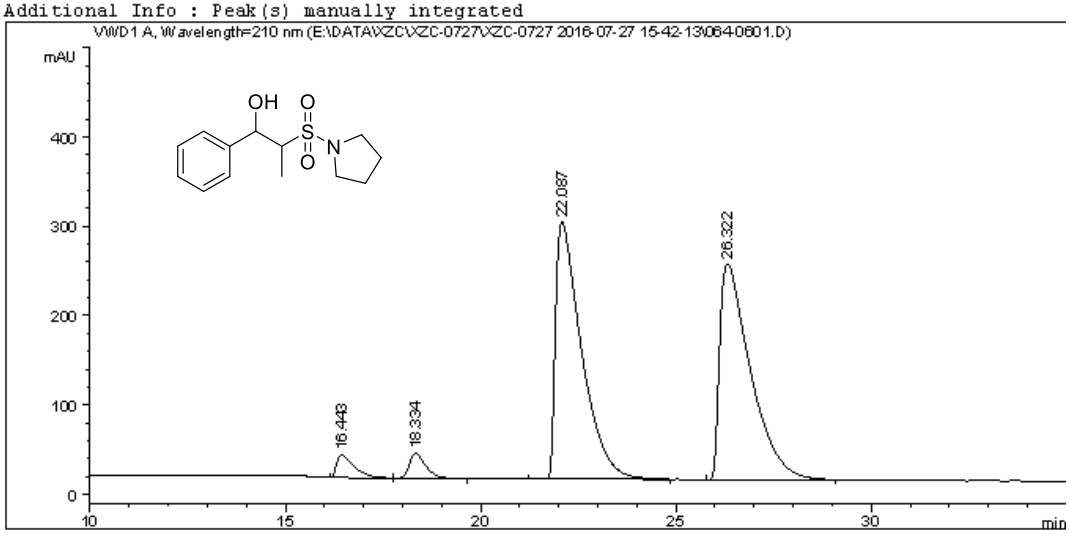
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :  17
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 53
    Injection Date  : 1/8/2018 11:10:16 PM                 Inj :  1
                                                     Inj Volume : 1.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-180108\XZC-180108-2 2018-01-08 14-01-51\VWD-IB(1-6)-90-
                      10-1ML-1UL-220NM-30MIN.M
    Last changed    : 1/8/2018 9:58:10 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-180108\XZC-180108-2 2018-01-08 14-01-51\VWD-IB(1-6)-90-
                      10-1ML-1UL-220NM-30MIN.M (Sequence Method)
    Last changed    : 1/31/2018 10:23:16 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=220 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  14.206 VB    0.6353 9.13525e4  2156.09497  95.6984
       2  18.211 BB    0.5664 3484.41943   91.67145   3.6502
       3  23.562 BB    0.7990  621.86285   11.26504   0.6514

    Totals :                  9.54588e4  2259.03146


    ======================================================================
```

Data File E:\DATA\XZC\XZC-0727\XZC-0727 2016-07-27 15-42-13\064-0601.D
Sample Name: XZC-5RING-RAC

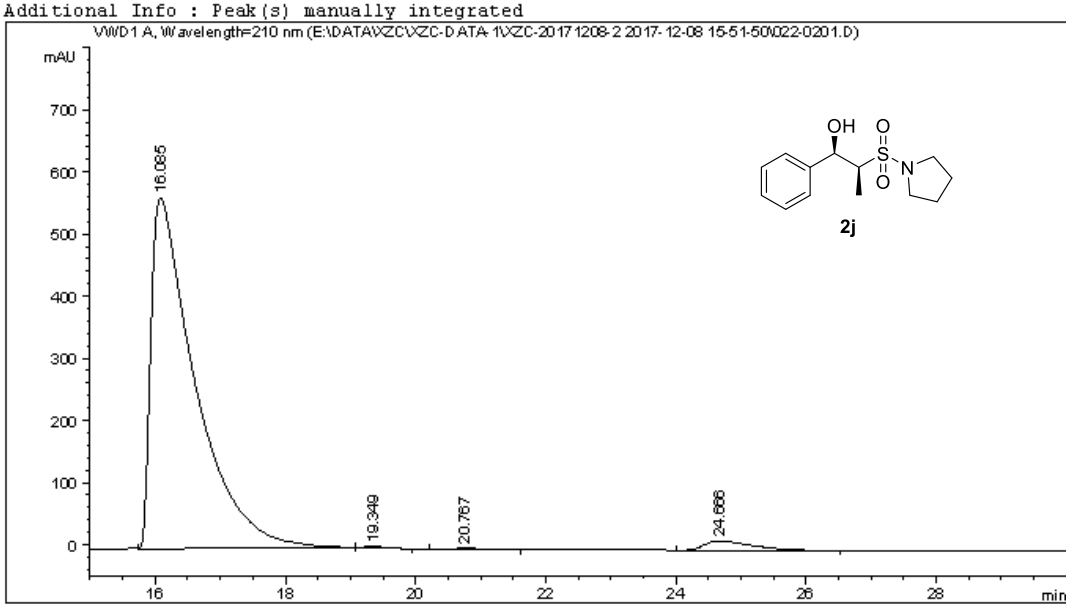
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   6
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 64
    Injection Date  : 7/27/2016 6:27:00 PM                Inj :   1
                                                   Inj Volume : 4.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-0727\XZC-0727 2016-07-27 15-42-13\VWD-IB(1-2)-95-5-1ML-
                      4UL-210NM-40MIN.M
    Last changed    : 7/27/2016 3:42:14 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-0727\XZC-0727 2016-07-27 15-42-13\VWD-IB(1-2)-95-5-1ML-
                      4UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 11/28/2017 8:08:22 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  16.443 BB    0.4612  789.61334   25.50612   2.8097
       2  18.334 BB    0.4444  819.18225   27.91368   2.9149
       3  22.087 BB    0.6821 1.32860e4   288.04010  47.2753
       4  26.322 BB    0.7972 1.32087e4   241.82739  47.0002

    Totals :                  2.81035e4   583.28729


    ======================================================================
                            *** End of Report ***
```

Data File E:\DATA\XZC\XZC-DATA-1\XZC-20171208-2 2017-12-08 15-51-50\022-0201.D
Sample Name: XZC-pyrrole

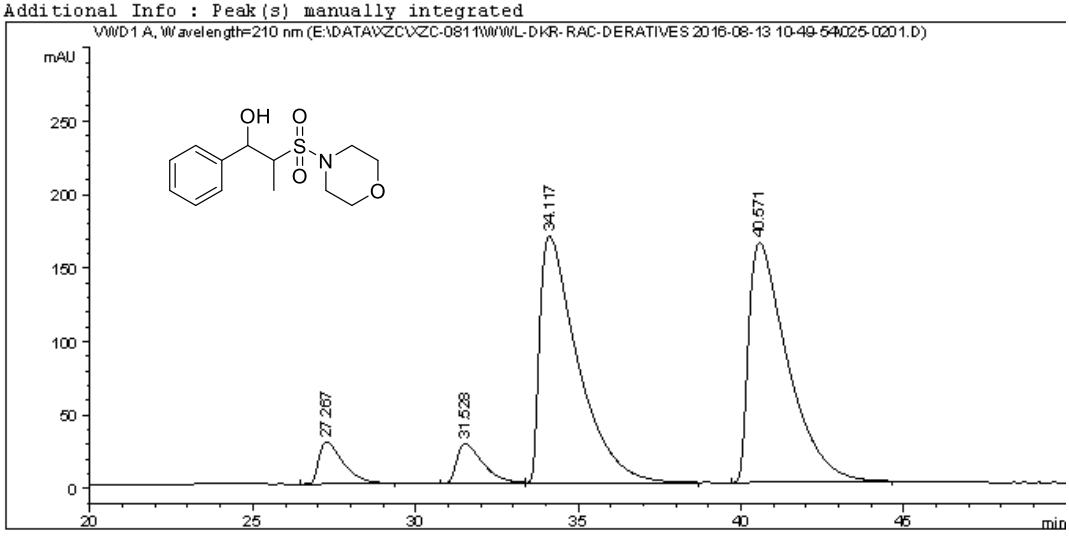
```
    ==================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 22
    Injection Date  : 12/8/2017 4:15:04 PM               Inj :   1
                                                   Inj Volume : 2.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-DATA-1\XZC-20171208-2 2017-12-08 15-51-50\VWD-IB(1-6)-95
                      -5-1ML-2UL-210NM-40MIN.M
    Last changed    : 12/8/2017 3:51:50 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-DATA-1\XZC-20171208-2 2017-12-08 15-51-50\VWD-IB(1-6)-95
                      -5-1ML-2UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 1/30/2018 9:00:12 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ==================================================================
                          Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1  16.085 VB    0.6635 2.64561e4   564.80981  96.7846
       2  19.349 BB    0.3974   45.41839    1.78188   0.1662
       3  20.767 BB    0.5119   66.05001    1.89840   0.2416
       4  24.666 BB    0.7469  767.45490   15.10091   2.8076

    Totals :                  2.73350e4   583.59101
```

Data File E:\DATA\XZC\XZC-0811\WWL-DKR-RAC-DERATIVES 2016-08-13 10-49-54\025-0201.D
Sample Name: XZC-morphine-RAC

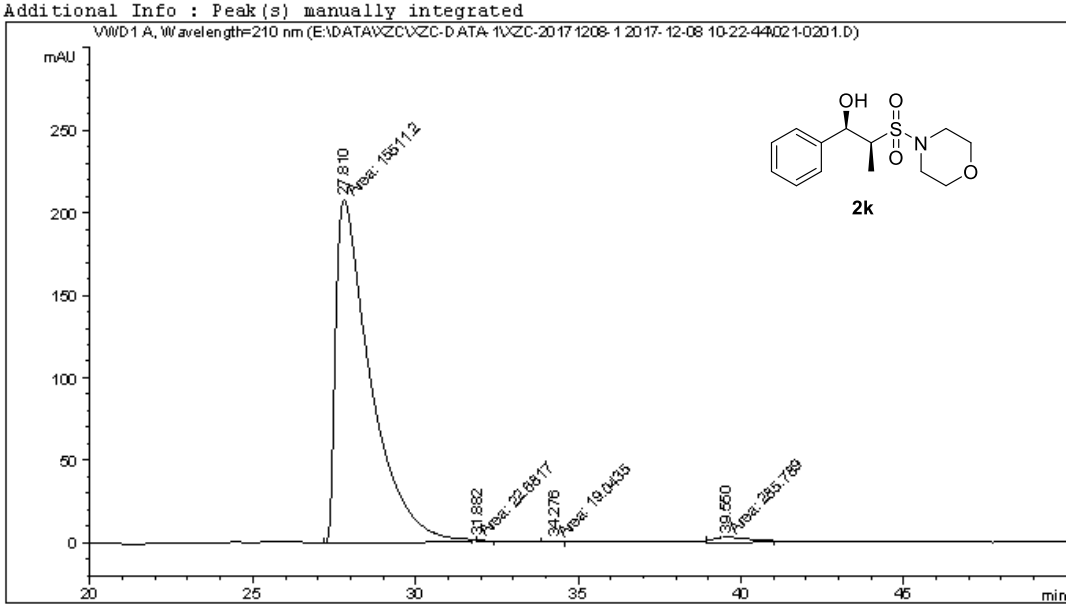
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 25
    Injection Date  : 8/13/2016 11:16:32 AM                 Inj :   1
                                                     Inj Volume : 4.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-0811\WWL-DKR-RAC-DERATIVES 2016-08-13 10-49-54\VWD-IB(1-
                      6)-95-5-1ML-4UL-210NM-60MIN.M
    Last changed    : 8/13/2016 10:49:54 AM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-0811\WWL-DKR-RAC-DERATIVES 2016-08-13 10-49-54\VWD-IB(1-
                      6)-95-5-1ML-4UL-210NM-60MIN.M (Sequence Method)
    Last changed    : 11/28/2017 8:04:12 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  27.267 BB    0.7899 1488.25549   28.65451   4.9443
       2  31.528 BB    0.8258 1473.23047   26.86329   4.8943
       3  34.117 BB    1.1739 1.35865e4   167.58055  45.1368
       4  40.571 BB    1.2328 1.35527e4   163.20480  45.0245

    Totals :                  3.01007e4   386.30315


    ======================================================================
                            *** End of Report ***
```

Data File E:\DATA\XZC\XZC-DATA-1\XZC-20171208-1 2017-12-08 10-22-44\021-0201.D
Sample Name: XZC-morph

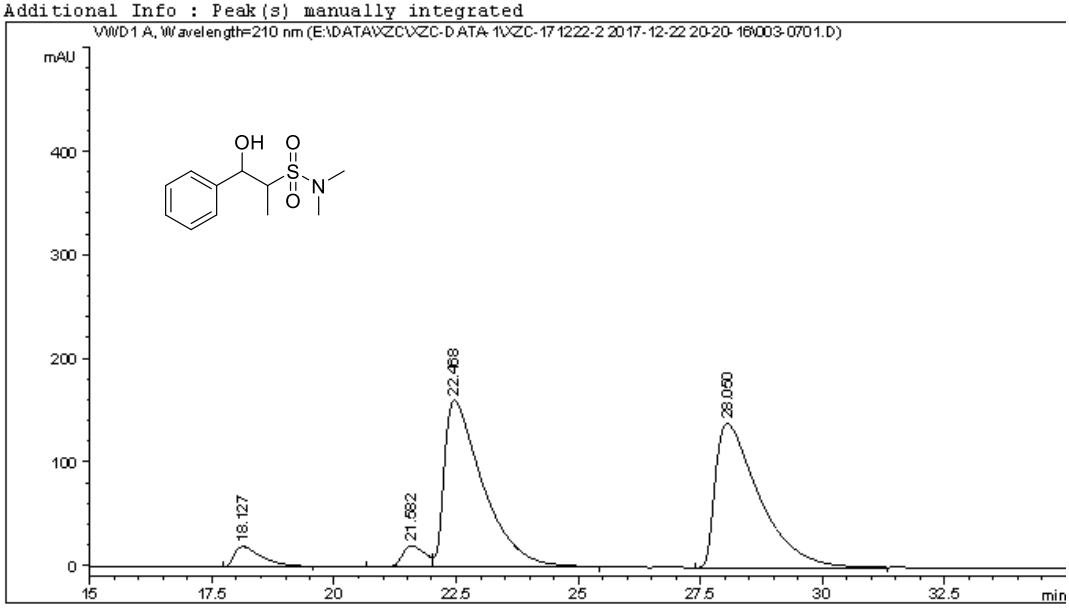
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 21
    Injection Date  : 12/8/2017 10:35:17 AM                Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-DATA-1\XZC-20171208-1 2017-12-08 10-22-44\VWD-IB(1-6)-95
                      -5-1ML-3UL-210NM-60MIN.M
    Last changed    : 12/8/2017 10:22:45 AM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-DATA-1\XZC-20171208-1 2017-12-08 10-22-44\VWD-IB(1-6)-95
                      -5-1ML-3UL-210NM-60MIN.M (Sequence Method)
    Last changed    : 1/31/2018 10:06:05 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  27.810 MM    1.2417 1.55112e4   208.20322  97.9322
       2  31.882 MM    0.3443   22.68172    1.09790   0.1432
       3  34.276 MM    0.6385   19.04350 4.97103e-1   0.1202
       4  39.550 MM    1.3278  285.78909    3.58713   1.8044

    Totals :                  1.58387e4   213.38535
```

Data File E:\DATA\XZC\XZC-DATA-1\XZC-171222-2 2017-12-22 20-20-16\003-0701.D
Sample Name: XZC-dm-RAC

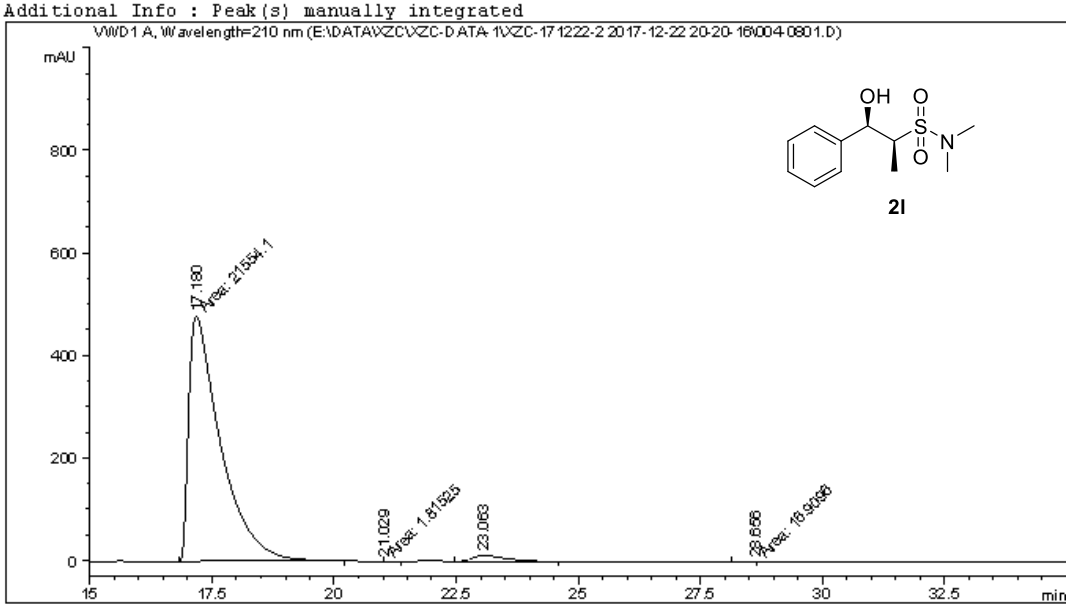
```
    ====================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   7
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 3
    Injection Date  : 12/22/2017 10:57:03 PM               Inj :   1
                                                     Inj Volume : 2.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-DATA-1\XZC-171222-2 2017-12-22 20-20-16\VWD-IB(1-6)-95-5
                      -1ML-2UL-210NM-40MIN.M
    Last changed    : 12/22/2017 8:20:17 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-DATA-1\XZC-171222-2 2017-12-22 20-20-16\VWD-IB(1-6)-95-5
                      -1ML-2UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 1/31/2018 11:16:57 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ====================================================================
                            Area Percent Report
    ====================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  18.127 BB    0.5675  721.49707   18.93785   3.8073
       2  21.582 BV    0.4938  647.35608   20.36981   3.4161
       3  22.468 VB    0.8100 8854.12109  160.89922  46.7233
       4  28.050 BB    0.9245 8727.15527  139.38730  46.0533

    Totals :                  1.8950le4   339.59417
```

Data File E:\DATA\XZC\XZC-DATA-1\XZC-171222-2 2017-12-22 20-20-16\004-0801.D
Sample Name: XZC-dm

```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   8
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 4
    Injection Date  : 12/22/2017 11:37:45 PM               Inj :   1
                                                     Inj Volume : 2.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-DATA-1\XZC-171222-2 2017-12-22 20-20-16\VWD-IB(1-6)-95-5
                      -1ML-2UL-210NM-40MIN.M
    Last changed    : 12/22/2017 8:20:17 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-DATA-1\XZC-171222-2 2017-12-22 20-20-16\VWD-IB(1-6)-95-5
                      -1ML-2UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 1/31/2018 11:21:07 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

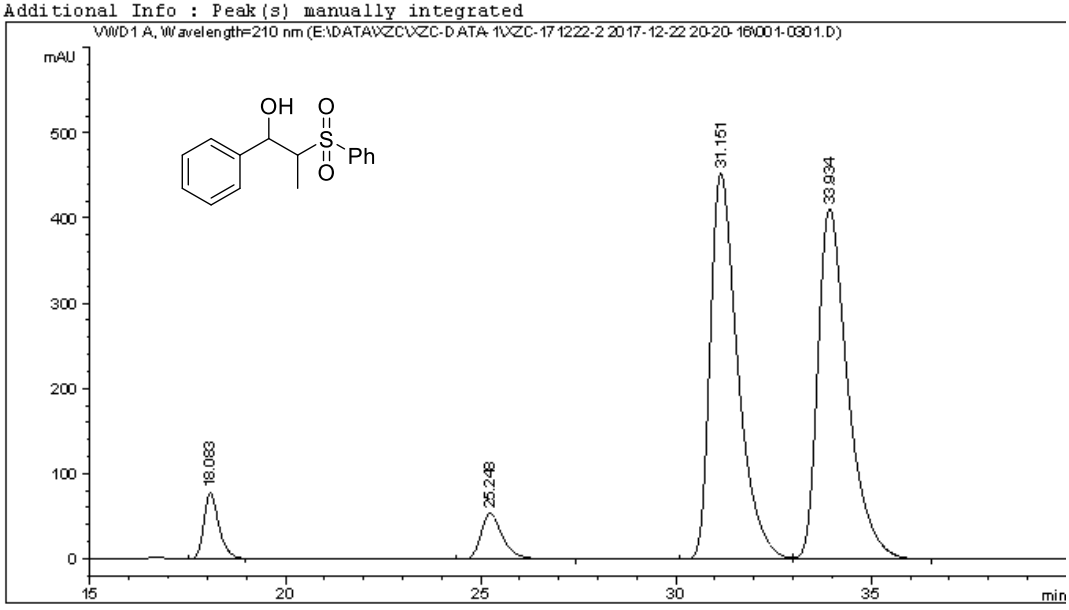


2l

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1  17.180 MM    0.7514 2.1554le4   478.10046  97.6305
       2  21.029 MM    0.1445    1.81525 1.48409e-1 8.222e-3
       3  23.063 BB    0.6628  504.38492   11.23520   2.2846
       4  28.656 MM    0.1596   16.90961    1.76546   0.0766

    Totals :                  2.20772e4   491.24953
```

Data File E:\DATA\XZC\XZC-DATA-1\XZC-171222-2 2017-12-22 20-20-16\001-0301.D
Sample Name: XZC-sulfon-RAC

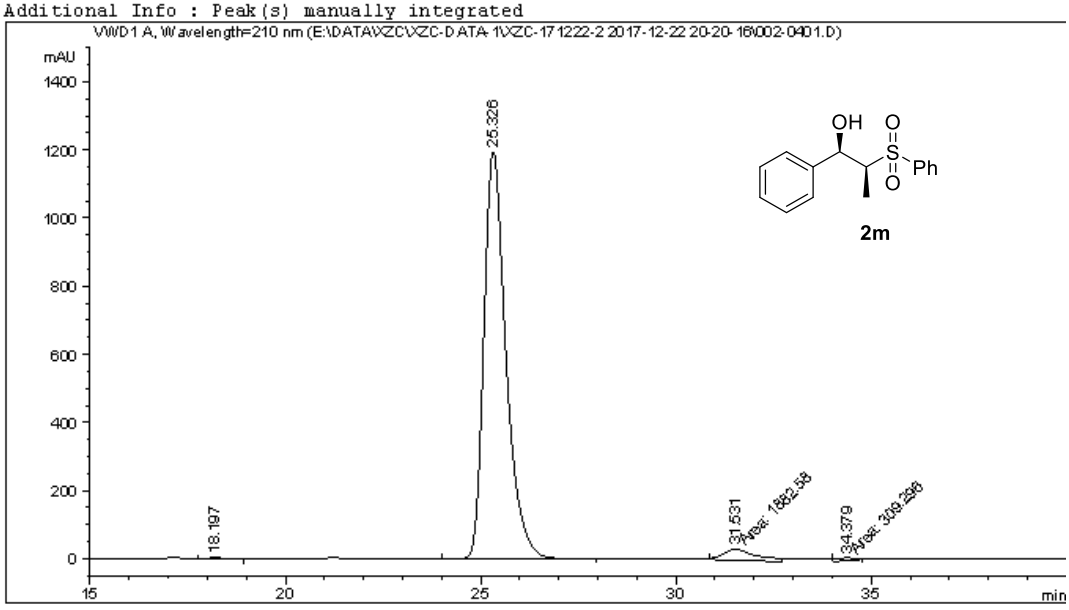
```
    ====================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   3
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 1
    Injection Date  : 12/22/2017 8:53:18 PM                Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-DATA-1\XZC-171222-2 2017-12-22 20-20-16\VWD-AD(1-2)-90-
                      10-1ML-3UL-210NM-45MIN.M
    Last changed    : 12/22/2017 8:20:16 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-DATA-1\XZC-171222-2 2017-12-22 20-20-16\VWD-AD(1-2)-90-
                      10-1ML-3UL-210NM-45MIN.M (Sequence Method)
    Last changed    : 1/30/2018 9:50:35 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ====================================================================
                            Area Percent Report
    ====================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  18.083 BB    0.4044 2075.11450   77.48622   4.2920
       2  25.248 BB    0.5879 2113.95703   54.09230   4.3724
       3  31.151 BV    0.7419 2.22281e4   453.47769  45.9753
       4  33.934 VB    0.8044 2.19307e4   411.07297  45.3602

    Totals :                  4.83479e4   996.12918
```

Data File E:\DATA\XZC\XZC-DATA-1\XZC-171222-2 2017-12-22 20-20-16\002-0401.D
Sample Name: XZC-sulfon

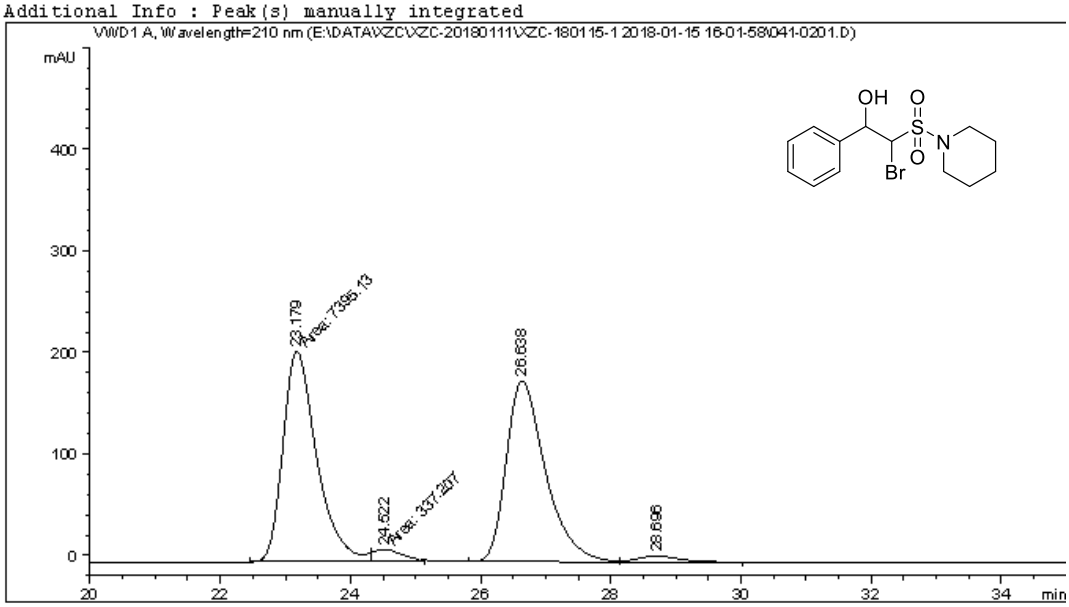
```
    ==================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   4
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 2
    Injection Date  : 12/22/2017 9:39:02 PM             Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-DATA-1\XZC-171222-2 2017-12-22 20-20-16\VWD-AD(1-2)-90-
                      10-1ML-3UL-210NM-45MIN.M
    Last changed    : 12/22/2017 8:20:16 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-DATA-1\XZC-171222-2 2017-12-22 20-20-16\VWD-AD(1-2)-90-
                      10-1ML-3UL-210NM-45MIN.M (Sequence Method)
    Last changed    : 1/30/2018 9:53:32 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ==================================================================
                          Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  18.197 BB    0.4040   66.87212    2.48476   0.1365
       2  25.326 BB    0.5923 4.6726le4  1194.72327  95.3889
       3  31.531 MM    0.9926 1882.57715   31.60878   3.8432
       4  34.379 MM    0.5903  309.29623    7.34431   0.6314

    Totals :                  4.89849e4  1236.16112
```

Data File E:\DATA\XZC\XZC-20180111\XZC-180115-1 2018-01-15 16-01-58\041-0201.D
Sample Name: XZC-Br-RAC

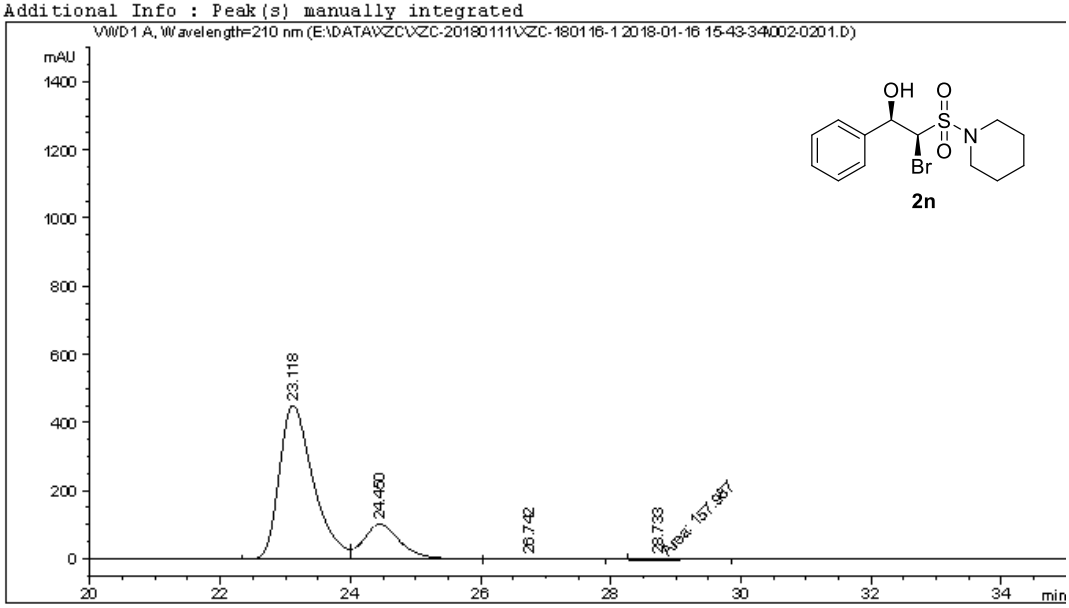
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 41
    Injection Date  : 1/15/2018 4:13:28 PM                 Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-20180111\XZC-180115-1 2018-01-15 16-01-58\VWD-AD(1-2)-90
                      -10-1ML-3UL-210NM-35MIN.M
    Last changed    : 1/15/2018 4:48:09 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\XZC\XZC-20180111\XZC-180115-1 2018-01-15 16-01-58\VWD-AD(1-2)-90
                      -10-1ML-3UL-210NM-35MIN.M (Sequence Method)
    Last changed    : 1/31/2018 11:02:16 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  23.179 MF    0.5972 7395.12744  206.38376  47.9120
       2  24.522 FM    0.4984  337.20685   11.27615   2.1847
       3  26.638 BV    0.6331 7447.60693  178.02249  48.2520
       4  28.696 VB    0.6426  254.87865    5.75562   1.6513

    Totals :                  1.54348e4   401.43802
```

Data File E:\DATA\XZC\XZC-20180111\XZC-180116-1 2018-01-16 15-43-34\002-0201.D
Sample Name: XZC-Br

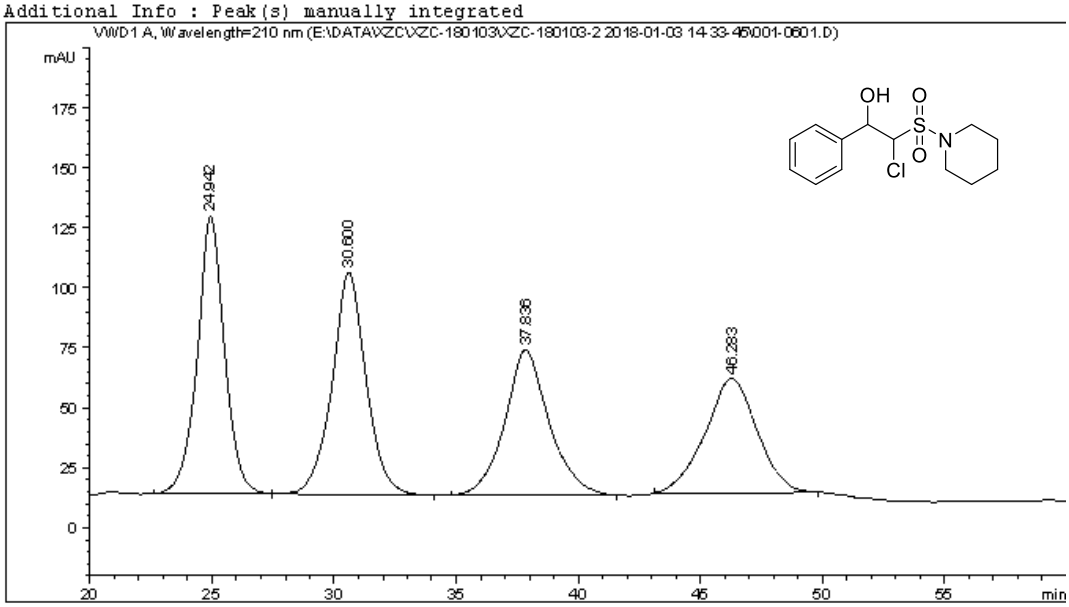
```
    ====================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 2
    Injection Date  : 1/16/2018 3:56:01 PM                  Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-20180111\XZC-180116-1 2018-01-16 15-43-34\VWD-AD(1-2)-90
                      -10-1ML-3UL-210NM-35MIN.M
    Last changed    : 1/16/2018 3:43:34 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-20180111\XZC-180116-1 2018-01-16 15-43-34\VWD-AD(1-2)-90
                      -10-1ML-3UL-210NM-35MIN.M (Sequence Method)
    Last changed    : 1/31/2018 11:05:36 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ====================================================================
                            Area Percent Report
    ====================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  23.118 BV    0.5486 1.63155e4   451.45810  79.3175
       2  24.450 VB    0.5889 4012.88306  102.25356  19.5085
       3  26.742 BB    0.6031   83.49436    2.05018   0.4059
       4  28.733 MM    1.0282  157.98688    2.56097   0.7680

    Totals :                  2.05699e4   558.32280
```

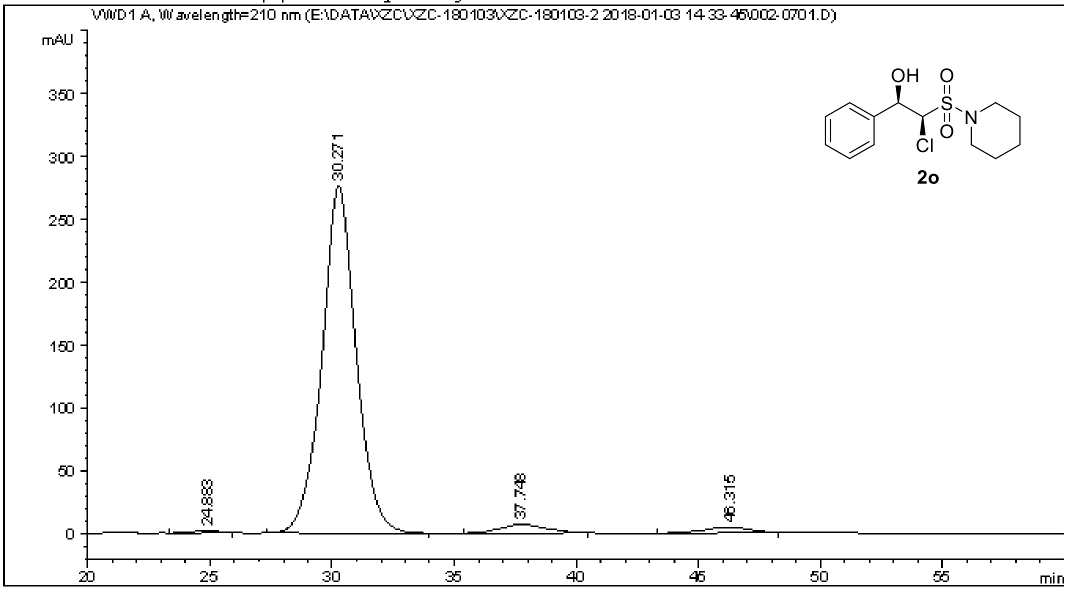
Data File E:\DATA\XZC\XZC-180103\XZC-180103-2 2018-01-03 14-33-45\001-0601.D
Sample Name: XZC-Cl-RAC

```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   6
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 1
    Injection Date  : 1/3/2018 4:02:18 PM                  Inj :   1
                                                     Inj Volume : 2.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-180103\XZC-180103-2 2018-01-03 14-33-45\VWD-IA(1-2)-95-5
                      -1ML-2UL-210NM-40MIN.M
    Last changed    : 1/3/2018 4:11:22 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\XZC\XZC-180103\XZC-180103-2 2018-01-03 14-33-45\VWD-IA(1-2)-95-5
                      -1ML-2UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 1/3/2018 7:22:33 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  24.942 BB    1.1373 8965.39063  115.53982  27.4710
       2  30.600 BB    1.4032 8999.07129   92.65170  27.5742
       3  37.836 BB    1.7684 7624.28271   60.53615  23.3617
       4  46.283 BB    2.1048 7047.13965   47.50086  21.5932

    Totals :                  3.26359e4   316.22852
```

```
Data File E:\DATA\XZC\XZC-180103\XZC-180103-2 2018-01-03 14-33-45\002-0701.D
Sample Name: XZC-Cl

    =================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   7
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 2
    Injection Date  : 1/3/2018 5:03:02 PM                 Inj :   1
                                                   Inj Volume : 2.000 µl
    Acq. Method     : E:\DATA\XZC\XZC-180103\XZC-180103-2 2018-01-03 14-33-45\VWD-IA(1-2)-95-5
                      -1ML-2UL-210NM-40MIN.M
    Last changed    : 1/3/2018 4:11:22 PM by SYSTEM
    Analysis Method : E:\DATA\XZC\XZC-180103\XZC-180103-2 2018-01-03 14-33-45\VWD-IA(1-2)-95-5
                      -1ML-2UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 1/3/2018 7:24:37 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    =================================================================
                             Area Percent Report
    =================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.883	BB	0.8341	153.94118	2.17922	0.5374
2	30.271	BB	1.4302	2.69259e4	276.73410	93.9914
3	37.748	BB	1.6306	938.47510	7.42008	3.2760
4	46.315	BB	1.5643	628.87866	4.79452	2.1953

Totals : 2.86472e4 291.12793

1260HPLC-VWD 1/3/2018 7:24:48 PM SYSTEM   Page 1 of 2

Reference:

1. John J. Piwinski *et al*, *Org. Lett.*, 2008, **10**, 2517–2520;

2. W. K. C. Park *et al*. *Bioorg. Med. Chem. Lett*., 2008, **18**, 1151–1156;

3. M.-Y. Chang *et al., Tetrahedron,* 2015, **71**, 782-791.