CHEMISTRY
A European Journal

Supporting Information

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Stereoselective Lewis Acid Mediated (3 + 2) Cycloadditions of *N*–H- and *N*–Sulfonylaziridines with Heterocumulenes

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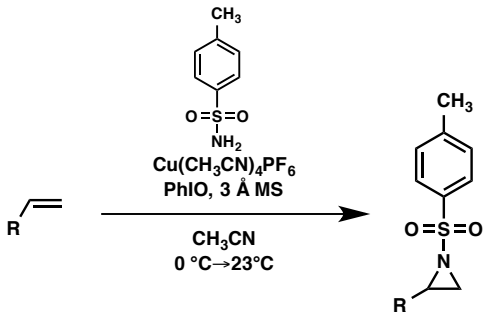
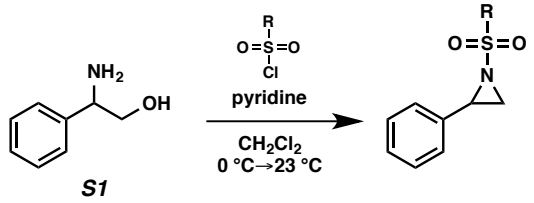
Materials and Methods

Unless stated otherwise, reactions were performed at ambient temperature (23 °C) in flame-dried or oven-dried glassware under an argon or nitrogen atmosphere using dry, deoxygenated solvents (distilled or passed over a column of activated alumina).[1] Commercially obtained reagents were used as received with the exception of tetra(*n*-butyl)ammonium bromide (TBAB), zinc(II) chloride, zinc(II) bromide, zinc(II) iodide, zinc(II) triflate, tin(II) triflate, lithium bromide, tetrakis(acetonitrile)copper(I) hexafluorophosphate, and tetrakis(triphenylphosphine)palladium(0), which were stored in a nitrogen-filled glovebox. Et_3N and pyridine were distilled from calcium hydride immediately prior to use. Methanol was distilled from magnesium methoxide immediately prior to use. Iodosobenzene[2] and diphenylcarbodiimide[3] were prepared by known methods. Reactions requiring external heat were modulated to the specified temperatures using an IKAmag temperature controller. Reaction progress was monitored by thin-layer chromatography (TLC) or Agilent 1290 UHPLC-LCMS. TLC was performed using E. Merck silica gel 60 F254 precoated plates (0.25 mm) and visualized by UV fluorescence quenching, potassium permanganate, or *p*-anisaldehyde staining. Silia*Flash* P60 Academic Silica gel (particle size 0.040-0.063 mm) was used for flash chromatography. ^1H and ^{13}C NMR spectra were recorded on a Varian Inova 500 spectrometer (500 MHz and 126 MHz, respectively) and are reported in terms of chemical shift relative to residual $CHCl_3$ (δ 7.26 and δ 77.16 ppm, respectively), $D_3CS(O)CHD_2$ (δ 2.50 and δ 39.52 ppm, respectively), or $CHDCl_2$ (δ 5.32 and δ 53.84 ppm, respectively). Data for ^1H NMR spectra are reported as follows: chemical shift (δ ppm) (multiplicity, coupling constant (Hz), integration). Abbreviations are used as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = complex multiplet, bs = broad singlet. Infrared (IR) spectra were recorded on a Perkin Elmer Paragon 1000 spectrometer and are reported in frequency of absorption (cm^{-1}). High-resolution mass spectra (HRMS) were obtained from the Caltech Mass Spectral Facility using a JEOL JMS-600H High Resolution Mass Spectrometer with fast atom bombardment (FAB+) ionization mode or were acquired using an Agilent 6200 Series TOF with an Agilent G1978A Multimode source in atmospheric pressure chemical ionization (APCI+), electrospray ionization (ESI+), or mixed (MultiMode: ESI-APCI) ionization mode. Optical rotations were measured on a JASCO P-2000 polarimeter using a 100 mm path length cell at 589 nm. Analytical supercritical fluid chromatography (SFC) was performed with a Mettler SFC supercritical CO_2 analytical chromatography system utilizing Chiralpak (AD-H or AS-H) or Chiralcel (OB-H or OD-H) columns (4.6 mm x 25 cm) obtained from Daicel Chemical Industries, Ltd.

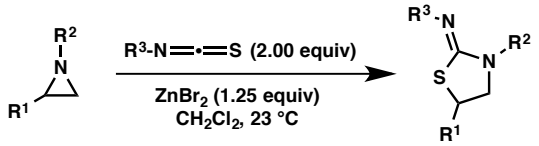
General Experimental Procedures



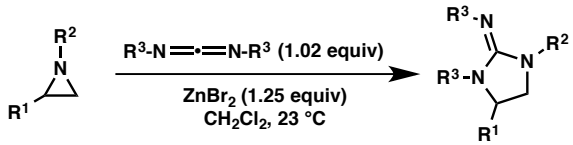
General Procedure A. *Direct aziridination of olefins.*[4]
To a flame-dried round-bottom flask with a stir bar were added *p*-toluenesulfonamide (5.60 mmol, 1.40 equiv), tetrakis(acetonitrile)copper(I) hexafluorophosphate (0.40 mmol, 0.10 equiv), the appropriate olefin (4.00 mmol, 1.00 equiv), activated 3 Å molecular sieves (2.40 g, 600 mg/mmol olefin), and acetonitrile (10 mL). The stirred suspension was cooled to 0 °C (ice/water bath) at which time iodosobenzene (5.60 mmol, 1.40 equiv) was added as a solid in one portion. The bath was immediately removed and the reaction mixture was allowed to warm to ambient temperature. Upon consumption of starting material (determined by TLC or LCMS analysis, ca. 12–48 h), the mixture was filtered through Celite, washing with acetonitrile (50 mL) and ethyl acetate (50 mL). The filtrate was concentrated in vacuo to give the crude product, which was purified by silica gel column chromatography (EtOAc in hexanes eluent).



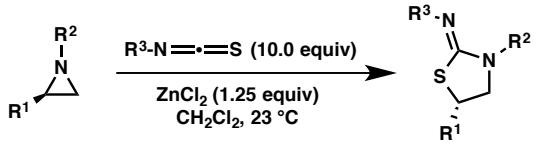
General Procedure B. *Ring closure of amino alcohols.*[5]
A flame-dried round-bottom flask with a stir bar was charged with 2-phenylglycinol (**S1**, 0.73 mmol, 1.00 equiv), which was then suspended in CH_2Cl_2 (500 μL) and pyridine (250 μL). The stirred suspension was cooled to 0 °C (ice/water bath) at which time the appropriate sulfonyl chloride (2.19 mmol, 3.00 equiv) was added in one portion. The bath was immediately removed and the reaction mixture was allowed to warm to ambient temperature. Upon completion (determined by TLC or LCMS analysis, ca. 1–5 h), the mixture was diluted with CH_2Cl_2 (12 mL), and washed with aqueous 2 N HCl (3 x 4 mL). The combined acidic aqueous layers were extracted with CH_2Cl_2 (1 x 4 mL). The organic layers were combined and carefully washed with aqueous 2 N KOH (6 x 8 mL). The combined basic aqueous layers were then extracted with CH_2Cl_2 (1 x 12 mL) and the combined organic layers were dried over sodium sulfate, filtered, and concentrated in vacuo. The crude residue was purified by silica gel column chromatography (EtOAc in hexanes eluent).



General Procedure C. *Isothiocyanate (3 + 2) cycloaddition with 2-subsituted aziridines.* To an oven-dried 1-dram vial equipped with a magnetic stir bar was added zinc(II) bromide (113 mg, 0.50 mmol, 1.25 equiv), freshly powdered with a mortar and pestle, in an inert atmosphere glovebox. The vial was sealed with a screw cap fitted with a Teflon septum, removed from the glovebox, and placed under an inert atmosphere. To a separate, oven-dried 1-dram vial was added the appropriate aziridine (0.40 mmol, 1.00 equiv). The vial was sealed with a screw cap fitted with a Teflon septum and anhydrous CH_2Cl_2 (0.60 mL) and isothiocyanate (0.80 mmol, 2.00 equiv) were added. The mixture was transferred to the first vial with a rinse of anhydrous CH_2Cl_2 (0.20 mL). The heterogeneous reaction mixture was then allowed to stir at ambient temperature. Upon consumption of the aziridine (determined by TLC or LCMS analysis), the reaction solution was diluted with CH_2Cl_2 (3 mL) and CH_3OH (1 mL), adsorbed onto Celite, and purified by silica gel column chromatography (acetone in hexanes eluent).



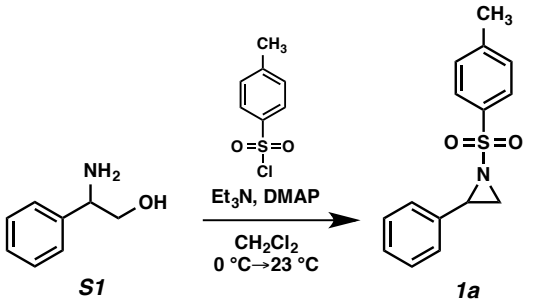
General Procedure D. *Carbodiimide (3 + 2) cycloaddition with 2-subsituted aziridines.* To an oven-dried 1-dram vial equipped with a magnetic stir bar was added zinc(II) bromide (113 mg, 0.50 mmol, 1.25 equiv), freshly powdered with a mortar and pestle, in an inert atmosphere glovebox. The vial was sealed with a screw cap fitted with a Teflon septum, removed from the glovebox, and placed under an inert atmosphere. To a separate, oven-dried 1-dram vial was added the appropriate aziridine (0.40 mmol, 1.00 equiv). The vial was sealed with a screw cap fitted with a Teflon septum and anhydrous CH_2Cl_2 (0.60 mL) and carbodiimide (0.41 mmol, 1.02 equiv) were added. The mixture was transferred to the first vial with a rinse of anhydrous CH_2Cl_2 (0.20 mL). The heterogeneous reaction mixture was then allowed to stir at ambient temperature. Upon consumption of the aziridine (determined by TLC or LCMS analysis), the reaction solution was diluted with CH_2Cl_2 (3 mL) and CH_3OH (1 mL), adsorbed onto Celite, and purified by silica gel column chromatography (acetone in hexanes or CH_3OH in CH_2Cl_2 eluent).



General Procedure E. *Stereoselective Isothiocyanate (3 + 2) cycloaddition with 2-subsituted aziridines.*

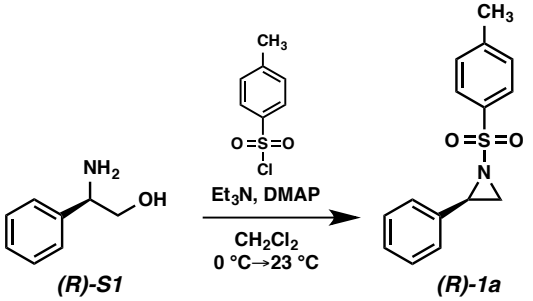
To an oven-dried 1-dram vial equipped with a magnetic stir bar was added powdered zinc(II) chloride (68 mg, 0.50 mmol, 1.25 equiv) in an inert atmosphere glovebox. The vial was sealed with a screw cap fitted with a Teflon septum, removed from the glovebox, and placed under an inert atmosphere. To a separate, oven-dried 1-dram vial was added the appropriate aziridine (0.40 mmol, 1.00 equiv). The vial was sealed with a screw cap fitted with a Teflon septum and anhydrous CH_2Cl_2 (0.60 mL) and isothiocyanate (4.00 mmol, 10.0 equiv) were added. The mixture was transferred to the first vial with a rinse of anhydrous CH_2Cl_2 (0.20 mL). The heterogeneous reaction mixture was then allowed to stir at ambient temperature. Upon consumption of the aziridine (determined by TLC or LCMS analysis), the reaction solution was diluted with CH_2Cl_2 (3 mL) and CH_3OH (1 mL), adsorbed onto Celite, and purified by silica gel column chromatography (acetone in hexanes).

Aziridine Synthesis and Characterization Data



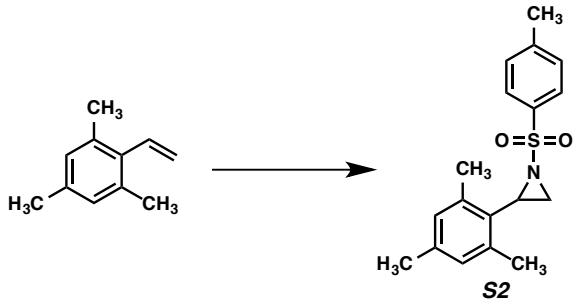
***N*-tosyl-2-phenylaziridine (1a):**

Aziridine **1a** was prepared according to General Procedure B from 2-phenylglycinol (**S1**): 85% yield; R_f = 0.25 (1:4 Acetone:Hexanes eluent); characterization data match those reported in the literature.[6]

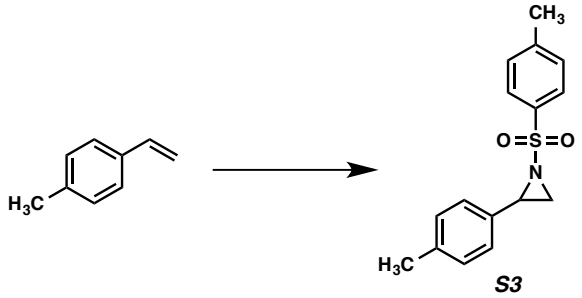


(*R*)-*N*-tosyl-2-phenylaziridine ((*R*)-1a):

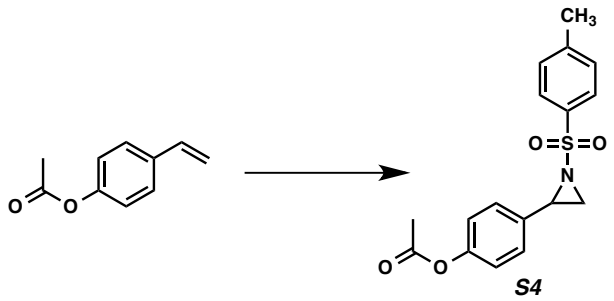
Aziridine **(*R*)-1a** was prepared according to a procedure modified from literature methods.[7] A flame-dried round-bottom flask with a stir bar was charged with (*R*)-(–)-2-phenylglycinol (**(*R*)-S1**, 5.00 g, 36.4 mmol, 1.00 equiv), *p*-toluenesulfonyl chloride (17.4 g, 91.1 mmol, 2.50 equiv), and 4-(dimethylamino)pyridine (DMAP, 445 mg, 3.64 mmol, 0.10 equiv). The solids were suspended in dichloromethane under nitrogen, and the flask was cooled in an ice-water bath. Triethylamine (Et_3N, 15.2 mL, 109 mmol, 3.00 equiv) was added dropwise, and the reaction mixture became clear and colorless. The flask was allowed to warm to room temperature and stir under nitrogen. Upon completion (as determined by LCMS analysis, ca. 8 h), the reaction was quenched by addition of saturated aqueous NH_4Cl (80 mL). The organic layer was removed and the aqueous layer extracted with dichloromethane (3 x 60 mL). The combined organic layers were dried over sodium sulfate, filtered, and concentrated in vacuo. The crude solid was purified by silica gel column chromatography (10% EtOAc in hexanes eluent) to give aziridine **(*R*)-1a** (6.34 g, 64% yield) as a fluffy white solid: characterization data are the same as above; $[\alpha]_D^{25.0}$ –108.6° (*c* 0.950, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralcel OB-H column, 10% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 7.5 minutes, minor retention time: 10.2 minutes, >99% ee).



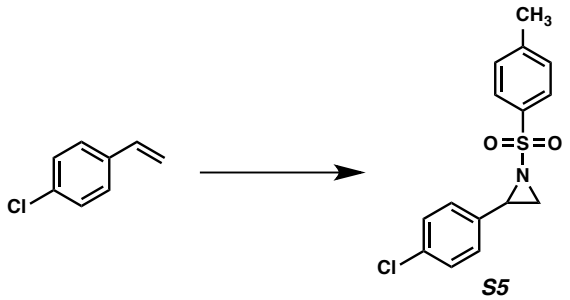
***N*-tosyl-2-mesitylaziridine (S2):**
Aziridine **S2** was prepared according to General Procedure A: 40% yield; R_f = 0.29 (1:9 EtOAc:Hexanes eluent); characterization data match those reported in the literature.[8]



***N*-tosyl-2-(*p*-tolyl)aziridine (S3):**
Aziridine **S3** was prepared according to General Procedure A: 75% yield; R_f = 0.34 (1:4 Acetone:Hexanes eluent); characterization data match those reported in the literature.[8]



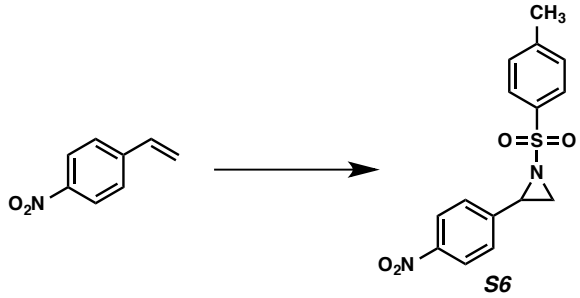
***N*-tosyl-2-(*p*-acetoxyphenyl)aziridine (S4):**
Aziridine **S4** was prepared according to General Procedure A: 76% yield; R_f = 0.32 (3:7 EtOAc:Hexanes eluent); characterization data for ^{1}H NMR, ^{13}C NMR, and IR spectra match those reported in the literature;[8a] HRMS (ESI+) *m/z* calc'd for $C_{17}H_{18}NO_4S$ $[M+H]^+$: 332.0951, found 332.0958.



S5

***N*-tosyl-2-(*p*-chlorophenyl)aziridine (S5):**

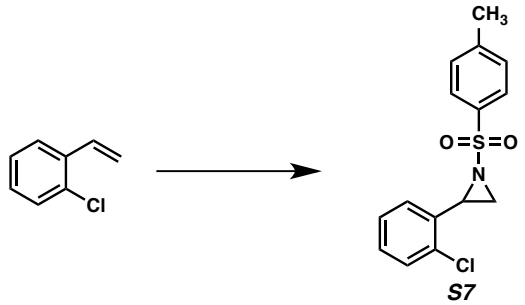
Aziridine **S5** was prepared according to General Procedure A: 82% yield; R_f = 0.30 (3:17 EtOAc:Hexanes eluent); characterization data match those reported in the literature.[8]



S6

***N*-tosyl-2-(*p*-nitrophenyl)aziridine (S6):**

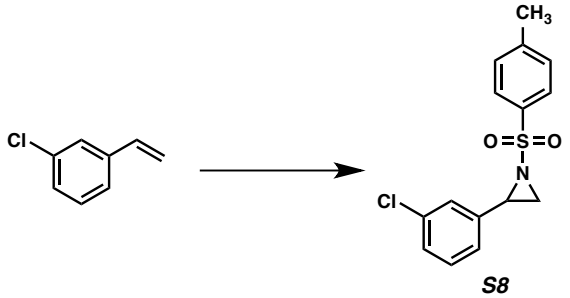
Aziridine **S6** was prepared according to General Procedure A: 31% yield; R_f = 0.27 (1:4 Acetone:Hexanes eluent); characterization data match those reported in the literature.[8b]



S7

***N*-tosyl-2-(*o*-chlorophenyl)aziridine (S7):**[9]

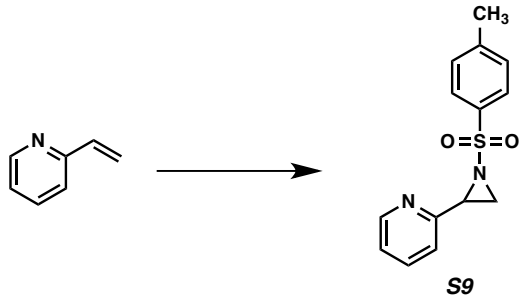
Aziridine **S7** was prepared according to General Procedure A: 90% yield; R_f = 0.45 (1:3 EtOAc:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.93–7.87 (m, 2H), 7.37–7.34 (m, 2H), 7.34–7.31 (m, 1H), 7.23–7.14 (m, 3H), 4.04 (dd, J = 7.2, 4.4 Hz, 1H), 3.03 (d, J = 7.2 Hz, 1H), 2.45 (s, 3H), 2.29 (d, J = 4.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 145.0, 134.8, 133.9, 133.2, 129.9, 129.4, 129.3, 128.2, 127.6, 127.1, 39.1, 35.8, 21.8; IR (Neat Film, NaCl) 3065, 1596, 1444, 1328, 1163, 1093, 913, 815, 759, 732 cm^{-1}; HRMS (FAB+) *m/z* calc'd for $C_{15}H_{15}{}^{35}ClNO_2S$ $[M+H]^+$: 308.0512, found 308.0520.



S8

***N*-tosyl-2-(*m*-chlorophenyl)aziridine (S8):**[9]

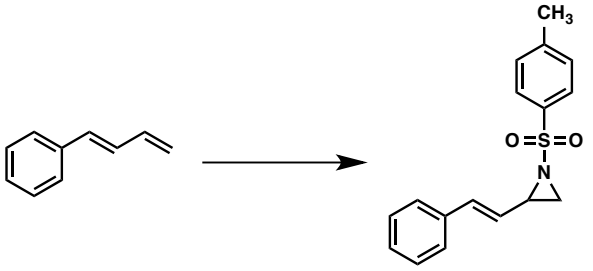
Aziridine **S8** was prepared according to General Procedure A: 97% yield; R_f = 0.46 (1:3 EtOAc:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.89–7.84 (m, 2H), 7.37–7.32 (m, 2H), 7.26–7.17 (m, 3H), 7.12 (dtd, *J* = 7.1, 1.5, 0.5 Hz, 1H), 3.73 (dd, *J* = 7.1, 4.4 Hz, 1H), 2.97 (d, *J* = 7.2 Hz, 1H), 2.44 (s, 3H), 2.35 (d, *J* = 4.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 145.0, 137.4, 134.9, 134.7, 130.0, 129.9, 128.6, 128.1, 126.7, 125.0, 40.2, 36.3, 21.8; IR (Neat Film, NaCl) 3062, 1597, 1451, 1326, 1161, 1092, 919, 786, 723 cm^{-1}; HRMS (FAB+) *m/z* calc'd for $C_{15}H_{15}{}^{35}ClNO_2S$ $[M+H]^+$: 308.0512, found 308.0515.



S9

***N*-tosyl-2-(*o*-pyridyl)aziridine (S9):**[10]

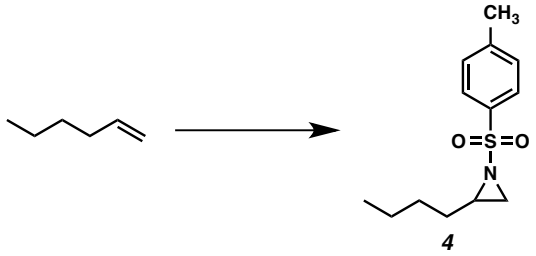
Aziridine **S9** was prepared according to General Procedure A: 68% yield; R_f = 0.34 (1:1 EtOAc:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.52 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 7.89–7.83 (m, 2H), 7.62 (td, *J* = 7.7, 1.8 Hz, 1H), 7.34–7.30 (m, 2H), 7.26 (dt, *J* = 7.8, 1.1 Hz, 1H), 7.19 (ddd, *J* = 7.6, 4.8, 1.2 Hz, 1H), 3.90 (dd, *J* = 7.2, 4.4 Hz, 1H), 2.97 (d, *J* = 7.2 Hz, 1H), 2.65 (d, *J* = 4.4 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 154.4, 149.7, 144.9, 136.9, 134.6, 129.9, 128.2, 123.4, 121.9, 41.4, 35.1, 21.8; IR (Neat Film, NaCl) 3064, 1594, 1477, 1437, 1326, 1204, 1161, 1092, 915, 804, 715 cm^{-1}; HRMS (ESI+) *m/z* calc'd for $C_{14}H_{15}N_2O_2S$ $[M+H]^+$: 275.0849, found 275.0835.



S10

***N*-tosyl-2-((*E*)-styryl)aziridine (S10):**

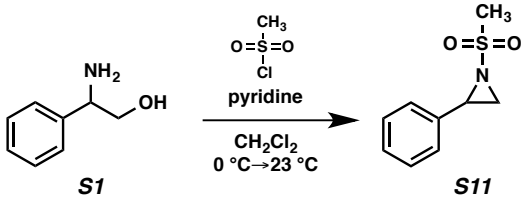
Aziridine **S10** was prepared according to General Procedure A: 11% yield; R_f = 0.18 (1:9 EtOAc:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.90–7.82 (m, 2H), 7.36–7.23 (m, 7H), 6.73 (d, *J* = 15.9 Hz, 1H), 5.84 (dd, *J* = 15.9, 7.9 Hz, 1H), 3.46 (dddd, *J* = 7.8, 7.1, 4.5, 0.7 Hz, 1H), 2.87 (d, *J* = 7.1 Hz, 1H), 2.44 (s, 3H), 2.32 (d, *J* = 4.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 144.8, 135.9, 135.2, 129.9, 128.8, 128.4, 128.0, 126.6, 126.6, 124.2, 41.4, 34.8, 21.8; IR (Neat Film, NaCl) 3287, 3028, 2924, 1597, 1494, 1450, 1323, 1160, 1090, 964, 939, 884, 815, 753, 714 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{17}H_{18}NO_2S$ $[M+H]^+$:300.1053, found 300.1057.



4

***N*-tosyl-2-(*n*-butyl)aziridine (4):**

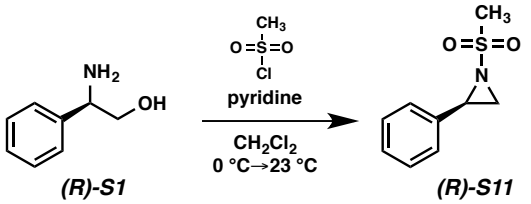
Aziridine **4** was prepared according to General Procedure A: 32% yield; R_f = 0.44 (1:3 EtOAc:Hexanes eluent); characterization data match those reported in the literature.[8b]



S1 ***S11***

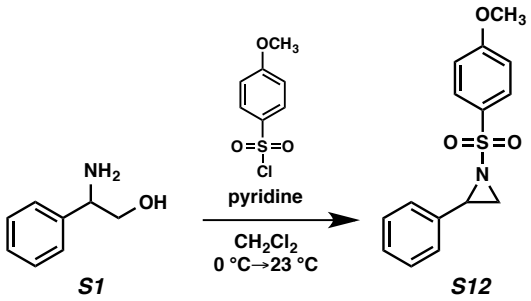
***N*-mesyl-2-phenylaziridine (S11):**

Aziridine **S11** was prepared according to General Procedure B from 2-phenylglycinol (**S1**); 88% yield; R_f = 0.29 (3:7 Acetone:Hexanes eluent); characterization data match those reported in the literature.[11]



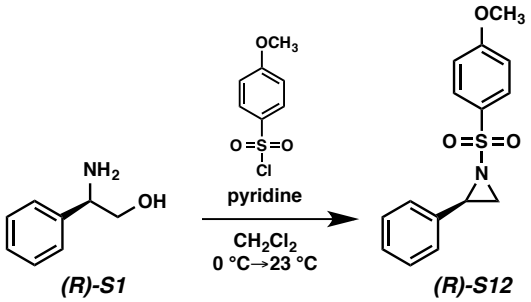
(*R*)-*N*-mesyl-2-phenylaziridine ((*R*)-S11):

Aziridine **(*R*)-S11** was prepared according to General Procedure B from (*R*)-(–)-2-phenylglycinol (**(*R*)-S1**): characterization data are the same as above; $[\alpha]_D^{25.0}$ –194.5° (*c* 0.500, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralpak AS-H column, 10% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 3.0 minutes, minor retention time: 3.3 minutes, 99% ee).



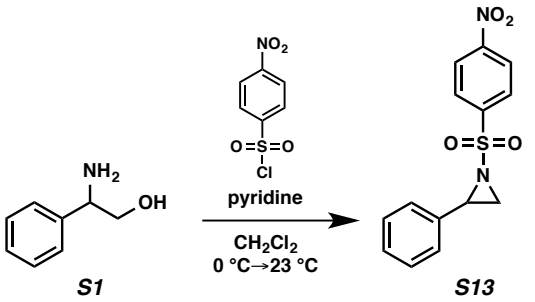
***N*-(*p*-methoxybenzenesulfonyl)-2-phenylaziridine (S12):**

Aziridine **S12** was prepared according to General Procedure B from 2-phenylglycinol (**S1**): 81% yield; R_f = 0.39 (3:7 Acetone:Hexanes eluent); characterization data match those reported in the literature.[6]



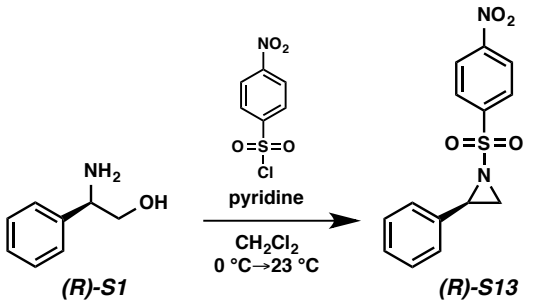
(*R*)-*N*-(*p*-methoxybenzenesulfonyl)-2-phenylaziridine ((*R*)-S12):

Aziridine **(*R*)-S12** was prepared according to General Procedure B from (*R*)-(–)-2-phenylglycinol (**(*R*)-S1**): characterization data are the same as above; $[\alpha]_D^{25.0}$ –78.0° (*c* 0.850, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralpak AS-H column, 10% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 10.0 minutes, minor retention time: 11.3 minutes, >99% ee).



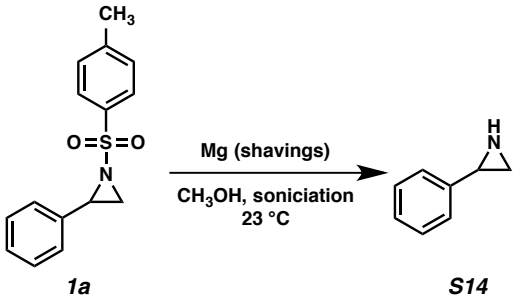
_N_-(_p_-nitrobenzenesulfonyl)-2-phenylaziridine (S13):

Aziridine **S13** was prepared according to General Procedure B from 2-phenylglycinol (**S1**): 76% yield; R_f = 0.24 (1:4 Acetone:Hexanes eluent); characterization data match those reported in the literature.[6]



(_R_)-_N_-(_p_-nitrobenzenesulfonyl)-2-phenylaziridine ((_R_)-S13):

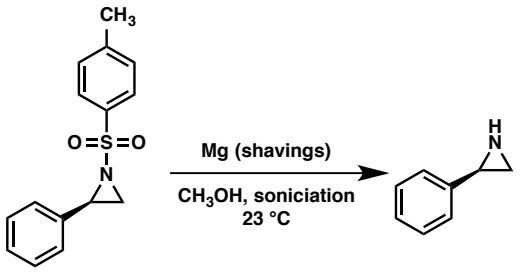
Aziridine **(*R*)-S13** was prepared according to General Procedure B from (*R*)-(–)-2-phenylglycinol (**(*R*)-S1**): characterization data are the same as above; $[\alpha]_D^{25.0}$ –58.4° (*c* 0.600, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralcel OD-H column, 10% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 8.9 minutes, minor retention time: 9.8 minutes, >99% ee).



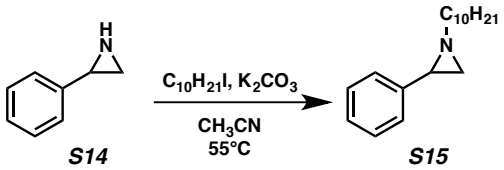
2-phenylaziridine (S14):

Aziridine **S14** was prepared according to literature methods from *N*-tosyl-2-phenylaziridine (**1a**).[12] To a suspension of magnesium metal shavings (474 mg, 19.5 mmol, 5.33 equiv) in CH_3OH (37 mL) was added a solution of aziridine **1a** (1.00 g, 3.66 mmol, 1.00 equiv) in CH_3OH (24 mL) quickly dropwise. The reaction mixture was then sonicated at ambient temperature until consumption of the starting material was complete (determined by TLC analysis, ca. 30 min). The resulting white suspension was poured over brine (200 mL) and extracted with CH_2Cl_2 (4 x 150 mL). The combined organic

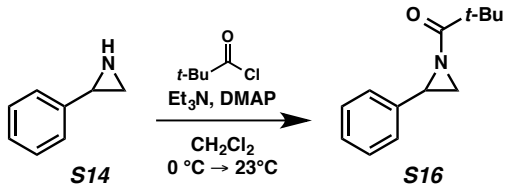
layers were dried over $MgSO_4$, filtered, and concentrated in vacuo to generate a white solid. The crude residue was purified by column chromatography (85% EtOAc and 3% Et_3N in hexanes→3%Et_3N in EtOAc eluent) to afford aziridine **S14** (342 mg, 78% yield) as a clear, colorless oil: R_f = 0.42 (EtOAc eluent); characterization data match those reported in the literature.[12]



(*R*)-2-phenylaziridine ((*R*)-S14):
Aziridine **(*R*)-S14** was prepared according to literature methods from (*R*)-*N*-tosyl-2-phenylaziridine (**(*R*)-1a**) as described above: characterization data are the same as above; $[\alpha]_D^{25.0}$ –59.4° (*c* 0.750, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralcel OD-H column, 10% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 7.8 minutes, minor retention time: 4.4 minutes, >99% ee).

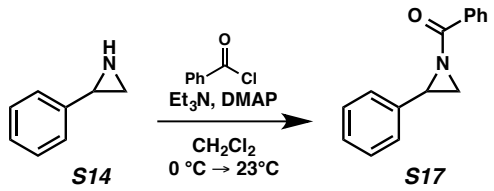


***N*-(*n*-decyl)-2-phenylaziridine (S15):**
Aziridine **S14** was prepared according to a procedure modified from literature methods.[13] To an oven-dried vial with a stir bar were added aziridine **S14** (113 mg, 0.95 mmol, 1.20 equiv) and acetonitrile (1.2 mL). Potassium carbonate (130 mg, 0.95 mmol, 1.20 equiv) and decyl iodide (170 μL, 0.79 mmol, 1.00 equiv) were then added, and the vial was sealed and heated to 55 °C. Upon consumption of starting material (determined by LCMS analysis, ca. 17 h), the reaction mixture was allowed to cool to room temperature, concentrated in vacuo, and the residue partitioned between diethyl ether and brine. The organic layer was separated and concentrated in vacuo to afford a gold oil. The crude residue was purified by column chromatography (5% EtOAc in hexanes eluent) to furnish alkylated aziridine **S15** (138 mg, 67% yield) as a clear, colorless oil: R_f = 0.33 (1:19 EtOAc:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.33–7.18 (m, 5H), 2.52–2.44 (m, 1H), 2.36–2.26 (m, 2H), 1.89 (dd, *J* = 3.4, 0.7 Hz, 1H), 1.65 (dd, *J* = 6.5, 0.7 Hz, 1H), 1.64–1.56 (m, 2H), 1.41–1.18 (m, 14H), 0.88 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 140.7, 128.4, 126.9, 126.3, 62.1, 41.4, 37.9, 32.1, 30.0, 29.8, 29.7, 29.7, 29.5, 27.6, 22.8, 14.3; IR (Neat Film, NaCl) 3036, 2925, 2853, 1606, 1495, 1467, 1377, 1207, 1084, 746 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{18}H_{30}N$ $[M+H]^+$: 260.2373, found 260.2378.



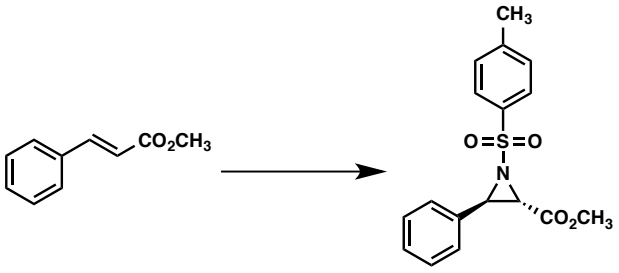
***N*-pivoyl-2-phenylaziridine (S16):**

To a stirred solution of 2-phenylaziridine (**S14**, 568 mg, 4.77 mmol, 1.00 equiv) in CH_2Cl_2 (12 mL) were added triethylamine (Et_3N, 0.39 mL, 5.25 mmol, 1.10 equiv) and trimethylacetyl chloride (1.17 mL, 9.54 mmol, 2.00 equiv) dropwise. The reaction mixture was cooled to 0 °C (ice/water bath) at which time 4-(dimethylamino)pyridine (DMAP, 59 mg, 0.49 mmol, 0.10 equiv) was added as a solid in one portion. The bath was immediately removed and the reaction mixture was allowed to warm to ambient temperature. Upon consumption of starting material (determined by TLC analysis, ca. 1 h), the reaction mixture was concentrated in vacuo to afford a gold oil. The crude residue was purified by column chromatography (20% EtOAc in hexanes eluent) to afford aziridine **S16** (204 mg, 21% yield) as a clear, colorless oil: R_f = 0.31 (1:4 EtOAc:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.38–7.33 (m, 2H), 7.32–7.28 (m, 1H), 7.27–7.24 (m, 2H), 5.44 (dd, *J* = 10.3, 7.8 Hz, 1H), 4.24 (dd, *J* = 14.2, 10.3 Hz, 1H), 3.74 (dd, *J* = 14.2, 7.8 Hz, 1H), 1.30 (s, 9H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 174.2, 141.8, 128.8, 128.1, 125.6, 80.7, 63.0, 33.4, 27.9; IR (Neat Film, NaCl) 2971, 2873, 1661, 1480, 1455, 1265, 1132, 988, 954, 759 cm^{-1}; HRMS (FAB+) *m/z* calc'd for $C_{13}H_{18}NO$ $[M+H]^+$: 204.1388, found 204.1385.



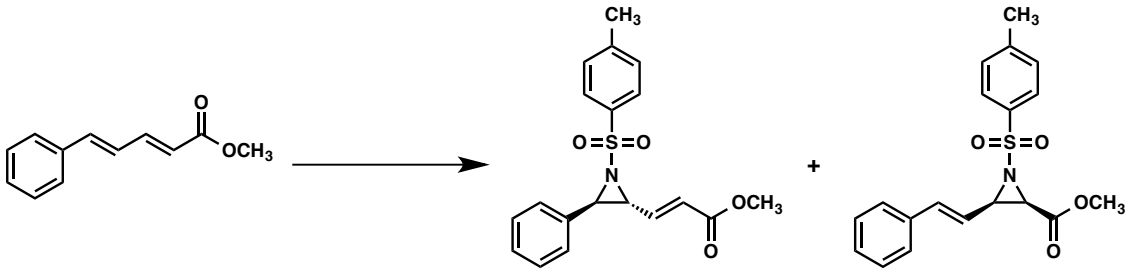
***N*-benzoyl-2-phenylaziridine (S17):**

To a stirred solution of 2-phenylaziridine (**S14**, 119 mg, 1.00 mmol, 1.00 equiv) in CH_2Cl_2 (2.5 mL) were added triethylamine (Et_3N, 0.16 mL, 1.10 mmol, 1.10 equiv) and benzoyl chloride (0.23 mL, 2.00 mmol, 2.00 equiv) dropwise. The reaction mixture was cooled to 0 °C (ice/water bath) at which time 4-(dimethylamino)pyridine (12 mg, 0.10 mmol, 0.10 equiv) was added as a solid in one portion. The bath was immediately removed and the reaction mixture was allowed to warm to ambient temperature. Upon consumption of starting material (determined by TLC analysis, ca. 1 h), the reaction mixture was concentrated in vacuo to afford a gold oil. The crude residue was purified by column chromatography (10% EtOAc with 1% Et_3N in hexanes eluent) to afford aziridine **S17** (222 mg, 99% yield) as a white amorphous solid: R_f = 0.40 (1:9 EtOAc:Hexanes eluent); characterization data match those reported in the literature.[14]



10

***trans*-methyl *N*-tosyl-3-phenylaziridine-2-carboxylate (10):**
Aziridine **10** was prepared according to General Procedure A: 52% yield; R_f = 0.29 (3:7 Acetone:Hexanes eluent); characterization data match those reported in the literature.[8b]

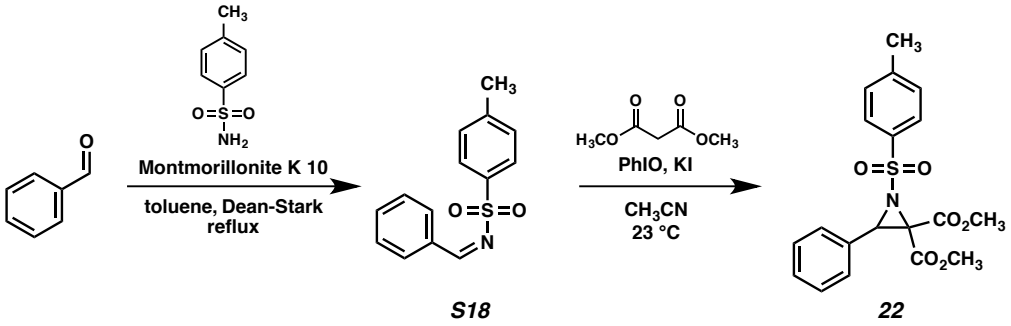


12 ***15***

***trans*-*N*-tosyl-2-((*E*)-2-(methoxycarbonyl)ethenyl)-3-phenylaziridine (12) and *cis*-methyl *N*-tosyl-3-((*E*)-styryl)aziridine-2-carboxylate (15):**
Aziridines **12** and **15** were prepared according to General Procedure A:

***trans*-*N*-tosyl-2-((*E*)-2-(methoxycarbonyl)ethenyl)-3-phenylaziridine (12):**
20% yield; R_f = 0.42 (3:7 EtOAc:Hexanes eluent); characterization data for ^{1}H and ^{13}C NMR spectra match those reported in the literature;[15] IR (Neat Film, NaCl) 3032, 2952, 2256, 1722, 1651, 1597, 1495, 1435, 1407, 1329, 1268, 1162, 1089, 1034, 980, 900, 865, 815, 766, 733 cm^{-1}; HRMS (ESI+) *m/z* calc'd for $C_{19}H_{20}NO_4S$ $[M+H]^+$: 358.1108, found 358.1108.

***cis*-methyl *N*-tosyl-3-((*E*)-styryl)aziridine-2-carboxylate (15):**
30% yield; R_f = 0.45 (3:7 EtOAc:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.90–7.83 (m, 2H), 7.37–7.24 (m, 7H), 6.81 (d, *J* = 16.0 Hz, 1H), 6.06 (dd, *J* = 16.0, 8.5 Hz, 1H), 3.74 (s, 3H), 3.72 (ddd, *J* = 8.5, 7.4, 0.6 Hz, 1H), 3.62 (d, *J* = 7.3 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 166.0, 145.3, 137.8, 135.7, 134.3, 130.1, 128.8, 128.7, 128.2, 126.8, 119.8, 52.9, 46.0, 42.0, 21.9; IR (Neat Film, NaCl) 3029, 2955, 2256, 1747, 1597, 1445, 1329, 1207, 1161, 1090, 1035, 969, 915, 802, 761, 734 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{19}H_{20}NO_4S$ $[M+H]^+$: 358.1108, found 358.1110.

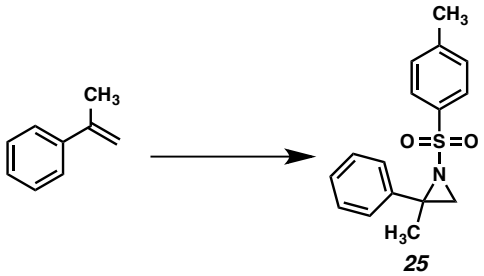


S18 ***22***

dimethyl *N*-tosyl-3-phenylaziridine-2,2-dicarboxylate (22):

Aziridine **22** was prepared according to literature methods from benzaldehyde over two steps. Procedure for the condensation of *p*-toluenesulfonamide onto benzaldehyde was followed from the literature.[16] A stirred suspension of benzaldehyde (1.02 mL, 10.0 mmol, 1.00 equiv), *p*-toluenesulfonamide (1.71 g, 10.0 mmol, 1.00 equiv), and montmorillonite K 10 (900 mg) in toluene (50 mL) was heated to reflux under a Dean-Stark apparatus. After 2.5 h, the consumption of starting material was complete (as determined by TLC analysis) and the reaction mixture was allowed to cool and filtered through Celite rinsing with toluene eluent (30 mL). The filtrate was concentrated in vacuo and the crude solids were purified by silica gel column chromatography (40% Et_2O in hexanes eluent), ensuring the product was eluted quickly,[17] to furnish imine **S18** (2.13 g, 82% yield) as a white solid: R_f = 0.32 (2:3 Et_2O:Hexanes eluent); characterization data matches those reported in the literature.[18]

Procedure for the oxidative cycloaddition of dimethyl malonate with imine **S18** was followed from the literature.[19] To a stirred solution of imine **S18** (648 mg, 2.50 mmol, 1.00 equiv) and dimethyl malonate (0.32 mL, 2.75 mmol, 1.10 equiv) in acetonitrile (5 mL) were added iodosobenzene (1.10 g, 5.00 mmol, 2.00 equiv) and potassium iodide (85 mg, 0.50 mmol, 0.20 equiv) as solids, each in a single portion. After 10 minutes, the consumption of starting material was complete (as determined by TLC analysis) and the reaction mixture was diluted with dichloromethane (20 mL), dry loaded onto Celite (2.5 g), and purified by silica gel column chromatography (25% EtOAc in hexanes eluent) to afford aziridine **22** (658 mg, 68% yield) as a viscous clear, colorless oil; R_f = 0.17 (1:4 EtOAc:Hexanes eluent); characterization data for ^1H and ^{13}C NMR and HRMS spectra match those reported in the literature;[20] IR (Neat Film, NaCl) 3281, 2956, 1749, 1435, 1344, 1234, 1165, 1092, 816.



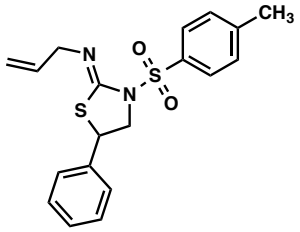
25

***N*-tosyl-2-methyl-2-phenylaziridine (26):**

Aziridine **26** was prepared according to General Procedure A: 32% yield; R_f = 0.44 (1:3 EtOAc:Hexanes eluent); characterization data match those reported in the literature.[8]

Iminothiazolidine Synthesis and Characterization Data

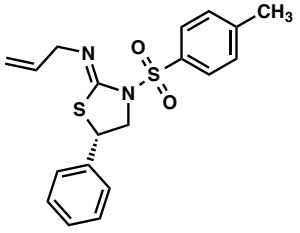
Unless otherwise stated, all iminothiazolidines were prepared according to General Procedure C and were isolated as amorphous white solids.



2a

(*Z*)-5-phenyl-3-tosyl-2-(allylimino)thiazolidine (2a):

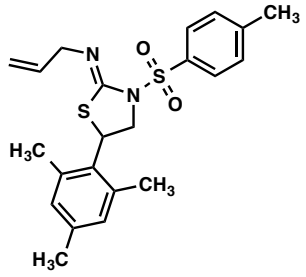
99% yield; R_f = 0.28 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.94–7.89 (m, 2H), 7.40–7.32 (m, 5H), 7.32–7.28 (m, 2H), 5.84 (ddt, *J* = 17.1, 10.3, 5.1 Hz, 1H), 5.12–4.98 (m, 2H), 4.80 (dd, *J* = 8.4, 6.3 Hz, 1H), 4.50 (dd, *J* = 10.3, 6.3 Hz, 1H), 3.94 (dd, *J* = 10.3, 8.5 Hz, 1H), 3.86 (ddt, *J* = 15.9, 5.1, 1.8 Hz, 1H), 3.77 (ddt, *J* = 15.9, 5.2, 1.8 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 151.2, 144.6, 136.8, 135.0, 134.9, 129.2, 129.1, 129.0, 128.8, 127.6, 115.3, 58.0, 56.6, 47.1, 21.8; IR (Neat Film, NaCl) 2923, 1653, 1596, 1355, 1168, 1108, 810, 764 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{19}H_{21}N_2O_2S_2$ $[M+H]^+$: 373.1039, found 373.1049.



(S)-2a

(*S*,*Z*)-5-phenyl-3-tosyl-2-(allylimino)thiazolidine ((*S*)-2a):

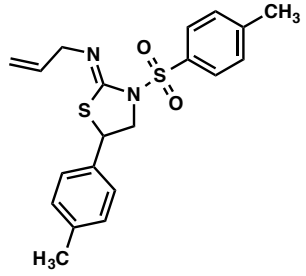
Thiazolidine **(*S*)-2a** was prepared according to General Procedure E: 99% yield; R_f = 0.28 (1:4 Acetone:Hexanes eluent); characterization data match those above; $[\alpha]_D^{25.0}$ –13.1° (*c* 1.600, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralpak AD-H, 30% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 5.4 minutes, minor retention time: 3.8 minutes, 94% ee).



2b

(*Z*)-5-mesityl-3-tosyl-2-(allylimino)thiazolidine (2b):

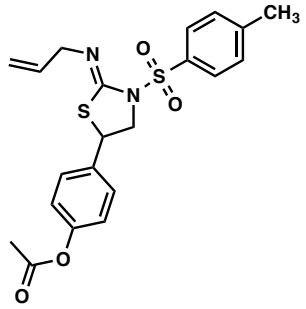
97% yield; R_f = 0.23 (1:4 Et_2O:Hexanes eluent); ^1H NMR ($CDCl_3$, 500 MHz) δ 7.99–7.91 (m, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 6.85 (s, 2H), 5.83 (ddt, *J* = 17.2, 10.3, 5.1 Hz, 1H), 5.43 (dd, *J* = 11.0, 7.6 Hz, 1H), 5.11–4.97 (m, 2H), 4.41 (dd, *J* = 10.4, 7.6 Hz, 1H), 4.14 (t, *J* = 10.7 Hz, 1H), 3.85 (ddt, *J* = 16.0, 5.1, 1.8 Hz, 1H), 3.73 (ddt, *J* = 16.0, 5.2, 1.7 Hz, 1H), 2.45 (s, 3H), 2.40 (s, 6H), 2.25 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 151.9, 144.6, 138.4, 138.0, 135.4, 135.2, 131.0, 129.3, 129.1, 127.3, 115.2, 58.0, 52.3, 42.4, 21.8, 21.6, 20.9; IR (Neat Film, NaCl) 2920, 1656, 1637, 1450, 1357, 1170, 1106, 1090, 858, 789 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{22}H_{27}N_2O_2S_2$ $[M+H]^+$: 415.1508, found 415.1519.



2c

(*Z*)-5-(*p*-tolyl)-3-tosyl-2-(allylimino)thiazolidine (2c):

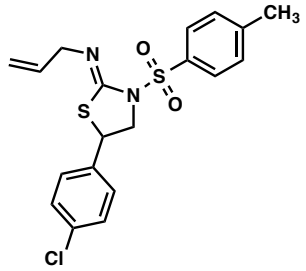
92% yield; R_f = 0.38 (1:4 Acetone:Hexanes eluent); ^1H NMR ($CDCl_3$, 500 MHz) δ 7.95–7.89 (m, 2H), 7.32–7.28 (m, 2H), 7.28–7.24 (m, 2H), 7.19–7.13 (m, 2H), 5.84 (ddt, *J* = 17.1, 10.3, 5.1 Hz, 1H), 5.06 (dq, *J* = 17.2, 1.9 Hz, 1H), 5.02 (dq, *J* = 10.3, 1.7 Hz, 1H), 4.77 (dd, *J* = 8.6, 6.3 Hz, 1H), 4.48 (dd, *J* = 10.3, 6.3 Hz, 1H), 3.91 (dd, *J* = 10.3, 8.7 Hz, 1H), 3.85 (ddt, *J* = 15.9, 5.1, 1.8 Hz, 1H), 3.76 (ddt, *J* = 15.9, 5.2, 1.8 Hz, 1H), 2.44 (s, 3H), 2.35 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 151.4, 144.6, 138.7, 135.1, 135.0, 133.7, 129.8, 129.2, 129.1, 127.5, 115.2, 58.0, 56.6, 47.0, 21.8, 21.2; IR (Neat Film, NaCl) 3007, 2922, 1657, 1639, 1597, 1514, 1358, 1170, 1110, 915, 814, 774, 732 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{20}H_{23}N_2O_2S_2$ $[M+H]^+$: 387.1195, found 387.1202.



2d

(*Z*)-5-(*p*-acetoxyphenyl)-3-tosyl-2-(allylimino)thiazolidine (2d):

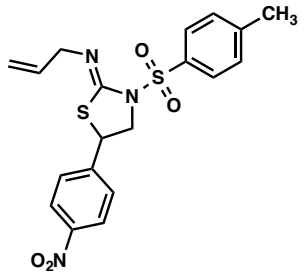
95% yield; R_f = 0.37 (3:7 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.93–7.87 (m, 2H), 7.42–7.34 (m, 2H), 7.32–7.27 (m, 2H), 7.10–7.04 (m, 2H), 5.83 (ddt, *J* = 17.1, 10.3, 5.1 Hz, 1H), 5.12–4.97 (m, 2H), 4.78 (dd, *J* = 8.3, 6.3 Hz, 1H), 4.47 (dd, *J* = 10.3, 6.3 Hz, 1H), 3.91 (dd, *J* = 10.3, 8.3 Hz, 1H), 3.84 (ddt, *J* = 15.9, 5.1, 1.8 Hz, 1H), 3.76 (ddt, *J* = 15.9, 5.2, 1.8 Hz, 1H), 2.43 (s, 3H), 2.30 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 169.4, 151.0, 150.8, 144.7, 135.0, 134.9, 134.5, 129.2, 129.1, 128.8, 122.3, 115.3, 58.0, 56.6, 46.5, 21.8, 21.2; IR (Neat Film, NaCl) 2922, 1760, 1657, 1505, 1360, 1202, 1169, 1107, 912, 811 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{21}H_{23}N_2O_4S_2$ $[M+H]^+$: 431.1094, found 431.1113.



2e

(*Z*)-5-(*p*-chlorophenyl)-3-tosyl-2-(allylimino)thiazolidine (2e):

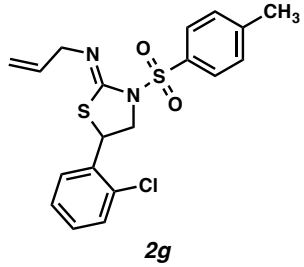
93% yield; R_f = 0.29 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.92–7.87 (m, 2H), 7.32–7.27 (m, 6H), 5.83 (ddt, *J* = 17.1, 10.3, 5.1 Hz, 1H), 5.10–4.99 (m, 2H), 4.75 (dd, *J* = 7.8, 6.3 Hz, 1H), 4.45 (dd, *J* = 10.3, 6.3 Hz, 1H), 3.93 (dd, *J* = 10.3, 7.8 Hz, 1H), 3.84 (ddt, *J* = 15.9, 5.1, 1.8 Hz, 1H), 3.77 (ddt, *J* = 15.9, 5.2, 1.8 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 150.7, 144.7, 135.7, 135.0, 134.9, 134.7, 129.3, 129.2, 129.1, 129.0, 115.4, 58.1, 56.4, 46.4, 21.8; IR (Neat Film, NaCl) 2924, 1651, 1597, 1493, 1354, 1168, 1090, 1014, 917, 809, 731 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{19}H_{20}{}^{35}ClN_2O_2S_2$ $[M+H]^+$: 407.0649, found 407.0665.



2f

(*Z*)-5-(*p*-nitrophenyl)-3-tosyl-2-(allylimino)thiazolidine (2f):

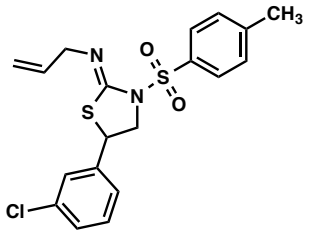
59% yield; R_f = 0.20 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.25–8.19 (m, 2H), 7.93–7.87 (m, 2H), 7.59–7.53 (m, 2H), 7.34–7.28 (m, 2H), 5.84 (ddt, *J* = 17.1, 10.3, 5.1 Hz, 1H), 5.12–5.01 (m, 2H), 4.84 (t, *J* = 6.5 Hz, 1H), 4.47 (dd, *J* = 10.5, 6.3 Hz, 1H), 4.06 (dd, *J* = 10.5, 6.7 Hz, 1H), 3.88–3.77 (m, 2H), 2.45 (d, *J* = 0.8 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 149.8, 148.1, 145.0, 134.8, 134.7, 129.4, 129.1, 128.6, 124.4, 115.6, 58.3, 55.9, 46.0, 21.8; IR (Neat Film, NaCl) 1656, 1597, 1521, 1347, 1169, 1107, 857, 813 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{19}H_{20}N_3O_4S_2$ $[M+H]^+$: 418.0890, found 418.0907.



2g

(*Z*)-5-(*o*-chlorophenyl)-3-tosyl-2-(allylimino)thiazolidine (2g):

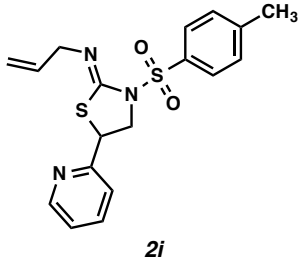
91% yield; R_f = 0.35 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.92–7.87 (m, 2H), 7.60–7.56 (m, 1H), 7.43–7.38 (m, 1H), 7.31–7.26 (m, 4H), 5.83 (ddt, *J* = 17.1, 10.3, 5.1 Hz, 1H), 5.19 (dd, *J* = 6.3, 5.2 Hz, 1H), 5.09–5.00 (m, 2H), 4.39 (dd, *J* = 10.5, 6.3 Hz, 1H), 4.20 (dd, *J* = 10.5, 5.2 Hz, 1H), 3.85 (ddt, *J* = 15.9, 5.1, 1.8 Hz, 1H), 3.79 (ddt, *J* = 15.9, 5.2, 1.8 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 150.8, 144.7, 135.6, 135.0, 134.9, 133.6, 130.0, 129.7, 129.3, 129.1, 128.1, 127.7, 115.3, 58.1, 54.9, 42.8, 21.8; IR (Neat Film, NaCl) 3067, 2881, 1657, 1597, 1470, 1444, 1361, 1284, 1171, 1109, 919, 811, 750 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{19}H_{20}{}^{35}ClN_2O_2S_2$ $[M+H]^+$: 407.0649, found 407.0665.



2h

(*Z*)-5-(*m*-chlorophenyl)-3-tosyl-2-(allylimino)thiazolidine (2h):

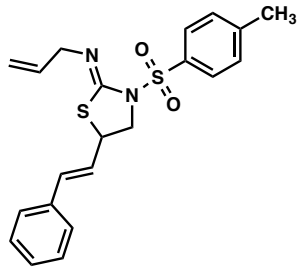
90% yield; R_f = 0.35 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.92–7.86 (m, 2H), 7.37–7.34 (m, 1H), 7.33–7.25 (m, 5H), 5.83 (ddt, *J* = 17.1, 10.3, 5.1 Hz, 1H), 5.09–5.00 (m, 2H), 4.74 (dd, *J* = 7.8, 6.3 Hz, 1H), 4.48 (dd, *J* = 10.4, 6.3 Hz, 1H), 3.94 (dd, *J* = 10.4, 7.8 Hz, 1H), 3.85 (ddt, *J* = 15.9, 5.1, 1.8 Hz, 1H), 3.77 (ddt, *J* = 15.9, 5.2, 1.8 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 150.6, 144.8, 139.3, 135.0, 134.9, 134.8, 130.5, 129.3, 129.1, 129.0, 127.8, 125.9, 115.4, 58.1, 56.4, 46.4, 21.8; IR (Neat Film, NaCl) 2923, 1656, 1596, 1479, 1360, 1169, 1110, 917, 812 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{19}H_{20}{}^{35}ClN_2O_2S_2$ $[M+H]^+$: 407.0649, found 407.0669.



2i

(*Z*)-5-(*o*-pyridyl)-3-tosyl-2-(allylimino)thiazolidine (2i):

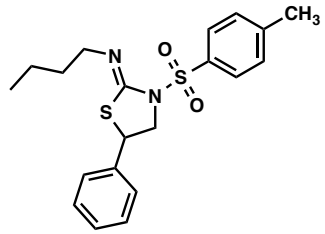
General Procedure C followed using 2.25 equivalents of zinc(II) bromide: 42% yield; R_f = 0.28 (1:1 EtOAc:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.58 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 7.86–7.79 (m, 2H), 7.64 (td, *J* = 7.7, 1.8 Hz, 1H), 7.38 (dq, *J* = 7.9, 0.9 Hz, 1H), 7.26–7.21 (m, 3H), 5.98–5.93 (m, 1H), 5.85 (ddt, *J* = 17.2, 10.3, 5.1 Hz, 1H), 5.10 (dq, *J* = 17.1, 1.8 Hz, 1H), 5.03 (dq, *J* = 10.3, 1.7 Hz, 1H), 3.88 (ddt, *J* = 15.9, 5.2, 1.8 Hz, 1H), 3.77 (ddt, *J* = 15.9, 5.1, 1.8 Hz, 1H), 3.69 (dd, *J* = 11.0, 7.2 Hz, 1H), 3.53 (dd, *J* = 11.0, 1.3 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 158.5, 152.2, 149.6, 144.6, 137.0, 136.1, 135.1, 129.2, 129.1, 123.1, 121.1, 115.3, 64.5, 58.4, 34.6, 21.8; IR (Neat Film, NaCl) 2921, 1655, 1638, 1590, 1352, 1169, 1110, 1088, 792 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{18}H_{20}N_3O_2S_2$ $[M+H]^+$: 374.0991, found 374.1006.



2j

(*Z*)-5-((*E*)-styryl)-3-tosyl-2-(allylimino)thiazolidine (2j):

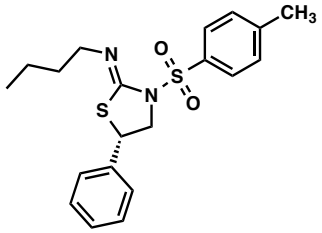
47% yield; R_f = 0.34 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.94–7.90 (m, 2H), 7.38–7.26 (m, 7H), 6.64 (dd, *J* = 15.6, 0.8 Hz, 1H), 6.13 (dd, *J* = 15.6, 8.9 Hz, 1H), 5.82 (ddt, *J* = 17.1, 10.3, 5.1 Hz, 1H), 5.09–4.97 (m, 2H), 4.42 (dddd, *J* = 8.9, 7.4, 6.0, 0.8 Hz, 1H), 4.34 (dd, *J* = 10.2, 6.0 Hz, 1H), 3.87 (dd, *J* = 10.2, 7.5 Hz, 1H), 3.82 (ddt, *J* = 15.8, 5.1, 1.8 Hz, 1H), 3.75 (ddt, *J* = 15.9, 5.2, 1.8 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 151.2, 144.7, 135.6, 135.0, 134.9, 134.4, 129.3, 129.1, 128.9, 128.6, 126.8, 124.6, 115.3, 58.1, 54.9, 46.2, 21.8; IR (Neat Film, NaCl) 2925, 2254, 1645, 1452, 1353, 1259, 1168, 1090, 1019, 915, 811, 753 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{21}H_{23}N_2O_2S_2$ $[M+H]^+$: 399.1195, found 399.1201.



2k

(*Z*)-5-phenyl-3-tosyl-2-((*n*-butyl)imino)thiazolidine (2k):

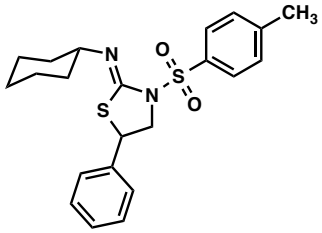
>99% yield; R_f = 0.36 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.92–7.87 (m, 2H), 7.40–7.32 (m, 5H), 7.31–7.27 (m, 2H), 4.78 (dd, *J* = 8.4, 6.3 Hz, 1H), 4.48 (dd, *J* = 10.2, 6.3 Hz, 1H), 3.91 (dd, *J* = 10.2, 8.4 Hz, 1H), 3.20 (dt, *J* = 12.6, 6.7 Hz, 1H), 3.08 (dt, *J* = 12.7, 6.8 Hz, 1H), 2.44 (s, 3H), 1.50 (dddd, *J* = 13.5, 8.7, 6.7, 2.2 Hz, 2H), 1.23–1.13 (m, 2H), 0.86 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 149.4, 144.5, 137.1, 135.1, 129.1, 129.1, 129.1, 128.8, 127.7, 56.4, 56.1, 47.0, 32.9, 21.8, 20.5, 14.0; IR (Neat Film, NaCl) 2955, 2928, 2870, 1658, 1455, 1357, 1170, 1096, 811, 765 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{20}H_{25}N_2O_2S_2$ $[M+H]^+$: 389.1352, found 389.1368.



(S)-2k

(*S*,*Z*)-5-phenyl-3-tosyl-2-(*n*-butylimino)thiazolidine ((*S*)-2k):

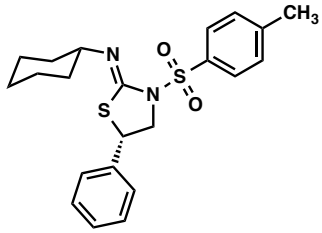
Thiazolidine **(*S*)-2k** was prepared according to General Procedure E: 94% yield; R_f = 0.36 (1:4 Acetone:Hexanes eluent); characterization data match those above; $[\alpha]_D^{25.0}$ –6.45° (*c* 2.800, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralpak AD-H column, 30% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 4.7 minutes, minor retention time: 3.6 minutes, 95% ee).



2l

(*Z*)-5-phenyl-3-tosyl-2-(cyclohexylimino)thiazolidine (2l):

94% yield; R_f = 0.41 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.95–7.89 (m, 2H), 7.41–7.31 (m, 5H), 7.31–7.27 (m, 2H), 4.76 (dd, *J* = 8.5, 6.3 Hz, 1H), 4.46 (dd, *J* = 10.3, 6.3 Hz, 1H), 3.87 (dd, *J* = 10.2, 8.5 Hz, 1H), 2.77 (tt, *J* = 9.5, 3.9 Hz, 1H), 2.44 (s, 3H), 1.79–1.62 (m, 3H), 1.58 (dddd, *J* = 12.8, 5.9, 3.6, 1.7 Hz, 2H), 1.40 (ddtd, *J* = 22.7, 16.6, 9.5, 4.6 Hz, 2H), 1.33–1.18 (m, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 147.2, 144.4, 137.2, 135.0, 129.3, 129.1, 129.0, 128.7, 127.6, 65.5, 56.1, 47.0, 33.6, 33.4, 25.8, 24.5, 24.5, 21.8; IR (Neat Film, NaCl) 2928, 2853, 1652, 1450, 1362, 1171, 1100, 812, 760 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{22}H_{27}N_2O_2S_2$ $[M+H]^+$: 415.1508, found 415.1493.

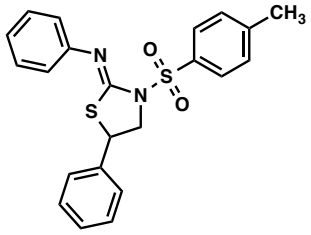


(S)-2l

(*S*,*Z*)-5-phenyl-3-tosyl-2-(cyclohexylimino)thiazolidine ((*S*)-2l):

Thiazolidine **(*S*)-2l** was prepared according to General Procedure E: 98% yield; R_f = 0.41 (1:4 Acetone:Hexanes eluent); characterization data match those above; $[\alpha]_D^{25.0}$ 0.72° (*c* 4.200, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralpak AS-H

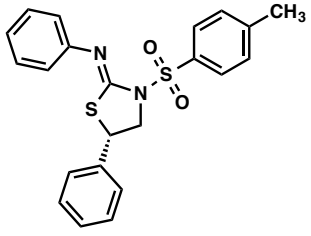
column, 30% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 5.1 minutes, minor retention time: 4.0 minutes, 92% ee).



2m

(*Z*)-5-phenyl-3-tosyl-2-(phenylimino)thiazolidine (2m):

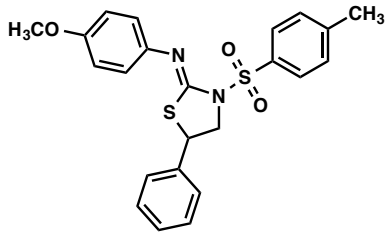
95% yield; R_f = 0.23 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.03–7.96 (m, 2H), 7.41–7.29 (m, 7H), 7.30–7.22 (m, 2H), 7.12–7.03 (m, 1H), 6.83–6.75 (m, 2H), 4.80 (dd, *J* = 8.5, 6.4 Hz, 1H), 4.60 (dd, *J* = 10.4, 6.4 Hz, 1H), 4.06 (dd, *J* = 10.4, 8.5 Hz, 1H), 2.49 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 152.3, 150.1, 145.0, 136.6, 134.7, 129.3, 129.2, 129.1, 129.0, 128.9, 127.6, 124.4, 120.9, 56.9, 47.1, 21.9; IR (Neat Film, NaCl) 3030, 1640, 1591, 1487, 1360, 1171, 1135, 1100, 763 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{22}H_{21}N_2O_2S_2$ $[M+H]^+$: 409.1039, found 409.1051.



(S)-2m

(*S*,*Z*)-5-phenyl-3-tosyl-2-(phenylimino)thiazolidine ((*S*)-2m):

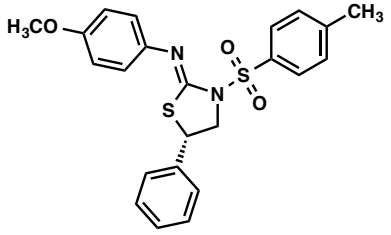
Thiazolidine **(*S*)-2m** was prepared according to General Procedure E: >99% yield; R_f = 0.23 (1:4 Acetone:Hexanes eluent); characterization data match those above; $[\alpha]_D^{25.0}$ 49.9° (*c* 3.400, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralpak AS-H column, 30% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 7.3 minutes, minor retention time: 5.7 minutes, 77% ee).



2n

(*Z*)-5-phenyl-3-tosyl-2-((*p*-methoxyphenyl)imino)thiazolidine (2n):

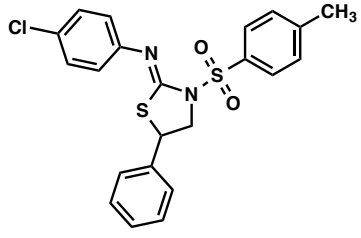
98% yield; R_f = 0.31 (3:7 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.03–7.94 (m, 2H), 7.39–7.28 (m, 7H), 6.85–6.79 (m, 2H), 6.79–6.73 (m, 2H), 4.79 (dd, *J* = 8.4, 6.4 Hz, 1H), 4.59 (dd, *J* = 10.4, 6.4 Hz, 1H), 4.05 (dd, *J* = 10.4, 8.5 Hz, 1H), 3.76 (s, 3H), 2.48 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 156.6, 151.9, 144.9, 143.4, 136.7, 134.8, 129.3, 129.2, 129.1, 128.8, 127.6, 121.9, 114.2, 56.7, 55.5, 47.0, 21.8; IR (Neat Film, NaCl) 2949, 1640, 1505, 1455, 1360, 1290, 1242, 1168, 1101, 1033, 910, 832, 811, 768, 733 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{23}H_{23}N_2O_3S_2$ $[M+H]^+$: 439.1145, found 439.1161.



(S)-2n

(*S*,*Z*)-5-phenyl-3-tosyl-2-(*p*-methoxyphenylimino)thiazolidine ((*S*)-2n):

Thiazolidine **(*S*)-2n** was prepared according to General Procedure E: 97% yield; R_f = 0.31 (3:7 Acetone:Hexanes eluent); characterization data match those above; $[\alpha]_D^{25.0}$ 61.6° (*c* 2.800, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralpak AS-H column, 30% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 9.1 minutes, minor retention time: 6.9 minutes, 90% ee).

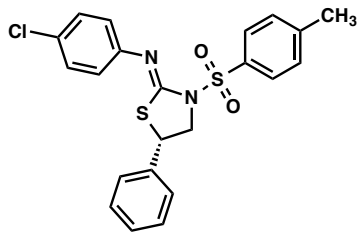


2o

(*Z*)-5-phenyl-3-tosyl-2-((*p*-chlorophenyl)imino)thiazolidine (2o):

92% yield; R_f = 0.29 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.01–7.93 (m, 2H), 7.39–7.30 (m, 7H), 7.25–7.18 (m, 2H), 6.76–6.70 (m, 2H), 4.81 (dd, *J* = 8.4, 6.4 Hz, 1H), 4.60 (dd, *J* = 10.4, 6.5 Hz, 1H), 4.07 (dd, *J* = 10.4, 8.5 Hz, 1H), 2.48 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 153.0, 148.5, 145.2, 136.4, 134.6, 129.7, 129.4,

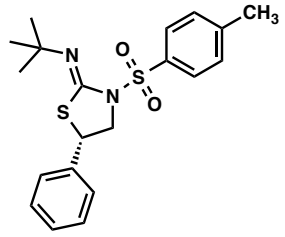
129.2, 129.2, 129.1, 129.0, 127.6, 122.3, 56.9, 47.2, 21.9; IR (Neat Film, NaCl) 2924, 1634, 1588, 1486, 1360, 1172, 1139, 1088, 833, 812 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{22}H_{20}{}^{35}ClN_2O_2S_2$ $[M+H]^+$: 443.0649, found 443.0664.



(S)-2o

(*S*,*Z*)-5-phenyl-3-tosyl-2-(*p*-chlorophenylimino)thiazolidine ((*S*)-2o):

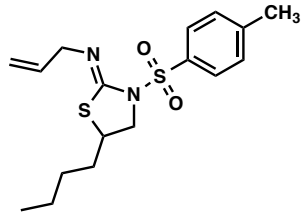
Thiazolidine **(*S*)-2o** was prepared according to General Procedure E: 99% yield; R_f = 0.29 (1:4 Acetone:Hexanes eluent); characterization data match those above; $[\alpha]_D{}^{25.0}$ 44.7° (*c* 4.950, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralpak AS-H column, 30% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 7.7 minutes, minor retention time: 6.1 minutes, 60% ee).



(S)-2p

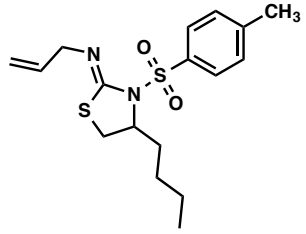
(*S*,*Z*)-5-phenyl-3-tosyl-2-(*t*-butylimino)thiazolidine ((*S*)-2p):

39% yield; R_f = 0.38 (1:4 Acetone:Hexanes eluent); ^1H NMR ($CDCl_3$, 500 MHz) δ 7.88–7.83 (m, 2H), 7.42–7.31 (m, 5H), 7.30–7.26 (m, 2H), 4.79 (dd, *J* = 8.4, 6.2 Hz, 1H), 4.47 (dd, *J* = 10.3, 6.2 Hz, 1H), 3.88 (dd, *J* = 10.3, 8.4 Hz, 1H), 2.44 (s, 3H), 1.17 (s, 9H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 144.2, 142.9, 137.3, 135.7, 129.4, 129.1, 128.8, 128.7, 127.7, 55.0, 54.7, 48.3, 28.9, 21.8; IR (Neat Film, NaCl) 2971, 1653, 1600, 1496, 1454, 1360, 1167, 1092, 810, 771, 701 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{20}H_{25}N_2O_2S_2$ $[M+H]^+$: 389.1352, found 389.1362; $[\alpha]_D{}^{25.0}$ 3.33° (*c* 1.900, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralpak IC-3 column, 30% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 6.2 minutes, minor retention time: 7.0 minutes, 75% ee).



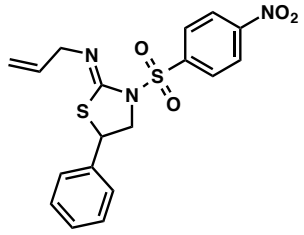
5

(*Z*)-5-(*n*-butyl)-3-tosyl-2-(allylimino)thiazolidine (5):[21]
18% yield; R_f = 0.44 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.94–7.86 (m, 2H), 7.30–7.26 (m, 2H), 5.80 (ddt, *J* = 17.1, 10.3, 5.1 Hz, 1H), 5.04–4.96 (m, 2H), 4.21 (dd, *J* = 10.0, 5.9 Hz, 1H), 3.81–3.73 (m, 2H), 3.70 (dd, *J* = 10.0, 7.1 Hz, 1H), 3.59 (ddt, *J* = 8.4, 7.0, 6.0 Hz, 1H), 2.42 (s, 3H), 1.82–1.70 (m, 1H), 1.71–1.60 (m, 1H), 1.42–1.27 (m, 4H), 0.90 (td, *J* = 7.4, 3.7 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 151.6, 144.5, 135.2, 130.0, 129.2, 129.0, 115.1, 58.0, 55.0, 44.0, 33.9, 30.1, 22.5, 21.8, 14.0; IR (Neat Film, NaCl) 2957, 2928, 2871, 1652, 1598, 1456, 1357, 1170, 1106, 918, 812 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{17}H_{25}N_2O_2S_2$ $[M+H]^+$: 353.1352, found 353.1364.



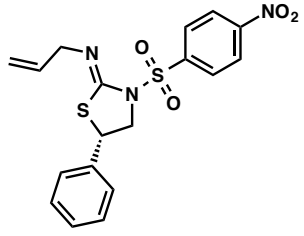
6

(*Z*)-4-(*n*-butyl)-3-tosyl-2-(allylimino)thiazolidine (6):[21]
56% yield; R_f = 0.44 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.95–7.85 (m, 2H), 7.29–7.24 (m, 2H), 5.80 (ddt, *J* = 17.1, 10.3, 5.2 Hz, 1H), 5.03 (dq, *J* = 17.2, 1.9 Hz, 1H), 4.99 (dq, *J* = 10.3, 1.8 Hz, 1H), 4.82–4.74 (m, 1H), 3.81 (ddt, *J* = 15.9, 5.2, 1.8 Hz, 1H), 3.70 (ddt, *J* = 15.9, 5.1, 1.8 Hz, 1H), 3.33 (dd, *J* = 11.0, 6.8 Hz, 1H), 2.94 (dd, *J* = 11.1, 0.8 Hz, 1H), 2.41 (s, 3H), 1.88–1.73 (m, 2H), 1.47–1.27 (m, 4H), 0.91 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 151.8, 144.2, 136.8, 135.1, 129.2, 128.9, 115.1, 61.2, 58.2, 33.1, 32.3, 28.7, 22.5, 21.7, 14.1; IR (Neat Film, NaCl) 2957, 2928, 2860, 1651, 1598, 1455, 1351, 1164, 1117, 1088, 918, 813 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{17}H_{25}N_2O_2S_2$ $[M+H]^+$: 353.1352, found 353.1358.



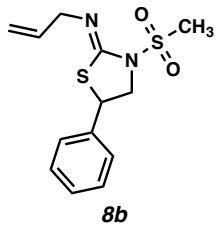
8a

(*Z*)-5-phenyl-3-(*p*-nitrobenzenesulfonyl)-2-(allylimino)thiazolidine (8a):
94% yield; R_f = 0.28 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.37–8.28 (m, 2H), 8.26–8.16 (m, 2H), 7.42–7.31 (m, 5H), 5.82 (ddt, *J* = 17.1, 10.4, 5.2 Hz, 1H), 5.11–5.03 (m, 2H), 4.86 (dd, *J* = 8.3, 6.3 Hz, 1H), 4.54 (dd, *J* = 10.3, 6.3 Hz, 1H), 3.98 (dd, *J* = 10.3, 8.4 Hz, 1H), 3.83 (ddt, *J* = 15.9, 5.2, 1.8 Hz, 1H), 3.75 (ddt, *J* = 15.8, 5.3, 1.7 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 151.1, 150.6, 143.6, 136.3, 134.6, 130.4, 129.2, 129.1, 127.6, 123.7, 115.7, 57.9, 56.5, 47.5; IR (Neat Film, NaCl) 3106, 1656, 1530, 1349, 1314, 1175, 1109, 854, 740 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{18}H_{18}N_3O_4S_2$ $[M+H]^+$: 404.0733, found 404.0742.



(S)-8a

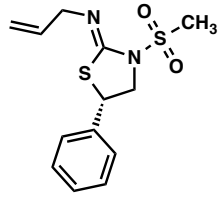
(*S*,*Z*)-5-phenyl-3-(*p*-nitrobenzenesulfonyl)-2-(allylimino)thiazolidine ((*S*)-8a):
Thiazolidine **(*S*)-8a** was prepared according to General Procedure E and was isolated as a white crystalline solid: 95% yield; R_f = 0.28 (1:4 Acetone:Hexanes eluent); characterization data match those above; colorless, translucent X-ray quality crystals were obtained by slow diffusion of 1% benzene in heptane into a solution of iminothiazolidine **(*S*)-8a** in ethyl acetate, mp: 70–72 °C; $[\alpha]_D^{25.0}$ 1.7° (*c* 2.250, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralcel OD-H column, 30% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 6.6 minutes, minor retention time: 5.5 minutes, 95% ee).



8b

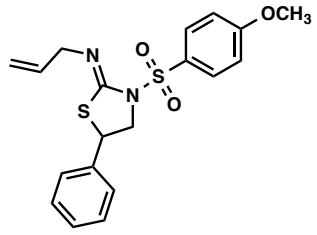
(*Z*)-5-phenyl-3-mesyl-2-(allylimino)thiazolidine (8b):
Thiazolidine **8b** was isolated as a clear, colorless oil: 91% yield; R_f = 0.40 (3:7 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.46–7.31 (m, 5H), 5.97 (ddt, *J* = 17.1, 10.3, 5.2 Hz, 1H), 5.27 (dq, *J* = 17.1, 1.8 Hz, 1H), 5.13 (dq, *J* = 10.3, 1.7 Hz, 1H),

4.84 (dd, J = 8.6, 6.3 Hz, 1H), 4.41 (dd, J = 10.4, 6.3 Hz, 1H), 3.99–3.90 (m, 3H), 3.38 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 153.0, 136.6, 134.9, 129.2, 129.0, 127.7, 115.8, 58.1, 55.6, 47.6, 40.5; IR (Neat Film, NaCl) 3011, 1656, 1651, 1346, 1163, 1113, 964, 764 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{13}H_{17}N_2O_2S_2$ $[M+H]^+$: 297.0726, found 297.0739.



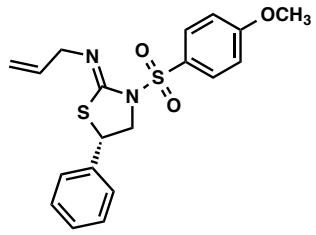
(S)-8b

(*S*,*Z*)-5-phenyl-3-mesyl-2-(allylimino)thiazolidine ((*S*)-8b):
Thiazolidine **(*S*)-8b** was prepared according to General Procedure E and was isolated as a clear, colorless oil: 95% yield; R_f = 0.40 (3:7 Acetone:Hexanes eluent); characterization data match those reported above; $[\alpha]_D^{25.0}$ –55.5° (*c* 2.200, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralpak AD-H column, 7% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 12.6 minutes, minor retention time: 11.3 minutes, 90% ee).



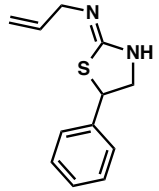
8c

(*Z*)-5-phenyl-3-(*p*-methoxybenzenesulfonyl)-2-(allylimino)thiazolidine (8c):
90% yield; R_f = 0.40 (3:7 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.01–7.93 (m, 2H), 7.42–7.29 (m, 5H), 6.98–6.93 (m, 2H), 5.85 (ddt, J = 17.1, 10.3, 5.2 Hz, 1H), 5.08 (dq, J = 17.1, 1.8 Hz, 1H), 5.03 (dq, J = 10.3, 1.7 Hz, 1H), 4.79 (dd, J = 8.4, 6.3 Hz, 1H), 4.49 (dd, J = 10.3, 6.3 Hz, 1H), 3.92 (dd, J = 10.3, 8.4 Hz, 1H), 3.88 (s, 3H), 3.88–3.83 (m, 1H), 3.77 (ddt, J = 15.9, 5.2, 1.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 163.8, 151.3, 136.9, 135.1, 131.4, 129.5, 129.2, 128.8, 127.7, 115.3, 113.8, 58.1, 56.6, 55.8, 47.1; IR (Neat Film, NaCl) 2927, 1655, 1595, 1497, 1356, 1262, 1162, 1110, 1090, 1025, 833, 810 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{19}H_{21}N_2O_3S_2$ $[M+H]^+$: 389.0988, found 389.1004.



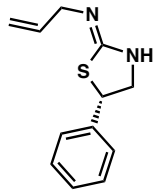
(S)-8c

(*S*,*Z*)-5-phenyl-3-(*p*-methoxybenzenesulfonyl)-2-(allylimino)thiazolidine ((*S*)-8c):
Thiazolidine **(*S*)-8c** was prepared according to General Procedure E: 94% yield; R_f = 0.40 (3:7 Acetone:Hexanes eluent); characterization data match those reported above; $[\alpha]_D^{25.0}$ –6.6° (*c* 2.000, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralpak AD-H column, 30% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 4.4 minutes, minor retention time: 6.6 minutes, 91% ee).



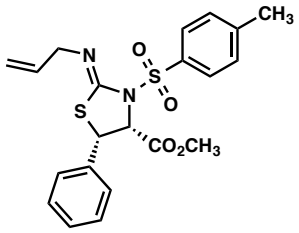
8d

(*Z*)-5-phenyl-2-(allylimino)thiazolidine (8d):
75% yield; R_f = 0.19 (3:7 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.40–7.36 (m, 2H), 7.35–7.30 (m, 2H), 7.29–7.26 (m, 1H), 5.94 (ddt, *J* = 17.2, 10.2, 5.5 Hz, 1H), 5.27 (dq, *J* = 17.1, 1.6 Hz, 1H), 5.18 (dq, *J* = 10.3, 1.4 Hz, 1H), 5.02 (dd, *J* = 7.8, 6.3 Hz, 1H), 4.34 (dd, *J* = 13.4, 7.8 Hz, 1H), 4.10 (dd, *J* = 13.4, 6.3 Hz, 1H), 3.97 (dt, *J* = 5.5, 1.6 Hz, 2H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 160.7, 141.3, 134.5, 128.9, 127.9, 127.4, 116.6, 68.4, 56.7, 47.3; IR (Neat Film, NaCl) 2924, 2853, 1612, 1454, 1260, 1023, 802, 758 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{12}H_{15}N_2S$ $[M+H]^+$: 219.0950, found 219.0950.



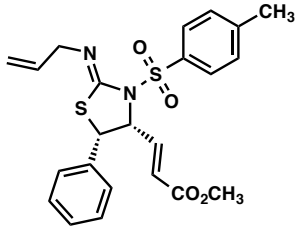
(S)-8d

(*S*,*Z*)-5-phenyl-2-(allylimino)thiazolidine ((*S*)-8d):
Thiazolidine **(*S*)-8d** was prepared according to General Procedure E: 31% yield; R_f = 0.19 (3:7 Acetone:Hexanes eluent); characterization data match those reported above; $[\alpha]_D^{25.0}$ 26.4° (*c* 0.200, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralcel OB-H column, 10% methanol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 3.9 minutes, minor retention time: 8.4 minutes, 34% ee).



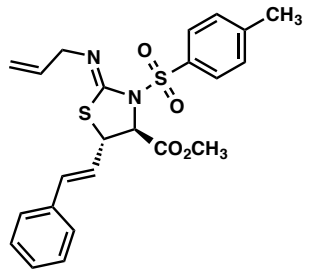
11

***cis*-methyl (*Z*)-5-phenyl-3-tosyl-2-(allylimino)thiazolidine-4-carboxylate (11):**
Thiazolidine **11** was isolated as a white crystalline solid and colorless, translucent X-ray quality crystals were obtained by slow diffusion of 1% benzene in heptane into a solution of iminothiazolidine **11** in ethyl acetate, mp: 107–109 °C: 88% yield; R_f = 0.32 (3:7 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.96–7.90 (m, 2H), 7.38–7.31 (m, 5H), 7.30–7.25 (m, 2H), 5.86 (ddt, *J* = 17.1, 10.3, 4.9 Hz, 1H), 5.33 (d, *J* = 8.0 Hz, 1H), 5.26 (d, *J* = 8.0 Hz, 1H), 5.07 (dq, *J* = 17.1, 1.9 Hz, 1H), 5.03 (dq, *J* = 10.4, 1.8 Hz, 1H), 3.91 (ddt, *J* = 16.1, 4.9, 1.8 Hz, 1H), 3.83 (ddt, *J* = 16.1, 4.8, 1.9 Hz, 1H), 3.25 (s, 3H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 168.0, 150.2, 144.7, 135.4, 134.8, 132.9, 129.7, 129.3, 128.9, 128.8, 128.4, 115.1, 65.7, 57.9, 52.1, 49.8, 21.8; IR (Neat Film, NaCl) 2952, 2253, 1748, 1660, 1595, 1444, 1353, 1166, 1107, 915, 811 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{21}H_{23}N_2O_4S_2$ $[M+H]^+$: 431.1094, found 431.1114.



13

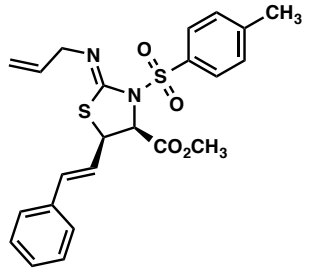
***cis*-(*Z*)-4-((*E*)-2-(methoxycarbonyl)ethenyl)-5-phenyl-3-tosyl-2-(allylimino)thiazolidine (13):**
62% yield; R_f = 0.43 (3:7 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.93–7.87 (m, 2H), 7.36–7.27 (m, 5H), 7.26–7.23 (m, 2H), 6.60 (dd, *J* = 15.6, 7.4 Hz, 1H), 5.88 (ddt, *J* = 17.1, 10.2, 5.0 Hz, 1H), 5.80 (dd, *J* = 15.7, 1.1 Hz, 1H), 5.42 (ddd, *J* = 7.5, 6.5, 1.1 Hz, 1H), 5.22 (d, *J* = 6.5 Hz, 1H), 5.11 (dq, *J* = 17.1, 1.9 Hz, 1H), 5.06 (dq, *J* = 10.3, 1.7 Hz, 1H), 3.90 (ddt, *J* = 16.0, 4.9, 1.8 Hz, 1H), 3.84 (ddt, *J* = 16.0, 5.1, 1.8 Hz, 1H), 3.66 (s, 3H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 165.6, 149.6, 144.7, 140.3, 135.9, 134.9, 132.2, 129.6, 129.2, 129.1, 129.0, 128.7, 125.8, 115.4, 65.3, 58.1, 52.8, 51.9, 21.8; IR (Neat Film, NaCl) 2951, 1726, 1659, 1436, 1360, 1276, 1168, 1109, 917, 812 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{23}H_{25}N_2O_4S_2$ $[M+H]^+$: 457.1250, found 457.1268.



16

***trans*-methyl (*Z*)-5-((*E*)-styryl)-3-tosyl-2-(allylimino)thiazolidine-4-carboxylate (16):**[22]

42% yield; R_f = 0.39 (3:7 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.98–7.93 (m, 2H), 7.34 (m, 4H), 7.32–7.27 (m, 1H), 7.25–7.20 (m, 2H), 6.62 (dd, *J* = 15.7, 0.9 Hz, 1H), 6.22 (dd, *J* = 15.6, 8.5 Hz, 1H), 5.84 (ddt, *J* = 17.1, 10.1, 4.9 Hz, 1H), 5.20 (d, *J* = 1.7 Hz, 1H), 5.07–4.99 (m, 2H), 4.57 (ddd, *J* = 8.5, 1.8, 1.0 Hz, 1H), 3.82 (ddd, *J* = 5.1, 3.5, 1.8 Hz, 2H), 3.80 (s, 3H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 169.4, 149.2, 144.6, 135.7, 135.5, 134.8, 133.2, 129.7, 128.9, 128.8, 128.6, 126.9, 125.9, 115.2, 66.9, 58.0, 53.4, 48.3, 21.8; IR (Neat Film, NaCl) 2954, 1756, 1661, 1597, 1495, 1435, 1354, 1167, 1113, 1089, 916, 813, 781, 754 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{23}H_{25}N_2O_4S_2$ $[M+H]^+$: 457.1250, found 457.1252.



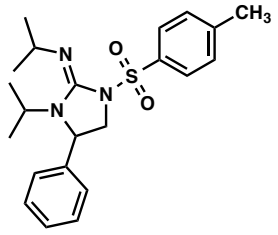
17

***cis*-methyl (*Z*)-5-((*E*)-styryl)-3-tosyl-2-(allylimino)thiazolidine-4-carboxylate (17):**[22]

31% yield; R_f = 0.39 (3:7 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.97–7.92 (m, 2H), 7.36–7.27 (m, 7H), 6.66 (dd, *J* = 15.6, 0.9 Hz, 1H), 6.00 (dd, *J* = 15.5, 9.1 Hz, 1H), 5.84 (ddt, *J* = 17.1, 10.3, 4.9 Hz, 1H), 5.27 (d, *J* = 7.6 Hz, 1H), 5.09–4.98 (m, 2H), 4.80 (ddd, *J* = 9.1, 7.6, 0.9 Hz, 1H), 3.85 (ddt, *J* = 16.1, 4.9, 1.9 Hz, 1H), 3.80 (ddt, *J* = 16.1, 4.8, 1.9 Hz, 1H), 3.68 (s, 3H), 2.43 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 168.2, 150.2, 144.7, 135.7, 135.5, 135.5, 134.8, 129.7, 129.0, 128.9, 128.8, 126.9, 121.2, 115.2, 64.5, 58.0, 52.6, 48.3, 21.8; IR (Neat Film, NaCl) 2952, 1750, 1661, 1597, 1495, 1450, 1354, 1206, 1169, 1121, 1089, 966, 916, 841, 813, 751 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{23}H_{25}N_2O_4S_2$ $[M+H]^+$: 457.1250, found 457.1253.

Iminoimidazolidine Synthesis and Characterization Data

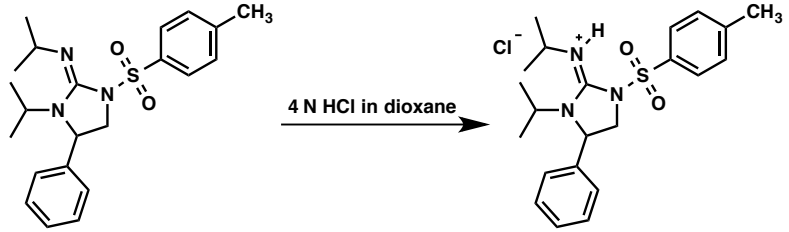
Unless otherwise stated, all iminothiazolidines were prepared according to General Procedure D and were isolated as amorphous white solids.



9a

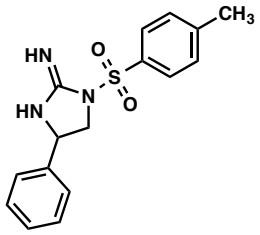
(*E*)-3-isopropyl-4-phenyl-1-tosyl-2-(isopropylimino)imidazolidine (9a):

Product was initially prepared according to General Procedure D, isolating the product as a salt after column chromatography (2%→5% CH_3OH in CH_2Cl_2eluent). The resulting white foam was dissolved in 20 mL CH_2Cl_2 and washed with aqueous 0.1 N NaOH (3 x 10 mL). The organic layer was dried over sodium sulfate, filtered, and concentrated in vacuo to give imidazolidine **9a** (88 mg, 55% yield) as a colorless oil.



9a ***9a·HCl***

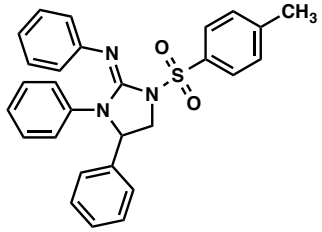
For the purpose of characterization, to a portion of iminoimidazolidine **9a** (ca. 0.20 mmol) as a neat oil was added 4 N HCl in dioxane (3 mL) immediately followed by Et_2O (40 mL) causing a white precipitate to form. The supernatant was decanted and the residual white solid was washed with Et_2O (3 x 10 mL) and dried in vacuo furnishing iminoimidazolidinium hydrochloride **9a•HCl** as a white solid: R_f = 0.39 (1:9 CH_3OH:CH_2Cl_2 eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 10.95 (bs, 1H), 7.69–7.59 (m, 2H), 7.30–7.24 (m, 3H), 7.18 (dd, *J* = 8.2, 6.9 Hz, 2H), 6.96–6.85 (m, 2H), 5.52–5.32 (m, 1H), 4.82–4.75 (m, 1H), 4.48–4.26 (m, 2H), 4.03 (dd, *J* = 12.0, 3.0 Hz, 1H), 2.46 (s, 3H), 1.70 (d, *J* = 6.4 Hz, 3H), 1.51 (d, *J* = 6.4 Hz, 3H), 1.28–1.21 (m, 3H), 0.95 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 154.7, 146.9, 137.9, 133.7, 130.8, 129.3, 128.8, 127.7, 125.9, 57.0, 56.1, 54.0, 51.3, 24.3, 22.2, 21.9, 21.3, 20.8; IR (Neat Film, NaCl) 2972, 1636, 1457, 1435, 1367, 1260, 1172, 1088, 1036, 907, 814, 729 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{22}H_{30}N_3O_2S$ $[M–Cl]^+$: 400.2053, found 400.2067.



9b

4-phenyl-1-tosyl-2-iminoimidazolidine (9b):

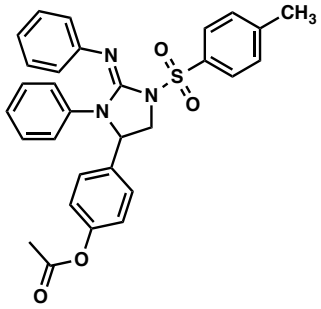
Prepared according to General Procedure D followed by purification by column chromatography using deactivated silica gel (1% Me_2NEt and 1% MeOH in CH_2Cl_2 eluent): 61% yield; R_f = 0.41 (1:9 CH_3OH:CH_2Cl_2 eluent); ^1H NMR (DMSO-d_6, 500 MHz) δ 7.86–7.79 (m, 2H), 7.46 (dd, *J* = 8.4, 0.9 Hz, 2H), 7.21–7.16 (m, 3H), 6.92 (dd, *J* = 6.7, 2.9 Hz, 2H), 4.77 (dd, *J* = 9.2, 6.5 Hz, 1H), 4.14 (t, *J* = 9.6 Hz, 1H), 3.35 (bs, 2H), 3.26 (dd, *J* = 9.9, 6.5 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (DMSO-d_6, 126 MHz) δ 151.2, 145.0, 143.6, 132.9, 130.1, 128.2, 127.5, 126.9, 125.9, 61.4, 55.2, 21.1; IR (Neat Film, NaCl) 3445, 2920, 1683, 1397, 1350, 1161, 1091, 1002 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{16}H_{18}N_3O_2S$ $[M+H]^+$: 316.1114, found 316.1126.



9c

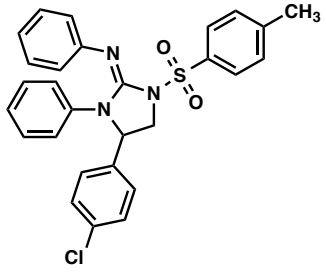
(*E*)-3,4-diphenyl-1-tosyl-2-(phenylimino)imidazolidine (9c):

96% yield; R_f = 0.22 (1:4 Acetone:Hexanes eluent); ^1H NMR ($CDCl_3$, 500 MHz) δ 8.03–7.96 (m, 2H), 7.37–7.28 (m, 5H), 7.24–7.15 (m, 2H), 6.82–6.73 (m, 5H), 6.60–6.48 (m, 3H), 6.42–6.34 (m, 2H), 4.77 (dd, *J* = 8.2, 5.7 Hz, 1H), 4.45 (dd, *J* = 9.9, 8.2 Hz, 1H), 3.94 (dd, *J* = 9.9, 5.8 Hz, 1H), 2.49 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 146.6, 144.6, 143.4, 139.9, 139.8, 135.0, 129.4, 129.3, 129.2, 128.8, 128.3, 127.8, 126.9, 125.8, 125.6, 121.9, 121.4, 64.9, 52.5, 21.9; IR (Neat Film, NaCl) 3027, 2924, 1667, 1593, 1488, 1354, 1166, 1089, 813, 759 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{28}H_{26}N_3O_2S$ $[M+H]^+$: 468.1740, found 468.1755.



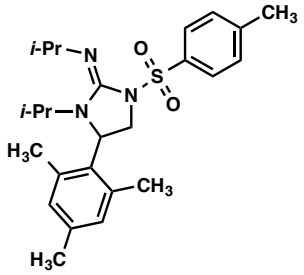
9d

(*E*)-4-(*p*-acetoxyphenyl)-3-phenyl-1-tosyl-2-(phenylimino)imidazolidine (9d):
99% yield; R_f = 0.28 (3:7 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.03–7.96 (m, 2H), 7.37–7.29 (m, 2H), 7.22–7.18 (m, 2H), 7.08–7.02 (m, 2H), 6.82–6.75 (m, 5H), 6.61–6.55 (m, 1H), 6.55–6.52 (m, 2H), 6.41–6.36 (m, 2H), 4.80 (dd, *J* = 8.1, 5.7 Hz, 1H), 4.44 (dd, *J* = 9.9, 8.1 Hz, 1H), 3.92 (dd, *J* = 9.9, 5.7 Hz, 1H), 2.48 (s, 3H), 2.30 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 169.4, 150.9, 146.1, 144.8, 143.5, 139.6, 137.2, 134.7, 129.4, 129.3, 128.4, 128.0, 127.9, 126.0, 125.7, 122.5, 122.0, 121.6, 64.4, 52.4, 21.9, 21.3; IR (Neat Film, NaCl) 3057, 2928, 1760, 1670, 1591, 1495, 1367, 1211, 1167, 1113, 1090, 1017, 911, 813, 763, 734 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{30}H_{28}N_3O_4S$ $[M+H]^+$: 526.1795, found 526.1800.



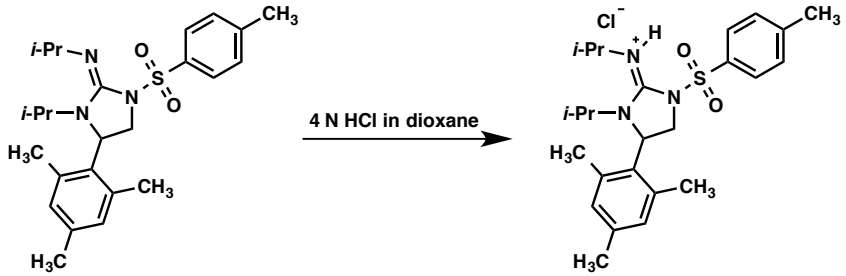
9e

(*E*)-4-(*p*-chlorophenyl)-3-phenyl-1-tosyl-2-(phenylimino)imidazolidine (9e):
87% yield; R_f = 0.19 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.03–7.95 (m, 2H), 7.35–7.31 (m, 2H), 7.30–7.27 (m, 2H), 7.16–7.12 (m, 2H), 6.83–6.75 (m, 5H), 6.61–6.56 (m, 1H), 6.53 (dd, *J* = 6.8, 2.9 Hz, 2H), 6.42–6.35 (m, 2H), 4.79 (dd, *J* = 8.1, 5.6 Hz, 1H), 4.44 (dd, *J* = 9.9, 8.1 Hz, 1H), 3.90 (dd, *J* = 9.9, 5.6 Hz, 1H), 2.49 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 146.0, 144.8, 143.4, 139.4, 138.2, 134.7, 134.6, 129.4, 129.4, 129.2, 128.4, 128.3, 127.9, 126.1, 125.7, 122.0, 121.7, 64.3, 52.3, 21.9; IR (Neat Film, NaCl) 3062, 1668, 1591, 1492, 1360, 1213, 1167, 1090, 1014, 910, 813, 761, 734 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{28}H_{25}{}^{35}ClN_3O_2S$ $[M+H]^+$: 502.1351, found 502.1355.



S19

(*E*)-3-isopropyl-4-mesityl-1-tosyl-2-(isopropylimino)imidazolidine (S19):
Product was initially prepared according to General Procedure D, isolating the product as the $H(ZnBr_3 \bullet CH_3OH)$ salt after column chromatography (2%→5% CH_3OH in CH_2Cl_2 eluent). A portion of this resulting white foam was crystallized, forming colorless, translucent X-ray quality crystals after slow evaporation from a solution of **S19** in CH_3OH, mp: 118–120 °C.

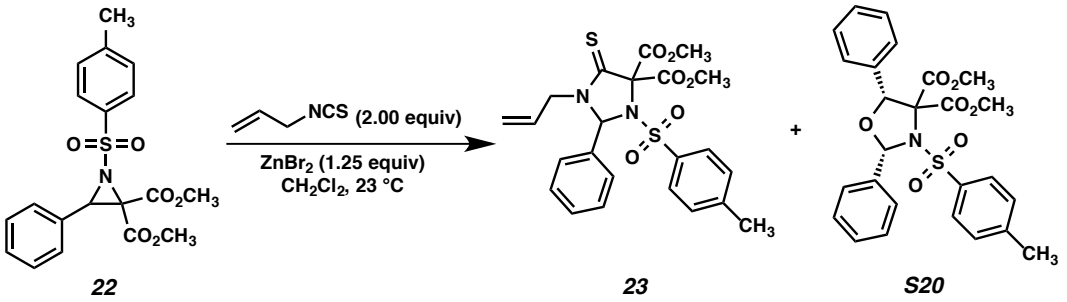


S19 ***S19·HCl***

The remaining portion of the white foam was dissolved in 20 mL CH_2Cl_2 and washed with aqueous 0.1 N NaOH (3 x 10 mL). The organic layer was dried over sodium sulfate, filtered, and concentrated in vacuo to give iminoimidazolidine **S19** as a colorless oil.

To neat **S19** was then added 4 N HCl in dioxane (3 mL) immediately followed by Et_2O (40 mL). The organics were then concentrated in vacuo to furnish iminoimidazolidinium hydrochloride **S19•HCl** as a white foam: R_f = 0.41 (1:9 MeOH:CH_2Cl_2 eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 10.98 (bs, 1H), 7.88 (d, J = 7.2 Hz, 2H), 7.52 (d, J = 7.1 Hz, 2H), 6.83 (s, 1H), 6.79 (s, 1H), 5.16 (bs, 1H), 4.56 (bs, 2H), 4.28 (bs, 1H), 3.92–3.81 (m, 1H), 2.52 (s, 3H), 2.23 (s, 3H), 2.20 (s, 3H), 2.03 (s, 3H), 1.72 (d, J = 6.0 Hz, 3H), 1.54 (d, J = 6.0 Hz, 3H), 0.94–0.80 (m, 6H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 155.1, 147.5, 139.7, 136.7, 136.2, 133.4, 132.6, 131.1, 130.5, 128.2, 127.8, 56.0, 54.9, 51.9, 50.9, 24.7, 22.0, 21.8, 20.9, 20.5, 20.5, 20.4, 19.7; IR (Neat Film, NaCl) 2925, 1640, 1441, 1366, 1276, 1171, 1089, 815 cm^{-1}; HRMS (APCI+) *m/z* calc'd for $C_{25}H_{36}N_3O_2S$ $[M–Cl]^+$: 442.2523, found 442.2514.

Preparation of Thioxoimidazolidine 23



22 ***23*** ***S20***

Imidazolidine **23** was prepared from diester aziridine **22** according to two procedures.

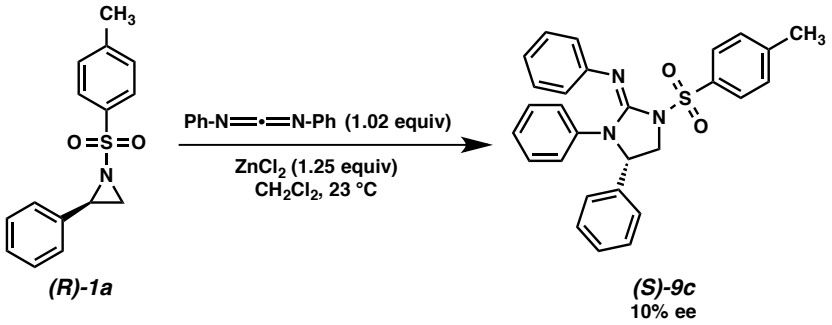
Initially, imidazolidine **23** was prepared according to General Procedure C. The reaction mixture was an intensely neon orange-red color throughout the duration of the reaction (ca. 11 h). Upon purification of the reaction mixture by silica gel column chromatography (20% acetone in hexanes eluent), imidazolidine **23** (70 mg, 36% yield) and *cis*-oxazolidine **S20** (48 mg, 24% yield) were both isolated as white crystalline solids.

Suspecting the formation of *cis*-oxazolidine **S20** was a result of partial hydrolysis of the ion-paired intermediate during the course of the reaction, imidazolidine **23** was subsequently prepared according to General Procedure C in the anhydrous environment of an inert atmosphere glovebox. The reaction mixture was an intensely neon orange-red color throughout the duration of the reaction (ca. 12 h) under these conditions as well. Upon purification of the reaction mixture by silica gel column chromatography (20% acetone in hexanes eluent), imidazolidine **23** (116 mg, 60% yield) was isolated in the absence of an isolable portion of *cis*-oxazolidine **S20**.

dimethyl 3-allyl-2-phenyl-4-thioxo-1-tosyl-imidazolidine-5,5-dicarboxylate (23):
Colorless, translucent X-ray quality crystals of imidazolidine **23** were obtained by slow diffusion of 1% benzene in heptane into a solution of imidazolidine **23** in ethyl acetate, mp: 147–150 °C: R_f = 0.41 (3:7 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.42–7.15 (m, 5H), 7.05–6.95 (m, 2H), 6.94–6.86 (m, 2H), 6.39 (s, 1H), 5.63 (dddd, *J* = 17.4, 10.3, 7.3, 4.3 Hz, 1H), 5.24 (ddt, *J* = 10.3, 1.8, 1.0 Hz, 1H), 5.10 (ddt, *J* = 17.2, 2.1, 1.2 Hz, 1H), 4.87–4.70 (m, 1H), 3.96 (s, 3H), 3.86 (s, 3H), 3.25 (ddt, *J* = 15.4, 7.4, 1.1 Hz, 1H), 2.28 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 186.5, 164.9, 164.3, 143.9, 136.7, 133.3, 130.6, 129.5, 129.0, 128.8, 128.3, 127.8, 120.1, 82.4, 82.3, 54.1, 53.9, 47.6, 21.6; IR (Neat Film, NaCl) 2952, 1794, 1771, 1489, 1354, 1257, 1162, 1090, 1061, 913, 850, 810, 777, 731 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{23}H_{25}N_2O_6S_2$ $[M+H]^+$: 489.1149, found 489.1164.

***cis*-dimethyl 2,5-diphenyl-3-tosyloxazolidine-4,4-dicarboxylate (S20):**
Colorless, translucent X-ray quality crystals of *cis*-oxazolidine **S20** were obtained by slow evaporation of a solution of *cis*-oxazolidine **S20** in ethyl acetate, mp: 145–147 °C: R_f = 0.50 (3:7 Acetone:Hexanes eluent); characterization data match those reported in the literature.[23]

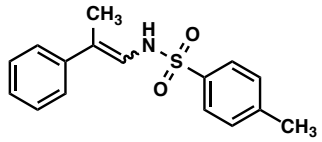
Stereoselective (3 + 2) Cycloaddition with Diphenylcarbodiimide



(R)-1a *(S)-9c* 10% ee

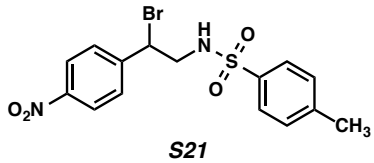
(*S*,*E*)-3,4-diphenyl-1-tosyl-2-(phenylimino)imidazolidine ((*S*)-9c):[24]
Imidazolidine **(*S*)-9c** was prepared according to General Procedure E using diphenylcarbodiimide (79 mg, 0.41 mmol, 1.02 equiv) in place of isothiocyanate:[25] 96% yield; R_f = 0.22 (1:4 Acetone:Hexanes eluent); characterization data match those reported above; $[\alpha]_D^{25.0}$ 46.6° (*c* 0.550, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralpak AS-H column, 30% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 9.6 minutes, minor retention time: 7.0 minutes, 10% ee).

(3 + 2) Cycloaddition Byproduct Characterization Data



27

4-methyl-*N*-(2-phenylprop-1-en-1-yl)benzenesulfonamide (27):
Sulfonamide **27** was prepared by General Procedure C from aziridine **26**: 65% combined yield as a 2:1 *Z*:*E* ratio of products as an amorphous white solid; R_f = 0.15 (1:4 Acetone:Hexanes eluent); ^{1}H and ^{13}C NMR spectra match those reported in the literature;[26] IR (Neat Film, NaCl) 3357, 3260, 1721, 1683, 1598, 1448, 1337, 1301, 1269, 1161, 1096, 904, 817, 761 cm^{-1}; HRMS (ESI+) *m/z* calc'd for $C_{16}H_{18}NO_2S$ $[M+H]^+$: 288.1053, found 288.1044.

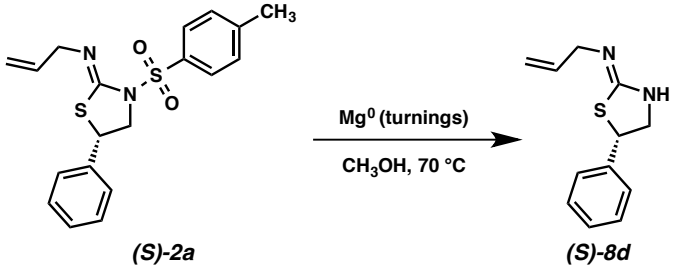


S21

1-bromo-1-(4-nitrophenyl)-2-(p-toluenesulfonamido)ethane (S21):[27]
Bromide **S21** was isolated as a byproduct of the reaction of aziridine **S6** under the reaction conditions specified in General Procedure C: 35% yield as an amorphous white solid; R_f = 0.15 (1:4 Acetone:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.24–8.14 (m, 2H), 7.75–7.67 (m, 2H), 7.53–7.46 (m, 2H), 7.35–7.29 (m, 2H), 5.02 (t, *J* = 7.1 Hz, 1H), 4.83 (dd, *J* = 7.4, 5.9 Hz, 1H), 3.64–3.50 (m, 2H), 2.45 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 148.1, 145.3, 144.3, 136.8, 130.1, 129.0, 127.1, 124.3, 50.5, 50.1, 21.7; IR (Neat Film, NaCl) 3278, 1598, 1522, 1423, 1346, 1157, 1092, 855, 814 cm^{-1}; HRMS (FAB+) *m/z* calc'd for $C_{15}H_{14}{}^{81}BrN_2O_4S$ $[(M–H_2)+H]^+$: 398.9837, found 398.9834.

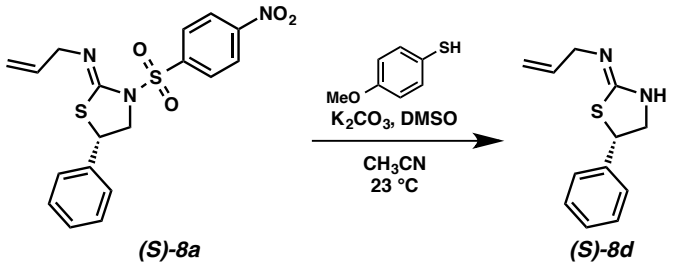
Deprotection of Iminothiazolidines (*S*)-2a and (*S*)-8a

*Desulfonylation of Tosylthiazolidine **(S)-2a***



Procedure for the desulfonylation of thiazolidine **(*S*)-2a** was adapted from the literature.[12] Iminothiazolidine **(*S*)-2a** (50 mg, 0.13 mmol, 1.00 equiv) was suspended in freshly distilled CH_3OH (2.2 mL) in an oven-dried vial with a stir bar and heated to 70 °C until a homogeneous solution was formed. Magnesium turnings (49 mg, 2.01 mmol, 15 equiv) were then added and the vial was sealed. The reaction mixture was stirred at 70 °C. Upon consumption of starting material (determined by LCMS analysis, ca. 30 min), the reaction mixture was allowed to cool to room temperature and filtered through Celite, washing with CH_2Cl_2 (20 mL) and CH_3OH (20 mL). The filtrate was adsorbed onto Celite and purified by silica gel column chromatography (30% acetone and 1% Et_3N in hexanes) to give iminothiazolidine **(*S*)-8d** (26 mg, 91% yield) as a white amorphous solid; characterization data match those reported above; $[\alpha]_D^{25.0}$ –61.2° (*c* 0.23, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralcel OB-H column, 10% methanol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 3.9 minutes, minor retention time: 8.4 minutes, 94% ee).

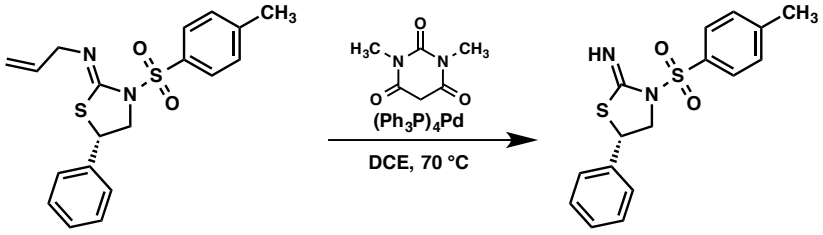
*Desulfonylation of (p-Nosyl)thiazolidine **(S)-8a***



Procedure for the desulfonylation of thiazolidine **(*S*)-8a** was adapted from the literature.[28] To a solution of iminothiazolidine **(*S*)-8a** (120 mg, 0.30 mmol, 1.00 equiv, 95% ee) and *p*-methoxythiophenol (110 µL, 0.89 mmol, 3.00 equiv) in acetonitrile (1.96 mL) was added DMSO (40 µL), followed by potassium carbonate (164 mg, 1.18 mmol, 4.00 equiv). The vial was loosely capped and the heterogeneous mixture was stirred at room temperature until the reaction was complete (determined by TLC analysis, ca. 3 h). The reaction mixture was concentrated and the residue partitioned between ethyl acetate and water. The organic layer was separated, washed with brine, dried over sodium sulfate, filtered, and concentrated in vacuo. The crude residue was purified by silica gel column chromatography (30% acetone and 1% Et_3N in hexanes eluent) to give

iminothiazolidine **(*S*)-8d** (60 mg, 93% yield) as a white amorphous solid; characterization data match those reported above; $[\alpha]_D^{25.0}$ –61.2° (*c* 0.23, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralcel OB-H column, 10% methanol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 3.9 minutes, minor retention time: 8.4 minutes, 94% ee).

*Deallylation of Tosylthiazolidine **(S)-2a***

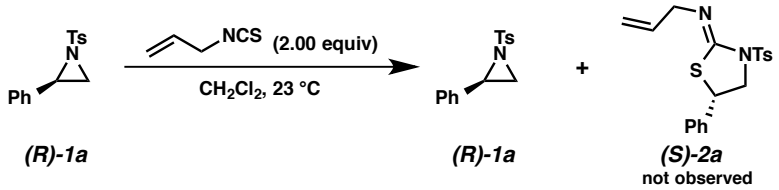


(S)-2a ***(S)-25***

Procedure for the deallylation of thiazolidine **(*S*)-2a** was adapted from the literature.[29] To a solution of iminothiazolidine **(*S*)-2a** (25 mg, 0.067 mmol, 1.00 equiv) in dichloroethane (750 μL) in an oven dried vial with a stir bar were added tetrakis(triphenylphosphine)palladium(0) (39 mg, 0.034 mmol, 0.50 equiv) and 1,3-dimethylbarbituric acid (157 mg, 1.01 mmol, 15.0 equiv). The vial was sealed and stirred at 70 °C until the reaction was complete (determined by LCMS analysis, ca. 1.5 h). The reaction mixture was diluted with CH_2Cl_2, adsorbed onto Celite, and purified by silica gel column chromatography (10% acetone and 1% Et_3N in hexanes) to give iminothiazolidine **(*S*)-25** (20 mg, 89% yield) as a white amorphous solid; R_f = 0.30 (3:7 Acetone:Hexanes eluent); ^1H NMR (CD_2Cl_2, 500 MHz) δ 7.83–7.78 (m, 2H), 7.38–7.34 (m, 2H), 7.34–7.31 (m, 5H), 4.77 (t, *J* = 7.0 Hz, 1H), 4.46 (dd, *J* = 10.5, 6.4 Hz, 1H), 4.01 (dd, *J* = 10.5, 7.6 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (CD_2Cl_2, 126 MHz) δ 160.3, 145.9, 137.3, 130.4, 129.8, 129.4, 129.0, 128.1, 127.8, 58.8, 21.8; IR (Neat Film, NaCl) 3311, 3031, 2922, 1622, 1597, 1494, 1454, 1358, 1168, 1089, 1054, 814 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{16}H_{17}N_2O_2S_2$ $[M+H]^+$: 333.0726, found 333.0736; $[\alpha]_D^{25.0}$ –10.0° (*c* 0.1, $CHCl_3$); enantiomeric excess was determined by analytical SFC (Chiralpak AD-H column, 30% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 7.3 minutes, minor retention time: 8.4 minutes, 39% ee).

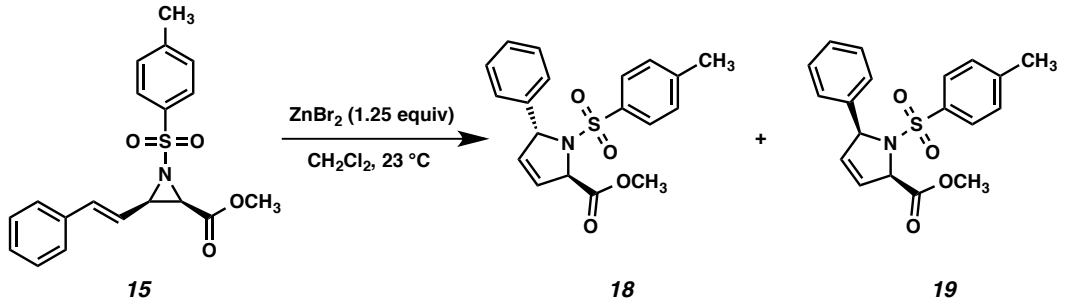
Control Reaction Experimental Procedures[30]

Lewis Acid Control



To an oven-dried 1-dram vial equipped with a magnetic stir bar were added (*R*)-*N*-tosyl-2-phenylaziridine (**(*R*)-1a**, 109 mg, 0.40 mmol, 1.00 equiv, >99% ee) and allyl isothiocyanate (79 μL, 0.80 mmol, 2.00 equiv). The vial was sealed with a screw cap fitted with a Teflon septum, placed under an inert atmosphere, and dissolved in anhydrous dichloromethane (0.80 mL). The heterogeneous reaction mixture was then allowed to stir at ambient temperature. Over the course of 96 hours, no formation of thiazolidine **(*S*)-2a** was observed. At 96 hours, the enantiomeric excess of the remaining aziridine **(*R*)-1a** was determined by analytical SFC (Chiralcel OB-H column, 10% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 7.5 minutes, minor retention time: 10.2 minutes, >99% ee).

Isomerization of Disubstituted Aziridines



To an oven-dried 1-dram vial equipped with a magnetic stir bar was added zinc(II) bromide (25 mg, 0.113 mmol, 1.25 equiv), freshly powdered with a mortar and pestle, in an inert atmosphere glovebox. The vial was sealed with a screw cap fitted with a Teflon septum, removed from the glovebox and placed under an inert atmosphere. To a separate, oven-dried 1-dram vial was added *cis*-aziridine **15** (32 mg, 0.090 mmol, 1.00 equiv). The vial was sealed with a screw cap fitted with a Teflon septum, and the mixture was transferred to the first vial as a solution in anhydrous dichloromethane (0.15 mL + 0.05 mL rinse). The heterogeneous reaction mixture was then allowed to stir at ambient temperature. Upon consumption of starting material (determined by LCMS, ca. 30 min), the reaction mixture directly purified by silica gel column chromatography (20% acetone in hexanes eluent) to furnish *trans*-pyrroline **18** (12 mg, 38% yield) and *cis*-pyrroline **19** (2 mg, 6% yield) as white amorphous solids.

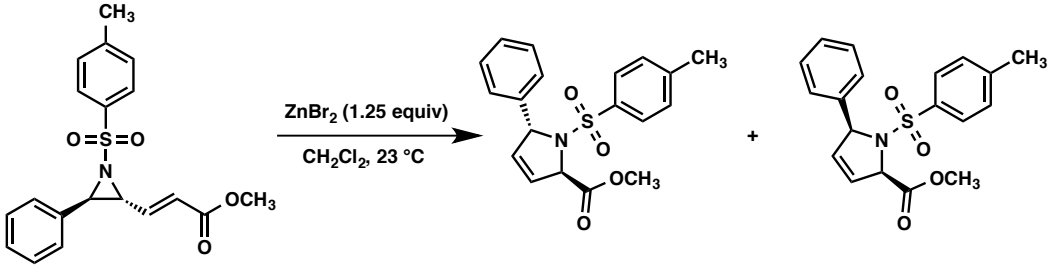
methyl *trans*-5-phenyl-1-tosyl-3-pyrroline-2-carboxylate (18):

R_f = 0.38 (3:7 EtOAc:Hexanes eluent); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.21–7.16 (m, 1H), 7.12–7.05 (m, 4H), 7.00–6.96 (m, 2H), 6.95–6.90 (m, 2H), 5.87 (dt, *J* = 6.2, 1.6 Hz, 1H),

5.84 (dt, *J* = 6.2, 1.8 Hz, 1H), 5.76 (dt, *J* = 6.2, 1.6 Hz, 1H), 5.18 (dt, *J* = 5.7, 1.7 Hz, 1H), 3.86 (s, 3H), 2.30 (s, 3H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 171.2, 142.6, 137.9, 136.9, 134.7, 129.0, 128.9, 128.4, 128.3, 126.8, 124.0, 70.5, 69.3, 53.0, 21.5; IR (Neat Film, NaCl) 2953, 1747, 1598, 1456, 1343, 1262, 1200, 1158, 1100, 1018, 813, 763 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{19}H_{20}NO_4S$ $[M+H]^+$: 358.1108, found 358.1106.

methyl *cis*-5-phenyl-1-tosyl-3-pyrroline-2-carboxylate (19):

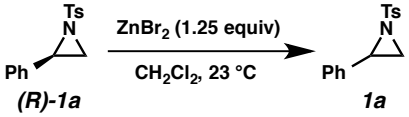
R_f = 0.47 (3:7 EtOAc:Hexanes eluent); characterization data match those reported in the literature.[31]



12 ***18*** not observed ***19*** not observed

To an oven-dried 1-dram vial equipped with a magnetic stir bar was added zinc(II) bromide (17 mg, 0.074 mmol, 1.25 equiv), freshly powdered with a mortar and pestle, in an inert atmosphere glovebox. The vial was sealed with a screw cap fitted with a Teflon septum, removed from the glovebox and placed under an inert atmosphere. To a separate, oven-dried 1-dram vial was added *trans*-aziridine **12** (21 mg, 0.059 mmol, 1.00 equiv). The vial was sealed with a screw cap fitted with a Teflon septum, and the mixture was transferred to the first vial as a solution in anhydrous dichloromethane (0.15 mL + 0.05 mL rinse). The heterogeneous reaction mixture was then allowed to stir at ambient temperature. The slow decomposition of aziridine **12** was complete after 96 h (determined by LCMS) and was characterized by the formation of no major products including neither *trans*-pyrroline **18** nor *cis*-pyrroline **19**.[32]

Racemization of Starting Material

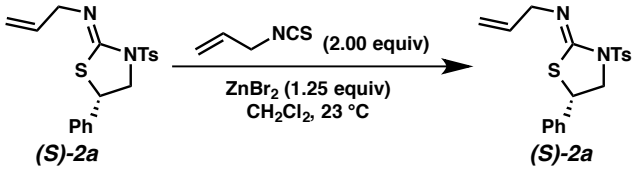


(R)-1a ***1a***

To an oven-dried 1-dram vial equipped with a magnetic stir bar was added zinc(II) bromide (113 mg, 0.50 mmol, 1.25 equiv), freshly powdered with a mortar and pestle, in an inert atmosphere glovebox. The vial was sealed with a screw cap fitted with a Teflon septum, removed from the glovebox and placed under an inert atmosphere. To a separate, oven-dried 1-dram vial was added *N*-tosyl-2-phenylaziridine (**(*R*)-1a**, 109 mg, 0.40 mmol, 1.00 equiv). The vial was sealed with a screw cap fitted with a Teflon septum, and the mixture was transferred to the first vial as a solution in anhydrous dichloromethane (0.60 mL + 0.20 mL rinse). The heterogeneous reaction mixture was then allowed to stir at ambient temperature. Racemization of the aziridine was complete after 10 minutes as

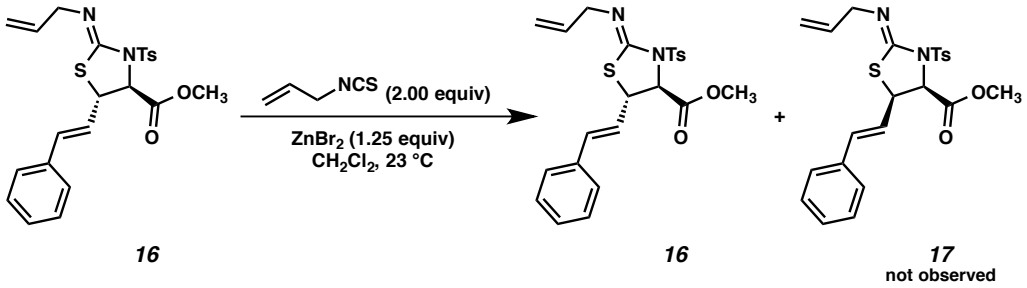
determined by analytical SFC (Chiralcel OB-H column, 10% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 7.5 minutes, minor retention time: 10.2 minutes).

Racemization of Product

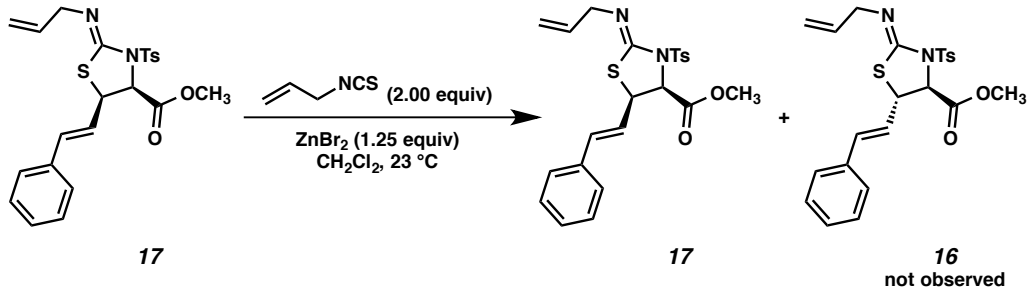


To an oven-dried 1-dram vial equipped with a magnetic stir bar was added zinc(II) bromide (31 mg, 0.14 mmol, 1.25 equiv), freshly powdered with a mortar and pestle, in an inert atmosphere glovebox. The vial was sealed with a screw cap fitted with a Teflon septum, removed from the glovebox and placed under an inert atmosphere. To a separate, oven-dried 1-dram vial were added the iminothiazolidine **(*S*)-2a** (40 mg, 0.11 mmol, 1.00 equiv, 94% ee) and allyl isothiocyanate (22 μL, 0.22 mmol, 2.00 equiv). The vial was sealed with a screw cap fitted with a Teflon septum, and the mixture was transferred to the first vial as a solution in anhydrous dichloromethane (0.15 mL + 0.10 mL rinse). The heterogeneous reaction mixture was then allowed to stir at ambient temperature. After 96 hours, the enantiomeric excess of thiazolidine **(*S*)-2a** was determined by analytical SFC (Chiralpak AD-H, 30% isopropyl alcohol in CO_2, 2.5 mL/min, λ = 254 nm, major retention time: 5.4 minutes, minor retention time: 3.8 minutes, 94% ee).

Isomerization of Thiazolidine Products



To an oven-dried 1-dram vial equipped with a magnetic stir bar was added zinc(II) bromide (10 mg, 0.044 mmol, 1.25 equiv), freshly powdered with a mortar and pestle, in an inert atmosphere glovebox. The vial was sealed with a screw cap fitted with a Teflon septum, removed from the glovebox and placed under an inert atmosphere. To a separate, oven-dried 1-dram vial were added the *trans*-iminothiazolidine **16** (16 mg, 0.035 mmol, 1.00 equiv) and allyl isothiocyanate (7 μL, 0.070 mmol, 2.00 equiv). The vial was sealed with a screw cap fitted with a Teflon septum, and the mixture was transferred to the first vial as a solution in anhydrous dichloromethane (0.10 mL + 0.05 mL rinse). The heterogeneous reaction mixture was then allowed to stir at ambient temperature. Over the course of 96 hours, no decomposition of *trans*-iminothiazolidine **16** or isomerization of *trans*-iminothiazolidine **16** to *cis*-iminothiazolidine **17** was observed (determined by LCMS).



17 ***17*** ***16***
not observed

To an oven-dried 1-dram vial equipped with a magnetic stir bar was added zinc(II) bromide (10 mg, 0.044 mmol, 1.25 equiv), freshly powdered with a mortar and pestle, in an inert atmosphere glovebox. The vial was sealed with a screw cap fitted with a Teflon septum, removed from the glovebox and placed under an inert atmosphere. To a separate, oven-dried 1-dram vial were added the *cis*-iminothiazolidine **17** (16 mg, 0.035 mmol, 1.00 equiv) and allyl isothiocyanate (7 μL, 0.070 mmol, 2.00 equiv). The vial was sealed with a screw cap fitted with a Teflon septum, and the mixture was transferred to the first vial as a solution in anhydrous dichloromethane (0.10 mL + 0.05 mL rinse). The heterogeneous reaction mixture was then allowed to stir at ambient temperature. Over the course of 96 hours, no decomposition of *cis*-iminothiazolidine **17** or isomerization of *cis*-iminothiazolidine **17** to *trans*-iminothiazolidine **16** was observed (determined by LCMS).

Notes and References

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[4] Procedure adapted from the literature and typically run on 3.0–4.0 mmol scale; see reference 2.
[5] Procedure adapted from the literature and typically run on 1.0–4.0 mmol scale, see: J. Farràs, X. Ginesta, P. W. Sutton, J. Taltavull, F. Egeler, P. Romea, F. Urpí, J. Vilarrasa, *Tetrahedron* **2001**, *57*, 7665-7674.
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[21] For the purpose of characterization, thiazolidines **5** and **6** were purified using and Agilent 1200 series preparative HPLC (Agilent Prep-SIL column (5 μm, 30 x 250 mm), 6% EtOAc in hexane, 50.00 mL/min, λ = 254 nm, compound **5**: 12.036 min, compound **6**: 11.372 min).
[22] For the purpose of characterization, *trans*-thiazolidine **16** and *cis*-thiazolidine **17** were purified using and Agilent 1200 series preparative HPLC (Agilent Prep-SIL column

(5 μm, 30 x 250 mm), 15% EtOAc in hexane, 50.00 mL/min, λ = 254 nm, *trans*-thiazolidine: 12.218 min, *cis*-thiazolidine: 8.845 min).
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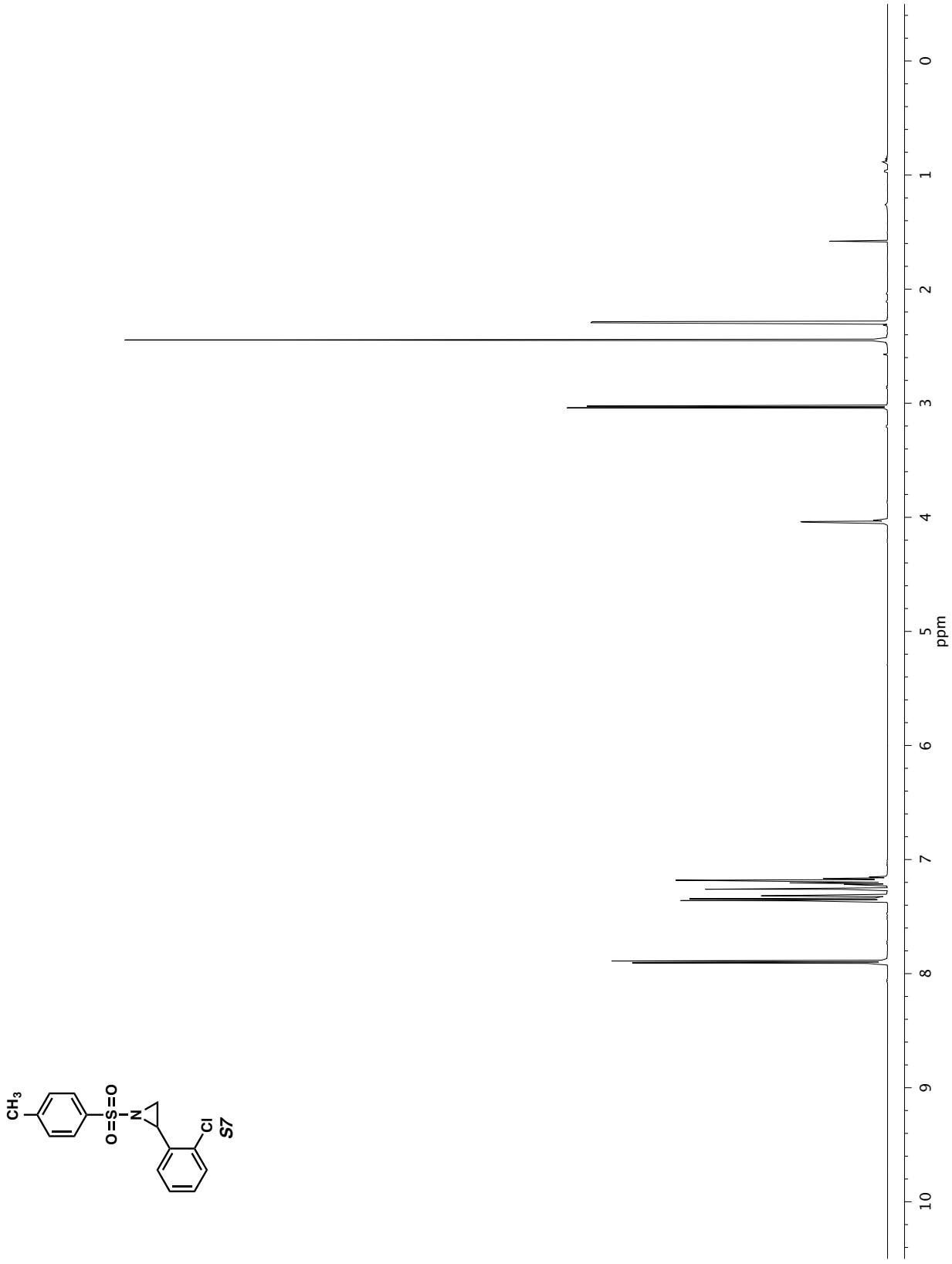
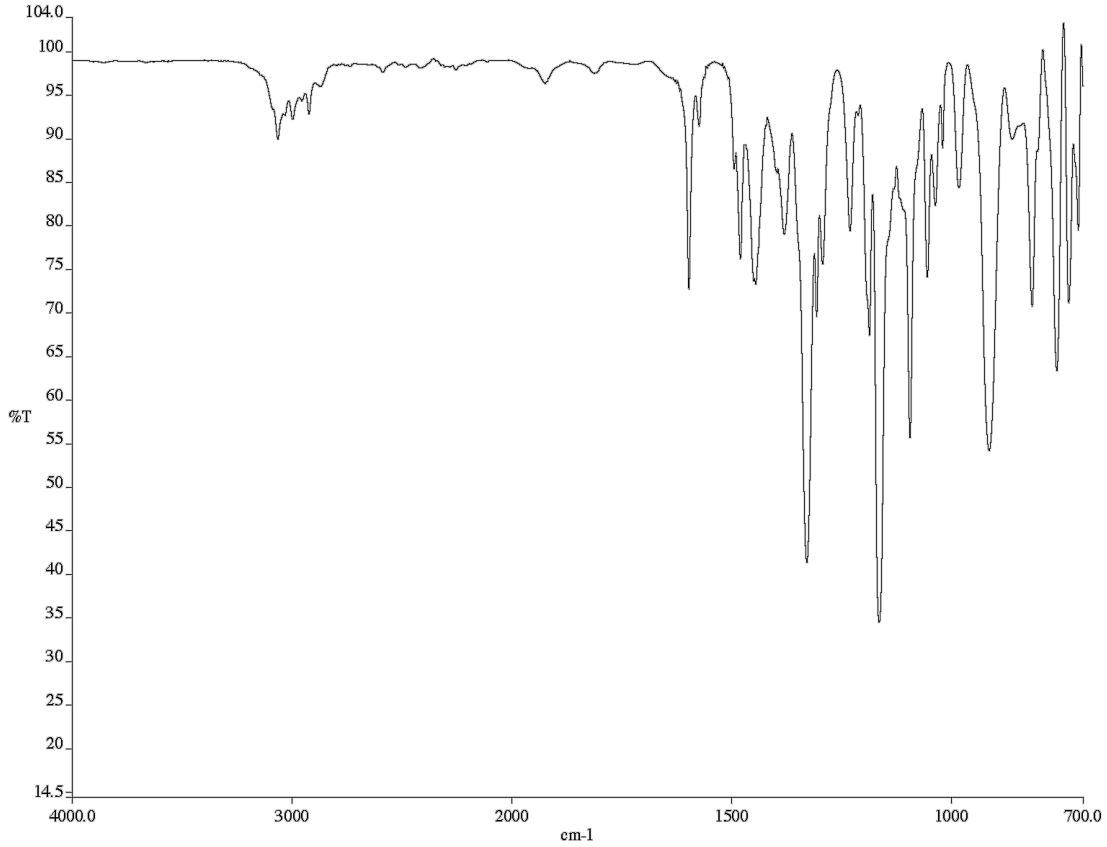
[32] Although the pyrroline products of the vinylaziridine-pyrroline rearrangement were not observed, aziridine **12** is known to readily undergo this transformation, see ref [10].

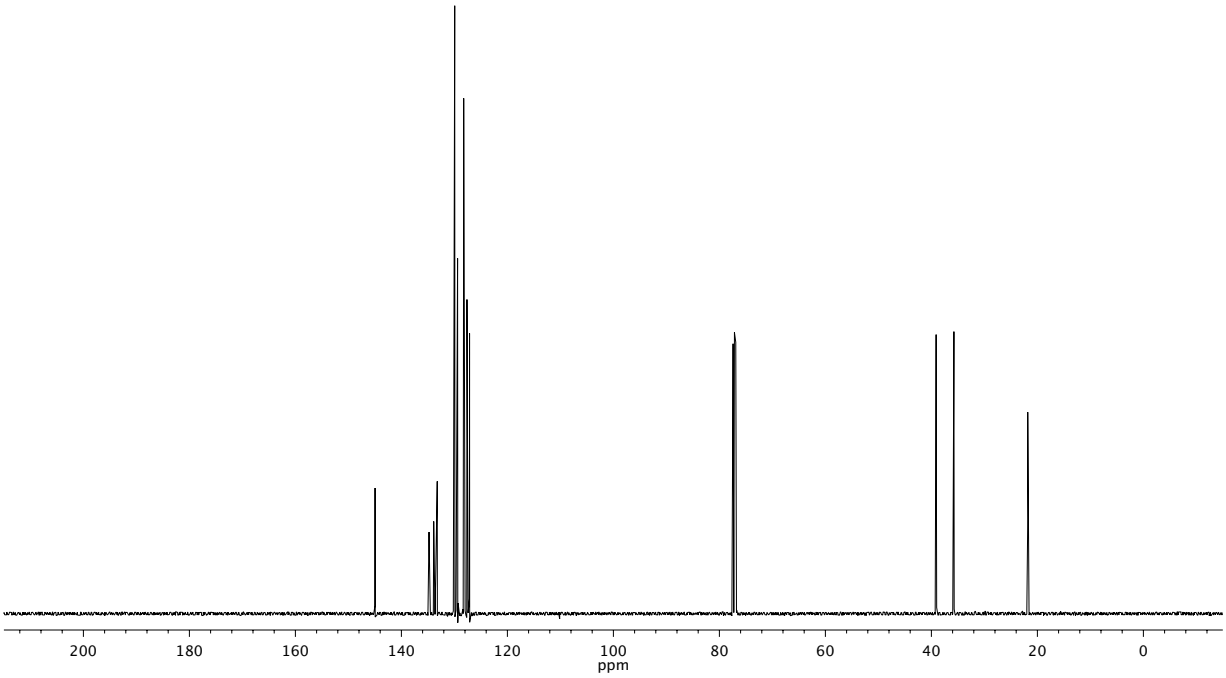
NMR & IR Spectra



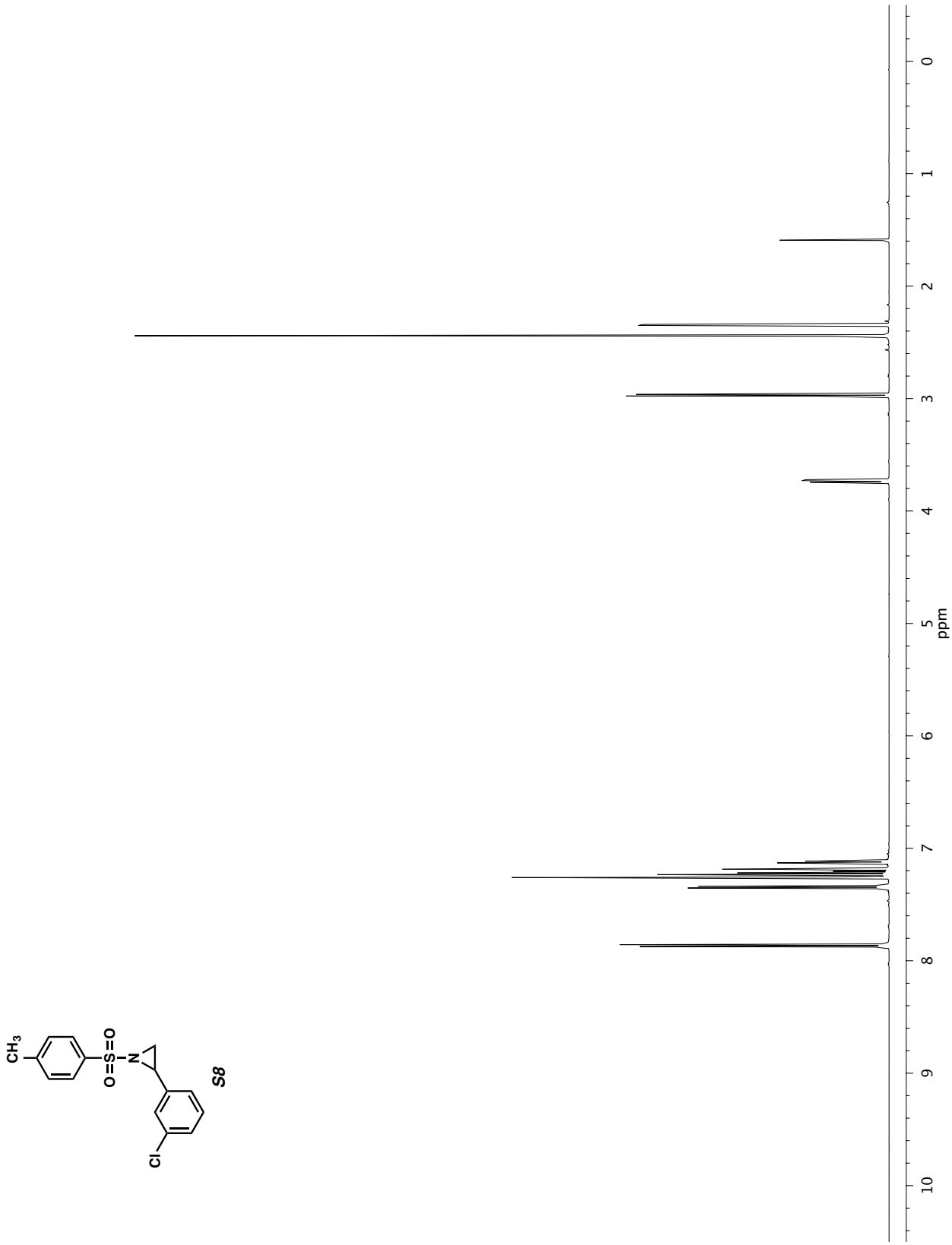
^{1}H NMR (500 MHz, $CDCl_3$) of compound **S7**.



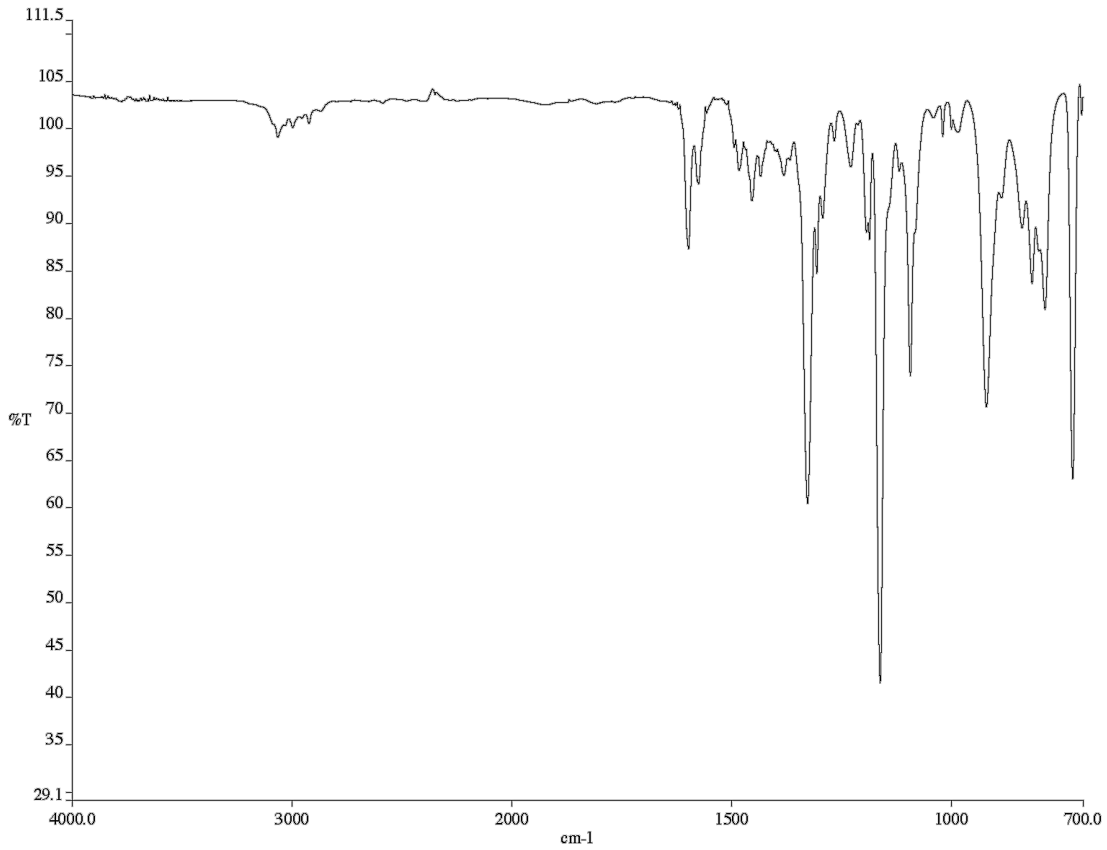
Infrared spectrum (Thin Film, NaCl) of compound **S7**.



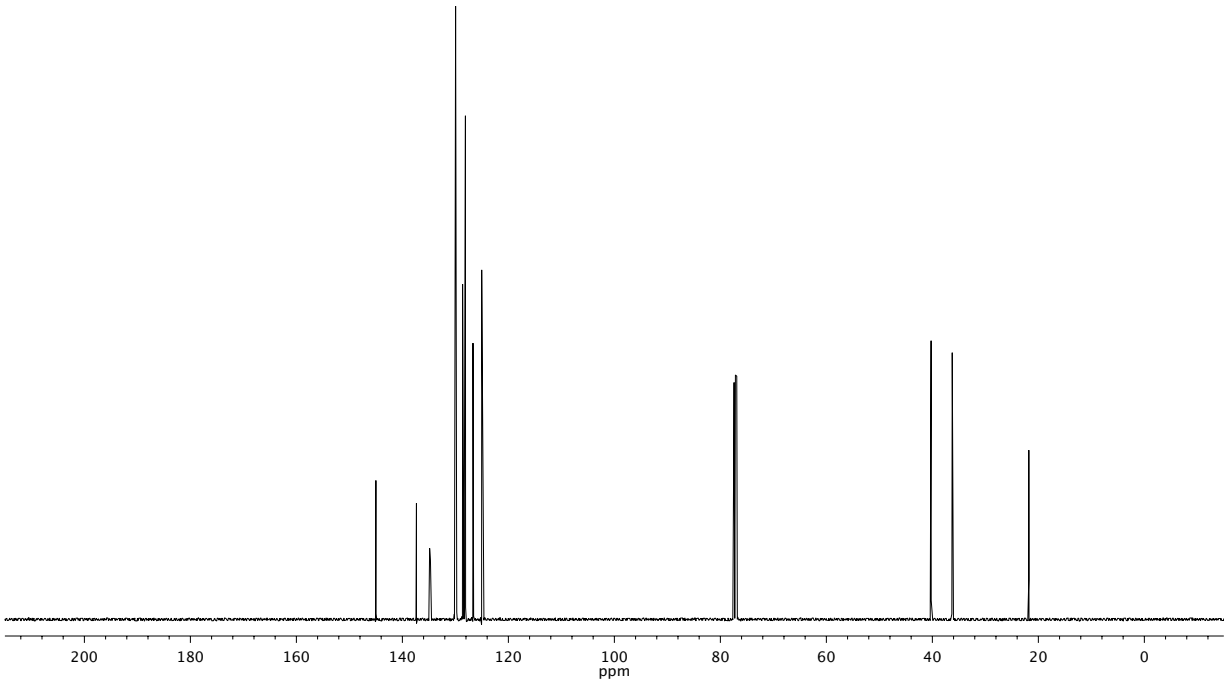
^{13}C NMR (126 MHz, $CDCl_3$) of compound **S7**.



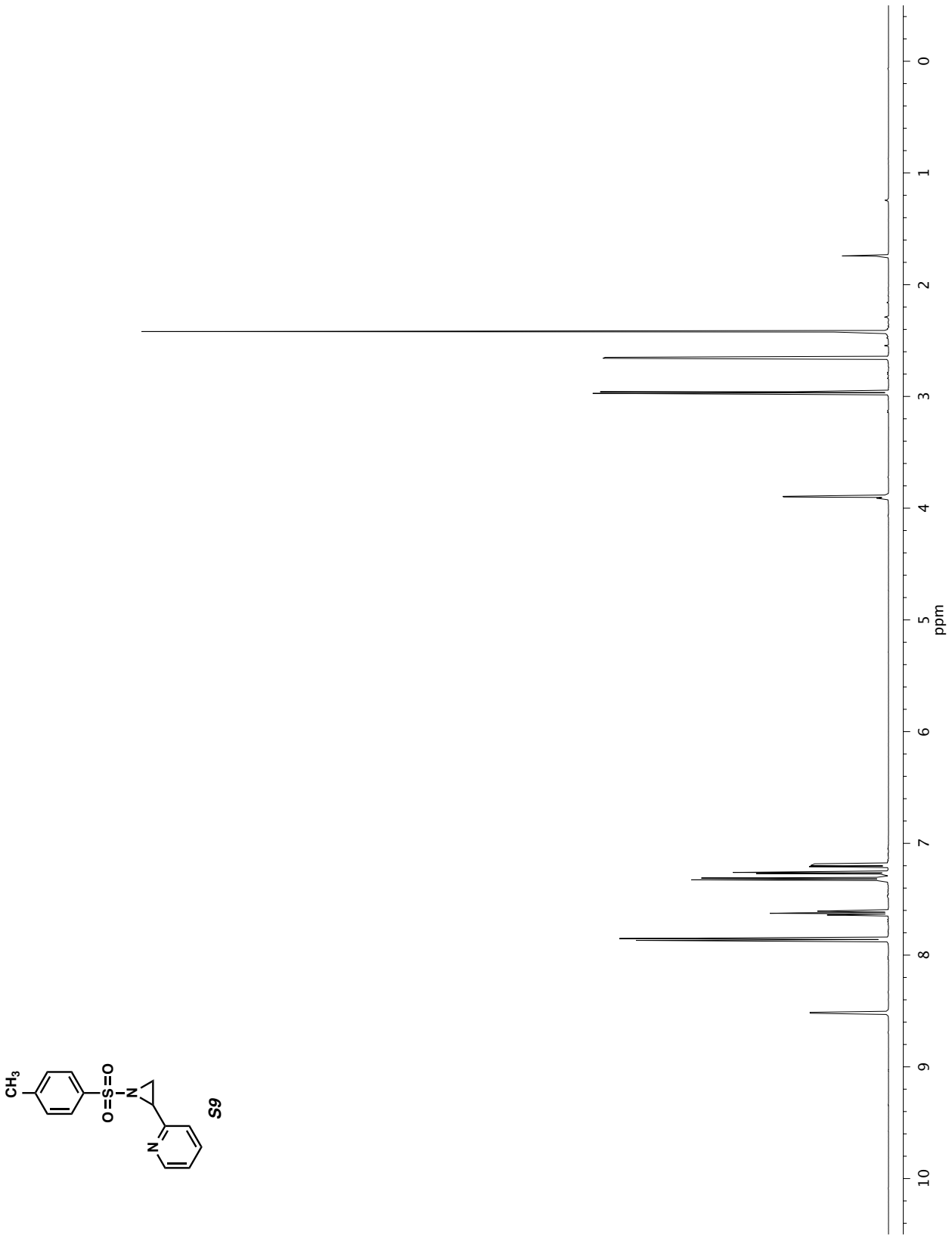
^{1}H NMR (500 MHz, $CDCl_3$) of compound **S8**.



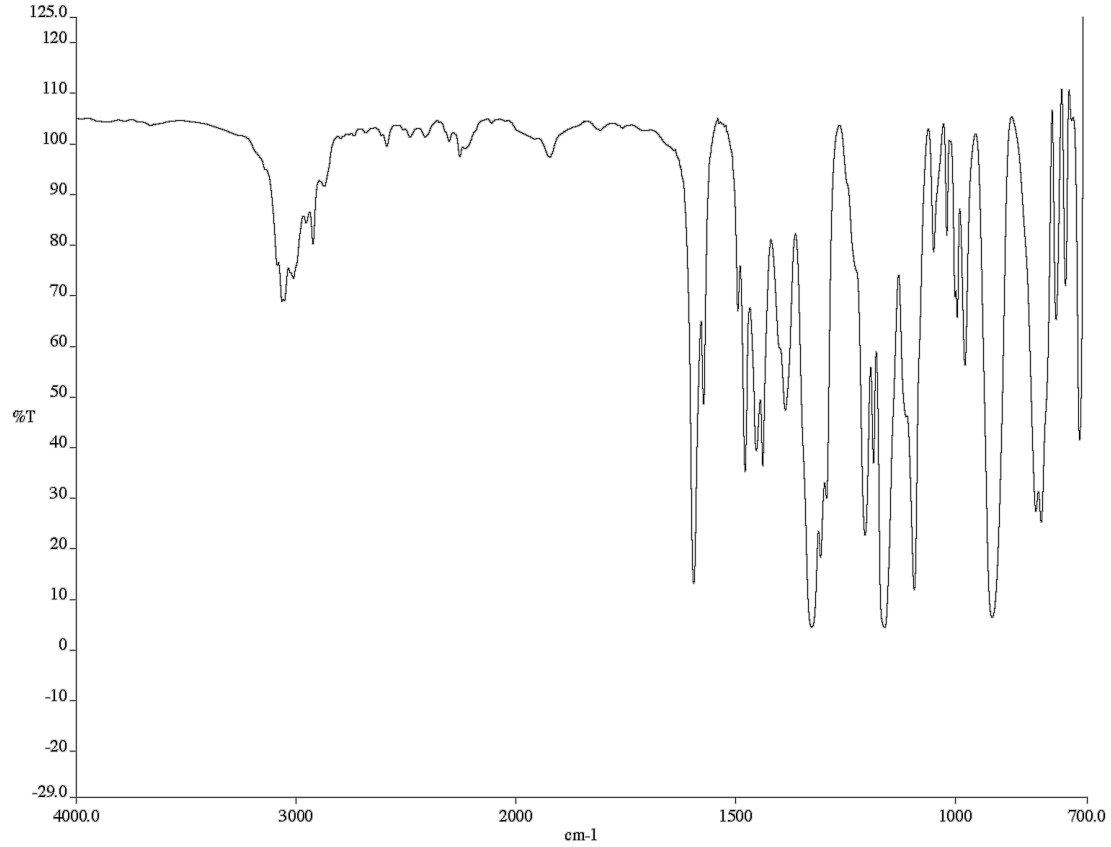
Infrared spectrum (Thin Film, NaCl) of compound **S8**.



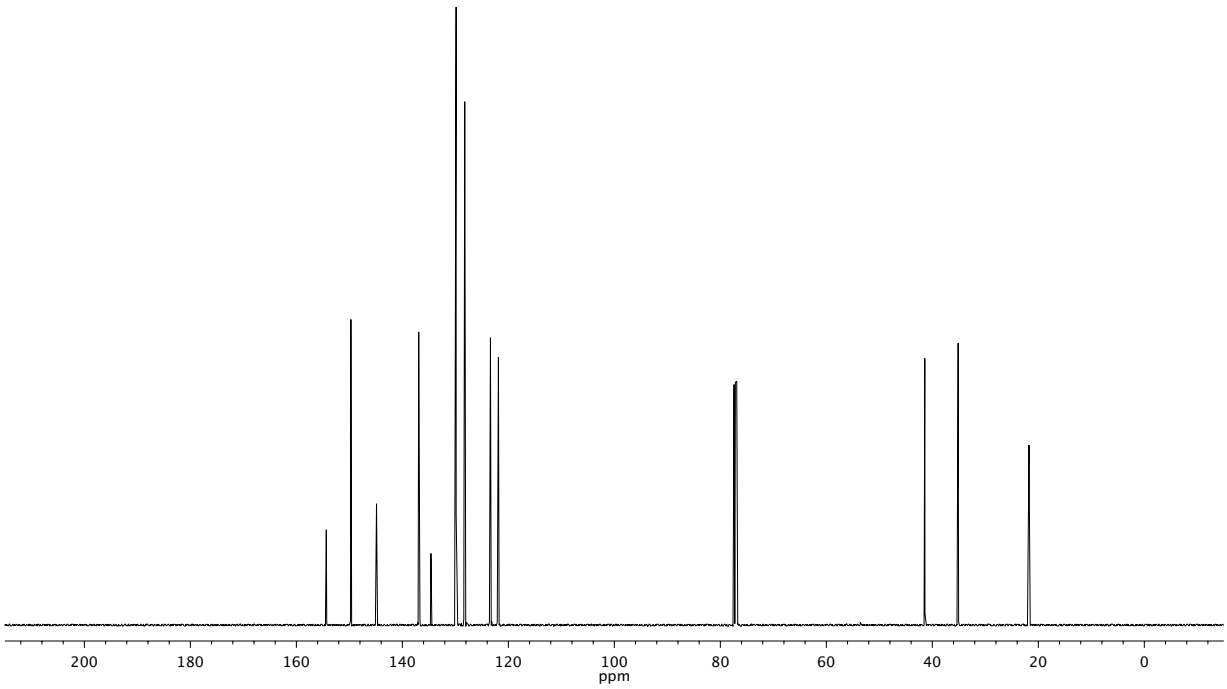
^{13}C NMR (126 MHz, $CDCl_3$) of compound **S8**.



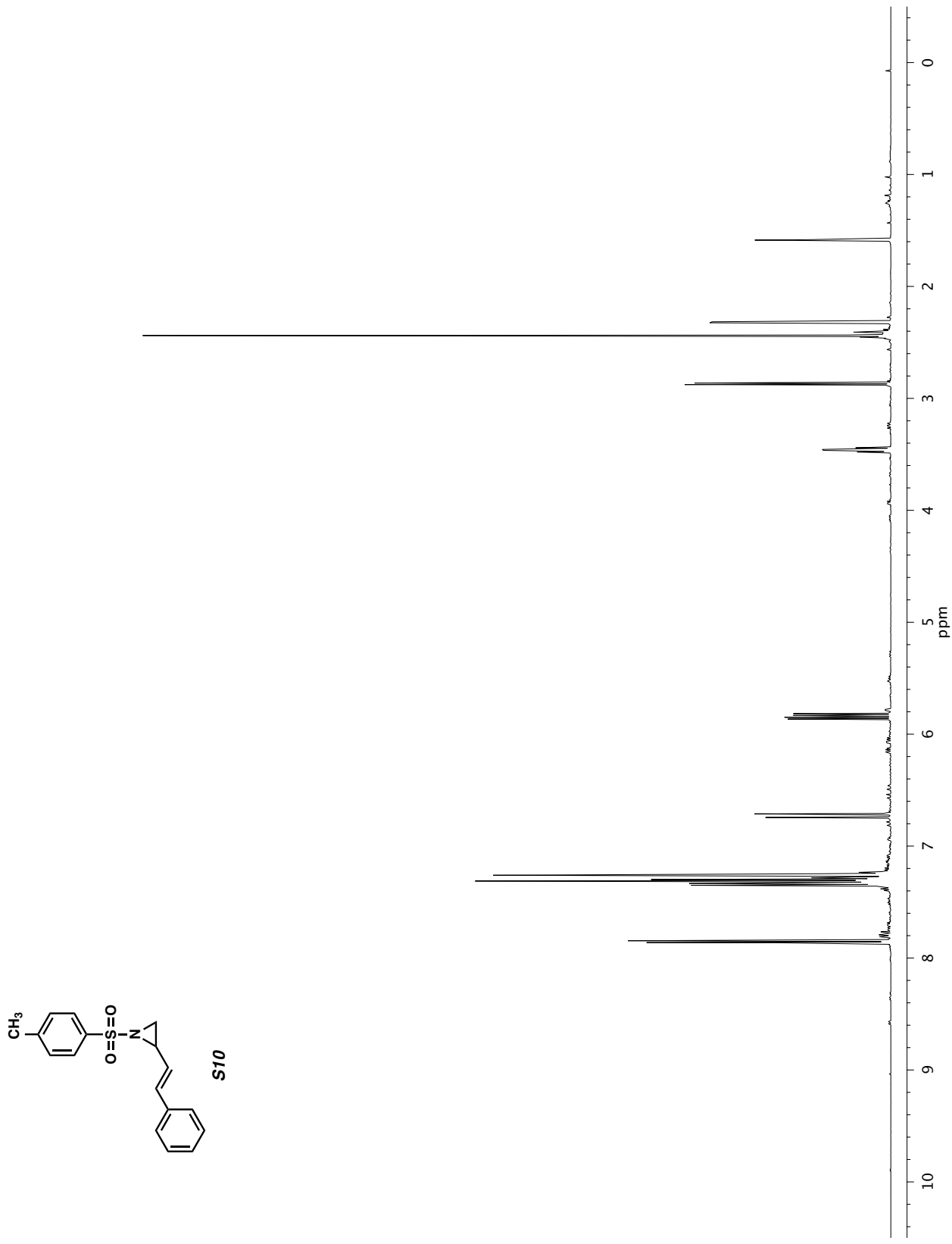
^{1}H NMR (500 MHz, $CDCl_3$) of compound **S9**.



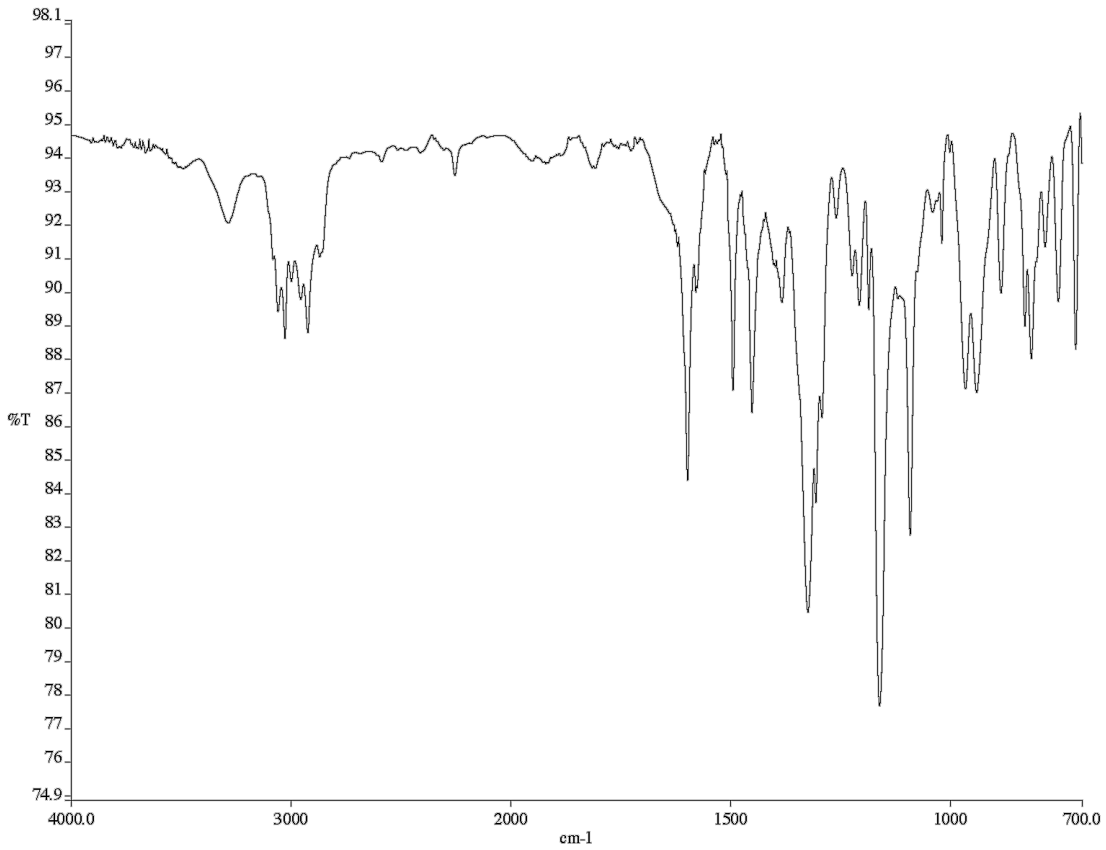
Infrared spectrum (Thin Film, NaCl) of compound **S9**.



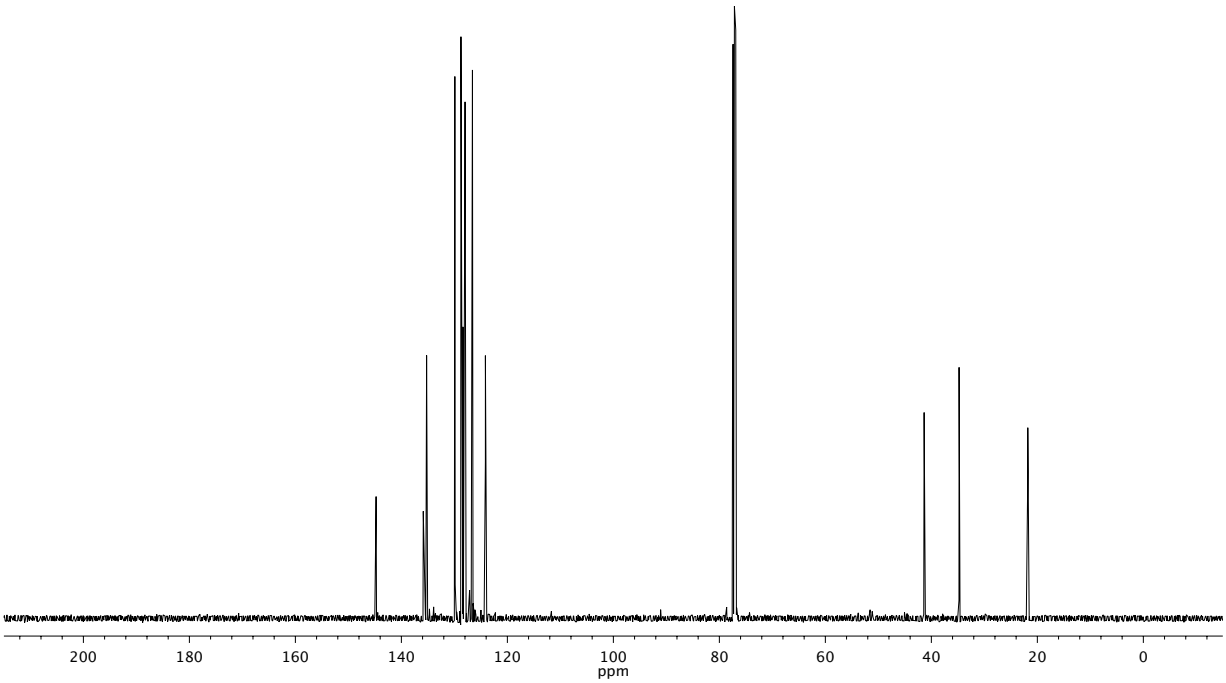
^{13}C NMR (126 MHz, $CDCl_3$) of compound **S9**.



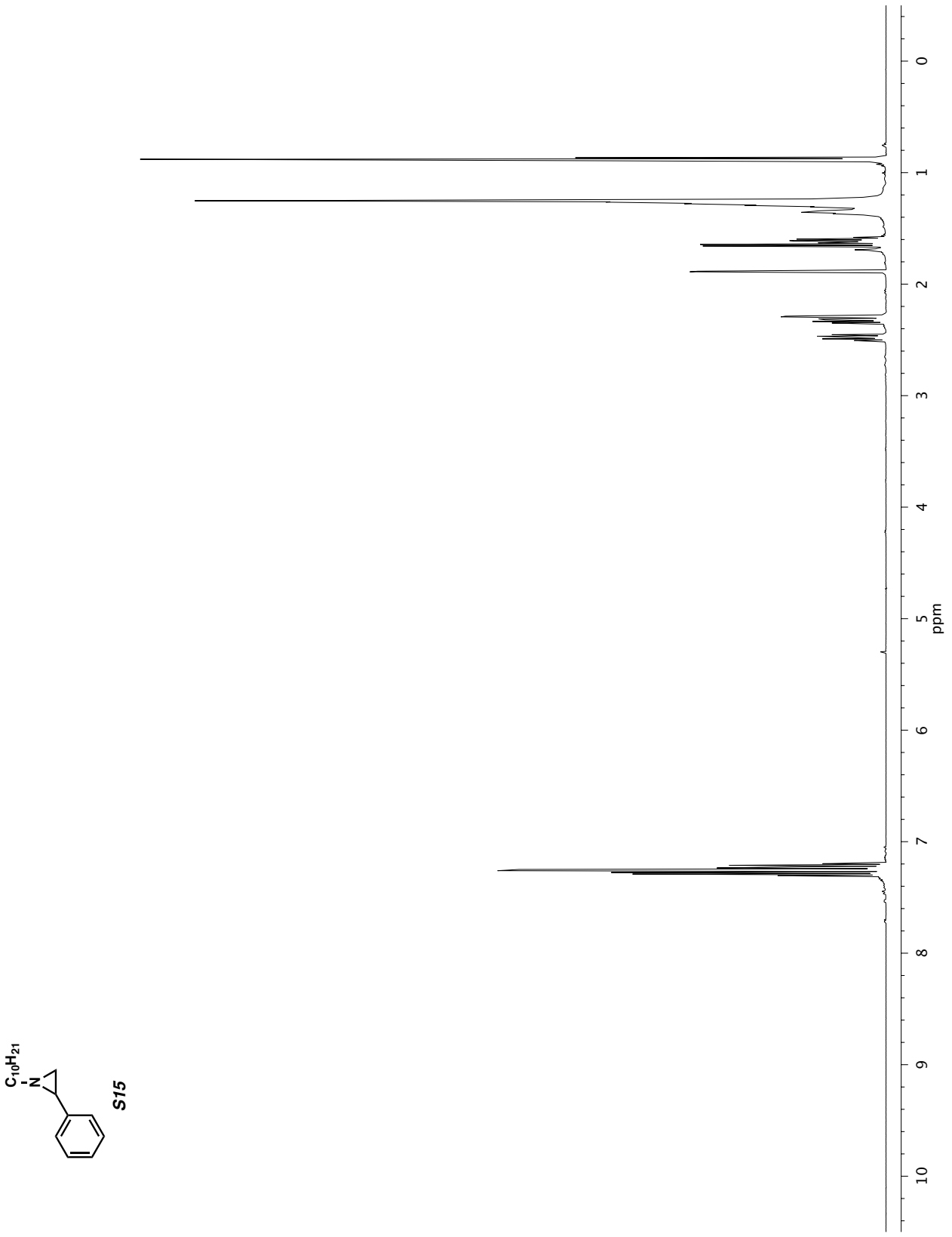
^{1}H NMR (500 MHz, $CDCl_3$) of compound **S10**.



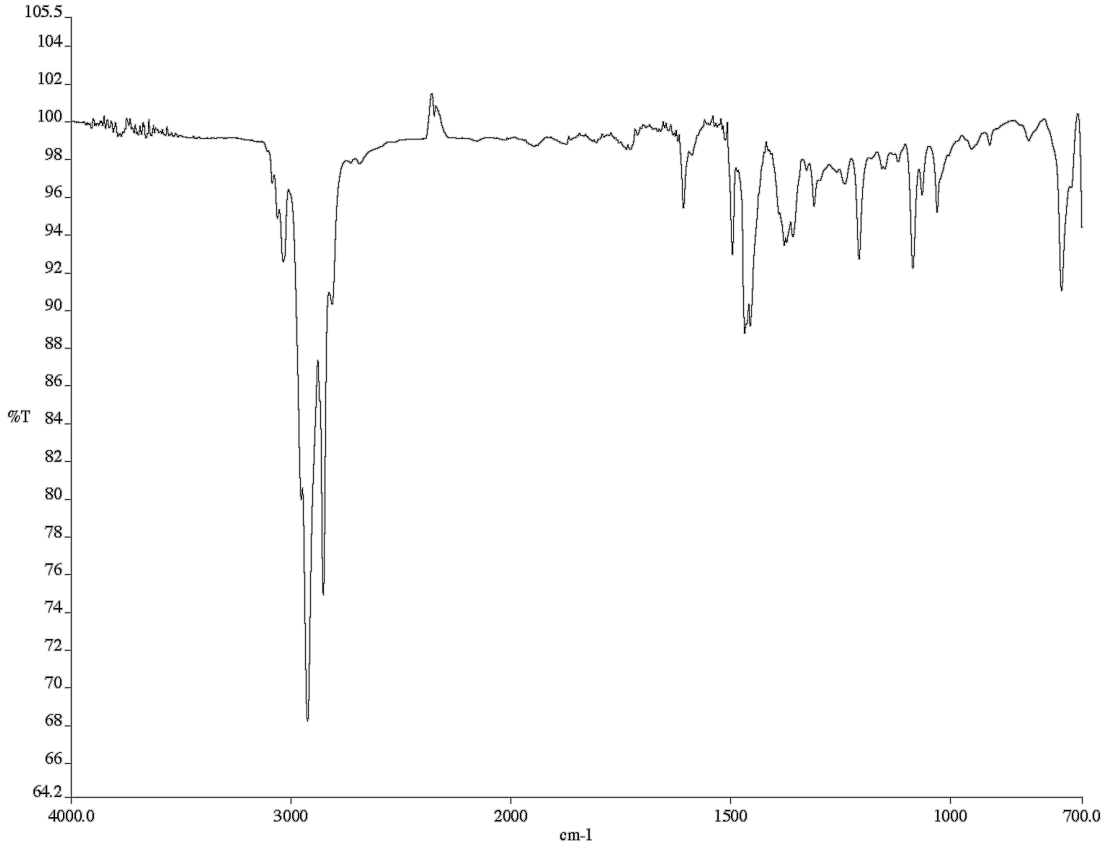
Infrared spectrum (Thin Film, NaCl) of compound **S10**.



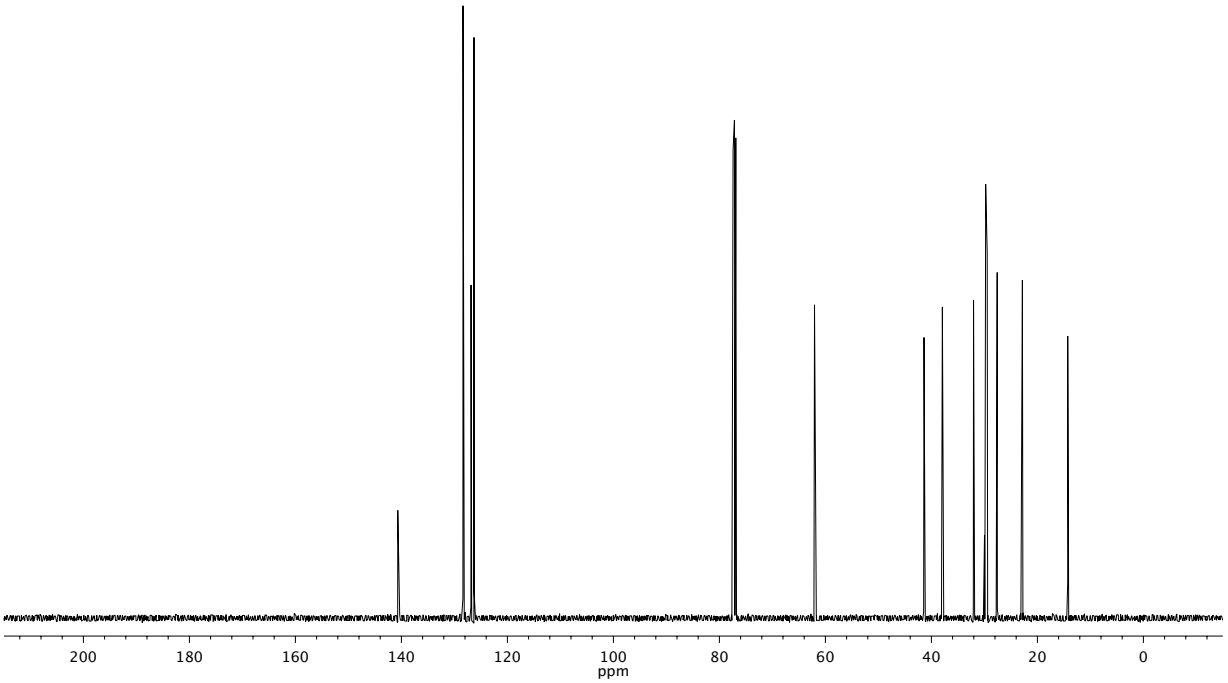
^{13}C NMR (126 MHz, $CDCl_3$) of compound **S10**.



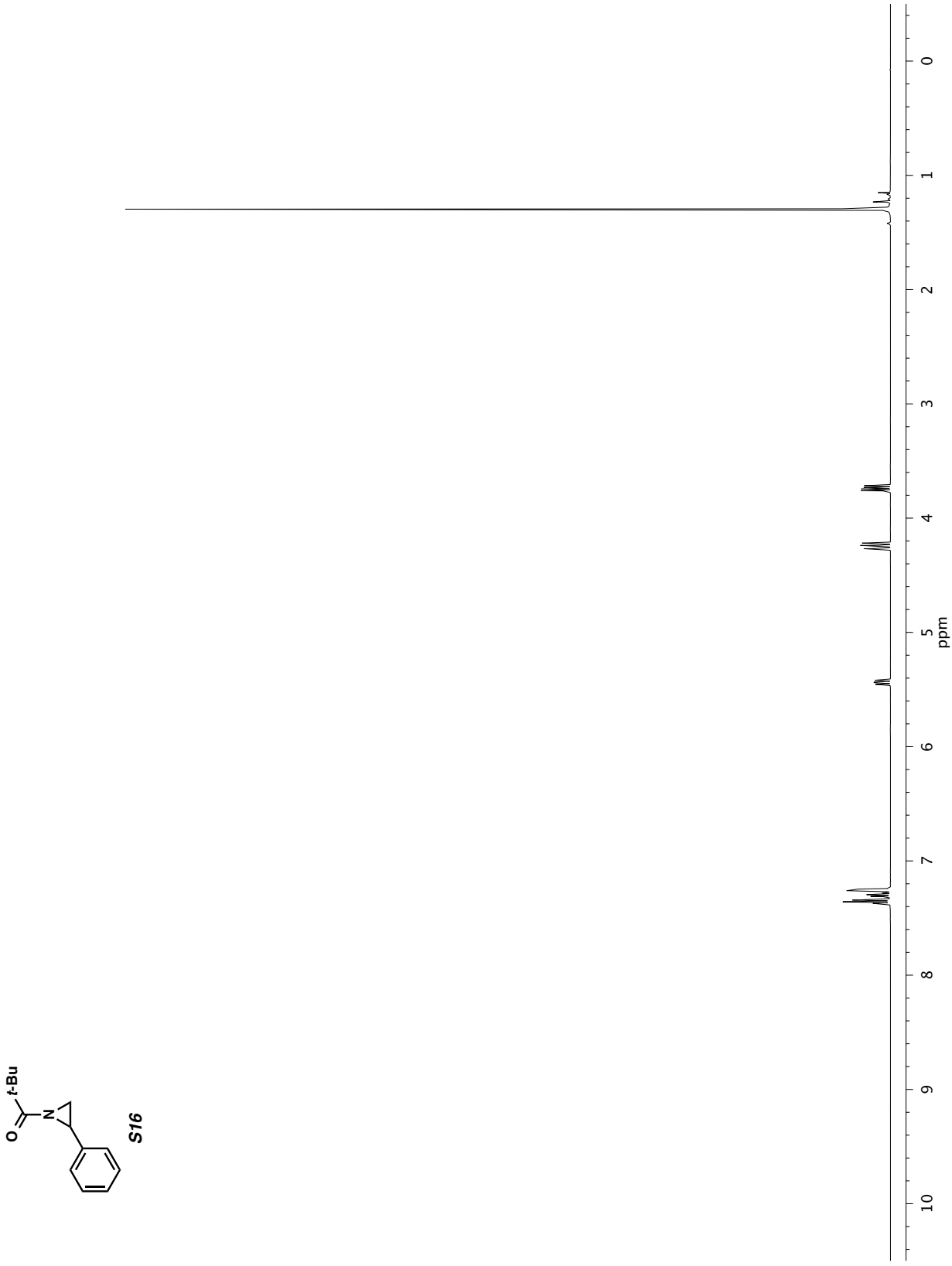
^{1}H NMR (500 MHz, $CDCl_3$) of compound **S15**.



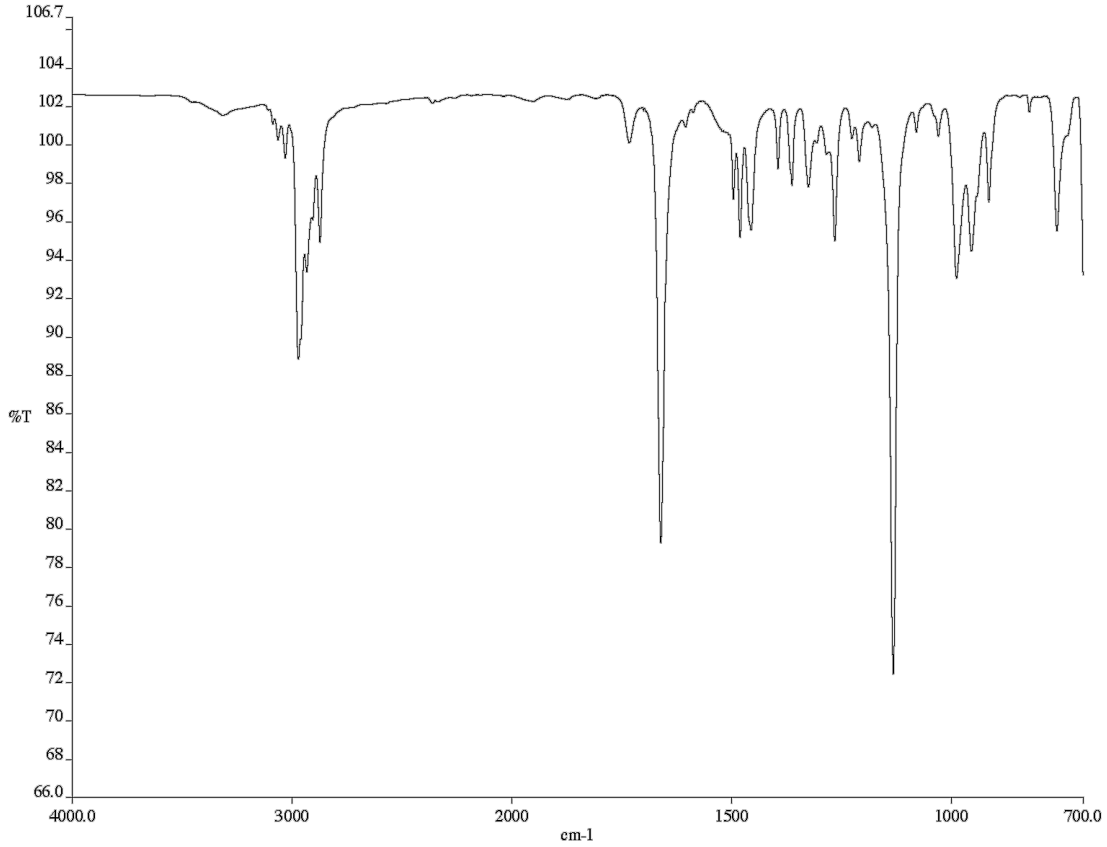
Infrared spectrum (Thin Film, NaCl) of compound **S15**.



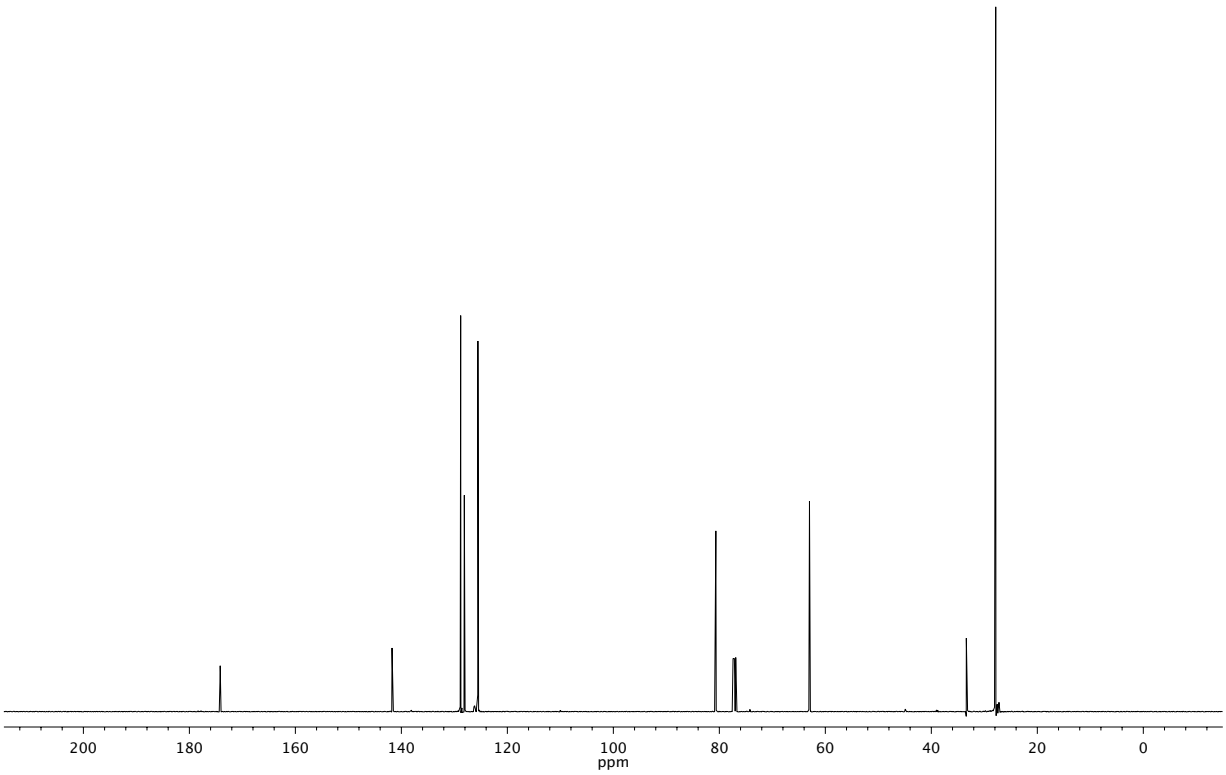
^{13}C NMR (126 MHz, $CDCl_3$) of compound **S15**.



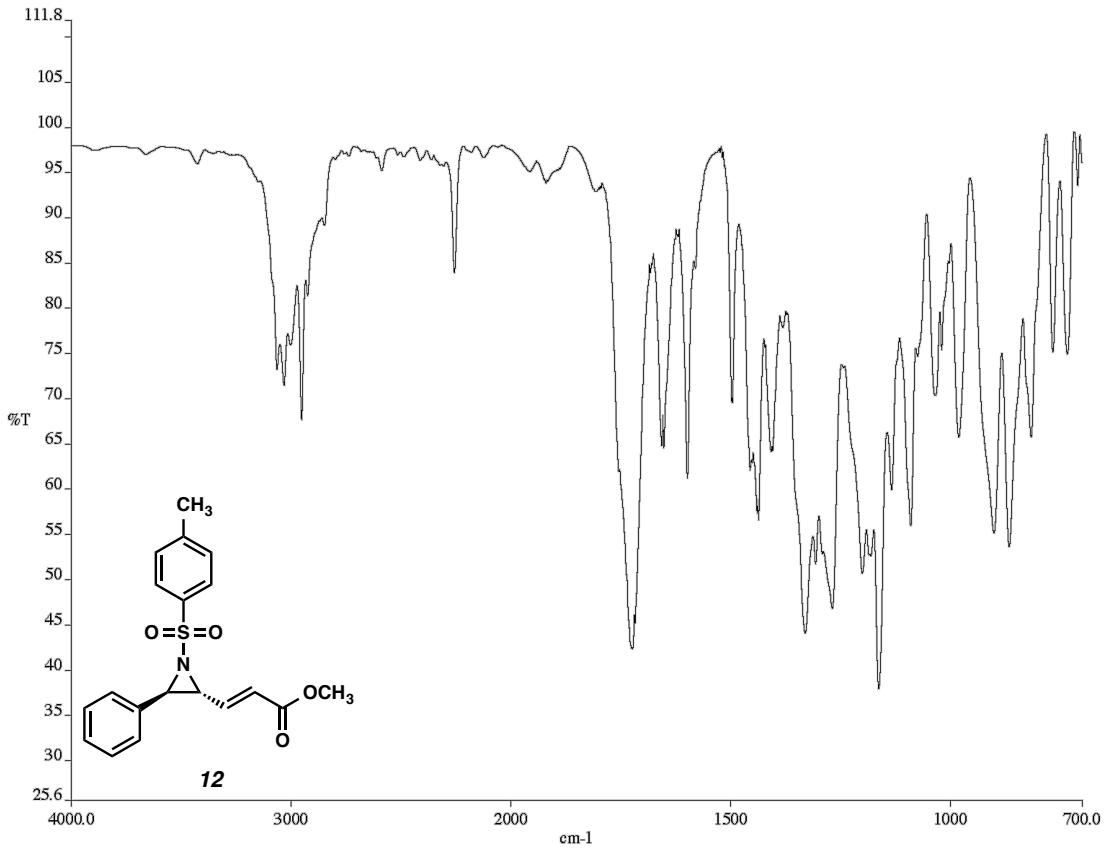
^{1}H NMR (500 MHz, $CDCl_3$) of compound **S16**.



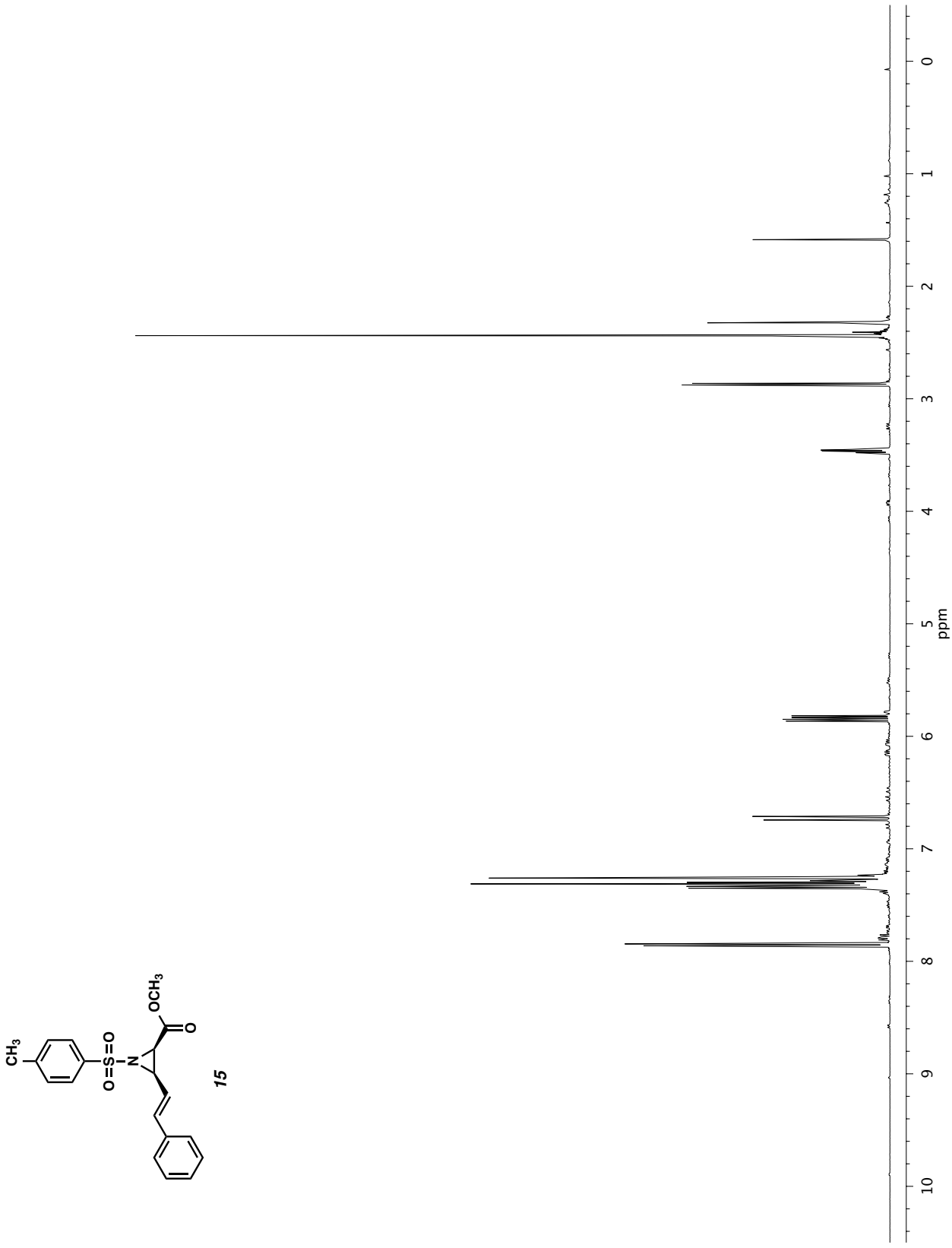
Infrared spectrum (Thin Film, NaCl) of compound **S16**.



^{13}C NMR (126 MHz, $CDCl_3$) of compound **S16**.

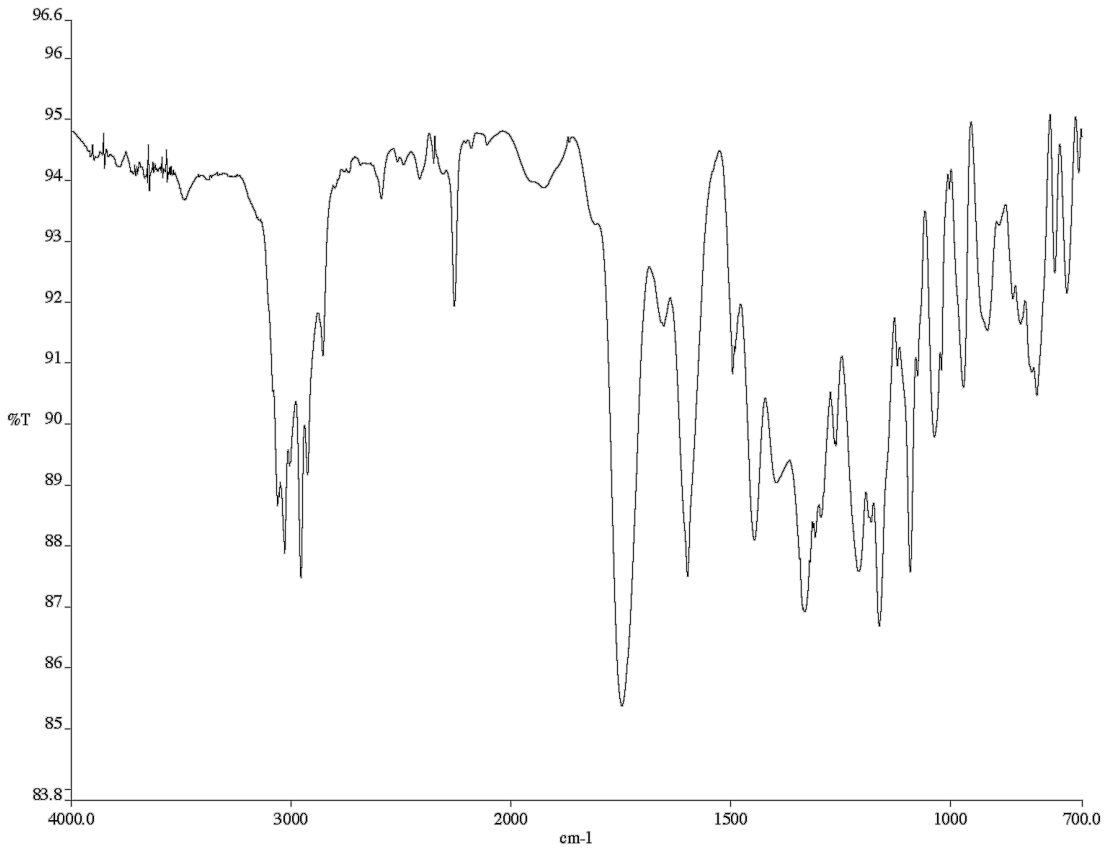


Infrared spectrum (Thin Film, NaCl) of compound **12**.

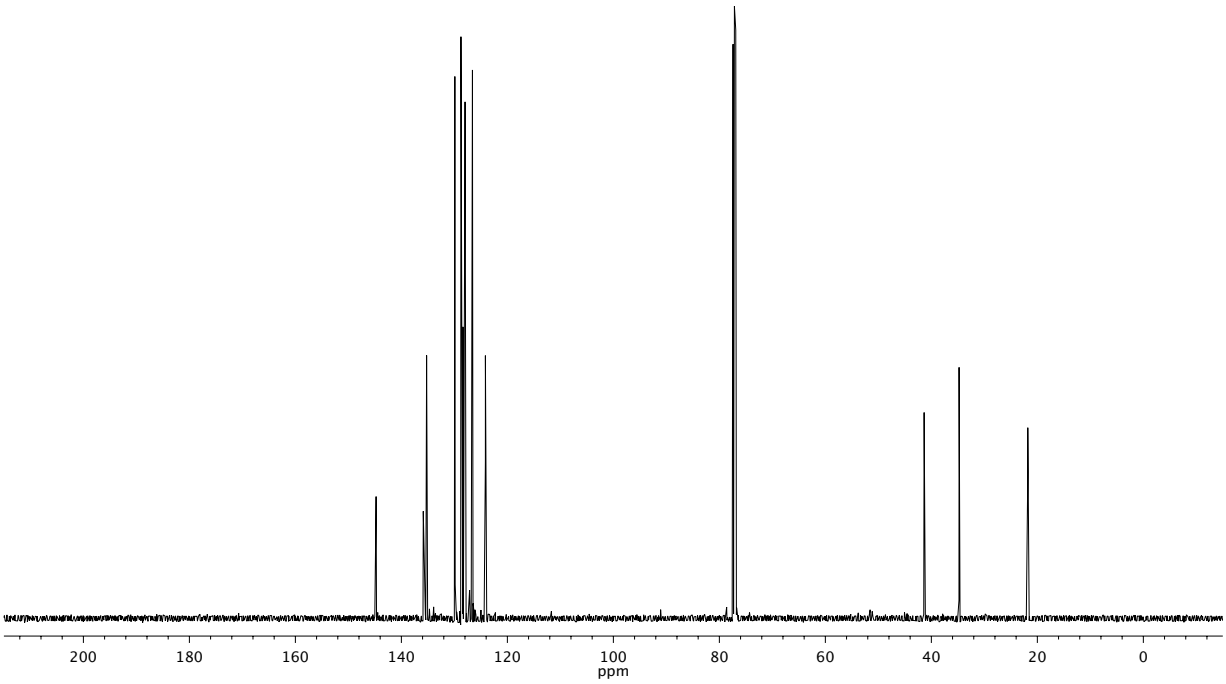


15

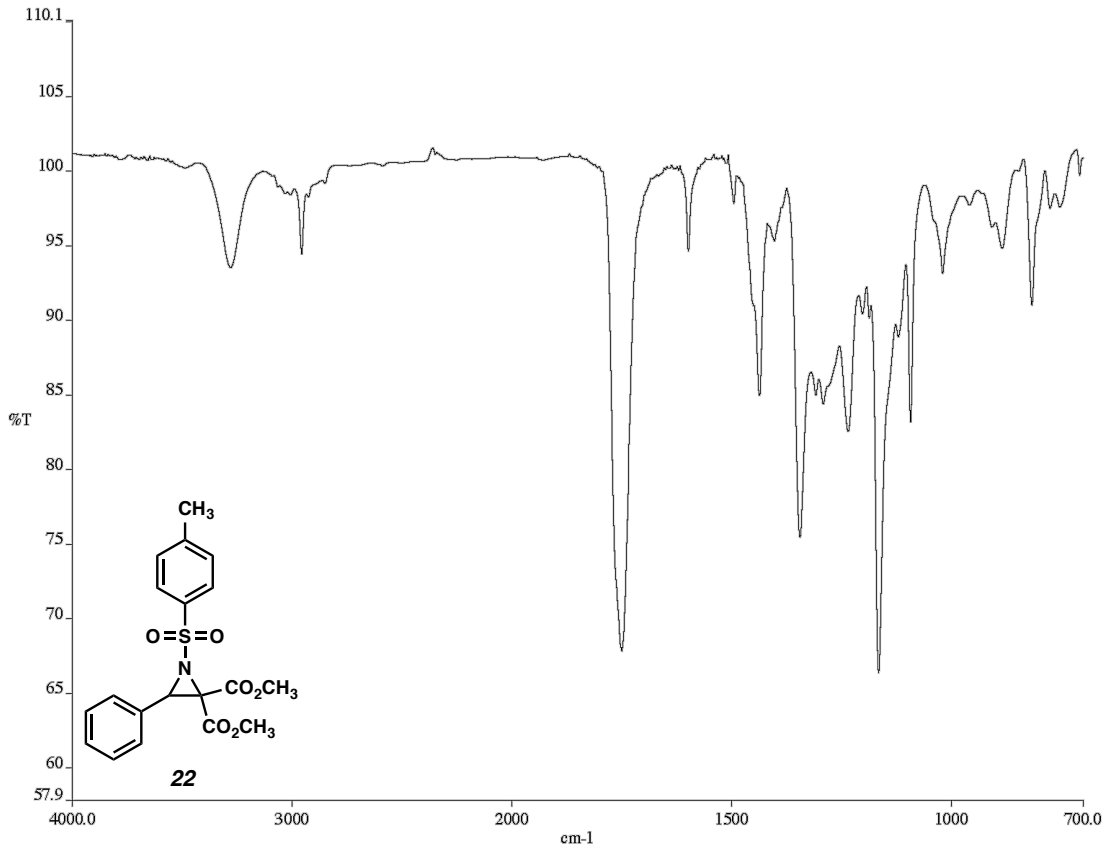
^{1}H NMR (500 MHz, $CDCl_3$) of compound **15**.



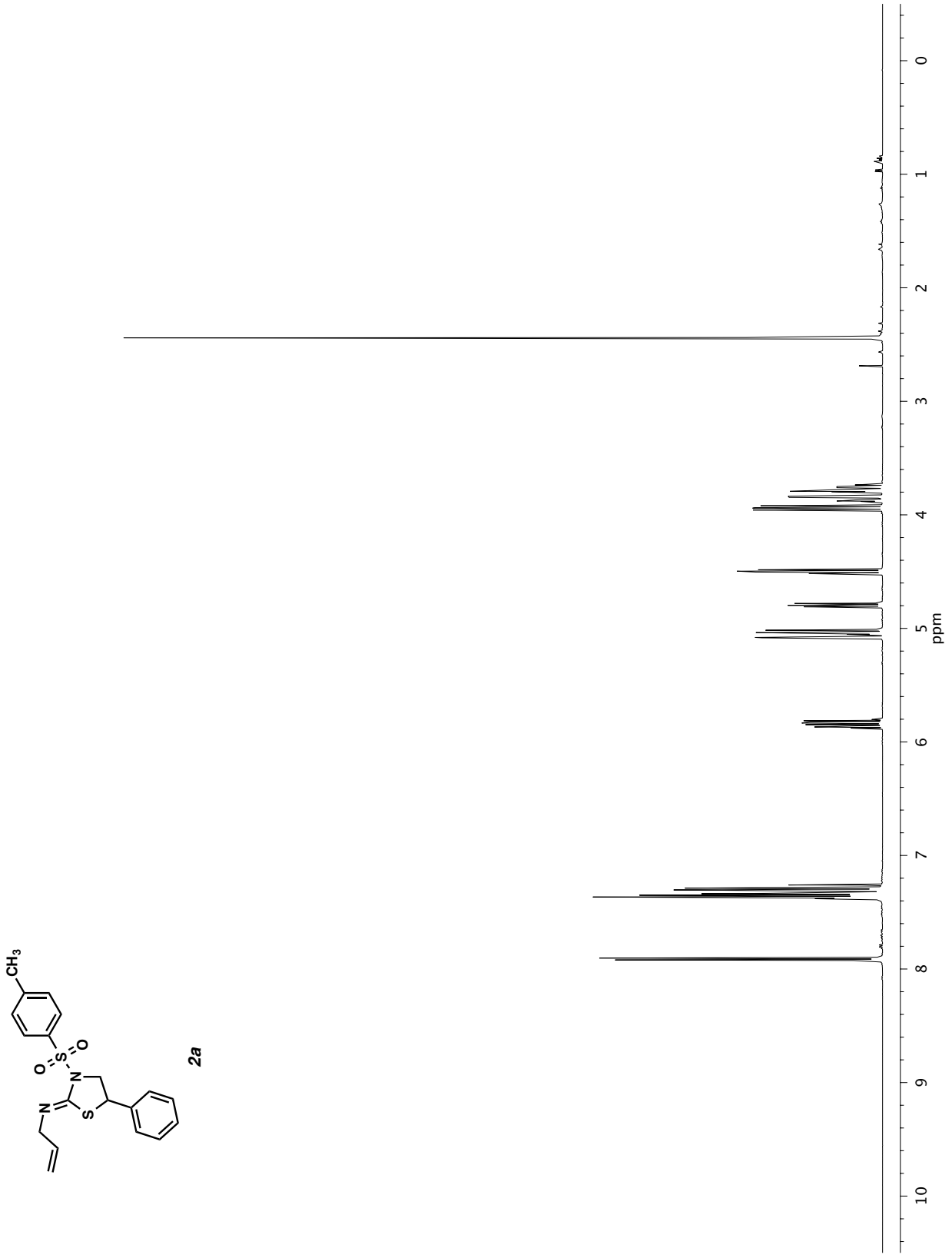
Infrared spectrum (Thin Film, NaCl) of compound **15**.



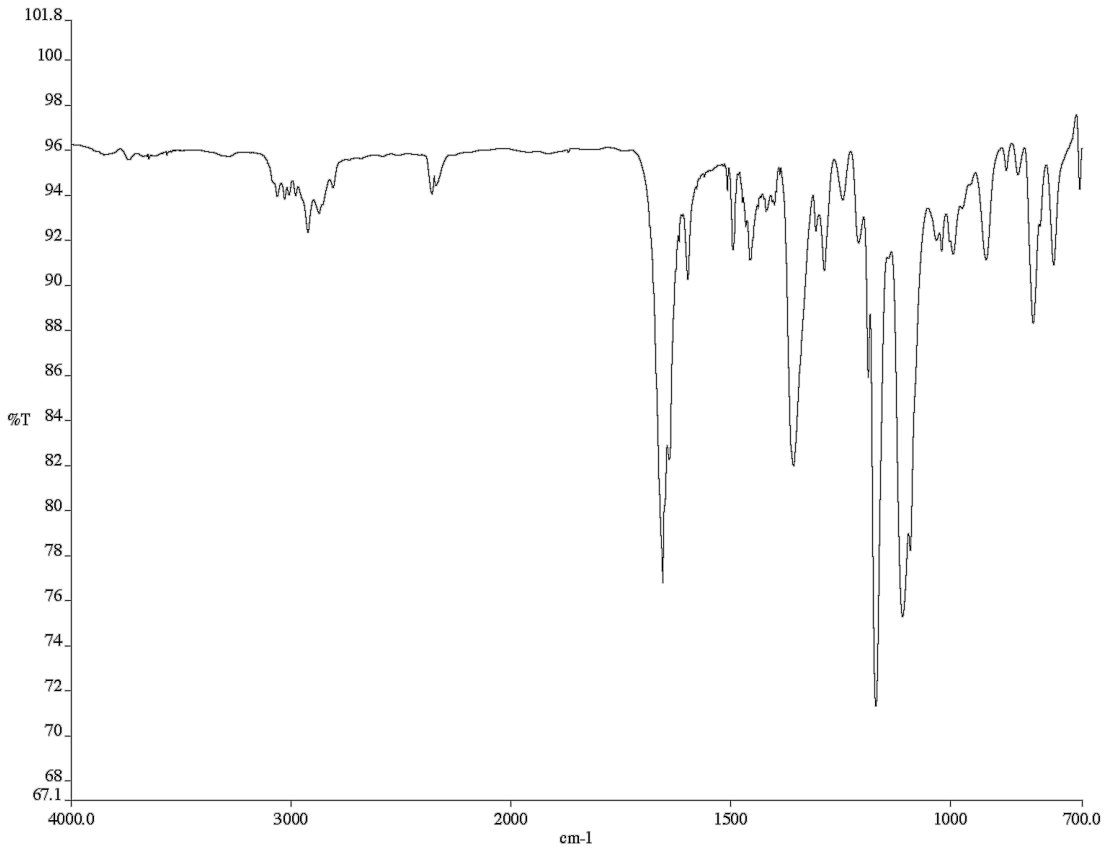
^{13}C NMR (126 MHz, $CDCl_3$) of compound **15**.



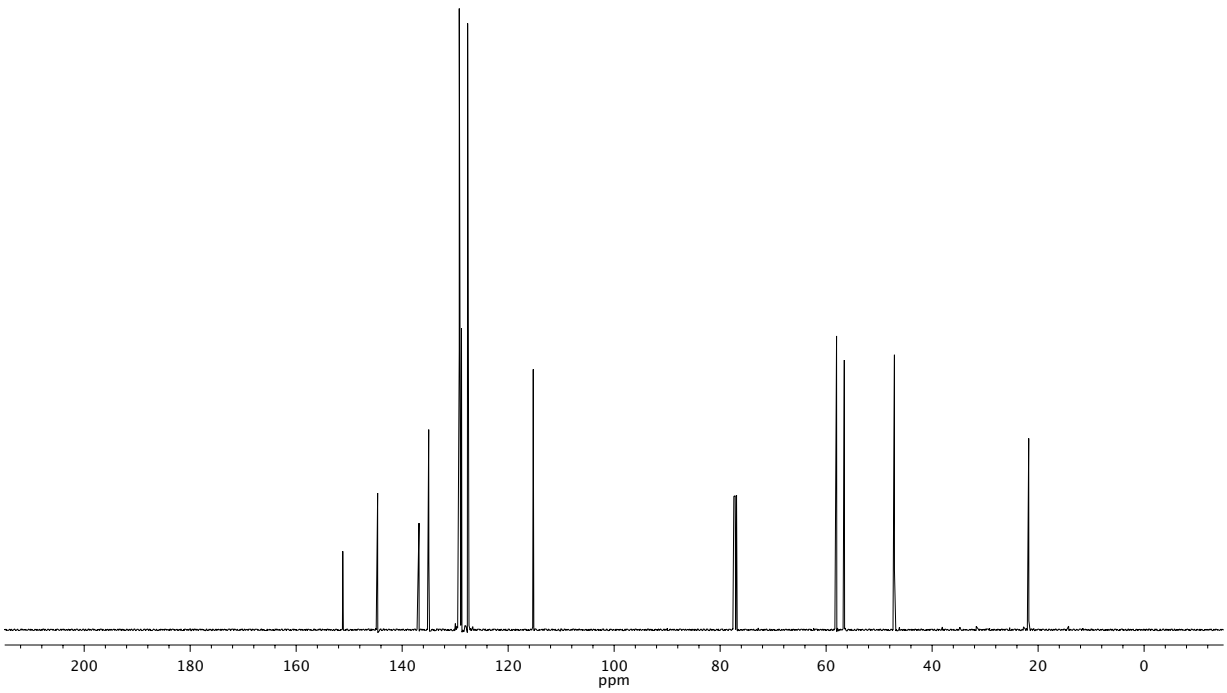
Infrared spectrum (Thin Film, NaCl) of compound **22**.



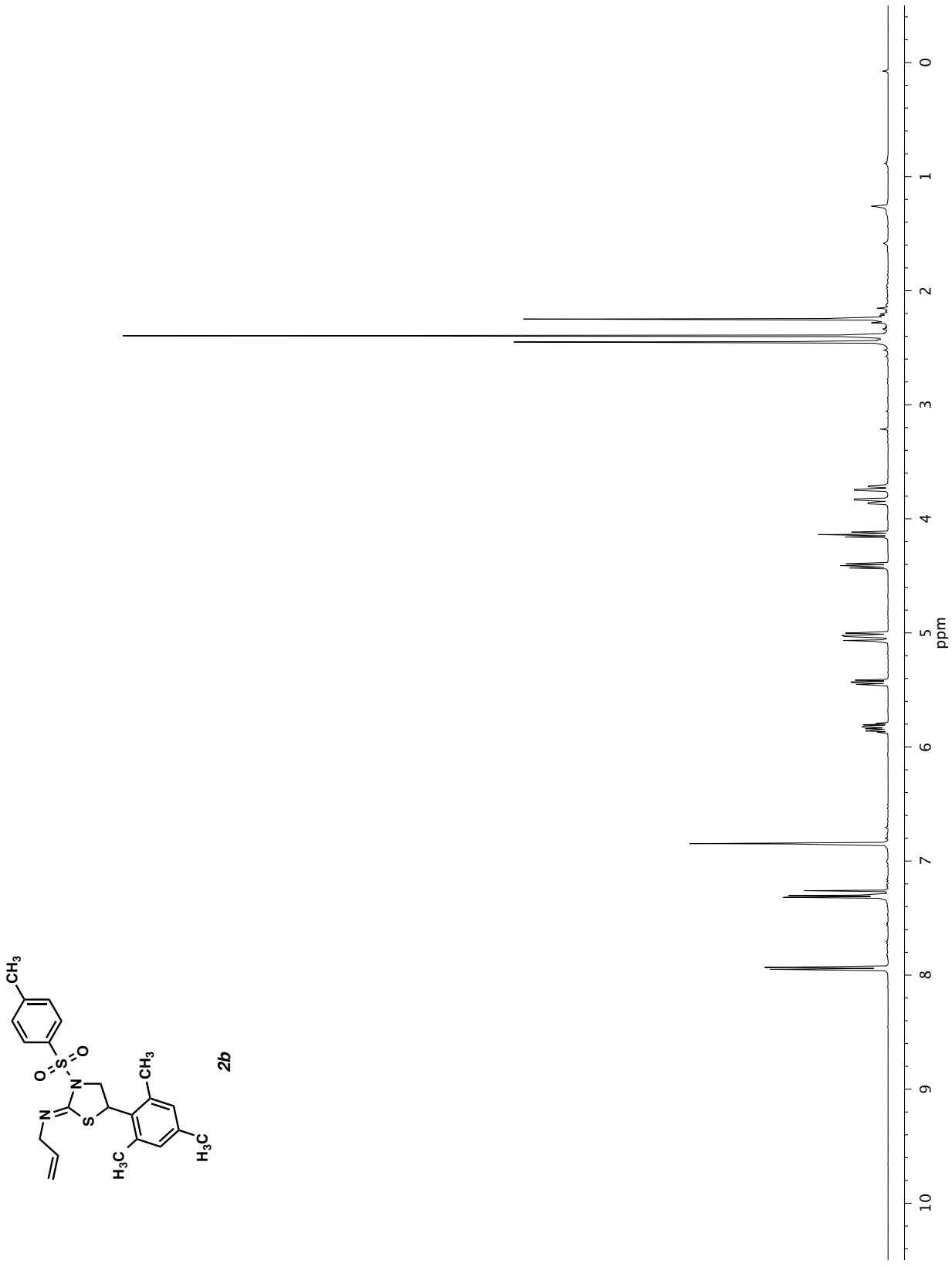
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2a**.



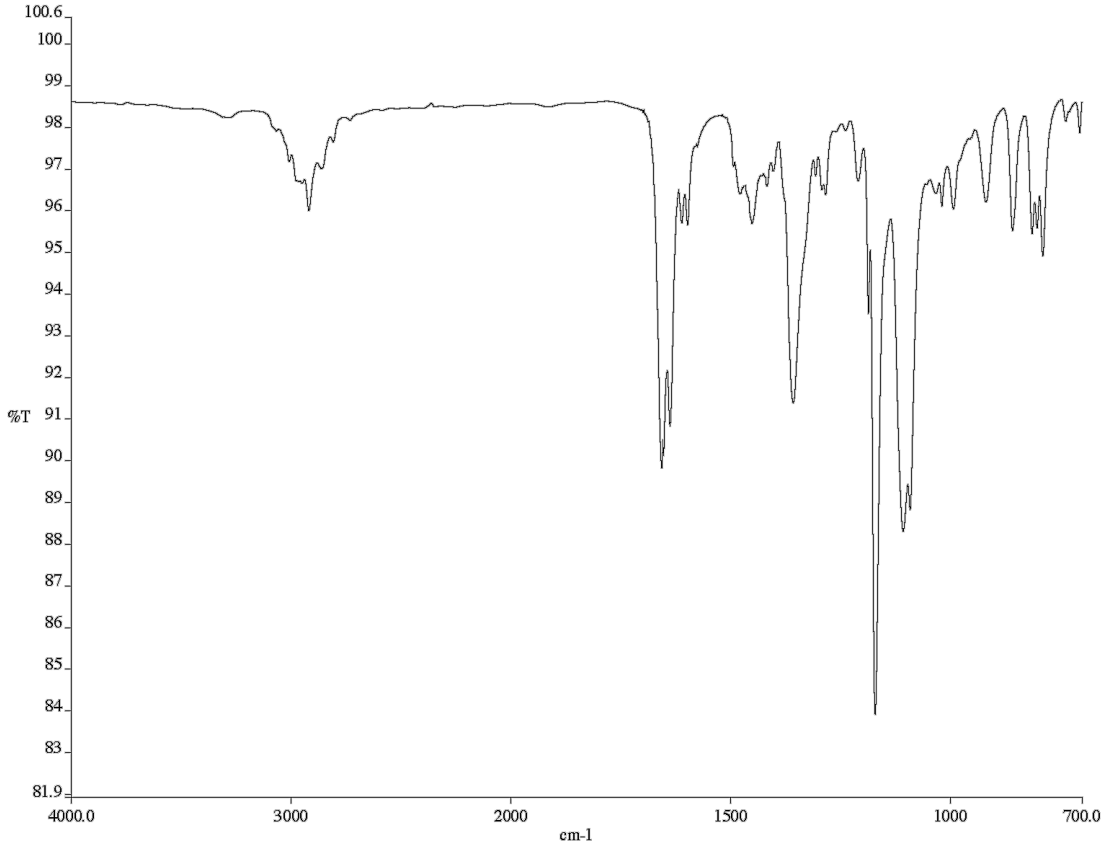
Infrared spectrum (Thin Film, NaCl) of compound **2a**.



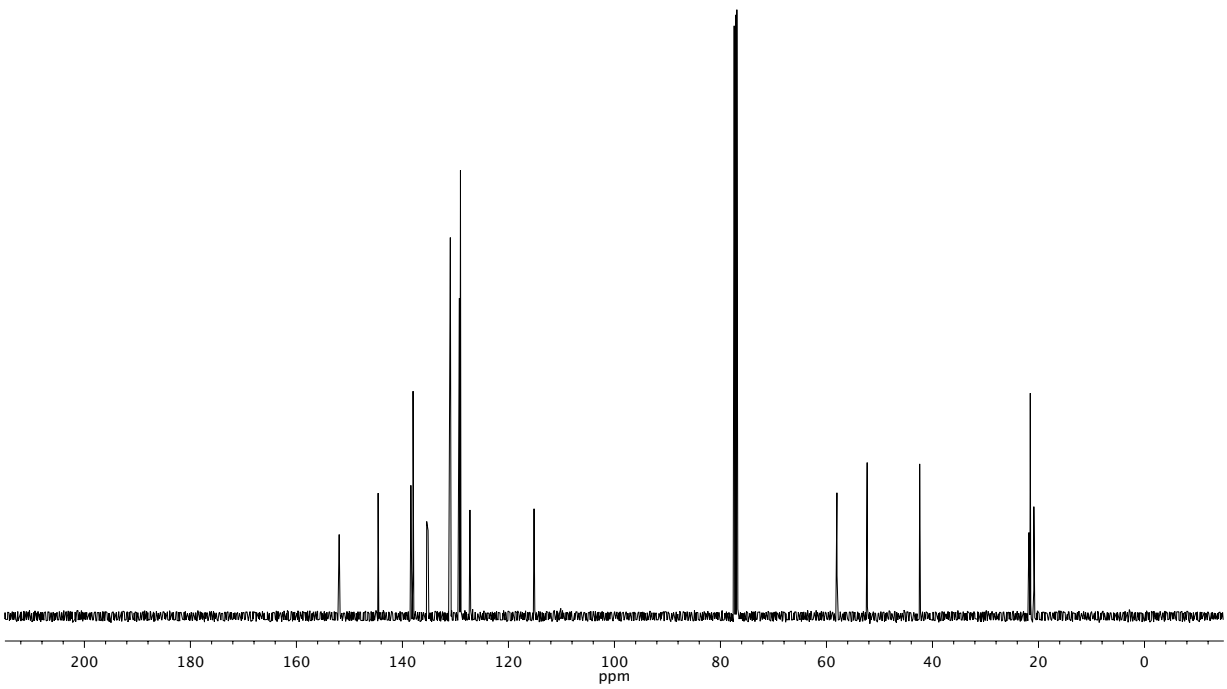
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2a**.



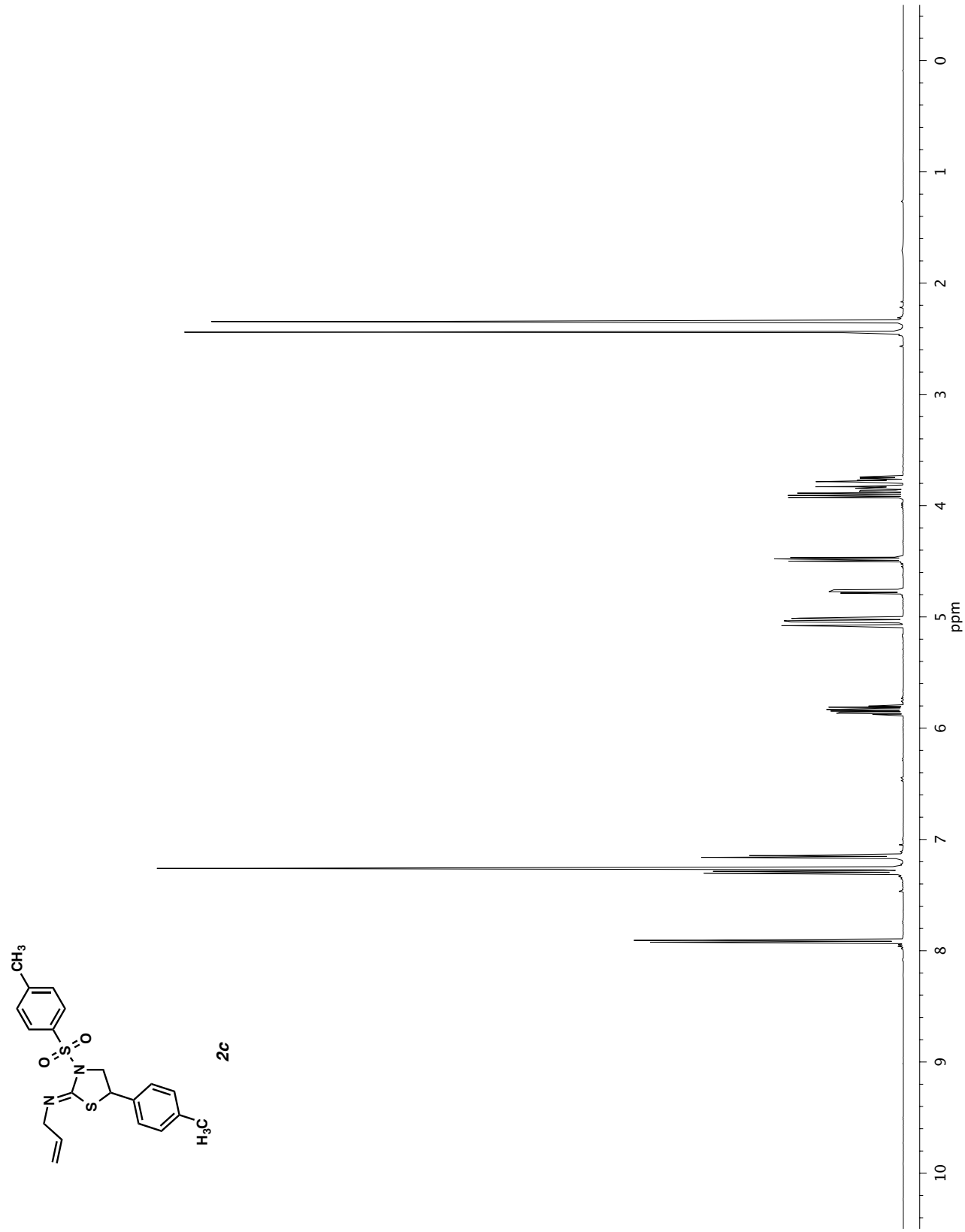
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2b**.



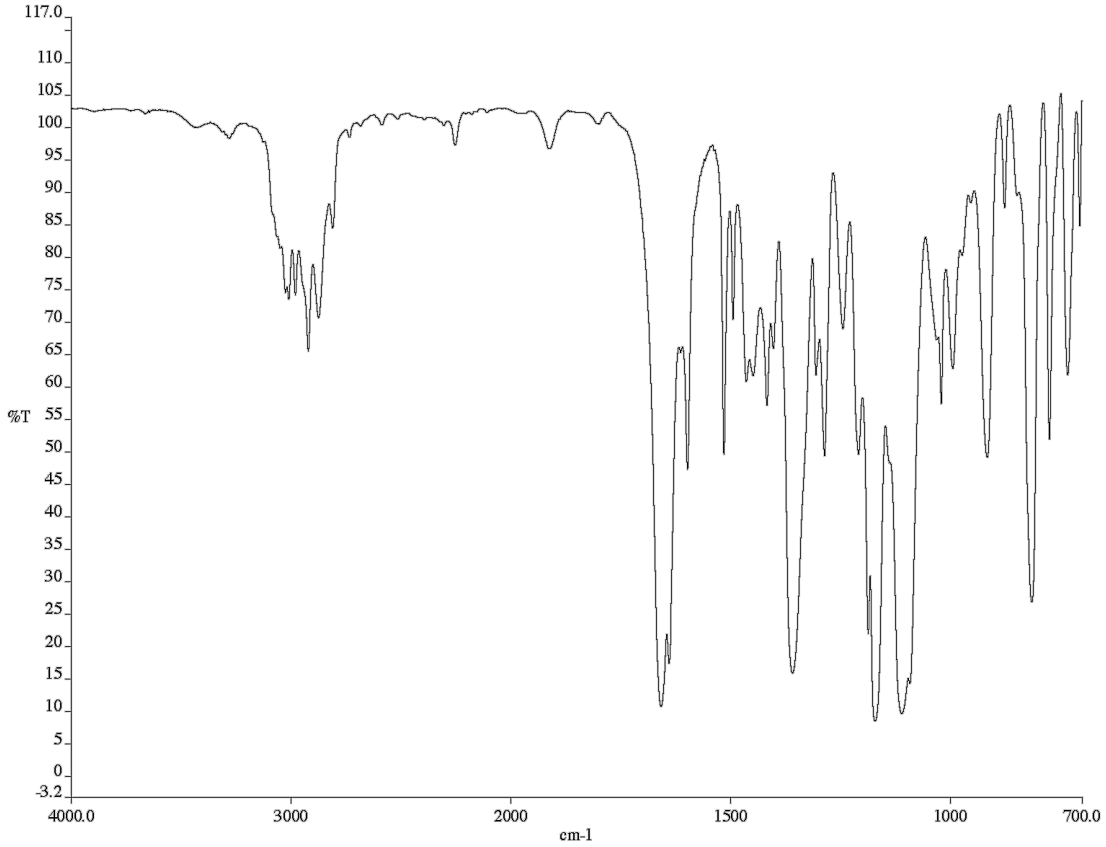
Infrared spectrum (Thin Film, NaCl) of compound **2b**.



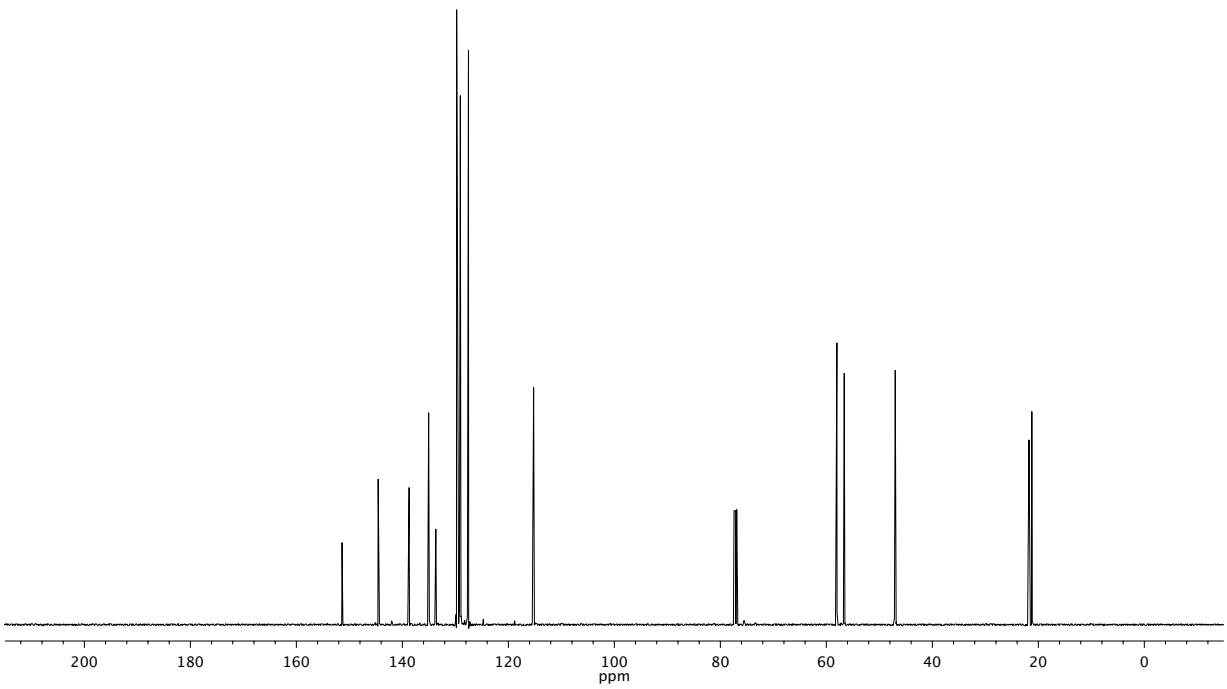
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2b**.



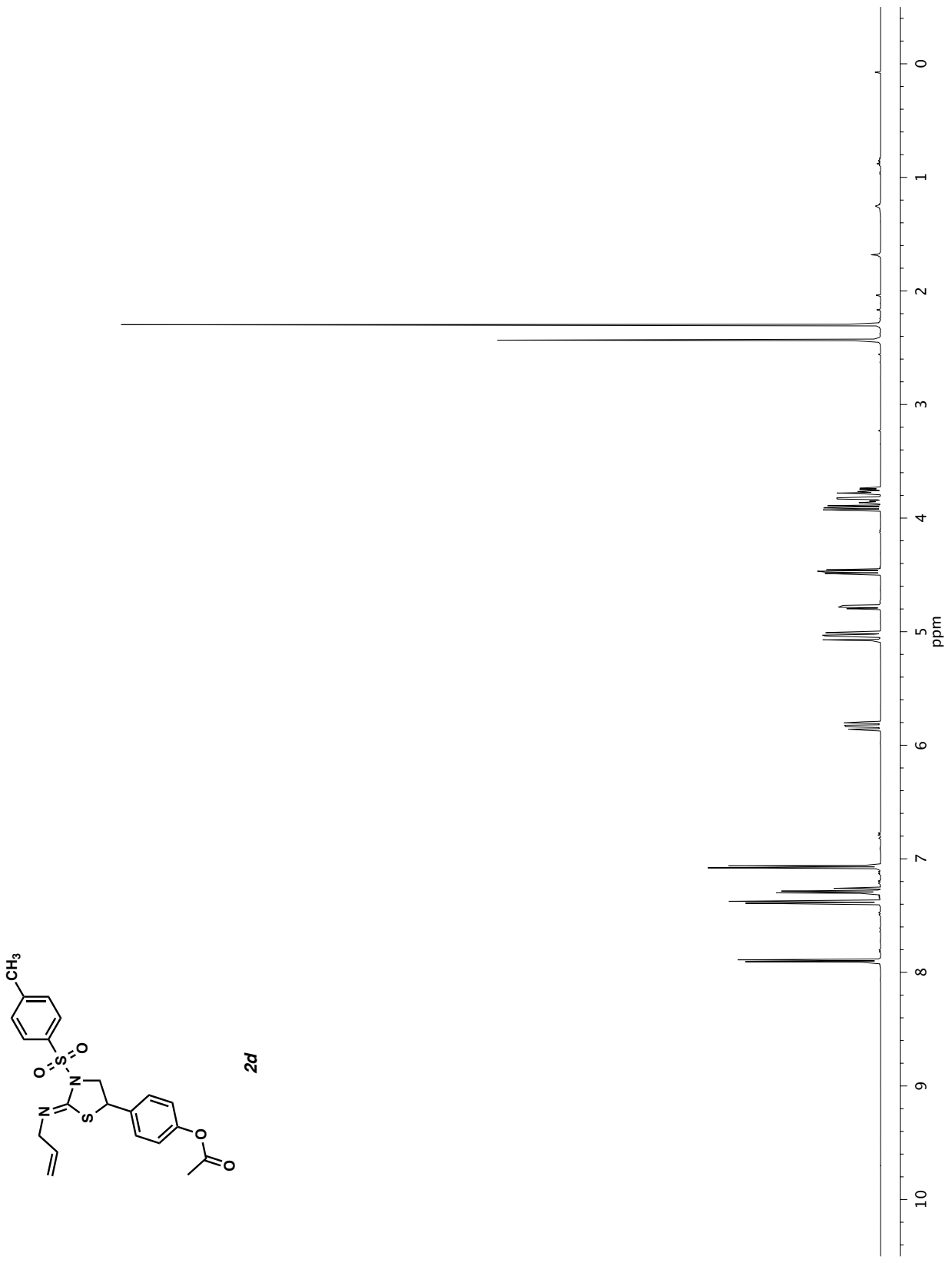
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2c**.



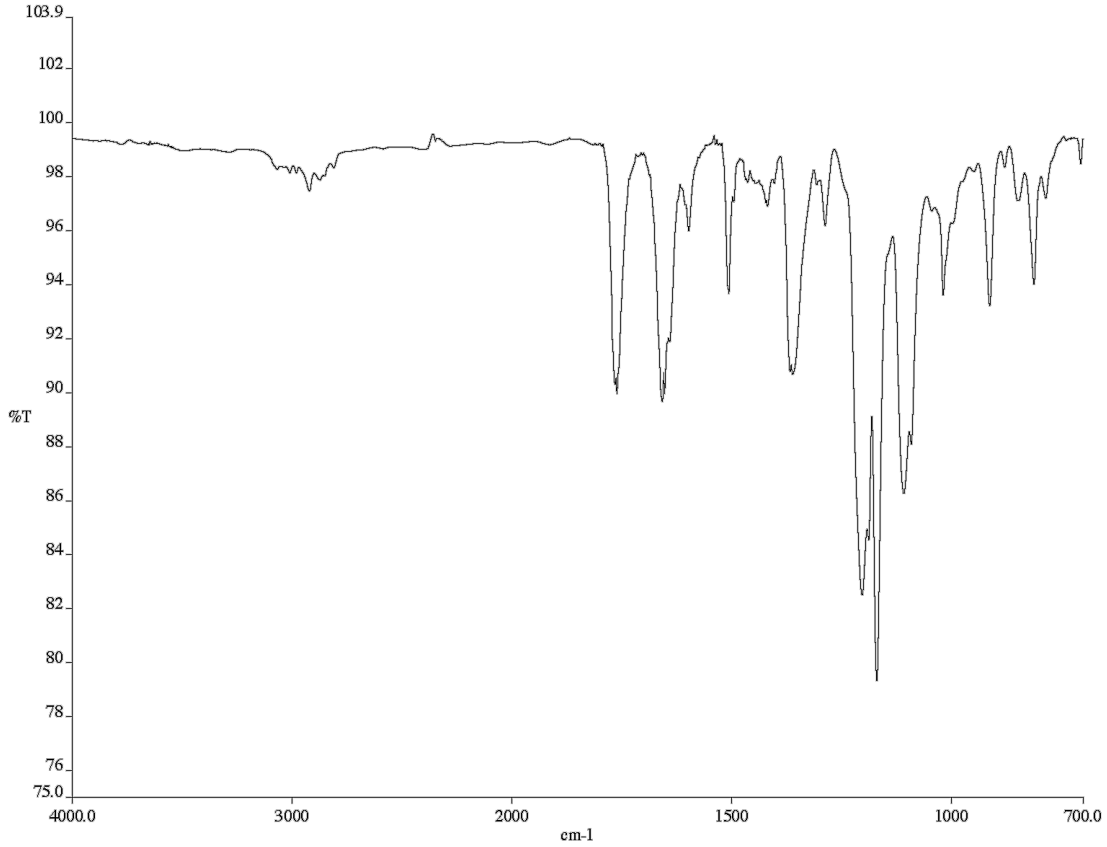
Infrared spectrum (Thin Film, NaCl) of compound **2c**.



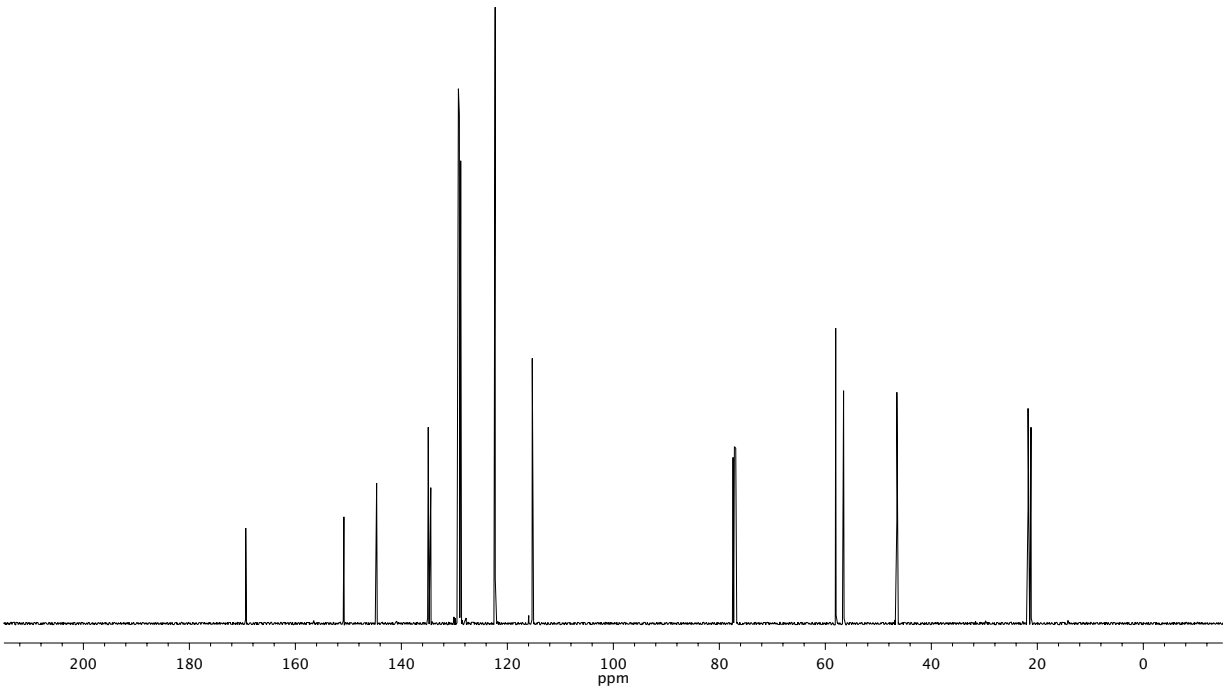
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2c**.



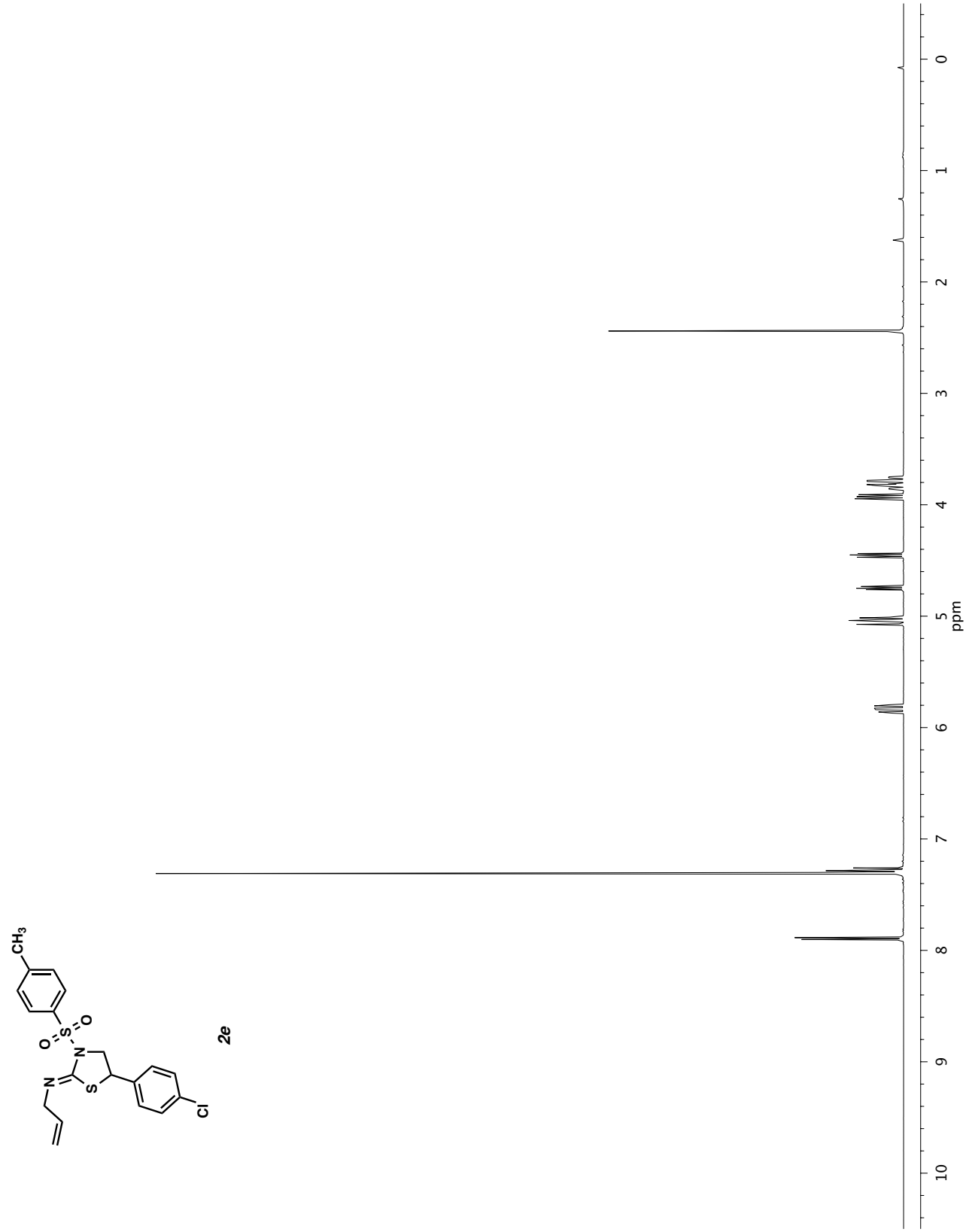
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2d**.



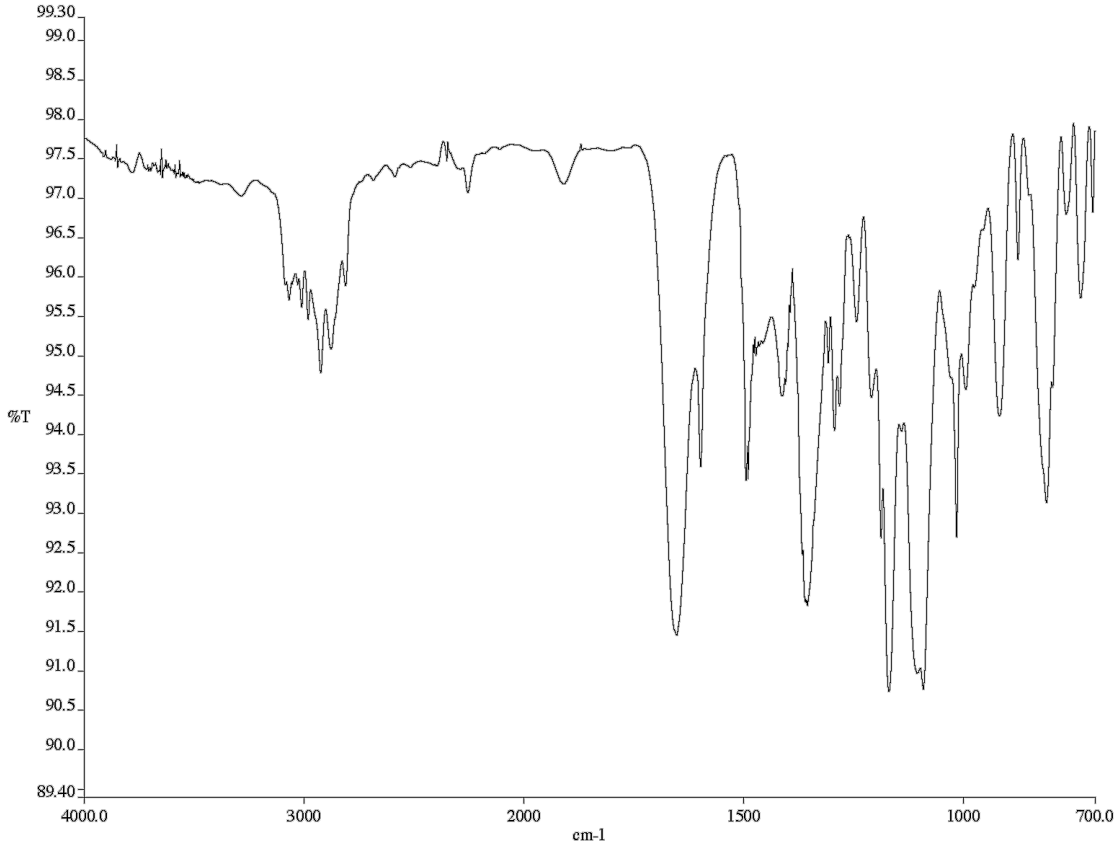
Infrared spectrum (Thin Film, NaCl) of compound **2d**.



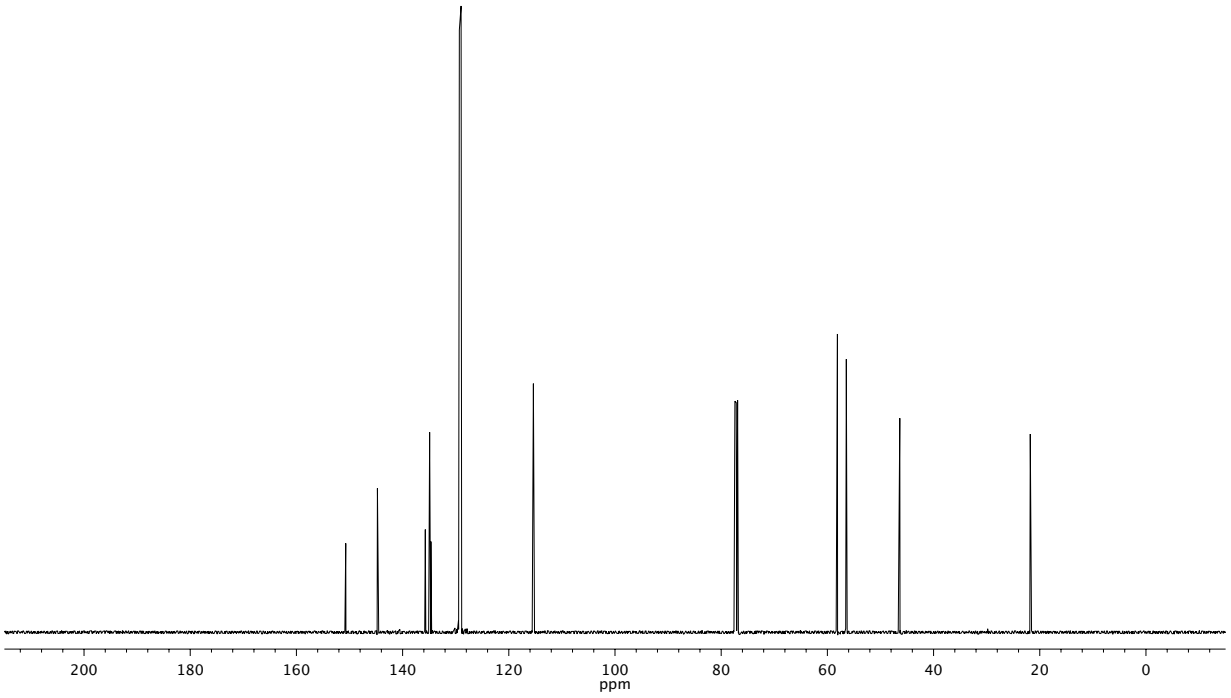
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2d**.



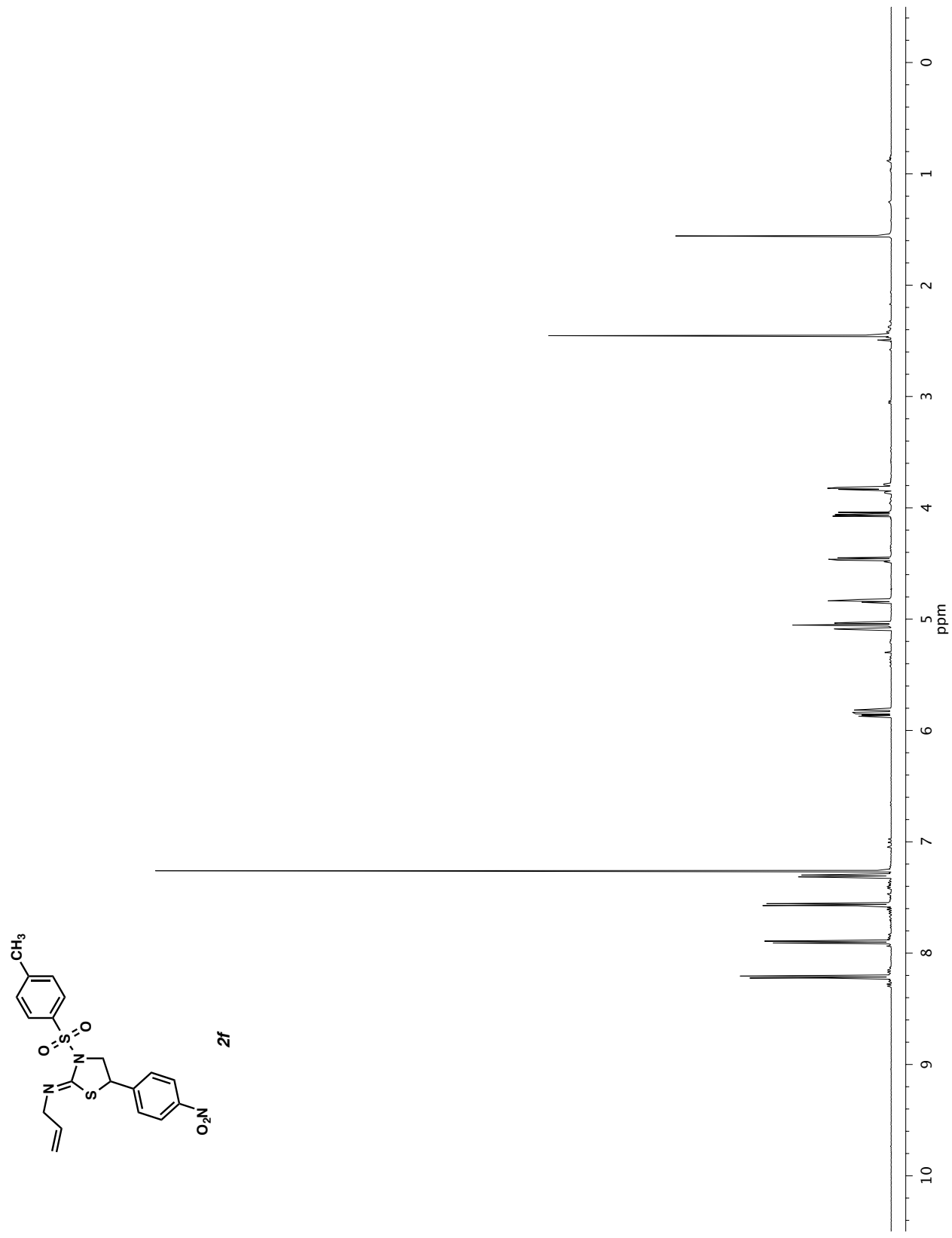
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2e**.



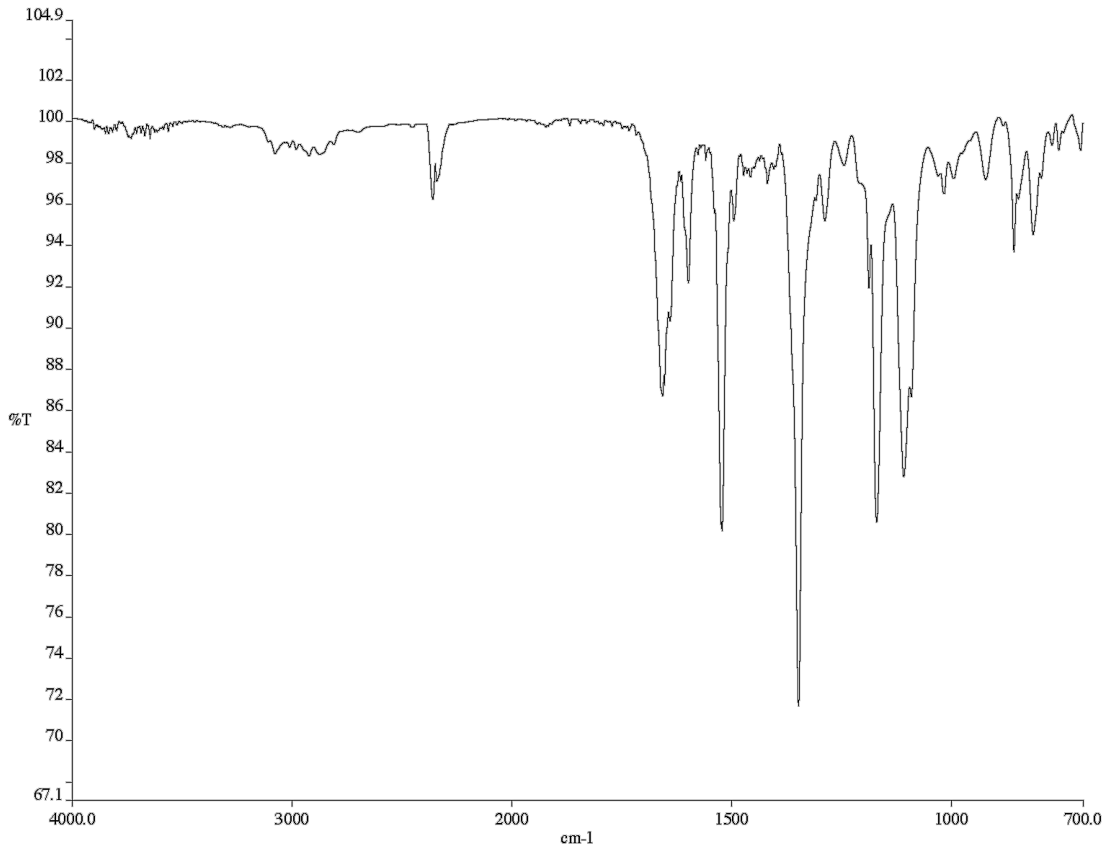
Infrared spectrum (Thin Film, NaCl) of compound **2e**.



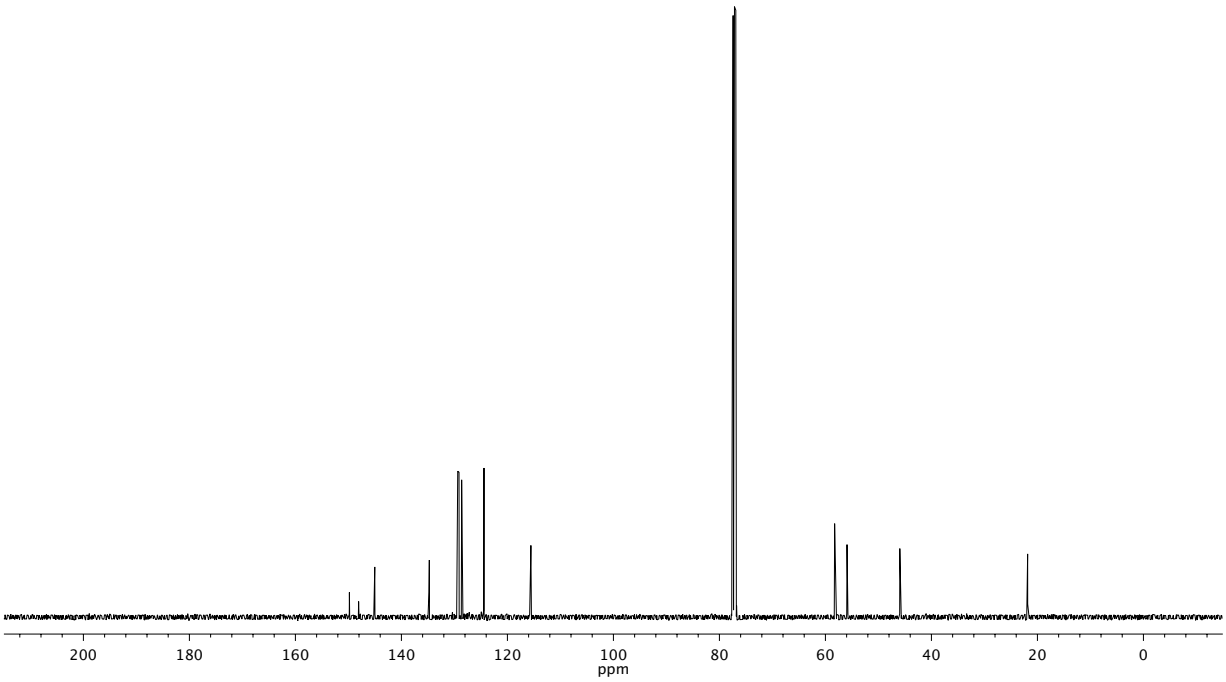
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2e**.



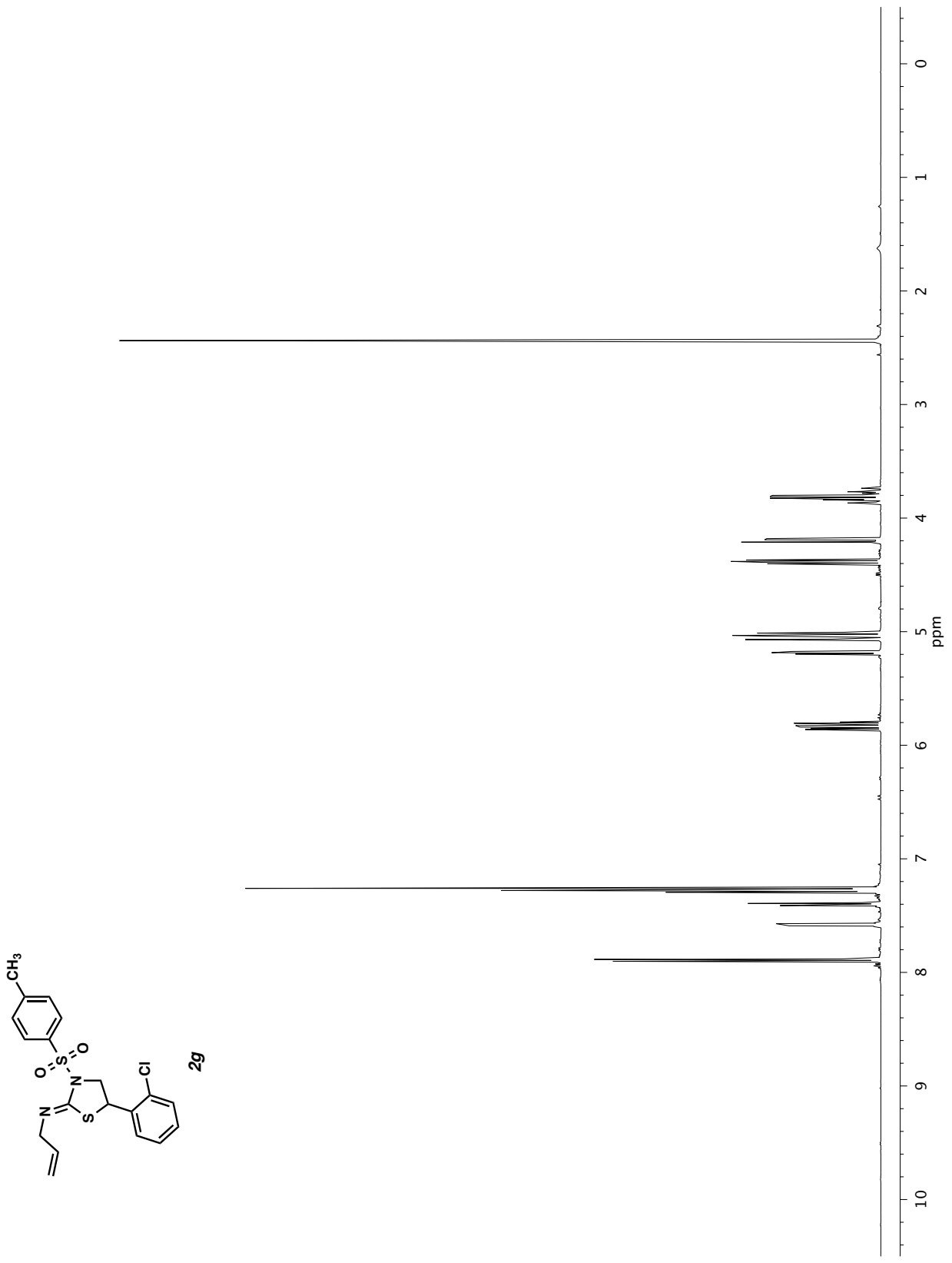
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2f**.



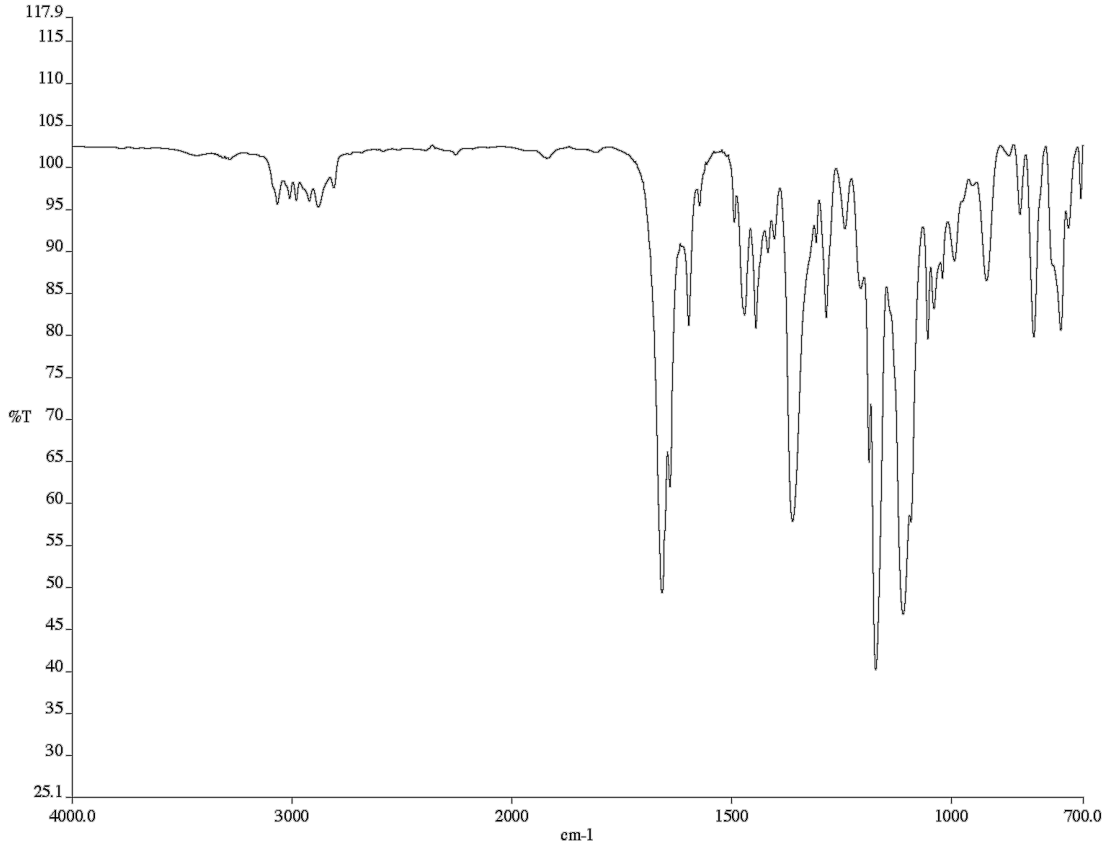
Infrared spectrum (Thin Film, NaCl) of compound **2f**.



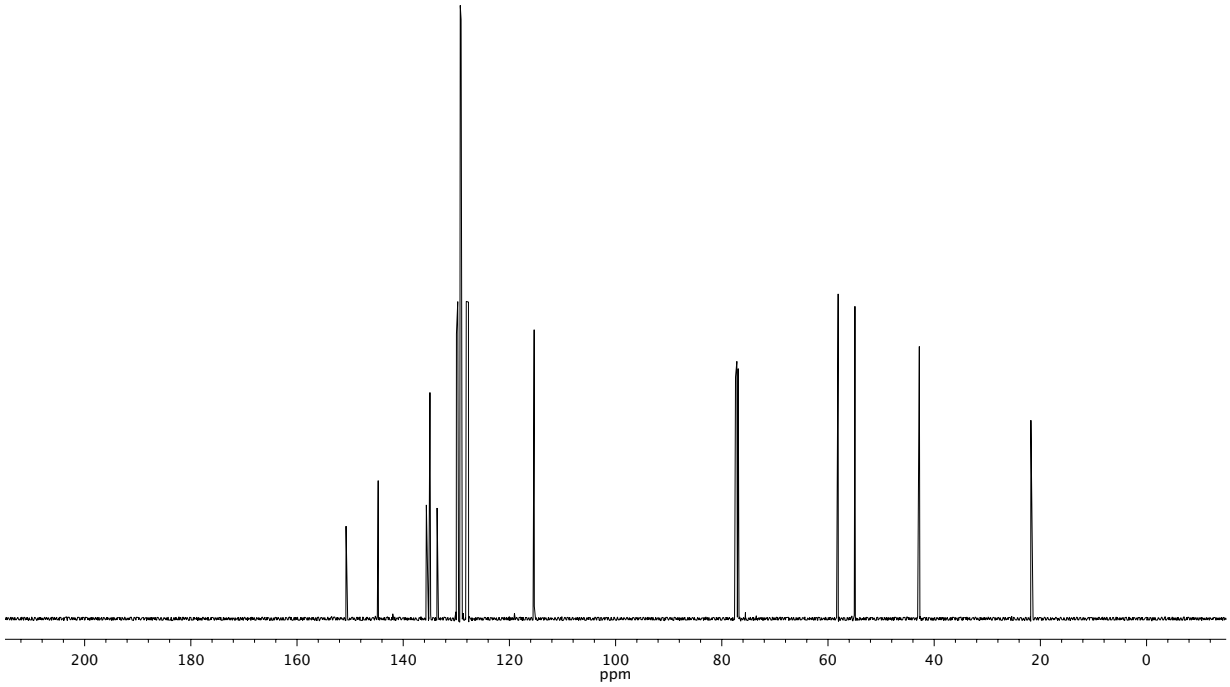
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2f**.



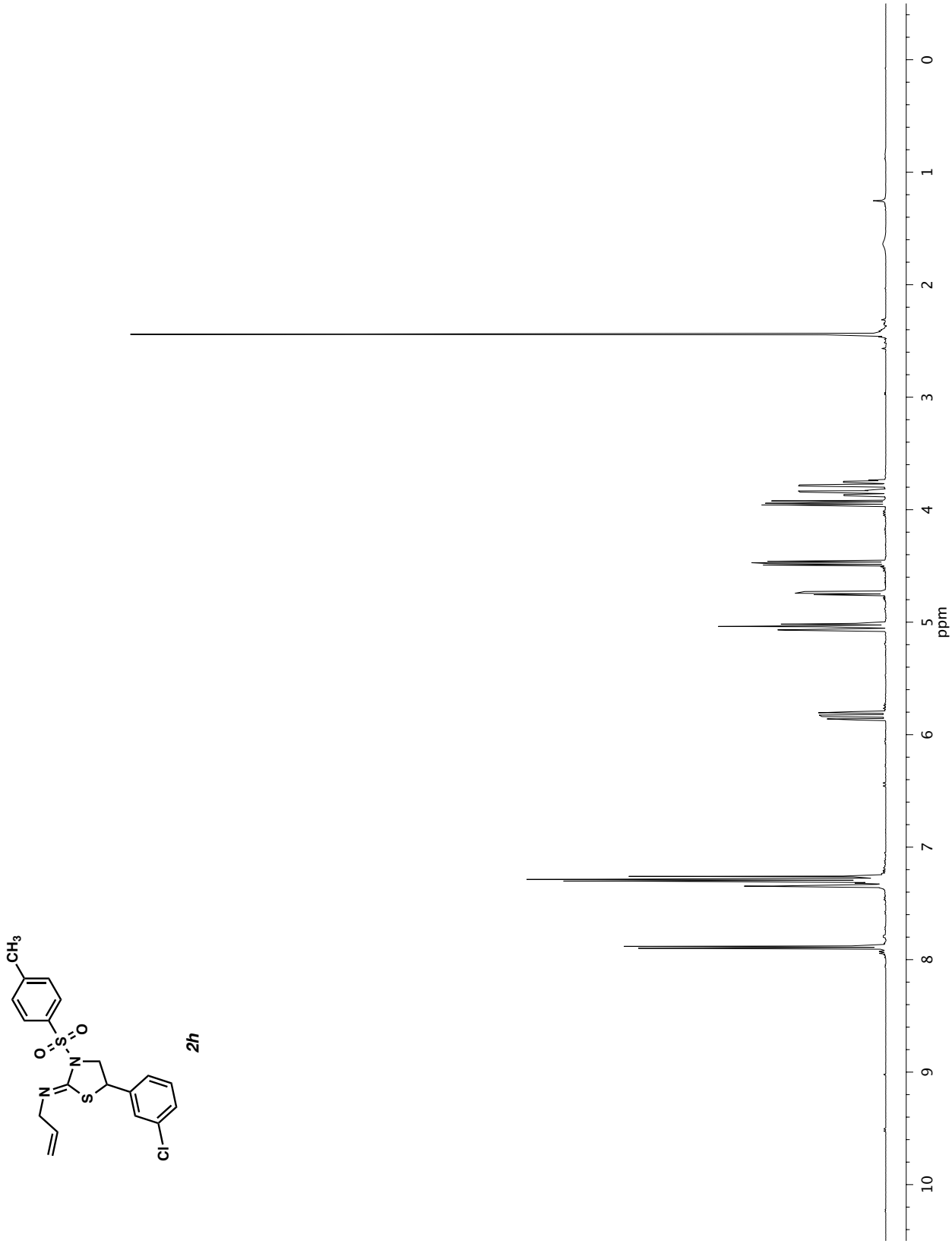
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2g**.



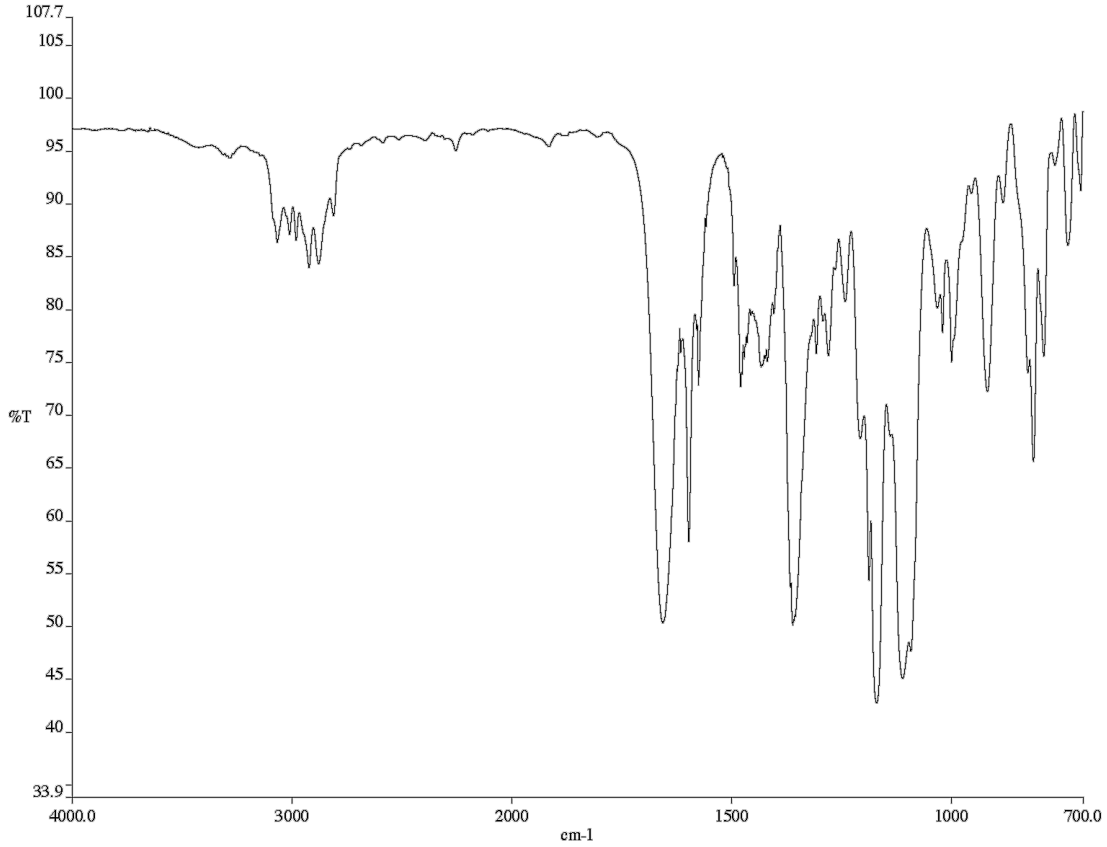
Infrared spectrum (Thin Film, NaCl) of compound **2g**.



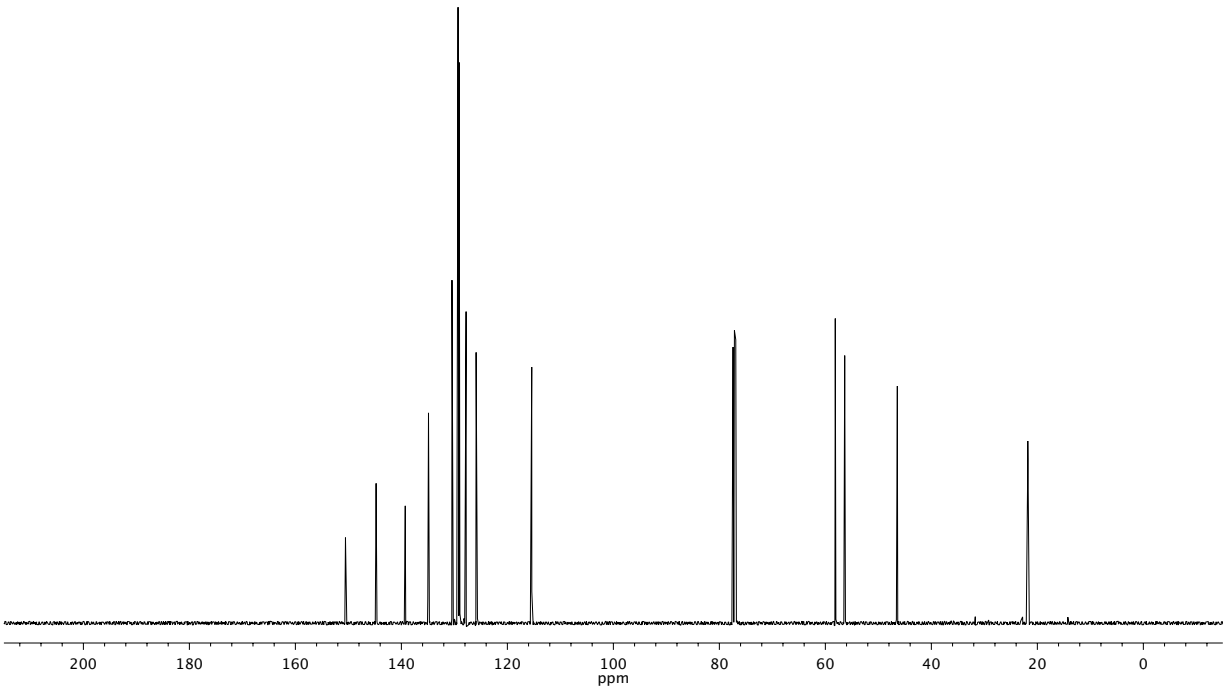
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2g**.



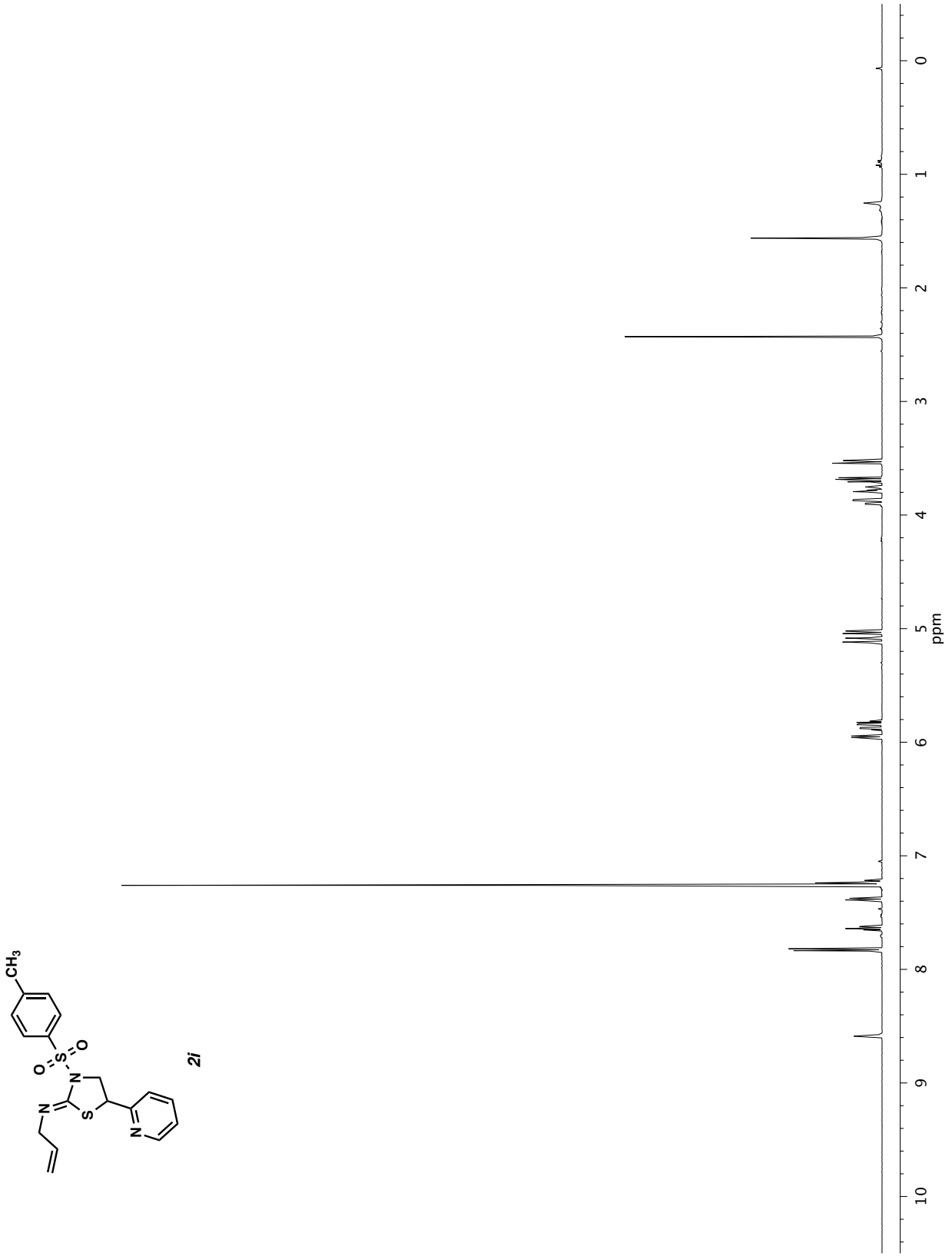
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2h**.



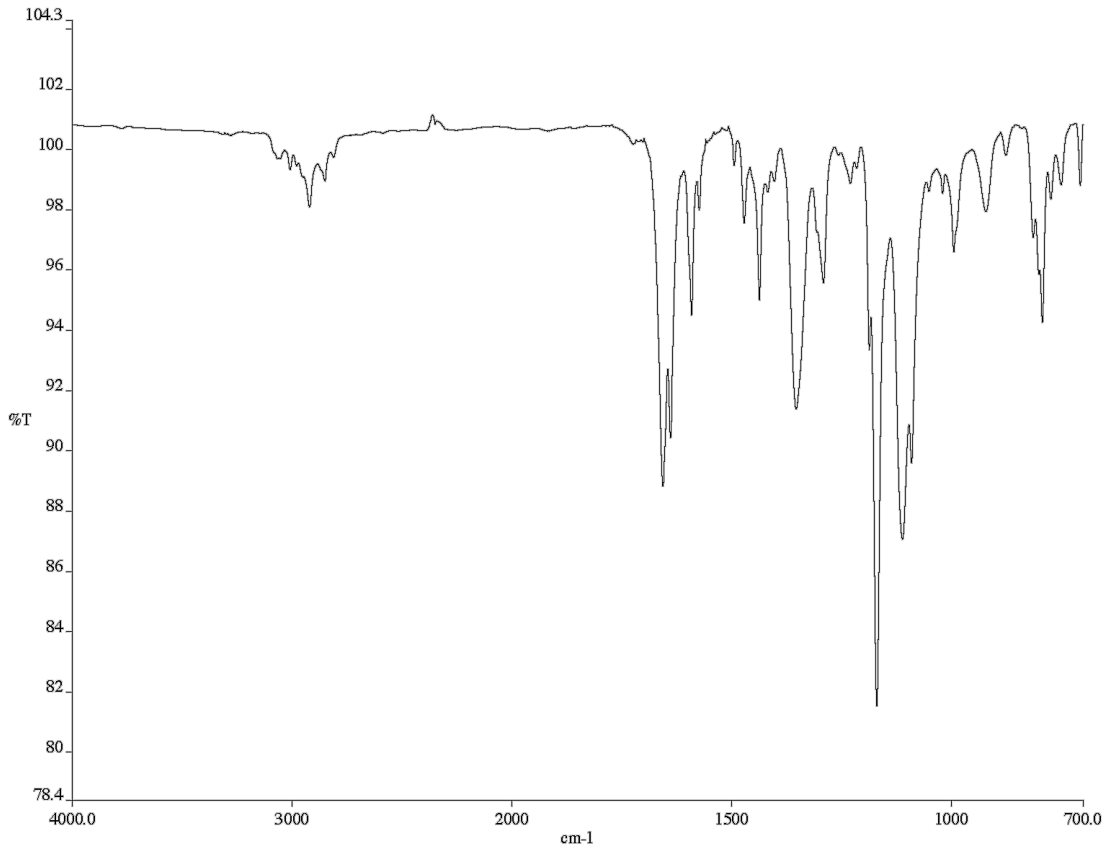
Infrared spectrum (Thin Film, NaCl) of compound **2h**.



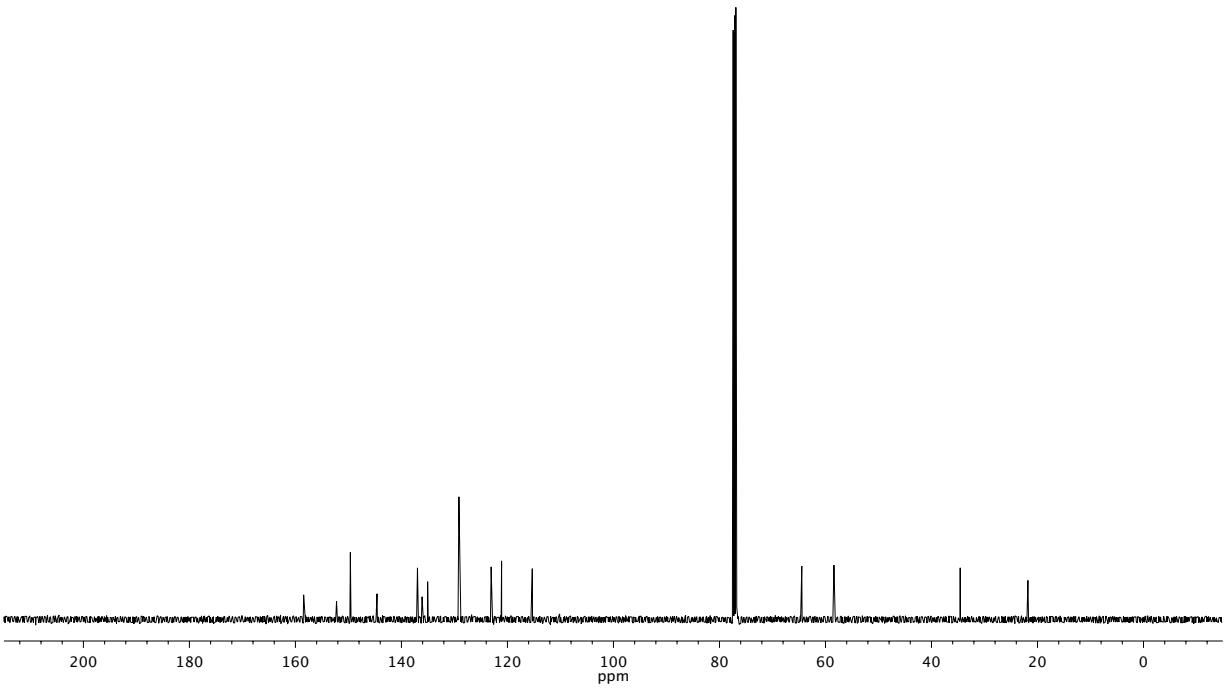
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2h**.



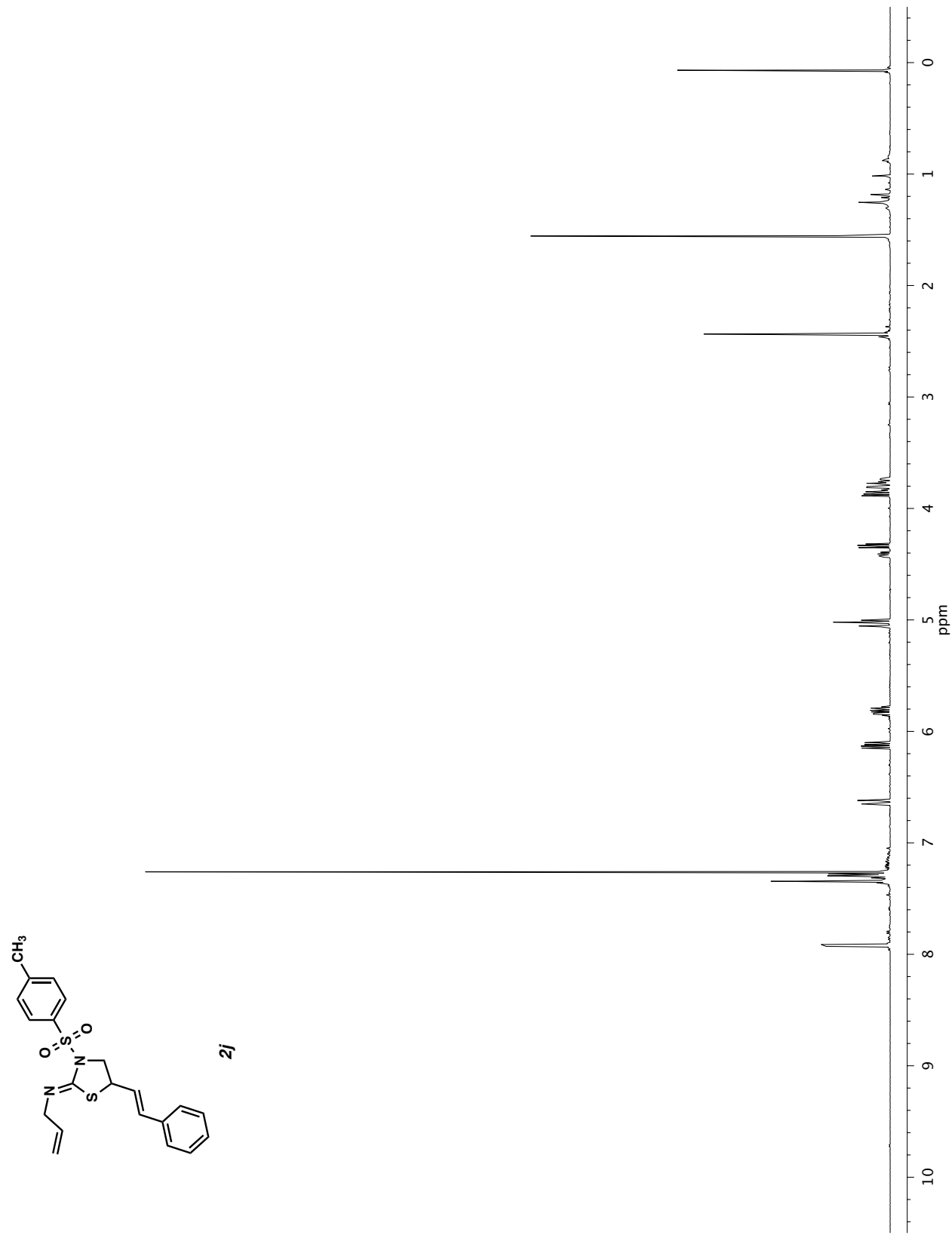
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2i**.



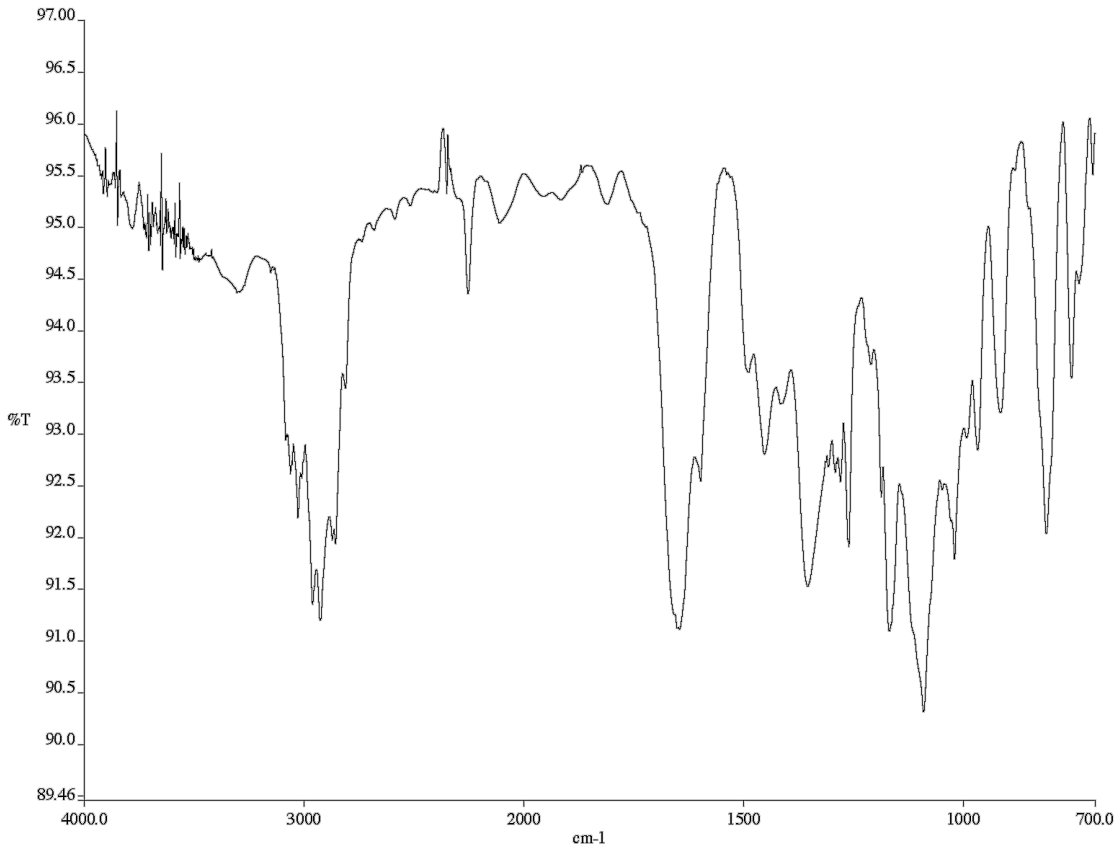
Infrared spectrum (Thin Film, NaCl) of compound **2i**.



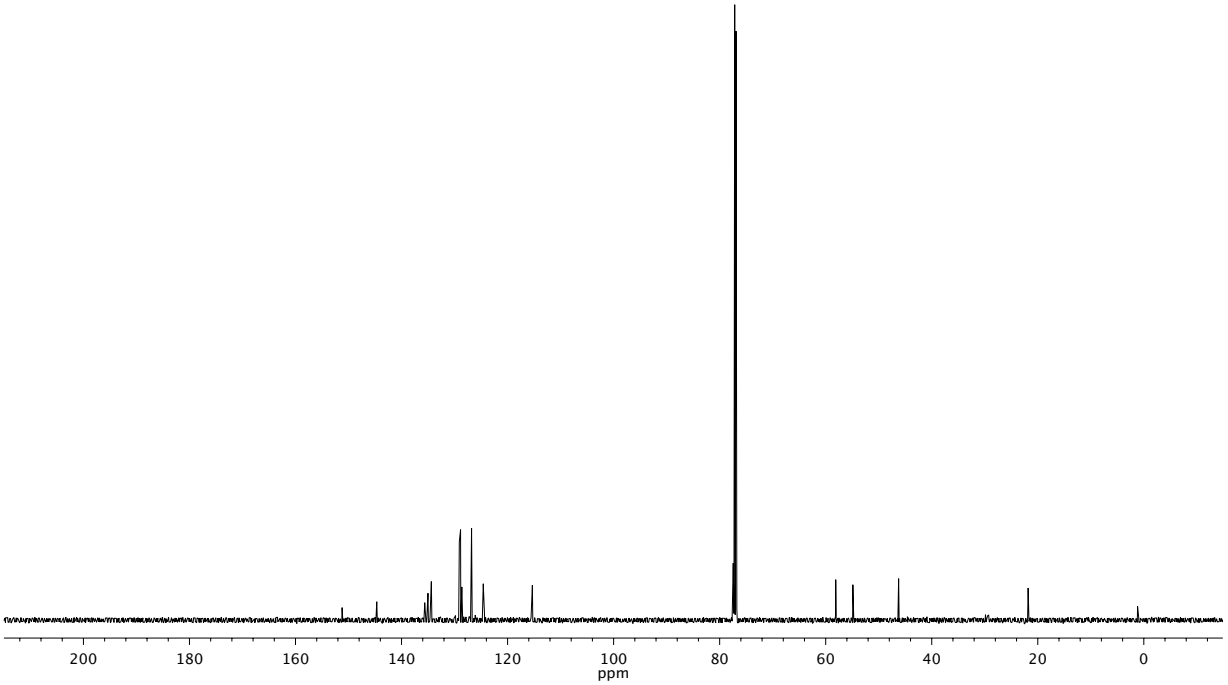
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2i**.



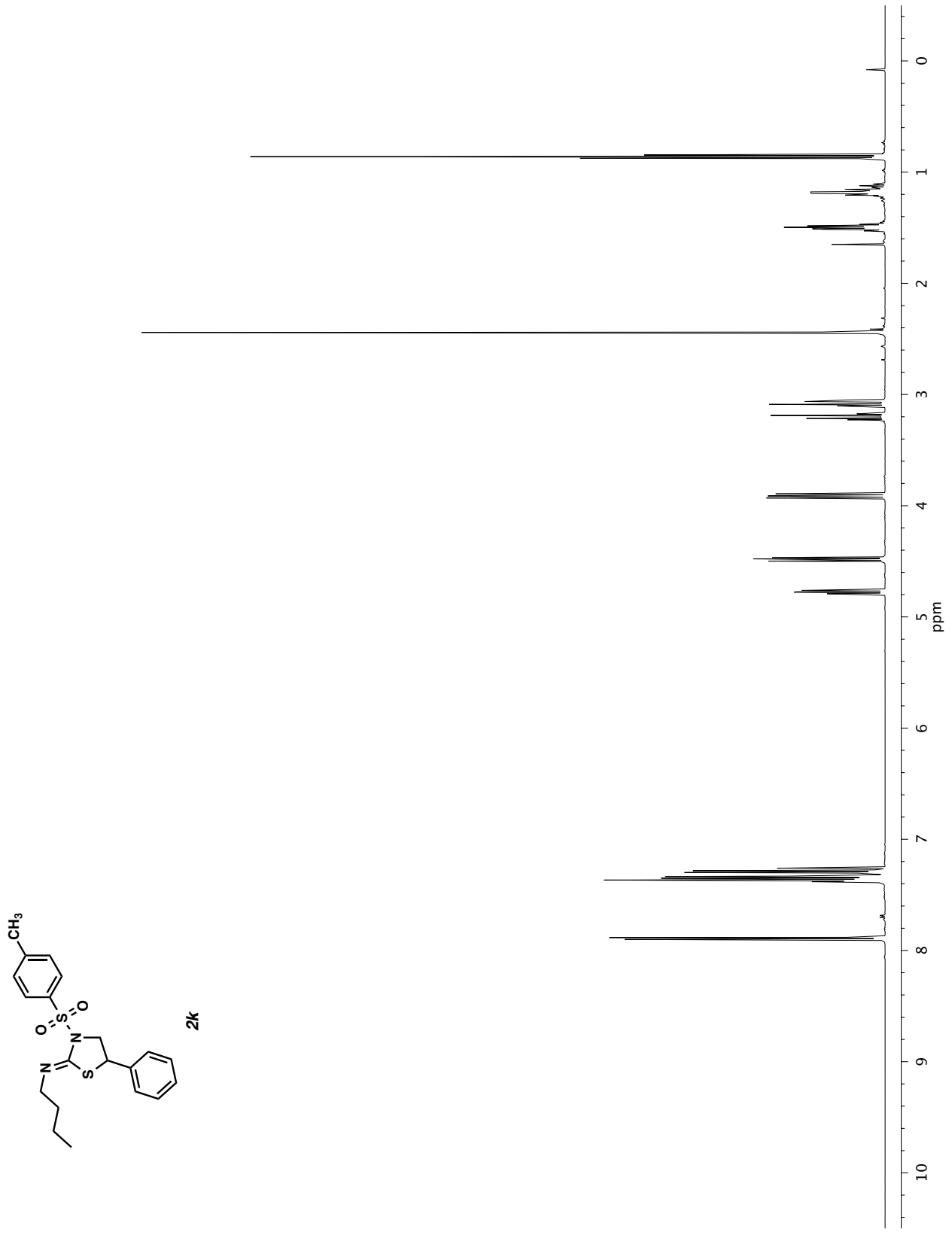
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2j**.



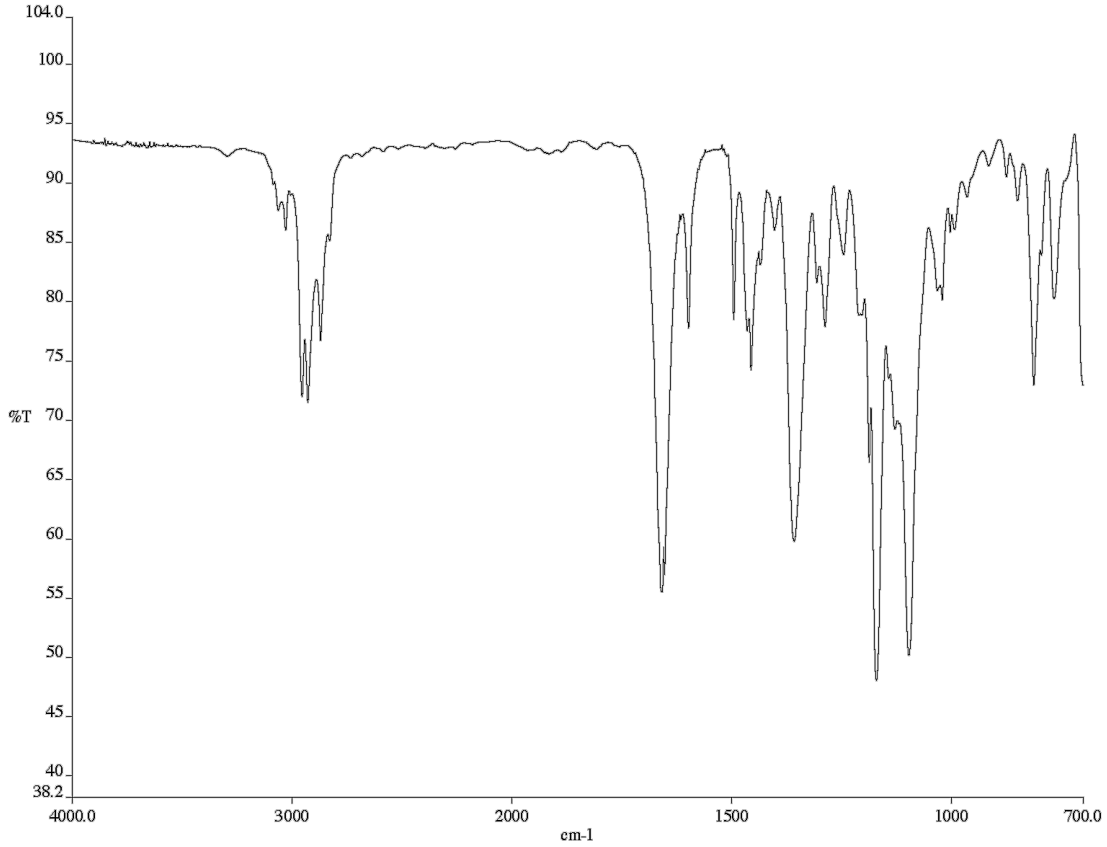
Infrared spectrum (Thin Film, NaCl) of compound **2j**.



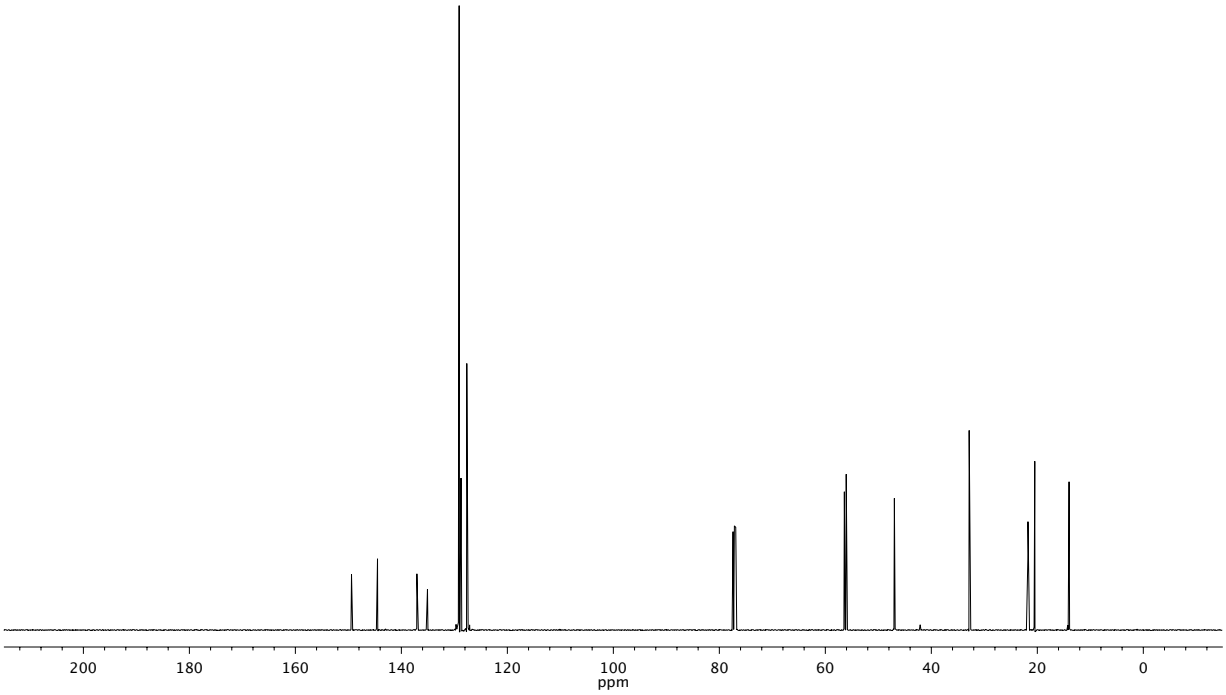
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2j**.



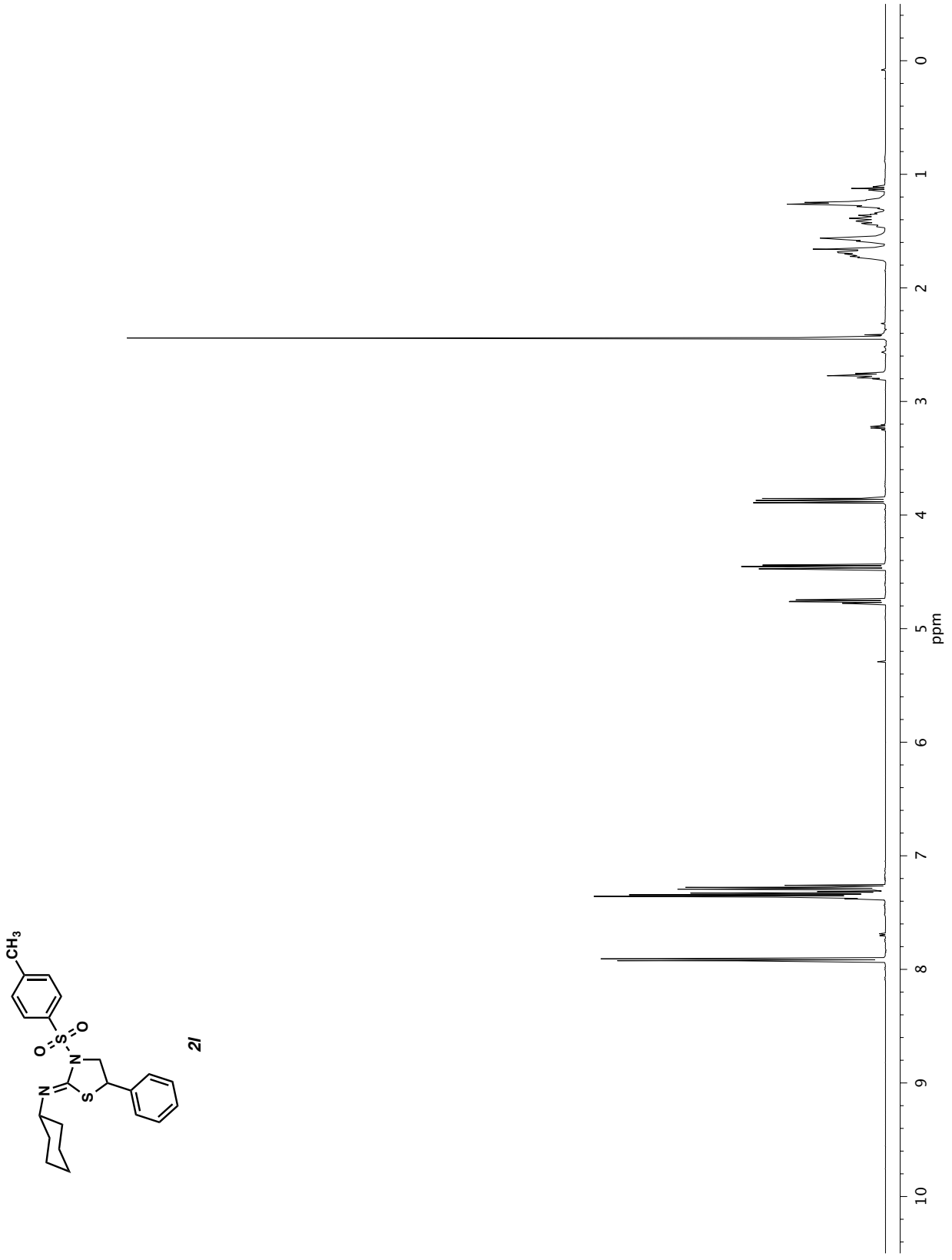
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2k**.



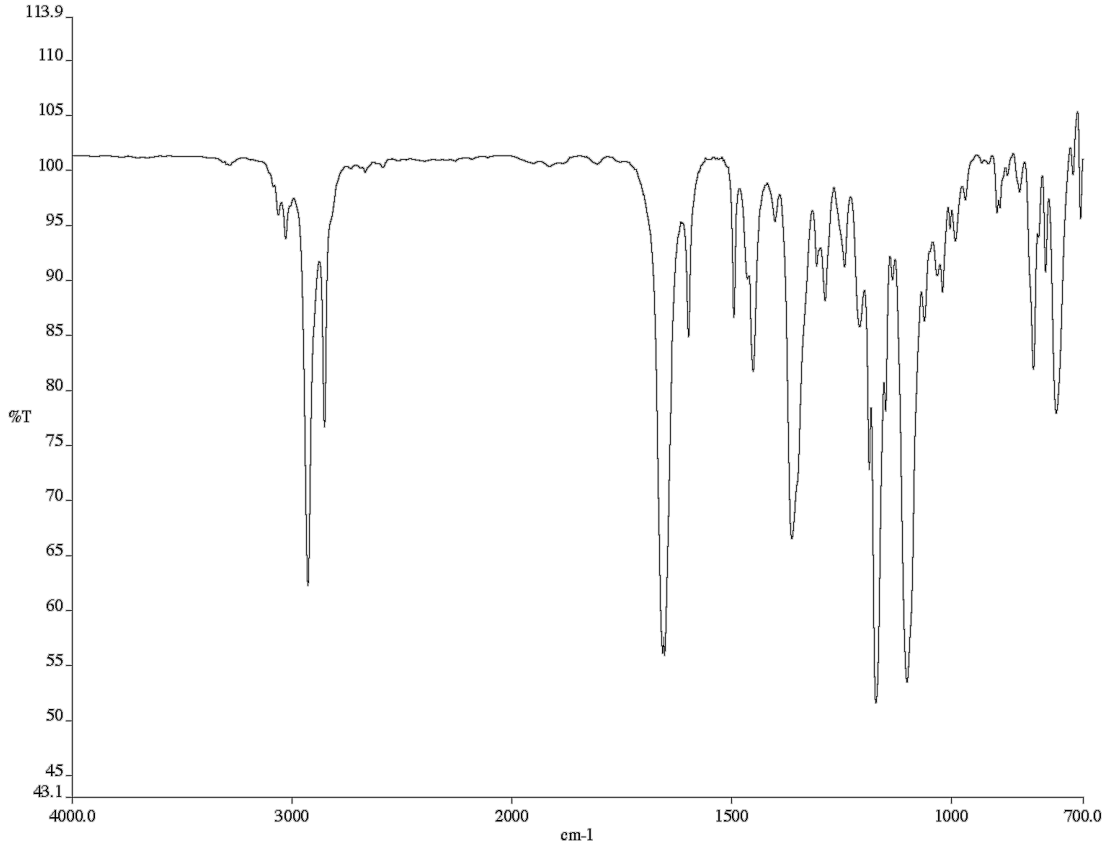
Infrared spectrum (Thin Film, NaCl) of compound **2k**.



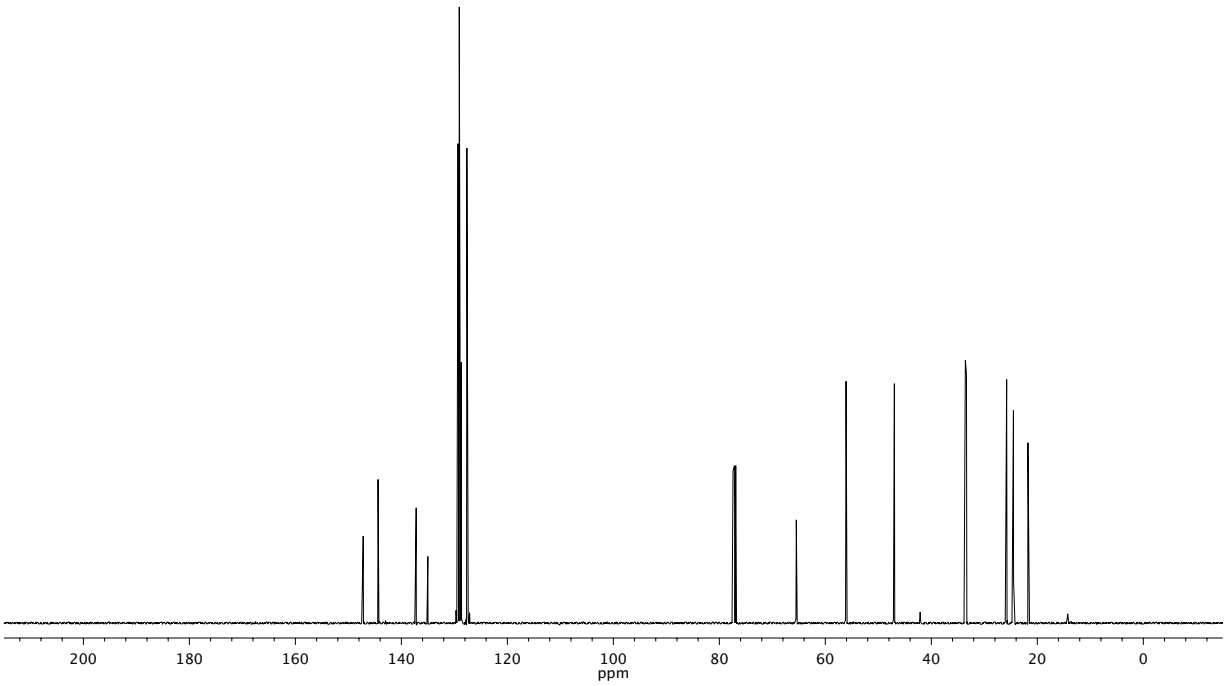
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2k**.



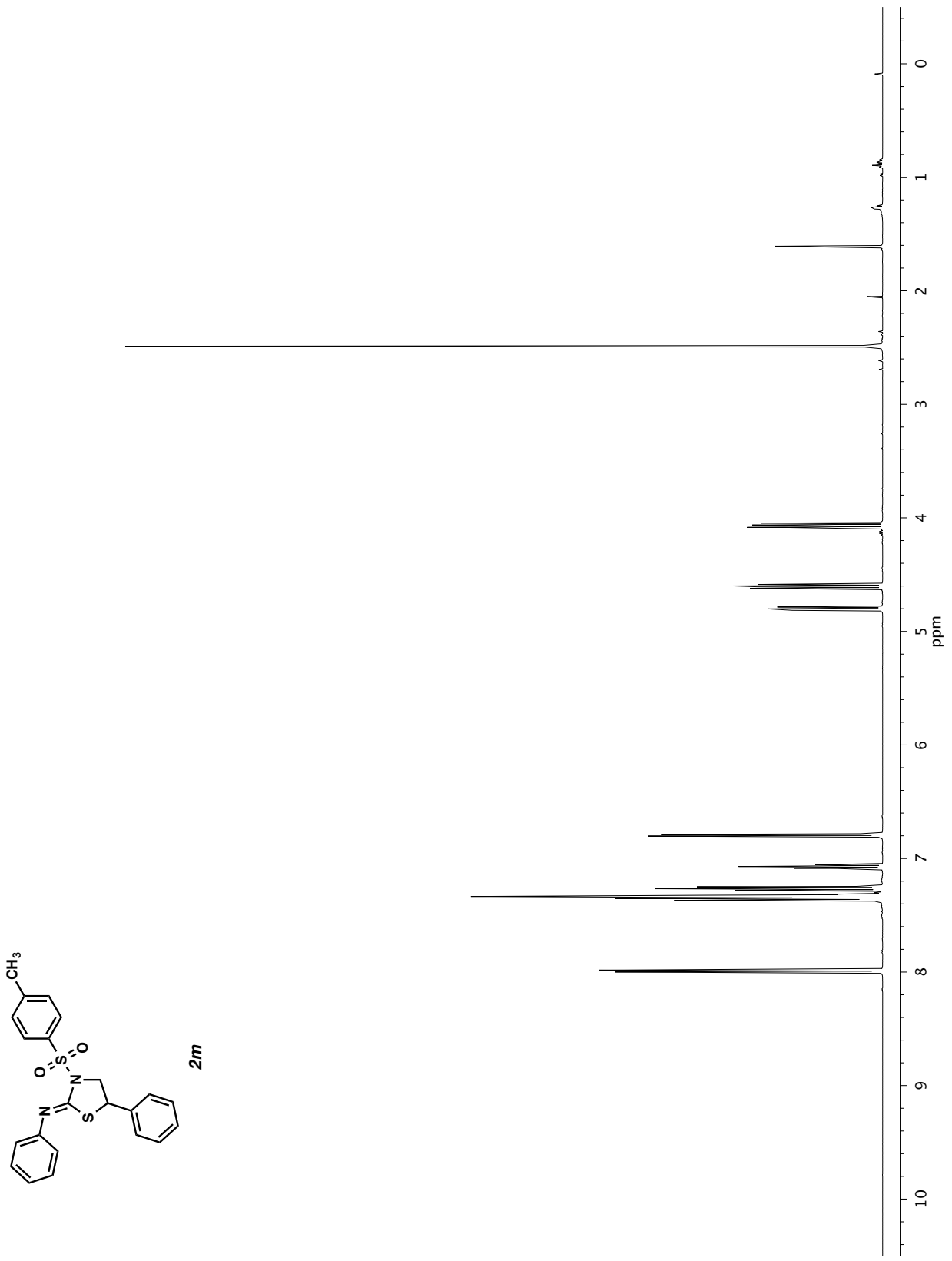
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2l**.



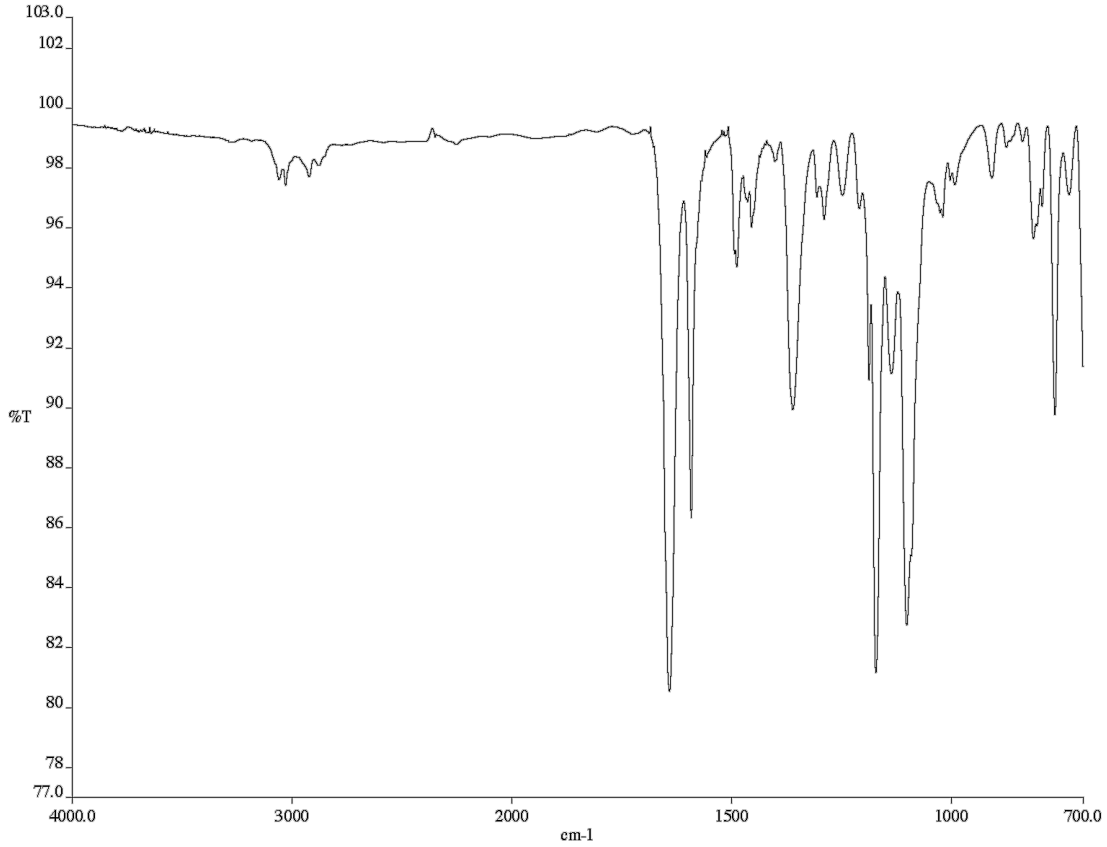
Infrared spectrum (Thin Film, NaCl) of compound **2l**.



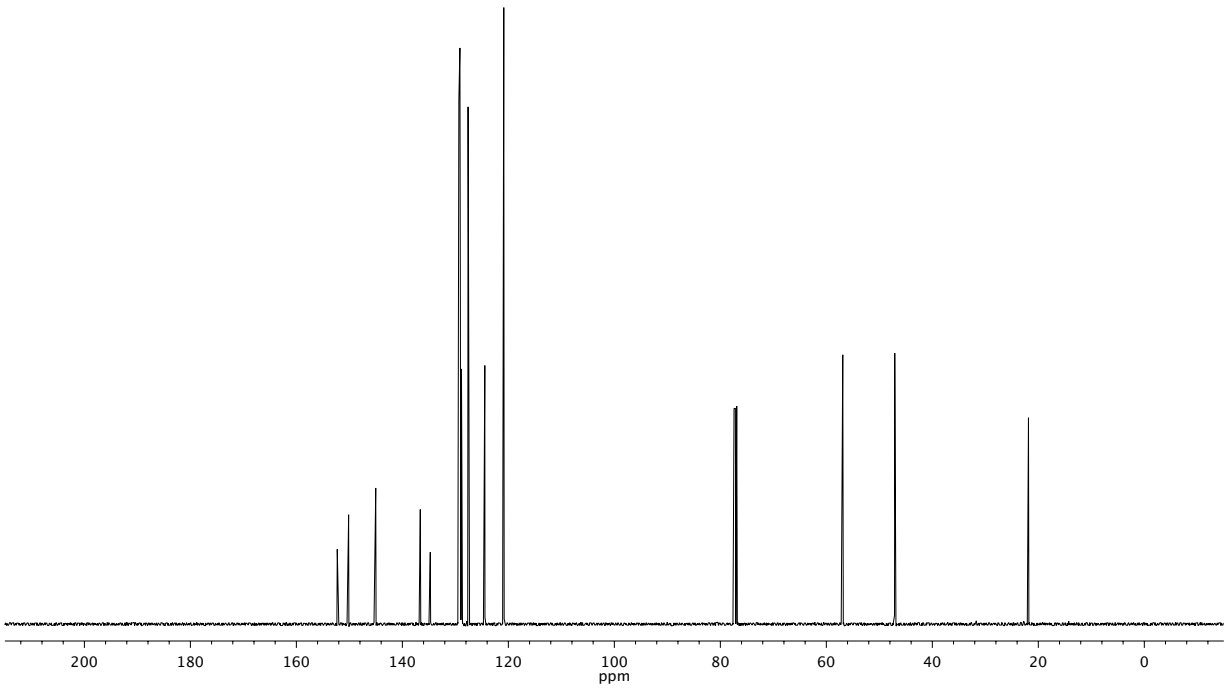
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2l**.



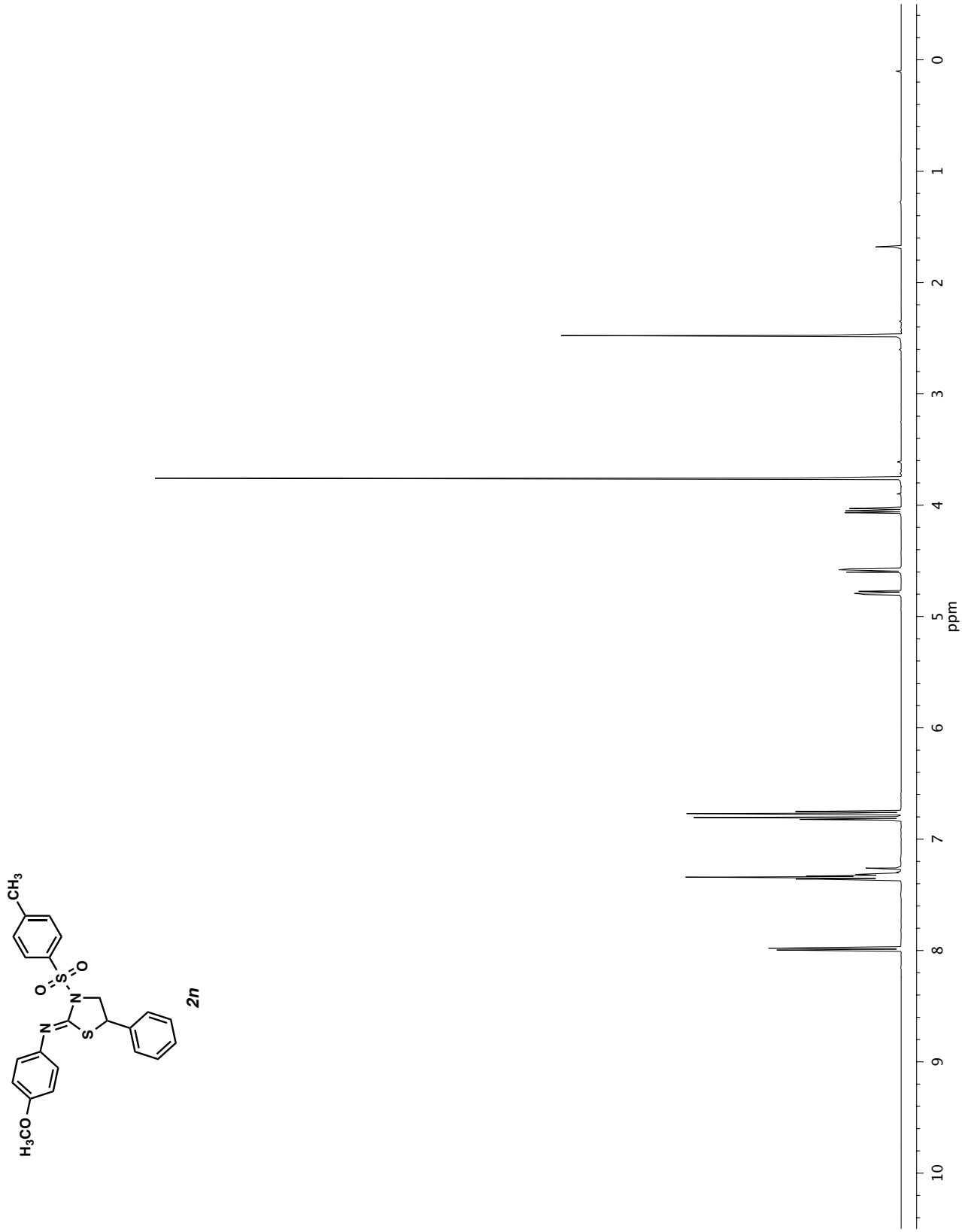
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2m**.



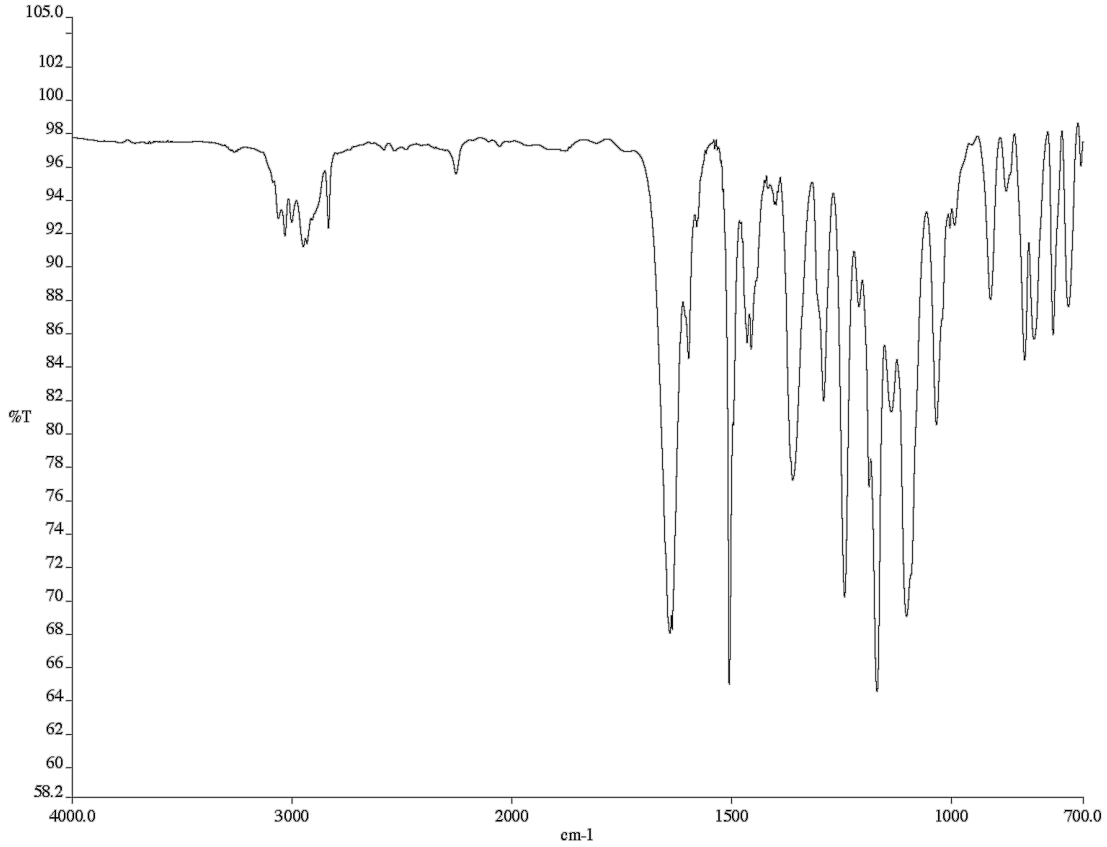
Infrared spectrum (Thin Film, NaCl) of compound **2m**.



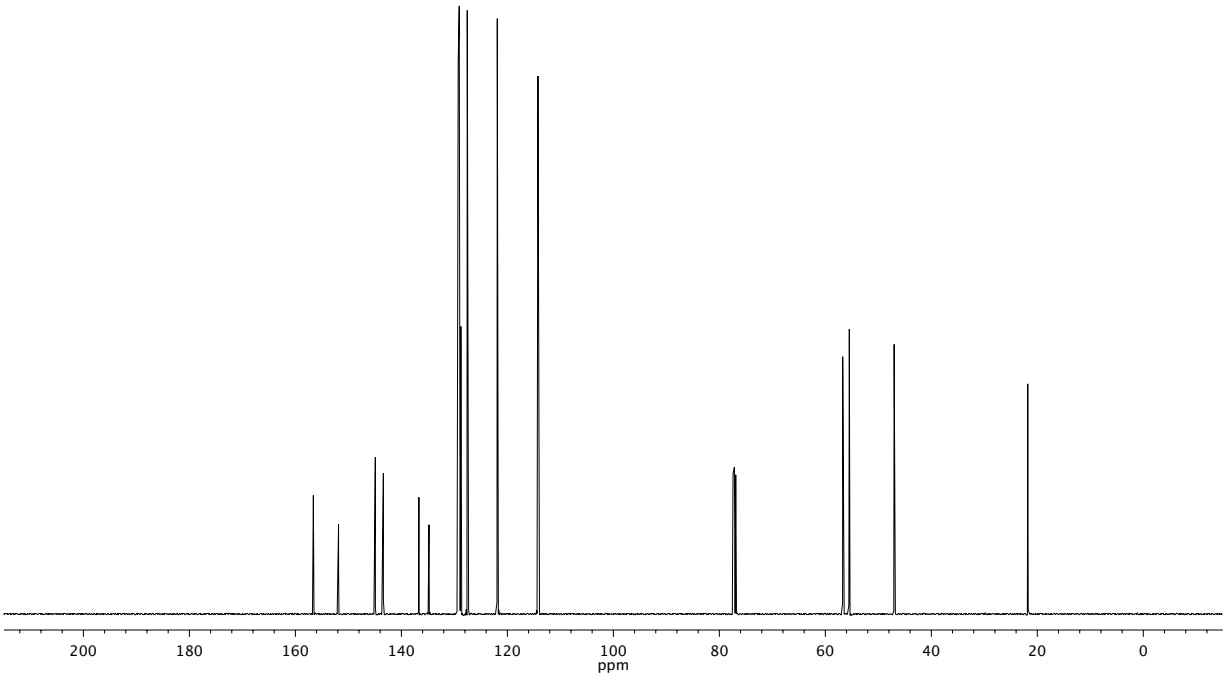
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2m**.



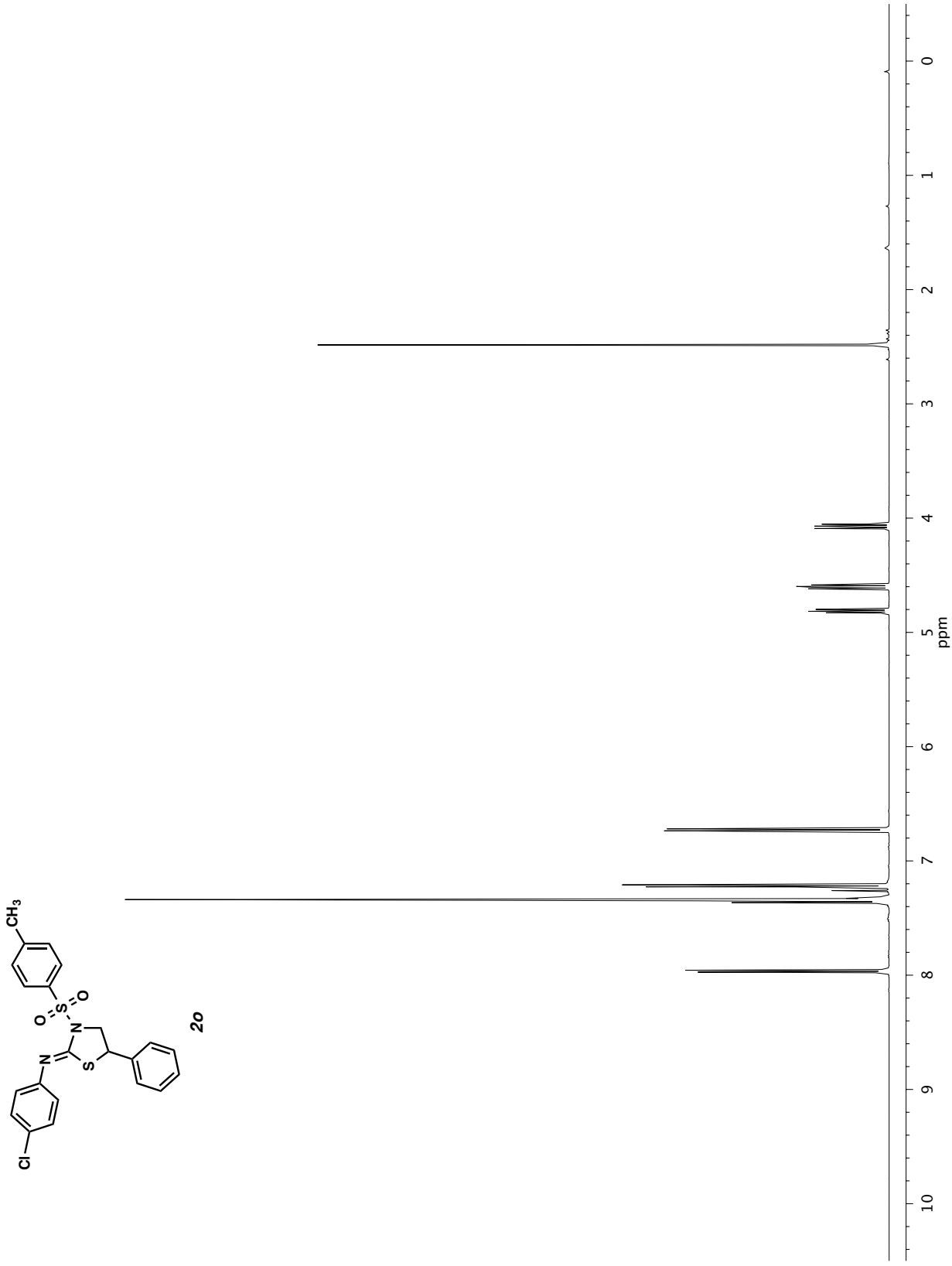
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2n**.



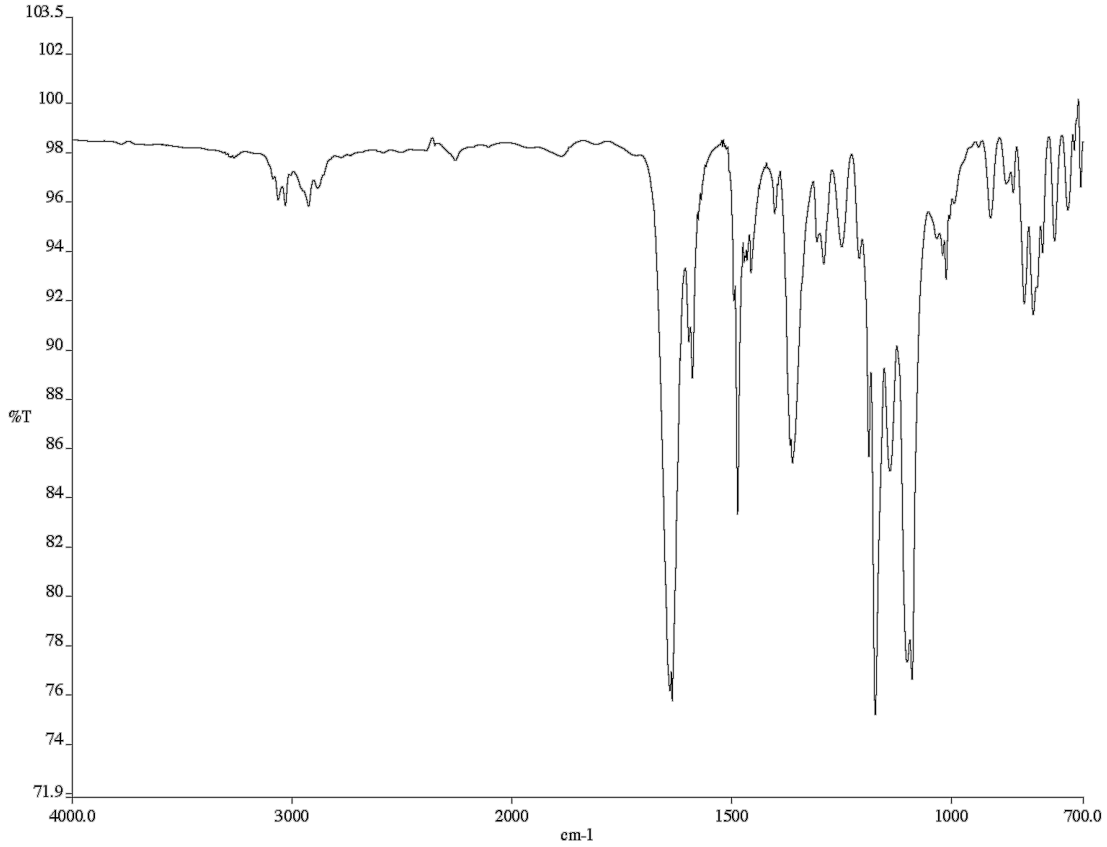
Infrared spectrum (Thin Film, NaCl) of compound **2n**.



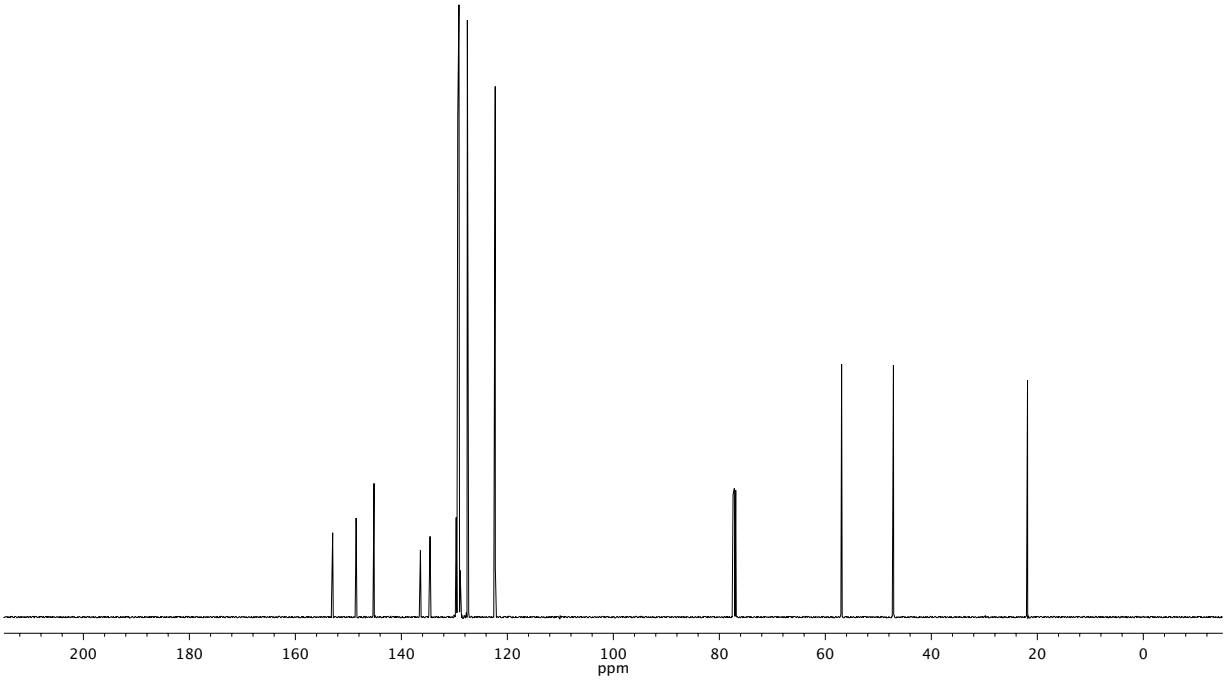
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2n**.



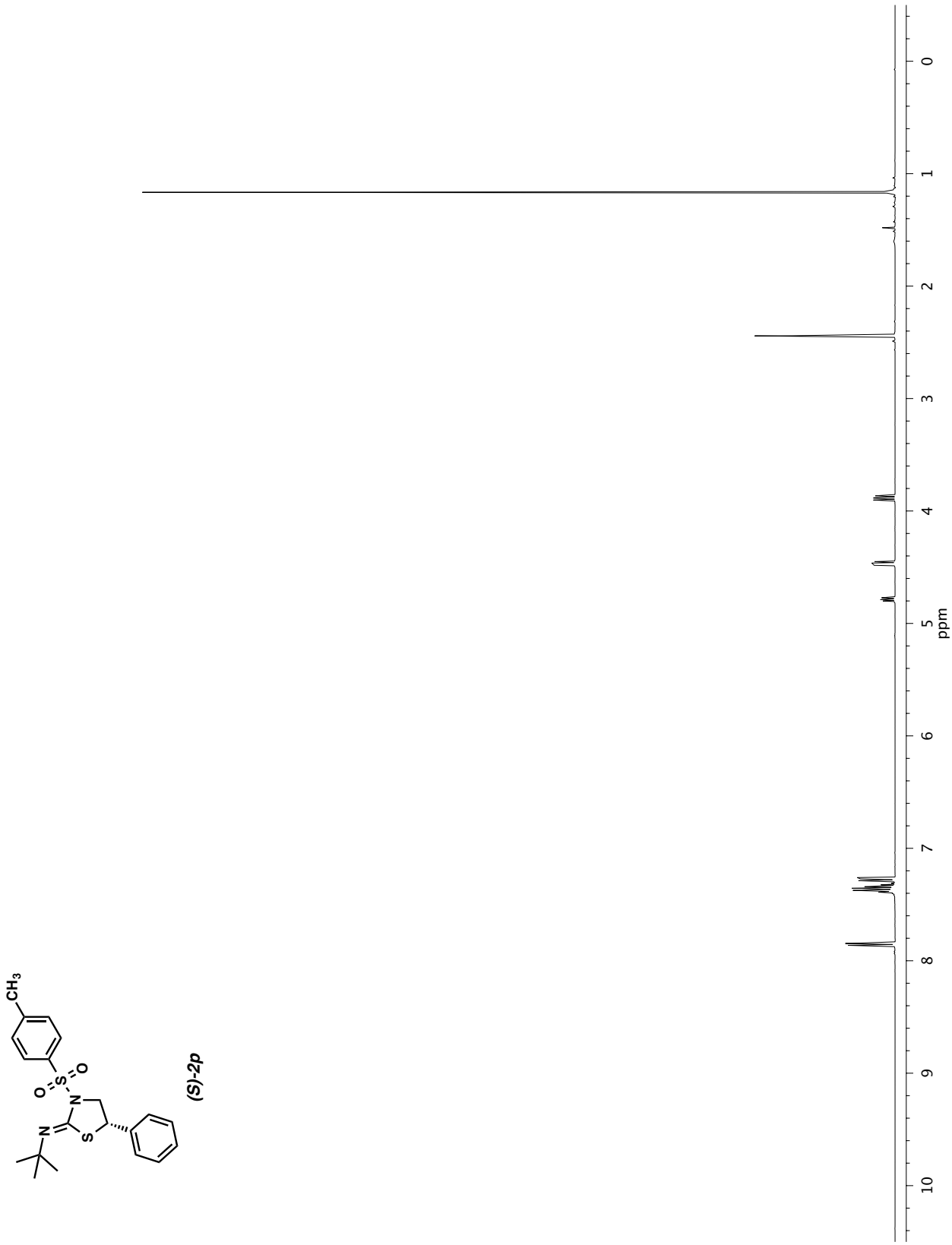
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2o**.



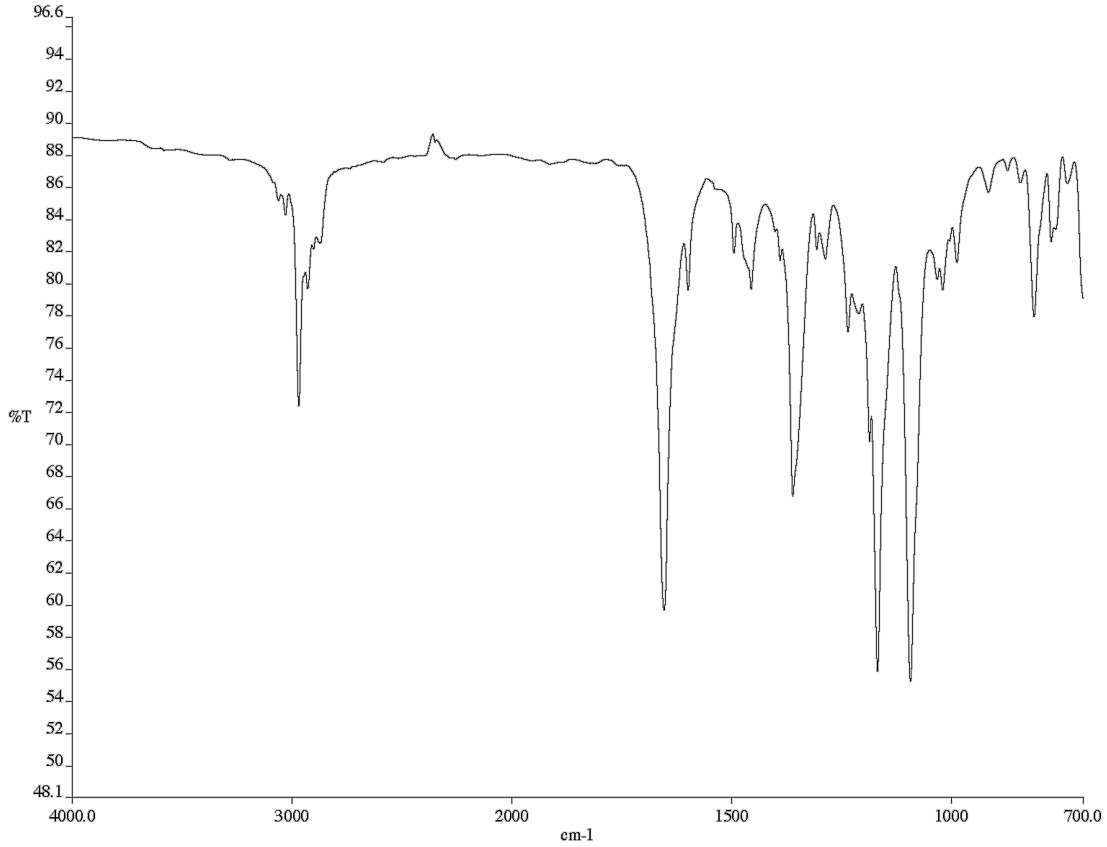
Infrared spectrum (Thin Film, NaCl) of compound **2o**.



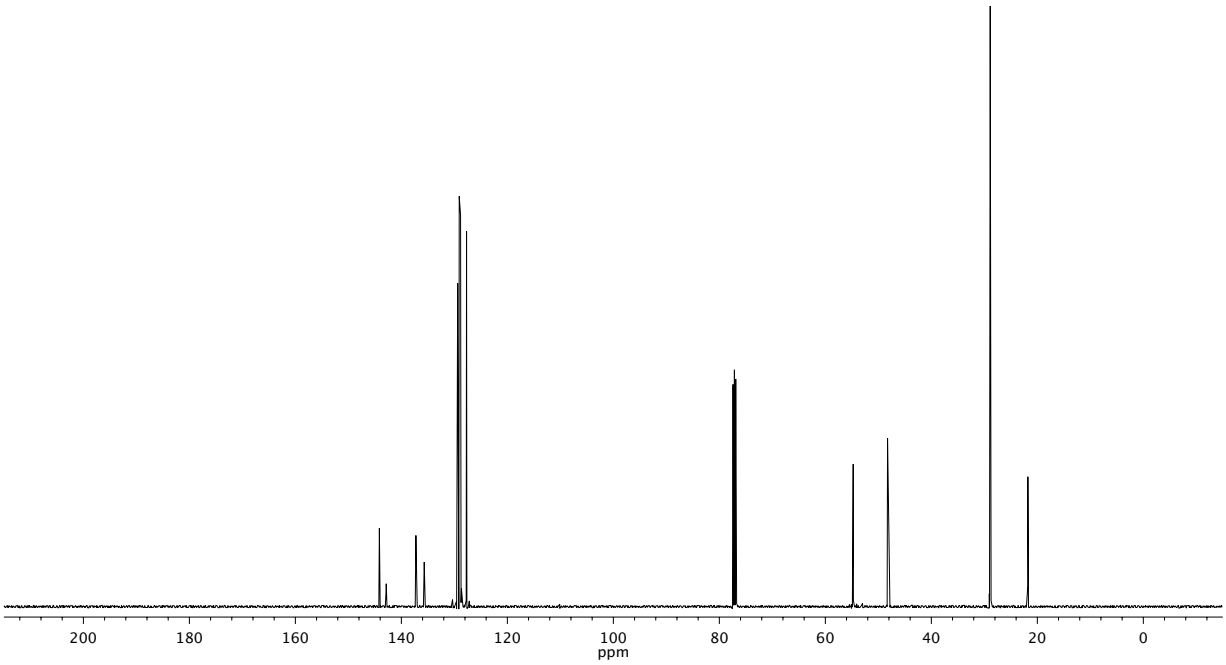
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2o**.



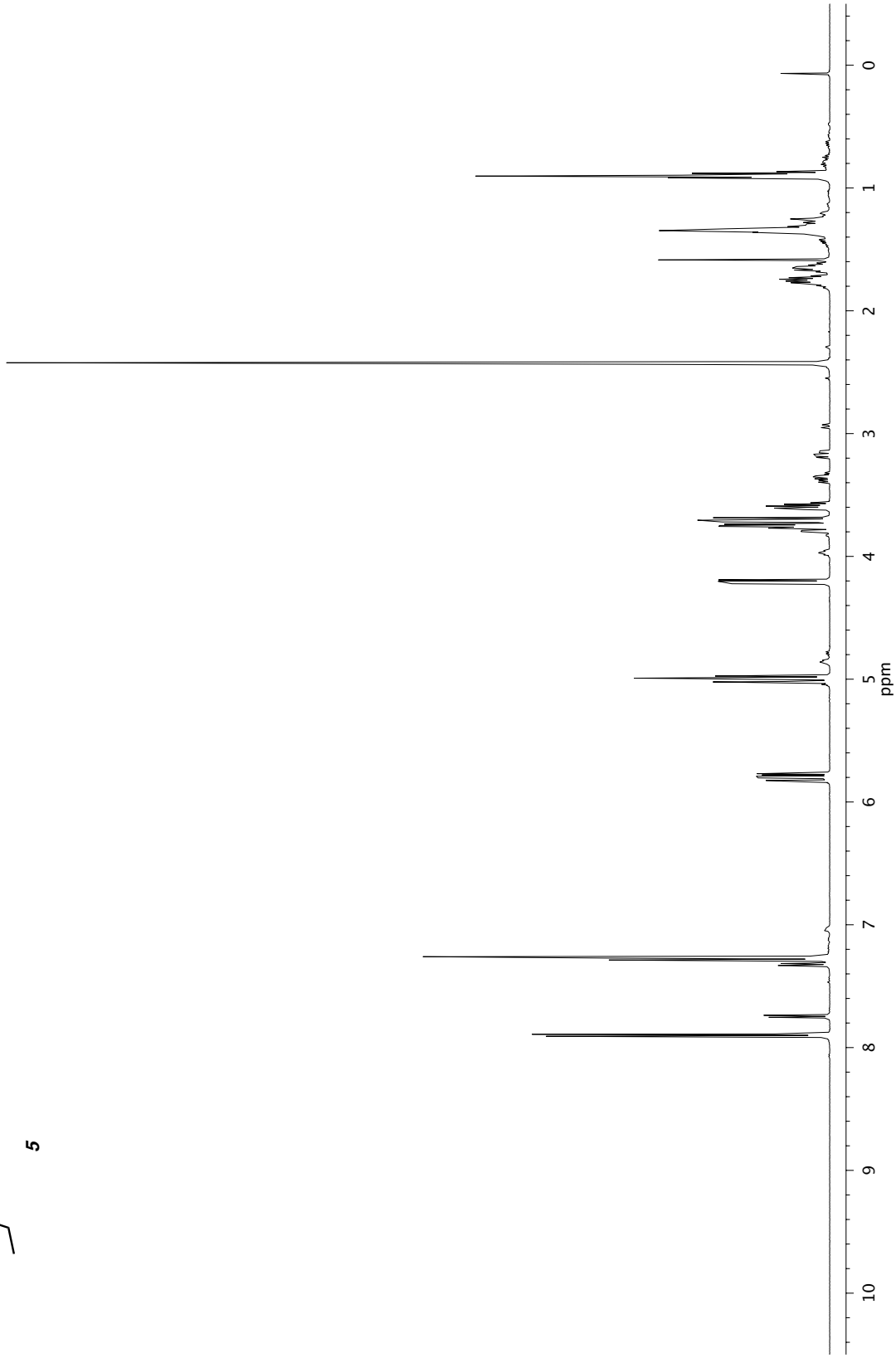
^{1}H NMR (500 MHz, $CDCl_3$) of compound **(*S*)-2p**.



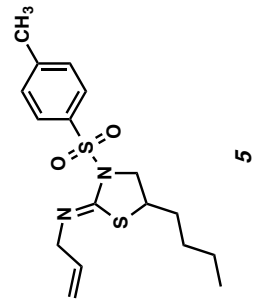
Infrared spectrum (Thin Film, NaCl) of compound **(*S*)-2p**.



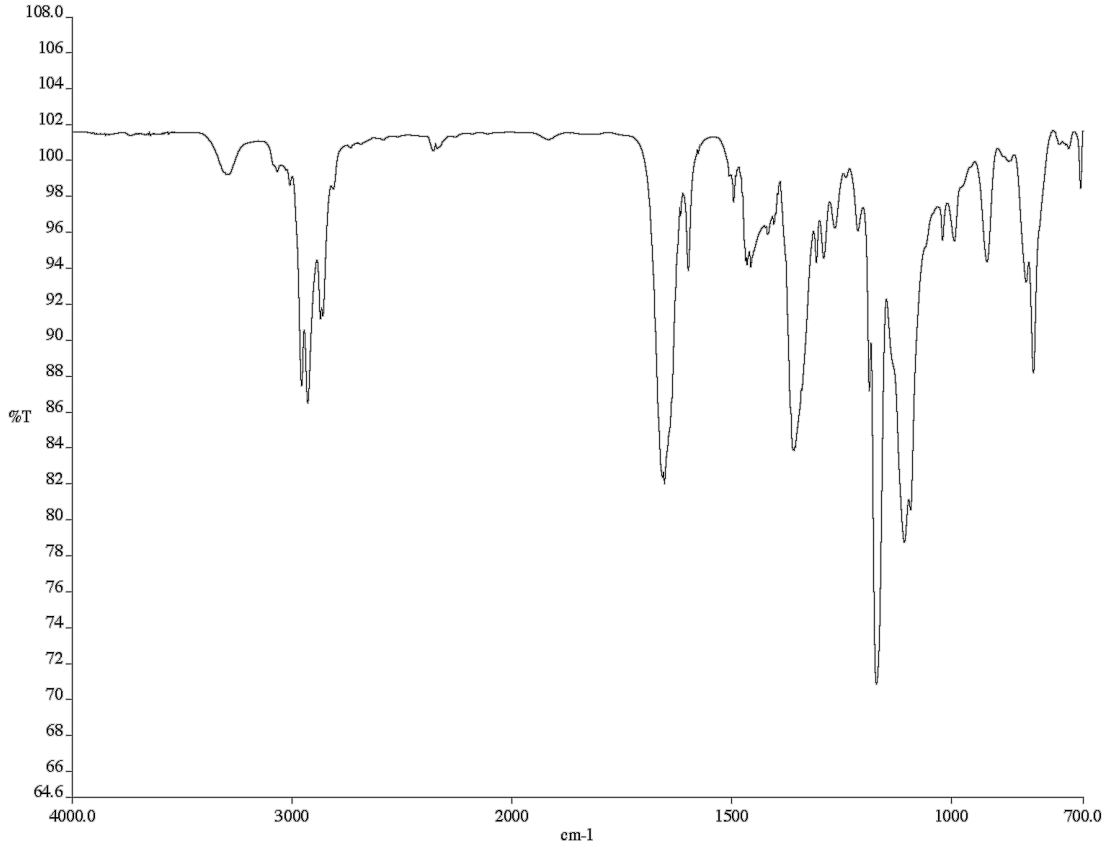
^{13}C NMR (126 MHz, $CDCl_3$) of compound **(*S*)-2p**.



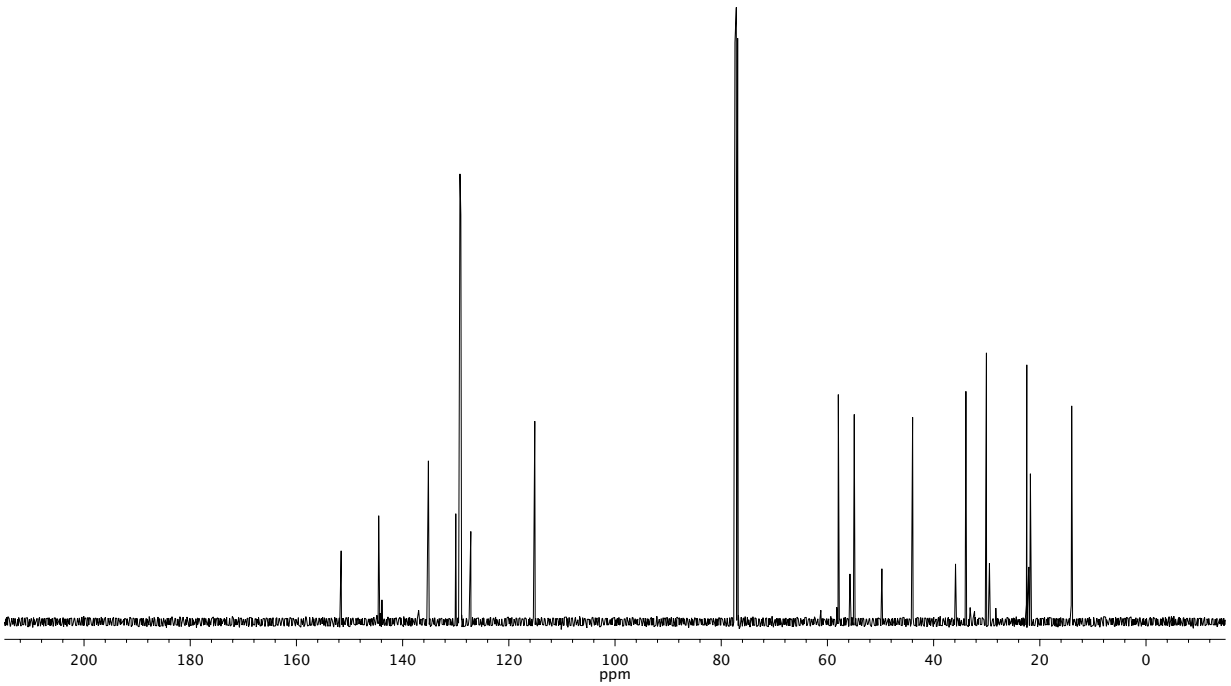
^{1}H NMR (500 MHz, $CDCl_3$) of compound **5**.



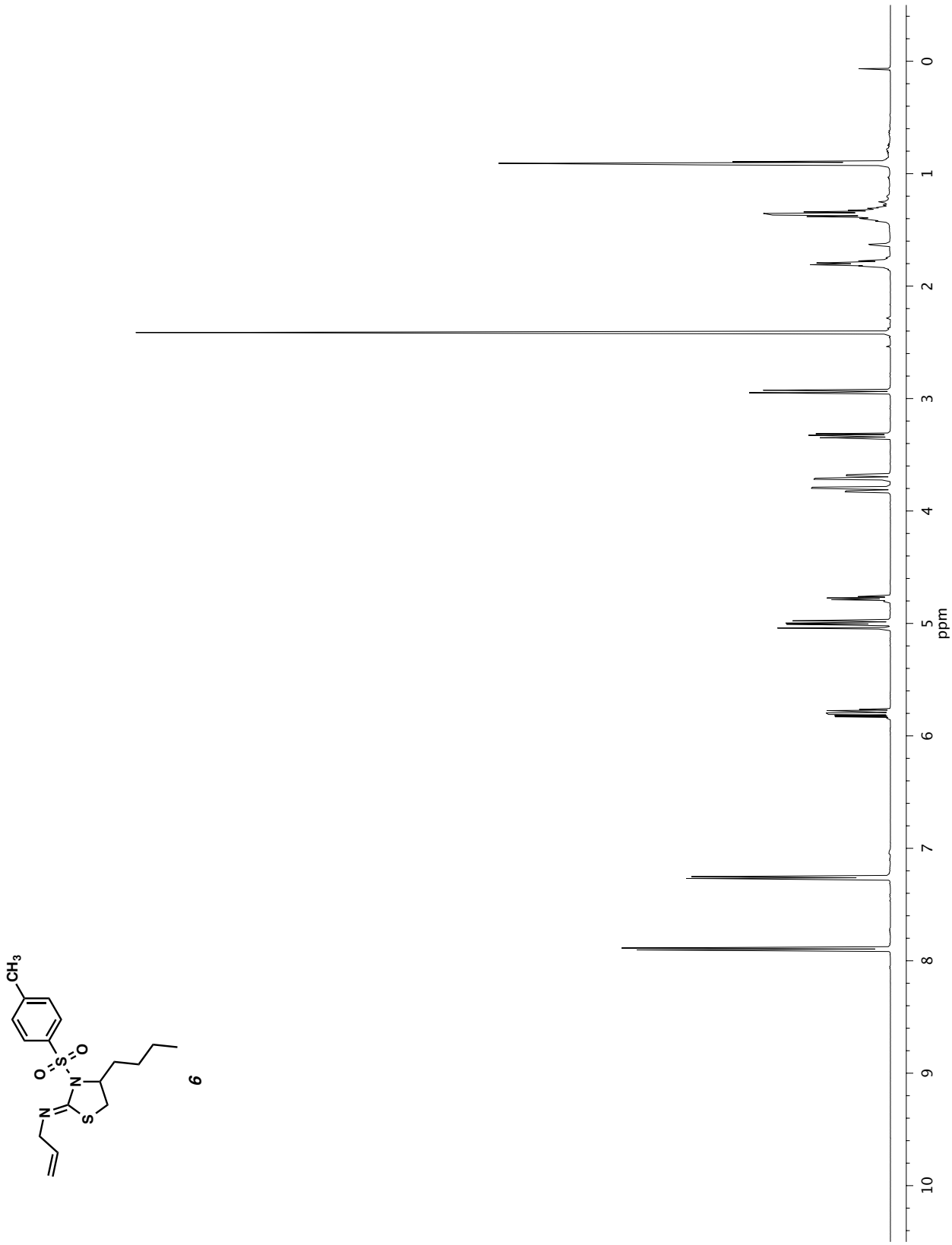
5



Infrared spectrum (Thin Film, NaCl) of compound **5**.

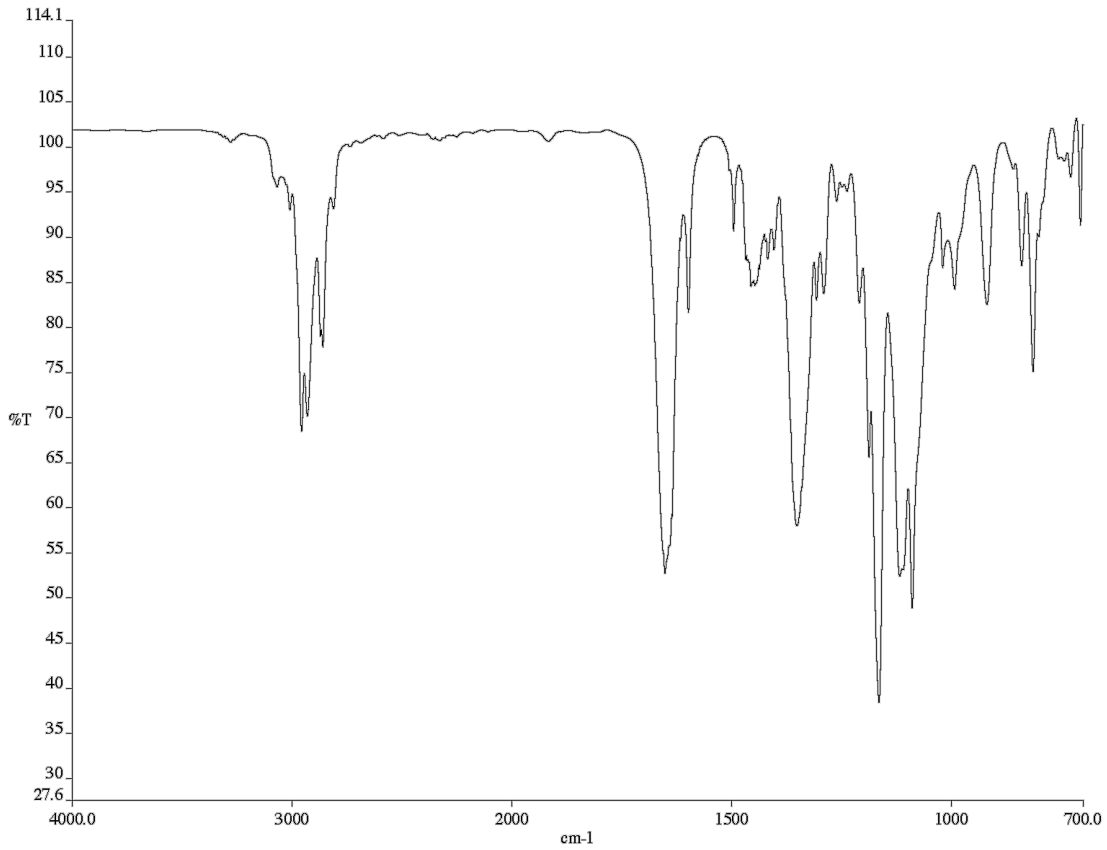


^{13}C NMR (126 MHz, $CDCl_3$) of compound **5**.

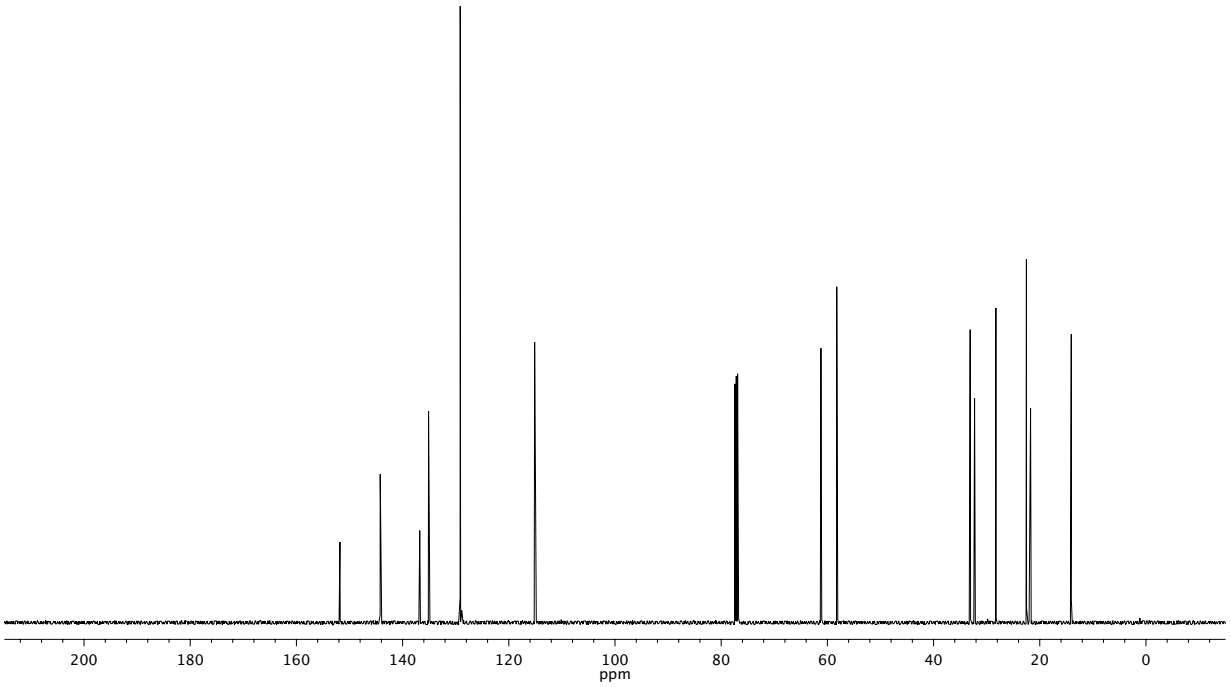


^{1}H NMR (500 MHz, $CDCl_3$) of compound **6**.

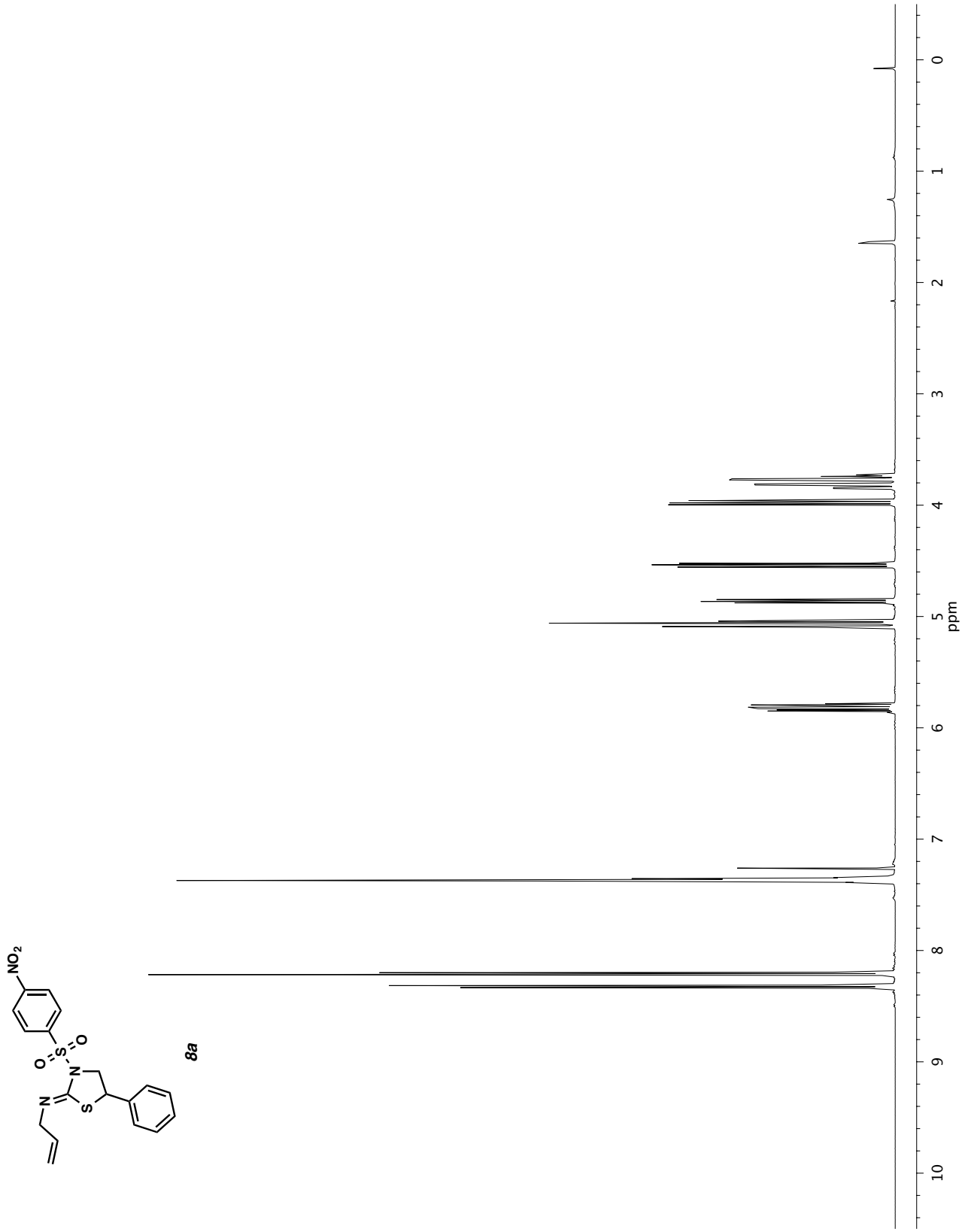
6



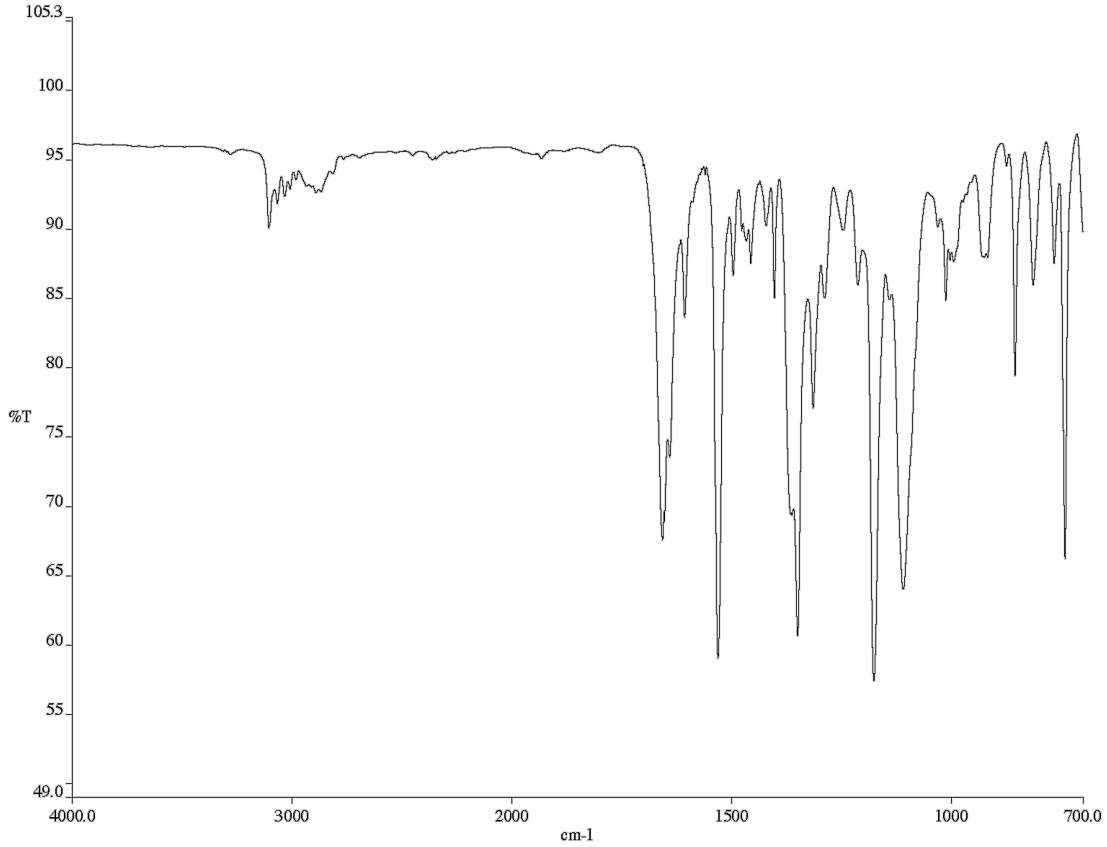
Infrared spectrum (Thin Film, NaCl) of compound **6**.



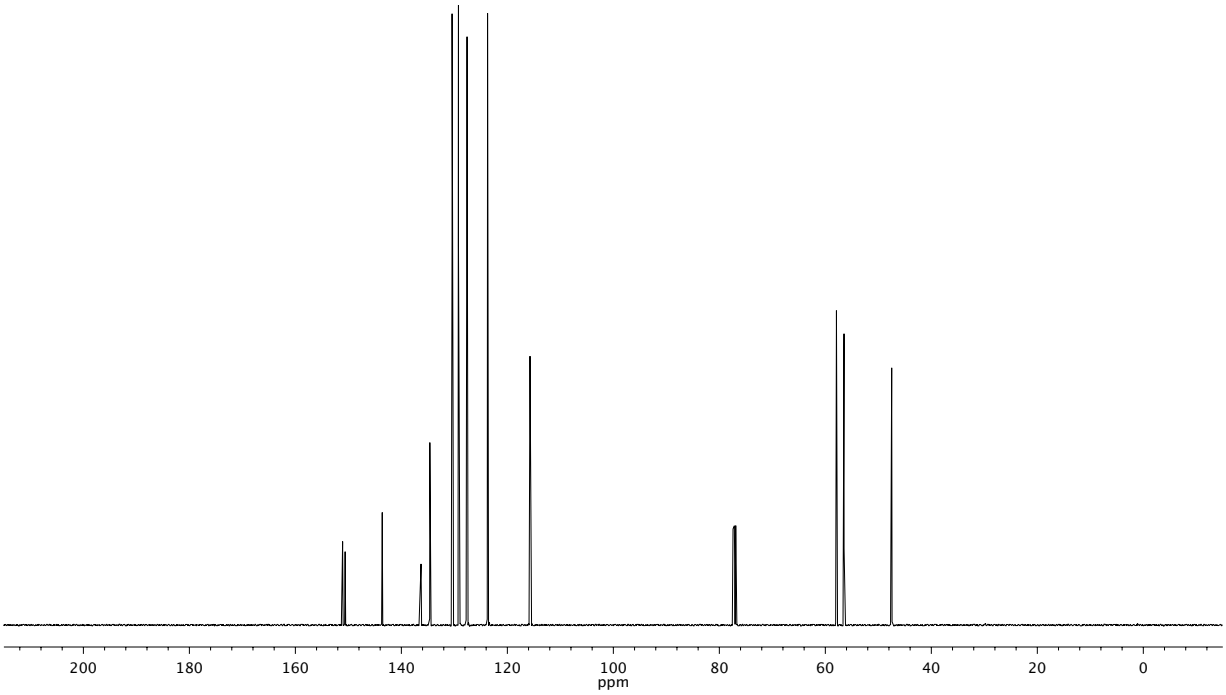
^{13}C NMR (126 MHz, $CDCl_3$) of compound **6**.



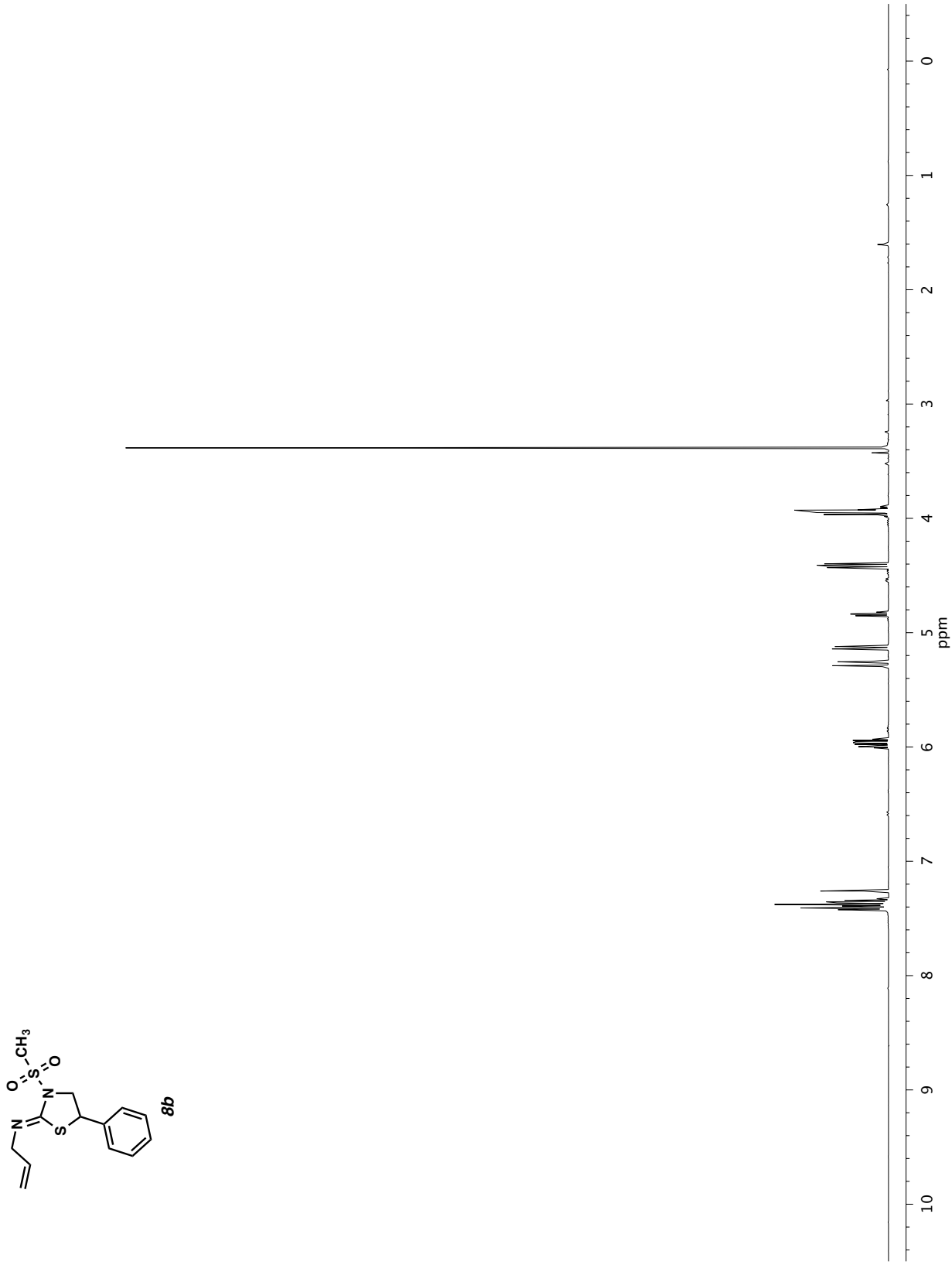
^{1}H NMR (500 MHz, $CDCl_3$) of compound **8a**.



Infrared spectrum (Thin Film, NaCl) of compound **8a**.

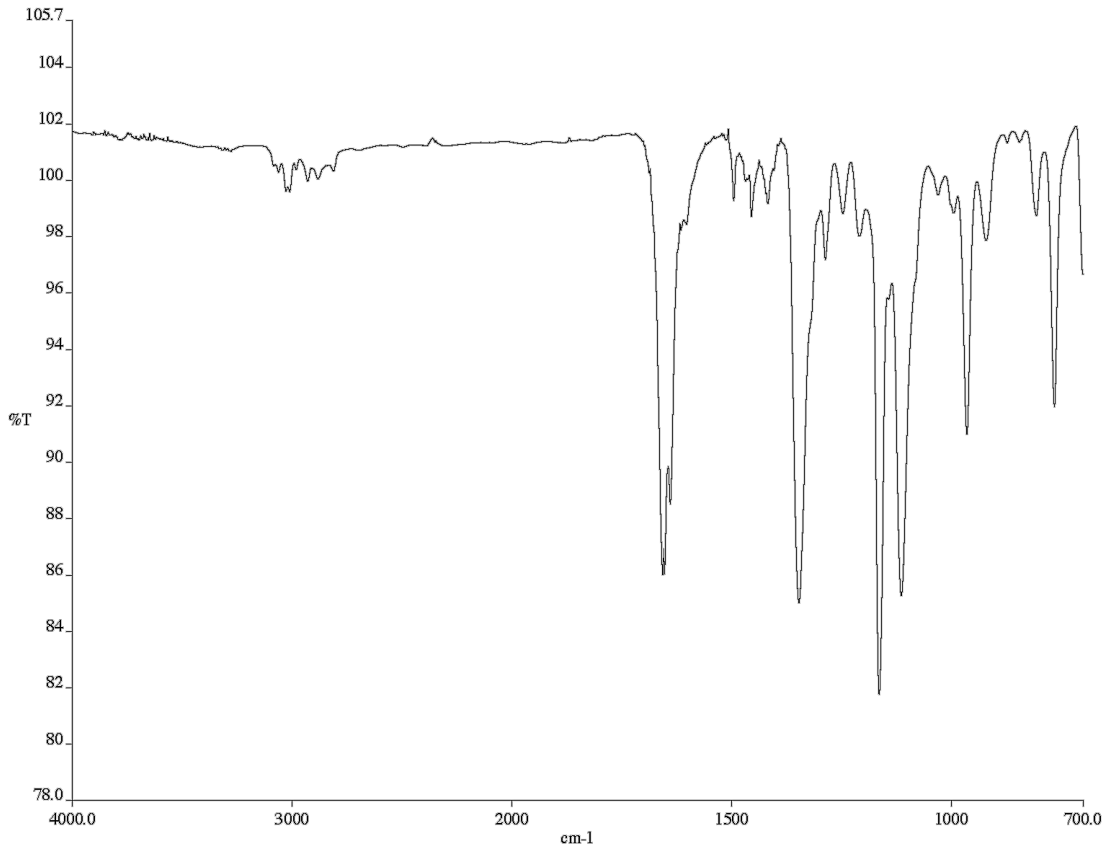


^{13}C NMR (126 MHz, $CDCl_3$) of compound **8a**.

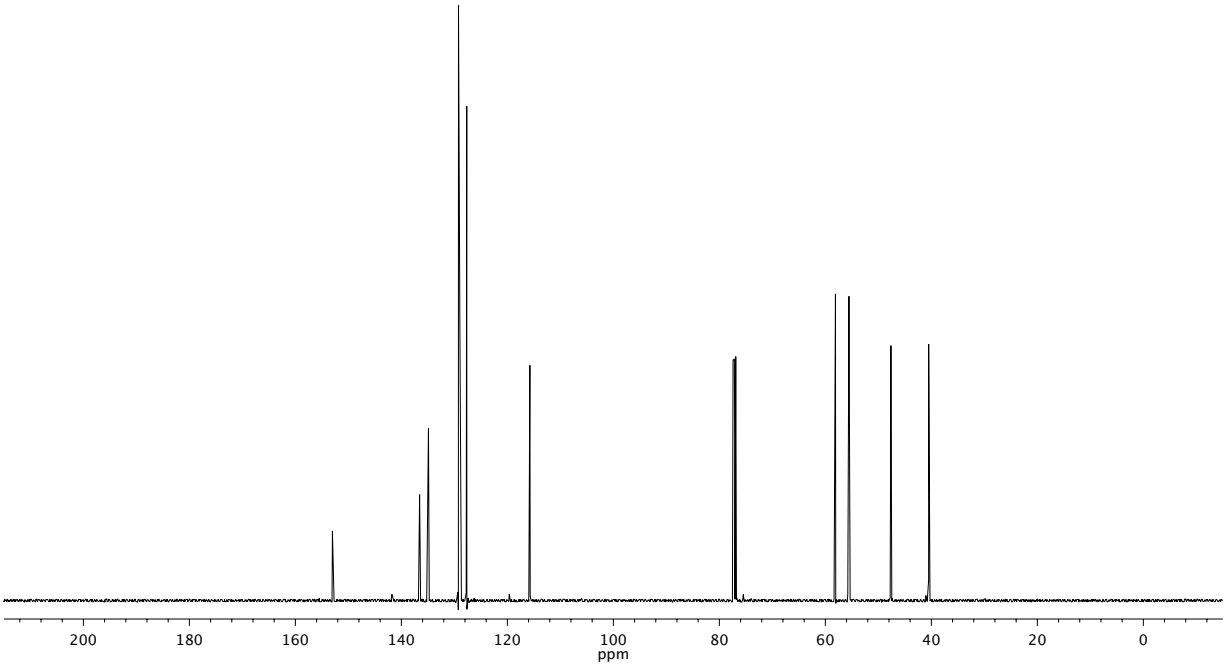


8b

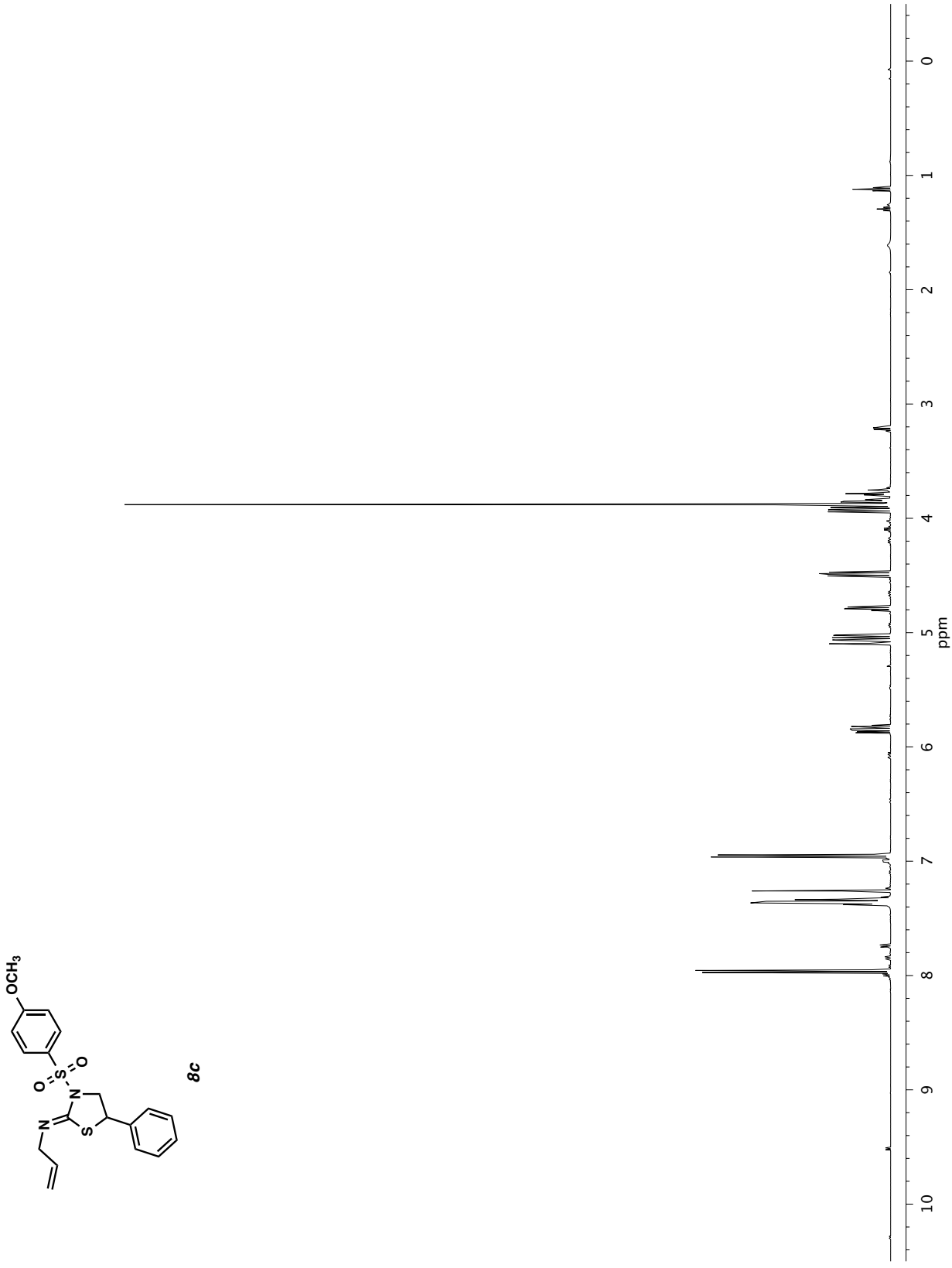
^{1}H NMR (500 MHz, $CDCl_3$) of compound **8b**.



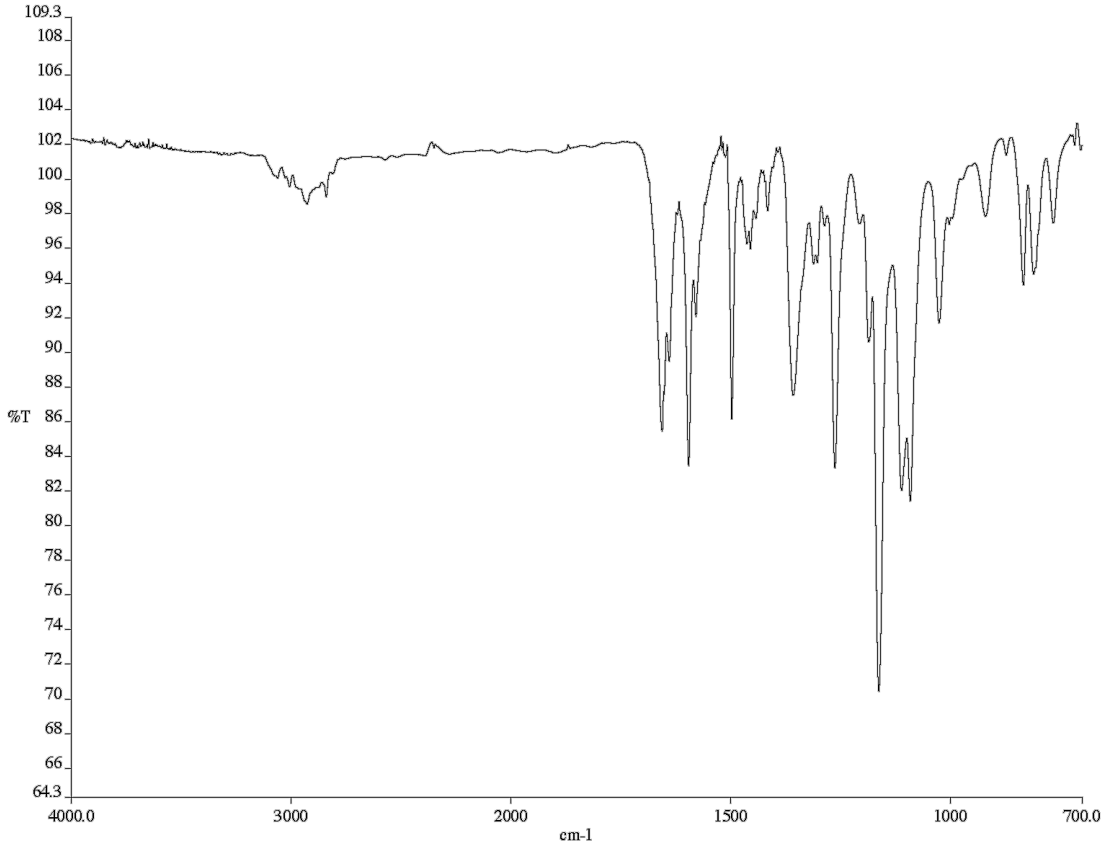
Infrared spectrum (Thin Film, NaCl) of compound **8b**.



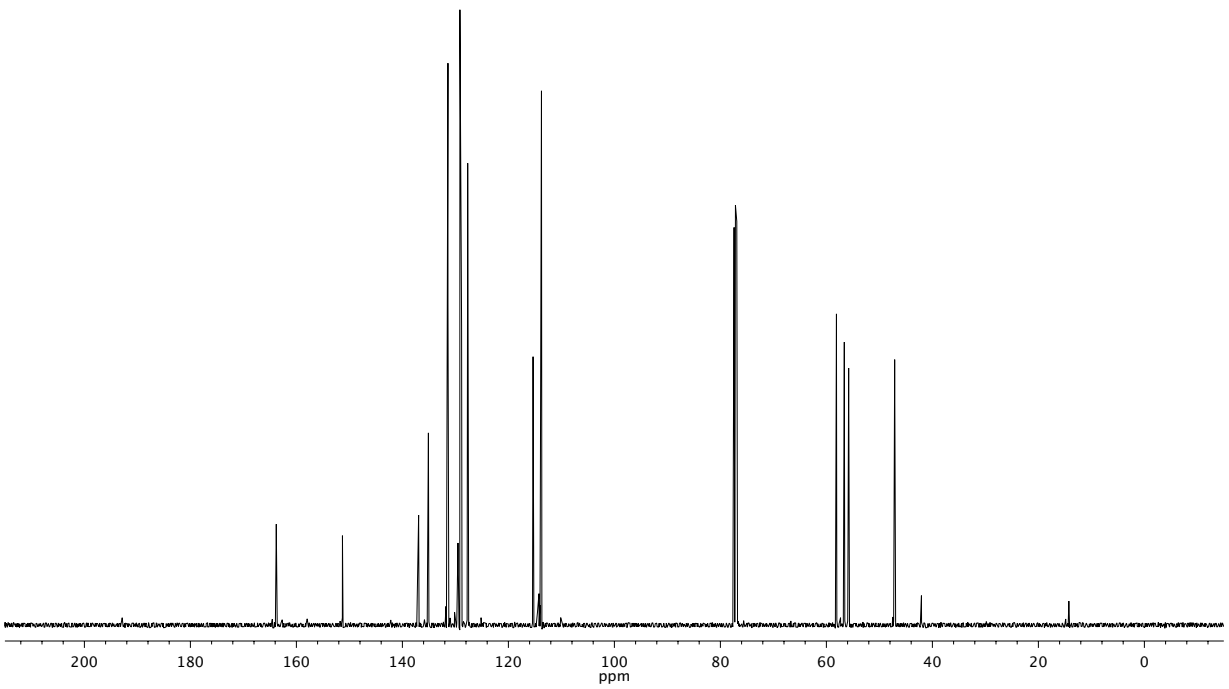
^{13}C NMR (126 MHz, $CDCl_3$) of compound **8b**.



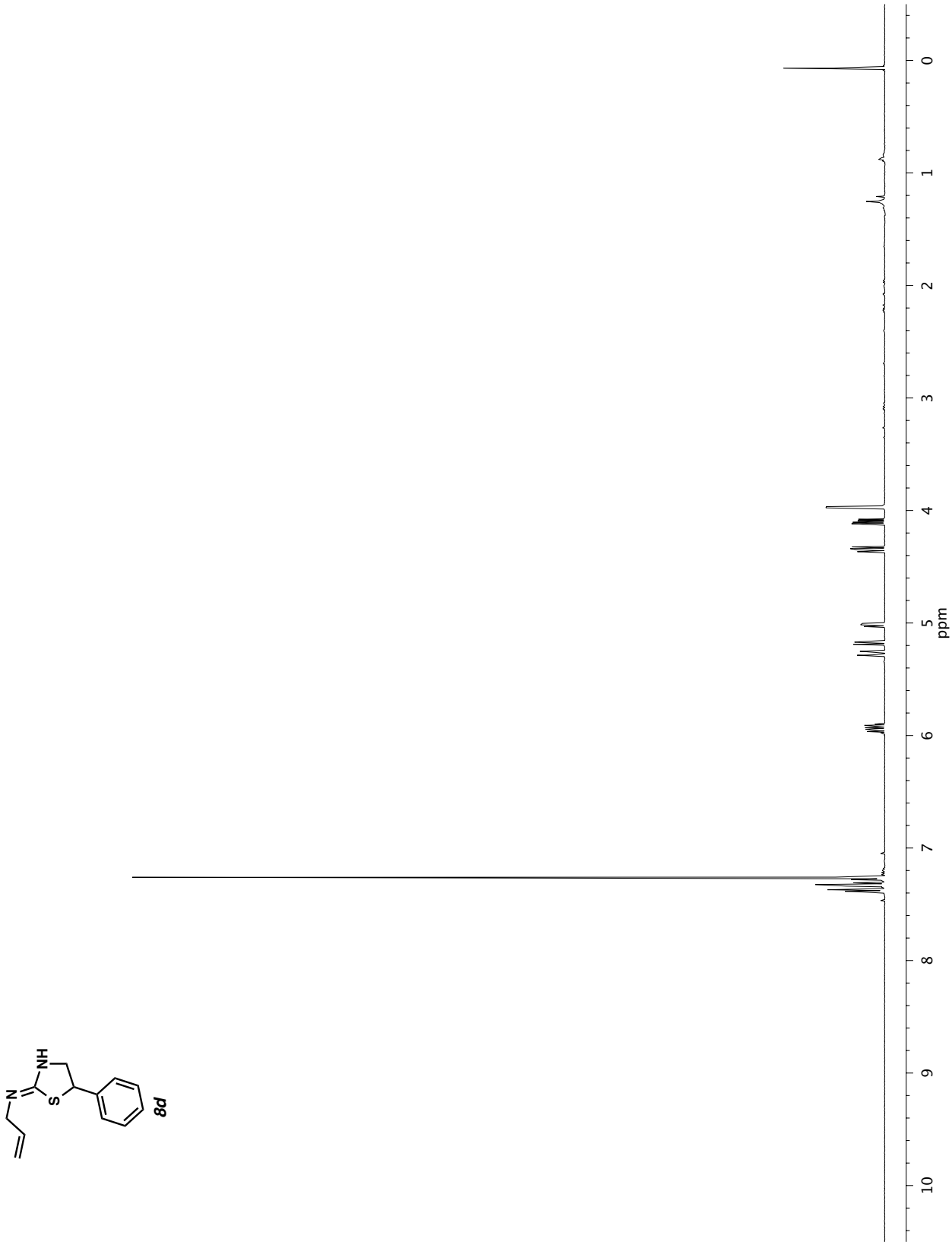
^{1}H NMR (500 MHz, $CDCl_3$) of compound **8c**.



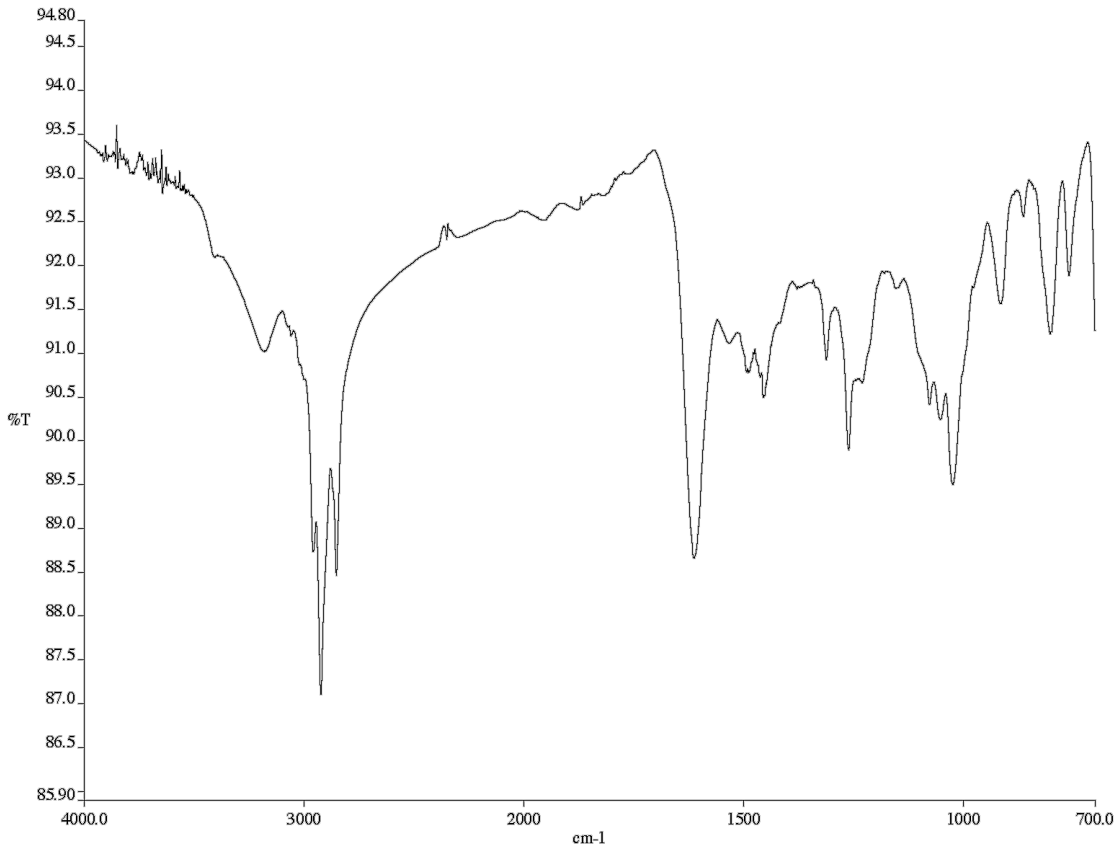
Infrared spectrum (Thin Film, NaCl) of compound **8c**.



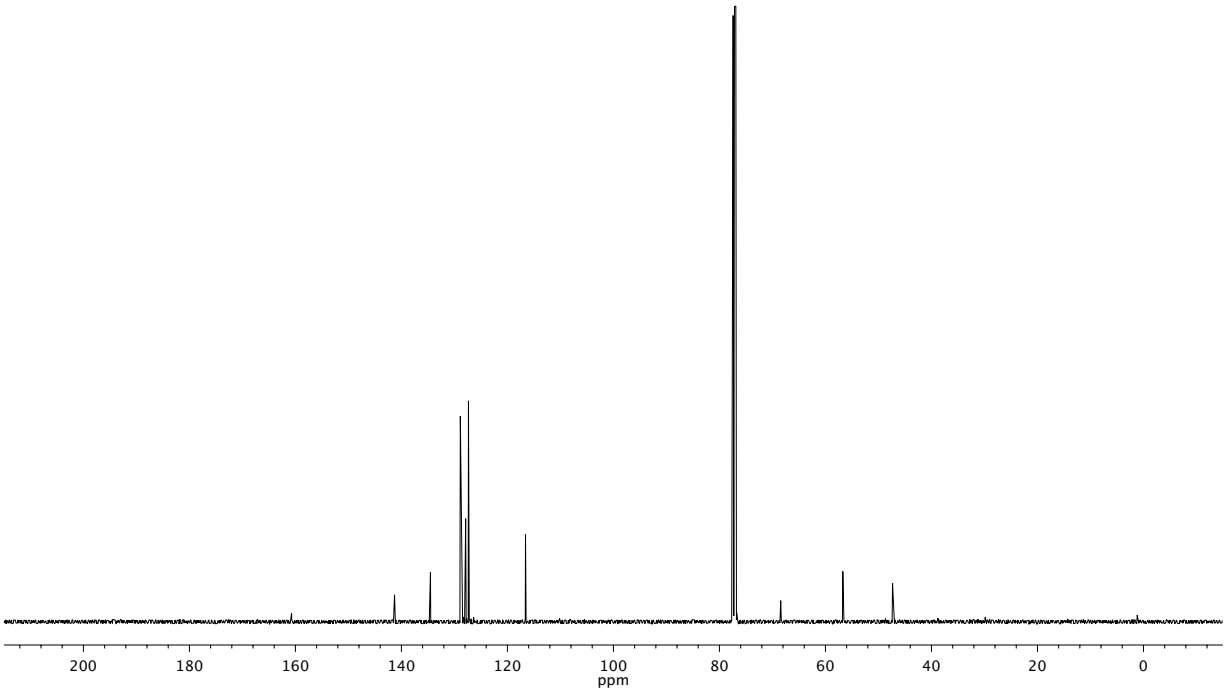
^{13}C NMR (126 MHz, $CDCl_3$) of compound **8c**.



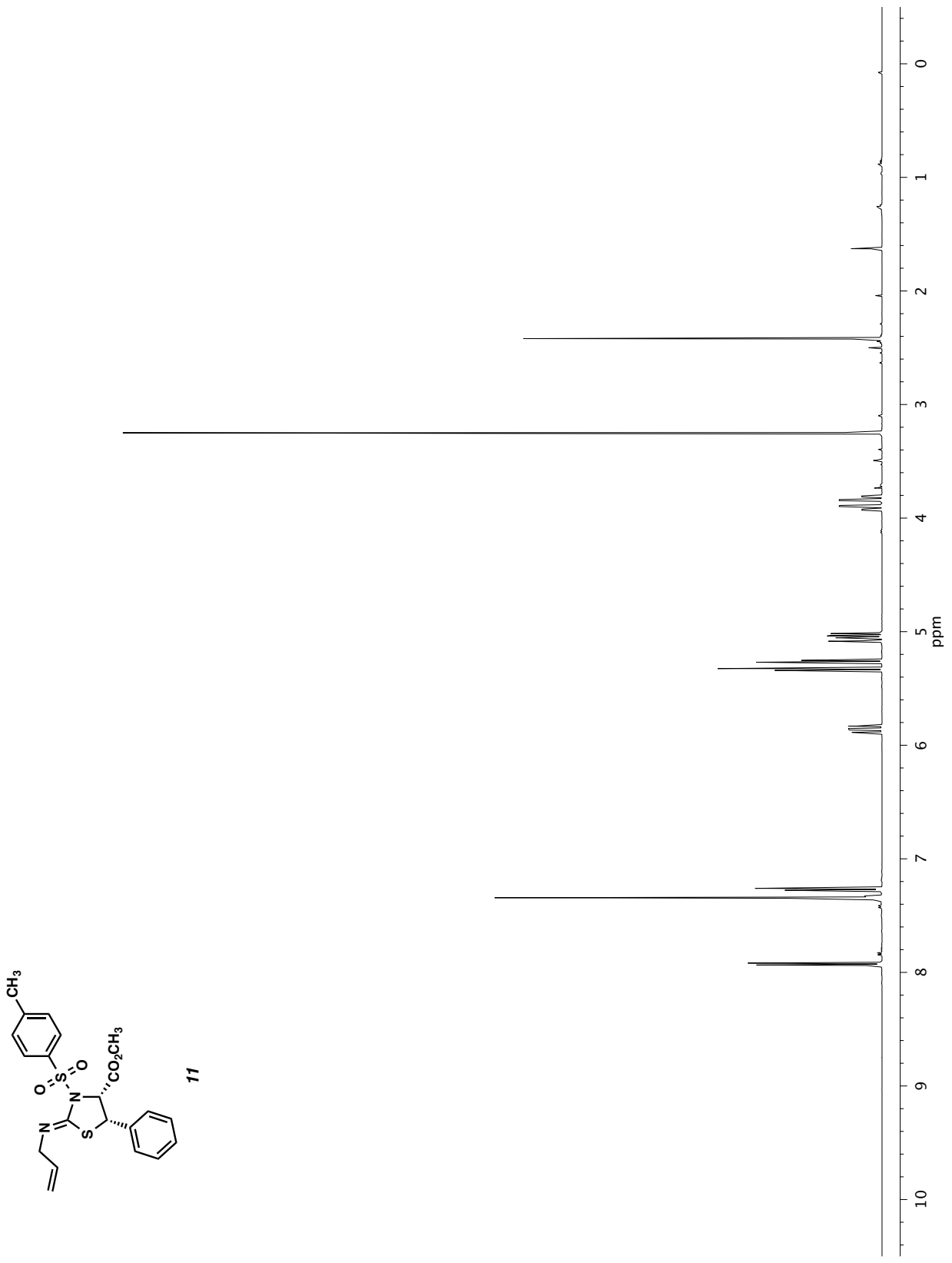
^{1}H NMR (500 MHz, $CDCl_3$) of compound **8d**.



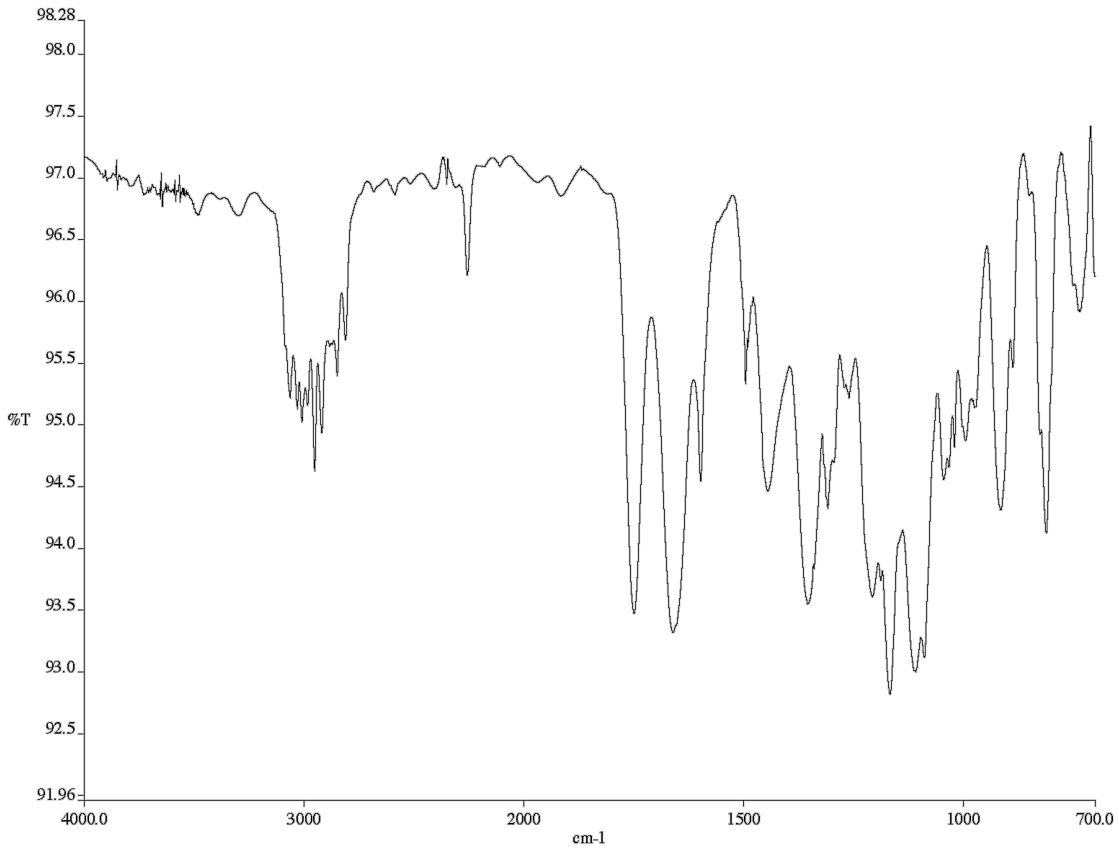
Infrared spectrum (Thin Film, NaCl) of compound **8d**.



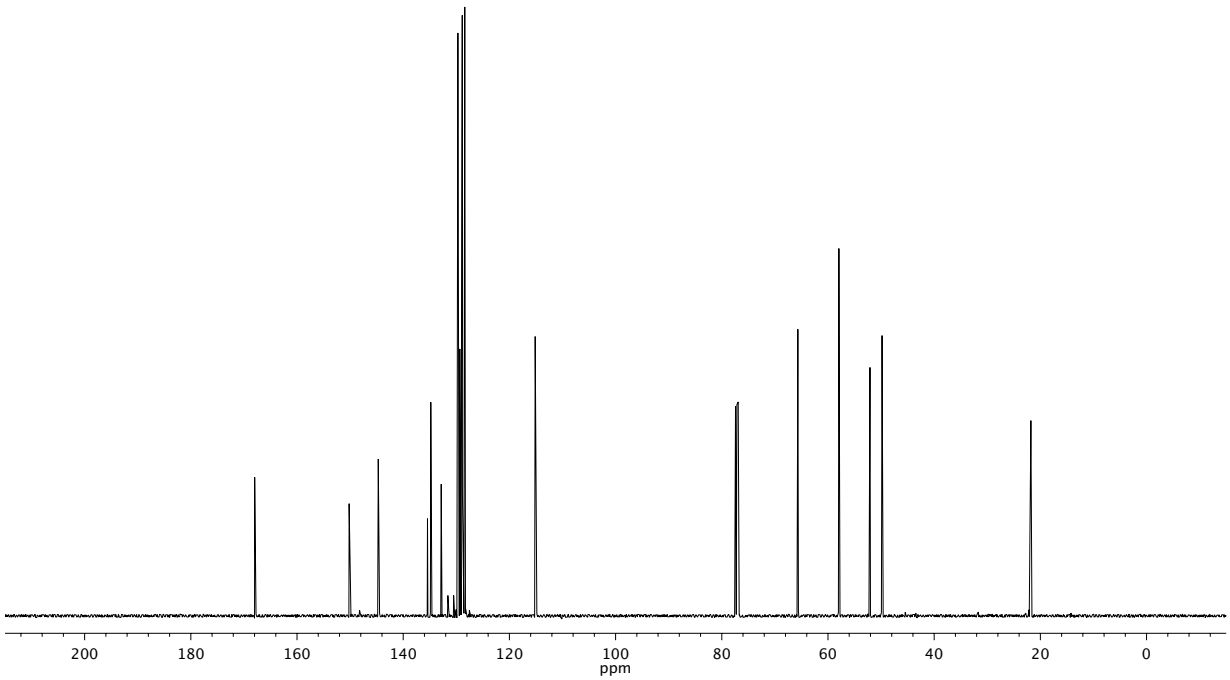
^{13}C NMR (126 MHz, $CDCl_3$) of compound **8d**.



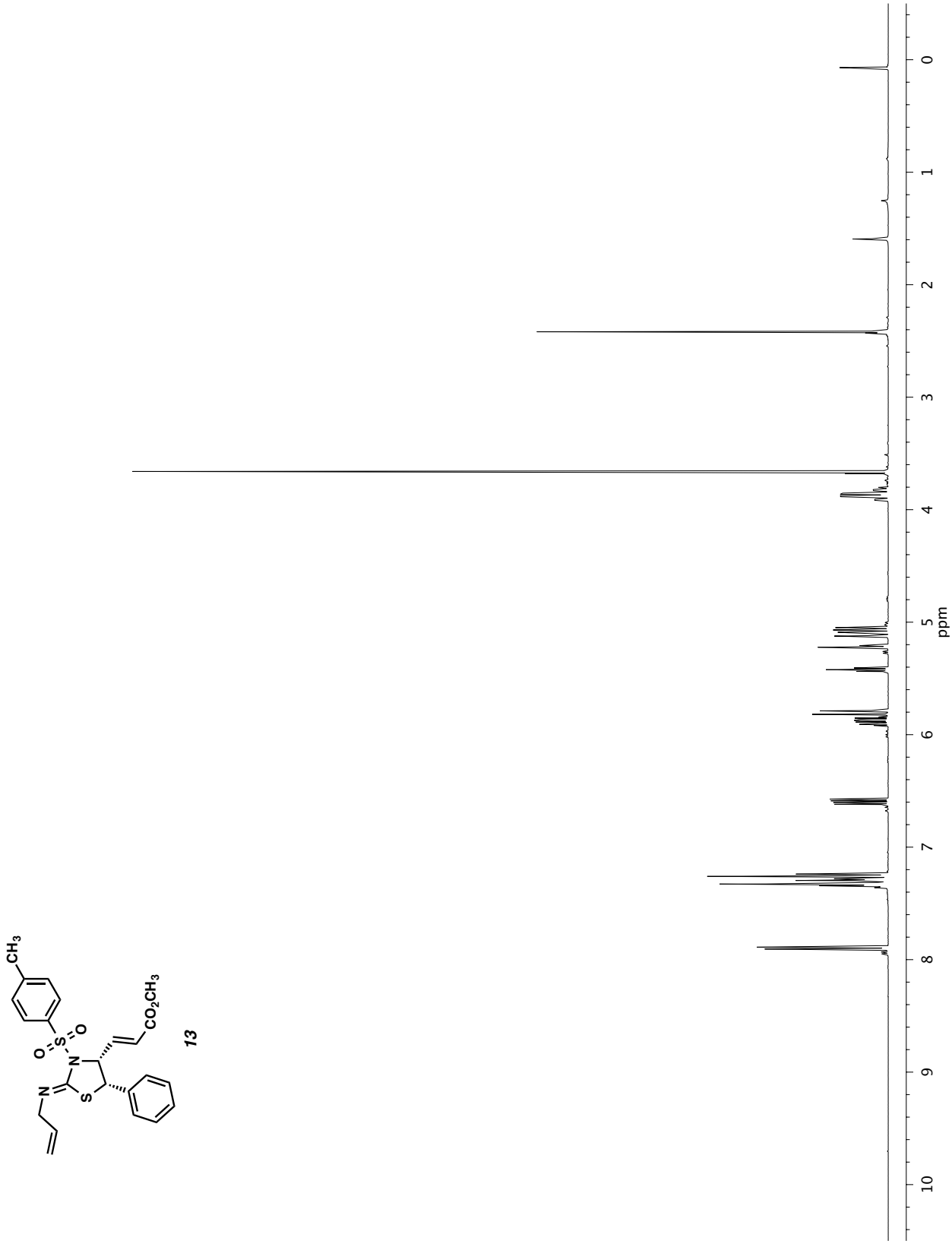
^{1}H NMR (500 MHz, $CDCl_3$) of compound **11**.



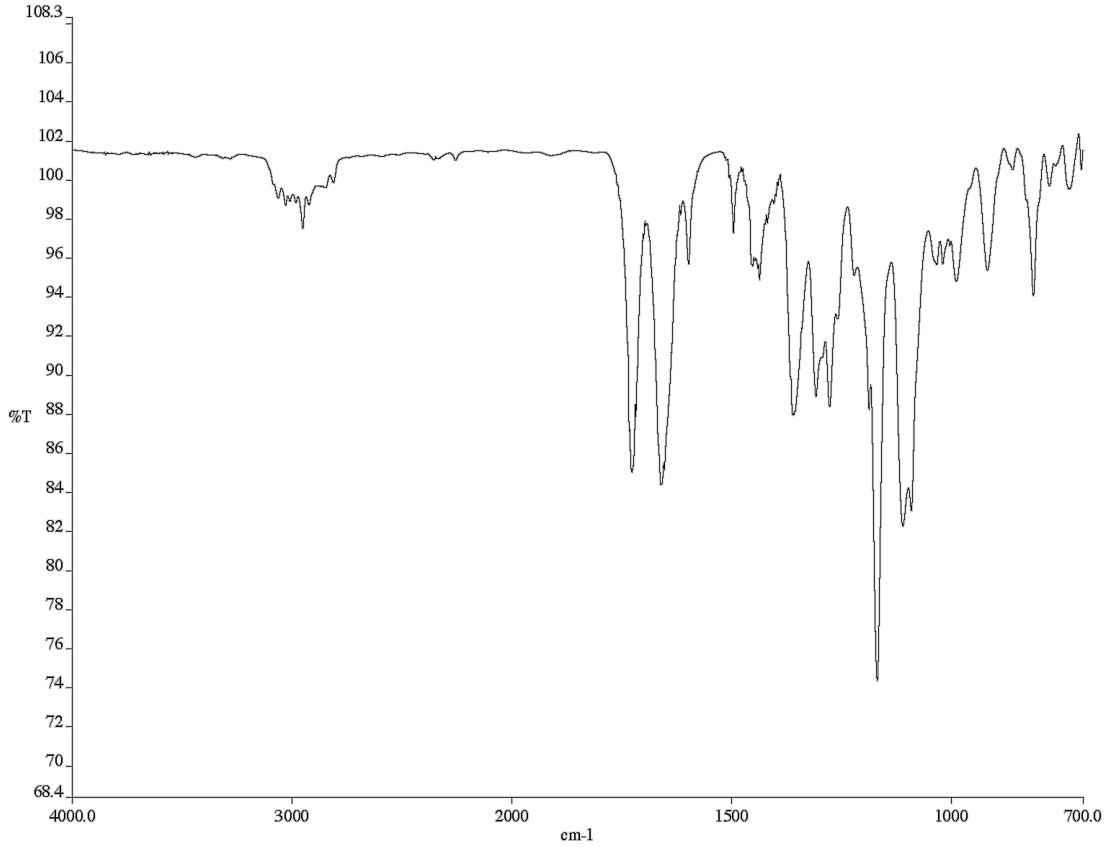
Infrared spectrum (Thin Film, NaCl) of compound **11**.



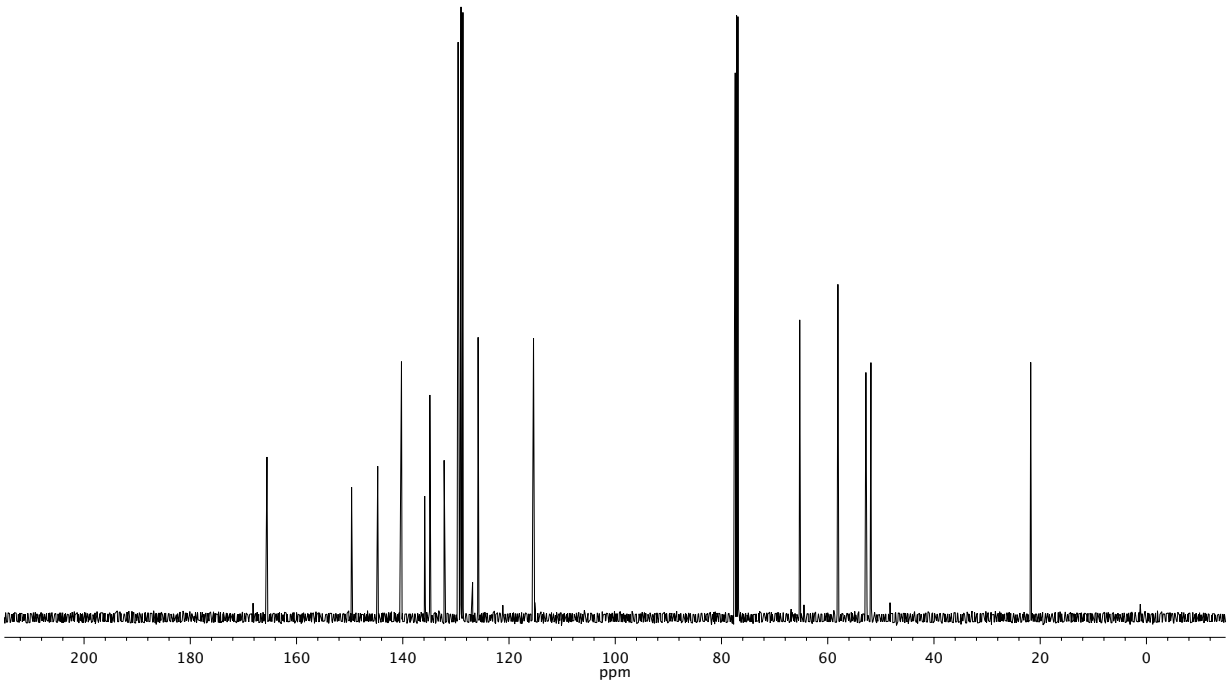
^{13}C NMR (126 MHz, $CDCl_3$) of compound **11**.



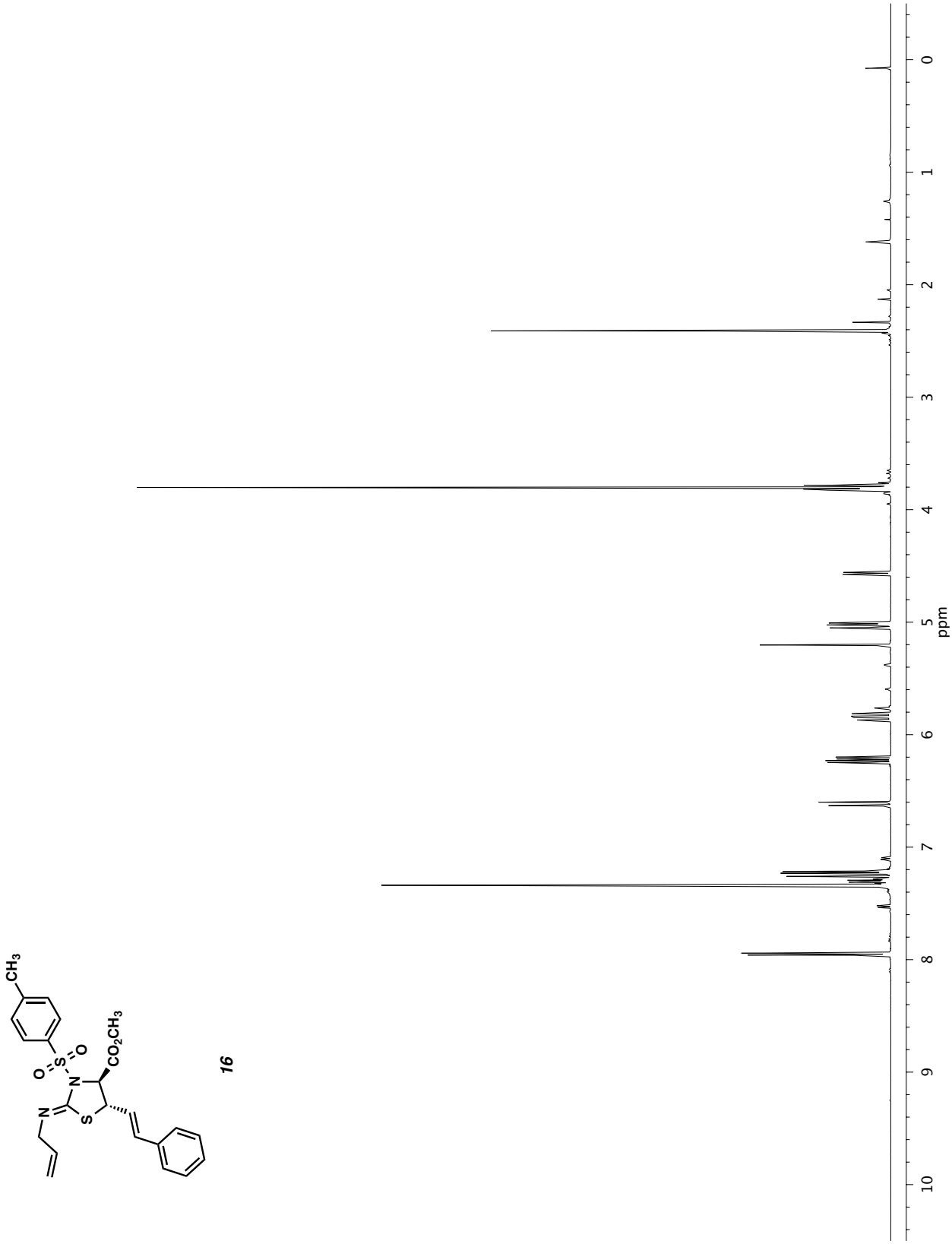
^{1}H NMR (500 MHz, $CDCl_3$) of compound **13**.



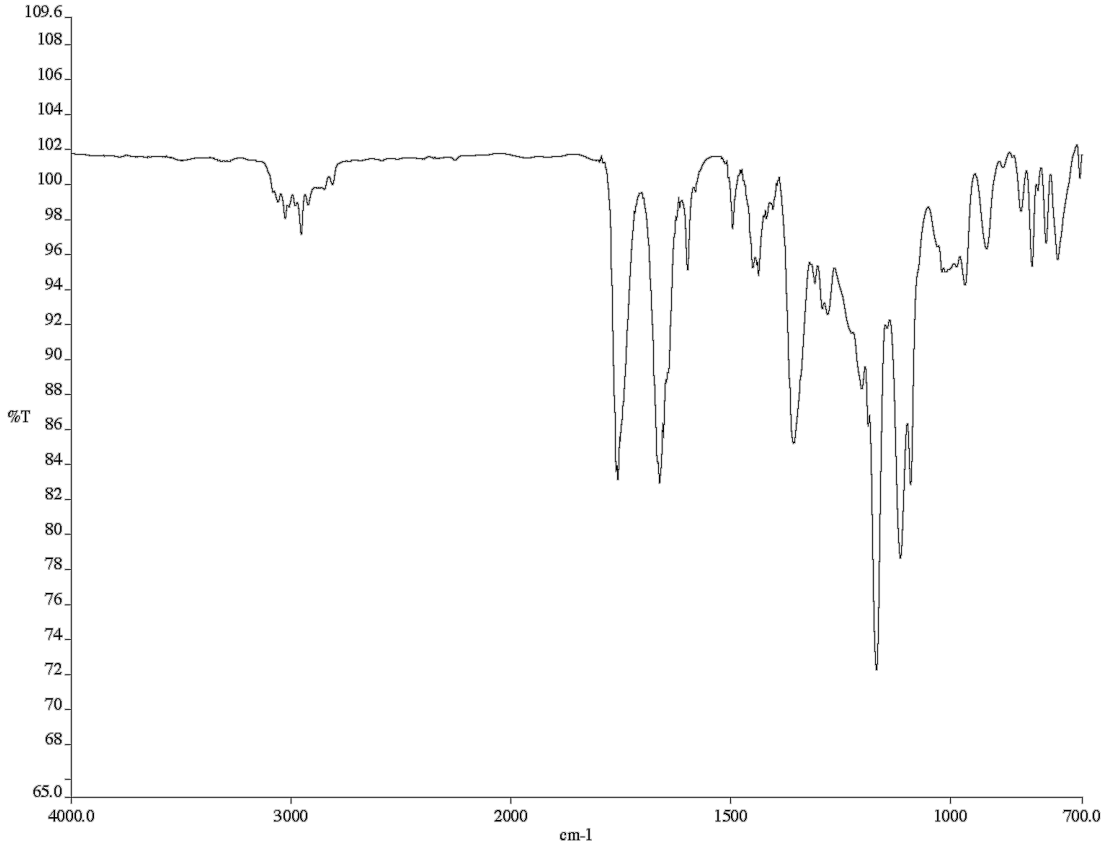
Infrared spectrum (Thin Film, NaCl) of compound **13**.



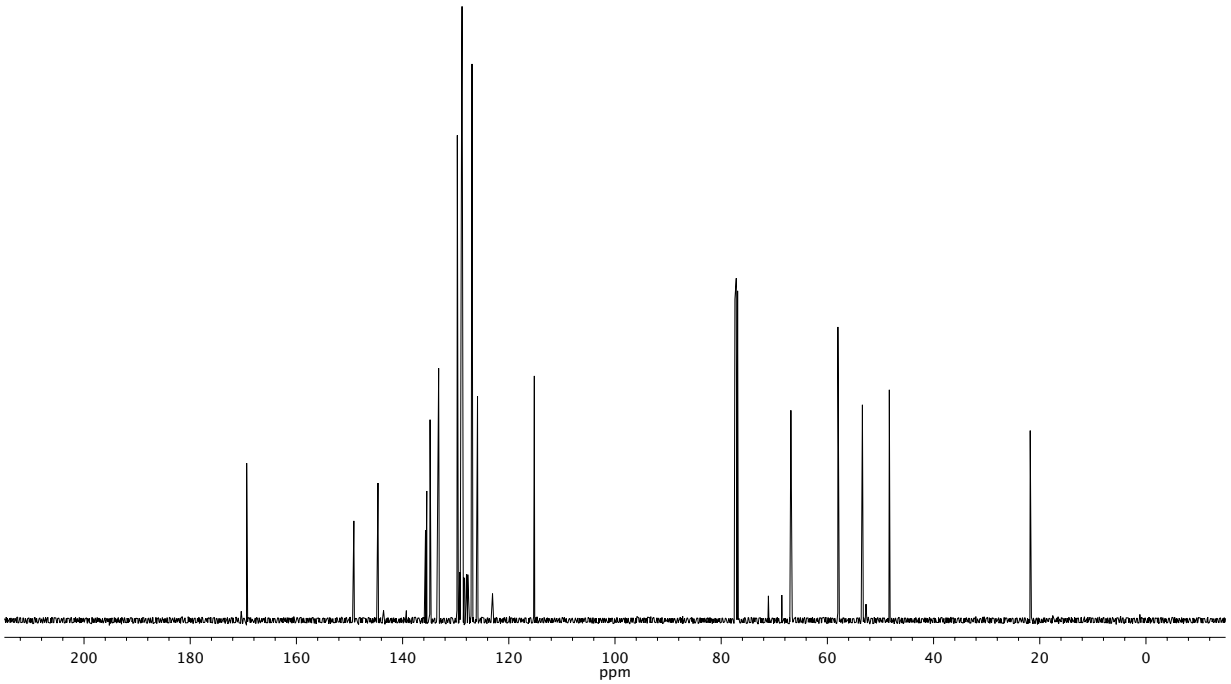
^{13}C NMR (126 MHz, $CDCl_3$) of compound **13**.



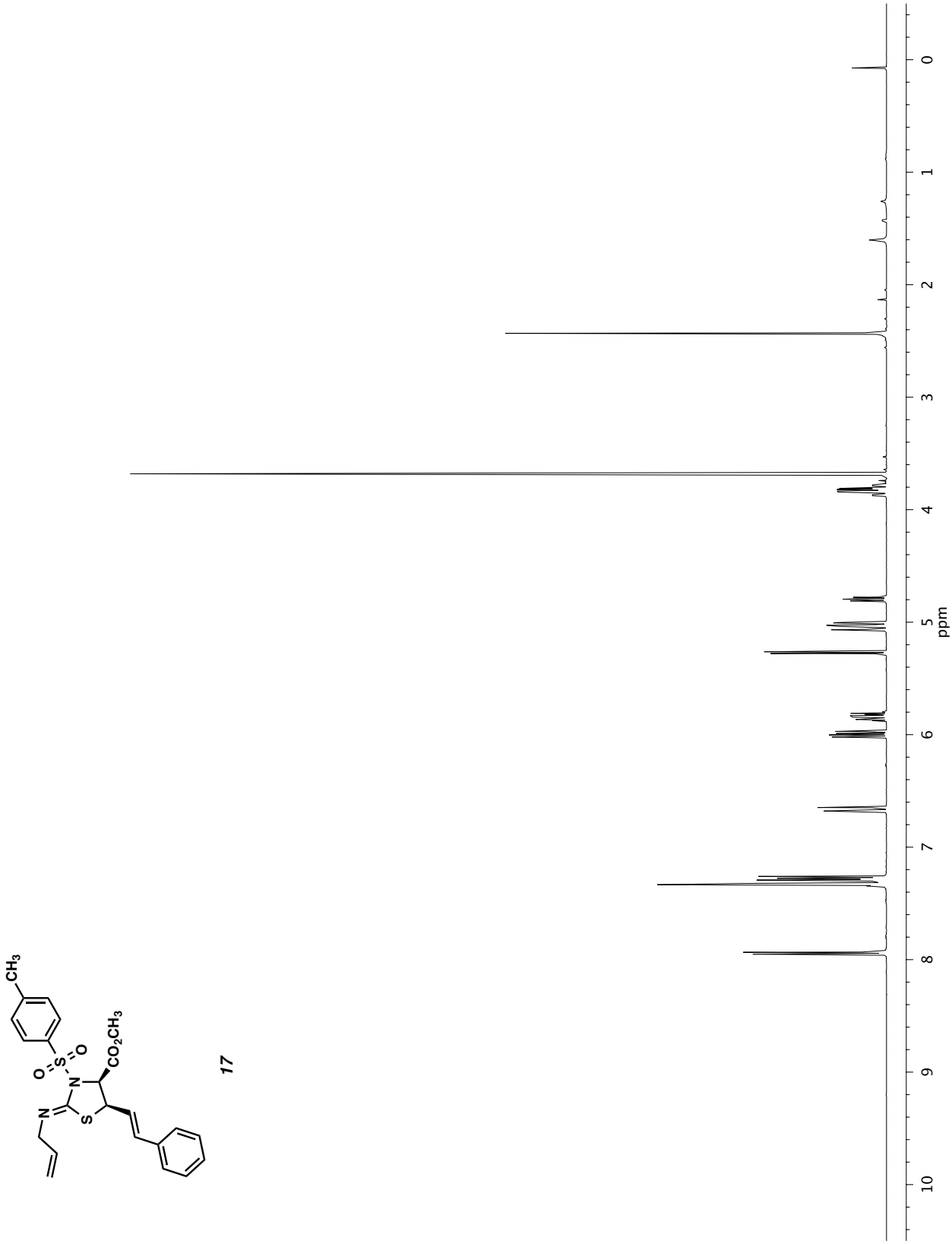
^{1}H NMR (500 MHz, $CDCl_3$) of compound **16**.



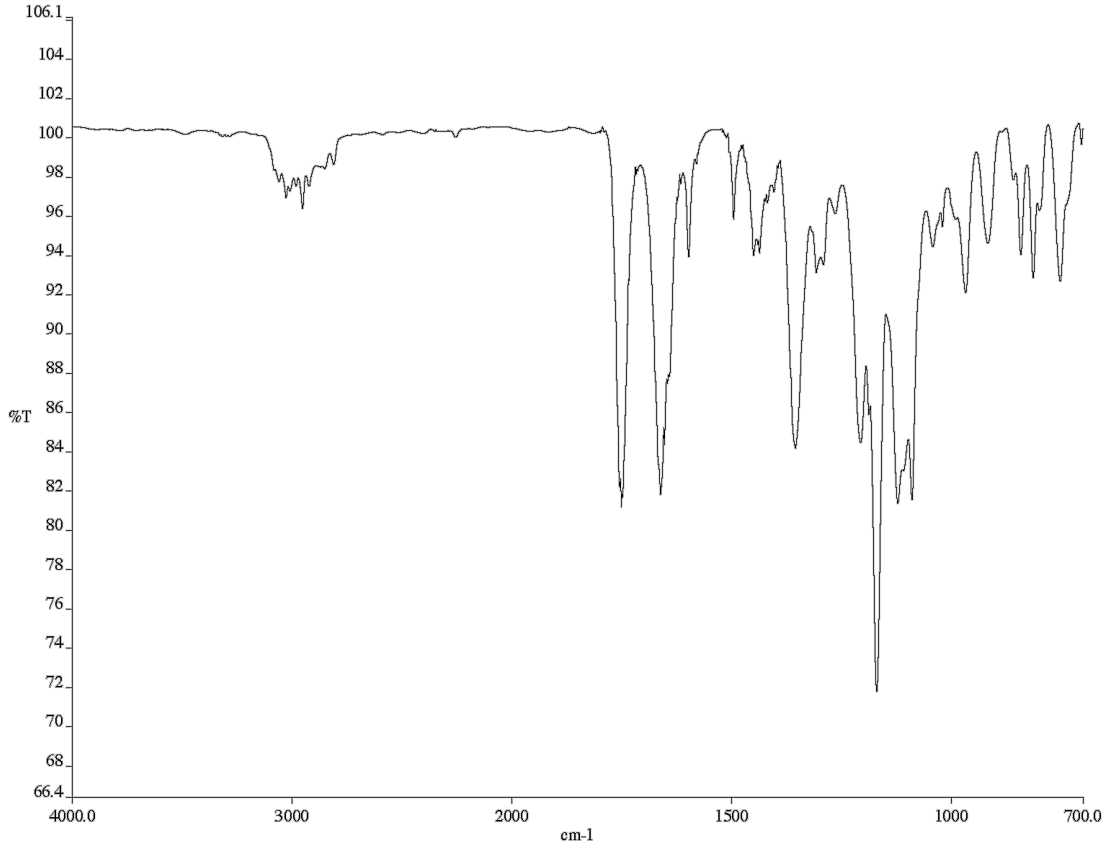
Infrared spectrum (Thin Film, NaCl) of compound **16**.



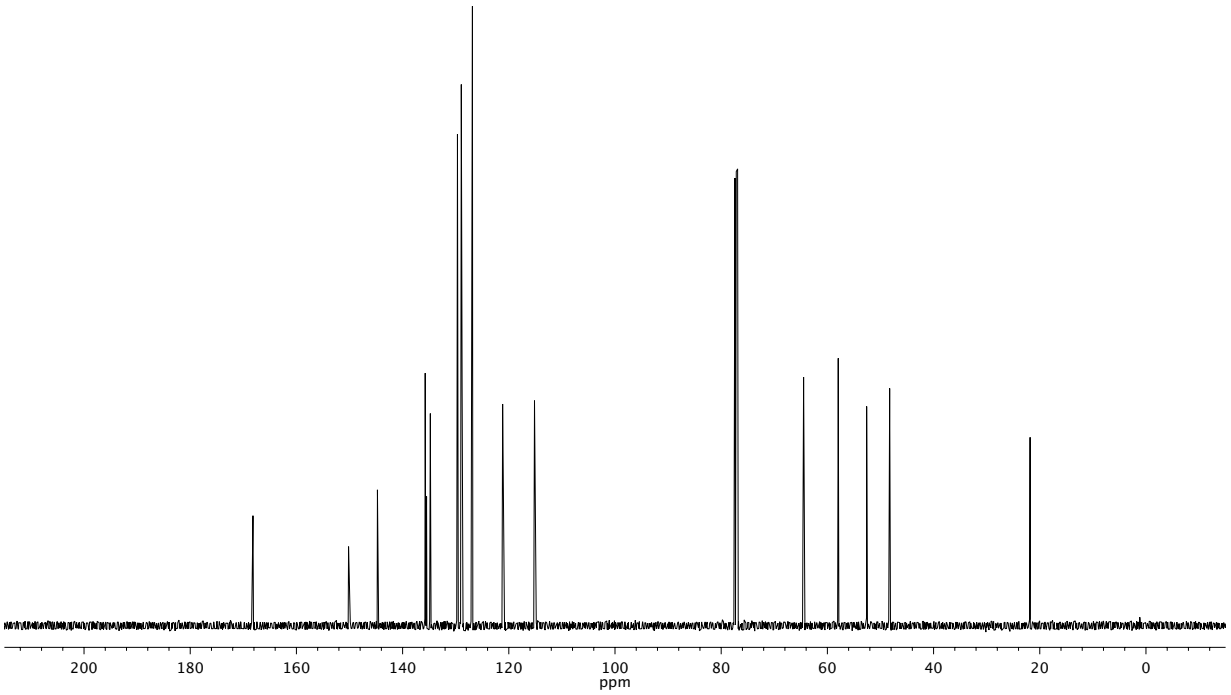
^{13}C NMR (126 MHz, $CDCl_3$) of compound **16**.



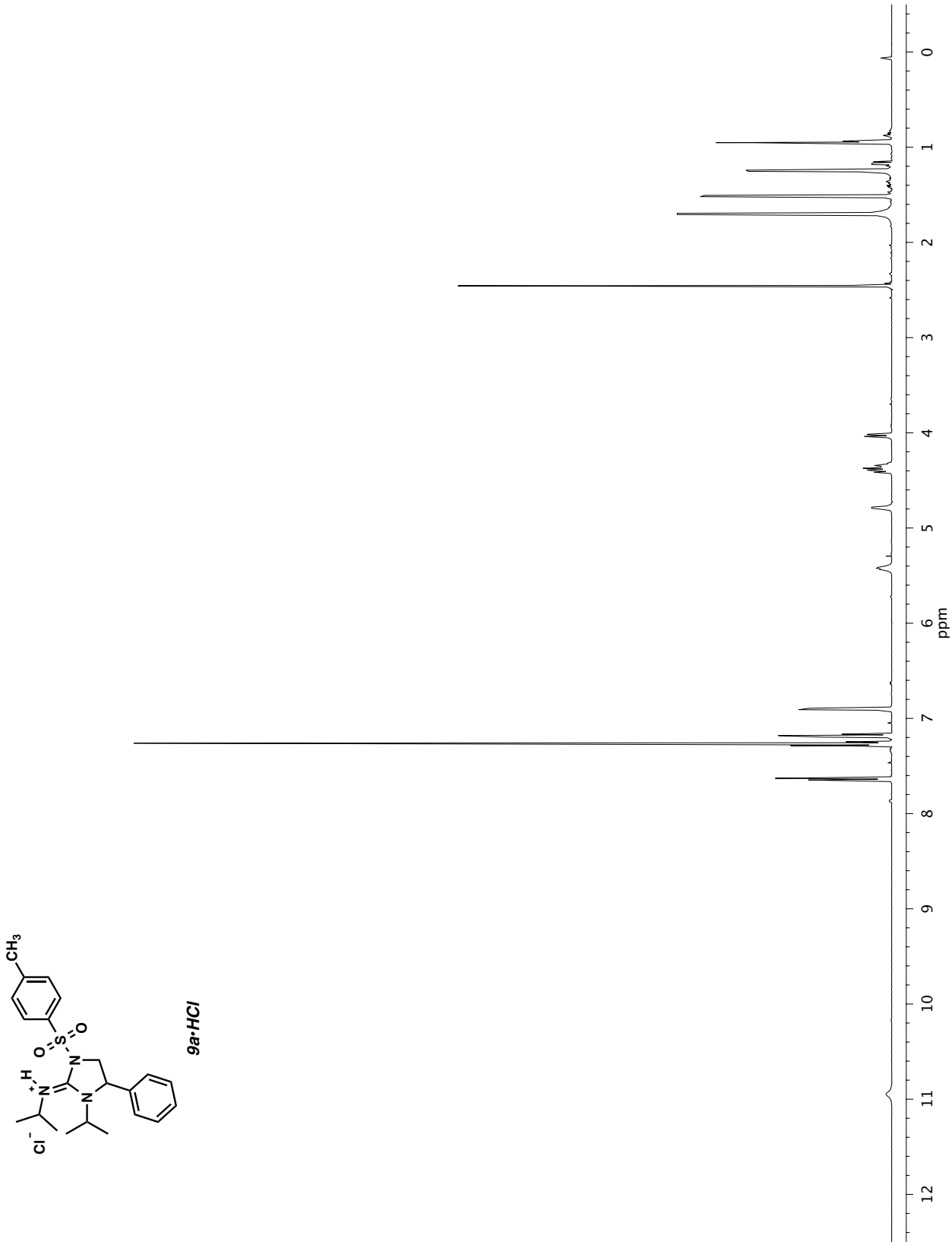
^{1}H NMR (500 MHz, $CDCl_3$) of compound **17**.



Infrared spectrum (Thin Film, NaCl) of compound **17**.

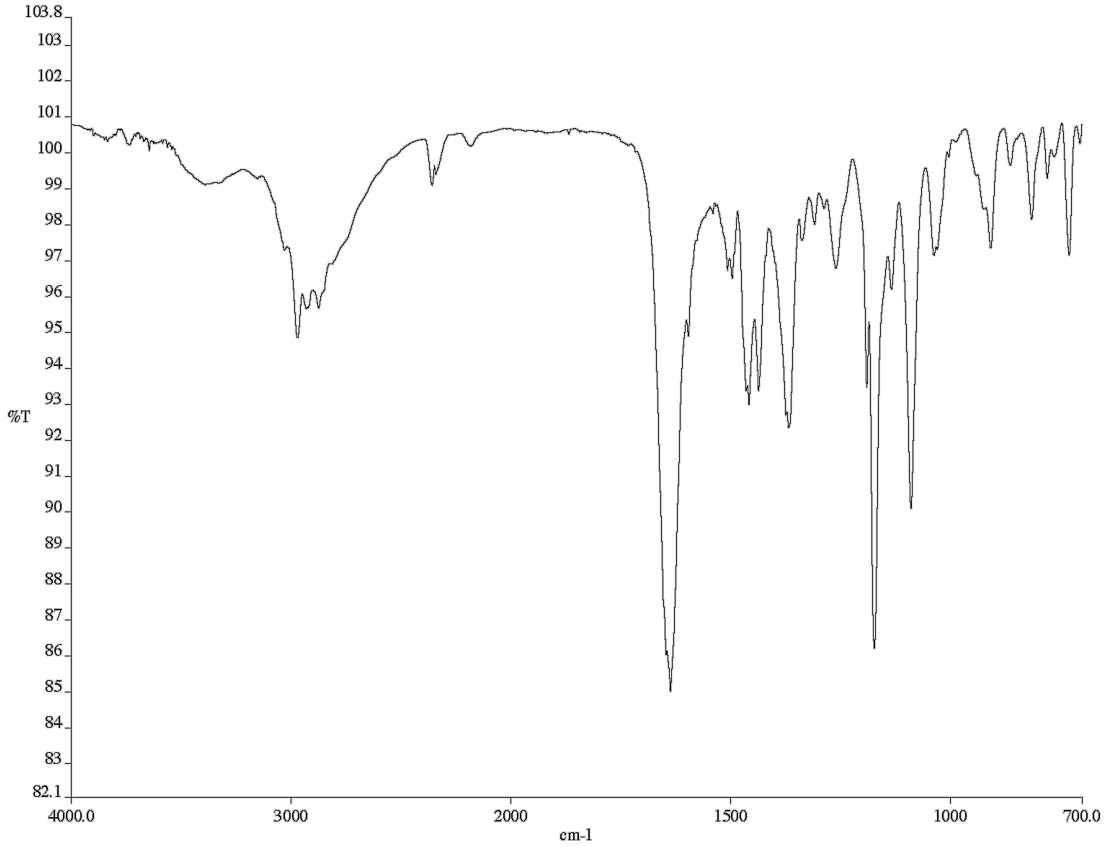


^{13}C NMR (126 MHz, $CDCl_3$) of compound **17**.

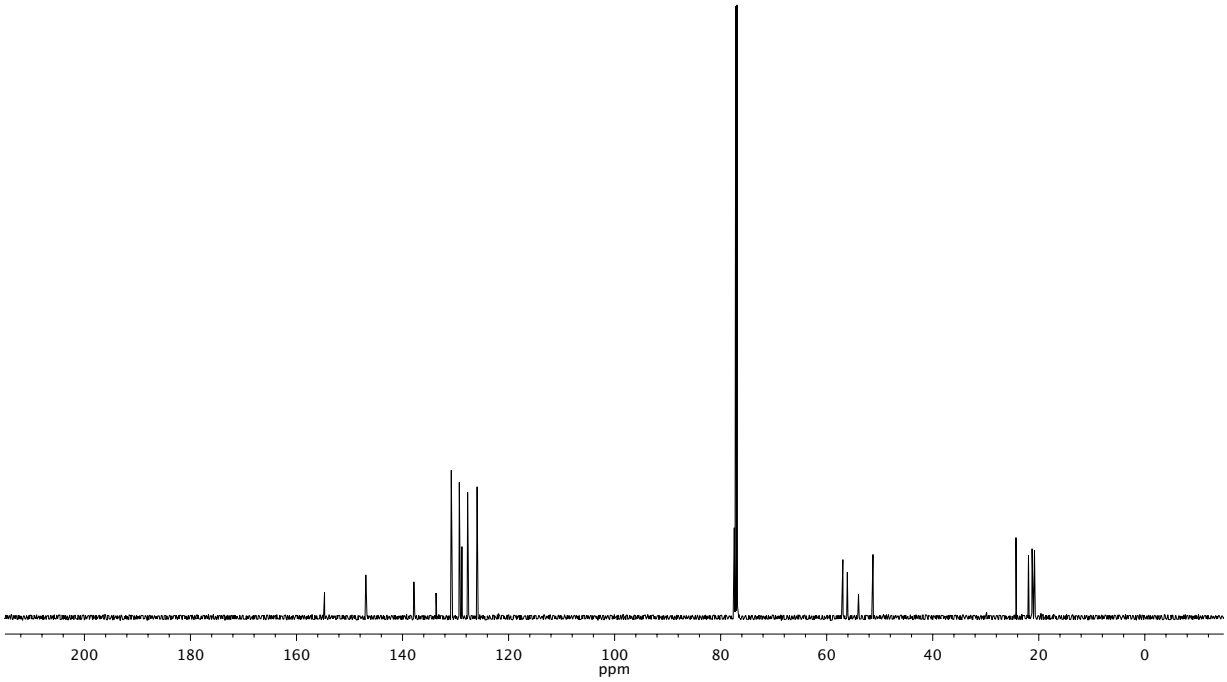


^{1}H NMR (500 MHz, $CDCl_3$) of compound **9a•HCl**.

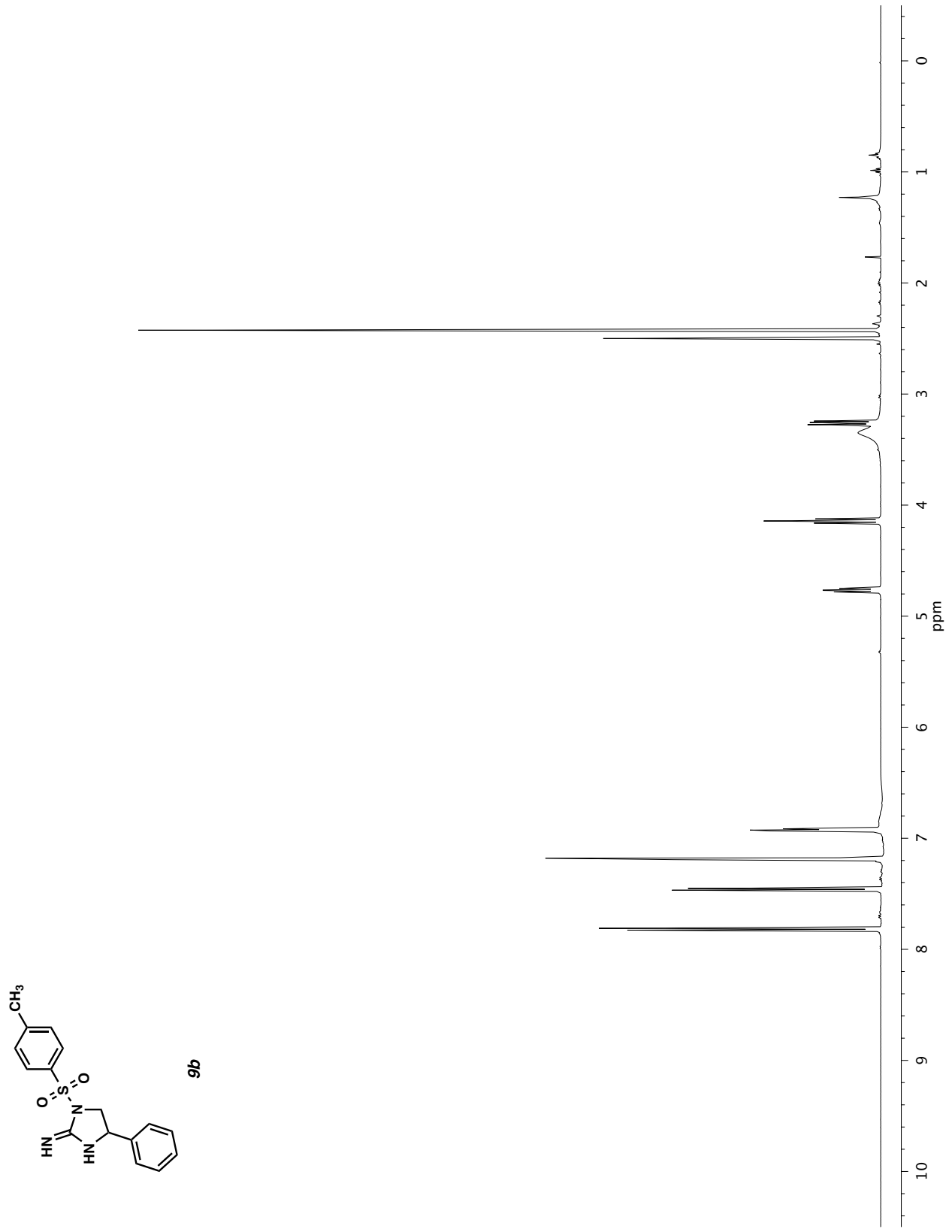
9a•HCl



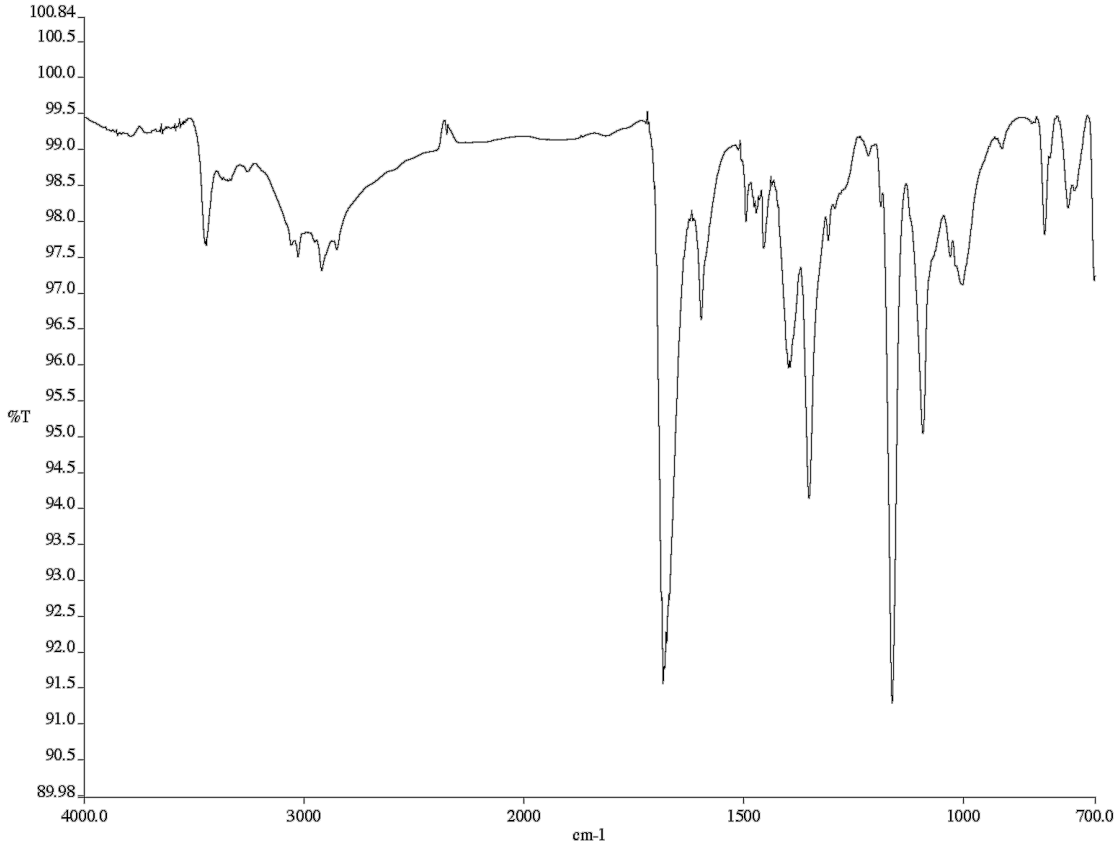
Infrared spectrum (Thin Film, NaCl) of compound **9a•HCl**.



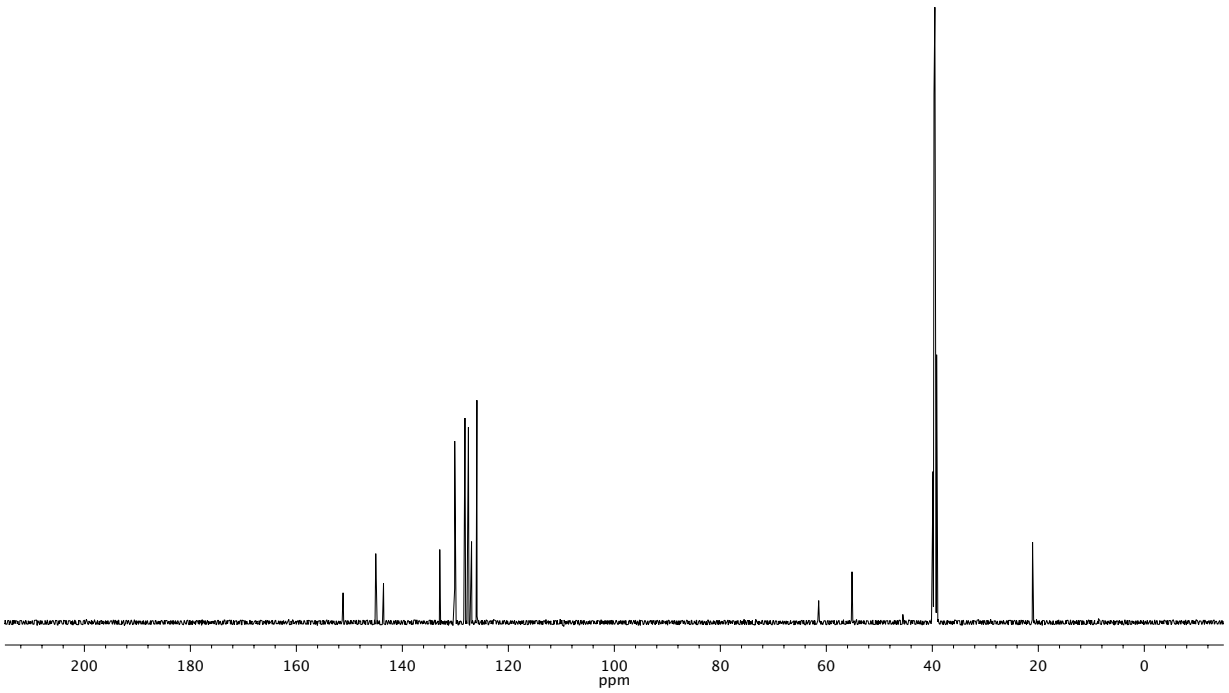
^{13}C NMR (126 MHz, $CDCl_3$) of compound **9a•HCl**.



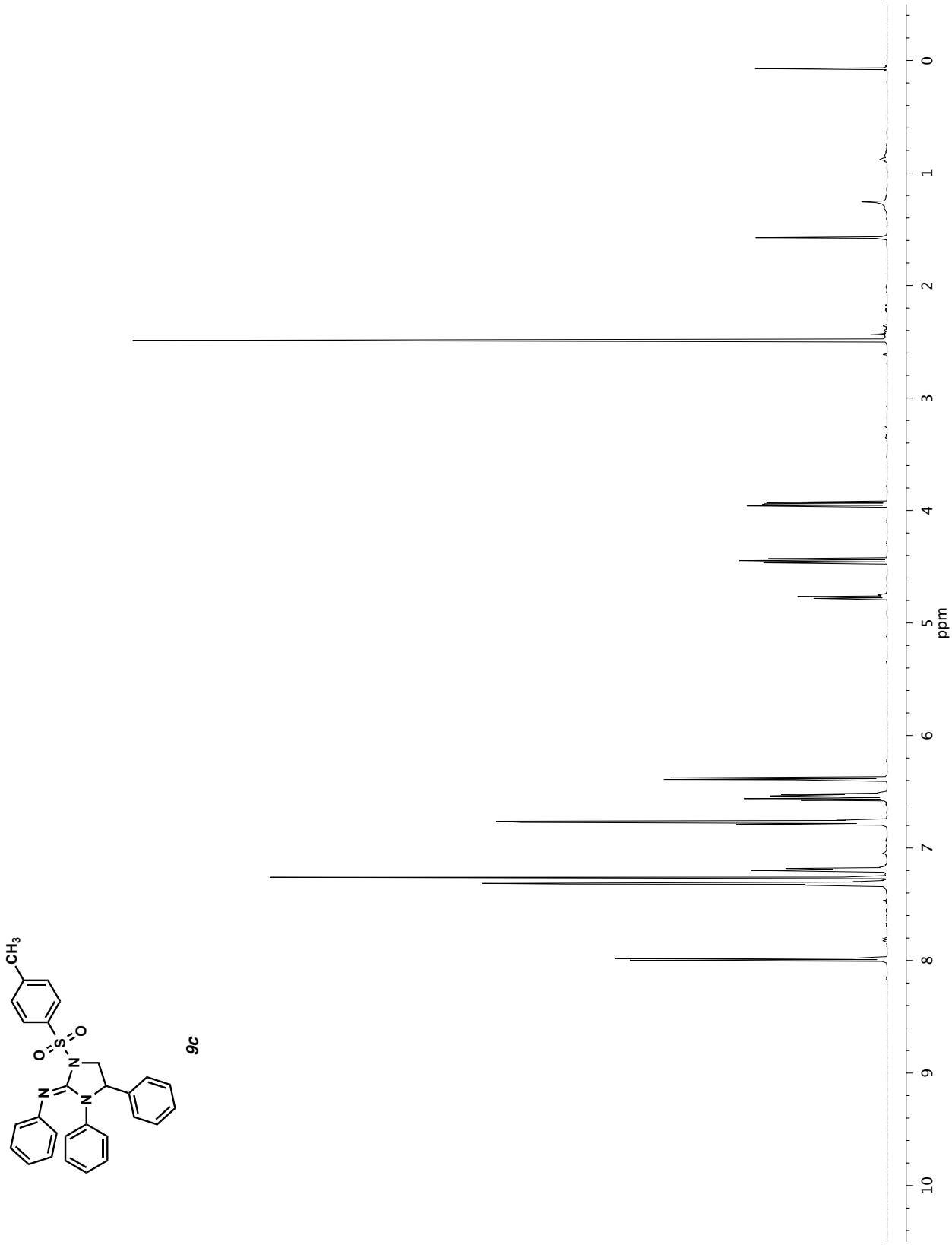
^{1}H NMR (500 MHz, $CDCl_3$) of compound **9b**.



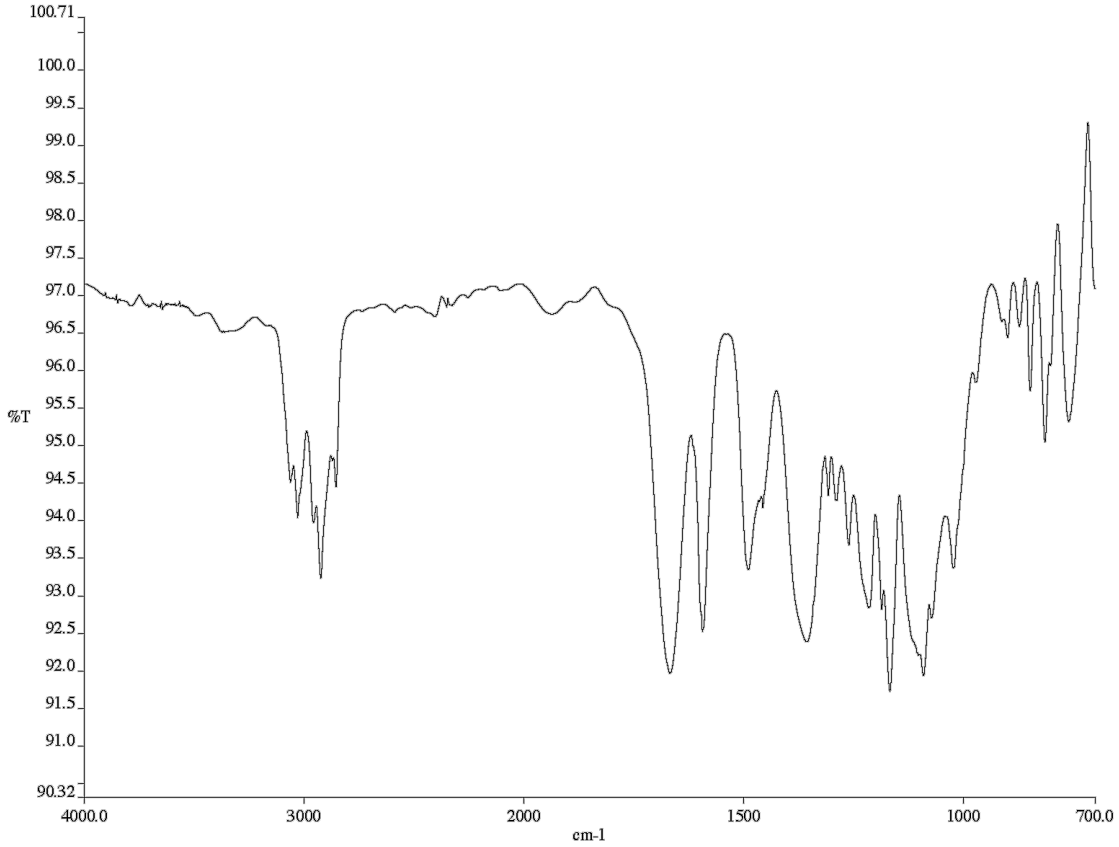
Infrared spectrum (Thin Film, NaCl) of compound **9b**.



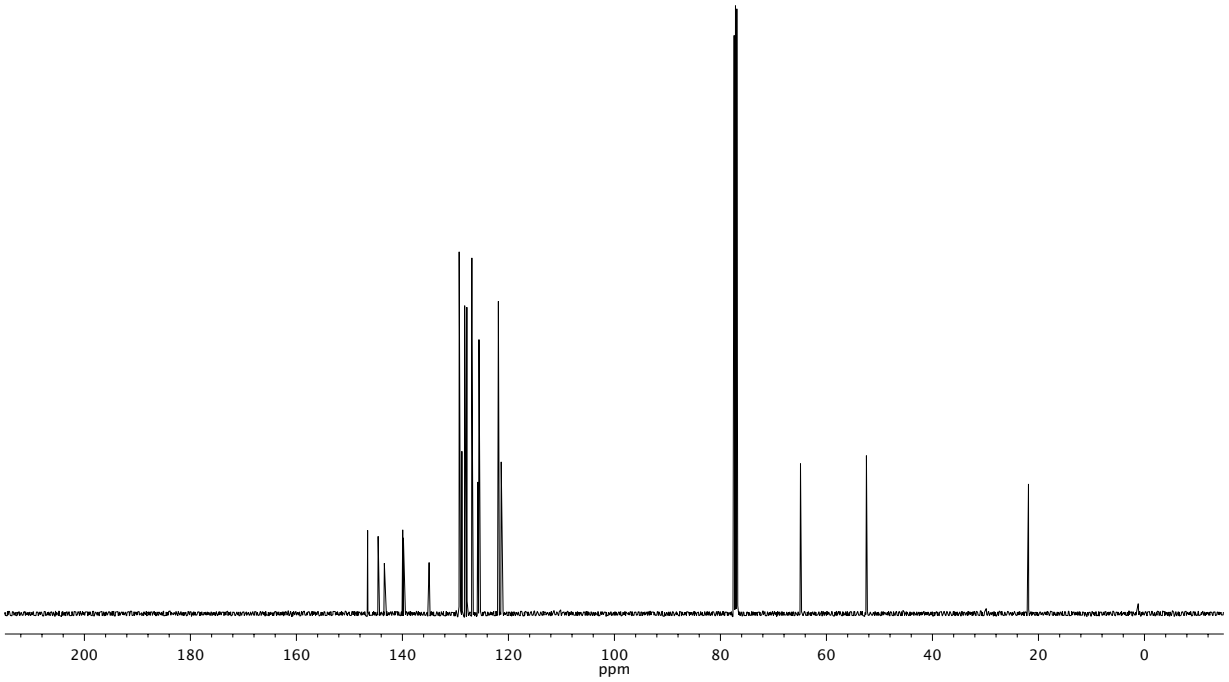
^{13}C NMR (126 MHz, $CDCl_3$) of compound **9b**.



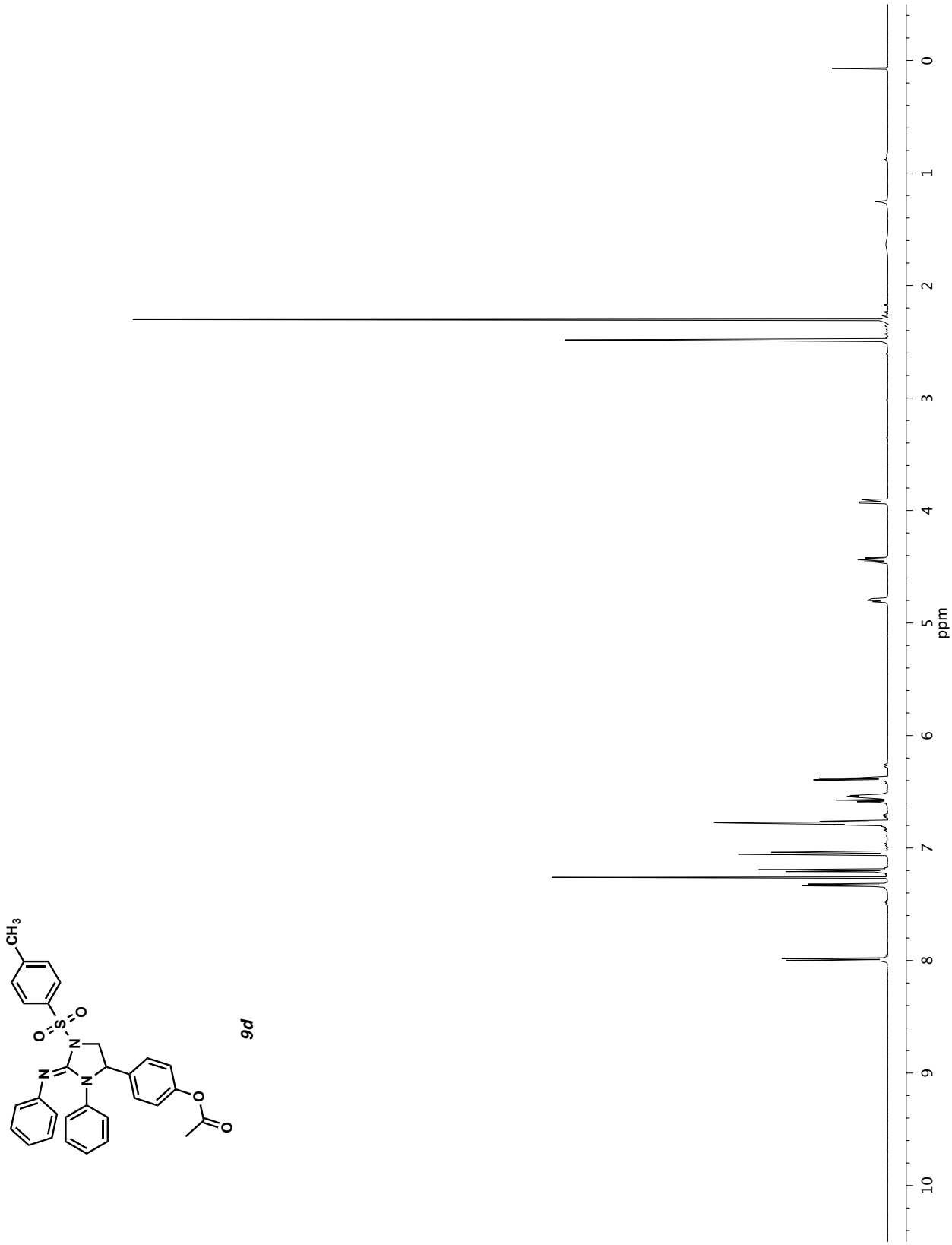
^{1}H NMR (500 MHz, $CDCl_3$) of compound **9c**.



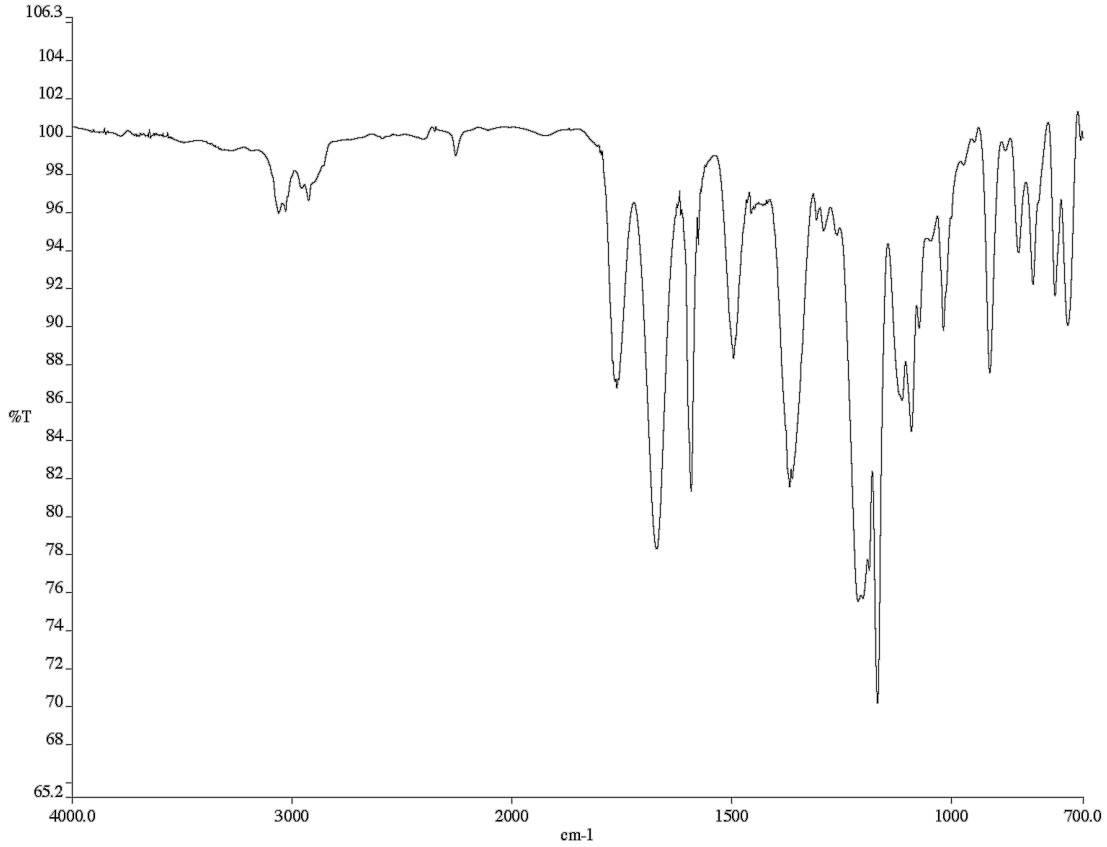
Infrared spectrum (Thin Film, NaCl) of compound **9c**.



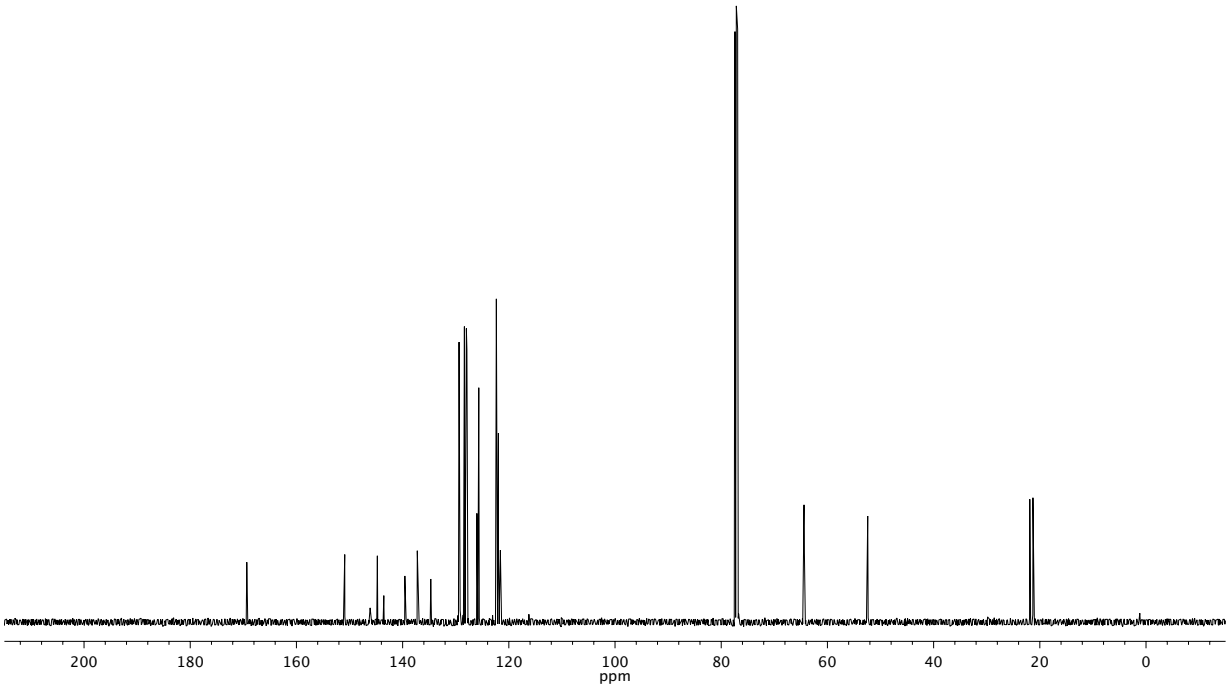
^{13}C NMR (126 MHz, $CDCl_3$) of compound **9c**.



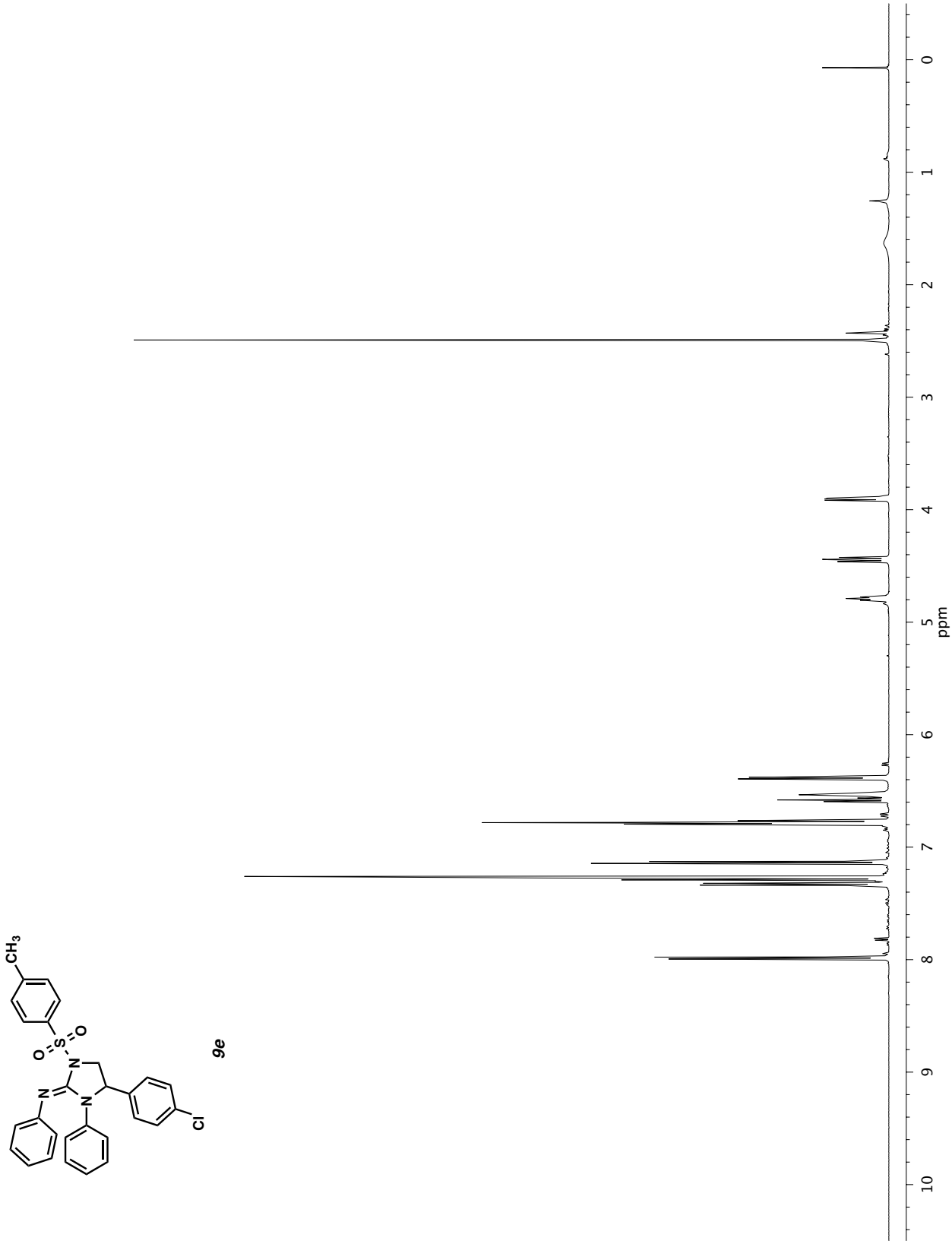
^{1}H NMR (500 MHz, $CDCl_3$) of compound **9d**.



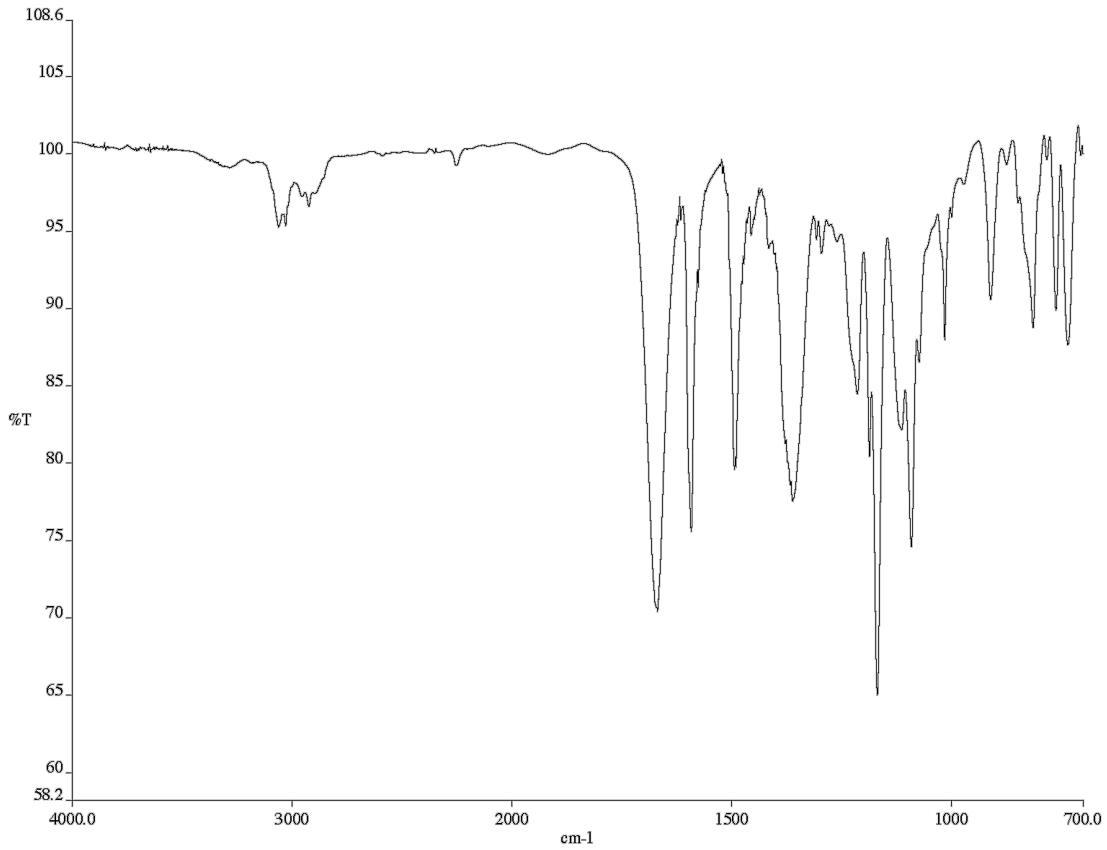
Infrared spectrum (Thin Film, NaCl) of compound **9d**.



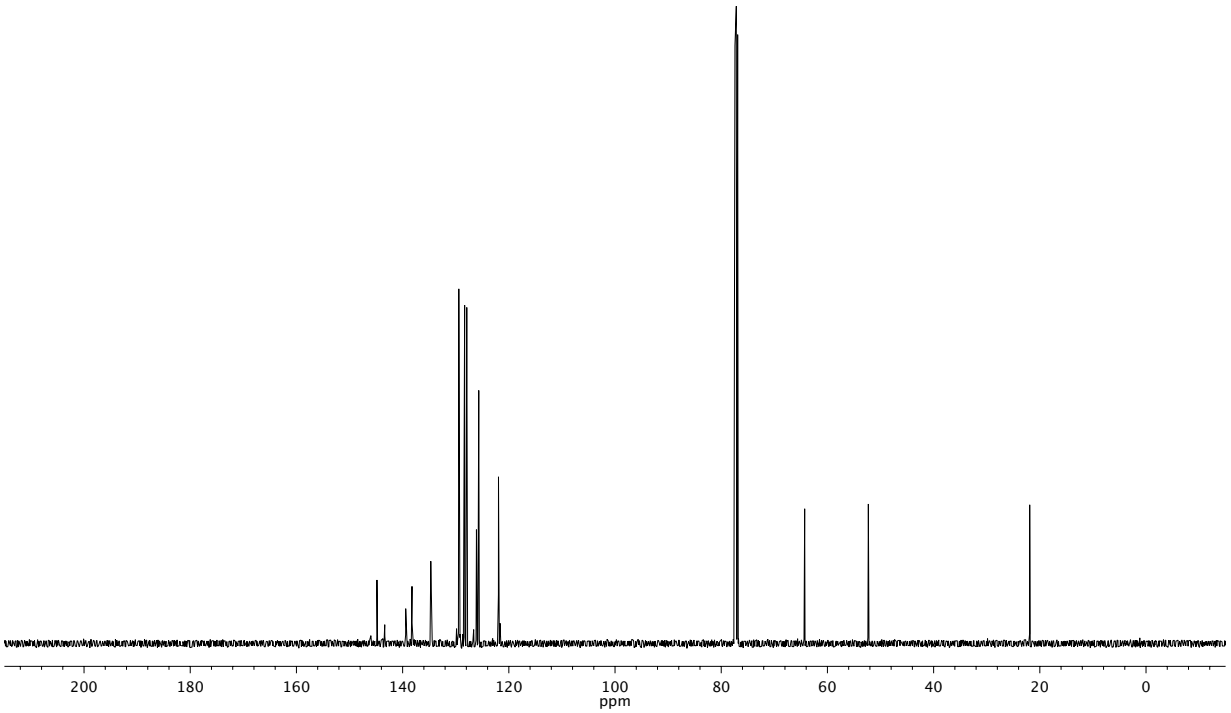
^{13}C NMR (126 MHz, $CDCl_3$) of compound **9d**.



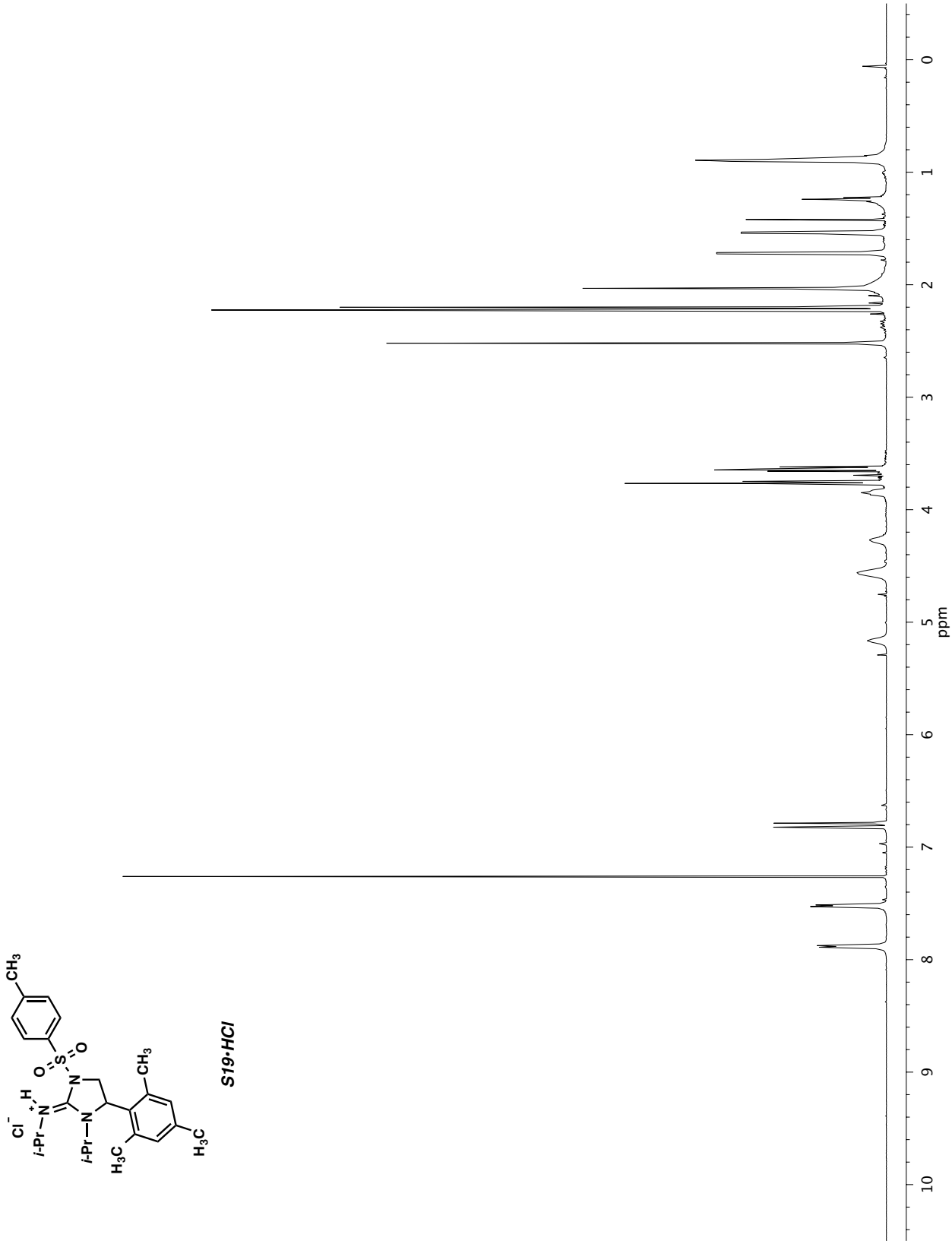
^{1}H NMR (500 MHz, $CDCl_3$) of compound **9e**.



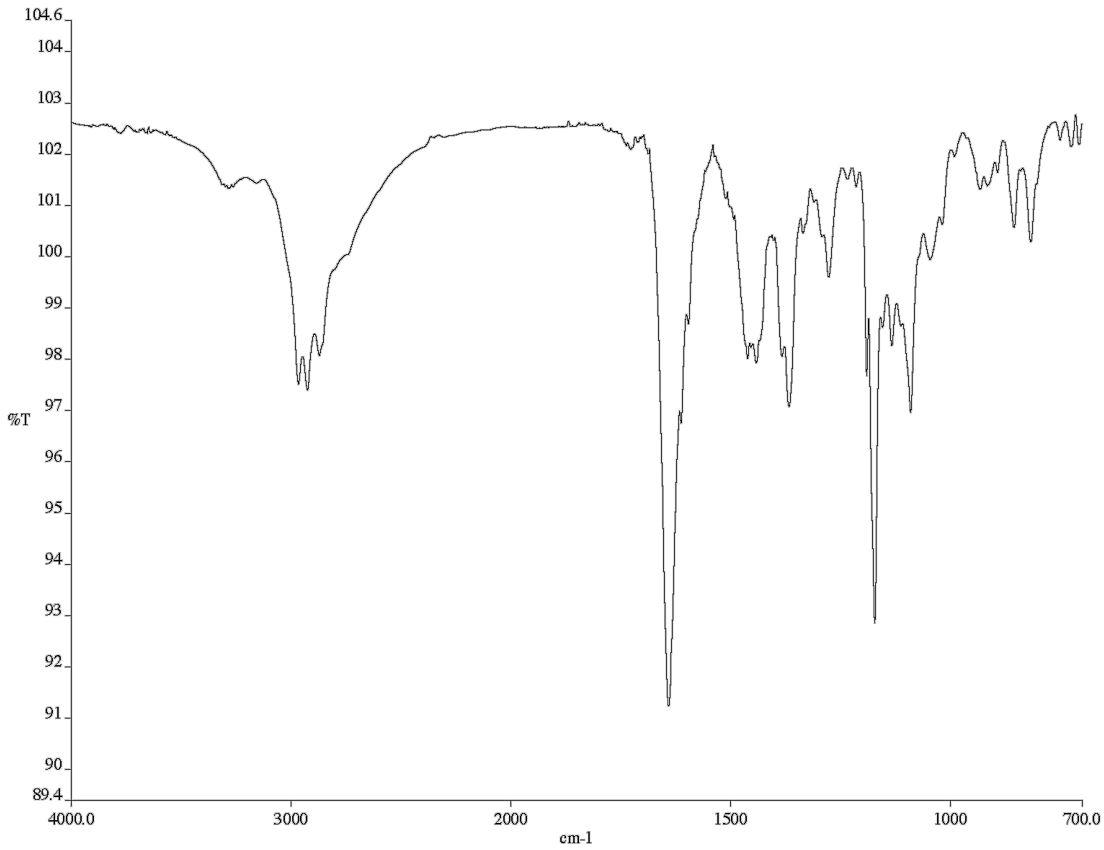
Infrared spectrum (Thin Film, NaCl) of compound **9e**.



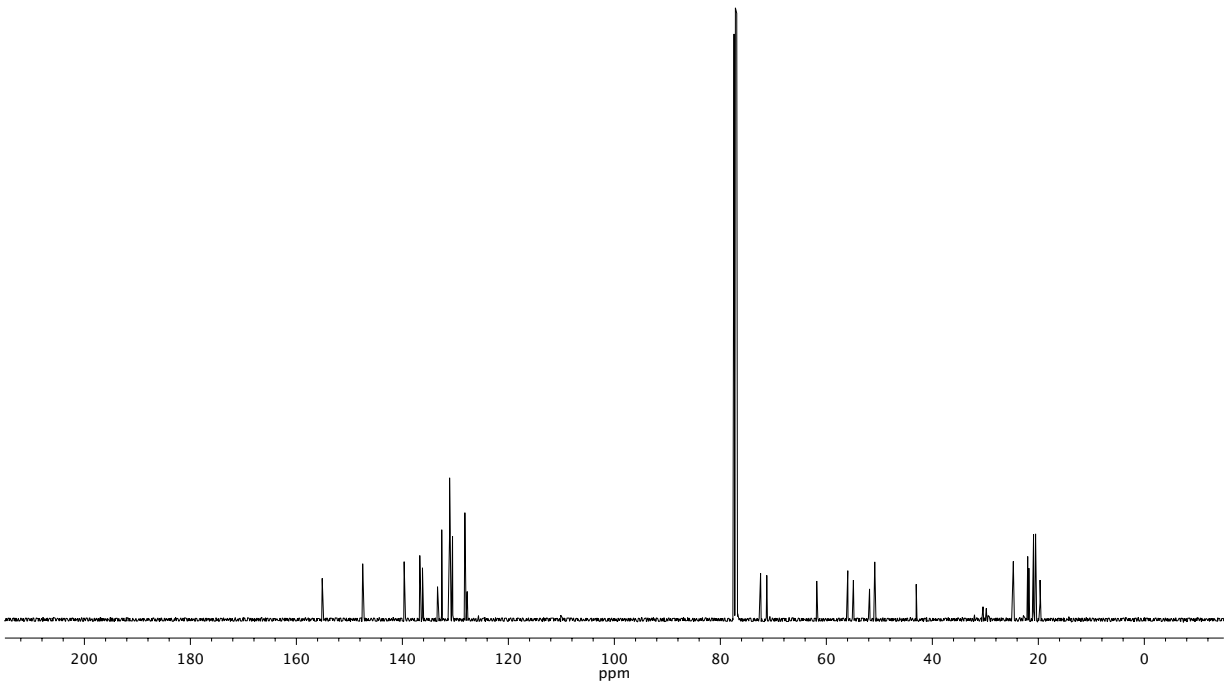
^{13}C NMR (126 MHz, $CDCl_3$) of compound **9e**.



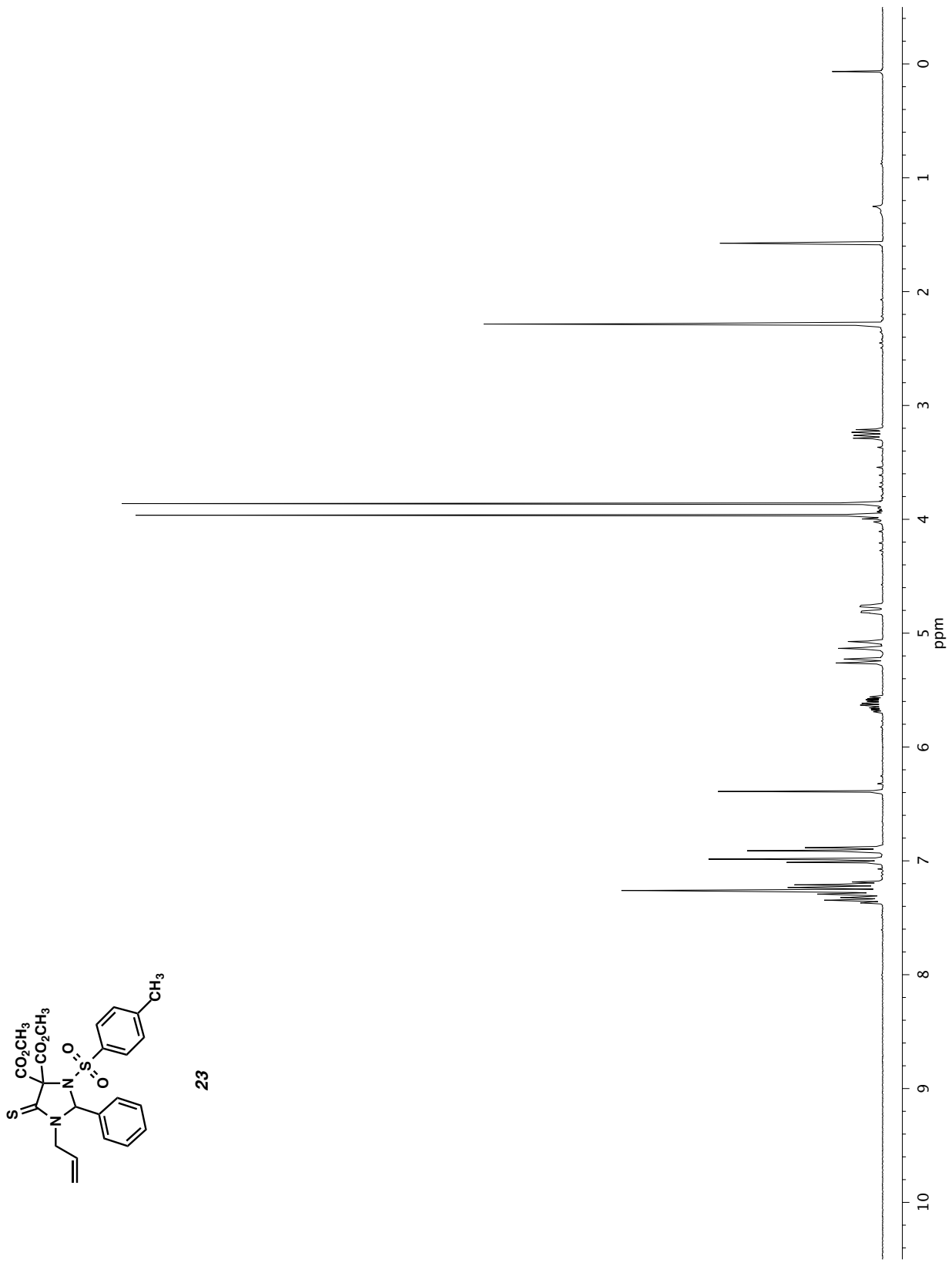
^{1}H NMR (500 MHz, $CDCl_3$) of compound **S19•HCl**.



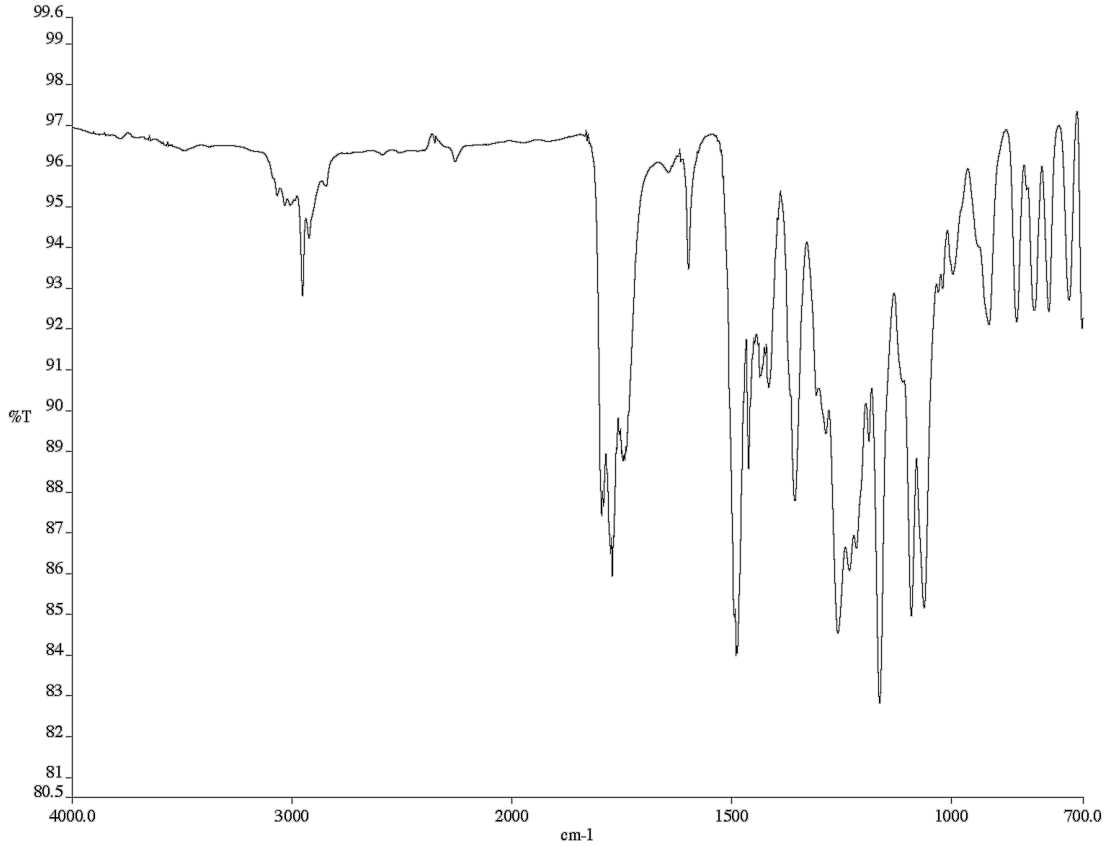
Infrared spectrum (Thin Film, NaCl) of compound **S19•HCl**.



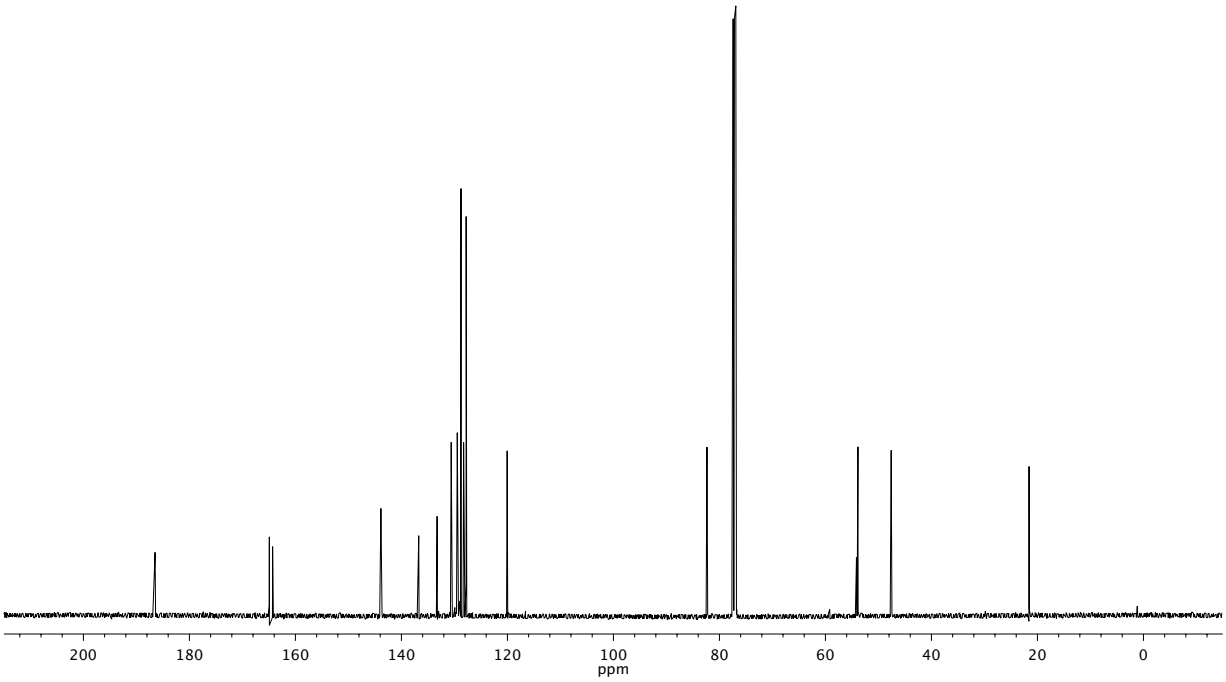
^{13}C NMR (126 MHz, $CDCl_3$) of compound **S19•HCl**.



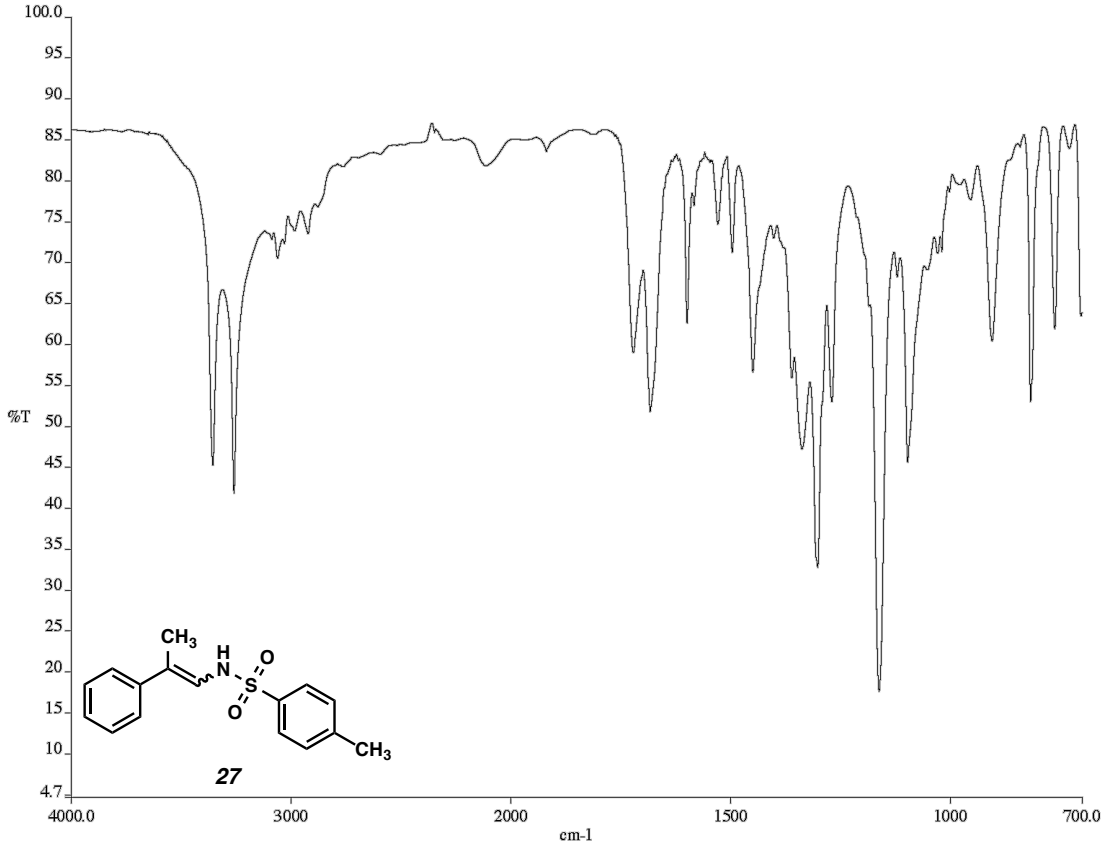
^{1}H NMR (500 MHz, $CDCl_3$) of compound **23**.



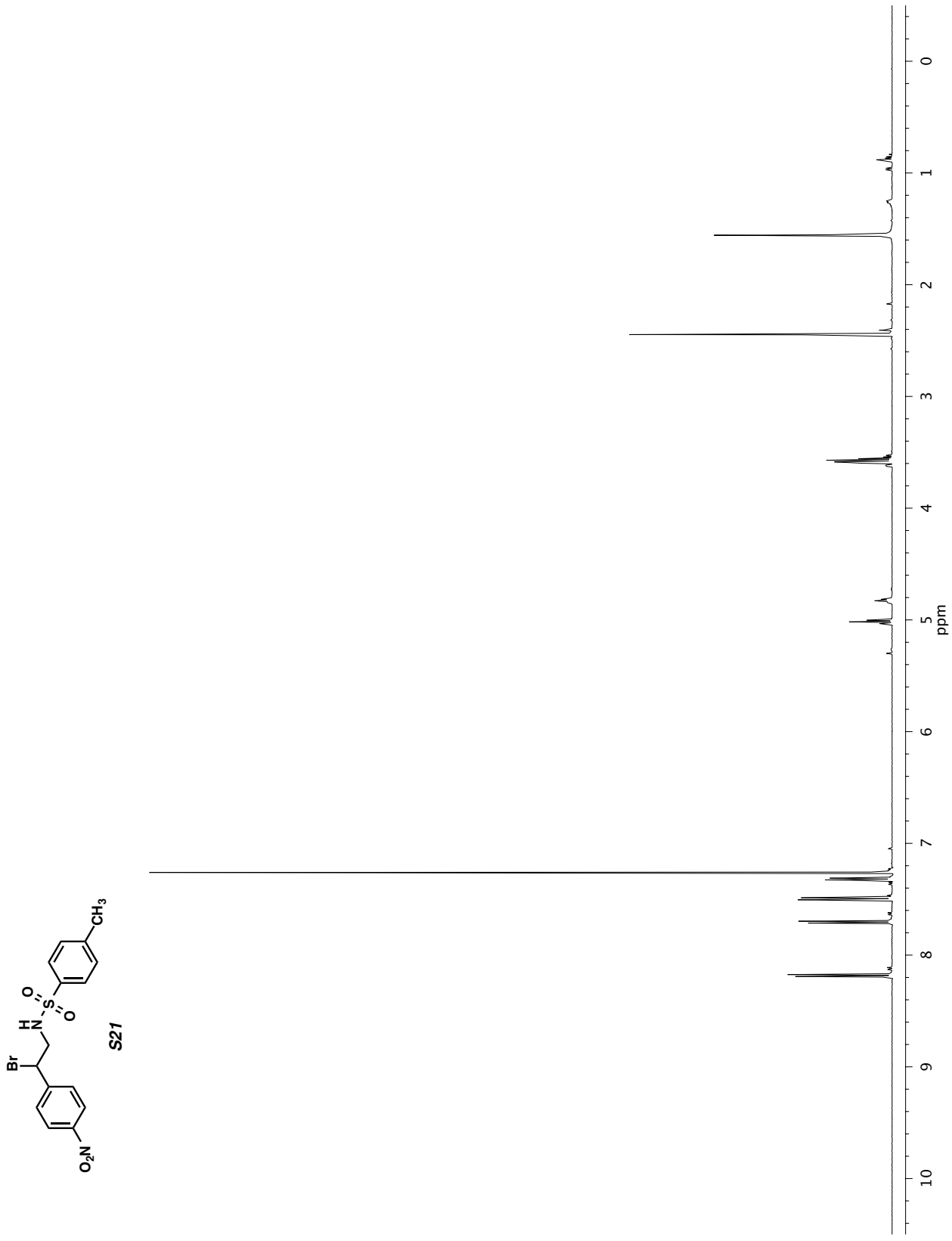
Infrared spectrum (Thin Film, NaCl) of compound **23**.



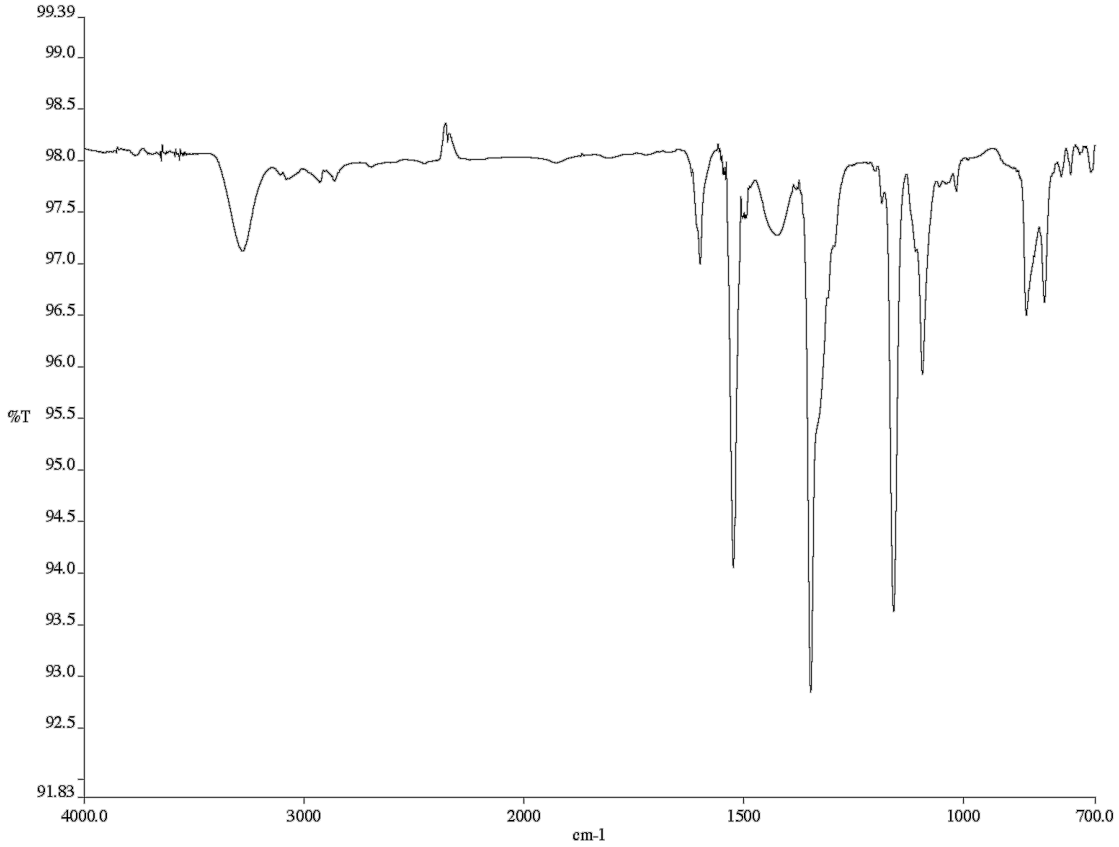
^{13}C NMR (126 MHz, $CDCl_3$) of compound **23**.



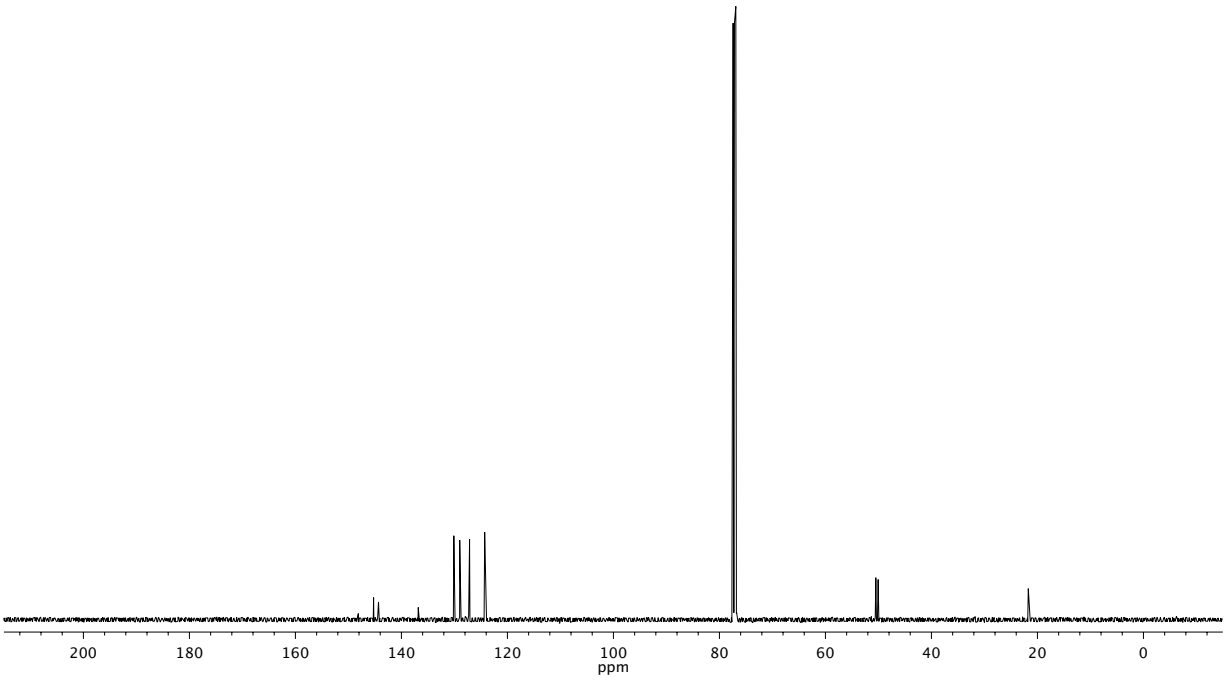
Infrared spectrum (Thin Film, NaCl) of compound **27**.



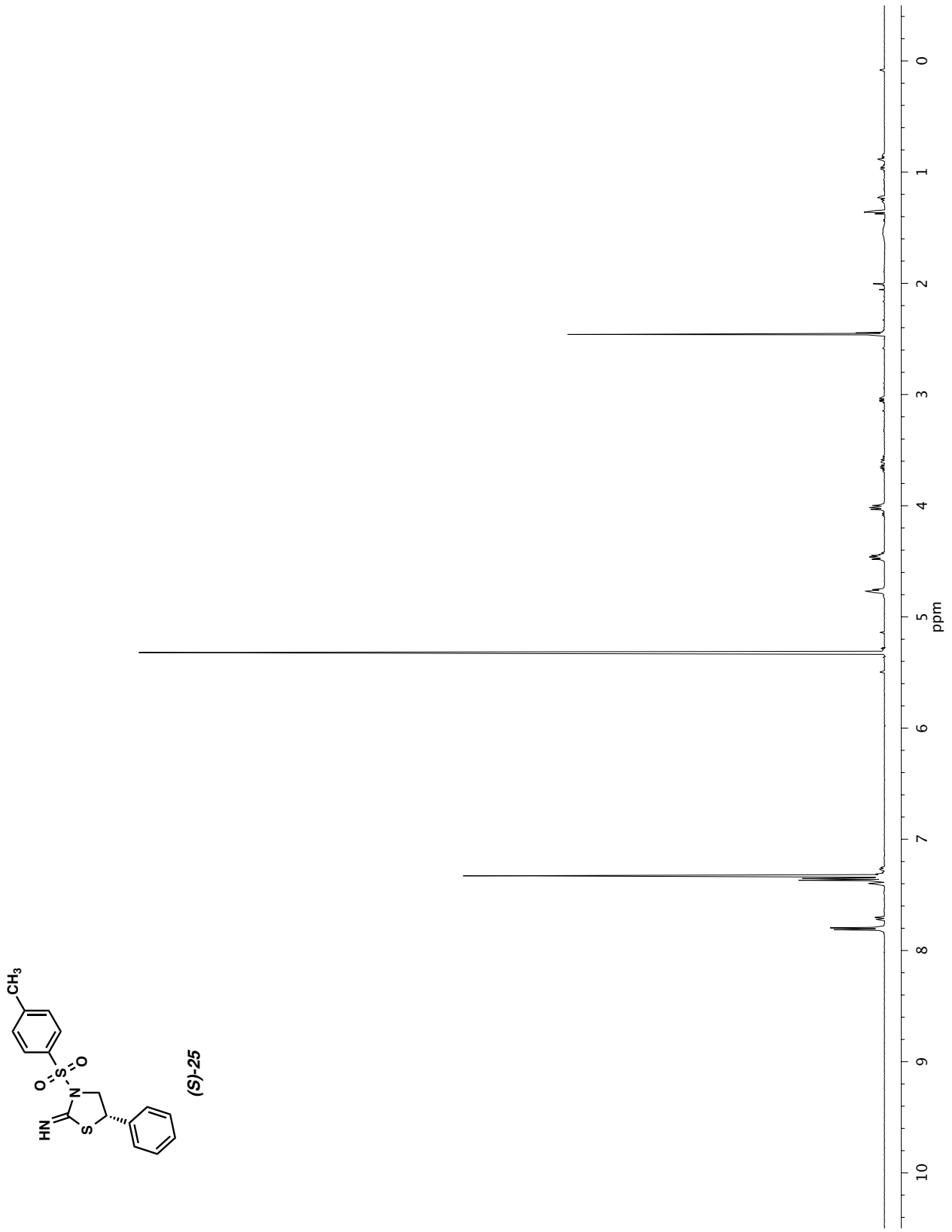
^{1}H NMR (500 MHz, $CDCl_3$) of compound **S21**.



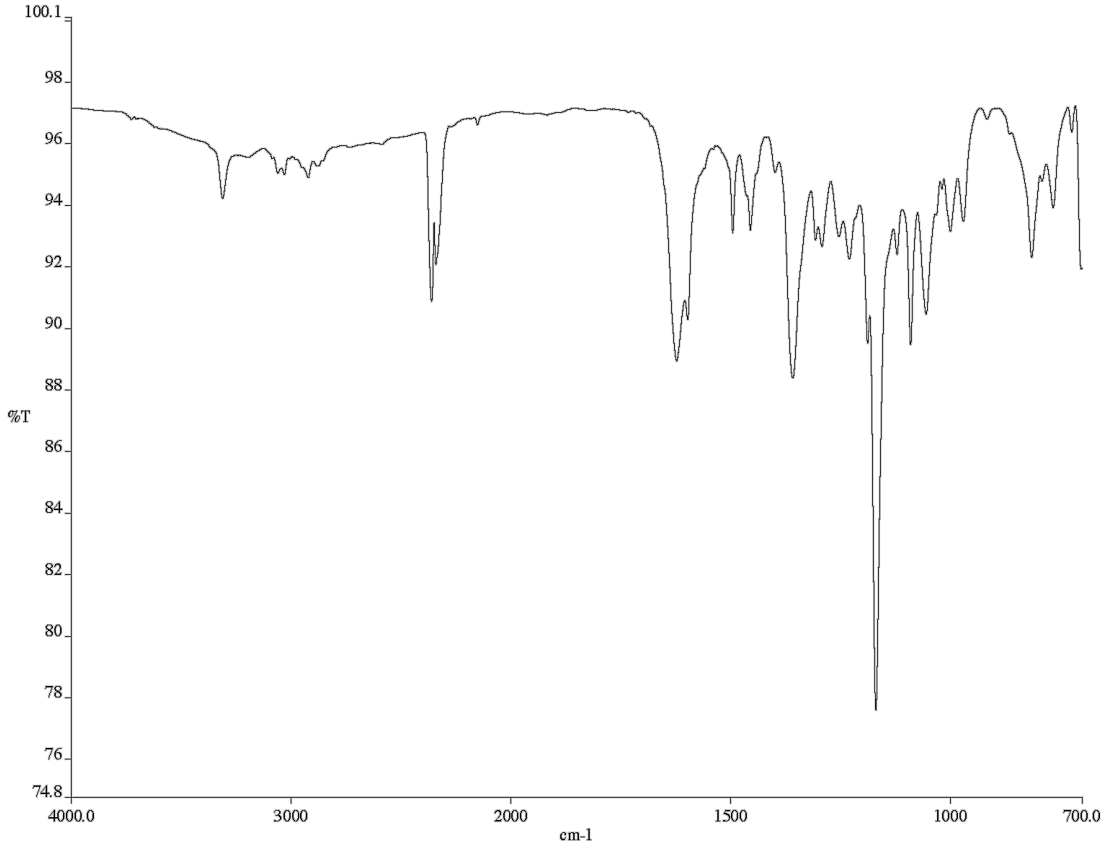
Infrared spectrum (Thin Film, NaCl) of compound **S21**.



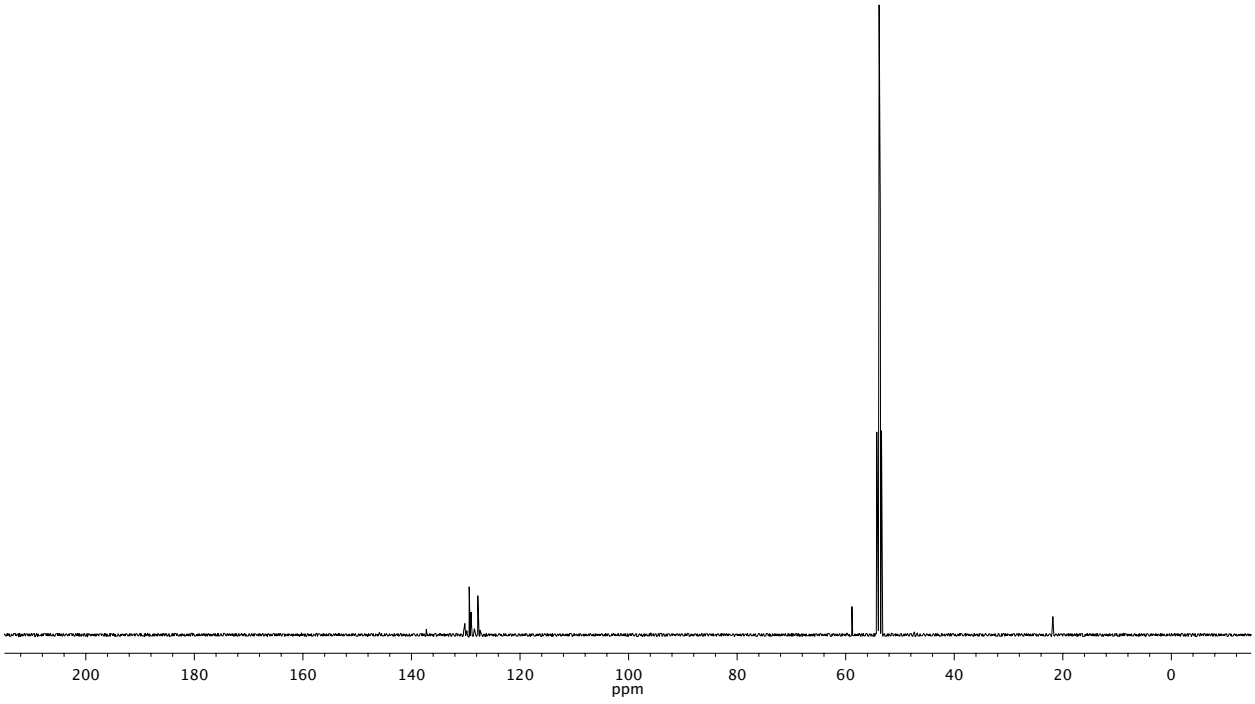
^{13}C NMR (126 MHz, $CDCl_3$) of compound **S21**.



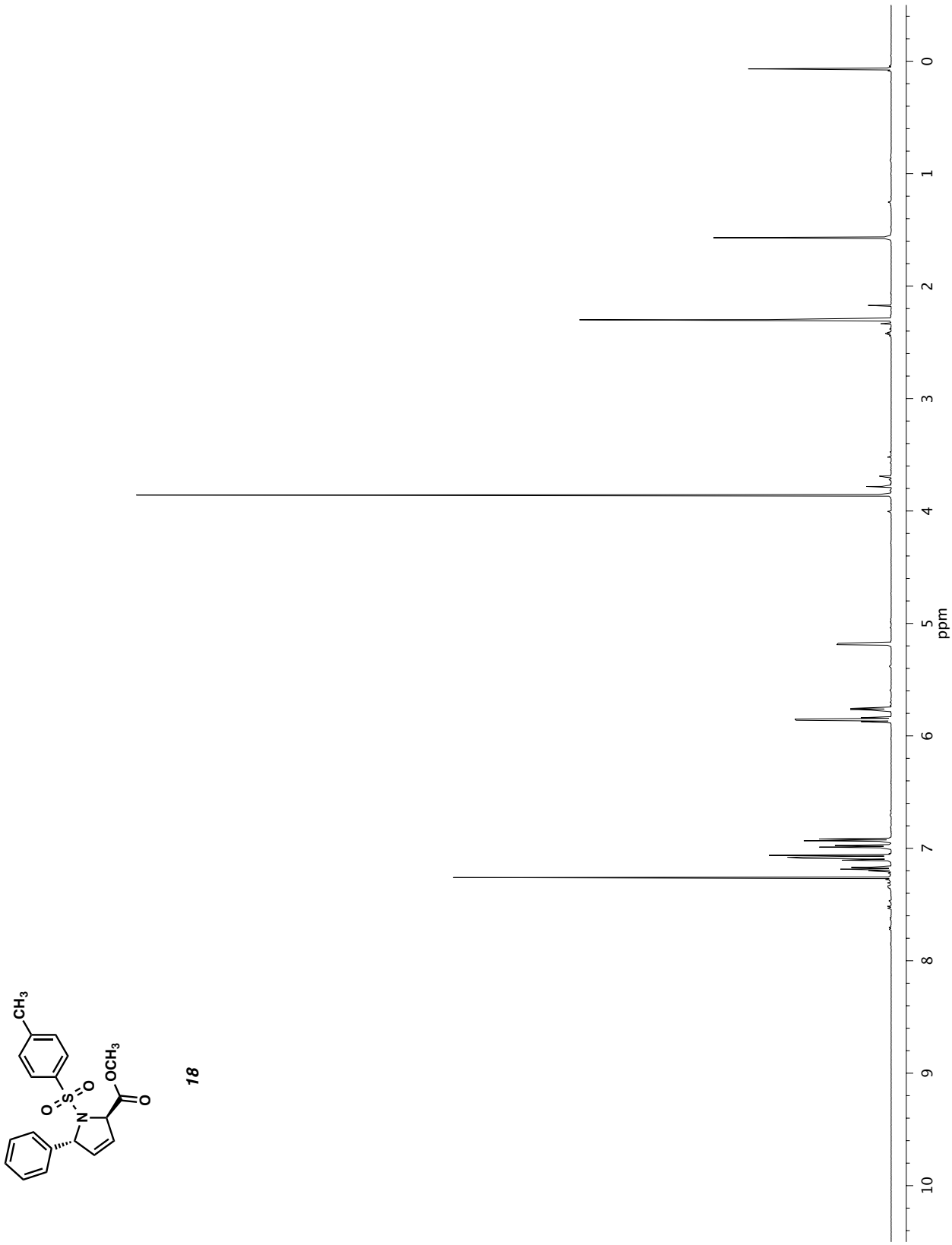
^{1}H NMR (500 MHz, CD_2Cl_2) of compound **(*S*)-25**.



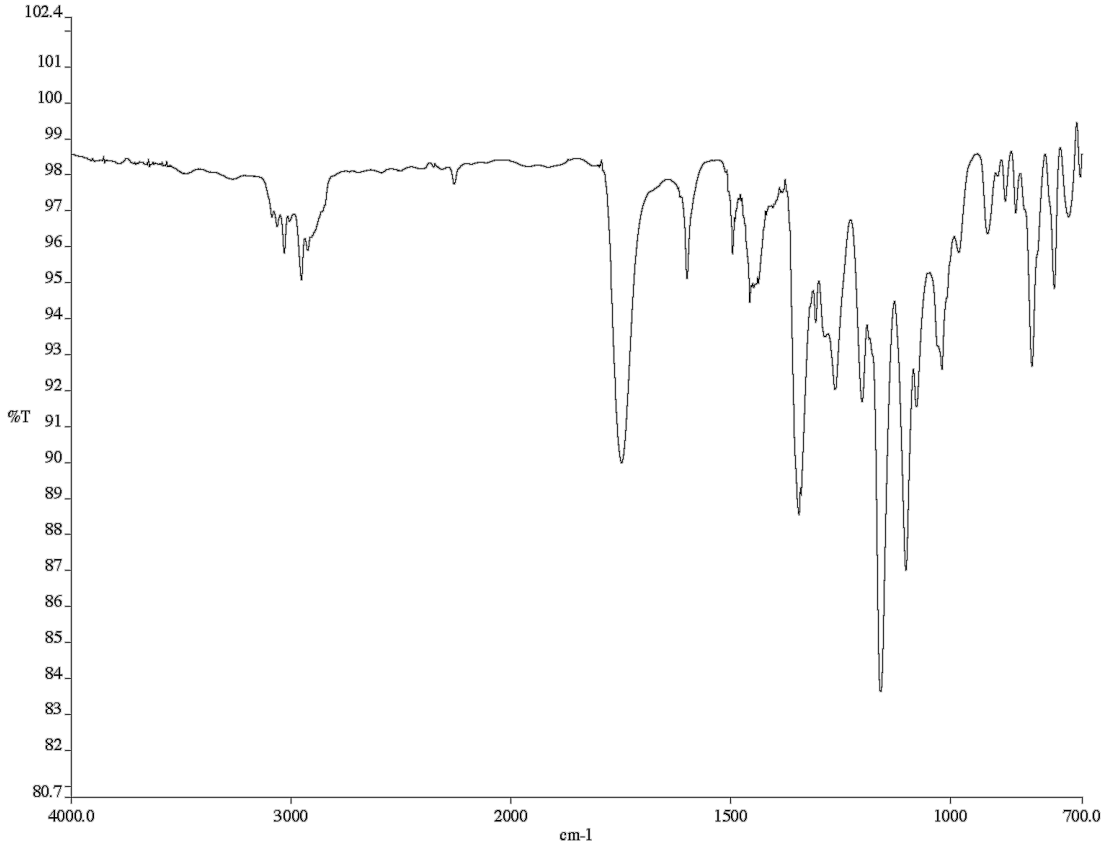
Infrared spectrum (Thin Film, NaCl) of compound **(*S*)-25**.



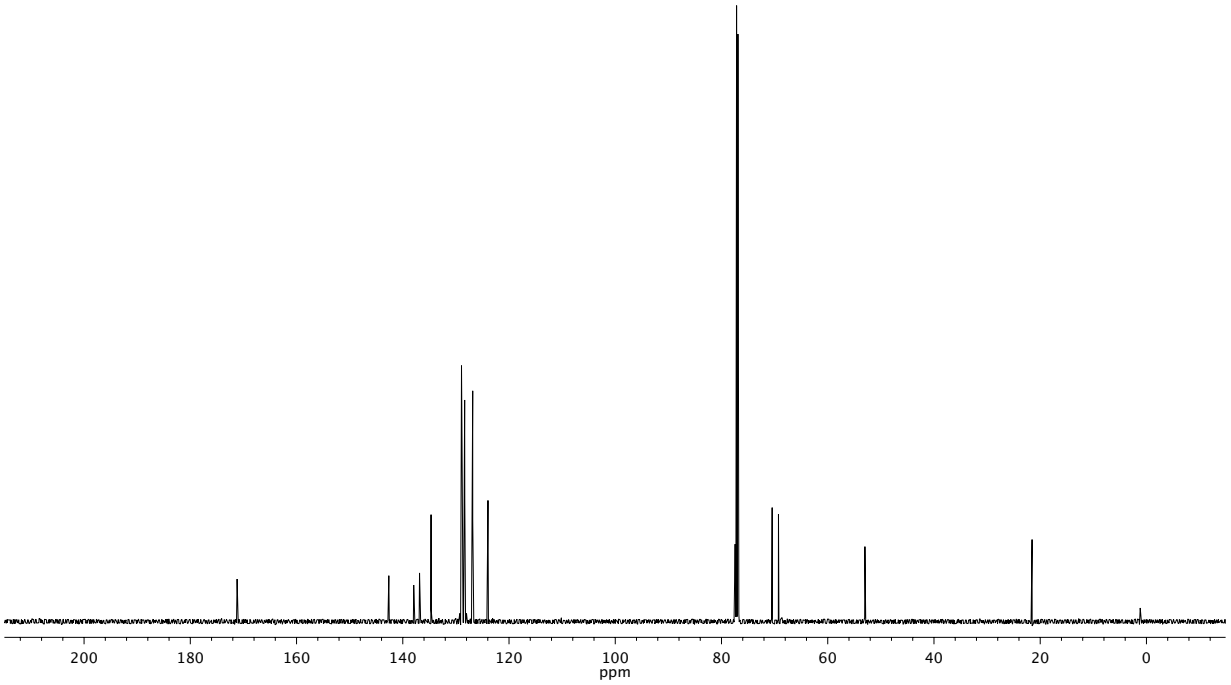
^{13}C NMR (126 MHz, CD_2Cl_2) of compound **(S)-25**.



^{1}H NMR (500 MHz, $CDCl_3$) of compound **18**.



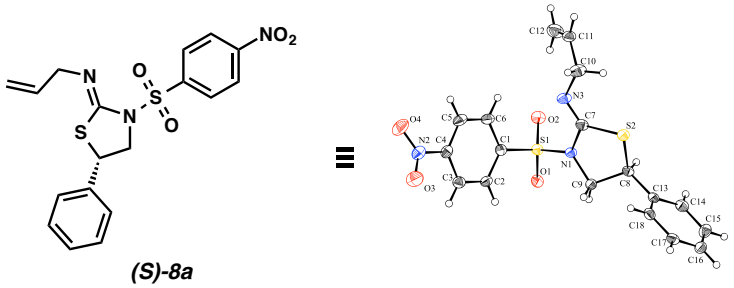
Infrared spectrum (Thin Film, NaCl) of compound **18**.



^{13}C NMR (126 MHz, $CDCl_3$) of compound **18**.

Crystallography Data

(*S*,*Z*)-5-phenyl-3-(*p*-nitrobenzenesulfonyl)-2-(allylimino)thiazolidine ((*S*)-8a):



Low-temperature diffraction data (and scans) were collected on a Bruker Kappa diffractometer coupled to a Apex II CCD detector with graphite monochromated Mo *K* radiation (= 0.71073 Å) for the structure of **(*S*)-8a**. The structure was solved by direct methods using SHELXS and refined against F^2 on all data by full-matrix least squares with SHELXL-2013 refinement using established techniques. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3- distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters.

Table 1. Crystal data and structure refinement for Compound **(*S*)-8a**.

Identification code	a13024
CCDC Deposition Number	973929
Empirical formula	C18 H17 N3 O4 S2
Formula weight	433.95
Crystallization solvent	Ethyl Acetate/Heptane/Benzene
Crystal shape	blade
Crystal color	colourless
Crystal size	0.04 x 0.11 x 0.40 mm
Preliminary photograph(s)	rotation
Type of diffractometer	Bruker APEX-II CCD
Wavelength	0.71073 Å MoK
Data collection temperature	100 K
Theta range for 9894 reflections used	

in lattice determination	2.34 to 26.36°	
Unit cell dimensions	a = 29.071(2) Å	α= 90°
	b = 6.0386(5) Å	β= 94.233(3)°
	c = 23.0477(19) Å	γ = 90°
Volume	4034.9(6) $Å^3$	
Z	8	
Crystal system	monoclinic	
Space group	C 1 2 1 (# 5)	
Density (calculated)	1.429 g/cm^3	
F(000)	1802	
Theta range for data collection	1.6 to 33.0°	
Completeness to theta = 25.000°	99.9%	
Index ranges	-42<=h<=44, -8<=k<=9, -35<=l<=35	
Reflections collected	71248	
Independent reflections	12862 [R_{int}= 0.0785]	
Reflections > 2s(I)	8839	
Average s(I)/(net I)	0.0814	
Absorption coefficient	0.30 mm^{-1}	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.8747	
Primary solution method	dual	
Hydrogen placement	geom	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12862 / 57 / 594	
Treatment of hydrogen atoms	constr	
Goodness-of-fit on F^2	1.01	
Final R indices [I>2s(I), 8839 reflections]	R1 = 0.0523, wR2 = 0.1051	
R indices (all data)	R1 = 0.0985, wR2 = 0.1215	
Type of weighting scheme used	calc	
Weighting scheme used	w=1/[^2^(Fo^2^)+(0.0559P)^2^+1.2322P] where	
	P=(Fo^2^+2Fc^2^)/3	
Max shift/error	0.001	
Average shift/error	0.000	
Absolute structure parameter	0.08(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.63 and -0.45 $e·Å^{-3}$	

Programs Used

Cell refinement	SAINT V8.32B (Bruker-AXS, 2007)
Data collection	APEX2 2013.6-2 (Bruker-AXS, 2007)
Data reduction	SAINT V8.32B (Bruker-AXS, 2007)
Structure solution	SHELXT (Sheldrick, 2012)
Structure refinement	SHELXL-2013/2 (Sheldrick, 2013)
Graphics	DIAMOND 3 (Crystal Impact, 1999)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for Compound **(*S*)-8a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
S(1)	8262(1)	-810(2)	7758(1)	19(1)
S(2)	7657(1)	76(2)	9340(1)	21(1)
O(1)	8012(1)	158(4)	7260(1)	22(1)
O(2)	8329(1)	-3134(4)	7794(1)	25(1)
O(3)	10067(1)	5822(5)	8110(1)	40(1)
O(4)	10425(1)	2713(5)	8234(1)	44(1)
N(1)	7986(1)	23(5)	8320(1)	20(1)
N(2)	10073(1)	3806(6)	8126(1)	28(1)
N(3)	8456(1)	-1870(5)	9026(1)	26(1)
C(1)	8809(1)	482(6)	7843(1)	20(1)
C(2)	8859(1)	2557(6)	7599(1)	20(1)
C(3)	9278(1)	3659(6)	7690(1)	24(1)
C(4)	9634(1)	2609(6)	8012(1)	23(1)
C(5)	9595(1)	498(6)	8237(1)	26(1)
C(6)	9177(1)	-574(6)	8158(1)	24(1)
C(7)	8098(1)	-772(6)	8892(1)	21(1)
C(8)	7276(1)	855(5)	8701(1)	18(1)
C(9)	7616(1)	1693(6)	8273(1)	20(1)
C(10)	8540(1)	-2675(7)	9616(1)	35(1)
C(11)	8739(1)	-4949(7)	9632(1)	26(1)
C(12)	8780(1)	-6214(7)	9179(2)	38(1)
C(13)	6914(1)	2514(6)	8844(1)	19(1)
C(14)	6448(1)	1979(6)	8723(1)	24(1)
C(15)	6108(1)	3500(6)	8831(1)	27(1)
C(16)	6225(1)	5531(6)	9070(1)	26(1)
C(17)	6686(1)	6055(6)	9207(1)	22(1)
C(18)	7027(1)	4541(5)	9093(1)	22(1)
S(1A)	1850(1)	2774(2)	7236(1)	24(1)
S(2A)	2370(2)	1779(14)	5621(2)	32(1)
S(2AA)	2253(3)	897(17)	5560(2)	29(1)
O(1A)	2091(1)	1685(4)	7716(1)	27(1)
O(2A)	1813(1)	5115(5)	7229(1)	31(1)

O(3A)	-335(1)	-199(6)	6712(2)	52(1)
O(4A)	-13(1)	-3389(5)	6842(1)	46(1)
N(1A)	2107(1)	1906(5)	6660(1)	25(1)
N(2A)	0(1)	-1372(6)	6830(1)	33(1)
N(3A)	1711(1)	4307(6)	5995(1)	32(1)
C(1A)	1291(1)	1635(6)	7142(1)	22(1)
C(2A)	1220(1)	-452(6)	7371(1)	26(1)
C(3A)	792(1)	-1444(6)	7274(2)	28(1)
C(4A)	450(1)	-287(7)	6954(2)	28(1)
C(5A)	509(1)	1817(7)	6744(2)	31(1)
C(6A)	940(1)	2785(7)	6830(1)	28(1)
C(7A)	1997(1)	2800(7)	6099(1)	25(1)
C(8A)	2550(1)	-700(8)	6107(2)	39(1)
C(9A)	2328(4)	-430(20)	6676(4)	32(2)
C(9AA)	2448(5)	360(20)	6736(6)	18(3)
C(10A)	1625(1)	5058(8)	5392(1)	38(1)
C(11A)	1359(2)	7136(9)	5353(2)	55(1)
C(12A)	1227(2)	8304(9)	5780(2)	66(2)
C(13A)	3068(1)	-809(7)	6117(1)	23(1)
C(14A)	3272(1)	-2798(6)	5960(1)	28(1)
C(15A)	3756(1)	-2909(9)	5974(2)	43(1)
C(16A)	4014(1)	-1147(10)	6144(2)	51(1)
C(17A)	3809(2)	801(9)	6298(2)	55(1)
C(18A)	3343(2)	954(7)	6286(2)	39(1)
C(19)	50(20)	8890(100)	4820(20)	234(16)
C(20)	-10(17)	6960(100)	5284(17)	235(14)
C(21)	-90(18)	5080(100)	4796(17)	219(12)
C(22)	168(14)	3320(90)	5179(15)	209(12)
C(23)	33(10)	1280(80)	4797(11)	170(10)
C(24)	9986(11)	1970(170)	10141(12)	340(30)
C(25)	10106(12)	3650(130)	9638(15)	360(30)
C(26)	10000	5830(130)	10000	360(30)
C(27)	9890(13)	7930(120)	9647(18)	370(30)
C(28)	9970(16)	9370(170)	10187(16)	340(30)

Table 3. Bond lengths [Å] and angles [°] for Compound **(*S*)-8a**.

S(1)-O(1)	1.437(2)
S(1)-O(2)	1.418(3)
S(1)-N(1)	1.653(3)
S(1)-C(1)	1.767(3)
S(2)-C(7)	1.780(3)
S(2)-C(8)	1.839(3)
O(3)-N(2)	1.218(4)
O(4)-N(2)	1.228(4)
N(1)-C(7)	1.416(4)
N(1)-C(9)	1.473(4)
N(2)-C(4)	1.472(4)
N(3)-C(7)	1.253(4)
N(3)-C(10)	1.447(4)
C(1)-C(2)	1.386(5)
C(1)-C(6)	1.401(4)
C(2)-H(2)	0.9500
C(2)-C(3)	1.389(5)
C(3)-H(3)	0.9500
C(3)-C(4)	1.382(4)
C(4)-C(5)	1.384(5)
C(5)-H(5)	0.9500
C(5)-C(6)	1.378(5)
C(6)-H(6)	0.9500
C(8)-H(8)	1.0000
C(8)-C(9)	1.533(4)
C(8)-C(13)	1.508(4)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10C)	0.9900
C(10)-H(10D)	0.9900
C(10)-C(11)	1.490(5)
C(11)-H(11)	0.9500
C(11)-C(12)	1.306(5)
C(12)-H(12C)	0.9500
C(12)-H(12D)	0.9500
C(13)-C(14)	1.399(4)
C(13)-C(18)	1.383(5)
C(14)-H(14)	0.9500
C(14)-C(15)	1.384(5)
C(15)-H(15)	0.9500
C(15)-C(16)	1.376(5)
C(16)-H(16)	0.9500
C(16)-C(17)	1.390(5)
C(17)-H(17)	0.9500
C(17)-C(18)	1.389(5)
C(18)-H(18)	0.9500
S(1A)-O(1A)	1.426(2)
S(1A)-O(2A)	1.418(3)
S(1A)-N(1A)	1.656(3)
S(1A)-C(1A)	1.763(3)
S(2A)-C(7A)	1.718(4)
S(2A)-C(8A)	1.919(6)

S(2AA)-C(7A)	1.886(7)
S(2AA)-C(8A)	1.763(6)
O(3A)-N(2A)	1.218(4)
O(4A)-N(2A)	1.219(4)
N(1A)-C(7A)	1.415(4)
N(1A)-C(9A)	1.548(12)
N(1A)-C(9AA)	1.364(14)
N(2A)-C(4A)	1.472(5)
N(3A)-C(7A)	1.243(5)
N(3A)-C(10A)	1.465(4)
C(1A)-C(2A)	1.388(5)
C(1A)-C(6A)	1.389(5)
C(2A)-H(2A)	0.9500
C(2A)-C(3A)	1.384(5)
C(3A)-H(3A)	0.9500
C(3A)-C(4A)	1.384(5)
C(4A)-C(5A)	1.375(6)
C(5A)-H(5A)	0.9500
C(5A)-C(6A)	1.383(5)
C(6A)-H(6A)	0.9500
C(8A)-H(8A)	1.0000
C(8A)-H(8AA)	1.0000
C(8A)-C(9A)	1.512(10)
C(8A)-C(9AA)	1.630(13)
C(8A)-C(13A)	1.506(5)
C(9A)-H(9AA)	0.9900
C(9A)-H(9AB)	0.9900
C(9AA)-H(9AC)	0.9900
C(9AA)-H(9AD)	0.9900
C(10A)-H(10A)	0.9900
C(10A)-H(10B)	0.9900
C(10A)-C(11A)	1.473(6)
C(11A)-H(11A)	0.9500
C(11A)-C(12A)	1.293(6)
C(12A)-H(12A)	0.9500
C(12A)-H(12B)	0.9500
C(13A)-C(14A)	1.399(5)
C(13A)-C(18A)	1.370(5)
C(14A)-H(14A)	0.9500
C(14A)-C(15A)	1.409(5)
C(15A)-H(15A)	0.9500
C(15A)-C(16A)	1.343(7)
C(16A)-H(16A)	0.9500
C(16A)-C(17A)	1.378(7)
C(17A)-H(17A)	0.9500
C(17A)-C(18A)	1.358(7)
C(18A)-H(18A)	0.9500
C(19)-C(19)#1	0.90(10)
C(19)-C(20)	1.60(2)
C(19)-C(20)#1	1.20(4)
C(19)-C(23)#2	1.45(4)
C(19)-C(23)#3	1.72(4)
C(20)-C(19)#1	1.20(4)
C(20)-C(20)#1	1.31(8)

C(20)-C(21)#1	1.19(4)
C(20)-C(21)	1.60(2)
C(21)-C(20)#1	1.19(4)
C(21)-C(21)#1	1.04(7)
C(21)-C(22)#1	1.09(4)
C(21)-C(22)	1.54(2)
C(22)-C(21)#1	1.09(4)
C(22)-C(22)#1	1.23(7)
C(22)-C(23)#1	1.37(4)
C(22)-C(23)	1.55(2)
C(23)-C(19)#4	1.72(4)
C(23)-C(19)#5	1.45(4)
C(23)-C(22)#1	1.37(4)
C(23)-C(23)#1	0.97(4)
C(24)-C(24)#6	0.66(5)
C(24)-C(25)	1.60(2)
C(24)-C(25)#6	1.18(5)
C(24)-C(28)#5	1.57(7)
C(24)-C(28)#7	1.75(6)
C(25)-C(24)#6	1.18(5)
C(25)-C(25)#6	1.82(7)
C(25)-C(26)	1.60(2)
C(26)-C(25)#6	1.60(2)
C(26)-C(27)#6	1.53(2)
C(26)-C(27)	1.53(2)
C(27)-C(27)#6	1.70(8)
C(27)-C(28)	1.52(2)
C(27)-C(28)#6	1.02(6)
C(28)-C(24)#8	1.75(6)
C(28)-C(24)#2	1.57(7)
C(28)-C(27)#6	1.02(6)
C(28)-C(28)#6	0.89(9)

O(1)-S(1)-N(1)	104.85(13)
O(1)-S(1)-C(1)	107.87(15)
O(2)-S(1)-O(1)	120.48(15)
O(2)-S(1)-N(1)	109.13(15)
O(2)-S(1)-C(1)	108.25(15)
N(1)-S(1)-C(1)	105.26(14)
C(7)-S(2)-C(8)	91.39(14)
C(7)-N(1)-S(1)	122.3(2)
C(7)-N(1)-C(9)	114.6(2)
C(9)-N(1)-S(1)	123.0(2)
O(3)-N(2)-O(4)	123.6(3)
O(3)-N(2)-C(4)	118.4(3)
O(4)-N(2)-C(4)	118.0(3)
C(7)-N(3)-C(10)	119.3(3)
C(2)-C(1)-S(1)	118.3(2)
C(2)-C(1)-C(6)	121.5(3)
C(6)-C(1)-S(1)	120.2(3)
C(1)-C(2)-H(2)	120.4
C(1)-C(2)-C(3)	119.3(3)
C(3)-C(2)-H(2)	120.4
C(2)-C(3)-H(3)	120.8

C(4)-C(3)-C(2)	118.3(3)
C(4)-C(3)-H(3)	120.8
C(3)-C(4)-N(2)	118.4(3)
C(3)-C(4)-C(5)	123.0(3)
C(5)-C(4)-N(2)	118.6(3)
C(4)-C(5)-H(5)	120.7
C(6)-C(5)-C(4)	118.6(3)
C(6)-C(5)-H(5)	120.7
C(1)-C(6)-H(6)	120.4
C(5)-C(6)-C(1)	119.2(3)
C(5)-C(6)-H(6)	120.4
N(1)-C(7)-S(2)	108.5(2)
N(3)-C(7)-S(2)	129.0(2)
N(3)-C(7)-N(1)	122.5(3)
S(2)-C(8)-H(8)	108.9
C(9)-C(8)-S(2)	102.8(2)
C(9)-C(8)-H(8)	108.9
C(13)-C(8)-S(2)	112.5(2)
C(13)-C(8)-H(8)	108.9
C(13)-C(8)-C(9)	114.6(3)
N(1)-C(9)-C(8)	103.2(2)
N(1)-C(9)-H(9A)	111.1
N(1)-C(9)-H(9B)	111.1
C(8)-C(9)-H(9A)	111.1
C(8)-C(9)-H(9B)	111.1
H(9A)-C(9)-H(9B)	109.1
N(3)-C(10)-H(10C)	109.3
N(3)-C(10)-H(10D)	109.3
N(3)-C(10)-C(11)	111.8(3)
H(10C)-C(10)-H(10D)	107.9
C(11)-C(10)-H(10C)	109.3
C(11)-C(10)-H(10D)	109.3
C(10)-C(11)-H(11)	117.4
C(12)-C(11)-C(10)	125.3(3)
C(12)-C(11)-H(11)	117.4
C(11)-C(12)-H(12C)	120.0
C(11)-C(12)-H(12D)	120.0
H(12C)-C(12)-H(12D)	120.0
C(14)-C(13)-C(8)	119.0(3)
C(18)-C(13)-C(8)	122.0(3)
C(18)-C(13)-C(14)	119.0(3)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-C(13)	120.2(3)
C(15)-C(14)-H(14)	119.9
C(14)-C(15)-H(15)	119.8
C(16)-C(15)-C(14)	120.4(3)
C(16)-C(15)-H(15)	119.8
C(15)-C(16)-H(16)	120.1
C(15)-C(16)-C(17)	119.8(3)
C(17)-C(16)-H(16)	120.1
C(16)-C(17)-H(17)	120.1
C(18)-C(17)-C(16)	119.9(3)
C(18)-C(17)-H(17)	120.1
C(13)-C(18)-C(17)	120.6(3)

C(13)-C(18)-H(18)	119.7
C(17)-C(18)-H(18)	119.7
O(1A)-S(1A)-N(1A)	104.59(15)
O(1A)-S(1A)-C(1A)	108.09(16)
O(2A)-S(1A)-O(1A)	120.09(16)
O(2A)-S(1A)-N(1A)	110.18(16)
O(2A)-S(1A)-C(1A)	108.57(17)
N(1A)-S(1A)-C(1A)	104.15(15)
C(7A)-S(2A)-C(8A)	93.6(2)
C(8A)-S(2AA)-C(7A)	93.3(2)
C(7A)-N(1A)-S(1A)	121.7(3)
C(7A)-N(1A)-C(9A)	115.8(5)
C(9A)-N(1A)-S(1A)	118.7(4)
C(9AA)-N(1A)-S(1A)	118.7(6)
C(9AA)-N(1A)-C(7A)	119.5(6)
O(3A)-N(2A)-O(4A)	124.1(4)
O(3A)-N(2A)-C(4A)	118.0(3)
O(4A)-N(2A)-C(4A)	117.9(3)
C(7A)-N(3A)-C(10A)	118.3(3)
C(2A)-C(1A)-S(1A)	118.0(3)
C(2A)-C(1A)-C(6A)	121.7(3)
C(6A)-C(1A)-S(1A)	120.3(3)
C(1A)-C(2A)-H(2A)	120.4
C(3A)-C(2A)-C(1A)	119.2(3)
C(3A)-C(2A)-H(2A)	120.4
C(2A)-C(3A)-H(3A)	121.0
C(2A)-C(3A)-C(4A)	118.0(3)
C(4A)-C(3A)-H(3A)	121.0
C(3A)-C(4A)-N(2A)	118.2(3)
C(5A)-C(4A)-N(2A)	118.4(3)
C(5A)-C(4A)-C(3A)	123.4(3)
C(4A)-C(5A)-H(5A)	120.8
C(4A)-C(5A)-C(6A)	118.4(4)
C(6A)-C(5A)-H(5A)	120.8
C(1A)-C(6A)-H(6A)	120.4
C(5A)-C(6A)-C(1A)	119.1(4)
C(5A)-C(6A)-H(6A)	120.4
N(1A)-C(7A)-S(2A)	109.7(3)
N(1A)-C(7A)-S(2AA)	107.2(3)
N(3A)-C(7A)-S(2A)	125.7(3)
N(3A)-C(7A)-S(2AA)	127.5(3)
N(3A)-C(7A)-N(1A)	124.0(3)
S(2A)-C(8A)-H(8A)	108.0
S(2AA)-C(8A)-H(8AA)	108.6
C(9A)-C(8A)-S(2A)	107.8(5)
C(9A)-C(8A)-H(8A)	108.0
C(9AA)-C(8A)-S(2AA)	108.1(6)
C(9AA)-C(8A)-H(8AA)	108.6
C(13A)-C(8A)-S(2A)	105.7(3)
C(13A)-C(8A)-S(2AA)	118.1(4)
C(13A)-C(8A)-H(8A)	108.0
C(13A)-C(8A)-H(8AA)	108.6
C(13A)-C(8A)-C(9A)	118.8(5)
C(13A)-C(8A)-C(9AA)	104.6(6)

N(1A)-C(9A)-H(9AA)	110.5
N(1A)-C(9A)-H(9AB)	110.5
C(8A)-C(9A)-N(1A)	106.3(7)
C(8A)-C(9A)-H(9AA)	110.5
C(8A)-C(9A)-H(9AB)	110.5
H(9AA)-C(9A)-H(9AB)	108.7
N(1A)-C(9AA)-C(8A)	109.4(9)
N(1A)-C(9AA)-H(9AC)	109.8
N(1A)-C(9AA)-H(9AD)	109.8
C(8A)-C(9AA)-H(9AC)	109.8
C(8A)-C(9AA)-H(9AD)	109.8
H(9AC)-C(9AA)-H(9AD)	108.2
N(3A)-C(10A)-H(10A)	109.2
N(3A)-C(10A)-H(10B)	109.2
N(3A)-C(10A)-C(11A)	112.0(3)
H(10A)-C(10A)-H(10B)	107.9
C(11A)-C(10A)-H(10A)	109.2
C(11A)-C(10A)-H(10B)	109.2
C(10A)-C(11A)-H(11A)	116.5
C(12A)-C(11A)-C(10A)	127.0(4)
C(12A)-C(11A)-H(11A)	116.5
C(11A)-C(12A)-H(12A)	120.0
C(11A)-C(12A)-H(12B)	120.0
H(12A)-C(12A)-H(12B)	120.0
C(14A)-C(13A)-C(8A)	118.4(4)
C(18A)-C(13A)-C(8A)	122.1(4)
C(18A)-C(13A)-C(14A)	119.5(3)
C(13A)-C(14A)-H(14A)	120.8
C(13A)-C(14A)-C(15A)	118.4(4)
C(15A)-C(14A)-H(14A)	120.8
C(14A)-C(15A)-H(15A)	119.8
C(16A)-C(15A)-C(14A)	120.4(4)
C(16A)-C(15A)-H(15A)	119.8
C(15A)-C(16A)-H(16A)	119.7
C(15A)-C(16A)-C(17A)	120.5(4)
C(17A)-C(16A)-H(16A)	119.7
C(16A)-C(17A)-H(17A)	119.9
C(18A)-C(17A)-C(16A)	120.2(4)
C(18A)-C(17A)-H(17A)	119.9
C(13A)-C(18A)-H(18A)	119.6
C(17A)-C(18A)-C(13A)	120.9(4)
C(17A)-C(18A)-H(18A)	119.6
C(19)#1-C(19)-C(20)#1	98(4)
C(19)#1-C(19)-C(20)	48(2)
C(19)#1-C(19)-C(23)#2	91(2)
C(19)#1-C(19)-C(23)#3	57.4(16)
C(20)#1-C(19)-C(20)	54(4)
C(20)#1-C(19)-C(23)#2	164(6)
C(20)-C(19)-C(23)#3	104(3)
C(20)#1-C(19)-C(23)#3	155(5)
C(23)#2-C(19)-C(20)	139(4)
C(23)#2-C(19)-C(23)#3	34.3(18)
C(19)#1-C(20)-C(19)	34(4)
C(19)#1-C(20)-C(20)#1	79(4)

C(19)-C(20)-C(21)	94(3)
C(19)#1-C(20)-C(21)	123(4)
C(20)#1-C(20)-C(19)	47.3(19)
C(20)#1-C(20)-C(21)	46.9(19)
C(21)#1-C(20)-C(19)	124(4)
C(21)#1-C(20)-C(19)#1	157(7)
C(21)#1-C(20)-C(20)#1	79(3)
C(21)#1-C(20)-C(21)	41(3)
C(20)#1-C(21)-C(20)	54(4)
C(20)#1-C(21)-C(22)	129(4)
C(21)#1-C(21)-C(20)#1	92(4)
C(21)#1-C(21)-C(20)	48(2)
C(21)#1-C(21)-C(22)	44.9(19)
C(21)#1-C(21)-C(22)#1	93(3)
C(22)#1-C(21)-C(20)#1	174(6)
C(22)#1-C(21)-C(20)	132(4)
C(22)-C(21)-C(20)	93(2)
C(22)#1-C(21)-C(22)	53(4)
C(21)#1-C(22)-C(21)	42(4)
C(21)#1-C(22)-C(22)#1	83(3)
C(21)#1-C(22)-C(23)#1	142(5)
C(21)#1-C(22)-C(23)	139(4)
C(21)-C(22)-C(23)	97(2)
C(22)#1-C(22)-C(21)	44.5(17)
C(22)#1-C(22)-C(23)#1	73(2)
C(22)#1-C(22)-C(23)	57.5(18)
C(23)#1-C(22)-C(21)	117(3)
C(23)#1-C(22)-C(23)	38.1(19)
C(19)#5-C(23)-C(19)#4	31(3)
C(19)#5-C(23)-C(22)	140(4)
C(22)-C(23)-C(19)#4	115(2)
C(22)#1-C(23)-C(19)#5	156(4)
C(22)#1-C(23)-C(19)#4	131(3)
C(22)#1-C(23)-C(22)	50(3)
C(23)#1-C(23)-C(19)#5	88(2)
C(23)#1-C(23)-C(19)#4	57.4(15)
C(23)#1-C(23)-C(22)	61(2)
C(23)#1-C(23)-C(22)#1	81.2(19)
C(24)#6-C(24)-C(25)#6	118(3)
C(24)#6-C(24)-C(25)	40(2)
C(24)#6-C(24)-C(28)#5	94(2)
C(24)#6-C(24)-C(28)#7	63.7(17)
C(25)#6-C(24)-C(25)	80(5)
C(25)#6-C(24)-C(28)#5	146(3)
C(25)-C(24)-C(28)#7	103(3)
C(25)#6-C(24)-C(28)#7	171(4)
C(28)#5-C(24)-C(25)	134(4)
C(28)#5-C(24)-C(28)#7	31(4)
C(24)#6-C(25)-C(24)	21.4(19)
C(24)-C(25)-C(25)#6	40(2)
C(24)#6-C(25)-C(25)#6	60(2)
C(24)#6-C(25)-C(26)	115(4)
C(26)-C(25)-C(24)	95(4)
C(26)-C(25)-C(25)#6	55.3(15)

C(25)-C(26)-C(25)#6	69(3)
C(27)-C(26)-C(25)	116.5(19)
C(27)#6-C(26)-C(25)	157(2)
C(27)-C(26)-C(25)#6	157(2)
C(27)#6-C(26)-C(25)#6	116.5(19)
C(27)#6-C(26)-C(27)	68(3)
C(26)-C(27)-C(27)#6	56.2(17)
C(28)#6-C(27)-C(26)	116(5)
C(28)-C(27)-C(26)	91(4)
C(28)#6-C(27)-C(27)#6	62(3)
C(28)-C(27)-C(27)#6	36(3)
C(28)#6-C(27)-C(28)	35(5)
C(24)#2-C(28)-C(24)#8	22.2(18)
C(27)#6-C(28)-C(24)#2	149(4)
C(27)-C(28)-C(24)#8	100(3)
C(27)-C(28)-C(24)#2	121(4)
C(27)#6-C(28)-C(24)#8	152(6)
C(27)#6-C(28)-C(27)	82(6)
C(28)#6-C(28)-C(24)#8	63.7(17)
C(28)#6-C(28)-C(24)#2	86(2)
C(28)#6-C(28)-C(27)	40(3)
C(28)#6-C(28)-C(27)#6	105(7)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1 #2 x,y+1,z #3 -x,y+1,-z+1 #4 -x,y-1,-z+1
#5 x,y-1,z #6 -x+2,y,-z+2 #7 -x+2,y-1,-z+2
#8 -x+2,y+1,-z+2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for Compound **(*S*)-8a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

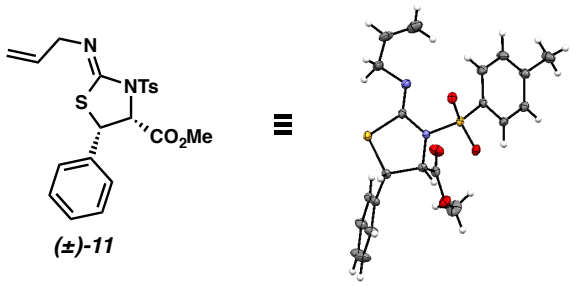
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	238(4)	213(4)	119(3)	-6(3)	17(3)	23(3)
S(2)	242(4)	282(4)	118(3)	15(3)	13(3)	50(3)
O(1)	256(11)	298(13)	112(9)	4(10)	11(8)	11(10)
O(2)	328(13)	232(13)	197(11)	-32(10)	9(10)	17(11)
O(3)	336(15)	298(16)	559(18)	-20(14)	-52(13)	-32(12)
O(4)	236(13)	475(18)	579(18)	-18(16)	-69(12)	67(14)
N(1)	236(13)	233(14)	117(11)	37(11)	22(9)	60(12)
N(2)	242(15)	320(20)	285(15)	-33(13)	-11(11)	40(13)
N(3)	339(16)	298(17)	139(12)	30(12)	2(11)	116(13)
C(1)	232(15)	216(19)	140(13)	-14(12)	31(11)	28(12)
C(2)	219(15)	213(18)	167(14)	-4(13)	9(11)	63(13)
C(3)	260(17)	233(19)	213(15)	9(13)	21(12)	27(13)
C(4)	212(15)	260(18)	214(15)	-36(14)	13(12)	33(14)
C(5)	243(17)	290(20)	239(17)	4(14)	-41(13)	88(14)
C(6)	283(17)	234(19)	210(15)	33(14)	14(12)	84(14)
C(7)	289(16)	198(16)	150(14)	2(14)	25(11)	21(14)
C(8)	230(15)	171(15)	133(13)	3(11)	4(11)	-2(12)
C(9)	206(15)	249(17)	130(13)	22(13)	14(11)	39(13)
C(10)	480(20)	430(30)	142(15)	30(15)	1(14)	196(19)
C(11)	307(17)	262(18)	198(15)	49(15)	29(13)	72(16)
C(12)	500(20)	260(20)	390(20)	26(18)	74(18)	21(18)
C(13)	229(15)	231(18)	113(13)	50(12)	28(11)	30(13)
C(14)	271(17)	259(18)	170(14)	19(13)	-21(12)	-16(14)
C(15)	195(16)	380(20)	218(16)	4(15)	-18(12)	29(14)
C(16)	247(17)	330(20)	194(15)	60(14)	44(12)	81(14)
C(17)	317(18)	165(16)	177(14)	3(13)	50(12)	8(13)
C(18)	233(16)	236(19)	186(14)	32(12)	36(12)	-16(13)
S(1A)	327(4)	267(5)	126(3)	-18(3)	-5(3)	-33(4)
S(2A)	324(16)	500(30)	143(9)	71(12)	55(9)	189(17)
S(2AA)	313(19)	400(30)	162(12)	-68(14)	22(11)	50(20)
O(1A)	313(13)	344(15)	152(11)	14(10)	-14(9)	-53(11)
O(2A)	425(14)	302(14)	193(11)	-37(11)	-40(10)	-56(12)
O(3A)	272(15)	510(20)	770(20)	-73(18)	-53(14)	63(14)
O(4A)	383(17)	385(19)	600(20)	13(16)	-35(14)	-55(14)
N(1A)	313(15)	304(16)	129(12)	11(12)	29(11)	-16(13)
N(2A)	288(17)	370(20)	343(17)	-34(14)	13(13)	-2(14)
N(3A)	427(18)	369(18)	152(13)	16(13)	-6(12)	57(15)
C(1A)	277(17)	226(18)	150(14)	-37(13)	39(12)	-15(14)
C(2A)	272(17)	330(20)	198(15)	25(14)	51(12)	18(14)
C(3A)	309(19)	280(20)	244(17)	29(14)	56(14)	0(14)
C(4A)	242(17)	340(20)	281(18)	-55(16)	41(13)	6(14)
C(5A)	303(19)	320(20)	300(19)	-35(17)	-45(15)	49(16)
C(6A)	366(19)	245(19)	239(16)	-45(16)	-8(14)	13(16)
C(7A)	248(16)	370(20)	113(13)	-1(15)	-10(11)	-51(16)
C(8A)	350(20)	620(30)	197(16)	42(18)	76(14)	120(20)
C(9A)	360(50)	390(70)	200(30)	20(40)	80(30)	150(40)
C(9AA)	260(60)	170(70)	110(40)	-40(40)	40(40)	60(40)

C(10A)	510(20)	520(30)	105(14)	-12(17)	-3(14)	130(20)
C(11A)	770(30)	660(30)	204(19)	90(20)	-10(20)	330(30)
C(12A)	1110(40)	550(30)	330(20)	60(20)	70(30)	370(30)
C(13A)	273(16)	291(18)	128(13)	27(14)	11(11)	69(15)
C(14A)	420(20)	270(20)	139(14)	41(13)	6(13)	-3(15)
C(15A)	370(20)	680(30)	245(18)	180(20)	48(16)	220(20)
C(16A)	290(20)	890(40)	360(20)	340(30)	-41(16)	-50(20)
C(17A)	610(30)	580(30)	420(20)	310(20)	-230(20)	-280(30)
C(18A)	650(30)	260(20)	240(18)	41(16)	-118(18)	-90(20)
C(19)	1400(200)	2800(400)	2700(300)	0(200)	-600(200)	-300(200)
C(20)	1970(190)	2600(400)	2500(200)	-50(180)	200(200)	-100(200)
C(21)	2200(200)	2200(300)	2200(200)	-100(160)	430(180)	70(190)
C(22)	2300(200)	2200(300)	1810(190)	320(160)	500(160)	300(180)
C(23)	1900(200)	2000(300)	1310(170)	170(140)	850(160)	450(190)
C(24)	950(140)	8800(900)	600(160)	500(200)	610(130)	400(300)
C(25)	1010(160)	8800(900)	1100(200)	300(200)	-70(140)	200(200)
C(26)	320(70)	8700(900)	1600(200)	0	-210(100)	0
C(27)	1240(180)	8500(900)	1300(200)	100(200)	60(160)	-400(200)
C(28)	1070(170)	8300(900)	860(190)	-100(300)	-550(170)	-700(300)

Table 5. Hydrogen coordinates (x 10^3) and isotropic displacement parameters (Å^{2}x 10^3) for Compound **(*S*)-8a**.

	x	y	z	U_{iso}
H(2)	861	322	737	24
H(3)	932	510	754	28
H(5)	985	-20	844	31
H(6)	914	-201	831	29
H(8)	712	-51	854	21
H(9A)	747	176	787	23
H(9B)	774	318	839	23
H(10C)	825	-268	981	42
H(10D)	876	-166	984	42
H(11)	885	-552	1000	31
H(12C)	868	-570	880	46
H(12D)	891	-765	923	46
H(14)	636	57	857	28
H(15)	579	314	874	32
H(16)	599	657	914	31
H(17)	677	744	938	26
H(18)	734	490	919	26
H(2A)	146	-119	759	32
H(3A)	74	-288	742	33
H(5A)	26	259	654	37
H(6A)	100	422	668	34
H(8A)	242	-207	591	46
H(8AA)	243	-224	609	46
H(9AA)	256	-55	701	38
H(9AB)	209	-158	672	38
H(9AC)	235	-83	700	21
H(9AD)	273	105	692	21
H(10A)	145	390	516	46
H(10B)	192	528	522	46
H(11A)	128	768	497	66
H(12A)	130	784	617	79
H(12B)	106	963	570	79
H(14A)	309	-405	585	33
H(15A)	390	-424	586	52
H(16A)	434	-124	616	62
H(17A)	400	204	641	66
H(18A)	320	230	640	47

cis-methyl (_Z_)-5-phenyl-3-tosyl-2-(allylimino)thiazolidine-4-carboxylate (11):



Low-temperature diffraction data (and scans) were collected on a Bruker Kappa diffractometer coupled to a Apex II CCD detector with graphite monochromated Mo *K* radiation (= 0.71073 Å) for the structure of **11**. The structure was solved by direct methods using SHELXS and refined against F^2 on all data by full-matrix least squares with SHELXL-2013 refinement using established techniques. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3- distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters.

Compound **11** crystallizes in the triclinic space group *P*-1 with one molecule in the asymmetric unit along with 0.389(2) molecules of benzene and 0.111(2) molecules of ethyl acetate. The partially occupied benzene and ethyl acetate molecules are located at mutually exclusive positions near a crystallographic inversion center and are disordered accordingly. This leads to non-integer values for the atoms in the empirical formula. The carbon atoms in the benzene were restrained to be flat. The 1,2- and 1,3- distances for the ethyl acetate were restrained to be similar to the distances in the ester moiety of the main molecule.

Table 1. Crystal data and structure refinement for Compound **11**.

Identification code	rac15	
CCDC Deposition Number	956878	
Empirical formula	C23.78 H25.22 N2 O4.22 S2	
Formula weight	470.68	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.0719(4) Å	α= 108.416(4)°.
	b = 10.9911(6) Å	β= 102.525(3)°.

	c = 14.6381(8) Å γ = 100.436(2)°.
Volume	1158.33(11) $Å^3$
Z	2
Density (calculated)	1.349 Mg/m^3
Absorption coefficient	0.264 mm^{-1}
F(000)	495
Crystal size	0.450 x 0.400 x 0.050 mm^3
Theta range for data collection	2.028 to 30.611°.
Index ranges	-11<=h<=11, -15<=k<=15, -20<=l<=20
Reflections collected	73111
Independent reflections	7117 [R(int) = 0.0401]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.6920
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7117 / 241 / 375
Goodness-of-fit on F^2	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0335, wR2 = 0.0852
R indices (all data)	R1 = 0.0411, wR2 = 0.0910
Extinction coefficient	n/a
Largest diff. peak and hole	0.519 and -0.298 $e·Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Compound **11**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	6720(1)	912(1)	6958(1)	19(1)
O(2)	7685(1)	-166(1)	5483(1)	18(1)
S(1)	7769(1)	1012(1)	6298(1)	14(1)
C(1)	9977(1)	1738(1)	7028(1)	15(1)
C(2)	10368(2)	2473(1)	8051(1)	22(1)
C(3)	12116(2)	2931(1)	8639(1)	25(1)
C(4)	13466(2)	2658(1)	8223(1)	21(1)
C(5)	13041(1)	1962(1)	7189(1)	20(1)
C(6)	11303(1)	1495(1)	6586(1)	18(1)
C(7)	15338(2)	3066(2)	8883(1)	30(1)
N(1)	7101(1)	1999(1)	5728(1)	14(1)
C(8)	6907(1)	3260(1)	6257(1)	16(1)
N(2)	7432(1)	3818(1)	7202(1)	20(1)
C(11)	6995(2)	5071(1)	7627(1)	27(1)
C(12)	8307(2)	6001(1)	8604(1)	30(1)
C(13)	9751(2)	5797(2)	9062(1)	37(1)
S(2)	5817(1)	3868(1)	5380(1)	19(1)
C(9)	5708(1)	2434(1)	4293(1)	15(1)
C(14)	5921(1)	2800(1)	3405(1)	17(1)
C(15)	4955(2)	1907(1)	2438(1)	25(1)
C(16)	5200(2)	2182(2)	1604(1)	33(1)
C(17)	6411(2)	3338(2)	1730(1)	31(1)
C(18)	7365(2)	4231(1)	2688(1)	24(1)
C(19)	7112(2)	3970(1)	3524(1)	18(1)
C(10)	7117(1)	1788(1)	4692(1)	14(1)
C(20)	8939(1)	2443(1)	4674(1)	17(1)
O(3)	9954(1)	3388(1)	5361(1)	27(1)
O(4)	9225(1)	1840(1)	3801(1)	25(1)
C(21)	10843(2)	2499(2)	3681(1)	39(1)
C(1S)	11128(19)	-483(17)	9748(10)	51(2)
C(2S)	10130(17)	77(11)	9173(10)	49(2)

C(3S)	8871(17)	592(13)	9507(10)	53(3)
C(4S)	8570(20)	585(17)	10386(11)	58(2)
C(5S)	9491(17)	-5(13)	10916(10)	53(2)
C(6S)	10810(18)	-484(13)	10638(9)	48(2)
C(1T)	11250(60)	-420(70)	9690(20)	54(4)
C(2T)	10990(40)	-780(20)	8564(14)	69(5)
O(1T)	12404(19)	-714(14)	10186(10)	63(3)
O(2T)	9820(20)	-163(16)	9947(14)	51(3)
C(3T)	10080(30)	210(30)	11027(16)	56(4)
C(4T)	8270(30)	370(20)	11135(15)	62(5)

Table 3. Bond lengths [Å] and angles [°] for Compound **11**.

O(1)-S(1)	1.4310(8)
O(2)-S(1)	1.4361(8)
S(1)-N(1)	1.6597(9)
S(1)-C(1)	1.7533(11)
C(1)-C(6)	1.3894(14)
C(1)-C(2)	1.3904(15)
C(2)-C(3)	1.3888(17)
C(2)-H(2)	0.9500
C(3)-C(4)	1.3931(16)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3938(16)
C(4)-C(7)	1.5053(16)
C(5)-C(6)	1.3880(15)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
N(1)-C(8)	1.4129(13)
N(1)-C(10)	1.4640(13)
C(8)-N(2)	1.2593(14)
C(8)-S(2)	1.7704(11)
N(2)-C(11)	1.4617(15)
C(11)-C(12)	1.4965(19)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.307(2)
C(12)-H(12)	0.9500
C(13)-H(13A)	0.9500
C(13)-H(13B)	0.9500
S(2)-C(9)	1.8239(11)
C(9)-C(14)	1.5114(14)
C(9)-C(10)	1.5510(14)
C(9)-H(9)	1.0000

C(14)-C(15)	1.3929(15)
C(14)-C(19)	1.3949(15)
C(15)-C(16)	1.3908(18)
C(15)-H(15)	0.9500
C(16)-C(17)	1.389(2)
C(16)-H(16)	0.9500
C(17)-C(18)	1.3827(18)
C(17)-H(17)	0.9500
C(18)-C(19)	1.3898(15)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(10)-C(20)	1.5249(14)
C(10)-H(10)	1.0000
C(20)-O(3)	1.1980(14)
C(20)-O(4)	1.3313(14)
O(4)-C(21)	1.4494(16)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(1S)-C(6S)	1.381(9)
C(1S)-C(2S)	1.396(10)
C(1S)-H(1S)	0.9500
C(2S)-C(3S)	1.358(9)
C(2S)-H(2S)	0.9500
C(3S)-C(4S)	1.363(10)
C(3S)-H(3S)	0.9500
C(4S)-C(5S)	1.348(11)
C(4S)-H(4S)	0.9500
C(5S)-C(6S)	1.354(9)
C(5S)-H(5S)	0.9500
C(6S)-H(6S)	0.9500
C(1T)-O(1T)	1.202(18)
C(1T)-O(2T)	1.340(18)
C(1T)-C(2T)	1.529(17)
C(2T)-H(2T1)	0.9800
C(2T)-H(2T2)	0.9800

C(2T)-H(2T3)	0.9800
O(2T)-C(3T)	1.458(18)
C(3T)-C(4T)	1.539(18)
C(3T)-H(3T1)	0.9900
C(3T)-H(3T2)	0.9900
C(4T)-H(4T1)	0.9800
C(4T)-H(4T2)	0.9800
C(4T)-H(4T3)	0.9800

O(1)-S(1)-O(2)	119.28(5)
O(1)-S(1)-N(1)	107.46(5)
O(2)-S(1)-N(1)	103.82(5)
O(1)-S(1)-C(1)	108.38(5)
O(2)-S(1)-C(1)	108.19(5)
N(1)-S(1)-C(1)	109.37(5)
C(6)-C(1)-C(2)	121.16(10)
C(6)-C(1)-S(1)	119.28(8)
C(2)-C(1)-S(1)	119.42(8)
C(3)-C(2)-C(1)	118.85(10)
C(3)-C(2)-H(2)	120.6
C(1)-C(2)-H(2)	120.6
C(2)-C(3)-C(4)	121.14(11)
C(2)-C(3)-H(3)	119.4
C(4)-C(3)-H(3)	119.4
C(3)-C(4)-C(5)	118.72(10)
C(3)-C(4)-C(7)	120.57(11)
C(5)-C(4)-C(7)	120.68(11)
C(6)-C(5)-C(4)	121.06(10)
C(6)-C(5)-H(5)	119.5
C(4)-C(5)-H(5)	119.5
C(5)-C(6)-C(1)	118.98(10)
C(5)-C(6)-H(6)	120.5
C(1)-C(6)-H(6)	120.5
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5

C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(8)-N(1)-C(10)	114.00(8)
C(8)-N(1)-S(1)	122.79(7)
C(10)-N(1)-S(1)	121.40(7)
N(2)-C(8)-N(1)	123.68(10)
N(2)-C(8)-S(2)	127.37(8)
N(1)-C(8)-S(2)	108.95(7)
C(8)-N(2)-C(11)	116.34(10)
N(2)-C(11)-C(12)	113.38(11)
N(2)-C(11)-H(11A)	108.9
C(12)-C(11)-H(11A)	108.9
N(2)-C(11)-H(11B)	108.9
C(12)-C(11)-H(11B)	108.9
H(11A)-C(11)-H(11B)	107.7
C(13)-C(12)-C(11)	126.39(12)
C(13)-C(12)-H(12)	116.8
C(11)-C(12)-H(12)	116.8
C(12)-C(13)-H(13A)	120.0
C(12)-C(13)-H(13B)	120.0
H(13A)-C(13)-H(13B)	120.0
C(8)-S(2)-C(9)	93.46(5)
C(14)-C(9)-C(10)	114.60(9)
C(14)-C(9)-S(2)	112.74(7)
C(10)-C(9)-S(2)	105.20(7)
C(14)-C(9)-H(9)	108.0
C(10)-C(9)-H(9)	108.0
S(2)-C(9)-H(9)	108.0
C(15)-C(14)-C(19)	119.35(10)
C(15)-C(14)-C(9)	118.64(10)
C(19)-C(14)-C(9)	121.95(9)
C(16)-C(15)-C(14)	119.89(11)
C(16)-C(15)-H(15)	120.1
C(14)-C(15)-H(15)	120.1
C(17)-C(16)-C(15)	120.38(12)

C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(18)-C(17)-C(16)	119.95(12)
C(18)-C(17)-H(17)	120.0
C(16)-C(17)-H(17)	120.0
C(17)-C(18)-C(19)	119.94(11)
C(17)-C(18)-H(18)	120.0
C(19)-C(18)-H(18)	120.0
C(18)-C(19)-C(14)	120.48(10)
C(18)-C(19)-H(19)	119.8
C(14)-C(19)-H(19)	119.8
N(1)-C(10)-C(20)	110.41(8)
N(1)-C(10)-C(9)	104.82(8)
C(20)-C(10)-C(9)	111.54(8)
N(1)-C(10)-H(10)	110.0
C(20)-C(10)-H(10)	110.0
C(9)-C(10)-H(10)	110.0
O(3)-C(20)-O(4)	125.32(10)
O(3)-C(20)-C(10)	123.43(10)
O(4)-C(20)-C(10)	111.24(9)
C(20)-O(4)-C(21)	114.48(11)
O(4)-C(21)-H(21A)	109.5
O(4)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
O(4)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(6S)-C(1S)-C(2S)	119.1(7)
C(6S)-C(1S)-H(1S)	120.5
C(2S)-C(1S)-H(1S)	120.5
C(3S)-C(2S)-C(1S)	118.6(7)
C(3S)-C(2S)-H(2S)	120.7
C(1S)-C(2S)-H(2S)	120.7
C(2S)-C(3S)-C(4S)	121.8(8)
C(2S)-C(3S)-H(3S)	119.1
C(4S)-C(3S)-H(3S)	119.1

C(5S)-C(4S)-C(3S)	119.2(8)
C(5S)-C(4S)-H(4S)	120.4
C(3S)-C(4S)-H(4S)	120.4
C(4S)-C(5S)-C(6S)	121.2(8)
C(4S)-C(5S)-H(5S)	119.4
C(6S)-C(5S)-H(5S)	119.4
C(5S)-C(6S)-C(1S)	120.0(8)
C(5S)-C(6S)-H(6S)	120.0
C(1S)-C(6S)-H(6S)	120.0
O(1T)-C(1T)-O(2T)	125(2)
O(1T)-C(1T)-C(2T)	120(2)
O(2T)-C(1T)-C(2T)	111.4(18)
C(1T)-C(2T)-H(2T1)	109.5
C(1T)-C(2T)-H(2T2)	109.5
H(2T1)-C(2T)-H(2T2)	109.5
C(1T)-C(2T)-H(2T3)	109.5
H(2T1)-C(2T)-H(2T3)	109.5
H(2T2)-C(2T)-H(2T3)	109.5
C(1T)-O(2T)-C(3T)	111.6(19)
O(2T)-C(3T)-C(4T)	102.8(17)
O(2T)-C(3T)-H(3T1)	111.2
C(4T)-C(3T)-H(3T1)	111.2
O(2T)-C(3T)-H(3T2)	111.2
C(4T)-C(3T)-H(3T2)	111.2
H(3T1)-C(3T)-H(3T2)	109.1
C(3T)-C(4T)-H(4T1)	109.5
C(3T)-C(4T)-H(4T2)	109.5
H(4T1)-C(4T)-H(4T2)	109.5
C(3T)-C(4T)-H(4T3)	109.5
H(4T1)-C(4T)-H(4T3)	109.5
H(4T2)-C(4T)-H(4T3)	109.5

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	17(1)	20(1)	26(1)	14(1)	11(1)	6(1)
O(2)	19(1)	13(1)	23(1)	5(1)	6(1)	5(1)
S(1)	13(1)	13(1)	18(1)	8(1)	6(1)	4(1)
C(1)	13(1)	17(1)	16(1)	7(1)	5(1)	5(1)
C(2)	19(1)	32(1)	18(1)	8(1)	9(1)	9(1)
C(3)	21(1)	38(1)	15(1)	6(1)	6(1)	7(1)
C(4)	16(1)	27(1)	18(1)	9(1)	4(1)	4(1)
C(5)	15(1)	25(1)	20(1)	6(1)	7(1)	6(1)
C(6)	16(1)	19(1)	16(1)	4(1)	6(1)	6(1)
C(7)	17(1)	46(1)	22(1)	10(1)	2(1)	4(1)
N(1)	16(1)	12(1)	15(1)	6(1)	5(1)	5(1)
C(8)	18(1)	14(1)	19(1)	9(1)	8(1)	6(1)
N(2)	27(1)	17(1)	18(1)	7(1)	9(1)	9(1)
C(11)	44(1)	21(1)	21(1)	6(1)	12(1)	17(1)
C(12)	44(1)	21(1)	24(1)	3(1)	17(1)	8(1)
C(13)	32(1)	32(1)	33(1)	-3(1)	11(1)	2(1)
S(2)	27(1)	18(1)	19(1)	10(1)	9(1)	12(1)
C(9)	14(1)	15(1)	17(1)	7(1)	4(1)	2(1)
C(14)	16(1)	18(1)	16(1)	7(1)	4(1)	4(1)
C(15)	25(1)	23(1)	19(1)	5(1)	3(1)	-2(1)
C(16)	38(1)	35(1)	16(1)	4(1)	4(1)	-2(1)
C(17)	36(1)	37(1)	19(1)	12(1)	10(1)	5(1)
C(18)	26(1)	25(1)	22(1)	12(1)	8(1)	3(1)
C(19)	20(1)	17(1)	17(1)	7(1)	5(1)	2(1)
C(10)	13(1)	13(1)	15(1)	4(1)	4(1)	2(1)
C(20)	14(1)	19(1)	21(1)	10(1)	6(1)	4(1)
O(3)	20(1)	28(1)	24(1)	9(1)	2(1)	-7(1)
O(4)	22(1)	28(1)	29(1)	9(1)	16(1)	8(1)
C(21)	27(1)	51(1)	51(1)	23(1)	27(1)	11(1)
C(1S)	55(4)	24(4)	77(4)	14(3)	33(3)	12(3)
C(2S)	84(6)	18(3)	38(3)	9(3)	18(3)	0(3)

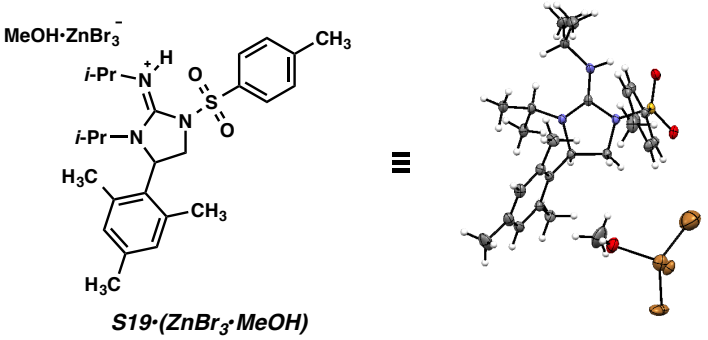
C(3S)	54(5)	22(3)	53(4)	0(3)	-16(3)	5(3)
C(4S)	52(5)	21(3)	87(5)	-2(3)	30(3)	6(3)
C(5S)	64(5)	35(4)	38(3)	-4(2)	16(3)	-13(3)
C(6S)	45(4)	38(5)	50(4)	25(4)	-5(3)	-5(3)
C(1T)	64(7)	30(9)	58(6)	10(8)	14(6)	3(7)
C(2T)	104(15)	48(10)	60(7)	23(9)	25(8)	30(10)
O(1T)	62(7)	50(7)	56(7)	6(6)	3(6)	9(6)
O(2T)	66(6)	25(6)	52(4)	13(4)	7(4)	8(5)
C(3T)	63(8)	33(9)	53(5)	5(7)	12(6)	-6(8)
C(4T)	58(9)	49(10)	41(8)	-12(8)	-6(6)	0(8)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for Compound **11**.

	x	y	z	U(eq)
H(2)	9455	2659	8342	27
H(3)	12396	3439	9338	30
H(5)	13956	1805	6891	24
H(6)	11024	1016	5883	21
H(7A)	15481	2462	9246	46
H(7B)	15613	3979	9367	46
H(7C)	16140	3022	8464	46
H(11A)	5821	4873	7734	33
H(11B)	6918	5519	7136	33
H(12)	8068	6820	8923	36
H(13A)	10049	4993	8773	44
H(13B)	10502	6453	9683	44
H(9)	4525	1788	4083	18
H(15)	4130	1113	2348	30
H(16)	4535	1575	946	40
H(17)	6585	3514	1157	37
H(18)	8191	5023	2775	29
H(19)	7755	4592	4182	22
H(10)	6777	813	4282	17
H(21A)	11839	2619	4251	59
H(21B)	10772	3370	3658	59
H(21C)	11013	1953	3053	59
H(1S)	12012	-858	9531	61
H(2S)	10329	97	8561	59
H(3S)	8179	967	9116	63
H(4S)	7723	992	10623	69
H(5S)	9209	-86	11495	64
H(6S)	11517	-821	11054	57
H(2T1)	12065	-360	8455	103
H(2T2)	10010	-464	8284	103

H(2T3)	10709	-1751	8229	103
H(3T1)	11018	1056	11413	67
H(3T2)	10402	-495	11258	67
H(4T1)	7342	-330	10569	93
H(4T2)	8170	1244	11135	93
H(4T3)	8157	295	11769	93

(*E*)-3-isopropyl-4-mesityl-1-tosyl-2-(isopropylimino)imidazolidinium zinc tribromide monomethanol salt (S19•($ZnBr_3$•MeOH)):



S19•(ZnBr$_3$•MeOH)

Low-temperature diffraction data (and scans) were collected on a Bruker Kappa diffractometer coupled to a Apex II CCD detector with graphite monochromated Mo *K* radiation (= 0.71073 Å) for the structure of compound **S19•($ZnBr_3$•MeOH)**. The structure was solved by direct methods using SHELXS and refined against F^2 on all data by full-matrix least squares with SHELXL-2013 using established refinement techniques. All non-hydrogen atoms were refined anisotropically. Unless otherwise noted, all hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl and hydroxide groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3- distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters.

Compound **S19•($ZnBr_3$•MeOH)** crystallizes in the triclinic space group *P*-1 with one molecule in the asymmetric unit along with one molecule of methanol. The coordinates for the hydrogen atoms on N3 and O3were taken from the difference Fourier synthesis and refined semi-freely with the help of a distance restraint, 0.91(2) and 0.83(2) Å respectively. An additional restraint was required for the hydrogen atom bound to O3 and the atoms Zn1, O3, C31 and H3O were restrained to be flat. All three bromine atoms were disordered over two positions. The solvent methanol had vey elongated ellipsoids and was disordered over two positions. The methanol is not very stable and the C-O distance was restrained to 1.43(2) Å. Additionally, the anisotropic displacement parameters for the two atoms in the second component of the disorder were constrained to be equivalent. Even with the disorder the methanol has elongated ellipsoids, however, refinement of additional components was not successful.

Table 1. Crystal data and structure refinement for Compound **S19•($ZnBr_3$•MeOH)**.

Identification code	rac14
CCDC Deposition Number	956877
Empirical formula	C27 H44 Br3 N3 O4 S Zn
Formula weight	811.81
Temperature	100(2) K

Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.5054(14) Å	α= 103.177(3)°.
	b = 12.5274(17) Å	β= 109.093(2)°.
	c = 14.785(2) Å	γ = 102.841(3)°.
Volume	1694.7(4) $Å^3$	
Z	2	
Density (calculated)	1.591 Mg/m^3	
Absorption coefficient	4.357 mm^{-1}	
F(000)	820	
Crystal size	0.580 x 0.380 x 0.270 mm^3	
Theta range for data collection	1.764 to 30.560°.	
Index ranges	-15<=h<=15, -17<=k<=17, -21<=l<=21	
Reflections collected	100294	
Independent reflections	10353 [R(int) = 0.0346]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.1292 and 0.0684	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10353 / 82 / 412	
Goodness-of-fit on F^2	1.096	
Final R indices [I>2sigma(I)]	R1 = 0.0332, wR2 = 0.0793	
R indices (all data)	R1 = 0.0418, wR2 = 0.0842	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.878 and -0.917 $e \cdot Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for Compound **S19•($ZnBr_3$•MeOH)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4177(2)	6547(2)	5223(1)	24(1)
O(2)	4429(2)	8386(1)	4821(1)	24(1)
S(1)	4213(1)	7168(1)	4530(1)	18(1)
C(1)	2695(2)	6459(2)	3406(2)	18(1)
C(2)	2284(2)	7039(2)	2722(2)	21(1)
C(3)	1068(2)	6464(2)	1841(2)	24(1)
C(4)	270(2)	5323(2)	1631(2)	24(1)
C(7)	-1077(2)	4724(3)	691(2)	33(1)
C(5)	717(2)	4751(2)	2324(2)	24(1)
C(6)	1922(2)	5310(2)	3212(2)	22(1)
N(1)	5573(2)	6976(2)	4235(1)	18(1)
C(8)	6315(2)	7626(2)	3813(2)	18(1)
N(3)	6281(2)	8679(2)	3862(2)	22(1)
C(11)	6662(2)	9434(2)	3284(2)	22(1)
C(12)	5359(3)	9741(2)	2755(2)	31(1)
C(13)	7911(3)	10511(2)	4005(2)	31(1)
N(2)	7008(2)	7029(2)	3402(1)	18(1)
C(14)	8269(2)	7560(2)	3202(2)	20(1)
C(15)	7914(2)	7273(2)	2070(2)	25(1)
C(16)	9538(2)	7195(2)	3714(2)	24(1)
C(9)	6792(2)	5874(2)	3547(2)	17(1)
C(21)	6427(2)	4851(2)	2623(2)	18(1)
C(22)	7171(2)	4051(2)	2748(2)	20(1)
C(27)	8267(2)	4165(2)	3761(2)	25(1)
C(23)	6873(2)	3098(2)	1914(2)	25(1)
C(24)	5860(2)	2920(2)	967(2)	28(1)
C(28)	5587(3)	1911(3)	62(2)	44(1)
C(25)	5097(2)	3697(2)	865(2)	26(1)
C(26)	5343(2)	4650(2)	1680(2)	21(1)
C(29)	4402(2)	5400(2)	1501(2)	28(1)
C(10)	5663(2)	5793(2)	4001(2)	19(1)

Zn(1)	727(1)	1039(1)	2621(1)	25(1)
O(3)	1824(2)	1549(2)	1805(2)	42(1)
C(31)	3303(4)	2206(4)	2288(4)	69(1)
Br(1)	-1687(2)	97(1)	1446(2)	31(1)
Br(2)	1081(1)	2756(1)	3849(1)	16(1)
Br(3)	1841(2)	-171(2)	3374(2)	30(1)
Br(1A)	-1582(4)	220(5)	1241(6)	39(1)
Br(2A)	1081(4)	2743(3)	3828(3)	83(3)
Br(3A)	1793(7)	-231(6)	3212(7)	47(1)
O(1S)	10478(14)	1719(7)	9938(6)	64(2)
C(1S)	8692(15)	1307(5)	9413(8)	65(3)
O(1T)	11160(20)	2063(15)	10107(8)	46(3)
C(1T)	9360(20)	1417(16)	9601(11)	46(3)

Table 3. Bond lengths [Å] and angles [°] for Compound **S19•($ZnBr_3$•MeOH)**.

O(1)-S(1)	1.4260(16)
O(2)-S(1)	1.4310(17)
S(1)-N(1)	1.6740(17)
S(1)-C(1)	1.748(2)
C(1)-C(2)	1.387(3)
C(1)-C(6)	1.398(3)
C(2)-C(3)	1.387(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.392(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.397(3)
C(4)-C(7)	1.504(3)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(5)-C(6)	1.384(3)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
N(1)-C(8)	1.389(2)
N(1)-C(10)	1.475(3)
C(8)-N(3)	1.314(3)
C(8)-N(2)	1.334(2)
N(3)-C(11)	1.485(3)
N(3)-H(3N)	0.868(17)
C(11)-C(12)	1.518(3)
C(11)-C(13)	1.524(3)
C(11)-H(11)	1.0000
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
N(2)-C(9)	1.490(3)

N(2)-C(14)	1.497(2)
C(14)-C(15)	1.525(3)
C(14)-C(16)	1.526(3)
C(14)-H(14)	1.0000
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(9)-C(21)	1.515(3)
C(9)-C(10)	1.538(3)
C(9)-H(9)	1.0000
C(21)-C(26)	1.407(3)
C(21)-C(22)	1.409(3)
C(22)-C(23)	1.397(3)
C(22)-C(27)	1.514(3)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(23)-C(24)	1.386(4)
C(23)-H(23)	0.9500
C(24)-C(25)	1.396(3)
C(24)-C(28)	1.512(3)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(25)-C(26)	1.395(3)
C(25)-H(25)	0.9500
C(26)-C(29)	1.512(3)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
Zn(1)-O(3)	2.030(2)

Zn(1)-Br(3A)	2.310(6)
Zn(1)-Br(2A)	2.314(4)
Zn(1)-Br(2)	2.3423(6)
Zn(1)-Br(3)	2.369(2)
Zn(1)-Br(1)	2.3860(13)
Zn(1)-Br(1A)	2.408(4)
O(3)-C(31)	1.428(4)
O(3)-H(3O)	0.816(18)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
O(1S)-C(1S)	1.680(8)
O(1S)-H(1S)	0.8400
C(1S)-H(1S1)	0.9800
C(1S)-H(1S2)	0.9800
C(1S)-H(1S3)	0.9800
O(1T)-C(1T)	1.704(14)
O(1T)-H(1T)	0.8400
C(1T)-H(1T1)	0.9800
C(1T)-H(1T2)	0.9800
C(1T)-H(1T3)	0.9800

O(1)-S(1)-O(2)	121.07(10)
O(1)-S(1)-N(1)	103.94(9)
O(2)-S(1)-N(1)	106.90(9)
O(1)-S(1)-C(1)	108.90(10)
O(2)-S(1)-C(1)	109.46(10)
N(1)-S(1)-C(1)	105.36(9)
C(2)-C(1)-C(6)	121.2(2)
C(2)-C(1)-S(1)	119.77(16)
C(6)-C(1)-S(1)	119.03(16)
C(3)-C(2)-C(1)	118.8(2)
C(3)-C(2)-H(2)	120.6
C(1)-C(2)-H(2)	120.6
C(2)-C(3)-C(4)	121.3(2)
C(2)-C(3)-H(3)	119.3

C(4)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	118.9(2)
C(3)-C(4)-C(7)	120.8(2)
C(5)-C(4)-C(7)	120.3(2)
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(5)-C(4)	120.9(2)
C(6)-C(5)-H(5)	119.6
C(4)-C(5)-H(5)	119.6
C(5)-C(6)-C(1)	119.0(2)
C(5)-C(6)-H(6)	120.5
C(1)-C(6)-H(6)	120.5
C(8)-N(1)-C(10)	110.49(16)
C(8)-N(1)-S(1)	127.75(15)
C(10)-N(1)-S(1)	117.14(13)
N(3)-C(8)-N(2)	129.07(18)
N(3)-C(8)-N(1)	120.52(18)
N(2)-C(8)-N(1)	110.40(18)
C(8)-N(3)-C(11)	131.07(17)
C(8)-N(3)-H(3N)	112.5(19)
C(11)-N(3)-H(3N)	116.4(19)
N(3)-C(11)-C(12)	108.11(18)
N(3)-C(11)-C(13)	109.48(19)
C(12)-C(11)-C(13)	111.6(2)
N(3)-C(11)-H(11)	109.2
C(12)-C(11)-H(11)	109.2
C(13)-C(11)-H(11)	109.2
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5

H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(8)-N(2)-C(9)	111.32(16)
C(8)-N(2)-C(14)	124.62(17)
C(9)-N(2)-C(14)	119.92(15)
N(2)-C(14)-C(15)	111.62(17)
N(2)-C(14)-C(16)	111.36(17)
C(15)-C(14)-C(16)	110.66(17)
N(2)-C(14)-H(14)	107.7
C(15)-C(14)-H(14)	107.7
C(16)-C(14)-H(14)	107.7
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
N(2)-C(9)-C(21)	116.28(16)
N(2)-C(9)-C(10)	103.46(15)
C(21)-C(9)-C(10)	114.31(16)
N(2)-C(9)-H(9)	107.4
C(21)-C(9)-H(9)	107.4
C(10)-C(9)-H(9)	107.4
C(26)-C(21)-C(22)	119.84(19)
C(26)-C(21)-C(9)	122.58(18)

C(22)-C(21)-C(9)	117.50(18)
C(23)-C(22)-C(21)	119.3(2)
C(23)-C(22)-C(27)	118.13(19)
C(21)-C(22)-C(27)	122.50(19)
C(22)-C(27)-H(27A)	109.5
C(22)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(22)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(24)-C(23)-C(22)	121.5(2)
C(24)-C(23)-H(23)	119.3
C(22)-C(23)-H(23)	119.3
C(23)-C(24)-C(25)	118.4(2)
C(23)-C(24)-C(28)	121.0(2)
C(25)-C(24)-C(28)	120.6(2)
C(24)-C(28)-H(28A)	109.5
C(24)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(24)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(26)-C(25)-C(24)	122.0(2)
C(26)-C(25)-H(25)	119.0
C(24)-C(25)-H(25)	119.0
C(25)-C(26)-C(21)	118.7(2)
C(25)-C(26)-C(29)	117.7(2)
C(21)-C(26)-C(29)	123.54(19)
C(26)-C(29)-H(29A)	109.5
C(26)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(26)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
N(1)-C(10)-C(9)	103.18(15)
N(1)-C(10)-H(10A)	111.1

C(9)-C(10)-H(10A)	111.1
N(1)-C(10)-H(10B)	111.1
C(9)-C(10)-H(10B)	111.1
H(10A)-C(10)-H(10B)	109.1
O(3)-Zn(1)-Br(3A)	102.1(2)
O(3)-Zn(1)-Br(2A)	104.27(11)
Br(3A)-Zn(1)-Br(2A)	116.2(3)
O(3)-Zn(1)-Br(2)	104.66(6)
O(3)-Zn(1)-Br(3)	105.41(9)
Br(2)-Zn(1)-Br(3)	110.95(5)
O(3)-Zn(1)-Br(1)	106.04(9)
Br(2)-Zn(1)-Br(1)	113.94(4)
Br(3)-Zn(1)-Br(1)	114.79(6)
O(3)-Zn(1)-Br(1A)	96.5(3)
Br(3A)-Zn(1)-Br(1A)	117.44(17)
Br(2A)-Zn(1)-Br(1A)	115.77(13)
C(31)-O(3)-Zn(1)	120.9(2)
C(31)-O(3)-H(3O)	120(3)
Zn(1)-O(3)-H(3O)	118(3)
O(3)-C(31)-H(31A)	109.5
O(3)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
O(3)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(1S)-O(1S)-H(1S)	109.5
O(1S)-C(1S)-H(1S1)	109.5
O(1S)-C(1S)-H(1S2)	109.5
H(1S1)-C(1S)-H(1S2)	109.5
O(1S)-C(1S)-H(1S3)	109.5
H(1S1)-C(1S)-H(1S3)	109.5
H(1S2)-C(1S)-H(1S3)	109.5
C(1T)-O(1T)-H(1T)	109.5
O(1T)-C(1T)-H(1T1)	109.5
O(1T)-C(1T)-H(1T2)	109.5
H(1T1)-C(1T)-H(1T2)	109.5

O(1T)-C(1T)-H(1T3)	109.5
H(1T1)-C(1T)-H(1T3)	109.5
H(1T2)-C(1T)-H(1T3)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Compound **S19•($ZnBr_3$•MeOH)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	21(1)	34(1)	21(1)	12(1)	12(1)	9(1)
O(2)	23(1)	23(1)	27(1)	3(1)	15(1)	6(1)
S(1)	16(1)	22(1)	19(1)	6(1)	11(1)	6(1)
C(1)	15(1)	22(1)	21(1)	8(1)	10(1)	7(1)
C(2)	21(1)	23(1)	26(1)	9(1)	13(1)	10(1)
C(3)	24(1)	33(1)	23(1)	12(1)	13(1)	15(1)
C(4)	17(1)	35(1)	21(1)	7(1)	10(1)	10(1)
C(7)	20(1)	49(2)	23(1)	8(1)	7(1)	7(1)
C(5)	18(1)	26(1)	28(1)	8(1)	10(1)	3(1)
C(6)	18(1)	24(1)	25(1)	10(1)	10(1)	6(1)
N(1)	15(1)	20(1)	20(1)	7(1)	11(1)	6(1)
C(8)	15(1)	21(1)	15(1)	3(1)	7(1)	3(1)
N(3)	26(1)	18(1)	26(1)	5(1)	19(1)	6(1)
C(11)	26(1)	19(1)	26(1)	6(1)	17(1)	6(1)
C(12)	35(1)	34(1)	34(1)	14(1)	19(1)	16(1)
C(13)	32(1)	21(1)	36(1)	6(1)	18(1)	1(1)
N(2)	15(1)	18(1)	20(1)	5(1)	10(1)	4(1)
C(14)	17(1)	22(1)	23(1)	6(1)	12(1)	4(1)
C(15)	28(1)	26(1)	25(1)	8(1)	17(1)	9(1)
C(16)	17(1)	30(1)	28(1)	9(1)	13(1)	5(1)
C(9)	14(1)	19(1)	20(1)	7(1)	8(1)	5(1)
C(21)	14(1)	19(1)	20(1)	6(1)	8(1)	4(1)
C(22)	16(1)	22(1)	25(1)	9(1)	12(1)	7(1)
C(27)	22(1)	34(1)	29(1)	16(1)	12(1)	15(1)
C(23)	24(1)	20(1)	36(1)	8(1)	18(1)	7(1)
C(24)	23(1)	24(1)	31(1)	0(1)	14(1)	1(1)
C(28)	38(1)	36(1)	42(2)	-11(1)	16(1)	4(1)
C(25)	19(1)	29(1)	22(1)	3(1)	7(1)	1(1)
C(26)	16(1)	23(1)	22(1)	7(1)	6(1)	4(1)
C(29)	21(1)	34(1)	26(1)	10(1)	4(1)	12(1)
C(10)	18(1)	22(1)	23(1)	9(1)	11(1)	8(1)

Zn(1)	24(1)	22(1)	29(1)	9(1)	12(1)	7(1)
O(3)	50(1)	47(1)	36(1)	19(1)	25(1)	11(1)
C(31)	53(2)	75(3)	85(3)	35(2)	44(2)	0(2)
Br(1)	27(1)	37(1)	25(1)	12(1)	7(1)	2(1)
Br(2)	18(1)	14(1)	17(1)	3(1)	8(1)	4(1)
Br(3)	31(1)	24(1)	36(1)	14(1)	12(1)	11(1)
Br(1A)	28(1)	42(1)	36(2)	9(1)	8(1)	4(1)
Br(2A)	85(3)	84(3)	96(4)	48(3)	40(2)	32(2)
Br(3A)	42(2)	36(1)	85(3)	32(2)	35(2)	27(1)
O(1S)	112(6)	44(3)	47(3)	14(3)	51(4)	17(4)
C(1S)	118(6)	31(2)	69(5)	15(3)	71(5)	16(4)
O(1T)	74(8)	40(5)	25(3)	15(3)	18(4)	14(5)
C(1T)	74(8)	40(5)	25(3)	15(3)	18(4)	14(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^{-3}) for Compound **S19•($ZnBr_3$•MeOH)**.

	x	y	z	U(eq)
H(2)	2826	7815	2855	25
H(3)	773	6857	1372	29
H(7A)	-1896	4599	880	49
H(7B)	-1048	3976	329	49
H(7C)	-1164	5207	252	49
H(5)	187	3969	2183	29
H(6)	2219	4918	3681	26
H(3N)	5930(30)	8950(20)	4288(19)	26
H(11)	6941	9000	2765	27
H(12A)	4592	9033	2276	47
H(12B)	5597	10263	2389	47
H(12C)	5047	10125	3259	47
H(13A)	7661	10915	4539	46
H(13B)	8132	11027	3630	46
H(13C)	8744	10285	4311	46
H(14)	8547	8420	3501	24
H(15A)	7648	6434	1758	37
H(15B)	8747	7664	1967	37
H(15C)	7118	7537	1759	37
H(16A)	9696	7321	4426	36
H(16B)	10389	7658	3672	36
H(16C)	9345	6373	3372	36
H(9)	7696	5909	4079	20
H(27A)	8580	3481	3698	38
H(27B)	7844	4227	4264	38
H(27C)	9085	4860	3978	38
H(23)	7376	2560	1999	30
H(28A)	6006	2192	-376	66
H(28B)	4559	1533	-317	66
H(28C)	6019	1353	294	66

H(25)	4387	3573	222	31
H(29A)	3713	5092	795	41
H(29B)	4989	6193	1641	41
H(29C)	3893	5402	1951	41
H(10A)	4736	5221	3507	23
H(10B)	5966	5574	4621	23
H(3O)	1370(40)	1460(30)	1211(15)	62
H(31A)	3421	3011	2631	103
H(31B)	3714	2180	1779	103
H(31C)	3791	1876	2786	103
H(1S)	10767	1332	9552	96
H(1S1)	8373	1939	9684	98
H(1S2)	8297	623	9573	98
H(1S3)	8364	1119	8677	98
H(1T)	11346	2769	10163	70
H(1T1)	8935	1883	9964	70
H(1T2)	9141	641	9663	70
H(1T3)	8973	1354	8884	70

Table 6. Hydrogen bonds for Compound **S19•($ZnBr_3$•MeOH)** [Å and °].

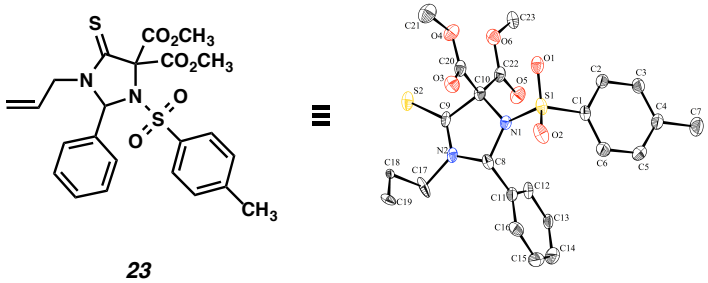
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...Br(3)#1	0.95	2.97	3.584(3)	123.6
C(2)-H(2)...Br(3A)#1	0.95	2.90	3.519(6)	123.9
C(6)-H(6)...Br(2)	0.95	2.81	3.545(2)	135.1
N(3)-H(3N)...O(2)	0.868(17)	2.05(2)	2.767(2)	140(3)
C(16)-H(16A)...Br(2)#2	0.98	2.93	3.855(2)	156.7
C(16)-H(16B)...Br(3)#3	0.98	3.01	3.872(3)	147.4
C(16)-H(16B)...Br(3A)#3	0.98	3.06	3.925(7)	147.6
C(9)-H(9)...Br(2)#2	1.00	2.82	3.523(2)	127.7
C(10)-H(10B)...Br(2)#2	0.99	3.08	3.550(2)	110.5
O(3)-H(3O)...O(1S)#4	0.816(18)	1.95(2)	2.741(7)	164(3)
O(3)-H(3O)...O(1T)#4	0.816(18)	1.92(3)	2.645(11)	148(4)
O(1S)-H(1S)...Br(1)#5	0.84	2.61	3.440(6)	170.0
C(1S)-H(1S2)...Br(1)#6	0.98	2.99	3.753(8)	136.0
C(1S)-H(1S3)...Br(3)#5	0.98	2.91	3.845(8)	159.8
C(1T)-H(1T3)...Br(3A)#5	0.98	2.85	3.749(18)	153.3

Symmetry transformations used to generate equivalent atoms:

#1 x,y+1,z #2 -x+1,-y+1,-z+1 #3 x+1,y+1,z

#4 x-1,y,z-1 #5 -x+1,-y,-z+1 #6 x+1,y,z+1

dimethyl 3-allyl-2-phenyl-4-thioxo-1-tosyl-imidazolidine-5,5-dicarboxylate (23):



23

Low-temperature diffraction data (and scans) were collected on a Bruker Kappa diffractometer coupled to a Apex II CCD detector with graphite monochromated Mo *K* radiation (= 0.71073 Å) for the structure of Compound **23**. The structure was solved by direct methods using SHELXS and refined against F^2 on all data by full-matrix least squares with SHELXL-2013 using established refinement techniques. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups).

Compound **23** crystallizes in the orthorhombic space group *Pbca* with one molecule in the asymmetric unit. A majority of the molecule was disordered over two positions. All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3- distances. All atoms were refined with the help of similarity as well as rigid bond restraints for anisotropic displacement parameters.

Table 1. Crystal data and structure refinement for Compound **23**.

Identification code	rac16	
CCDC Deposition Number	973927	
Empirical formula	C23 H24 N2 O6 S2	
Formula weight	488.56	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 7.5481(4) Å	α= 90°.
	b = 21.3568(13) Å	β= 90°.
	c = 28.1256(18) Å	γ = 90°.
Volume	4533.9(5) $Å^3$	
Z	8	

Density (calculated)	1.431 Mg/m^3
Absorption coefficient	0.278 mm^{-1}
F(000)	2048
Crystal size	0.400 x 0.250 x 0.150 mm^3
Theta range for data collection	1.907 to 30.677°.
Index ranges	-10<=h<=10, -30<=k<=30, -39<=l<=40
Reflections collected	98231
Independent reflections	7007 [R(int) = 0.0490]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.6817
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7007 / 1023 / 507
Goodness-of-fit on F^2	1.116
Final R indices [I>2sigma(I)]	R1 = 0.0505, wR2 = 0.1269
R indices (all data)	R1 = 0.0597, wR2 = 0.1324
Extinction coefficient	n/a
Largest diff. peak and hole	0.662 and -0.538 $e \cdot Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Compound **23**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5335(2)	1620(1)	1380(1)	26(1)
O(2)	4409(2)	2342(1)	726(1)	31(1)
S(1)	4127(1)	2069(1)	1184(1)	21(1)
C(1)	3945(2)	2681(1)	1599(1)	20(1)
C(2)	4527(2)	2582(1)	2061(1)	22(1)
C(3)	4518(2)	3079(1)	2378(1)	24(1)
C(4)	3935(2)	3668(1)	2242(1)	26(1)
C(5)	3339(3)	3752(1)	1780(1)	32(1)
C(6)	3336(3)	3263(1)	1455(1)	28(1)
C(7)	3924(3)	4209(1)	2587(1)	37(1)
N(1)	2138(13)	1760(4)	1128(4)	18(1)
C(8)	877(12)	1912(3)	744(3)	21(1)
C(11)	-60(19)	2527(4)	804(4)	21(1)
C(12)	-830(30)	2682(7)	1243(5)	21(2)
C(13)	-1790(30)	3228(7)	1286(4)	21(2)
C(14)	-1950(20)	3623(6)	896(4)	33(2)
C(15)	-1186(18)	3468(5)	464(4)	32(2)
C(16)	-231(16)	2926(4)	418(4)	26(1)
N(2)	-368(12)	1385(3)	805(3)	20(1)
C(17)	-1909(11)	1330(3)	484(2)	29(2)
C(18)	-1271(4)	782(1)	140(1)	11(1)
C(19)	-1060(4)	1020(2)	-290(1)	20(1)
C(9)	88(11)	951(4)	1108(4)	21(1)
S(2)	-891(4)	277(1)	1228(1)	28(1)
C(10)	1879(10)	1142(3)	1327(2)	18(1)
C(20)	3219(6)	664(2)	1106(2)	23(1)
O(3)	3612(9)	724(3)	689(2)	27(1)
O(4)	3688(6)	201(2)	1380(2)	26(1)
C(21)	4655(6)	-280(2)	1124(2)	39(1)
C(22)	1640(20)	1198(6)	1871(3)	21(1)
O(5)	720(20)	1617(8)	2024(6)	28(2)

O(6)	2335(18)	750(5)	2130(2)	27(1)
C(23)	2074(14)	822(5)	2643(3)	26(1)
N(1A)	2257(12)	1661(4)	1182(4)	17(1)
C(8A)	967(11)	1778(3)	803(3)	16(1)
C(11A)	53(16)	2403(4)	818(4)	17(1)
C(12A)	-880(30)	2594(7)	1223(5)	22(2)
C(13A)	-1780(30)	3161(7)	1216(4)	28(2)
C(14A)	-1815(18)	3529(5)	811(4)	31(2)
C(15A)	-907(16)	3334(4)	410(4)	31(1)
C(16A)	12(14)	2775(4)	415(4)	23(1)
N(2A)	-258(11)	1253(3)	881(3)	17(1)
C(17A)	-1788(11)	1187(3)	566(2)	23(1)
C(18A)	-1586(8)	1051(4)	20(2)	64(2)
C(19A)	-321(12)	812(4)	-170(3)	92(3)
C(9A)	244(10)	839(3)	1203(3)	17(1)
S(2A)	-720(4)	172(1)	1345(1)	22(1)
C(10A)	1983(9)	1075(3)	1432(2)	18(1)
C(20A)	3358(5)	561(2)	1297(2)	19(1)
O(3A)	4024(5)	193(2)	1558(2)	29(1)
O(4A)	3553(8)	579(2)	823(2)	25(1)
C(21A)	4614(4)	87(2)	615(2)	33(1)
C(22A)	1630(20)	1207(6)	1960(2)	20(1)
O(5A)	920(20)	1681(7)	2086(5)	33(2)
O(6A)	2257(17)	779(5)	2248(2)	28(1)
C(23A)	1896(15)	893(5)	2748(3)	36(2)

Table 3. Bond lengths [Å] and angles [°] for Compound **23**.

O(1)-S(1)	1.4335(14)
O(2)-S(1)	1.4295(14)
S(1)-N(1)	1.648(9)
S(1)-N(1A)	1.659(8)
S(1)-C(1)	1.7562(16)
C(1)-C(6)	1.387(2)
C(1)-C(2)	1.387(2)
C(2)-C(3)	1.387(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.388(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.387(3)
C(4)-C(7)	1.508(2)
C(5)-C(6)	1.386(3)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
N(1)-C(10)	1.446(8)
N(1)-C(8)	1.476(8)
C(8)-N(2)	1.476(8)
C(8)-C(11)	1.500(8)
C(8)-H(8)	1.0000
C(11)-C(16)	1.385(8)
C(11)-C(12)	1.407(9)
C(12)-C(13)	1.378(9)
C(12)-H(12)	0.9500
C(13)-C(14)	1.387(9)
C(13)-H(13)	0.9500
C(14)-C(15)	1.383(8)
C(14)-H(14)	0.9500
C(15)-C(16)	1.371(7)
C(15)-H(15)	0.9500

C(16)-H(16)	0.9500
N(2)-C(9)	1.307(6)
N(2)-C(17)	1.477(7)
C(17)-C(18)	1.593(5)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.323(4)
C(18)-H(18)	0.9500
C(19)-H(19A)	0.9500
C(19)-H(19B)	0.9500
C(9)-C(10)	1.542(8)
C(9)-S(2)	1.653(6)
C(10)-C(22)	1.544(8)
C(10)-C(20)	1.567(7)
C(20)-O(3)	1.215(6)
C(20)-O(4)	1.301(6)
O(4)-C(21)	1.451(6)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-O(5)	1.209(9)
C(22)-O(6)	1.312(9)
O(6)-C(23)	1.464(7)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
N(1A)-C(10A)	1.450(7)
N(1A)-C(8A)	1.466(7)
C(8A)-N(2A)	1.469(7)
C(8A)-C(11A)	1.503(7)
C(8A)-H(8A)	1.0000
C(11A)-C(16A)	1.383(7)
C(11A)-C(12A)	1.400(9)
C(12A)-C(13A)	1.387(9)
C(12A)-H(12A)	0.9500
C(13A)-C(14A)	1.384(9)

C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.384(8)
C(14A)-H(14A)	0.9500
C(15A)-C(16A)	1.381(6)
C(15A)-H(15A)	0.9500
C(16A)-H(16A)	0.9500
N(2A)-C(9A)	1.320(5)
N(2A)-C(17A)	1.463(7)
C(17A)-C(18A)	1.569(6)
C(17A)-H(17C)	0.9900
C(17A)-H(17D)	0.9900
C(18A)-C(19A)	1.207(7)
C(18A)-H(18A)	0.9500
C(19A)-H(19C)	0.9500
C(19A)-H(19D)	0.9500
C(9A)-C(10A)	1.546(7)
C(9A)-S(2A)	1.649(6)
C(10A)-C(22A)	1.535(7)
C(10A)-C(20A)	1.557(7)
C(20A)-O(3A)	1.187(5)
C(20A)-O(4A)	1.342(5)
O(4A)-C(21A)	1.444(6)
C(21A)-H(21D)	0.9800
C(21A)-H(21E)	0.9800
C(21A)-H(21F)	0.9800
C(22A)-O(5A)	1.199(9)
C(22A)-O(6A)	1.310(8)
O(6A)-C(23A)	1.452(7)
C(23A)-H(23D)	0.9800
C(23A)-H(23E)	0.9800
C(23A)-H(23F)	0.9800

O(2)-S(1)-O(1)	121.63(8)
O(2)-S(1)-N(1)	102.3(4)
O(1)-S(1)-N(1)	110.4(3)
O(2)-S(1)-N(1A)	109.8(3)

O(1)-S(1)-N(1A)	101.0(2)
O(2)-S(1)-C(1)	107.88(8)
O(1)-S(1)-C(1)	106.97(8)
N(1)-S(1)-C(1)	106.8(4)
N(1A)-S(1)-C(1)	109.0(4)
C(6)-C(1)-C(2)	120.95(15)
C(6)-C(1)-S(1)	119.99(13)
C(2)-C(1)-S(1)	118.93(12)
C(3)-C(2)-C(1)	119.01(15)
C(3)-C(2)-H(2)	120.5
C(1)-C(2)-H(2)	120.5
C(2)-C(3)-C(4)	121.20(16)
C(2)-C(3)-H(3)	119.4
C(4)-C(3)-H(3)	119.4
C(5)-C(4)-C(3)	118.54(16)
C(5)-C(4)-C(7)	120.23(17)
C(3)-C(4)-C(7)	121.22(17)
C(6)-C(5)-C(4)	121.41(16)
C(6)-C(5)-H(5)	119.3
C(4)-C(5)-H(5)	119.3
C(5)-C(6)-C(1)	118.88(16)
C(5)-C(6)-H(6)	120.6
C(1)-C(6)-H(6)	120.6
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(10)-N(1)-C(8)	113.4(6)
C(10)-N(1)-S(1)	116.9(6)
C(8)-N(1)-S(1)	124.7(6)
N(2)-C(8)-N(1)	99.1(5)
N(2)-C(8)-C(11)	110.7(7)
N(1)-C(8)-C(11)	114.5(8)
N(2)-C(8)-H(8)	110.7

N(1)-C(8)-H(8)	110.7
C(11)-C(8)-H(8)	110.7
C(16)-C(11)-C(12)	120.3(7)
C(16)-C(11)-C(8)	119.6(8)
C(12)-C(11)-C(8)	120.0(8)
C(13)-C(12)-C(11)	119.6(9)
C(13)-C(12)-H(12)	120.2
C(11)-C(12)-H(12)	120.2
C(12)-C(13)-C(14)	119.3(9)
C(12)-C(13)-H(13)	120.3
C(14)-C(13)-H(13)	120.3
C(15)-C(14)-C(13)	120.9(8)
C(15)-C(14)-H(14)	119.5
C(13)-C(14)-H(14)	119.5
C(16)-C(15)-C(14)	120.2(7)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(15)-C(16)-C(11)	119.6(7)
C(15)-C(16)-H(16)	120.2
C(11)-C(16)-H(16)	120.2
C(9)-N(2)-C(8)	116.7(5)
C(9)-N(2)-C(17)	123.3(6)
C(8)-N(2)-C(17)	119.5(6)
N(2)-C(17)-C(18)	101.0(6)
N(2)-C(17)-H(17A)	111.6
C(18)-C(17)-H(17A)	111.6
N(2)-C(17)-H(17B)	111.6
C(18)-C(17)-H(17B)	111.6
H(17A)-C(17)-H(17B)	109.4
C(19)-C(18)-C(17)	108.0(4)
C(19)-C(18)-H(18)	126.0
C(17)-C(18)-H(18)	126.0
C(18)-C(19)-H(19A)	120.0
C(18)-C(19)-H(19B)	120.0
H(19A)-C(19)-H(19B)	120.0
N(2)-C(9)-C(10)	107.7(5)

N(2)-C(9)-S(2)	129.3(5)
C(10)-C(9)-S(2)	122.8(5)
N(1)-C(10)-C(9)	101.9(5)
N(1)-C(10)-C(22)	109.1(7)
C(9)-C(10)-C(22)	108.3(8)
N(1)-C(10)-C(20)	110.8(6)
C(9)-C(10)-C(20)	103.6(6)
C(22)-C(10)-C(20)	121.3(6)
O(3)-C(20)-O(4)	125.8(4)
O(3)-C(20)-C(10)	118.1(5)
O(4)-C(20)-C(10)	115.8(5)
C(20)-O(4)-C(21)	112.4(4)
O(4)-C(21)-H(21A)	109.5
O(4)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
O(4)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
O(5)-C(22)-O(6)	124.8(10)
O(5)-C(22)-C(10)	118.5(10)
O(6)-C(22)-C(10)	116.5(7)
C(22)-O(6)-C(23)	114.6(7)
O(6)-C(23)-H(23A)	109.5
O(6)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
O(6)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(10A)-N(1A)-C(8A)	113.8(5)
C(10A)-N(1A)-S(1)	125.0(5)
C(8A)-N(1A)-S(1)	118.5(6)
N(1A)-C(8A)-N(2A)	100.3(5)
N(1A)-C(8A)-C(11A)	115.8(6)
N(2A)-C(8A)-C(11A)	112.6(6)
N(1A)-C(8A)-H(8A)	109.2
N(2A)-C(8A)-H(8A)	109.2

C(11A)-C(8A)-H(8A)	109.2
C(16A)-C(11A)-C(12A)	119.2(7)
C(16A)-C(11A)-C(8A)	119.8(6)
C(12A)-C(11A)-C(8A)	120.8(7)
C(13A)-C(12A)-C(11A)	119.4(9)
C(13A)-C(12A)-H(12A)	120.3
C(11A)-C(12A)-H(12A)	120.3
C(14A)-C(13A)-C(12A)	121.0(8)
C(14A)-C(13A)-H(13A)	119.5
C(12A)-C(13A)-H(13A)	119.5
C(15A)-C(14A)-C(13A)	119.3(7)
C(15A)-C(14A)-H(14A)	120.4
C(13A)-C(14A)-H(14A)	120.4
C(16A)-C(15A)-C(14A)	120.1(7)
C(16A)-C(15A)-H(15A)	119.9
C(14A)-C(15A)-H(15A)	119.9
C(15A)-C(16A)-C(11A)	121.0(6)
C(15A)-C(16A)-H(16A)	119.5
C(11A)-C(16A)-H(16A)	119.5
C(9A)-N(2A)-C(17A)	125.3(5)
C(9A)-N(2A)-C(8A)	115.6(5)
C(17A)-N(2A)-C(8A)	118.6(5)
N(2A)-C(17A)-C(18A)	122.3(7)
N(2A)-C(17A)-H(17C)	106.8
C(18A)-C(17A)-H(17C)	106.8
N(2A)-C(17A)-H(17D)	106.8
C(18A)-C(17A)-H(17D)	106.8
H(17C)-C(17A)-H(17D)	106.6
C(19A)-C(18A)-C(17A)	126.1(8)
C(19A)-C(18A)-H(18A)	117.0
C(17A)-C(18A)-H(18A)	117.0
C(18A)-C(19A)-H(19C)	120.0
C(18A)-C(19A)-H(19D)	120.0
H(19C)-C(19A)-H(19D)	120.0
N(2A)-C(9A)-C(10A)	108.1(4)
N(2A)-C(9A)-S(2A)	128.1(5)

C(10A)-C(9A)-S(2A)	123.7(4)
N(1A)-C(10A)-C(22A)	109.4(7)
N(1A)-C(10A)-C(9A)	101.6(4)
C(22A)-C(10A)-C(9A)	108.5(7)
N(1A)-C(10A)-C(20A)	113.3(6)
C(22A)-C(10A)-C(20A)	118.7(5)
C(9A)-C(10A)-C(20A)	103.7(5)
O(3A)-C(20A)-O(4A)	125.9(4)
O(3A)-C(20A)-C(10A)	126.7(4)
O(4A)-C(20A)-C(10A)	107.2(4)
C(20A)-O(4A)-C(21A)	116.2(4)
O(4A)-C(21A)-H(21D)	109.5
O(4A)-C(21A)-H(21E)	109.5
H(21D)-C(21A)-H(21E)	109.5
O(4A)-C(21A)-H(21F)	109.5
H(21D)-C(21A)-H(21F)	109.5
H(21E)-C(21A)-H(21F)	109.5
O(5A)-C(22A)-O(6A)	124.5(10)
O(5A)-C(22A)-C(10A)	121.2(9)
O(6A)-C(22A)-C(10A)	114.1(6)
C(22A)-O(6A)-C(23A)	114.6(7)
O(6A)-C(23A)-H(23D)	109.5
O(6A)-C(23A)-H(23E)	109.5
H(23D)-C(23A)-H(23E)	109.5
O(6A)-C(23A)-H(23F)	109.5
H(23D)-C(23A)-H(23F)	109.5
H(23E)-C(23A)-H(23F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Compound **23**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	19(1)	26(1)	34(1)	-10(1)	3(1)	-3(1)
O(2)	26(1)	47(1)	19(1)	-7(1)	6(1)	-12(1)
S(1)	16(1)	27(1)	21(1)	-8(1)	5(1)	-7(1)
C(1)	20(1)	20(1)	19(1)	-4(1)	2(1)	-5(1)
C(2)	25(1)	19(1)	22(1)	0(1)	-1(1)	-3(1)
C(3)	28(1)	24(1)	21(1)	-4(1)	-2(1)	-2(1)
C(4)	26(1)	20(1)	31(1)	-6(1)	0(1)	-2(1)
C(5)	41(1)	19(1)	34(1)	1(1)	-7(1)	2(1)
C(6)	36(1)	26(1)	22(1)	1(1)	-6(1)	-2(1)
C(7)	41(1)	28(1)	41(1)	-14(1)	-2(1)	0(1)
N(1)	15(2)	17(2)	22(3)	-3(2)	3(2)	-2(2)
C(8)	18(2)	25(3)	19(2)	-4(2)	-1(2)	-6(2)
C(11)	17(2)	19(3)	26(2)	-7(2)	-2(2)	0(2)
C(12)	24(3)	20(4)	19(2)	-7(2)	3(2)	-10(3)
C(13)	23(2)	18(3)	23(3)	-10(2)	-3(3)	-1(2)
C(14)	43(3)	24(4)	32(4)	-8(3)	-3(3)	4(3)
C(15)	38(4)	28(4)	31(3)	-1(3)	-7(2)	6(2)
C(16)	27(3)	32(4)	18(2)	-2(3)	-2(2)	1(3)
N(2)	17(2)	17(3)	26(3)	-11(2)	2(2)	2(2)
C(17)	16(2)	51(4)	21(2)	-22(3)	0(2)	-7(2)
C(18)	8(1)	11(1)	15(1)	-4(1)	-2(1)	2(1)
C(19)	14(1)	32(2)	14(2)	-5(1)	-3(1)	10(1)
C(9)	14(2)	15(3)	33(4)	-10(2)	2(2)	-2(2)
S(2)	24(1)	24(1)	35(1)	-9(1)	6(1)	-9(1)
C(10)	16(2)	19(2)	20(2)	-7(2)	4(2)	1(1)
C(20)	14(2)	21(2)	35(3)	-8(2)	2(2)	-3(1)
O(3)	26(2)	32(3)	24(2)	-9(2)	4(2)	3(2)
O(4)	27(2)	21(2)	31(2)	-2(2)	10(2)	3(1)
C(21)	34(2)	33(2)	51(3)	-5(2)	9(2)	5(2)
C(22)	18(2)	18(2)	26(3)	-3(2)	4(3)	-6(2)
O(5)	36(3)	25(3)	24(4)	-7(2)	8(3)	3(3)

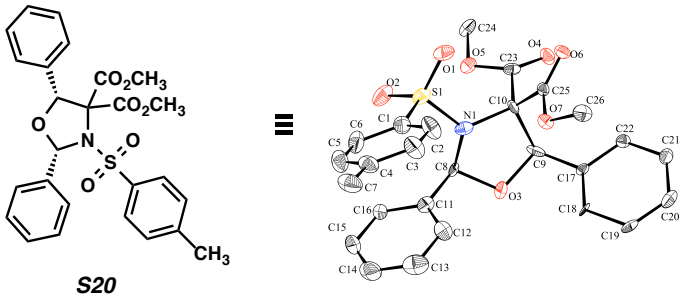
O(6)	31(2)	29(2)	21(3)	-7(2)	0(3)	1(1)
C(23)	25(2)	27(2)	27(3)	-7(2)	-1(2)	-7(2)
N(1A)	14(2)	16(2)	21(2)	-2(2)	-3(1)	-3(2)
C(8A)	17(2)	15(2)	16(2)	-3(2)	3(1)	0(2)
C(11A)	17(2)	15(2)	18(2)	-2(2)	-2(1)	-5(2)
C(12A)	19(3)	17(3)	29(3)	-6(2)	1(2)	-2(3)
C(13A)	25(2)	26(3)	32(4)	-14(3)	2(3)	-4(2)
C(14A)	31(3)	21(3)	42(4)	-10(2)	-9(3)	2(2)
C(15A)	33(4)	28(4)	31(3)	2(3)	-4(2)	6(2)
C(16A)	22(3)	20(3)	26(2)	-1(2)	-6(2)	1(2)
N(2A)	15(2)	11(2)	26(2)	-4(2)	-2(1)	-1(2)
C(17A)	18(2)	27(2)	24(2)	-6(2)	-3(2)	0(1)
C(18A)	55(3)	89(5)	50(3)	-38(3)	-13(3)	3(3)
C(19A)	107(6)	83(5)	87(6)	-44(4)	53(5)	-25(4)
C(9A)	16(2)	15(2)	21(3)	-4(1)	3(1)	1(2)
S(2A)	22(1)	18(1)	26(1)	0(1)	-1(1)	-7(1)
C(10A)	14(2)	14(2)	24(2)	1(2)	-1(2)	-4(1)
C(20A)	16(1)	16(2)	26(2)	0(2)	-1(2)	-3(1)
O(3A)	27(2)	22(1)	40(2)	1(2)	-8(2)	3(1)
O(4A)	24(1)	25(2)	27(2)	-11(2)	2(2)	2(1)
C(21A)	16(1)	24(2)	59(2)	-27(2)	6(1)	0(1)
C(22A)	18(2)	21(2)	21(2)	-2(2)	2(2)	-7(2)
O(5A)	50(5)	23(3)	26(4)	-4(2)	6(3)	5(3)
O(6A)	33(2)	32(2)	20(3)	-3(2)	-8(3)	6(1)
C(23A)	37(3)	53(4)	19(3)	-3(3)	-6(2)	7(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for Compound **23**.

	x	y	z	U(eq)
H(2)	4925	2180	2158	26
H(3)	4920	3014	2694	29
H(5)	2924	4152	1683	38
H(6)	2923	3327	1140	34
H(7A)	2760	4236	2740	55
H(7B)	4166	4599	2416	55
H(7C)	4838	4142	2829	55
H(8)	1472	1890	427	25
H(12)	-697	2412	1509	26
H(13)	-2345	3334	1579	26
H(14)	-2581	4005	926	39
H(15)	-1326	3739	199	39
H(16)	310	2823	123	31
H(17A)	-2122	1724	307	35
H(17B)	-2996	1213	660	35
H(18)	-1076	358	229	14
H(19A)	-1288	1452	-345	24
H(19B)	-680	760	-544	24
H(21A)	5017	-609	1346	59
H(21B)	5708	-95	976	59
H(21C)	3893	-459	877	59
H(23A)	2690	483	2810	40
H(23B)	805	803	2715	40
H(23C)	2550	1226	2746	40
H(8A)	1560	1725	487	19
H(12A)	-896	2339	1499	26
H(13A)	-2382	3298	1494	33
H(14A)	-2456	3912	809	38
H(15A)	-915	3585	132	37
H(16A)	624	2643	137	27

H(17C)	-2485	1578	595	27
H(17D)	-2531	848	699	27
H(18A)	-2549	1167	-179	77
H(19C)	673	689	15	111
H(19D)	-320	748	-504	111
H(21D)	4647	139	269	50
H(21E)	4094	-321	693	50
H(21F)	5821	109	742	50
H(23D)	2360	545	2938	54
H(23E)	614	927	2797	54
H(23F)	2470	1283	2847	54

cis-dimethyl 2,5-diphenyl-3-tosyloxazolidine-4,4-dicarboxylate (S20):



Low-temperature diffraction data (and scans) were collected on a Bruker Kappa diffractometer coupled to a Apex II CCD detector with graphite monochromated Mo *K* radiation (= 0.71073 Å) for the structure of **S20**. The structure was solved by direct methods using SHELXS and refined against F^2 on all data by full-matrix least squares with SHELXL-2013 refinement using established techniques. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3- distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters.

Table 1. Crystal Data and Structure Analysis Details for Compound **S20**.

Empirical formula	C26 H25 N O7 S	
CCDC Deposition Number	973928	
Formula weight	495.53	
Crystallization solvent	Ethyl Acetate	
Crystal shape	block	
Crystal color	colourless	
Crystal size	0.34 x 0.39 x 0.41 mm	
Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker APEX-II CCD	
Wavelength	0.71073 Å MoK	
Data collection temperature	100 K	
Theta range for 9033 reflections used in lattice determination	2.40 to 34.83°	
Unit cell dimensions	a = 26.2830(13) Å	α= 90°
	b = 10.5471(5) Å	β= 90°
	c = 8.4772(4) Å	γ = 90°

Volume	2350.0(2) Å^3
Z	4
Crystal system	orthorhombic
Space group	P c a 21 (# 29)
Density (calculated)	1.401 g/cm^3
F(000)	1040
Theta range for data collection	1.9 to 35.2°
Completeness to theta = 25.000°	99.8%
Index ranges	-42<=h<=41, -16<=k<=16, -13<=l<=13
Reflections collected	85187
Independent reflections	10087 [R_{int}= 0.0399]
Reflections > 2s(I)	9439
Average s(I)/(net I)	0.0240
Absorption coefficient	0.19 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.9213
Primary solution method	dual
Hydrogen placement	geom
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10087 / 13 / 538
Treatment of hydrogen atoms	constr
Goodness-of-fit on F^2	1.19
Final R indices [I>2s(I), 9439 reflections]	R1 = 0.0430, wR2 = 0.1033
R indices (all data)	R1 = 0.0470, wR2 = 0.1048
Type of weighting scheme used	calc
Max shift/error	0.001
Average shift/error	0.000
Absolute structure parameter	0.044(12)
Extinction coefficient	n/a
Largest diff. peak and hole	0.33 and -0.36 e·Å^{-3}

Programs Used

Cell refinement	SAINT V8.32B (Bruker-AXS, 2007)
Data collection	APEX2 2013.6-2 (Bruker-AXS, 2007)
Data reduction	SAINT V8.32B (Bruker-AXS, 2007)
Structure solution	SHELXT (Sheldrick, 2012)

Structure refinement	SHELXL-2013/2 (Sheldrick, 2013)
Graphics	DIAMOND 3 (Crystal Impact, 1999)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for Compound **S20**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
S(1)	8926(1)	6201(1)	5357(1)	24(1)
O(1)	8757(1)	5962(1)	6946(2)	28(1)
O(2)	8828(1)	5297(2)	4131(2)	35(1)
N(1)	8669(1)	7567(1)	4885(2)	21(1)
C(1)	9589(1)	6443(2)	5403(3)	26(1)
C(2)	9800(1)	7205(3)	6560(3)	36(1)
C(3)	10325(1)	7313(3)	6651(3)	38(1)
C(4)	10644(1)	6666(2)	5619(2)	32(1)
C(5)	10424(1)	5912(2)	4466(3)	37(1)
C(6)	9899(1)	5798(2)	4339(3)	32(1)
C(7)	11214(1)	6743(3)	5801(3)	41(1)
O(3)	8454(4)	9290(10)	3416(13)	31(2)
O(4)	7331(1)	7845(3)	6401(4)	23(1)
O(5)	7789(6)	6381(13)	5033(14)	20(1)
O(6)	8103(1)	8362(3)	8651(3)	20(1)
O(7)	8770(1)	9307(3)	7484(3)	18(1)
C(8)	8655(4)	7986(7)	3269(11)	13(2)
C(9)	8056(7)	9322(18)	4700(20)	22(3)
C(10)	8209(5)	8173(18)	5850(20)	16(2)
C(11)	9116(4)	8065(15)	2442(16)	21(2)
C(12)	9471(3)	8980(7)	2868(7)	26(1)
C(13)	9938(2)	9060(6)	2102(10)	40(1)
C(14)	10053(3)	8198(8)	966(11)	44(2)
C(15)	9701(3)	7272(7)	552(10)	44(2)
C(16)	9233(3)	7206(6)	1270(9)	29(1)
C(17)	8091(3)	10654(7)	5427(12)	13(1)
C(18)	8430(3)	11443(5)	4959(11)	16(1)
C(19)	8464(3)	12722(6)	5697(9)	24(1)
C(20)	8107(2)	13055(4)	6806(6)	25(1)
C(21)	7731(2)	12188(4)	7246(5)	19(1)
C(22)	7720(2)	10989(4)	6570(5)	16(1)
C(23)	7715(2)	7381(7)	5901(9)	17(1)
C(24)	7324(6)	5619(14)	5180(20)	23(2)
C(25)	8350(2)	8604(3)	7505(4)	14(1)
C(26)	8860(2)	10020(4)	8925(4)	26(1)
O(3A)	8459(2)	9216(8)	3393(7)	13(1)
O(4A)	7556(1)	7446(3)	7202(4)	30(1)
O(5A)	7767(6)	6217(12)	5341(14)	22(1)
O(6A)	8992(1)	9186(3)	7025(4)	23(1)
O(7A)	8266(1)	8980(3)	8372(3)	22(1)
C(8A)	8668(6)	8051(11)	3175(15)	37(3)
C(9A)	8106(5)	9189(15)	4546(18)	13(2)

C(10A)	8303(5)	8102(13)	5730(17)	11(1)
C(11A)	9229(3)	8166(12)	2597(11)	17(1)
C(12A)	9556(2)	8999(5)	3331(6)	19(1)
C(13A)	10052(2)	9131(4)	2790(6)	26(1)
C(14A)	10225(2)	8406(6)	1527(6)	31(1)
C(15A)	9903(3)	7558(7)	790(6)	30(1)
C(16A)	9402(2)	7438(6)	1290(7)	25(1)
C(17A)	8008(3)	10427(7)	5241(10)	15(1)
C(18A)	8397(5)	11464(10)	5114(14)	45(3)
C(19A)	8298(3)	12553(7)	5784(10)	38(2)
C(20A)	7868(3)	12772(5)	6675(6)	39(1)
C(21A)	7503(2)	11837(5)	6819(5)	36(1)
C(22A)	7578(2)	10668(4)	6104(5)	26(1)
C(23A)	7845(2)	7284(7)	6149(8)	16(1)
C(24A)	7299(7)	5528(16)	5250(30)	41(4)
C(25A)	8564(2)	8793(3)	7139(4)	14(1)
C(26A)	8481(2)	9837(5)	9541(4)	31(1)

Table 3. Bond lengths [Å] and angles [°] for Compound **S20**.

S(1)-O(1)	1.4406(16)
S(1)-O(2)	1.4334(17)
S(1)-N(1)	1.6401(16)
S(1)-C(1)	1.762(2)
N(1)-C(8)	1.440(10)
N(1)-C(10)	1.592(12)
N(1)-C(8A)	1.537(13)
N(1)-C(10A)	1.326(11)
C(1)-C(2)	1.384(3)
C(1)-C(6)	1.393(3)
C(2)-H(2)	0.9500
C(2)-C(3)	1.386(3)
C(3)-H(3)	0.9500
C(3)-C(4)	1.390(3)
C(4)-C(5)	1.386(4)
C(4)-C(7)	1.510(3)
C(5)-H(5)	0.9500
C(5)-C(6)	1.389(4)
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
O(3)-C(8)	1.478(14)
O(3)-C(9)	1.51(2)
O(4)-C(23)	1.198(8)
O(5)-C(23)	1.301(19)
O(5)-C(24)	1.47(2)
O(6)-C(25)	1.196(5)
O(7)-C(25)	1.330(5)
O(7)-C(26)	1.454(5)
C(8)-H(8)	1.0000
C(8)-C(11)	1.403(16)
C(9)-H(9)	1.0000
C(9)-C(10)	1.60(3)
C(9)-C(17)	1.54(2)
C(10)-C(23)	1.546(18)
C(10)-C(25)	1.52(2)
C(11)-C(12)	1.389(12)
C(11)-C(16)	1.379(16)
C(12)-H(12)	0.9500
C(12)-C(13)	1.393(10)
C(13)-H(13)	0.9500
C(13)-C(14)	1.359(12)
C(14)-H(14)	0.9500
C(14)-C(15)	1.389(11)
C(15)-H(15)	0.9500
C(15)-C(16)	1.374(9)
C(16)-H(16)	0.9500
C(17)-C(18)	1.283(10)
C(17)-C(22)	1.418(11)
C(18)-H(18)	0.9500
C(18)-C(19)	1.490(9)

C(19)-H(19)	0.9500
C(19)-C(20)	1.374(9)
C(20)-H(20)	0.9500
C(20)-C(21)	1.396(6)
C(21)-H(21)	0.9500
C(21)-C(22)	1.389(6)
C(22)-H(22)	0.9500
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
O(3A)-C(8A)	1.358(15)
O(3A)-C(9A)	1.348(18)
O(4A)-C(23A)	1.185(8)
O(5A)-C(23A)	1.334(17)
O(5A)-C(24A)	1.43(2)
O(6A)-C(25A)	1.203(5)
O(7A)-C(25A)	1.320(4)
O(7A)-C(26A)	1.455(5)
C(8A)-H(8A)	1.0000
C(8A)-C(11A)	1.558(17)
C(9A)-H(9A)	1.0000
C(9A)-C(10A)	1.61(2)
C(9A)-C(17A)	1.456(19)
C(10A)-C(23A)	1.523(15)
C(10A)-C(25A)	1.558(16)
C(11A)-C(12A)	1.378(11)
C(11A)-C(16A)	1.423(12)
C(12A)-H(12A)	0.9500
C(12A)-C(13A)	1.391(7)
C(13A)-H(13A)	0.9500
C(13A)-C(14A)	1.393(7)
C(14A)-H(14A)	0.9500
C(14A)-C(15A)	1.380(8)
C(15A)-H(15A)	0.9500
C(15A)-C(16A)	1.390(8)
C(16A)-H(16A)	0.9500
C(17A)-C(18A)	1.500(13)
C(17A)-C(22A)	1.371(11)
C(18A)-H(18A)	0.9500
C(18A)-C(19A)	1.307(14)
C(19A)-H(19A)	0.9500
C(19A)-C(20A)	1.379(11)
C(20A)-H(20A)	0.9500
C(20A)-C(21A)	1.381(9)
C(21A)-H(21A)	0.9500
C(21A)-C(22A)	1.388(6)
C(22A)-H(22A)	0.9500
C(24A)-H(24D)	0.9800
C(24A)-H(24E)	0.9800
C(24A)-H(24F)	0.9800
C(26A)-H(26D)	0.9800

C(26A)-H(26E)	0.9800
C(26A)-H(26F)	0.9800

O(1)-S(1)-N(1)	104.74(9)
O(1)-S(1)-C(1)	108.06(10)
O(2)-S(1)-O(1)	120.43(10)
O(2)-S(1)-N(1)	109.52(9)
O(2)-S(1)-C(1)	106.81(11)
N(1)-S(1)-C(1)	106.53(8)
C(8)-N(1)-S(1)	120.8(3)
C(8)-N(1)-C(10)	110.1(8)
C(10)-N(1)-S(1)	122.7(7)
C(10A)-N(1)-C(8A)	111.5(8)
C(2)-C(1)-S(1)	119.77(16)
C(2)-C(1)-C(6)	120.5(2)
C(6)-C(1)-S(1)	119.58(17)
C(1)-C(2)-H(2)	120.4
C(1)-C(2)-C(3)	119.1(2)
C(3)-C(2)-H(2)	120.4
C(2)-C(3)-H(3)	119.2
C(2)-C(3)-C(4)	121.6(2)
C(4)-C(3)-H(3)	119.2
C(3)-C(4)-C(7)	120.5(2)
C(5)-C(4)-C(3)	118.4(2)
C(5)-C(4)-C(7)	121.1(2)
C(4)-C(5)-H(5)	119.4
C(4)-C(5)-C(6)	121.2(2)
C(6)-C(5)-H(5)	119.4
C(1)-C(6)-H(6)	120.4
C(5)-C(6)-C(1)	119.2(2)
C(5)-C(6)-H(6)	120.4
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(8)-O(3)-C(9)	109.2(11)
C(23)-O(5)-C(24)	105.8(12)
C(25)-O(7)-C(26)	114.3(3)
N(1)-C(8)-O(3)	102.4(6)
N(1)-C(8)-H(8)	109.6
O(3)-C(8)-H(8)	109.6
C(11)-C(8)-N(1)	118.1(8)
C(11)-C(8)-O(3)	107.2(10)
C(11)-C(8)-H(8)	109.6
O(3)-C(9)-H(9)	110.4
O(3)-C(9)-C(10)	104.1(13)
O(3)-C(9)-C(17)	105.5(12)
C(10)-C(9)-H(9)	110.4
C(17)-C(9)-H(9)	110.4
C(17)-C(9)-C(10)	115.7(13)
N(1)-C(10)-C(9)	100.7(11)
C(23)-C(10)-N(1)	115.9(12)

C(23)-C(10)-C(9)	102.4(12)
C(25)-C(10)-N(1)	114.0(11)
C(25)-C(10)-C(9)	113.2(13)
C(25)-C(10)-C(23)	109.7(10)
C(12)-C(11)-C(8)	119.4(11)
C(16)-C(11)-C(8)	120.9(9)
C(16)-C(11)-C(12)	119.6(10)
C(11)-C(12)-H(12)	119.5
C(11)-C(12)-C(13)	120.9(8)
C(13)-C(12)-H(12)	119.5
C(12)-C(13)-H(13)	120.5
C(14)-C(13)-C(12)	119.0(6)
C(14)-C(13)-H(13)	120.5
C(13)-C(14)-H(14)	119.9
C(13)-C(14)-C(15)	120.1(6)
C(15)-C(14)-H(14)	119.9
C(14)-C(15)-H(15)	119.4
C(16)-C(15)-C(14)	121.3(7)
C(16)-C(15)-H(15)	119.4
C(11)-C(16)-H(16)	120.5
C(15)-C(16)-C(11)	119.0(7)
C(15)-C(16)-H(16)	120.5
C(18)-C(17)-C(9)	120.7(11)
C(18)-C(17)-C(22)	121.8(7)
C(22)-C(17)-C(9)	117.4(9)
C(17)-C(18)-H(18)	120.0
C(17)-C(18)-C(19)	119.9(9)
C(19)-C(18)-H(18)	120.0
C(18)-C(19)-H(19)	120.7
C(20)-C(19)-C(18)	118.6(5)
C(20)-C(19)-H(19)	120.7
C(19)-C(20)-H(20)	120.1
C(19)-C(20)-C(21)	119.9(4)
C(21)-C(20)-H(20)	120.1
C(20)-C(21)-H(21)	120.0
C(22)-C(21)-C(20)	120.1(4)
C(22)-C(21)-H(21)	120.0
C(17)-C(22)-H(22)	120.2
C(21)-C(22)-C(17)	119.7(4)
C(21)-C(22)-H(22)	120.2
O(4)-C(23)-O(5)	131.1(9)
O(4)-C(23)-C(10)	119.8(8)
O(5)-C(23)-C(10)	107.1(10)
O(5)-C(24)-H(24A)	109.5
O(5)-C(24)-H(24B)	109.5
O(5)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
O(6)-C(25)-O(7)	125.5(3)
O(6)-C(25)-C(10)	123.6(7)
O(7)-C(25)-C(10)	110.8(7)
O(7)-C(26)-H(26A)	109.5
O(7)-C(26)-H(26B)	109.5

O(7)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(9A)-O(3A)-C(8A)	111.0(10)
C(23A)-O(5A)-C(24A)	125.9(13)
C(25A)-O(7A)-C(26A)	113.7(3)
N(1)-C(8A)-H(8A)	112.3
N(1)-C(8A)-C(11A)	108.6(9)
O(3A)-C(8A)-N(1)	100.0(8)
O(3A)-C(8A)-H(8A)	112.3
O(3A)-C(8A)-C(11A)	110.8(10)
C(11A)-C(8A)-H(8A)	112.3
O(3A)-C(9A)-H(9A)	107.5
O(3A)-C(9A)-C(10A)	104.2(11)
O(3A)-C(9A)-C(17A)	113.3(11)
C(10A)-C(9A)-H(9A)	107.5
C(17A)-C(9A)-H(9A)	107.5
C(17A)-C(9A)-C(10A)	116.3(11)
N(1)-C(10A)-C(9A)	101.5(10)
N(1)-C(10A)-C(23A)	117.3(10)
N(1)-C(10A)-C(25A)	107.1(9)
C(23A)-C(10A)-C(9A)	107.1(9)
C(23A)-C(10A)-C(25A)	115.7(9)
C(25A)-C(10A)-C(9A)	106.7(9)
C(12A)-C(11A)-C(8A)	119.8(9)
C(12A)-C(11A)-C(16A)	119.7(7)
C(16A)-C(11A)-C(8A)	120.4(8)
C(11A)-C(12A)-H(12A)	120.0
C(11A)-C(12A)-C(13A)	120.0(6)
C(13A)-C(12A)-H(12A)	120.0
C(12A)-C(13A)-H(13A)	119.8
C(12A)-C(13A)-C(14A)	120.3(5)
C(14A)-C(13A)-H(13A)	119.8
C(13A)-C(14A)-H(14A)	119.9
C(15A)-C(14A)-C(13A)	120.2(5)
C(15A)-C(14A)-H(14A)	119.9
C(14A)-C(15A)-H(15A)	119.9
C(14A)-C(15A)-C(16A)	120.2(5)
C(16A)-C(15A)-H(15A)	119.9
C(11A)-C(16A)-H(16A)	120.3
C(15A)-C(16A)-C(11A)	119.5(6)
C(15A)-C(16A)-H(16A)	120.3
C(9A)-C(17A)-C(18A)	120.4(10)
C(22A)-C(17A)-C(9A)	121.8(8)
C(22A)-C(17A)-C(18A)	117.7(8)
C(17A)-C(18A)-H(18A)	120.8
C(19A)-C(18A)-C(17A)	118.3(11)
C(19A)-C(18A)-H(18A)	120.8
C(18A)-C(19A)-H(19A)	118.4
C(18A)-C(19A)-C(20A)	123.2(8)
C(20A)-C(19A)-H(19A)	118.4
C(19A)-C(20A)-H(20A)	120.0
C(19A)-C(20A)-C(21A)	119.9(5)

C(21A)-C(20A)-H(20A)	120.0
C(20A)-C(21A)-H(21A)	120.1
C(20A)-C(21A)-C(22A)	119.8(5)
C(22A)-C(21A)-H(21A)	120.1
C(17A)-C(22A)-C(21A)	121.0(5)
C(17A)-C(22A)-H(22A)	119.5
C(21A)-C(22A)-H(22A)	119.5
O(4A)-C(23A)-O(5A)	114.2(8)
O(4A)-C(23A)-C(10A)	126.9(8)
O(5A)-C(23A)-C(10A)	118.7(9)
O(5A)-C(24A)-H(24D)	109.5
O(5A)-C(24A)-H(24E)	109.5
O(5A)-C(24A)-H(24F)	109.5
H(24D)-C(24A)-H(24E)	109.5
H(24D)-C(24A)-H(24F)	109.5
H(24E)-C(24A)-H(24F)	109.5
O(6A)-C(25A)-O(7A)	124.5(3)
O(6A)-C(25A)-C(10A)	120.7(5)
O(7A)-C(25A)-C(10A)	114.6(5)
O(7A)-C(26A)-H(26D)	109.5
O(7A)-C(26A)-H(26E)	109.5
O(7A)-C(26A)-H(26F)	109.5
H(26D)-C(26A)-H(26E)	109.5
H(26D)-C(26A)-H(26F)	109.5
H(26E)-C(26A)-H(26F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Compound **S20**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	307(2)	186(2)	231(2)	33(2)	-63(2)	-10(2)
O(1)	299(7)	260(6)	277(7)	110(5)	-33(6)	3(5)
O(2)	504(10)	189(6)	359(8)	-28(6)	-108(7)	-39(6)
N(1)	222(7)	202(6)	190(6)	63(5)	-40(5)	-31(5)
C(1)	303(8)	267(8)	212(7)	15(7)	-14(8)	46(6)
C(2)	286(10)	507(13)	276(10)	-125(9)	36(8)	-28(9)
C(3)	307(11)	485(13)	337(11)	-73(10)	37(9)	-18(10)
C(4)	296(9)	390(10)	257(10)	110(8)	35(7)	86(8)
C(5)	410(12)	399(12)	294(10)	26(9)	30(9)	217(10)
C(6)	417(11)	278(9)	275(9)	-42(7)	-51(8)	135(9)
C(7)	304(10)	553(15)	381(12)	187(11)	61(9)	93(10)
O(3)	460(40)	160(30)	310(40)	0(20)	120(30)	110(30)
O(4)	174(12)	241(13)	269(14)	-59(11)	87(10)	-40(10)
O(5)	190(17)	160(30)	240(40)	-20(20)	-30(20)	-50(20)
O(6)	217(12)	216(13)	152(11)	5(9)	47(9)	-27(10)
O(7)	153(13)	231(13)	161(11)	-15(10)	-1(10)	-22(11)
C(8)	230(30)	62(19)	100(30)	-50(18)	-40(20)	-7(18)
C(9)	150(30)	330(60)	170(40)	120(40)	70(20)	30(30)
C(10)	160(50)	180(30)	140(20)	-39(17)	70(30)	0(30)
C(11)	240(40)	190(20)	200(30)	0(20)	-60(20)	-20(30)
C(12)	250(30)	340(20)	200(30)	-40(20)	-40(20)	-1(19)
C(13)	240(20)	470(30)	510(40)	130(30)	-50(20)	-60(20)
C(14)	290(30)	460(40)	590(50)	160(40)	210(30)	110(30)
C(15)	500(40)	320(30)	490(40)	40(30)	300(40)	140(30)
C(16)	410(40)	180(20)	280(20)	-15(17)	140(30)	0(20)
C(17)	90(30)	90(20)	200(30)	15(18)	7(19)	-23(16)
C(18)	220(20)	15(15)	230(30)	-4(13)	16(19)	2(14)
C(19)	320(30)	90(20)	330(20)	38(15)	50(20)	-60(18)
C(20)	340(20)	119(15)	290(20)	-3(14)	-48(18)	14(15)
C(21)	245(17)	156(15)	180(16)	-8(13)	-10(14)	27(13)
C(22)	171(16)	153(15)	149(15)	-6(11)	-8(12)	-31(12)
C(23)	190(30)	180(20)	140(20)	25(15)	-25(17)	-80(20)
C(24)	220(30)	130(20)	350(50)	10(30)	-40(30)	-10(30)
C(25)	133(15)	148(13)	145(15)	4(11)	12(12)	34(12)
C(26)	303(19)	281(18)	184(16)	-36(13)	-26(13)	-96(15)
O(3A)	140(20)	190(30)	70(20)	66(16)	-31(17)	-61(18)
O(4A)	256(14)	344(14)	299(15)	-66(12)	118(12)	-107(12)
O(5A)	260(20)	140(30)	270(40)	0(20)	-50(30)	-14(18)
O(6A)	177(13)	288(13)	215(12)	-71(10)	12(10)	-61(10)
O(7A)	191(11)	331(15)	125(10)	-33(10)	4(9)	-16(10)
C(8A)	500(60)	380(50)	210(30)	200(30)	-110(30)	-90(30)
C(9A)	70(30)	190(20)	120(30)	32(17)	-20(30)	-40(30)
C(10A)	150(40)	90(20)	90(30)	0(17)	30(20)	-30(20)
C(11A)	220(40)	210(30)	90(20)	-4(17)	10(20)	20(30)
C(12A)	210(20)	216(16)	150(20)	-35(17)	29(16)	-32(15)
C(13A)	225(18)	255(18)	290(20)	37(15)	101(16)	-5(14)
C(14A)	260(20)	390(20)	290(20)	84(19)	134(17)	40(20)

C(15A)	320(30)	390(30)	182(17)	24(19)	100(20)	120(20)
C(16A)	310(30)	270(30)	175(16)	2(16)	17(19)	21(19)
C(17A)	140(30)	140(30)	170(20)	58(19)	-45(16)	-15(17)
C(18A)	500(50)	630(60)	210(30)	0(30)	10(30)	250(40)
C(19A)	540(50)	150(20)	440(30)	31(19)	-160(30)	-80(30)
C(20A)	660(40)	220(20)	290(20)	-85(19)	-130(30)	210(20)
C(21A)	550(30)	320(20)	207(17)	30(16)	42(19)	250(20)
C(22A)	310(20)	248(18)	212(18)	64(14)	66(15)	117(16)
C(23A)	160(30)	163(16)	140(20)	-14(14)	-3(16)	-17(18)
C(24A)	420(50)	300(50)	510(80)	-30(50)	-110(50)	-210(30)
C(25A)	146(15)	150(13)	116(12)	12(10)	-2(12)	17(12)
C(26A)	312(18)	480(20)	150(14)	-139(15)	-44(13)	16(17)

Table 5. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for Compound **S20**.

	x	y	z	U_{iso}
H(2)	959	765	728	43
H(3)	1047	784	744	45
H(5)	1064	546	375	44
H(6)	975	529	354	39
H(7A)	1131	760	612	62
H(7B)	1138	654	479	62
H(7C)	1133	614	661	62
H(8)	841	745	266	16
H(9)	771	918	425	26
H(12)	939	956	369	31
H(13)	1017	971	237	48
H(14)	1037	823	45	53
H(15)	979	667	-24	52
H(16)	899	658	96	35
H(18)	866	1121	414	19
H(19)	873	1330	541	29
H(20)	811	1387	727	30
H(21)	748	1242	801	23
H(22)	747	1040	687	19
H(24A)	737	481	462	35
H(24B)	704	608	471	35
H(24C)	725	545	629	35
H(26A)	909	1074	870	38
H(26B)	902	947	971	38
H(26C)	854	1034	933	38
H(8A)	846	751	246	44
H(9A)	778	889	407	15
H(12A)	944	948	421	23
H(13A)	1028	972	329	31
H(14A)	1057	850	117	38
H(15A)	1003	706	-6	36
H(16A)	918	687	76	30
H(18A)	871	1133	456	54
H(19A)	853	1323	565	45
H(20A)	782	1356	719	47
H(21A)	720	1199	740	43
H(22A)	733	1003	622	31
H(24D)	706	597	455	62
H(24E)	715	547	631	62
H(24F)	736	467	485	62
H(26D)	851	1069	909	47
H(26E)	882	954	985	47
H(26F)	826	986	1047	47