Lewis Acid Mediated (3 + 2) Cycloadditions of Donor-Acceptor Cyclopropanes with Heterocumulenes

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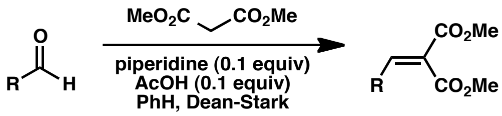
Materials and Methods. Unless stated otherwise, reactions were performed in flame-dried or oven-dried glassware under an argon or nitrogen atmosphere using dry, deoxygenated solvents (distilled or passed over a column of activated alumina).[1] Diazodimethylmalonate was prepared according to the method of Davies and coworkers.[2] Commercially obtained reagents were used as received with the exception of tin(II) triflate and iron(III) chloride, which were stored in a nitrogen-filled glovebox. Thin-layer chromatography (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. ^{1}H and ^{13}C NMR spectra were recorded on a Varian 400 (at 400 MHz and 100 MHz, respectively) or on a Varian Mercury 500 (at 500 MHz and 126 MHz, respectively) and are reported relative to $CHCl_3$ (δ 7.26 & 77.16 ppm, respectively) or tetramethylsilane (0.00 ppm). Data for ^{1}H 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, hept = heptet, m = complex multiplet, app = apparent. IR spectra were recorded on a Perkin Elmer Paragon 1000 Spectrometer and are reported in frequency of absorption (cm^{-1}). HRMS were acquired using an Agilent 6200 Series TOF with an Agilent G1978A Multimode source in electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI) or mixed (MM) ionization mode; HRMS were also acquired using a JEOL JMS-600H with fast atom bombardment (FAB). Optical rotations were recorded on a JASCO P-2000 Polarimeter. Enantiomeric excesses were determined by chiral HPLC (Agilent 1100 Series) or chiral SFC (Thar).

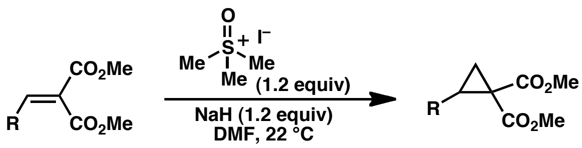
[1] Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518–1520.

[2] Baum, J. S.; Shook, D. A.; Davies, H. M. L.; Smith, D. *Synth. Commun.* **1987**, *17*, 1709–1716.

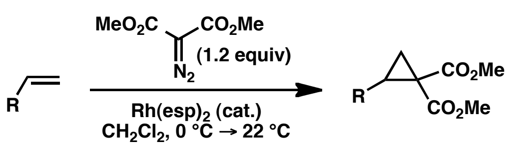
General Experimental Procedures



General Procedure A. *Knoevenagel condensation.*
A round-bottom flask was charged with the appropriate aldehyde (14.4 mmol), followed by benzene (85 mL), dimethyl malonate (15.8 mmol), piperidine (1.44 mmol), and acetic acid (1.44 mmol). The flask was equipped with a Dean-Stark trap and condenser and the solution heated to reflux. Upon completion (as determined by TLC analysis), evaporation of the solvent gave the crude product, which was purified by silica gel column chromatography.

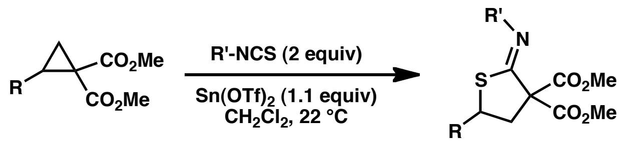


General Procedure B. *Corey-Chaykovsky cyclopropanation.*
Sodium hydride (2.56 mmol, 60% dispersion in mineral oil) was suspended in anhydrous DMF (4 mL) in a flame-dried round-bottom flask under nitrogen. Trimethylsulfoxonium iodide (2.56 mmol) was added, and the solution stirred at ambient temperature for 1 hour. A solution of the appropriate benzylidene malonate (2.13 mmol) in anhydrous DMF (2 mL) was added, and the reaction mixture allowed to stir at room temperature. Upon completion (as determined by TLC analysis), the solution was poured onto a mixture of ice and 2 M $HCl_{(aq)}$ (10 mL) and extracted with diethyl ether (3 x 30 mL). The combined organic layers were washed once with brine, dried over magnesium sulfate, filtered and concentrated *in vacuo* to give the crude product, which was purified by silica gel column chromatography.

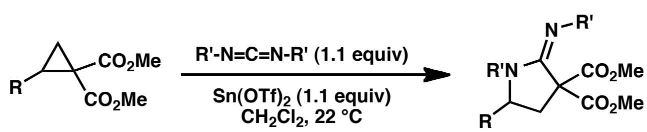


General Procedure C. *Styrene cyclopropanation.*
$Rh(esp)_2$ (0.3 mg) was added to a flame-dried round-bottom flask, which was then evacuated and backfilled with nitrogen three times. The appropriate styrene (5.0 mmol) and anhydrous dichloromethane (5 mL) were then added and the solution was stirred under nitrogen and cooled in an ice bath. A solution of diazodimethylmalonate (6.0 mmol) in anhydrous dichloromethane (5 mL) was added dropwise over 20 minutes. The reaction solution was then allowed to warm to ambient temperature. Upon completion (as determined by TLC analysis), the crude product was adsorbed onto silica gel and purified by column chromatography. When traces of the rhodium catalyst remained after chromatography (as determined by a blue discoloration), the product was dissolved in anhydrous benzene (1.5 mL) in a flame-dried round-bottom flask. A solution of

tetrakis(hydroxymethyl)phosphonium hydroxide (10 μL, 1M in isopropanol) was added,[3] and the mixture was stirred at 60 °C for 12 hours. The solution was then cooled to room temperature, diluted with diethyl ether (20 mL), washed once with water and once with brine, dried over magnesium sulfate, filtered and concentrated to give the purified product.



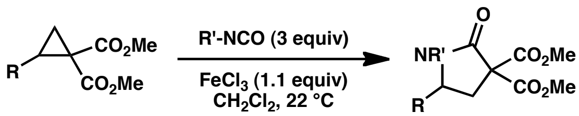
General Procedure D. *Isothiocyanate (3 + 2) reaction with D-A cyclopropanes*
To an oven-dried 1 dram vial equipped with a magnetic stir bar was added tin(II) trifluoromethanesulfonate (0.44 mmol) in an inert atmosphere glovebox. The vial was sealed with a screw cap fitted with a Teflon septum, removed from the glovebox and placed under a nitrogen atmosphere. To a separate, oven-dried 1 dram vial were added the appropriate cyclopropane (0.4 mmol) and isothiocyanate (0.8 mmol). 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 (1 mL + 0.33 mL rinse). The heterogeneous reaction mixture was then allowed to stir at ambient temperature under nitrogen. Upon consumption of the cyclopropane (as determined by TLC analysis), the reaction solution was diluted with dichloromethane (3 mL) and methanol (1 mL), adsorbed onto Celite, and purified by silica gel column chromatography. The products of this reaction were often found to be unstable during prolonged storage (~1 week) at ambient temperature; the decomposition products have not been identified.



General Procedure E. *Carbodiimide (3 + 2) reaction with D-A cyclopropanes*
To an oven-dried 1 dram vial equipped with a magnetic stir bar was added tin(II) trifluoromethanesulfonate (0.44 mmol) 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 a nitrogen atmosphere. To a separate, oven-dried 1 dram vial were added the appropriate cyclopropane (0.4 mmol) and carbodiimide (0.44 mmol). 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 (1 mL + 0.33 mL rinse). The heterogeneous reaction mixture was then allowed to stir at ambient temperature under nitrogen. Upon consumption of the cyclopropane (as determined by TLC analysis), the reaction solution was diluted with dichloromethane (3 mL) and methanol (1 mL), adsorbed onto Celite, and purified by silica gel column chromatography. The product obtained after column chromatography is an amidinium salt, which is dissolved in DCM,

[3] Pederson, R. L.; Fellows, I. M.; Ung, T. A.; Ishihara, H.; Hajela, S. P. *Adv. Synth. Catal.* **2002**, *344*, 728–735.

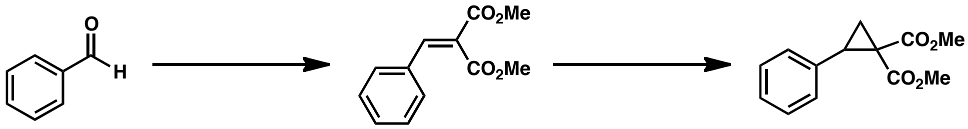
and washed with aqueous sodium hydroxide (0.1 M) and brine, then dried over sodium sulfate, filtered, and concentrated *in vacuo* to yield the free amidine base.



General Procedure F. *Isocyanate (3 + 2) reaction with D-A cyclopropanes, Method A.* To a flame-dried 10 mL flask equipped with a magnetic stir bar was added iron(III) chloride (0.44 mmol) in an inert atmosphere glovebox. The flask was sealed with a Teflon septum, removed from were glovebox and placed under a nitrogen atmosphere. To an oven-dried 1 dram vial were added the appropriate cyclopropane (0.4 mmol) and isocyanate (1.2 mmol). The vial was sealed with a screw cap fitted with a Teflon septum, and this mixture was transferred to the reaction flask as a solution in anhydrous dichloromethane (1 mL + 0.33 mL rinse). The solution was then allowed to stir at ambient temperature under nitrogen. Upon consumption of the cyclopropane (as determined by TLC analysis), the reaction solution was diluted with dichloromethane, adsorbed onto Celite, and purified by silica gel column chromatography.

General Procedure G. *Isocyanate (3 + 2) reaction with D-A cyclopropanes, Method B.* To an oven-dried 1 dram vial equipped with a magnetic stir bar was added iron (III) chloride (0.44 mmol) and oven-dried 4Å molecular sieves (50 mg). The vial was sealed with a screw cap fitted with a rubber septum, and was placed under a nitrogen atmosphere. To a second oven-dried 1 dram vial was added the appropriate cyclopropane (0.4 mmol) and isocyanate (1.2 mmol). The vial was sealed with a screw cap fitted with a Teflon septum and this mixture was transferred to the first vial as a solution in anhydrous dichloromethane (1 mL + 0.33 mL rinse). The mixture was then allowed to stir at ambient temperature under nitrogen. Upon consumption of the cyclopropane (as determined by TLC analysis), the reaction mixture was partitioned between dichloromethane and saturated aqueous sodium bicarbonate. The layers were separated and the aqueous phase was washed twice with dichloromethane. The combined organic layers were washed with brine, dried over magnesium sulfate, filtered, and concentrated *in vacuo*. The crude product was purified by column chromatography.

Cyclopropane Characterization Data

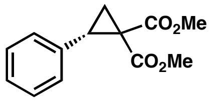


S1 ***3***

dimethyl 2-phenylcyclopropane-1,1-dicarboxylate

Benzylidene dimethylmalonate **S1** was prepared according to General Method A: 99% yield. R_f = 0.60 (3:1 Hexanes:EtOAc eluent). Characterization data matches those reported in the literature.[4]

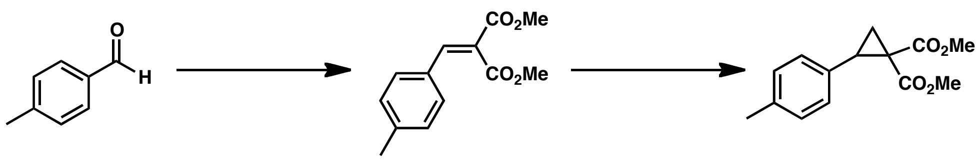
Cyclopropane **3** was prepared according to General Method B: 66% yield. R_f = 0.60 (3:1 Hexanes:EtOAc eluent). Characterization data matches those reported in the literature.[5]



(S)-3

(*S*)-dimethyl 2-phenylcyclopropane-1,1-dicarboxylate

Cyclopropane (*S*)**-3** was prepared according to literature methods.[6] $[\alpha]_D^{25.0}$ -133.17° (*c* 0.99, $CHCl_3$, >98% ee).



S2 ***S3***

dimethyl 2-(*p*-tolyl)cyclopropane-1,1-dicarboxylate

Benzylidene dimethylmalonate **S2** was prepared according to General Method A: 30% yield. R_f = 0.19 (3:1 Heaxanes:EtOAc eluent). Characterization data matches those reported in the literature.[7]

Cyclopropane **S3** was prepared according to General Method B: 77% yield. R_f = 0.60 (3:1 Hexanes:EtOAc). Characterization data matches those reported in the literature.[8]

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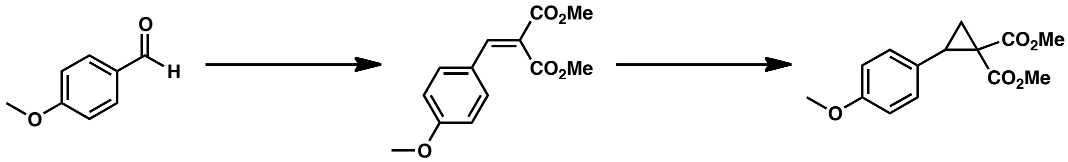
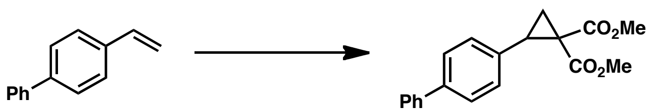
[4] Smith, III, A. B.; Liu, Z. *Org. Lett.* **2008**, *10*, 4363–4365.
[5] Goudreau, S. R.; Marcoux, D.; Charette, A. B. *J. Org. Chem.* **2009**, *74*, 470–473.
[6] Davies, H. M. L.; Bruzinski, P. R.; Lake, D. H.; Kong, N.; Fall, M. J. *J. Am. Chem. Soc.* **1996**, *118*, 6897–6907.
[7] Rappoport, Z.; Gazit, A. *J. Org. Chem.* **1986**, *51*, 4107–4111.
[8] Davies, H. M. L.; Panaro, S. A. *Tetrahedron* **2000**, *56*, 4871–4880.



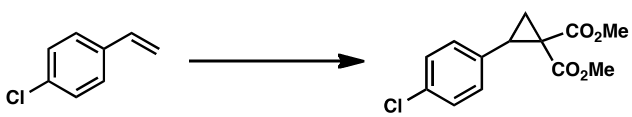
S4 **S5**

dimethyl 2-(4-methoxyphenyl)cyclopropane-1,1-dicarboxylate
Benzylidene dimethylmalonate **S4** was prepared according to General Method A: 92% yield. R_f = 0.27 (3:1 Hexanes:EtOAc eluent). Characterization data matches those reported in the literature.[9]
Cyclopropane **S5** was prepared according to General Method B: 95% yield. R_f = 0.40 (3:1 Hexanes:EtOAc eluent). Characterization data matches those reported in the literature.[10]



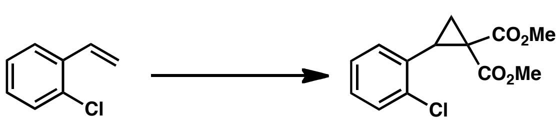
S6

dimethyl 2-([1,1'-biphenyl]-4-yl)cyclopropane-1,1-dicarboxylate
Cyclopropane **S6** was prepared according to General Method C: 99% yield. R_f = 0.48 (3:1 Hexanes:EtOAc eluent). Characterization data matches those reported in the literature.[11]



S7

dimethyl 2-(4-chlorophenyl)cyclopropane-1,1-dicarboxylate
Cyclopropane **S7** was prepared according to General Method C: 99% yield. R_f = 0.53 (3:1 Hexanes:EtOAc eluent). Characterization data matches those reported in the literature.[10]



S8

dimethyl 2-(2-chlorophenyl)cyclopropane-1,1-dicarboxylate
Cyclopropane **S8** was prepared according to General Method C: 60% yield. R_f = 0.50 (3:1 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39–7.33 (m, 1H), 7.22–7.15 (m, 2H), 7.11–7.07 (m, 1H), 3.81 (s, 3H), 3.36 (s, 4H), 2.26 (dd, *J* = 8.3, 5.2 Hz, 1H), 1.79 (dd, *J* = 9.1, 5.2 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.0, 167.1, 136.6, 132.8, 129.3, 129.0, 128.9, 126.5, 53.0, 52.4, 36.5, 31.3, 19.0; IR (Neat Film, NaCl) 3001, 2953,

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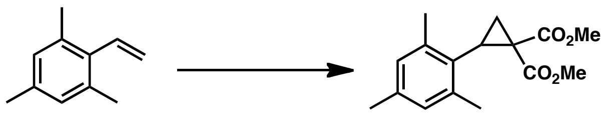
[9] Srgel, S.; Tokunaga, N.; Sasaki, K.; Okamoto, K.; Hayashi, T. *Org. Lett.* **2008**, *10*, 589–592.
[10] De Simone, F.; Saget, T.; Benfatti, F.; Almeida, S.; Waser, J. *Chem.–Eur. J.* **2011**, *51*, 14527–14538.
[11] Chagarovskiy, A. O.; Ivanova, O. A.; Rakhmankulov, E. R.; Budynina, E. M.; Trushkov, I. V.; Melnikov, M. Y. *Adv. Synth. Catal.* **2010**, *352*, 3179–3184.

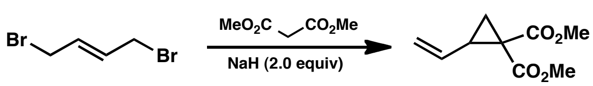
1732, 1483, 1435, 1377, 1331, 1288, 1219, 1131, 1055, 894, 785, 754 cm^{-1}; HRMS (ESI) *m/z* calc'd for $C_{13}H_{14}{}^{35}ClO_4$ $[M+H]^+$: 269.0575, found 269.0573.



S9

dimethyl 2-mesitylcyclopropane-1,1-dicarboxylate

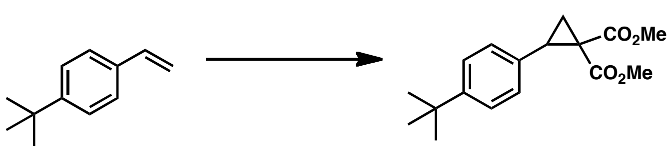
Cyclopropane **S9** was prepared according to General Method C: 71% yield. R_f = 0.40 (3:1 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.81 (s, 2H), 3.83 (s, 3H), 3.34 (s, 3H), 3.10–3.02 (app t, *J* = 9.3 Hz, 1H), 2.42–2.36 (dd, *J* = 8.9, 4.9 Hz, 1H), 2.32 (s, 6H), 2.22 (s, 3H), 1.97–1.89 (dd, *J* = 9.6, 4.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.8, 168.0, 136.6, 129.2, 128.5, 52.9, 52.2, 35.3, 32.0, 24.0, 21.0; IR (Neat Film, NaCl) 2953, 2921, 1728, 1612, 1437, 1372, 1328, 1287, 1224, 1196, 1128, 1096, 1032, 1015, 992, 894, 852, 782, 718 cm^{-1}; HRMS (Low Voltage MM: ESI-APCI) *m/z* calc'd for $C_{16}H_{21}O_4$ $[M+H]^+$: 277.1434, found 277.1420.



S10

dimethyl 2-vinylcyclopropane-1,1-dicarboxylate

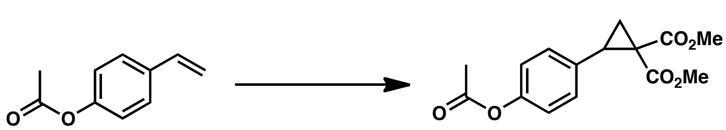
Cyclopropane **S10** was prepared according to the method of Johnson and coworkers.[12]



S11

dimethyl 2-(4-(*tert*-butyl)phenyl)cyclopropane-1,1-dicarboxylate

Cyclopropane **S11** was prepared according to General Method C: 89% yield. R_f = 0.50 (3:1 Hexanes:EtOAc eluent). Characterization data matches those reported in the literature.[13]



S12

dimethyl 2-(4-acetoxyphenyl)cyclopropane-1,1-dicarboxylate

Cyclopropane **S12** was prepared according to General Method C: 67% yield. R_f = 0.30 (3:1 Hexanes:EtOAc eluent). Characterization data matches those reported in the literature.[14]

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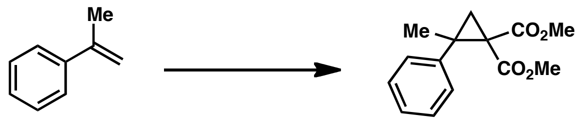
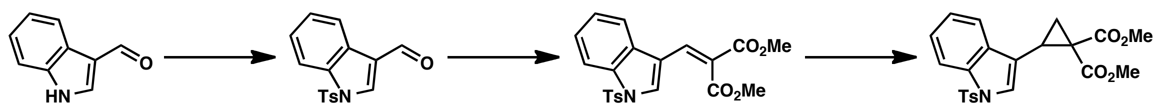
[12] Parsons, A. T.; Campbell, M. J.; Johnson, J. S. *Org. Lett.* **2008**, *10*, 2541–2544.
[13] Perreault, C.; Goudreau, S. R.; Zimmer, L. E.; Charette, A. B.; *Org. Lett.* **2008**, *10*, 689–692.



S13

dimethyl 2-methyl-2-phenylcyclopropane-1,1-dicarboxylate
Cyclopropane **S13** was prepared according to General Method C: 41% yield. $R_f = 0.53$ (3:1 Hexanes:EtOAc eluent). Characterization data matches those reported in the literature.[15]



S14 ***S15*** ***S16*** ***S17***

dimethyl 2-(1-tosyl-1*H*-indol-3-yl)cyclopropane-1,1-dicarboxylate
N-Tosylindole-3-carboxaldehyde (**S15**) was prepared according to literature methods from indole-3-carbodaldehyde (**S14**).[16]
Benzylidene dimethylmalonate **S16** was prepared according to General Method A: 75% yield. $R_f = 0.20$ (3:1 Hexanes:EtOAc eluent). Characterization data matches those reported in the literature.[17]
Cyclopropane **S17** was prepared according to General Method B: 95% yield. $R_f = 0.30$ (3:1 Hexanes:EtOAc eluent).[17]

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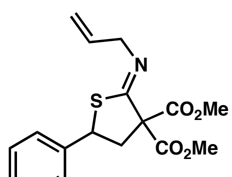
[14] Pohlhaus, P. D.; Sanders, S. D.; Parsons, A. T.; Li, W.; Johnson, J. S.; *J. Am. Chem. Soc.* **2008**, *130*, 8642–8650.
[15] Georgakopoulou, G.; Kalogiros, C.; Hadjiarapoglou, L. P. *Synlett* **2001**, 1843–1846.
[16] Guo, X.; Hu, W.; Cheng, S.; Wang, L.; Chang, J. *Synth. Commun.* **2006**, *36*, 781–788.
[17] Ivanova, O. A.; Budynina, E. M.; Chagarovskiy, A. O.; Rakhmankulov, E. R.; Trushkov, I. V.; Semeykin, A. V.; Shimanovskii, N. L.; Melnikov, M. Y. *Chem.–Eur. J.* **2011**, *17*, 11738–11742.

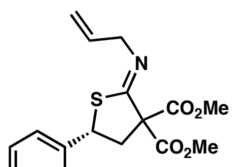
Thioimidate Characterization Data

Unless stated otherwise, all thioimidates were prepared according to General Method D



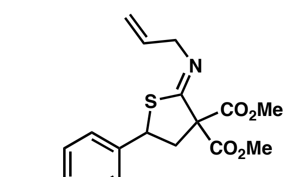
2a

(*Z*)-dimethyl 2-(allylimino)-5-phenyldihydrothiophene-3,3(2*H*)-dicarboxylate (2a): 92% yield. R_f = 0.45 (7:3 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46–7.40 (m, 2H), 7.39–7.34 (m, 2H), 7.33–7.29 (m, 1H), 5.99 (ddt, *J* = 17.1, 10.4, 5.2 Hz, 1H), 5.26 (dq, *J* = 17.2, 1.8 Hz, 1H), 5.13 (dq, *J* = 10.4, 1.7 Hz, 1H), 4.73 (dd, *J* = 11.7, 4.9 Hz, 1H), 4.00 (dtd, *J* = 5.5, 1.8, 0.7 Hz, 2H), 3.88 (s, 3H), 3.81 (s, 3H), 3.12 (dd, *J* = 13.0, 4.9 Hz, 1H), 2.90 (dd, *J* = 13.0, 11.7 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.4, 168.1, 166.0, 138.2, 134.0, 129.0, 128.5, 127.8, 116.0, 71.0, 59.8, 53.8, 53.6, 50.9, 44.3; IR (Neat Film, NaCl) 3010, 2952, 1738, 1652, 1495, 1435, 1269, 1227, 1169, 1098, 1064, 977, 921, 862, 842, 799, 765 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{17}H_{20}NO_4S$ $[M+H]^+$: 334.1108, found 334.1113.



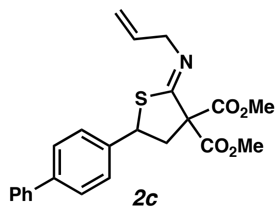
(R)-2a

(*R*,*Z*)-dimethyl 2-(allylimino)-5-phenyldihydrothiophene-3,3(2H)-dicarboxylate ((*R*)-*2a*): Characterization data is same as above; $[\alpha]_D^{25.0}$ 8.8° (*c* 0.445, $CHCl_3$, 95% ee).



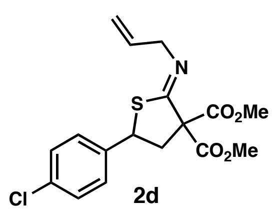
2b

dimethyl 1-allyl-5-(4-methoxyphenyl)-2-thioxopyrrolidine-3,3-dicarboxylate (2b): 98% yield. R_f = 0.49 (7:3 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38–7.32 (m, 2H), 6.90–6.85 (m, 2H), 6.03–5.92 (m, 1H), 5.24 (dq, *J* = 17.2, 1.8 Hz, 1H), 5.12 (dq, *J* = 10.4, 1.7 Hz, 1H), 4.71 (dd, *J* = 11.8, 4.8 Hz, 1H), 3.99 (dt, *J* = 5.2, 1.8 Hz, 2H), 3.87 (s, 3H), 3.81 (s, 3H), 3.80 (s, 3H), 3.07 (dd, *J* = 13.0, 4.9 Hz, 1H), 2.87 (dd, *J* = 13.0, 11.8 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.4, 168.1, 166.5, 159.7, 134.0, 130.0, 129.0, 116.0, 114.3, 71.1, 59.7, 55.5, 53.8, 53.6, 50.6, 44.5; IR (Neat Film, NaCl) 3003, 2953, 2837, 1736, 1638, 1610, 1513, 1435, 1305, 1250, 1175, 1098, 1070, 1032, 922, 831, 792 cm^{-1}; HRMS (Low Voltage MM: ESI-APCI) *m/z* calc'd for $C_{18}H_{22}NO_5S$ $[M+H]^+$: 364.1213, found 364.1193.



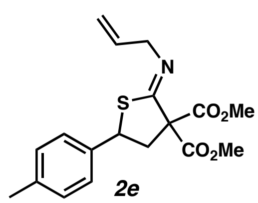
2c

(*Z*)-dimethyl 5-([1,1'-biphenyl]-4-yl)-2-(allylimino)dihydrothiophene-3,3(2*H*)-dicarboxylate (2c): 80% yield. R_f = 0.53 (7:3 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62–7.56 (m, 4H), 7.53–7.49 (m, 2H), 7.48–7.42 (m, 2H), 7.39–7.33 (m, 1H), 6.00 (ddt, *J* = 17.2, 10.4, 5.2 Hz, 1H), 5.27 (dq, *J* = 17.1, 1.8 Hz, 1H), 5.14 (dq, *J* = 10.3, 1.7 Hz, 1H), 4.79 (dd, *J* = 11.7, 4.9 Hz, 1H), 4.02 (dt, *J* = 5.2, 1.8 Hz, 2H), 3.89 (s, 3H), 3.83 (s, 3H), 3.16 (dd, *J* = 13.0, 4.9 Hz, 1H), 2.94 (dd, *J* = 13.0, 11.7 Hz, 1H);; ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.3, 168.0, 166.2, 141.4, 140.4, 137.0, 133.8, 128.9, 128.2, 127.6, 127.1, 116.0, 71.0, 59.6, 53.7, 53.5, 50.6, 44.2; IR (Neat Film, NaCl) 3029, 2952, 1736, 1651, 1639, 1487, 1435, 1412, 1279, 1263, 1226, 1168, 1099, 1070, 1008, 977, 920, 836, 799, 767, 738 cm^{-1}; HRMS (Low Voltage MM: ESI-APCI) *m/z* calc'd for $C_{23}H_{24}NO_4S$ [M+H]$^+$: 410.1421, found 410.1408.



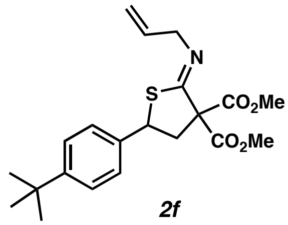
2d

(*Z*)-dimethyl 2-(allylimino)-5-(4-chlorophenyl)dihydrothiophene-3,3(2*H*)-dicarboxylate (2d): 66% yield. R_f = 0.49 (7:3 Hexanes:EtOAc eluent); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.19 (m, 4H), 5.97 (ddt, *J* = 17.1, 10.4, 5.1 Hz, 1H), 5.23 (dq, *J* = 17.2, 1.9 Hz, 1H), 5.12 (dq, *J* = 10.4, 1.7 Hz, 1H), 4.69 (dd, *J* = 11.6, 4.9 Hz, 1H), 3.98 (dt, *J* = 5.1, 1.8 Hz, 2H), 3.86 (s, 3H), 3.79 (s, 3H), 3.09 (dd, *J* = 13.0, 5.0 Hz, 1H), 2.82 (dd, *J* = 13.0, 11.6 Hz, 1H).; ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 167.8, 165.3, 136.7, 134.2, 133.8, 129.0, 129.0, 115.9, 70.8, 59.7, 53.7, 53.4, 50.0, 44.1; IR (Neat Film, NaCl) 2953, 1733, 1652, 1637, 1491, 1434, 1266, 1221, 1167, 1090, 1068, 1011 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{17}H_{19}{}^{35}ClNO_4S$ [M+H]$^+$: 368.0718, found 368.0729.



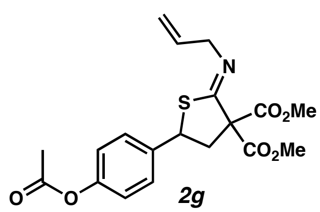
2e

(Z)-dimethyl 2-(allylimino)-5-(p-tolyl)dihydrothiophene-3,3(2H)-dicarboxylate (2e): 99% yield. R_f = 0.47 (7:3 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33–7.29 (m, 2H), 7.19–7.15 (m, 2H), 5.98 (ddt, *J* = 17.2, 10.4, 5.2 Hz, 1H), 5.25 (dq, *J* = 17.2, 1.8 Hz, 1H), 5.14 (dq, *J* = 10.4, 1.7 Hz, 1H), 4.72 (dd, *J* = 11.8, 4.8 Hz, 1H), 4.01 (dt, *J* = 5.2, 1.8 Hz, 2H), 3.88 (s, 3H), 3.82 (s, 3H), 3.10 (dd, *J* = 13.1, 4.9 Hz, 1H), 2.88 (dd, *J* = 13.0, 11.8 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ168.2, 168.0, 138.5, 134.9, 133.7, 129.7, 127.7, 116.3, 71.1, 59.5, 53.9, 53.7, 51.1, 44.5, 21.3; IR (Neat Film, NaCl) 3011, 2952, 1737, 1652, 1639, 1515, 1435, 1278, 1269, 1257, 1228, 1169, 1071, 1018, 978, 921, 864, 848, 818, 790 cm^{-1}; HRMS (Low Voltage MM: ESI-APCI) *m/z* calc'd for $C_{18}H_{22}NO_4S$ $[M+H]^+$: 348.1264, found 348.1254.



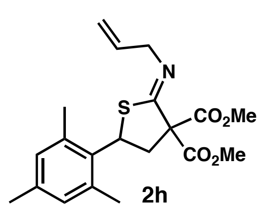
2f

(*Z*)-dimethyl 2-(allylimino)-5-(4-(*tert*-butyl)phenyl)dihydrothiophene-3,3(2*H*)-dicarboxylate (2f): 41% yield. R_f = 0.30 (3:1 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41–7.32 (m, 4H), 5.98 (ddt, *J* = 17.1, 10.4, 5.2 Hz, 1H), 5.25 (dq, *J* = 17.2, 1.8 Hz, 1H), 5.13 (dq, *J* = 10.4, 1.7 Hz, 1H), 4.71 (dd, *J* = 11.8, 4.9 Hz, 1H), 3.99 (dt, *J* = 5.1, 1.7 Hz, 2H), 3.88 (s, 3H), 3.81 (s, 3H), 3.07 (dd, J = 13.0, 4.9 Hz, 1H), 2.90 (dd, J = 13.0, 11.8 Hz, 1H) 1.31 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.5, 168.2, 166.3, 151.6, 135.1, 134.1, 127.5, 125.9, 116.0, 71.1, 59.8, 53.8, 53.6, 50.7, 44.3, 34.8, 31.4; IR (Neat Film, NaCl) 2955, 2904, 2868, 1737, 1652, 1639, 1509, 1435, 1363, 1280, 1267, 1227, 1168, 1111, 1070, 1016, 978, 920, 828 cm^{-1}; HRMS (Low Voltage MM: ESI-APCI) *m/z* calc'd for $C_{21}H_{28}NO_4S$ $[M+H]^+$: 390.1734, found 390.1726.



2g

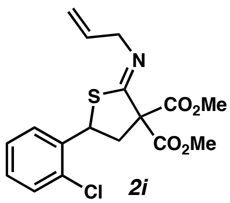
(*Z*)-dimethyl 5-(4-acetoxyphenyl)-2-(allylimino)dihydrothiophene-3,3(2*H*)-dicarboxylate (2g): 84% yield. R_f = 0.20 (3:1 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49–7.41 (m, 2H), 7.12–7.05 (m, 2H), 5.97 (ddt, *J* = 17.2, 10.3, 5.2 Hz, 1H), 5.25 (dq, *J* = 17.2, 1.8 Hz, 1H), 5.13 (dq, *J* = 10.4, 1.7 Hz, 1H), 4.72 (dd, *J* = 11.6, 4.9 Hz, 1H), 3.99 (ddd, *J* = 7.0, 1.7, 1.0 Hz, 2H), 3.87 (s, 3H), 3.80 (s, 3H), 3.11 (dd, *J* = 13.1, 4.9 Hz, 1H), 2.85 (dd, *J* = 13.1, 11.6 Hz, 1H), 2.30 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.5, 168.4, 168.0, 165.8, 150.6, 135.8, 134.0, 129.0, 122.2, 116.0, 71.0, 59.8, 53.8, 53.6, 50.3, 44.5, 21.3; IR (Neat Film, NaCl) 2953, 1736, 1649, 1639, 1507, 1436, 1370, 1280, 1257, 1194, 1167, 1099, 1016, 911, 851 cm^{-1}; HRMS (Low Voltage MM: ESI-APCI) *m/z* calc'd for $C_{19}H_{22}NO_6S$ $[M+H]^+$: 392.1162, found 392.1159.



2h

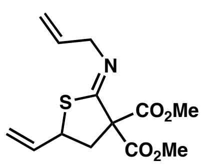
(*Z*)-dimethyl 2-(allylimino)-5-mesityldihydrothiophene-3,3(2*H*)-dicarboxylate (2h): 85% yield. White, translucent crystals were obtained by slow diffusion of 1% benzene in heptane into a solution of thioimidate **2h** in ethyl acetate, M.P.: 89–91 °C; R_f = 0.52 (7:3 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.87–6.84 (m, 2H), 5.99 (ddt, *J* =

17.2, 10.4, 5.2 Hz, 1H), 5.32 (dd, *J* = 12.5, 5.3 Hz, 1H), 5.24 (dq, *J* = 17.2, 1.8 Hz, 1H), 5.13 (dq, *J* = 10.4, 1.7 Hz, 1H), 4.02 (dtd, *J* = 5.2, 1.8, 0.8 Hz, 2H), 3.90 (s, 3H), 3.84 (s, 3H), 3.24 (dd, *J* = 13.3, 12.5 Hz, 1H), 2.93 (dd, *J* = 13.3, 5.3 Hz, 1H), 2.46 (s, 6H), 2.25 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.5, 168.3, 166.8, 137.9, 134.0, 130.9, 129.2, 116.0, 71.1, 59.8, 53.8, 53.6, 46.2, 40.0, 21.3, 20.9; IR (Neat Film, NaCl) 3010, 2952, 2918, 1737, 1649, 1638, 1611, 1435, 1267, 1230, 1203, 1167, 1097, 1073, 1015, 976, 921, 954, 822, 799, 774, 739 cm^{-1}; HRMS (Low Voltage MM: ESI-APCI) *m/z* calc'd for $C_{20}H_{26}NO_4S$ $[M+H]^+$: 376.1577, found 376.1563.



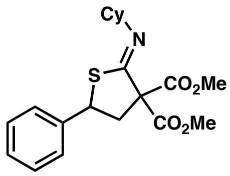
2i

(*Z*)-dimethyl 2-(allylimino)-5-(2-chlorophenyl)dihydrothiophene-3,3(2*H*)-dicarboxylate (2i): 84% yield. R_f = 0.48 (7:3 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.38 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.31 (td, *J* = 7.6, 1.4 Hz, 1H), 7.23 (td, *J* = 7.6, 1.7, 1H), 5.98 (ddt, *J* = 17.2, 10.4, 5.2 Hz, 1H), 5.30–5.22 (m, 2H), 5.14 (dq, *J* = 10.4, 1.7 Hz, 1H), 4.03 (td, *J* = 4.4, 2.0 Hz, 2H), 3.88 (s, 3H), 3.77 (s, 3H), 3.19 (dd, *J* = 13.0, 5.1 Hz, 1H), 2.84 (dd, *J* = 13.0, 11.0 Hz, 1H);; ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.1, 168.0, 165.7, 135.8, 134.0, 133.9, 130.0, 129.5, 128.5, 127.5, 116.1, 70.6, 59.7, 53.8, 53.6, 47.0, 42.6; IR (Neat Film, NaCl) 3011, 2953, 1737, 1651, 1639, 1435, 1279, 1256, 1228, 1171, 1130, 1100, 1069, 1051, 1038, 977, 921, 760 cm^{-1}; HRMS (Low Voltage MM: ESI-APCI) *m/z* calc'd for $C_{17}H_{19}{}^{35}ClNO_4S$ $[M+H]^+$: 368.0718, found 368.0700.



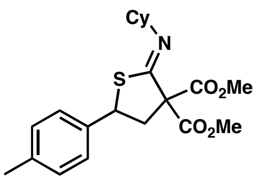
2j

(*Z*)-dimethyl 2-(allylimino)-5-vinyldihydrothiophene-3,3(2*H*)-dicarboxylate (2j): 99% yield. R_f = 0.45 (7:3 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.95 (ddt, *J* = 17.2, 10.4, 5.2 Hz, 1H), 5.80 (ddd, *J* = 16.9, 10.0, 8.4 Hz, 1H), 5.33 (dq, *J* = 16.9, 0.8 Hz, 1H), 5.23 (ddd, *J* = 17.3, 1.8, 0.6 Hz, 1H), 5.19 (d, *J* = 10.1. 1H), 5.13 (ddd, *J* = 10.4, 1.7, 0.7 Hz, 1H), 4.22 (m, 1H), 3.98 (dd, *J* = 5.2, 2.0 Hz, 2H), 3.84 (s, 3H), 3.81 (d, *J* = 0.6 Hz, 3H), 2.97 (ddd, *J* = 13.1, 5.1, 0.8 Hz, 1H), 2.61 (dd, *J* = 13.1, 10.6 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.1, 168.0, 135.7, 133.6, 118.9, 116.3, 70.5, 59.4, 53.8, 53.7, 50.3, 42.2; IR (Neat Film, NaCl) 2952, 1735, 1649, 1638, 1434, 1328, 1272, 1254, 1169, 1139, 1097, 1068, 987, 923, 859, 787, 728 cm^{-1}; HRMS (Low Voltage MM: ESI-APCI) *m/z* calc'd for $C_{13}H_{18}NO_4S$ $[M+H]^+$: 284.0951, found 284.0962.



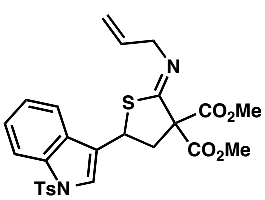
2k

(*Z*)-dimethyl 2-(cyclohexylimino)-5-phenyldihydrothiophene-3,3(2*H*)-dicarboxylate (2k): 91% yield. R_f = 0.40 (3:1 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46–7.42 (m, 2H), 7.36 (ddd, *J* = 8.2, 7.1, 0.9 Hz, 2H), 7.30 (m, 1H), 4.69 (dd, *J* = 11.7, 4.9 Hz, 1H), 3.87 (s, 3H), 3.78 (s, 3H), 3.08 (dd, *J* = 13.0, 4.9 Hz, 1H), 2.98 (tt, *J* = 10.1, 3.6 Hz, 1H), 2.85 (dd, *J* = 13.0, 11.7 Hz, 1H), 1.85–1.72 (m, 4H), 1.65–1.57 (m, 1H), 1.57–1.44 (m, 2H), 1.37–1.20 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.6, 168.3, 161.5, 138.6, 128.9, 128.4, 127.8, 70.8, 67.1, 53.7, 53.4, 50.6, 44.0, 32.8, 31.7, 25.8, 24.7, 24.6; IR (Neat Film, NaCl) 2930, 2854, 1738, 1651, 1435, 1168, 1067, 973, 912, 764 cm^{-1}; HRMS (ESI) *m/z* calc'd for $C_{20}H_{26}NO_4S$ [M+H]$^+$: 376.1577, found 356.1589.



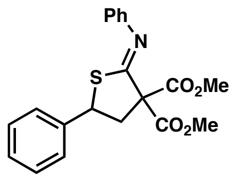
2l

(*Z*)-dimethyl 2-(cyclohexylimino)-5-(*p*-tolyl)dihydrothiophene-3,3(2*H*)-dicarboxylate (2l): 99% yield. R_f = 0.63 (2:1 Hexanes: EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35–7.29 (m, 2H), 7.18–7.14 (m, 2H), 4.67 (dd, *J* = 11.8, 4.8 Hz, 1H), 3.86 (s, 3H), 3.78 (s, 3H), 3.05 (dd, *J* = 13.0, 4.9 Hz, 1H), 2.98 (tt, *J* = 10.1, 3.6 Hz, 1H), 2.83 (dd, *J* = 13.0, 11.8 Hz, 1H), 2.35 (s, 3H), 1.83–1.72 (m, 4H), 1.65–1.57 (m, 1H), 1.56–1.44 (m, 2H), 1.38–1.21 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.7, 168.3, 161.5, 138.2, 135.5, 129.6, 127.6, 70.9, 67.0, 53.6, 53.4, 50.4, 44.0, 32.8, 31.7, 25.8, 24.7, 24.5, 21.2; IR (Neat Film, NaCl) 2929, 2853, 1735, 1648, 1434, 1255, 1167, 1071, 973, 818 cm^{-1}; HRMS (APCI) *m/z* calc'd for $C_{21}H_{28}NO_4S$ [M+H]$^+$: 390.1734, found 390.1738.



2m

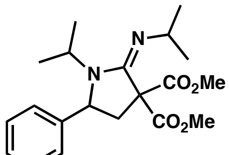
(*Z*)-dimethyl 2-(allylimino)-5-(1-tosyl-1*H*-indol-3-yl)dihydrothiophene-3,3(2*H*)-dicarboxylate (XX): 77% yield. R_f = 0.80 (1:1 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 168.1, 167.9, 166.2, 145.4, 135.5, 135.1, 133.6, 130.2, 128.9, 127.1, 125.5, 123.9, 123.5, 119.9, 116.3, 114.0, 77.4, 70.5, 59.7, 53.9, 53.7, 42.7, 41.7, 21.7; ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.1, 167.9, 166.2, 145.4, 135.5, 135.1, 133.6, 130.2, 128.9, 127.1, 125.5, 123.9, 123.5, 119.9, 116.3, 114.0, 77.4, 70.5, 59.7, 53.9, 53.7, 42.7, 41.7, 21.7; IR (Neat Film, NaCl) 2953, 1738, 1639, 1447, 1372, 1275, 1175, 1126, 1095, 974, 912, 733 cm^{-1}; HRMS (ESI) *m/z* calc'd for $C_{26}H_{27}N_2O_6S_2$ [M+H]$^+$: 527.1305, found 527.1298.



5

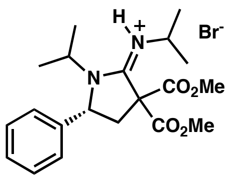
(*Z*)-dimethyl 5-phenyl-2-(phenylimino)dihydrothiophene-3,3(2*H*)-dicarboxylate (5): Prepared using General Method F, using phenylisothiocyanate. 89% yield. R_f = 0.60 (3:1 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41–7.37 (m, 2H), 7.36–7.31 (m, 4H), 7.30–7.27 (m, 1H), 7.16–7.11 (m, 1H), 7.05–7.01 (m, 2H), 4.76 (dd, *J* = 11.7, 4.9 Hz, 1H), 3.97 (s, 3H), 3.87 (s, 3H), 3.19 (dd, *J* = 13.1, 4.9 Hz, 1H), 2.99 (dd, *J* = 13.1, 11.7 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.3, 167.9, 167.8, 151.0, 137.8, 129.1, 129.0, 128.5, 127.8, 125.3, 120.2, 71.4, 54.0, 53.8, 51.2, 43.9; IR (Neat Film, NaCl) 3030, 2952, 1735, 1638, 1593, 1486, 1434, 1268, 1224, 1170, 1063, 973, 763 cm^{-1}; HRMS (ESI) *m/z* calc'd for $C_{20}H_{20}NO_4S$ [M+H]$^+$: 370.1108, found 370.1098.

Characterization Data for Amidines
All amidines were synthesized according to General Method E.



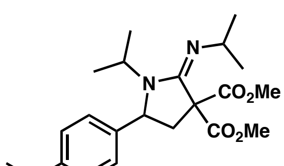
6a

(*E*)-dimethyl 1-isopropyl-2-(isopropylimino)-5-phenylpyrrolidine-3,3-dicarboxylate (6a): 98% yield. R_f = 0.39 (9:1 CH_2Cl_2:MeOH eluent); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.18 (m, 5H), 4.52 (t, *J* = 7.1 Hz, 1H), 3.99 (p, *J* = 6.8 Hz, 1H), 3.79 (s, 3H), 3.70 (s, 3H), 3.50 (hept, *J* = 6.0 Hz, 1H), 2.95 (dd, *J* = 12.8, 7.0 Hz, 1H), 2.33 (dd, *J* = 12.8, 7.2 Hz, 1H), 1.15 (d, *J* = 6.8 Hz, 3H), 1.11 (d, *J* = 6.0 Hz, 3H), 1.05 (d, *J* = 5.9 Hz, 3H), 0.88 (d, *J* = 6.9 Hz, 3H).; ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 169.2, 151.3, 143.8, 128.5, 127.8, 127.0, 60.5, 59.8, 53.1, 52.9, 51.4, 47.3, 43.4, 24.7, 24.3, 19.6, 19.2; IR (Neat Film, NaCl) 2963, 1731, 1659, 1436, 1261, 1212, 1063, 969 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{20}H_{29}N_2O_4$ $[M+H]^+$: 361.2122, found 361.2018.



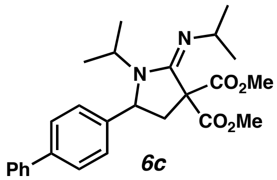
(R)-6a·HBr

(*R*,*E*)-dimethyl 1-isopropyl-2-(isopropylimino)-5-phenylpyrrolidine-3,3-dicarboxylate (*(R)-6a•HBr*): Acetyl bromide (22 μL, 0.3 mmol) was dissolved in dichloromethane (3 mL) in a 10 mL round bottom flask. Methanol (41 μL, 1 mmol) was added to the solution and this mixture was transferred into a second flask containing a solution of amidine (*R*)-**6a** (72 mg, 0.2 mmol). The mixture was concentrated in vacuo and crystallized by vapor diffusion of diethyl ether into dichloromethane to produce fine colorless needles suitable for X-ray crystallography. $[\alpha]_D^{25.0}$ 8.8° (*c* 0.445, $CHCl_3$, >98% ee).

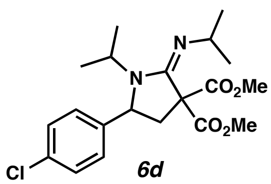


6b

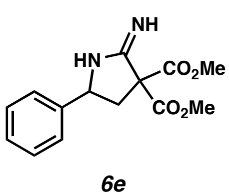
(*E*)-dimethyl 1-isopropyl-2-(isopropylimino)-5-(4-methoxyphenyl)pyrrolidine-3,3-dicarboxylate (6b): 98% yield. R_f = 0.42 (9:1 CH_2Cl_2:MeOH eluent); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.16 (m, 2H), 6.89 – 6.79 (m, 2H), 4.50 (br t, *J* = 6.9 Hz, 1H), 4.07 – 3.95 (br m, 1H), 3.79 (s, 3H), 3.77 (s, 3H), 3.72 (s, 3H), 3.49 (p, *J* = 6.0 Hz, 1H), 2.93 (br dd, *J* = 12.8, 6.9 Hz, 1H), 2.30 (br dd, *J* = 12.9, 7.3 Hz, 1H), 1.14 (br d, *J* = 6.9 Hz, 4H), 1.11 (d, *J* = 4.3 Hz, 2H), 1.05 (d, *J* = 6.0 Hz, 3H), 0.87 (d, *J* = 6.9 Hz, 3H).; ^{13}C NMR (101 MHz, $CDCl_3$) δ169.5, 169.0, 159.3, 151.6, 135.2, 128.2, 113.9, 60.7, 59.6, 55.3, 53.2, 53.0, 51.4, 47.4, 43.4, 24.5, 24.1, 19.7, 19.2.; IR (Neat Film, NaCl) 2963, 2928, 1736, 1654, 1612, 1513, 1249, 1214, 1172, 1081 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{21}H_{31}N_2O_5$ $[M+H]^+$: 391.2227, found 391.2208.



(*E*)-dimethyl 5-([1,1'-biphenyl]-4-yl)-1-isopropyl-2-(isopropylimino)pyrrolidine-3,3-dicarboxylate (6c): 92% yield. R_f = 0.42 (9:1 CH_2Cl_2:MeOH eluent); ^1H NMR (500 MHz, $CDCl_3$) δ 7.63–7.53 (m, 4H), 7.47–7.38 (m, 4H), 7.37–7.32 (m, 1H), 4.59 (t, *J* = 7.1 Hz, 1H), 4.04 (hept, *J* = 6.9 Hz, 1H), 3.83 (s, 3H), 3.74 (s, 3H), 3.53 (hept, *J* = 5.9 Hz, 1H), 3.00 (dd, *J* = 12.8, 7.0 Hz, 1H), 2.37 (dd, *J* = 12.8, 7.3 Hz, 1H), 1.20 (d, *J* = 6.8 Hz, 3H), 1.15 (d, *J* = 6.0 Hz, 3H), 1.08 (d, *J* = 5.9 Hz, 3H), 0.95 (d, *J* = 6.9 Hz, 3H);; ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.7, 169.2, 151.4, 142.9, 140.8, 140.7, 128.9, 127.5, 127.4, 127.2, 127.1, 60.6, 59.6, 53.2, 53.0, 51.5, 47.4, 43.4, 24.7, 24.4, 19.8, 19.2; IR (Neat Film, NaCl) 2964, 1733, 1658, 1486, 1435, 1375, 1358, 1264, 1216, 1165, 1126, 1076, 1008, 973, 841, 767, 733 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{26}H_{33}N_2O_4$ $[M+H]^+$: 437.2435, found 437.2411.

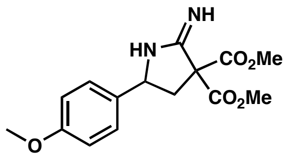


(*E*)-dimethyl 5-(4-chlorophenyl)-1-isopropyl-2-(isopropylimino)pyrrolidine-3,3-dicarboxylate (6d): 78% yield. R_f = 0.40 (9:1 CH_2Cl_2:MeOH eluent); ^1H NMR (500 MHz, $CDCl_3$) δ 7.30–7.23 (m, 4H), 4.50 (t, *J* = 7.1 Hz, 1H), 4.00 (hept, *J* = 6.9 Hz, 1H), 3.80 (s, 3H), 3.71 (s, 3H), 3.48 (hept, *J* = 5.9 Hz, 1H), 2.95 (dd, *J* = 12.8, 7.1 Hz, 1H), 2.27 (dd, *J* = 12.9, 7.1 Hz, 1H), 1.13 (d, *J* = 6.7 Hz, 3H), 1.09 (d, *J* = 6.0 Hz, 3H), 1.04 (d, *J* = 5.9 Hz, 3H), 0.86 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.6, 169.1, 151.2, 142.6, 133.4, 128.7, 128.3, 60.4, 59.1, 53.2, 53.0, 51.5, 47.3, 43.3, 24.7, 24.3, 19.9, 19.1; IR (Neat Film, NaCl) 2965, 1733, 1658, 1489, 1435, 1376, 1359, 1269, 1214, 1165, 1126, 1088, 1014, 974, 831 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{20}H_{28}{}^{35}ClN_2O_4$ $[M+H]^+$: 395.1732, found 395.1755.



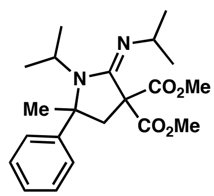
dimethyl 2-imino-5-phenylpyrrolidine-3,3-dicarboxylate (6e): 78% yield. R_f = 0.45 (9:1 CH_2Cl_2:MeOH eluent); ^1H NMR (500 MHz, $CDCl_3$) δ7.34–7.27 (m, 3H), 7.25–7.21 (m, 2H), 4.99 (dd, *J* = 8.2, 6.9 Hz, 1H), 3.83 (s, 3H), 3.77 (s, 3H), 3.10 (dd, *J* = 13.6, 7.0 Hz, 1H), 2.37 (dd, *J* = 13.6, 8.1 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.9, 168.3, 160.2, 144.2, 128.6, 127.1, 126.4, 68.4, 67.4, 53.6, 53.4, 42.8; IR (Neat Film, NaCl)

3449, 3028, 1729, 1665, 1600, 1435, 1386, 1354, 1279, 1243, 1201, 1154, 1114, 1075, 765 cm^{-1}; HRMS (FAB+) *m/z* calc'd for $C_{14}H_{17}N_2O_4$ $[M+H]^+$: 277.1188, found 277.1176.



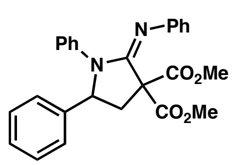
6f

dimethyl 2-imino-5-(4-methoxyphenyl)pyrrolidine-3,3-dicarboxylate (6f): 68% yield. R_f = 0.47 (9:1 CH_2Cl_2:MeOH eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23–7.16 (m, 2H), 6.84 (dd, *J* = 6.8, 1.9 Hz, 2H), 4.97–4.88 (m, 1H), 3.82 (s, 3H), 3.78 (s, 3H), 3.76 (s, 3H), 3.06 (dd, *J* = 13.6, 6.9 Hz, 1H) 2.34 (dd, *J* = 13.6, 8.1 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.9, 168.3, 160.1, 158.7, 136.3, 127.5, 113.9, 113.9, 67.8, 67.4, 55.4, 53.6, 53.4, 42.9; IR (Neat Film, NaCl) 3464, 3374, 3102, 2955, 2838, 1738, 1662, 1612, 1514, 1439, 1351, 1247, 1213, 1175, 1105, 1077, 1034, 831, 733 cm^{-1}; HRMS (FAB+) *m/z* calc'd for $C_{15}H_{19}N_2O_5$ $[M+H]^+$: 307.1294, found 307.1287.



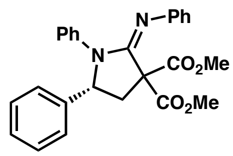
6g

(*E*)-dimethyl 1-isopropyl-2-(isopropylimino)-5-methyl-5-phenylpyrrolidine-3,3-dicarboxylate (6g): 58% yield. R_f =0.35 (10:1 $CHCl_3$:MeOH eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48–7.44 (m, 2H), 7.38–7.33 (m, 2H), 7.29–7.24 (m, 1H), 3.85 (s, 3H), 3.71 (s, 3H), 3.44 (dt, *J* = 11.8, 5.9 Hz, 1H), 3.09 ? 2.99 (hept, *J* = 6.7 Hz, 1H), 2.83–2.72 (m, 2H), 1.61 (s, 3H), 1.35 (dd, *J* = 17.2, 6.7 Hz, 6H), 1.10 (dd, *J* = 18.8, 5.9 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.5, 170.2, 148.5, 146.8, 128.3, 127.2, 126.7, 64.8, 60.3, 53.2, 53.1, 51.4, 50.5, 47.1, 24.9, 24.8, 24.5, 19.9, 19.1; IR (Neat Film, NaCl) 2963, 1731, 1654, 1375, 1251, 1217, 1090 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{21}H_{31}N_2O_4$ $[M+H]^+$: 375.2278, found 375.2297.



6h

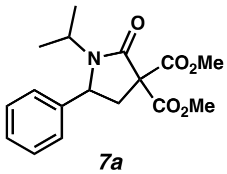
(*E*)-dimethyl 1,5-diphenyl-2-(phenylimino)pyrrolidine-3,3-dicarboxylate (6h): 79% yield. R_f =0.32 (10:1 CH_2Cl_2:MeOH eluent); ^{1}H NMR (400 MHz, DMSO-d6, 80 °C) δ 7.34 – 7.16 (m, 8H), 7.10 (dt, *J* = 15.2, 7.6 Hz, 5H), 6.95 (t, *J* = 7.4 Hz, 1H), 6.80 (t, *J* = 7.3 Hz, 1H), 6.71 (d, *J* = 7.7 Hz, 2H), 5.28 (t, *J* = 7.0 Hz, 1H), 3.66 (s, 3H) 3.45 (s, 3H), 3.17 (dd, *J* = 13.0, 7.2 Hz, 1H), 3.05 (s, 1H), 2.71 (dd, *J* = 13.0, 6.9 Hz, 1H);^{13}C NMR (101 MHz, DMSO-d6, 100 °C) δ 168.5, 168.2, 152.0, 148.4, 148.3, 140.9, 129.6, 129.5, 129.4, 129.3, 129.2, 129.1, 129.0, 128.9, 128.8, 128.7, 128.2, 128.2, 128.1, 128.0, 127.7, 127.5, 127.4, 127.3, 127.2, 126.6, 125.9, 124.6, 122.0, 121.9, 120.9, 64.1, 63.1, 62.7, 55.3, 54.5, 54.3, 53.4, 52.6, 52.4, 51.9, 43.0; IR (Neat Film, NaCl) 3062, 3027, 2948, 1730, 1661, 1592, 1493, 1372, 1263, 1051 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{26}H_{25}N_2O_4$ $[M+H]^+$: 429.1809, found 429.1825.



(R)-6h

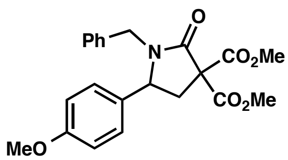
(*R*,*E*)-dimethyl 1,5-diphenyl-2-(phenylimino)pyrrolidine-3,3-dicarboxylate ((*R*)-6h): Characterization data same as above; $[\alpha]_D^{25.0}$ 36.7° (*c* 0.805, $CHCl_3$, 88% ee).

Characterization data for Lactams



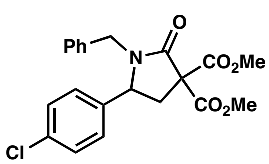
7a

dimethyl 1-isopropyl-2-oxo-5-phenylpyrrolidine-3,3-dicarboxylate (7a): Prepared according to General Method F. 72% yield. R_f = 0.46 (1:1 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39–7.26 (m, 5H), 4.64 (t, *J* = 7.3 Hz, 1H), 3.83 (s, 3H), 3.81 (s, 3H), 3.80–3.71 (m, 1H), 3.02 (dd, *J* = 13.8, 7.7 Hz, 1H), 2.59 (dd, *J* = 13.8, 6.9 Hz, 1H), 1.25 (d, *J* = 6.9 Hz, 3H), 1.01 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.3, 168.1, 167.2, 141.0, 129.0, 128.6, 127.2, 63.4, 59.7, 53.7, 53.5, 47.1, 38.4, 19.8, 19.7; IR (Neat Film, NaCl) 2954, 1735, 1703, 1495, 1457, 1434, 1367, 1342, 1259, 1218, 1130, 1090, 1065, 998, 966, 919, 894, 774 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{17}H_{22}NO_5$ $[M+H]^+$: 320.1492, found 320.1490.



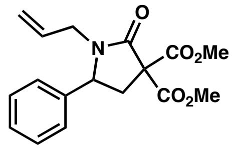
7b

dimethyl 1-butyl-2-oxo-5-(4-methoxyphenyl)pyrrolidine-3,3-dicarboxylate (7b): Prepared according to General Method F. 62% yield. R_f = 0.39 (1:1 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30–7.23 (m, 3H), 7.08–7.02 (m, 4H), 6.94–6.87 (m, 2H), 5.11 (d, *J* = 14.5 Hz, 1H), 4.31 (t, *J* = 7.6 Hz, 1H), 3.87 (s, 3H), 3.84 (s, 3H), 3.81 (s, 3H), 3.46 (d, *J* = 14.6 Hz, 1H), 2.94 (dd, *J* = 13.8, 7.2 Hz, 1H), 2.65 (dd, *J* = 13.8, 8.1 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ168.1, 167.9, 167.1, 160.0, 135.5, 130.4, 128.8, 128.7, 128.6, 127.9, 114.6, 63.4, 58.3, 55.5, 53.7, 53.6, 45.2, 38.1; IR (Neat Film, NaCl) 2953, 1735, 1705, 1513, 1434, 1281, 1247 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{22}H_{24}NO_6$ $[M+H]^+$: 398.1598, found 398.1581.



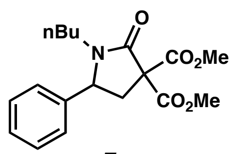
7c

dimethyl 1-butyl-2-oxo-5-(4-chlorophenyl)pyrrolidine-3,3-dicarboxylate (7c): Prepared according to General Method F. 78% yield. R_f = 0.41 (1:1 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39–7.33 (m, 2H), 7.29–7.24 (m, 3H), 7.10–7.05 (m, 2H), 7.04–7.00 (m, 2H), 5.13 (d, *J* = 14.6 Hz, 1H), 4.33 (t, *J* = 7.6 Hz, 1H), 3.87 (s, 3H), 3.83 (s, 3H), 3.46 (d, *J* = 14.6 Hz, 1H), 2.97 (dd, *J* = 13.9, 7.4 Hz, 1H), 2.60 (dd, *J* = 13.9, 7.8 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.9, 167.7, 167.2, 137.3, 135.1, 134.7, 129.5, 128.8, 128.7, 128.6, 128.0, 63.2, 58.1, 53.8, 53.7, 45.3, 37.9; IR (Neat Film, NaCl) 2953, 1736, 1708, 1435, 1242, 1204, 1090 cm^{-1}; HRMS (MM: ESI-APCI) *m/z* calc'd for $C_{21}H_{21}{}^{35}ClNO_5$ $[M+H]^+$: 402.1103, found 402.1084.



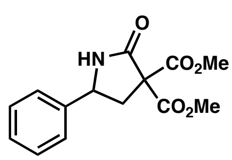
7d

dimethyl 1-allyl-2-oxo-5-phenylpyrrolidine-3,3-dicarboxylate (7d): Prepared according to General Method G. 42% yield. R_f = 0.52 (1:1 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42–7.29 (m, 3H), 7.24–7.18 (m, 2H), 5.71–5.52 (m, 1H), 5.12 (ddt, *J* = 10.1, 1.3, 0.7 Hz, 1H), 4.99–4.91 (m, 1H), 4.64 (t, *J* = 7.5 Hz, 1H), 4.40 (m, 1H), 3.90–3.84 (m, 3H), 3.82 (d, *J* = 0.9 Hz, 3H), 3.15–3.02 (m, 2H), 2.62 (dd, *J* = 13.8, 7.4 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.0, 167.9, 166.8, 138.9, 131.0, 129.2, 128.8, 127.3, 118.9, 63.1, 59.1, 53.8, 53.6, 44.1, 38.0; IR (Neat Film, NaCl) 2953, 1735, 1707, 1433, 1245, 1214, 1070 cm^{-1}; HRMS (FAB+) *m/z* calc'd for $C_{17}H_{20}NO_5$ $[M+H]^+$: 318.1341, found 318.1356.



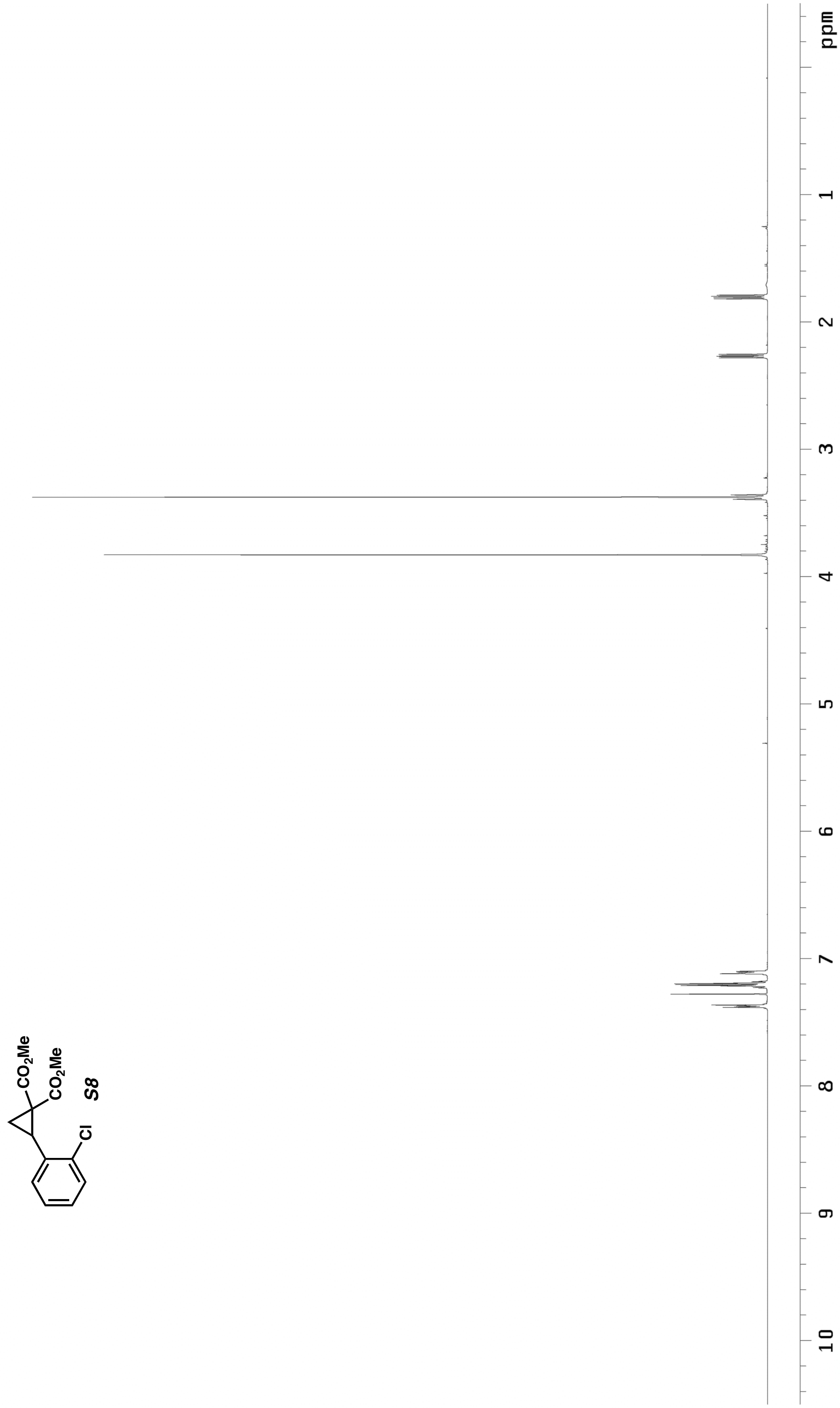
7e

dimethyl 1-butyl-2-oxo-5-phenylpyrrolidine-3,3-dicarboxylate (7e): Prepared according to General Method G. 58% yield. R_f = 0.10 (4:1 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40–7.31 (m, 3H), 7.25–7.20 (m, 2H), 4.63 (t, *J* = 7.5 Hz, 1H), 3.84 (s, 3H), 3.81 (s, 3H), 3.70 (dt, *J* = 13.7, 7.9 Hz, 1H), 3.06 (dd, *J* = 13.7, 7.3 Hz, 1H), 2.57–2.53 (m, 2H), 1.43–1.30 (m, 2H), 1.29–1.10 (m, 2H), 0.82 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.1, 168.0, 166.9, 139.1, 129.2, 128.7, 127.1, 63.2, 59.5, 53.7, 53.6, 41.1, 38.3, 28.6, 19.8, 13.7; IR (Neat Film, NaCl) 2957, 2873, 1732, 1708, 1495, 1456, 1435, 1370, 1278, 1242, 1202, 1108, 1090, 1070, 893, 771 cm^{-1}; HRMS (FAB+) *m/z* calc'd for $C_{18}H_{24}NO_5$ $[M+H]^+$: 334.1654, found 334.1646.

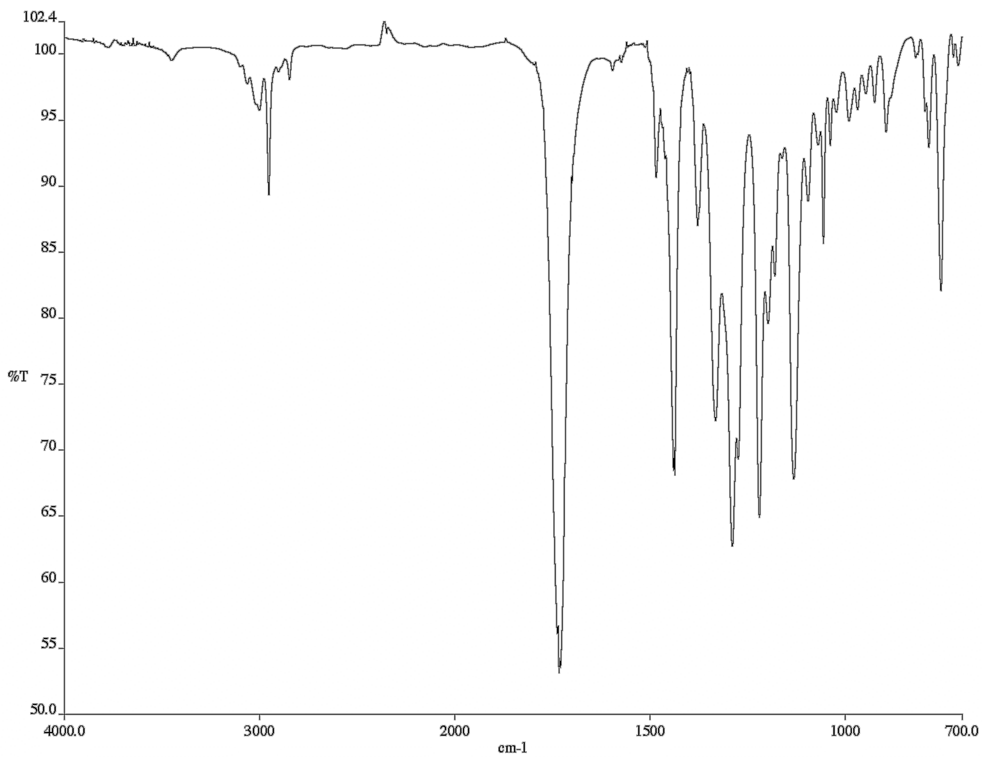


7f

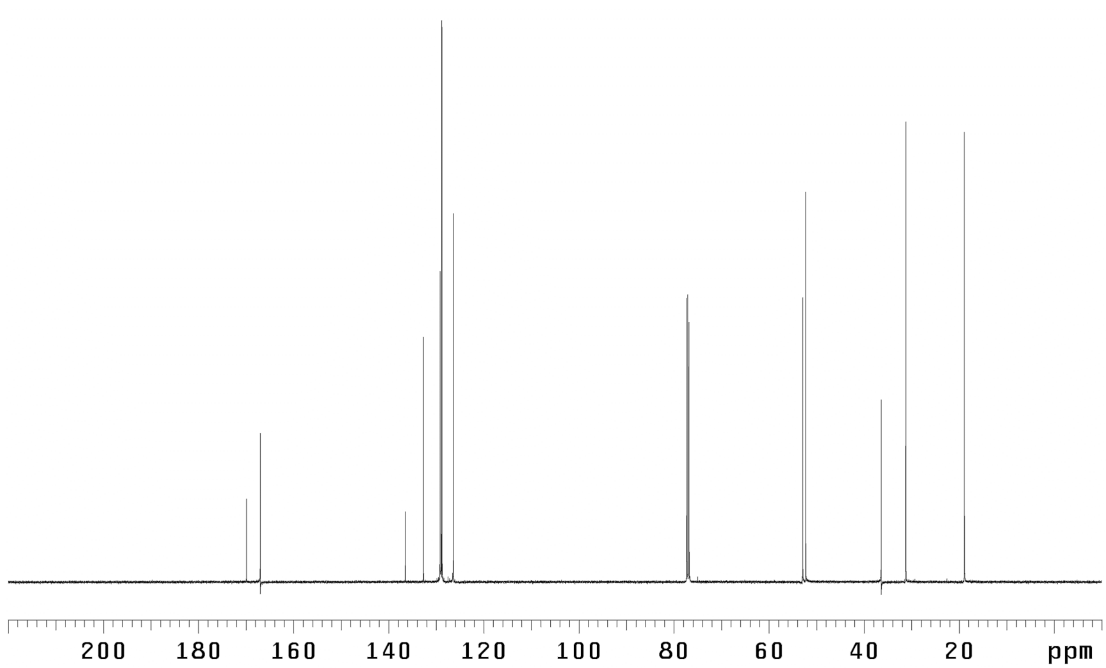
dimethyl 2-oxo-5-phenylpyrrolidine-3,3-dicarboxylate (7f): Prepared according to General Method G. 49% yield. R_f = 0.48 (1:1 Hexanes:EtOAc eluent); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40–7.33 (m, 2H), 7.33–7.28 (m, 3H), 6.93–6.69 (bs, 1H), 4.75 (t, *J* = 7.4 Hz, 1H), 3.85 (d, *J* = 1.6 Hz, 3H), 3.77 (dd, *J* = 2.1, 0.9 Hz, 3H), 3.18 (ddt, *J* = 13.6, 7.2, 0.8 Hz, 1H), 2.63 (ddd, *J* = 13.5, 7.8, 1.8 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.5, 167.5, 167.4, 140.3, 129.0, 128.4, 126.0, 63.2, 55.4, 53.7, 53.6, 40.4; IR (Neat Film, NaCl) 3251, 2955, 1729, 1435, 1250, 1208, 1060 cm^{-1}; HRMS (FAB+) *m/z* calc'd for $C_{14}H_{16}NO_5$ $[M+H]^+$: 278.1028, found 278.1042.



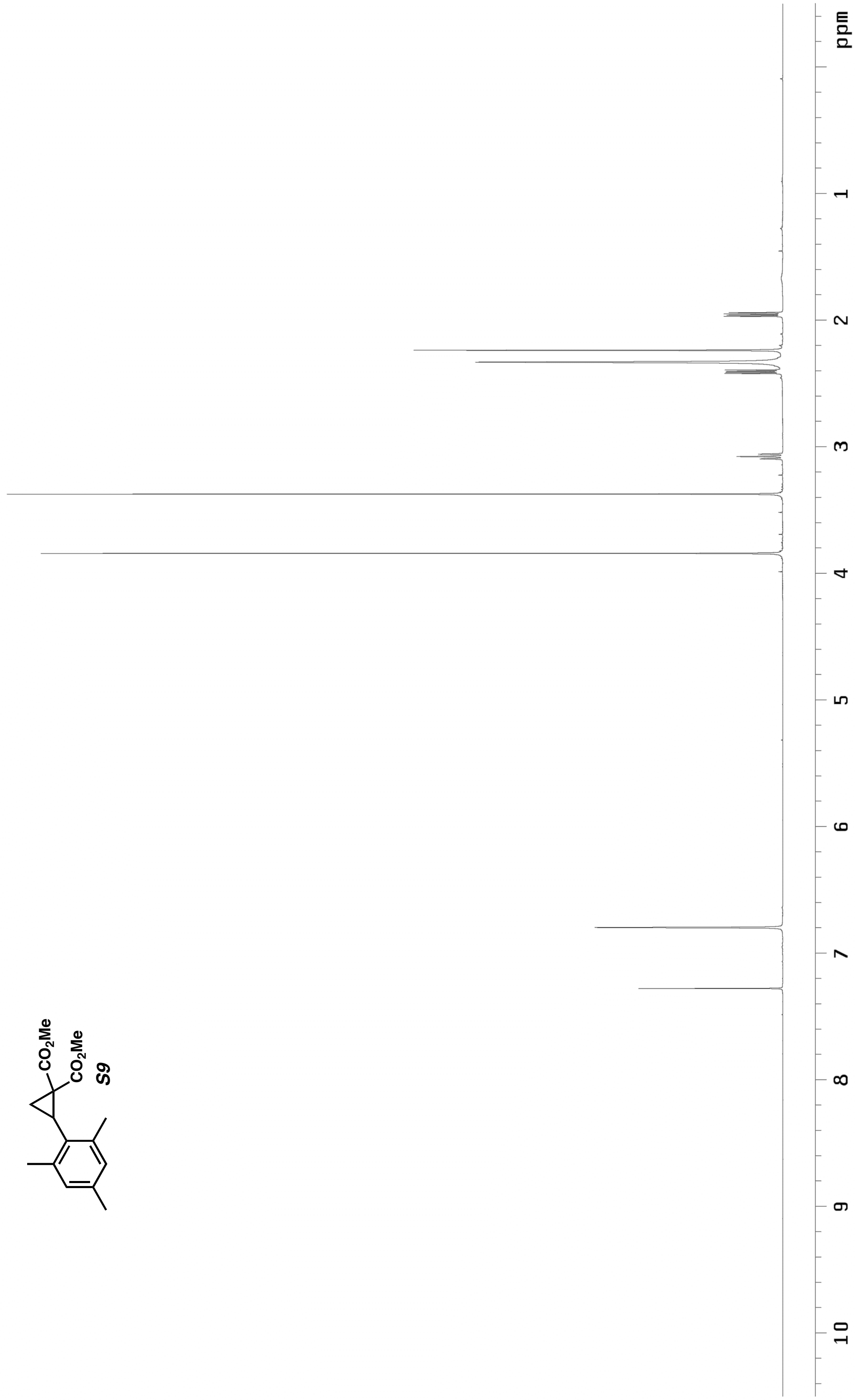
[1]H NMR (500 MHz, $CDCl_3$) of compound **S8**.



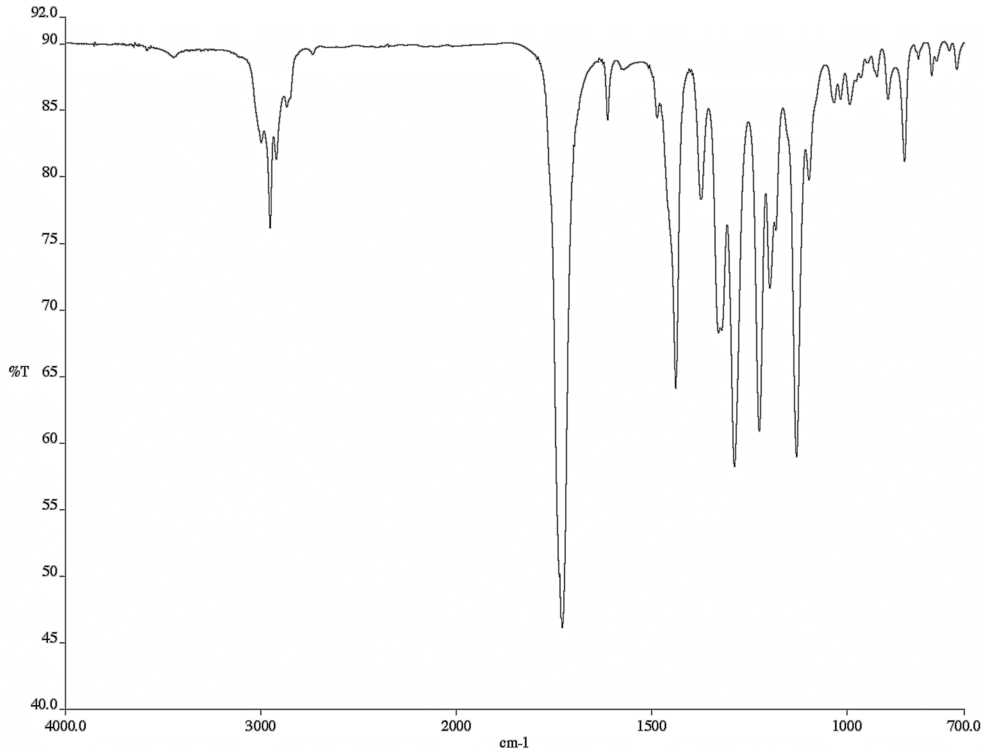
Infrared spectrum (thin film/NaCl) of compound **S8**.



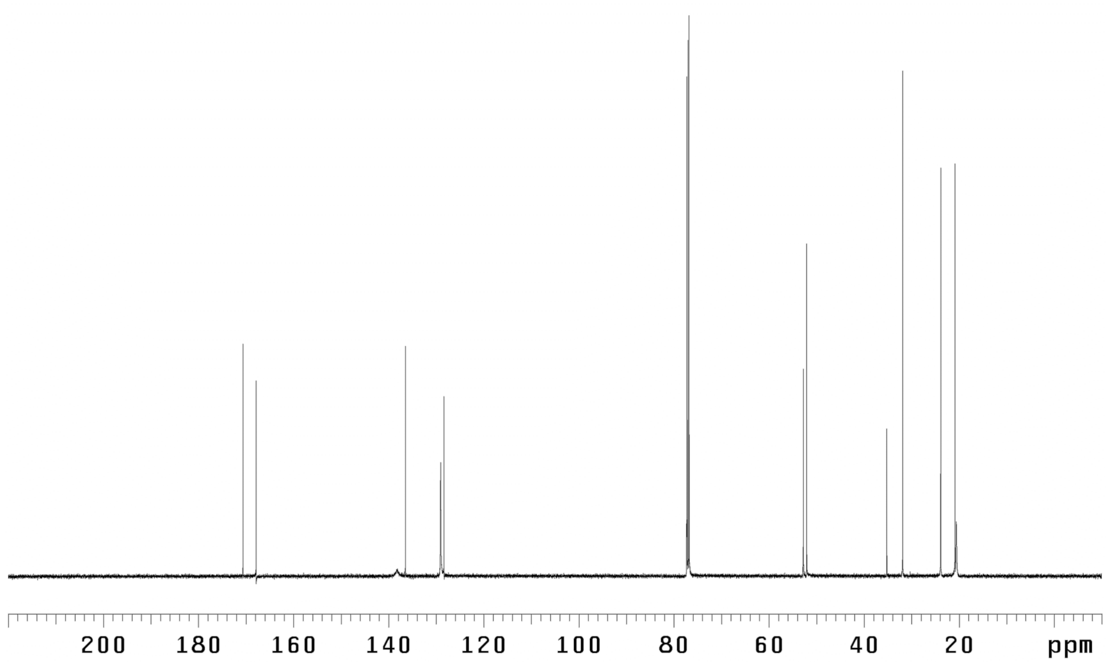
^{13}C NMR (126 MHz, $CDCl_3$) of compound **S8**.



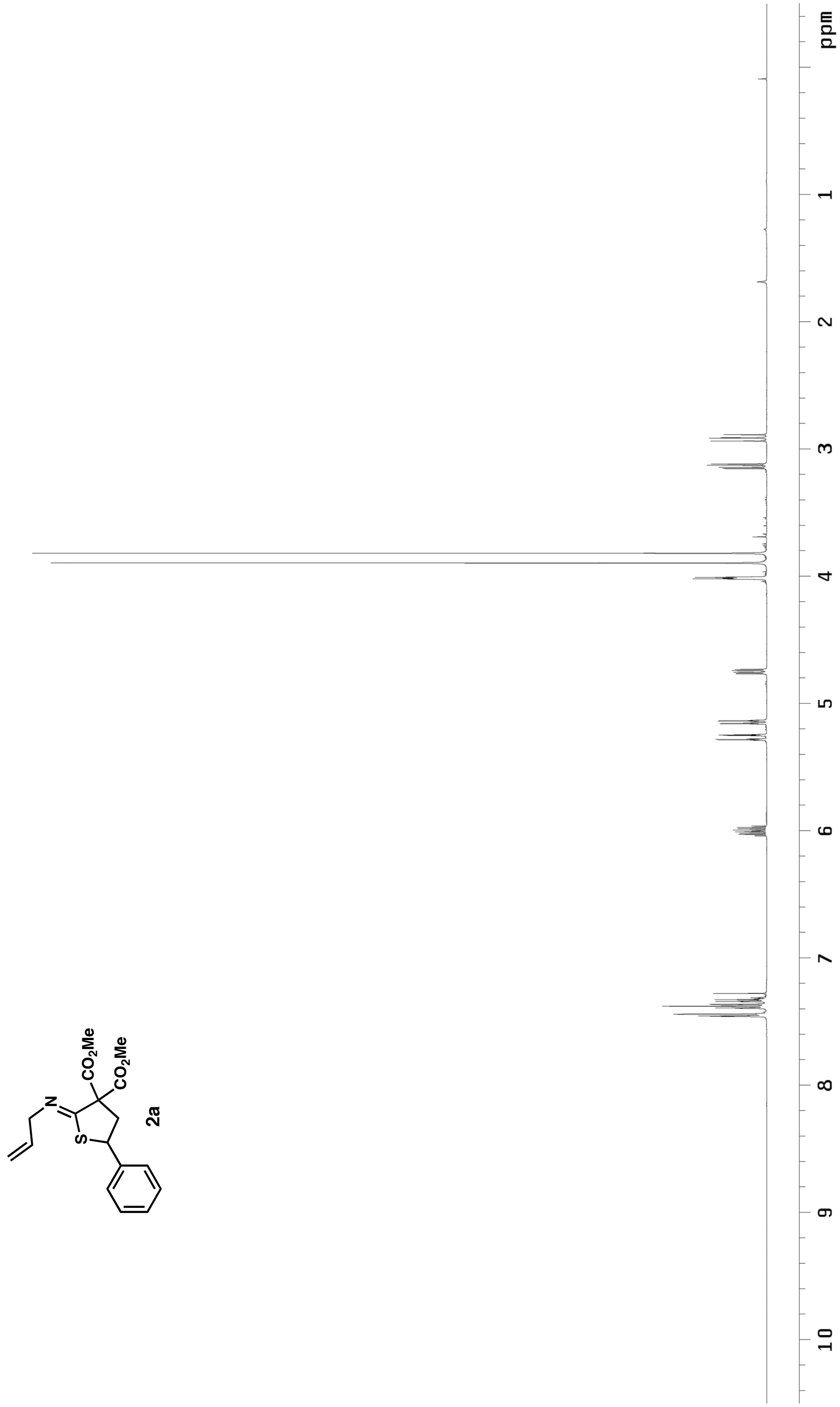
[1]H NMR (500 MHz, $CDCl_3$) of compound **S9**.



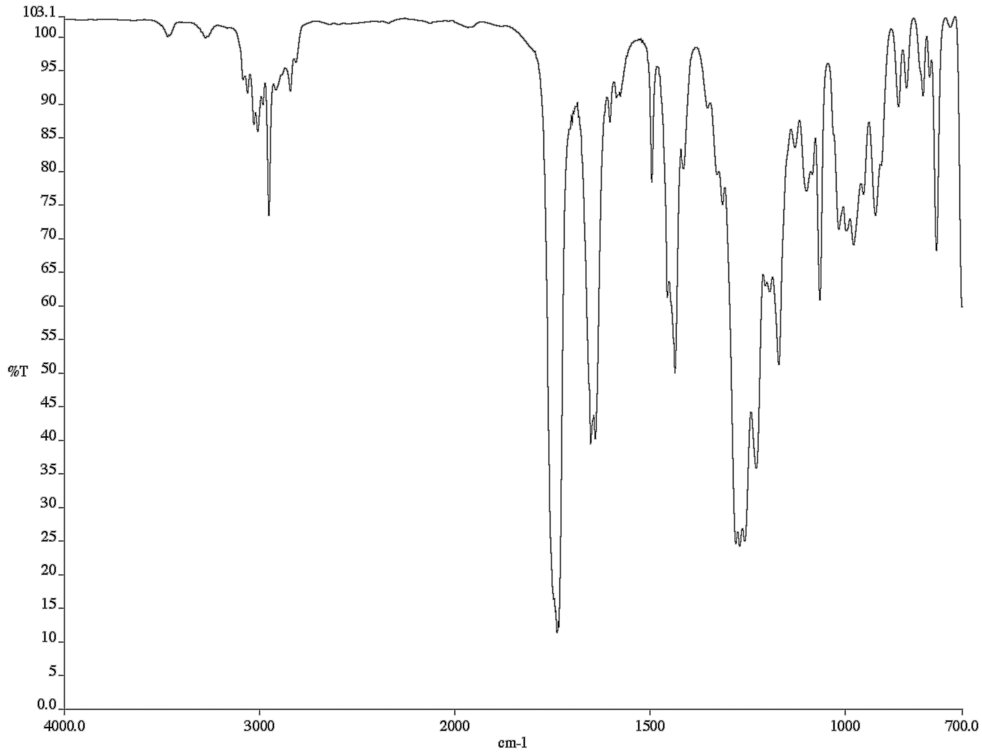
Infrared spectrum (thin film/NaCl) of compound **S9**.



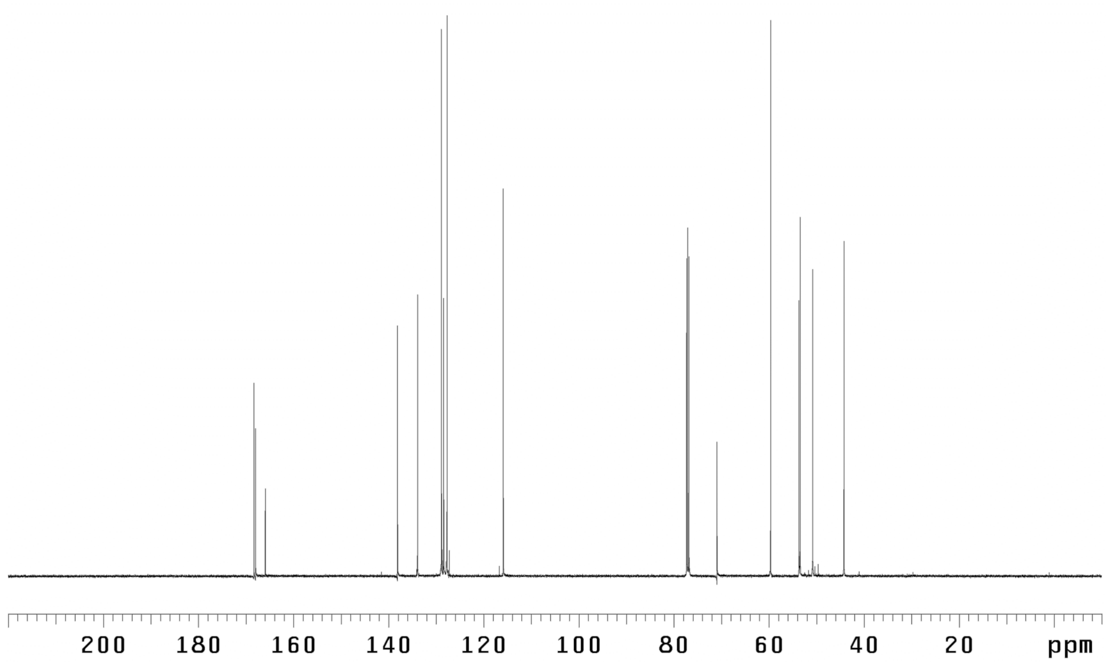
^{13}C NMR (126 MHz, $CDCl_3$) of compound **S9**.



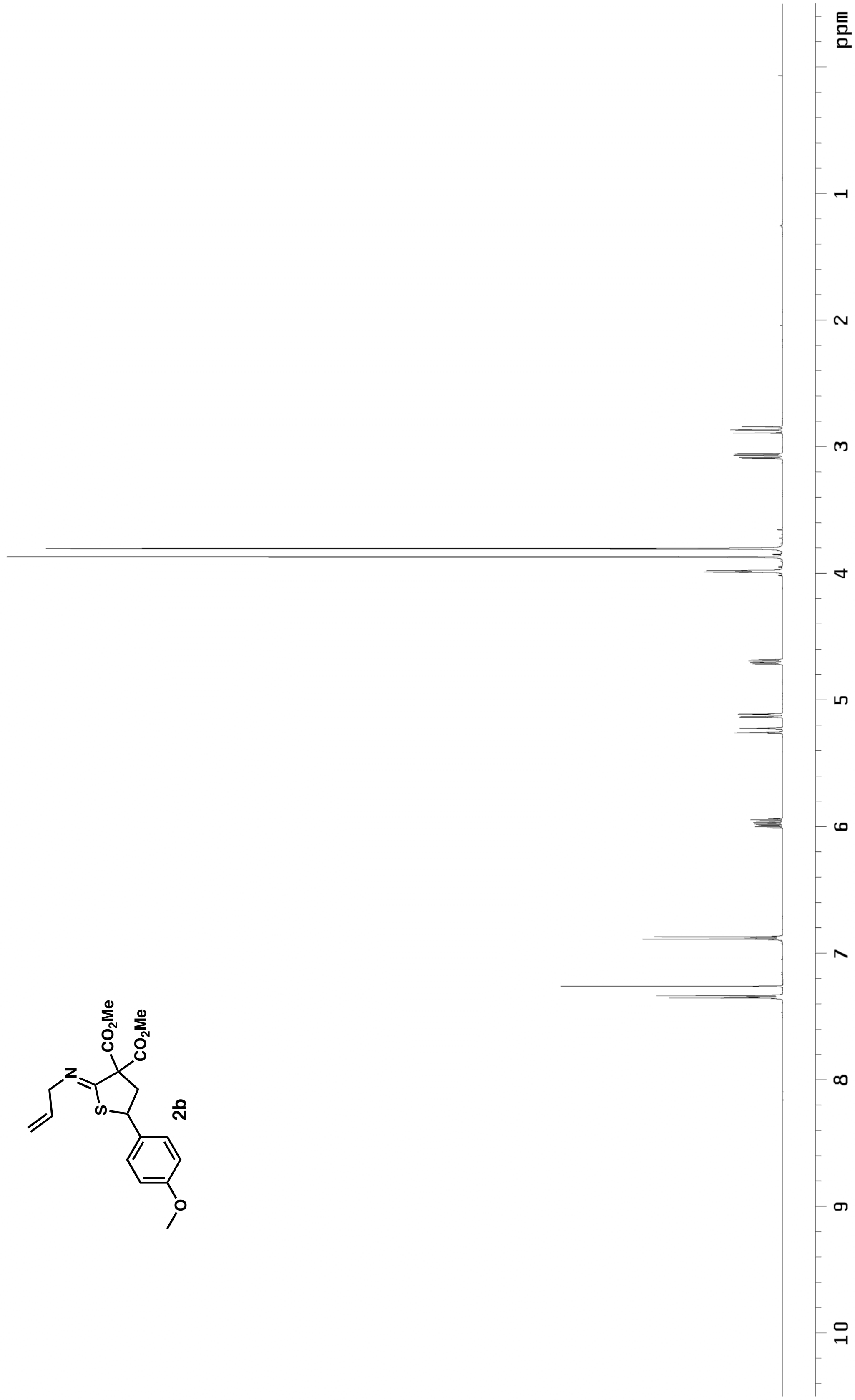
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2a**.



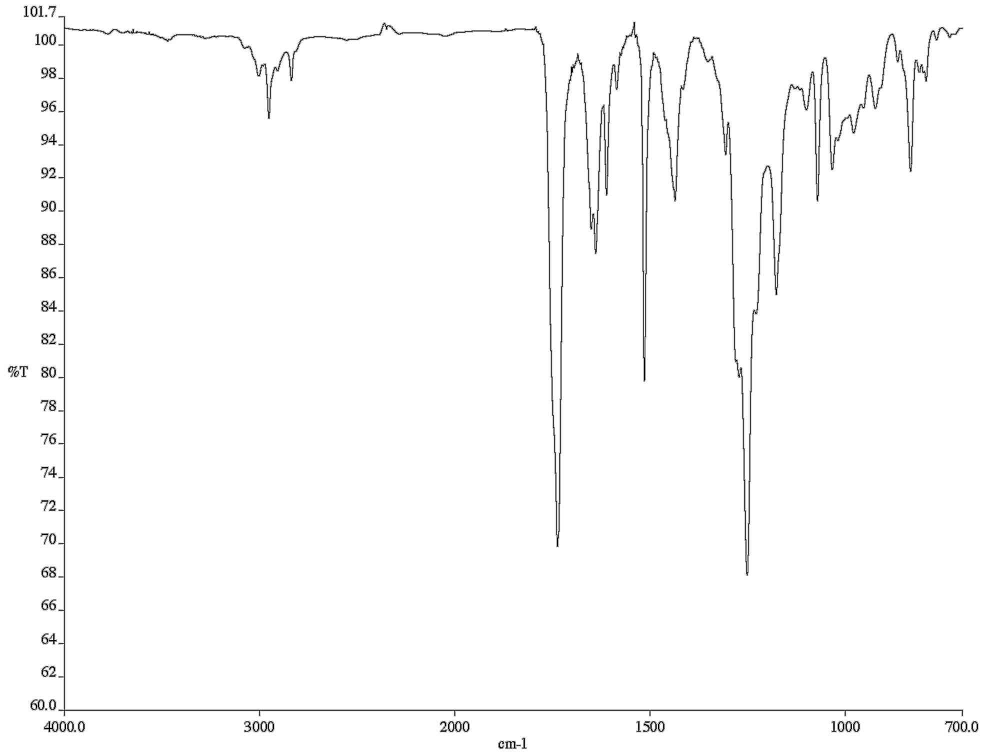
Infrared spectrum (thin film/NaCl) of compound **2a**.



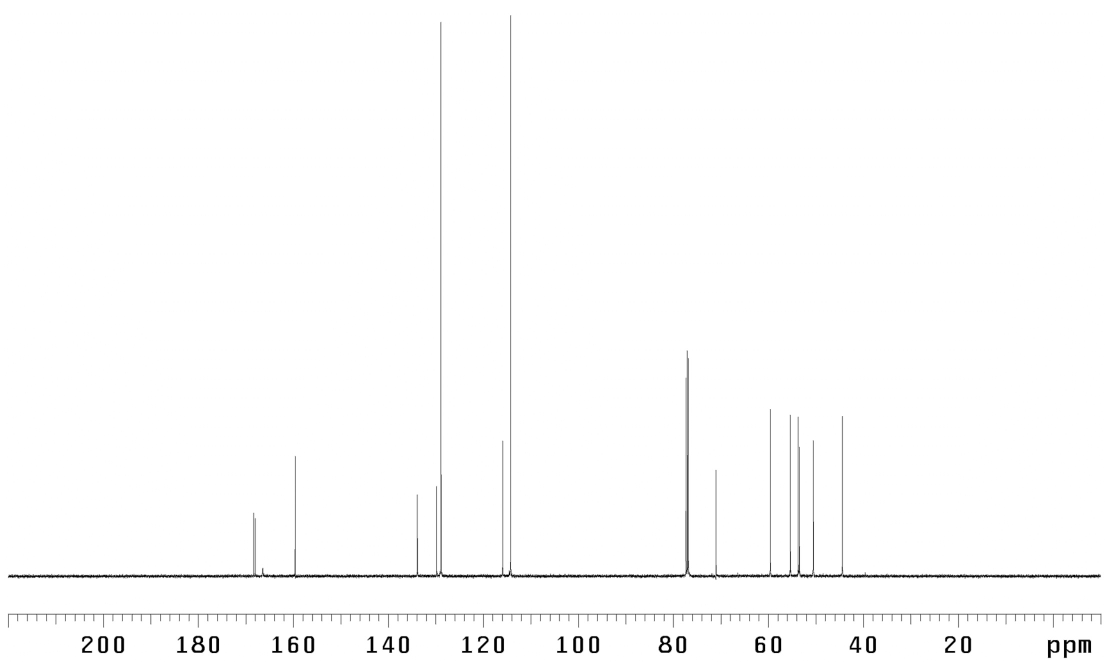
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2a**.



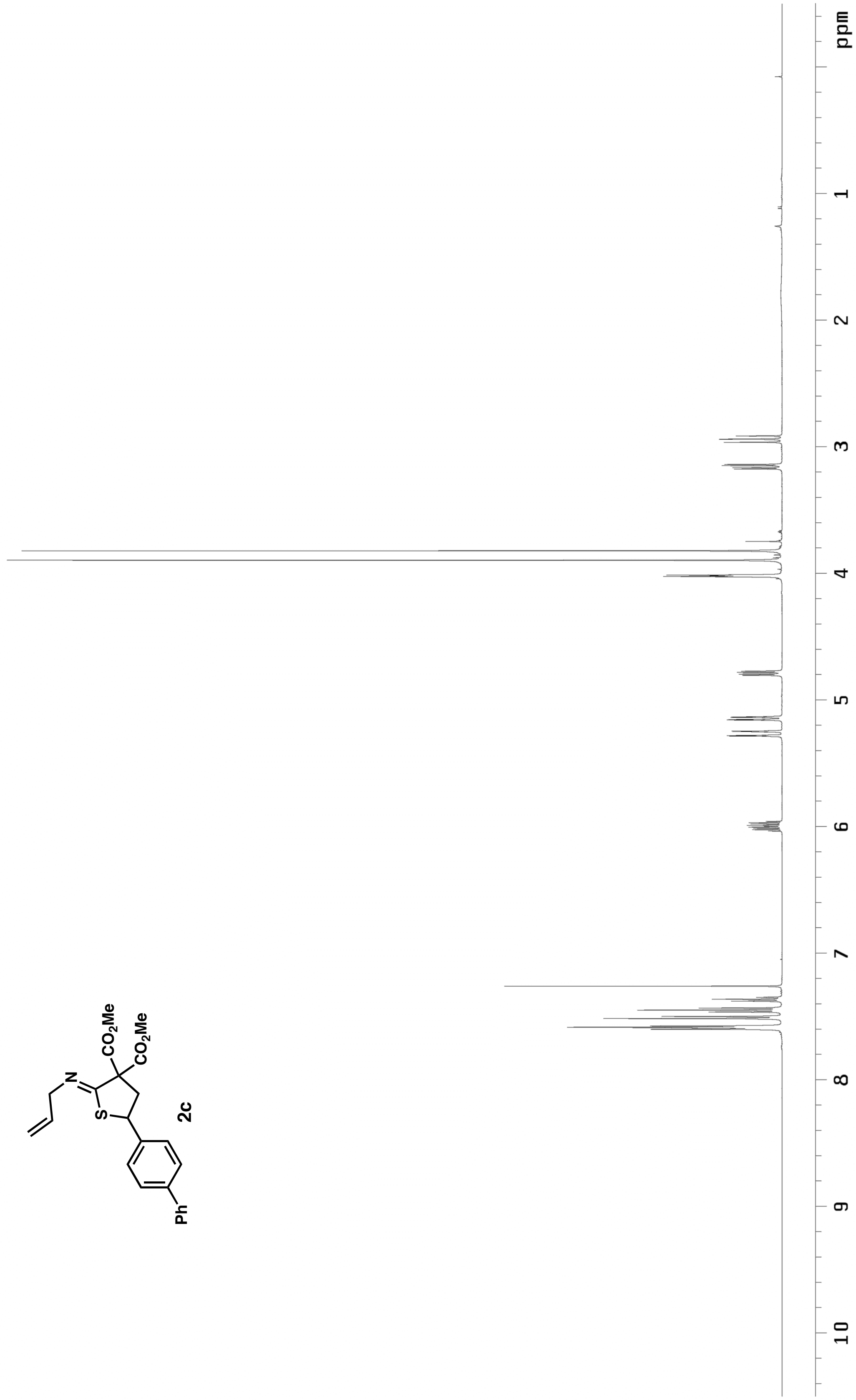
[1]H NMR (500 MHz, $CDCl_3$) of compound **2b**.



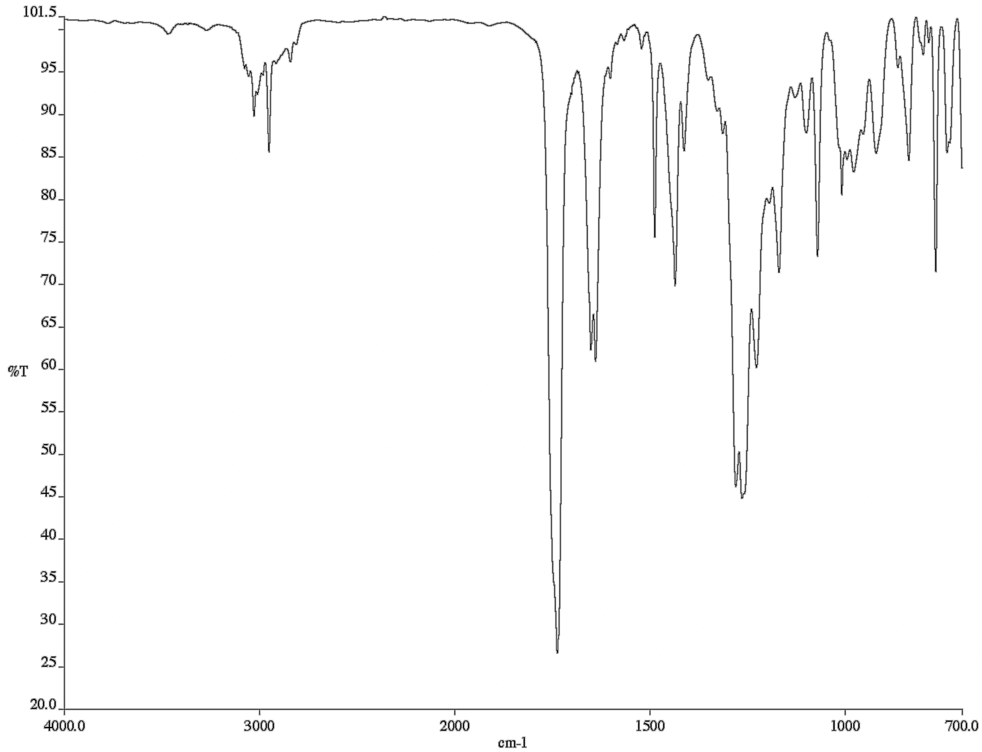
Infrared spectrum (thin film/NaCl) of compound **2b**.



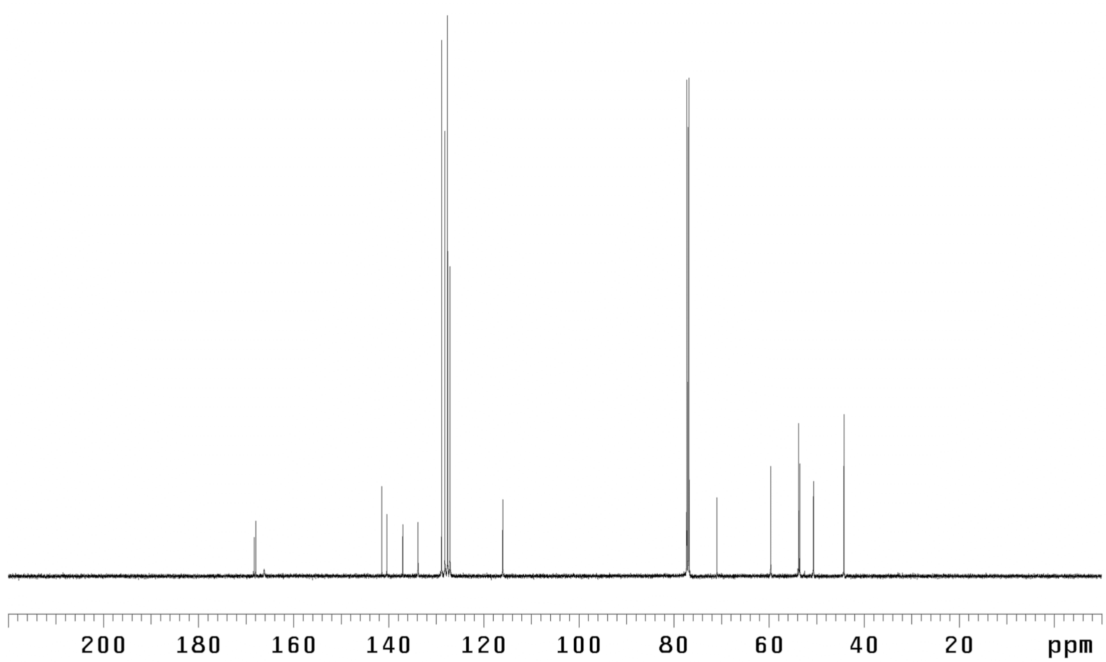
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2b**.



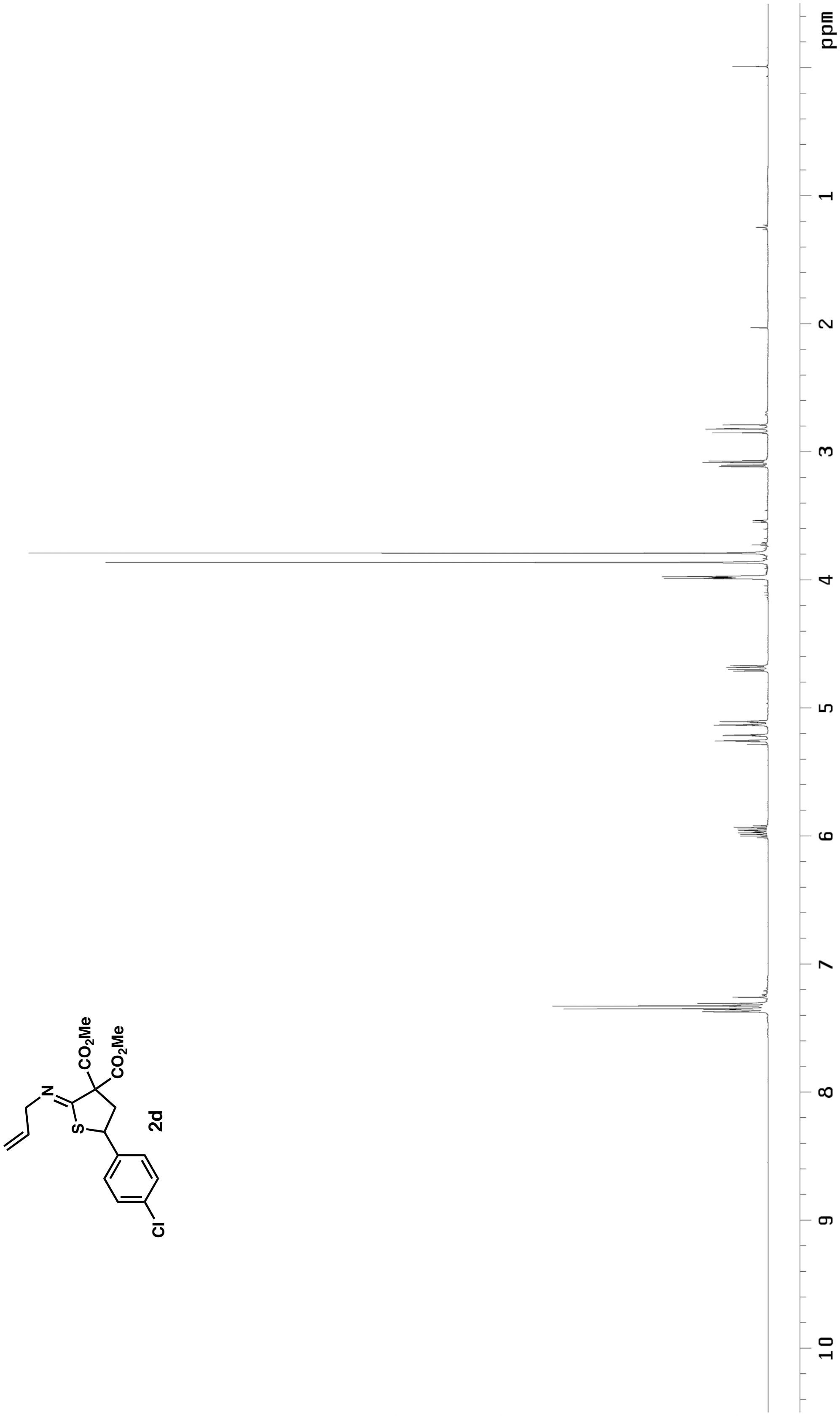
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2c**.



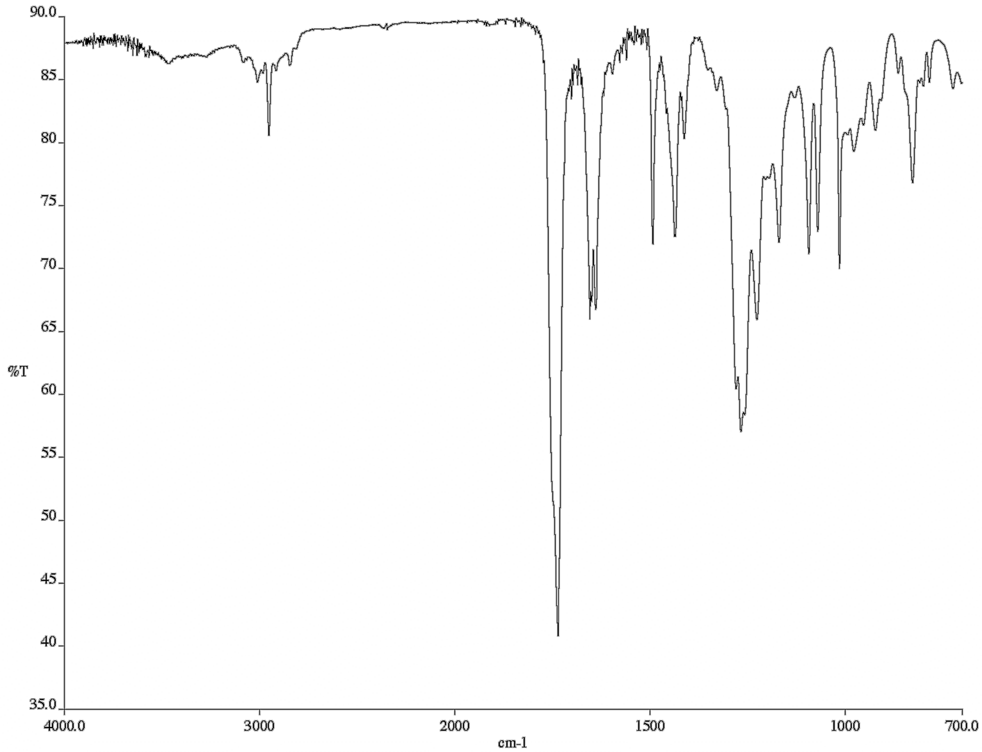
Infrared spectrum (thin film/NaCl) of compound **2c**.



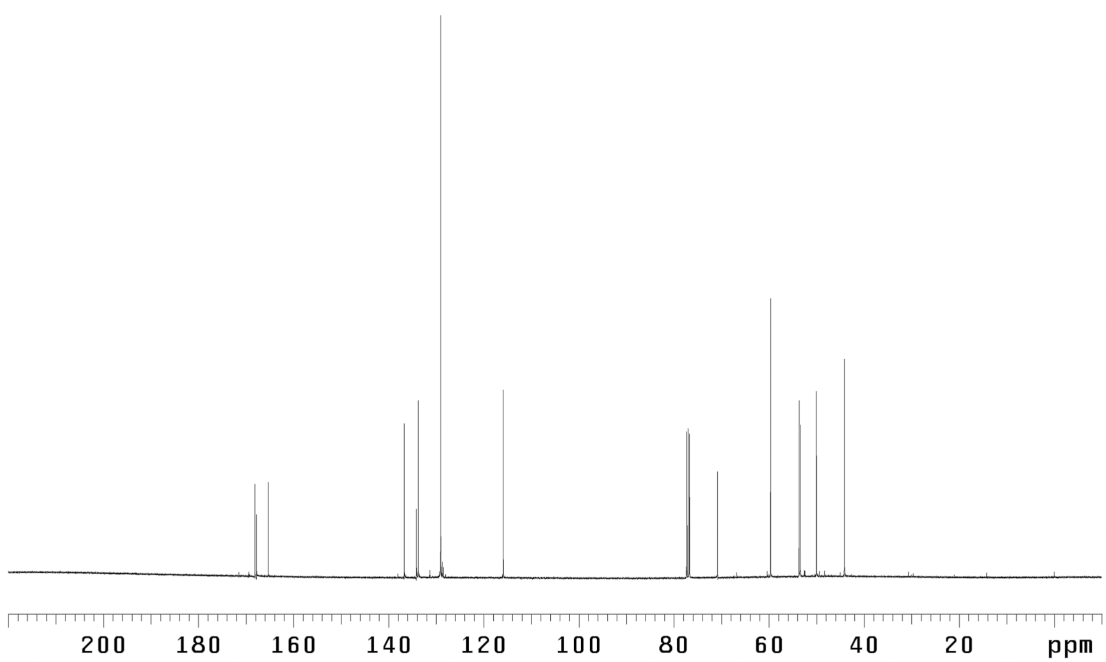
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2c**.



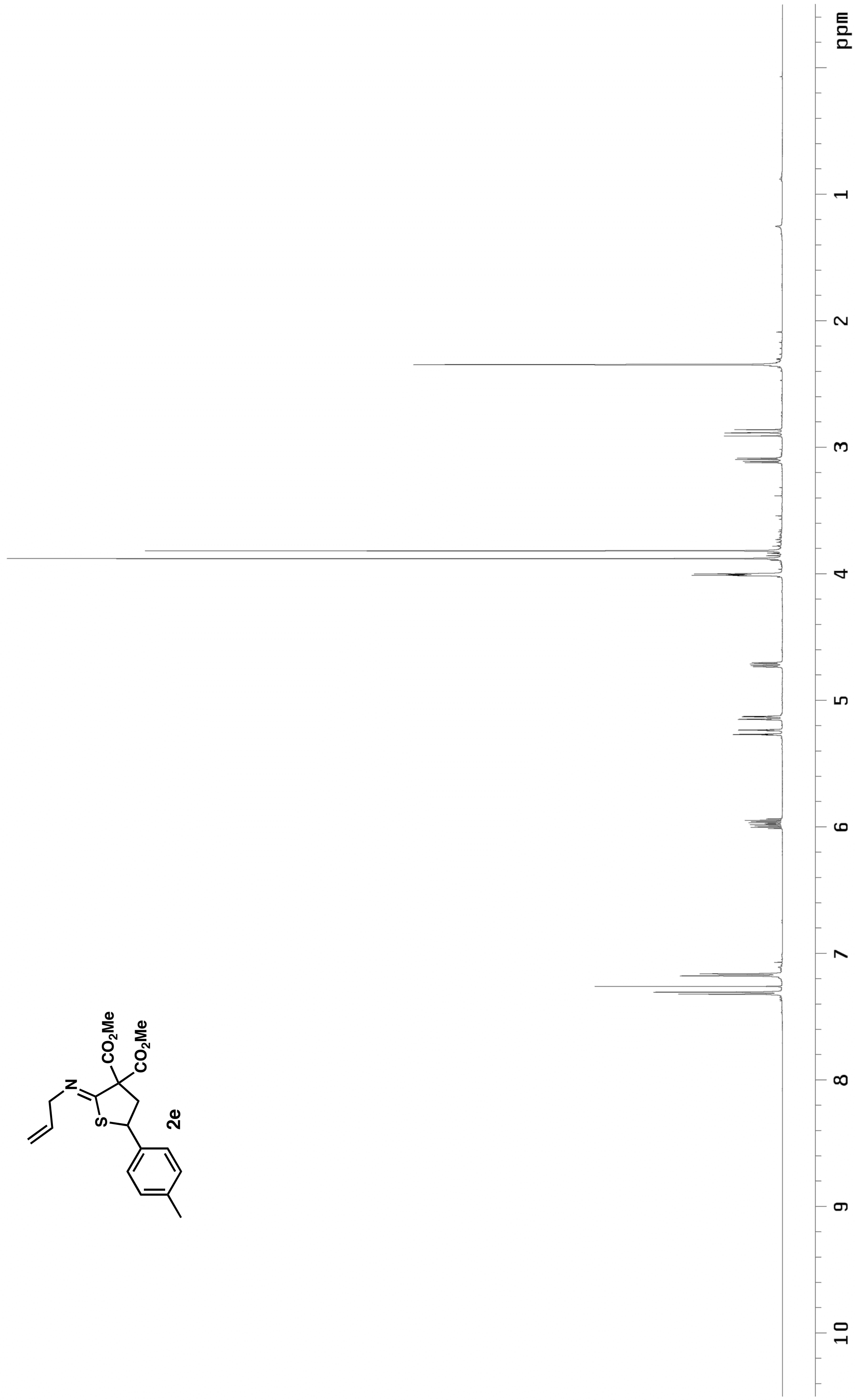
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2d**.



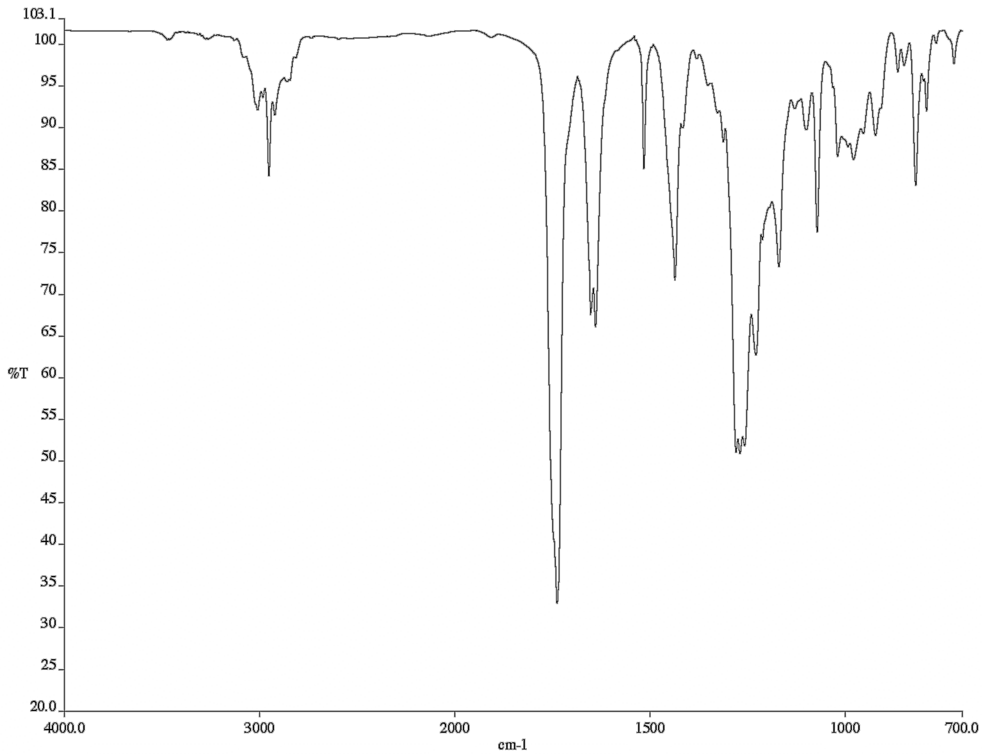
Infrared spectrum (thin film/NaCl) of compound **2d**.



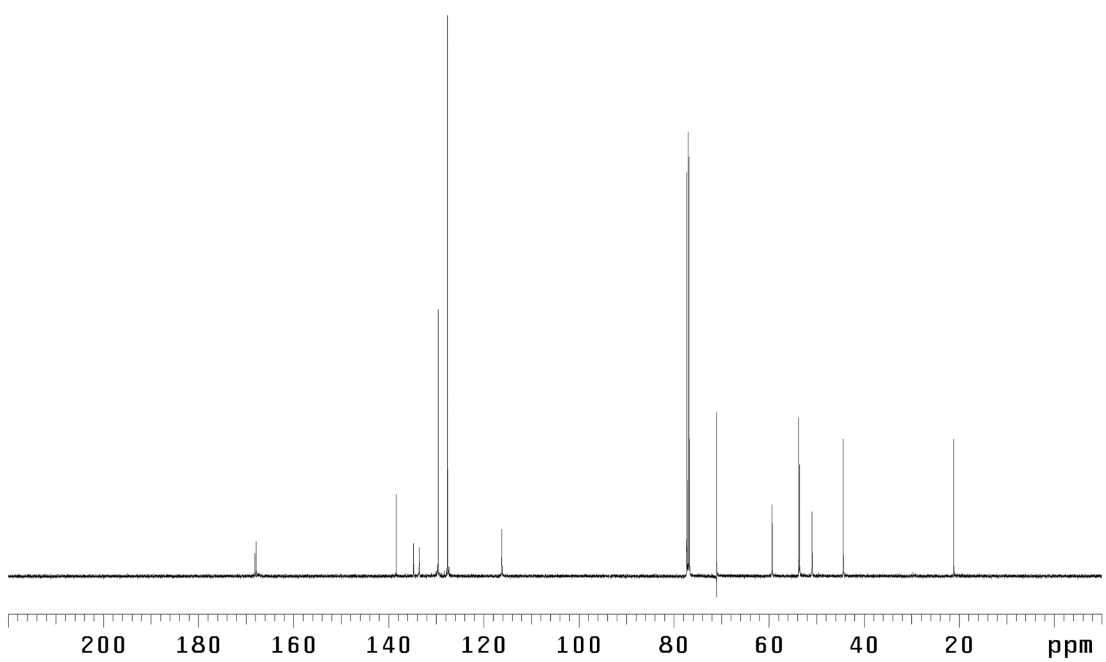
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2d**.



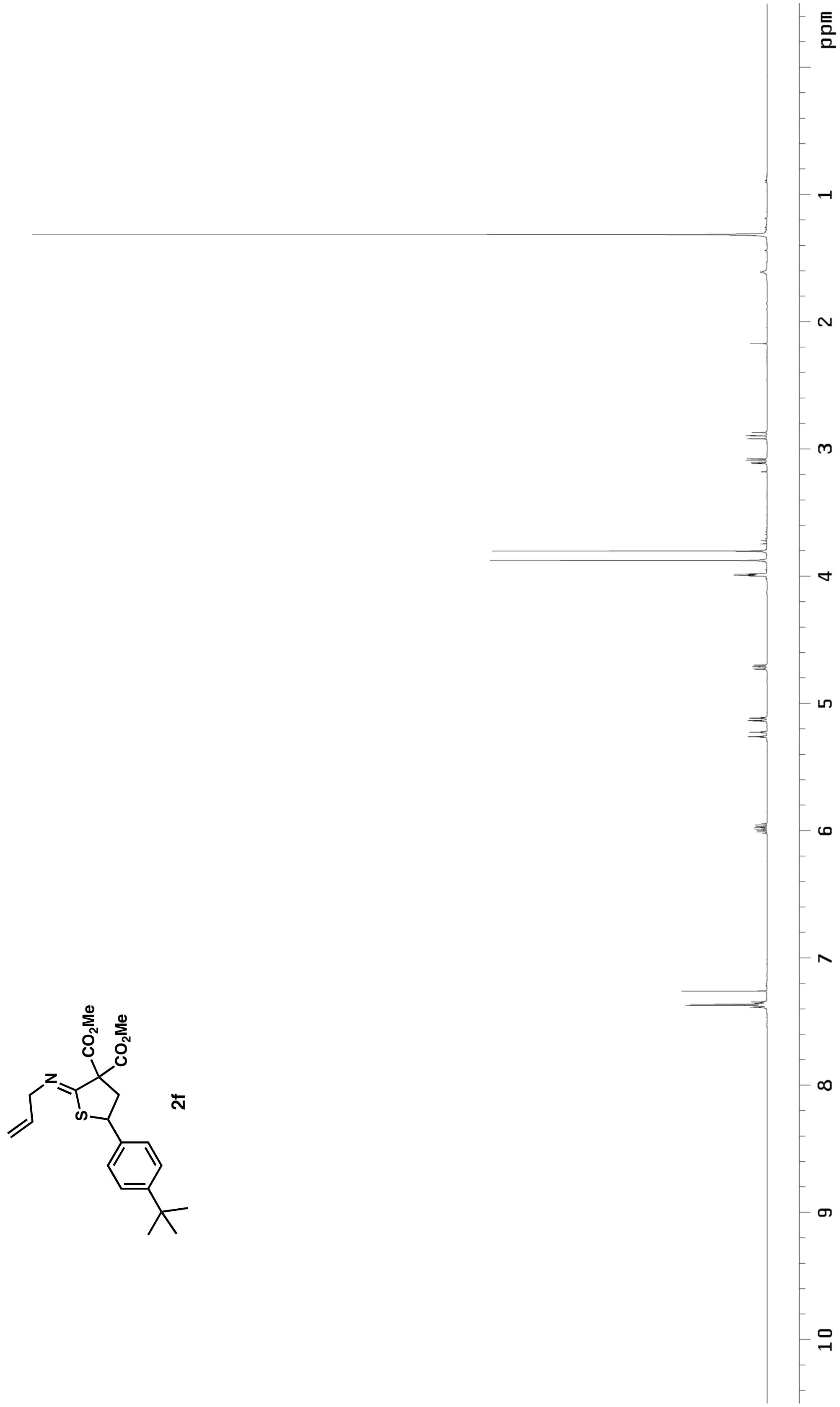
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2e**.



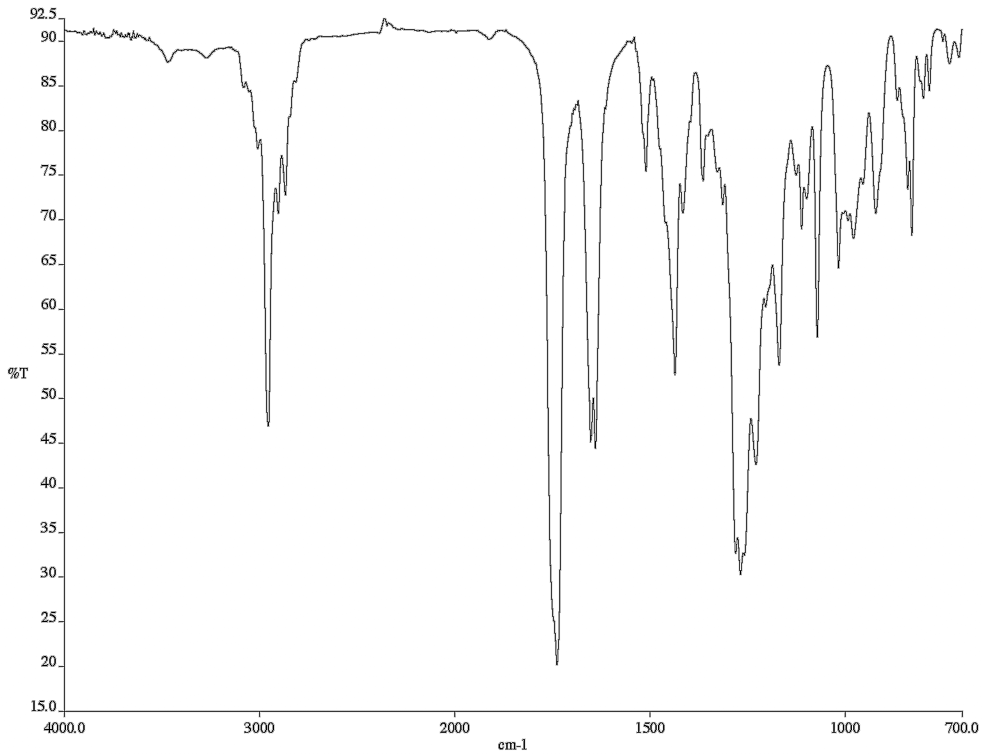
Infrared spectrum (thin film/NaCl) of compound **2e**.



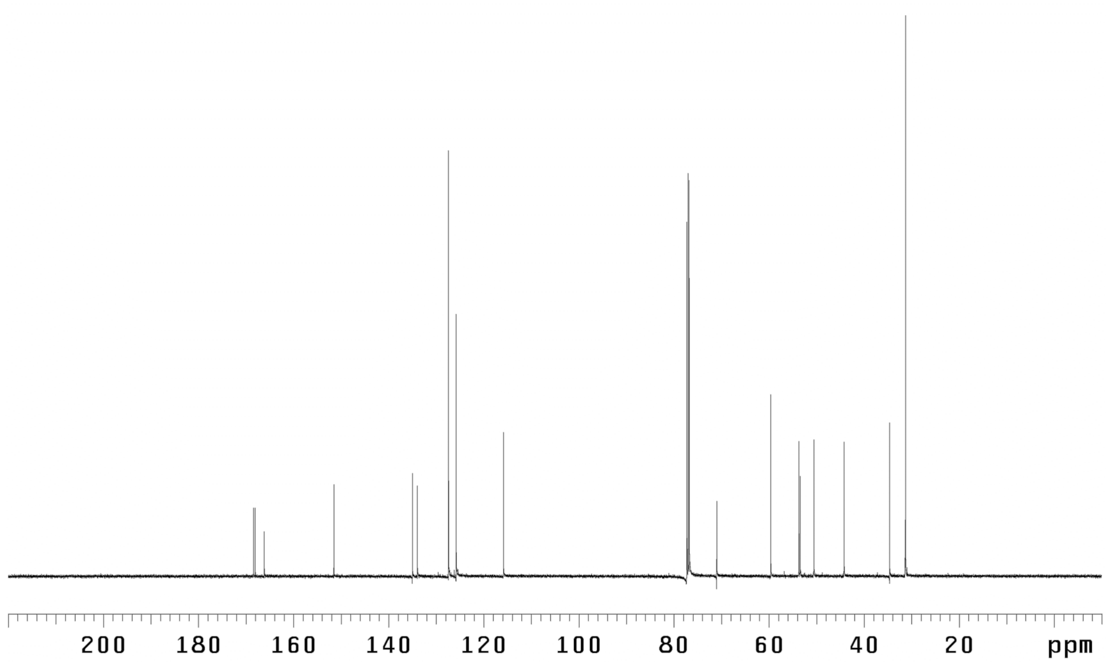
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2e**.



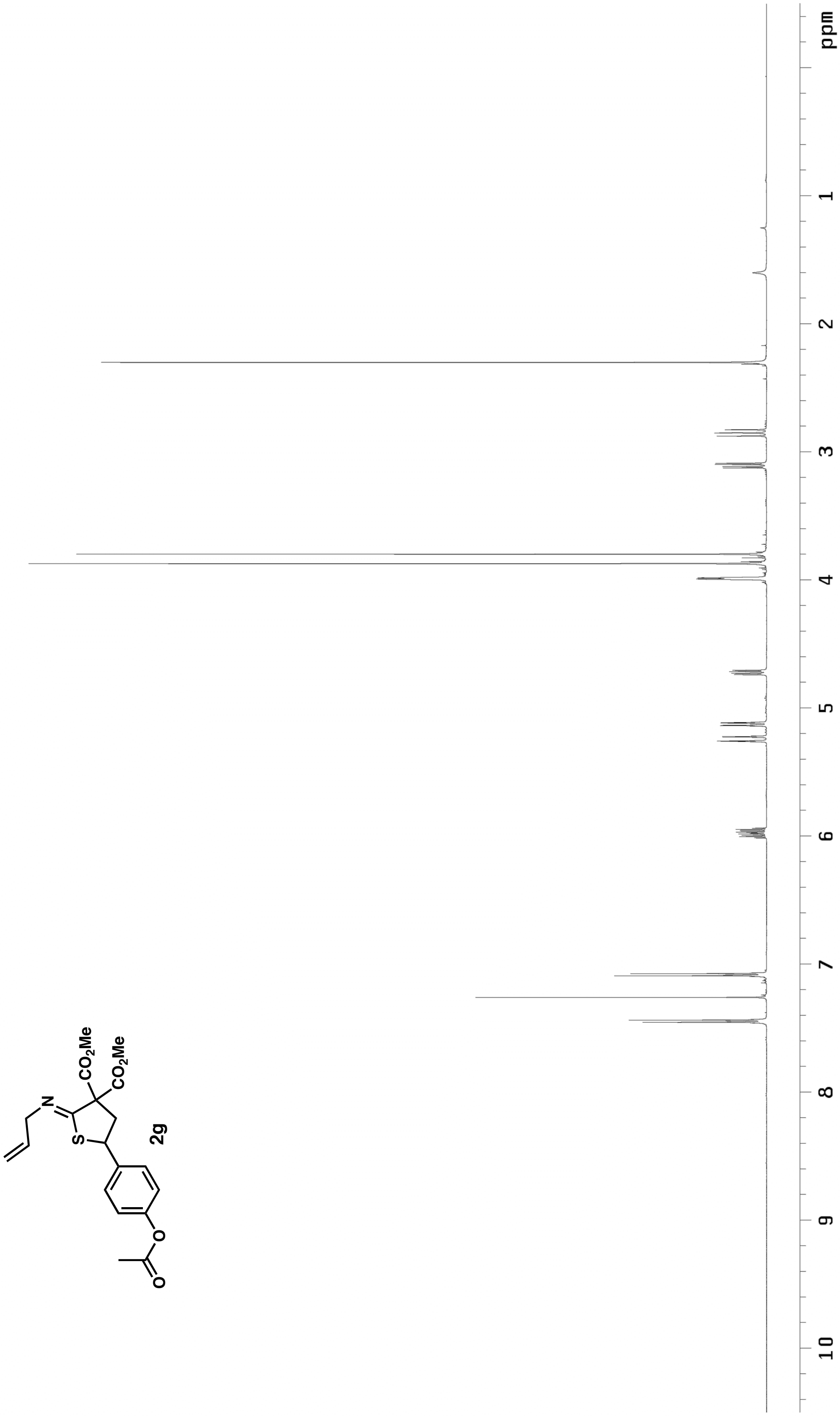
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2f**.



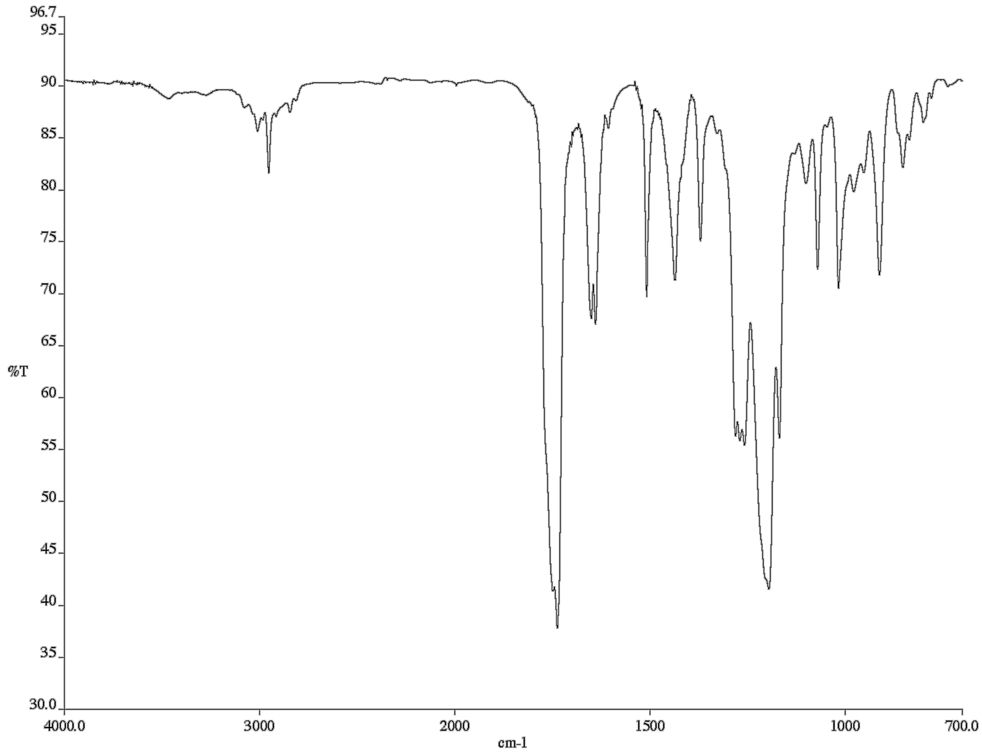
Infrared spectrum (thin film/NaCl) of compound **2f**.



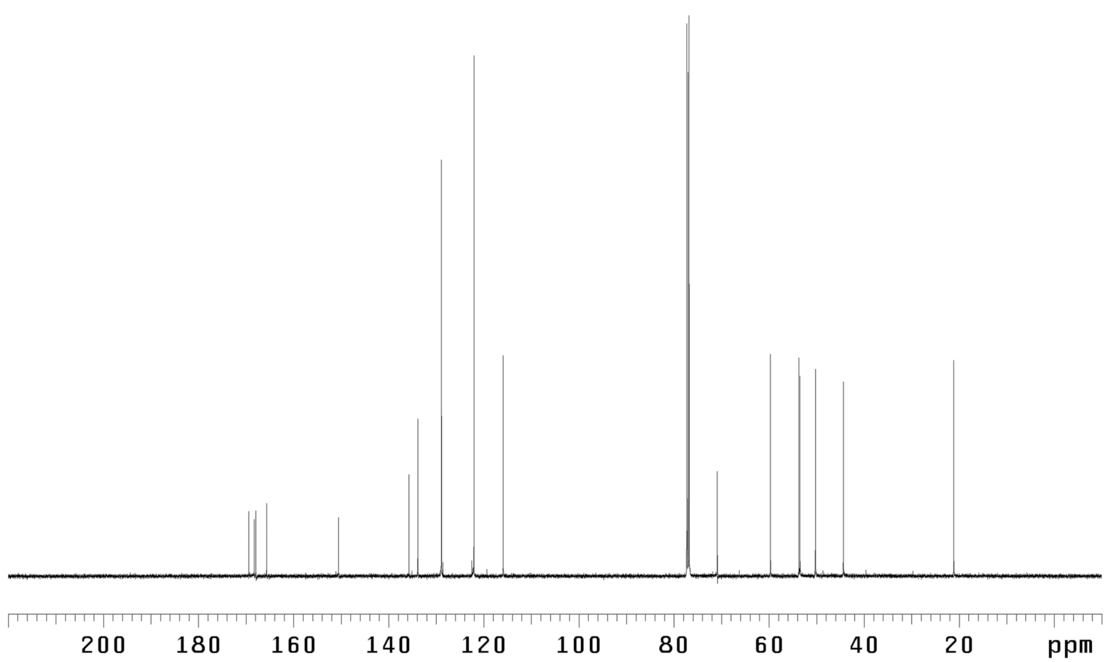
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2f**.



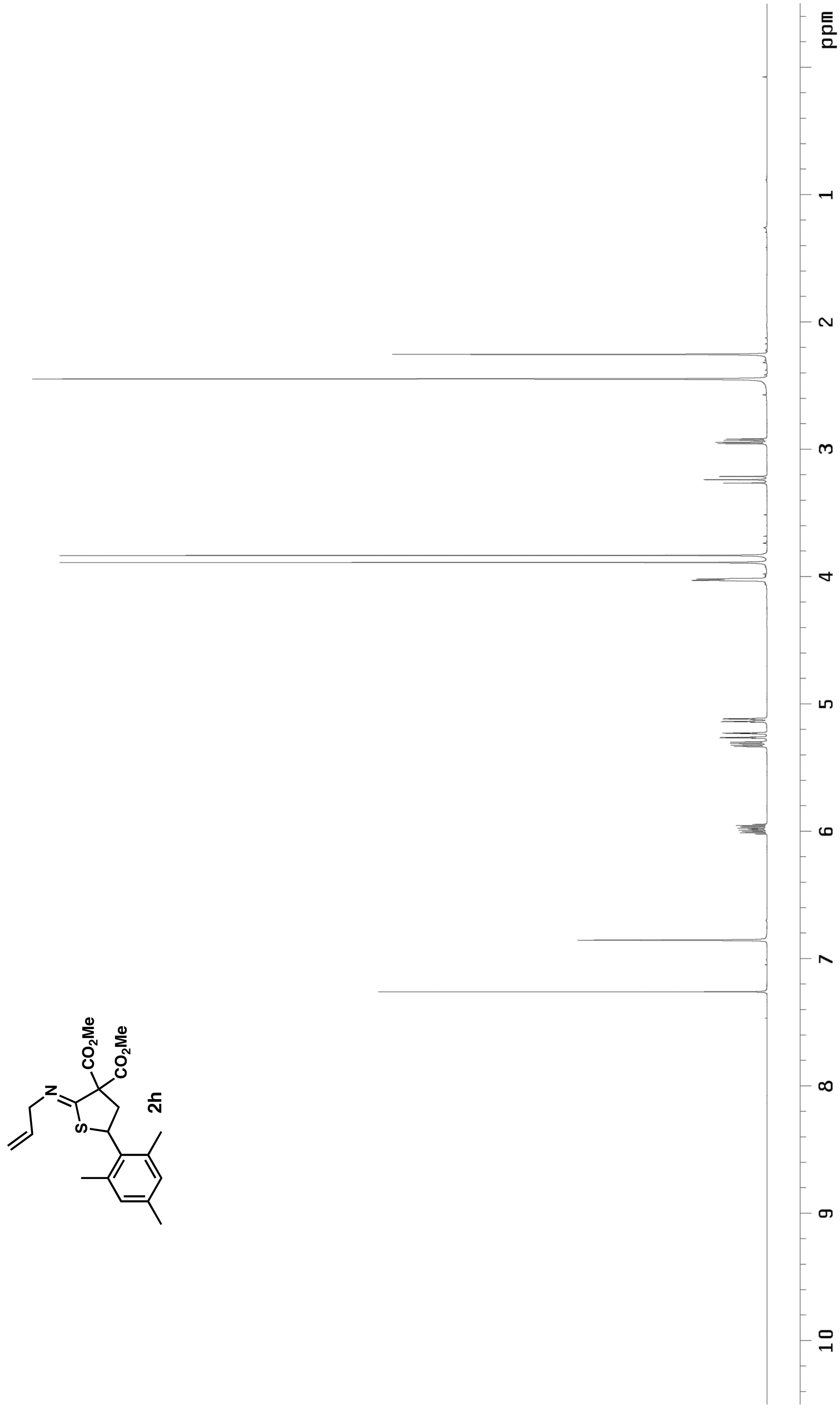
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2g**.



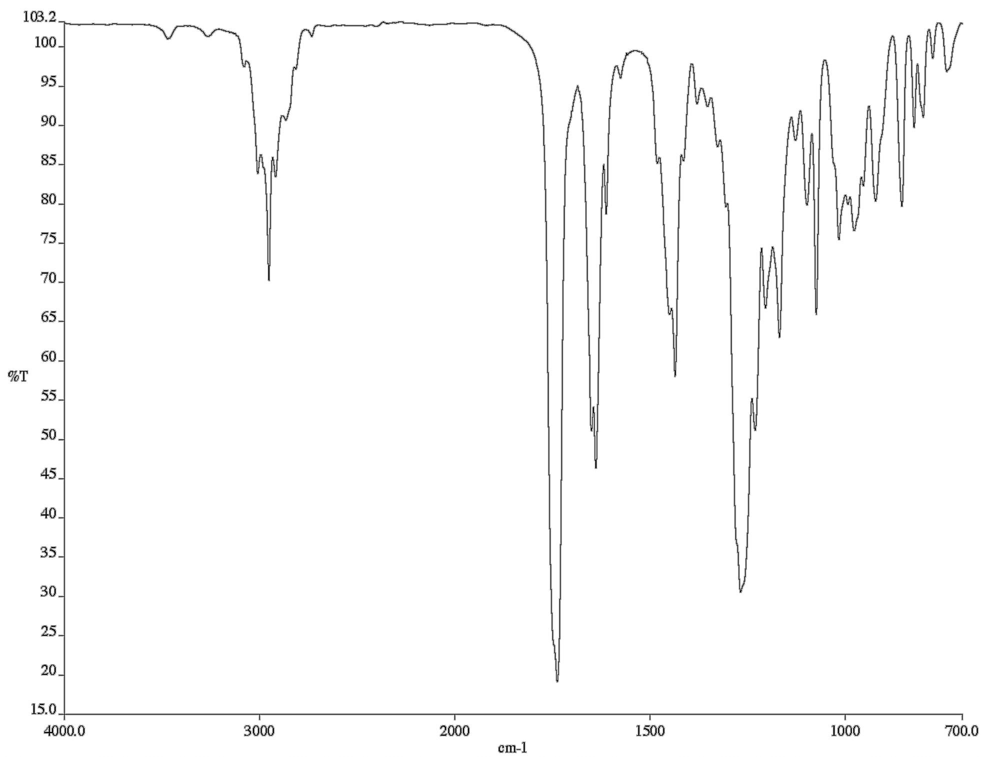
Infrared spectrum (thin film/NaCl) of compound **2g**.



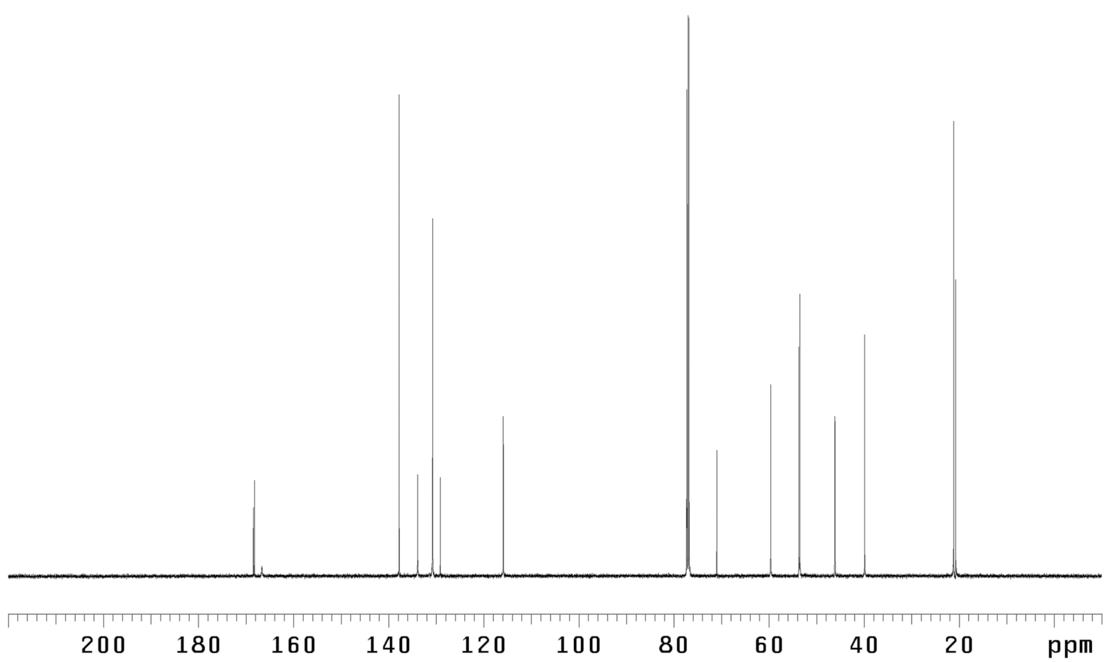
^{13}C NMR (500 MHz, $CDCl_3$) of compound **2g**.



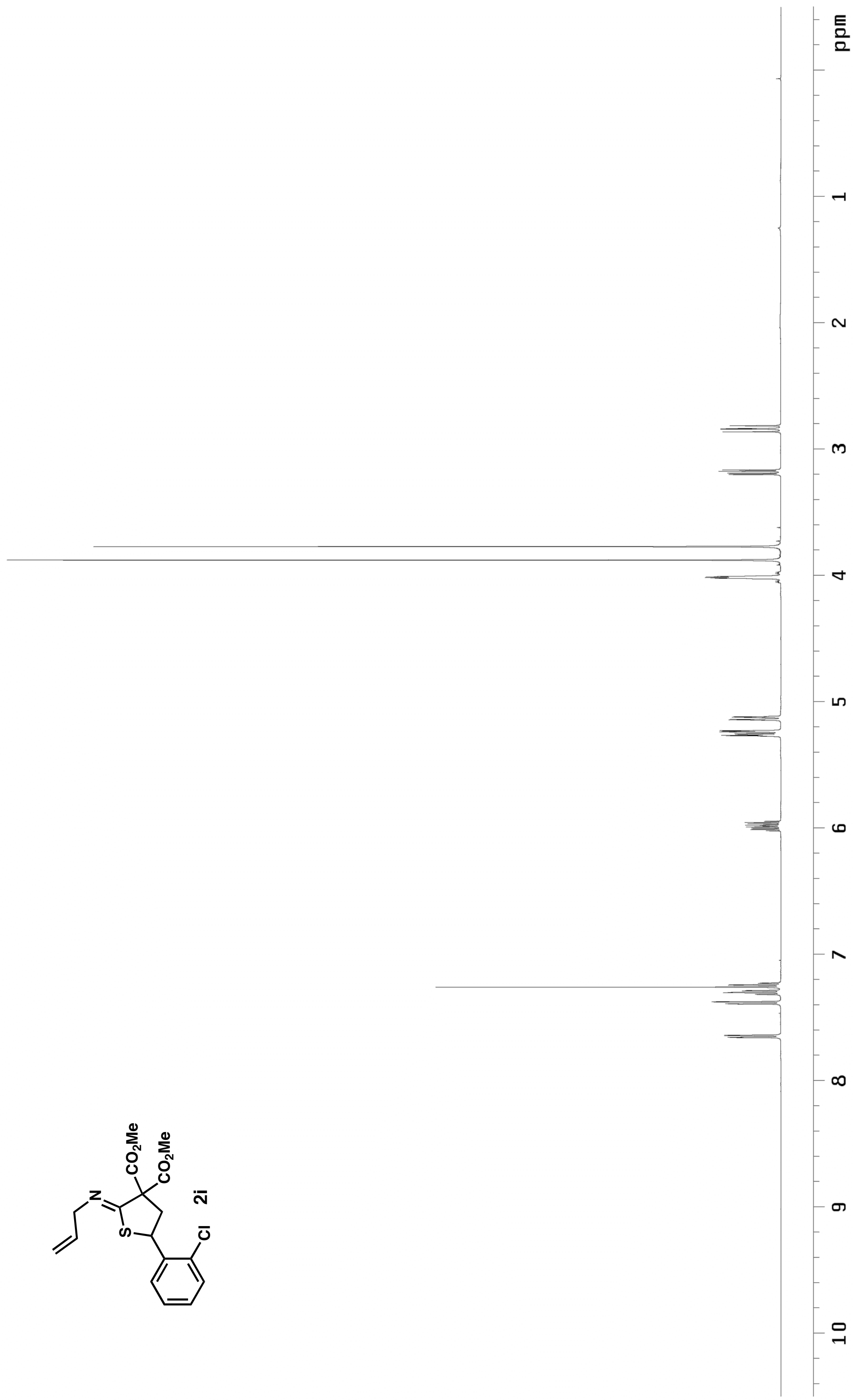
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2h**.



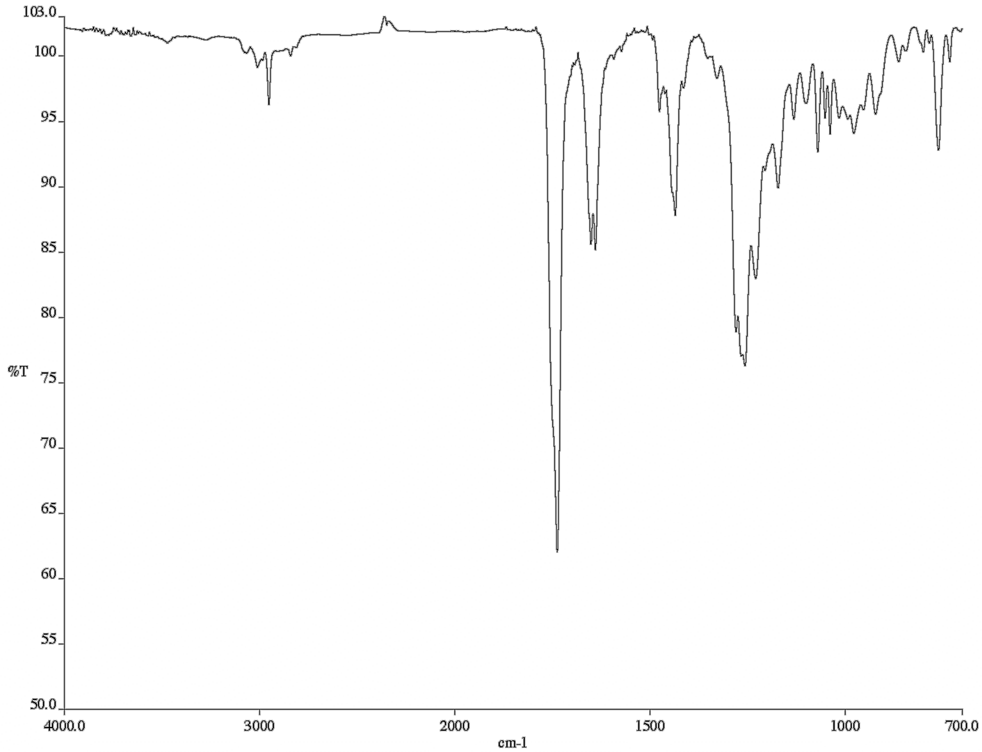
Infrared spectrum (thin film/NaCl) of compound **2h**.



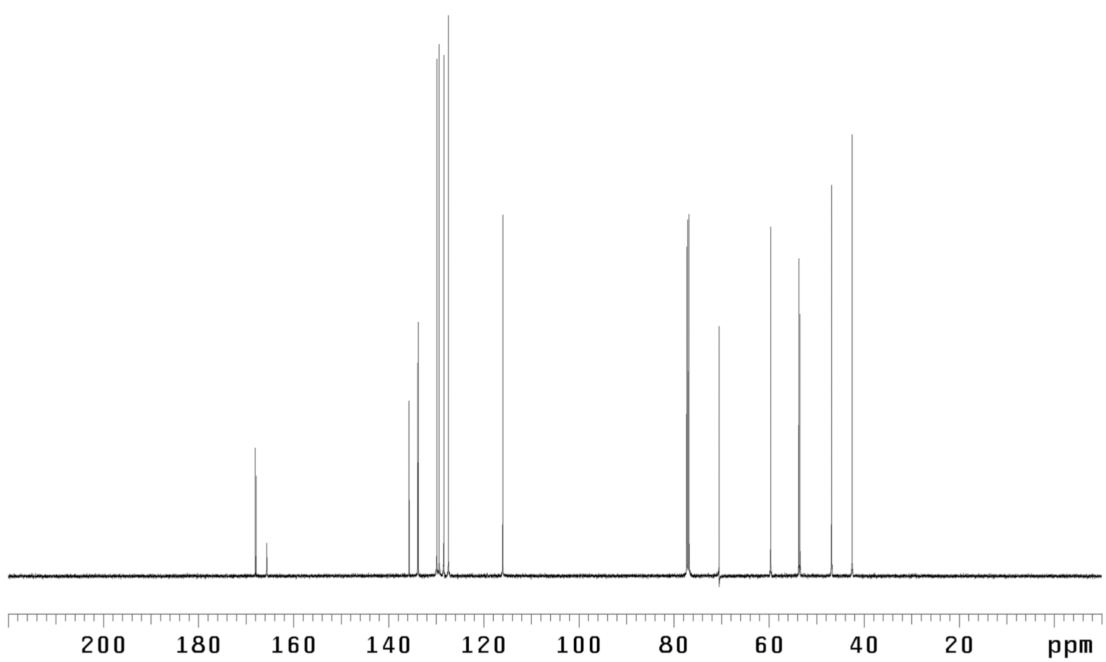
^{13}C NMR (500 MHz, $CDCl_3$) of compound **2h**.



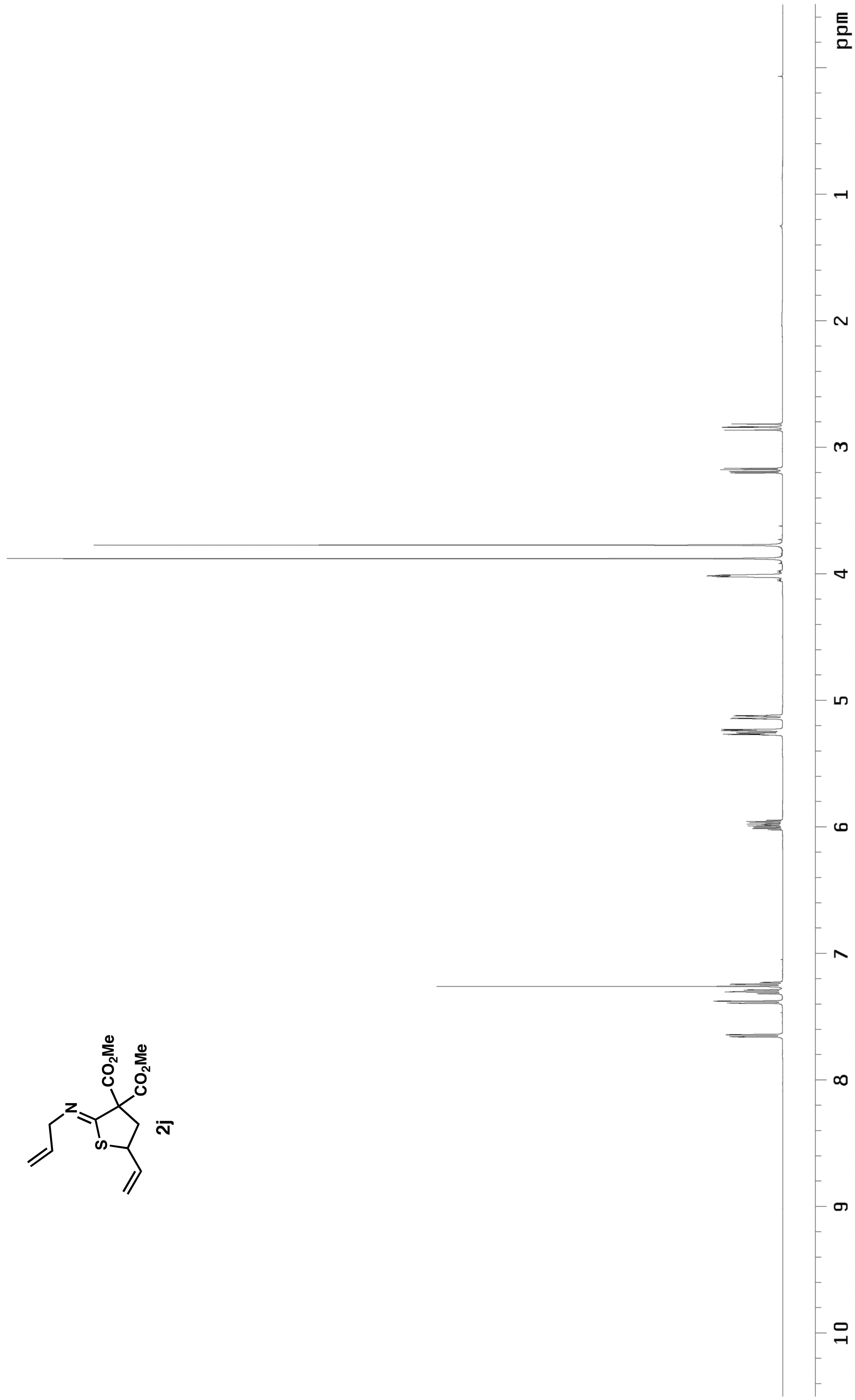
^1H NMR (500 MHz, $CDCl_3$) of compound **2i**.



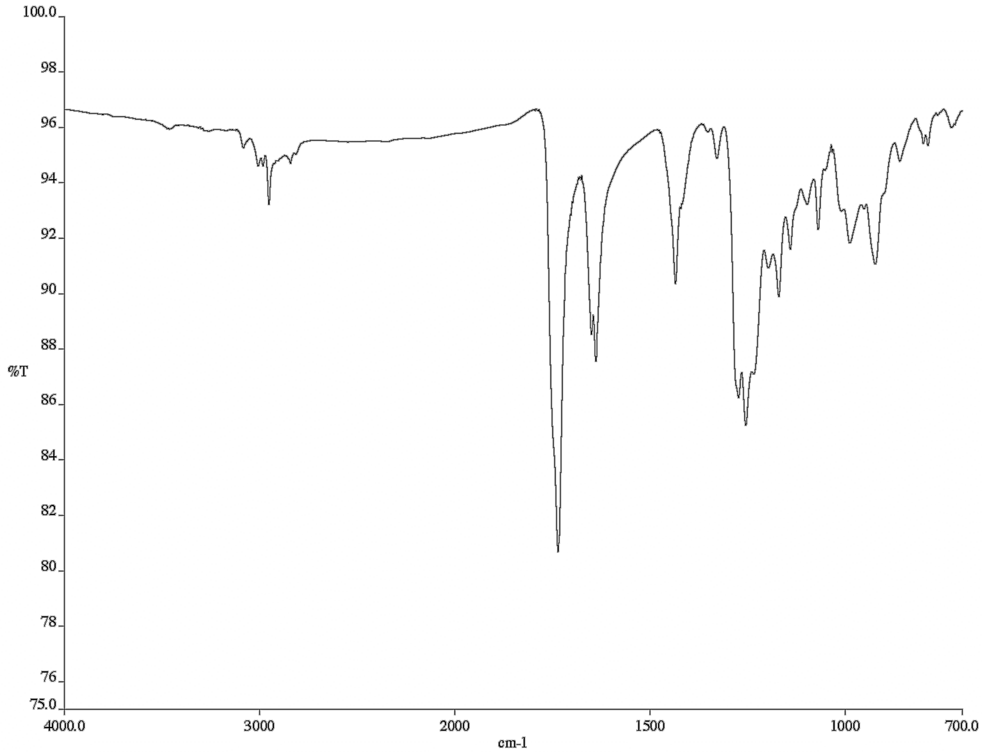
Infrared spectrum (thin film/NaCl) of compound **2i**.



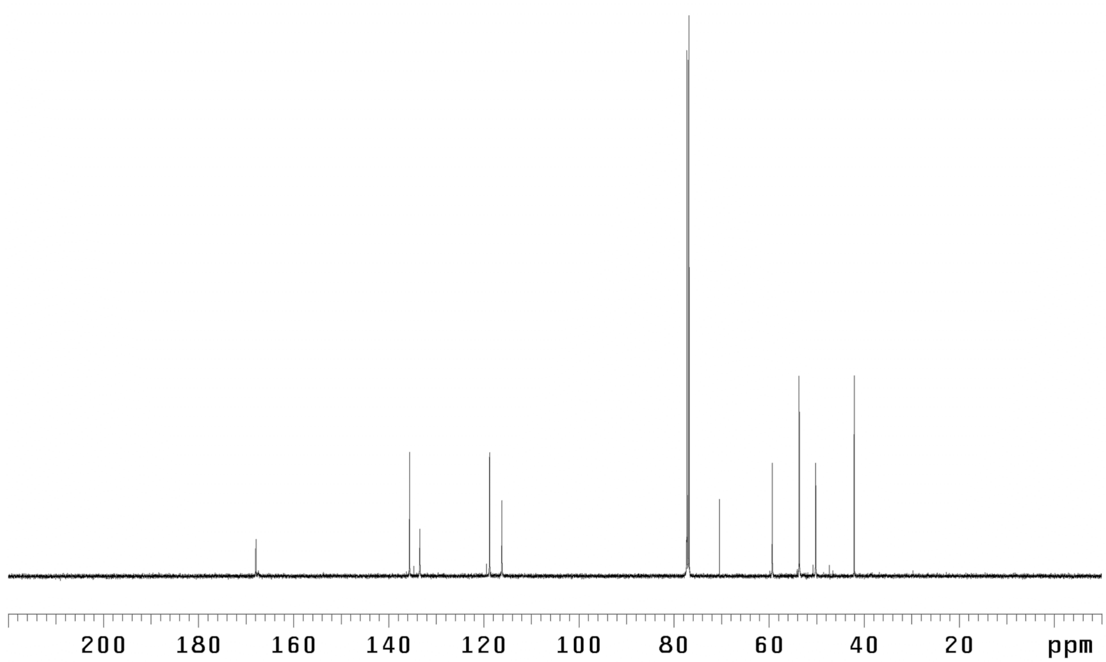
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2i**.



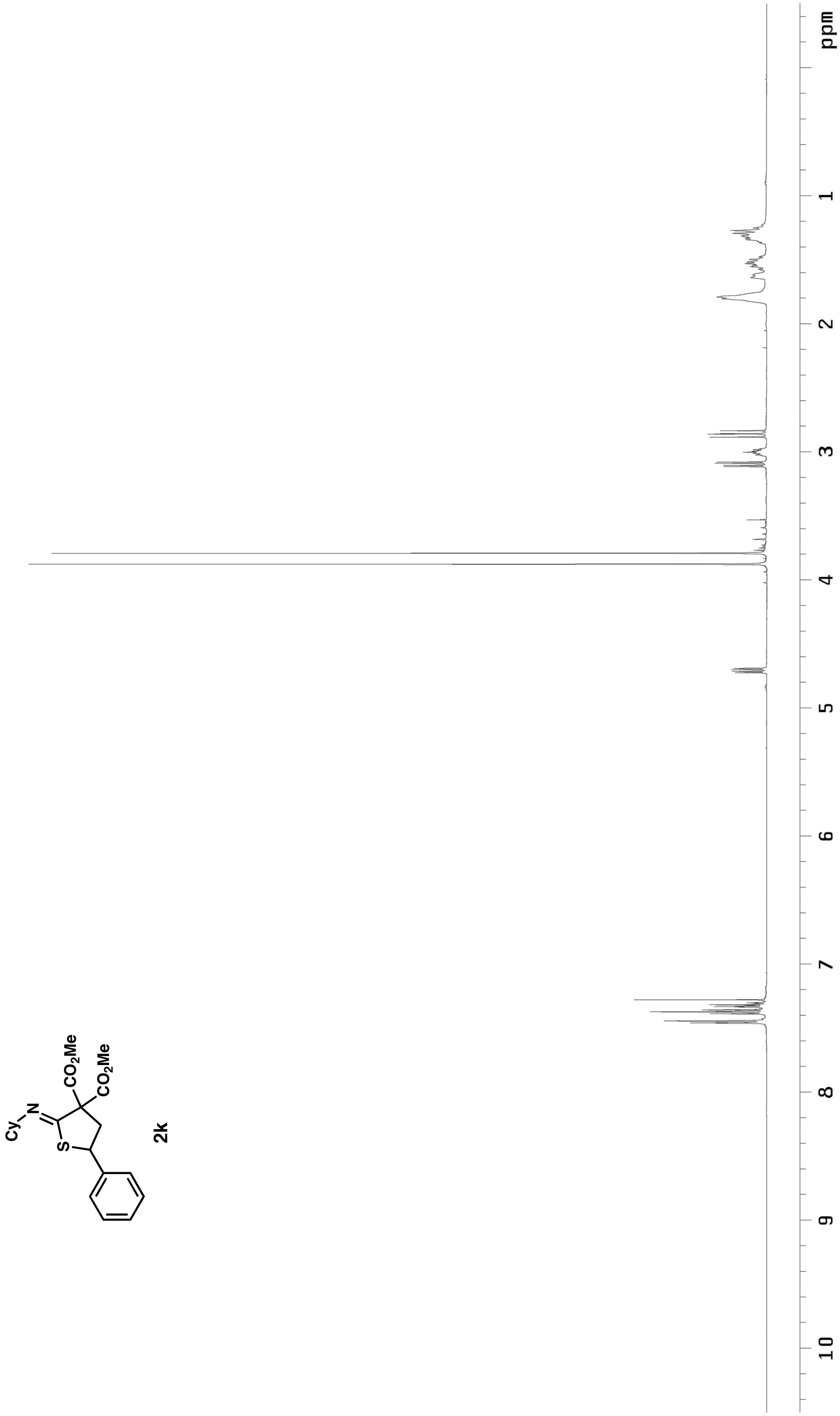
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2j**.



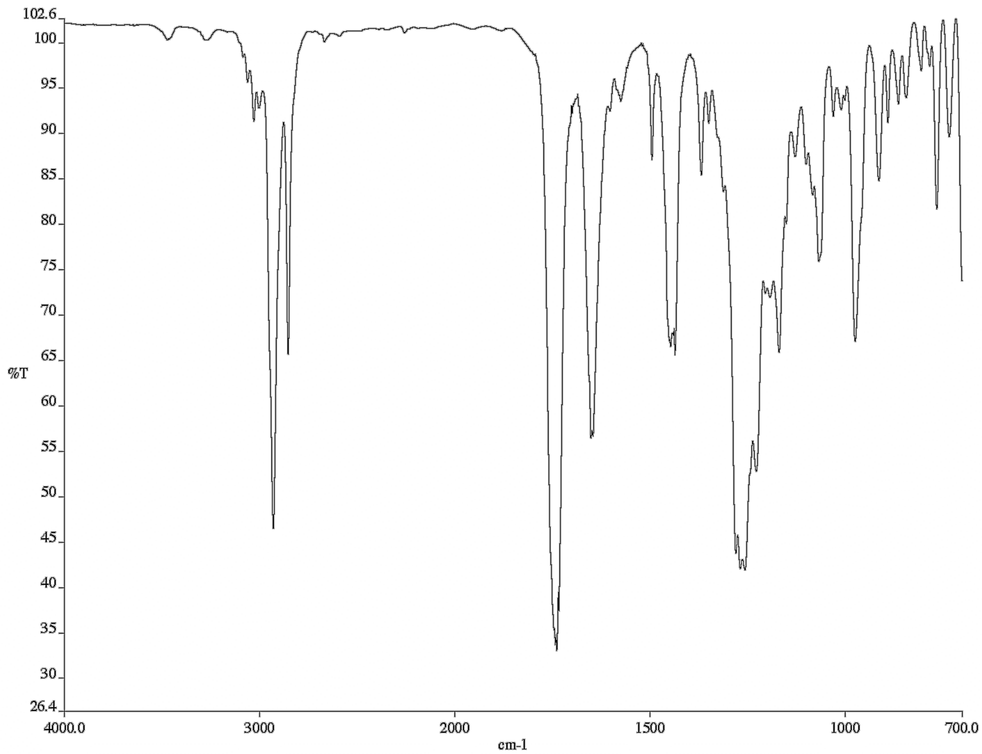
Infrared spectrum (thin film/NaCl) of compound **2j**.



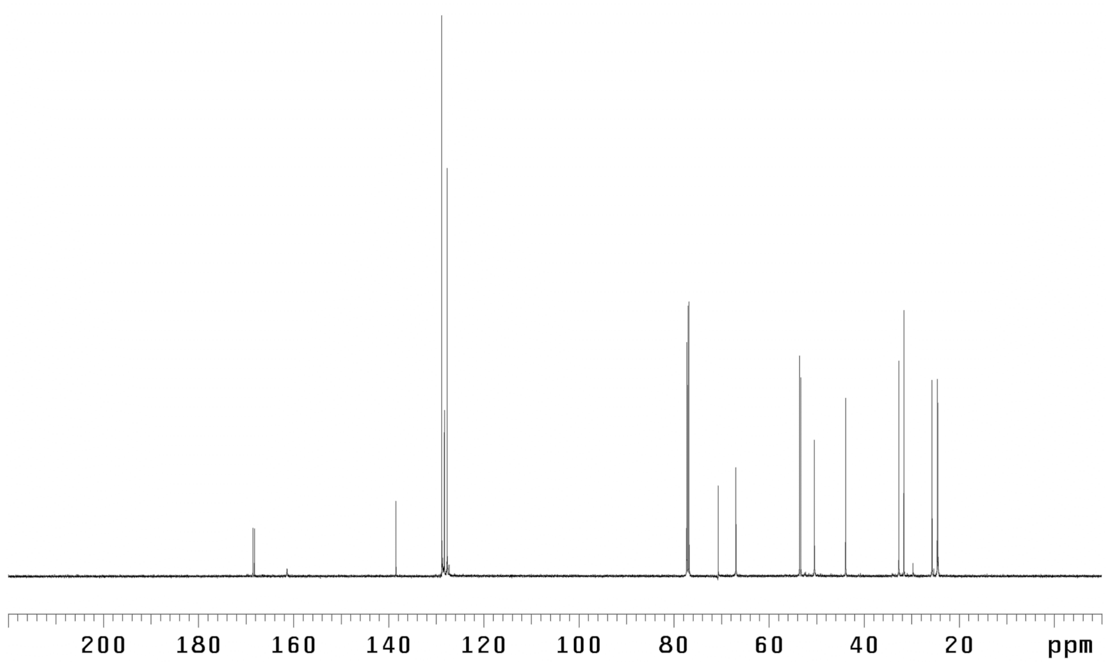
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2j**.



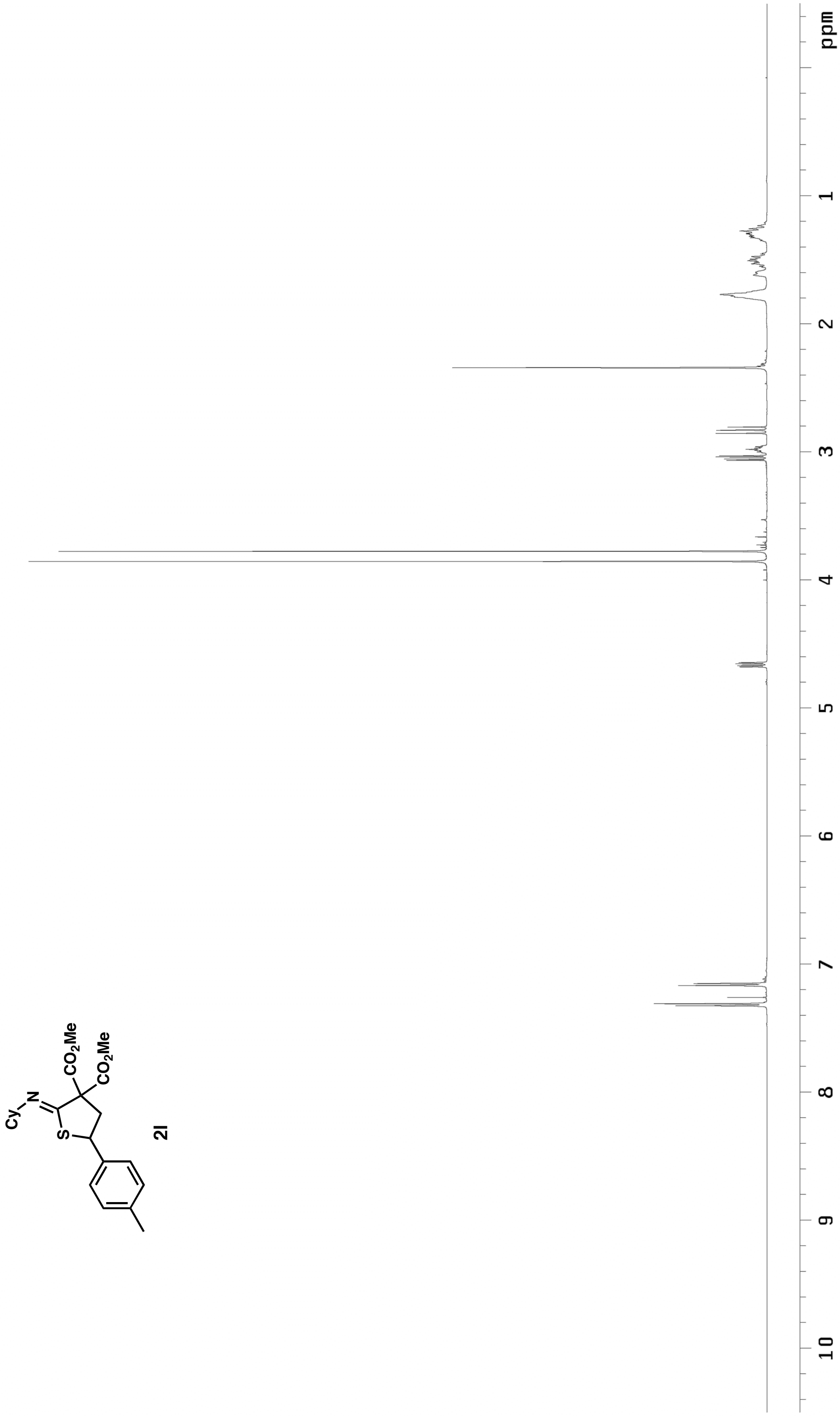
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2k**.



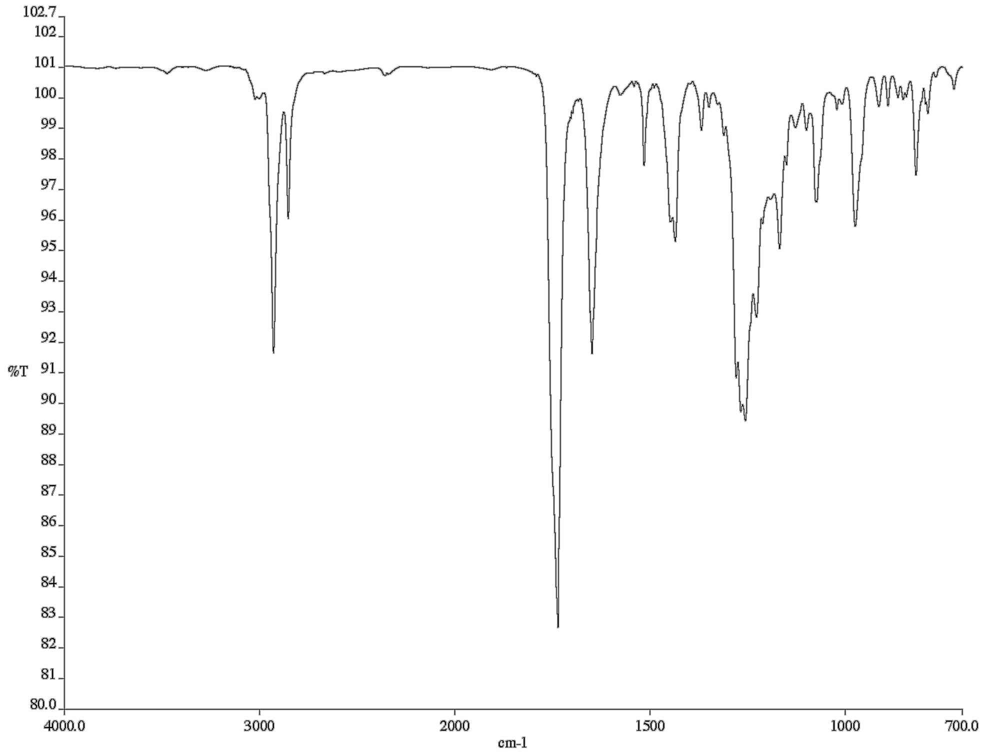
Infrared spectrum (thin film/NaCl) of compound **2k**.



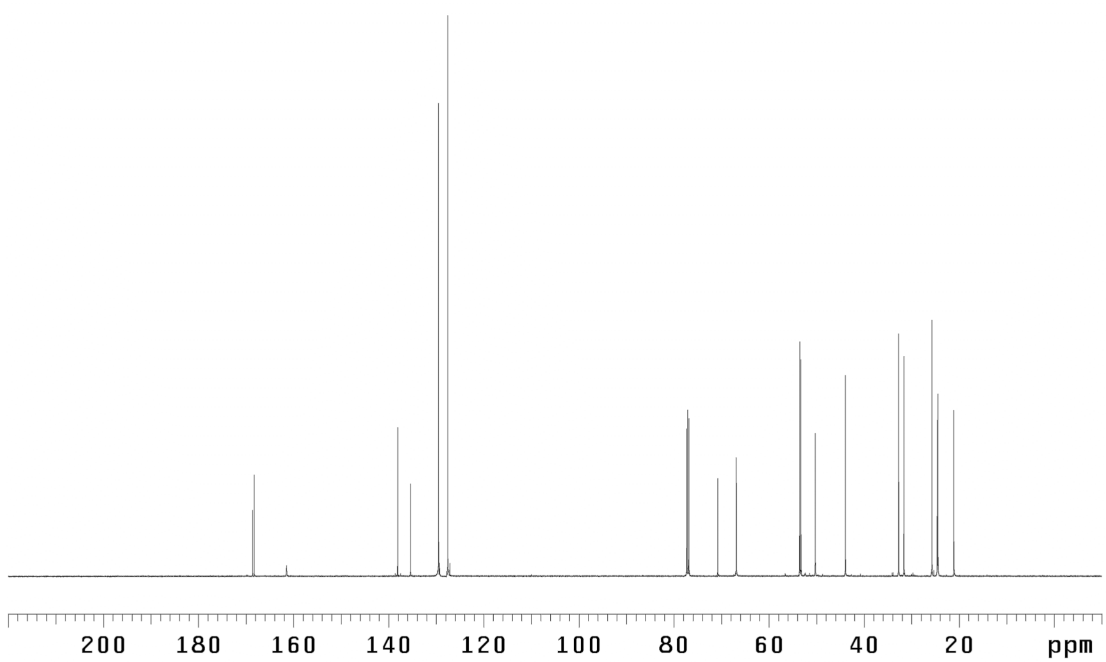
^{13}C NMR (500 MHz, $CDCl_3$) of compound **2k**.



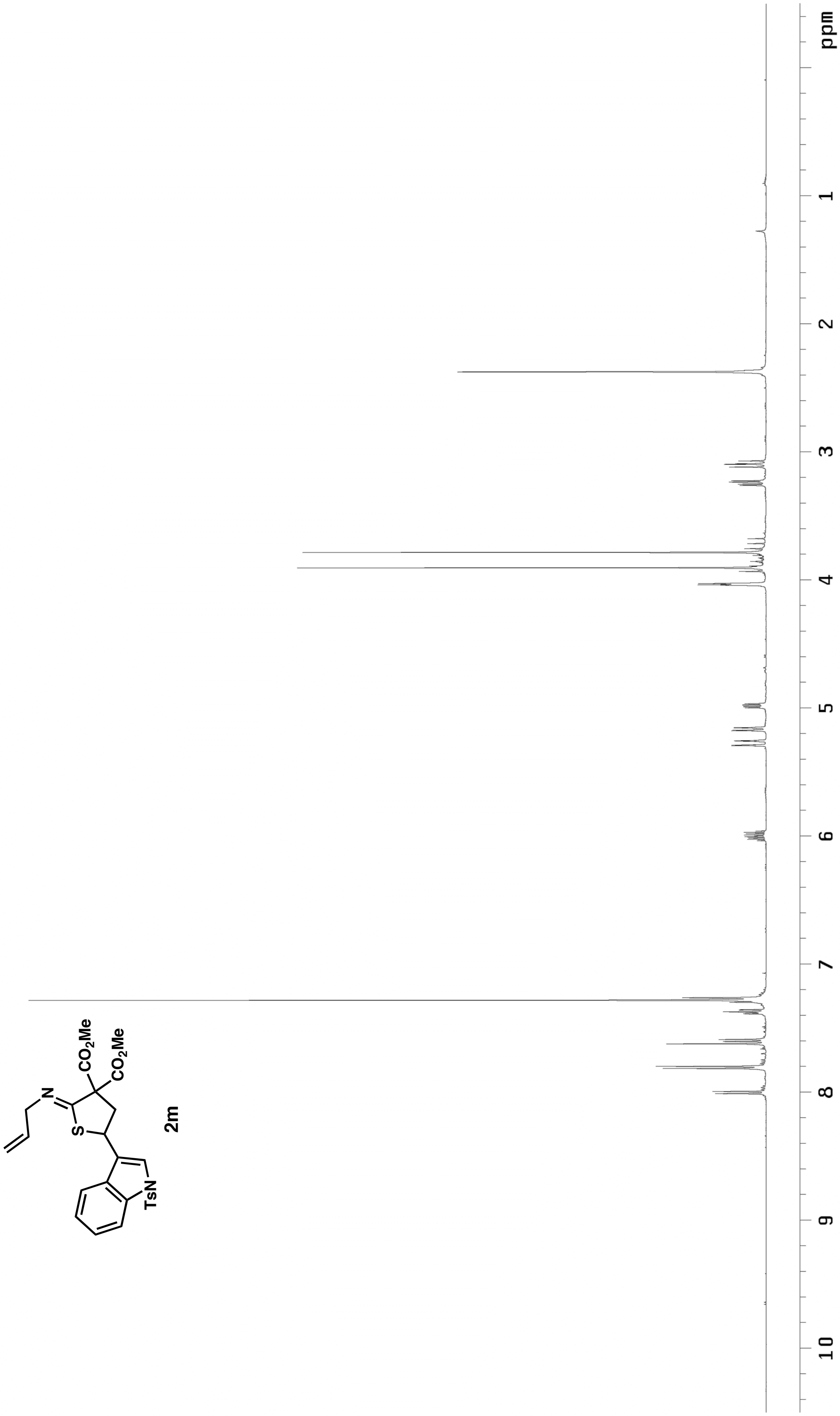
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2l**.



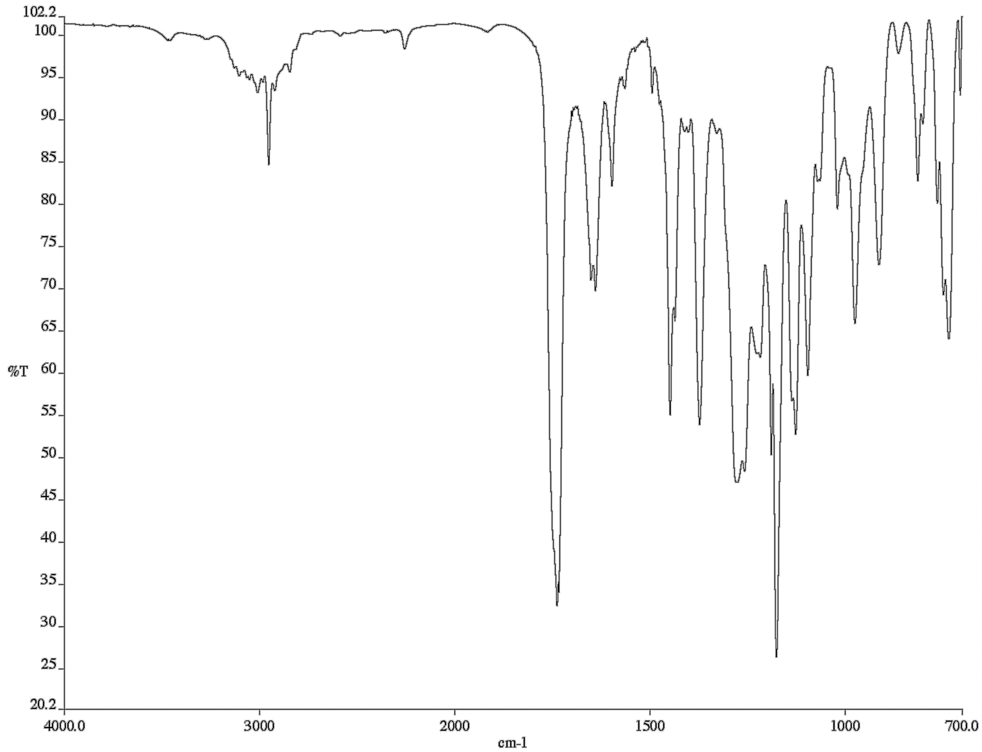
Infrared spectrum (thin film/NaCl) of compound **2l**.



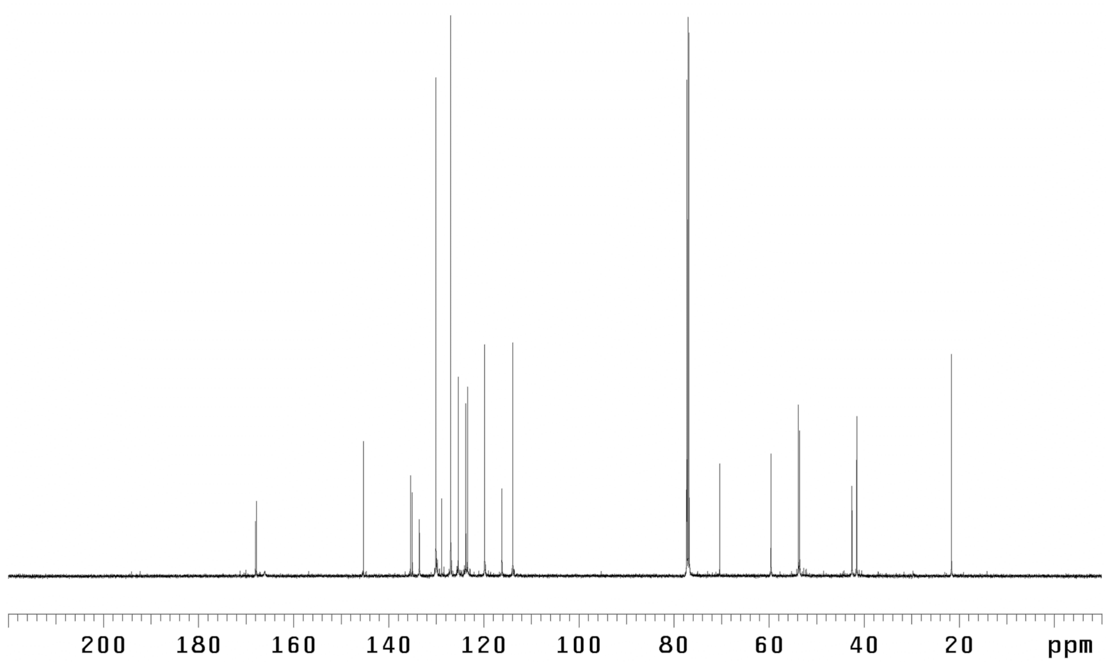
^{13}C NMR (126 MHz, $CDCl_3$) of compound **2l**.



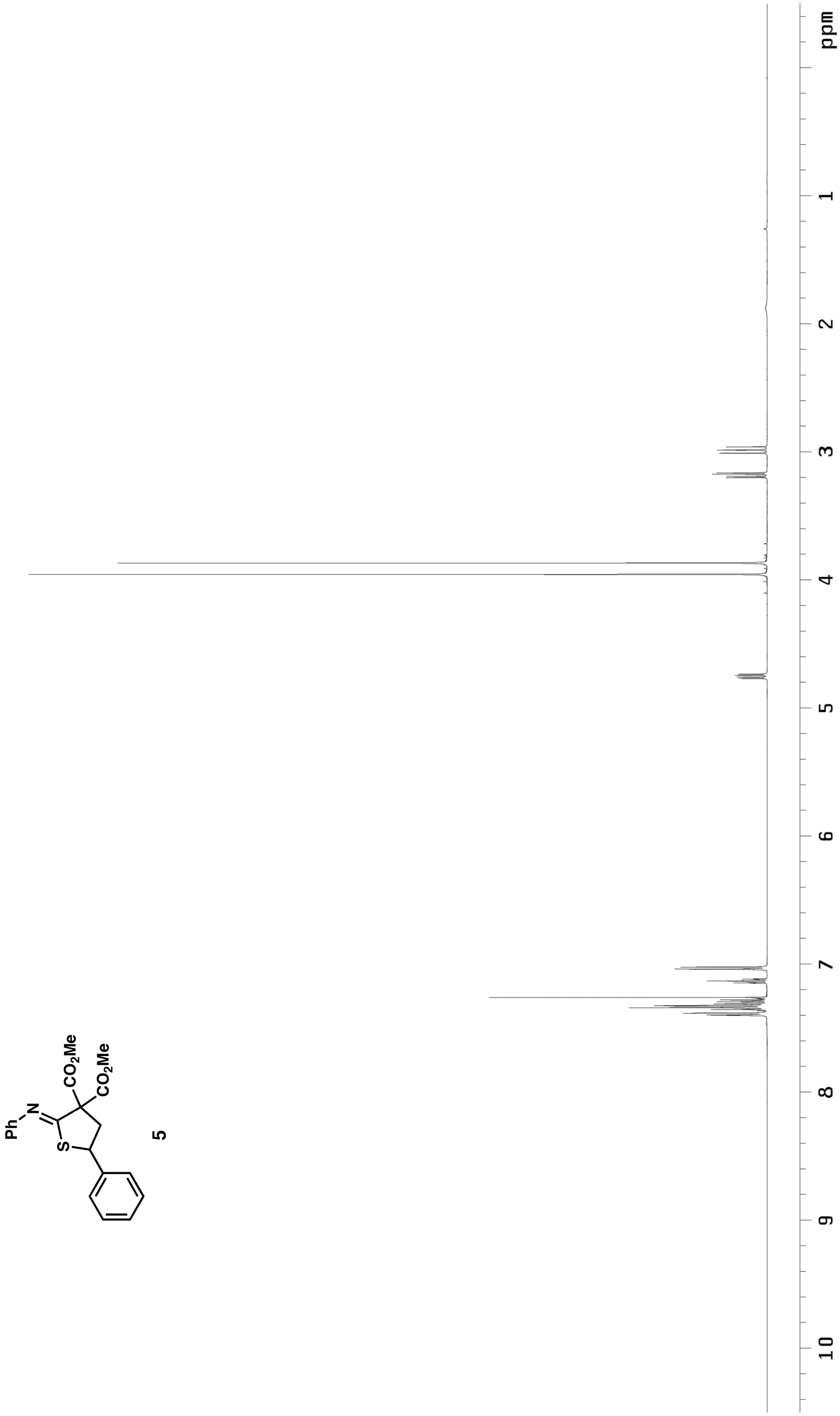
^{1}H NMR (500 MHz, $CDCl_3$) of compound **2m**.



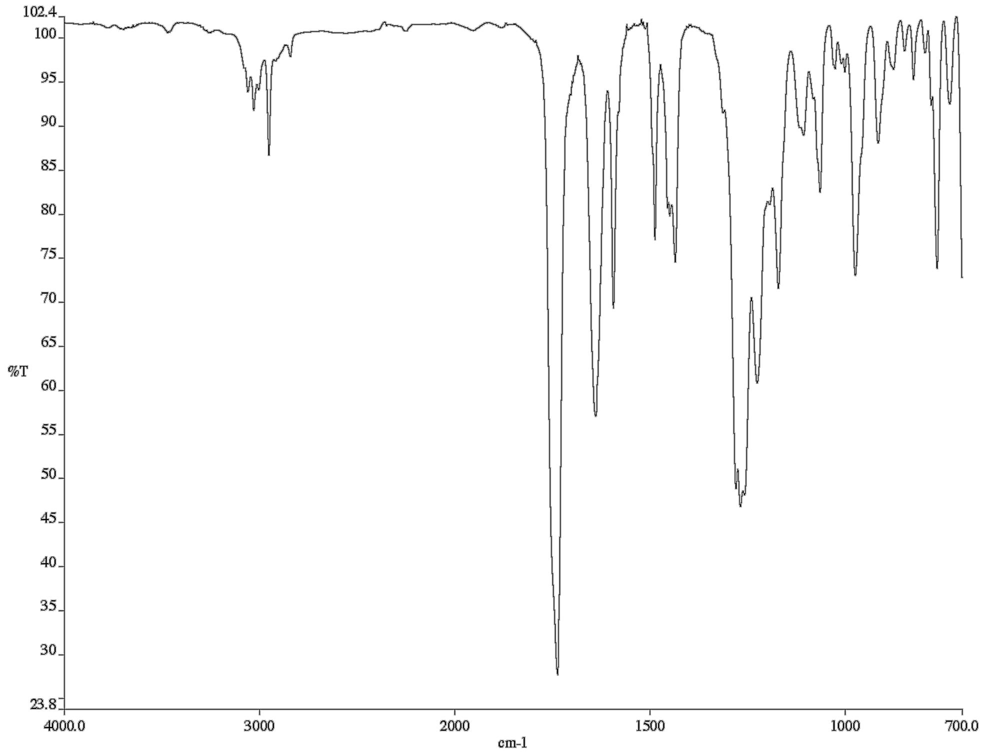
Infrared spectrum (thin film/NaCl) of compound **2m**.



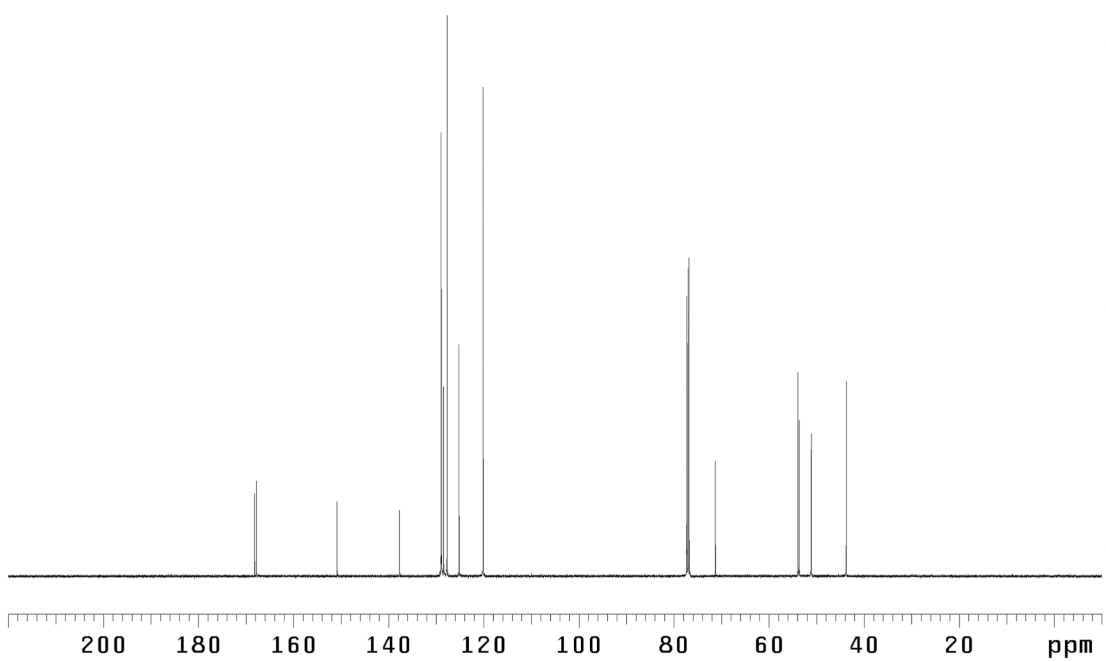
[13]C NMR (126 MHz, $CDCl_3$) of compound **2m**.



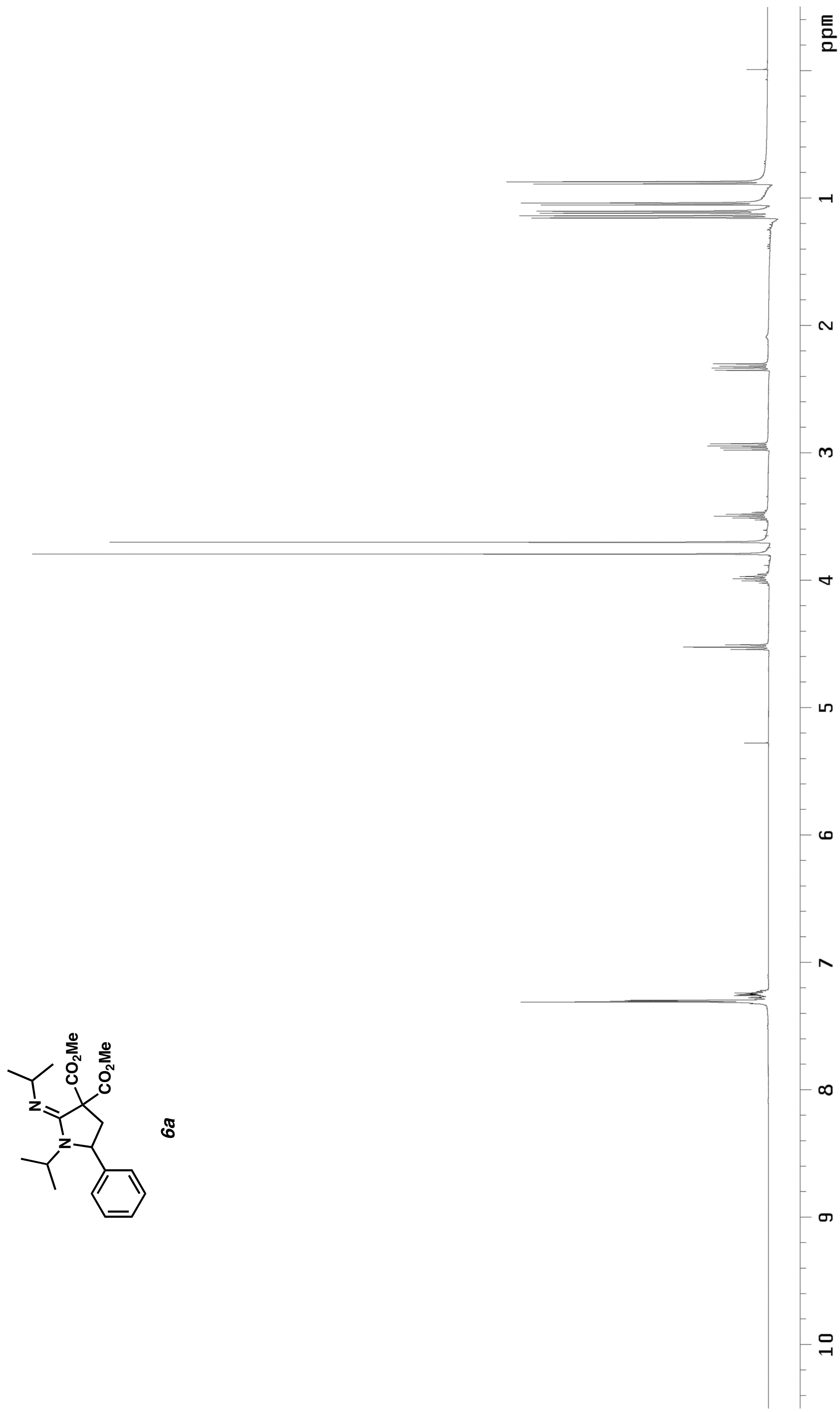
^{1}H NMR (500 MHz, $CDCl_3$) of compound **5**.



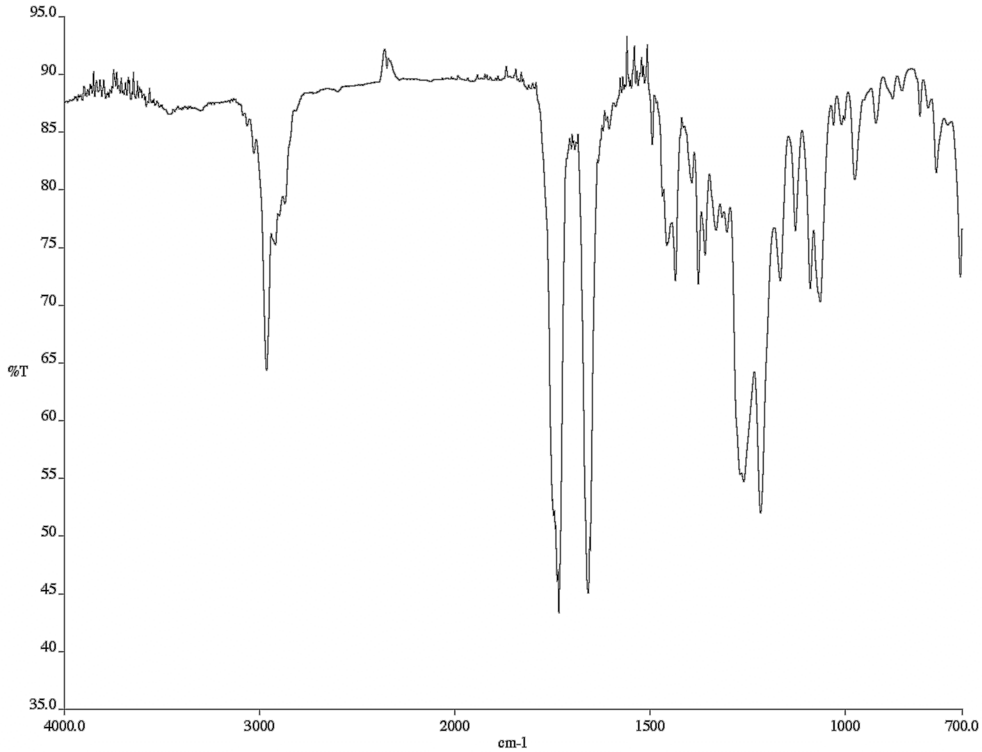
Infrared spectrum (thin film/NaCl) of compound **5**.



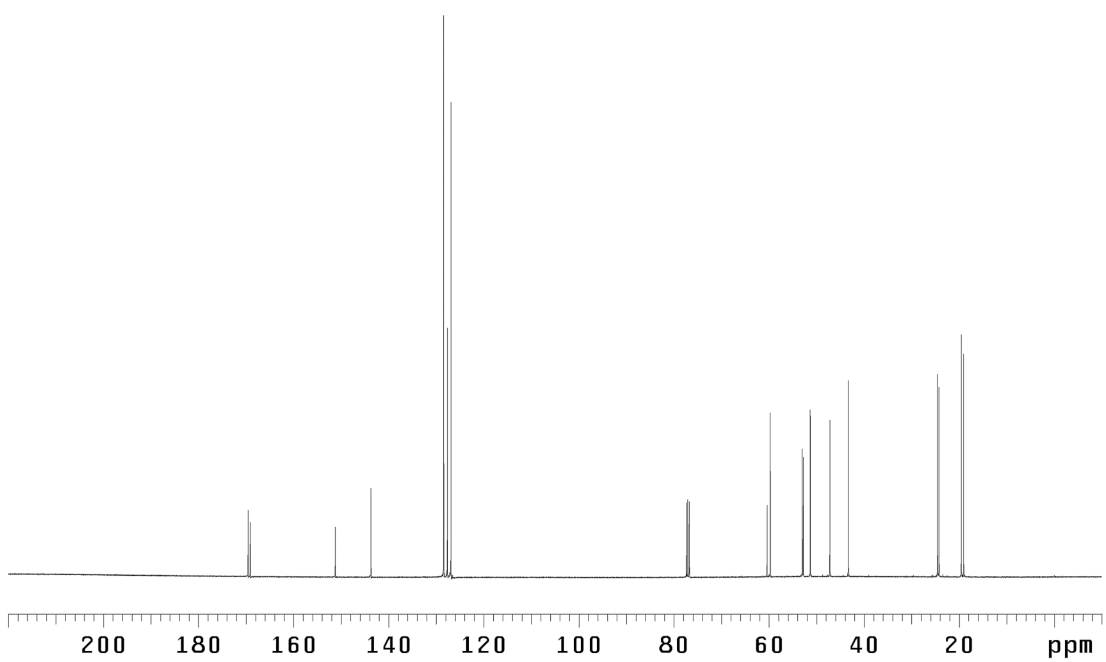
^{13}C NMR (126 MHz, $CDCl_3$) of compound **5**.



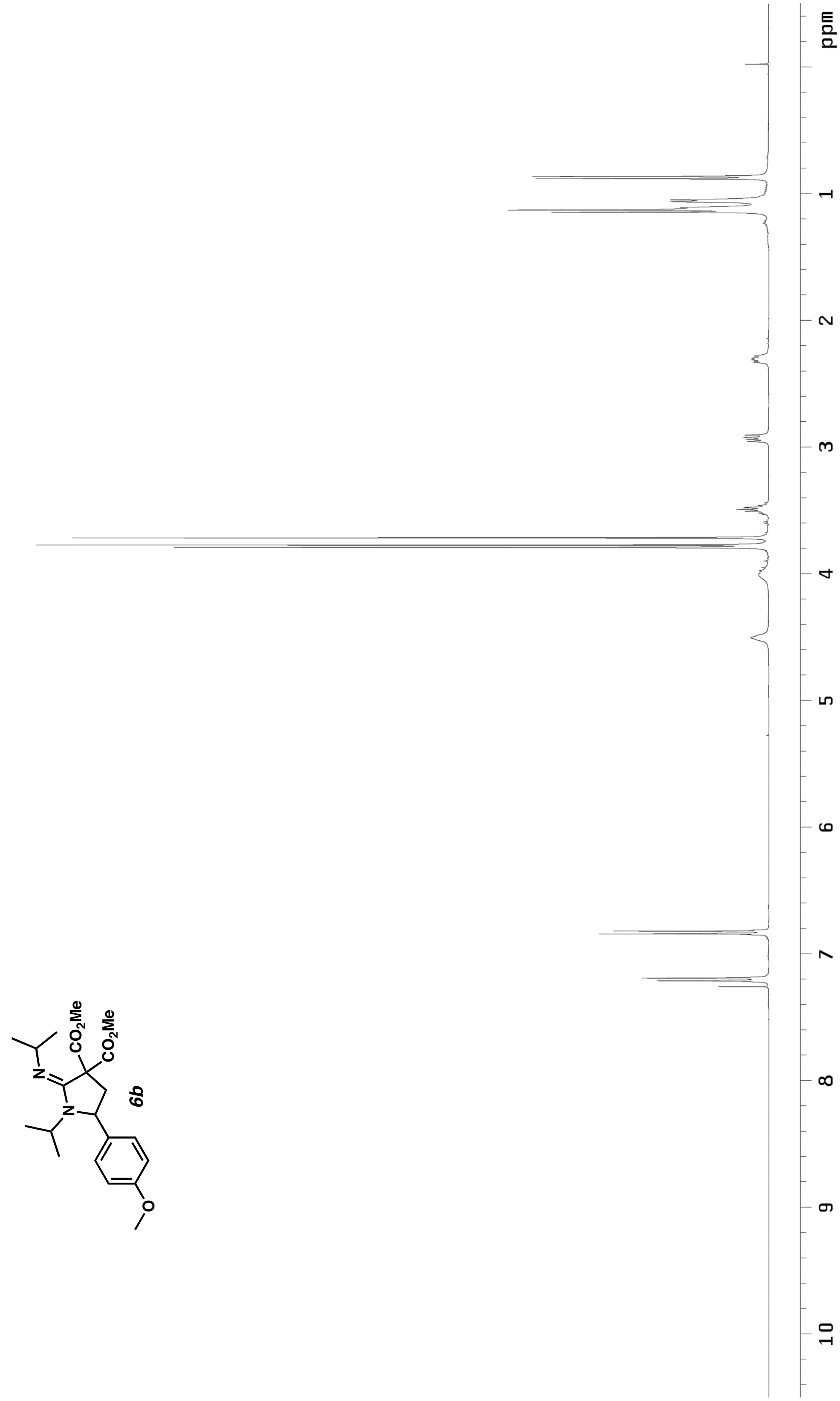
^{1}H NMR (400 MHz, XX) of compound **6a**.



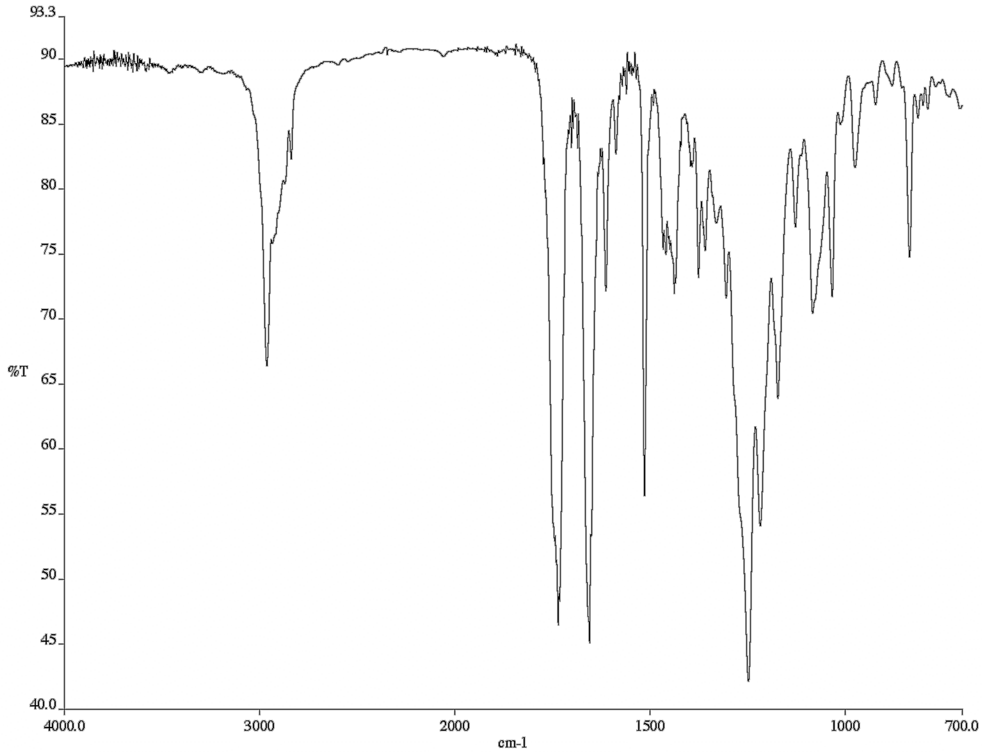
Infrared spectrum (thin film/NaCl) of compound **6a**.



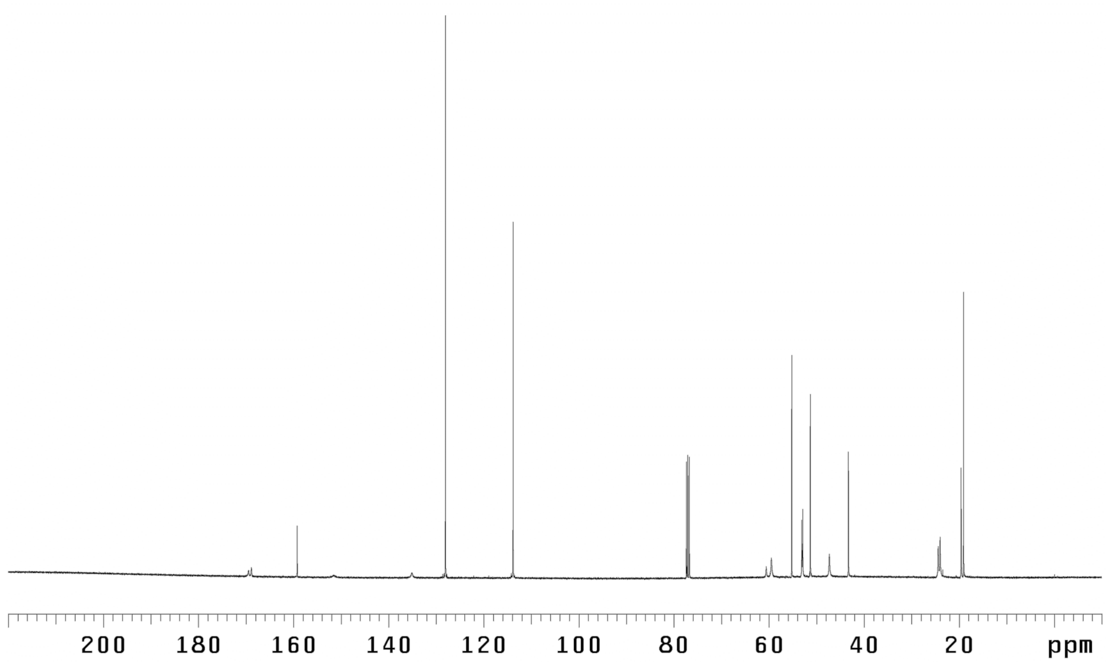
^{13}C NMR (101 MHz, $CDCl_3$) of compound **6a**.



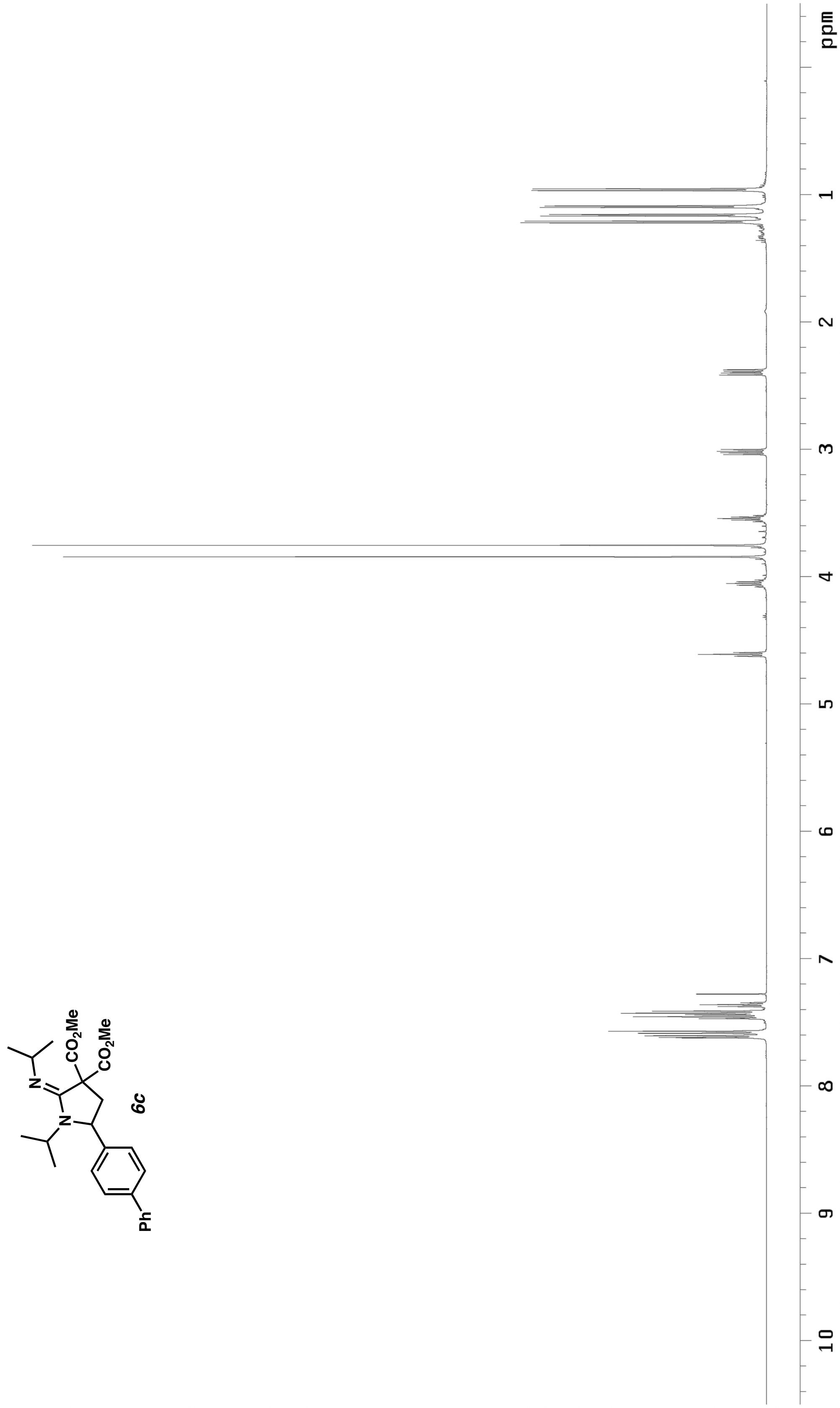
^{1}H NMR (400 MHz, $CDCl_3$) of compound **6b**.



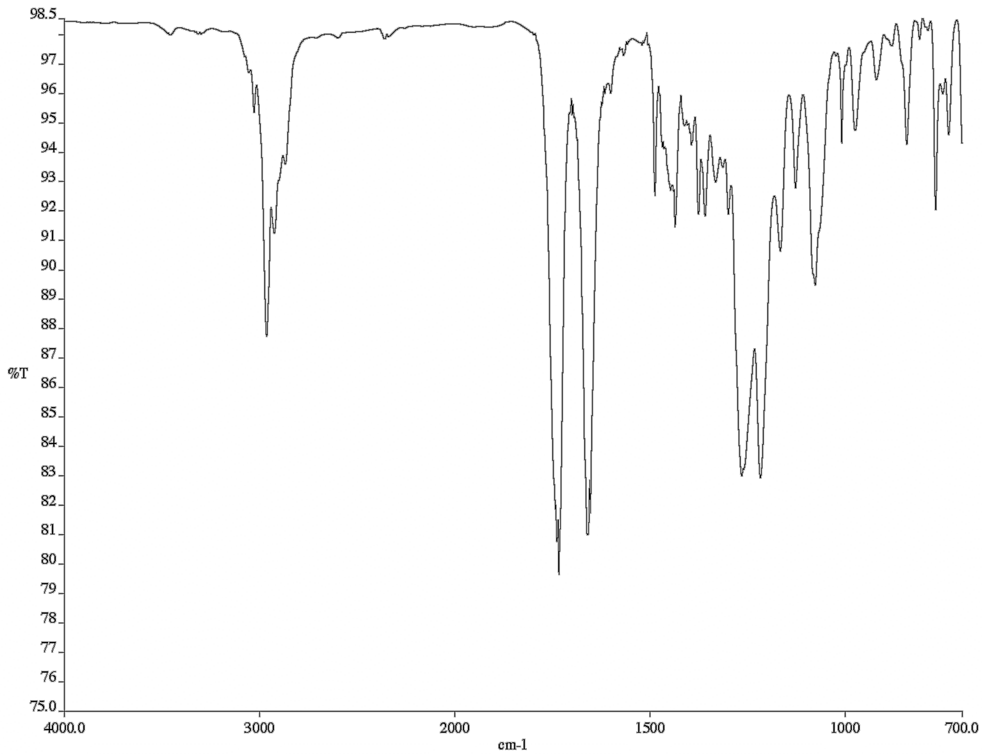
Infrared spectrum (thin film/NaCl) of compound **6b**.



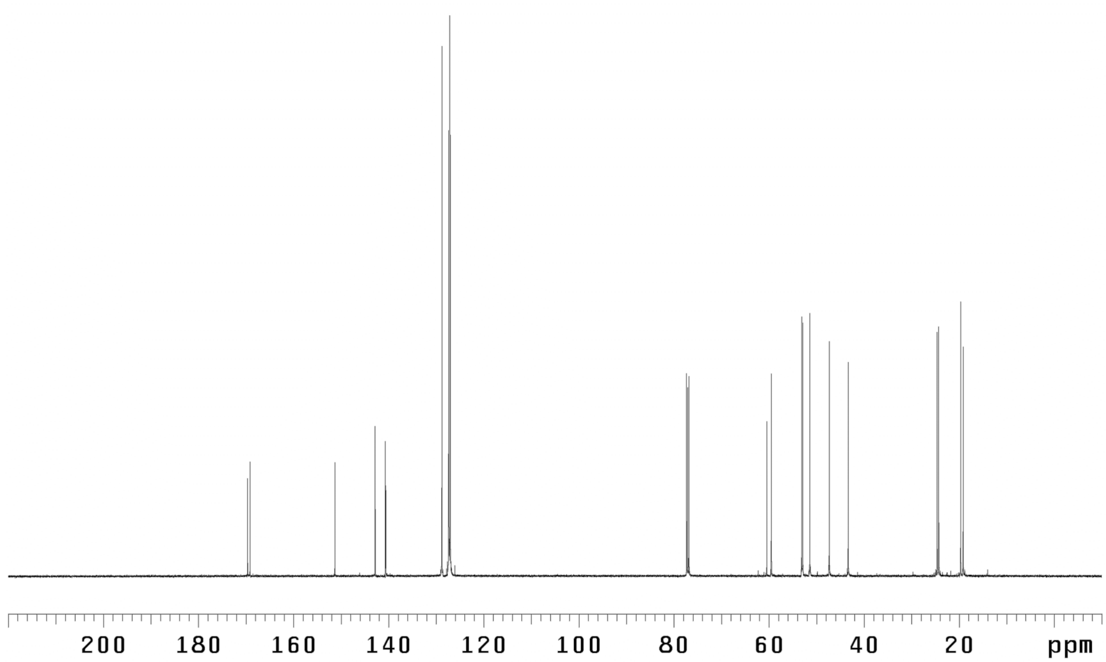
^{13}C NMR (101 MHz, $CDCl_3$) of compound **6b**.



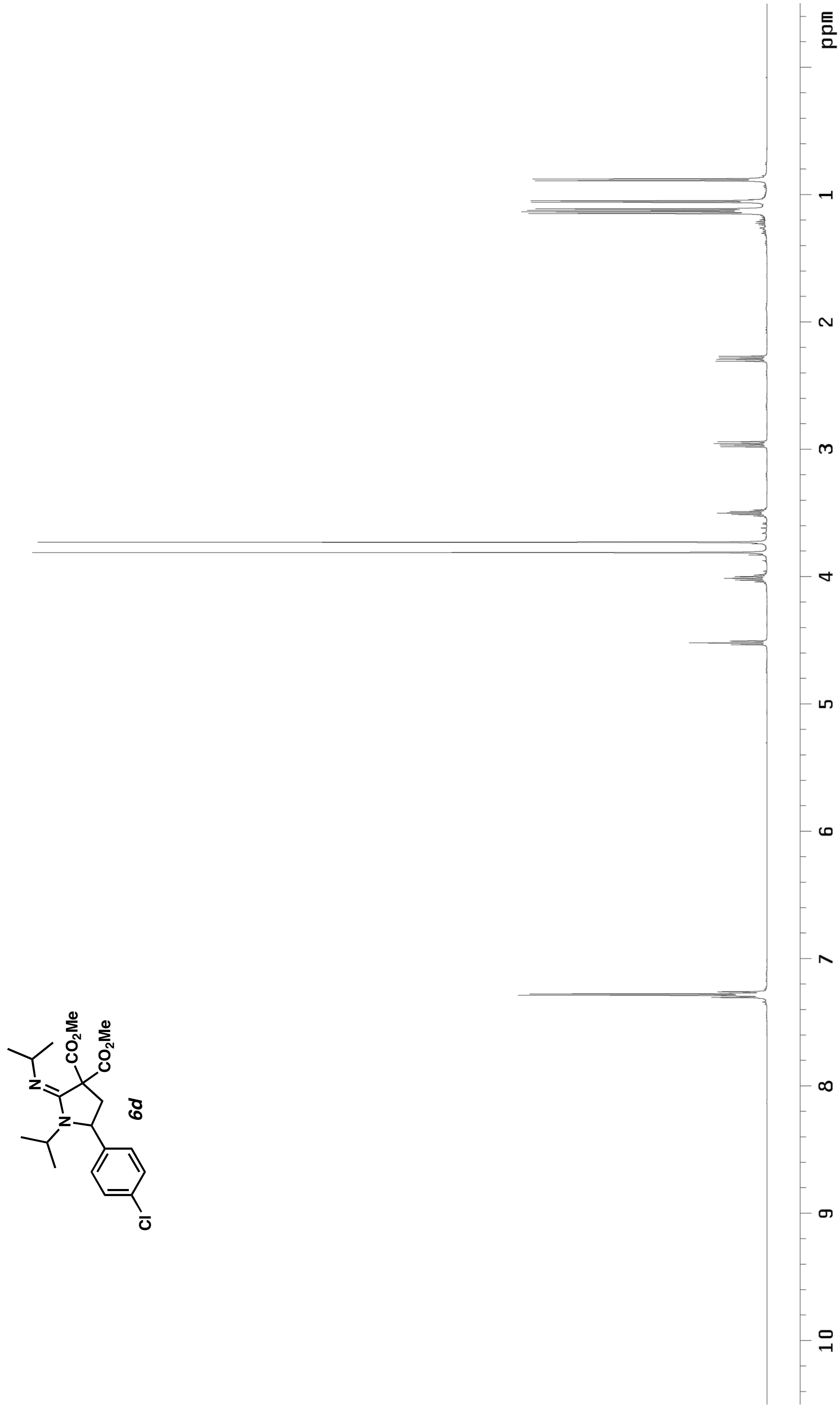
^{1}H NMR (500 MHz, $CDCl_3$) of compound **6c**.



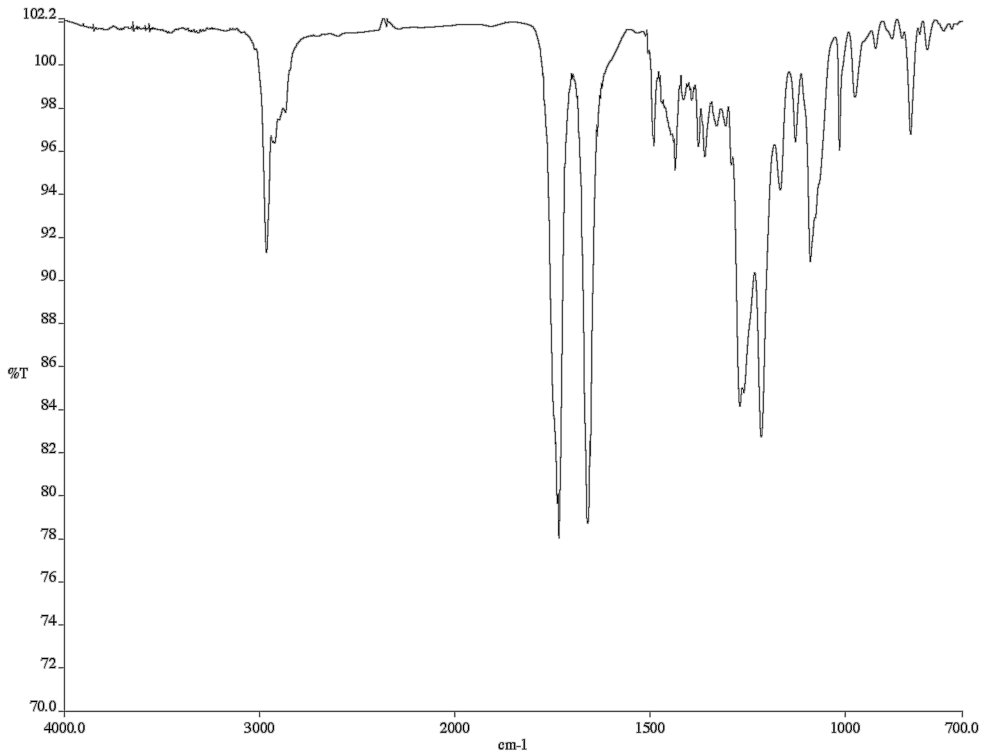
Infrared spectrum (thin film/NaCl) of compound **6c**.



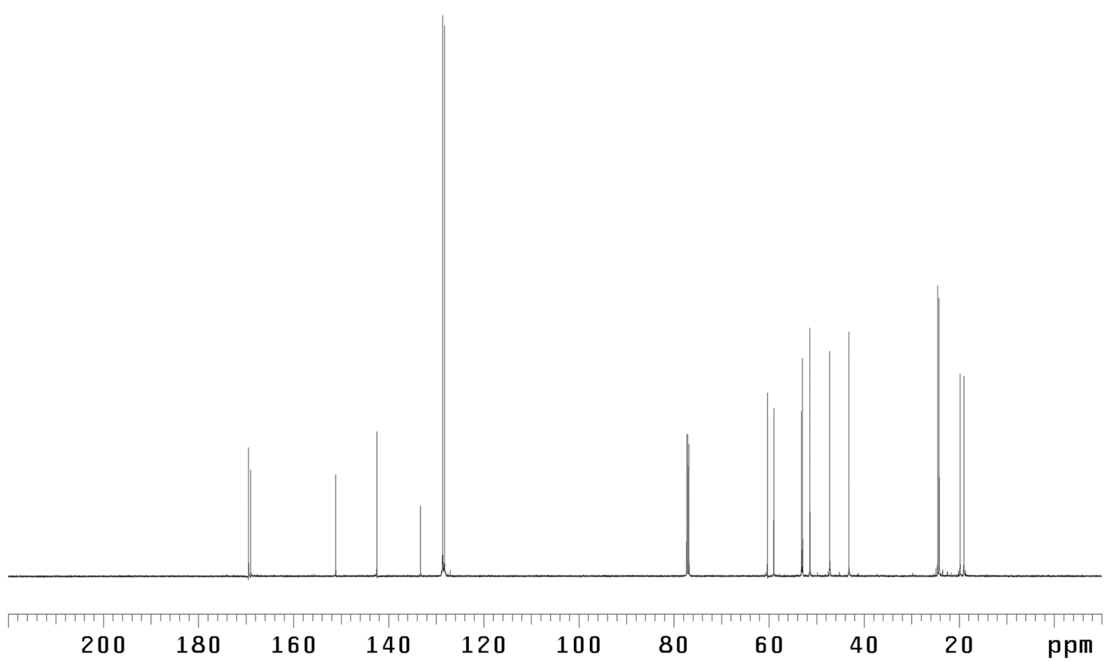
^{13}C NMR (126 MHz, $CDCl_3$) of compound **6c**.



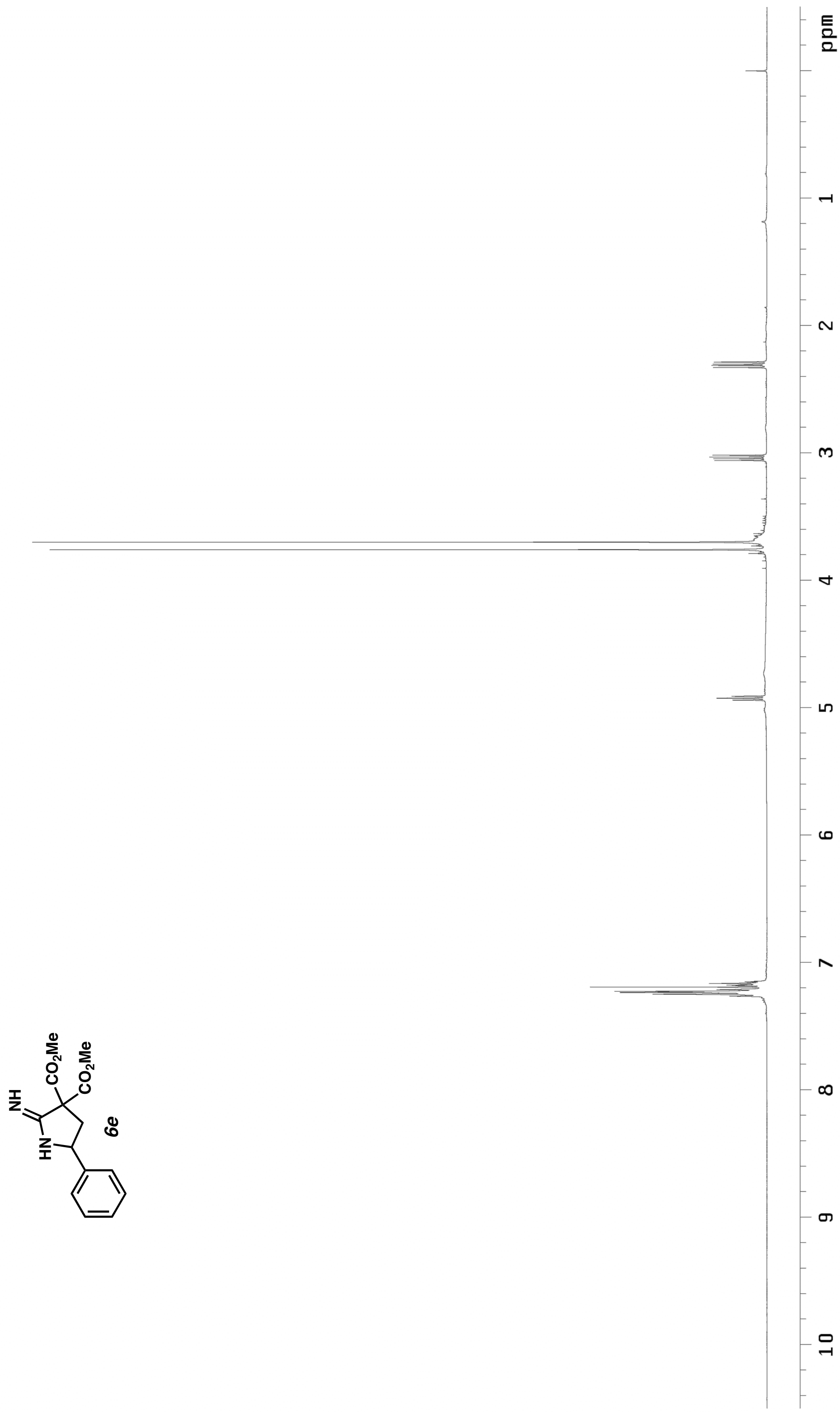
^{1}H NMR (500 MHz, $CDCl_3$) of compound **6d**.



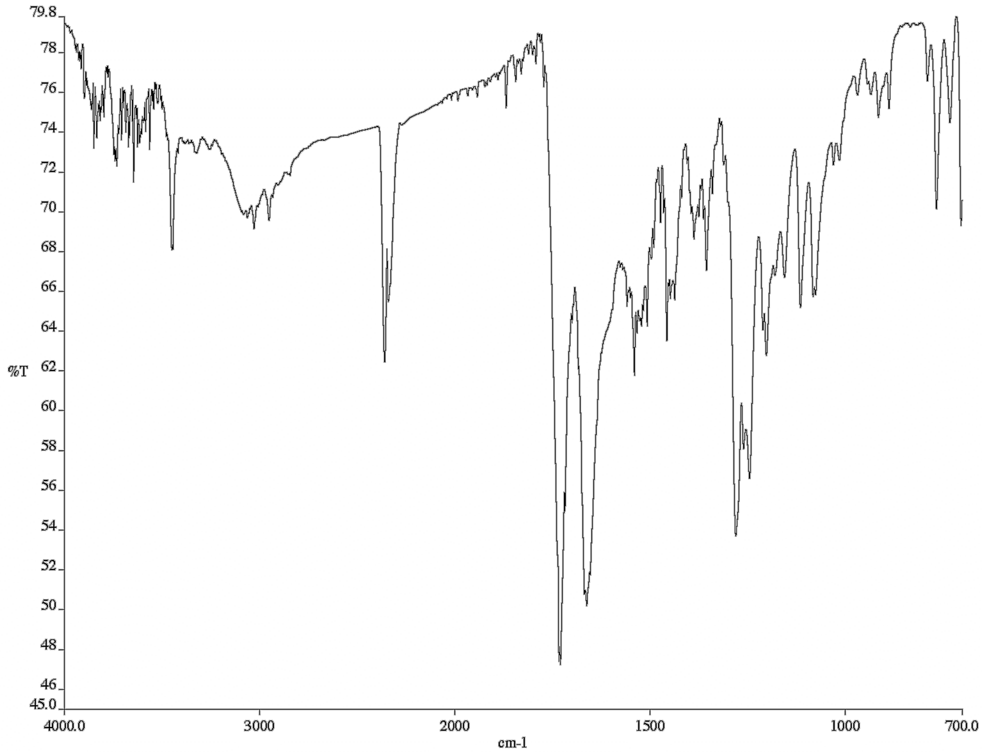
Infrared spectrum (thin film/NaCl) of compound **6d**.



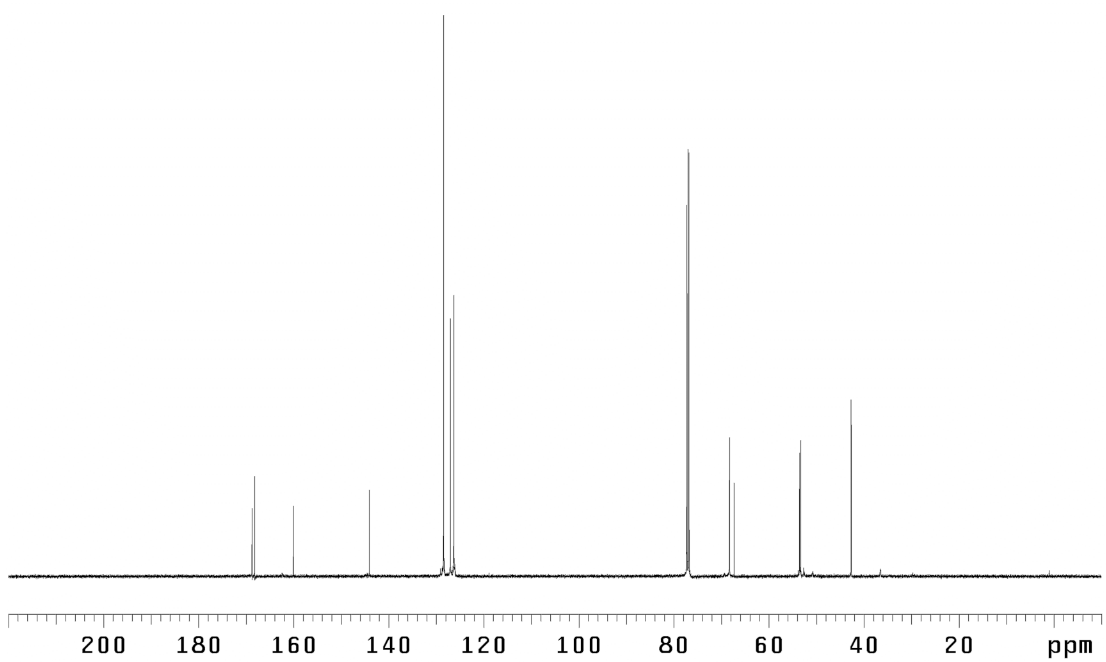
^{13}C NMR (126 MHz, $CDCl_3$) of compound **6d**.



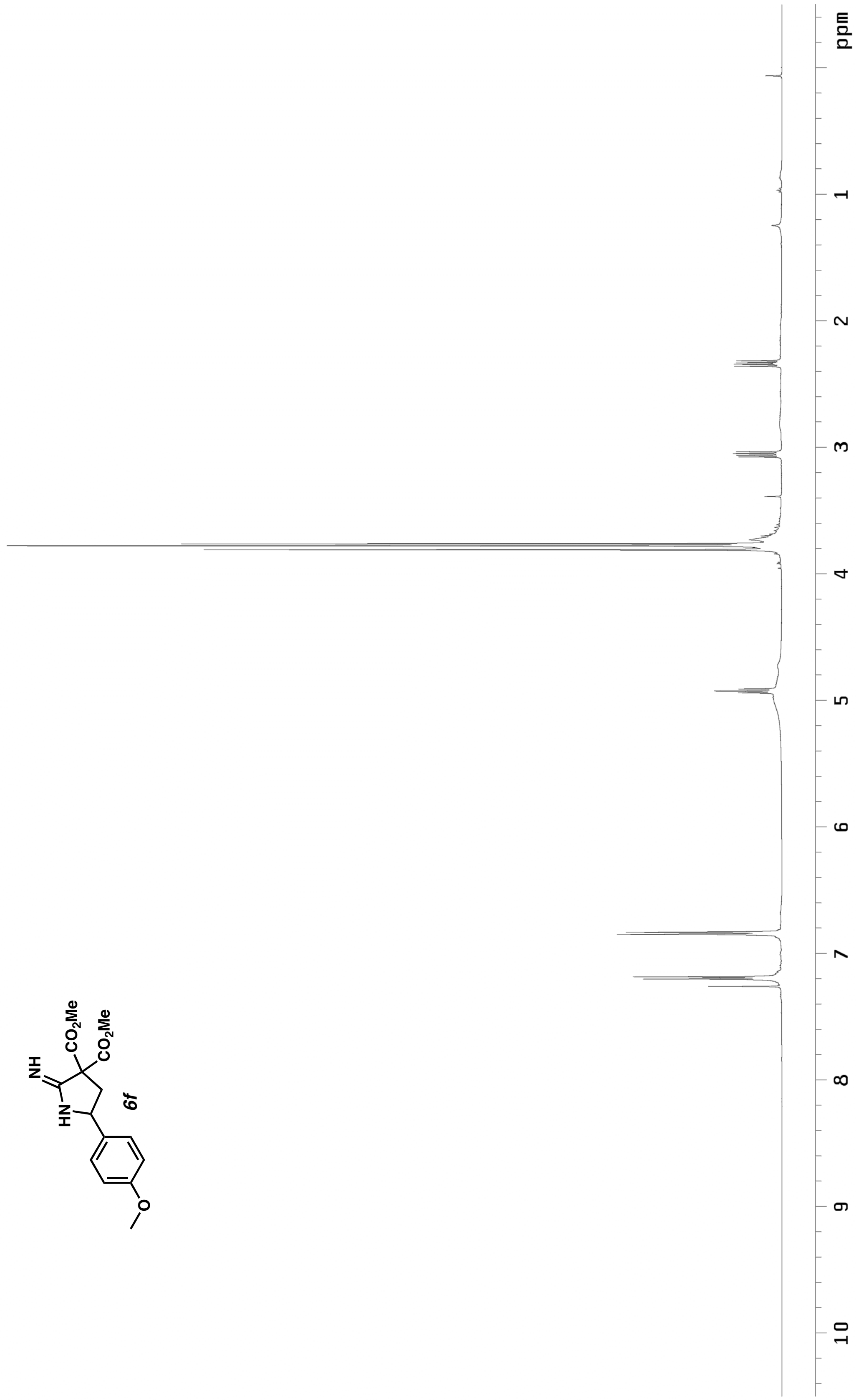
^{1}H NMR (500 MHz, $CDCl_3$) of compound **6e**.



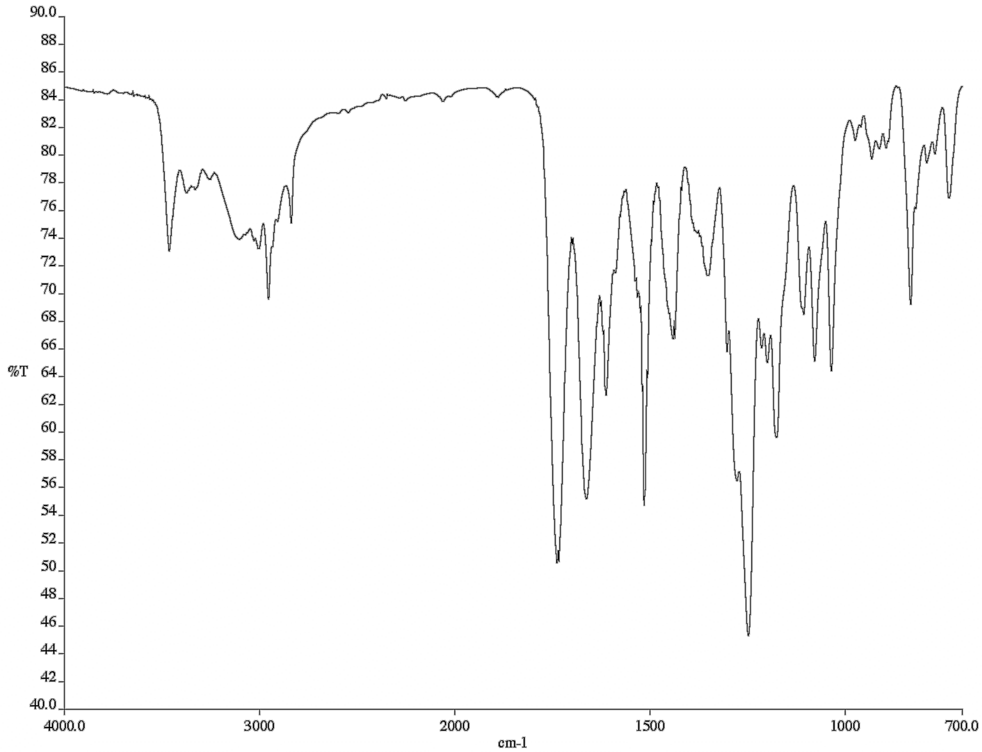
Infrared spectrum (thin film/NaCl) of compound **6e**.



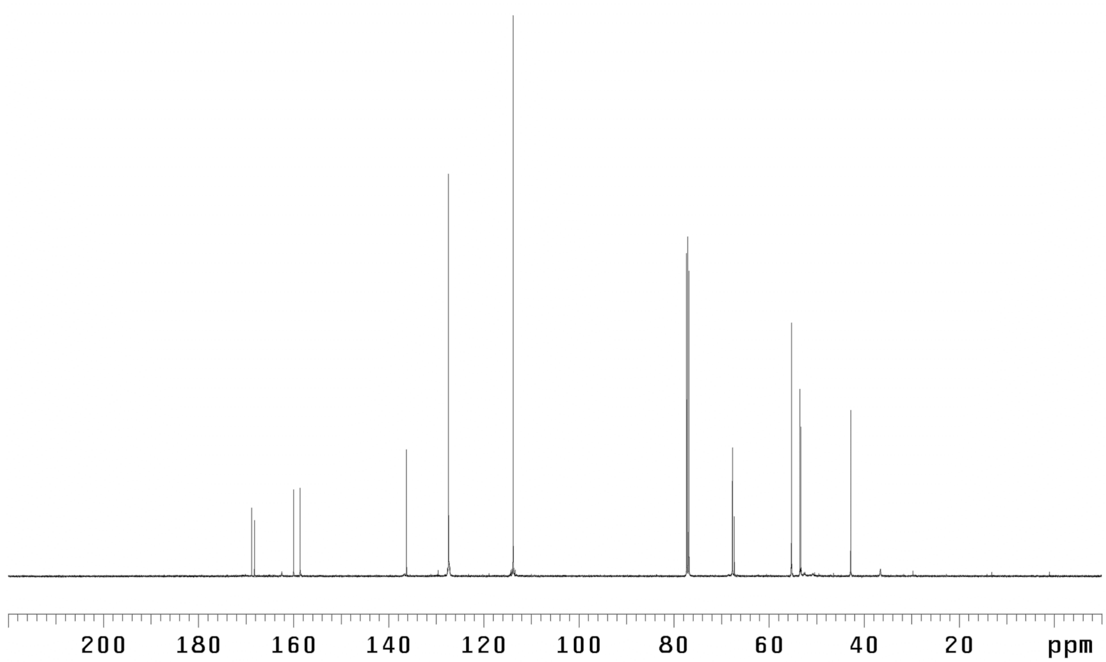
^{13}C NMR (126 MHz, $CDCl_3$) of compound **6e**.



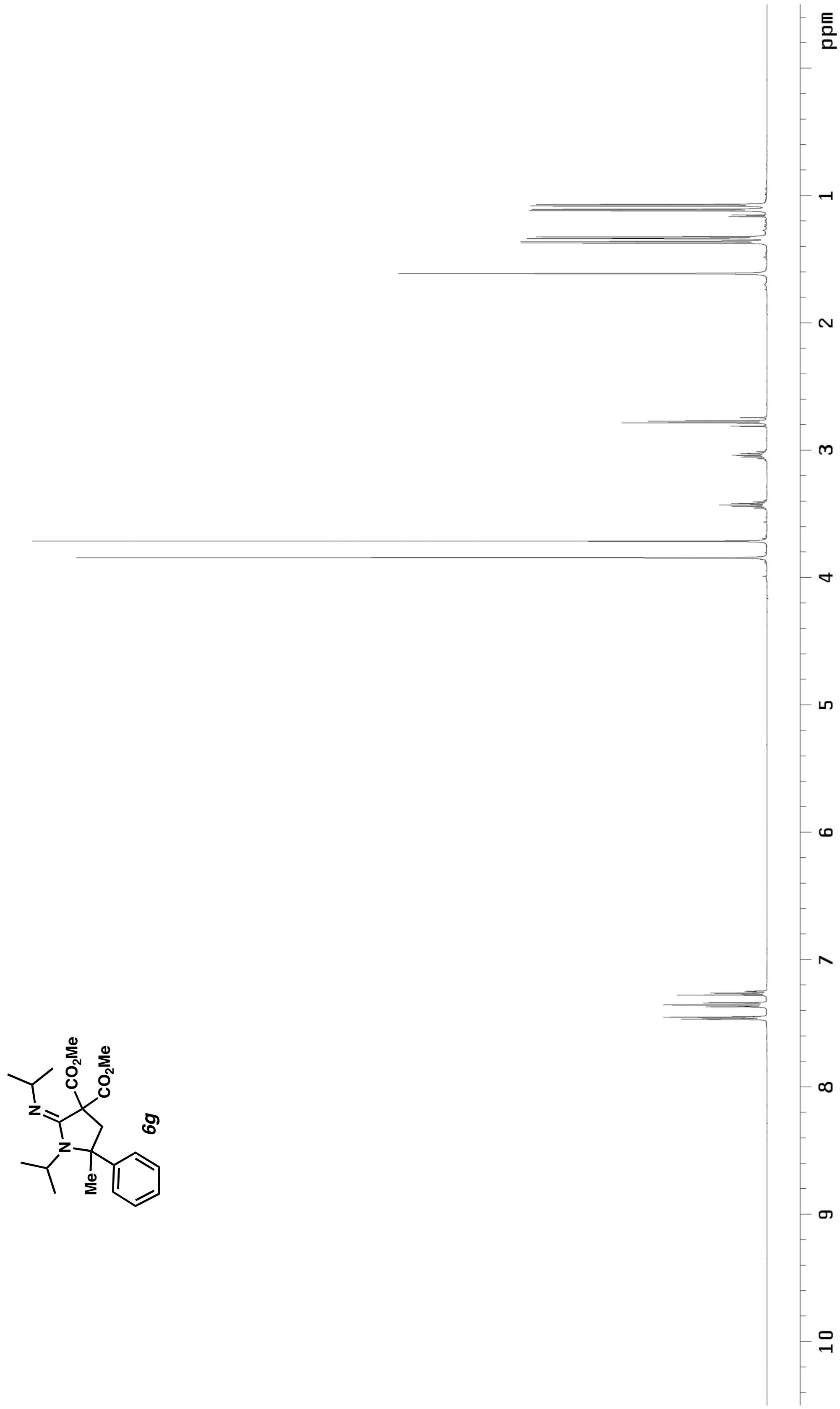
^{1}H NMR (500 MHz, $CDCl_3$) of compound **6f**.



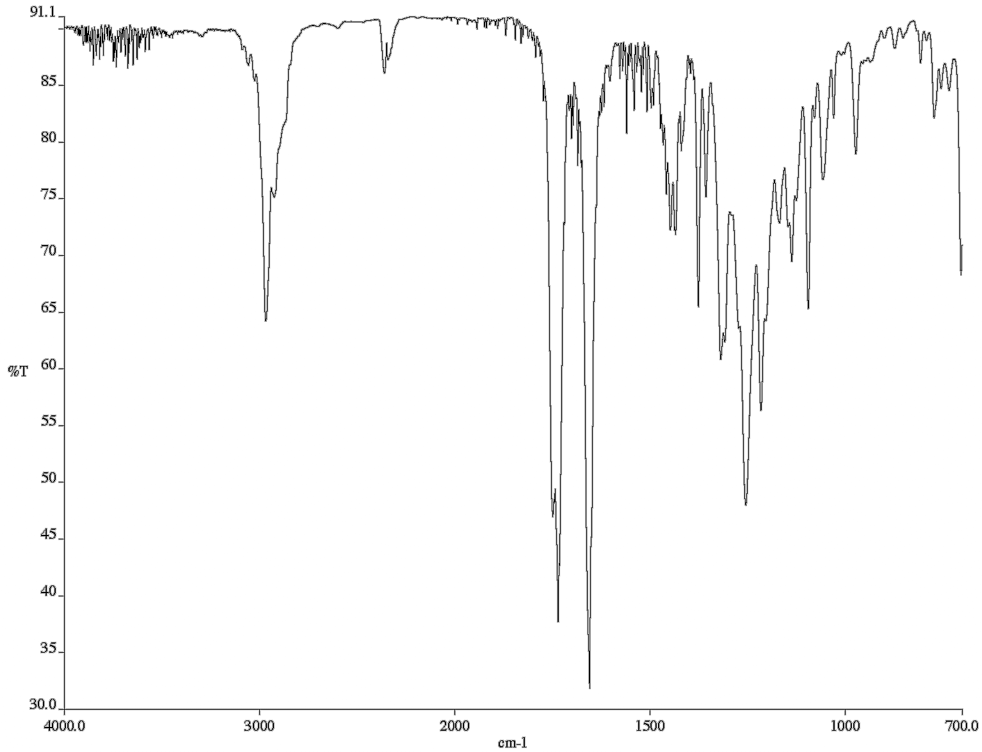
Infrared spectrum (thin film/NaCl) of compound **6f**.



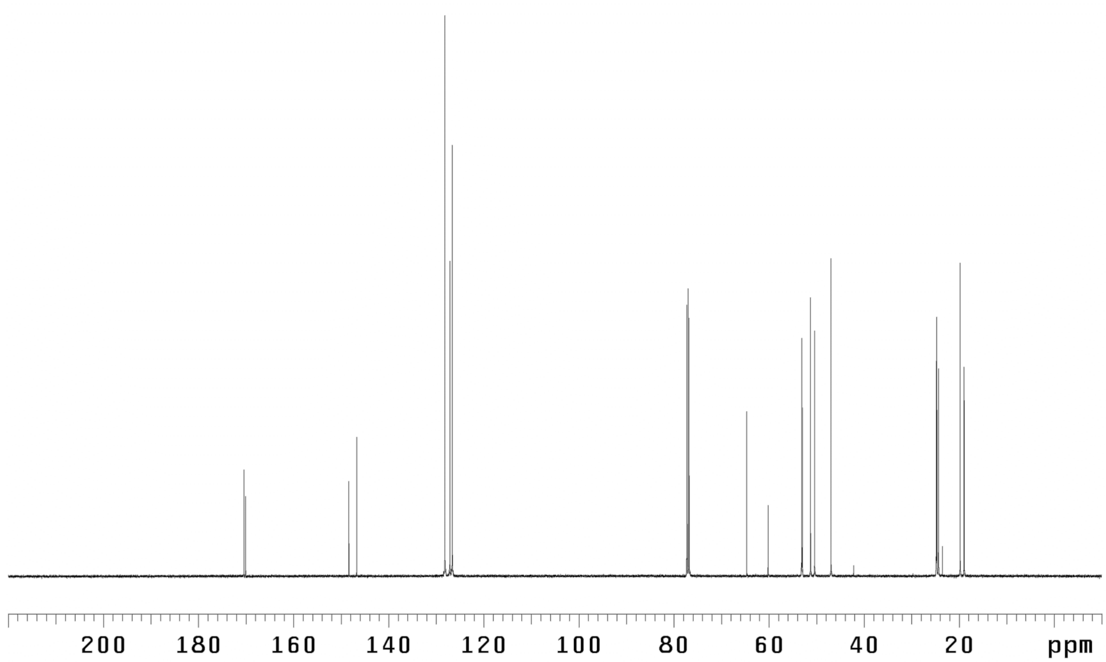
^{13}C NMR (126 MHz, $CDCl_3$) of compound **6f**.



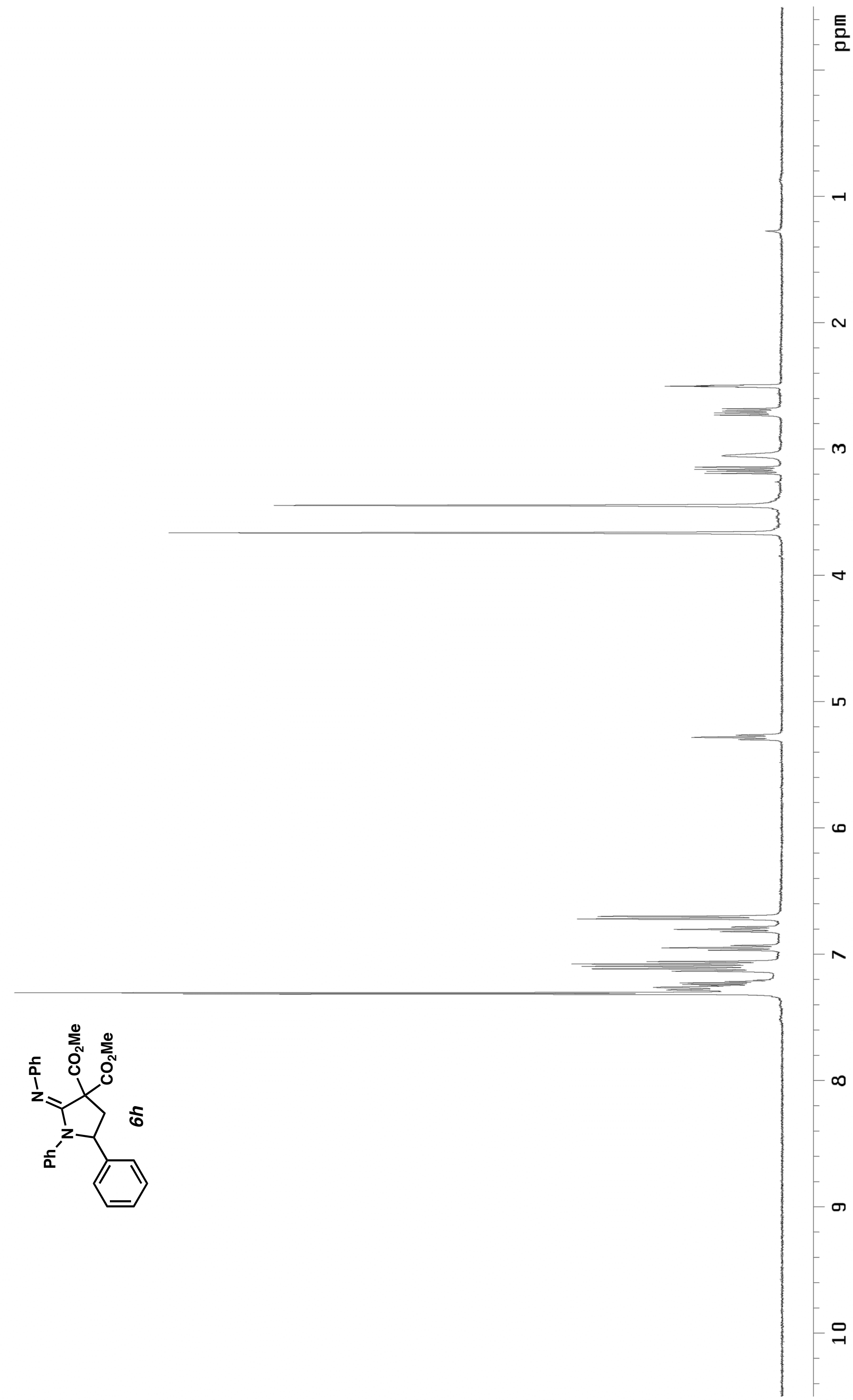
^{1}H NMR (500 MHz, $CDCl_3$) of compound **6g**.



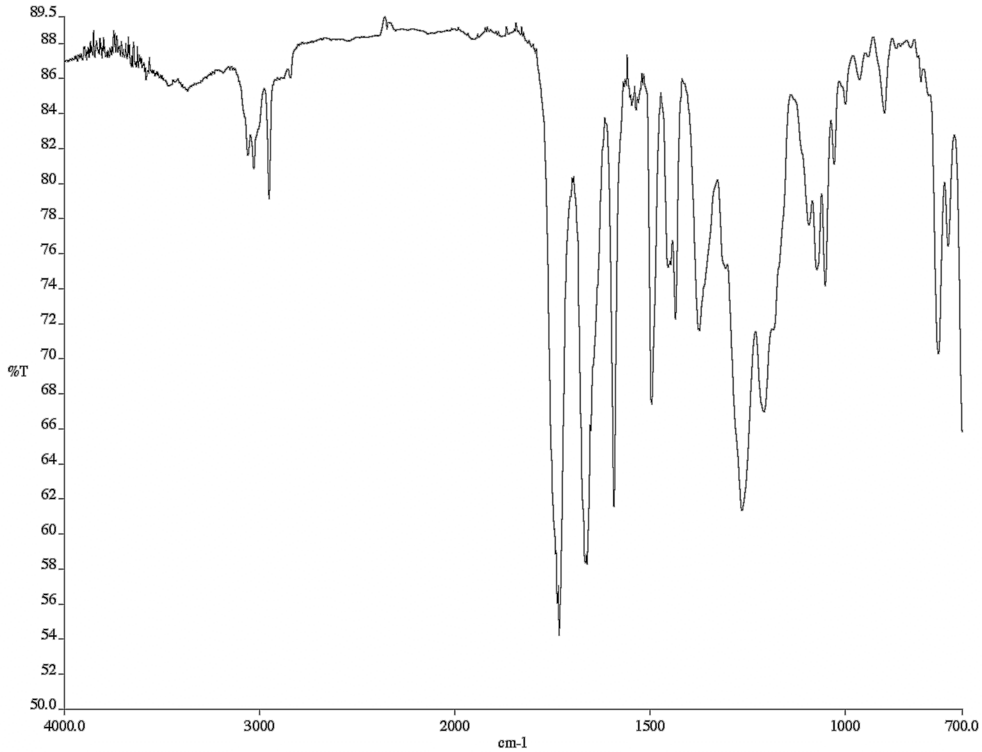
Infrared spectrum (thin film/NaCl) of compound **6g**.



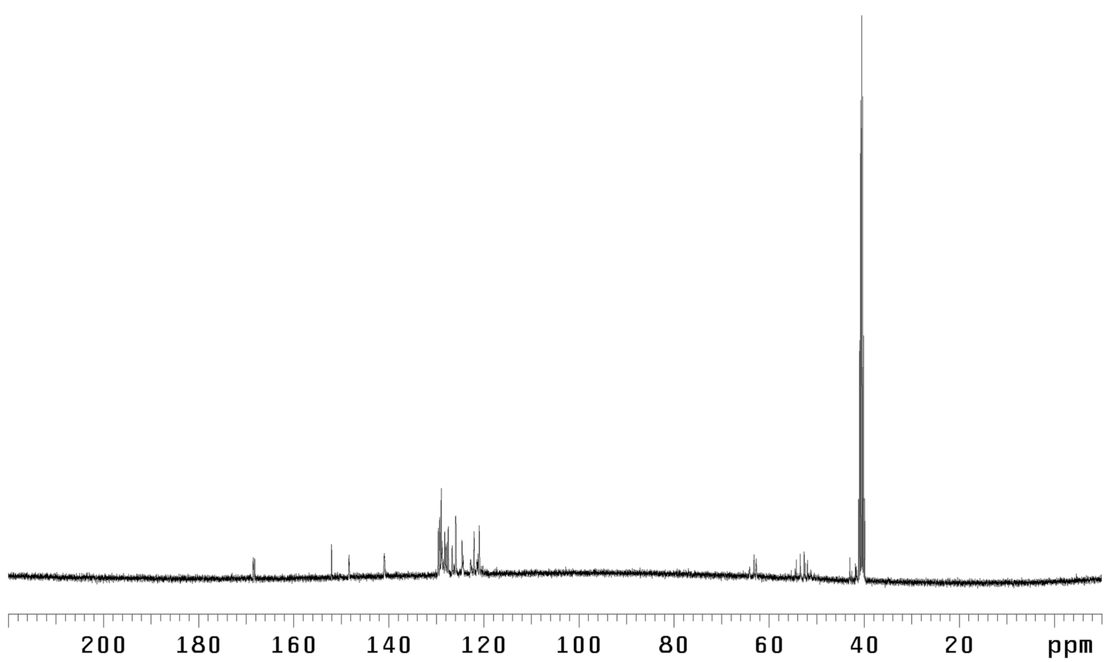
^{13}C NMR (126 MHz, $CDCl_3$) of compound **6g**.



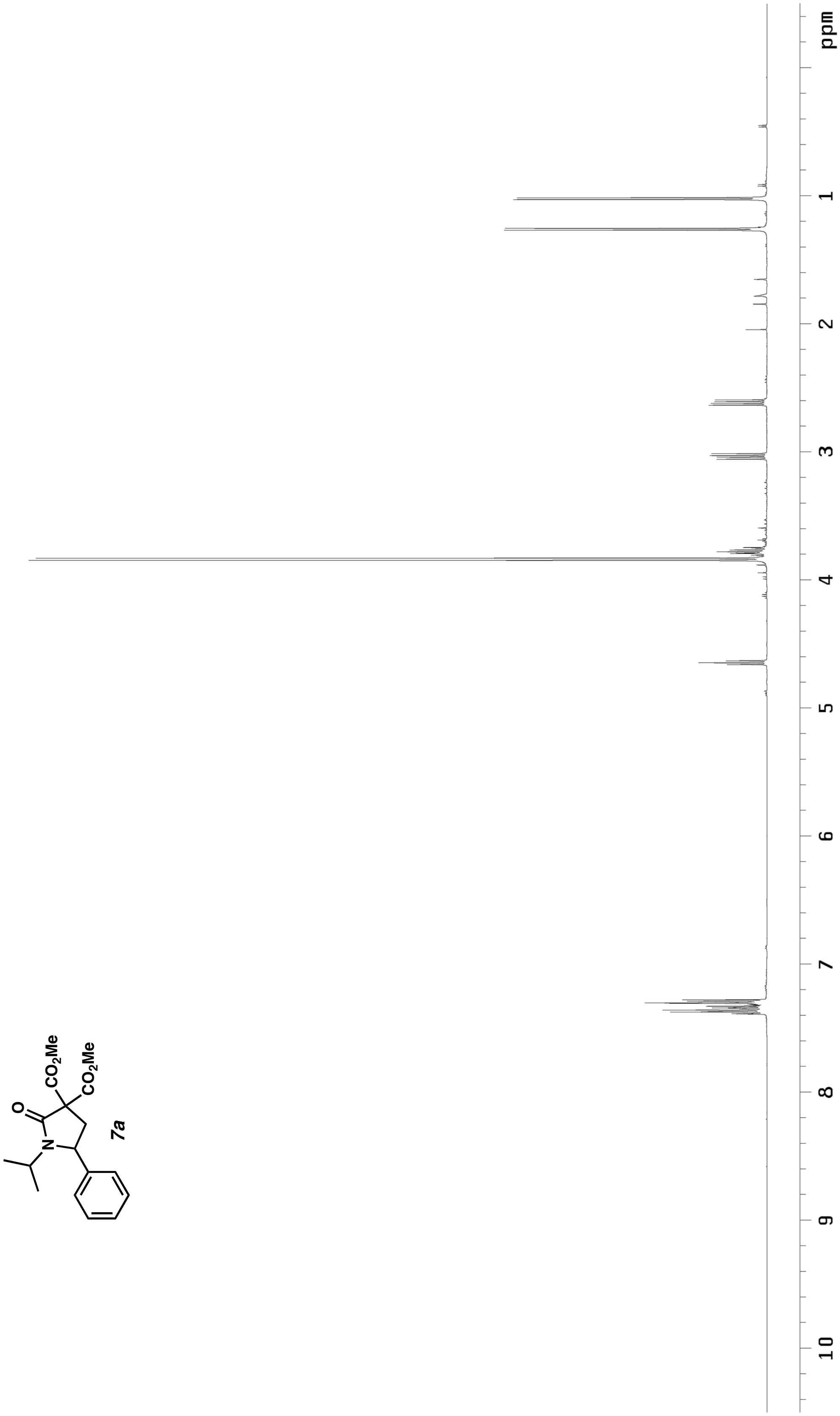
^{1}H NMR (400 MHz, DMSO-d6, 80 °C) of compound **6h**.



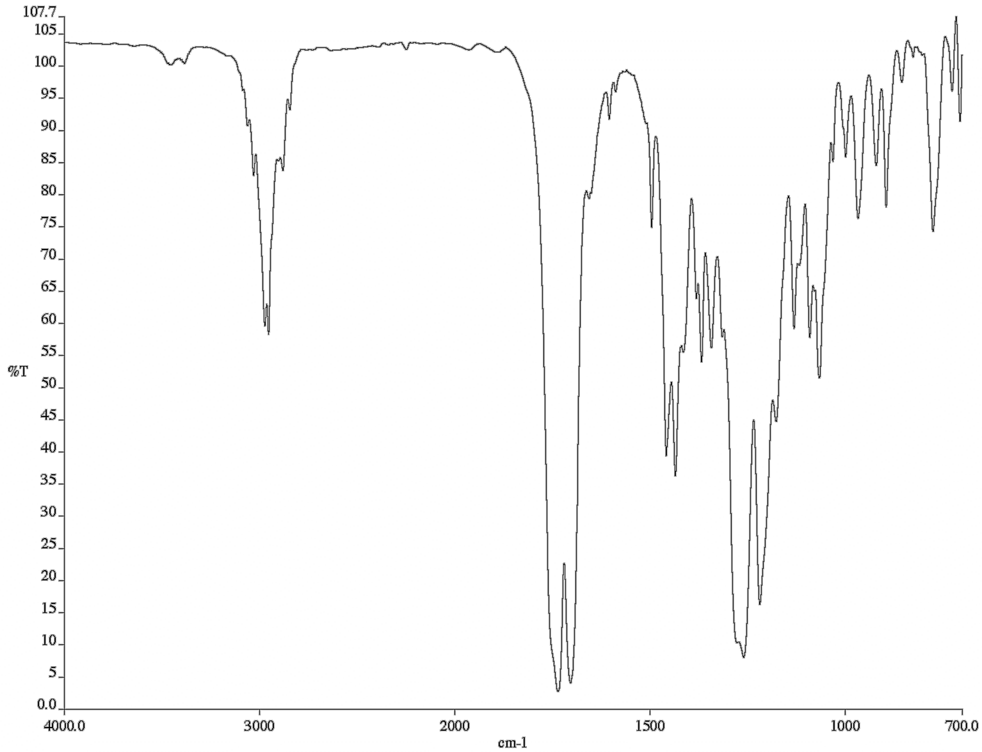
Infrared spectrum (thin film/NaCl) of compound **6h**.



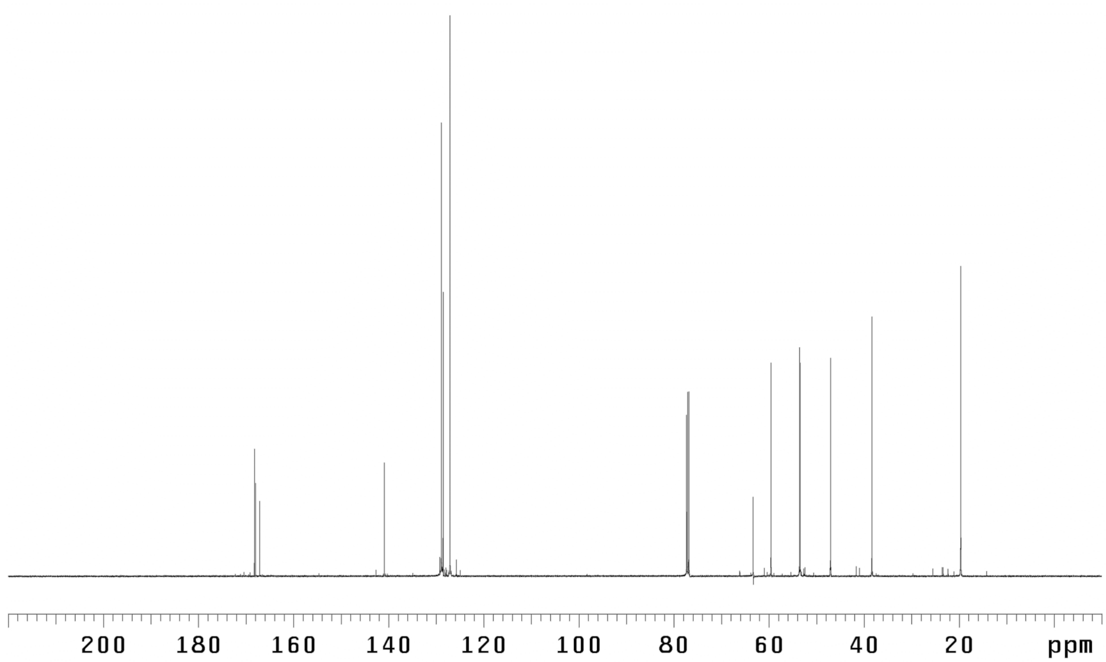
^{13}C NMR (101 MHz, DMSO-d6, 100 °C) of compound **6h**.



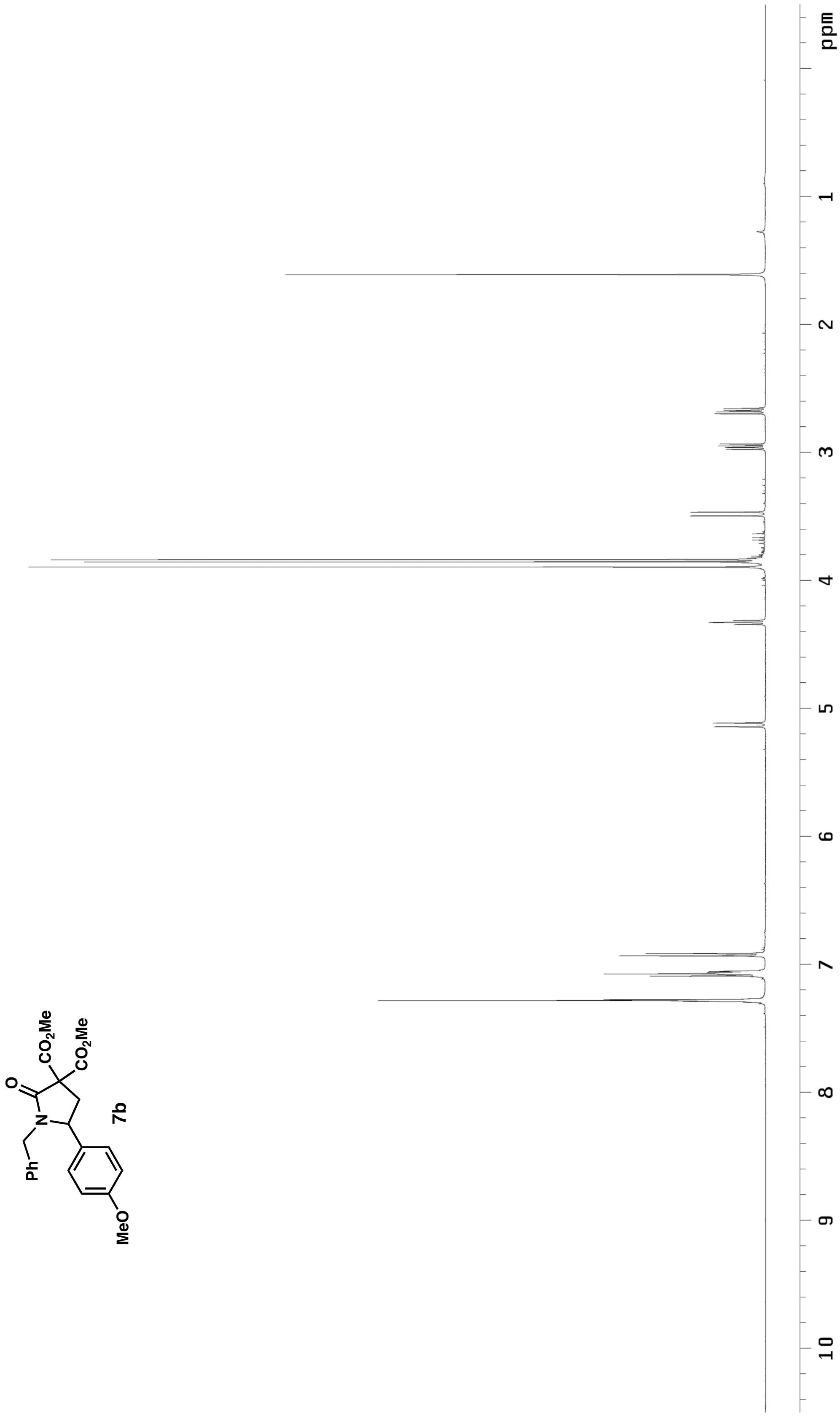
^{1}H NMR (500 MHz, CDCl3) of compound **7a**.



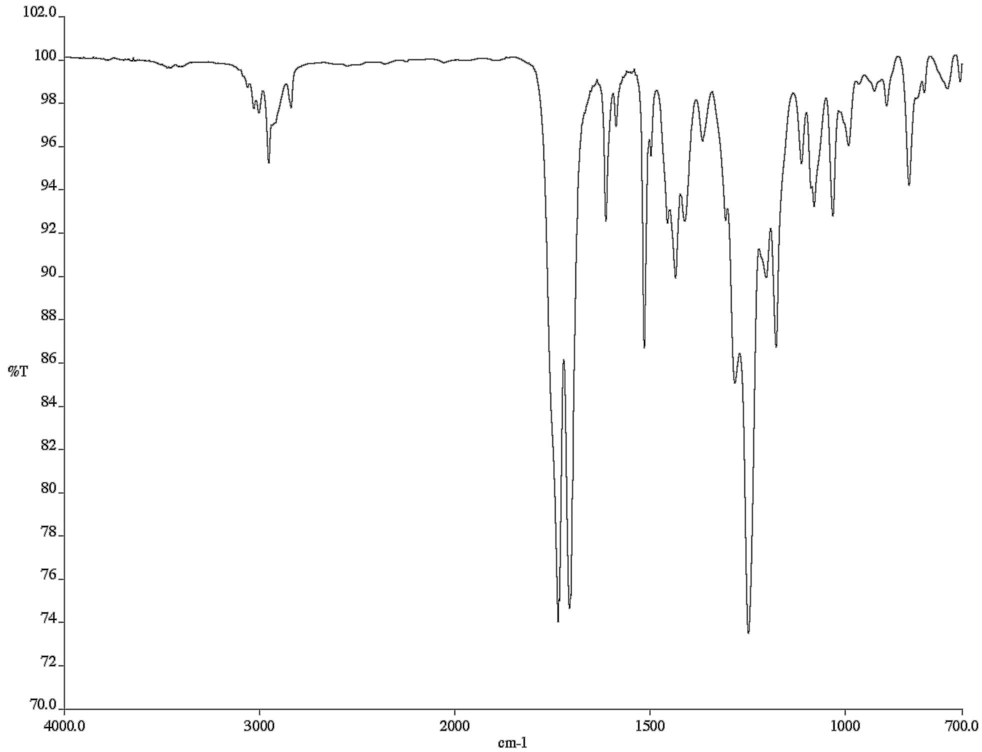
Infrared spectrum (thin film/NaCl) of compound **7a**.



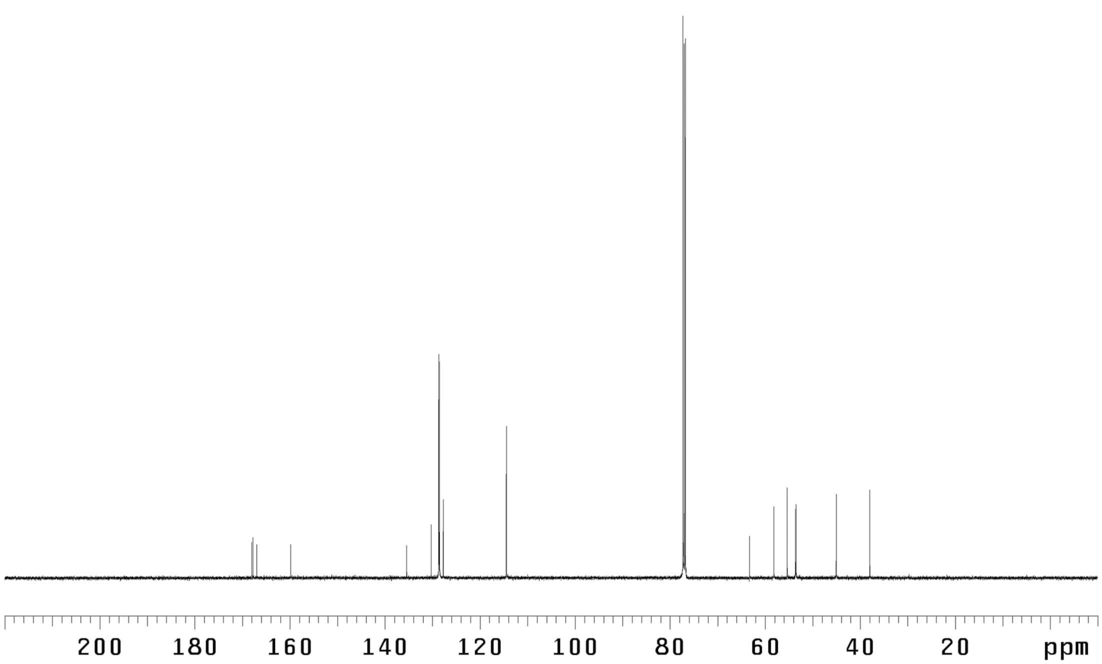
^{13}C NMR (126 MHz, $CDCl_3$) of compound **7a**.



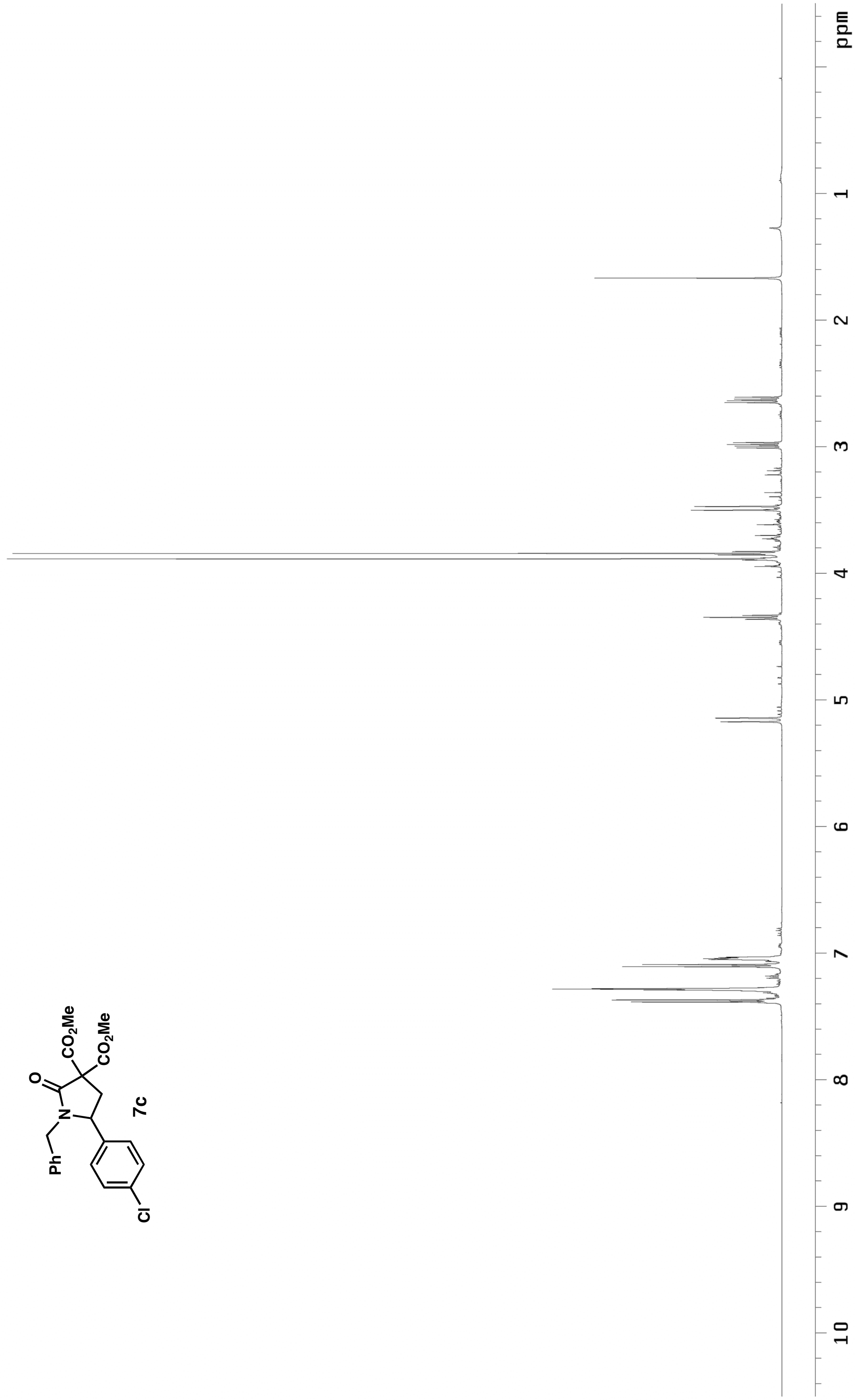
^{1}H NMR (500 MHz, $CDCl_3$) of compound **7b**.



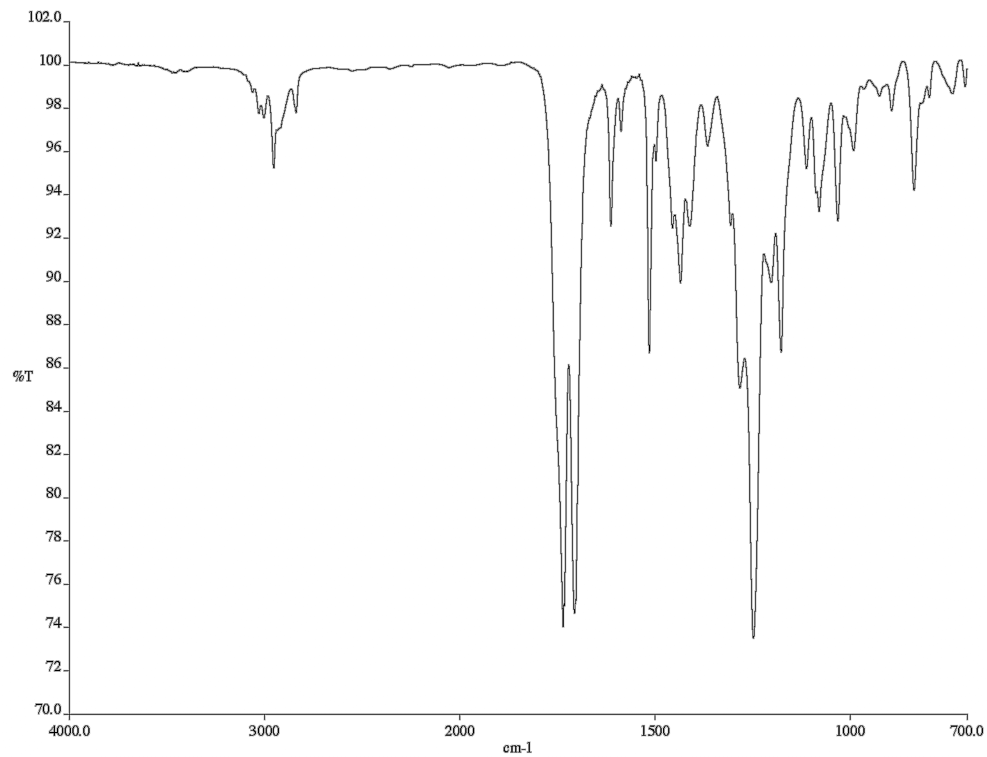
Infrared spectrum (thin film/NaCl) of compound **7b**.



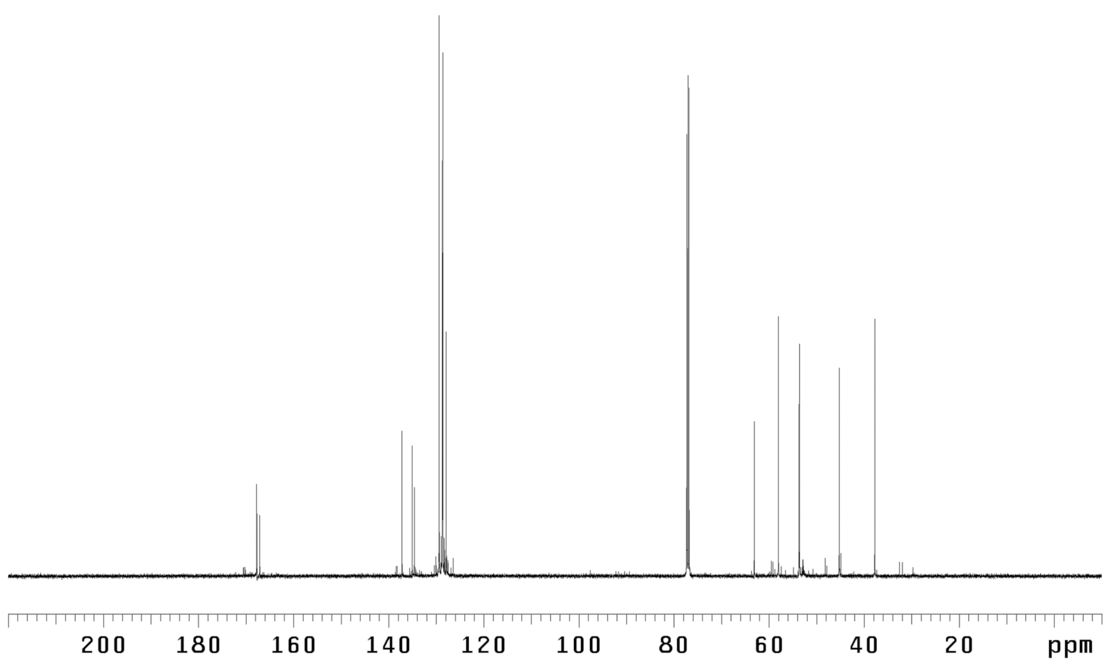
^{13}C NMR (126 MHz, $CDCl_3$) of compound **7b**.



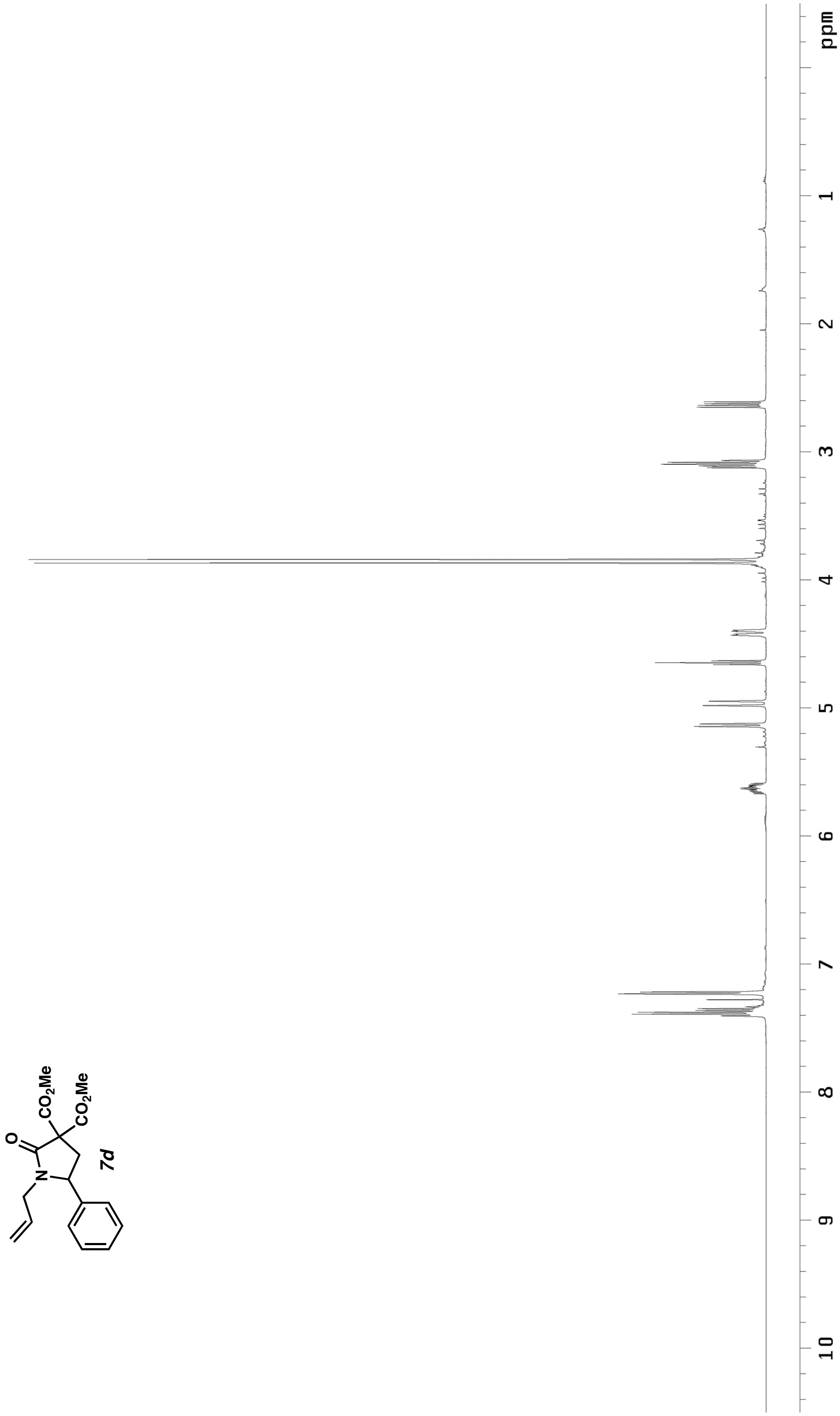
^{1}H NMR (500 MHz, $CDCl_3$) of compound **7c**.



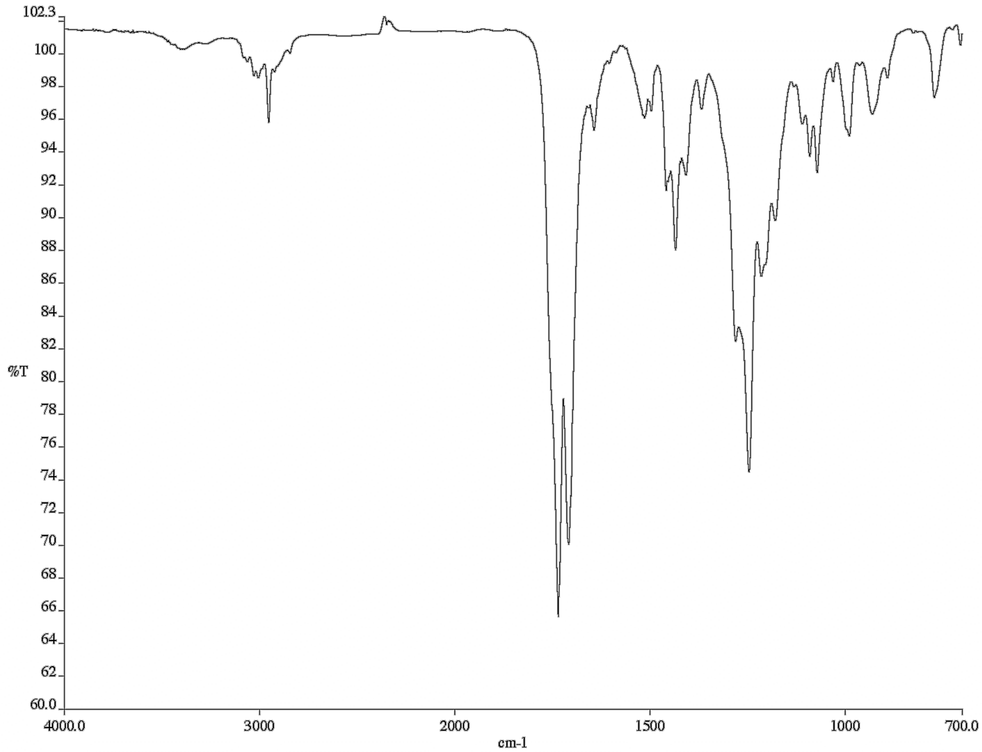
Infrared spectrum (thin film/NaCl) of compound **7c**.



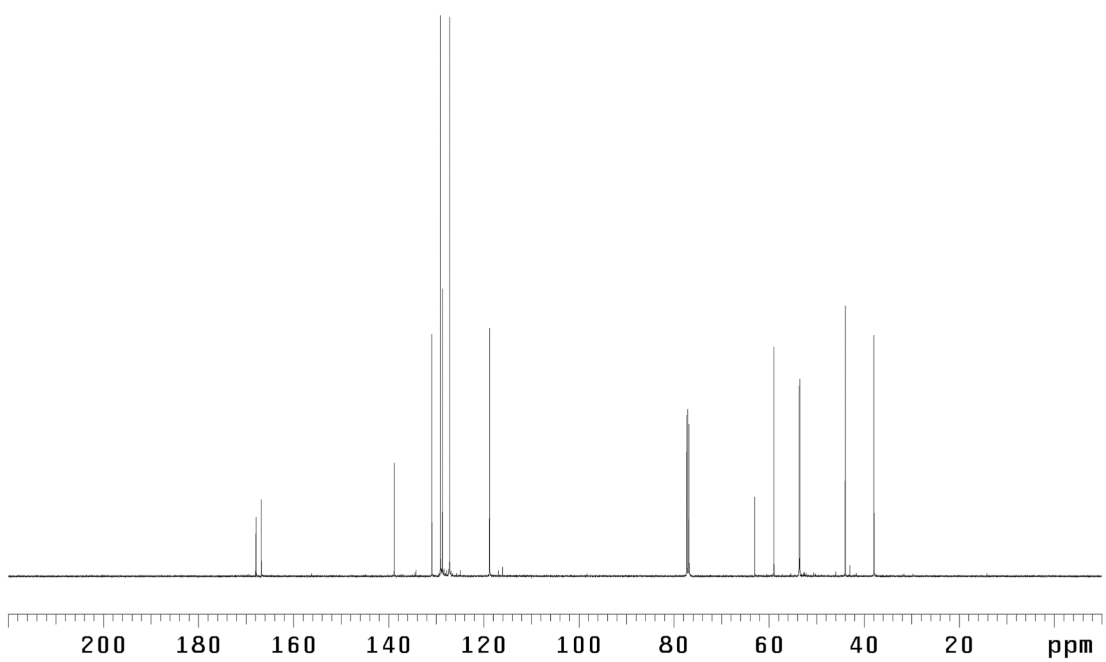
[13]C NMR (126 MHz, $CDCl_3$) of compound **7c**.



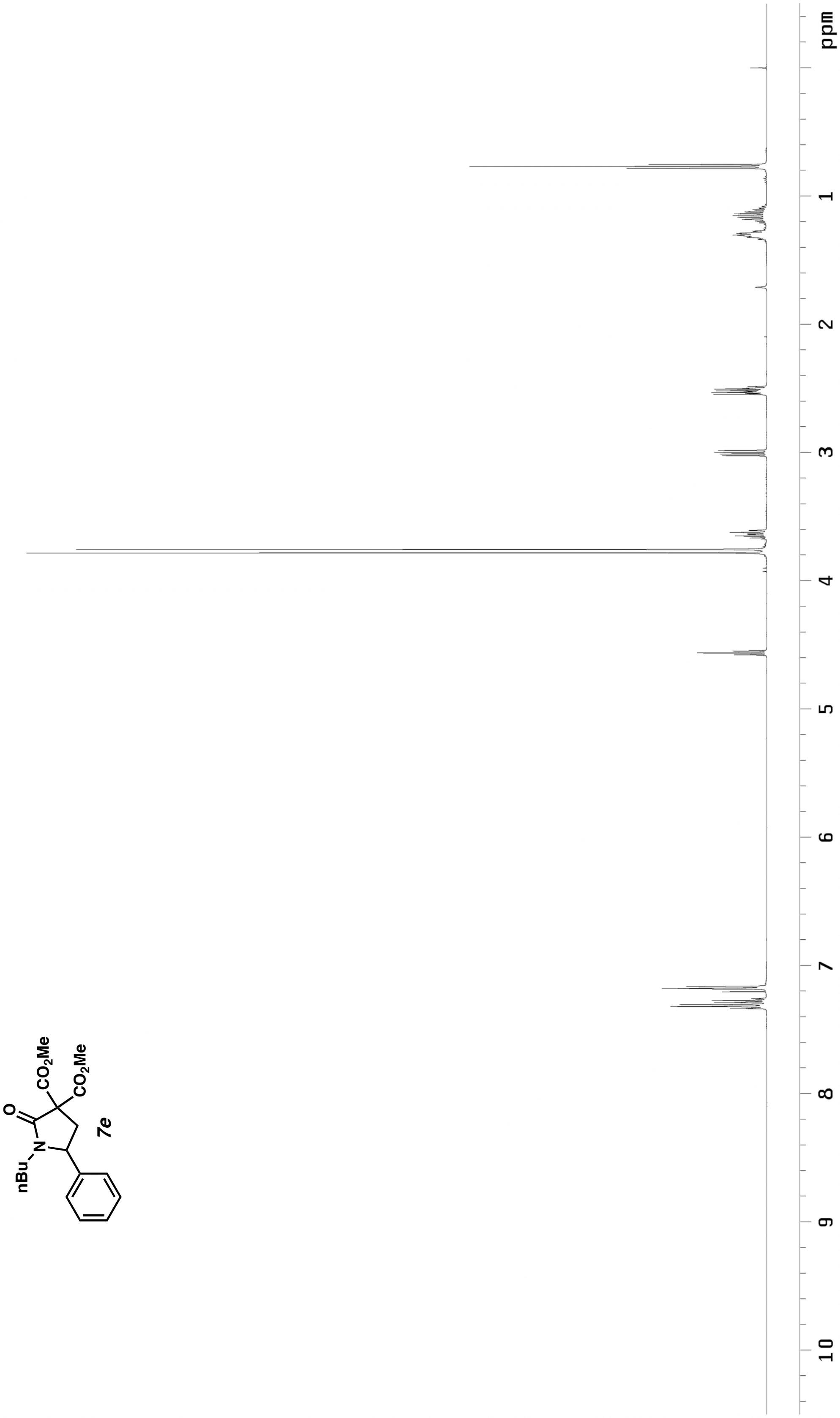
^1H NMR (500 MHz, $CDCl_3$) of compound **7d**.



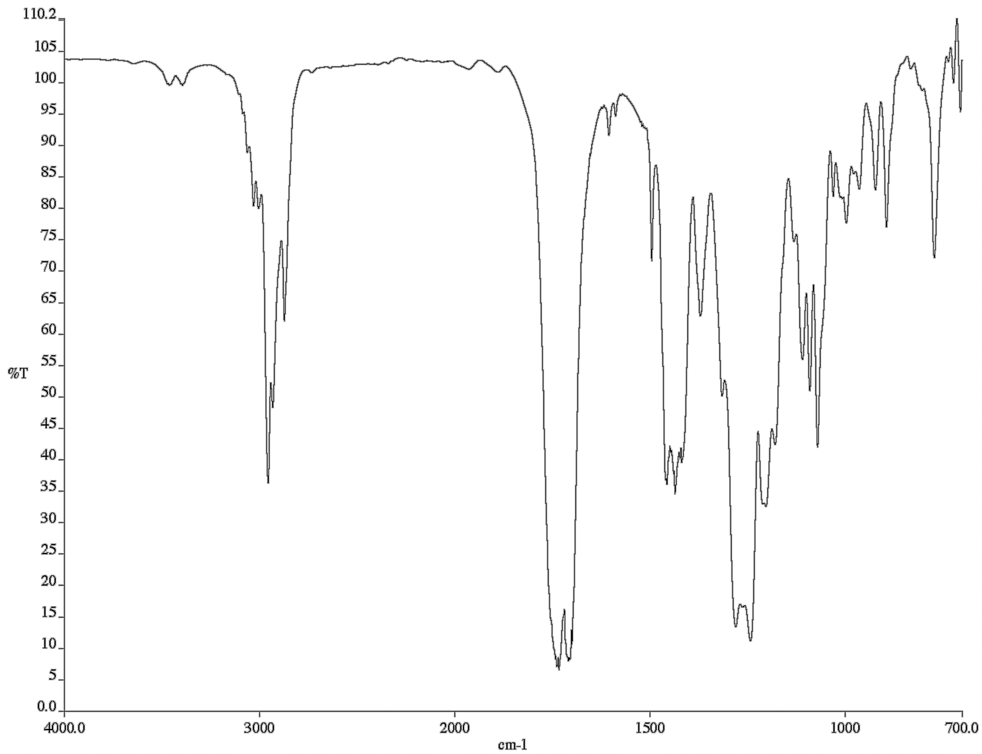
Infrared spectrum (thin film/NaCl) of compound **7d**.



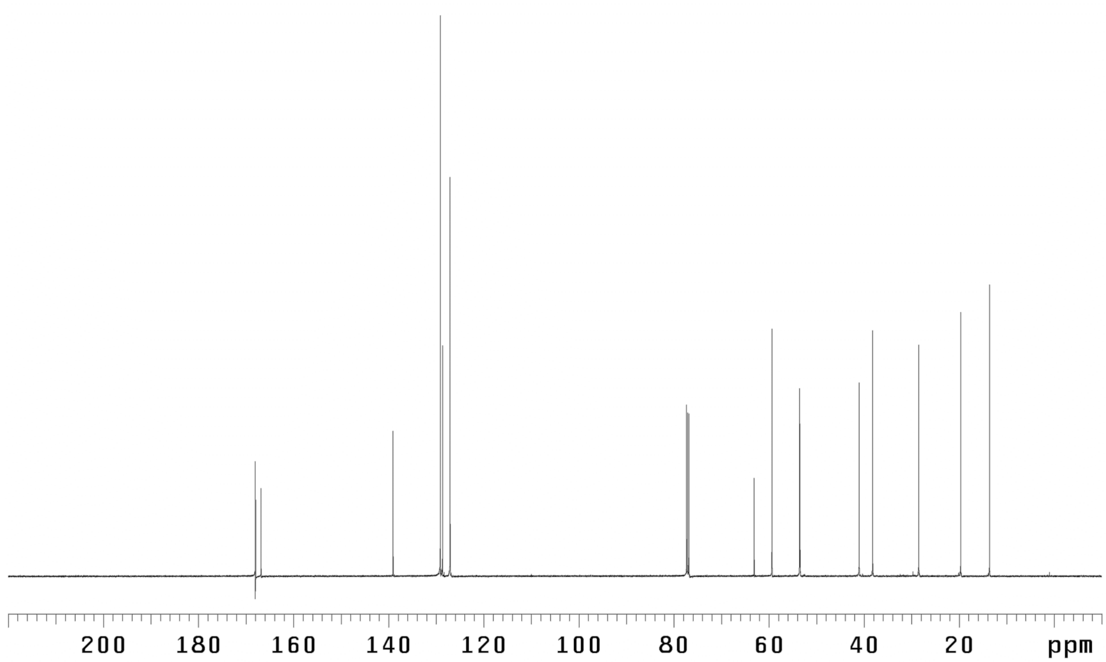
^{13}C NMR (126 MHz, $CDCl_3$) of compound **7d**.



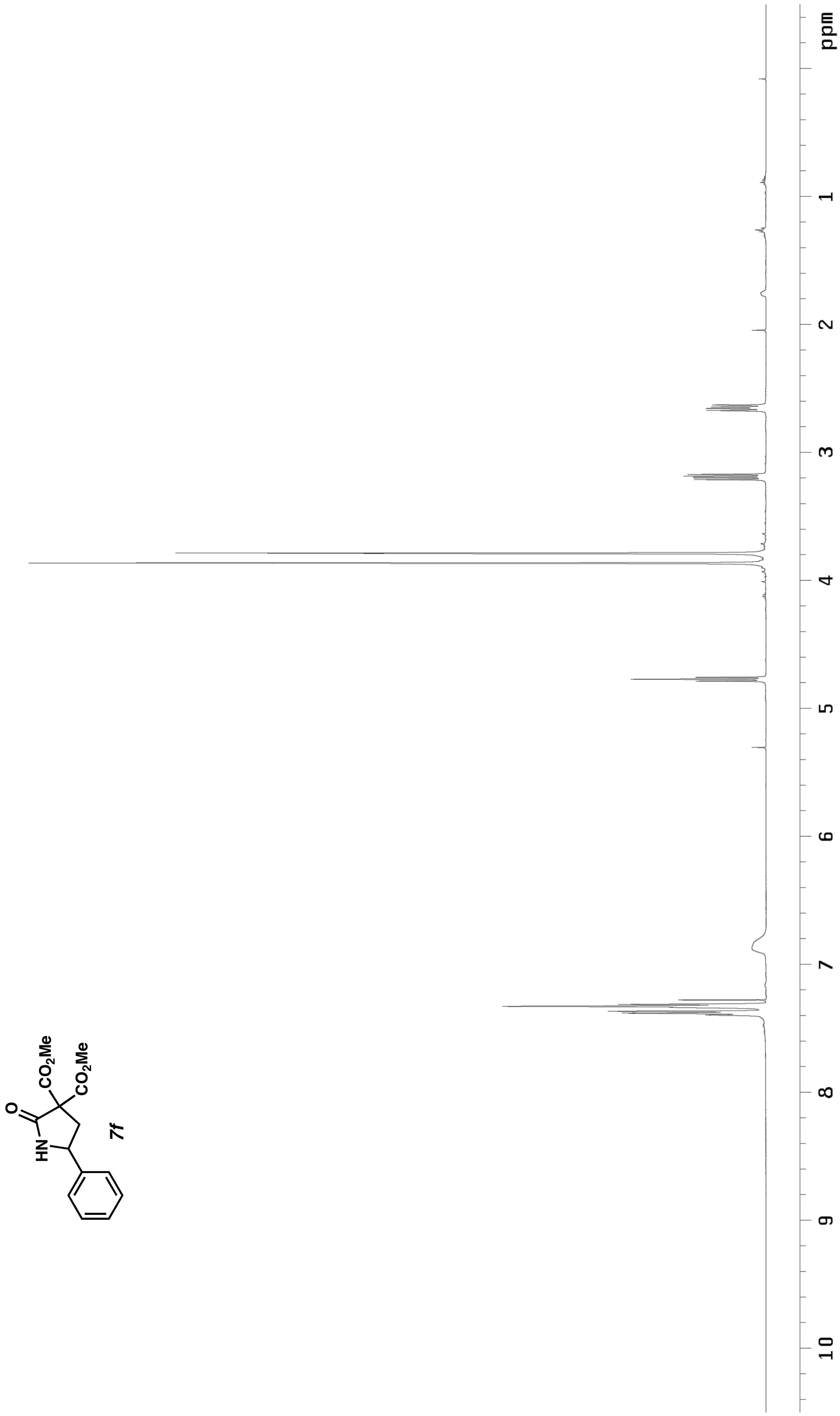
^{1}H NMR (500 MHz, $CDCl_3$) of compound **7e**.



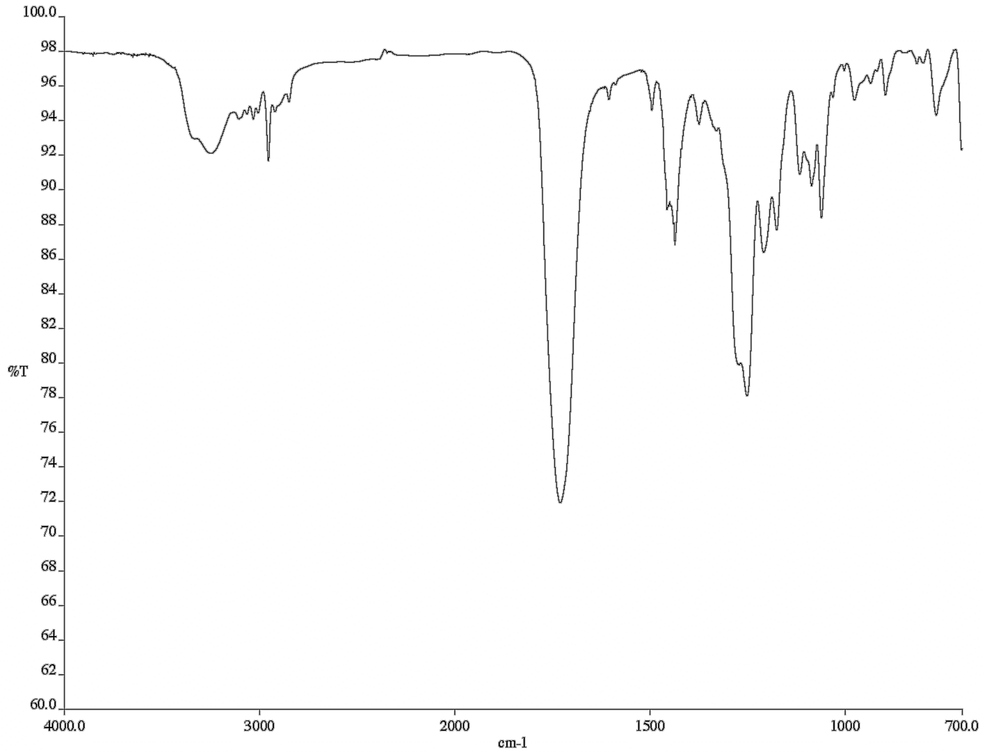
Infrared spectrum (thin film/NaCl) of compound **7e**.



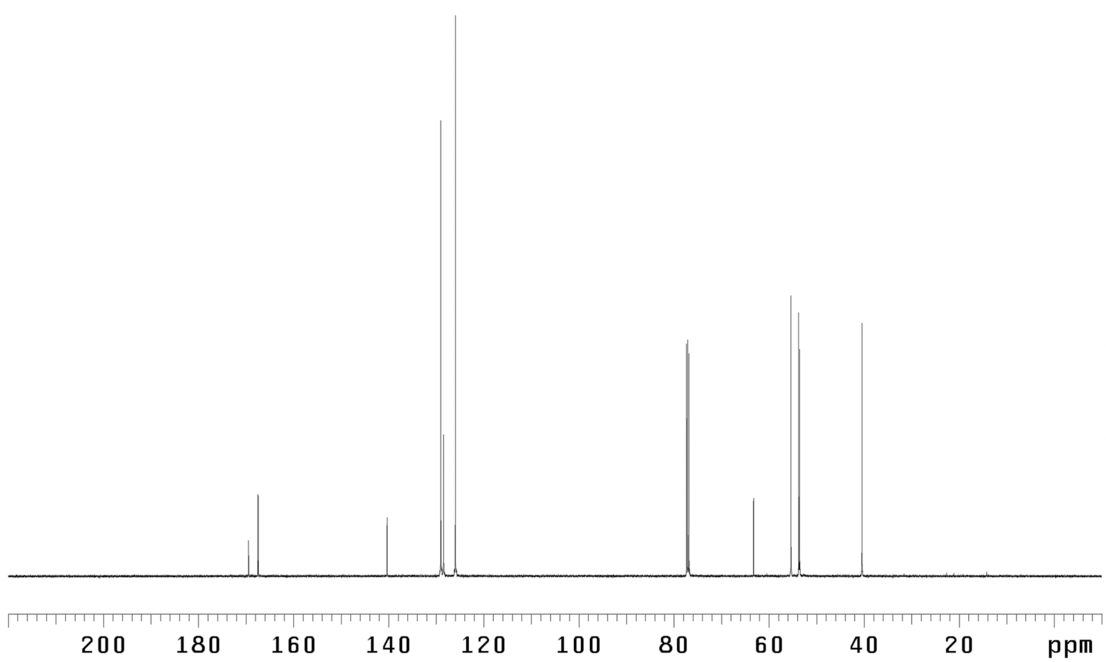
[13]C NMR (126 MHz, $CDCl_3$) of compound **7e**.



^1H NMR (500 MHz, $CDCl_3$) of compound **7f**.

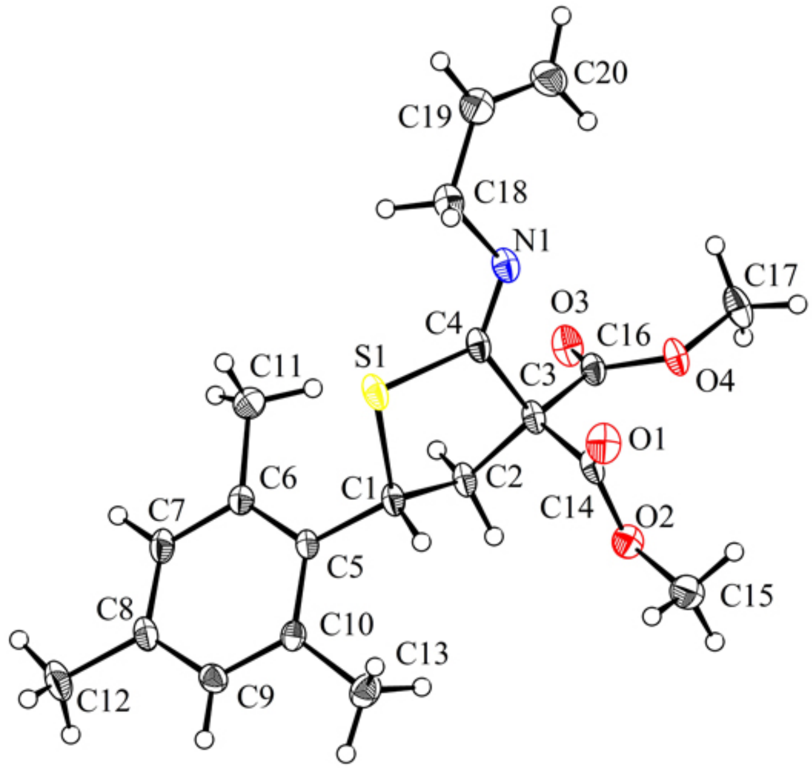


Infrared spectrum (thin film/NaCl) of compound **7f**.



^{13}C NMR (126 MHz, $CDCl_3$) of compound **7f**.

Table 1. Crystal Data and Structure Analysis Details for 2h.



Empirical formula	C20 H25 N O4 S
Formula weight	375.47
Crystallization solvent	Benzene/Heptane/Ethyl Acetate
Crystal shape	?
Crystal color	colourless
Crystal size	0.08 x 0.19 x 0.46 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker KAPPA APEX II	
Wavelength	0.71073 ≈ MO K	
Data collection temperature	100.15 K	
Theta range for 5787 reflections used in lattice determination	2.521 to 31.600∞	
Unit cell dimensions	a = 14.5982(10) ≈	α= 90∞

	b = 16.1620(12) ≈	β= 92.145(4)∞
	c = 8.2014(6) ≈	γ = 90∞
Volume	1933.7(2) ≈³	
Z	4	
Crystal system	monoclinic	
Space group	P 1 21/c 1 (# 14)	
Density (calculated)	1.290 g/cm³	
F(000)	800	
Theta range for data collection	1.4 to 37.4∞	
Completeness to theta = 25.00∞	100.0%	
Index ranges	-24 ≤ h ≤ 24, 0 ≤ k ≤ 27, 0 ≤ l ≤ 13	
Data collection scan type	narrow and scans	
Reflections collected	15085	
Independent reflections	15085 [R_{int}= 0.0000]	
Reflections > 2σ(I)	10418	
Average σ(I)/(net I)	0.0676	
Absorption coefficient	0.19 mm⁻¹	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9848 and 0.9170	
Reflections monitored for decay	0	
Decay of standards	0%	

Structure Solution and Refinement

Primary solution method	direct
Secondary solution method	difmap
Hydrogen placement	geom
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15085 / 0 / 241
Treatment of hydrogen atoms	constr
Goodness-of-fit on F^2	1.06
Final R indices [I>2σ(I), 10418 reflections]	R1 = 0.0592, wR2 = 0.1221
R indices (all data)	R1 = 0.1034, wR2 = 0.1431
Type of weighting scheme used	calc
Weighting scheme used	calc
w=1/[^2^(Fo^2^)+(0.0645P)^2^+0.3700P]	where P=(Fo^2^+2Fc^2^)/3
Max shift/error	0.001
Average shift/error	0.000

Largest diff. peak and hole	0.49 and -0.37 e∑≈$^{-3}$

	Programs Used
Cell refinement	SAINT V8.18C (Bruker-AXS, 2007)
Data collection	APEX2 2012.2-0 (Bruker-AXS, 2007)
Data reduction	SAINT V8.18C (Bruker-AXS, 2007)
Structure solution	SHELXS-97 (Sheldrick, 1990)
Structure refinement	SHELXL-97 (Sheldrick, 1997)
Graphics	DIAMOND 3 (Crystal Impact, 1999)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (≈^{2}x 10^3) for rac13. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
S(1)	7001(1)	6892(1)	2895(1)	22(1)
O(1)	8360(1)	6282(1)	6404(1)	27(1)
O(2)	7480(1)	5212(1)	7100(1)	22(1)
O(3)	7866(1)	4219(1)	2706(1)	26(1)
O(4)	8857(1)	4560(1)	4768(1)	22(1)
N(1)	8660(1)	6157(1)	2476(1)	20(1)
C(1)	6183(1)	6259(1)	4018(2)	18(1)
C(2)	6567(1)	5375(1)	4014(2)	18(1)
C(3)	7607(1)	5456(1)	4275(2)	17(1)
C(4)	7894(1)	6152(1)	3131(2)	18(1)
C(5)	5192(1)	6358(1)	3430(1)	15(1)
C(6)	4890(1)	6274(1)	1789(1)	18(1)
C(7)	3969(1)	6418(1)	1363(2)	20(1)
C(8)	3336(1)	6643(1)	2493(2)	20(1)
C(9)	3634(1)	6687(1)	4121(2)	19(1)
C(10)	4541(1)	6543(1)	4608(1)	17(1)
C(11)	5514(1)	6056(1)	420(2)	26(1)
C(12)	2354(1)	6831(1)	1995(2)	29(1)
C(13)	4795(1)	6554(1)	6414(1)	24(1)
C(14)	7874(1)	5710(1)	6034(2)	18(1)
C(15)	7719(1)	5383(1)	8800(2)	26(1)
C(16)	8111(1)	4667(1)	3805(2)	18(1)
C(17)	9433(1)	3862(1)	4390(2)	29(1)
C(18)	8876(1)	6851(1)	1424(2)	23(1)
C(19)	9690(1)	6694(1)	428(2)	27(1)
C(20)	10218(1)	6036(1)	521(2)	31(1)

Table 3. Bond lengths [≈] and angles [∞] for rac13.

S(1)-C(1)	1.8457(13)
S(1)-C(4)	1.7750(12)
O(1)-C(14)	1.1975(14)
O(2)-C(14)	1.3343(15)
O(2)-C(15)	1.4511(15)
O(3)-C(16)	1.1997(14)
O(4)-C(16)	1.3320(15)
O(4)-C(17)	1.4486(16)
N(1)-C(4)	1.2587(17)
N(1)-C(18)	1.4571(16)
C(1)-H(1)	1.0000
C(1)-C(2)	1.5343(16)
C(1)-C(5)	1.5167(17)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(2)-C(3)	1.5308(17)
C(3)-C(4)	1.5333(17)
C(3)-C(14)	1.5361(17)
C(3)-C(16)	1.5297(16)
C(5)-C(6)	1.4066(16)
C(5)-C(10)	1.4121(18)
C(6)-C(7)	1.3959(18)
C(6)-C(11)	1.5136(19)
C(7)-H(7)	0.9500
C(7)-C(8)	1.3812(19)
C(8)-C(9)	1.3904(17)
C(8)-C(12)	1.5075(18)
C(9)-H(9)	0.9500
C(9)-C(10)	1.3892(17)
C(10)-C(13)	1.5126(16)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
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
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800

C(15)-H(15C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(18)-C(19)	1.489(2)
C(19)-H(19)	0.9500
C(19)-C(20)	1.313(2)
C(20)-H(20A)	0.9500
C(20)-H(20B)	0.9500

C(4)-S(1)-C(1)	93.31(6)
C(14)-O(2)-C(15)	114.91(10)
C(16)-O(4)-C(17)	116.24(10)
C(4)-N(1)-C(18)	118.20(11)
S(1)-C(1)-H(1)	106.7
C(2)-C(1)-S(1)	105.80(9)
C(2)-C(1)-H(1)	106.7
C(5)-C(1)-S(1)	114.20(8)
C(5)-C(1)-H(1)	106.7
C(5)-C(1)-C(2)	116.22(10)
C(1)-C(2)-H(2A)	110.5
C(1)-C(2)-H(2B)	110.5
H(2A)-C(2)-H(2B)	108.7
C(3)-C(2)-C(1)	106.28(9)
C(3)-C(2)-H(2A)	110.5
C(3)-C(2)-H(2B)	110.5
C(2)-C(3)-C(4)	105.66(9)
C(2)-C(3)-C(14)	111.69(10)
C(4)-C(3)-C(14)	108.25(9)
C(16)-C(3)-C(2)	112.20(10)
C(16)-C(3)-C(4)	108.18(10)
C(16)-C(3)-C(14)	110.60(9)
N(1)-C(4)-S(1)	127.60(9)
N(1)-C(4)-C(3)	122.25(10)
C(3)-C(4)-S(1)	110.15(9)
C(6)-C(5)-C(1)	123.69(11)
C(6)-C(5)-C(10)	118.76(11)
C(10)-C(5)-C(1)	117.55(10)
C(5)-C(6)-C(11)	123.86(11)
C(7)-C(6)-C(5)	119.14(11)
C(7)-C(6)-C(11)	116.99(11)

C(6)-C(7)-H(7)	118.7
C(8)-C(7)-C(6)	122.59(11)
C(8)-C(7)-H(7)	118.7
C(7)-C(8)-C(9)	117.69(11)
C(7)-C(8)-C(12)	121.68(12)
C(9)-C(8)-C(12)	120.63(12)
C(8)-C(9)-H(9)	119.1
C(10)-C(9)-C(8)	121.88(11)
C(10)-C(9)-H(9)	119.1
C(5)-C(10)-C(13)	121.74(11)
C(9)-C(10)-C(5)	119.79(11)
C(9)-C(10)-C(13)	118.41(11)
C(6)-C(11)-H(11A)	109.5
C(6)-C(11)-H(11B)	109.5
C(6)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(8)-C(12)-H(12A)	109.5
C(8)-C(12)-H(12B)	109.5
C(8)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(10)-C(13)-H(13A)	109.5
C(10)-C(13)-H(13B)	109.5
C(10)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
O(1)-C(14)-O(2)	124.42(11)
O(1)-C(14)-C(3)	124.85(12)
O(2)-C(14)-C(3)	110.72(10)
O(2)-C(15)-H(15A)	109.5
O(2)-C(15)-H(15B)	109.5
O(2)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
O(3)-C(16)-O(4)	125.53(11)
O(3)-C(16)-C(3)	124.03(11)
O(4)-C(16)-C(3)	110.43(10)
O(4)-C(17)-H(17A)	109.5

O(4)-C(17)-H(17B)	109.5
O(4)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
N(1)-C(18)-H(18A)	109.0
N(1)-C(18)-H(18B)	109.0
N(1)-C(18)-C(19)	112.84(11)
H(18A)-C(18)-H(18B)	107.8
C(19)-C(18)-H(18A)	109.0
C(19)-C(18)-H(18B)	109.0
C(18)-C(19)-H(19)	117.1
C(20)-C(19)-C(18)	125.79(13)
C(20)-C(19)-H(19)	117.1
C(19)-C(20)-H(20A)	120.0
C(19)-C(20)-H(20B)	120.0
H(20A)-C(20)-H(20B)	120.0

Symmetry transformations used to generate equivalent atoms:

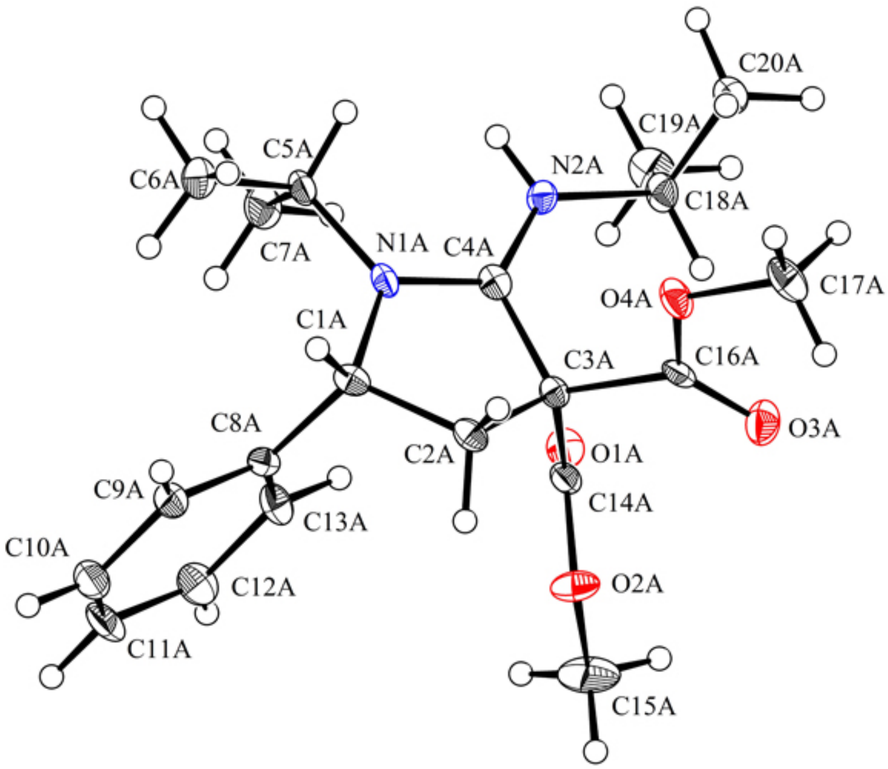
Table 4. Anisotropic displacement parameters (≈^{2}x 10^4) for rac13. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 $a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	146(1)	147(1)	372(2)	67(1)	-20(1)	19(1)
O(1)	275(6)	192(4)	326(5)	-16(4)	-66(4)	-65(4)
O(2)	204(5)	218(4)	232(4)	-6(3)	-28(3)	-45(3)
O(3)	261(5)	201(4)	313(5)	-57(4)	-71(4)	32(4)
O(4)	175(5)	176(4)	300(5)	-10(3)	-55(3)	60(3)
N(1)	170(5)	157(4)	275(5)	8(4)	-34(4)	-1(4)
C(1)	140(6)	152(5)	228(5)	21(4)	-52(4)	-1(4)
C(2)	142(6)	134(5)	259(6)	23(4)	-55(4)	-3(4)
C(3)	136(6)	125(5)	245(5)	10(4)	-47(4)	5(4)
C(4)	160(6)	127(5)	256(6)	6(4)	-50(5)	11(4)
C(5)	138(5)	139(5)	181(5)	20(4)	-28(4)	4(4)
C(6)	174(6)	184(5)	173(5)	13(4)	-19(4)	7(4)
C(7)	185(6)	211(6)	210(5)	35(4)	-70(5)	-12(5)
C(8)	145(6)	157(5)	286(6)	54(4)	-41(5)	-6(4)
C(9)	177(6)	168(5)	237(5)	19(4)	25(5)	20(4)
C(10)	192(6)	127(5)	180(5)	16(4)	-14(4)	13(4)
C(11)	258(7)	331(7)	186(5)	-2(5)	10(5)	35(6)
C(12)	152(6)	289(7)	436(8)	87(6)	-65(6)	12(5)
C(13)	311(8)	249(6)	171(5)	-12(5)	-13(5)	31(5)
C(14)	130(6)	132(5)	272(6)	0(4)	-39(4)	27(4)
C(15)	236(7)	302(7)	241(6)	-38(5)	-11(5)	-12(5)
C(16)	158(6)	137(5)	248(6)	31(4)	-22(5)	14(4)
C(17)	232(7)	237(7)	401(8)	-37(6)	-48(6)	116(5)
C(18)	207(7)	182(5)	301(6)	22(5)	-30(5)	-21(5)
C(19)	219(7)	292(7)	309(7)	32(5)	-34(5)	-87(5)
C(20)	211(7)	391(8)	323(7)	-5(6)	2(6)	-20(6)

Table 5. Hydrogen coordinates (x 10^3) and isotropic displacement parameters (≈^{2}x 10^3) for rac13.

	x	y	z	U_{iso}
H(1)	622	645	518	21
H(2A)	631	504	490	22
H(2B)	641	510	296	22
H(7)	377	636	25	24
H(9)	320	682	492	23
H(11A)	516	576	-44	39
H(11B)	601	570	84	39
H(11C)	578	656	-2	39
H(12A)	227	677	81	44
H(12B)	221	740	230	44
H(12C)	195	645	255	44
H(13A)	424	663	704	37
H(13B)	522	701	665	37
H(13C)	509	603	672	37
H(15A)	839	538	896	39
H(15B)	745	496	949	39
H(15C)	748	593	910	39
H(17A)	907	335	441	44
H(17B)	994	382	520	44
H(17C)	968	394	330	44
H(18A)	899	735	211	28
H(18B)	834	697	68	28
H(19)	984	711	-34	33
H(20A)	1009	561	128	37
H(20B)	1072	599	-17	37

Table 1. Crystal Data and Structure Analysis Details for (*R*)-6a•HBr.



Empirical formula	C20 H31 Br N2 O5
Formula weight	459.38
Crystallization solvent	diethyl ether / dichloromethane
Crystal shape	prism
Crystal color	colourless
Crystal size	0.17 x 0.18 x 0.47 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker KAPPA APEX II	
Wavelength	0.71073 ≈ MO K	
Data collection temperature	100.15 K	
Theta range for 9397 reflections used in lattice determination	2.620 to 31.334∞	
Unit cell dimensions	a = 8.0748(6) ≈ b = 15.1323(12) ≈	α= 98.815(5)∞ β= 92.189(5)∞

	c = 29.190(2) ≈	γ = 105.250(4)∞
Volume	3388.9(5) $≈^3$	
Z	6	
Crystal system	triclinic	
Space group	P 1 (# 1)	
Density (calculated)	1.351 g/cm^3	
F(000)	1440	
Theta range for data collection	1.7 to 35.3∞	
Completeness to theta = 25.00∞	99.7%	
Index ranges	-12 ≤ h ≤ 12, -24 ≤ k ≤ 24, -46 ≤ l ≤ 45	
Data collection scan type	narrow and scans	
Reflections collected	161414	
Independent reflections	54469 [R_{int}= 0.0430]	
Reflections > 2σ(I)	44420	
Average σ(I)/(net I)	0.0781	
Absorption coefficient	1.85 mm^{-1}	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.8047	
Reflections monitored for decay	0	
Decay of standards	0%	

Structure Solution and Refinement

Primary solution method	direct
Secondary solution method	difmap
Hydrogen placement	geom
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	54469 / 21 / 1585
Treatment of hydrogen atoms	mixed
Goodness-of-fit on F^2	1.65
Final R indices [I>2σ(I), 44420 reflections]	R1 = 0.0568, wR2 = 0.1138
R indices (all data)	R1 = 0.0743, wR2 = 0.1159
Type of weighting scheme used	calc
Weighting scheme used	calc w=1/[^2^(Fo^2^)+(0.0000P)^2^+0.0000P] where
P=(Fo^2^+2Fc^2^)/3	
Max shift/error	0.001
Average shift/error	0.000
Absolute structure parameter	0.029(3)

Largest diff. peak and hole	3.05 and -1.34 e∑≈$^{-3}$

	Programs Used
Cell refinement	SAINT V8.18C (Bruker-AXS, 2007)
Data collection	APEX2_2011.2-3 (Bruker-AXS, 2007)
Data reduction	SAINT V8.18C (Bruker-AXS, 2007)
Structure solution	SHELXS-97 (Sheldrick, 1990)
Structure refinement	
Graphics	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (≈^{2}x 10^3) for afg04. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
O(1A)	5205(3)	3297(1)	8553(1)	18(1)
O(2A)	8042(3)	3464(1)	8523(1)	23(1)
O(3A)	7013(3)	1830(2)	9013(1)	23(1)
O(4A)	6394(3)	573(1)	8452(1)	19(1)
N(1A)	4511(3)	1542(2)	7520(1)	13(1)
N(2A)	2967(3)	1288(2)	8164(1)	14(1)
C(1A)	6285(4)	1836(2)	7379(1)	14(1)
C(2A)	7391(4)	1877(2)	7827(1)	14(1)
C(3A)	6203(4)	1976(2)	8227(1)	12(1)
C(4A)	4428(4)	1573(2)	7975(1)	14(1)
C(5A)	2951(4)	1256(2)	7188(1)	16(1)
C(6A)	3358(5)	925(2)	6694(1)	24(1)
C(7A)	2076(4)	2039(2)	7207(1)	23(1)
C(8A)	6672(4)	2728(2)	7175(1)	15(1)
C(9A)	7542(4)	2761(2)	6775(1)	18(1)
C(10A)	8003(4)	3575(2)	6590(1)	21(1)
C(11A)	7600(4)	4364(2)	6807(1)	23(1)
C(12A)	6731(4)	4340(2)	7206(1)	22(1)
C(13A)	6259(4)	3527(2)	7390(1)	18(1)
C(14A)	6408(4)	2992(2)	8455(1)	14(1)
C(15A)	8393(5)	4430(2)	8746(1)	34(1)
C(16A)	6583(4)	1461(2)	8621(1)	14(1)
C(17A)	6827(5)	27(2)	8784(1)	25(1)
C(18A)	2705(4)	1332(2)	8666(1)	18(1)
C(19A)	1333(5)	1853(2)	8773(1)	26(1)
C(20A)	2143(4)	350(2)	8781(1)	23(1)
O(1B)	2761(3)	3136(1)	5141(1)	17(1)
O(2B)	5580(3)	3478(1)	5045(1)	21(1)
O(3B)	5020(3)	2039(1)	5691(1)	20(1)
O(4B)	4388(3)	642(1)	5224(1)	15(1)
N(1B)	2497(3)	1144(2)	4168(1)	13(1)

N(2B)	861(3)	1029(2)	4810(1)	13(1)
C(1B)	4227(4)	1579(2)	4036(1)	12(1)
C(2B)	5323(4)	1771(2)	4507(1)	14(1)
C(3B)	4061(4)	1890(2)	4879(1)	11(1)
C(4B)	2345(4)	1315(2)	4624(1)	10(1)
C(5B)	1134(4)	495(2)	3828(1)	16(1)
C(6B)	1108(6)	-489(2)	3872(1)	34(1)
C(7B)	1377(5)	664(2)	3331(1)	25(1)
C(8B)	4279(4)	2426(2)	3819(1)	16(1)
C(9B)	5329(4)	2597(2)	3455(1)	20(1)
C(10B)	5427(5)	3384(2)	3252(1)	27(1)
C(11B)	4507(5)	4012(2)	3411(1)	27(1)
C(12B)	3444(5)	3838(2)	3769(1)	29(1)
C(13B)	3321(4)	3048(2)	3970(1)	21(1)
C(14B)	4016(4)	2910(2)	5039(1)	14(1)
C(15B)	5731(5)	4454(2)	5218(1)	35(1)
C(16B)	4545(4)	1538(2)	5321(1)	11(1)
C(17B)	4834(4)	217(2)	5610(1)	19(1)
C(18B)	562(4)	1128(2)	5308(1)	16(1)
C(19B)	-769(4)	1662(2)	5395(1)	24(1)
C(20B)	24(5)	159(2)	5438(1)	23(1)
O(1C)	7414(3)	3248(1)	1843(1)	18(1)
O(2C)	10170(3)	3462(1)	1676(1)	20(1)
O(3C)	9486(3)	1908(1)	2270(1)	18(1)
O(4C)	8375(3)	559(1)	1779(1)	17(1)
N(1C)	6577(3)	1420(2)	803(1)	12(1)
N(2C)	5107(3)	1248(2)	1469(1)	14(1)
C(1C)	8322(4)	1713(2)	645(1)	14(1)
C(2C)	9463(4)	1764(2)	1090(1)	14(1)
C(3C)	8351(4)	1926(2)	1498(1)	12(1)
C(4C)	6541(4)	1503(2)	1260(1)	12(1)
C(5C)	4995(4)	1095(2)	474(1)	16(1)
C(6C)	5401(5)	735(2)	-8(1)	25(1)
C(7C)	4090(4)	1873(2)	480(1)	23(1)
C(8C)	8674(4)	2610(2)	448(1)	14(1)
C(9C)	9607(4)	2662(2)	57(1)	17(1)
C(10C)	10051(4)	3492(2)	-124(1)	22(1)
C(11C)	9592(4)	4260(2)	85(1)	21(1)
C(12C)	8658(4)	4211(2)	475(1)	19(1)
C(13C)	8190(4)	3389(2)	650(1)	17(1)
C(14C)	8566(4)	2959(2)	1696(1)	15(1)
C(15C)	10528(5)	4459(2)	1838(1)	28(1)
C(16C)	8817(4)	1481(2)	1902(1)	13(1)
C(17C)	8809(5)	56(2)	2138(1)	24(1)
C(18C)	4905(4)	1339(2)	1975(1)	15(1)
C(19C)	3653(5)	1915(2)	2094(1)	24(1)
C(20C)	4316(4)	374(2)	2103(1)	20(1)
O(1D)	1240(3)	5108(1)	6240(1)	20(1)
O(2D)	3700(3)	4743(1)	6402(1)	20(1)
O(3D)	4660(3)	6149(1)	5724(1)	18(1)
O(4D)	5282(3)	7583(1)	6158(1)	16(1)
N(1D)	3160(3)	7177(2)	7194(1)	15(1)
N(2D)	1547(3)	7222(2)	6524(1)	14(1)
C(1D)	4426(4)	6735(2)	7354(1)	16(1)

C(2D)	5261(4)	6488(2)	6909(1)	15(1)
C(3D)	3823(4)	6343(2)	6516(1)	13(1)
C(4D)	2718(4)	6949(2)	6737(1)	12(1)
C(5D)	2529(5)	7876(2)	7495(1)	21(1)
C(6D)	3492(7)	8846(2)	7419(1)	44(1)
C(7D)	2737(6)	7782(3)	8001(1)	40(1)
C(8D)	3631(4)	5924(2)	7600(1)	16(1)
C(9D)	4577(4)	5780(2)	7978(1)	19(1)
C(10D)	3931(5)	5037(2)	8204(1)	24(1)
C(11D)	2319(5)	4419(2)	8048(1)	24(1)
C(12D)	1365(4)	4564(2)	7676(1)	24(1)
C(13D)	2023(4)	5321(2)	7453(1)	19(1)
C(14D)	2742(4)	5328(2)	6366(1)	14(1)
C(15D)	2805(5)	3759(2)	6283(1)	26(1)
C(16D)	4603(4)	6663(2)	6069(1)	18(1)
C(17D)	6055(4)	7985(2)	5766(1)	20(1)
C(18D)	1059(4)	7056(2)	6019(1)	16(1)
C(19D)	-850(4)	6519(2)	5928(1)	22(1)
C(20D)	1460(5)	7990(2)	5849(1)	23(1)
O(1E)	8189(3)	5002(1)	2884(1)	17(1)
O(2E)	10789(3)	4812(1)	3084(1)	20(1)
O(3E)	11510(3)	6349(1)	2459(1)	19(1)
O(4E)	11784(3)	7706(1)	2936(1)	16(1)
N(1E)	9306(3)	6863(2)	3901(1)	14(1)
N(2E)	7912(3)	7004(2)	3214(1)	13(1)
C(1E)	10840(4)	6612(2)	4078(1)	15(1)
C(2E)	11850(4)	6544(2)	3643(1)	16(1)
C(3E)	10485(4)	6346(2)	3224(1)	13(1)
C(4E)	9125(4)	6767(2)	3441(1)	12(1)
C(5E)	8093(4)	7202(2)	4207(1)	17(1)
C(6E)	8924(5)	7597(2)	4695(1)	24(1)
C(7E)	6434(4)	6429(2)	4205(1)	25(1)
C(8E)	10401(4)	5743(2)	4298(1)	14(1)
C(9E)	11448(4)	5716(2)	4684(1)	18(1)
C(10E)	11196(5)	4923(2)	4890(1)	24(1)
C(11E)	9887(4)	4130(2)	4696(1)	25(1)
C(12E)	8829(4)	4150(2)	4313(1)	22(1)
C(13E)	9087(4)	4951(2)	4113(1)	20(1)
C(14E)	9677(4)	5308(2)	3044(1)	13(1)
C(15E)	10098(5)	3806(2)	2945(1)	28(1)
C(16E)	11305(4)	6788(2)	2820(1)	13(1)
C(17E)	12685(5)	8211(2)	2588(1)	22(1)
C(18E)	7528(4)	6881(2)	2704(1)	14(1)
C(19E)	5668(4)	6298(2)	2585(1)	19(1)
C(20E)	7882(4)	7829(2)	2556(1)	20(1)
O(1F)	3235(3)	5134(1)	-412(1)	19(1)
O(2F)	5671(3)	4755(1)	-225(1)	18(1)
O(3F)	6672(3)	6143(1)	-899(1)	18(1)
O(4F)	7152(3)	7587(1)	-500(1)	16(1)
N(1F)	5150(3)	7135(2)	573(1)	13(1)
N(2F)	3519(3)	7236(2)	-81(1)	12(1)
C(1F)	6479(4)	6698(2)	719(1)	14(1)
C(2F)	7291(4)	6503(2)	261(1)	14(1)
C(3F)	5819(4)	6356(2)	-119(1)	12(1)

C(4F)	4727(4)	6948(2)	117(1)	12(1)
C(5F)	4508(5)	7803(2)	905(1)	21(1)
C(6F)	5459(6)	8792(2)	852(1)	36(1)
C(7F)	4692(5)	7654(2)	1401(1)	27(1)
C(8F)	5722(4)	5850(2)	939(1)	16(1)
C(9F)	6733(5)	5676(2)	1296(1)	21(1)
C(10F)	6146(5)	4885(2)	1498(1)	26(1)
C(11F)	4527(5)	4264(2)	1334(1)	32(1)
C(12F)	3517(5)	4448(2)	988(1)	30(1)
C(13F)	4112(4)	5250(2)	793(1)	22(1)
C(14F)	4735(4)	5344(2)	-269(1)	14(1)
C(15F)	4757(5)	3776(2)	-342(1)	23(1)
C(16F)	6572(4)	6673(2)	-552(1)	11(1)
C(17F)	7860(4)	7967(2)	-903(1)	20(1)
C(18F)	3033(4)	7127(2)	-582(1)	15(1)
C(19F)	1129(4)	6619(2)	-683(1)	21(1)
C(20F)	3407(5)	8094(2)	-714(1)	23(1)
Br(1A)	8079(1)	123(1)	6649(1)	21(1)
Br(1B)	6474(1)	134(1)	3290(1)	18(1)
Br(1C)	137(1)	-30(1)	-14(1)	21(1)
Br(1D)	8418(1)	8234(1)	7949(1)	23(1)
Br(1E)	4521(1)	8396(1)	4618(1)	20(1)
Br(1F)	358(1)	8210(1)	1391(1)	21(1)
O(5A)	9657(3)	349(1)	7734(1)	19(1)
O(5B)	7574(3)	112(2)	4381(1)	21(1)
O(5C)	1767(3)	255(2)	1077(1)	20(1)
O(5D)	9265(3)	8257(2)	6859(1)	25(1)
O(5E)	5655(3)	8046(1)	3544(1)	18(1)
O(5F)	1187(3)	8178(2)	296(1)	24(1)

Table 3. Bond lengths [≈] and angles [∞] for afg04.

O(1A)-C(14A)	1.207(4)
O(2A)-C(14A)	1.316(4)
O(2A)-C(15A)	1.456(3)
O(3A)-C(16A)	1.189(3)
O(4A)-C(16A)	1.326(3)
O(4A)-C(17A)	1.454(4)
N(1A)-C(1A)	1.479(4)
N(1A)-C(4A)	1.327(3)
N(1A)-C(5A)	1.483(4)
N(2A)-H(2A)	0.8800
N(2A)-C(4A)	1.319(4)
N(2A)-C(18A)	1.482(4)
C(1A)-H(1A)	1.0000
C(1A)-C(2A)	1.539(4)
C(1A)-C(8A)	1.521(4)
C(2A)-H(2AA)	0.9900
C(2A)-H(2AB)	0.9900
C(2A)-C(3A)	1.555(4)
C(3A)-C(4A)	1.513(4)
C(3A)-C(14A)	1.541(4)
C(3A)-C(16A)	1.548(4)
C(5A)-H(5A)	1.0000
C(5A)-C(6A)	1.531(4)
C(5A)-C(7A)	1.527(4)
C(6A)-H(6AA)	0.9800
C(6A)-H(6AB)	0.9800
C(6A)-H(6AC)	0.9800
C(7A)-H(7AA)	0.9800
C(7A)-H(7AB)	0.9800
C(7A)-H(7AC)	0.9800
C(8A)-C(9A)	1.386(4)
C(8A)-C(13A)	1.401(4)
C(9A)-H(9A)	0.9500
C(9A)-C(10A)	1.388(4)
C(10A)-H(10A)	0.9500
C(10A)-C(11A)	1.386(5)
C(11A)-H(11A)	0.9500
C(11A)-C(12A)	1.382(4)
C(12A)-H(12A)	0.9500
C(12A)-C(13A)	1.385(4)
C(13A)-H(13A)	0.9500
C(15A)-H(15G)	0.9800
C(15A)-H(15H)	0.9800
C(15A)-H(15I)	0.9800
C(17A)-H(17G)	0.9800
C(17A)-H(17H)	0.9800
C(17A)-H(17I)	0.9800
C(18A)-H(18A)	1.0000
C(18A)-C(19A)	1.535(5)
C(18A)-C(20A)	1.529(4)
C(19A)-H(19G)	0.9800

C(19A)-H(19H)	0.9800
C(19A)-H(19I)	0.9800
C(20A)-H(20G)	0.9800
C(20A)-H(20H)	0.9800
C(20A)-H(20I)	0.9800
O(1B)-C(14B)	1.186(4)
O(2B)-C(14B)	1.325(3)
O(2B)-C(15B)	1.456(4)
O(3B)-C(16B)	1.204(3)
O(4B)-C(16B)	1.314(3)
O(4B)-C(17B)	1.458(3)
N(1B)-C(1B)	1.473(4)
N(1B)-C(4B)	1.332(3)
N(1B)-C(5B)	1.485(3)
N(2B)-H(2B)	0.8800
N(2B)-C(4B)	1.330(4)
N(2B)-C(18B)	1.473(3)
C(1B)-H(1B)	1.0000
C(1B)-C(2B)	1.552(4)
C(1B)-C(8B)	1.505(4)
C(2B)-H(2BA)	0.9900
C(2B)-H(2BB)	0.9900
C(2B)-C(3B)	1.540(4)
C(3B)-C(4B)	1.524(4)
C(3B)-C(14B)	1.552(4)
C(3B)-C(16B)	1.544(4)
C(5B)-H(5B)	1.0000
C(5B)-C(6B)	1.509(5)
C(5B)-C(7B)	1.523(4)
C(6B)-H(6BA)	0.9800
C(6B)-H(6BB)	0.9800
C(6B)-H(6BC)	0.9800
C(7B)-H(7BA)	0.9800
C(7B)-H(7BB)	0.9800
C(7B)-H(7BC)	0.9800
C(8B)-C(9B)	1.398(4)
C(8B)-C(13B)	1.401(4)
C(9B)-H(9B)	0.9500
C(9B)-C(10B)	1.395(4)
C(10B)-H(10B)	0.9500
C(10B)-C(11B)	1.391(5)
C(11B)-H(11B)	0.9500
C(11B)-C(12B)	1.391(5)
C(12B)-H(12B)	0.9500
C(12B)-C(13B)	1.393(4)
C(13B)-H(13B)	0.9500
C(15B)-H(15D)	0.9800
C(15B)-H(15E)	0.9800
C(15B)-H(15F)	0.9800
C(17B)-H(17D)	0.9800
C(17B)-H(17E)	0.9800
C(17B)-H(17F)	0.9800
C(18B)-H(18B)	1.0000
C(18B)-C(19B)	1.513(5)

C(18B)-C(20B)	1.527(4)
C(19B)-H(19D)	0.9800
C(19B)-H(19E)	0.9800
C(19B)-H(19F)	0.9800
C(20B)-H(20D)	0.9800
C(20B)-H(20E)	0.9800
C(20B)-H(20F)	0.9800
O(1C)-C(14C)	1.194(4)
O(2C)-C(14C)	1.327(4)
O(2C)-C(15C)	1.457(3)
O(3C)-C(16C)	1.192(3)
O(4C)-C(16C)	1.334(3)
O(4C)-C(17C)	1.470(4)
N(1C)-C(1C)	1.476(4)
N(1C)-C(4C)	1.322(3)
N(1C)-C(5C)	1.492(4)
N(2C)-H(2C)	0.8800
N(2C)-C(4C)	1.324(4)
N(2C)-C(18C)	1.481(3)
C(1C)-H(1C)	1.0000
C(1C)-C(2C)	1.544(4)
C(1C)-C(8C)	1.517(4)
C(2C)-H(2CA)	0.9900
C(2C)-H(2CB)	0.9900
C(2C)-C(3C)	1.546(4)
C(3C)-C(4C)	1.524(4)
C(3C)-C(14C)	1.544(4)
C(3C)-C(16C)	1.525(4)
C(5C)-H(5C)	1.0000
C(5C)-C(6C)	1.510(4)
C(5C)-C(7C)	1.539(4)
C(6C)-H(6CA)	0.9800
C(6C)-H(6CB)	0.9800
C(6C)-H(6CC)	0.9800
C(7C)-H(7CA)	0.9800
C(7C)-H(7CB)	0.9800
C(7C)-H(7CC)	0.9800
C(8C)-C(9C)	1.392(4)
C(8C)-C(13C)	1.391(4)
C(9C)-H(9C)	0.9500
C(9C)-C(10C)	1.403(4)
C(10C)-H(10C)	0.9500
C(10C)-C(11C)	1.373(5)
C(11C)-H(11C)	0.9500
C(11C)-C(12C)	1.390(4)
C(12C)-H(12C)	0.9500
C(12C)-C(13C)	1.383(4)
C(13C)-H(13C)	0.9500
C(15C)-H(15A)	0.9800
C(15C)-H(15B)	0.9800
C(15C)-H(15C)	0.9800
C(17C)-H(17A)	0.9800
C(17C)-H(17B)	0.9800
C(17C)-H(17C)	0.9800

C(18C)-H(18C)	1.0000
C(18C)-C(19C)	1.516(5)
C(18C)-C(20C)	1.522(4)
C(19C)-H(19A)	0.9800
C(19C)-H(19B)	0.9800
C(19C)-H(19C)	0.9800
C(20C)-H(20A)	0.9800
C(20C)-H(20B)	0.9800
C(20C)-H(20C)	0.9800
O(1D)-C(14D)	1.197(4)
O(2D)-C(14D)	1.333(4)
O(2D)-C(15D)	1.454(3)
O(3D)-C(16D)	1.184(4)
O(4D)-C(16D)	1.335(3)
O(4D)-C(17D)	1.462(3)
N(1D)-C(1D)	1.460(4)
N(1D)-C(4D)	1.335(3)
N(1D)-C(5D)	1.478(4)
N(2D)-H(2D)	0.8800
N(2D)-C(4D)	1.300(4)
N(2D)-C(18D)	1.477(4)
C(1D)-H(1D)	1.0000
C(1D)-C(2D)	1.529(4)
C(1D)-C(8D)	1.525(4)
C(2D)-H(2DA)	0.9900
C(2D)-H(2DB)	0.9900
C(2D)-C(3D)	1.549(4)
C(3D)-C(4D)	1.531(4)
C(3D)-C(14D)	1.541(4)
C(3D)-C(16D)	1.559(4)
C(5D)-H(5D)	1.0000
C(5D)-C(6D)	1.523(5)
C(5D)-C(7D)	1.514(4)
C(6D)-H(6DA)	0.9800
C(6D)-H(6DB)	0.9800
C(6D)-H(6DC)	0.9800
C(7D)-H(7DA)	0.9800
C(7D)-H(7DB)	0.9800
C(7D)-H(7DC)	0.9800
C(8D)-C(9D)	1.394(4)
C(8D)-C(13D)	1.384(4)
C(9D)-H(9D)	0.9500
C(9D)-C(10D)	1.385(4)
C(10D)-H(10D)	0.9500
C(10D)-C(11D)	1.400(5)
C(11D)-H(11D)	0.9500
C(11D)-C(12D)	1.384(5)
C(12D)-H(12D)	0.9500
C(12D)-C(13D)	1.397(4)
C(13D)-H(13D)	0.9500
C(15D)-H(15P)	0.9800
C(15D)-H(15Q)	0.9800
C(15D)-H(15R)	0.9800
C(17D)-H(17P)	0.9800

C(17D)-H(17Q)	0.9800
C(17D)-H(17R)	0.9800
C(18D)-H(18D)	1.0000
C(18D)-C(19D)	1.533(4)
C(18D)-C(20D)	1.527(4)
C(19D)-H(19P)	0.9800
C(19D)-H(19Q)	0.9800
C(19D)-H(19R)	0.9800
C(20D)-H(20P)	0.9800
C(20D)-H(20Q)	0.9800
C(20D)-H(20R)	0.9800
O(1E)-C(14E)	1.215(4)
O(2E)-C(14E)	1.325(4)
O(2E)-C(15E)	1.462(3)
O(3E)-C(16E)	1.200(3)
O(4E)-C(16E)	1.325(3)
O(4E)-C(17E)	1.465(3)
N(1E)-C(1E)	1.485(4)
N(1E)-C(4E)	1.327(3)
N(1E)-C(5E)	1.486(4)
N(2E)-H(2E)	0.8800
N(2E)-C(4E)	1.317(4)
N(2E)-C(18E)	1.481(4)
C(1E)-H(1E)	1.0000
C(1E)-C(2E)	1.541(4)
C(1E)-C(8E)	1.515(4)
C(2E)-H(2EA)	0.9900
C(2E)-H(2EB)	0.9900
C(2E)-C(3E)	1.553(4)
C(3E)-C(4E)	1.520(4)
C(3E)-C(14E)	1.533(4)
C(3E)-C(16E)	1.532(4)
C(5E)-H(5E)	1.0000
C(5E)-C(6E)	1.514(4)
C(5E)-C(7E)	1.528(4)
C(6E)-H(6EA)	0.9800
C(6E)-H(6EB)	0.9800
C(6E)-H(6EC)	0.9800
C(7E)-H(7EA)	0.9800
C(7E)-H(7EB)	0.9800
C(7E)-H(7EC)	0.9800
C(8E)-C(9E)	1.394(4)
C(8E)-C(13E)	1.394(4)
C(9E)-H(9E)	0.9500
C(9E)-C(10E)	1.396(4)
C(10E)-H(10E)	0.9500
C(10E)-C(11E)	1.398(5)
C(11E)-H(11E)	0.9500
C(11E)-C(12E)	1.390(5)
C(12E)-H(12E)	0.9500
C(12E)-C(13E)	1.396(4)
C(13E)-H(13E)	0.9500
C(15E)-H(15M)	0.9800
C(15E)-H(15N)	0.9800

C(15E)-H(15O)	0.9800
C(17E)-H(17M)	0.9800
C(17E)-H(17N)	0.9800
C(17E)-H(17O)	0.9800
C(18E)-H(18E)	1.0000
C(18E)-C(19E)	1.525(4)
C(18E)-C(20E)	1.520(4)
C(19E)-H(19M)	0.9800
C(19E)-H(19N)	0.9800
C(19E)-H(19O)	0.9800
C(20E)-H(20M)	0.9800
C(20E)-H(20N)	0.9800
C(20E)-H(20O)	0.9800
O(1F)-C(14F)	1.209(4)
O(2F)-C(14F)	1.328(4)
O(2F)-C(15F)	1.451(3)
O(3F)-C(16F)	1.212(3)
O(4F)-C(16F)	1.321(3)
O(4F)-C(17F)	1.459(3)
N(1F)-C(1F)	1.481(4)
N(1F)-C(4F)	1.329(3)
N(1F)-C(5F)	1.497(4)
N(2F)-H(2F)	0.8800
N(2F)-C(4F)	1.316(4)
N(2F)-C(18F)	1.473(3)
C(1F)-H(1F)	1.0000
C(1F)-C(2F)	1.533(4)
C(1F)-C(8F)	1.517(4)
C(2F)-H(2FA)	0.9900
C(2F)-H(2FB)	0.9900
C(2F)-C(3F)	1.542(4)
C(3F)-C(4F)	1.526(4)
C(3F)-C(14F)	1.537(4)
C(3F)-C(16F)	1.513(4)
C(5F)-H(5F)	1.0000
C(5F)-C(6F)	1.526(5)
C(5F)-C(7F)	1.506(4)
C(6F)-H(6FA)	0.9800
C(6F)-H(6FB)	0.9800
C(6F)-H(6FC)	0.9800
C(7F)-H(7FA)	0.9800
C(7F)-H(7FB)	0.9800
C(7F)-H(7FC)	0.9800
C(8F)-C(9F)	1.398(4)
C(8F)-C(13F)	1.383(4)
C(9F)-H(9F)	0.9500
C(9F)-C(10F)	1.394(4)
C(10F)-H(10F)	0.9500
C(10F)-C(11F)	1.410(5)
C(11F)-H(11F)	0.9500
C(11F)-C(12F)	1.381(6)
C(12F)-H(12F)	0.9500
C(12F)-C(13F)	1.397(4)
C(13F)-H(13F)	0.9500

C(15F)-H(15J)	0.9800
C(15F)-H(15K)	0.9800
C(15F)-H(15L)	0.9800
C(17F)-H(17J)	0.9800
C(17F)-H(17K)	0.9800
C(17F)-H(17L)	0.9800
C(18F)-H(18F)	1.0000
C(18F)-C(19F)	1.521(4)
C(18F)-C(20F)	1.527(4)
C(19F)-H(19J)	0.9800
C(19F)-H(19K)	0.9800
C(19F)-H(19L)	0.9800
C(20F)-H(20J)	0.9800
C(20F)-H(20K)	0.9800
C(20F)-H(20L)	0.9800
O(5A)-H(5AA)	0.846(17)
O(5A)-H(5AB)	0.830(17)
O(5B)-H(5BA)	0.863(17)
O(5B)-H(5BB)	0.845(17)
O(5C)-H(5CA)	0.882(17)
O(5C)-H(5CB)	0.850(17)
O(5D)-H(5DA)	0.874(18)
O(5D)-H(5DB)	0.895(17)
O(5E)-H(5EA)	0.857(17)
O(5E)-H(5EB)	0.891(17)
O(5F)-H(5FA)	0.866(19)
O(5F)-H(5FB)	0.896(18)

C(14A)-O(2A)-C(15A)	115.9(3)
C(16A)-O(4A)-C(17A)	115.2(2)
C(1A)-N(1A)-C(5A)	123.7(2)
C(4A)-N(1A)-C(1A)	113.8(2)
C(4A)-N(1A)-C(5A)	122.5(2)
C(4A)-N(2A)-H(2A)	116.3
C(4A)-N(2A)-C(18A)	127.4(3)
C(18A)-N(2A)-H(2A)	116.3
N(1A)-C(1A)-H(1A)	108.2
N(1A)-C(1A)-C(2A)	102.6(2)
N(1A)-C(1A)-C(8A)	113.9(2)
C(2A)-C(1A)-H(1A)	108.2
C(8A)-C(1A)-H(1A)	108.2
C(8A)-C(1A)-C(2A)	115.3(2)
C(1A)-C(2A)-H(2AA)	110.7
C(1A)-C(2A)-H(2AB)	110.7
C(1A)-C(2A)-C(3A)	105.2(2)
H(2AA)-C(2A)-H(2AB)	108.8
C(3A)-C(2A)-H(2AA)	110.7
C(3A)-C(2A)-H(2AB)	110.7
C(4A)-C(3A)-C(2A)	101.9(2)
C(4A)-C(3A)-C(14A)	109.6(2)
C(4A)-C(3A)-C(16A)	114.3(2)
C(14A)-C(3A)-C(2A)	113.6(2)
C(14A)-C(3A)-C(16A)	106.5(2)
C(16A)-C(3A)-C(2A)	111.1(2)

N(1A)-C(4A)-C(3A)	110.6(2)
N(2A)-C(4A)-N(1A)	122.7(3)
N(2A)-C(4A)-C(3A)	126.8(2)
N(1A)-C(5A)-H(5A)	107.5
N(1A)-C(5A)-C(6A)	111.8(3)
N(1A)-C(5A)-C(7A)	110.5(2)
C(6A)-C(5A)-H(5A)	107.5
C(7A)-C(5A)-H(5A)	107.5
C(7A)-C(5A)-C(6A)	111.9(3)
C(5A)-C(6A)-H(6AA)	109.5
C(5A)-C(6A)-H(6AB)	109.5
C(5A)-C(6A)-H(6AC)	109.5
H(6AA)-C(6A)-H(6AB)	109.5
H(6AA)-C(6A)-H(6AC)	109.5
H(6AB)-C(6A)-H(6AC)	109.5
C(5A)-C(7A)-H(7AA)	109.5
C(5A)-C(7A)-H(7AB)	109.5
C(5A)-C(7A)-H(7AC)	109.5
H(7AA)-C(7A)-H(7AB)	109.5
H(7AA)-C(7A)-H(7AC)	109.5
H(7AB)-C(7A)-H(7AC)	109.5
C(9A)-C(8A)-C(1A)	118.4(3)
C(9A)-C(8A)-C(13A)	119.2(3)
C(13A)-C(8A)-C(1A)	122.3(3)
C(8A)-C(9A)-H(9A)	119.8
C(8A)-C(9A)-C(10A)	120.4(3)
C(10A)-C(9A)-H(9A)	119.8
C(9A)-C(10A)-H(10A)	120.0
C(11A)-C(10A)-C(9A)	120.0(3)
C(11A)-C(10A)-H(10A)	120.0
C(10A)-C(11A)-H(11A)	119.9
C(12A)-C(11A)-C(10A)	120.1(3)
C(12A)-C(11A)-H(11A)	119.9
C(11A)-C(12A)-H(12A)	119.9
C(11A)-C(12A)-C(13A)	120.1(3)
C(13A)-C(12A)-H(12A)	119.9
C(8A)-C(13A)-H(13A)	119.9
C(12A)-C(13A)-C(8A)	120.1(3)
C(12A)-C(13A)-H(13A)	119.9
O(1A)-C(14A)-O(2A)	125.7(3)
O(1A)-C(14A)-C(3A)	123.3(3)
O(2A)-C(14A)-C(3A)	111.1(2)
O(2A)-C(15A)-H(15G)	109.5
O(2A)-C(15A)-H(15H)	109.5
O(2A)-C(15A)-H(15I)	109.5
H(15G)-C(15A)-H(15H)	109.5
H(15G)-C(15A)-H(15I)	109.5
H(15H)-C(15A)-H(15I)	109.5
O(3A)-C(16A)-O(4A)	126.2(3)
O(3A)-C(16A)-C(3A)	123.8(2)
O(4A)-C(16A)-C(3A)	110.0(2)
O(4A)-C(17A)-H(17G)	109.5
O(4A)-C(17A)-H(17H)	109.5
O(4A)-C(17A)-H(17I)	109.5

H(17G)-C(17A)-H(17H)	109.5
H(17G)-C(17A)-H(17I)	109.5
H(17H)-C(17A)-H(17I)	109.5
N(2A)-C(18A)-H(18A)	109.3
N(2A)-C(18A)-C(19A)	107.7(3)
N(2A)-C(18A)-C(20A)	109.9(2)
C(19A)-C(18A)-H(18A)	109.3
C(20A)-C(18A)-H(18A)	109.3
C(20A)-C(18A)-C(19A)	111.3(3)
C(18A)-C(19A)-H(19G)	109.5
C(18A)-C(19A)-H(19H)	109.5
C(18A)-C(19A)-H(19I)	109.5
H(19G)-C(19A)-H(19H)	109.5
H(19G)-C(19A)-H(19I)	109.5
H(19H)-C(19A)-H(19I)	109.5
C(18A)-C(20A)-H(20G)	109.5
C(18A)-C(20A)-H(20H)	109.5
C(18A)-C(20A)-H(20I)	109.5
H(20G)-C(20A)-H(20H)	109.5
H(20G)-C(20A)-H(20I)	109.5
H(20H)-C(20A)-H(20I)	109.5
C(14B)-O(2B)-C(15B)	115.1(3)
C(16B)-O(4B)-C(17B)	115.6(2)
C(1B)-N(1B)-C(5B)	122.4(2)
C(4B)-N(1B)-C(1B)	113.4(2)
C(4B)-N(1B)-C(5B)	123.9(2)
C(4B)-N(2B)-H(2B)	116.3
C(4B)-N(2B)-C(18B)	127.4(2)
C(18B)-N(2B)-H(2B)	116.3
N(1B)-C(1B)-H(1B)	109.3
N(1B)-C(1B)-C(2B)	101.5(2)
N(1B)-C(1B)-C(8B)	112.3(2)
C(2B)-C(1B)-H(1B)	109.3
C(8B)-C(1B)-H(1B)	109.3
C(8B)-C(1B)-C(2B)	114.9(2)
C(1B)-C(2B)-H(2BA)	110.8
C(1B)-C(2B)-H(2BB)	110.8
H(2BA)-C(2B)-H(2BB)	108.9
C(3B)-C(2B)-C(1B)	104.9(2)
C(3B)-C(2B)-H(2BA)	110.8
C(3B)-C(2B)-H(2BB)	110.8
C(2B)-C(3B)-C(14B)	114.4(2)
C(2B)-C(3B)-C(16B)	110.6(2)
C(4B)-C(3B)-C(2B)	101.5(2)
C(4B)-C(3B)-C(14B)	110.4(2)
C(4B)-C(3B)-C(16B)	113.9(2)
C(16B)-C(3B)-C(14B)	106.2(2)
N(1B)-C(4B)-C(3B)	110.4(2)
N(2B)-C(4B)-N(1B)	122.7(2)
N(2B)-C(4B)-C(3B)	126.9(2)
N(1B)-C(5B)-H(5B)	108.1
N(1B)-C(5B)-C(6B)	108.7(3)
N(1B)-C(5B)-C(7B)	112.4(2)
C(6B)-C(5B)-H(5B)	108.1

C(6B)-C(5B)-C(7B)	111.1(3)
C(7B)-C(5B)-H(5B)	108.1
C(5B)-C(6B)-H(6BA)	109.5
C(5B)-C(6B)-H(6BB)	109.5
C(5B)-C(6B)-H(6BC)	109.5
H(6BA)-C(6B)-H(6BB)	109.5
H(6BA)-C(6B)-H(6BC)	109.5
H(6BB)-C(6B)-H(6BC)	109.5
C(5B)-C(7B)-H(7BA)	109.5
C(5B)-C(7B)-H(7BB)	109.5
C(5B)-C(7B)-H(7BC)	109.5
H(7BA)-C(7B)-H(7BB)	109.5
H(7BA)-C(7B)-H(7BC)	109.5
H(7BB)-C(7B)-H(7BC)	109.5
C(9B)-C(8B)-C(1B)	118.6(3)
C(9B)-C(8B)-C(13B)	118.9(3)
C(13B)-C(8B)-C(1B)	122.4(3)
C(8B)-C(9B)-H(9B)	120.0
C(10B)-C(9B)-C(8B)	120.0(3)
C(10B)-C(9B)-H(9B)	120.0
C(9B)-C(10B)-H(10B)	119.6
C(11B)-C(10B)-C(9B)	120.8(3)
C(11B)-C(10B)-H(10B)	119.6
C(10B)-C(11B)-H(11B)	120.3
C(10B)-C(11B)-C(12B)	119.3(3)
C(12B)-C(11B)-H(11B)	120.3
C(11B)-C(12B)-H(12B)	119.9
C(11B)-C(12B)-C(13B)	120.2(3)
C(13B)-C(12B)-H(12B)	119.9
C(8B)-C(13B)-H(13B)	119.7
C(12B)-C(13B)-C(8B)	120.6(3)
C(12B)-C(13B)-H(13B)	119.7
O(1B)-C(14B)-O(2B)	125.7(3)
O(1B)-C(14B)-C(3B)	124.5(2)
O(2B)-C(14B)-C(3B)	109.8(2)
O(2B)-C(15B)-H(15D)	109.5
O(2B)-C(15B)-H(15E)	109.5
O(2B)-C(15B)-H(15F)	109.5
H(15D)-C(15B)-H(15E)	109.5
H(15D)-C(15B)-H(15F)	109.5
H(15E)-C(15B)-H(15F)	109.5
O(3B)-C(16B)-O(4B)	127.1(3)
O(3B)-C(16B)-C(3B)	123.2(2)
O(4B)-C(16B)-C(3B)	109.7(2)
O(4B)-C(17B)-H(17D)	109.5
O(4B)-C(17B)-H(17E)	109.5
O(4B)-C(17B)-H(17F)	109.5
H(17D)-C(17B)-H(17E)	109.5
H(17D)-C(17B)-H(17F)	109.5
H(17E)-C(17B)-H(17F)	109.5
N(2B)-C(18B)-H(18B)	108.8
N(2B)-C(18B)-C(19B)	108.8(3)
N(2B)-C(18B)-C(20B)	108.3(2)
C(19B)-C(18B)-H(18B)	108.8

C(19B)-C(18B)-C(20B)	113.3(3)
C(20B)-C(18B)-H(18B)	108.8
C(18B)-C(19B)-H(19D)	109.5
C(18B)-C(19B)-H(19E)	109.5
C(18B)-C(19B)-H(19F)	109.5
H(19D)-C(19B)-H(19E)	109.5
H(19D)-C(19B)-H(19F)	109.5
H(19E)-C(19B)-H(19F)	109.5
C(18B)-C(20B)-H(20D)	109.5
C(18B)-C(20B)-H(20E)	109.5
C(18B)-C(20B)-H(20F)	109.5
H(20D)-C(20B)-H(20E)	109.5
H(20D)-C(20B)-H(20F)	109.5
H(20E)-C(20B)-H(20F)	109.5
C(14C)-O(2C)-C(15C)	116.4(2)
C(16C)-O(4C)-C(17C)	114.6(2)
C(1C)-N(1C)-C(5C)	122.5(2)
C(4C)-N(1C)-C(1C)	114.1(2)
C(4C)-N(1C)-C(5C)	123.3(2)
C(4C)-N(2C)-H(2C)	116.0
C(4C)-N(2C)-C(18C)	128.0(2)
C(18C)-N(2C)-H(2C)	116.0
N(1C)-C(1C)-H(1C)	108.9
N(1C)-C(1C)-C(2C)	101.6(2)
N(1C)-C(1C)-C(8C)	113.8(2)
C(2C)-C(1C)-H(1C)	108.9
C(8C)-C(1C)-H(1C)	108.9
C(8C)-C(1C)-C(2C)	114.5(2)
C(1C)-C(2C)-H(2CA)	110.6
C(1C)-C(2C)-H(2CB)	110.6
C(1C)-C(2C)-C(3C)	105.5(2)
H(2CA)-C(2C)-H(2CB)	108.8
C(3C)-C(2C)-H(2CA)	110.6
C(3C)-C(2C)-H(2CB)	110.6
C(4C)-C(3C)-C(2C)	101.2(2)
C(4C)-C(3C)-C(14C)	109.0(2)
C(4C)-C(3C)-C(16C)	115.9(2)
C(14C)-C(3C)-C(2C)	114.2(2)
C(16C)-C(3C)-C(2C)	110.4(2)
C(16C)-C(3C)-C(14C)	106.4(2)
N(1C)-C(4C)-N(2C)	123.3(3)
N(1C)-C(4C)-C(3C)	110.4(2)
N(2C)-C(4C)-C(3C)	126.3(2)
N(1C)-C(5C)-H(5C)	107.5
N(1C)-C(5C)-C(6C)	111.3(3)
N(1C)-C(5C)-C(7C)	110.1(2)
C(6C)-C(5C)-H(5C)	107.5
C(6C)-C(5C)-C(7C)	112.6(3)
C(7C)-C(5C)-H(5C)	107.5
C(5C)-C(6C)-H(6CA)	109.5
C(5C)-C(6C)-H(6CB)	109.5
C(5C)-C(6C)-H(6CC)	109.5
H(6CA)-C(6C)-H(6CB)	109.5
H(6CA)-C(6C)-H(6CC)	109.5

H(6CB)-C(6C)-H(6CC)	109.5
C(5C)-C(7C)-H(7CA)	109.5
C(5C)-C(7C)-H(7CB)	109.5
C(5C)-C(7C)-H(7CC)	109.5
H(7CA)-C(7C)-H(7CB)	109.5
H(7CA)-C(7C)-H(7CC)	109.5
H(7CB)-C(7C)-H(7CC)	109.5
C(9C)-C(8C)-C(1C)	117.5(2)
C(13C)-C(8C)-C(1C)	123.6(2)
C(13C)-C(8C)-C(9C)	118.8(3)
C(8C)-C(9C)-H(9C)	120.0
C(8C)-C(9C)-C(10C)	119.9(3)
C(10C)-C(9C)-H(9C)	120.0
C(9C)-C(10C)-H(10C)	119.8
C(11C)-C(10C)-C(9C)	120.4(3)
C(11C)-C(10C)-H(10C)	119.8
C(10C)-C(11C)-H(11C)	120.0
C(10C)-C(11C)-C(12C)	119.9(3)
C(12C)-C(11C)-H(11C)	120.0
C(11C)-C(12C)-H(12C)	120.1
C(13C)-C(12C)-C(11C)	119.8(3)
C(13C)-C(12C)-H(12C)	120.1
C(8C)-C(13C)-H(13C)	119.4
C(12C)-C(13C)-C(8C)	121.1(3)
C(12C)-C(13C)-H(13C)	119.4
O(1C)-C(14C)-O(2C)	125.9(3)
O(1C)-C(14C)-C(3C)	123.2(3)
O(2C)-C(14C)-C(3C)	110.9(2)
O(2C)-C(15C)-H(15A)	109.5
O(2C)-C(15C)-H(15B)	109.5
O(2C)-C(15C)-H(15C)	109.5
H(15A)-C(15C)-H(15B)	109.5
H(15A)-C(15C)-H(15C)	109.5
H(15B)-C(15C)-H(15C)	109.5
O(3C)-C(16C)-O(4C)	126.0(3)
O(3C)-C(16C)-C(3C)	124.1(2)
O(4C)-C(16C)-C(3C)	109.9(2)
O(4C)-C(17C)-H(17A)	109.5
O(4C)-C(17C)-H(17B)	109.5
O(4C)-C(17C)-H(17C)	109.5
H(17A)-C(17C)-H(17B)	109.5
H(17A)-C(17C)-H(17C)	109.5
H(17B)-C(17C)-H(17C)	109.5
N(2C)-C(18C)-H(18C)	108.7
N(2C)-C(18C)-C(19C)	109.0(2)
N(2C)-C(18C)-C(20C)	109.0(2)
C(19C)-C(18C)-H(18C)	108.7
C(19C)-C(18C)-C(20C)	112.7(3)
C(20C)-C(18C)-H(18C)	108.7
C(18C)-C(19C)-H(19A)	109.5
C(18C)-C(19C)-H(19B)	109.5
C(18C)-C(19C)-H(19C)	109.5
H(19A)-C(19C)-H(19B)	109.5
H(19A)-C(19C)-H(19C)	109.5

H(19B)-C(19C)-H(19C)	109.5
C(18C)-C(20C)-H(20A)	109.5
C(18C)-C(20C)-H(20B)	109.5
C(18C)-C(20C)-H(20C)	109.5
H(20A)-C(20C)-H(20B)	109.5
H(20A)-C(20C)-H(20C)	109.5
H(20B)-C(20C)-H(20C)	109.5
C(14D)-O(2D)-C(15D)	115.9(3)
C(16D)-O(4D)-C(17D)	114.6(2)
C(1D)-N(1D)-C(5D)	123.8(2)
C(4D)-N(1D)-C(1D)	113.7(2)
C(4D)-N(1D)-C(5D)	122.3(2)
C(4D)-N(2D)-H(2D)	116.2
C(4D)-N(2D)-C(18D)	127.6(3)
C(18D)-N(2D)-H(2D)	116.2
N(1D)-C(1D)-H(1D)	108.5
N(1D)-C(1D)-C(2D)	102.4(2)
N(1D)-C(1D)-C(8D)	112.9(2)
C(2D)-C(1D)-H(1D)	108.5
C(8D)-C(1D)-H(1D)	108.5
C(8D)-C(1D)-C(2D)	115.6(2)
C(1D)-C(2D)-H(2DA)	110.9
C(1D)-C(2D)-H(2DB)	110.9
C(1D)-C(2D)-C(3D)	104.1(2)
H(2DA)-C(2D)-H(2DB)	109.0
C(3D)-C(2D)-H(2DA)	110.9
C(3D)-C(2D)-H(2DB)	110.9
C(2D)-C(3D)-C(16D)	110.7(2)
C(4D)-C(3D)-C(2D)	102.1(2)
C(4D)-C(3D)-C(14D)	111.0(2)
C(4D)-C(3D)-C(16D)	112.7(2)
C(14D)-C(3D)-C(2D)	114.5(2)
C(14D)-C(3D)-C(16D)	106.1(2)
N(1D)-C(4D)-C(3D)	109.1(2)
N(2D)-C(4D)-N(1D)	124.0(3)
N(2D)-C(4D)-C(3D)	126.9(2)
N(1D)-C(5D)-H(5D)	108.5
N(1D)-C(5D)-C(6D)	109.5(3)
N(1D)-C(5D)-C(7D)	111.0(3)
C(6D)-C(5D)-H(5D)	108.5
C(7D)-C(5D)-H(5D)	108.5
C(7D)-C(5D)-C(6D)	110.9(3)
C(5D)-C(6D)-H(6DA)	109.5
C(5D)-C(6D)-H(6DB)	109.5
C(5D)-C(6D)-H(6DC)	109.5
H(6DA)-C(6D)-H(6DB)	109.5
H(6DA)-C(6D)-H(6DC)	109.5
H(6DB)-C(6D)-H(6DC)	109.5
C(5D)-C(7D)-H(7DA)	109.5
C(5D)-C(7D)-H(7DB)	109.5
C(5D)-C(7D)-H(7DC)	109.5
H(7DA)-C(7D)-H(7DB)	109.5
H(7DA)-C(7D)-H(7DC)	109.5
H(7DB)-C(7D)-H(7DC)	109.5

C(9D)-C(8D)-C(1D)	118.6(3)
C(13D)-C(8D)-C(1D)	121.9(3)
C(13D)-C(8D)-C(9D)	119.5(3)
C(8D)-C(9D)-H(9D)	119.7
C(10D)-C(9D)-C(8D)	120.7(3)
C(10D)-C(9D)-H(9D)	119.7
C(9D)-C(10D)-H(10D)	120.3
C(9D)-C(10D)-C(11D)	119.5(3)
C(11D)-C(10D)-H(10D)	120.3
C(10D)-C(11D)-H(11D)	119.9
C(12D)-C(11D)-C(10D)	120.1(3)
C(12D)-C(11D)-H(11D)	119.9
C(11D)-C(12D)-H(12D)	120.1
C(11D)-C(12D)-C(13D)	119.9(3)
C(13D)-C(12D)-H(12D)	120.1
C(8D)-C(13D)-C(12D)	120.3(3)
C(8D)-C(13D)-H(13D)	119.9
C(12D)-C(13D)-H(13D)	119.9
O(1D)-C(14D)-O(2D)	125.5(3)
O(1D)-C(14D)-C(3D)	123.7(3)
O(2D)-C(14D)-C(3D)	110.8(2)
O(2D)-C(15D)-H(15P)	109.5
O(2D)-C(15D)-H(15Q)	109.5
O(2D)-C(15D)-H(15R)	109.5
H(15P)-C(15D)-H(15Q)	109.5
H(15P)-C(15D)-H(15R)	109.5
H(15Q)-C(15D)-H(15R)	109.5
O(3D)-C(16D)-O(4D)	127.4(3)
O(3D)-C(16D)-C(3D)	124.0(3)
O(4D)-C(16D)-C(3D)	108.5(2)
O(4D)-C(17D)-H(17P)	109.5
O(4D)-C(17D)-H(17Q)	109.5
O(4D)-C(17D)-H(17R)	109.5
H(17P)-C(17D)-H(17Q)	109.5
H(17P)-C(17D)-H(17R)	109.5
H(17Q)-C(17D)-H(17R)	109.5
N(2D)-C(18D)-H(18D)	108.8
N(2D)-C(18D)-C(19D)	108.8(2)
N(2D)-C(18D)-C(20D)	108.8(2)
C(19D)-C(18D)-H(18D)	108.8
C(20D)-C(18D)-H(18D)	108.8
C(20D)-C(18D)-C(19D)	112.7(3)
C(18D)-C(19D)-H(19P)	109.5
C(18D)-C(19D)-H(19Q)	109.5
C(18D)-C(19D)-H(19R)	109.5
H(19P)-C(19D)-H(19Q)	109.5
H(19P)-C(19D)-H(19R)	109.5
H(19Q)-C(19D)-H(19R)	109.5
C(18D)-C(20D)-H(20P)	109.5
C(18D)-C(20D)-H(20Q)	109.5
C(18D)-C(20D)-H(20R)	109.5
H(20P)-C(20D)-H(20Q)	109.5
H(20P)-C(20D)-H(20R)	109.5
H(20Q)-C(20D)-H(20R)	109.5

C(14E)-O(2E)-C(15E)	115.7(2)
C(16E)-O(4E)-C(17E)	115.6(2)
C(1E)-N(1E)-C(5E)	123.7(2)
C(4E)-N(1E)-C(1E)	113.6(2)
C(4E)-N(1E)-C(5E)	122.7(3)
C(4E)-N(2E)-H(2E)	116.0
C(4E)-N(2E)-C(18E)	128.1(3)
C(18E)-N(2E)-H(2E)	116.0
N(1E)-C(1E)-H(1E)	108.6
N(1E)-C(1E)-C(2E)	102.3(2)
N(1E)-C(1E)-C(8E)	113.7(2)
C(2E)-C(1E)-H(1E)	108.6
C(8E)-C(1E)-H(1E)	108.6
C(8E)-C(1E)-C(2E)	114.8(2)
C(1E)-C(2E)-H(2EA)	110.7
C(1E)-C(2E)-H(2EB)	110.7
C(1E)-C(2E)-C(3E)	105.2(2)
H(2EA)-C(2E)-H(2EB)	108.8
C(3E)-C(2E)-H(2EA)	110.7
C(3E)-C(2E)-H(2EB)	110.7
C(4E)-C(3E)-C(2E)	101.4(2)
C(4E)-C(3E)-C(14E)	109.2(2)
C(4E)-C(3E)-C(16E)	114.9(2)
C(14E)-C(3E)-C(2E)	113.6(2)
C(16E)-C(3E)-C(2E)	109.9(2)
C(16E)-C(3E)-C(14E)	107.9(2)
N(1E)-C(4E)-C(3E)	110.5(2)
N(2E)-C(4E)-N(1E)	123.4(3)
N(2E)-C(4E)-C(3E)	126.1(2)
N(1E)-C(5E)-H(5E)	107.7
N(1E)-C(5E)-C(6E)	111.4(3)
N(1E)-C(5E)-C(7E)	110.5(2)
C(6E)-C(5E)-H(5E)	107.7
C(6E)-C(5E)-C(7E)	111.8(3)
C(7E)-C(5E)-H(5E)	107.7
C(5E)-C(6E)-H(6EA)	109.5
C(5E)-C(6E)-H(6EB)	109.5
C(5E)-C(6E)-H(6EC)	109.5
H(6EA)-C(6E)-H(6EB)	109.5
H(6EA)-C(6E)-H(6EC)	109.5
H(6EB)-C(6E)-H(6EC)	109.5
C(5E)-C(7E)-H(7EA)	109.5
C(5E)-C(7E)-H(7EB)	109.5
C(5E)-C(7E)-H(7EC)	109.5
H(7EA)-C(7E)-H(7EB)	109.5
H(7EA)-C(7E)-H(7EC)	109.5
H(7EB)-C(7E)-H(7EC)	109.5
C(9E)-C(8E)-C(1E)	117.9(2)
C(13E)-C(8E)-C(1E)	123.2(3)
C(13E)-C(8E)-C(9E)	118.8(3)
C(8E)-C(9E)-H(9E)	119.2
C(8E)-C(9E)-C(10E)	121.6(3)
C(10E)-C(9E)-H(9E)	119.2
C(9E)-C(10E)-H(10E)	120.6

C(9E)-C(10E)-C(11E)	118.8(3)
C(11E)-C(10E)-H(10E)	120.6
C(10E)-C(11E)-H(11E)	120.0
C(12E)-C(11E)-C(10E)	120.0(3)
C(12E)-C(11E)-H(11E)	120.0
C(11E)-C(12E)-H(12E)	119.8
C(11E)-C(12E)-C(13E)	120.5(3)
C(13E)-C(12E)-H(12E)	119.8
C(8E)-C(13E)-C(12E)	120.2(3)
C(8E)-C(13E)-H(13E)	119.9
C(12E)-C(13E)-H(13E)	119.9
O(1E)-C(14E)-O(2E)	125.6(2)
O(1E)-C(14E)-C(3E)	122.3(3)
O(2E)-C(14E)-C(3E)	112.1(2)
O(2E)-C(15E)-H(15M)	109.5
O(2E)-C(15E)-H(15N)	109.5
O(2E)-C(15E)-H(15O)	109.5
H(15M)-C(15E)-H(15N)	109.5
H(15M)-C(15E)-H(15O)	109.5
H(15N)-C(15E)-H(15O)	109.5
O(3E)-C(16E)-O(4E)	126.0(3)
O(3E)-C(16E)-C(3E)	123.6(2)
O(4E)-C(16E)-C(3E)	110.3(2)
O(4E)-C(17E)-H(17M)	109.5
O(4E)-C(17E)-H(17N)	109.5
O(4E)-C(17E)-H(17O)	109.5
H(17M)-C(17E)-H(17N)	109.5
H(17M)-C(17E)-H(17O)	109.5
H(17N)-C(17E)-H(17O)	109.5
N(2E)-C(18E)-H(18E)	108.7
N(2E)-C(18E)-C(19E)	108.1(2)
N(2E)-C(18E)-C(20E)	109.4(2)
C(19E)-C(18E)-H(18E)	108.7
C(20E)-C(18E)-H(18E)	108.7
C(20E)-C(18E)-C(19E)	113.2(3)
C(18E)-C(19E)-H(19M)	109.5
C(18E)-C(19E)-H(19N)	109.5
C(18E)-C(19E)-H(19O)	109.5
H(19M)-C(19E)-H(19N)	109.5
H(19M)-C(19E)-H(19O)	109.5
H(19N)-C(19E)-H(19O)	109.5
C(18E)-C(20E)-H(20M)	109.5
C(18E)-C(20E)-H(20N)	109.5
C(18E)-C(20E)-H(20O)	109.5
H(20M)-C(20E)-H(20N)	109.5
H(20M)-C(20E)-H(20O)	109.5
H(20N)-C(20E)-H(20O)	109.5
C(14F)-O(2F)-C(15F)	115.7(2)
C(16F)-O(4F)-C(17F)	116.4(2)
C(1F)-N(1F)-C(5F)	122.3(2)
C(4F)-N(1F)-C(1F)	113.4(2)
C(4F)-N(1F)-C(5F)	123.9(2)
C(4F)-N(2F)-H(2F)	116.3
C(4F)-N(2F)-C(18F)	127.5(2)

C(18F)-N(2F)-H(2F)	116.3
N(1F)-C(1F)-H(1F)	109.2
N(1F)-C(1F)-C(2F)	101.6(2)
N(1F)-C(1F)-C(8F)	112.3(2)
C(2F)-C(1F)-H(1F)	109.2
C(8F)-C(1F)-H(1F)	109.2
C(8F)-C(1F)-C(2F)	115.1(2)
C(1F)-C(2F)-H(2FA)	110.9
C(1F)-C(2F)-H(2FB)	110.9
C(1F)-C(2F)-C(3F)	104.4(2)
H(2FA)-C(2F)-H(2FB)	108.9
C(3F)-C(2F)-H(2FA)	110.9
C(3F)-C(2F)-H(2FB)	110.9
C(4F)-C(3F)-C(2F)	101.8(2)
C(4F)-C(3F)-C(14F)	110.5(2)
C(14F)-C(3F)-C(2F)	115.0(2)
C(16F)-C(3F)-C(2F)	109.2(2)
C(16F)-C(3F)-C(4F)	114.2(2)
C(16F)-C(3F)-C(14F)	106.4(2)
N(1F)-C(4F)-C(3F)	109.5(2)
N(2F)-C(4F)-N(1F)	123.0(3)
N(2F)-C(4F)-C(3F)	127.5(2)
N(1F)-C(5F)-H(5F)	108.0
N(1F)-C(5F)-C(6F)	108.8(3)
N(1F)-C(5F)-C(7F)	112.4(3)
C(6F)-C(5F)-H(5F)	108.0
C(7F)-C(5F)-H(5F)	108.0
C(7F)-C(5F)-C(6F)	111.4(3)
C(5F)-C(6F)-H(6FA)	109.5
C(5F)-C(6F)-H(6FB)	109.5
C(5F)-C(6F)-H(6FC)	109.5
H(6FA)-C(6F)-H(6FB)	109.5
H(6FA)-C(6F)-H(6FC)	109.5
H(6FB)-C(6F)-H(6FC)	109.5
C(5F)-C(7F)-H(7FA)	109.5
C(5F)-C(7F)-H(7FB)	109.5
C(5F)-C(7F)-H(7FC)	109.5
H(7FA)-C(7F)-H(7FB)	109.5
H(7FA)-C(7F)-H(7FC)	109.5
H(7FB)-C(7F)-H(7FC)	109.5
C(9F)-C(8F)-C(1F)	117.4(3)
C(13F)-C(8F)-C(1F)	122.6(3)
C(13F)-C(8F)-C(9F)	120.0(3)
C(8F)-C(9F)-H(9F)	119.9
C(10F)-C(9F)-C(8F)	120.3(3)
C(10F)-C(9F)-H(9F)	119.9
C(9F)-C(10F)-H(10F)	120.5
C(9F)-C(10F)-C(11F)	119.0(3)
C(11F)-C(10F)-H(10F)	120.5
C(10F)-C(11F)-H(11F)	119.7
C(12F)-C(11F)-C(10F)	120.6(3)
C(12F)-C(11F)-H(11F)	119.7
C(11F)-C(12F)-H(12F)	120.1
C(11F)-C(12F)-C(13F)	119.8(3)

C(13F)-C(12F)-H(12F)	120.1
C(8F)-C(13F)-C(12F)	120.3(3)
C(8F)-C(13F)-H(13F)	119.8
C(12F)-C(13F)-H(13F)	119.8
O(1F)-C(14F)-O(2F)	125.8(2)
O(1F)-C(14F)-C(3F)	123.1(3)
O(2F)-C(14F)-C(3F)	111.1(2)
O(2F)-C(15F)-H(15J)	109.5
O(2F)-C(15F)-H(15K)	109.5
O(2F)-C(15F)-H(15L)	109.5
H(15J)-C(15F)-H(15K)	109.5
H(15J)-C(15F)-H(15L)	109.5
H(15K)-C(15F)-H(15L)	109.5
O(3F)-C(16F)-O(4F)	124.5(2)
O(3F)-C(16F)-C(3F)	123.4(2)
O(4F)-C(16F)-C(3F)	112.0(2)
O(4F)-C(17F)-H(17J)	109.5
O(4F)-C(17F)-H(17K)	109.5
O(4F)-C(17F)-H(17L)	109.5
H(17J)-C(17F)-H(17K)	109.5
H(17J)-C(17F)-H(17L)	109.5
H(17K)-C(17F)-H(17L)	109.5
N(2F)-C(18F)-H(18F)	109.5
N(2F)-C(18F)-C(19F)	109.5(2)
N(2F)-C(18F)-C(20F)	108.1(2)
C(19F)-C(18F)-H(18F)	109.5
C(19F)-C(18F)-C(20F)	110.7(3)
C(20F)-C(18F)-H(18F)	109.5
C(18F)-C(19F)-H(19J)	109.5
C(18F)-C(19F)-H(19K)	109.5
C(18F)-C(19F)-H(19L)	109.5
H(19J)-C(19F)-H(19K)	109.5
H(19J)-C(19F)-H(19L)	109.5
H(19K)-C(19F)-H(19L)	109.5
C(18F)-C(20F)-H(20J)	109.5
C(18F)-C(20F)-H(20K)	109.5
C(18F)-C(20F)-H(20L)	109.5
H(20J)-C(20F)-H(20K)	109.5
H(20J)-C(20F)-H(20L)	109.5
H(20K)-C(20F)-H(20L)	109.5
H(5AA)-O(5A)-H(5AB)	117(3)
H(5BA)-O(5B)-H(5BB)	113(3)
H(5CA)-O(5C)-H(5CB)	109(2)
H(5DA)-O(5D)-H(5DB)	105(2)
H(5EA)-O(5E)-H(5EB)	107(2)
H(5FA)-O(5F)-H(5FB)	107(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (≈^{2}x 10^4) for afg04. 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(1A)	246(12)	132(9)	182(10)	11(8)	35(9)	80(8)
O(2A)	202(12)	132(9)	284(12)	-45(8)	-6(10)	-9(8)
O(3A)	331(14)	195(10)	173(11)	39(8)	-26(9)	90(9)
O(4A)	285(12)	137(9)	176(10)	71(8)	42(9)	65(8)
N(1A)	177(13)	123(10)	105(10)	40(8)	46(9)	41(9)
N(2A)	155(12)	152(11)	102(10)	1(8)	21(9)	42(9)
C(1A)	149(14)	90(11)	175(13)	15(9)	50(11)	44(10)
C(2A)	140(14)	140(12)	166(13)	42(10)	68(11)	49(10)
C(3A)	147(14)	99(11)	127(12)	30(9)	28(10)	48(9)
C(4A)	192(15)	94(11)	134(12)	6(9)	48(11)	67(10)
C(5A)	163(15)	194(13)	128(13)	75(10)	35(11)	34(11)
C(6A)	268(18)	294(16)	135(14)	33(12)	30(13)	16(14)
C(7A)	220(17)	257(16)	255(16)	115(13)	-14(13)	95(13)
C(8A)	149(14)	127(12)	145(13)	25(10)	14(11)	4(10)
C(9A)	168(15)	212(14)	163(13)	51(11)	30(11)	29(11)
C(10A)	199(16)	235(15)	212(15)	95(12)	31(12)	45(12)
C(11A)	228(17)	202(14)	290(17)	162(12)	62(14)	43(12)
C(12A)	259(17)	168(13)	260(16)	73(11)	35(13)	94(12)
C(13A)	190(16)	203(13)	187(14)	96(11)	63(12)	100(11)
C(14A)	140(14)	141(12)	161(13)	67(10)	21(11)	28(10)
C(15A)	360(20)	110(13)	450(20)	-96(14)	49(18)	-22(13)
C(16A)	117(14)	129(12)	180(13)	69(10)	40(11)	3(10)
C(17A)	302(19)	203(14)	296(17)	153(13)	75(14)	93(13)
C(18A)	193(16)	232(14)	115(13)	25(11)	59(11)	65(12)
C(19A)	259(18)	254(16)	277(17)	30(13)	97(14)	104(14)
C(20A)	185(16)	288(16)	213(16)	120(12)	7(13)	4(13)
O(1B)	177(11)	139(9)	201(11)	-4(8)	21(9)	82(8)
O(2B)	154(11)	78(8)	366(13)	-25(8)	34(10)	-8(7)
O(3B)	257(12)	180(10)	138(10)	-21(8)	-66(9)	43(9)
O(4B)	246(12)	108(8)	107(9)	31(7)	-2(8)	55(8)
N(1B)	116(12)	124(10)	121(10)	30(8)	7(9)	-3(8)
N(2B)	113(12)	158(11)	100(10)	4(8)	13(9)	1(9)
C(1B)	119(13)	108(11)	130(12)	20(9)	38(10)	4(9)
C(2B)	114(13)	121(11)	168(13)	28(10)	7(11)	21(10)
C(3B)	104(13)	107(11)	104(11)	5(9)	-30(10)	13(9)
C(4B)	115(13)	72(10)	113(12)	21(9)	9(10)	35(9)
C(5B)	144(14)	199(13)	96(12)	-27(10)	6(10)	-10(11)
C(6B)	490(20)	151(14)	245(17)	-70(12)	-74(17)	-43(15)
C(7B)	207(17)	349(18)	140(14)	29(12)	38(12)	-12(14)
C(8B)	162(15)	128(12)	167(13)	19(10)	-22(11)	-9(10)
C(9B)	205(16)	190(14)	179(14)	59(11)	19(12)	-31(12)
C(10B)	277(19)	219(15)	241(16)	117(12)	7(14)	-80(13)
C(11B)	350(20)	161(14)	267(17)	92(12)	-67(15)	-32(13)
C(12B)	400(20)	211(15)	274(18)	68(13)	-41(15)	112(14)
C(13B)	270(18)	165(13)	208(15)	52(11)	16(13)	69(12)
C(14B)	155(14)	87(11)	158(13)	29(9)	11(11)	16(10)

C(15B)	340(20)	73(13)	550(20)	-81(14)	87(18)	-24(13)
C(16B)	122(13)	81(11)	116(12)	1(9)	15(10)	-4(9)
C(17B)	277(17)	193(13)	122(13)	67(10)	20(12)	100(12)
C(18B)	198(16)	172(13)	74(12)	-18(10)	23(11)	7(11)
C(19B)	122(15)	279(16)	282(17)	-48(13)	56(13)	44(12)
C(20B)	232(17)	285(16)	180(15)	103(12)	63(13)	32(13)
O(1C)	224(12)	106(9)	222(11)	35(8)	32(9)	54(8)
O(2C)	191(12)	114(9)	264(11)	14(8)	58(9)	-16(8)
O(3C)	211(12)	148(9)	152(10)	8(7)	-45(8)	31(8)
O(4C)	276(12)	117(9)	126(9)	37(7)	7(8)	61(8)
N(1C)	160(12)	110(10)	107(10)	28(8)	49(9)	39(9)
N(2C)	150(12)	162(11)	83(10)	17(8)	14(9)	30(9)
C(1C)	205(15)	133(12)	116(12)	57(10)	76(11)	71(11)
C(2C)	175(15)	139(12)	130(12)	40(9)	53(11)	63(10)
C(3C)	117(13)	100(11)	131(12)	9(9)	13(10)	27(9)
C(4C)	156(14)	80(11)	120(12)	33(9)	20(10)	37(10)
C(5C)	183(15)	176(13)	95(12)	27(10)	4(11)	27(11)
C(6C)	291(19)	258(16)	136(14)	-22(12)	0(13)	3(13)
C(7C)	197(17)	208(14)	280(17)	79(12)	-25(13)	51(12)
C(8C)	176(15)	122(12)	119(12)	32(9)	19(11)	39(10)
C(9C)	222(16)	183(13)	124(13)	54(10)	83(11)	51(11)
C(10C)	269(18)	221(14)	201(15)	137(12)	107(13)	49(13)
C(11C)	280(18)	154(13)	213(15)	108(11)	56(13)	43(12)
C(12C)	275(17)	124(12)	199(14)	51(10)	31(12)	73(11)
C(13C)	246(17)	155(13)	161(13)	49(10)	98(12)	102(11)
C(14C)	205(15)	111(12)	96(12)	29(9)	1(11)	-5(10)
C(15C)	320(20)	139(13)	348(19)	12(12)	154(16)	-19(13)
C(16C)	98(14)	131(12)	192(14)	64(10)	31(11)	54(10)
C(17C)	350(20)	200(14)	228(15)	150(12)	56(14)	115(13)
C(18C)	160(15)	214(13)	83(12)	53(10)	0(10)	29(11)
C(19C)	311(19)	283(16)	89(13)	-87(11)	12(12)	92(14)
C(20C)	206(16)	223(15)	157(14)	76(11)	13(12)	10(12)
O(1D)	206(12)	167(10)	223(11)	30(8)	2(9)	26(8)
O(2D)	223(12)	110(9)	280(12)	53(8)	49(9)	69(8)
O(3D)	225(12)	131(9)	181(10)	15(8)	12(9)	35(8)
O(4D)	216(11)	87(8)	170(10)	36(7)	16(8)	4(8)
N(1D)	224(14)	153(11)	80(10)	19(8)	-16(9)	79(9)
N(2D)	181(13)	132(10)	105(10)	19(8)	5(9)	63(9)
C(1D)	184(15)	166(13)	128(13)	35(10)	-17(11)	64(11)
C(2D)	134(14)	177(13)	175(13)	64(10)	-15(11)	77(11)
C(3D)	118(13)	113(11)	148(13)	17(9)	2(10)	22(10)
C(4D)	167(14)	70(10)	127(12)	23(9)	-21(10)	26(10)
C(5D)	310(18)	229(14)	132(13)	-30(11)	-18(12)	167(13)
C(6D)	750(30)	164(15)	360(20)	-54(14)	0(20)	124(18)
C(7D)	780(30)	490(20)	120(15)	39(14)	63(17)	510(20)
C(8D)	174(15)	148(12)	171(13)	43(10)	-12(11)	77(11)
C(9D)	209(16)	158(13)	192(14)	28(11)	-26(12)	59(11)
C(10D)	312(19)	235(15)	202(15)	74(12)	-17(14)	108(13)
C(11D)	308(19)	221(15)	211(15)	116(12)	57(14)	76(13)
C(12D)	223(17)	249(15)	206(15)	93(12)	-12(13)	-12(13)
C(13D)	159(15)	240(14)	152(14)	86(11)	-33(11)	2(12)
C(14D)	174(15)	132(12)	115(12)	57(9)	36(11)	20(10)
C(15D)	330(20)	115(13)	308(18)	33(12)	31(15)	43(12)
C(16D)	137(15)	141(13)	296(17)	48(12)	79(13)	57(11)

C(17D)	227(17)	170(13)	199(15)	86(11)	30(12)	31(12)
C(18D)	166(15)	187(13)	120(13)	29(10)	-25(11)	64(11)
C(19D)	229(17)	246(15)	180(15)	49(12)	-67(13)	67(13)
C(20D)	274(18)	202(14)	207(15)	74(12)	-23(13)	51(12)
O(1E)	127(11)	105(9)	242(11)	17(8)	-31(9)	-22(7)
O(2E)	186(11)	130(9)	271(12)	11(8)	-32(9)	54(8)
O(3E)	205(12)	141(9)	192(10)	5(8)	50(9)	13(8)
O(4E)	206(11)	121(9)	142(9)	41(7)	-18(8)	-3(8)
N(1E)	182(13)	111(10)	108(11)	17(8)	-20(9)	32(9)
N(2E)	147(12)	147(11)	117(11)	22(8)	4(9)	62(9)
C(1E)	146(14)	134(12)	139(13)	24(10)	-37(11)	-6(10)
C(2E)	113(14)	146(12)	192(14)	63(10)	-21(11)	-20(10)
C(3E)	118(13)	97(11)	149(12)	26(9)	-8(10)	-6(9)
C(4E)	113(13)	91(11)	131(12)	15(9)	-13(10)	-22(9)
C(5E)	233(16)	159(13)	131(13)	39(10)	28(11)	78(11)
C(6E)	330(20)	286(16)	104(13)	37(11)	-32(13)	89(14)
C(7E)	231(18)	286(17)	260(17)	79(13)	89(14)	70(13)
C(8E)	150(14)	136(12)	139(12)	34(10)	-17(10)	33(10)
C(9E)	159(15)	203(13)	176(14)	60(11)	-20(11)	35(11)
C(10E)	284(19)	223(15)	235(16)	93(12)	-43(13)	83(13)
C(11E)	278(18)	203(14)	275(17)	115(12)	-25(14)	54(13)
C(12E)	209(17)	175(13)	258(16)	114(12)	-28(13)	-8(12)
C(13E)	185(16)	198(14)	208(15)	85(11)	-32(12)	43(12)
C(14E)	168(14)	113(11)	108(12)	32(9)	3(10)	30(10)
C(15E)	330(20)	83(12)	420(20)	14(12)	-59(16)	79(12)
C(16E)	115(13)	116(11)	167(13)	44(10)	15(11)	15(10)
C(17E)	259(18)	179(14)	194(15)	105(11)	14(13)	-8(12)
C(18E)	173(15)	177(13)	87(12)	35(10)	-15(10)	75(11)
C(19E)	150(15)	196(14)	222(15)	-15(11)	-45(12)	65(11)
C(20E)	226(17)	224(14)	194(15)	100(12)	23(12)	93(12)
O(1F)	190(12)	151(10)	243(11)	61(8)	13(9)	47(8)
O(2F)	231(12)	101(9)	213(11)	20(8)	15(9)	35(8)
O(3F)	243(12)	163(9)	150(10)	-4(8)	55(9)	67(8)
O(4F)	257(12)	107(8)	99(9)	34(7)	29(8)	12(8)
N(1F)	168(13)	136(10)	110(10)	33(8)	-17(9)	80(9)
N(2F)	141(12)	133(10)	98(10)	20(8)	-12(9)	52(9)
C(1F)	147(14)	163(12)	135(12)	46(10)	1(11)	71(10)
C(2F)	167(14)	134(12)	121(12)	35(9)	7(11)	39(10)
C(3F)	126(13)	91(11)	132(12)	27(9)	-2(10)	16(9)
C(4F)	140(14)	81(11)	132(12)	26(9)	10(10)	17(9)
C(5F)	326(18)	192(14)	160(14)	0(11)	9(13)	160(13)
C(6F)	630(30)	219(16)	240(17)	2(13)	13(18)	172(17)
C(7F)	380(20)	330(17)	125(14)	-28(12)	-34(14)	192(15)
C(8F)	225(16)	146(12)	131(13)	35(10)	39(11)	85(11)
C(9F)	310(18)	229(15)	174(14)	68(11)	42(13)	174(13)
C(10F)	430(20)	278(16)	180(15)	111(12)	94(14)	237(15)
C(11F)	550(30)	199(15)	261(17)	104(13)	208(17)	145(15)
C(12F)	430(20)	203(15)	258(17)	91(13)	153(16)	59(15)
C(13F)	246(18)	229(15)	183(15)	69(12)	45(13)	60(13)
C(14F)	157(14)	123(12)	128(12)	21(9)	13(11)	24(10)
C(15F)	350(20)	72(11)	238(15)	8(10)	62(14)	23(12)
C(16F)	132(14)	155(12)	50(11)	17(9)	-21(10)	62(10)
C(17F)	238(17)	216(14)	155(14)	107(11)	27(12)	22(12)
C(18F)	177(15)	168(12)	99(12)	22(10)	-28(11)	61(11)

C(19F)	215(17)	139(13)	200(15)	-5(11)	-47(13)	-39(11)
C(20F)	351(19)	240(15)	129(13)	76(11)	-9(13)	130(13)
Br(1A)	265(2)	205(1)	172(1)	6(1)	-6(1)	118(1)
Br(1B)	212(2)	209(1)	143(1)	38(1)	18(1)	89(1)
Br(1C)	286(2)	173(1)	186(2)	-11(1)	-24(1)	92(1)
Br(1D)	242(2)	223(2)	175(2)	45(1)	22(1)	-12(1)
Br(1E)	225(2)	166(1)	142(1)	0(1)	31(1)	-40(1)
Br(1F)	212(2)	228(2)	157(1)	45(1)	-2(1)	10(1)
O(5A)	202(12)	160(10)	207(11)	8(8)	11(9)	47(8)
O(5B)	155(11)	210(10)	200(11)	29(8)	-5(9)	-74(9)
O(5C)	189(12)	159(10)	246(12)	43(8)	21(9)	55(9)
O(5D)	342(15)	272(12)	219(12)	50(9)	23(10)	202(11)
O(5E)	200(12)	176(10)	162(10)	29(8)	54(9)	63(8)
O(5F)	253(13)	291(12)	214(12)	35(9)	37(10)	159(10)

Table 5. Hydrogen coordinates (x 10^3) and isotropic displacement parameters (≈^{2}x 10^3) for afg04.

	x	y	z	U_{iso}
H(2A)	204	104	797	17
H(1A)	646	133	714	16
H(2AA)	842	242	787	17
H(2AB)	776	130	782	17
H(5A)	213	72	729	19
H(6AA)	404	146	657	37
H(6AB)	228	64	650	37
H(6AC)	402	47	670	37
H(7AA)	186	224	753	35
H(7AB)	98	182	702	35
H(7AC)	282	256	709	35
H(9A)	782	222	663	22
H(10A)	859	359	632	25
H(11A)	792	492	668	27
H(12A)	646	488	735	26
H(13A)	565	351	766	21
H(15G)	784	477	855	51
H(15H)	964	472	878	51
H(15I)	794	446	905	51
H(17G)	691	-57	862	37
H(17H)	593	-8	900	37
H(17I)	793	36	896	37
H(18A)	381	168	885	21
H(19G)	173	248	870	38
H(19H)	114	190	910	38
H(19I)	25	151	859	38
H(20G)	99	3	863	35
H(20H)	211	38	912	35
H(20I)	296	1	867	35
H(2B)	-4	75	461	16
H(1B)	460	112	381	15
H(2BA)	580	124	454	16
H(2BB)	628	234	453	16
H(5B)	0	59	391	20
H(6BA)	226	-58	383	50
H(6BB)	27	-92	363	50
H(6BC)	78	-61	418	50
H(7BA)	134	130	331	37
H(7BB)	45	22	312	37
H(7BC)	249	58	324	37
H(9B)	598	218	334	25
H(10B)	613	349	300	32
H(11B)	460	456	328	33
H(12B)	280	426	388	35
H(13B)	258	293	421	25
H(15D)	494	467	503	53
H(15E)	692	482	520	53

H(15F)	543	453	554	53
H(17D)	488	-42	549	28
H(17E)	396	20	584	28
H(17F)	596	58	576	28
H(18B)	166	149	549	19
H(19D)	-33	229	532	36
H(19E)	-101	171	572	36
H(19F)	-183	134	520	36
H(20D)	-108	-19	527	35
H(20E)	-10	21	577	35
H(20F)	90	-16	536	35
H(2C)	416	99	128	16
H(1C)	849	121	40	17
H(2CA)	1052	228	112	17
H(2CB)	979	118	109	17
H(5C)	419	57	59	19
H(6CA)	606	125	-15	37
H(6CB)	432	43	-20	37
H(6CC)	608	29	1	37
H(7CA)	386	208	80	34
H(7CB)	300	164	28	34
H(7CC)	483	240	36	34
H(9C)	994	214	-9	21
H(10C)	1067	352	-39	26
H(11C)	991	482	-4	25
H(12C)	834	474	62	23
H(13C)	753	336	91	21
H(15A)	1026	476	158	42
H(15B)	1175	471	195	42
H(15C)	982	457	209	42
H(17A)	855	-61	201	36
H(17B)	813	14	240	36
H(17C)	1004	30	224	36
H(18C)	605	167	215	18
H(19A)	412	254	202	36
H(19B)	349	197	243	36
H(19C)	254	161	192	36
H(20A)	317	5	195	30
H(20B)	427	43	244	30
H(20C)	513	2	200	30
H(2D)	98	754	670	16
H(1D)	531	721	758	19
H(2DA)	563	591	691	18
H(2DB)	628	700	687	18
H(5D)	128	777	740	26
H(6DA)	471	898	753	65
H(6DB)	300	931	760	65
H(6DC)	339	888	709	65
H(7DA)	236	712	803	60
H(7DB)	204	812	818	60
H(7DC)	395	804	812	60
H(9D)	568	620	808	22
H(10D)	458	495	846	29
H(11D)	188	390	820	28

H(12D)	26	415	757	28
H(13D)	136	542	720	23
H(15P)	229	362	596	38
H(15Q)	190	360	649	38
H(15R)	363	339	631	38
H(17P)	515	793	552	30
H(17Q)	688	765	564	30
H(17R)	665	864	587	30
H(18D)	176	667	586	19
H(19P)	-101	589	600	33
H(19Q)	-123	649	560	33
H(19R)	-153	684	613	33
H(20P)	67	834	598	34
H(20Q)	132	788	551	34
H(20R)	265	834	596	34
H(2E)	725	727	339	16
H(1E)	1153	714	432	18
H(2EA)	1241	603	363	19
H(2EB)	1274	713	364	19
H(5E)	778	772	408	20
H(6EA)	909	709	485	36
H(6EB)	818	791	487	36
H(6EC)	1004	804	468	36
H(7EA)	600	615	388	38
H(7EB)	557	669	436	38
H(7EC)	667	595	437	38
H(9E)	1236	625	481	22
H(10E)	1190	492	516	29
H(11E)	972	358	483	30
H(12E)	792	362	419	26
H(13E)	836	496	385	23
H(15M)	935	367	266	42
H(15N)	943	355	319	42
H(15O)	1105	352	290	42
H(17M)	1192	808	230	32
H(17N)	1372	801	252	32
H(17O)	1302	888	271	32
H(18E)	830	654	255	17
H(19M)	557	566	263	29
H(19N)	533	629	226	29
H(19O)	491	656	279	29
H(20M)	708	816	269	30
H(20N)	772	775	222	30
H(20O)	907	819	266	30
H(2F)	294	753	11	15
H(1F)	736	716	95	17
H(2FA)	771	594	25	17
H(2FB)	827	704	23	17
H(5F)	326	770	82	25
H(6FA)	669	891	94	54
H(6FB)	499	923	105	54
H(6FC)	530	887	53	54
H(7FA)	413	700	142	40
H(7FB)	415	806	160	40

H(7FC)	592	780	150	40
H(9F)	782	610	140	26
H(10F)	683	477	174	31
H(11F)	413	372	146	38
H(12F)	242	403	88	35
H(13F)	341	538	56	26
H(15J)	426	364	-66	34
H(15K)	383	363	-14	34
H(15L)	556	340	-30	34
H(17J)	696	780	-116	30
H(17K)	882	771	-100	30
H(17L)	828	864	-82	30
H(18F)	373	676	-76	18
H(19J)	93	599	-62	31
H(19K)	78	660	-101	31
H(19L)	45	695	-49	31
H(20J)	267	844	-55	34
H(20K)	318	804	-105	34
H(20L)	462	843	-62	34
H(5AA)	998(5)	-14(2)	771(1)	29
H(5AB)	915(5)	48(2)	797(1)	29
H(5BA)	681(4)	-35(2)	445(1)	32
H(5BB)	758(5)	62(1)	454(1)	32
H(5CA)	145(5)	-29(1)	117(1)	29
H(5CB)	114(4)	59(2)	119(1)	29
H(5DA)	897(5)	875(2)	681(1)	38
H(5DB)	901(5)	820(2)	715(1)	38
H(5EA)	601(5)	860(2)	349(1)	26
H(5EB)	528(5)	808(2)	383(1)	26
H(5FA)	230(2)	832(3)	35(1)	35
H(5FB)	75(5)	820(3)	57(1)	35