Palladium-Catalyzed Construction of Quaternary Stereocenters by Enantioselective Arylation of γ-Lactams with Aryl Chlorides and Bromides

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Materials and Methods

Unless otherwise stated, reactions were performed in flame-dried glassware under an argon or nitrogen atmosphere using dry, deoxygenated solvents. Solvents were dried by passage through an activated alumina column under argon. Reaction progress was monitored by thin-layer chromatography (TLC) or Agilent 1290 UHPLC-MS. TLC was performed using E. Merck silica gel 60 F254 precoated glass plates (0.25 mm) and visualized by UV fluorescence quenching, *p*-anisaldehyde, or $KMnO_4$ staining. Silicycle Silia*Flash*® P60 Academic Silica gel (particle size 40–63 nm) was used for flash chromatography. ^{1}H NMR spectra were recorded on a Bruker Avance HD 400 MHz or Varian Mercury 300 MHz spectrometers and are reported relative to residual $CHCl_3$ (δ 7.26 ppm). ^{13}C NMR spectra were recorded on a Bruker Avance HD 400 MHz spectrometer (100 MHz) and are reported relative to residual $CHCl_3$ (δ 77.36 ppm). ^{19}F NMR spectra were recorded on a Varian Mercury 300 MHz spectrometer (282 MHz). Data for ^{1}H NMR are reported as follows: chemical shift (δ ppm) (multiplicity, coupling constant (Hz), integration). Multiplicities are reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, sept = septuplet, m = multiplet, br s = broad singlet, br d = broad doublet, app = apparent. Data for ^{13}C NMR are reported in terms of chemical shifts (δ ppm). IR spectra were obtained using a Perkin Elmer Spectrum BXII spectrometer or Nicolet 6700 FTIR spectrometer using thin films deposited on NaCl plates and reported in frequency of absorption (cm^{-1}). Optical rotations were measured with a Jasco P-2000 polarimeter operating on the sodium D-line (589 nm), using a 100 mm path-length cell and are reported as: $[\alpha]_D^T$ (concentration in 10 mg/1 mL, solvent). Analytical SFC was performed with a Mettler SFC supercritical CO_2 analytical chromatography system utilizing Chiralpak (AD-H) or Chiralcel (OD-H) columns (4.6 mm x 25 cm) obtained from Daicel Chemical Industries, Ltd. High resolution mass spectra (HRMS) were obtained from Agilent 6200 Series TOF with an Agilent G1978A

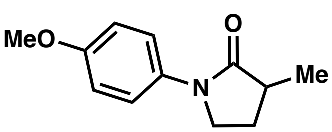
Multimode source in electrospray ionization (ESI+), atmospheric pressure chemical ionization (APCI+), or mixed ionization mode (MM: ESI-APCI+).

Reagents were purchased from Sigma-Aldrich, Acros Organics, Strem, or Alfa Aesar and used as received unless otherwise stated.

List of Abbreviations

ee – enantiomeric excess, SFC – supercritical fluid chromatography, TLC – thin-layer chromatography, IPA – isopropanol, MTBE – methyl *tert*-butyl ether, PE – petroleum ether, DMAP – 4-dimethylaminopyridine, EtOAc – ethyl acetate, LiHMDS – lithium bis(trimethylsilyl)amide, NaHMDS – sodium bis(trimethylsilyl)amide, PMP – *p*-methoxy phenyl, pmdba – 4,4'-dimethoxydibenzylideneacetone, THF – tetrahydrofuran, DMEDA – 1,2-dimethylethylenediamine.

N-substituted lactams synthesized and tested



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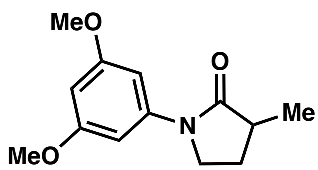

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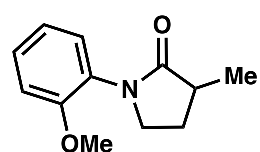

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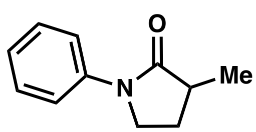

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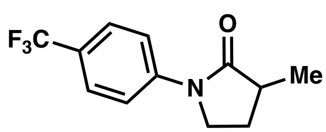

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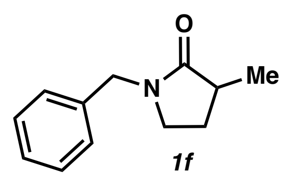

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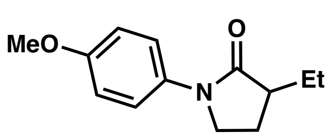

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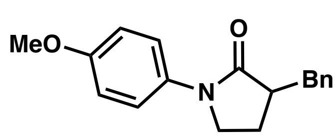

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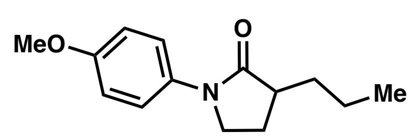

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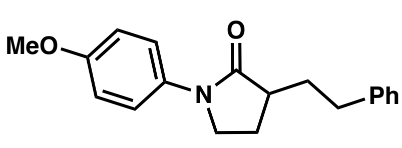

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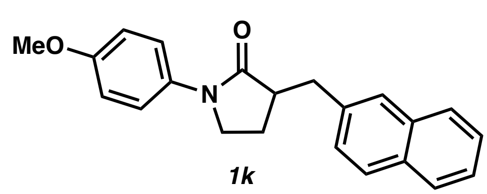
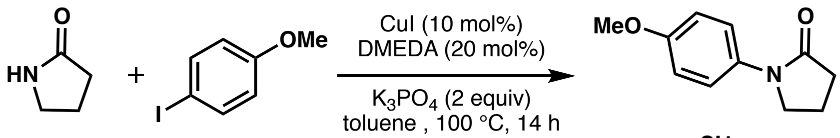


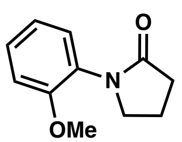
1k

Synthesis of *N*-substituted lactam starting material



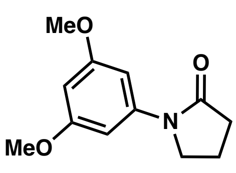
SI1

1-(4-methoxyphenyl)pyrrolidin-2-one (SI1):[1] To a solution of CuI (1.904 g, 10 mmol, 0.1 equiv) in toluene (100 mL, 1.0 M) was added DMEDA (2.15 mL, 20 mmol, 0.2 equiv), 4-iodoanisole (23.4 g, 100 mmol, 1 equiv), 2-pyrrolidinone (9.11 mL, 120 mmol, 1.2 equiv), and anhydrous K_3PO_4 (42.5 g, 200 mmol, 2 equiv). The resultant mixture was heated to 100 °C and allowed to stir for 14 hours. The reaction was cooled, diluted with EtOAc, and filtered through celite. The filtrate was concentrated and recrystallized from 20% EtOAc in hexanes to afford **SI1** as a colorless solid (16.0 g, 83.7 mmol, 84% yield); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 – 7.43 (m, 2H), 6.96 – 6.84 (m, 2H), 3.92 – 3.73 (m, 5H), 2.59 (dd, *J* = 8.5, 7.7 Hz, 2H), 2.25 – 2.07 (m, 2H). All characterization data match those reported.[1]



SI2

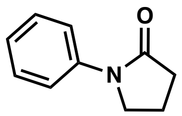
1-(2-methoxyphenyl)pyrrolidin-2-one (SI2):[1] Compound **SI2** was prepared from 2-pyrrolidinone using a previously reported procedure; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.26 (m, 2H), 7.04 – 6.90 (m, 2H), 3.84 (s, 3H), 3.76 (t, *J* = 7.1 Hz, 2H), 2.56 (dd, *J* = 8.5, 7.7 Hz, 2H), 2.19 (tt, *J* = 7.7, 6.9 Hz, 2H). All characterization data match those reported.[1]



SI3

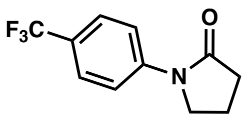
1-(3,5-dimethoxyphenyl)pyrrolidin-2-one (SI3):[1] Compound **SI3** was prepared from 2-pyrrolidinone using a previously reported procedure; ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.86

(d, J = 2.2 Hz, 2H), 6.27 (t, J = 2.2 Hz, 1H), 3.83 (t, J = 7.0 Hz, 2H), 3.80 (s, 6H), 2.61 (dd, J = 8.5, 7.7 Hz, 2H), 2.15 (tt, J = 7.8, 7.0 Hz, 2H). All characterization data match those reported.[1]



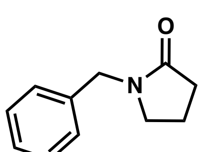
SI4

1-phenylpyrrolidin-2-one (SI4):[2] Compound **SI4** was prepared from 2-pyrrolidinone using a previously reported procedure. All characterization data match those reported.[2]



SI5

1-(4-(trifluoromethyl)phenyl)pyrrolidin-2-one (SI5): 2-pyrrolidinone (23.5 mmol, 2.0 g), Cs_2CO_3 (1.07 g, 32.9 mmol, 1.4 equiv), Xantphos (460 mg, 0.80 mmol, 3.3 mol%), $Pd(OAc)_2$ (106 mg, 0.47 mmol, 2.0 mol%), and 4-bromobenzotrifluoride (4.22 mL, 30.6 mmol, 1.3 equiv) in dioxane (70 mL) under inert atmosphere were heated to 100 °C for 24 h. The reaction was then cooled to ambient temperature, filtered through a plug of silica, and concentrated. The filtrate was recrystallized from 20% EtOAc in hexanes to afford **SI5** as a colorless solid (4.52 g, 19.7 mmol, 84% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 – 7.74 (m, 2H), 7.64 – 7.59 (m, 2H), 3.90 (t, J = 7.0 Hz, 2H), 2.65 (dd, J = 8.5, 7.8 Hz, 2H), 2.28 – 2.14 (m, 2H). All characterization data match those reported.

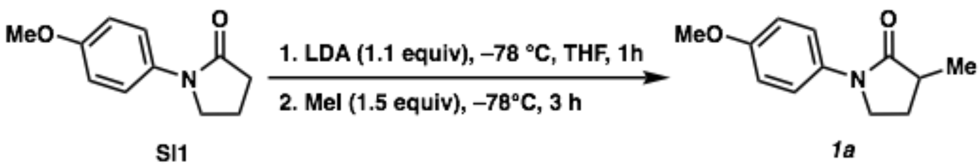


SI6

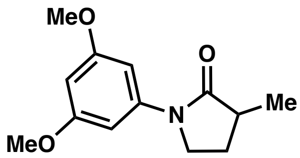
1-benzylpyrrolidin-2-one (SI6): To a flame-dried round-bottom flask under argon was added 2-pyrrolidinone (3.38 g, 39.7 mmol, 1.0 equiv), DMAP (243 mg, 1.39 mmol, 0.05 equiv), dichloromethane (60 mL), and triethylamine (8.30 mL, 60 mmol, 1.5 equiv). The resulting solution was cooled to 0 °C and benzyl chloride (5.54 mL, 47.7 mmol, 1.2 equiv) was added dropwise. The reaction was allowed to warm to ambient temperature and stirred for one hour. The crude reaction mixture was quenched with saturated NH_4Cl solution , extracted three times, then the combine organic layers were washed with saturated $NaHCO_3$ solution. The organic layer was dried over Na_2SO_4 and concentrated. The filtrate was recrystallized from 25% EtOAc in hexanes to afford **SI6** as a colorless solid (3.64 g, 20.8 mmol, 48% yield); ^1H NMR (300 MHz, $CDCl_3$) δ 7.26 (m, 5H), 4.45 (s, 2H), 3.26 (dd, J = 7.5, 6.7 Hz, 2H), 2.45 (dd, J = 8.6, 7.6 Hz, 2H), 2.07 – 1.90 (m, 2H). All characterization data match those reported.[4]

Synthesis of Nucleophiles: Experimental Procedures and Spectroscopic Data

General Procedure 1: α-alkylation of *N*-substituted lactams with alkyl halides:

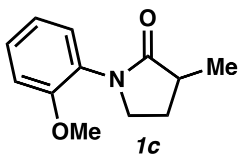


1-(4-methoxyphenyl)-3-methylpyrrolidin-2-one (1a): To a solution of *i*-Pr_2NH (3.45 mL, 24.7 mmol, 1.1 equiv) in THF (22.5 mL) at 0 °C was added a solution *n*-BuLi (2.57 M in hexanes, 9.63 mL, 24.7 mmol, 1.1 equiv) dropwise. The resulting mixture was stirred at 0 °C for 20 min, then cooled to –78 °C. A solution of 1-(4-methoxyphenyl)pyrrolidin-2-one (4.30 g, 22.5 mmol, 1.0 equiv) in THF (60 mL) was added dropwise *via* cannula. The reaction was allowed to stir for 1 h at –78 °C, then a solution of MeI (2.10 mL, 33.75 mmol, 1.5 equiv) in MTBE (17 mL) was added dropwise *via* cannula. The resulting mixture was stirred for 3 h at –78 °C. The reaction was quenched with a saturated aqueous NH_4Cl solution and allowed to warm to ambient temperature. The aqueous layer was extracted four times with EtOAc, and the resulting organic layers were dried over Na_2SO_4 and concentrated. The resulting crude oil was purified by column chromatography (40% EtOAc in hexanes) to afford **1a** as a colorless solid (4.0 g, 19.5 mmol, 89% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, J = 9.1 Hz, 2H), 6.90 (d, J = 9.1 Hz, 1H), 3.80 (s, 3H), 3.78 – 3.68 (m, 1H), 2.74 – 2.57 (m, 1H), 2.36 (dddd, J = 12.3, 8.5, 6.7, 3.6 Hz, 1H), 1.76 (ddt, J = 12.5, 9.4, 8.6 Hz, 1H), 1.30 (d, J = 7.1 Hz, 3H). All characterization data match those reported.[1]



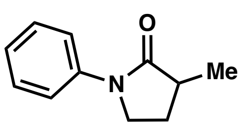
1b

1-(3,5-dimethoxyphenyl)-3-methylpyrrolidin-2-one (1b): Compound **1b** was prepared from **SI3** using a previously reported procedure;[1] ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.91 (d, *J* = 2.2 Hz, 2H), 6.26 (t, *J* = 2.2 Hz, 1H), 3.80 (s, 6H), 3.74 (dd, *J* = 8.8, 5.0 Hz, 2H), 2.67 (ddq, *J* = 9.7, 8.2, 7.0 Hz, 1H), 2.35 (ddt, *J* = 12.3, 8.4, 5.0 Hz, 1H), 1.75 (ddt, *J* = 12.4, 9.6, 8.8 Hz, 1H), 1.30 (d, *J* = 7.1 Hz, 3H). All characterization data match those reported.[1]



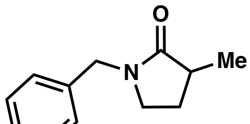
1c

1-(2-methoxyphenyl)-3-methylpyrrolidin-2-one (1c): Compound **1c** was prepared from **SI2** using a previously reported procedure;[1] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 (m, 2H), 7.08 – 6.89 (m, 2H), 3.83 (s, 3H), 3.76 – 3.60 (m, 2H), 2.64 (tq, *J* = 8.7, 7.1 Hz, 1H), 2.37 (dddd, *J* = 12.2, 8.5, 7.3, 3.5 Hz, 1H), 1.81 (dq, *J* = 12.4, 8.5 Hz, 1H), 1.31 (d, *J* = 7.2 Hz, 3H). All characterization data match those reported.[1]



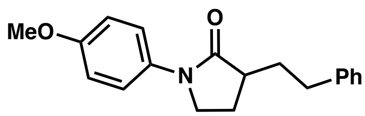
1d

3-methyl-1-phenylpyrrolidin-2-one (1d): Compound **1d** was prepared from **SI4** and iodomethane using General Procedure 1. The filtrate was recrystallized from 25% EtOAc in hexanes to afford **1d** as a colorless solid (3.2 g, 18.3 mmol, 74% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 – 7.61 (m, 2H), 7.41 – 7.33 (m, 2H), 7.14 (tt, *J* = 7.4, 1.1 Hz, 1H), 3.85 – 3.72 (m, 2H), 2.68 (ddq, *J* = 9.5, 8.5, 7.1 Hz, 1H), 2.38 (dddd, *J* = 12.2, 8.5, 6.6, 3.5 Hz, 1H), 1.78 (ddt, *J* = 12.4, 9.5, 8.6 Hz, 1H), 1.32 (d, *J* = 7.1 Hz, 3H). All characterization data match those reported.[5]



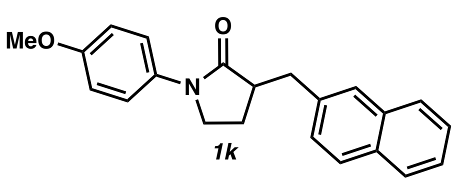
1f

1-benzyl-3-methylpyrrolidin-2-one (1f): Compound **1f** was prepared from **SI6** and iodomethane using General Procedure 1. The resulting crude oil was purified by column chromatography (5% MeOH in CH_2Cl_2) to afford **1f** as a yellow oil (4.1 g, 21.7 mmol, 70% yield); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.26 (s, 5H), 4.45 (d, *J* = 3.7 Hz, 2H), 3.23 – 3.09 (m, 2H), 2.52 (ddt, *J* = 15.8, 8.7, 7.1 Hz, 1H), 2.21 (dddd, *J* = 12.6, 8.7, 6.0, 4.8 Hz, 1H), 1.68 – 1.50 (m, 1H), 1.24 (d, *J* = 7.1 Hz, 3H). All characterization data match those reported.[6]



1j

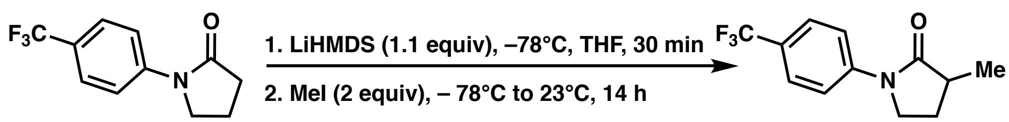
1-(4-methoxyphenyl)-3-phenethylpyrrolidin-2-one (1j): Compound **1j** was prepared from **SI1** and (2-iodoethyl)benzene using General Procedure 1. The resulting crude oil was purified by column chromatography (40% EtOAc in hexanes) to afford **1j** as a colorless solid (487 mg, 1.65 mmol, 33% yield); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58 – 7.47 (m, 2H), 7.36 – 7.14 (m, 5H), 6.96 – 6.83 (m, 2H), 3.80 (s, 3H), 3.78 – 3.69 (m, 2H), 2.93 – 2.66 (m, 2H), 2.59 (qd, *J* = 9.1, 4.7 Hz, 1H), 2.40 – 2.24 (m, 2H), 1.91 – 1.68 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.8, 156.8, 141.9, 133.2, 128.8, 126.3, 121.9, 114.3, 55.8, 47.5, 42.8, 33.7, 33.3, 25.4; IR (Neat Film, NaCl) 2930, 2855, 1677, 1518, 1456, 1393, 1318, 1255, 1224, 1181, 1121, 1034, 825, 752, 717, 699 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{19}H_{22}NO_2^+$ $[M+H]^+$: 296.1645, found 296.1646.



1k

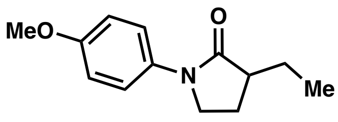
1-(4-methoxyphenyl)-3-(naphthalen-2-ylmethyl)pyrrolidin-2-one (1k): Product **1k** was prepared from **SI1** 2-(bromomethyl)naphthalene using General Procedure 1 and purified by column chromatography (33% EtOAc in hexanes) to provide **1k** as a colorless solid (430 mg, 1.30 mmol, 52% yield); ^{1}H NMR (500 MHz, CDCl3) δ 7.80 – 7.83 (m, 1H), 7.77 – 7.80 (m, 2H), 7.68 – 7.69 (m, 1H), 7.48 – 7.51 (m, 2H), 7.42 – 7.47 (m, 2H), 7.39 (dd, J = 8.4, 1.7 Hz, 1H), 6.89 – 6.92 (m, 2H), 3.81 (s, 3H), 3.68 (dt, J = 9.5, 7.8 Hz, 1H), 3.56 (ddd, J = 9.6, 8.7, 3.4 Hz, 1H), 3.47 (dd, J = 13.0, 3.4 Hz, 1H), 2.95 – 3.05 (m, 2H), 2.17 (dddd, J = 12.7, 8.4, 7.5, 3.3 Hz, 1H), 1.91 (dq, J = 12.7, 8.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 174.9, 156.7, 137.0, 133.7, 132.8, 132.4, 128.3, 127.8, 127.7, 127.6, 127.5, 126.2, 125.6, 121.9, 114.2, 55.6, 47.3, 45.0, 37.4, 24.3; IR (Neat Film, NaCl) 3048, 3014, 2953, 2836, 1677, 1516, 1399, 1328, 1285, 1256, 1180, 1032, 900, 824, 739 cm–1; HRMS (MM) m/z calc'd for $C_{22}H_{22}NO_2^+$ $[M+H]^+$: 332.1645, found 332.1648.

General Procedure 2: α-alkylation of N-substituted lactams with alkyl iodides:



1e

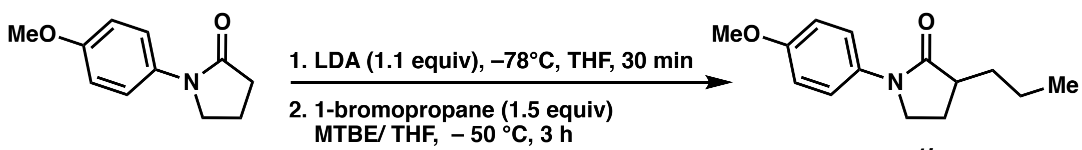
3-methyl-1-(4-(trifluoromethyl)phenyl)pyrrolidin-2-one (1e): To a solution of LiHMDS (1.61 g, 9.60 mmol, 1.1 equiv) in THF (44 mL) at –78 °C was added a solution of 1-(4-(trifluoromethyl)phenyl)pyrrolidin-2-one (2.0 g, 8.93 mmol, 1.0 equiv) in THF (4 mL) dropwise. The solution was stirred –78°C for 30 minutes, then iodomethane (1.11 mL, 17.86 mmol, 2 equiv) was added dropwise. The reaction was stirred at –48 °C for 30 minutes, then allowed to warm to ambient temperature overnight. The reaction mixture was quenched with a saturated NH_4Cl solution, and extracted with EtOAc three times. The combined organic extracts were washed with saturated $NaHCO_3$ solution, dried over Na_2SO_4, and concentrated. The resulting crude oil was purified by column chromatography (10% EtOAc in hexanes) to afford **1e** as a colorless solid (1.30 g, 5.34 mmol, 61% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 – 7.77 (m, 2H), 7.64 – 7.59 (m, 2H), 3.85 – 3.77 (m, 2H), 2.71 (ddq, J = 9.8, 8.5, 7.1 Hz, 1H), 2.42 (dddd, J = 12.7, 8.5, 5.7, 4.3 Hz, 1H), 1.81 (ddt, J = 12.5, 9.8, 8.7 Hz, 1H), 1.33 (d, J = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.10, 142.53, 125.96 (q, J = 3.7 Hz), 118.93, 46.31, 38.38, 26.86, 16.06; ^{19}F NMR (282 MHz, $CDCl_3$) δ –62.1; (Neat Film, NaCl) 2977, 1697, 1393, 1329, 1221, 1195, 1164, 1113, 1070, 908, 859, 842, 821, 731, 715 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{12}H_{13}F_3NO^+$ $[M+H]^+$: 244.0944, found 244.0947.



1h

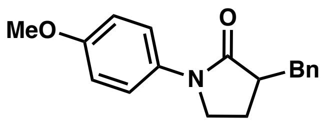
3-ethyl-1-(4-methoxyphenyl)pyrrolidin-2-one (1h): Compound **1h** was prepared from iodoethane using General Procedure 2. The resulting crude oil was purified by column chromatography (20% EtOAc in hexanes) to afford **1h** as a colorless solid (1.18 g, 5.38 mmol, 54% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 – 7.49 (m, 2H), 6.93 – 6.80 (m, 2H), 3.80 (s, 3H), 3.78 – 3.71 (m, 2H), 2.54 (qd, *J* = 8.9, 4.3 Hz, 1H), 2.32 (dddd, *J* = 12.5, 8.7, 7.1, 3.7 Hz, 1H), 1.98 (dqd, *J* = 13.6, 7.5, 4.3 Hz, 1H), 1.81 (dq, *J* = 12.5, 8.6 Hz, 1H), 1.58 – 1.47 (m, 1H), 1.02 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.0, 156.7, 133.2, 121.8, 114.3, 55.8, 44.9, 24.6, 24.5, 11.8; (Neat Film, NaCl) 3054, 2957, 2935, 2875, 2837, 1682, 1613, 1514, 1486, 1464, 1430, 1398, 1326, 1288, 1252, 1225, 1181, 1121, 1100, 1032, 829, 736, 704, 612 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{13}H_{18}NO_2^+$ [M+H]$^+$: 220.1332, found 220.1322.

General Procedure 3: α-alkylation of PMP-pyrrolidinone with alkyl bromides:



1i

1-(4-methoxyphenyl)-3-propylpyrrolidin-2-one (1i): To a solution of *i*-Pr_2NH (0.77 mL, 5.5 mmol, 1.1 equiv) in THF (5.0 mL) at 0 °C was added a solution *n*-BuLi (2.57 M in hexanes, 2.2 mL, 5.5 mmol, 1.1 equiv) dropwise. The resulting mixture was stirred at 0 °C for 20 min, then cooled to –78 °C. A solution of 1-(4-methoxyphenyl)pyrrolidin-2-one **SI1** (956 mg, 5.0 mmol, 1.0 equiv) in THF (12.5 mL) was added dropwise *via* cannula. The reaction was allowed to stir for 1 h at –78 °C, then a solution of 1-bromopropane (0.68 mL, 7.5 mmol, 1.5 equiv) in MTBE (4 mL) was added dropwise *via* cannula. The resulting mixture was stirred for 3 h at –50 °C. The reaction was then quenched with saturated NH_4Cl solution and allowed to warm to ambient temperature. The aqueous layer was extracted four times with EtOAc, and the resulting organic layers were dried over Na_2SO_4 and concentrated. The resulting crude oil was purified by column chromatography (40% EtOAc in hexanes) to afford **1i** as a colorless solid (210 mg, 0.90 mmol, 20% yield); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.56 – 7.46 (m, 2H), 6.94 – 6.86 (m, 2H), 3.80 (s, 3H), 3.78 – 3.70 (m, 2H), 2.59 (qd, J = 8.8, 4.1 Hz, 1H), 2.31 (dddd, J = 12.7, 8.7, 6.6, 4.1 Hz, 1H), 1.94 (qd, J = 5.9, 4.9, 3.4 Hz, 1H), 1.79 (dq, J = 12.5, 8.6 Hz, 1H), 1.52 – 1.34 (m, 3H), 0.97 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.2, 156.7, 133.3, 121.8, 114.3, 55.8, 47.5, 43.4, 33.8, 25.2, 20.8, 14.4; IR (Neat Film, NaCl) 2955, 2927, 2859, 2837, 1681, 1613, 1517, 1480, 1464, 1398, 1324, 1291, 1252, 1223, 1181, 1123, 1099, 1032, 909, 828, 732, 646, 614 cm^{-1}; HRMS (MM) m/z calc'd for $C_{14}H_{20}NO_2^+$ $[M+H]^+$: 234.1489, found 234.1494.



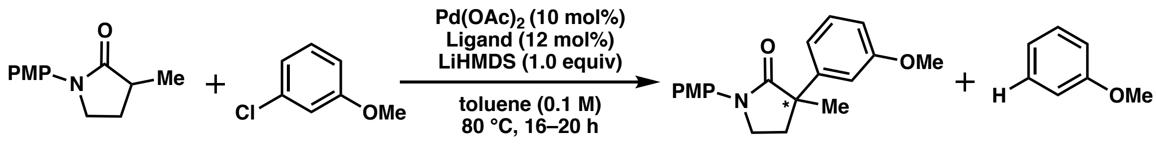
1g

3-benzyl-1-(4-methoxyphenyl)pyrrolidin-2-one (1g): Compound **1g** was prepared from benzyl bromide using General Procedure 3. The resulting crude oil was purified by column chromatography (20% EtOAc in hexanes) to afford **1g** as a colorless solid (2.25 g, 8.00 mmol, 80% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 – 7.44 (m, 2H), 7.33 – 7.28 (m, 2H), 7.26 – 7.21 (m, 3H), 6.95 – 6.86 (m, 2H), 3.81 (s, 3H), 3.68 (dt, J = 9.5, 7.7 Hz, 1H), 3.55 (ddd, J = 9.5, 8.6, 3.5 Hz, 1H), 3.31 (dd, J = 13.6, 4.0 Hz, 1H), 2.96 – 2.88 (m, 1H), 2.80 (dd, J = 13.7, 9.4 Hz, 1H), 2.17 (dddd, J = 12.3, 8.6, 7.5, 3.5 Hz, 1H), 1.86 (dq, J = 12.7, 8.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 175.1, 156.9, 139.7, 133.1, 129.4, 128.8, 126.7, 122.0, 114.3, 55.8, 47.5, 45.3, 37.4, 24.5; IR (Neat Film, NaCl) 2950, 2924, 2857, 2835, 1674, 1615, 1514, 1494, 1455, 1443, 1396, 1324, 1284, 1256, 1226, 1180, 1125, 1088, 1032, 824, 748, 733, 701, 618 cm^{-1}; HRMS (MM) m/z calc'd for $C_{18}H_{20}NO_2^+$ $[M+H]^+$: 282.1489, found 282.1500.

Additional Ligand Screen Results:

Procedure for evaluating ligands in the Pd-catalyzed α-arylation of lactam 1a: n = the number of reactions in the screen. In the glovebox, $Pd(OAc)_2$ (1.10n mg, 0.005n mmol, 0.100 equiv), toluene (0.25n mL), and a stir bar were added to a 4-mL vial A. To a separate 4-mL vial B was added LiHMDS (8.37n mg, 0.050n mmol, 1.00 equiv), lactam 15 (12.3n mg, 0.060n mmol, 1.20 equiv), toluene (0.25n mL), and a stir bar. The contents of A and B were stirred for ~2 minutes. To a separate vial was added the ligand (0.006 mmol, 0.120 equiv) and a stir bar followed by 0.25 mL of solution A. The ligand/Pd mixture was stirred for 10 minutes and 3-chloroanisole (7.1 mg, 6.1 μL, 0.050 mmol, 1.00 equiv) and 0.25 mL of solution B were added. The vial was sealed with a PTFE-lined cap and removed from the glovebox. The reaction mixture was heated at 80 °C and stirred for 16–20 h. The vial was cooled to room temperature and opened to air. A solution of 1,3,5-trimethoxybenzene (8.41 mg, 0.050 mmol, 1.00 equiv) in Et_2O (0.1 mL) was added as an internal standard. The reaction mixture was filtered through a short silica plug eluting with Et_2O (2 mL). An aliquot of the eluate was then removed for GC determination of 3-chloroanisole conversion with respect to 1,3,5-trimethoxybenzene. The remaining eluate was concentrated by rotary evaporator and dissolved in $CDCl_3$ to determine a ^1H NMR yield with respect to 1,3,5-trimethoxybenzene. Then, the sample was concentrated and purified by preparative TLC (30% EtOAc/hexanes). The purified product was then dissolved in hexanes for SFC analysis on a Chiralcel AD column (40% IPA/hexanes, 2.5 mL/min).

All racemic material was synthesized using the procedure described above, but with 10 mol% Pd(P*t*-Bu$_3$)$_2$ as the Pd catalyst.



1a 1.2 equiv

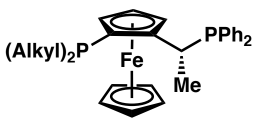
2i 1.0 equiv

3ai

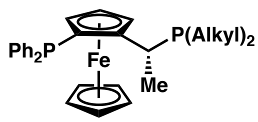
A

Entry	Ligand	Conv. (%)[a]	Yield (%)[b]	A (%)[a]	ee (%)[c]
1	SL-J004-1	61	27	5	45
2	SL-J502-1	37	< 5	28	–
3	SL-J002-1	88	8	40	–
4	SL-J004-1	62	16	6	18
5	SL-J009-1	41	< 5	25	–
6	SL-J015-1	24	20	5	–10
7	SL-J404-2	66	24	19	–8
8	SL-M004-1	65	47	12	–34
9	SL-M009-1	59	43	12	–48
10	SL-M003-1	14	8	19	–55
11	SL-M012-1	59	< 5	35	–
12	SL-M004-1	35	13	13	54
13	SL-W002-1	4	< 5	4	–
14	SL-W003-1	45	18	13	2
15	SL-W008-1	7	< 5	4	–
16	SL-T001-1	46	21	19	16
17	SL-T002-1	75	38	9	–12
18	(*R*)-SEGPHOS	< 5	< 5	5	–
19	(*S*)-*t*-Bu-Phox	< 5	< 5	< 5	–
20	(*R*)-Diop	8	7	< 5	–
21	(*S*,*R*)-Tangphos	58	6	10	–

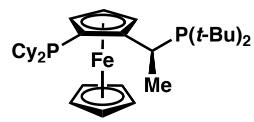
[a]Determined by GC using 1,3,5-trimethoxybenzene as an internal standard. [b]Determined by ^{1}HNMR using 1,3,5-trimethoxybenzene as an internal standard. [c]Determined by SFC, AD column, 40% IPA, 2.5 mL/min method.



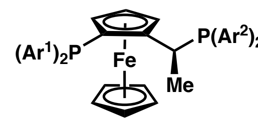
SL-J004-1: Alkyl = Cy
SL-J502-1: Alkyl = *t-Bu*



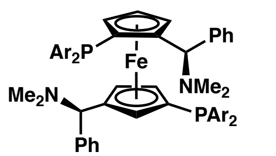
SL-J002-1: Alkyl = *t*-Bu
SL-J001-1: Alkyl = Cy



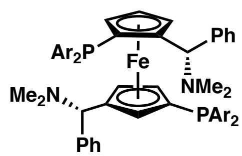
SL-J009-1



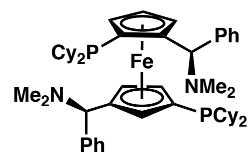
SL-J015-2: Ar[1] = 2-furyl, Ar[2] = 3,5-xylyl
SL-J404-2: Ar[1] = 3,5-xylyl, Ar[2] = 1-naphthyl



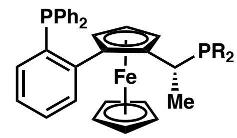
SL-M004-1: Ar = 4-methoxy-3,-5-dimethylphenyl
SL-M009-1: Ar = 3,-5-dixylyl
SL-M003-1: Ar = 3,5-ditrifluoromethylphenyl



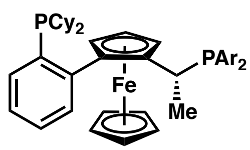
SL-M012-2: Ar = 2-tolyl
SL-M001-2: Ar = phenyl



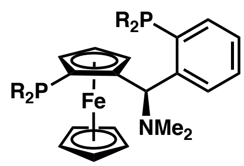
SL-M002-1



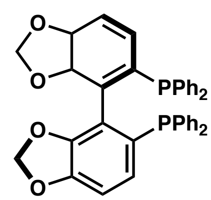
SL-W002-1: R = Ph
SL-W003-1: R = Cy



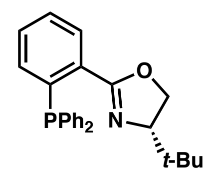
SL-W008-1: Ar = 3,5-ditrifluoromethylphenyl



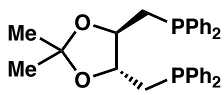
SL-T001-1: R = Ph
SL-T002-1: R = Cy



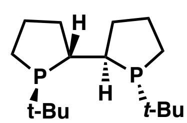
(*R*)-SEGPHOS



(*S*)-*t*-Bu-PHOX



(*R*,*R*)-DIOP



(*S*,*S'*,*R*,*R'*)-TangPhos

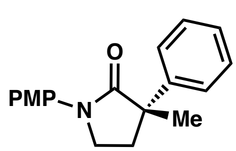
General Procedures for Pd-Catalyzed α-arylation of γ-lactams:

Method A: In a nitrogen-filled glovebox, to an oven-dried 4 mL vial equipped with a stir bar was added 1,1′-Bis[(2*S*,5*S*)-2,5-diethylphospholano]ferrocene **L1** (7.06 mg, 15 μmol, 0.075 equiv) and $Pd_2(pmdba)_3$ (5.5 mg, 5 μmol, 0.025 equiv), and dioxane (0.4 mL). The vial was capped with a PTFE-lined septum cap and stirred at 40 °C. After 20 minutes, the mixture was cooled to ambient temperature and the corresponding aryl chloride **2** (1.0 equiv) was added. A solution of protected-lactam **1** (1.5 equiv) and LiHMDS (50.2 mg, 0.3 mmol, 1.5 equiv) was then added to the resulting mixture, and the reaction sealed with electrical tape and stirred at 100 °C for 6 h, unless otherwise noted. The solution was cooled to ambient temperature, quenched with saturated NH_4Cl solution, and extracted with EtOAc five times. The combined organic layers were dried over Na_2SO_4 and concentrated. The crude reaction mixture was purified by silica gel flash chromatography to furnish the product.

Method B: In a nitrogen-filled glovebox, to an oven-dried 4 mL vial equipped with a stir bar was added 1,1′-Bis[(2*S*,5*S*)-2,5-dimethylphospholano]ferrocene **L2** (7.06 mg, 15 μmol, 0.075 equiv) and $Pd_2(pmdba)_3$ (5.5 mg, 5 μmol, 0.025 equiv), and dioxane (0.4 mL). The vial was capped with a PTFE-lined septum cap and stirred at 40 °C. After 20 minutes, the mixture was cooled to ambient temperature and the corresponding aryl bromide **2** (1.0 equiv) was added. A solution of protected-lactam **1** (1.5 equiv) and NaHMDS (55.0 mg, 0.3 mmol, 1.5 equiv) was added to the resulting mixture, and the reaction sealed with electrical tape and stirred at 80 °C for 15 h, unless otherwise noted. The solution was cooled to ambient temperature, quenched with saturated NH_4Cl solution, and extracted with EtOAc five times. The combined organic layers were dried over Na_2SO_4 and concentrated. The crude reaction mixture was purified by silica gel flash chromatography to furnish the product.

Spectroscopic Data for Products from Catalytic Reactions

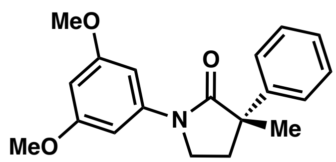
<u>*Please note*</u> that the absolute configuration was determined only for compound **3ab** *via* x-ray crystallographic analysis. The absolute configuration for all other products has been inferred by analogy.



3aa

(*S*)-1-(4-methoxyphenyl)-3-methyl-3-phenylpyrrolidin-2-one (3aa): Product **3aa** was prepared using Method A and purified by column chromatography (25% EtOAc in hexanes) to provide a colorless oil (34.9 mg, 0.124 mmol, 65% yield); 94% *ee*; $[\alpha]_D^{25}$ – 284.5 (*c* 0.98, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.42 (m, 2H), 7.40 – 7.30 (m, 2H), 7.32 – 7.12 (m, 3H), 6.91 – 6.79 (m, 2H), 3.73 (s, 3H), 3.64 (qdd, *J* = 9.6, 8.0, 5.3 Hz, 2H), 2.50 (ddd, J = 12.7, 6.7, 3.9 Hz, 1H), 2.20 (dt, J = 12.7, 8.0 Hz, 1H), 1.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.6, 156.9, 143.6, 133.3, 128.9, 127.2, 126.4, 121.8, 114.3, 55.8, 50.3, 45.9, 35.2, 25.8; IR (Neat Film, NaCl) 3057, 2932, 2963, 2874, 1690, 1511, 1429, 1463, 1396, 1321, 1299, 1248, 1181, 1088, 1070, 1032, 881, 829, 768, 699, 634 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{18}H_{20}NO_2^+$ $[M+H]^+$: 282.1489, found 282.1490; SFC Conditions: 20% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 5.69, major = 6.73.

Method B: Product **3aa** was prepared using Method B. The crude product was purified by column chromatography to provide a yellow solid (46.9 mg, 0.167 mmol, 83% yield); 92% *ee*; $[\alpha]_D^{25}$ –284.0 (*c* 0.70, $CHCl_3$); SFC Conditions: 20% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 5.70, major = 6.70.

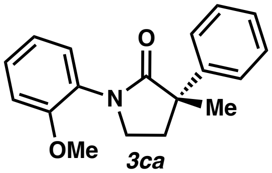


3ba

(*S*)-1-(3,5-dimethoxyphenyl)-3-methyl-3-phenylpyrrolidin-2-one (3ba): Product **3ba** was prepared using general Method A, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography (33% EtOAc in hexanes) to provide a colorless oil (33.1 mg, 0.106 mmol, 53% yield); 89% *ee*; $[\alpha]_D^{25}$ –123.4 (*c* 1.00, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.43 (m, 2H), 7.32 – 7.36 (m, 2H), 7.25 (ddt, J = 8.0, 6.6, 1.2 Hz, 1H), 6.98 (d, J = 2.2 Hz, 2H), 6.29 (t, J = 2.2 Hz, 1H), 3.80 (s, 6H), 3.75 (ddd, J = 9.6, 8.1, 3.7 Hz, 1H), 3.70 (ddd, J = 9.6, 8.1, 6.9 Hz, 1H), 2.58 (ddd, J = 12.7, 6.9, 3.7 Hz, 1H), 2.26 (dt, J = 12.7, 8.1 Hz, 1H), 1.64 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.3, 161.2, 143.2, 141.8, 129.0, 127.2, 126.4, 98.3, 97.0, 55.7, 50.9, 45.7, 34.8, 25.7; IR (Neat Film, NaCl) 3057, 2962, 2934, 2841, 1699, 1598, 1479, 1459, 1447, 1391, 1275, 1249, 1208, 1155, 1067, 835, 701 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{19}H_{22}NO_3^+$ $[M+H]^+$: 312.1594, found 312.1594; SFC Conditions: 20% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 5.29, major= 6.47.

Method B: Product **3ba** was prepared using Method B, allowing the reaction to stir for 20 h. The crude reaction was purified by column chromatography to provide a yellow solid (52.9 mg, 0.170 mmol, 85% yield); 92% *ee*; $[\alpha]_D^{25}$ –141.0 (*c* 1.00, $CHCl_3$); SFC

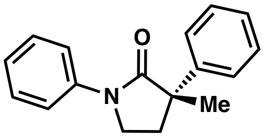
Conditions: 20% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 5.31, major= 6.44.



3ca

(*S*)-1-(2-methoxyphenyl)-3-methyl-3-phenylpyrrolidin-2-one (3ca): Product **3ca** was prepared using general Method A, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography (33% EtOAc in hexanes) to provide a colorless oil (18.3 mg, 65 μmol, 33% yield); 79% *ee*; $[\alpha]_D^{25}$ – 44.7 (*c* 1.00, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 – 7.55 (m, 2H), 7.34 – 7.38 (m, 2H), 7.24 – 7.30 (m, 3H), 6.95 – 7.01 (m, 2H), 3.83 (s, 3H), 3.63 – 3.71 (m, 2H), 2.56 (ddd, *J* = 12.6, 6.9, 4.5 Hz, 1H), 2.34 (dt, *J* = 12.5, 7.7 Hz, 1H), 1.66 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.8, 155.3, 144.2, 129.1, 129.0, 128.7, 127.9, 126.9, 126.7, 121.2, 112.4, 55.9, 49.1, 46.9, 36.7, 25.6; IR (Neat Film, NaCl) 3060, 2964, 2927, 1698, 1597, 1504, 1461, 1406, 1304, 1280, 1252, 1122, 1025, 752, 700 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{18}H_{20}NO_2^+$ $[M+H]^+$: 282.1489, found 282.1492; SFC Conditions: 20% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 210 nm, t_R (min): minor = 4.85, major = 6.04.

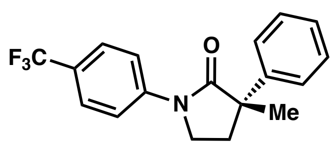
Method B: Product **3ba** was prepared using Method B, allowing the reaction to stir for 20 h. The crude reaction was purified by column chromatography to provide a yellow solid (26.7 mg, 0.1 mmol, 47% yield); 90% *ee*; $[\alpha]_D^{25}$ –64.5 (*c* 0.84, $CHCl_3$); SFC Conditions: 20% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 210 nm, t_R (min): minor = 4.80, major= 5.83.



3da

(*S*)-3-methyl-1,3-diphenylpyrrolidin-2-one (3da): Product **3da** was prepared using general Method A, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography (33% EtOAc in hexanes) to provide a yellow oil (29.3 mg, 0.117 mmol, 58% yield); 90% *ee*; $[\alpha]_D^{25}$ –87.2 (*c* 1.00, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 – 7.72 (m, 2H), 7.44 – 7.46 (m, 2H), 7.37 – 7.41 (m, 2H), 7.33 – 7.37 (m, 2H), 7.24 – 7.28 (m, 1H), 7.15 – 7.18 (m, 1H), 3.79 (ddd, *J* = 9.6, 8.0, 3.7 Hz, 1H), 3.74 (ddd, *J* = 9.6, 8.1, 6.9 Hz, 1H), 2.60 (ddd, *J* = 12.6, 6.8, 3.7 Hz, 1H), 2.29 (dt, *J* = 12.7, 8.0 Hz, 1H), 1.65 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.0, 143.4, 139.9, 129.1, 128.9, 127.2, 126.4, 124.8, 120.1, 50.5, 45.5, 35.0, 25.7; IR (Neat Film, NaCl) 3061, 3030, 2967, 2928, 2875, 1710, 1694, 1597, 1494, 1458, 1445, 1393, 1304, 1225, 1091, 1072, 1031, 901, 878, 759, 699 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{17}H_{18}NO^+$ $[M+H]^+$: 252.1383, found 252.1385; SFC Conditions: 10% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 9.96, major = 10.52.

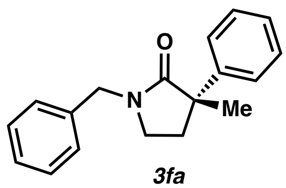
Method B: Product **3da** was prepared using Method B, allowing the reaction to stir for 20 h. The crude reaction mixture was purified by column chromatography to provide a yellow oil (45.8 mg, 0.182 mmol, 91% yield); 93% *ee*; $[\alpha]_D^{25}$ –82.6 (*c* 1.00, $CHCl_3$); SFC Conditions: 10% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 10.51, major = 11.01.



3ea

(*S*)-3-methyl-3-phenyl-1-(4-(trifluoromethyl)phenyl)pyrrolidin-2-one (3ea): Product **3ea** was prepared using general Method A, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography (33% EtOAc in hexanes) to provide a yellow oil (25.3 mg, 79 µmol, 40% yield); 73% *ee*; $[\alpha]_D^{25}$ –92.0 (*c* 1.00, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 – 7.87 (m, 2H), 7.61 – 7.65 (m, 2H), 7.41 – 7.43 (m, 2H), 7.33 – 7.37 (m, 2H), 7.25 – 7.28 (m, 1H), 3.81 (ddd, *J* = 9.5, 8.0, 3.6 Hz, 1H), 3.75 (ddd, *J* = 9.5, 8.2, 6.9 Hz, 1H), 2.65 (ddd, *J* = 12.8, 6.9, 3.6 Hz, 1H), 2.31 (dt, *J* = 12.8, 8.1 Hz, 1H), 1.65 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.6, 142.9, 129.1, 127.4, 126.6 – 126.2 (m), 125.5, 123.4, 119.4, 50.7, 45.3, 34.7, 25.8; ^{19}F (282 MHz, CDCl3) δ –62.1; IR (Neat Film, NaCl) 2925, 1700, 1614, 1520, 1490, 1457, 1387, 1321, 1222, 1163, 1117, 1064, 1012, 839, 765, 698 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{18}H_{17}F_3NO^+$ $[M+H]^+$: 320.1257, found 320.1260; SFC Conditions: 20% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 3.03, major = 3.23.

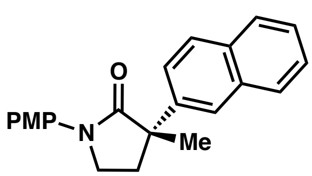
Method B: Product **3ea** was prepared using Method B, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography to provide a yellow oil (40.9 mg, 0.128 mmol, 64% yield); 56% *ee*; $[\alpha]_D^{25}$ –16.9 (*c* 1.00, $CHCl_3$); SFC Conditions: 20% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 2.95, major = 3.14.



3fa

(*S*)-1-benzyl-3-methyl-3-phenylpyrrolidin-2-one (3fa): Product **3fa** was prepared using Method A, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography (33% EtOAc in hexanes) to provide a yellow oil (23.0 mg, 87 μmol, 43% yield); 95% *ee*; $[\alpha]_D^{25}$ –21.4 (*c* 1.00, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.43 (m, 2H), 7.30 – 7.31 (m, 4H), 7.27 – 7.30 (m, 1H), 7.22 – 7.26 (m, 3H), 4.55 (d, *J* = 14.7 Hz, 1H), 4.52 (d, *J* = 14.9 Hz, 1H), 3.15 – 3.22 (m, 2H), 2.41 (ddd, *J* = 12.8, 6.7, 5.2 Hz, 1H), 2.12 (ddd, *J* = 12.8, 7.9, 7.1 Hz, 1H), 1.58 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.7, 144.1, 136.9, 129.0, 128.8, 128.5, 127.9, 127.0, 126.4, 49.1, 47.3, 43.7, 35.7, 25.4; IR (Neat Film, NaCl) 3059, 3028, 2964, 2925, 2868, 1686, 1494, 1425, 1269, 1078, 1029, 766, 747, 699 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{18}H_{20}NO^+$ $[M+H]^+$: 266.1539, found 266.1541; SFC Conditions: 20% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 210 nm, t_R (min): minor = 6.24, major = 6.48.

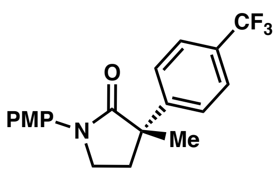
Method B: Product **3fa** was prepared using Method B, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography to provide a yellow oil (29.1 mg, 0.110 mmol, 55% yield); 92% *ee*; $[\alpha]_D^{25}$ –17.7 (*c* 1.00, $CHCl_3$); SFC Conditions: 20% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 210 nm, t_R (min): minor = 6.14, major = 6.47.



3ab

(*S*)-1-(4-methoxyphenyl)-3-methyl-3-(naphthalen-2-yl)pyrrolidin-2-one (3ab): Product **3ab** was prepared using Method A and purified by column chromatography (25% EtOAc in hexanes) to provide a colorless oil (54.8 mg, 0.165 mmol, 83% yield); 94% *ee*; $[\alpha]_D^{25}$ –159.0 (*c* 0.70, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.83 (m, 2H), 7.82 – 7.78 (m, 2H), 7.63 – 7.58 (m, 3H), 7.50 – 7.41 (m, 2H), 6.96 – 6.90 (m, 2H), 3.81 (s, 3H), 3.78 – 3.70 (m, 2H), 2.70 (ddd, *J* = 12.6, 6.6, 4.0 Hz, 1H), 2.35 (dt, *J* = 12.7, 8.0 Hz, 1H), 1.73 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.5, 156.9, 140.9, 133.5, 133.2, 132.6, 128.8, 128.4, 127.8, 126.5, 126.2, 125.0, 124.9, 122.0, 114.4, 55.8, 50.6, 46.0, 35.2, 25.8; IR (Neat Film, NaCl) 3054, 2964, 2834, 1689, 1512, 1396, 1290, 1299, 1248, 1182, 1093, 1033, 951, 859, 827, 751, 639 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{22}H_{22}NO_2^+$ $[M+H]^+$: 332.1645, found 332.1649; SFC Conditions: SFC Conditions: 30% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 5.71, major = 7.18.

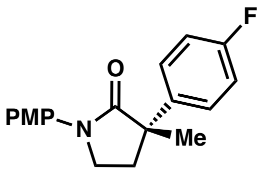
Method B: Product **3ab** was prepared using Method B. The crude product was purified by column chromatography to provide a colorless oil (50 mg, 0.151 mmol, 75% yield); 93% *ee*; $[\alpha]_D^{25}$ –176.0 (*c* 0.70, $CHCl_3$); SFC Conditions: 30% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 5.69, major = 7.12.



3ac

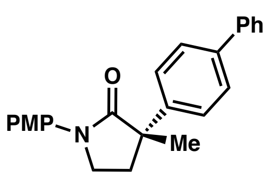
(*S*)-1-(4-methoxyphenyl)-3-methyl-3-(4-(trifluoromethyl)phenyl)pyrrolidin-2-one (3ac): Product **3ac** was prepared using Method A and purified by column chromatography (25% EtOAc in hexanes) to provide a colorless oil (61.5 mg, 0.176 mmol, 88% yield); 94% *ee*; $[\alpha]_D^{25}$ –109.8 (*c* 0.70, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.49 (m, 6H), 7.03 – 6.80 (m, 2H), 3.81 (s, 3H), 3.80 (m, 2H), 2.57 (ddd, *J* = 12.8, 7.1, 4.4 Hz, 1H), 2.32 (ddd, *J* = 12.8, 7.9, 7.2 Hz, 1H), 1.65 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.8, 157.1 147.8, 132.9, 129.5 (q, *J* = 32.5 Hz), 127.0, 125.9 (q, *J* = 3.8 Hz), 122.0, 114.4, 55.8, 50.3, 45.8, 34.9, 25.6; ^{19}F NMR (282 MHz, $CDCl_3$) δ –62.5; IR (Neat Film, NaCl) 2965, 2935, 1691, 1618, 1513, 1455, 1444, 1398, 1328, 1300, 1250, 1165, 1121, 1078, 1068, 1035, 1016, 829, 708, 618 cm^{-1}; HRMS (MM) *m/z* calc'd for

$C_{19}H_{19}F_3NO_2^+$ [M+H]$^+$: 350.1362, found 350.1367; SFC Conditions: 30% IPA, 2.5 mL/min, Chiralpak AD-H column, λ = 254 nm, t_R (min): minor: 3.80, major = 7.12.



3ad

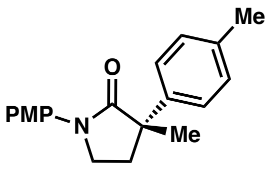
(*S*)-3-(4-fluorophenyl)-1-(4-methoxyphenyl)-3-methylpyrrolidin-2-one (3ad): Product **3ad** was prepared using Method A and purified by column chromatography (25% EtOAc in hexanes) to provide a colorless oil (19.5 mg, 65 μmol, 33% yield); 93% *ee*; $[\alpha]_D^{25}$ –109.9 (*c* 0.6, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.50 (m, 2H), 7.47 – 7.34 (m, 2H), 7.07 – 6.96 (m, 2H), 6.96 – 6.87 (m, 2H), 3.81 (s, 3H), 3.85 – 3.63 (m, 2H), 2.59 – 2.48 (m, 1H), 2.28 (dt, *J* = 12.7, 7.8 Hz, 1H), 1.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.4, 163.2, 160.8, 157.0, 139.4 (d, *J* = 3.2 Hz), 128.1 (d, *J* = 8.0 Hz), 121.9, 115.7 (d, *J* = 21.2 Hz), 114.4, 55.8, 49.8, 45.8, 35.2, 25.9; ^{19}F NMR (282 MHz, $CDCl_3$) δ –116.2; IR (Neat Film, NaCl) 2959, 2926, 1689, 1602, 1509, 1463,1454, 1443, 1397, 1299, 1290, 1248, 1181, 1165, 1085, 1072, 1034, 1015, 830, 750, 621 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{18}H_{19}FNO_2^+$ [M+H]$^+$: 300.1394, found 300.1404; SFC Conditions: 30% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 210 nm, t_R (min): minor = 2.78, major = 3.11.



3ae

(*S*)-3-([1,1'-biphenyl]-4-yl)-1-(4-methoxyphenyl)-3-methylpyrrolidin-2-one (3ae): Product **3ae** was prepared using method A and purified by column chromatography (25% EtOAc in hexanes) to provide a colorless oil (55.4 mg, 0.155 mmol, 78% yield); 97% *ee*; $[\alpha]_D^{25}$ –129.1 (*c* 0.94, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.53 (m, 6H), 7.54 – 7.48 (m, 2H), 7.47 – 7.40 (m, 2H), 7.37 – 7.30 (m, 1H), 6.95 – 6.88 (m, 2H), 3.81 (s, 3H), 3.79 – 3.70 (m, 2H), 2.63 (ddd, *J* = 12.7, 6.5, 4.3 Hz, 1H), 2.31 (d, *J* = 12.7 Hz, 1H), 1.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ176.6, 156.9, 142.7, 141.0, 140.1, 133.2, 129.1, 127.6, 127.4, 126.9, 121.9, 114.4, 55.8, 53.8, 50.1, 45.9, 35.1, 25.7; IR (Neat Film, NaCl)

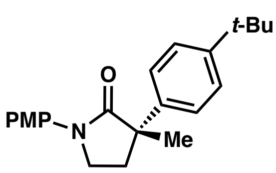
3028, 2963, 2932, 1689, 1511, 1486, 1396, 1289, 1299, 1248, 1181, 1086, 1034, 1007, 829, 768, 733 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{24}H_{24}NO_2^+$ [M+H]$^+$: 358.1802, found 358.1808; SFC Conditions: 30% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min):, minor = 7.40, major = 8.83.



3af

(*S*)-1-(4-methoxyphenyl)-3-methyl-3-(*p*-tolyl)pyrrolidin-2-one (3af): Product **3af** was prepared using Method A and purified by column chromatography (25% EtOAc in hexanes) to provide a colorless oil (28.8 mg, 98 µmol, 49% yield); 91% *ee*; $[\alpha]_D^{25}$ –64.6 (*c* 0.50, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 – 7.52 (m, 2H), 7.35 – 7.29 (m, 2H), 7.20 – 7.11 (m, 2H), 6.96 – 6.87 (m, 2H), 3.81 (s, 3H), 3.76 – 3.63 (m, 2H), 2.56 (ddd, *J* = 12.7, 6.5, 3.9 Hz, 1H), 2.32 (s, 3H), 2.26 (dt, *J* = 12.6, 8.1 Hz, 1H), 1.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.8, 156.8, 140.6, 136.8, 133.3, 129.6, 126.3, 121.8, 114.3, 55.8, 50.0, 45.9, 35.2, 25.8, 21.3; IR (Neat Film, NaCl) 2960, 1689, 1511, 1452, 1395, 1289, 1249, 1182, 1086, 1031, 828, 749 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{19}H_{22}NO_2^+$ [M+H]$^+$: 296.1645, found 296.1650; SFC Conditions: 30% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 3.29, major = 3.63.

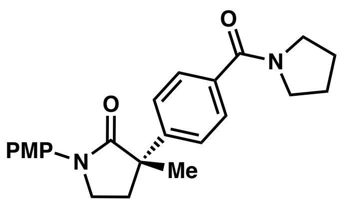
Method B: Product **3af** was prepared using Method B. The crude product was purified by column chromatography to provide a colorless oil (33.6 mg, 0.114 mmol, 57% yield); 95% *ee*; $[\alpha]_D^{25}$ –125.8 (*c* 0.70, $CHCl_3$); SFC Conditions: 30% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 3.56, major = 3.93.



3ag

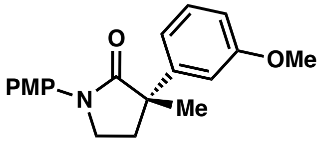
(*S*)-3-(4-(*tert*-butyl)phenyl)-1-(4-methoxyphenyl)-3-methylpyrrolidin-2-one (3ag): Product **3ag** was prepared using Method A and purified by column chromatography (25% EtOAc in hexanes) to provide a colorless oil (39.9 mg, 0.118 mmol, 60% yield); 91% *ee*; $[\alpha]_D^{25}$ –121.0 (*c* 0.93, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.55 (m, 2H), 7.35

(d, J = 0.6 Hz, 4H), 6.97 – 6.84 (m, 2H), 3.80 (s, 3H), 3.73 (ddd, J = 8.2, 5.4, 3.1 Hz, 2H), 2.58 (ddd, J = 12.6, 6.4, 4.3 Hz, 1H), 2.26 (dt, J = 12.7, 7.9 Hz, 1H), 1.62 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.9, 156.8, 149.9, 140.5, 133.4, 126.1, 125.8, 121.8, 114.3, 55.8, 49.9, 45.9, 35.1, 34.7, 31.6, 25.7; IR (Neat Film, NaCl) 2962, 2869, 1693, 1512, 1396, 1363, 1321, 1290, 1299, 1249, 1182, 1121, 1086, 1034, 829, 796, 758, 618 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{22}H_{28}NO_2^+$ [M+H]$^+$: 338.2115, found 338.2120; SFC Conditions: 30% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): major = 3.35, minor = 4.06.



3ah

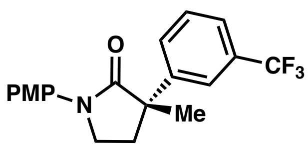
(*S*)-1-(4-methoxyphenyl)-3-methyl-3-(4-(pyrrolidine-1 carbonyl)phenyl)pyrrolidin-2-one (3ah): Product **3ah** was prepared using Method B and purified by column chromatography (25% EtOAc in hexanes) to provide a colorless oil (65.9 mg, 0.174 mmol, 87% yield); 81% *ee*; $[\alpha]_D^{25}$ –89.2 (*c* 0.70, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.54 (m, 2H), 7.51 – 7.43 (m, 4H), 6.97 – 6.89 (m, 2H), 3.80 (s, 3H), 3.77 – 3.66 (m, 2H), 3.63 (t, J = 7.0 Hz, 2H), 3.42 (t, J = 6.6 Hz, 2H), 2.54 (ddd, J = 12.7, 6.9, 3.9 Hz, 1H), 2.28 (dt, J = 12.7, 7.9 Hz, 1H), 2.00 – 1.92 (m, 2H), 1.91 – 1.79 (m, 2H), 1.63 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.3, 169.7, 157.0, 145.4, 136.1, 133.0, 127.7, 126.4, 121.9, 114.4, 55.8, 50.3, 50.0, 46.5, 45.9, 35.1, 26.7, 25.6, 24.8; IR (Neat Film, NaCl) 2968, 2876, 1689, 1623, 1562, 1512, 1426, 1398, 1298, 1249, 1182, 1116, 1085, 1033, 933, 830, 749, 707, 663 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{23}H_{27}N_2O_3^+$ [M+H]$^+$: 379.2016, found 379.2011; SFC Conditions: 30% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 9.00, major =10.34.



3ai

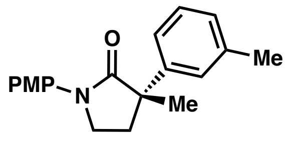
(*S*)-3-(3-methoxyphenyl)-1-(4-methoxyphenyl)-3-methylpyrrolidin-2-one (3ai):

Product **3ai** was prepared using Method A and purified by column chromatography (25% EtOAc in hexanes) to provide a colorless oil (43.0 mg, 0.138 mmol, 69% yield); 86% *ee*; $[\alpha]_D^{25}$ –109.9 (*c* 0.70, $CHCl_3$); ^1H NMR (300 MHz, $CDCl_3$) δ 7.62 – 7.53 (m, 2H), 7.30 – 7.21 (m, 1H), 7.05 – 6.98 (m, 2H), 6.95 – 6.86 (m, 2H), 6.79 (ddd, *J* = 8.2, 2.3, 1.1 Hz, 1H), 3.80 (s, 3H), 3.79 (s, 3H), 3.77 – 3.67 (m, 2H), 2.57 (ddd, *J* = 12.7, 6.5, 4.2 Hz, 1H), 2.26 (dt, *J* = 12.7, 8.0 Hz, 1H), 1.62 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.5, 160.1, 156.9, 145.3, 133.2, 129.9, 121.9, 118.8, 114.4, 112.8, 112.1, 55.8, 55.6, 50.3, 45.9, 35.2, 25.8; IR (Neat Film, NaCl) 3052, 2962, 2935, 2836, 1693, 1682, 1600, 1582, 1513, 1488, 1456, 1464, 1430, 1395, 1320, 1290, 1247, 1181, 1124, 1089, 1036, 932, 914, 882, 829, 792, 751, 701, 667, 637 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{19}H_{22}NO_3^+$ $[M+H]^+$: 312.1594, found 312.1590; SFC Conditions: 30% IPA, 4.0 mL/min, Chiralpak AD-H column, λ = 254 nm, t_R (min): minor = 4.06, major = 5.81.



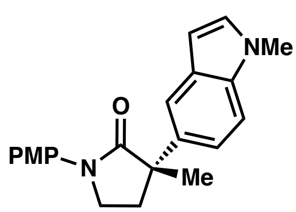
3aj

(*S*)-1-(4-methoxyphenyl)-3-methyl-3-(3-(trifluoromethyl)phenyl)pyrrolidin-2-one (3aj): Product **3aj** was prepared using Method A and purified by column chromatography (20% EtOAc in hexanes) to provide a colorless oil (53.3 mg, 0.153 mmol, 75% yield); 96% *ee*; $[\alpha]_D^{25}$ –105.7 (*c* 0.93, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.70 (m, 1H), 7.67 (dddd, *J* = 7.8, 1.9, 1.3, 0.6 Hz, 1H), 7.61 – 7.40 (m, 4H), 6.97 – 6.89 (m, 2H), 3.81 (s, 4H), 3.75 – 3.69 (m, 1H), 2.58 (ddd, *J* = 12.8, 7.3, 4.7 Hz, 1H), 2.33 (ddd, *J* = 12.9, 7.9, 6.9 Hz, 1H), 1.65 (d, *J* = 1.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.9, 157.1, 144.8, 132.9, 131.2 (q, *J* = 32.0 Hz), 130.2, 129.4, 127.0, 126.2 – 125.6 (m), 124.3 – 124.0 (m), 123.2 (q, *J* = 3.8 Hz), 122.0, 114.4, 55.8, 50.1, 45.9, 34.9, 25.7; ^{19}F NMR (282 MHz, $CDCl_3$) δ –62.5; IR (Neat Film, NaCl) 2932, 2962, 2838, 1721, 1692, 1681, 1512, 1504, 1493, 1442, 1400, 1329, 1299, 1249, 1163, 1119, 1075, 1034, 829, 802, 702 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{19}H_{19}F_3NO_2^+$ $[M+H]^+$: 350.1362, found 350.1359; SFC Conditions: 30% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 2.52, major = 2.97.



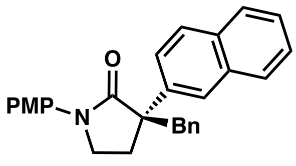
3ak

(*S*)-1-(4-methoxyphenyl)-3-methyl-3-(*m*-tolyl)pyrrolidin-2-one (3ak): Product **3ak** was prepared using Method B and purified by column chromatography (25% EtOAc in hexanes) to provide a colorless oil (41.4 mg, 0.140 mmol, 70% yield); 97% *ee*; $[\alpha]_D^{25}$ –209.3 (*c* 0.79, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 9.2 Hz, 2H), 7.31 – 7.18 (m, 3H), 7.06 (t, *J* = 5.5 Hz, 1H), 6.92 (d, *J* = 9.2 Hz, 2H), 3.81 (s, 3H), 3.76 – 3.67 (m, 2H), 2.64 – 2.51 (m, 1H), 2.35 (s, 3H), 2.26 (dt, *J* = 12.7, 8.0 Hz, 1H), 1.62 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.7, 156.8, 143.5, 138.5, 133.3, 128.8, 127.9, 127.2, 123.4, 121.8, 114.3, 55.8, 50.2, 45.9, 35.3, 25.8, 22.0; IR (Neat Film, NaCl) 2962, 2962, 1690, 1606, 1586, 1512, 1488, 1444, 1429, 1396, 1321, 1299, 1249, 1182, 1124, 1086, 1034, 932, 882, 829, 788, 750, 704, 641, 612; HRMS (MM) *m/z* calc'd for $C_{19}H_{22}NO_2^+$ $[M+H]^+$: 296.1645, found 296.1645; SFC Conditions: 30% IPA, 2.5 mL/min, Chiralpak AD-H column, λ = 254 nm, t_R (min): major = 5.47, minor = 7.72.



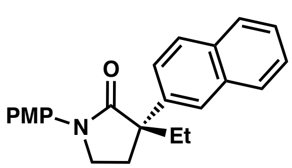
3al

(*S*)-1-(4-methoxyphenyl)-3-methyl-3-(1-methyl-1*H*-indol-6-yl)pyrrolidin-2-one (3al): Product **3al** was prepared using Method B and purified by column chromatography (25% EtOAc in hexanes) to provide a colorless oil (29.2 mg, 87 µmol, 44% yield); 92% *ee*; $[\alpha]_D^{25}$ –94.5 (*c* 0.70, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 1.9, 0.8 Hz, 1H), 7.64 – 7.56 (m, 2H), 7.38 – 7.27 (m, 2H), 7.03 (d, *J* = 3.1 Hz, 1H), 6.95 – 6.88 (m, 2H), 6.44 (dd, *J* = 3.1, 0.8 Hz, 1H), 3.81 (s, 3H), 3.77 (s, 3H), 3.71 (dd, *J* = 8.3, 4.9 Hz, 2H), 2.67 (dt, *J* = 12.6, 5.0 Hz, 1H), 2.31 (dt, *J* = 12.6, 8.3 Hz, 1H), 1.69 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.3, 156.7, 135.9, 134.3, 133.5, 129.5, 128.7, 121.8, 120.5, 118.3, 114.3, 109.7, 101.4, 55.8, 50.4, 46.0, 35.8, 33.2, 26.5; IR (Neat Film, NaCl) 2961, 1688, 1614, 1511, 1490, 1394, 1294, 1248, 1181, 1124, 1089, 1034, 884, 827, 798, 730, 654 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{21}H_{23}N_2O_2^+$ $[M+H]^+$: 335.1754, found 335.1752; SFC Conditions: 30% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 2.75, major = 5.48.



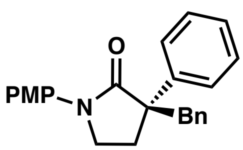
3gb

(*S*)-3-benzyl-1-(4-methoxyphenyl)-3-(naphthalen-2-yl)pyrrolidin-2-one (3gb): Product **3gb** was prepared using general Method A, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography (33% EtOAc in hexanes) to provide a colorless solid (47.7 mg, 0.117 mmol, 59% yield); 91% *ee*; $[\alpha]_D^{25}$ –172.6 (*c* 1.00, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, *J* = 2.0 Hz, 1H), 7.86 (d, *J* = 8.8 Hz, 1H), 7.80 – 7.85 (m, 2H), 7.72 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.46 – 7.49 (m, 2H), 7.41 – 7.45 (m, 2H), 7.21 – 7.23 (m, 3H), 7.15 – 7.17 (m, 2H), 6.87 – 6.90 (m, 2H), 3.79 (s, 3H), 3.51 – 3.56 (m, 2H), 3.24 – 3.29 (m, 2H), 2.60 (ddd, *J* = 12.9, 7.1, 3.7 Hz, 1H), 2.48 (dt, *J* = 13.0, 7.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 175.1, 157.0, 139.4, 137.6, 133.5, 133.0, 132.7, 130.8, 128.6, 128.6, 128.5, 127.7, 127.0, 126.4, 126.3, 125.6, 125.6, 122.3, 114.3, 55.8, 55.2, 46.1, 45.7, 30.2; IR (Neat Film, NaCl) 3058, 2951, 2929, 2836, 1687, 1600, 1512, 1454, 1397, 1321, 1299, 1249, 1181, 1036, 828, 749, 703 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{28}H_{26}NO_2^+$ $[M+H]^+$: 408.1958, found 408.1962; SFC Conditions: 30% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): major = 8.16, minor = 9.63.



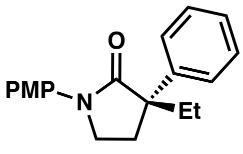
3hb

(*S*)-3-ethyl-1-(4-methoxyphenyl)-3-(naphthalen-2-yl)pyrrolidin-2-one (3hb). Product **3hb** was prepared using Method A, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography (33% EtOAc in hexanes) to provide yellow oil (31.3 mg, 91 μmol, 46% yield); 93% *ee*; $[\alpha]_D^{25}$ –167.2 (*c* 1.00, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$) δ 7.91 – 7.93 (br s, 1H), 7.80 – 7.85 (m, 3H), 7.70 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.54 – 7.57 (m, 2H), 7.44 – 7.49 (m, 2H), 6.88 – 6.92 (m, 2H), 3.80 (s, 3H), 3.74 – 3.77 (m, 2H), 2.74 (ddd, J = 12.8, 5.6, 4.0 Hz, 1H), 2.41 (dt, J = 12.7, 8.5 Hz, 1H), 2.18 – 2.25 (m, 1H), 2.03 – 2.10 (m, 1H), 0.93 (t, J = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 175.8, 156.8, 138.8, 133.5, 133.2, 132.6, 128.6, 128.4, 127.7, 126.4, 126.2, 125.6 – 125.3 (m), 122.0, 114.3, 55.8, 54.3, 46.1, 32.3, 30.5, 9.5; IR (Neat Film, NaCl) 3055, 2963, 2932, 2877, 1687, 1512, 1464, 1396, 1298, 1249, 1181, 1035, 828, 750 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{23}H_{24}NO_2^+$ [M+H]$^+$: 346.1802, found 346.1805; SFC Conditions: 30% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 210 nm, t_R (min): minor = 5.01, major = 6.05.



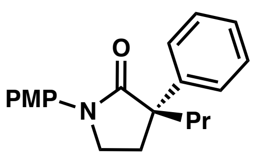
3ga

(*S*)-3-benzyl-1-(4-methoxyphenyl)-3-phenylpyrrolidin-2-one (3ga): Product **3ga** was prepared using Method B, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography (33% EtOAc in hexanes) to provide a colorless oil (29.0 mg, 81 μmol, 41% yield); 90% *ee*; $[\alpha]_D^{25}$ –90.0 (*c* 1.00, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 – 7.56 (m, 2H), 7.40 – 7.43 (m, 2H), 7.33 – 7.37 (m, 2H), 7.25 – 7.28 (m, 1H), 7.20 – 7.24 (m, 3H), 7.11 – 7.13 (m, 2H), 6.85 – 6.89 (m, 2H), 3.79 (s, 3H), 3.49 (dt, J = 9.4, 7.4 Hz, 1H), 3.44 (d, J = 13.4 Hz, 1H), 3.23 (ddd, J = 9.3, 8.1, 3.9 Hz, 1H), 3.14 (d, J = 13.5 Hz, 1H), 2.48 (ddd, J = 12.9, 7.1, 3.9 Hz, 1H), 2.39 (dt, J = 13.0, 7.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 175.2, 156.9, 142.2, 137.7, 133.0, 130.7, 128.8, 128.5, 127.4, 127.1, 127.0, 122.2, 114.3, 55.8, 55.0, 46.0, 45.8, 30.1; IR (Neat Film, NaCl) 3059, 3027, 2925, 1687, 1507, 1455, 1397, 1319, 1298, 1249, 1181, 1034, 828, 701 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{24}H_{24}NO_2^+$ [M+H]$^+$: 358.1802, found 358.1805; SFC Conditions: 25% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): major = 6.45, minor = 7.11.



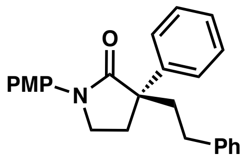
3ha

(*S*)-3-ethyl-1-(4-methoxyphenyl)-3-phenylpyrrolidin-2-one (3ha): Product **3ha** was prepared using Method B, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography (33% EtOAc in hexanes) to provide a light yellow oil (29.5 mg, 0.100 mmol, 50% yield); 89% *ee*; $[\alpha]_D^{25}$ –77.2 (*c* 1.00, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 – 7.56 (m, 2H), 7.43 – 7.52 (m, 2H), 7.31 – 7.36 (m, 2H), 7.22 – 7.27 (m, 1H), 6.87 – 6.91 (m, 2H), 3.79 (s, 3H), 3.65 – 3.75 (m, 2H), 2.60 (ddd, *J* = 12.9, 6.5, 3.2 Hz, 1H), 2.33 (dt, *J* = 12.9, 8.5 Hz, 1H), 2.05 – 2.13 (m, 1H), 1.93 – 2.00 (m, 1H), 0.88 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 175.9, 156.8, 141.5, 133.3, 128.8, 127.2, 126.9, 121.9, 114.3, 55.8, 54.1, 46.1, 32.4, 30.5, 9.5; IR (Neat Film, NaCl) 3056, 2962, 2931, 1687, 1512, 1444, 1396, 1322, 1296, 1249, 1181, 1118, 1097, 1034, 829, 764, 700 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{19}H_{22}NO_2^+$ $[M+H]^+$: 296.1645, found 296.1638; SFC Conditions: 20% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): major = 5.32, minor = 6.46.



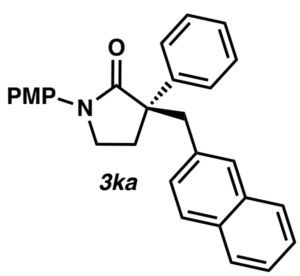
3ia

(*S*)-1-(4-methoxyphenyl)-3-phenyl-3-propylpyrrolidin-2-one (3ia): Product **3ia** was prepared using Method B, allowing the reaction to stir for 20 h. The product was purified by column chromatography (15% EtOAc in hexanes) to provide a colorless oil (27.6 mg, 89 μmol, 45% yield); 90% *ee*; $[\alpha]_D^{25}$ –120.0 (*c* 0.70, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) 7.57 – 7.48 (m, 4H), 7.37 – 7.30 (m, 2H), 7.26 – 7.21 (m, 1H), 6.93 – 6.85 (m, 2H), 3.79 (s, 3H), 3.75 – 3.65 (m, 2H), 2.62 (ddd, *J* = 12.9, 6.3, 3.4 Hz, 1H), 2.33 (dt, *J* = 12.9, 8.5 Hz, 1H), 2.04 (ddd, *J* = 13.7, 11.1, 5.9 Hz, 1H), 1.93 – 1.82 (m, 1H), 1.34 – 1.20 (m, 2H), 0.90 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.9, 156.8, 141.7, 133.3, 128.8, 127.1, 126.8, 121.8, 114.3, 55.8, 53.7, 46.1, 42.0, 31.0, 18.4, 14.8; IR (Neat Film, NaCl) 2957, 2932, 2872, 1687, 1512, 1463, 1444, 1430, 1396, 1322, 1298, 1249, 1181, 1098, 1034, 883, 829, 964, 731, 700, 638 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{20}H_{24}NO_2^+$ $[M+H]^+$: 310.1802, found 310.1807; SFC Conditions: 40% IPA, 2.5 mL/min, Chiralpak AD-H column, λ = 210 nm, t_R (min): minor = 2.94 , major = 3.47.



3ja

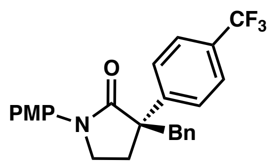
(*S*)-1-(4-methoxyphenyl)-3-phenethyl-3-phenylpyrrolidin-2-one (3ja): Product **3ja** was prepared using Method B, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography (25% EtOAc in hexanes) to provide a colorless oil (39.9 mg, 0.107 mmol, 54% yield); 78% *ee*; $[\alpha]_D^{25}$ –95.7 (*c* 0.70, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.49 (m, 4H), 7.41 – 7.31 (m, 2H), 7.29 – 7.23 (m, 3H), 7.20 – 7.09 (m, 3H), 6.96 – 6.84 (m, 2H), 3.80 (s, 3H), 3.79 – 3.67 (m, 2H), 2.71 – 2.60 (m, 2H), 2.51 (td, *J* = 12.7, 4.7 Hz, 1H), 2.44 – 2.34 (m, 2H), 2.21 (ddd, *J* = 13.5, 12.2, 4.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.6, 156.9, 142.3, 141.2, 133.2, 129.0, 128.7, 127.4, 126.9, 126.1, 121.9, 114.3, 55.8, 53.7, 46.1, 41.5, 31.4; IR (Neat Film, NaCl) 2961, 1688, 1614, 1511, 1490, 1394, 1294, 1248, 1181, 1124, 1089, 1034, 884, 827, 798, 730, 654 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{25}H_{26}NO_2^+$ $[M+H]^+$: 372.1958, found 372.1961; SFC Conditions: 30% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 5.03, major = 5.40.



3ka

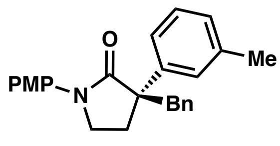
(*S*)-1-(4-methoxyphenyl)-3-(naphthalen-2-ylmethyl)-3-phenylpyrrolidin-2-one (3ka). Product **3ka** was prepared using Method B, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography (33% EtOAc in hexanes) to provide a colorless oil (48.0 mg, 0.118 mmol, 59% yield); 94% *ee*; $[\alpha]_D^{25}$ –128.4 (*c* 1.00, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$) δ 7.77 – 7.81 (m, 1H), 7.72 – 7.75 (m, 1H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.60 (br s, 1H), 7.56 – 7.59 (m, 2H), 7.42 – 7.46 (m, 2H), 7.34 – 7.41

(m, 4H), 7.27 – 7.30 (m, 1H), 7.22 (dd, J = 8.4, 1.8 Hz, 1H), 6.84 – 6.87 (m, 2H), 3.79 (s, 3H), 3.62 (d, J = 13.5 Hz, 1H), 3.50 (ddd, J = 9.4, 8.0, 7.0 Hz, 1H), 3.31 (d, J = 13.5 Hz, 1H), 3.24 (ddd, J = 9.4, 8.0, 3.6 Hz, 1H), 2.50 (ddd, J = 12.9, 7.0, 3.6 Hz, 1H), 2.44 (dt, J = 12.9, 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 175.2, 156.9, 142.0, 135.4, 133.6, 133.0, 132.6, 129.4, 129.1, 128.9, 128.0, 127.9, 127.9, 127.4, 127.1, 126.2, 125.9, 122.2, 114.3, 55.8, 55.2, 46.1, 45.9, 30.0; IR (Neat Film, NaCl) 3054, 2952, 2836, 1688, 1511, 1463, 1397, 1321, 1299, 1249, 1181, 1034, 909, 828, 729, 699 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{28}H_{26}NO_2^+$ [M+H]$^+$: 408.1958, found 408.1954; SFC Conditions: 10% IPA, 2.5 mL/min, Chiralcel OD-H column, λ = 254 nm, t_R (min): minor = 10.69, major = 11.15.



3gc

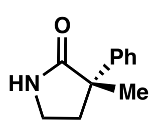
(*S*)-3-benzyl-1-(4-methoxyphenyl)-3-(4-(trifluoromethyl)phenyl)pyrrolidin-2-one (3gc). Product **3gc** was prepared using general Method A, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography (25% EtOAc in hexanes) to provide a colorless oil (60.3 mg, 0.142 mmol, 71% yield); 94% *ee*; $[\alpha]_D^{25}$ –188.3 (*c* 1.00, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 – 7.72 (m, 2H), 7.59 – 7.63 (m, 2H), 7.37 – 7.41 (m, 2H), 7.22 – 7.25 (m, 3H), 7.11 – 7.13 (m, 2H), 6.87 – 6.90 (m, 2H), 3.80 (s, 3H), 3.49 (t, J = 7.2 Hz, 1H), 3.45 (d, J = 11.3 Hz, 1H), 3.22 (ddd, J = 9.4, 7.2, 5.4 Hz, 1H), 3.13 (d, J = 13.4 Hz, 1H), 2.45 – 2.53 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 174.5, 157.1, 146.5, 136.9, 132.6, 130.6, 129.5 (q, J = 32.5 Hz), 128.6, 127.5, 127.3, 125.7 (q, J = 3.8 Hz), 123.4, 122.3, 114.3, 55.8, 54.9, 45.9, 45.9, 30.0; ^{19}F NMR (282 MHz, $CDCl_3$) δ –62.5; IR (Neat Film, NaCl) 3062, 2954, 2926, 2838, 1687, 1616, 1513, 1442, 1400, 1327, 1300, 1251, 1167, 1123, 1072, 1037, 1018, 829, 703 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{25}H_{23}F_3NO_2^+$ [M+H]$^+$: 426.1675, found 426.1677; SFC Conditions: 15% IPA, 2.5 mL/min, Chiralpak AD-H column, λ = 254 nm, t_R (min): major = 5.17, minor = 5.93.



3gd

(*S*)-3-benzyl-1-(4-methoxyphenyl)-3-(*m*-tolyl)pyrrolidin-2-one (3gd): Product **3gd** was prepared using Method B, allowing the reaction to stir for 20 h. The crude product was purified by column chromatography (33% EtOAc in hexanes) to provide a colorless oil (47.6 mg, 0.128 mmol, 64% yield); 93% *ee*; $[\alpha]_D^{25}$ –179.0 (*c* 1.00, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 16.1 Hz, 2H), 7.39 (s, 1H), 7.32 (s, 1H), 7.25 (m, 4H), 7.16 (m, 2H), 7.10 (s, 1H), 6.87 (d, *J* = 16.1 Hz, 2H), 3.80 (s, 3H), 3.50 (dt, *J* = 9.3, 7.4 Hz, 1H), 3.45 (d, *J* = 13.4 Hz, 1H), 3.21 (ddd, *J* = 9.2, 8.1, 3.8 Hz, 1H), 3.12 (d, *J* = 13.4 Hz, 1H), 2.47 (ddd, *J* = 12.9, 7.1, 3.8 Hz, 1H), 2.41 (s, 1H), 2.37 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 175.2, 156.9, 142.2, 138.4, 137.8, 133.1, 130.8, 128.6, 128.4, 128.1, 127.8, 127.0, 124.0, 122.2, 114.3, 55.8, 55.0, 46.0, 45.8, 30.1, 22.0; IR (Neat Film, NaCl) 2923, 1686, 1604, 1584, 1511, 1453, 1299, 1249, 1180, 1119, 1099, 1036, 890, 828, 787, 738, 703, 613 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{25}H_{26}NO_2^+$ $[M+H]^+$: 372.1958, found 372.1960; SFC Conditions: 15% IPA, 2.5 mL/min, Chiralpak AD-H column, λ = 254 nm, t_R (min): major = 8.44, minor = 7.00.

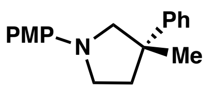
Product Transformations



4

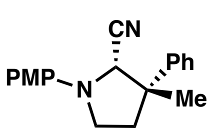
(*S*)-3-methyl-3-phenylpyrrolidin-2-one (4): To a solution of **3aa** (30.2 mg, 93% *ee*; 0.107 mmol, 1.0 equiv) in acetonitrile (2.2 mL) at 0 °C was added a solution of ceric ammonium nitrate (88 mg, 0.161 mmol, 1.5 equiv) in de-ionized water (2.2 mL) dropwise. The resulting mixture was stirred for 30 minutes at 0 °C. Upon consumption of the starting material, the reaction was diluted with water and extracted with EtOAc three times. The combined organic extracts were dried over Na_2SO_4 and the product was purified by column chromatography (5% MeOH in CH_2Cl_2) to afford **4** as a yellow solid (13.6 mg, 78 µmol, 73% yield). [✔]$_D^{25}$ –80.8 (*c* 0.665, $CHCl_3$); ^{1}H NMR (400 MHz,

$CDCl_3$) δ 7.47 – 7.39 (m, 2H), 7.39 – 7.30 (m, 2H), 7.26 (s, 1H), 6.88 (d, J = 22.5 Hz, 1H), 3.45 – 3.23 (m, 2H), 2.51 (ddd, J = 12.3, 7.3, 4.6 Hz, 1H), 2.25 (ddd, J = 12.7, 8.0, 6.8 Hz, 1H), 1.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 181.8, 143.7, 128.9, 127.1, 126.4, 48.2, 39.4, 38.3, 24.8, 19.4; IR (Neat Film, NaCl) 3056, 3026, 2960, 2931, 2830, 1619, 1601, 1515, 1488, 1496, 1464, 1445, 1366, 1281, 1240, 1180, 1081, 1042, 967, 811, 764, 700 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{11}H_{14}NO^+$ $[M+H]^+$: 176.1070, found 176.1068.



5

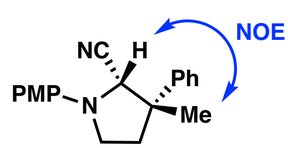
(*S*)-1-(4-methoxyphenyl)-3-methyl-3-phenylpyrrolidine (5): To a solution of **3aa** (46.3 mg, 93% *ee*, 0.170 mmol, 1.0 equiv) in diethyl ether (1.65 mL) at 0 °C was added $LiAlH_4$ (31.2 mg, 0.820 mmol, 5 equiv). The reaction was stirred at 0 °C for 5 min then allowed to warm to ambient temperature. After 15 h the reaction was quenched with H_2O and extracted with EtOAc seven times. The combined organic layers were dried over Na_2SO_4 and concentrated *in vacuo*. The crude product was purified by column chromatography (10% EtOAc in hexanes) to afford **5** as a light grey solid (41.1 mg, 0.154 mmol, 93% yield); [✔]$_D^{25}$ –85.2 (*c* 0.70, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ δ 7.40 – 7.30 (m, 5H), 7.26 – 7.21 (m, 1H), 6.88 (d, J = 9.0 Hz, 2H), 6.56 (d, J = 8.1 Hz, 2H), 3.78 (s, 3H), 3.60 – 3.42 (m, 3H), 3.38 (t, J = 10.5 Hz, 1H), 2.38 – 2.25 (m, 1H), 2.24 – 2.14 (m, 1H), 1.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.4, 143.1, 128.7, 126.5, 126.1, 115.5, 112.3, 60.4, 56.4, 47.6, 46.1, 38.5, 28.6; IR (Neat Film, NaCl) 3056, 3026, 2960, 2931, 2830, 1619, 1601, 1515, 1488, 1496, 1464, 1445, 1366, 1281, 1240, 1180, 1081, 1042, 967, 811, 764, 700 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{18}H_{22}NO^+$ $[M+H]^+$: 268.1696, found 268.1702.



6

(2*S*,3*S*)-1-(4-methoxyphenyl)-3-methyl-3-phenylpyrrolidine-2-carbonitrile (6): To a solution of **3aa** (38.5 mg, 93% *ee*, 0.137 mmol, 1 equiv) in THF (14 mL) was added a solution of $LiBEt_3H$ (1 M in THF, 0.42 mL, 3 equiv) dropwise at –78 °C. The resulting solution was stirred at –78 °C for 2 hours then warmed to ambient temperature and allowed to stir for 8 hours. The reaction was cooled to 0 °C and acetic acid (164 μL, 2.9 mmol, 21 equiv) was added dropwise. After 10 min, KCN (171 μL, 4.8 M solution, 0.82 mmol, 6.0 equiv), celite, and Na_2SO_4 were added successively. The reaction was stirred at 0 °C for 5 hours, quenched with anhydrous K_2CO_3, and filtered through celite. The solvent was removed and the crude product was purified by column chromatography (20% EtOAc in hexanes) to afford **6** as a colorless solid (17.5 mg, 60 μmol, 43% yield, 93:7 dr); $[\alpha]_D^{25}$ –233.7 (*c* 0.70, $CHCl_3$); δ ^1H NMR (400 MHz, CD_2Cl_2) δ 7.35 – 7.30 (m, 4H), 7.28 – 7.20 (m, 1H), 6.88 – 6.82 (m, 2H), 6.66 – 6.59 (m, 2H), 4.67 (s, 1H), 3.72 (s, 3H), 3.49 (td, *J* = 8.6, 4.1 Hz, 1H), 3.34 (dt, *J* = 8.8, 7.5 Hz, 1H), 2.51 (dddd, *J* = 12.3, 7.5, 4.2, 0.8 Hz, 1H), 2.31 (ddd, *J* = 13.0, 8.4, 7.6 Hz, 1H), 1.71 (s, 3H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ 152.6, 144.5, 139.7, 128.8, 127.1, 125.3, 117.9, 114.9, 113.6, 60.4, 55.7, 49.5, 47.3, 37.0, 25.7; IR (Neat Film, NaCl) 3048, 2929, 2860, 1514, 1456, 146 cm^{-1}; HRMS (MM) *m/z* calc'd for $C_{19}H_{21}N_2O^+$ $[M+H]^+$: 293.1648, found 293.1642; Please note that the NMR data listed is for the major diastereomer.

Stereochemical Assignment:



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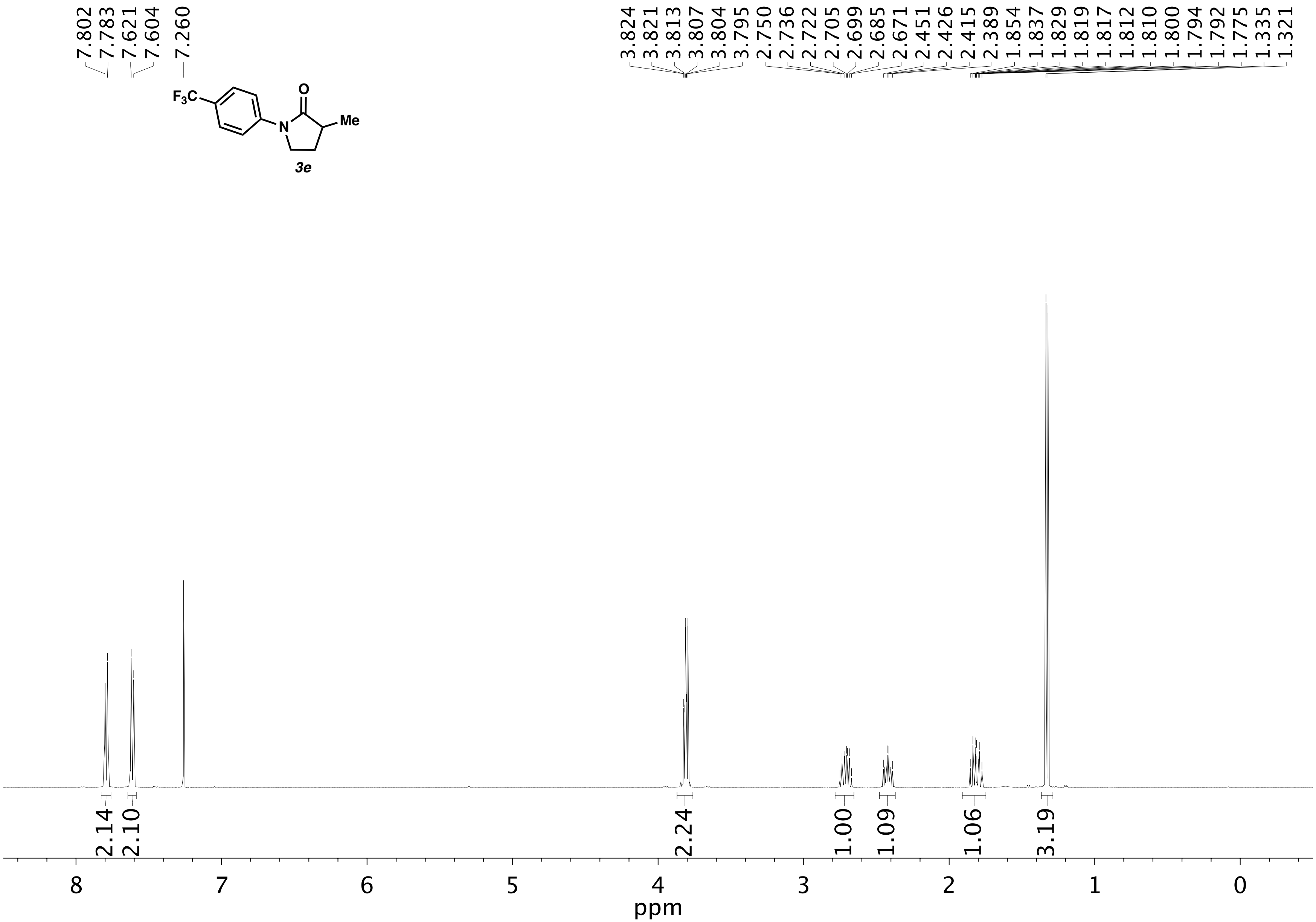
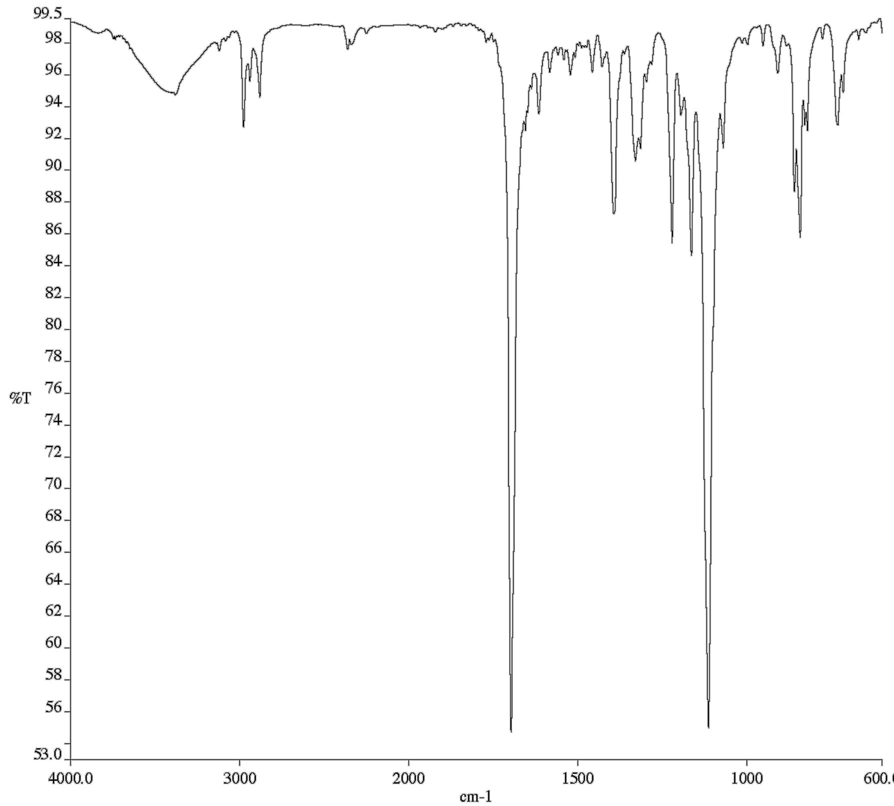
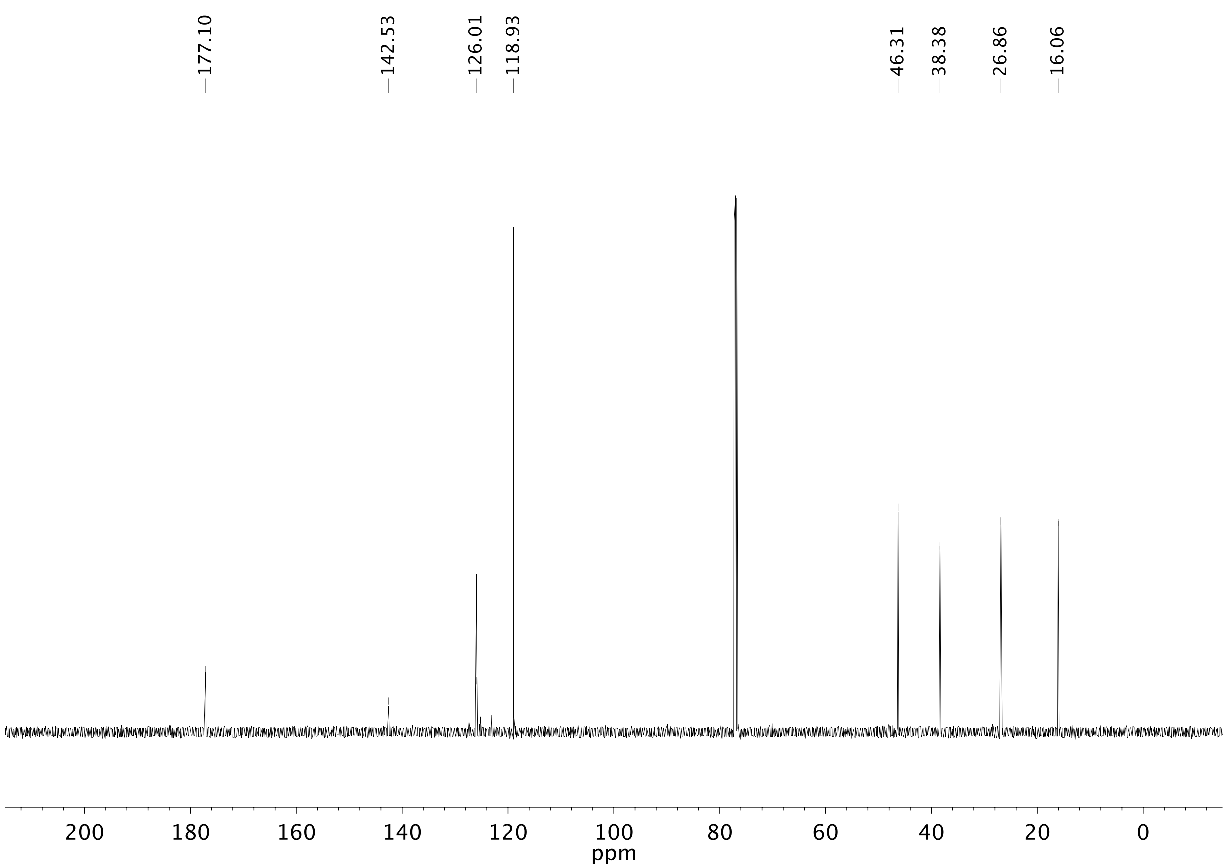


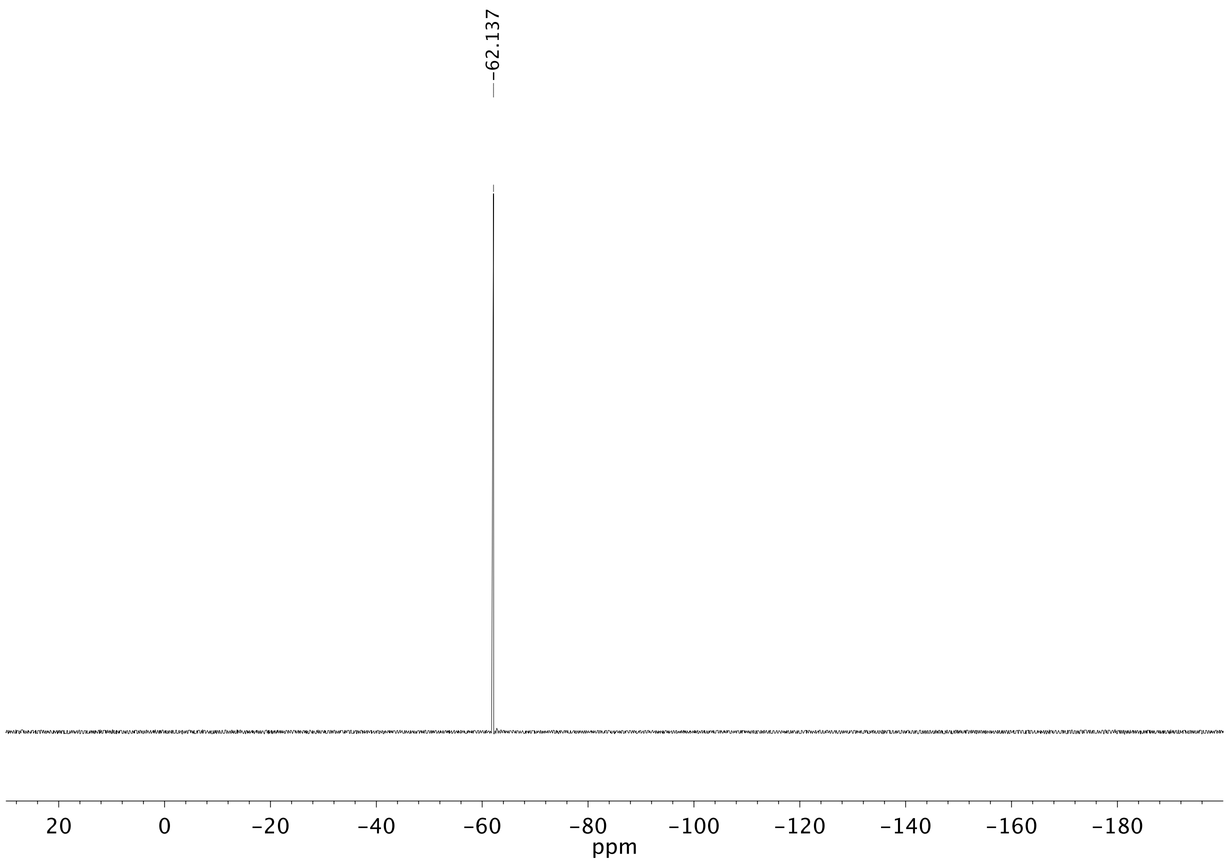
^{1}H NMR (400 MHz, $CDCl_3$) of compound **1e**



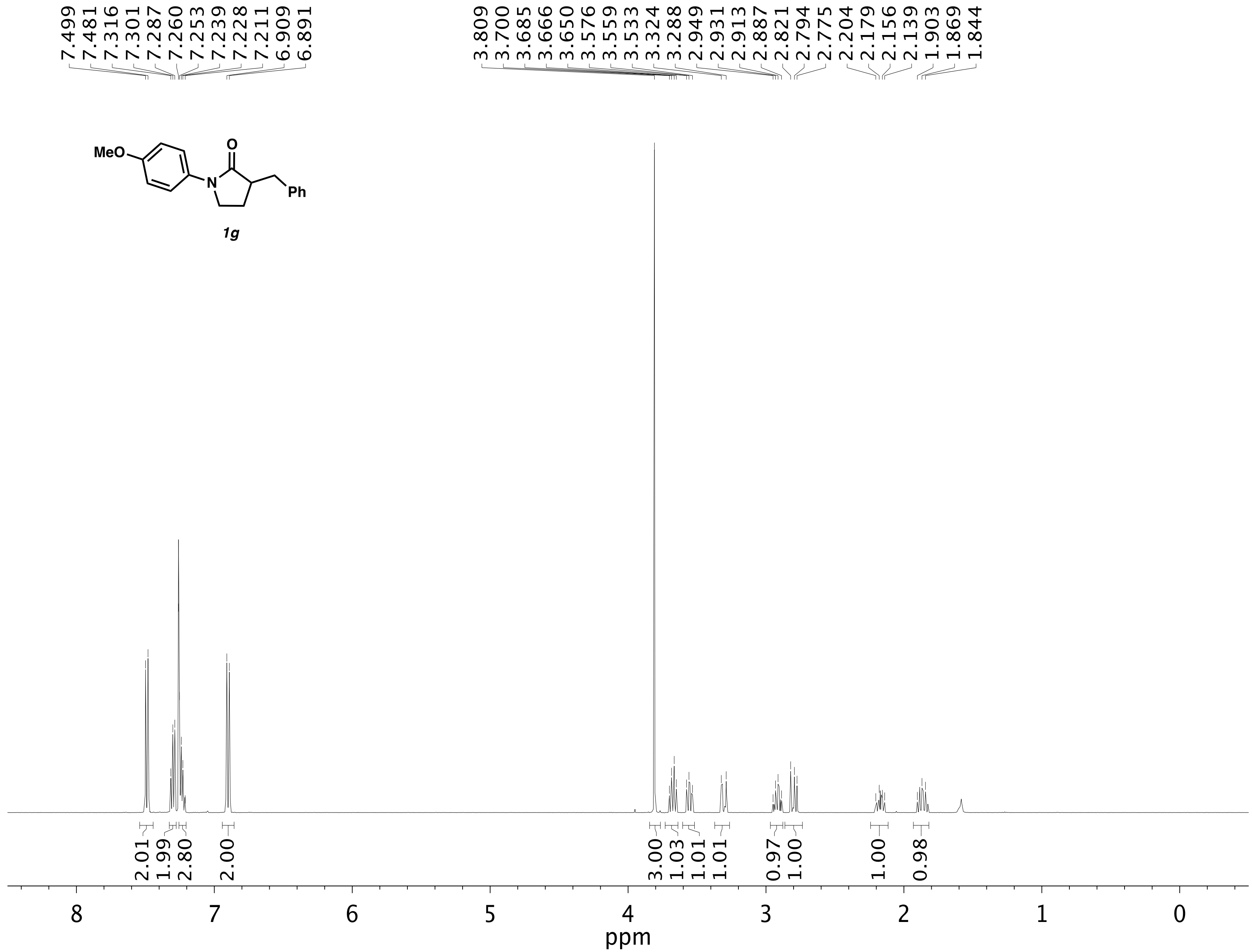
Infrared spectrum (Thin Film, NaCl) of compound **1e**



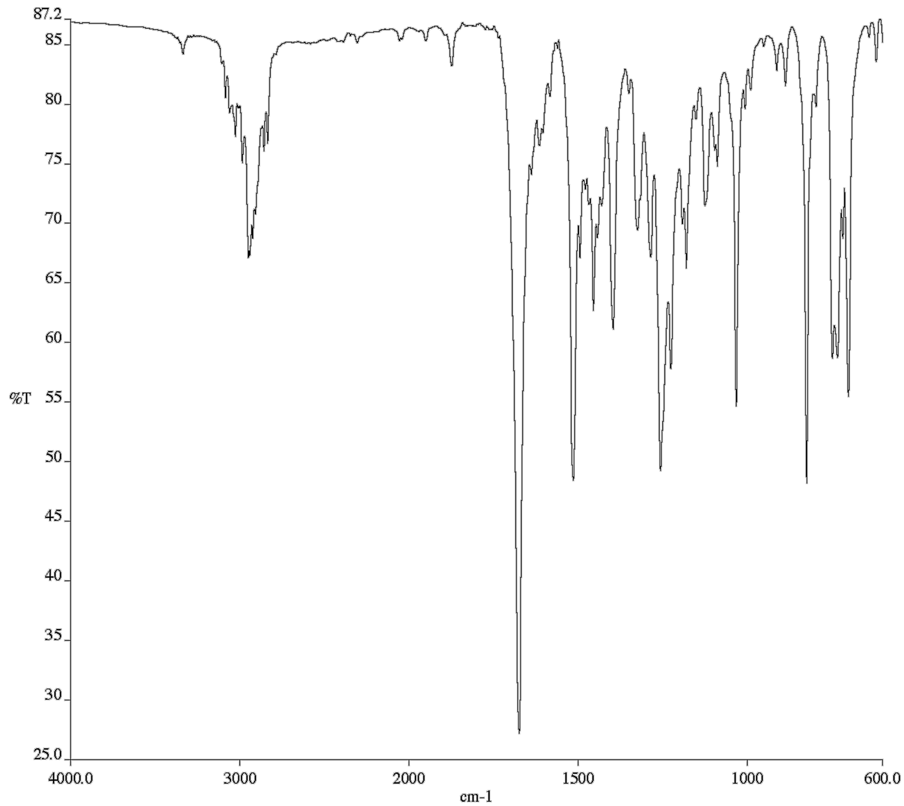
^{13}C NMR (125 MHz, $CDCl_3$) of compound **1e**



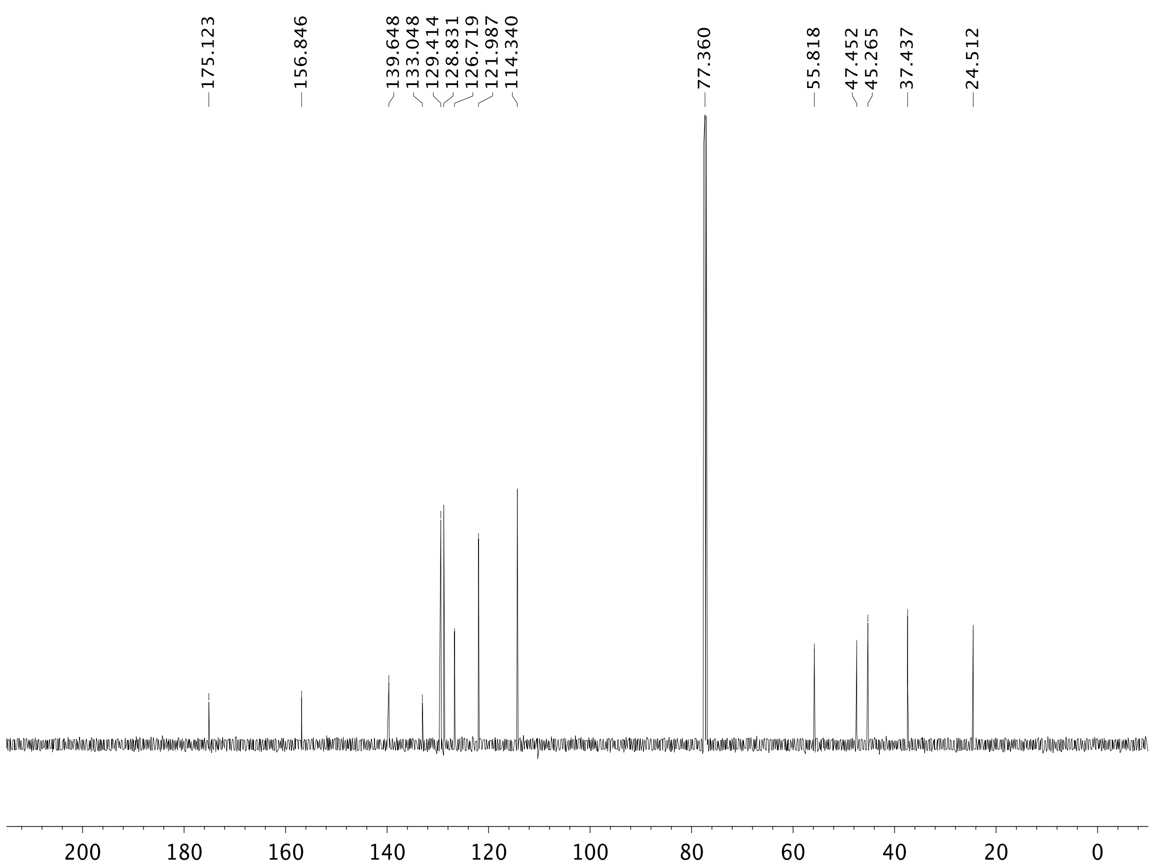
^{19}F NMR (282 MHz, $CDCl_3$) of compound **1e**



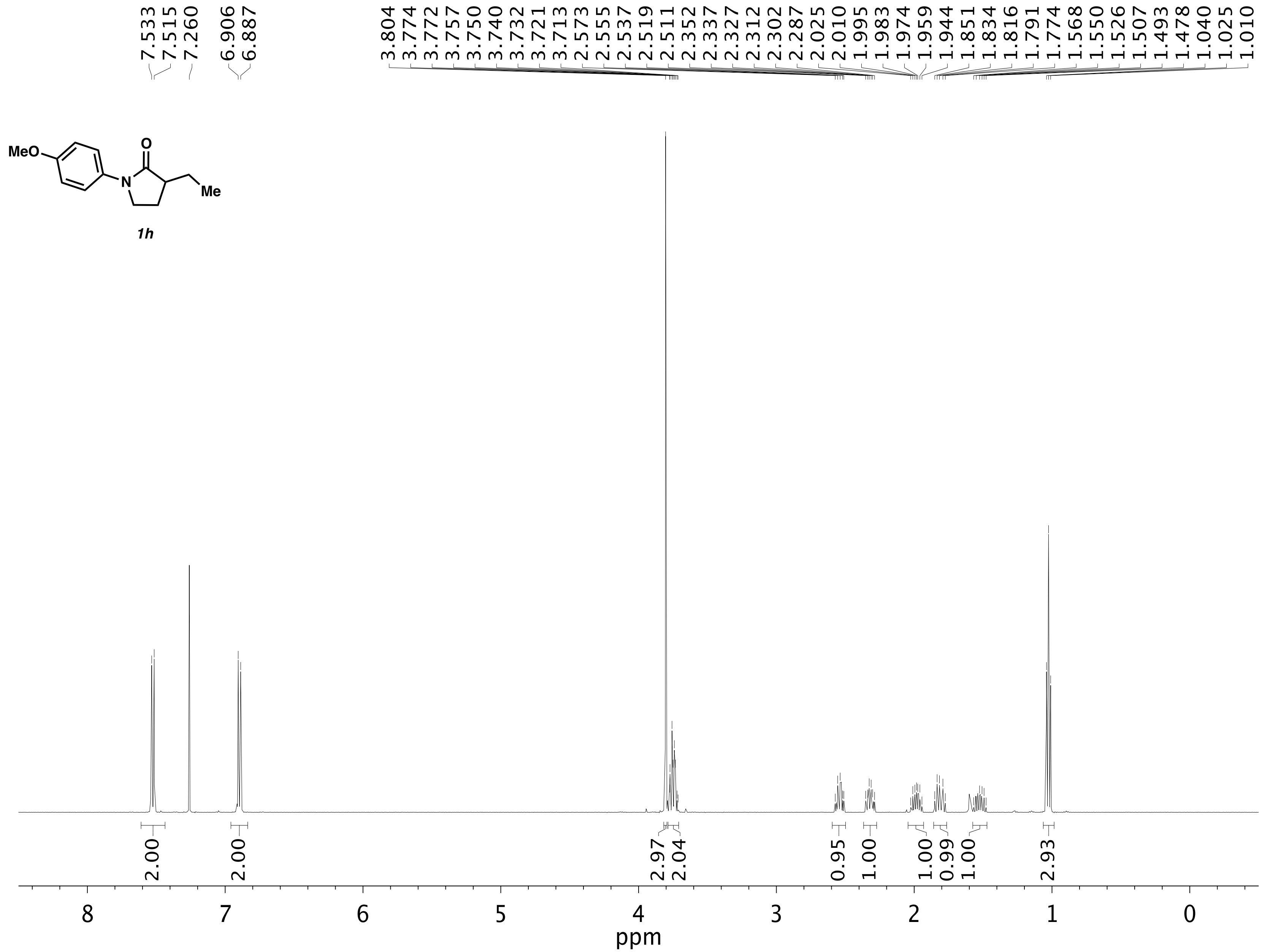
^{1}H NMR (500 MHz, $CDCl_3$) of compound **1g**



Infrared spectrum (Thin Film, NaCl) of compound **1g**

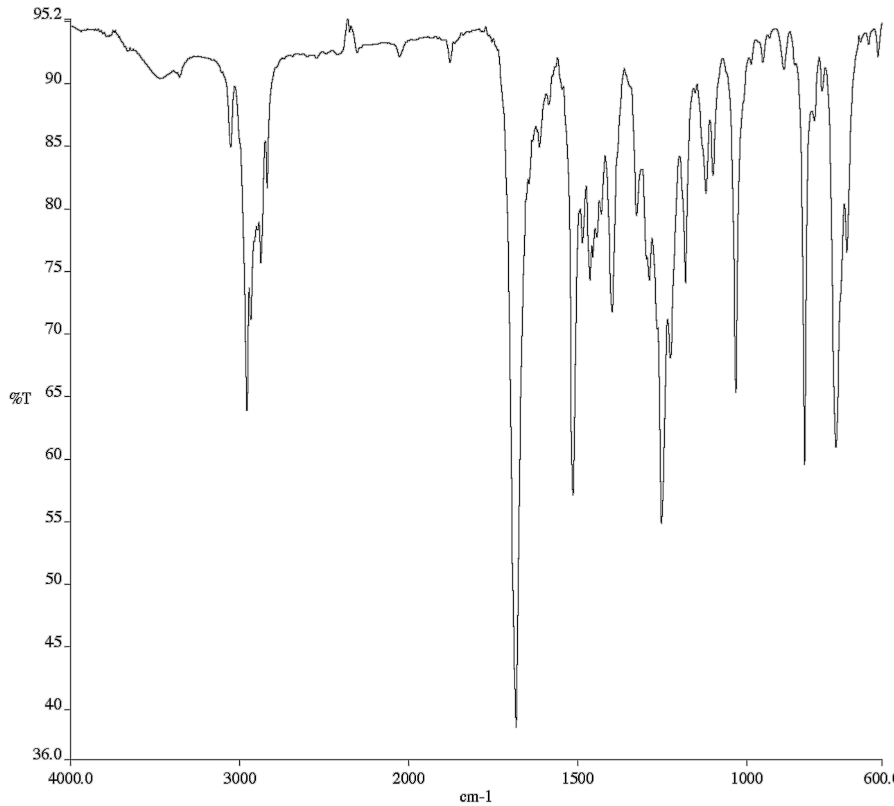


^{13}C NMR (125 MHz, $CDCl_3$) of compound **1g**

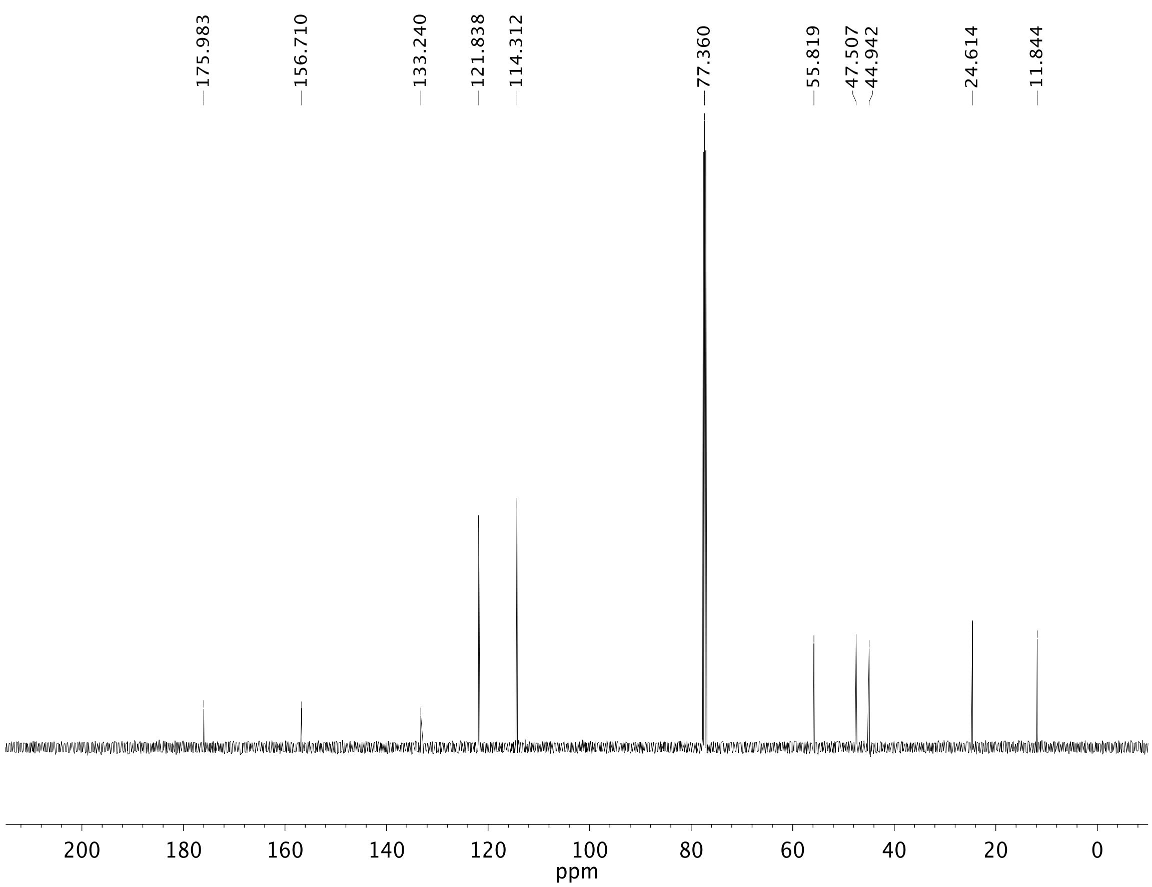


1h

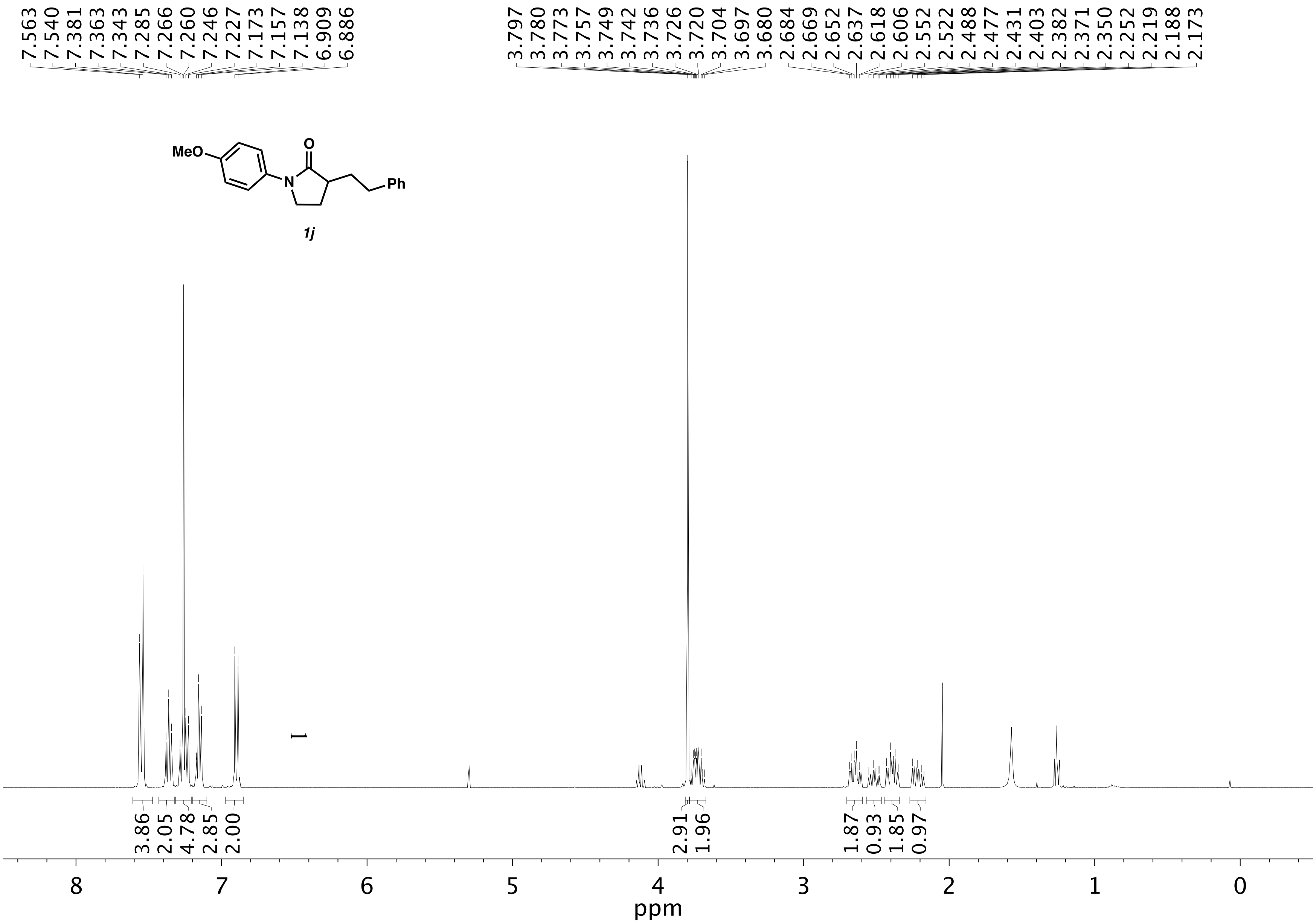
^{1}H NMR (500 MHz, $CDCl_3$) of compound **1h**



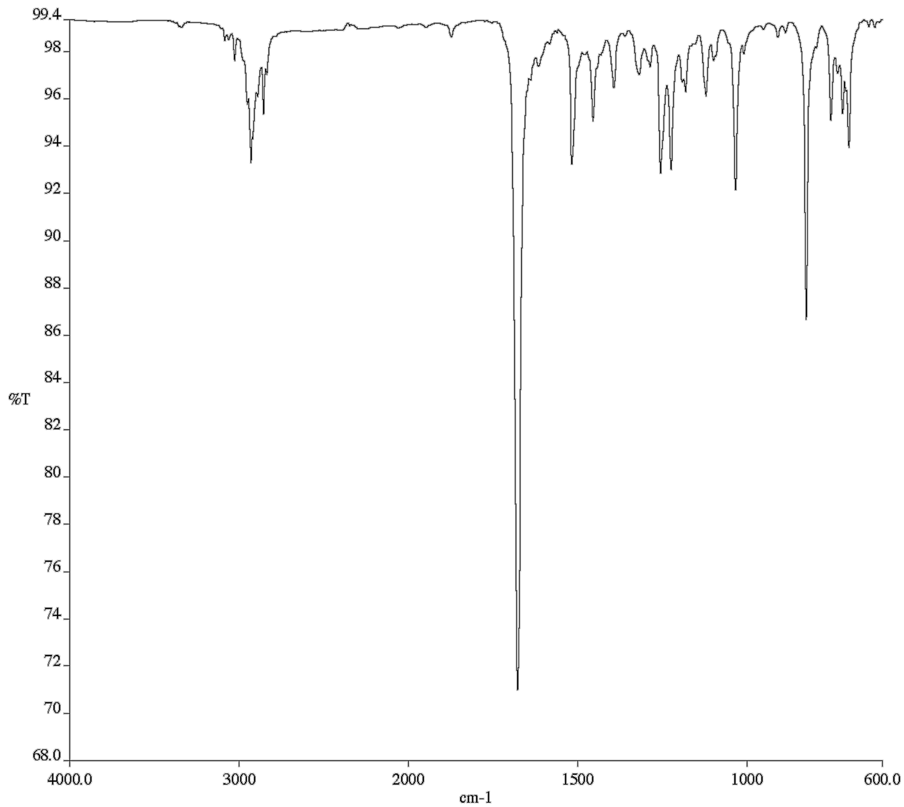
Infrared spectrum (Thin Film, NaCl) of compound **1h**



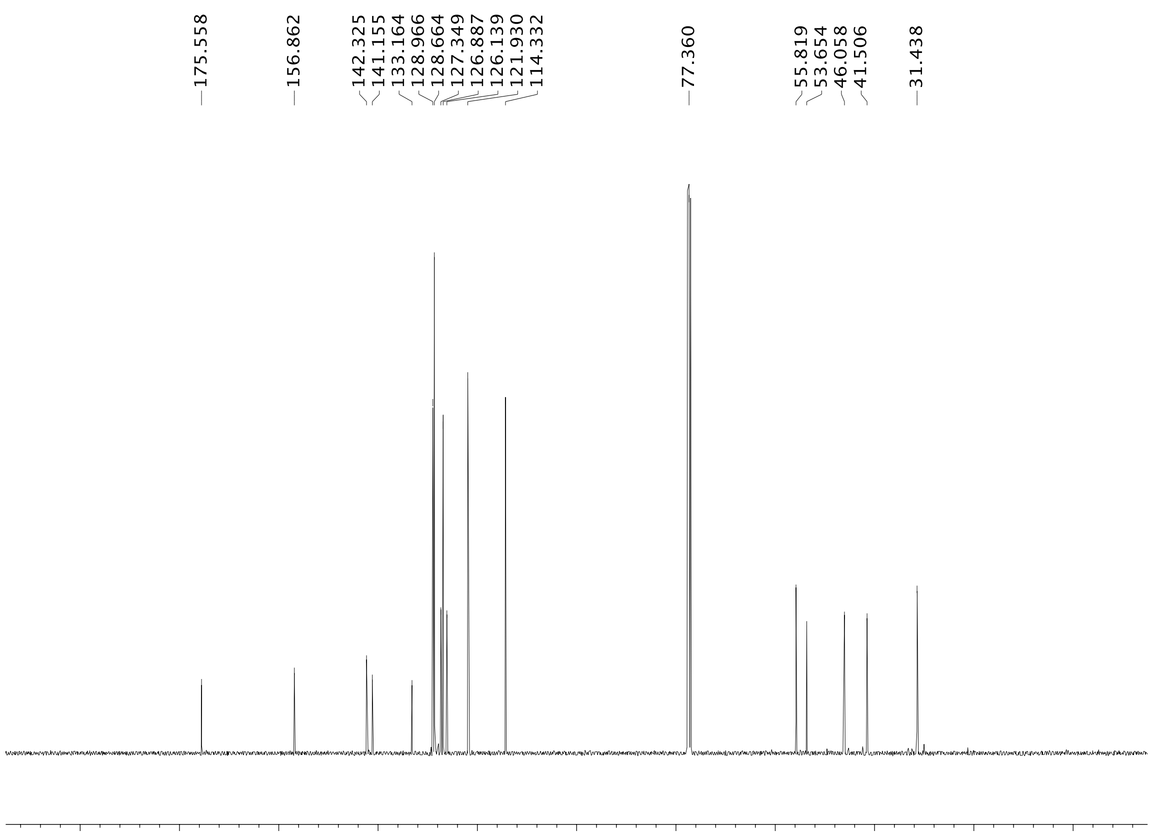
^{13}C NMR (125 MHz, $CDCl_3$) of compound **1h**



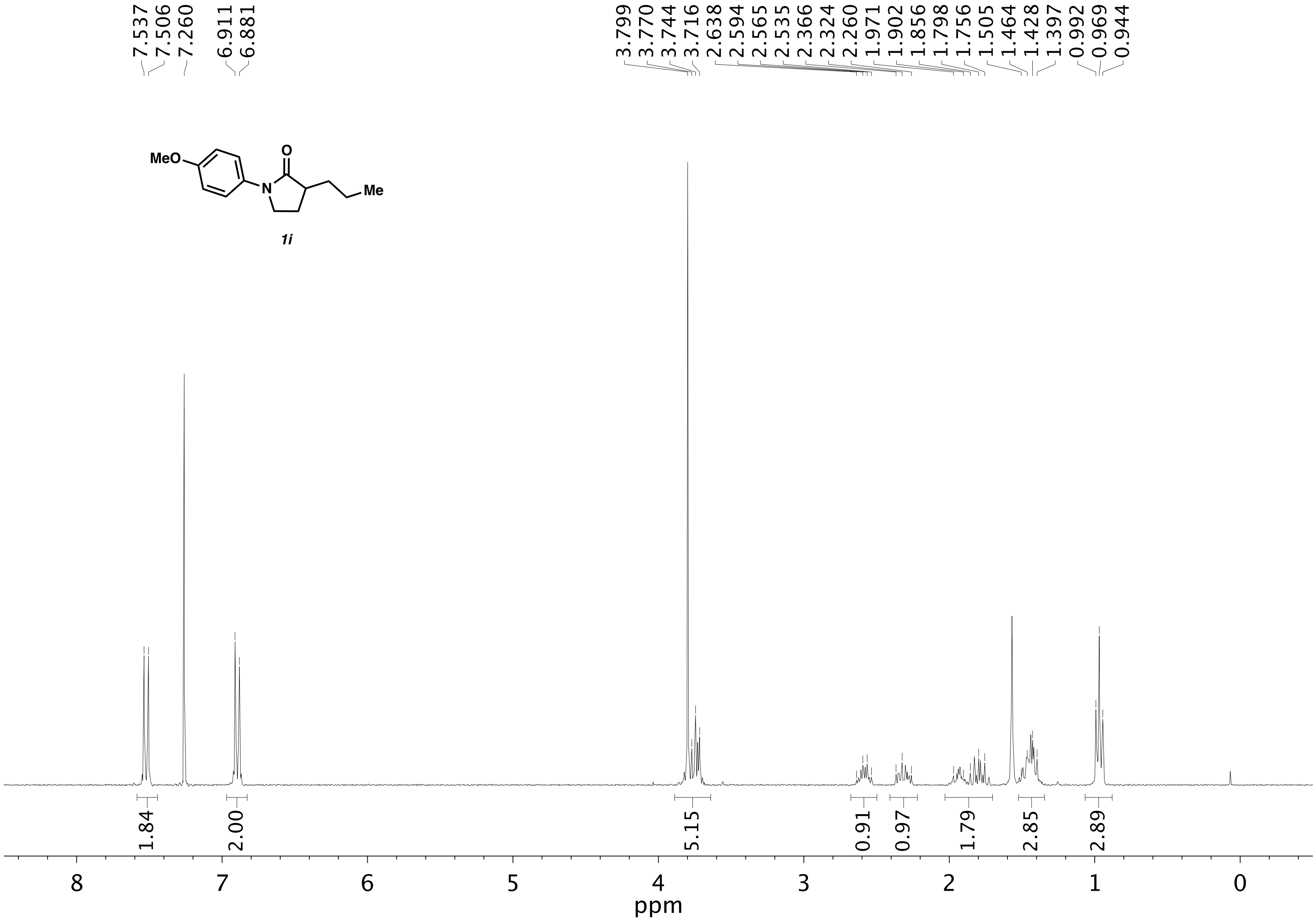
^{1}H NMR (300 MHz, $CDCl_3$) of compound **1j**



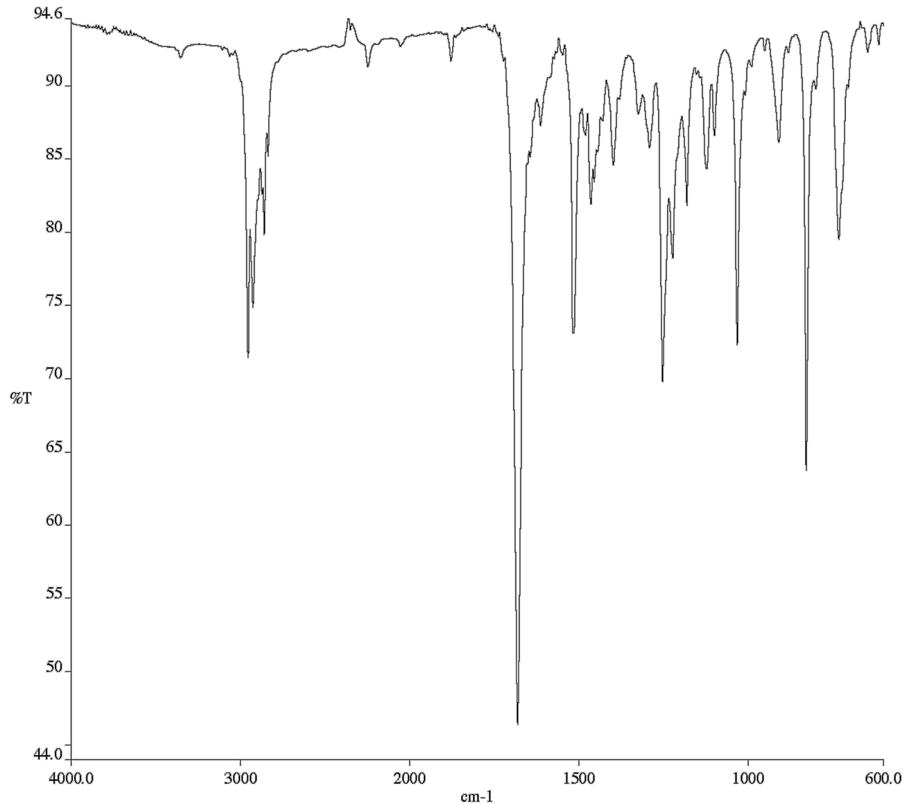
Infrared spectrum (Thin Film, NaCl) of compound **1j**



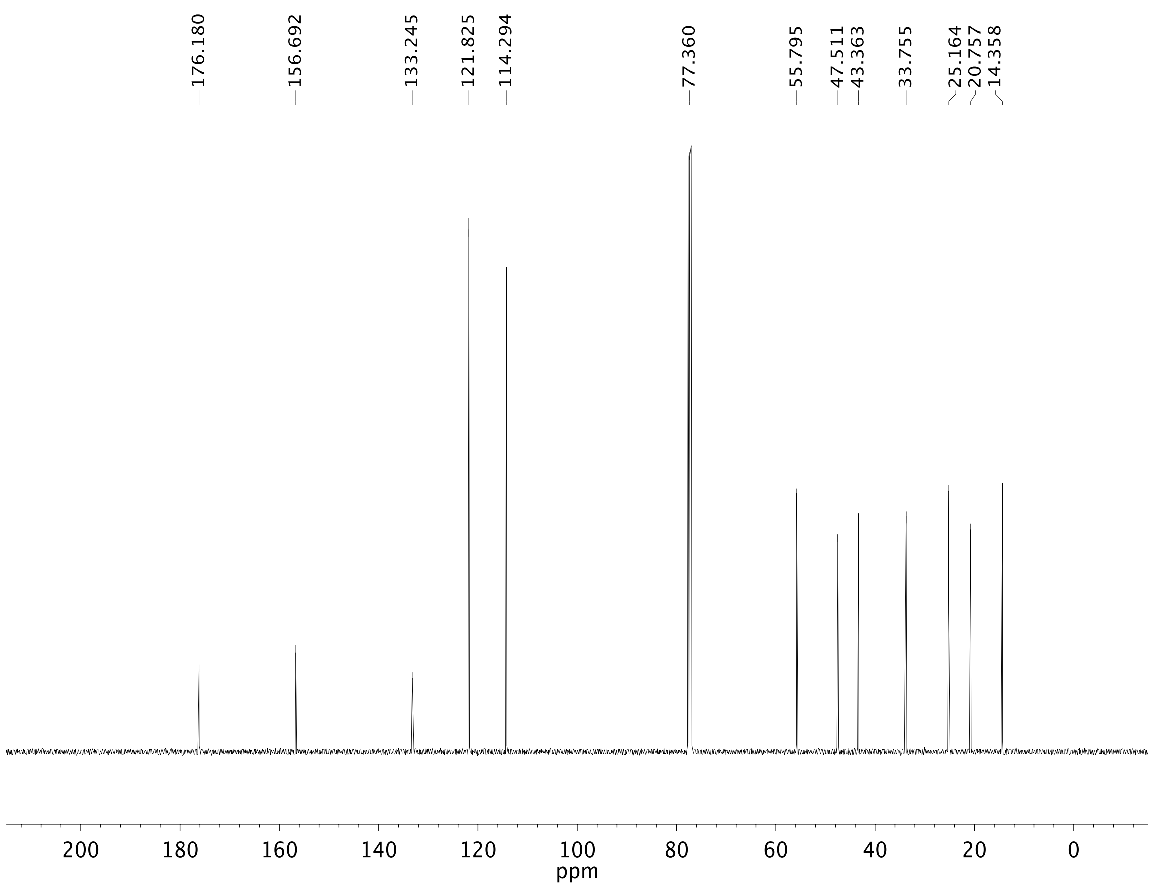
^{13}C NMR (100 MHz, $CDCl_3$) of compound **1j**



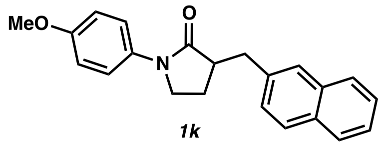
^{1}H NMR (300 MHz, $CDCl_3$) of compound **1i**



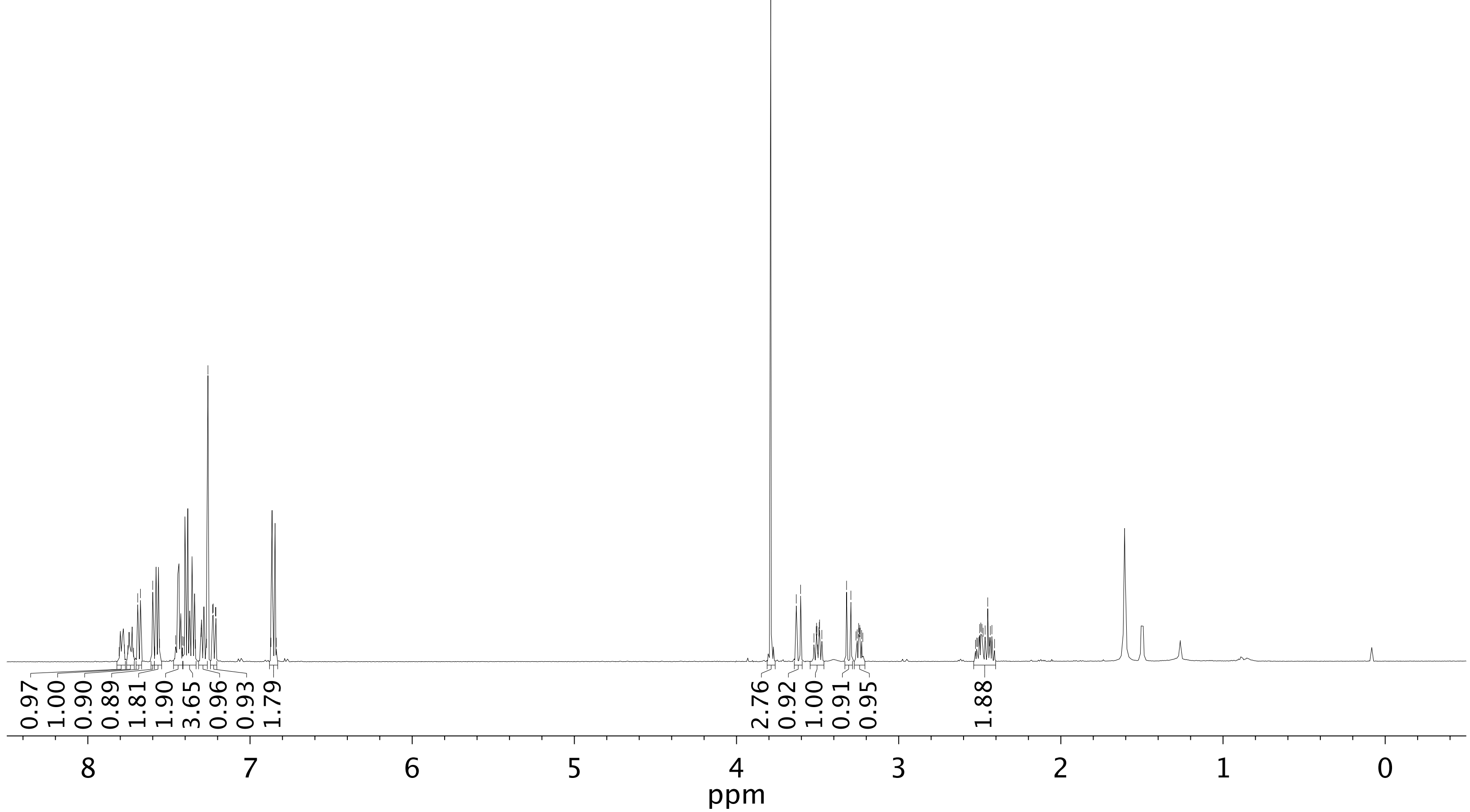
Infrared spectrum (Thin Film, NaCl) of compound **1i**



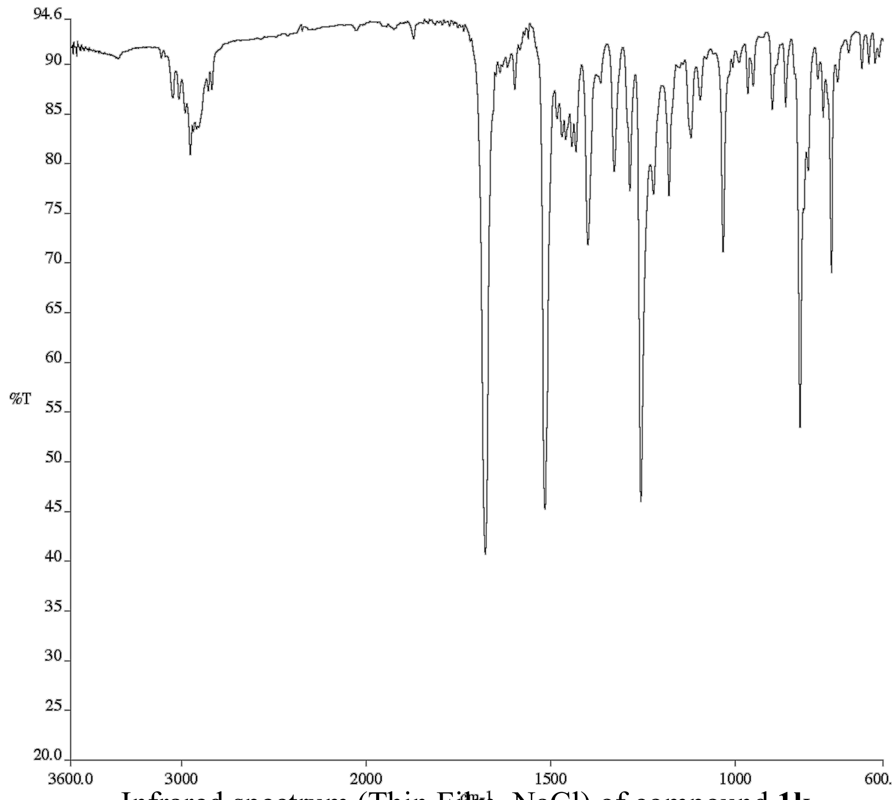
^{13}C NMR (100 MHz, $CDCl_3$) of compound **1i**



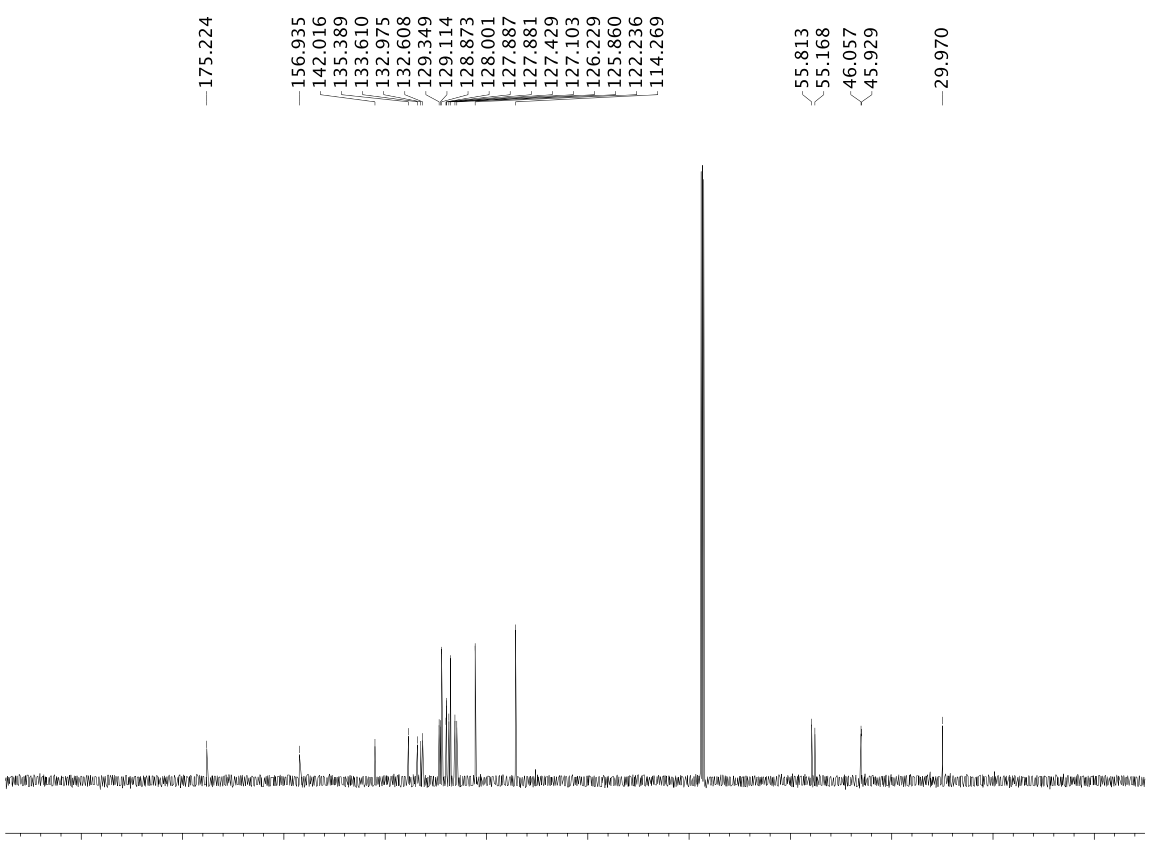
1k



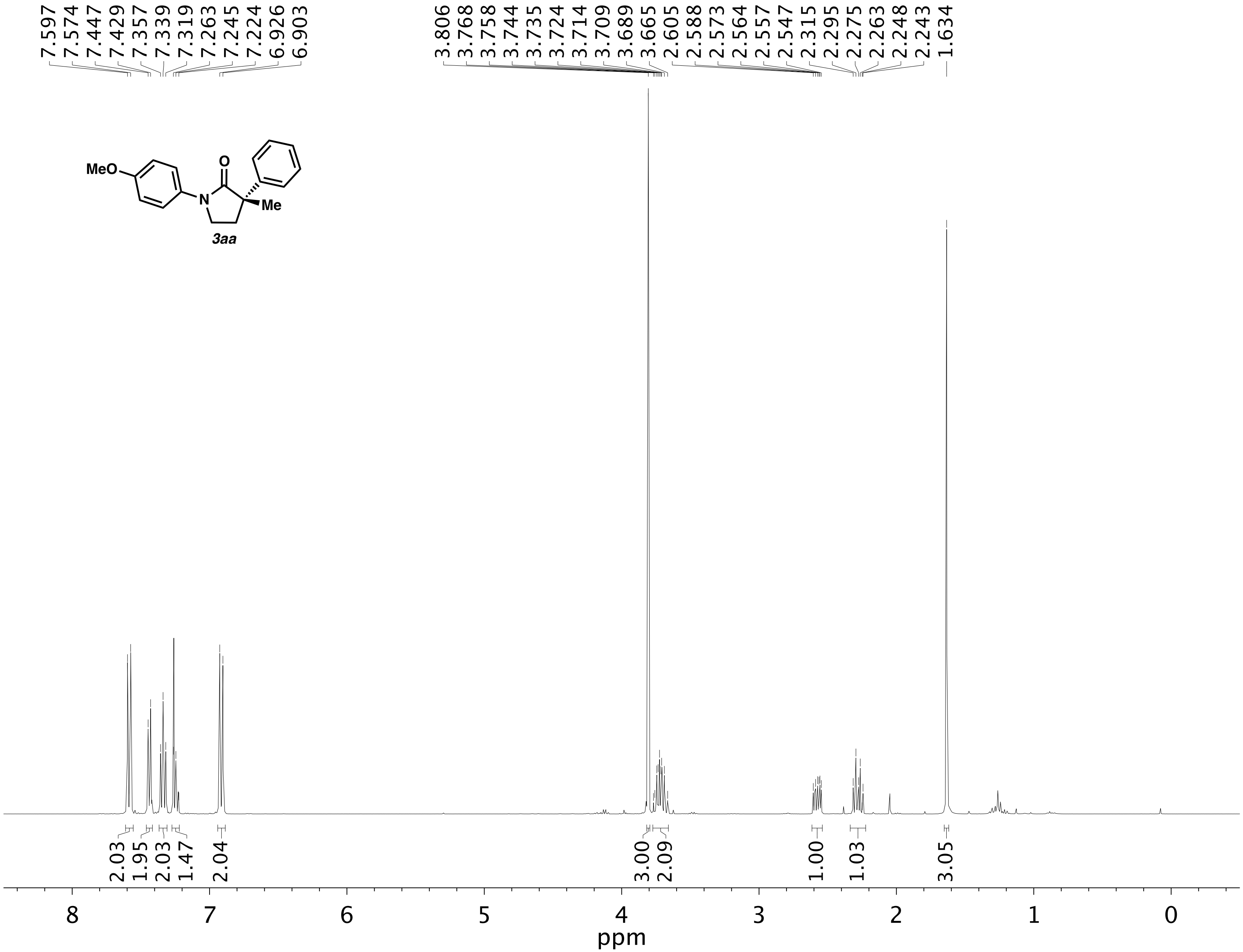
^{1}H NMR (500 MHz, $CDCl_3$) of compound **1k**



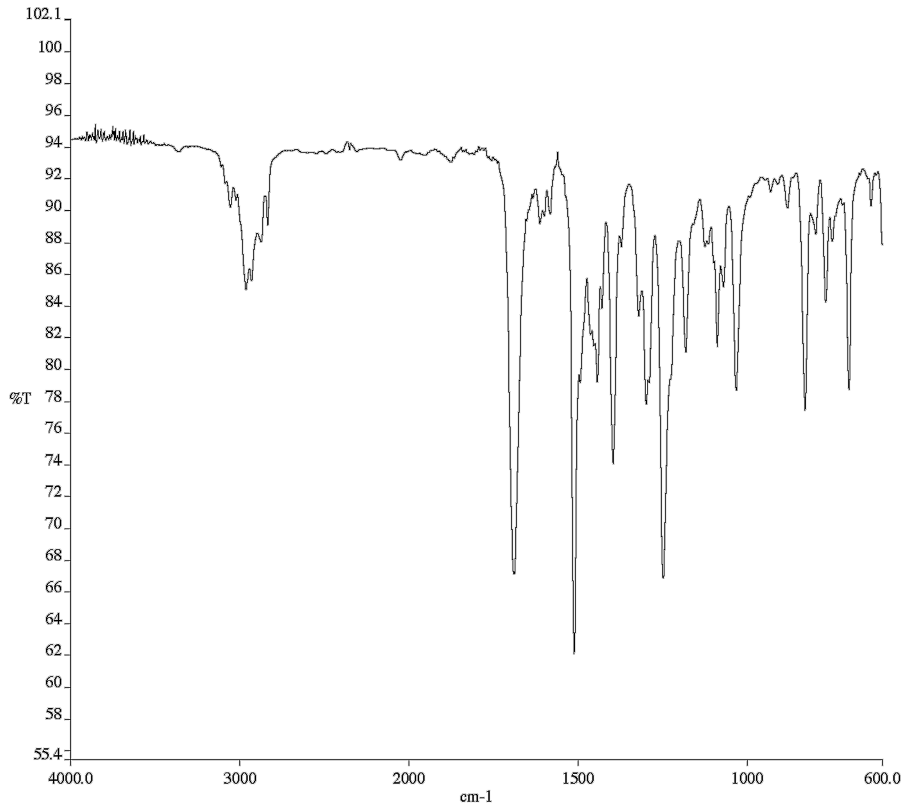
Infrared spectrum (Thin Film, NaCl) of compound **1k**



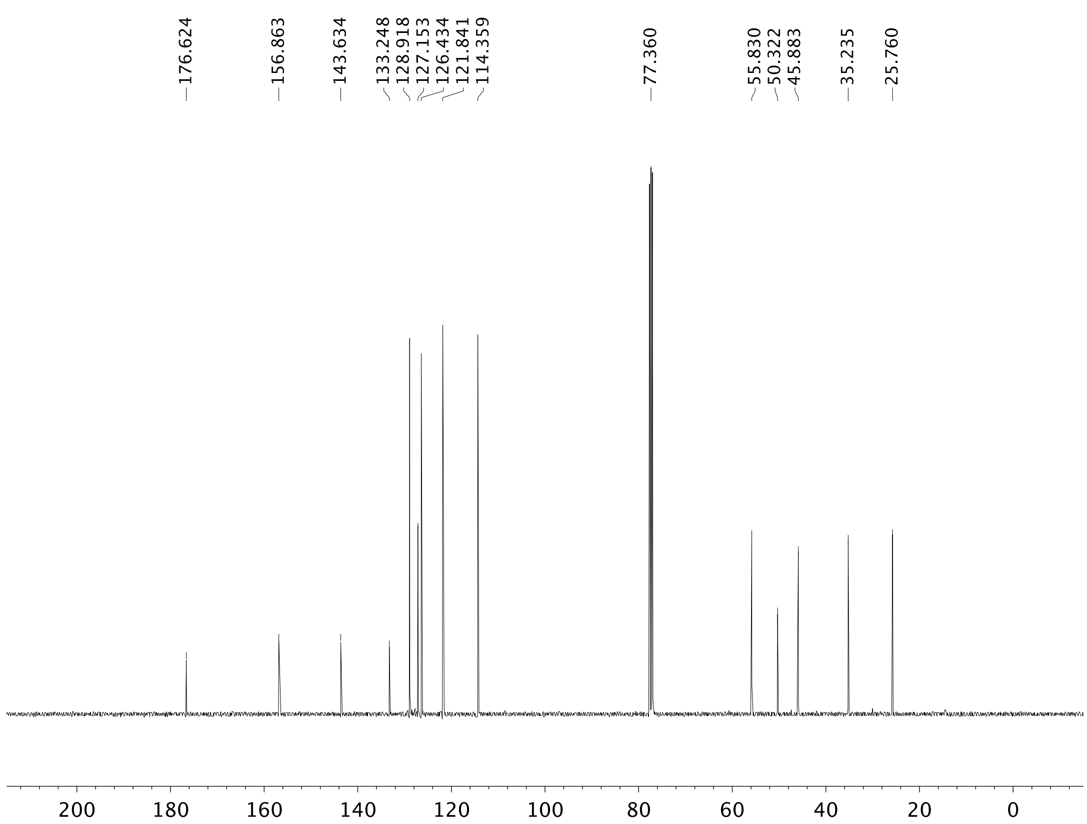
^{13}C NMR (125 MHz, $CDCl_3$) of compound **1k**



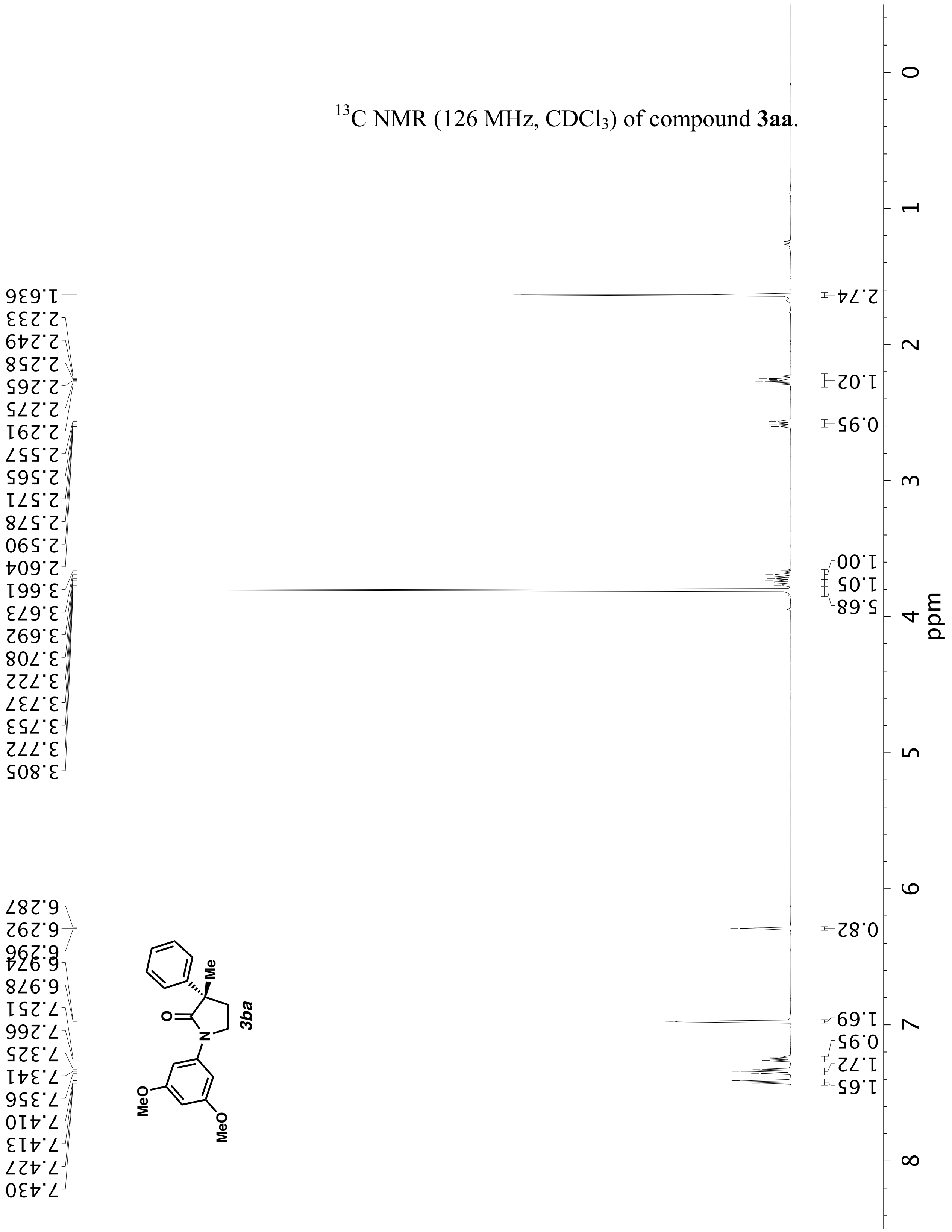
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3aa**



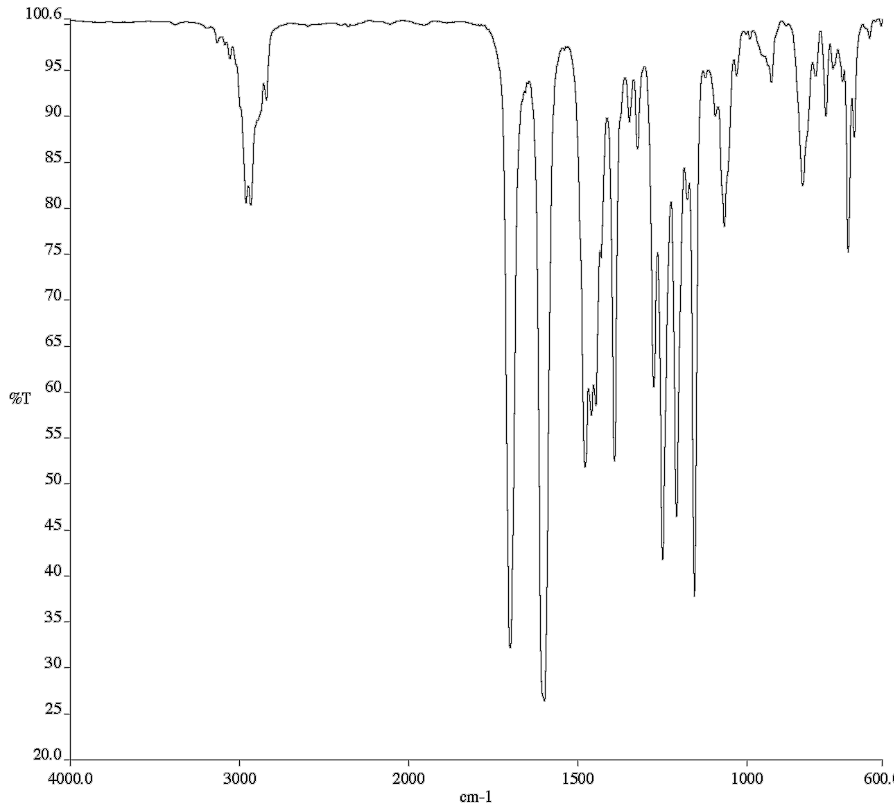
Infrared spectrum (Thin Film, NaCl) of compound **3aa**.



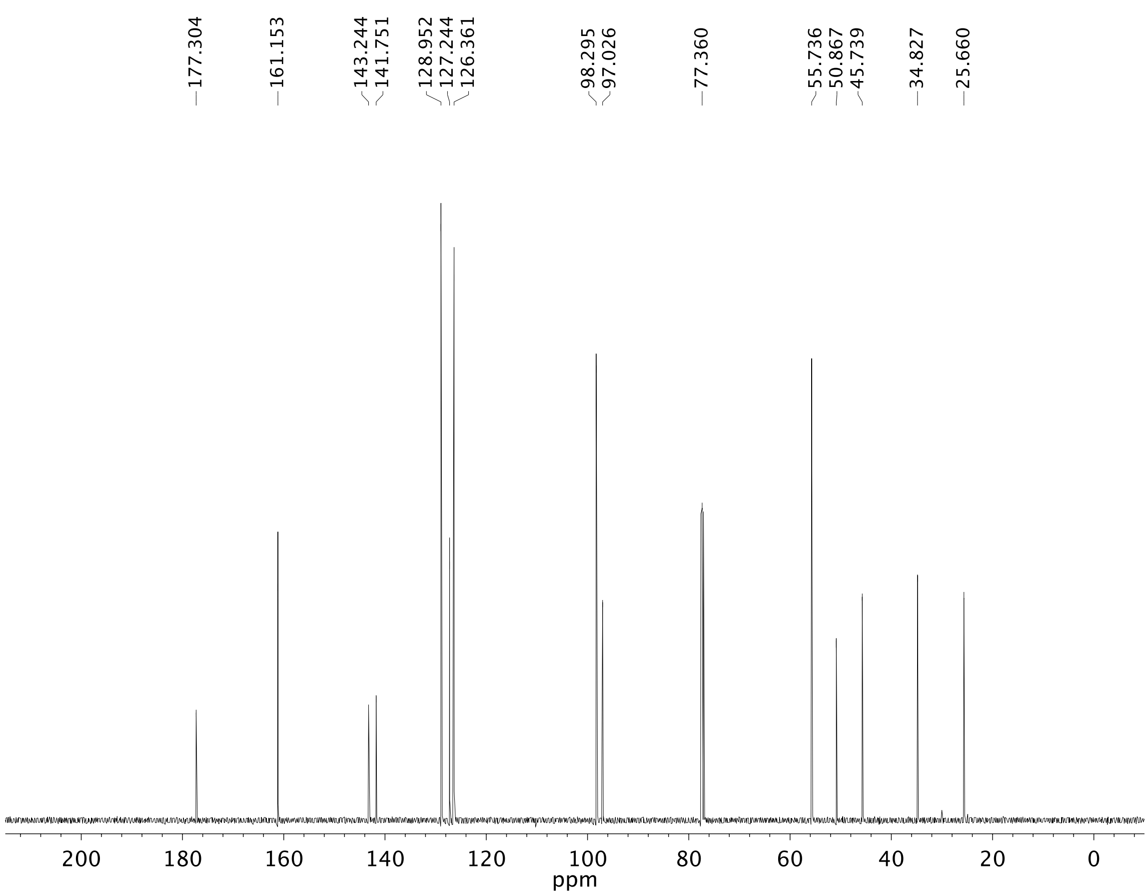
^{13}C NMR (126 MHz, CDCl$_3$) of compound **3aa**.



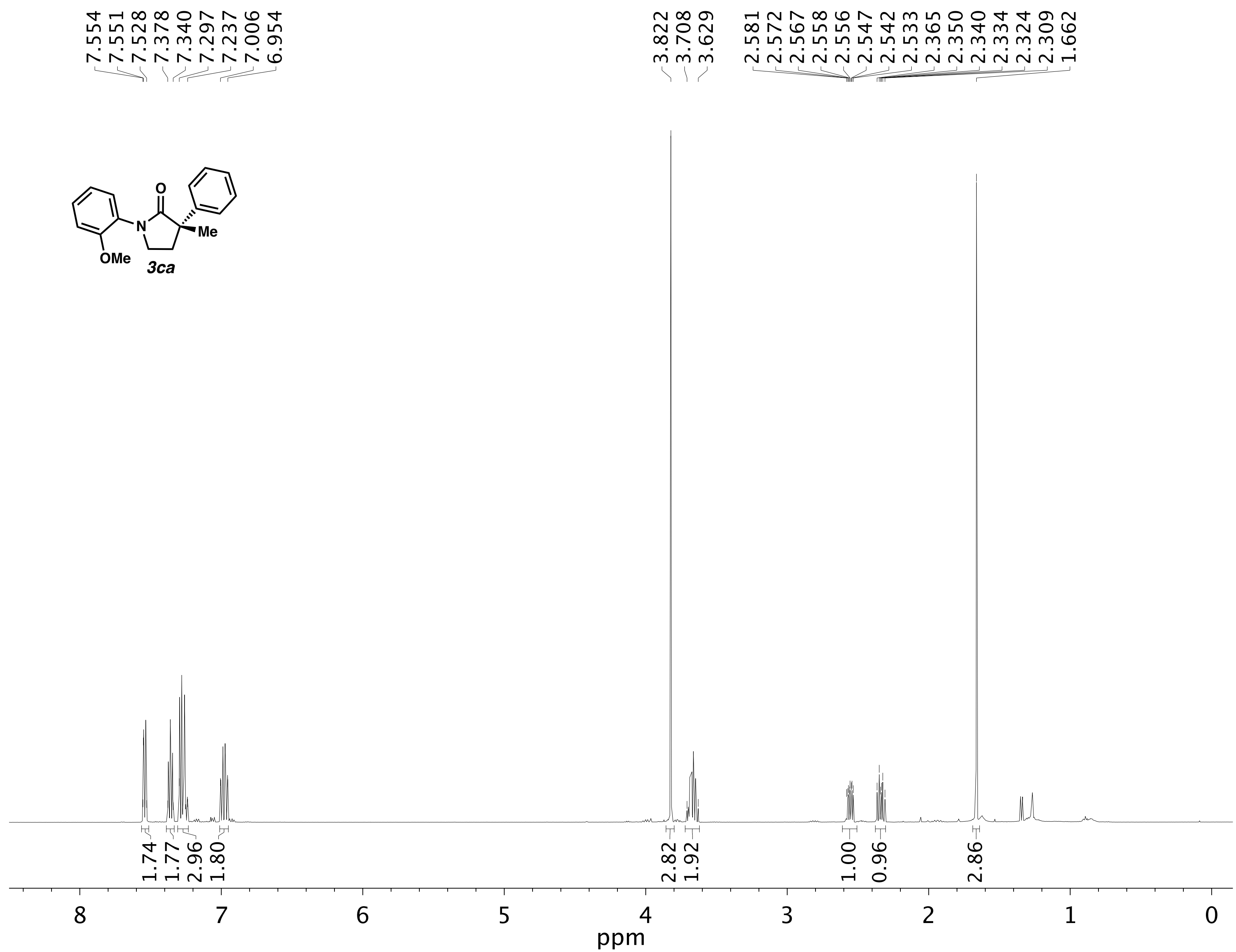
^{1}H NMR (500 MHz, CDCl$_3$) of compound **3ba**



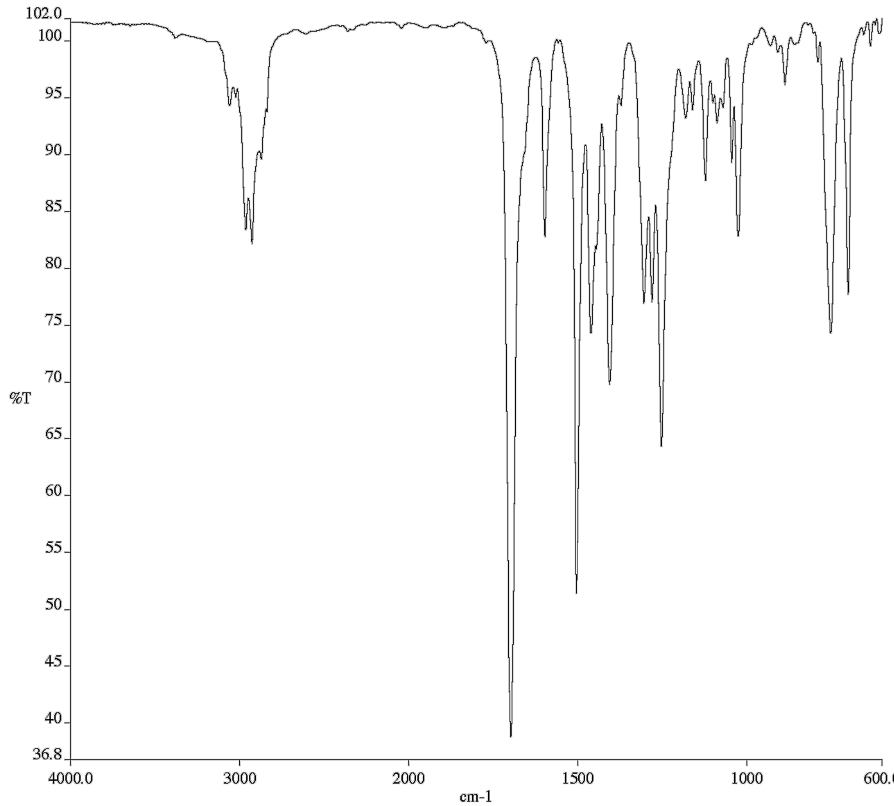
Infrared spectrum (Thin Film, NaCl) of compound **3ba**.



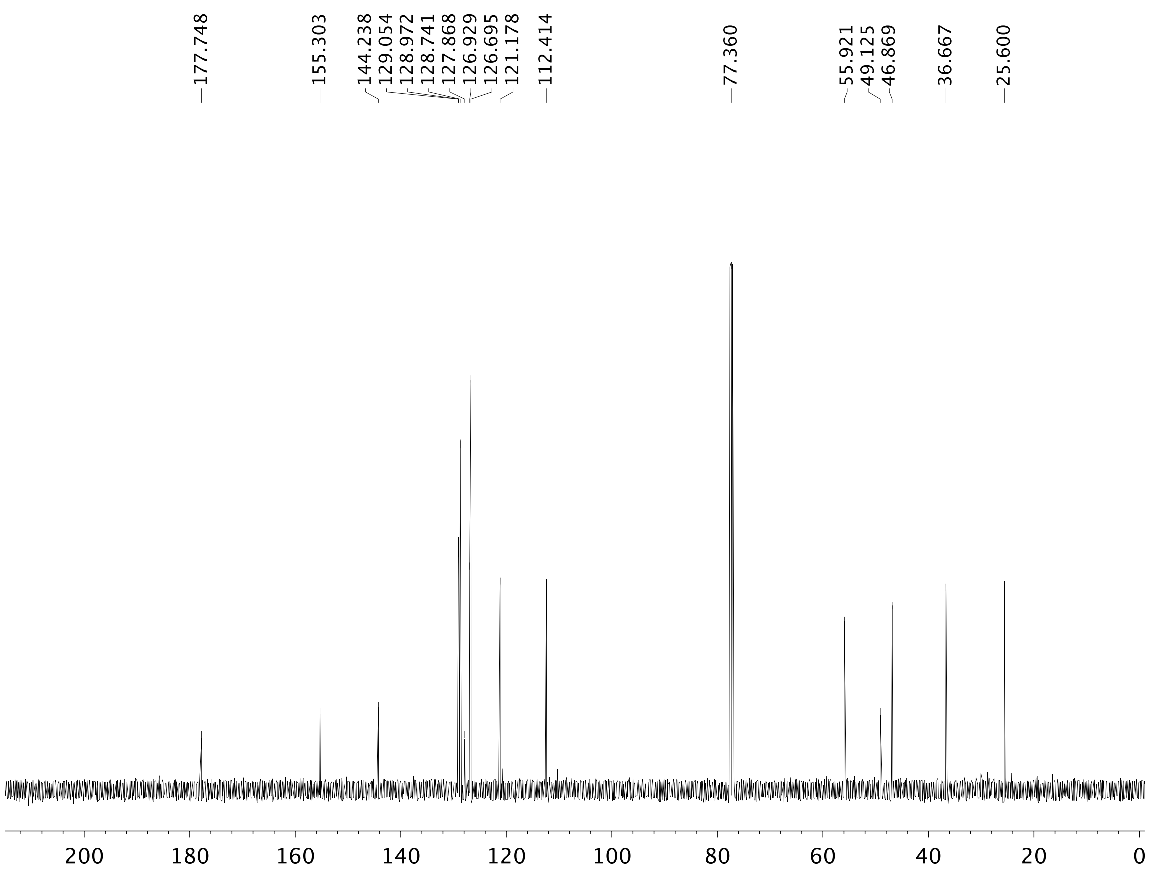
^{13}C NMR (125 MHz, $CDCl_3$) of compound **3ba**



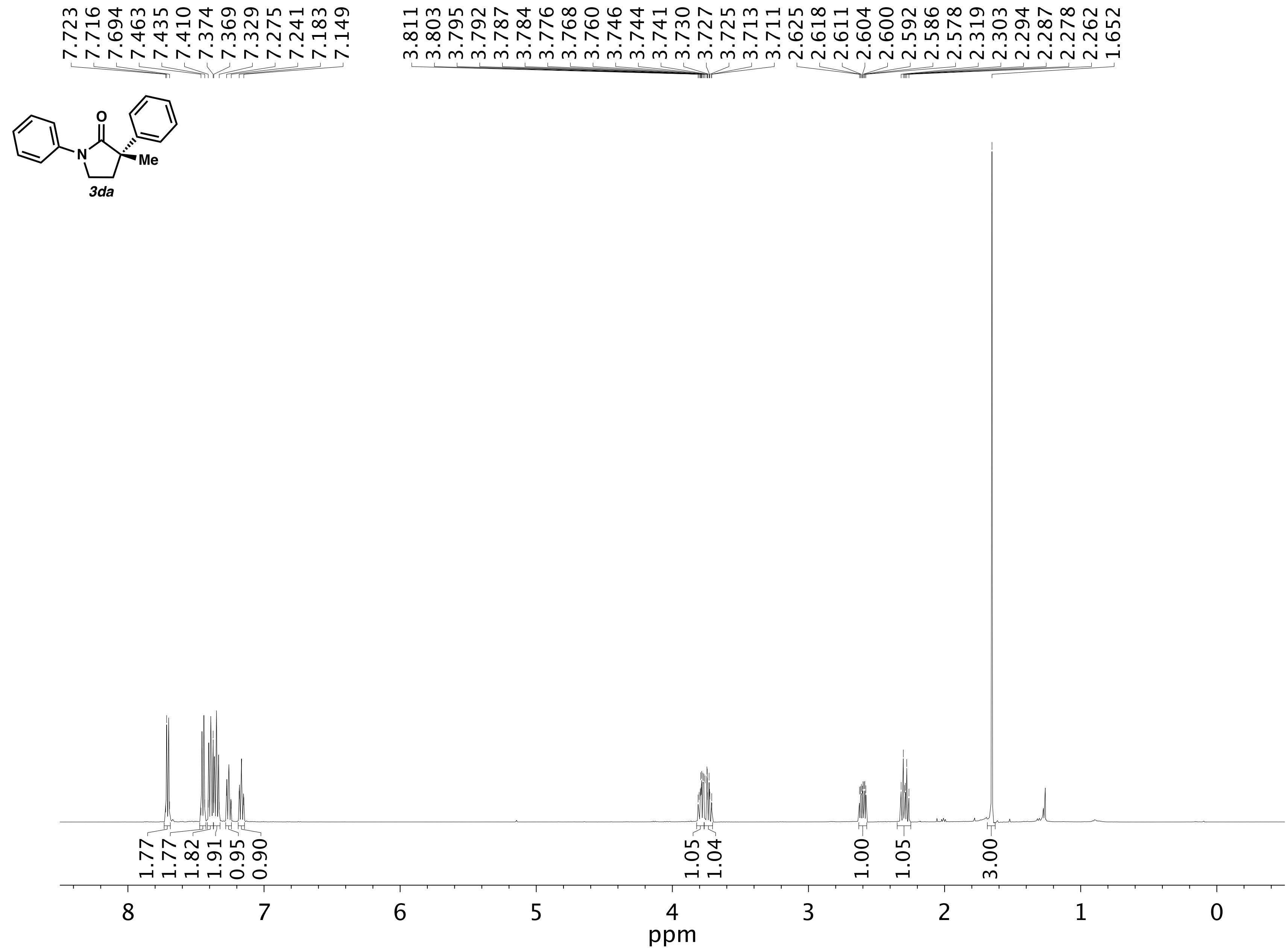
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3ca**



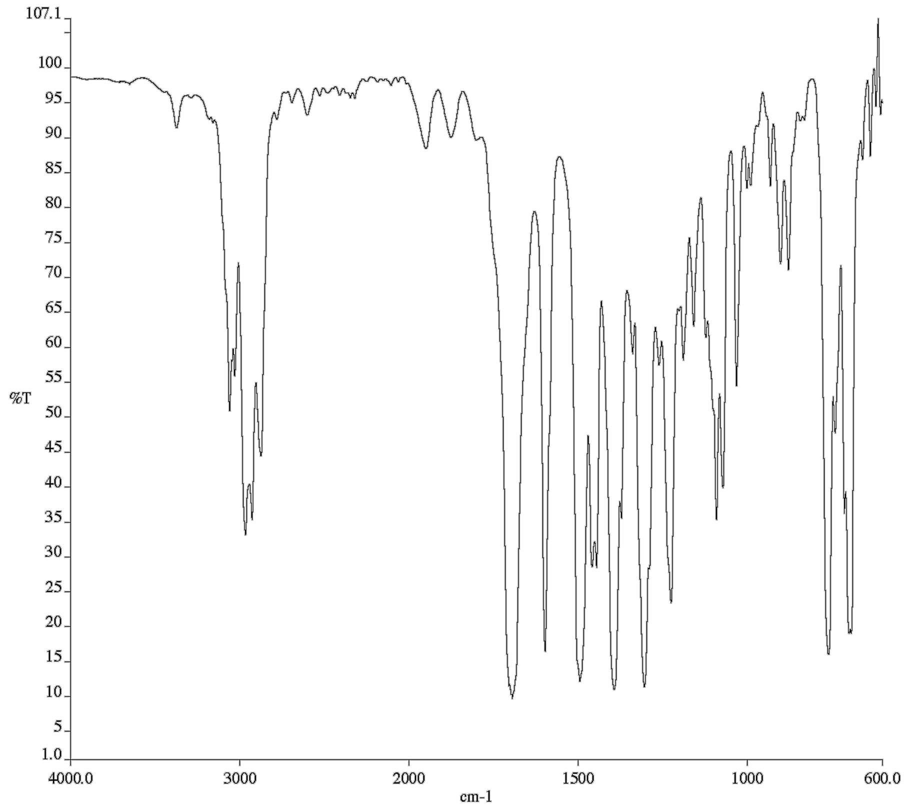
Infrared spectrum (Thin Film, NaCl) of compound **3ca**.



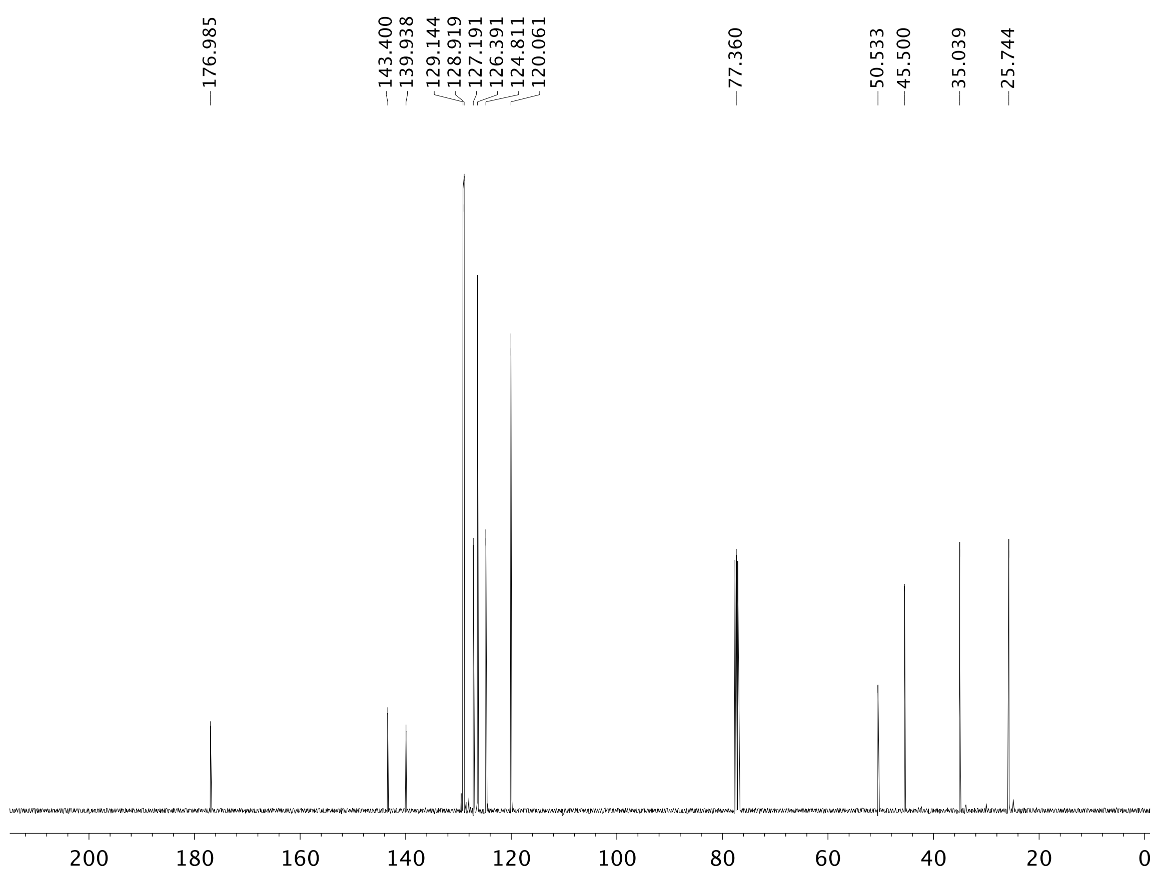
^{13}C NMR (125 MHz, $CDCl_3$) of compound **3ca**



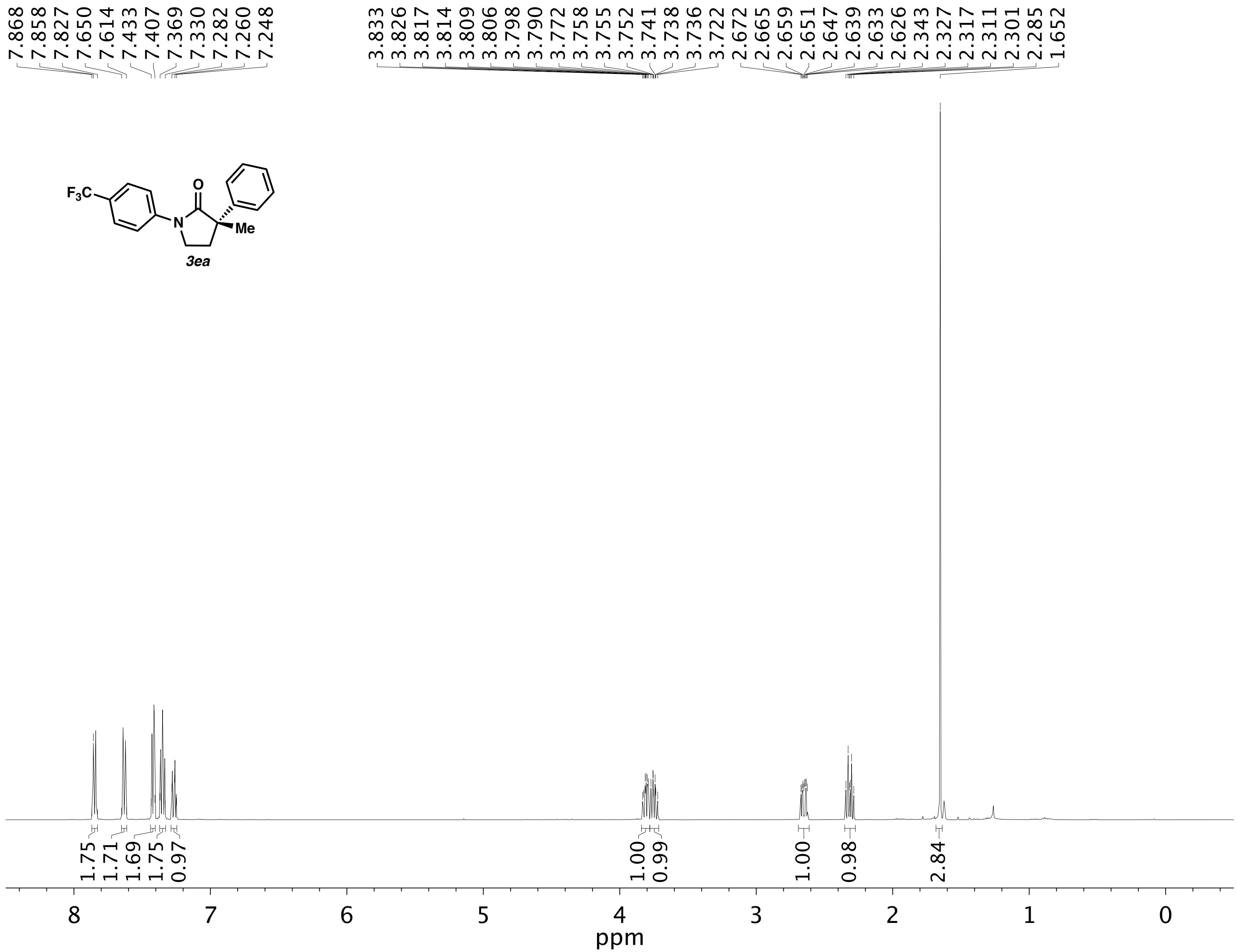
[1]H NMR (500 MHz, $CDCl_3$) of compound **3da**



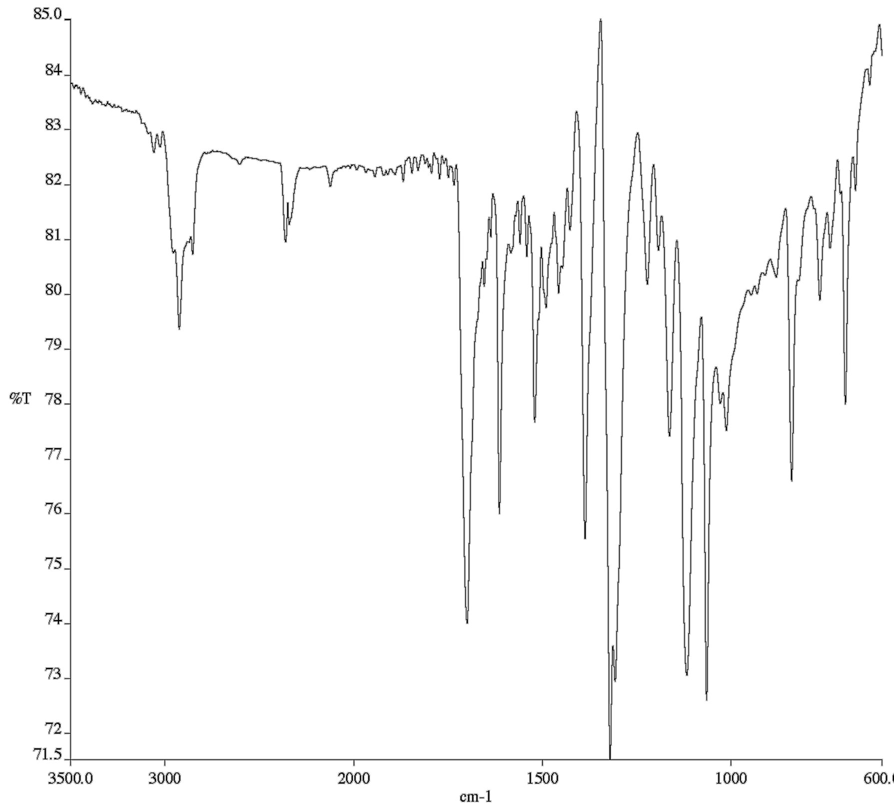
Infrared spectrum (Thin Film, NaCl) of compound **3da**.



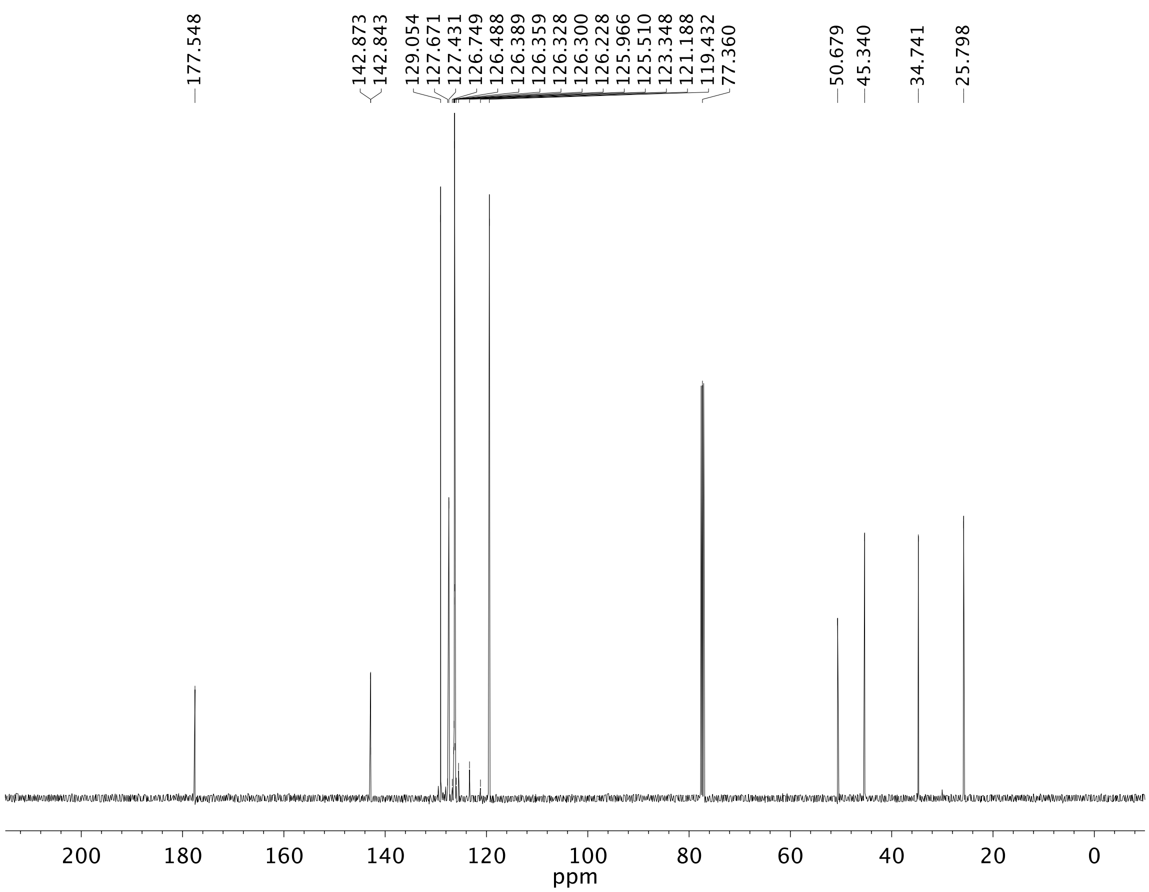
^{13}C NMR (125 MHz, $CDCl_3$) of compound **3da**



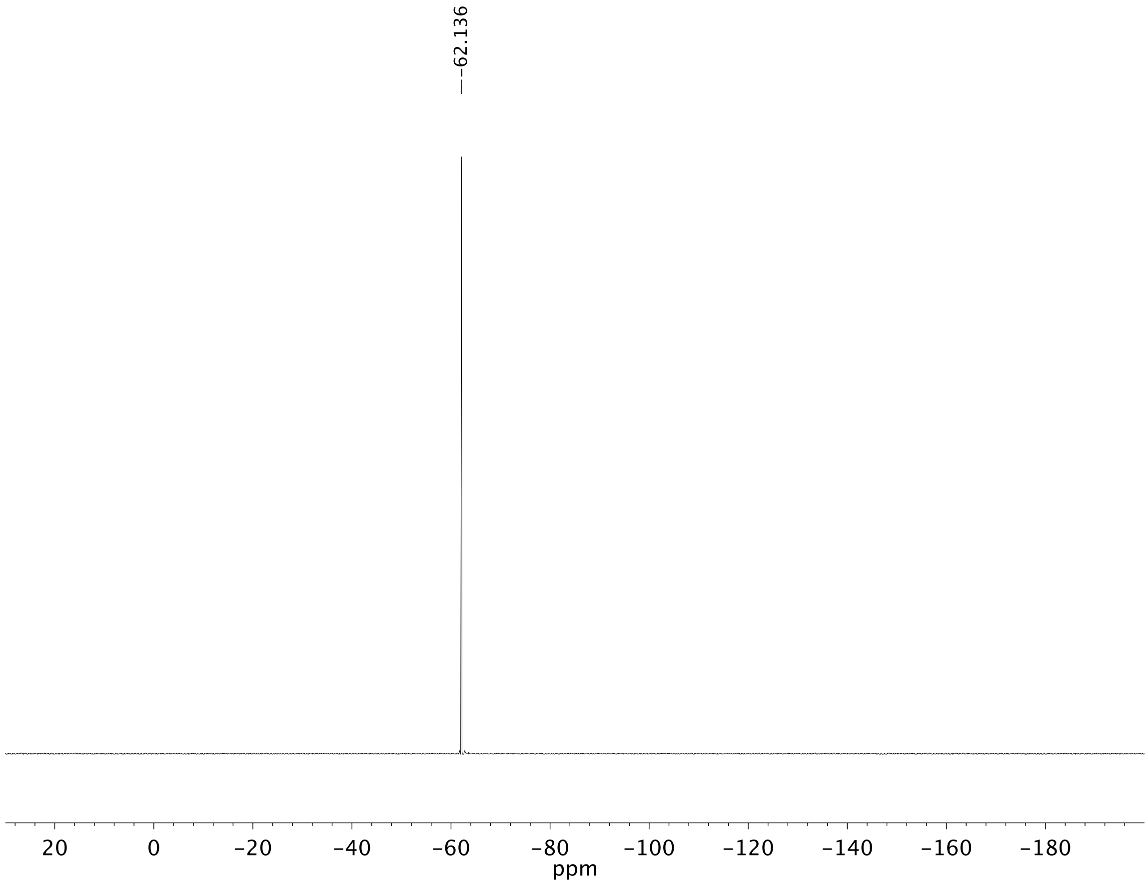
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3ea**



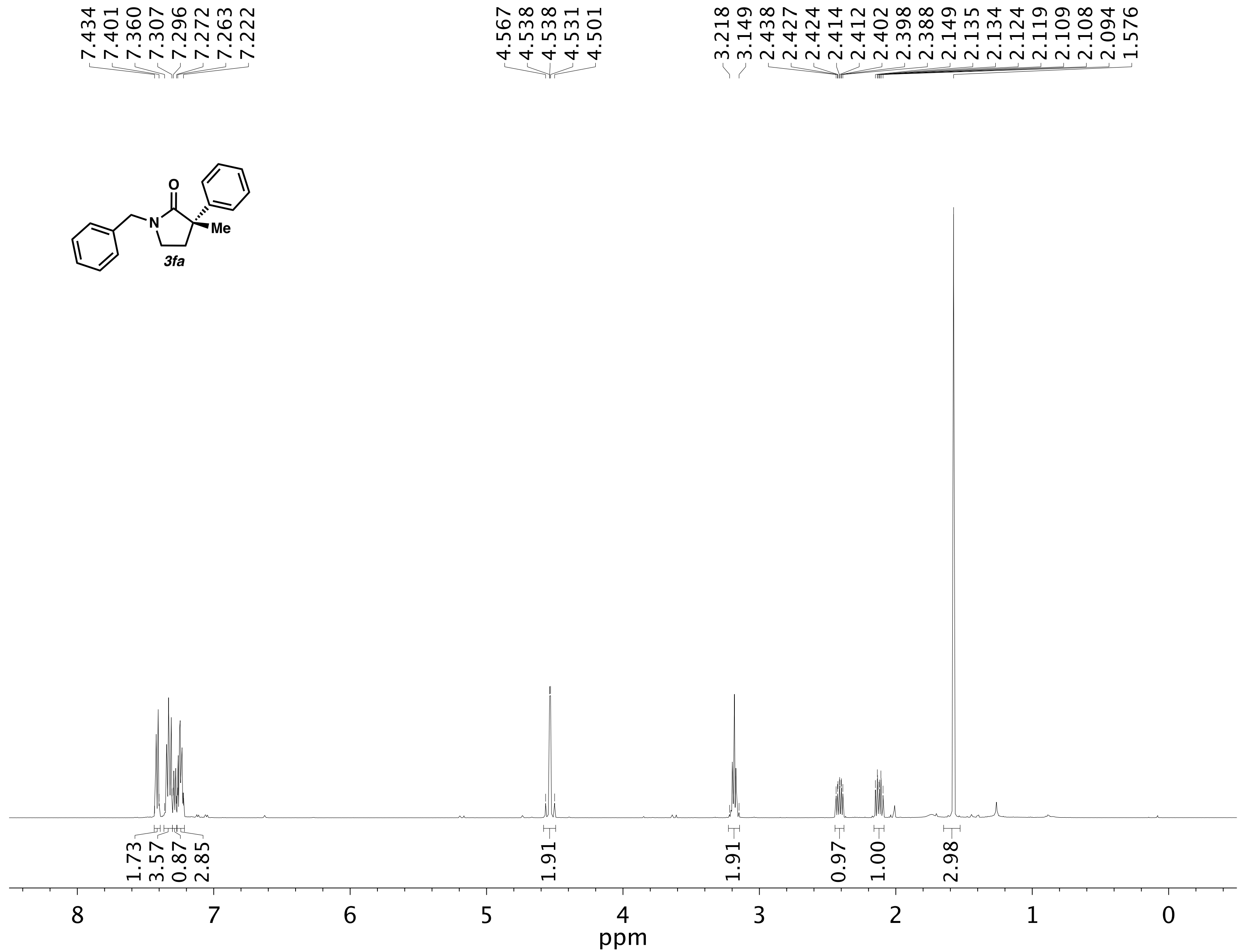
Infrared spectrum (Thin Film, NaCl) of compound **3ea**.



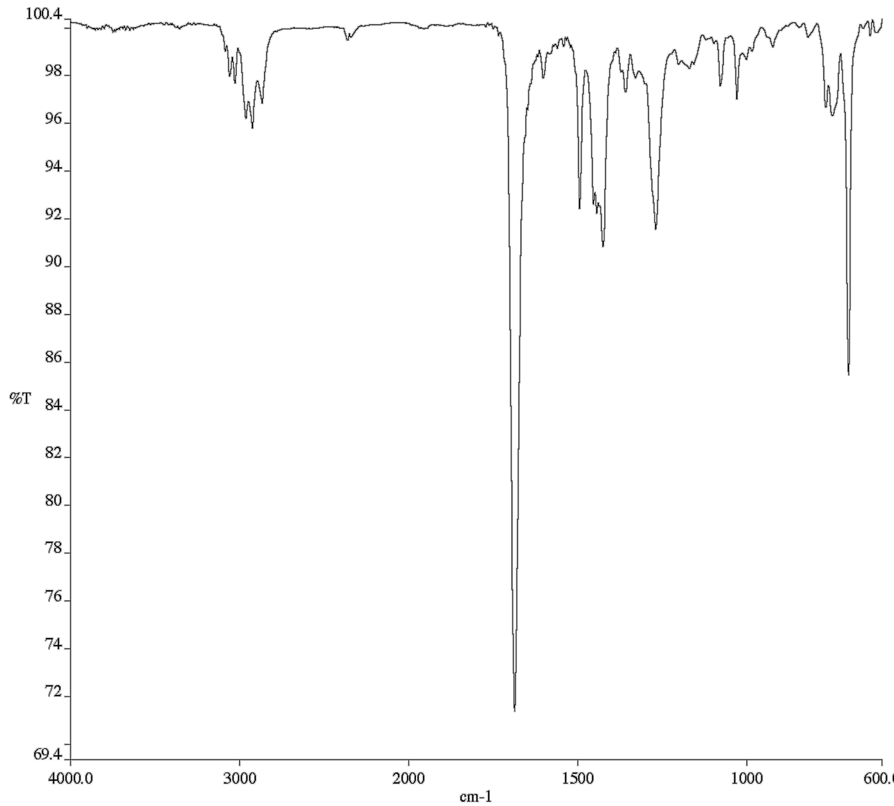
^{13}C NMR (125 MHz, $CDCl_3$) of compound **3ea**



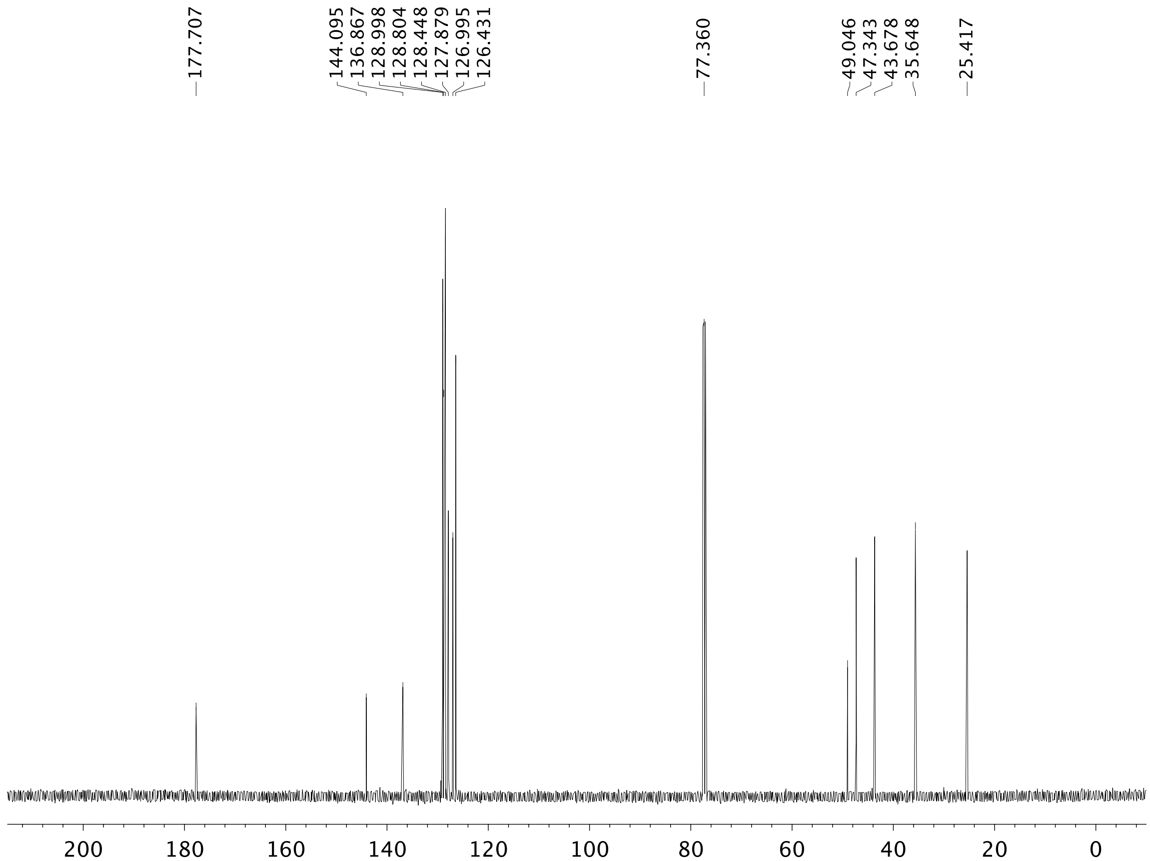
^{19}F NMR (282 MHz, $CDCl_3$) of compound **3ea**



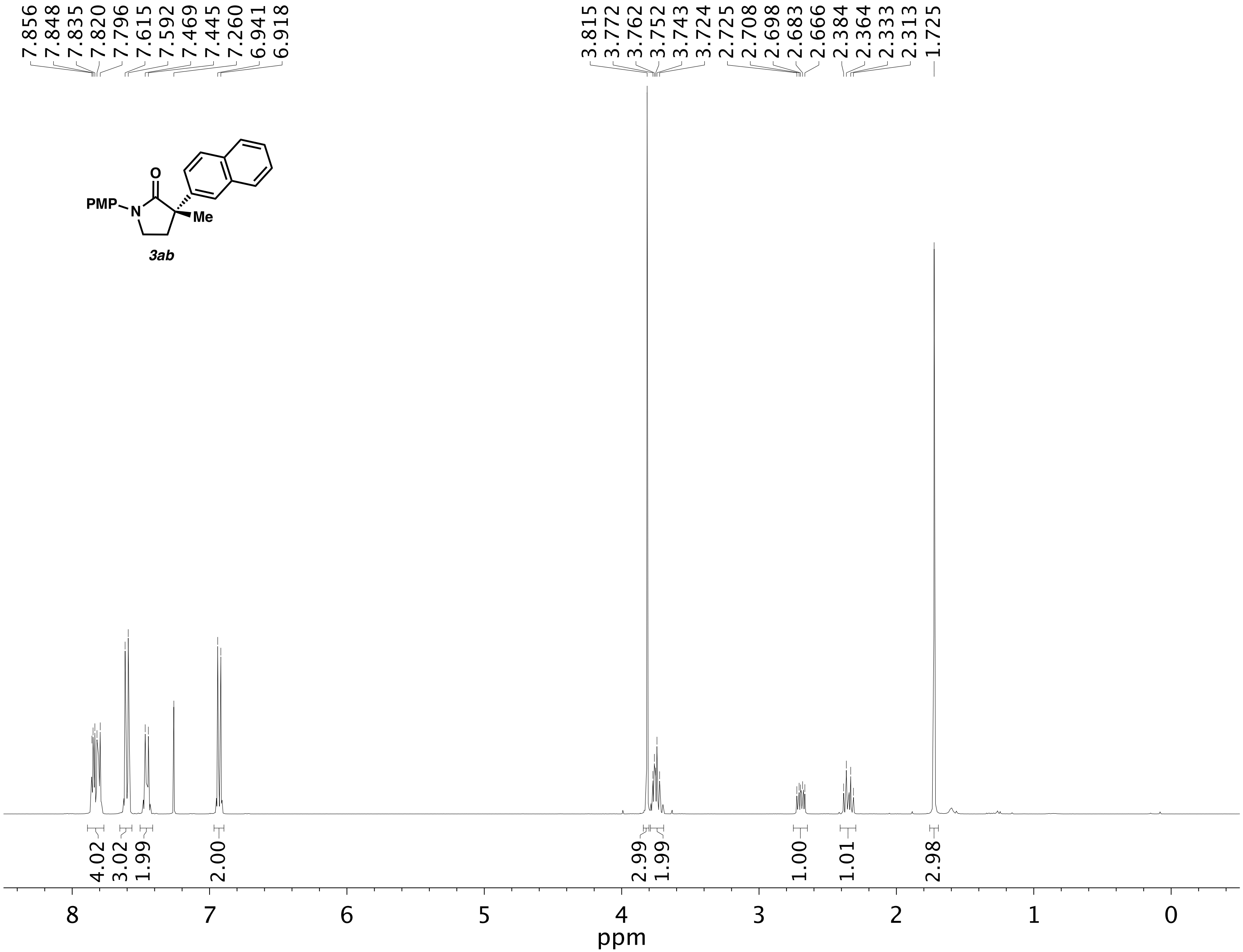
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3fa**



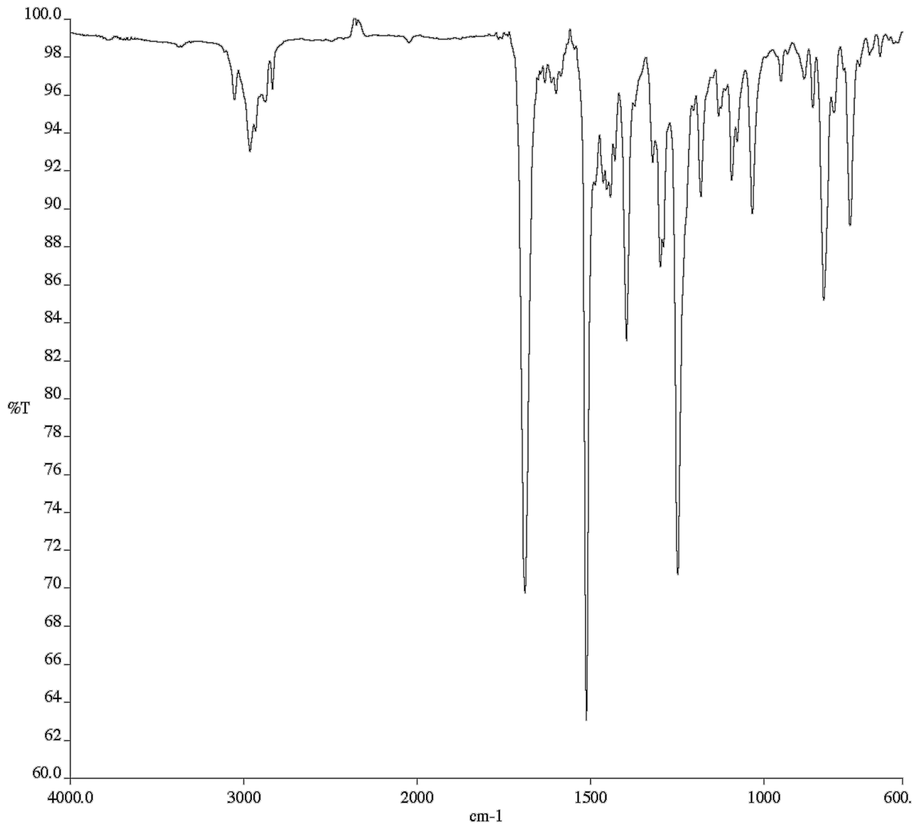
Infrared spectrum (Thin Film, NaCl) of compound **3fa**.



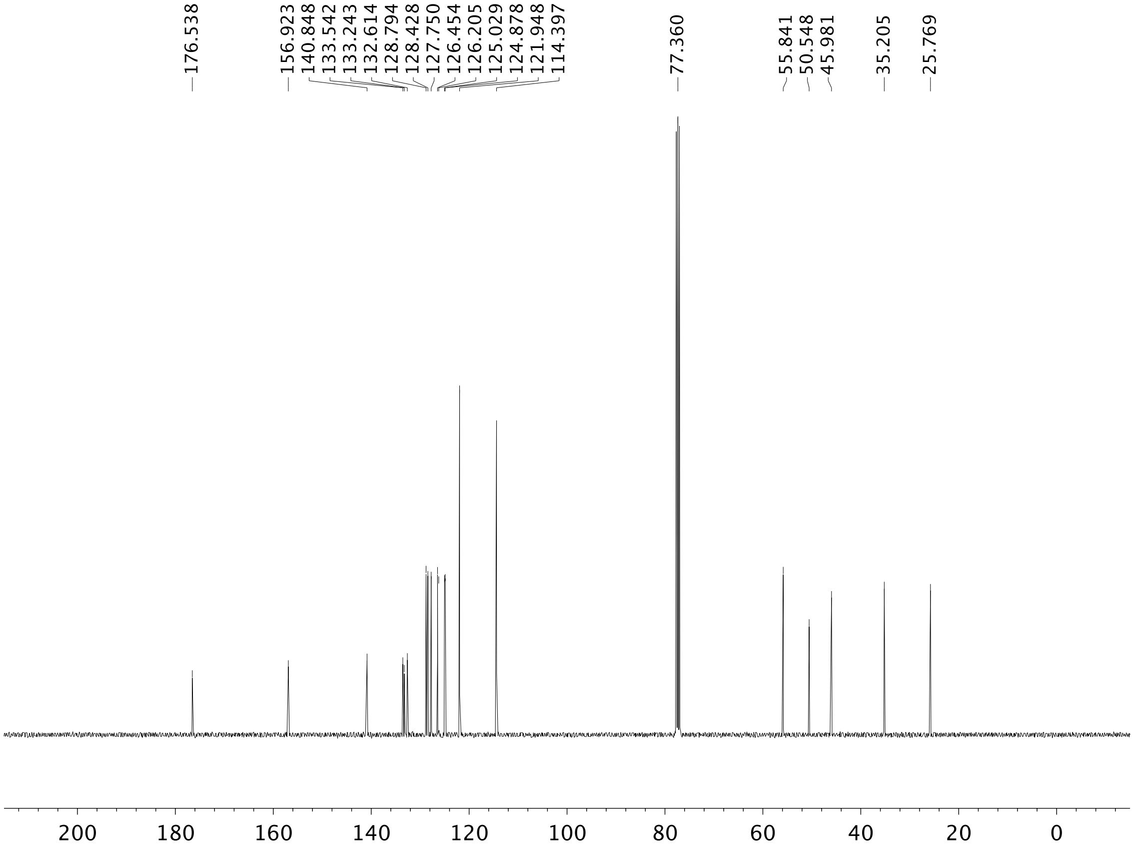
^{13}C NMR (125 MHz, $CDCl_3$) of compound **3fa**



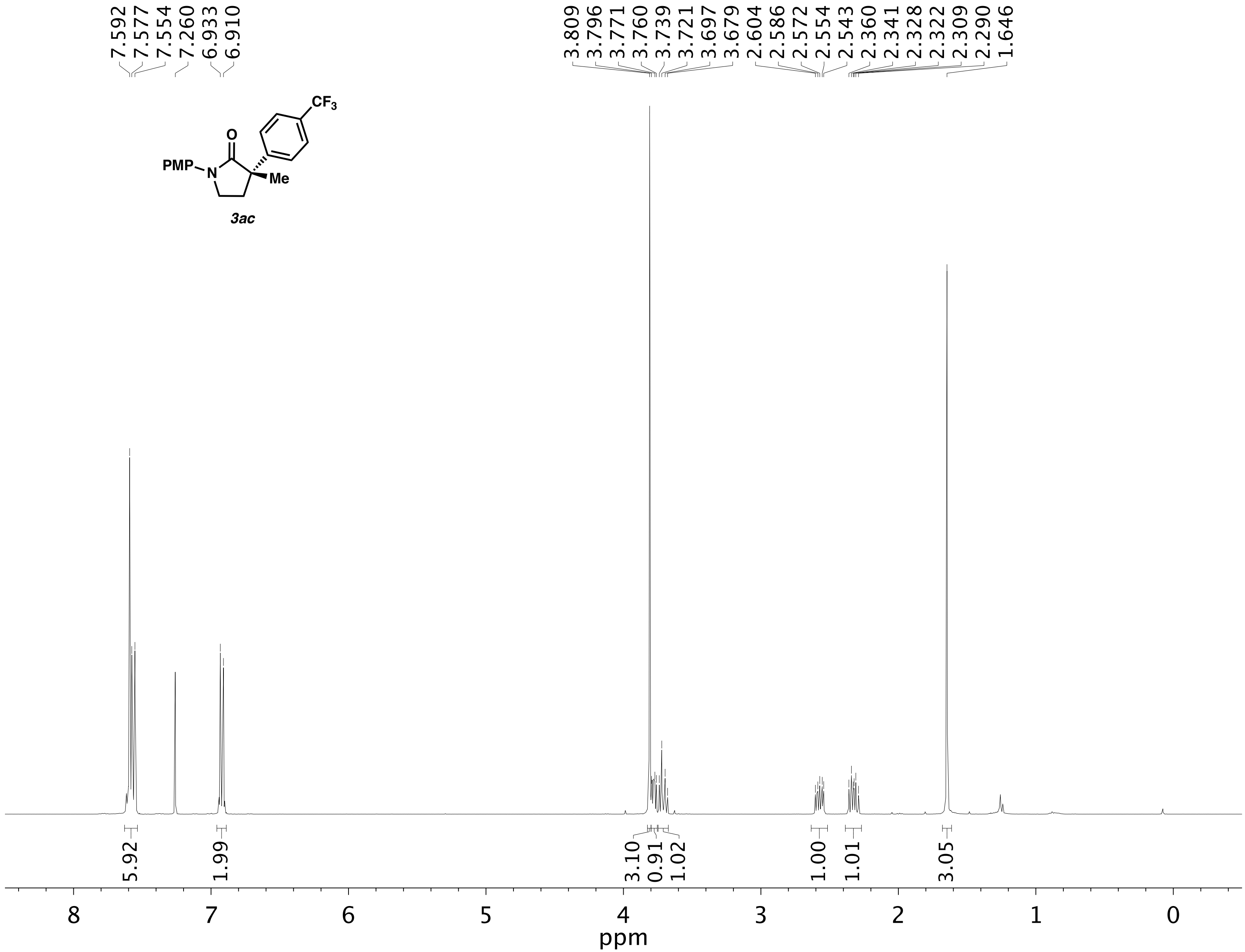
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ab**



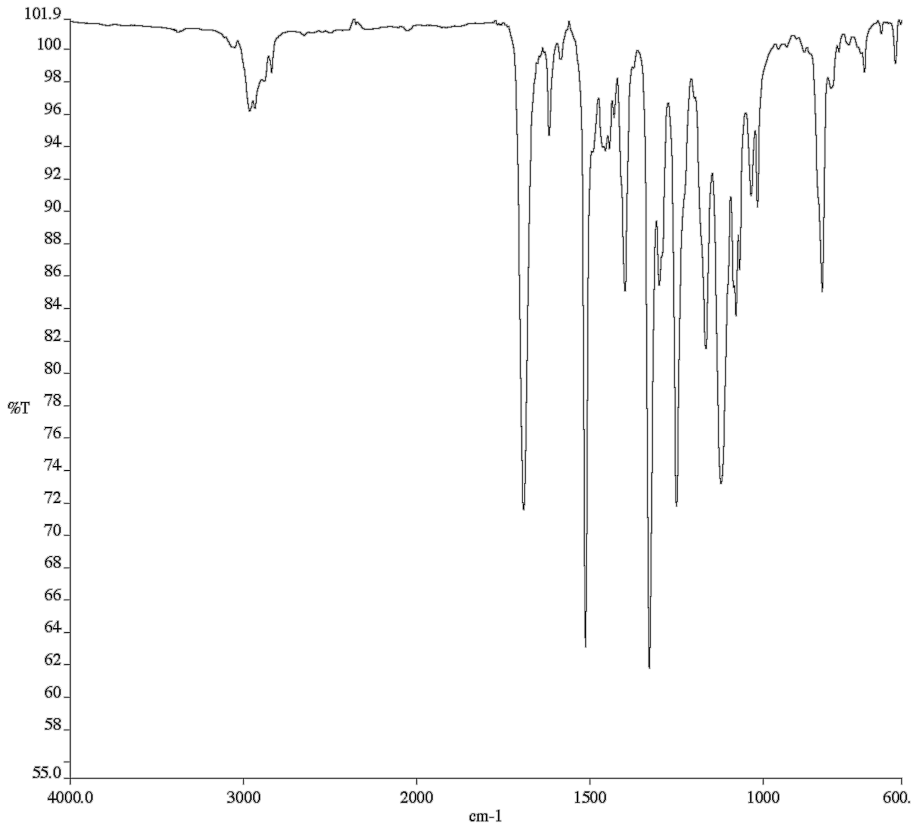
Infrared spectrum (Thin Film, NaCl) of compound **3ab**



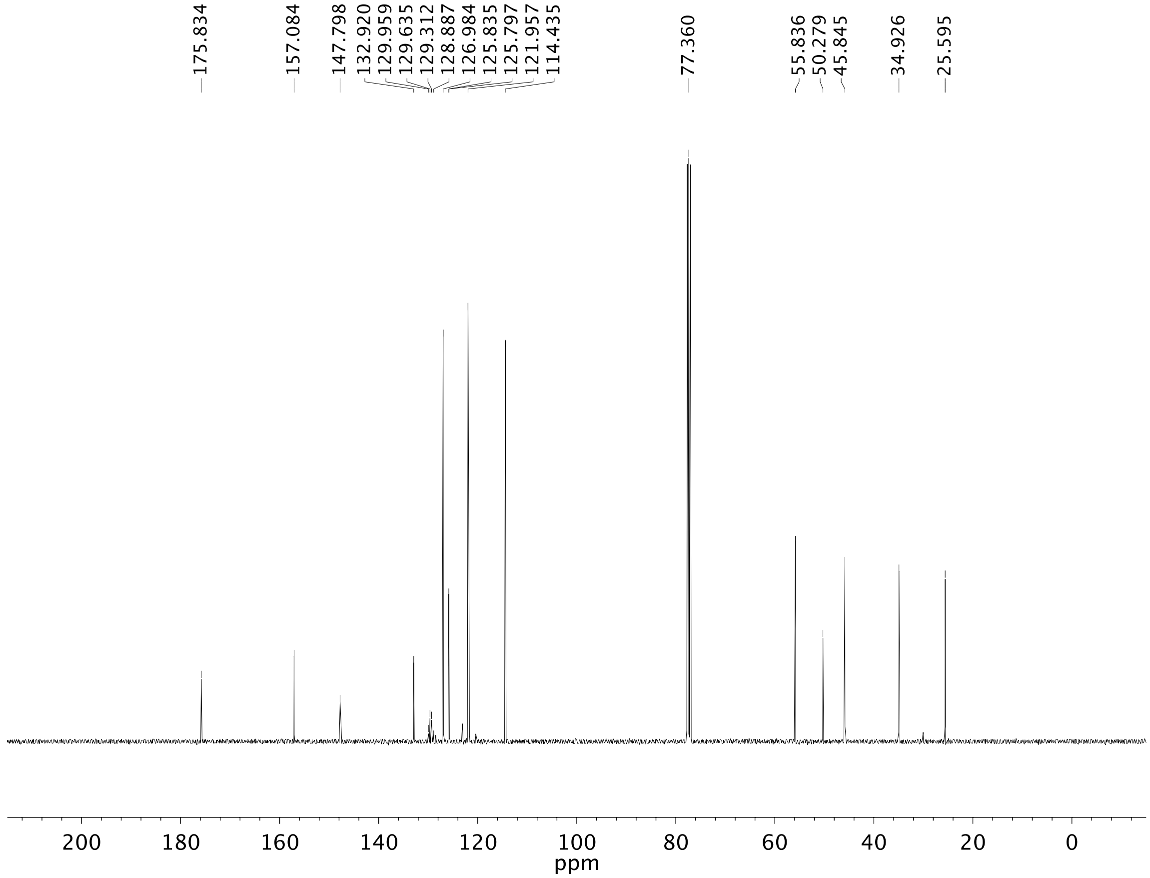
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ab**.



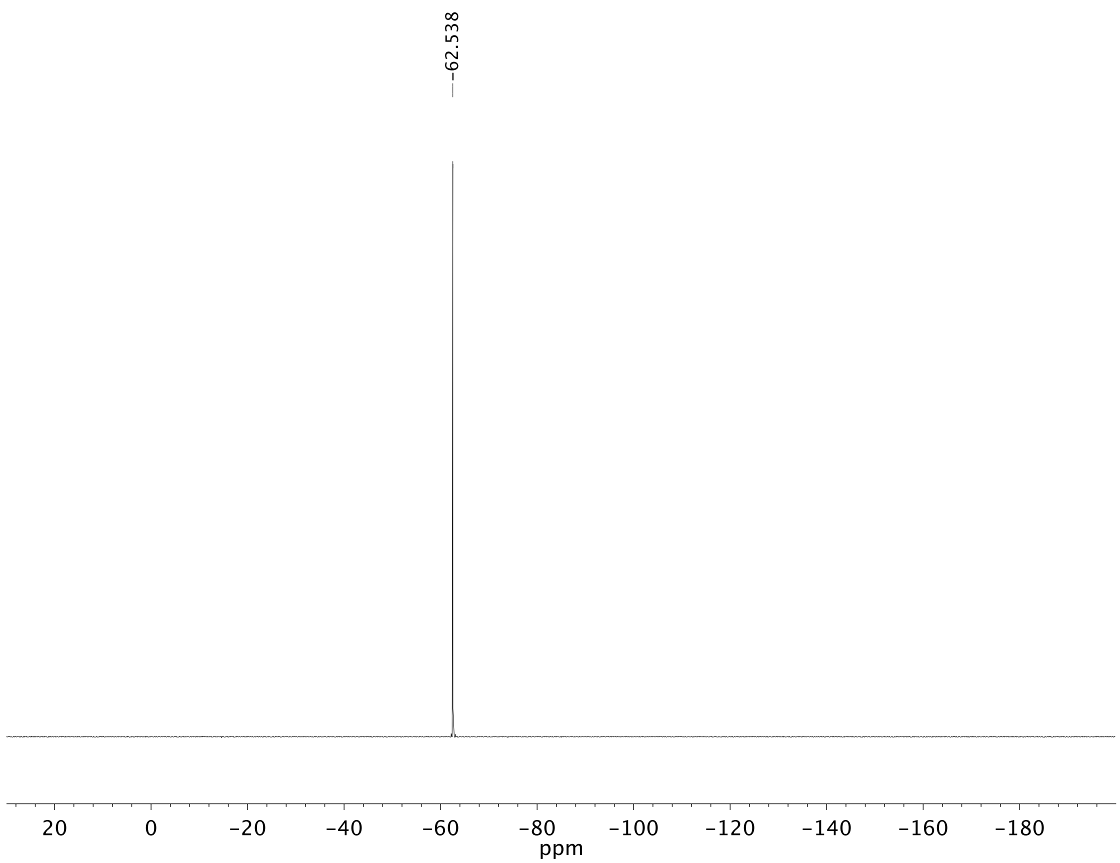
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ac**



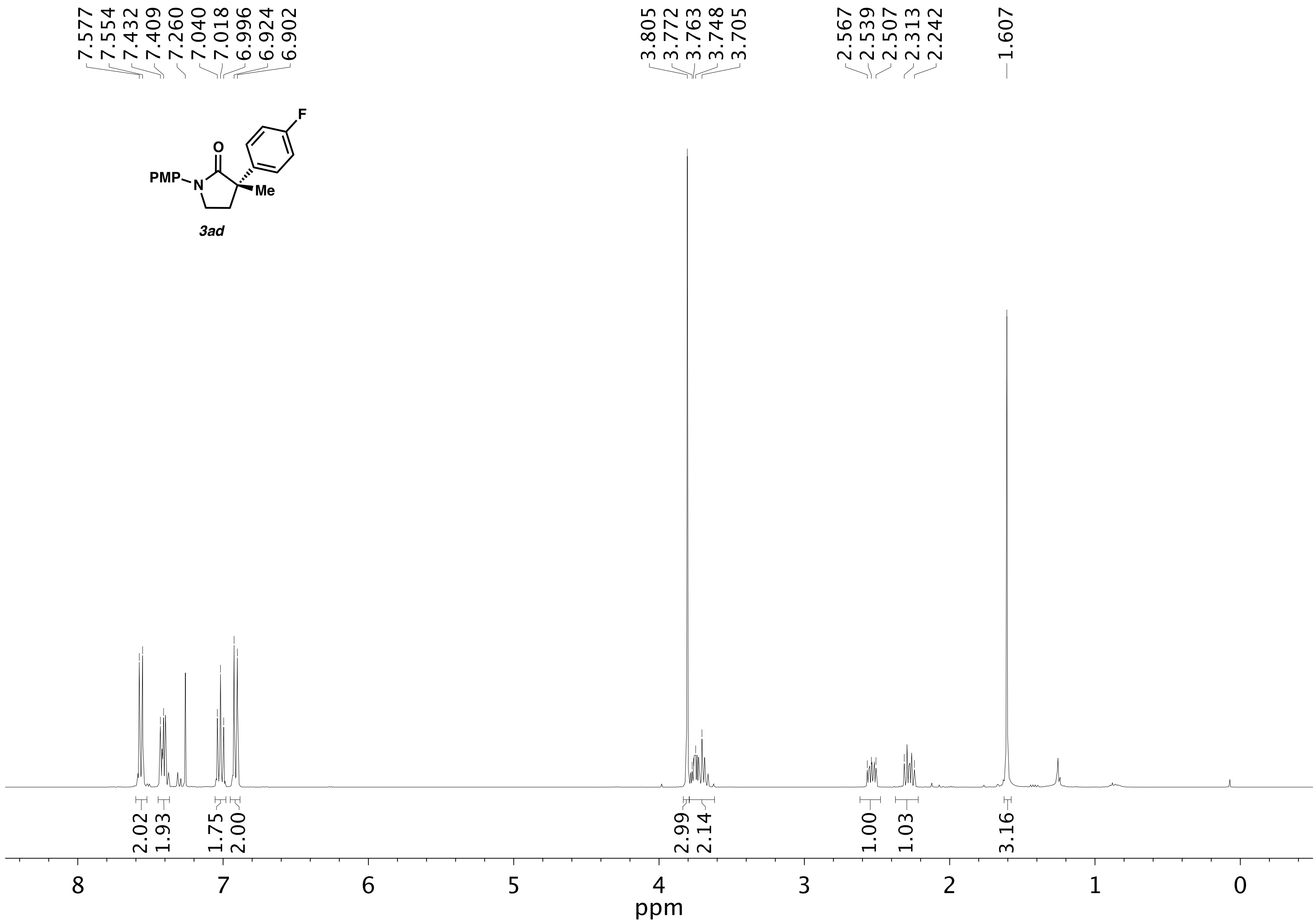
Infrared spectrum (Thin Film, NaCl) of compound **3ac**



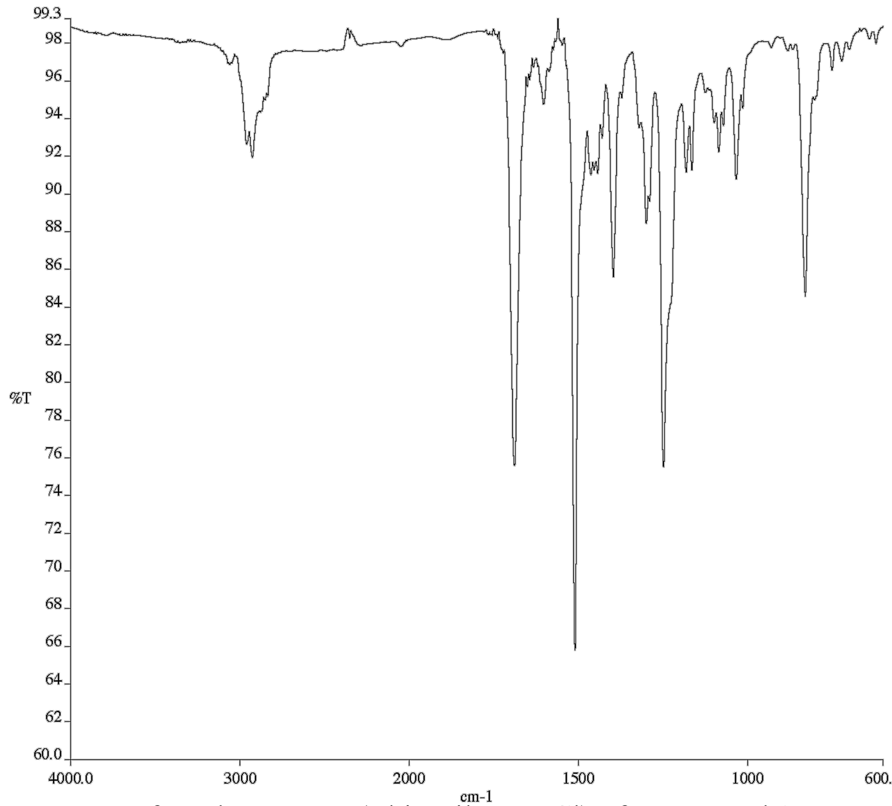
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ac**



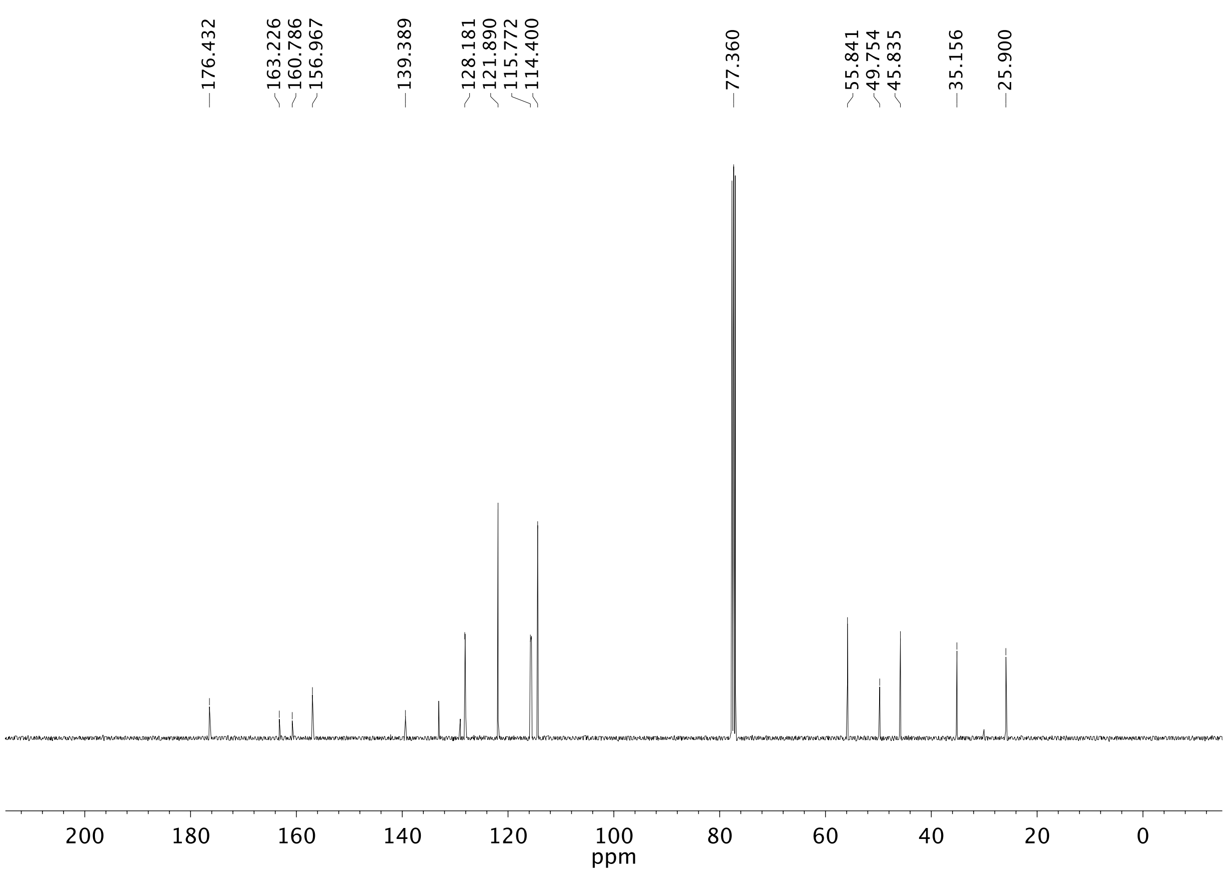
^{19}F NMR (282 MHz, $CDCl_3$) of compound **3ac**



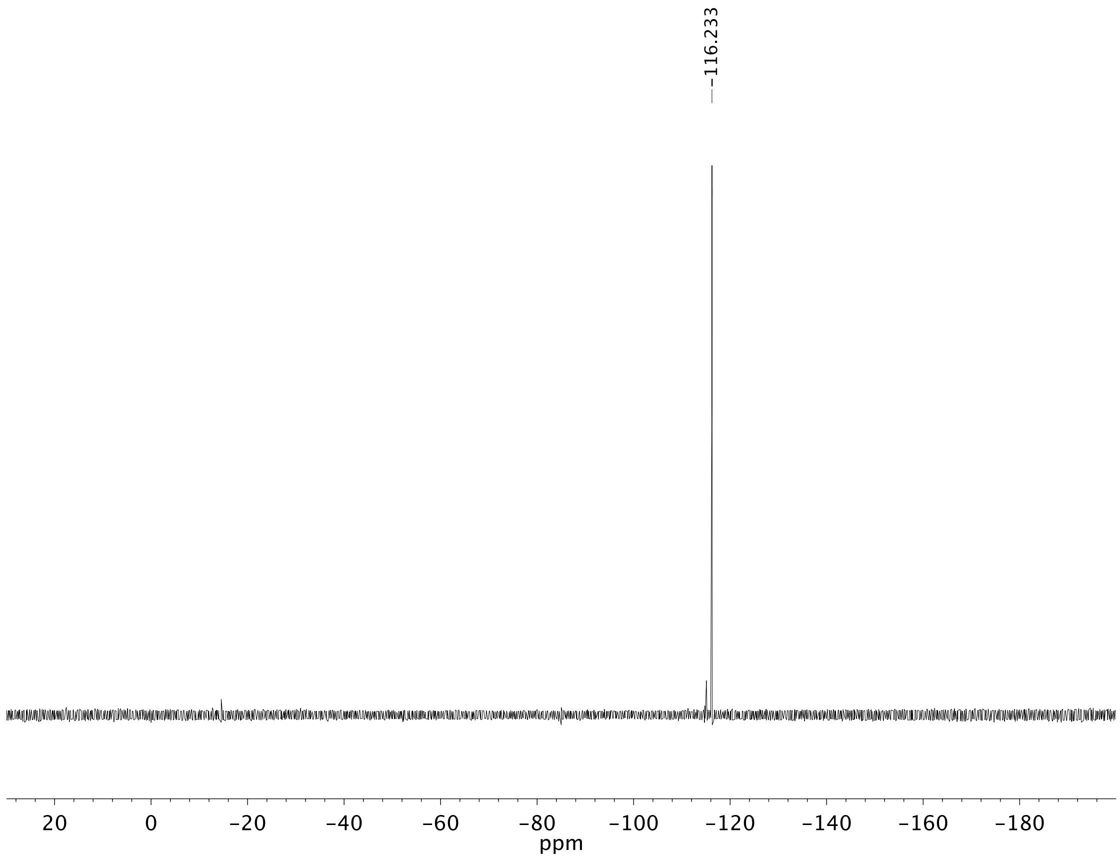
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ad**



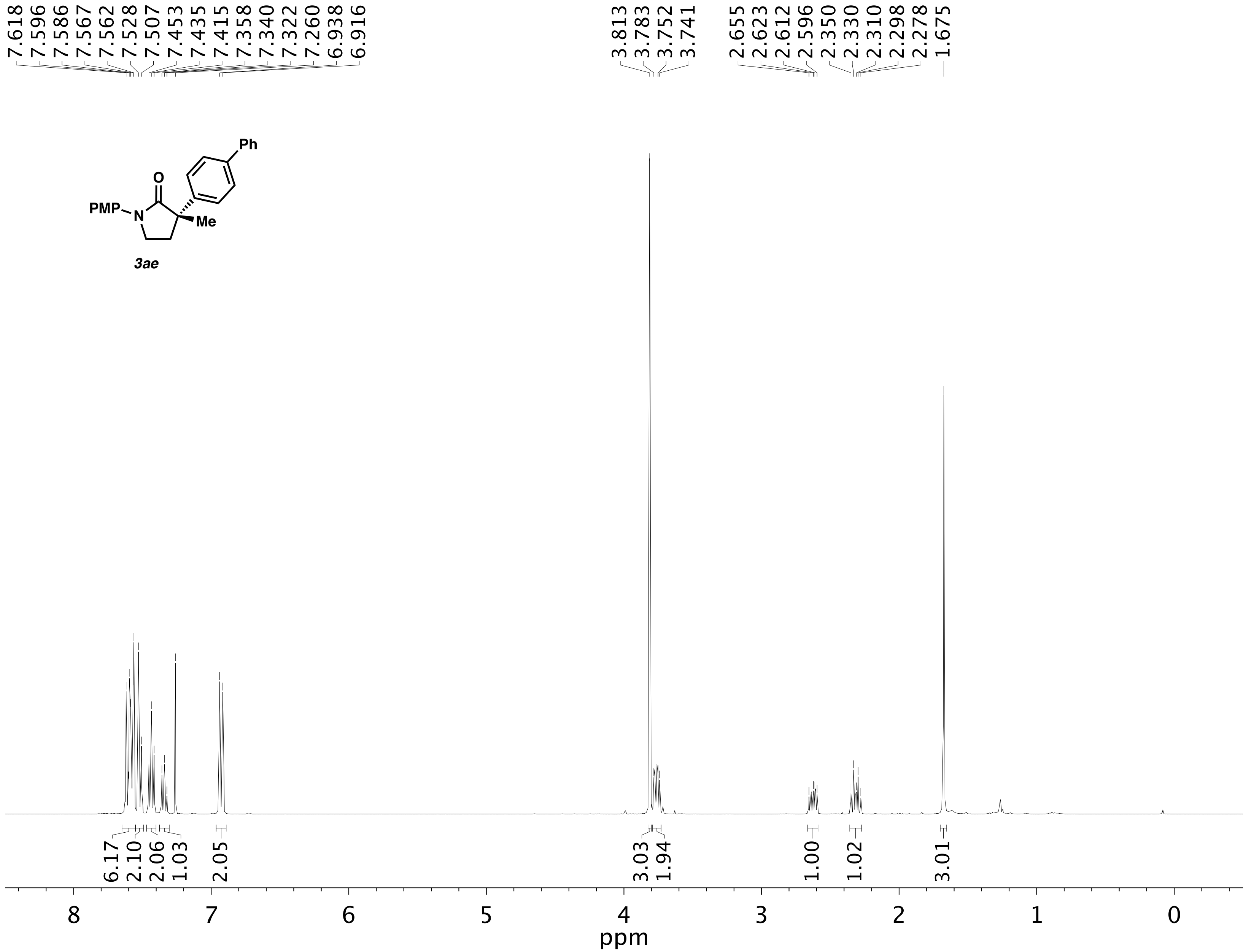
Infrared spectrum (Thin Film, NaCl) of compound **3ad**.



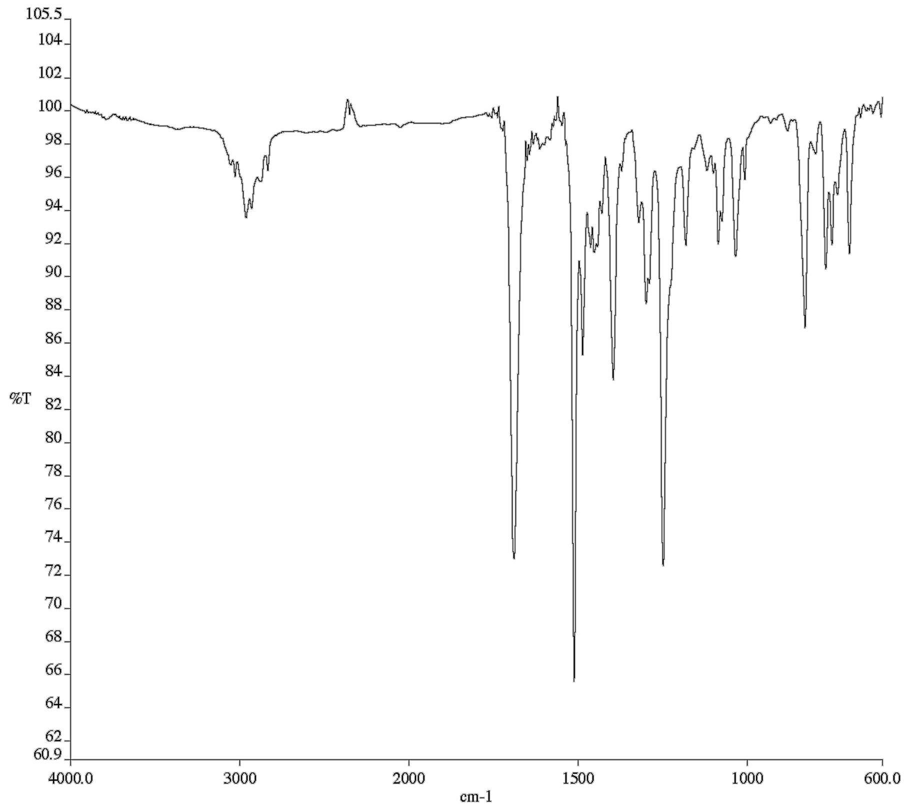
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ad**



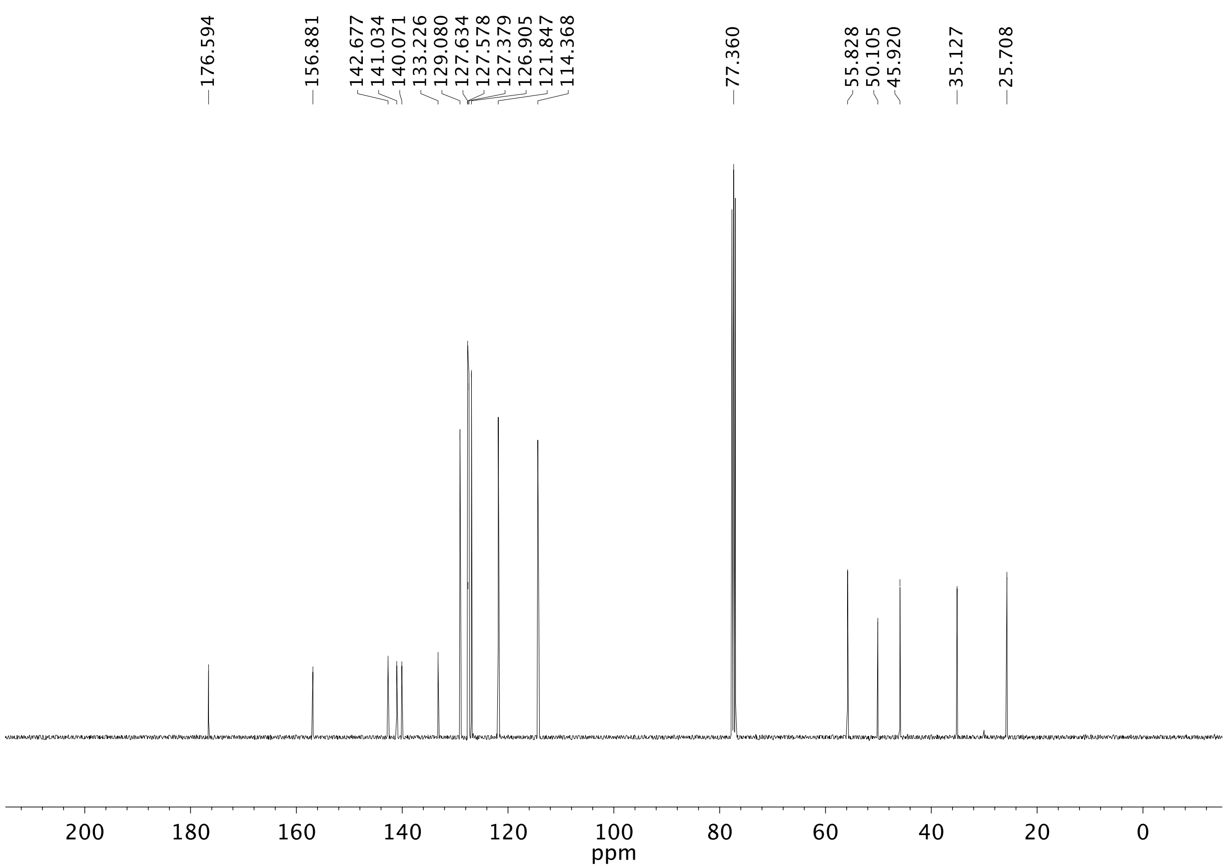
^{19}F NMR (282 MHz, $CDCl_3$) of compound **3ad**



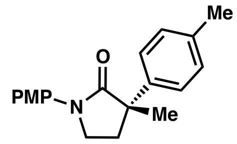
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ae**



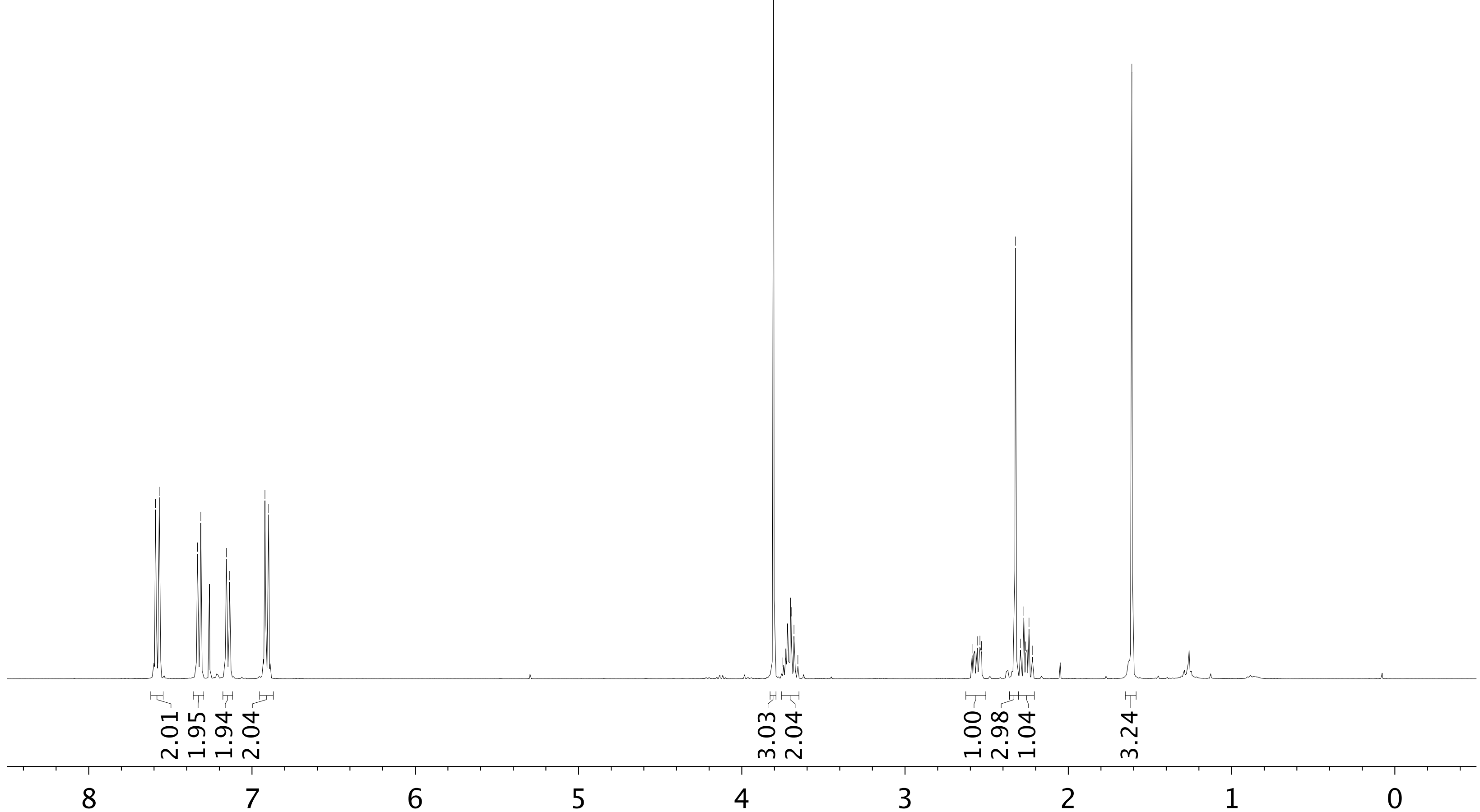
Infrared spectrum (Thin Film, NaCl) of compound **3ae**.



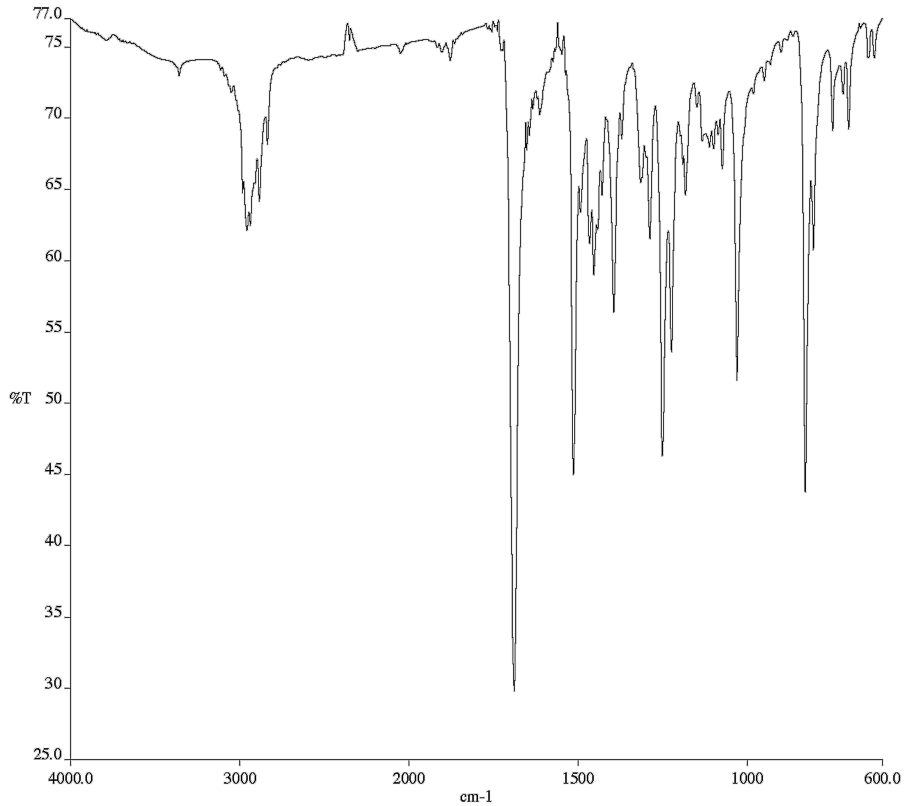
^{13}C NMR (126 100 MHz, $CDCl_3$) of compound **3ae**



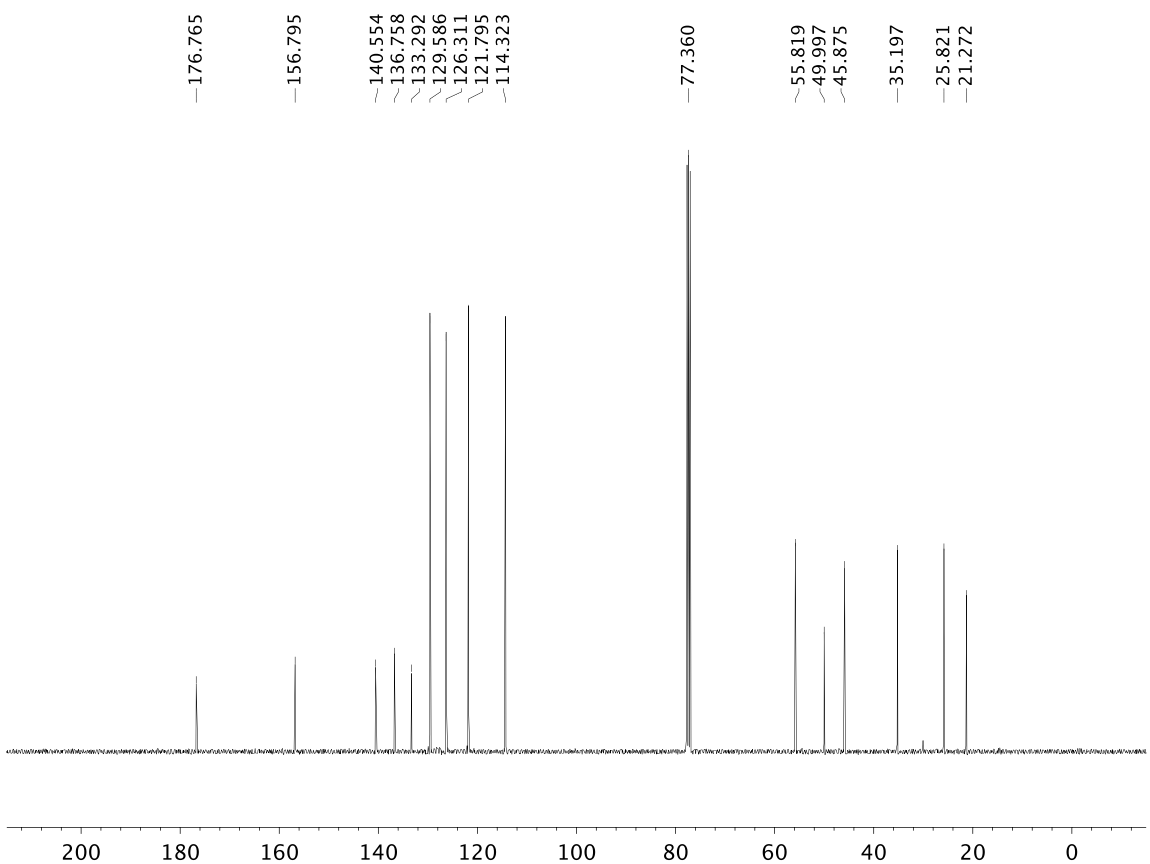
3af



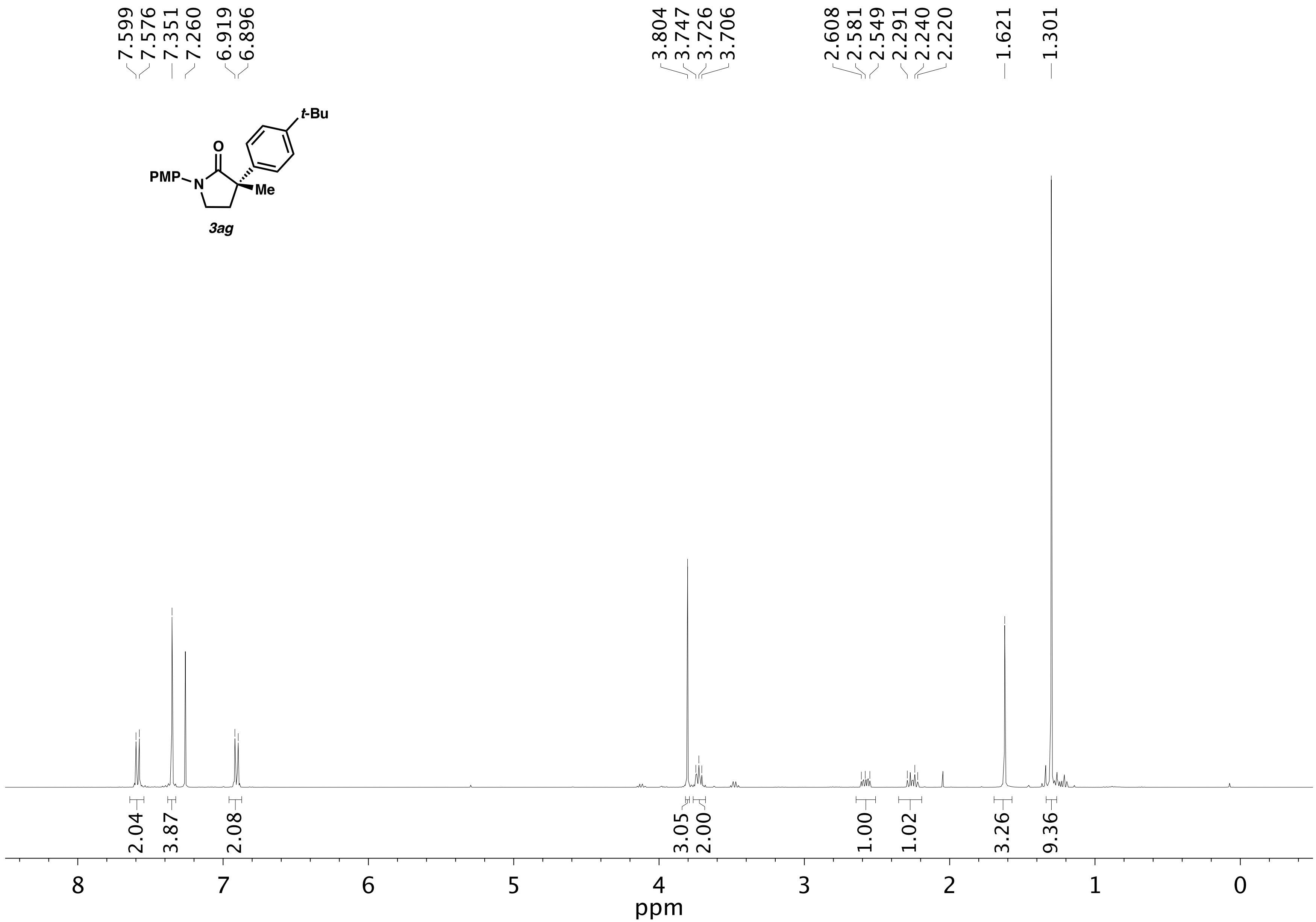
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3af**



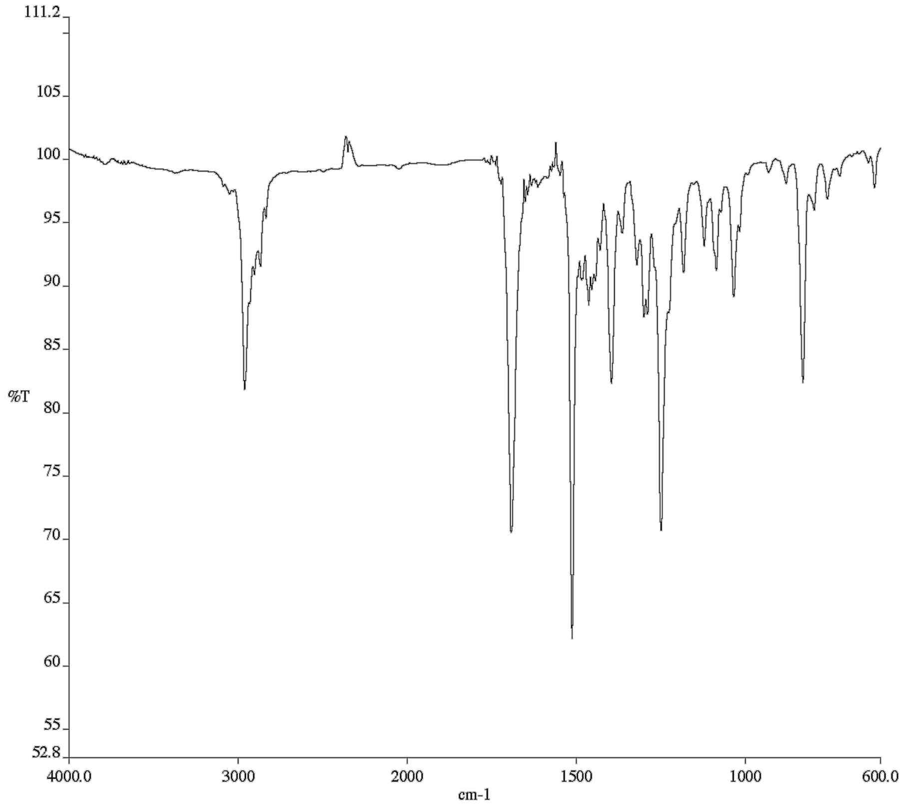
Infrared spectrum (Thin Film, NaCl) of compound **3af**.



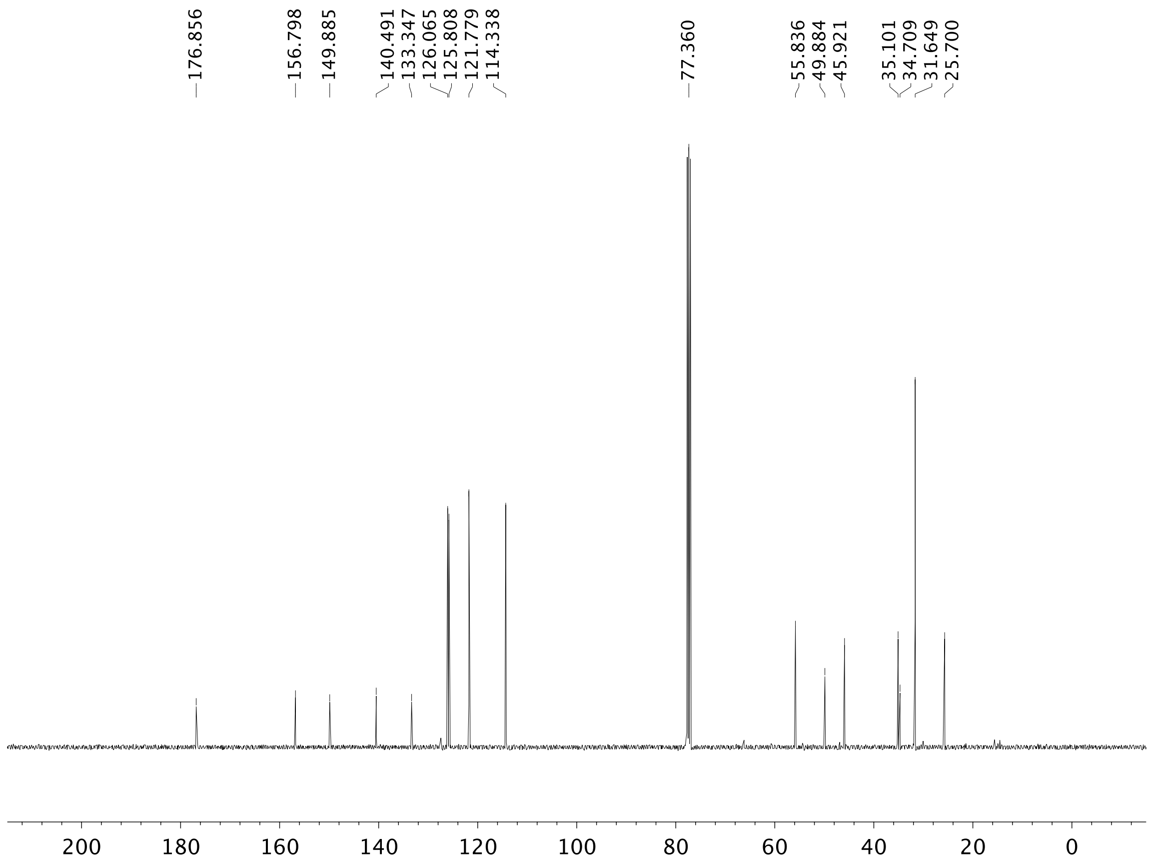
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3af**



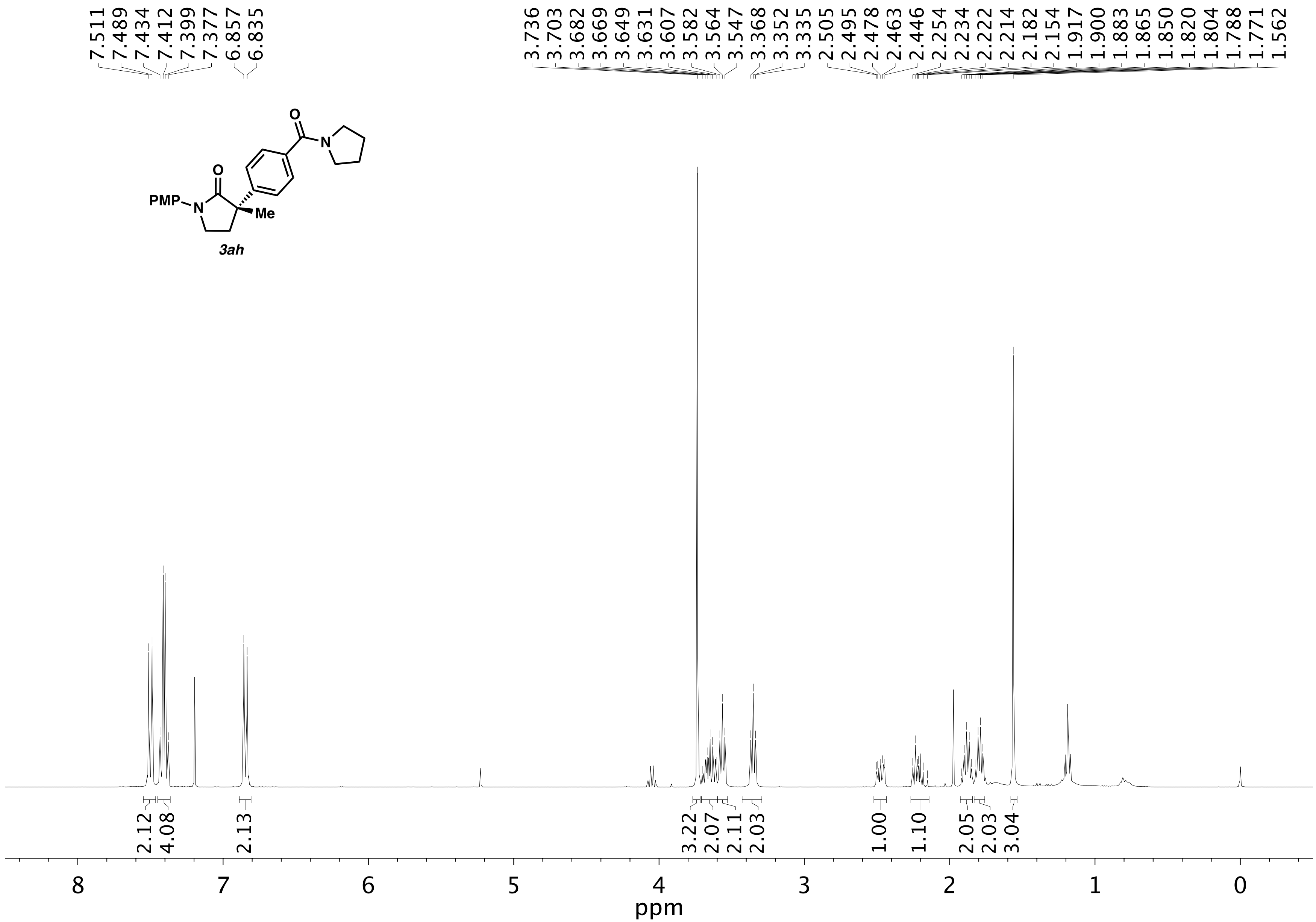
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ag**



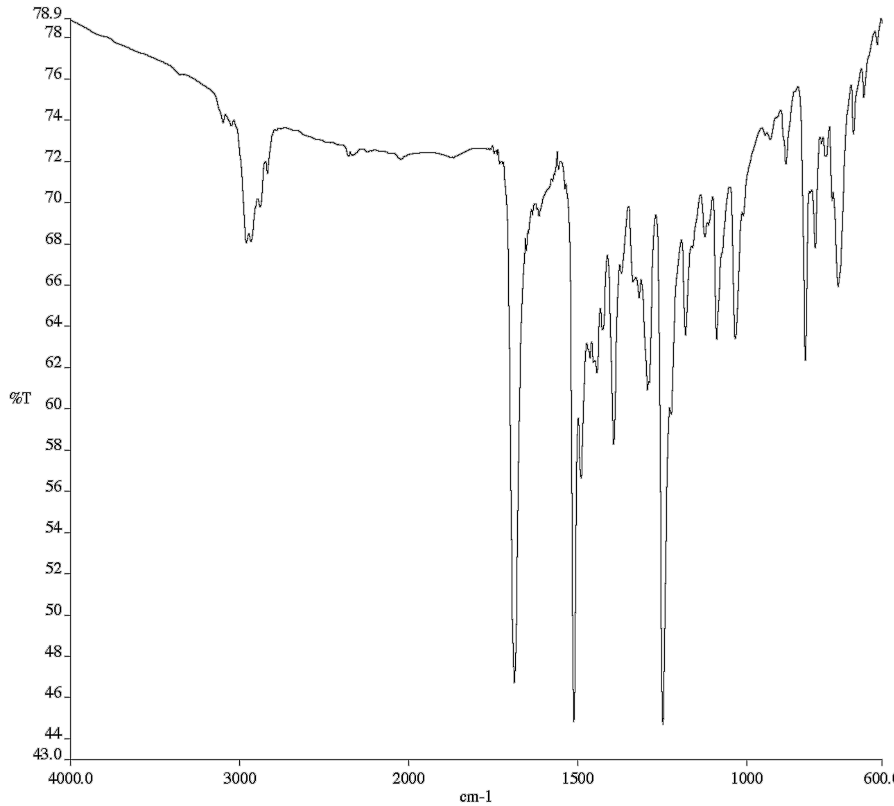
Infrared spectrum (Thin Film, NaCl) of compound **3ag**.



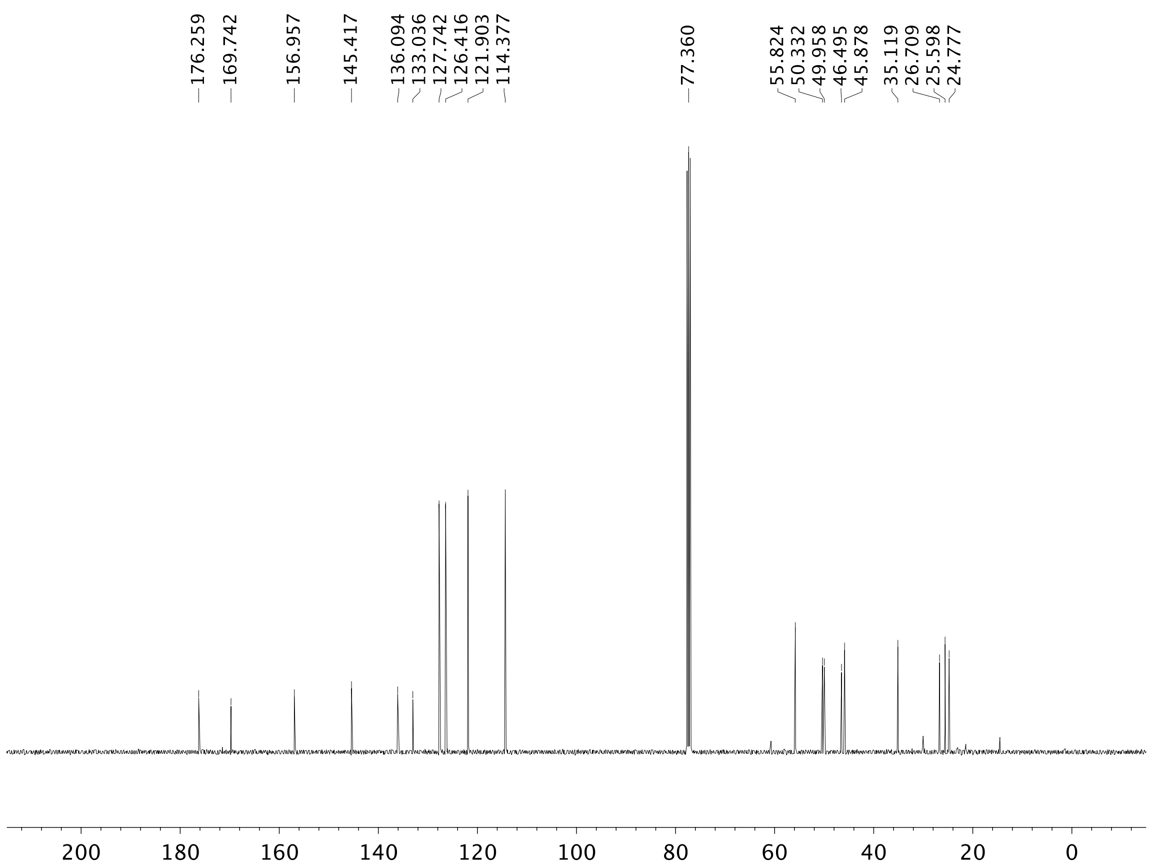
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ag**



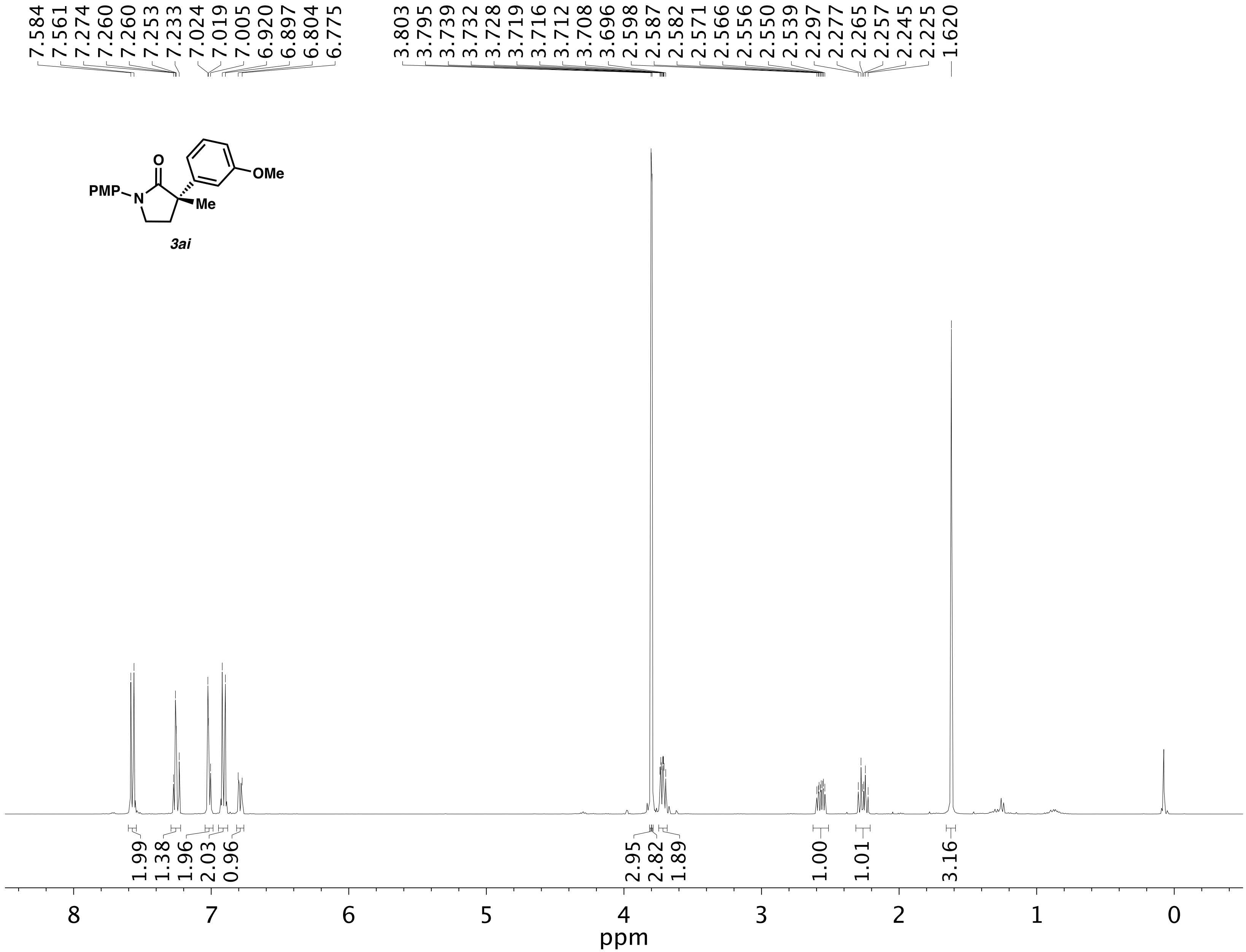
^1H NMR (400 MHz, $CDCl_3$) of compound **3ah**



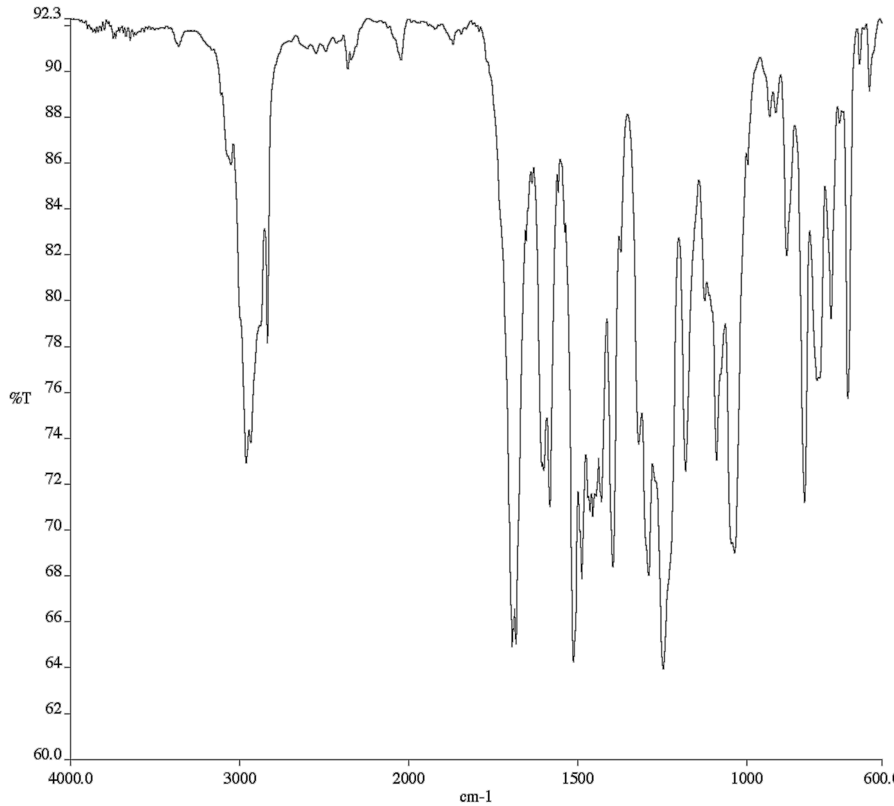
Infrared spectrum (Thin Film, NaCl) of compound **3ah**.



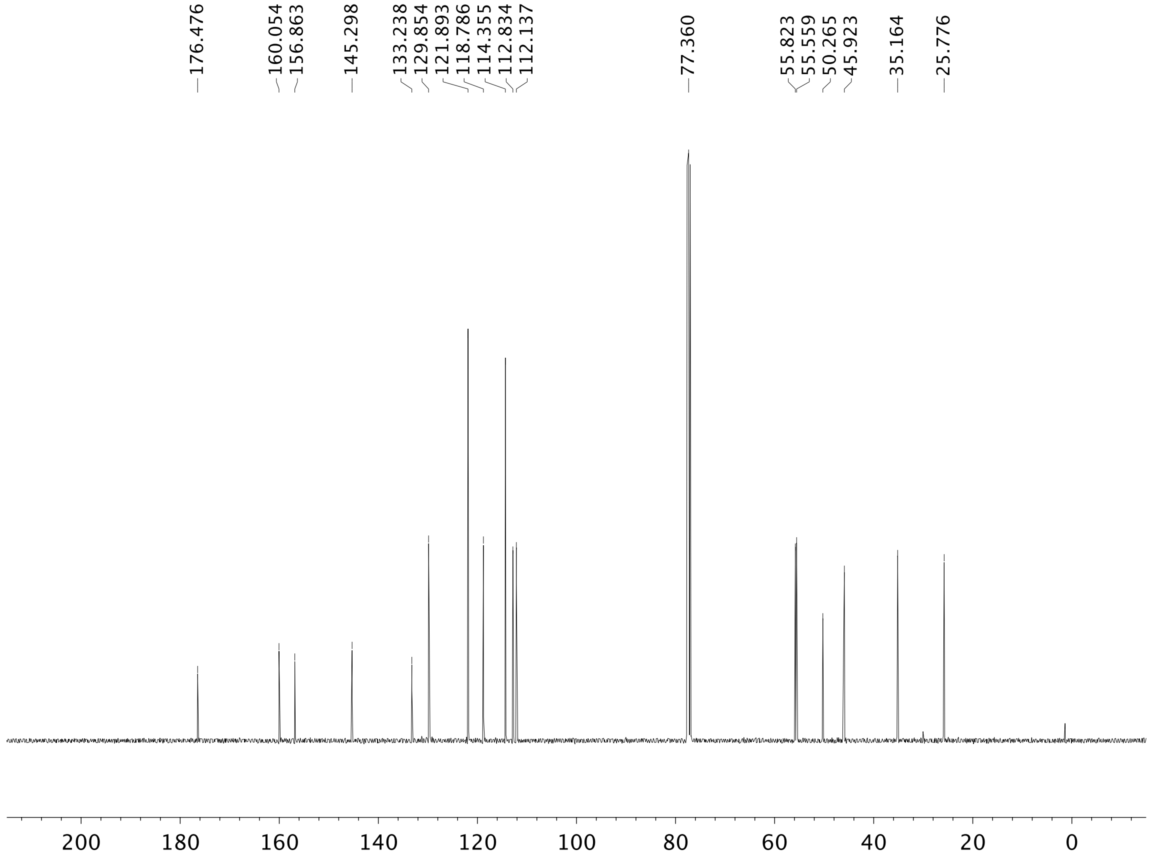
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ah**



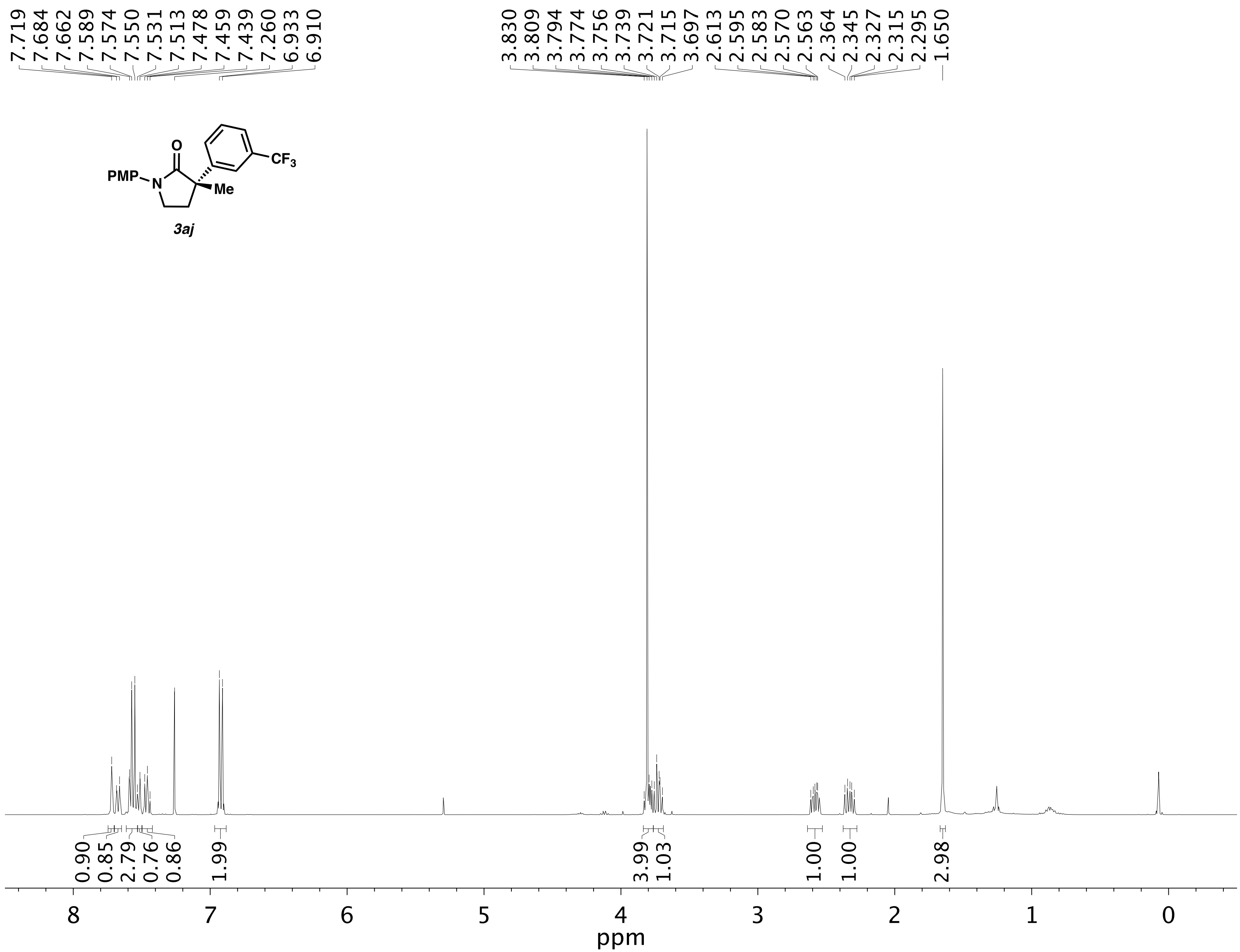
^{1}H NMR (300 MHz, $CDCl_3$) of compound **3ai**



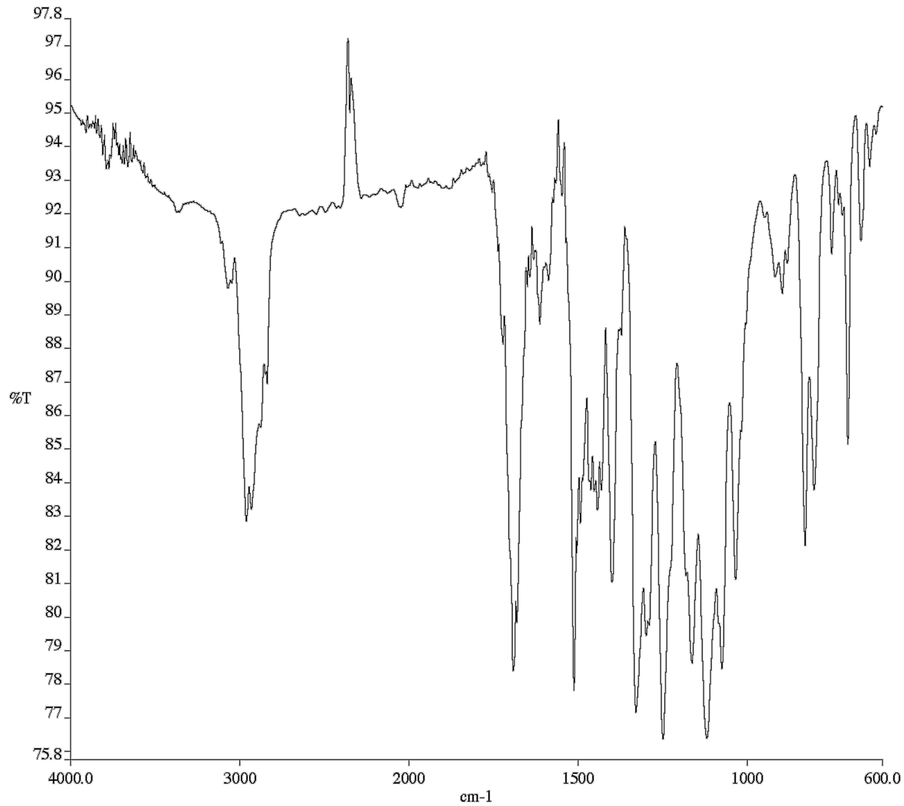
Infrared spectrum (Thin Film, NaCl) of compound **3ai**.



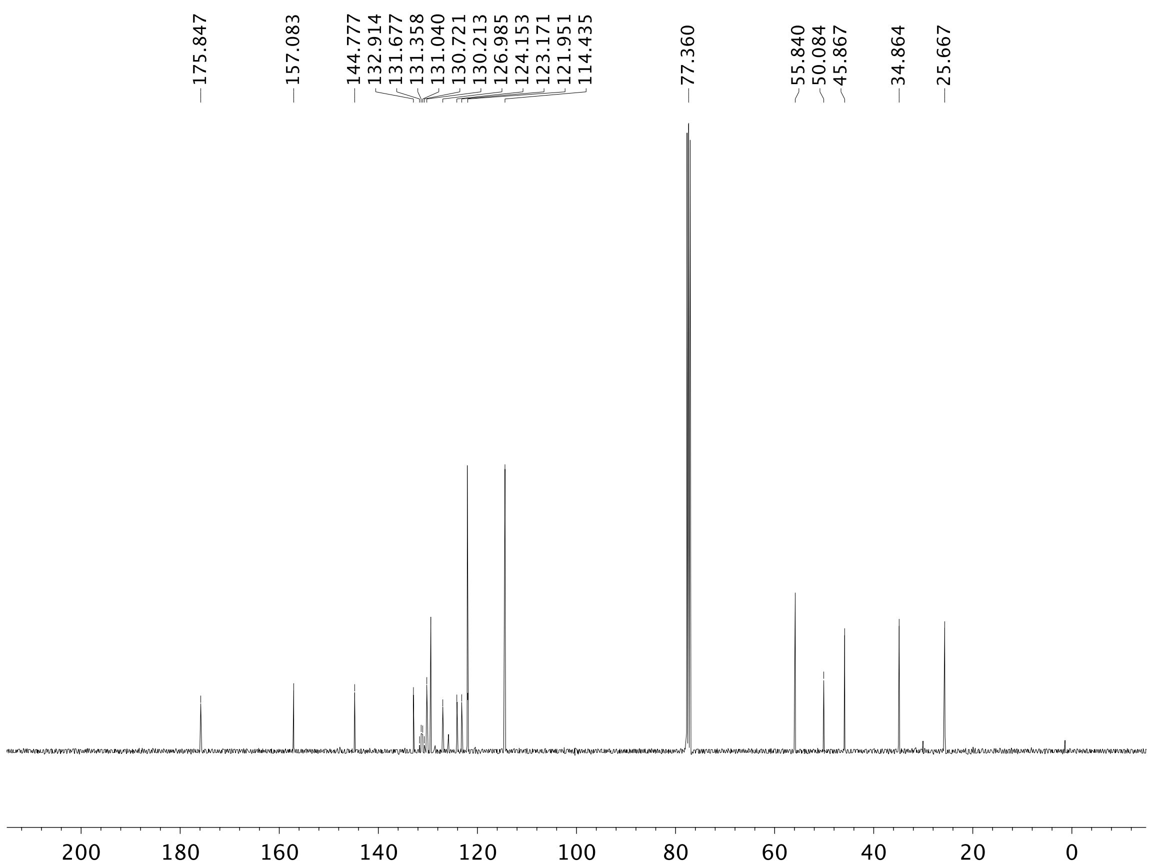
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ai**



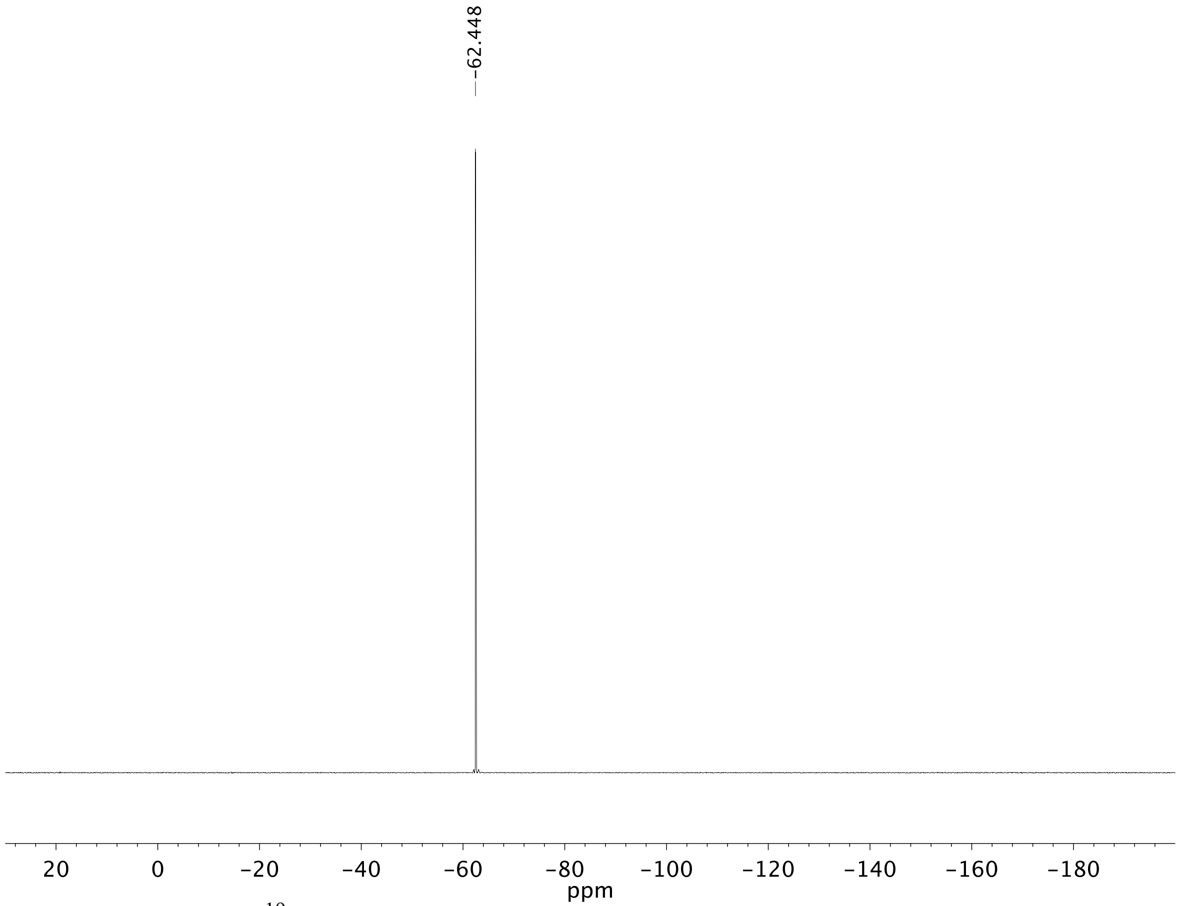
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3aj**



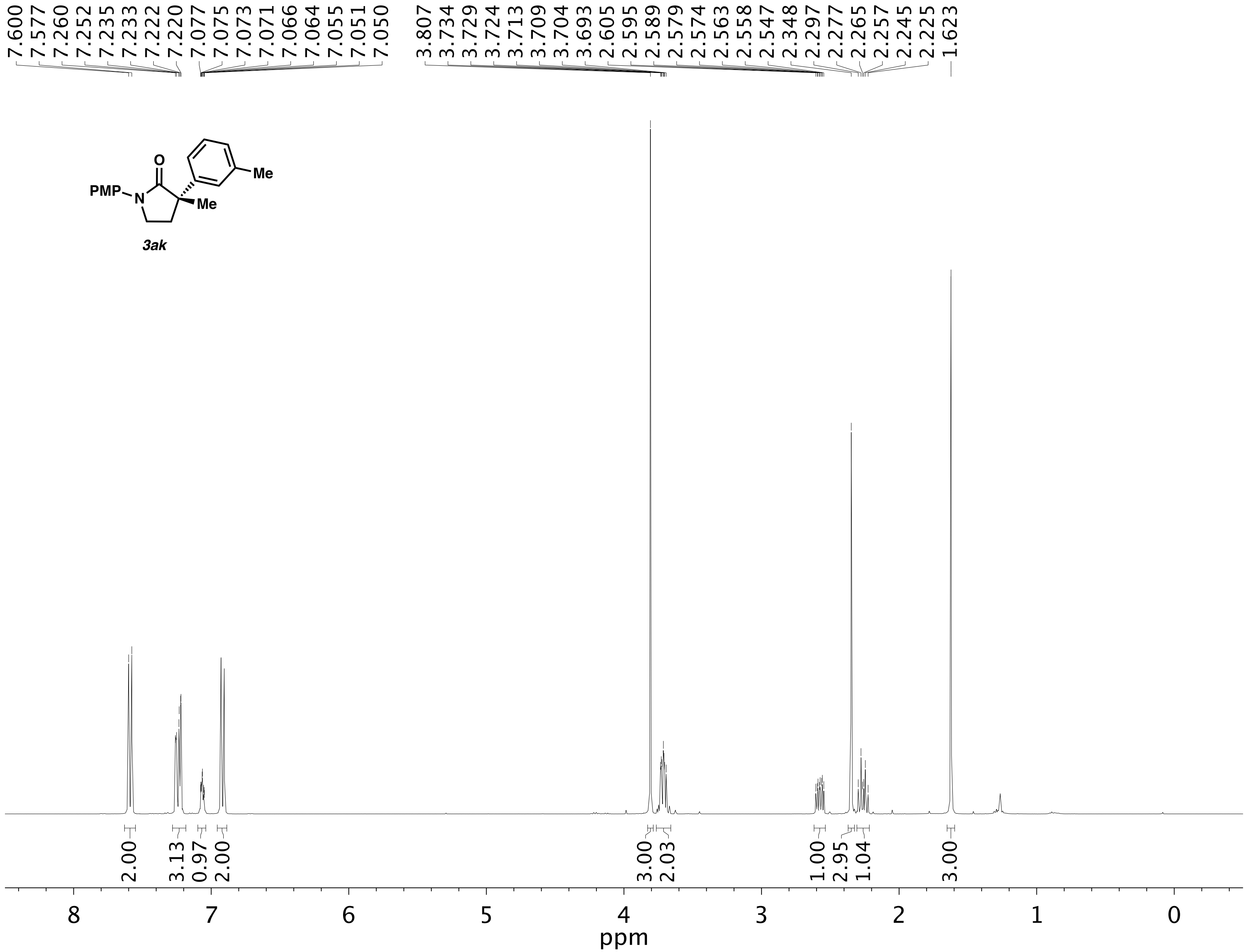
Infrared spectrum (Thin Film, NaCl) of compound **3aj**



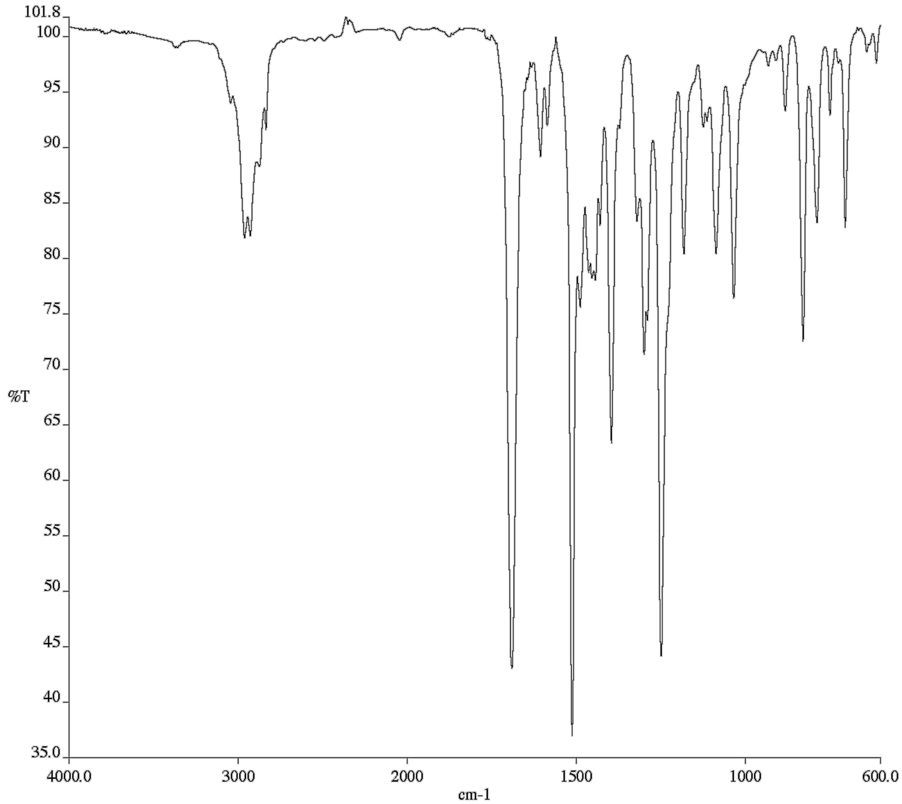
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3aj**



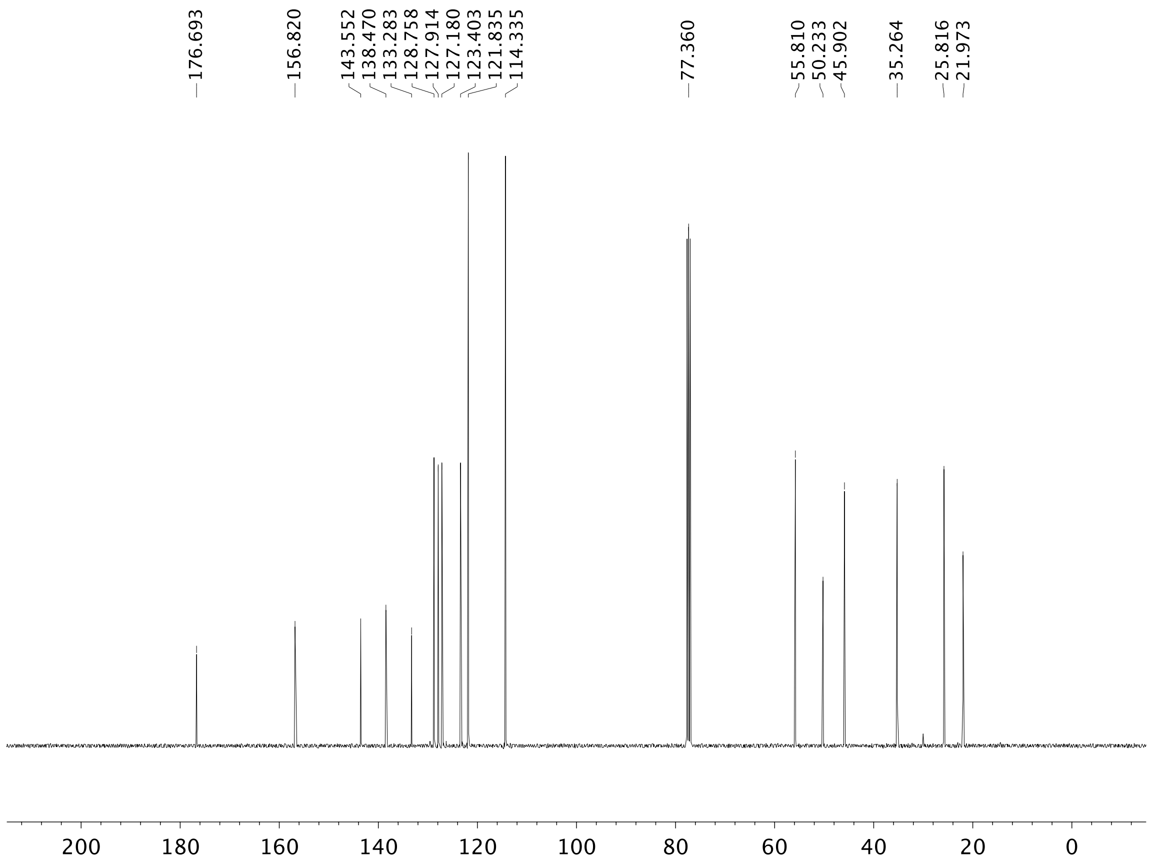
^{19}F NMR (282 MHz, $CDCl_3$) of compound **3aj**



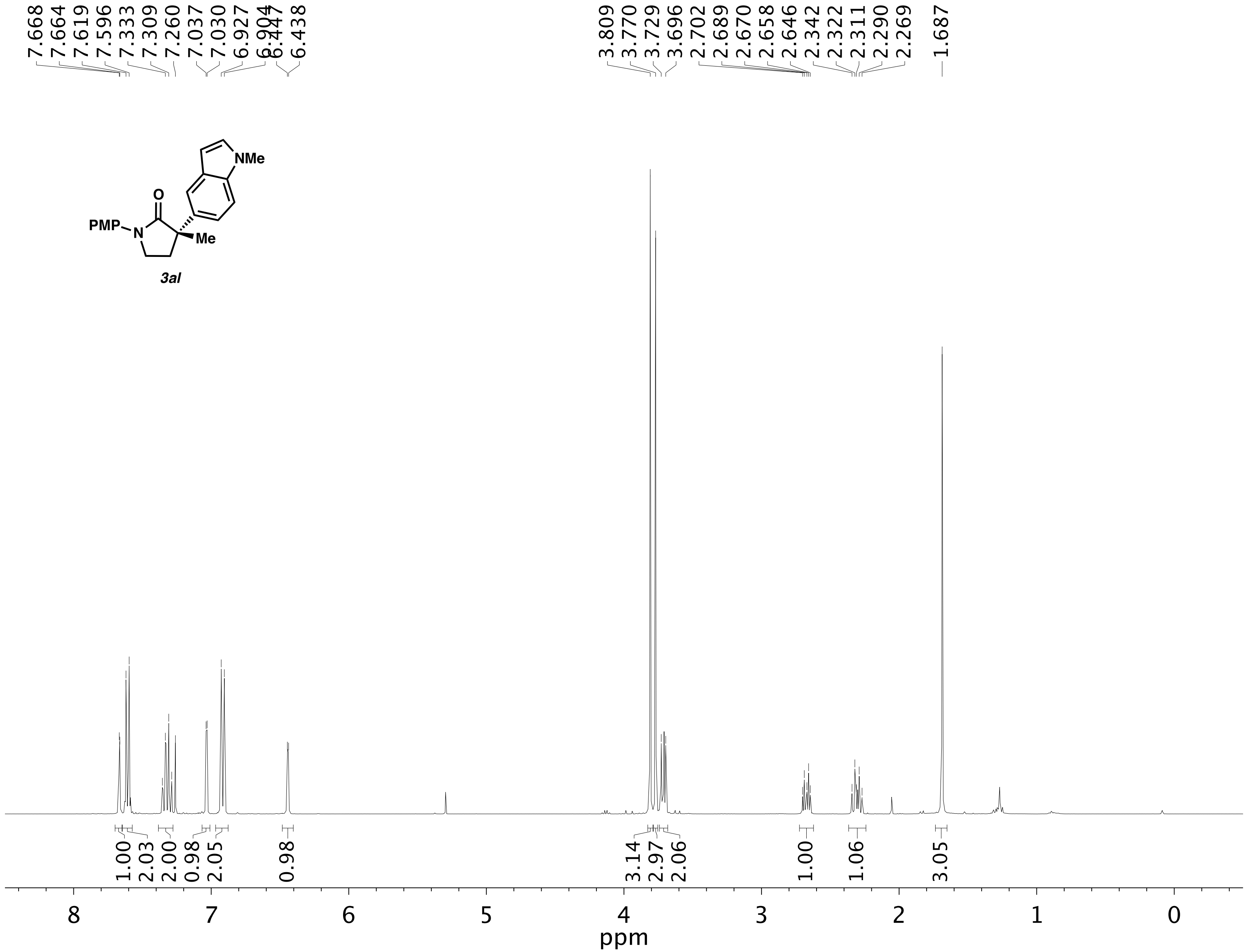
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ak**



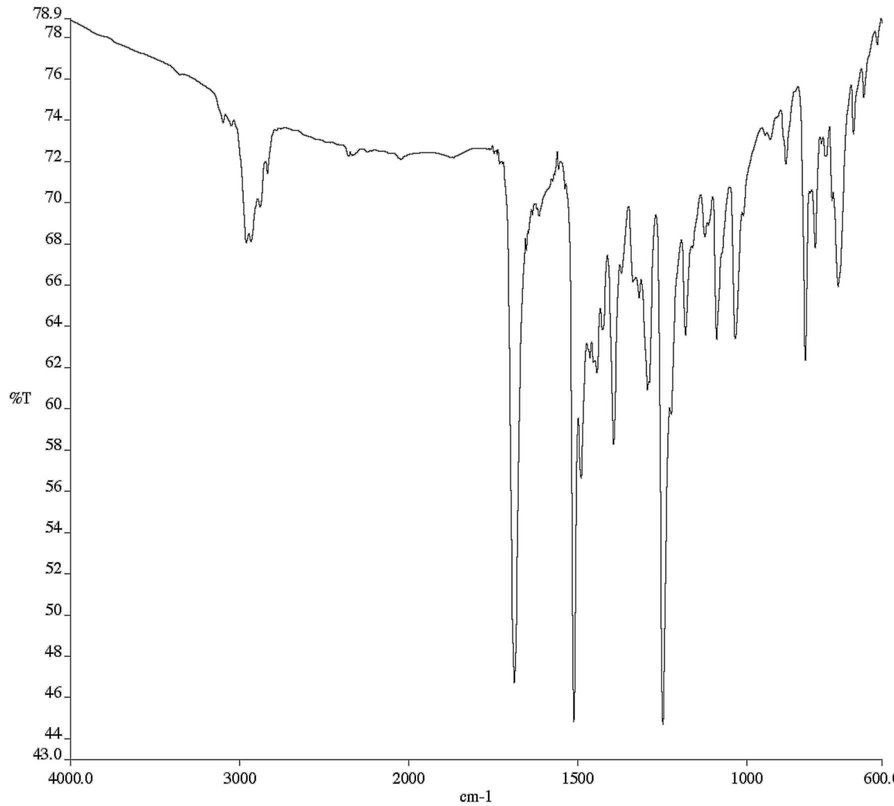
Infrared spectrum (Thin Film, NaCl) of compound **3ak**.



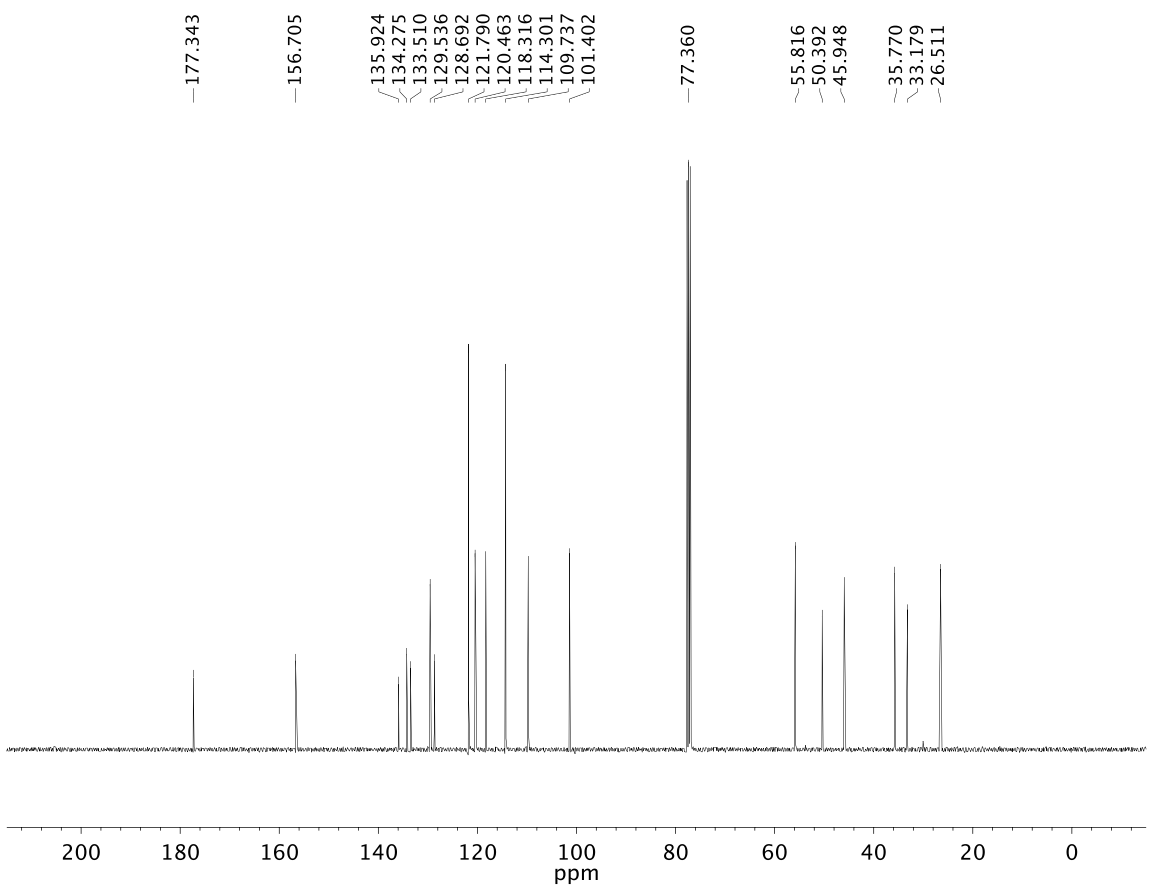
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ak**



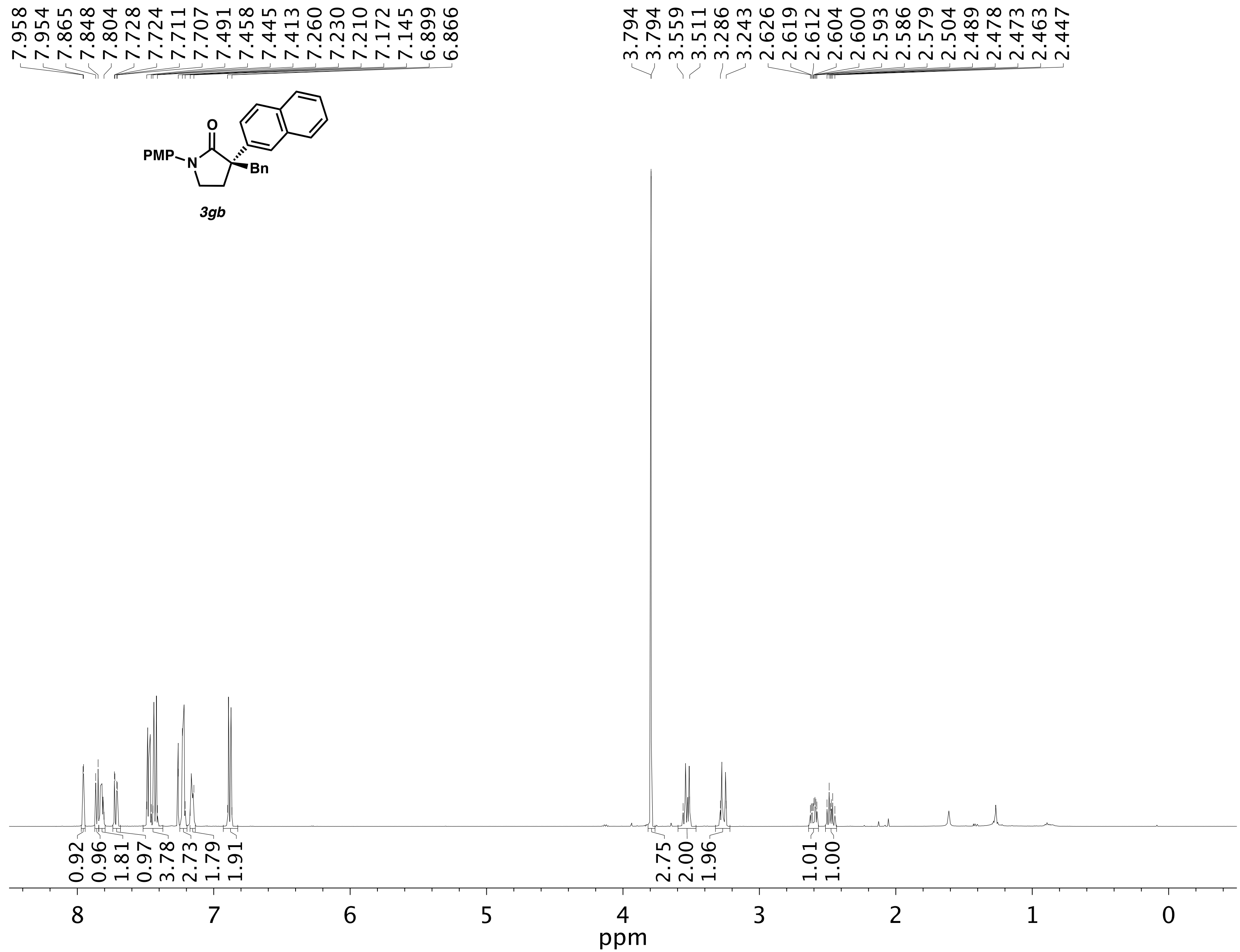
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3al**



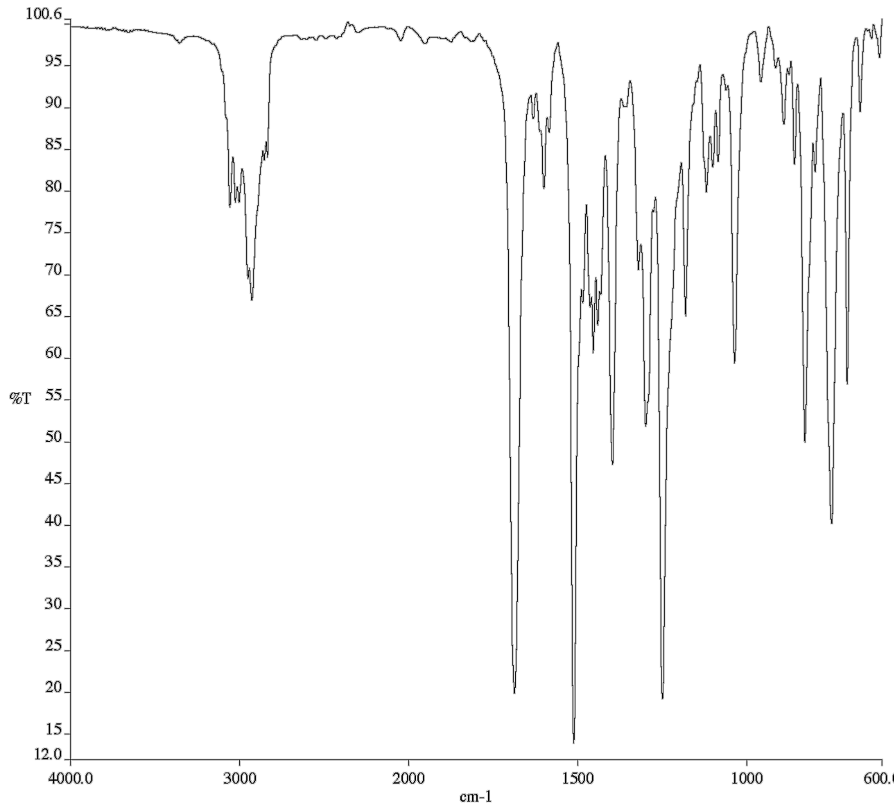
Infrared spectrum (Thin Film, NaCl) of compound **3al**



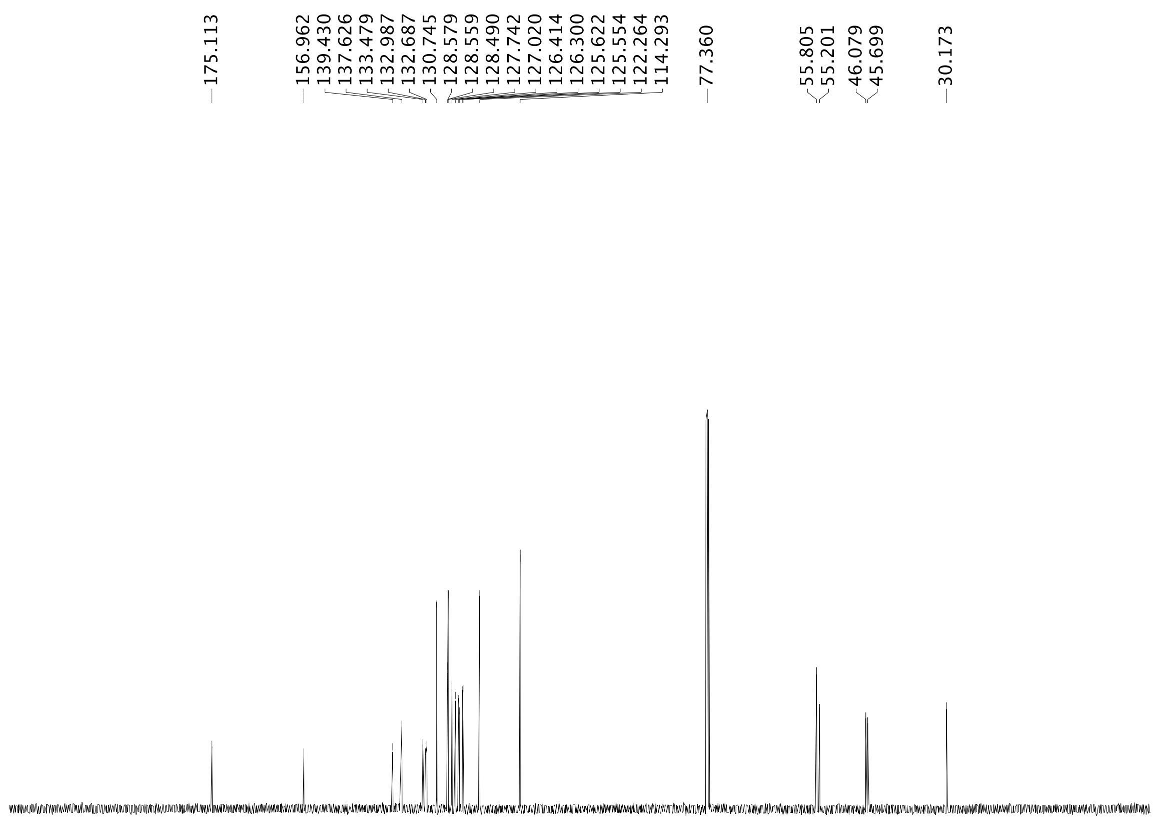
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3al**



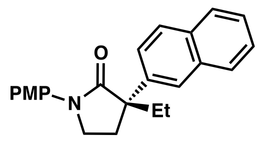
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3gb**



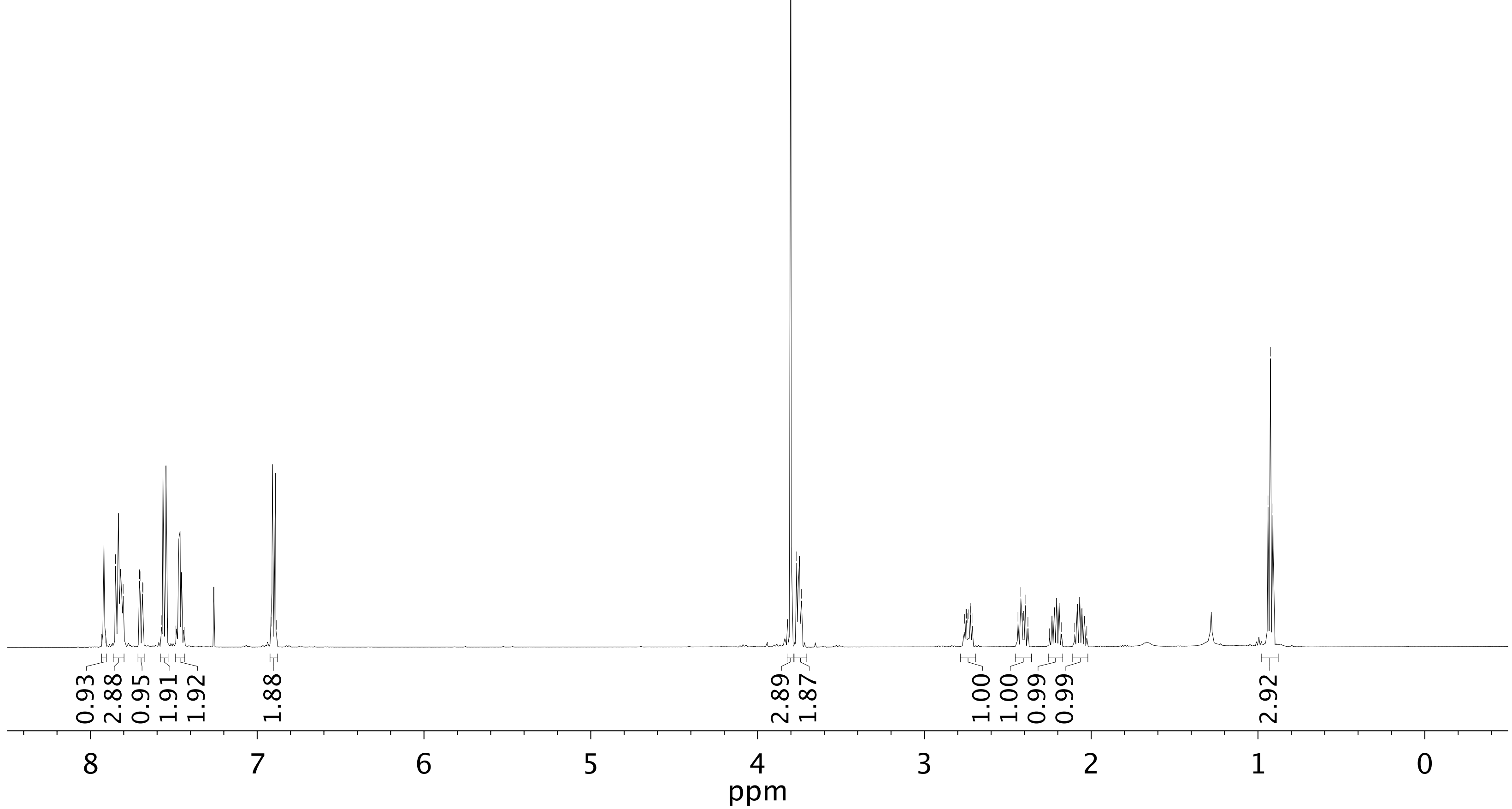
Infrared spectrum (Thin Film, NaCl) of compound **3gb**.



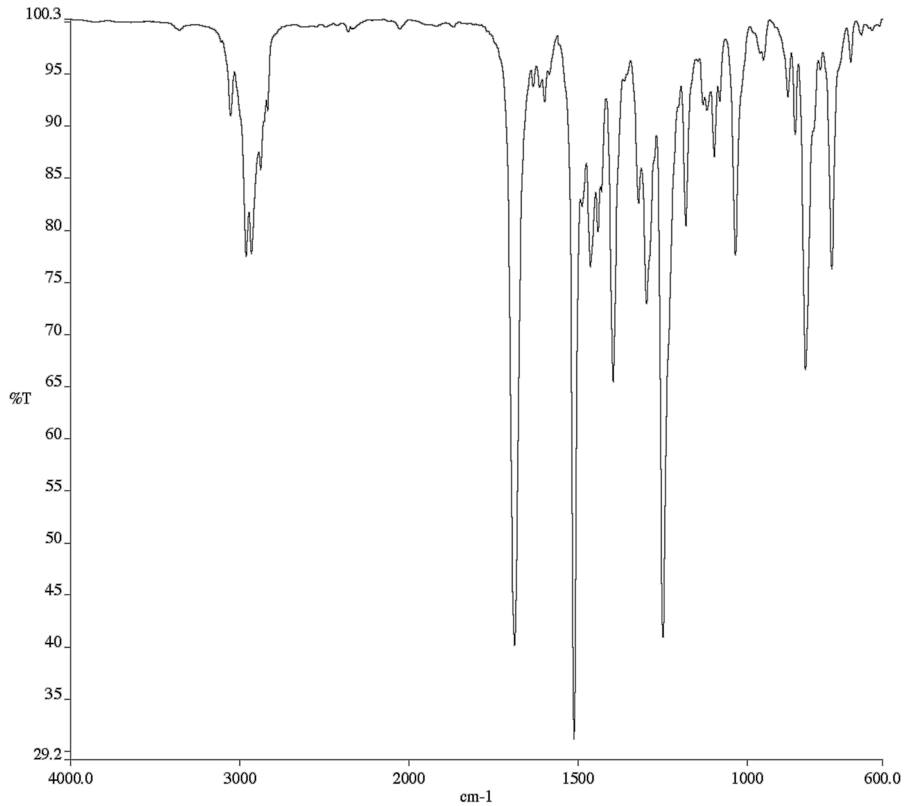
^{13}C NMR (125 MHz, $CDCl_3$) of compound **3gb**



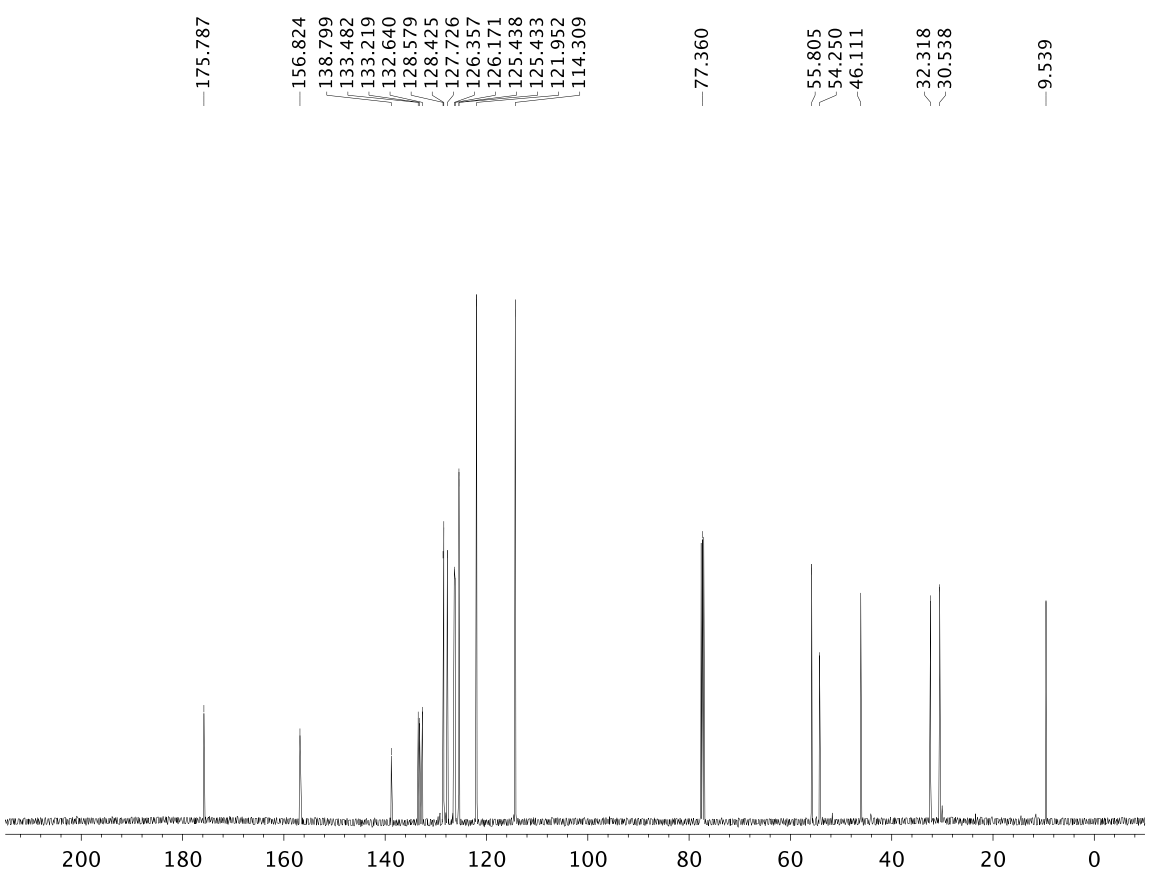
3hb



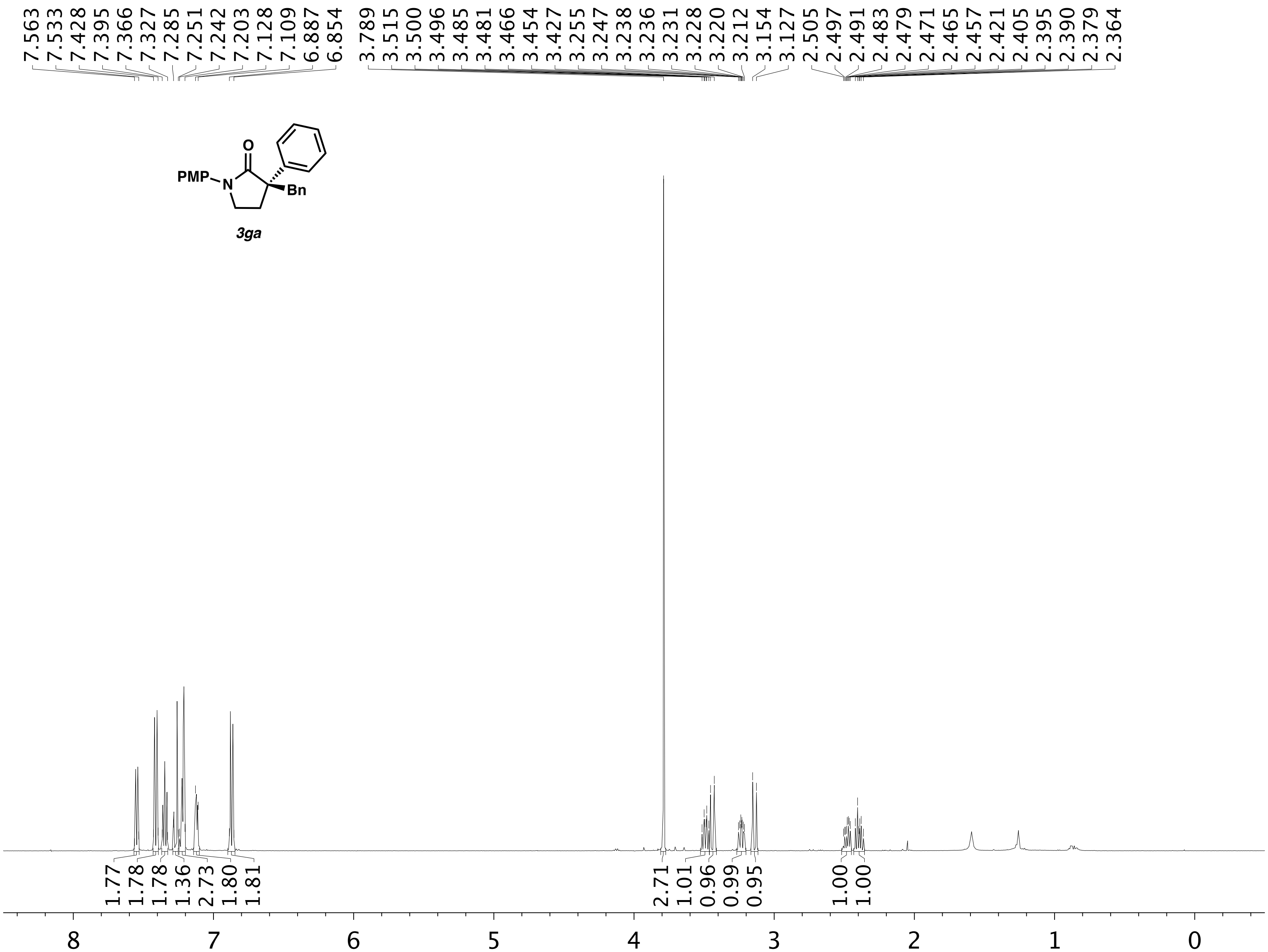
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3hb**



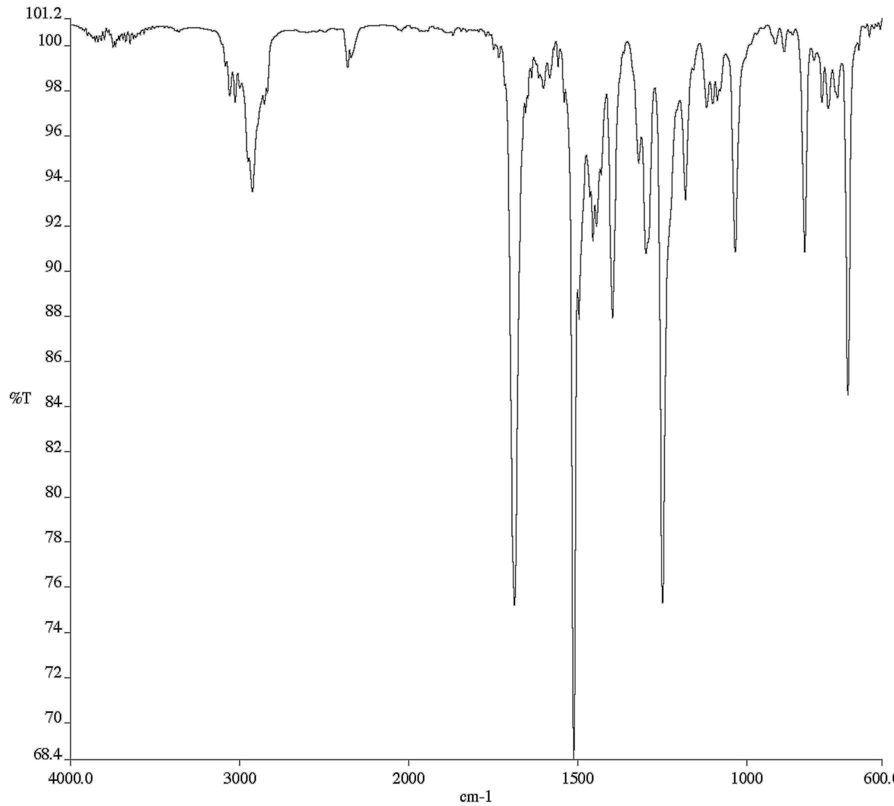
Infrared spectrum (Thin Film, NaCl) of compound **3hb**.



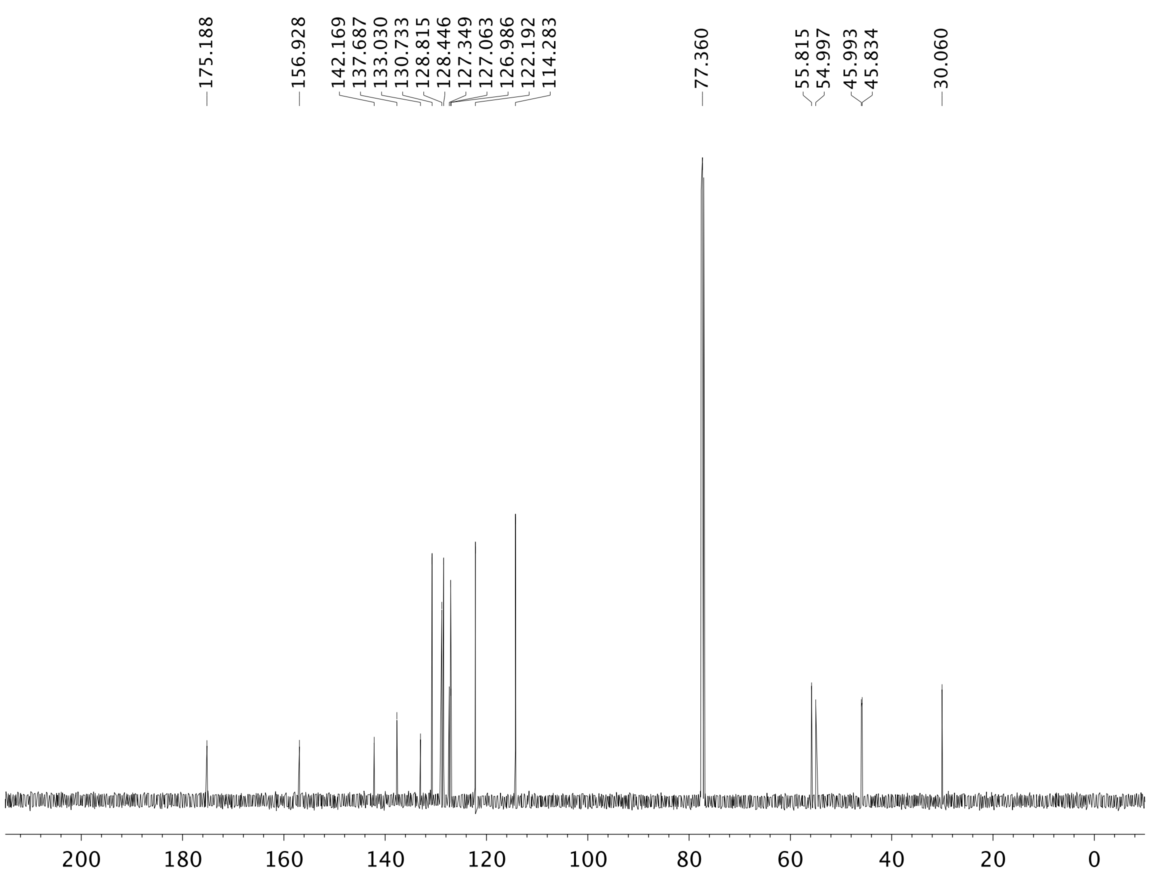
^{13}C NMR (125 MHz, $CDCl_3$) of compound **3hb**



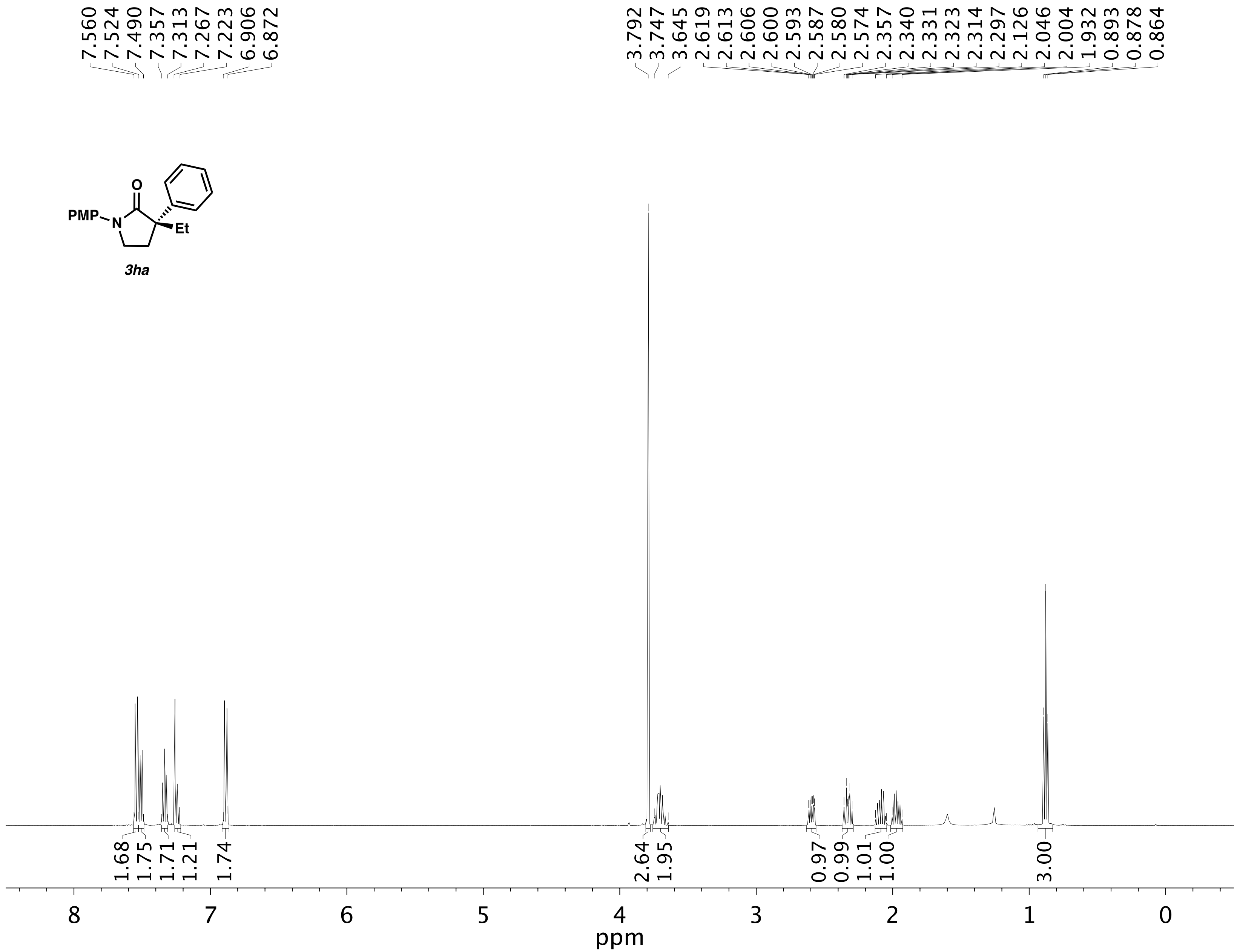
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3ga**



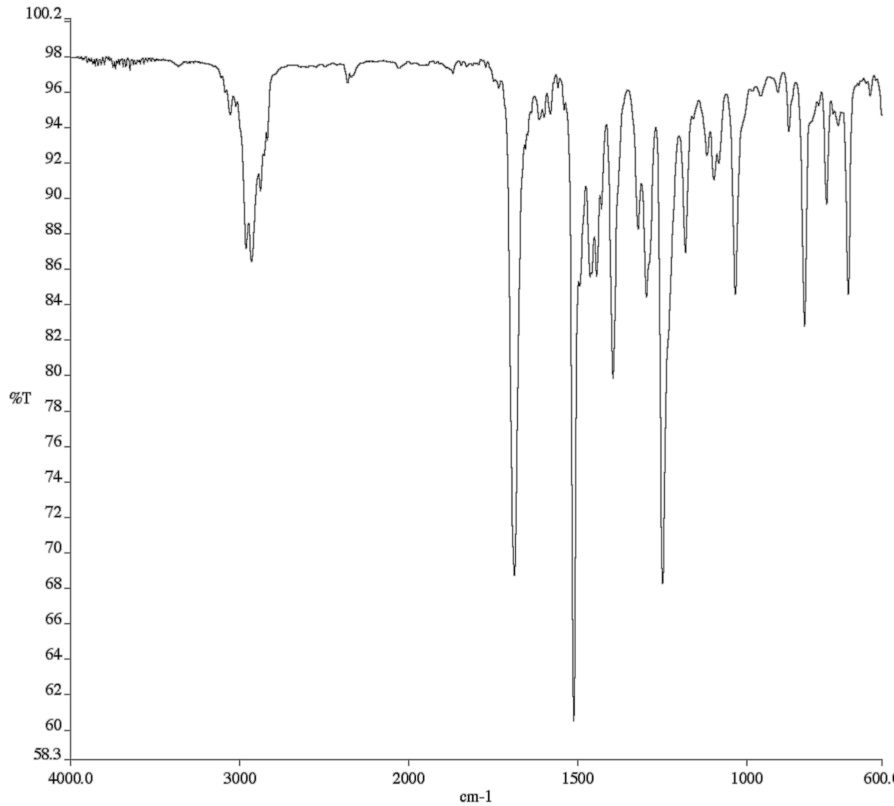
Infrared spectrum (Thin Film, NaCl) of compound **3ga**.



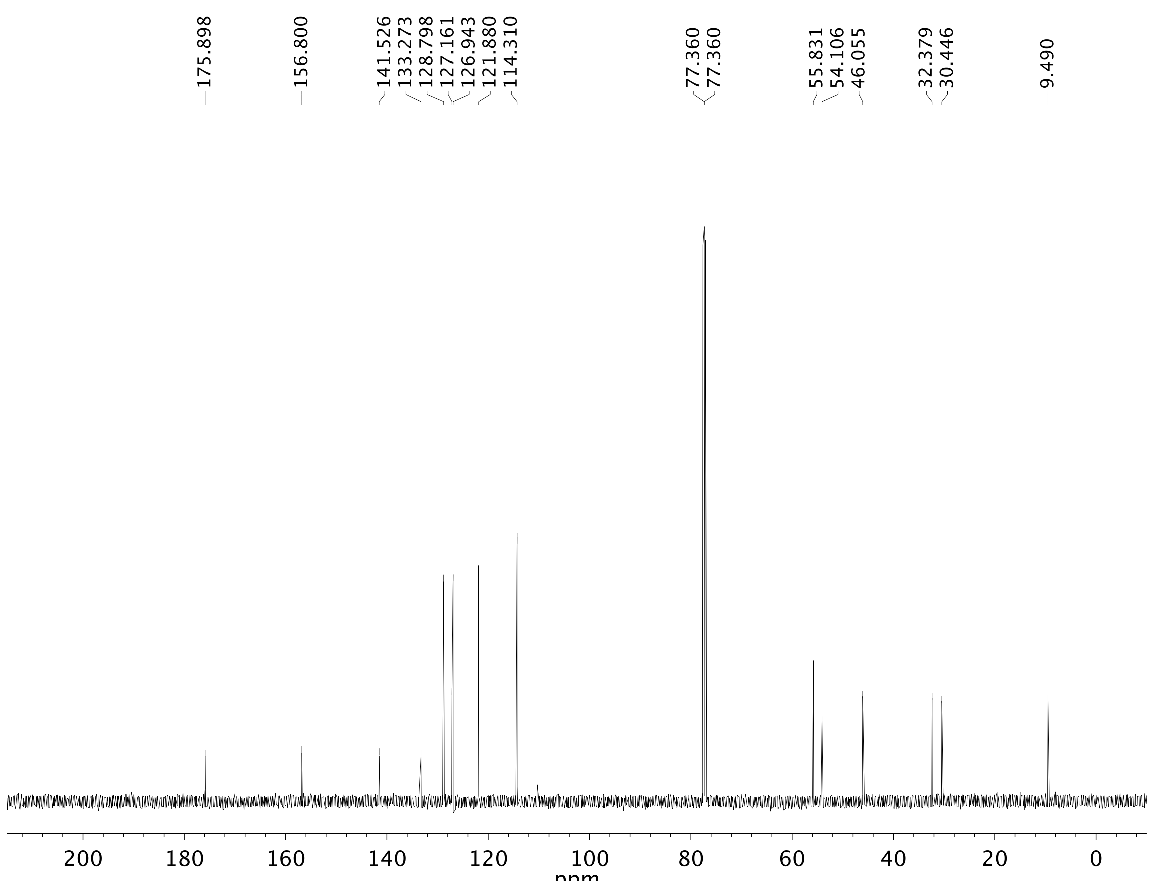
^{13}C NMR (125 MHz, $CDCl_3$) of compound **3ga**



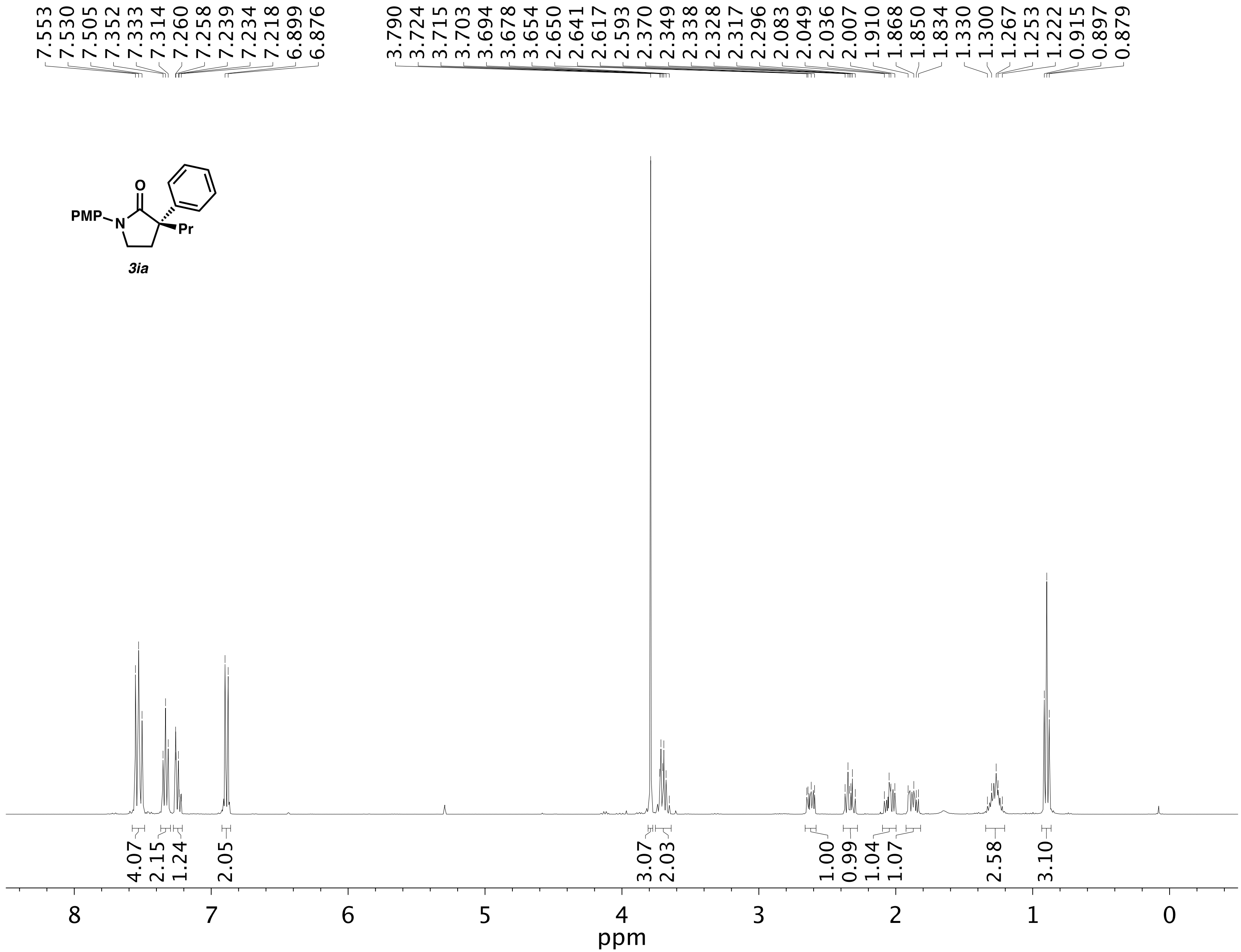
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3ha**



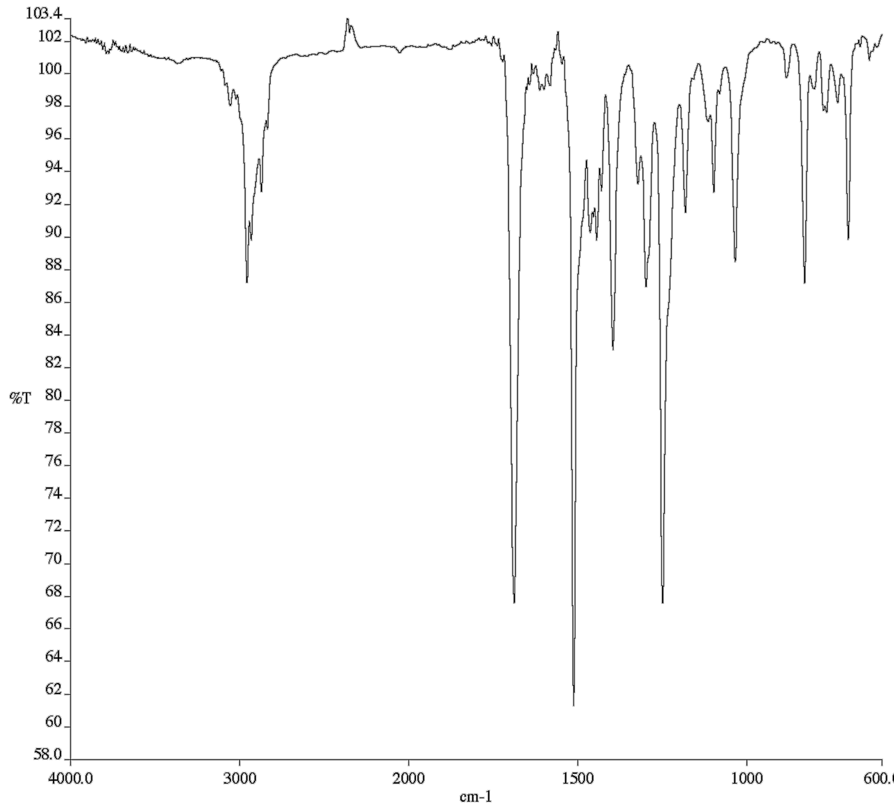
Infrared spectrum (Thin Film, NaCl) of compound **3ha**.



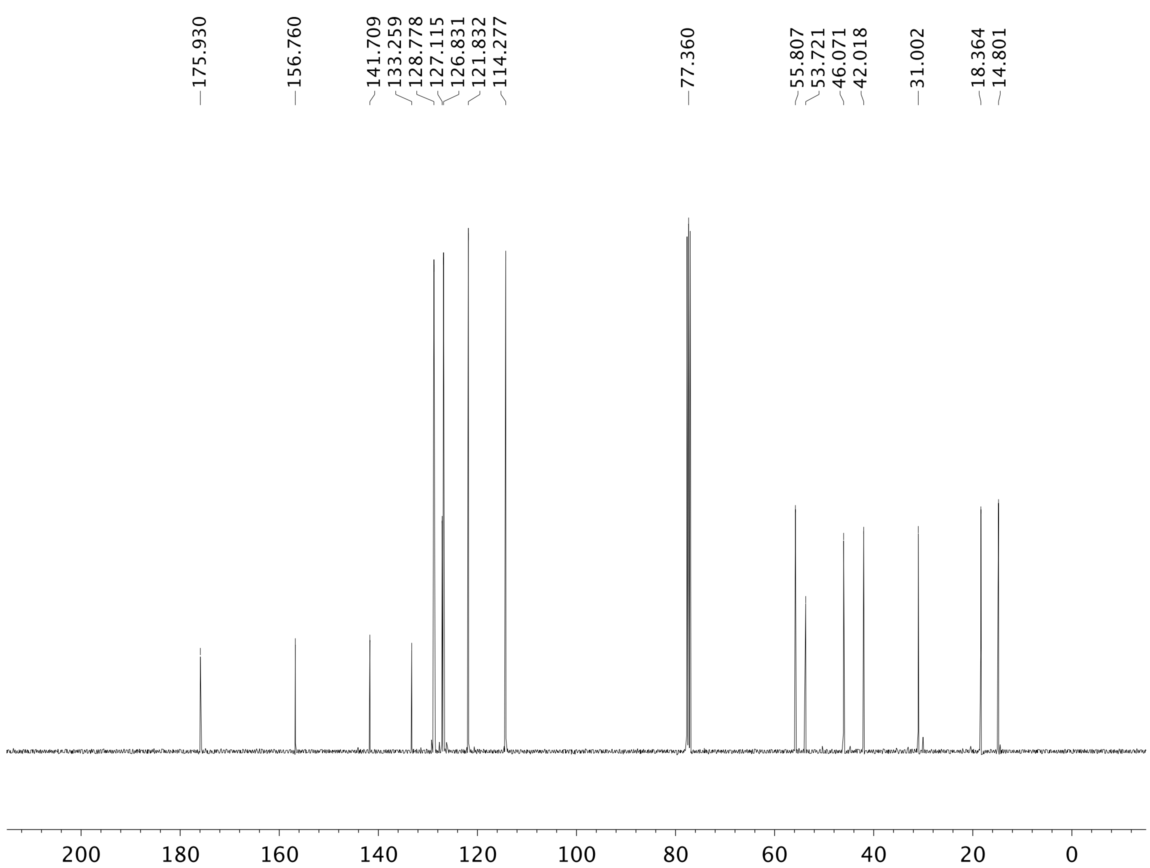
^{13}C NMR (125 MHz, $CDCl_3$) of compound **3ha**



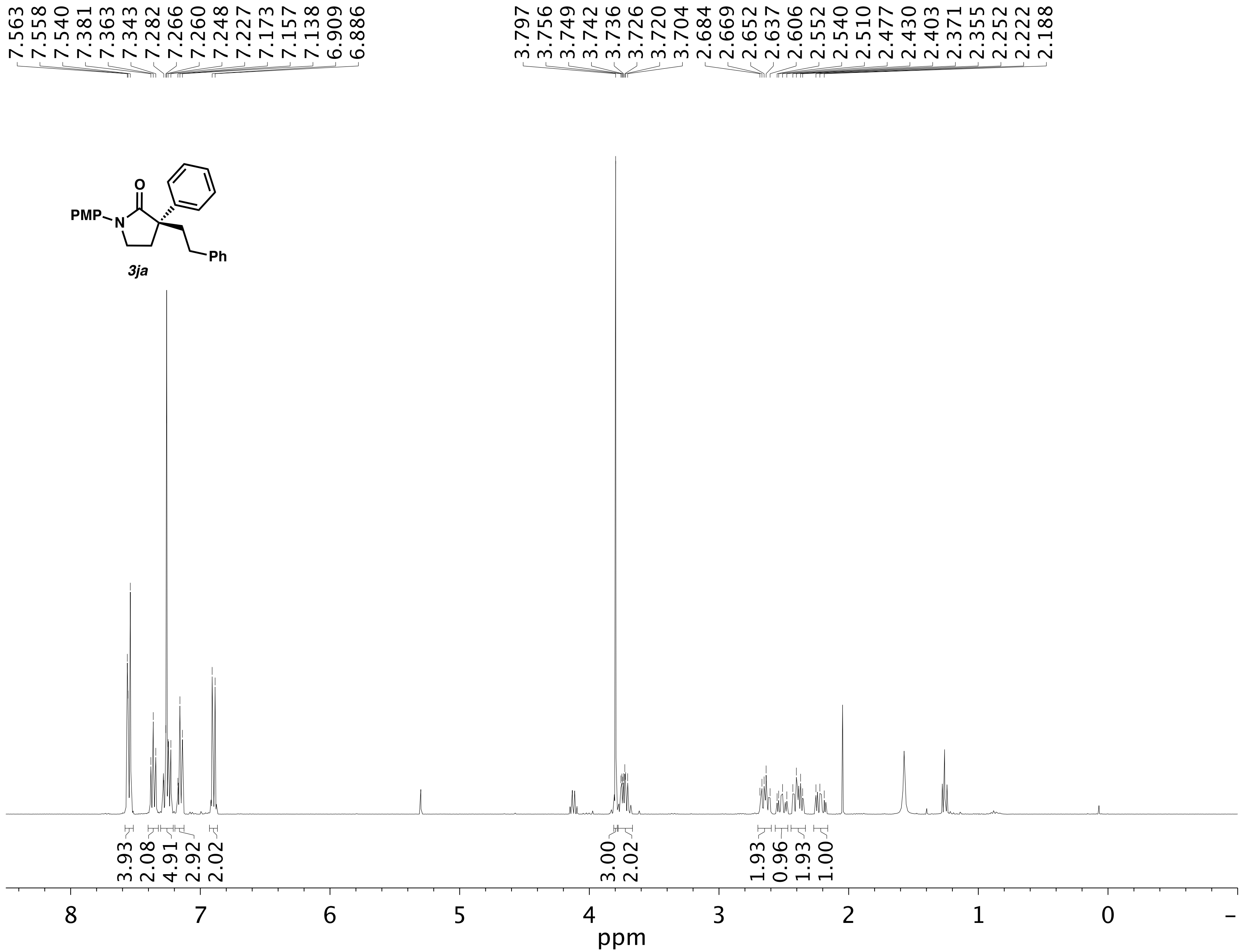
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ia**



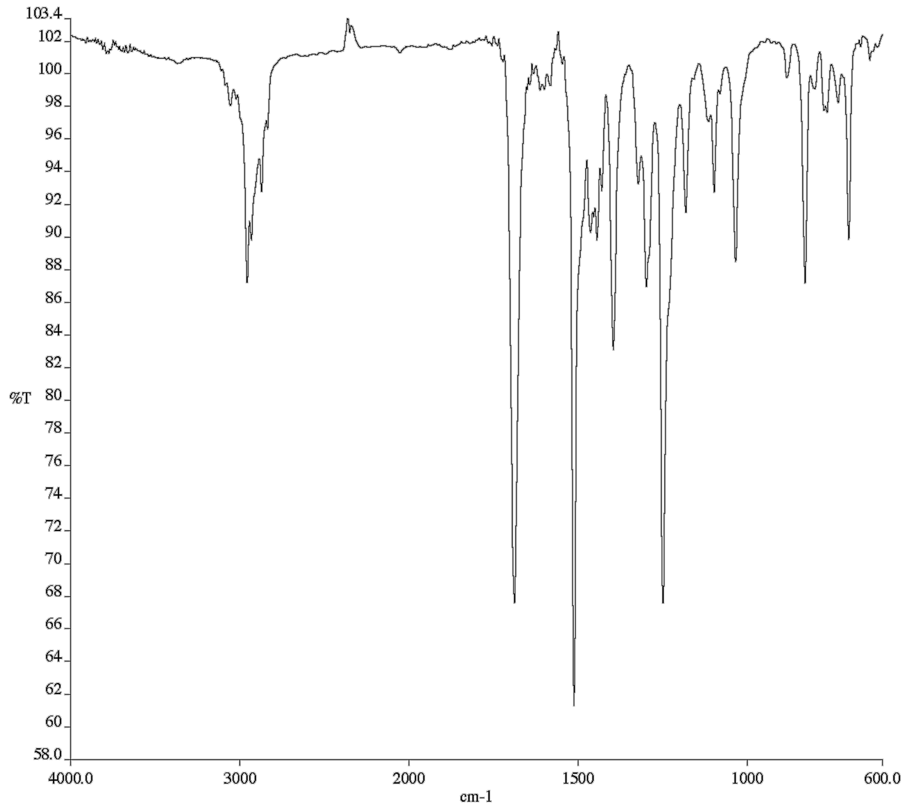
Infrared spectrum (Thin Film, NaCl) of compound **3ia**.



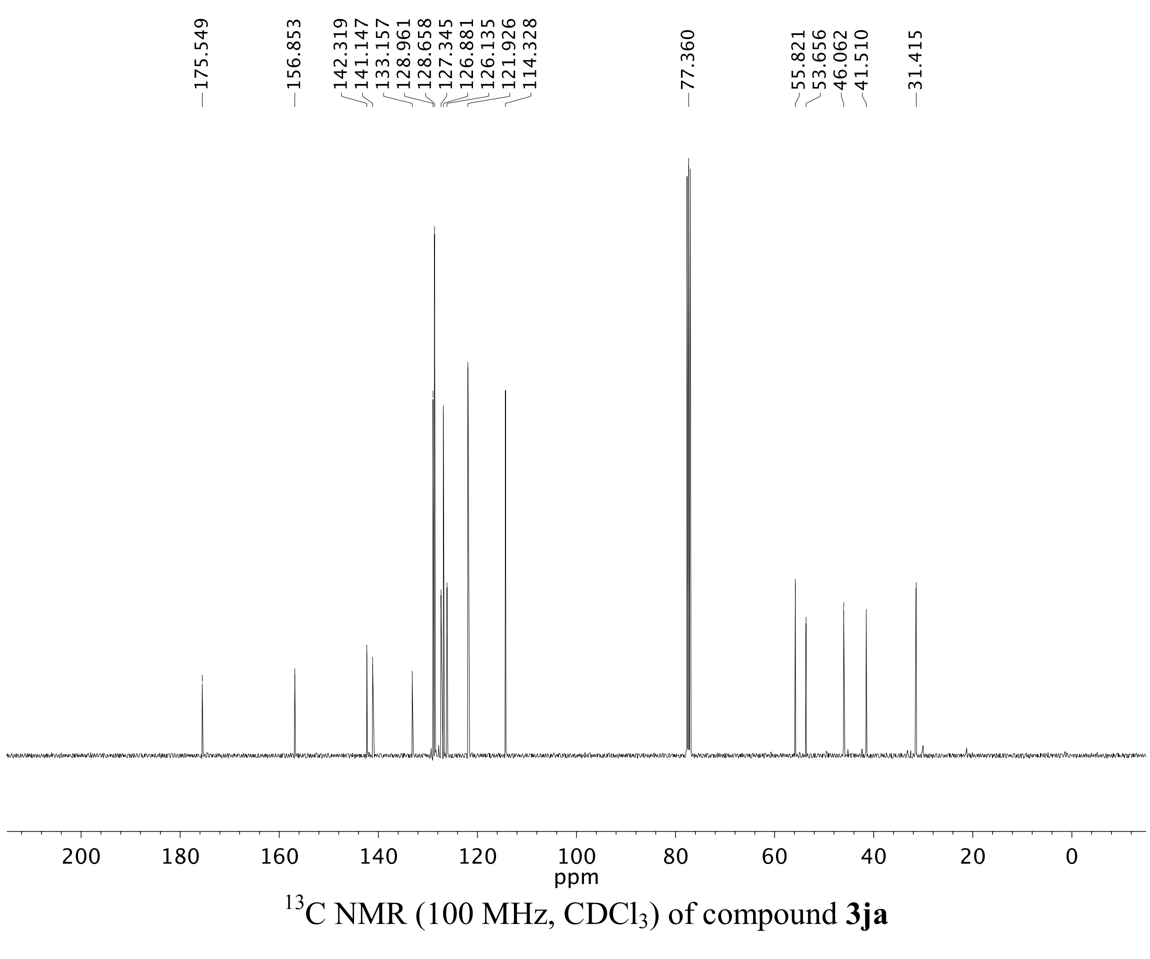
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ia**



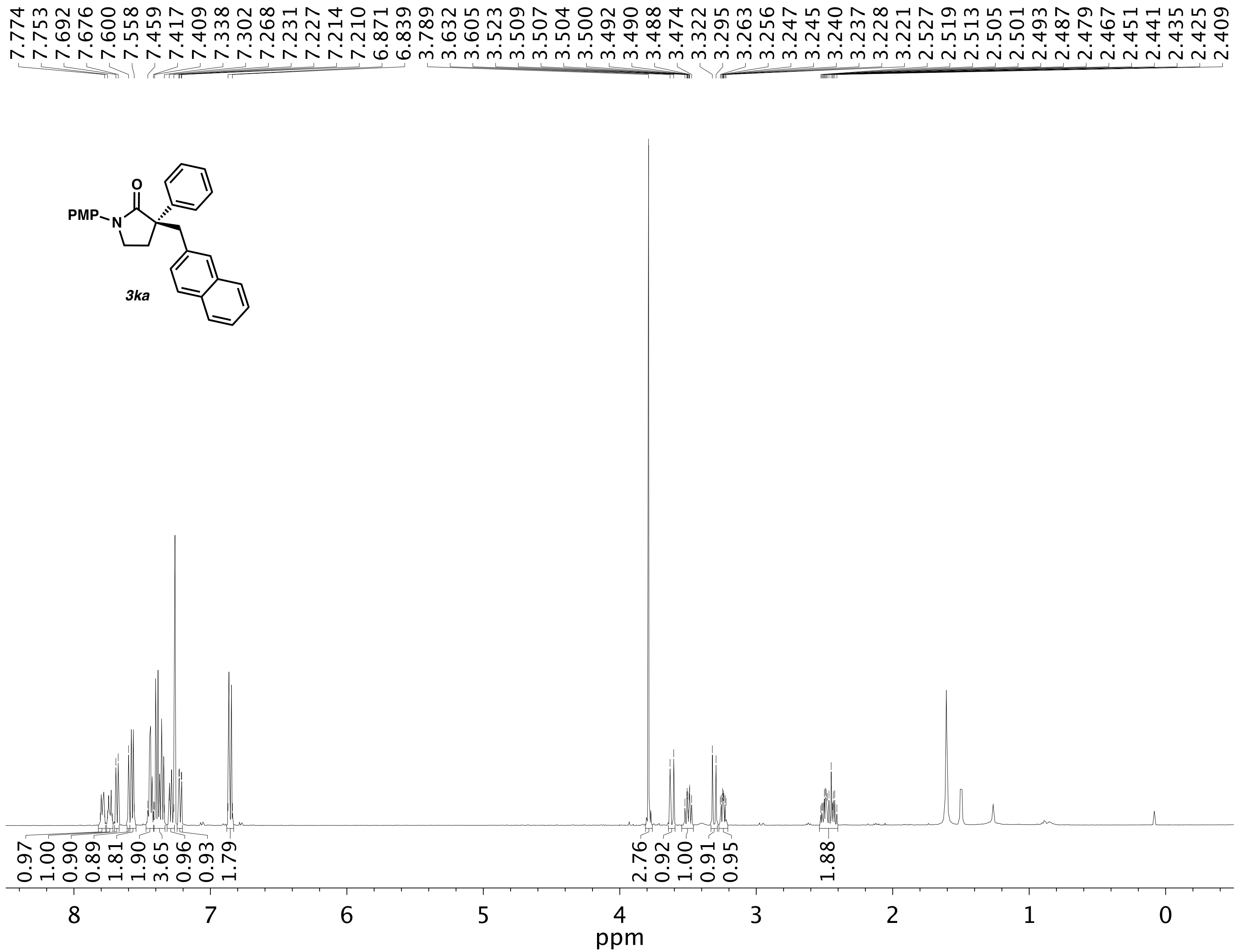
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ja**



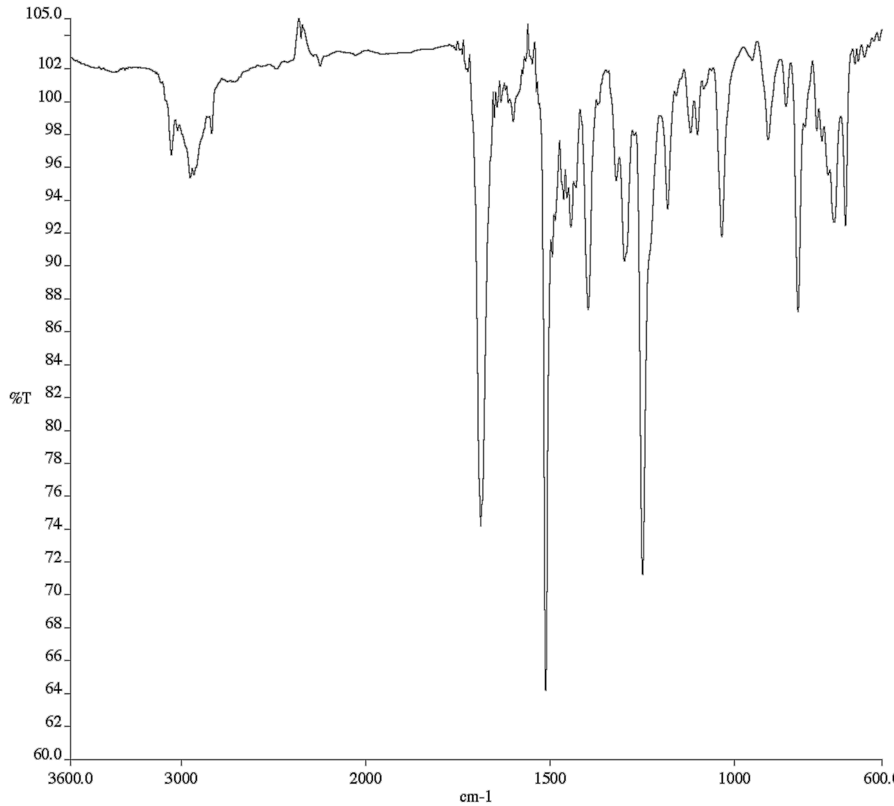
Infrared spectrum (Thin Film, NaCl) of compound **3ja**.



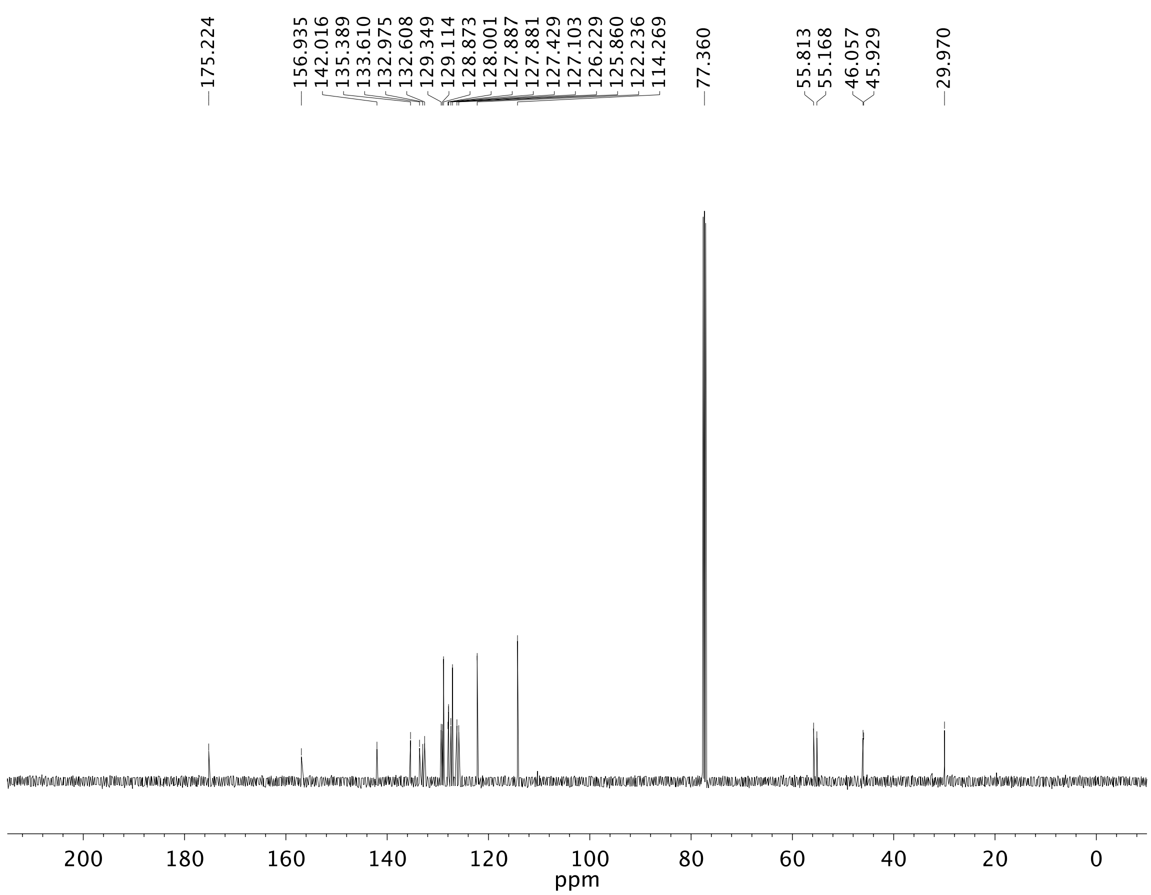
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ja**



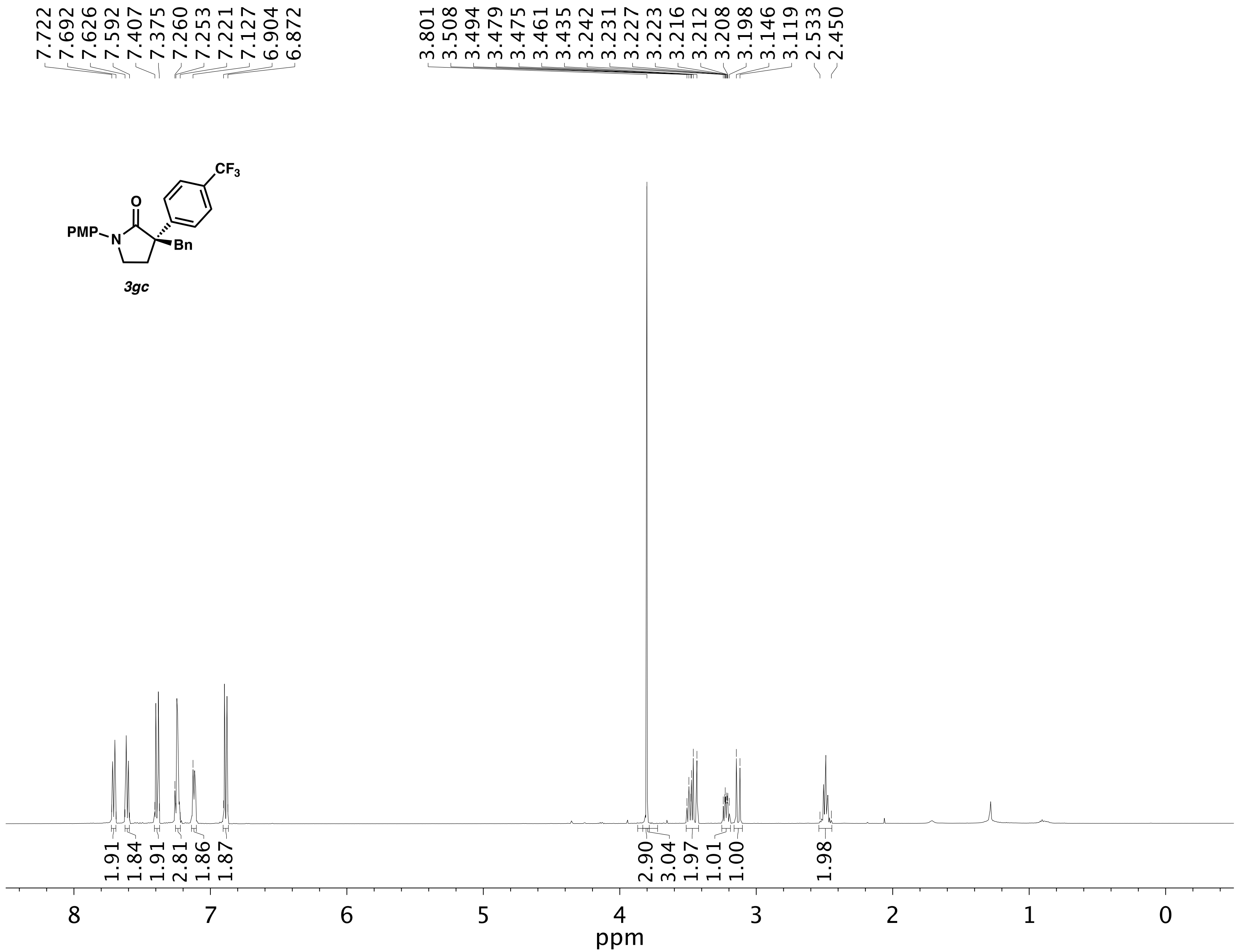
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3ka**



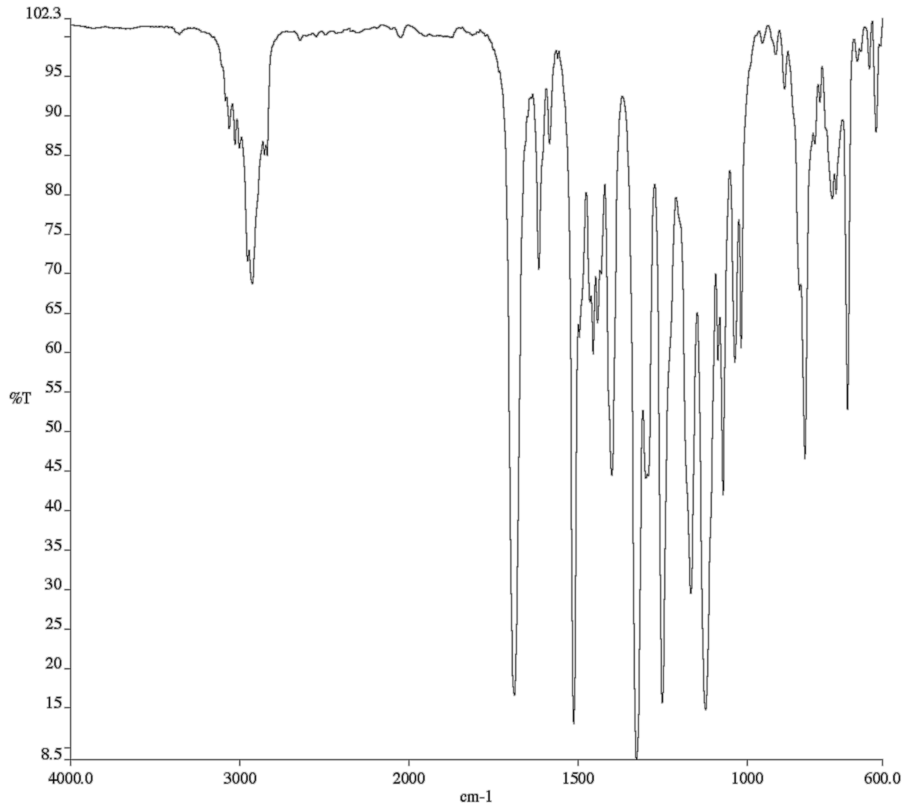
Infrared spectrum (Thin Film, NaCl) of compound **3ka**.



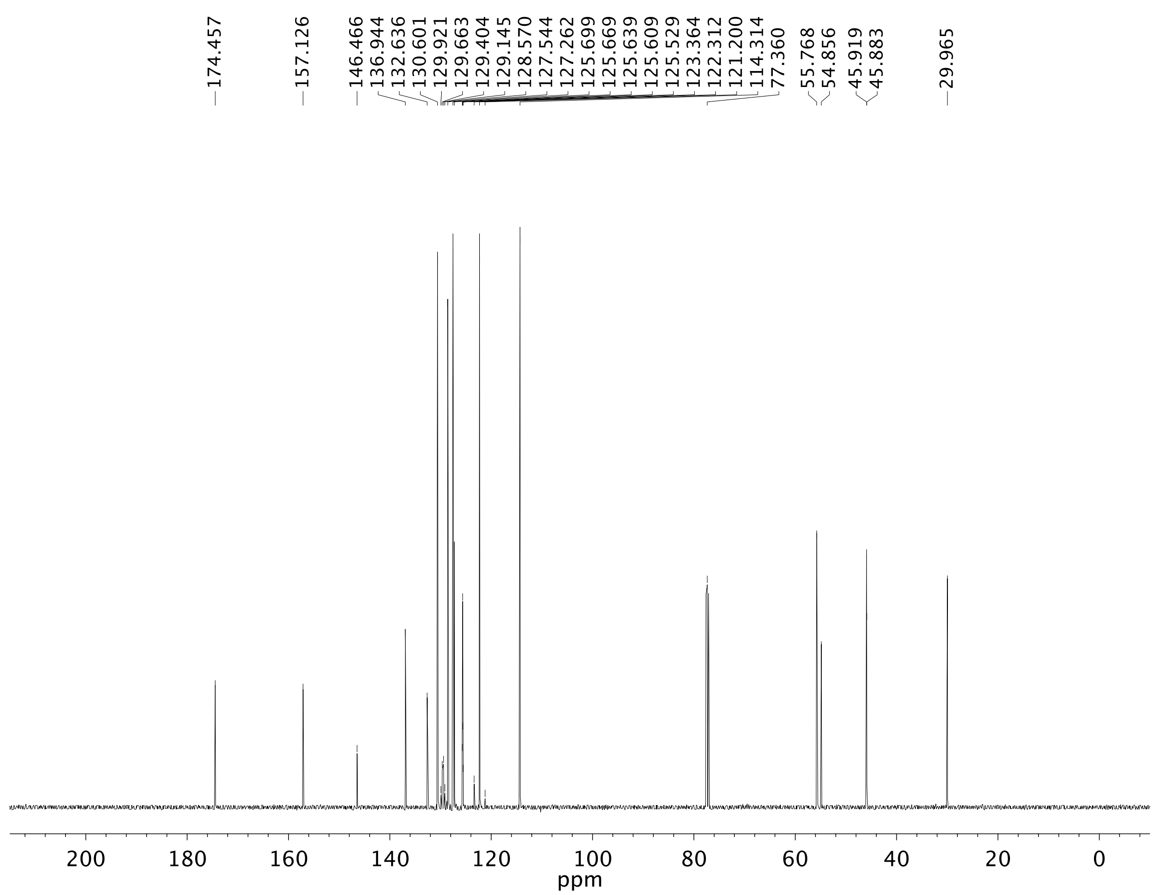
^{13}C NMR (125 MHz, $CDCl_3$) of compound **3ka**



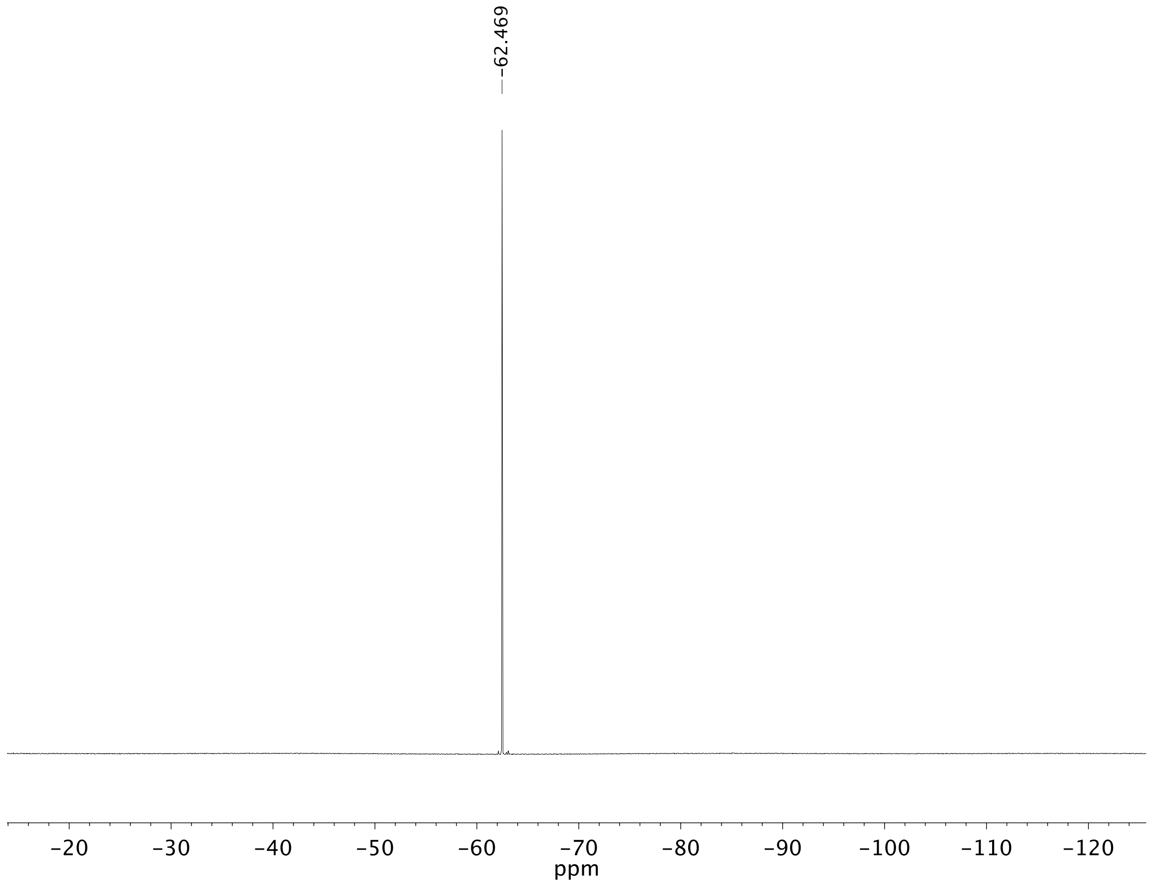
[1]H NMR (500 MHz, $CDCl_3$) of compound **3gc**



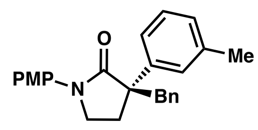
Infrared spectrum (Thin Film, NaCl) of compound **3gc**



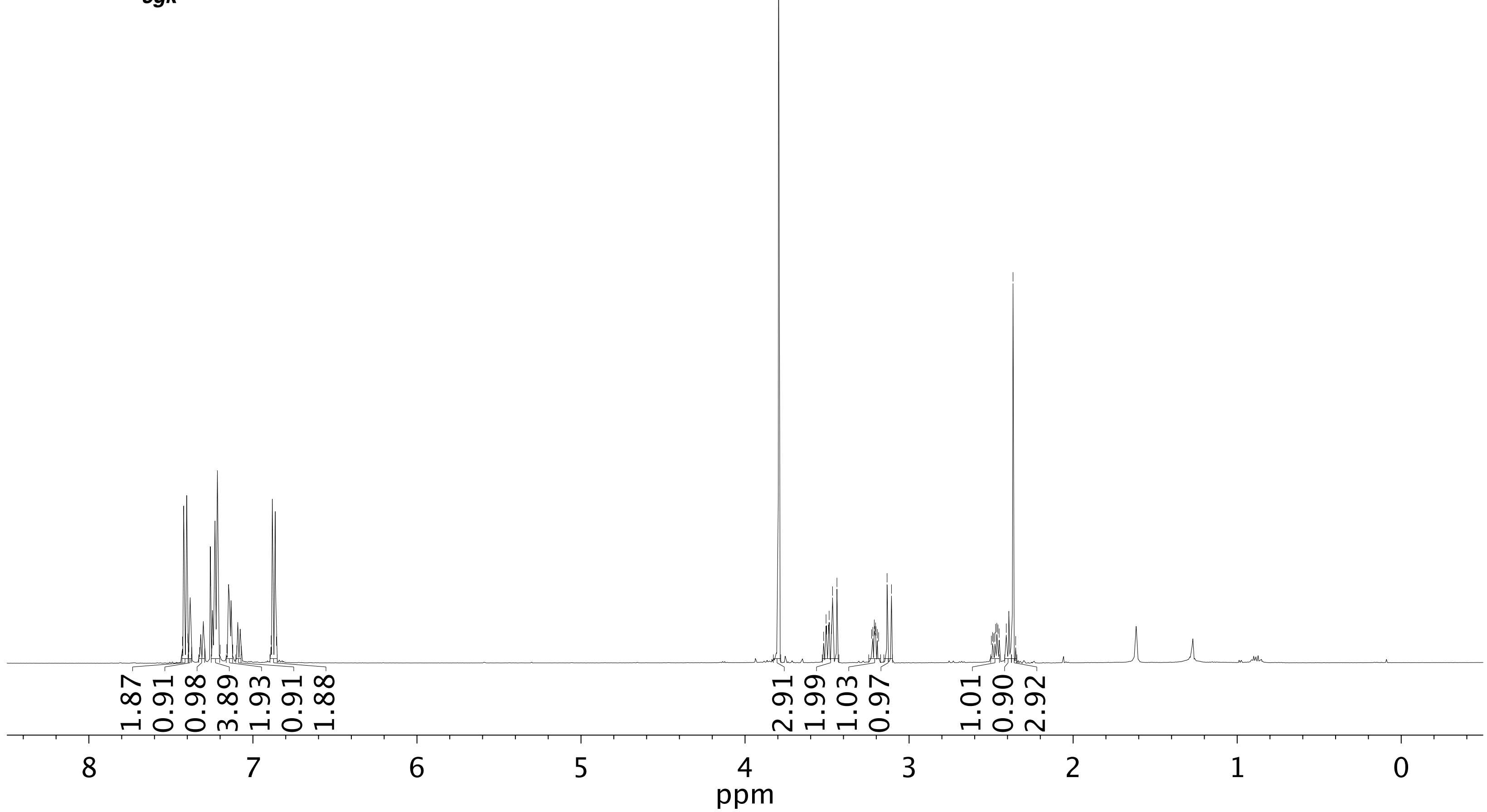
^{13}C NMR (125 MHz, $CDCl_3$) of compound **3gc**



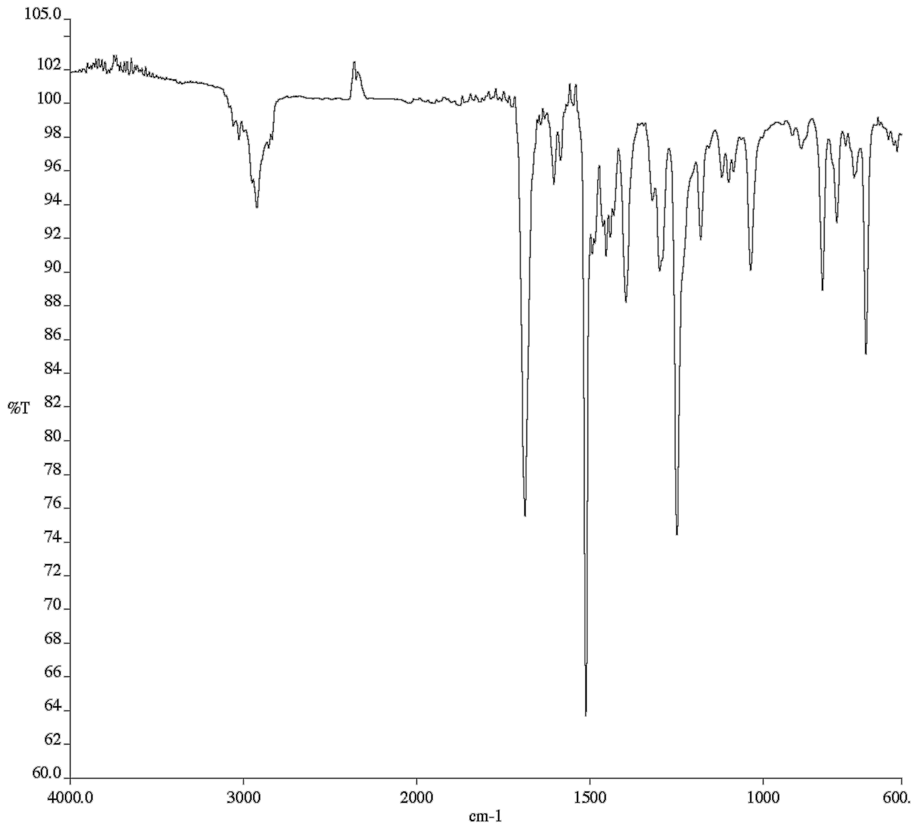
^{19}F NMR (282 MHz, $CDCl_3$) of compound **3gc**



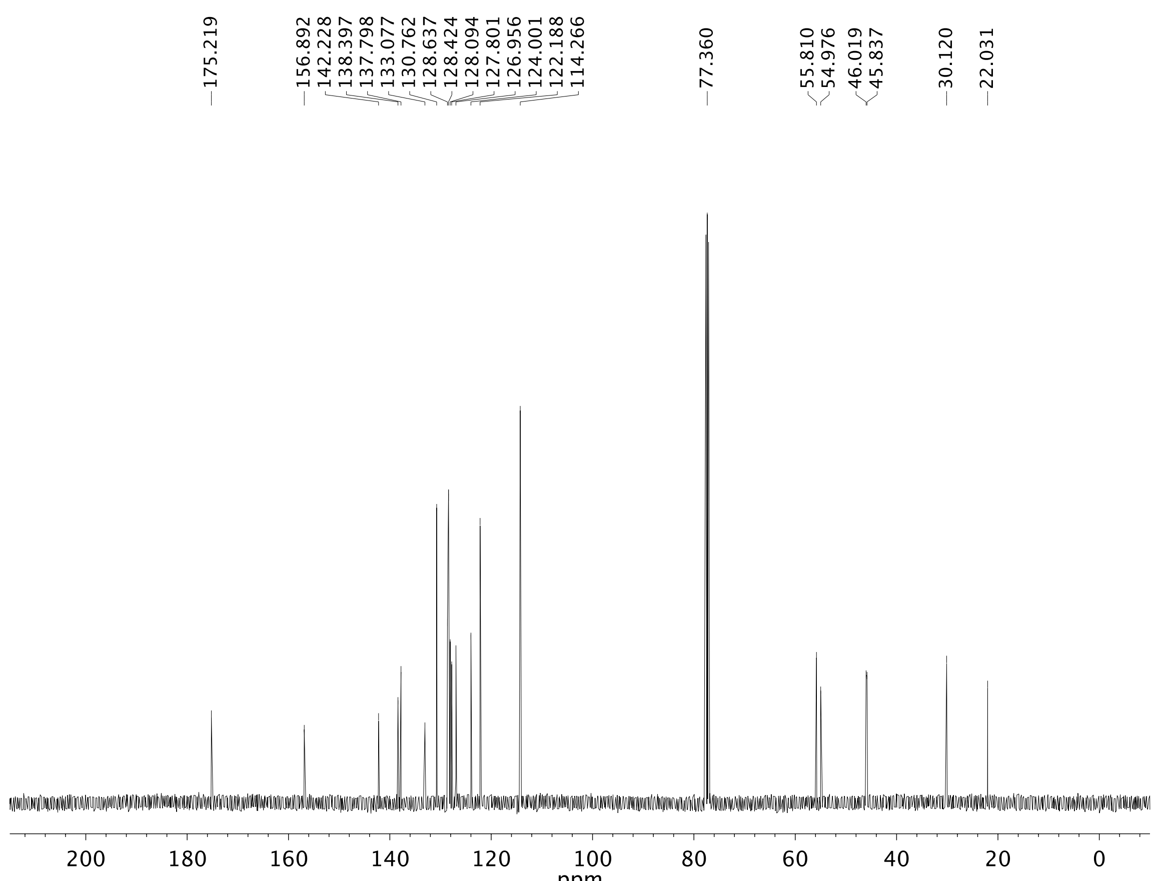
3gk



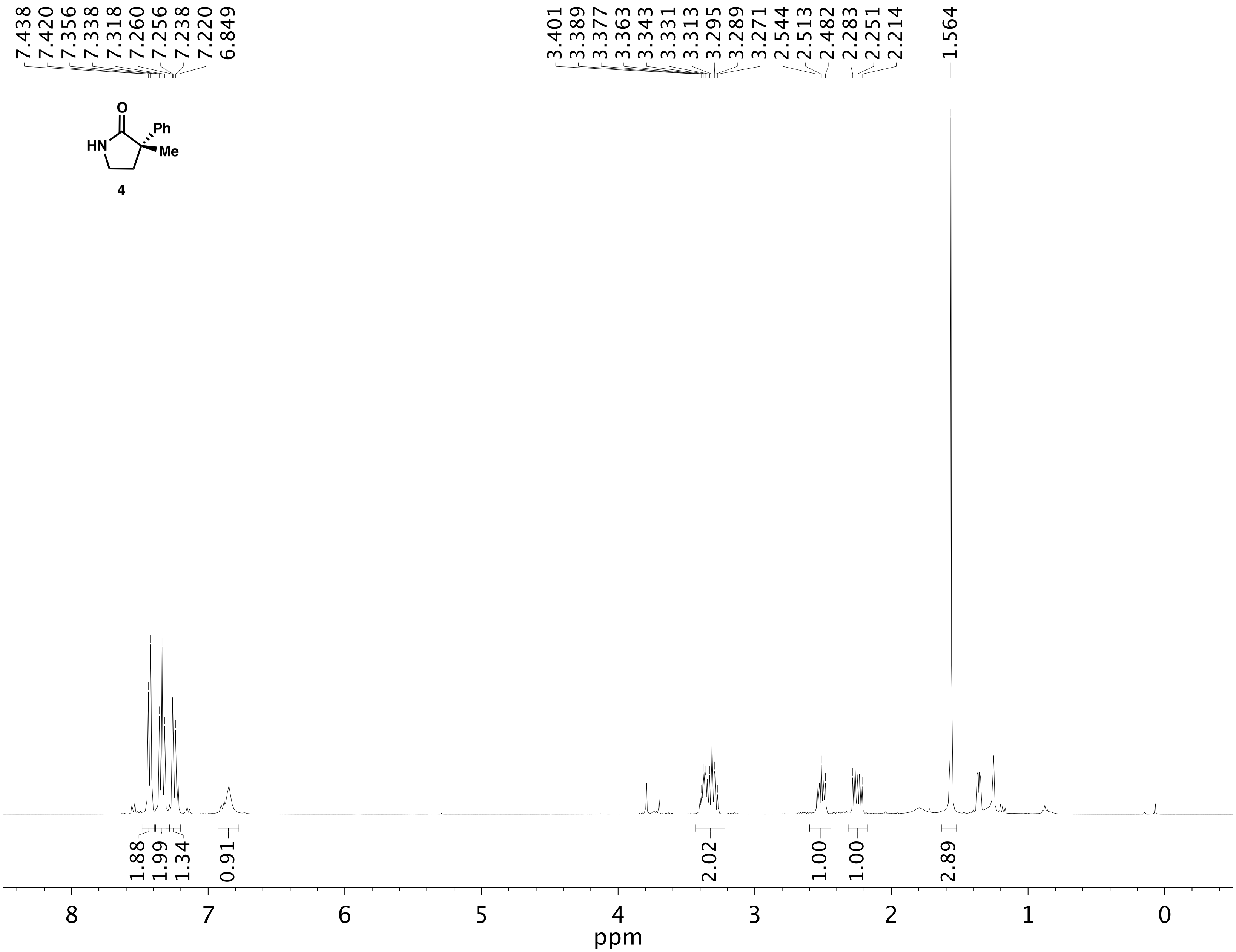
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3gk**



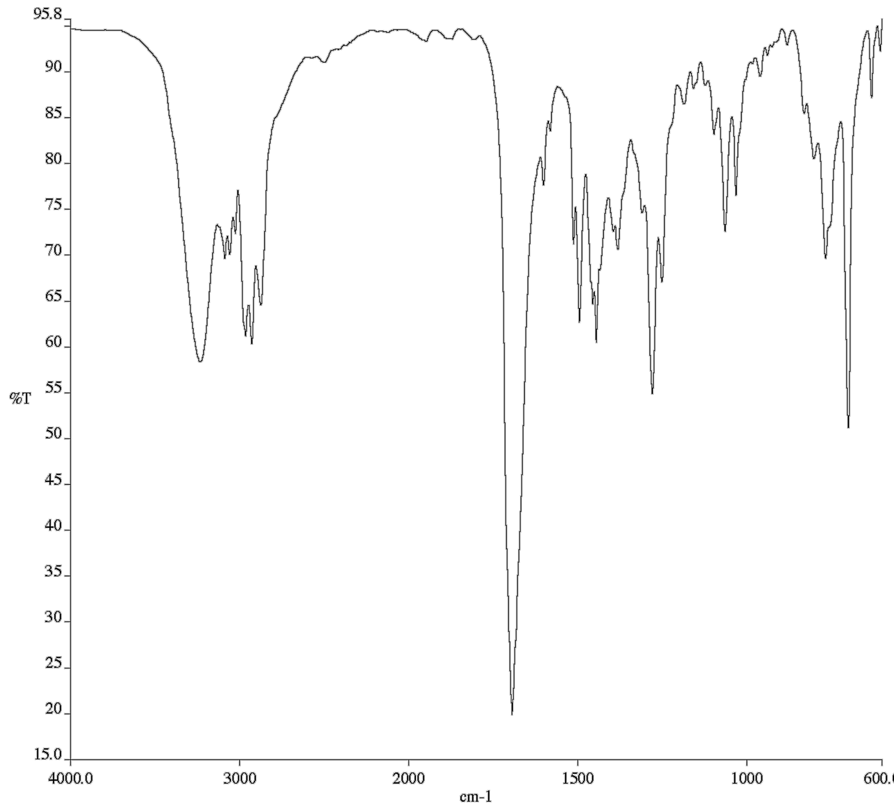
Infrared spectrum (Thin Film, NaCl) of compound **3gk**.



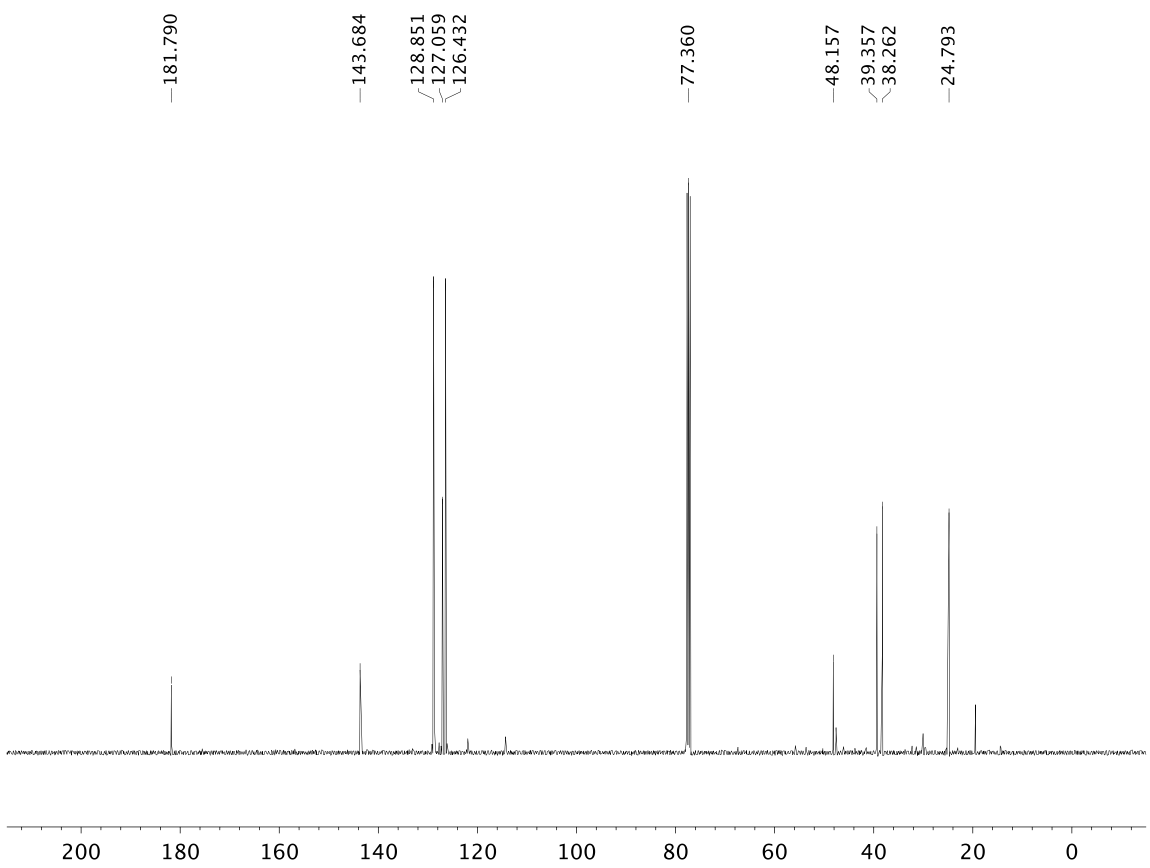
^{13}C NMR (125 MHz, $CDCl_3$) of compound **3gk**



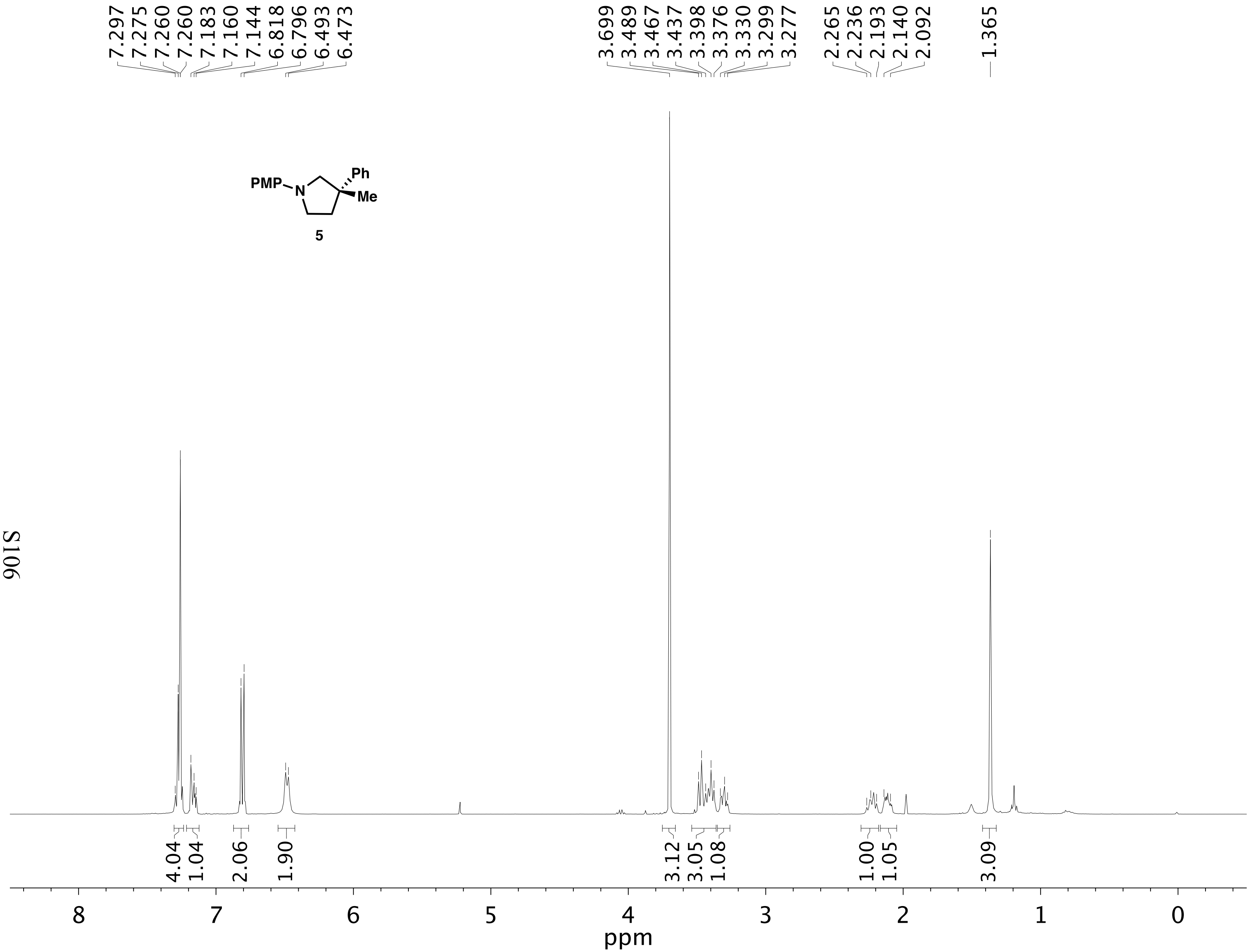
^{1}H NMR (400 MHz, $CDCl_3$) of compound **4**



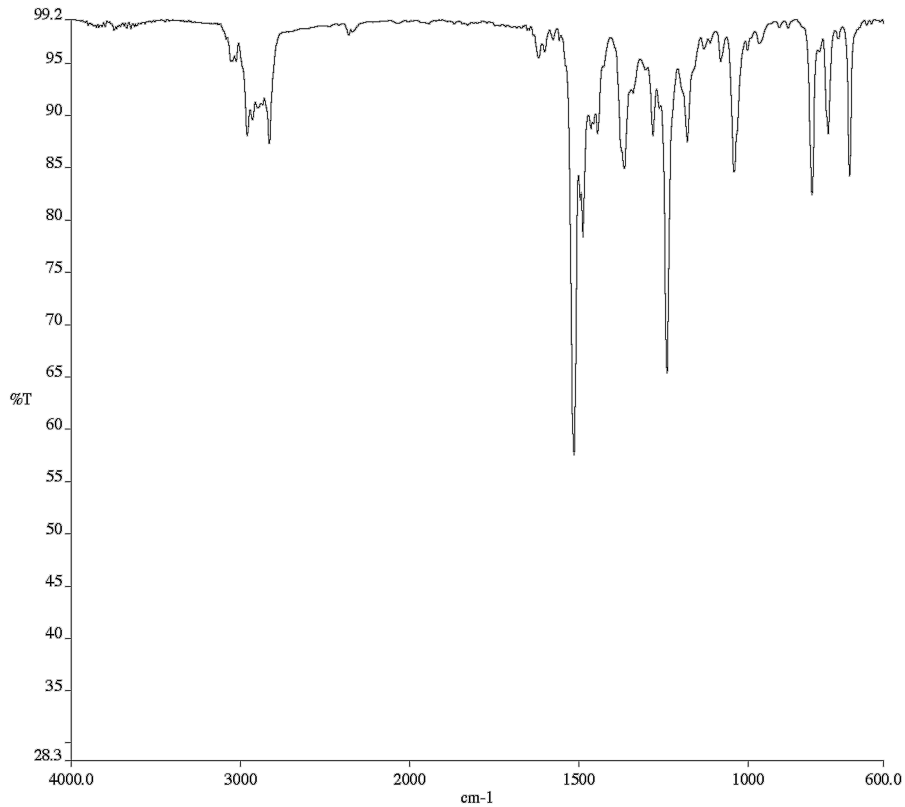
Infrared spectrum (Thin Film, NaCl) of compound **4**



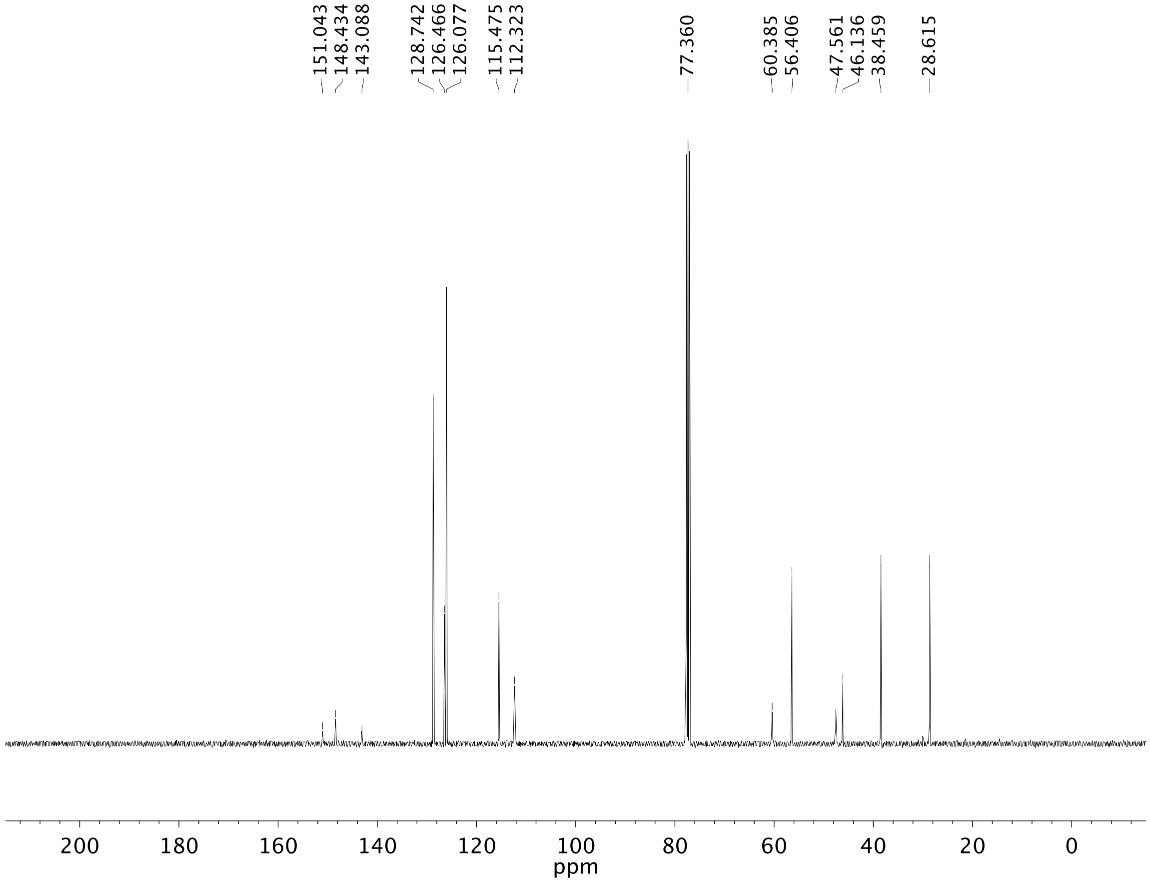
^{13}C NMR (100 MHz, $CDCl_3$) of compound **4**



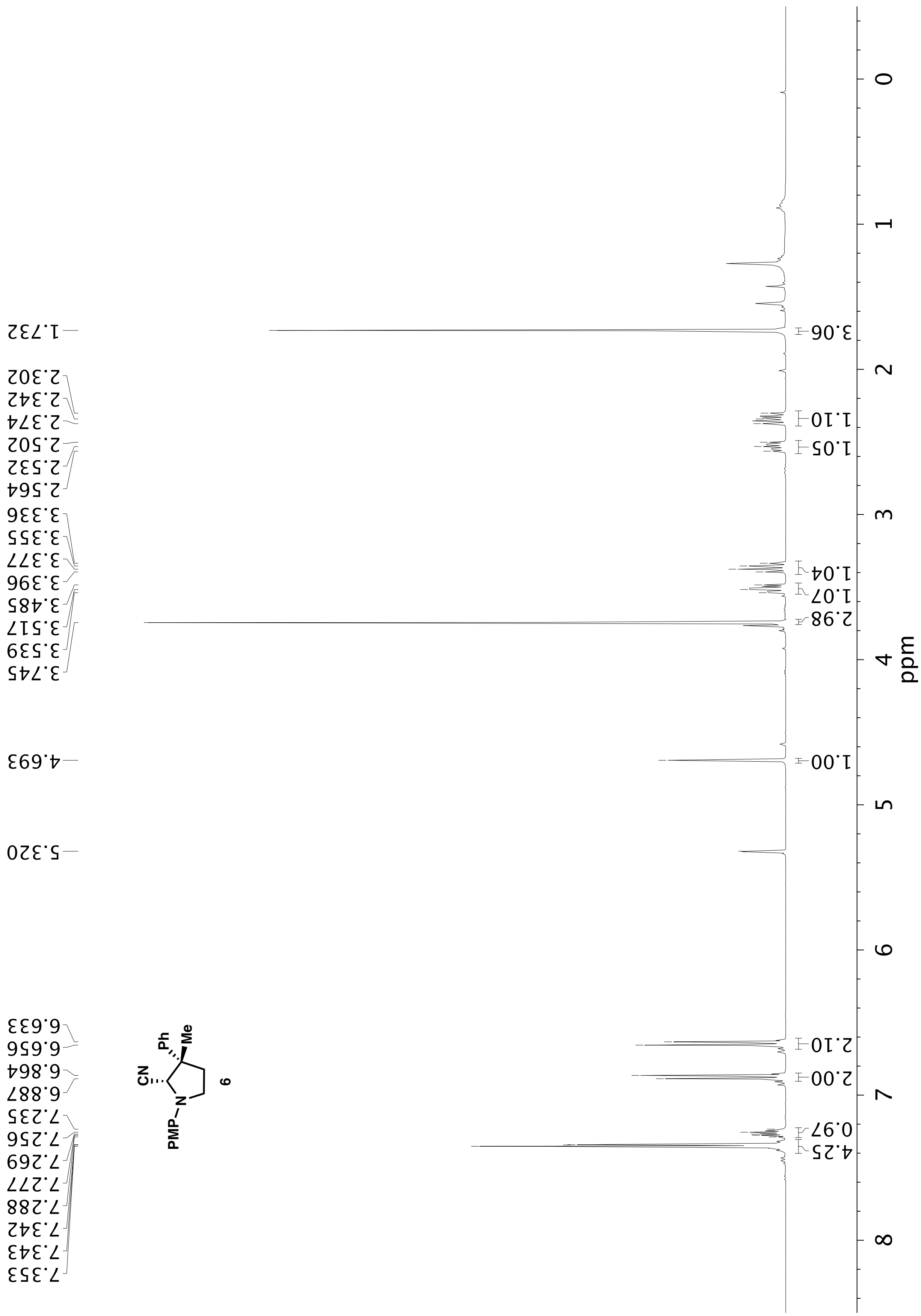
^{1}H NMR (400 MHz, $CDCl_3$) of compound **5**



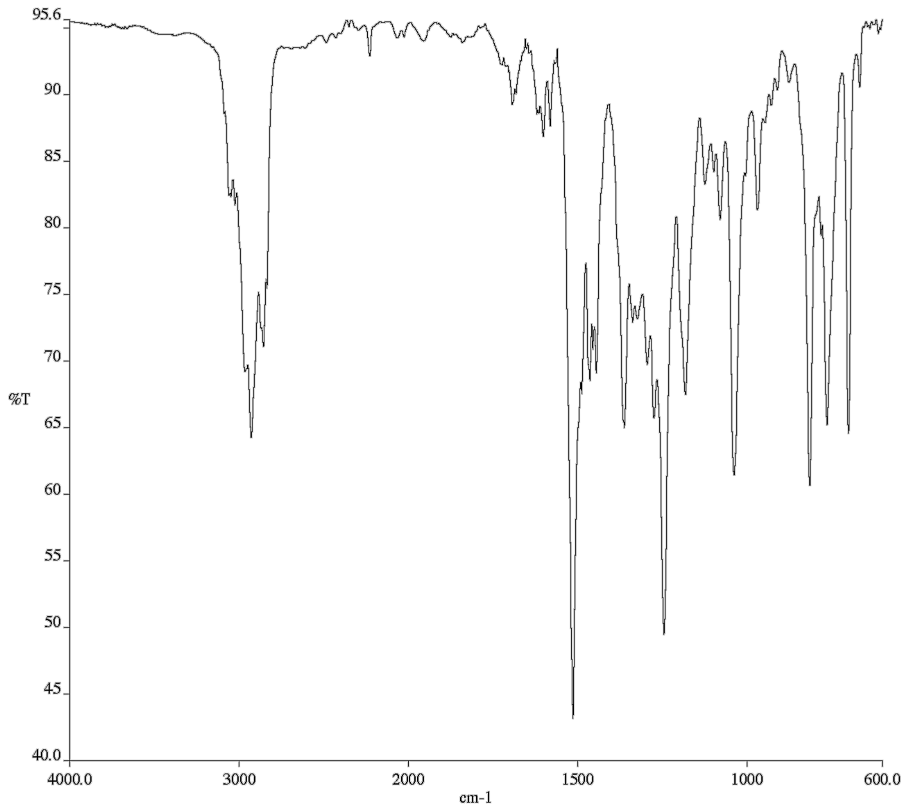
Infrared spectrum (Thin Film, NaCl) of compound **5**



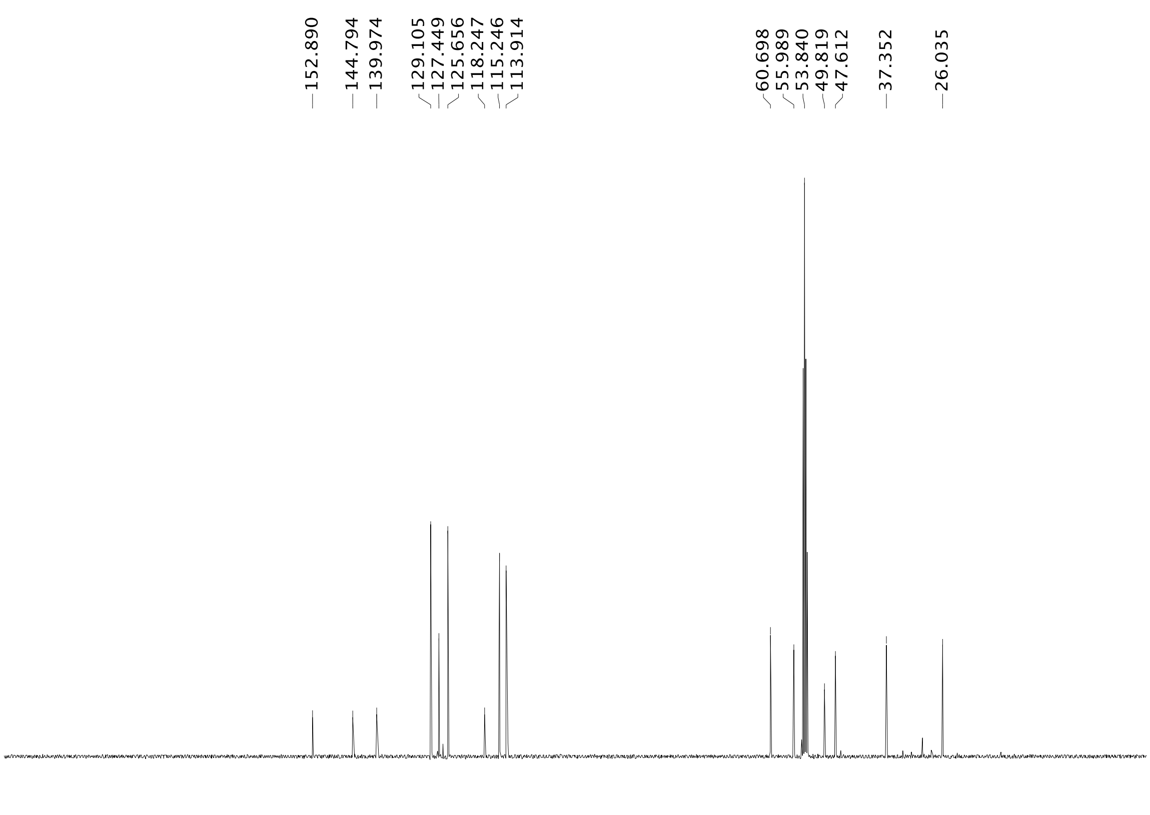
^{13}C NMR (100 MHz, $CDCl_3$) of compound **5**



^{1}H NMR (400 MHz, CD_2Cl_2) of compound **6**



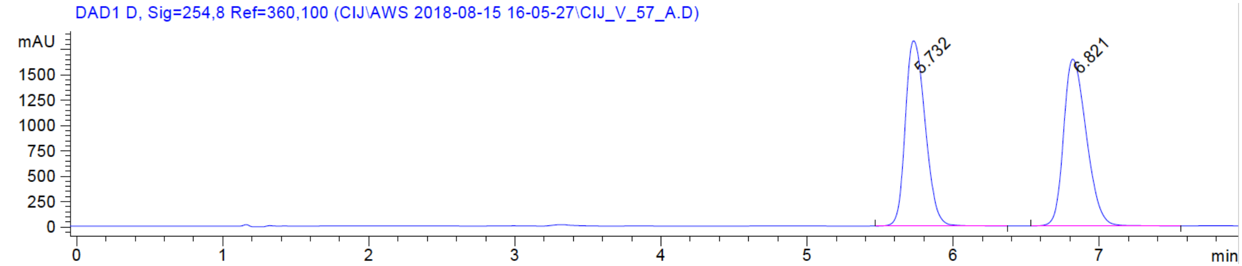
Infrared spectrum (Thin Film, NaCl) of compound **6**



^{13}C NMR (100 MHz, CD_2Cl_2) of compound **6**

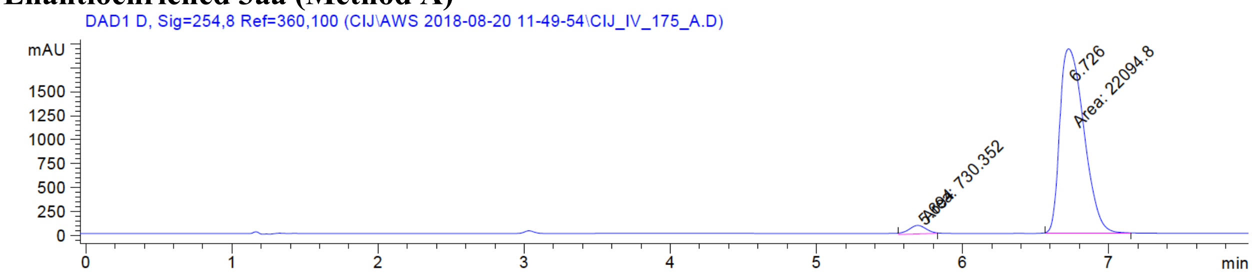
SFC Traces of Racemic and Enantioenriched Compounds

Racemic 3aa



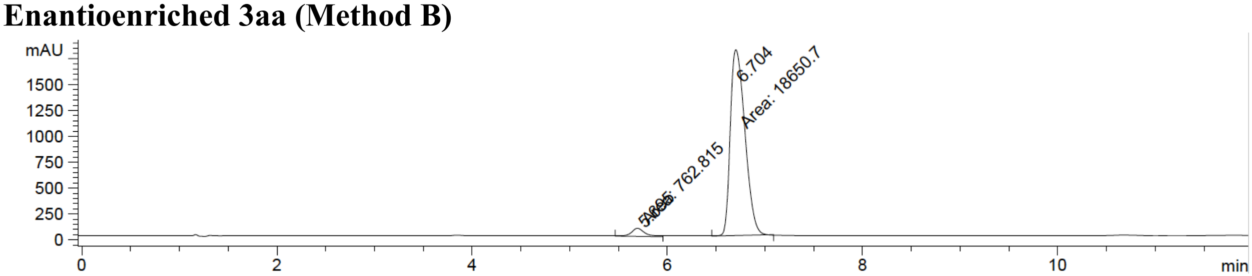
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.732	BB	0.1507	1.73046e4	1823.55408	49.1835
2	6.821	BB	0.1711	1.78791e4	1641.45984	50.8165

Enantioenriched 3aa (Method A)



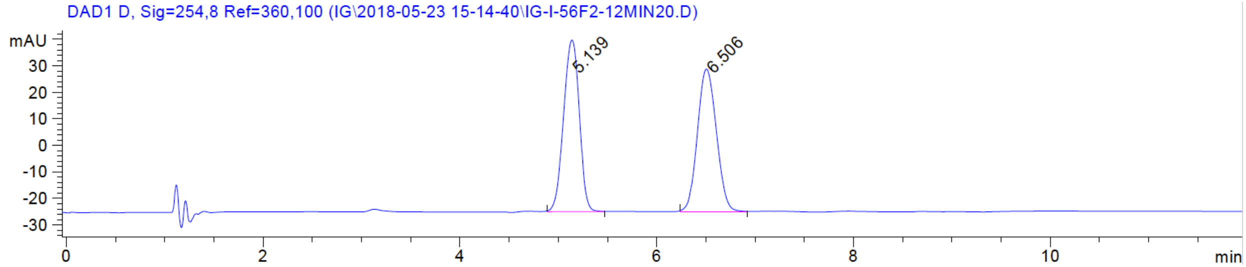
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.694	MM	0.1370	730.35217	88.85317	3.1998
2	6.726	MM	0.1916	2.20948e4	1922.27869	96.8002

Enantioenriched 3aa (Method B)



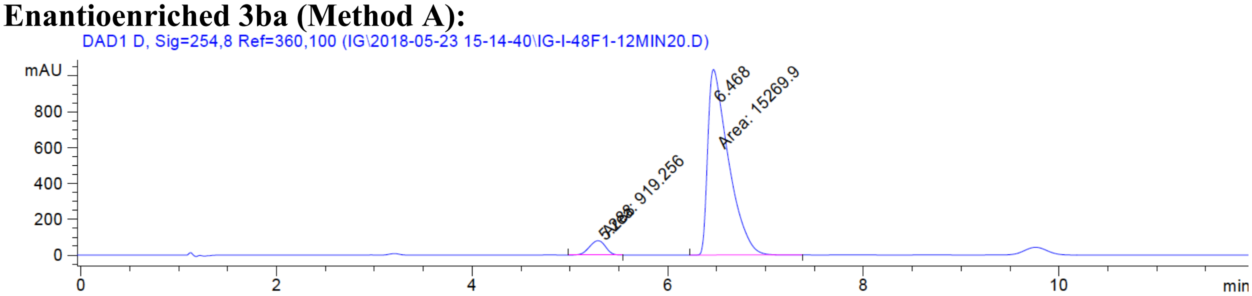
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.695	MM	0.1634	762.81488	77.81515	3.9293
2	6.704	MM	0.1731	1.86507e4	1795.67065	96.0707

Racemic 3ba:



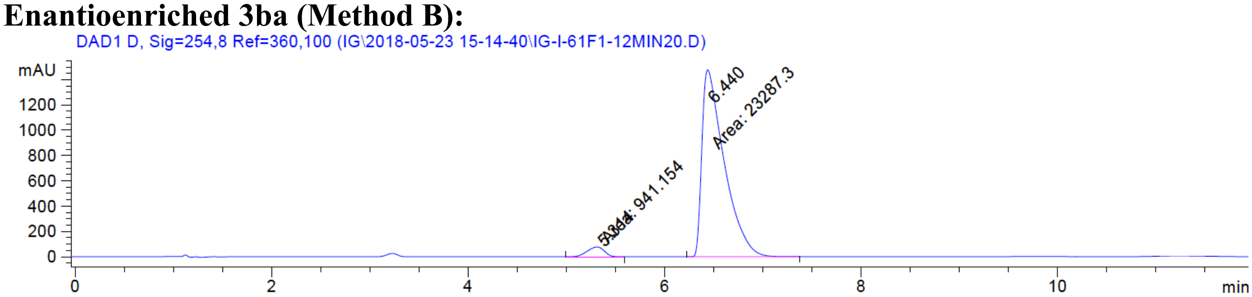
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.139	BB	0.1779	720.65485	64.72079	50.0934
2	6.506	BB	0.2079	717.96631	53.71758	49.9066

Enantioenriched 3ba (Method A):



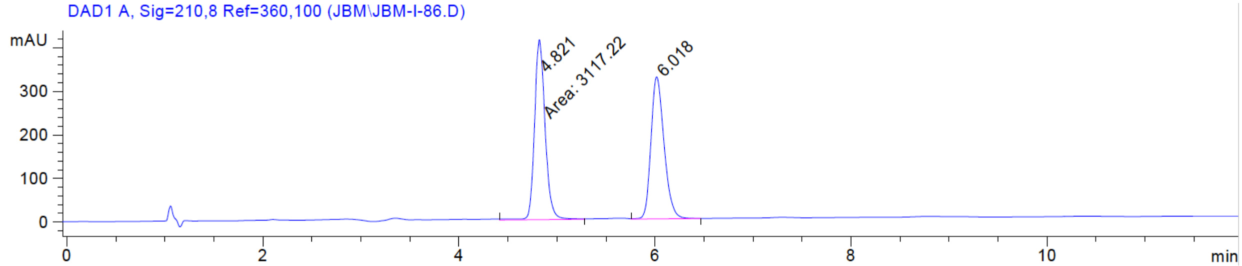
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.288	MM	0.1910	919.25604	80.21479	5.6782
2	6.468	MM	0.2454	1.52699e4	1037.26819	94.3218

Enantioenriched 3ba (Method B):



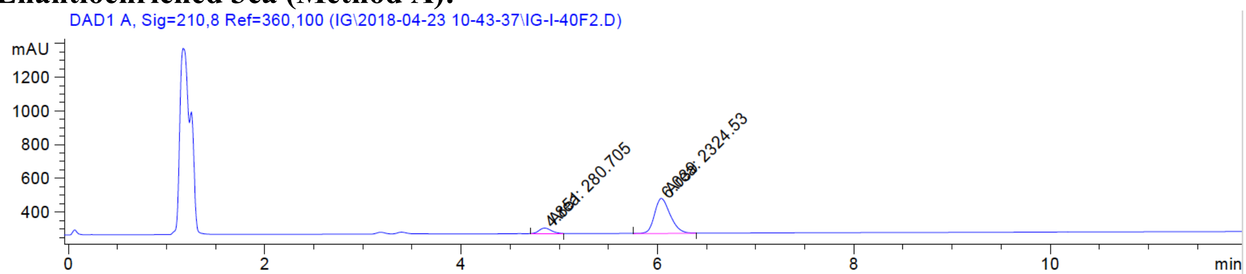
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.314	MM	0.2012	941.15393	77.94627	3.8845
2	6.440	MM	0.2624	2.32873e4	1479.37891	96.1155

Racemic 3ca:



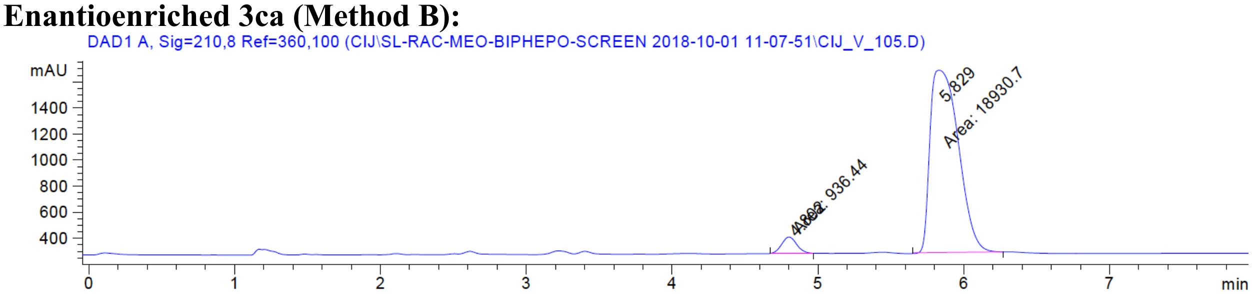
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.821	MM	0.1252	3117.21655	414.82434	50.6649
2	6.018	VB	0.1447	3035.40259	325.73962	49.3351

Enantioenriched 3ca (Method A):



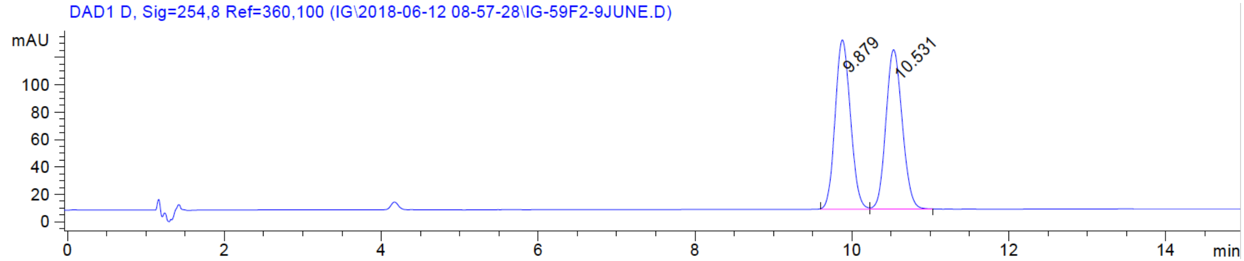
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.851	MM	0.1428	280.70517	32.76271	10.7747
2	6.039	MM	0.1861	2324.52930	208.16582	89.2253

Enantioenriched 3ca (Method B):



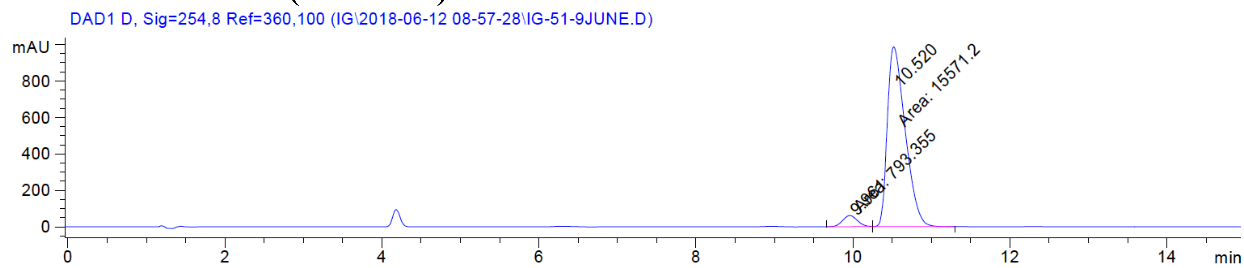
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.802	MM	0.1220	936.44037	127.97585	4.7135
2	5.829	MM	0.2253	1.89307e4	1400.13245	95.2865

Racemic 3da:



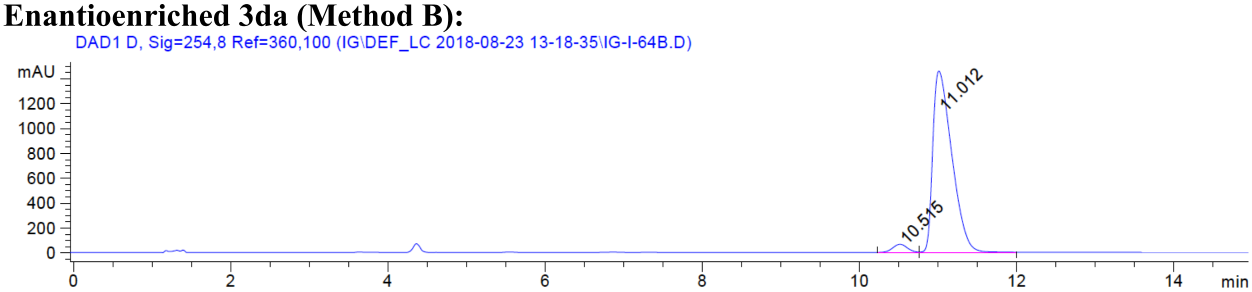
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.879	BV	0.2103	1676.87537	123.57167	49.8413
2	10.531	VB	0.2252	1687.55713	116.35130	50.1587

Enantioenriched 3da (Method A):



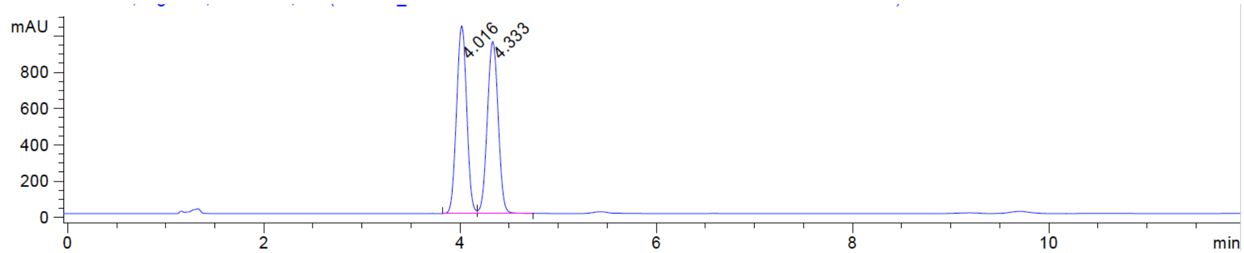
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.961	MM	0.2186	793.35480	60.49282	4.8480
2	10.520	MM	0.2633	1.55712e4	985.72064	95.1520

Enantioenriched 3da (Method B):



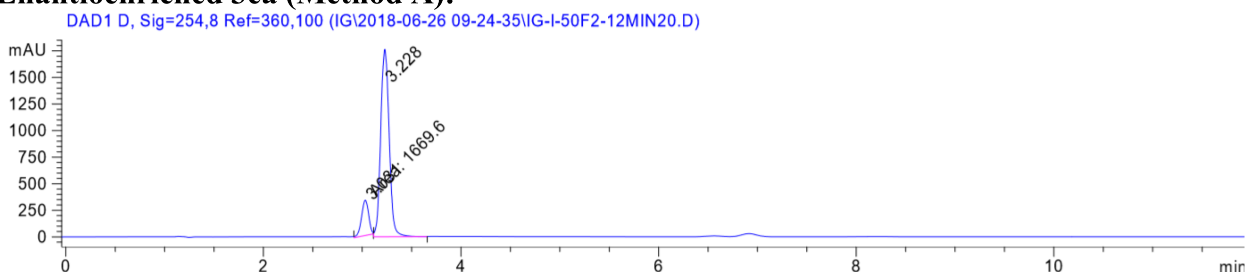
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.515	BV	0.1999	855.45862	65.70339	3.3678
2	11.012	VBA	0.2606	2.45459e4	1456.71838	96.6322

Racemic 3ea



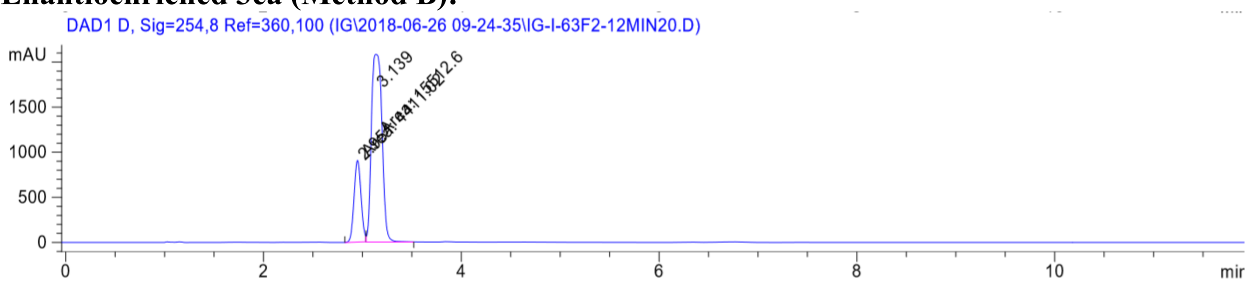
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.016	BV	0.1161	7452.02637	1034.19238	50.5540
2	4.333	VB	0.1218	7288.71240	947.14972	49.4460

Enantioenriched 3ea (Method A):



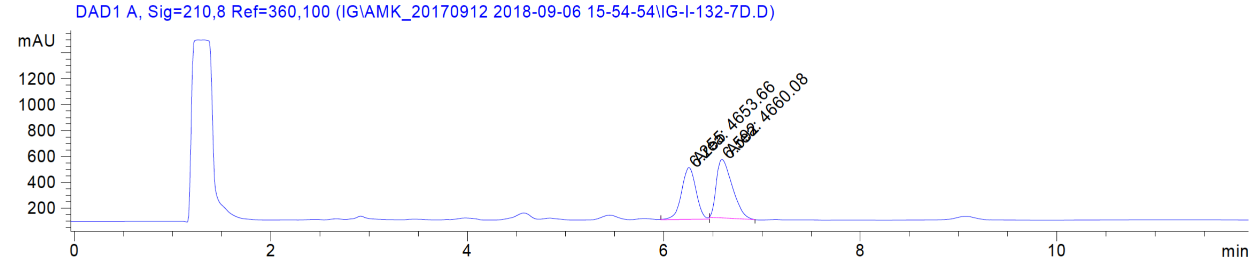
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.031	MM	0.0833	1669.59949	334.15417	13.5659
2	3.228	VB	0.0942	1.06377e4	1767.28540	86.4341

Enantioenriched 3ea (Method B):



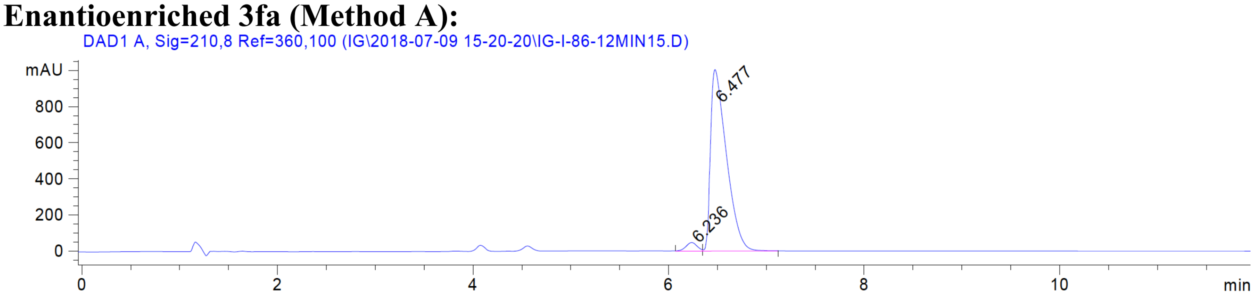
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.951	MM	0.0809	4411.02246	908.98328	22.1397
2	3.139	MM	0.1243	1.55126e4	2080.52515	77.8603

Racemic 3fa:



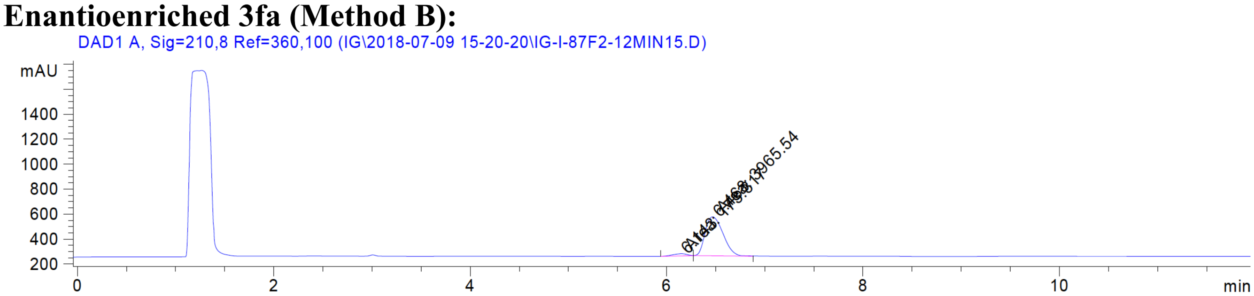
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.255	MM	0.1853	4653.66064	418.65048	49.9655
2	6.592	MM	0.1770	4660.08008	438.68570	50.0345

Enantioenriched 3fa (Method A):



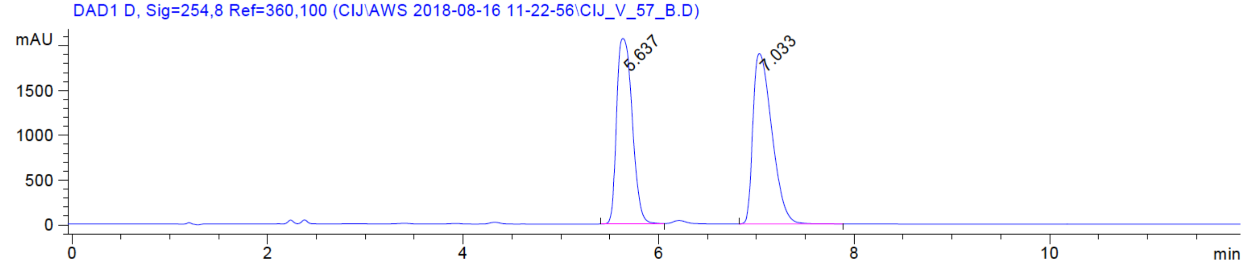
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.236	BV	0.1242	311.98120	47.82814	2.6593
2	6.477	VB	0.1724	1.14197e4	1006.15845	97.3407

Enantioenriched 3fa (Method B):



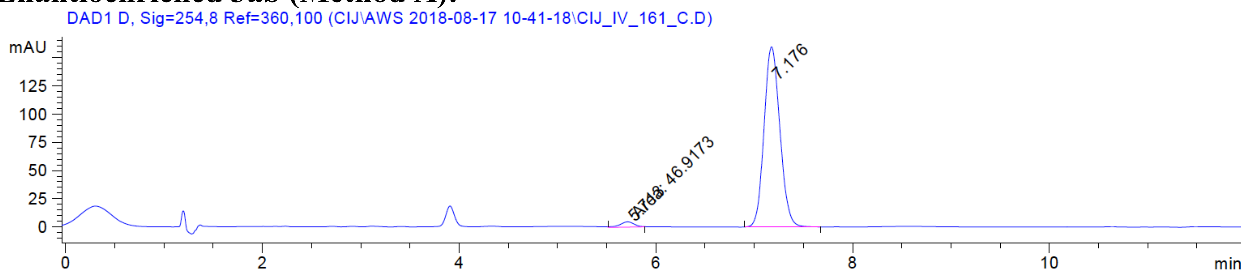
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.143	MM	0.1710	173.31717	16.89257	4.1876
2	6.468	MM	0.2115	3965.54468	312.46899	95.8124

Racemic 3ab



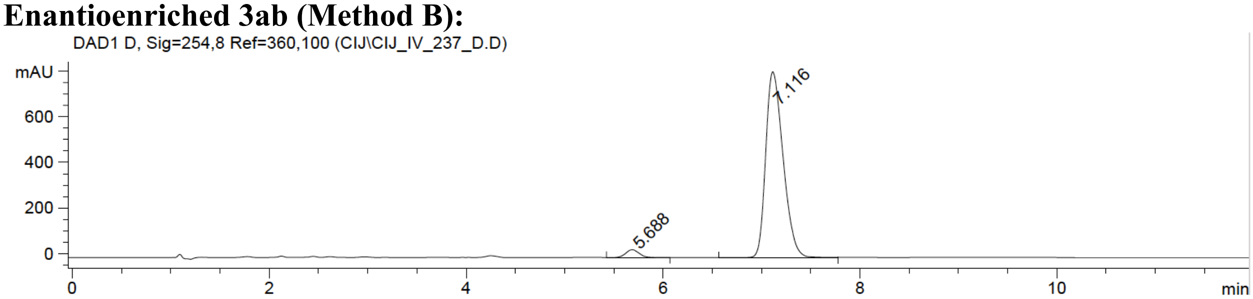
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.637	BV	0.1773	2.29310e4	2069.20288	47.2262
2	7.033	BB	0.2093	2.56246e4	1900.44934	52.7738

Enantioenriched 3ab (Method A):



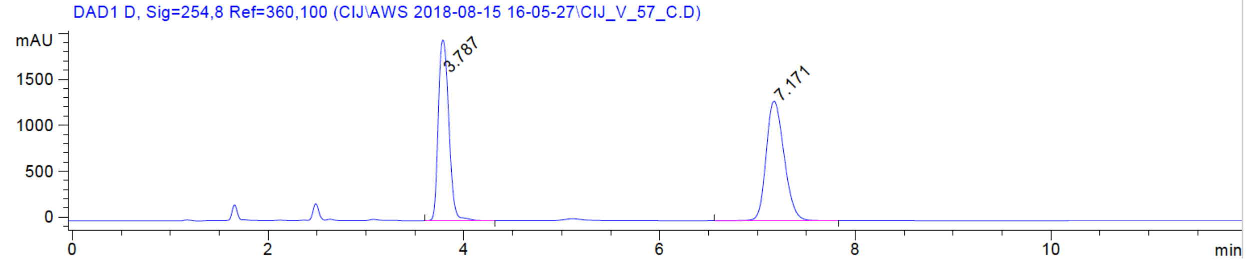
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.713	MM	0.1657	46.91730	4.71817	2.5642
2	7.176	BB	0.1744	1782.80688	159.48334	97.4358

Enantioenriched 3ab (Method B):



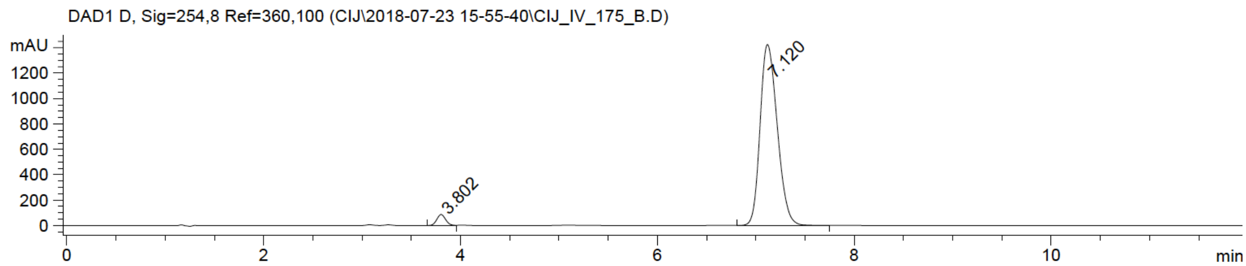
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.688	VB	0.1535	355.71619	35.33065	3.4483
2	7.116	BB	0.1907	9960.10352	814.19574	96.5517

Racemic 3ac



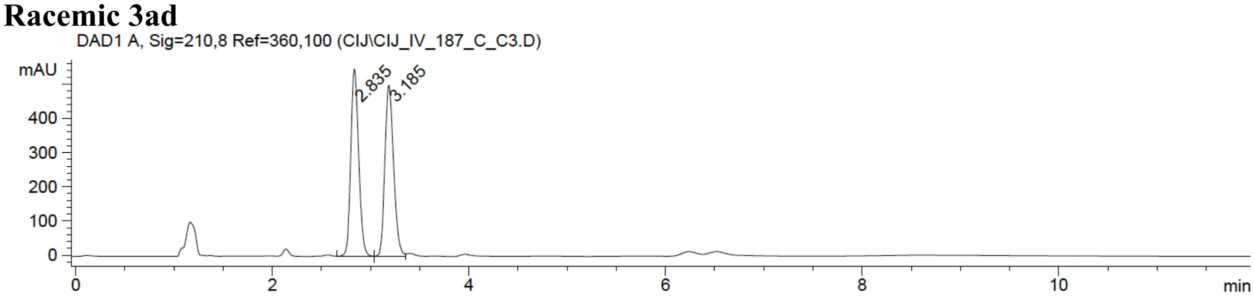
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.787	BB	0.1191	1.46599e4	1964.33459	46.9531
2	7.171	BB	0.2006	1.65625e4	1300.21704	53.0469

Enantioenriched 3ac



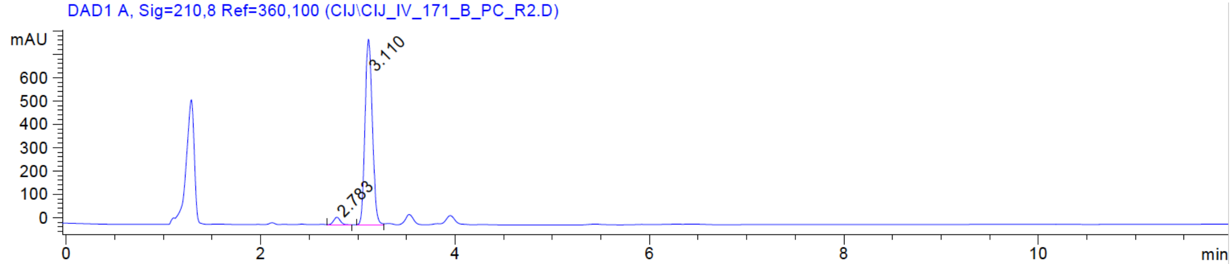
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.802	BV	0.0974	548.64478	87.19595	3.0727
2	7.120	VB	0.1897	1.73069e4	1424.59058	96.9273

Racemic 3ad



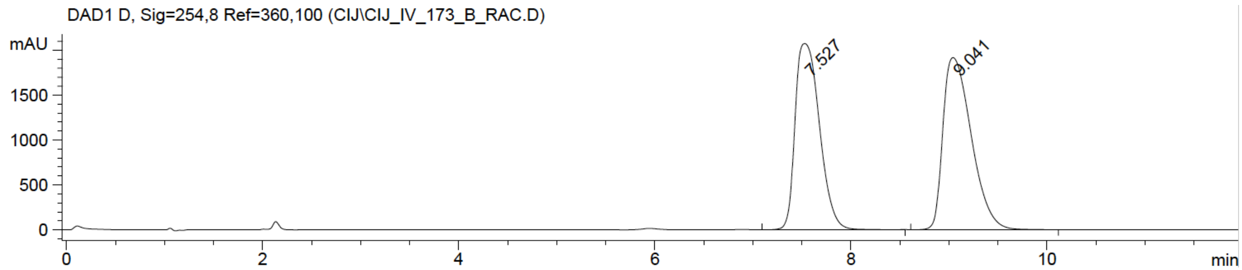
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.835	VV	0.0859	3100.32373	548.77954	50.0235
2	3.185	VV	0.0941	3097.40625	501.10672	49.9765

Enantioenriched 3ad



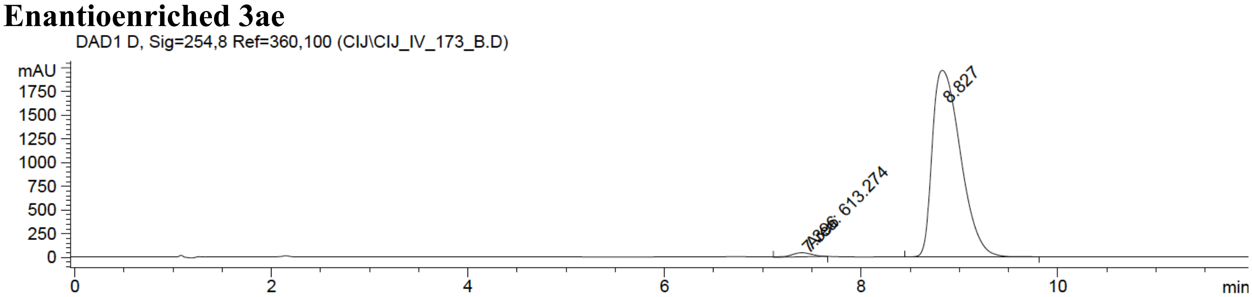
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.783	VB	0.0728	151.04274	32.14610	3.4828
2	3.110	BV	0.0834	4185.71582	795.92487	96.5172

Racemic 3ae



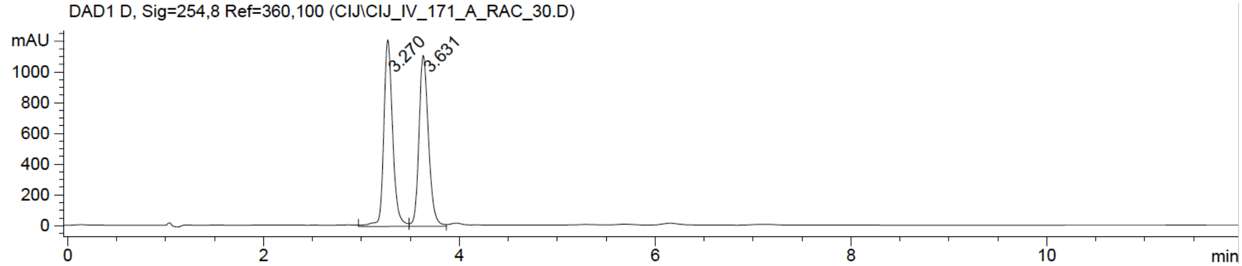
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.527	VB	0.2739	3.59289e4	2076.07275	48.2410
2	9.041	BB	0.3145	3.85490e4	1917.55591	51.7590

Enantioenriched 3ae



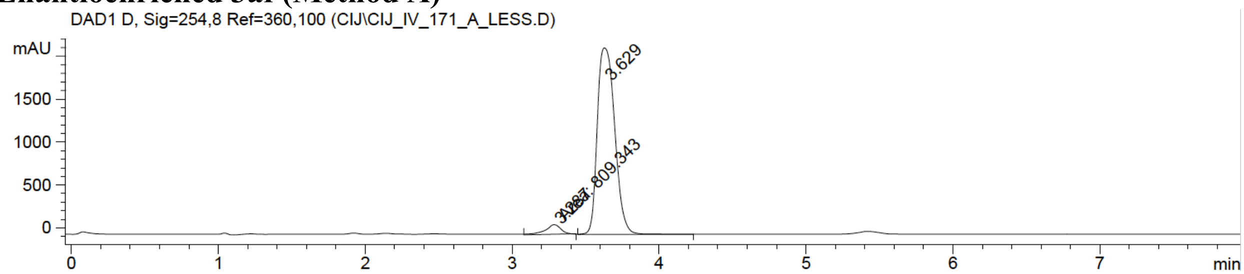
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.396	MM	0.2348	613.27362	43.52377	1.5376
2	8.827	BB	0.3149	3.92727e4	1967.01807	98.4624

Racemic 3af



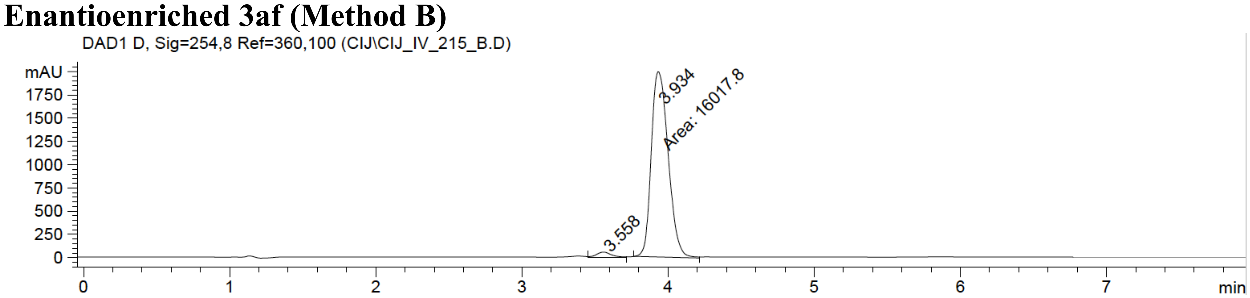
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.270	VV	0.0959	7697.81494	1214.51843	50.5270
2	3.631	VV	0.1029	7537.22900	1113.83862	49.4730

Enantioenriched 3af (Method A)



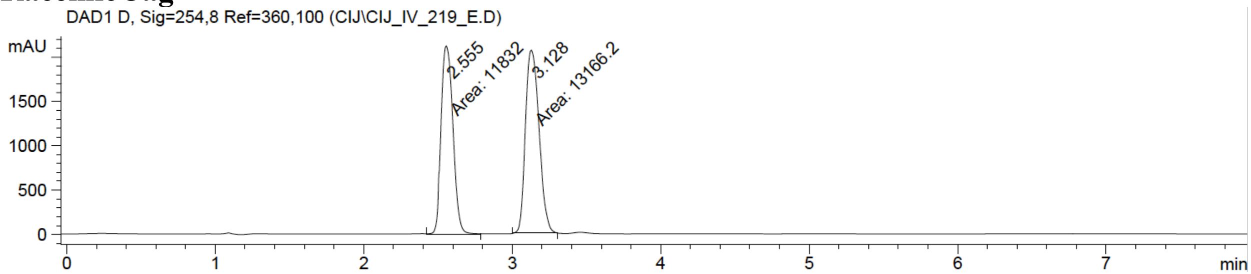
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.287	MM	0.1208	809.34290	111.69874	4.3034
2	3.629	VB	0.1326	1.79977e4	2173.46069	95.6966

Enantioenriched 3af (Method B)



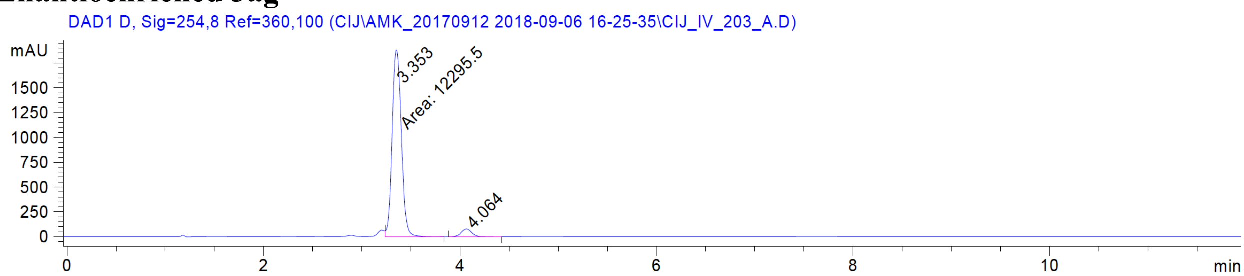
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.558	VV	0.1047	370.16199	54.85843	2.2587
2	3.934	MM	0.1339	1.60178e4	1993.98669	97.7413

Racemic 3ag



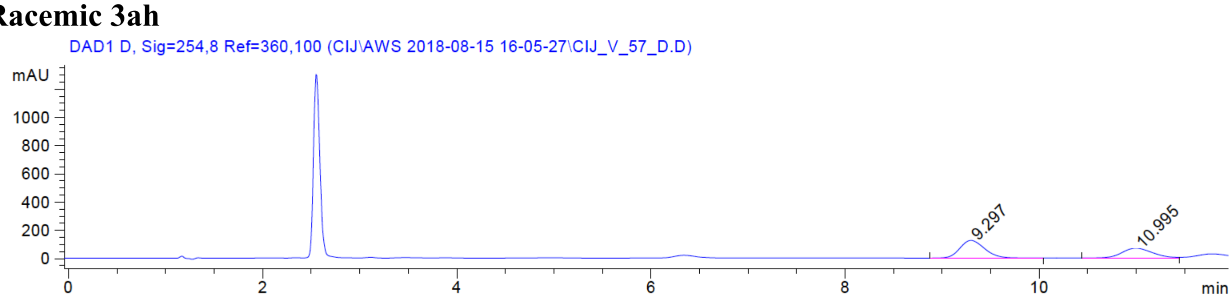
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.555	MM	0.0928	1.18320e4	2124.87231	47.3314
2	3.128	MM	0.1061	1.31662e4	2067.63916	52.6686

Enantioenriched 3ag



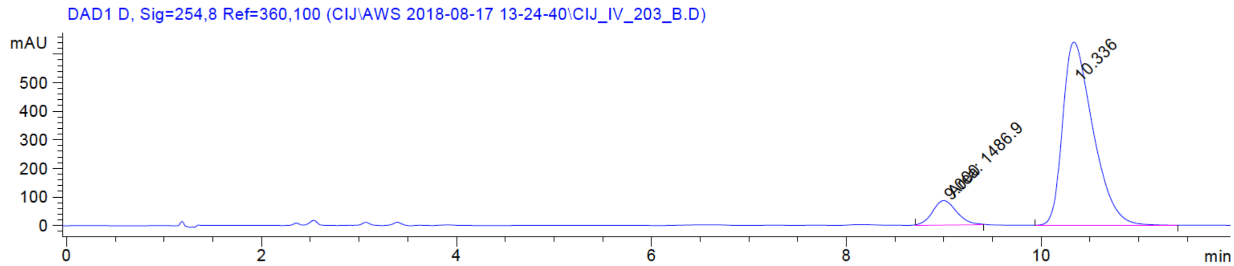
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.353	FM	0.1085	1.22955e4	1888.93799	95.4138
2	4.064	BB	0.1163	591.00110	78.10308	4.5862

Racemic 3ah



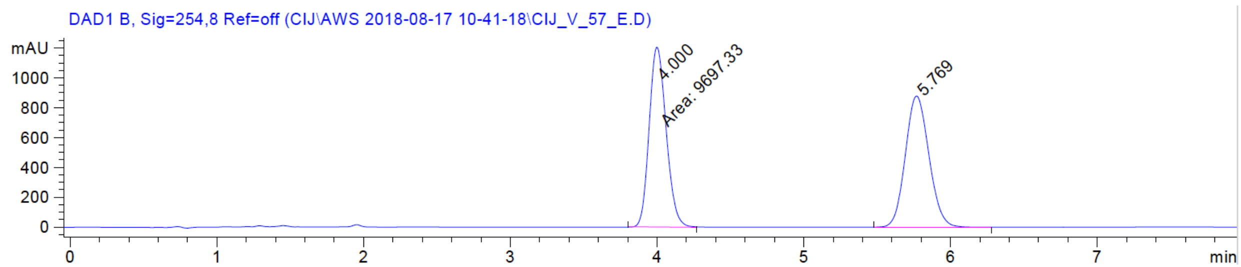
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.297	BB	0.2749	2219.42676	125.12122	59.0963
2	10.995	BV	0.3407	1536.18433	69.81071	40.9037

Enantioenriched 3ah



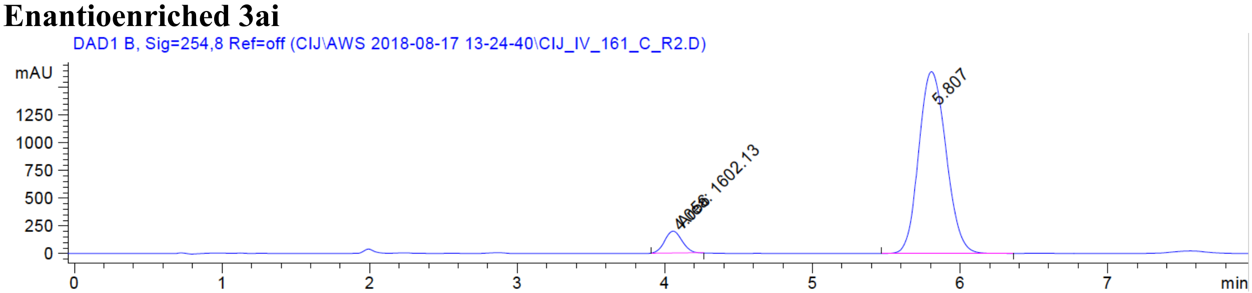
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.000	MM	0.2883	1486.90210	85.95448	9.6858
2	10.336	BB	0.3285	1.38644e4	640.68628	90.3142

Racemic 3ai



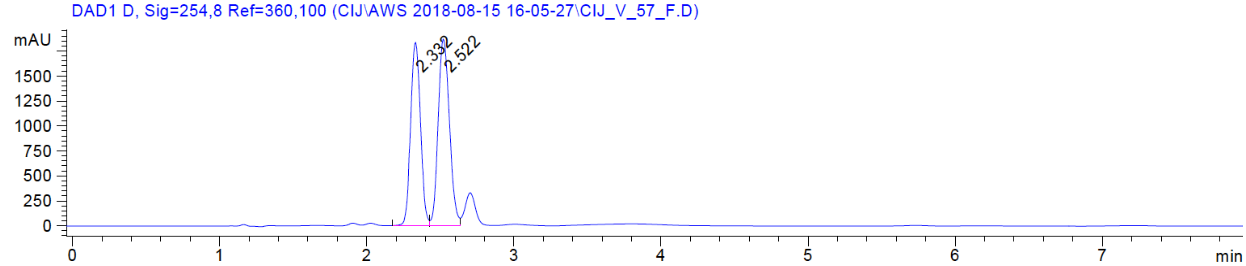
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.000	MM	0.1337	9697.33105	1208.43311	49.6496
2	5.769	BB	0.1747	9834.22070	878.10040	50.3504

Enantioenriched 3ai



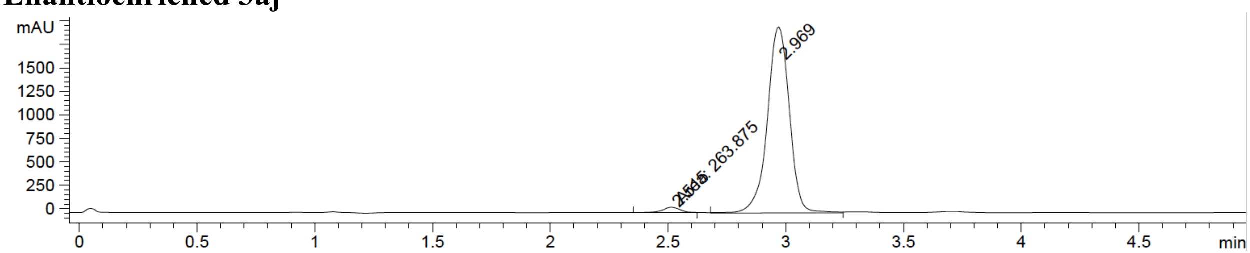
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.056	MM	0.1349	1602.13367	197.90459	7.0340
2	5.807	BB	0.2025	2.11748e4	1641.31360	92.9660

Racemic 3aj



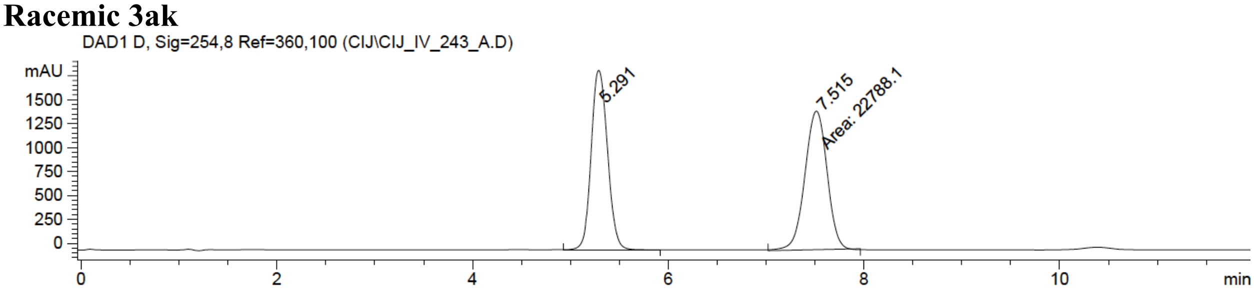
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.332	BV	0.0750	8584.59863	1821.74634	46.2517
2	2.522	VV	0.0826	9976.01562	1860.31799	53.7483

Enantioenriched 3aj



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.515	MM	0.0810	263.87479	54.30037	2.0037
2	2.969	VV	0.1021	1.29057e4	1978.46008	97.9963

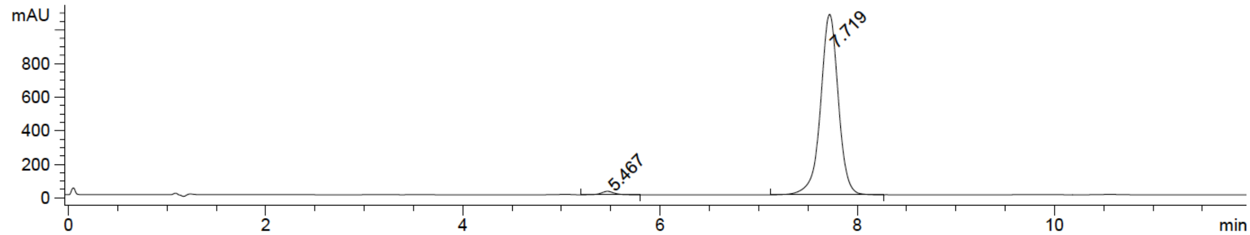
Racemic 3ak



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.291	VB	0.1837	2.18013e4	1874.45410	48.8934
2	7.515	MM	0.2621	2.27881e4	1448.80847	51.1066

Enantioenriched 3ak

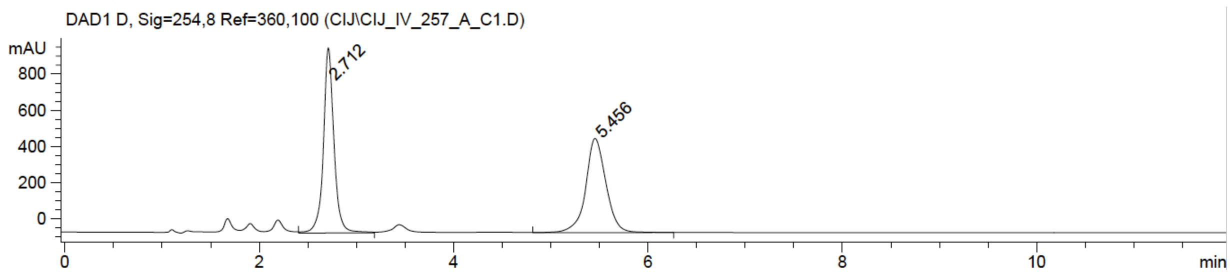
DAD1 D, Sig=254,8 Ref=360,100 (KELLYZ\2018-06-08 11-06-07\CIJ_IV_235_A.D)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.467	VB	0.1411	196.88924	21.06404	1.4419
2	7.719	BB	0.1900	1.34582e4	1075.12634	98.5581

Racemic 3al

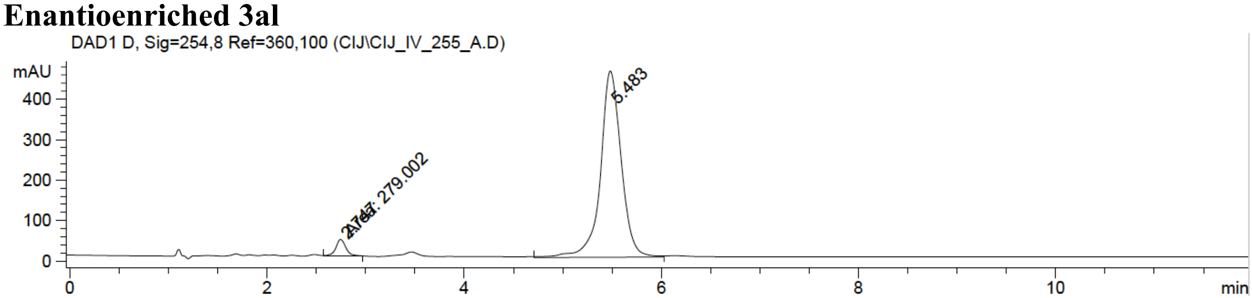
DAD1 D, Sig=254,8 Ref=360,100 (CIJ\CIJ_IV_257_A_C1.D)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.712	VV	0.1122	7731.06787	1023.18335	50.5629
2	5.456	VB	0.2196	7558.94238	519.99438	49.4371

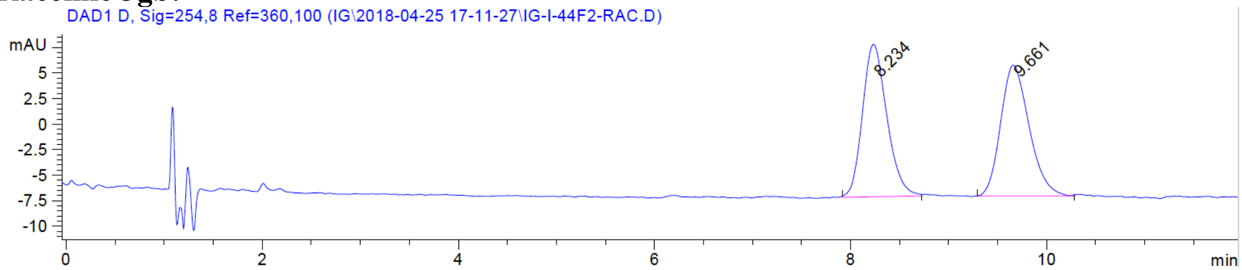
Enantioenriched 3al

DAD1 D, Sig=254,8 Ref=360,100 (CIJ\CIJ_IV_255_A.D)



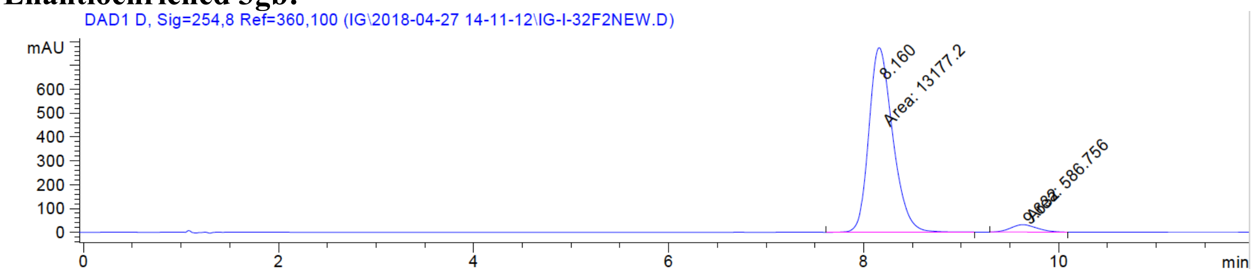
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.747	MM	0.1151	279.00238	40.41557	3.9607
2	5.483	BV	0.2215	6765.28516	460.20511	96.0393

Racemic 3gb:



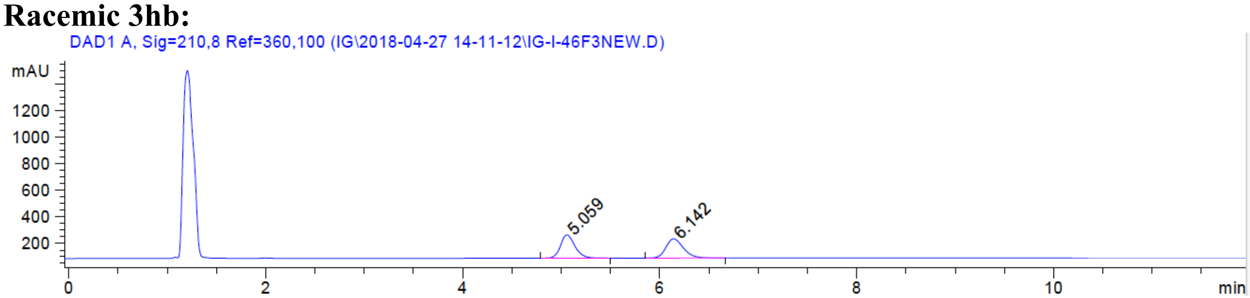
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.234	BB	0.2636	258.12427	14.94135	49.9168
2	9.661	BB	0.3157	258.98459	12.82095	50.0832

Enantioenriched 3gb:



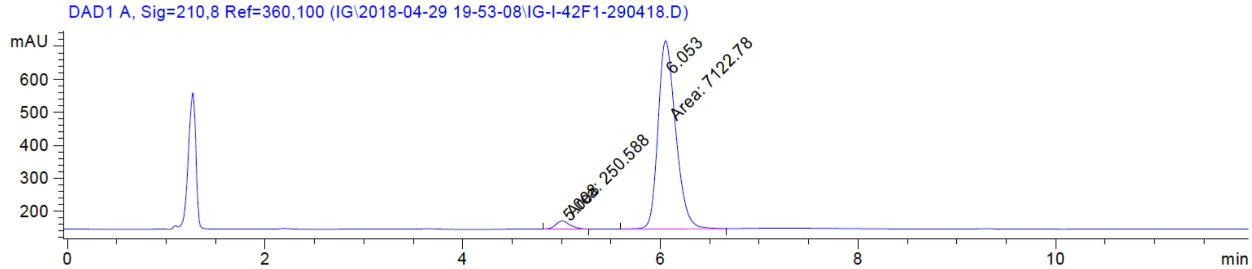
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.160	MM	0.2835	1.31772e4	774.70050	95.7370
2	9.632	MM	0.3140	586.75641	31.14583	4.2630

Racemic 3hb:



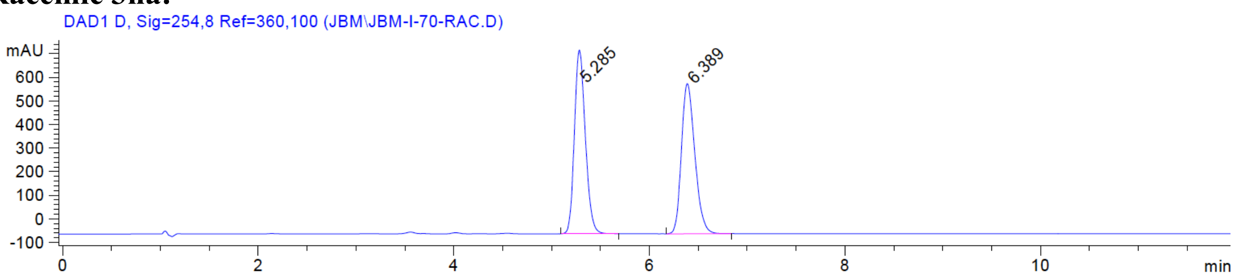
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.059	BB	0.1548	1790.89502	175.89771	50.1022
2	6.142	BB	0.1916	1783.58618	144.91161	49.8978

Enantioenriched 3hb:



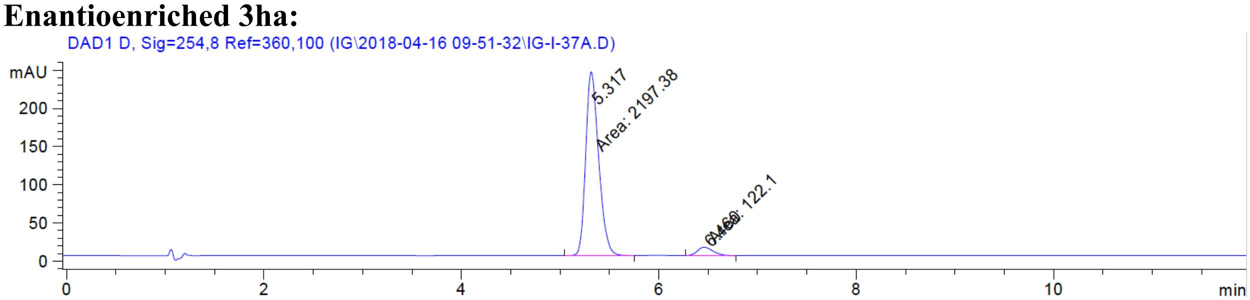
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.008	MM	0.1695	250.58771	24.64256	3.3986
2	6.053	MM	0.2078	7122.77539	571.42010	96.6014

Racemic 3ha:



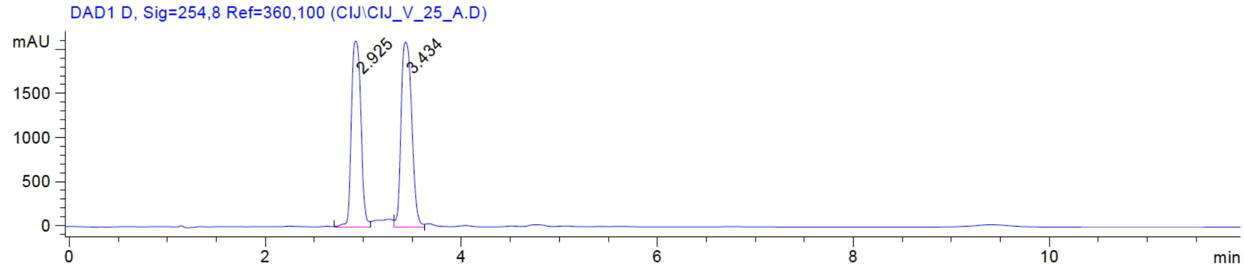
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.285	BB	0.1232	6085.81885	778.67822	50.0746
2	6.389	BB	0.1472	6067.69775	636.37927	49.9254

Enantioenriched 3ha:



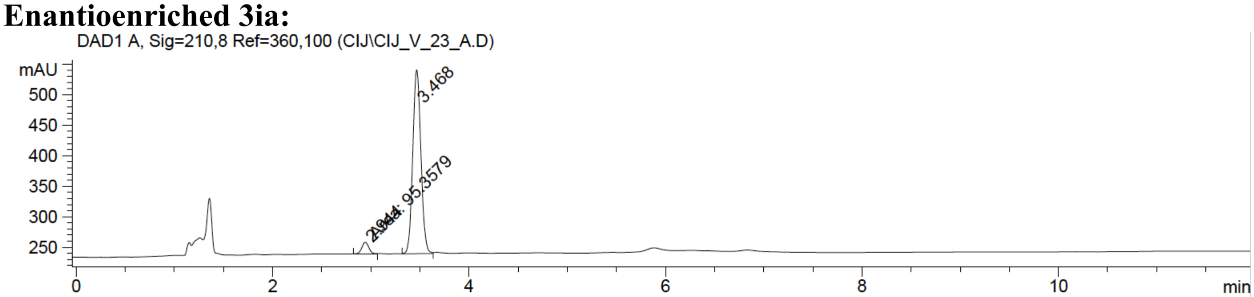
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.317	MM	0.1520	2197.37671	240.95227	94.7359
2	6.460	MM	0.1844	122.10018	11.03627	5.2641

Racemic 3ia:



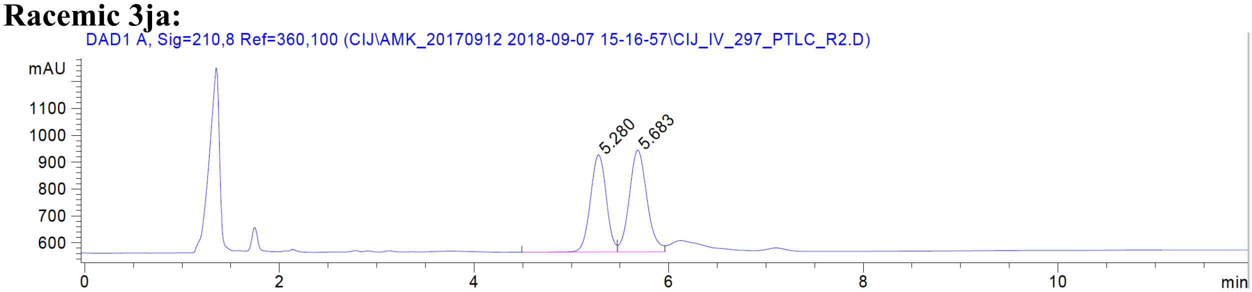
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.925	VV	0.1105	1.41847e4	2109.47583	47.0185
2	3.434	VV	0.1247	1.59837e4	2101.68701	52.9815

Enantioenriched 3ia:



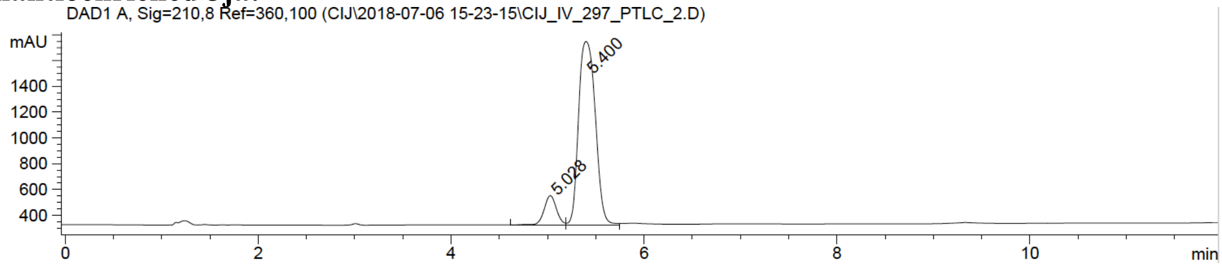
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.944	MM	0.0826	95.35790	19.23708	5.1820
2	3.468	BV	0.0915	1744.83435	301.61948	94.8180

Racemic 3ja:



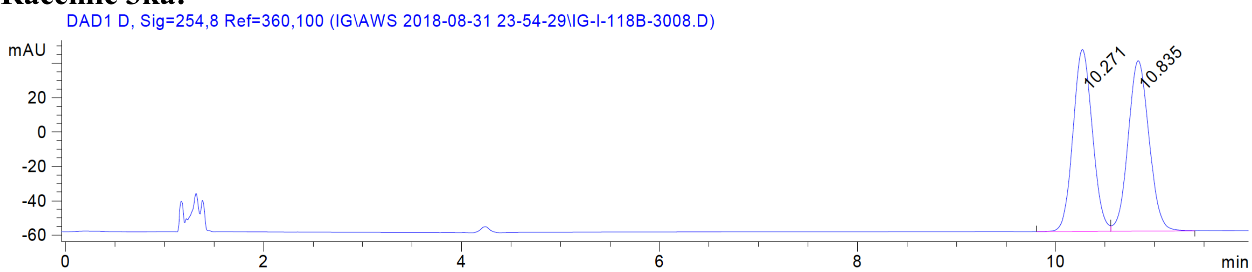
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.280	BV	0.1759	4091.06519	361.79446	46.0818
2	5.683	VV	0.1956	4786.76318	378.41559	53.9182

Enantioenriched 3ja:



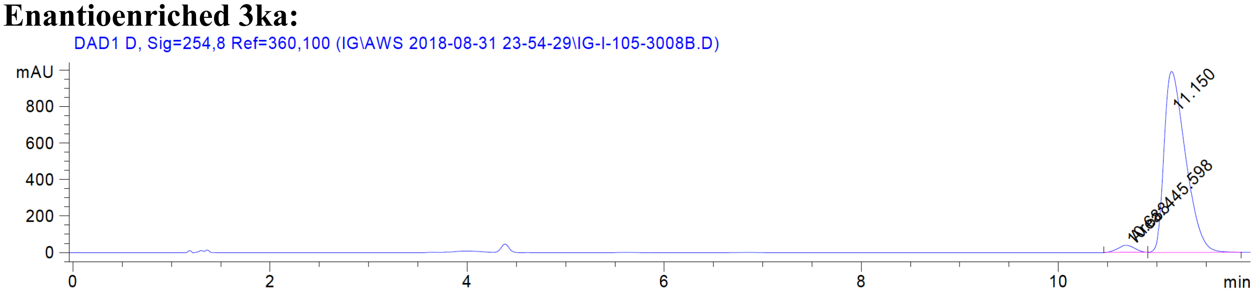
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.028	VV	0.1439	2123.26978	229.58139	10.9278
2	5.400	VV	0.1976	1.73067e4	1425.71802	89.0722

Racemic 3ka:



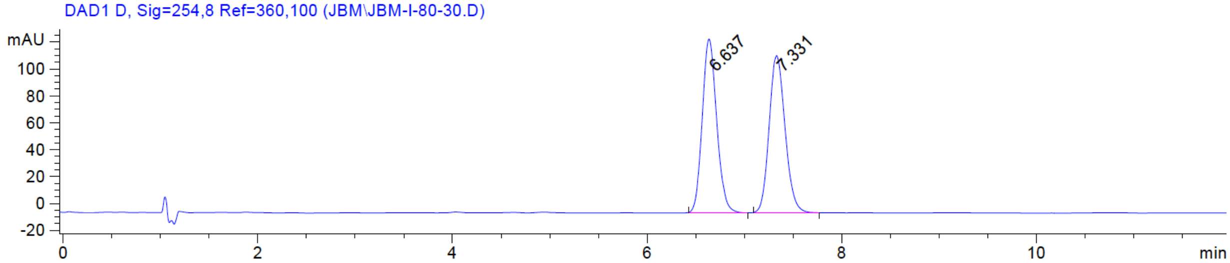
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.271	VV	0.2127	1439.08911	105.81954	49.6707
2	10.835	VV	0.2275	1458.16992	99.20084	50.3293

Enantioenriched 3ka:



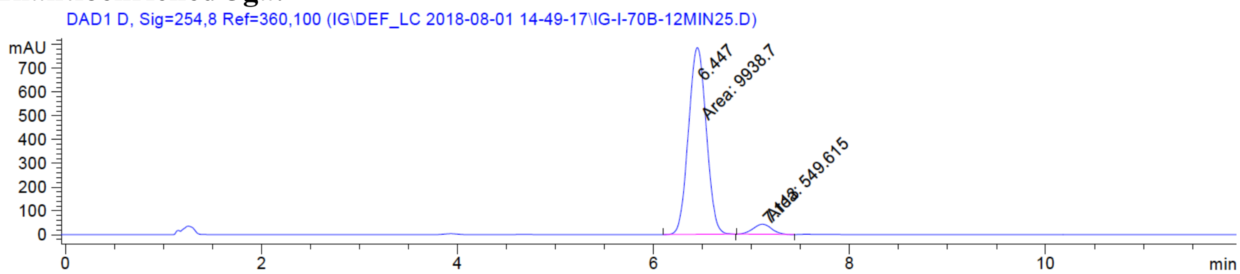
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.688	MM	0.1932	445.59821	38.44982	2.8725
2	11.150	VB	0.2332	1.50668e4	992.22070	97.1275

Racemic 3ga:



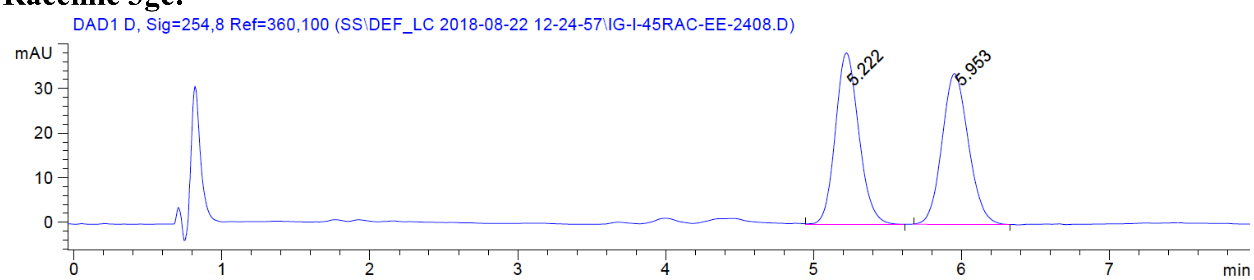
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.637	BB	0.1607	1336.68604	129.16518	50.0423
2	7.331	BB	0.1772	1334.42639	116.91229	49.9577

Enantioenriched 3ga:



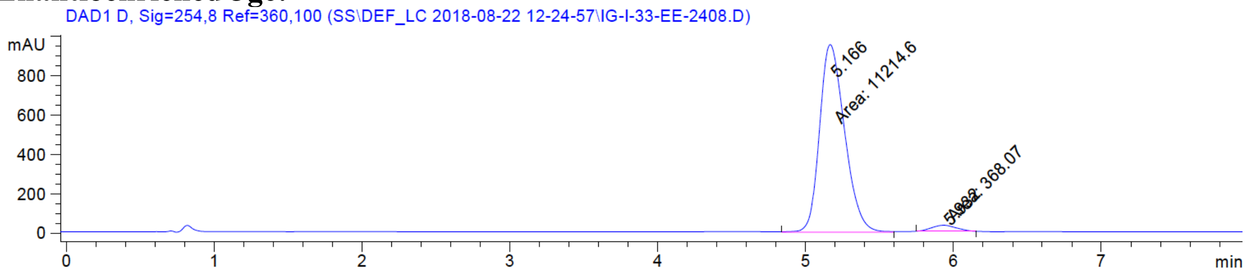
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.447	MM	0.2107	9938.70117	786.14569	94.7597
2	7.113	MM	0.2174	549.61450	42.14084	5.2403

Racemic 3gc:



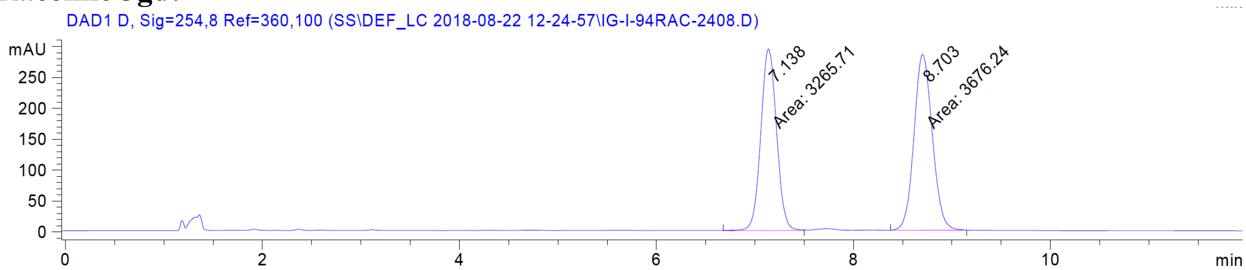
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.222	VB	0.1689	424.83261	38.45545	50.2150
2	5.953	BB	0.1932	421.19498	33.84225	49.7850

Enantioenriched 3gc:



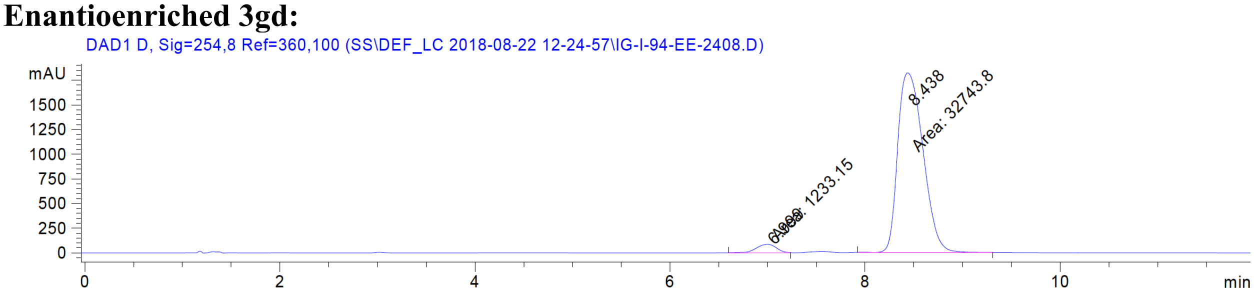
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.166	MM	0.1963	1.12146e4	952.25464	96.8222
2	5.932	MM	0.1985	368.06973	30.90477	3.1778

Racemic 3gd:



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.138	MM	0.1849	3265.71362	294.33276	47.0432
2	8.703	MM	0.2151	3676.23511	284.81070	52.9568

Enantioenriched 3gd:



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.999	MM	0.2375	1233.14587	86.52834	3.6294
2	8.438	MM	0.2999	3.27438e4	1819.75952	96.3706

Crystallographic Data:

Materials and Methods:

For crystal structure determination of ***3ab*:** Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Bruker AXS D8 VENTURE KAPPA diffractometer coupled to a PHOTON 100 CMOS detector with Cu K_α radiation (λ = 1.54178 Å) from an IμS micro-source for the structure of compound P17471. The structure was solved by direct methods using SHELXS[1] and refined against F^2 on all data by full-matrix least squares with SHELXL-2016[1] using established refinement techniques.[1] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms they are linked to (1.5 times for methyl groups).

For crystal structure determination of Pd/**L4** complex: A crystal was mounted on a polyimide MiTeGen loop with STP Oil Treatment and placed under a nitrogen stream. Low temperature (100K) X-ray data were collected with a Bruker AXS D8 VENTURE KAPPA diffractometer running at 50 kV and 1mA (Mo K_α = 0.71073 Å; PHOTON II CPAD detector and Helios focusing multilayer mirror optics). All diffractometer manipulations, including data collection, integration, and scaling were carried out using the Bruker APEX3 software. An absorption correction was applied using SADABS. The space group was determined and the structure solved by intrinsic phasing using XT. Refinement was full-matrix least squares on F^2 using XL. All non-hydrogen atoms were refined using anisotropic displacement parameters. Hydrogen atoms were placed in idealized positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed at 1.2 times (1.5 times for methyl groups) the U_{eq} value of the bonded atom.

References:

1. G. M. Sheldrick, *Acta Cryst.* **1990**, A46, 467.

2. G. M. Sheldrick, *Acta Cryst.* **2015**, C71, 3.
3. P. Müller, *Crystallography Reviews* **2009**, *15*, 57.

X-ray Crystal structure Data for Arylated Product *3ab*: Product ***3ab*** was crystallized from EtOAc in hexanes at ambient temperature *via* slow evaporation.

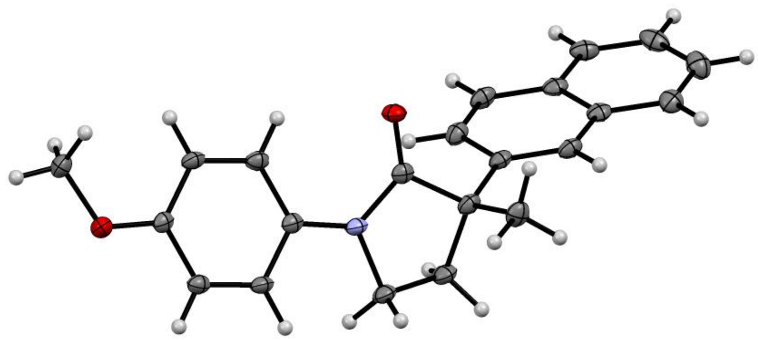


Table 1. Crystal data and structure refinement for V18128.

Identification code	V18128	
Empirical formula	C22 H21 N O2	
Formula weight	331.40	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 6.1796(3) Å	α = 90°.
	b = 7.7424(4) Å	β = 90°.
	c = 34.9981(18) Å	γ = 90°.
Volume	1674.48(15) Å^3	
Z	4	
Density (calculated)	1.315 Mg/m^3	
Absorption coefficient	0.662 mm^{-1}	
F(000)	704	
Crystal size	0.500 x 0.200 x 0.050 mm^3	
Theta range for data collection	2.525 to 74.537°.	
Index ranges	-7<=h<=7, -9<=k<=9, -43<=l<=43	
Reflections collected	15394	

Independent reflections	3423 [R(int) = 0.0559]
Completeness to theta = 67.679°	99.9%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7528 and 0.4845
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3423 / 0 / 228
Goodness-of-fit on F^2	1.142
Final R indices [I>2sigma(I)]	R1 = 0.0419, wR2 = 0.1076
R indices (all data)	R1 = 0.0434, wR2 = 0.1083
Absolute structure parameter	0.17(9)
Extinction coefficient	n/a
Largest diff. peak and hole	0.215 and -0.302 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for V18128. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3102(3)	3420(2)	3552(1)	20(1)
C(1)	4333(3)	4646(3)	3530(1)	16(1)
C(2)	6048(3)	5153(3)	3827(1)	18(1)
C(5)	7930(4)	3889(3)	3763(1)	23(1)
C(21)	5192(3)	5139(3)	4235(1)	17(1)
C(22)	6379(3)	4486(3)	4533(1)	19(1)
C(23)	5648(4)	4624(3)	4918(1)	18(1)
C(24)	6887(4)	3964(3)	5226(1)	23(1)
C(25)	6135(4)	4082(3)	5595(1)	27(1)
C(26)	4144(4)	4895(3)	5669(1)	26(1)
C(27)	2910(4)	5554(3)	5378(1)	23(1)
C(28)	3633(4)	5434(3)	4994(1)	19(1)
C(29)	2412(4)	6077(3)	4681(1)	21(1)
C(30)	3175(4)	5943(3)	4316(1)	21(1)
C(3)	6667(4)	6991(3)	3702(1)	22(1)
C(4)	6306(4)	6988(3)	3270(1)	20(1)
N(1)	4552(3)	5731(2)	3219(1)	17(1)
C(11)	3510(3)	5571(3)	2860(1)	17(1)
C(12)	1606(4)	4621(3)	2809(1)	18(1)
C(13)	597(3)	4557(3)	2453(1)	18(1)
C(14)	1476(3)	5434(3)	2142(1)	16(1)
O(2)	637(3)	5431(2)	1780(1)	21(1)
C(17)	-1408(4)	4619(3)	1726(1)	22(1)
C(15)	3386(4)	6368(3)	2190(1)	18(1)
C(16)	4384(4)	6441(3)	2543(1)	18(1)

Table 3. Bond lengths [Å] and angles [°] for V18128.

O(1)-C(1)	1.219(3)
C(1)-N(1)	1.382(3)
C(1)-C(2)	1.535(3)
C(2)-C(21)	1.525(3)
C(2)-C(5)	1.537(3)
C(2)-C(3)	1.537(3)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(21)-C(22)	1.372(3)
C(21)-C(30)	1.421(3)
C(22)-C(23)	1.423(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.418(3)
C(23)-C(28)	1.420(3)
C(24)-C(25)	1.375(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.407(4)
C(25)-H(25)	0.9500
C(26)-C(27)	1.371(4)
C(26)-H(26)	0.9500
C(27)-C(28)	1.418(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.422(3)
C(29)-C(30)	1.366(3)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(3)-C(4)	1.527(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-N(1)	1.468(3)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
N(1)-C(11)	1.416(3)

C(11)-C(12)	1.399(3)
C(11)-C(16)	1.406(3)
C(12)-C(13)	1.394(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.394(3)
C(13)-H(13)	0.9500
C(14)-O(2)	1.366(3)
C(14)-C(15)	1.395(3)
O(2)-C(17)	1.424(3)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(15)-C(16)	1.382(3)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500

O(1)-C(1)-N(1)	125.7(2)
O(1)-C(1)-C(2)	126.05(19)
N(1)-C(1)-C(2)	108.06(18)
C(21)-C(2)-C(1)	113.12(17)
C(21)-C(2)-C(5)	113.27(18)
C(1)-C(2)-C(5)	105.12(17)
C(21)-C(2)-C(3)	111.11(17)
C(1)-C(2)-C(3)	102.47(18)
C(5)-C(2)-C(3)	111.11(19)
C(2)-C(5)-H(5A)	109.5
C(2)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(2)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(22)-C(21)-C(30)	118.7(2)
C(22)-C(21)-C(2)	121.98(19)
C(30)-C(21)-C(2)	119.13(19)
C(21)-C(22)-C(23)	121.4(2)
C(21)-C(22)-H(22)	119.3

C(23)-C(22)-H(22)	119.3
C(24)-C(23)-C(28)	119.2(2)
C(24)-C(23)-C(22)	121.4(2)
C(28)-C(23)-C(22)	119.4(2)
C(25)-C(24)-C(23)	120.5(2)
C(25)-C(24)-H(24)	119.7
C(23)-C(24)-H(24)	119.7
C(24)-C(25)-C(26)	120.0(2)
C(24)-C(25)-H(25)	120.0
C(26)-C(25)-H(25)	120.0
C(27)-C(26)-C(25)	121.0(2)
C(27)-C(26)-H(26)	119.5
C(25)-C(26)-H(26)	119.5
C(26)-C(27)-C(28)	120.3(2)
C(26)-C(27)-H(27)	119.9
C(28)-C(27)-H(27)	119.9
C(27)-C(28)-C(23)	119.0(2)
C(27)-C(28)-C(29)	122.7(2)
C(23)-C(28)-C(29)	118.3(2)
C(30)-C(29)-C(28)	120.8(2)
C(30)-C(29)-H(29)	119.6
C(28)-C(29)-H(29)	119.6
C(29)-C(30)-C(21)	121.4(2)
C(29)-C(30)-H(30)	119.3
C(21)-C(30)-H(30)	119.3
C(4)-C(3)-C(2)	104.11(17)
C(4)-C(3)-H(3A)	110.9
C(2)-C(3)-H(3A)	110.9
C(4)-C(3)-H(3B)	110.9
C(2)-C(3)-H(3B)	110.9
H(3A)-C(3)-H(3B)	109.0
N(1)-C(4)-C(3)	103.28(17)
N(1)-C(4)-H(4A)	111.1
C(3)-C(4)-H(4A)	111.1
N(1)-C(4)-H(4B)	111.1
C(3)-C(4)-H(4B)	111.1

H(4A)-C(4)-H(4B)	109.1
C(1)-N(1)-C(11)	126.92(18)
C(1)-N(1)-C(4)	112.28(18)
C(11)-N(1)-C(4)	120.13(17)
C(12)-C(11)-C(16)	118.2(2)
C(12)-C(11)-N(1)	122.88(19)
C(16)-C(11)-N(1)	118.90(19)
C(13)-C(12)-C(11)	120.71(19)
C(13)-C(12)-H(12)	119.6
C(11)-C(12)-H(12)	119.6
C(12)-C(13)-C(14)	120.44(19)
C(12)-C(13)-H(13)	119.8
C(14)-C(13)-H(13)	119.8
O(2)-C(14)-C(13)	125.07(19)
O(2)-C(14)-C(15)	115.79(18)
C(13)-C(14)-C(15)	119.1(2)
C(14)-O(2)-C(17)	117.49(17)
O(2)-C(17)-H(17A)	109.5
O(2)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
O(2)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(15)-C(14)	120.52(19)
C(16)-C(15)-H(15)	119.7
C(14)-C(15)-H(15)	119.7
C(15)-C(16)-C(11)	121.0(2)
C(15)-C(16)-H(16)	119.5
C(11)-C(16)-H(16)	119.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for V18128. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	20(1)	16(1)	25(1)	2(1)	1(1)	-6(1)
C(1)	14(1)	14(1)	22(1)	-2(1)	3(1)	3(1)
C(2)	12(1)	18(1)	25(1)	-2(1)	0(1)	0(1)
C(5)	16(1)	26(1)	25(1)	-2(1)	3(1)	5(1)
C(21)	14(1)	14(1)	24(1)	-3(1)	1(1)	-3(1)
C(22)	13(1)	17(1)	26(1)	-3(1)	2(1)	0(1)
C(23)	18(1)	12(1)	26(1)	-3(1)	2(1)	-2(1)
C(24)	23(1)	16(1)	30(1)	-2(1)	-2(1)	1(1)
C(25)	35(1)	20(1)	26(1)	0(1)	-3(1)	2(1)
C(26)	37(1)	15(1)	24(1)	-1(1)	6(1)	-2(1)
C(27)	22(1)	16(1)	31(1)	-3(1)	8(1)	-2(1)
C(28)	18(1)	12(1)	27(1)	-2(1)	2(1)	-3(1)
C(29)	13(1)	18(1)	32(1)	-5(1)	3(1)	2(1)
C(30)	17(1)	18(1)	27(1)	-2(1)	-3(1)	1(1)
C(3)	19(1)	20(1)	28(1)	-1(1)	-1(1)	-7(1)
C(4)	16(1)	18(1)	27(1)	0(1)	-1(1)	-6(1)
N(1)	14(1)	14(1)	23(1)	1(1)	2(1)	-4(1)
C(11)	13(1)	12(1)	24(1)	0(1)	2(1)	2(1)
C(12)	14(1)	16(1)	24(1)	1(1)	4(1)	0(1)
C(13)	12(1)	15(1)	26(1)	-1(1)	3(1)	-1(1)
C(14)	12(1)	13(1)	24(1)	-1(1)	1(1)	3(1)
O(2)	16(1)	23(1)	23(1)	4(1)	-2(1)	-2(1)
C(17)	15(1)	25(1)	27(1)	3(1)	-3(1)	-1(1)
C(15)	15(1)	15(1)	26(1)	3(1)	4(1)	1(1)
C(16)	12(1)	14(1)	28(1)	2(1)	3(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for V18128.

	x	y	z	U(eq)
H(5A)	9143	4205	3929	34
H(5B)	8393	3943	3495	34
H(5C)	7454	2713	3823	34
H(22)	7718	3929	4482	22
H(24)	8248	3437	5177	27
H(25)	6960	3614	5799	32
H(26)	3646	4989	5925	31
H(27)	1565	6093	5434	27
H(29)	1049	6607	4726	25
H(30)	2340	6397	4111	25
H(3A)	5734	7860	3828	27
H(3B)	8198	7243	3764	27
H(4A)	5871	8146	3178	24
H(4B)	7629	6621	3133	24
H(12)	996	4013	3018	22
H(13)	-700	3912	2422	21
H(17A)	-1264	3373	1768	34
H(17B)	-1909	4827	1464	34
H(17C)	-2457	5097	1907	34
H(15)	4007	6959	1979	22
H(16)	5680	7088	2572	22

Table 6. Torsion angles [°] for V18128.

O(1)-C(1)-C(2)-C(21)	-46.6(3)
N(1)-C(1)-C(2)-C(21)	138.58(18)
O(1)-C(1)-C(2)-C(5)	77.5(3)
N(1)-C(1)-C(2)-C(5)	-97.33(19)
O(1)-C(1)-C(2)-C(3)	-166.3(2)
N(1)-C(1)-C(2)-C(3)	18.9(2)
C(1)-C(2)-C(21)-C(22)	138.2(2)
C(5)-C(2)-C(21)-C(22)	18.7(3)
C(3)-C(2)-C(21)-C(22)	-107.2(2)
C(1)-C(2)-C(21)-C(30)	-46.7(3)
C(5)-C(2)-C(21)-C(30)	-166.21(19)
C(3)-C(2)-C(21)-C(30)	67.9(2)
C(30)-C(21)-C(22)-C(23)	-1.0(3)
C(2)-C(21)-C(22)-C(23)	174.10(19)
C(21)-C(22)-C(23)-C(24)	-179.3(2)
C(21)-C(22)-C(23)-C(28)	0.9(3)
C(28)-C(23)-C(24)-C(25)	1.0(3)
C(22)-C(23)-C(24)-C(25)	-178.8(2)
C(23)-C(24)-C(25)-C(26)	-1.4(3)
C(24)-C(25)-C(26)-C(27)	1.1(4)
C(25)-C(26)-C(27)-C(28)	-0.4(3)
C(26)-C(27)-C(28)-C(23)	0.0(3)
C(26)-C(27)-C(28)-C(29)	179.3(2)
C(24)-C(23)-C(28)-C(27)	-0.3(3)
C(22)-C(23)-C(28)-C(27)	179.5(2)
C(24)-C(23)-C(28)-C(29)	-179.7(2)
C(22)-C(23)-C(28)-C(29)	0.1(3)
C(27)-C(28)-C(29)-C(30)	179.6(2)
C(23)-C(28)-C(29)-C(30)	-1.0(3)
C(28)-C(29)-C(30)-C(21)	0.9(3)
C(22)-C(21)-C(30)-C(29)	0.1(3)
C(2)-C(21)-C(30)-C(29)	-175.1(2)
C(21)-C(2)-C(3)-C(4)	-150.71(18)
C(1)-C(2)-C(3)-C(4)	-29.6(2)

C(5)-C(2)-C(3)-C(4)	82.2(2)
C(2)-C(3)-C(4)-N(1)	29.8(2)
O(1)-C(1)-N(1)-C(11)	-4.3(3)
C(2)-C(1)-N(1)-C(11)	170.57(18)
O(1)-C(1)-N(1)-C(4)	-174.9(2)
C(2)-C(1)-N(1)-C(4)	0.0(2)
C(3)-C(4)-N(1)-C(1)	-19.0(2)
C(3)-C(4)-N(1)-C(11)	169.66(18)
C(1)-N(1)-C(11)-C(12)	21.1(3)
C(4)-N(1)-C(11)-C(12)	-168.92(19)
C(1)-N(1)-C(11)-C(16)	-160.7(2)
C(4)-N(1)-C(11)-C(16)	9.3(3)
C(16)-C(11)-C(12)-C(13)	-0.7(3)
N(1)-C(11)-C(12)-C(13)	177.52(19)
C(11)-C(12)-C(13)-C(14)	0.3(3)
C(12)-C(13)-C(14)-O(2)	178.80(19)
C(12)-C(13)-C(14)-C(15)	0.4(3)
C(13)-C(14)-O(2)-C(17)	6.8(3)
C(15)-C(14)-O(2)-C(17)	-174.67(18)
O(2)-C(14)-C(15)-C(16)	-179.30(19)
C(13)-C(14)-C(15)-C(16)	-0.7(3)
C(14)-C(15)-C(16)-C(11)	0.4(3)
C(12)-C(11)-C(16)-C(15)	0.3(3)
N(1)-C(11)-C(16)-C(15)	-177.95(19)

Symmetry transformations used to generate equivalent atoms:

X-ray Crystal structure Data for Pd/L4 complex: The desired product was crystallized from dioxane at ambient temperature under N_2 atmosphere.

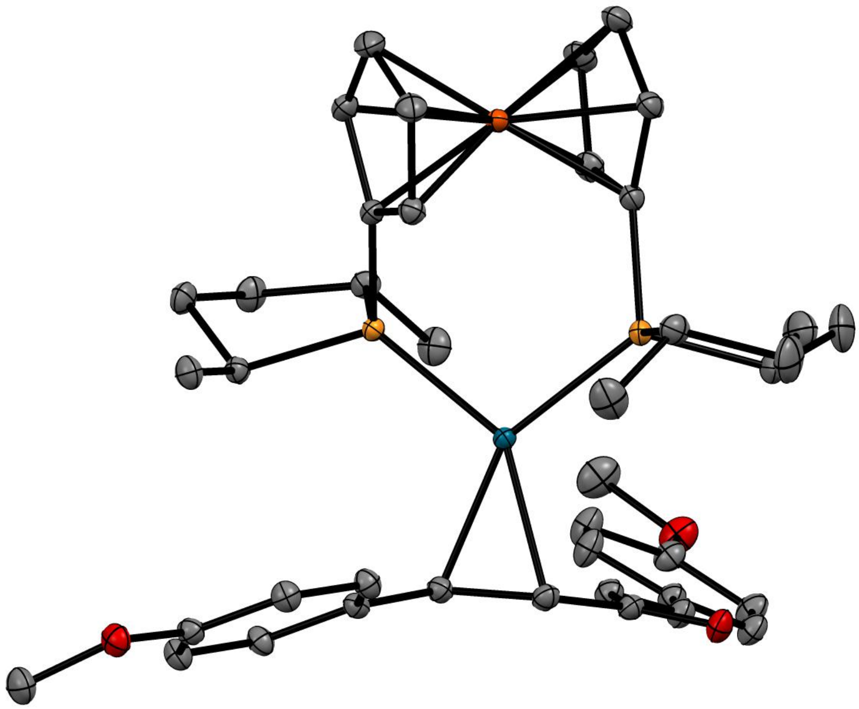


Table 1. Crystal data and structure refinement for v18320.

Identification code	v18320	
Empirical formula	C45 H58 Fe O5 P2 Pd	
Formula weight	903.10	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 11.4377(19) Å	a= 102.706(12)°
	b = 12.9524(19) Å	b= 97.356(16)°
	c = 14.383(3) Å	g = 90.123(13)°
Volume	2060.5(6) $Å^3$	
Z	2	
Density (calculated)	1.456 g/cm^3	
Absorption coefficient	0.911 mm^{-1}	
F(000)	940	

Crystal size	0.22 x 0.21 x 0.16 mm^3
Theta range for data collection	2.463 to 60.741°.
Index ranges	-27 £ h £ 27, -31 £ k £ 31, -35 £ l £ 35
Reflections collected	761601
Independent reflections	122367 [R(int) = 0.0434]
Completeness to theta = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9961 and 0.9523
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	122367 / 3 / 985
Goodness-of-fit on F^2	1.027
Final R indices [I>2sigma(I)]	R1 = 0.0322, wR2 = 0.0704
R indices (all data)	R1 = 0.0492, wR2 = 0.0788
Absolute structure parameter [Flack]	0.004(2)
Extinction coefficient	n/a
Largest diff. peak and hole	4.760 and -2.265 e.Å^{-3}

Table 2. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters (Å^{2}x 10^4) for v18320. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	66302(2)	76561(2)	13310(2)	98(1)
Fe(1)	101781(2)	79532(2)	24779(2)	113(1)
P(1)	77429(2)	92194(2)	18578(2)	107(1)
P(2)	79432(2)	62950(2)	13324(2)	116(1)
O(1)	35675(9)	102732(8)	47613(7)	194(1)
O(2)	47599(9)	54258(7)	-3074(7)	185(1)
O(3)	66651(12)	81266(10)	-47409(8)	245(2)
C(1)	48505(9)	70000(8)	8966(8)	142(1)
C(2)	48417(9)	81293(8)	11766(8)	133(1)
C(3)	44752(8)	86701(8)	21062(7)	129(1)
C(4)	39970(10)	96739(8)	21963(8)	148(1)
C(5)	36668(10)	102337(9)	30659(8)	162(1)
C(6)	38383(10)	97917(9)	38721(8)	150(1)
C(7)	43174(10)	87888(9)	37969(8)	163(1)

C(8)	46244(10)	82352(9)	29252(8)	156(1)
C(9)	30681(14)	112850(11)	48511(11)	233(2)
C(10)	49188(9)	64054(8)	-790(8)	143(1)
C(11)	52127(11)	69958(10)	-8035(9)	156(2)
C(12)	51813(10)	65205(9)	-17361(8)	167(2)
C(13)	55158(10)	69989(9)	-24961(8)	165(2)
C(14)	60938(14)	79891(10)	-23061(9)	221(2)
C(15)	64722(15)	84033(11)	-30348(9)	235(2)
C(16)	62747(12)	78209(10)	-39813(9)	192(2)
C(17)	56621(13)	68470(12)	-41961(9)	217(2)
C(18)	52974(13)	64452(12)	-34600(10)	201(2)
C(19)	72900(20)	91291(14)	-45351(13)	328(3)
C(20)	77475(10)	51844(10)	2496(9)	189(2)
C(21)	84260(14)	53215(14)	-5599(11)	269(3)
C(22)	80131(18)	41884(11)	6354(15)	318(3)
C(23)	74330(20)	43240(11)	15504(16)	345(4)
C(24)	77954(10)	54210(9)	21901(10)	180(2)
C(25)	69277(15)	57873(12)	29127(12)	252(2)
C(26)	84142(10)	98172(9)	9735(8)	159(1)
C(27)	79083(13)	93252(12)	-654(9)	224(2)
C(28)	81897(12)	110239(10)	12363(11)	213(2)
C(29)	79295(11)	113368(9)	22734(10)	195(2)
C(30)	70992(9)	104740(8)	24247(8)	149(1)
C(31)	69132(12)	105680(10)	34682(10)	201(2)
C(32)	89843(8)	91030(7)	27445(7)	125(1)
C(33)	101569(10)	95684(9)	29299(9)	169(2)
C(34)	108213(11)	91287(11)	36489(10)	211(2)
C(35)	100739(14)	83994(13)	39224(10)	209(2)
C(36)	89390(10)	83824(9)	33700(8)	156(1)
C(37)	95133(8)	66319(8)	14991(8)	131(1)
C(38)	104718(9)	63658(8)	21480(9)	158(1)
C(39)	115067(9)	69536(9)	20759(10)	184(2)
C(40)	112081(11)	75730(11)	13823(11)	181(2)
C(41)	99866(9)	73785(9)	10265(8)	151(1)
Pd(1B)	33505(2)	19811(2)	86721(2)	97(1)
Fe(1B)	-1861(2)	16576(2)	75190(2)	115(1)

P(1B)	22117(2)	32635(2)	81434(2)	102(1)
P(2B)	20536(2)	5905(2)	86561(2)	119(1)
O(3B)	32914(10)	54630(9)	147589(7)	216(2)
O(1B)	65209(8)	29095(8)	52638(6)	168(1)
O(2B)	51746(9)	6078(7)	103341(7)	176(1)
C(1B)	51319(9)	15755(8)	91206(8)	135(1)
C(2B)	51356(9)	25618(8)	88273(7)	126(1)
C(3B)	55273(8)	26435(8)	79057(7)	122(1)
C(4B)	59970(9)	36052(8)	78095(7)	139(1)
C(5B)	63509(10)	37319(8)	69447(8)	150(1)
C(6B)	62243(9)	28821(8)	61512(7)	133(1)
C(7B)	57586(10)	19113(8)	62318(7)	146(1)
C(8B)	54175(9)	17930(8)	70964(8)	142(1)
C(9B)	71124(13)	38421(11)	51718(10)	214(2)
C(10B)	50331(9)	14694(8)	100937(7)	132(1)
C(11B)	47387(10)	24269(9)	108040(8)	145(2)
C(12B)	47741(10)	24182(9)	117387(7)	151(1)
C(13B)	44527(9)	32752(9)	124988(7)	146(1)
C(14B)	39291(12)	42022(10)	123235(8)	190(2)
C(15B)	35415(13)	49582(10)	130555(9)	203(2)
C(16B)	36820(10)	48005(9)	139918(8)	167(2)
C(17B)	42476(11)	39065(10)	141926(8)	181(2)
C(18B)	46209(12)	31602(11)	134546(9)	167(2)
C(19B)	26642(16)	63661(13)	145818(12)	274(3)
C(20B)	22290(11)	-705(10)	96843(9)	183(2)
C(21B)	16251(15)	4839(15)	105328(11)	267(3)
C(22B)	18170(18)	-12224(12)	92382(13)	292(3)
C(23B)	23741(17)	-15387(11)	83119(13)	288(3)
C(24B)	21757(10)	-6686(9)	77401(9)	172(2)
C(25B)	31380(15)	-6459(12)	70993(12)	258(2)
C(26B)	15192(9)	42820(8)	90217(8)	143(1)
C(27B)	20266(13)	43219(11)	100653(9)	204(2)
C(28B)	17228(11)	53626(9)	87583(9)	181(2)
C(29B)	19902(10)	51709(8)	77198(9)	165(2)
C(30B)	28477(9)	42602(7)	75925(7)	126(1)
C(31B)	30851(11)	38519(10)	65614(8)	170(2)

C(32B)	9938(8)	26815(7)	72422(7)	121(1)
C(33B)	-1900(9)	30135(9)	70174(9)	161(2)
C(34B)	-8155(10)	21847(10)	63016(9)	187(2)
C(35B)	-348(12)	13412(11)	60707(10)	171(2)
C(36B)	10763(9)	16456(8)	66412(7)	135(1)
C(37B)	4871(9)	8555(8)	85202(8)	134(1)
C(38B)	-5002(9)	2653(8)	79092(9)	157(1)
C(39B)	-15140(10)	9071(10)	79812(10)	184(2)
C(40B)	-11816(12)	18825(11)	86406(11)	187(2)
C(41B)	454(10)	18537(9)	89766(8)	158(1)
O(4)	94593(18)	77923(10)	70024(11)	372(3)
O(5)	92141(13)	56432(10)	60551(11)	329(3)
C(42)	99870(30)	73967(17)	61717(16)	512(7)
C(43)	92730(30)	64705(18)	55379(15)	427(5)
C(44)	86782(15)	60419(12)	68985(14)	280(3)
C(45)	93548(15)	69988(12)	75181(11)	251(2)
O(4B)	8282(12)	21933(9)	33615(11)	297(2)
O(5B)	4502(14)	43546(10)	33786(12)	334(3)
C(42B)	7350(30)	29334(19)	42100(17)	503(7)
C(43B)	-570(30)	38262(18)	40050(20)	561(8)
C(44B)	5650(20)	36016(16)	25116(13)	328(3)
C(45B)	13115(18)	27100(14)	27149(15)	325(3)

Table 3. Bond lengths [Å] and angles [°] for v18320.

Pd(1)-P(1)	2.3154(5)
Pd(1)-P(2)	2.3185(4)
Pd(1)-C(1)	2.1655(11)
Pd(1)-C(2)	2.1351(10)
Fe(1)-C(32)	2.0300(10)
Fe(1)-C(33)	2.0508(11)
Fe(1)-C(34)	2.0606(13)
Fe(1)-C(35)	2.0494(15)
Fe(1)-C(36)	2.0296(12)
Fe(1)-C(37)	2.0370(11)
Fe(1)-C(38)	2.0445(11)
Fe(1)-C(39)	2.0552(12)
Fe(1)-C(40)	2.0616(14)
Fe(1)-C(41)	2.0392(12)
P(1)-C(26)	1.8674(11)
P(1)-C(30)	1.8503(11)
P(1)-C(32)	1.8130(10)
P(2)-C(20)	1.8624(12)
P(2)-C(24)	1.8704(12)
P(2)-C(37)	1.8203(11)
O(1)-C(6)	1.3682(14)
O(1)-C(9)	1.4170(18)
O(2)-C(10)	1.2455(13)
O(3)-C(16)	1.3654(17)
O(3)-C(19)	1.434(2)
C(1)-H(1)	1.0000
C(1)-C(2)	1.4296(15)
C(1)-C(10)	1.4563(16)
C(2)-H(2)	1.0000
C(2)-C(3)	1.4789(15)
C(3)-C(4)	1.3976(14)
C(3)-C(8)	1.4054(15)
C(4)-H(4)	0.9500
C(4)-C(5)	1.3985(15)

C(5)-H(5)	0.9500
C(5)-C(6)	1.3947(16)
C(6)-C(7)	1.3985(16)
C(7)-H(7)	0.9500
C(7)-C(8)	1.3884(16)
C(8)-H(8)	0.9500
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.4910(17)
C(11)-H(11)	0.9500
C(11)-C(12)	1.3431(17)
C(12)-H(12)	0.9500
C(12)-C(13)	1.4591(17)
C(13)-C(14)	1.3974(17)
C(13)-C(18)	1.4043(17)
C(14)-H(14)	0.9500
C(14)-C(15)	1.3913(19)
C(15)-H(15)	0.9500
C(15)-C(16)	1.3936(18)
C(16)-C(17)	1.395(2)
C(17)-H(17)	0.9500
C(17)-C(18)	1.386(2)
C(18)-H(18)	0.9500
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20)	1.0000
C(20)-C(21)	1.520(2)
C(20)-C(22)	1.529(2)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(22)-C(23)	1.525(3)

C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(23)-C(24)	1.537(2)
C(24)-H(24)	1.0000
C(24)-C(25)	1.530(2)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26)	1.0000
C(26)-C(27)	1.5270(18)
C(26)-C(28)	1.5551(18)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(28)-C(29)	1.525(2)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(29)-C(30)	1.5341(16)
C(30)-H(30)	1.0000
C(30)-C(31)	1.5211(18)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-C(33)	1.4378(15)
C(32)-C(36)	1.4368(15)
C(33)-H(33)	0.9500
C(33)-C(34)	1.4251(17)
C(34)-H(34)	0.9500
C(34)-C(35)	1.423(2)
C(35)-H(35)	0.9500
C(35)-C(36)	1.4299(18)
C(36)-H(36)	0.9500
C(37)-C(38)	1.4397(14)
C(37)-C(41)	1.4392(15)

C(38)-H(38)	0.9500
C(38)-C(39)	1.4332(16)
C(39)-H(39)	0.9500
C(39)-C(40)	1.4217(18)
C(40)-H(40)	0.9500
C(40)-C(41)	1.4269(17)
C(41)-H(41)	0.9500
Pd(1B)-P(1B)	2.3119(4)
Pd(1B)-P(2B)	2.3252(5)
Pd(1B)-C(1B)	2.1589(10)
Pd(1B)-C(2B)	2.1417(11)
Fe(1B)-C(32B)	2.0251(10)
Fe(1B)-C(33B)	2.0400(11)
Fe(1B)-C(34B)	2.0628(12)
Fe(1B)-C(35B)	2.0625(14)
Fe(1B)-C(36B)	2.0340(11)
Fe(1B)-C(37B)	2.0307(11)
Fe(1B)-C(38B)	2.0471(11)
Fe(1B)-C(39B)	2.0568(12)
Fe(1B)-C(40B)	2.0612(14)
Fe(1B)-C(41B)	2.0380(12)
P(1B)-C(26B)	1.8685(11)
P(1B)-C(30B)	1.8486(10)
P(1B)-C(32B)	1.8144(11)
P(2B)-C(20B)	1.8553(11)
P(2B)-C(24B)	1.8756(12)
P(2B)-C(37B)	1.8190(11)
O(3B)-C(16B)	1.3655(15)
O(3B)-C(19B)	1.4269(19)
O(1B)-C(6B)	1.3698(13)
O(1B)-C(9B)	1.4226(16)
O(2B)-C(10B)	1.2439(13)
C(1B)-H(1B)	1.0000
C(1B)-C(2B)	1.4309(14)
C(1B)-C(10B)	1.4545(15)
C(2B)-H(2B)	1.0000

C(2B)-C(3B)	1.4773(14)
C(3B)-C(4B)	1.3970(14)
C(3B)-C(8B)	1.4079(14)
C(4B)-H(4B)	0.9500
C(4B)-C(5B)	1.3986(15)
C(5B)-H(5B)	0.9500
C(5B)-C(6B)	1.3927(15)
C(6B)-C(7B)	1.3983(15)
C(7B)-H(7B)	0.9500
C(7B)-C(8B)	1.3892(15)
C(8B)-H(8B)	0.9500
C(9B)-H(9BA)	0.9800
C(9B)-H(9BB)	0.9800
C(9B)-H(9BC)	0.9800
C(10B)-C(11B)	1.4926(16)
C(11B)-H(11B)	0.9500
C(11B)-C(12B)	1.3423(15)
C(12B)-H(12B)	0.9500
C(12B)-C(13B)	1.4605(16)
C(13B)-C(14B)	1.4005(16)
C(13B)-C(18B)	1.4042(16)
C(14B)-H(14B)	0.9500
C(14B)-C(15B)	1.3898(17)
C(15B)-H(15B)	0.9500
C(15B)-C(16B)	1.3953(16)
C(16B)-C(17B)	1.3947(16)
C(17B)-H(17B)	0.9500
C(17B)-C(18B)	1.3820(18)
C(18B)-H(18B)	0.9500
C(19B)-H(19D)	0.9800
C(19B)-H(19E)	0.9800
C(19B)-H(19F)	0.9800
C(20B)-H(20B)	1.0000
C(20B)-C(21B)	1.521(2)
C(20B)-C(22B)	1.536(2)
C(21B)-H(21D)	0.9800

C(21B)-H(21E)	0.9800
C(21B)-H(21F)	0.9800
C(22B)-H(22C)	0.9900
C(22B)-H(22D)	0.9900
C(22B)-C(23B)	1.526(3)
C(23B)-H(23C)	0.9900
C(23B)-H(23D)	0.9900
C(23B)-C(24B)	1.5359(18)
C(24B)-H(24B)	1.0000
C(24B)-C(25B)	1.527(2)
C(25B)-H(25D)	0.9800
C(25B)-H(25E)	0.9800
C(25B)-H(25F)	0.9800
C(26B)-H(26B)	1.0000
C(26B)-C(27B)	1.5281(17)
C(26B)-C(28B)	1.5529(16)
C(27B)-H(27D)	0.9800
C(27B)-H(27E)	0.9800
C(27B)-H(27F)	0.9800
C(28B)-H(28C)	0.9900
C(28B)-H(28D)	0.9900
C(28B)-C(29B)	1.5299(18)
C(29B)-H(29C)	0.9900
C(29B)-H(29D)	0.9900
C(29B)-C(30B)	1.5307(14)
C(30B)-H(30B)	1.0000
C(30B)-C(31B)	1.5203(15)
C(31B)-H(31D)	0.9800
C(31B)-H(31E)	0.9800
C(31B)-H(31F)	0.9800
C(32B)-C(33B)	1.4403(14)
C(32B)-C(36B)	1.4380(14)
C(33B)-H(33B)	0.9500
C(33B)-C(34B)	1.4303(17)
C(34B)-H(34B)	0.9500
C(34B)-C(35B)	1.4219(19)

C(35B)-H(35B)	0.9500
C(35B)-C(36B)	1.4255(16)
C(36B)-H(36B)	0.9500
C(37B)-C(38B)	1.4418(15)
C(37B)-C(41B)	1.4395(15)
C(38B)-H(38B)	0.9500
C(38B)-C(39B)	1.4295(16)
C(39B)-H(39B)	0.9500
C(39B)-C(40B)	1.421(2)
C(40B)-H(40B)	0.9500
C(40B)-C(41B)	1.4279(18)
C(41B)-H(41B)	0.9500
O(4)-C(42)	1.404(3)
O(4)-C(45)	1.406(2)
O(5)-C(43)	1.438(3)
O(5)-C(44)	1.425(2)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(42)-C(43)	1.504(3)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(44)-C(45)	1.504(2)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
O(4B)-C(42B)	1.392(3)
O(4B)-C(45B)	1.422(3)
O(5B)-C(43B)	1.422(3)
O(5B)-C(44B)	1.425(2)
C(42B)-H(42C)	0.9900
C(42B)-H(42D)	0.9900
C(42B)-C(43B)	1.526(4)
C(43B)-H(43C)	0.9900
C(43B)-H(43D)	0.9900
C(44B)-H(44C)	0.9900

C(44B)-H(44D)	0.9900
C(44B)-C(45B)	1.496(3)
C(45B)-H(45C)	0.9900
C(45B)-H(45D)	0.9900

P(1)-Pd(1)-P(2)	106.356(16)
C(1)-Pd(1)-P(1)	143.96(3)
C(1)-Pd(1)-P(2)	109.62(3)
C(2)-Pd(1)-P(1)	105.15(3)
C(2)-Pd(1)-P(2)	148.17(3)
C(2)-Pd(1)-C(1)	38.82(4)
C(32)-Fe(1)-C(33)	41.26(4)
C(32)-Fe(1)-C(34)	69.15(5)
C(32)-Fe(1)-C(35)	69.43(5)
C(32)-Fe(1)-C(37)	113.61(4)
C(32)-Fe(1)-C(38)	146.99(4)
C(32)-Fe(1)-C(39)	170.14(5)
C(32)-Fe(1)-C(40)	130.66(5)
C(32)-Fe(1)-C(41)	107.12(4)
C(33)-Fe(1)-C(34)	40.56(5)
C(33)-Fe(1)-C(39)	131.72(5)
C(33)-Fe(1)-C(40)	109.28(5)
C(34)-Fe(1)-C(40)	117.11(6)
C(35)-Fe(1)-C(33)	68.49(6)
C(35)-Fe(1)-C(34)	40.50(6)
C(35)-Fe(1)-C(39)	116.52(6)
C(35)-Fe(1)-C(40)	148.76(6)
C(36)-Fe(1)-C(32)	41.46(4)
C(36)-Fe(1)-C(33)	69.02(5)
C(36)-Fe(1)-C(34)	68.72(5)
C(36)-Fe(1)-C(35)	41.04(5)
C(36)-Fe(1)-C(37)	106.30(5)
C(36)-Fe(1)-C(38)	114.76(5)
C(36)-Fe(1)-C(39)	148.06(5)
C(36)-Fe(1)-C(40)	169.65(5)
C(36)-Fe(1)-C(41)	130.02(5)

C(37)-Fe(1)-C(33)	147.48(4)
C(37)-Fe(1)-C(34)	169.64(5)
C(37)-Fe(1)-C(35)	129.96(6)
C(37)-Fe(1)-C(38)	41.31(4)
C(37)-Fe(1)-C(39)	69.34(5)
C(37)-Fe(1)-C(40)	69.33(5)
C(37)-Fe(1)-C(41)	41.35(4)
C(38)-Fe(1)-C(33)	170.61(4)
C(38)-Fe(1)-C(34)	131.43(5)
C(38)-Fe(1)-C(35)	108.24(6)
C(38)-Fe(1)-C(39)	40.92(5)
C(38)-Fe(1)-C(40)	68.62(5)
C(39)-Fe(1)-C(34)	109.74(5)
C(39)-Fe(1)-C(40)	40.41(5)
C(41)-Fe(1)-C(33)	115.94(5)
C(41)-Fe(1)-C(34)	148.68(5)
C(41)-Fe(1)-C(35)	169.49(6)
C(41)-Fe(1)-C(38)	68.89(5)
C(41)-Fe(1)-C(39)	68.43(5)
C(41)-Fe(1)-C(40)	40.72(5)
C(26)-P(1)-Pd(1)	119.76(4)
C(30)-P(1)-Pd(1)	122.07(4)
C(30)-P(1)-C(26)	93.82(5)
C(32)-P(1)-Pd(1)	112.02(3)
C(32)-P(1)-C(26)	103.74(5)
C(32)-P(1)-C(30)	102.26(5)
C(20)-P(2)-Pd(1)	116.06(4)
C(20)-P(2)-C(24)	94.15(6)
C(24)-P(2)-Pd(1)	117.30(4)
C(37)-P(2)-Pd(1)	117.98(3)
C(37)-P(2)-C(20)	103.77(5)
C(37)-P(2)-C(24)	104.19(5)
C(6)-O(1)-C(9)	116.77(10)
C(16)-O(3)-C(19)	116.61(12)
Pd(1)-C(1)-H(1)	116.3
C(2)-C(1)-Pd(1)	69.44(6)

C(2)-C(1)-H(1)	116.3
C(2)-C(1)-C(10)	124.48(10)
C(10)-C(1)-Pd(1)	101.73(7)
C(10)-C(1)-H(1)	116.3
Pd(1)-C(2)-H(2)	114.8
C(1)-C(2)-Pd(1)	71.74(6)
C(1)-C(2)-H(2)	114.8
C(1)-C(2)-C(3)	121.34(10)
C(3)-C(2)-Pd(1)	112.06(7)
C(3)-C(2)-H(2)	114.8
C(4)-C(3)-C(2)	119.37(9)
C(4)-C(3)-C(8)	117.78(9)
C(8)-C(3)-C(2)	122.82(9)
C(3)-C(4)-H(4)	119.1
C(3)-C(4)-C(5)	121.76(10)
C(5)-C(4)-H(4)	119.1
C(4)-C(5)-H(5)	120.3
C(6)-C(5)-C(4)	119.41(10)
C(6)-C(5)-H(5)	120.3
O(1)-C(6)-C(5)	124.49(10)
O(1)-C(6)-C(7)	115.82(10)
C(5)-C(6)-C(7)	119.68(10)
C(6)-C(7)-H(7)	119.9
C(8)-C(7)-C(6)	120.27(10)
C(8)-C(7)-H(7)	119.9
C(3)-C(8)-H(8)	119.5
C(7)-C(8)-C(3)	121.09(10)
C(7)-C(8)-H(8)	119.5
O(1)-C(9)-H(9A)	109.5
O(1)-C(9)-H(9B)	109.5
O(1)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
O(2)-C(10)-C(1)	121.48(11)
O(2)-C(10)-C(11)	120.17(10)

C(1)-C(10)-C(11)	118.33(9)
C(10)-C(11)-H(11)	119.1
C(12)-C(11)-C(10)	121.73(11)
C(12)-C(11)-H(11)	119.1
C(11)-C(12)-H(12)	116.7
C(11)-C(12)-C(13)	126.55(11)
C(13)-C(12)-H(12)	116.7
C(14)-C(13)-C(12)	122.56(10)
C(14)-C(13)-C(18)	117.35(12)
C(18)-C(13)-C(12)	120.04(11)
C(13)-C(14)-H(14)	119.1
C(15)-C(14)-C(13)	121.74(11)
C(15)-C(14)-H(14)	119.1
C(14)-C(15)-H(15)	120.2
C(14)-C(15)-C(16)	119.58(12)
C(16)-C(15)-H(15)	120.2
O(3)-C(16)-C(15)	124.30(13)
O(3)-C(16)-C(17)	115.81(11)
C(15)-C(16)-C(17)	119.87(12)
C(16)-C(17)-H(17)	120.2
C(18)-C(17)-C(16)	119.65(11)
C(18)-C(17)-H(17)	120.2
C(13)-C(18)-H(18)	119.1
C(17)-C(18)-C(13)	121.72(13)
C(17)-C(18)-H(18)	119.1
O(3)-C(19)-H(19A)	109.5
O(3)-C(19)-H(19B)	109.5
O(3)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
P(2)-C(20)-H(20)	106.9
C(21)-C(20)-P(2)	115.09(10)
C(21)-C(20)-H(20)	106.9
C(21)-C(20)-C(22)	115.47(12)
C(22)-C(20)-P(2)	104.93(10)

C(22)-C(20)-H(20)	106.9
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	110.5
C(20)-C(22)-H(22B)	110.5
H(22A)-C(22)-H(22B)	108.7
C(23)-C(22)-C(20)	106.14(12)
C(23)-C(22)-H(22A)	110.5
C(23)-C(22)-H(22B)	110.5
C(22)-C(23)-H(23A)	110.0
C(22)-C(23)-H(23B)	110.0
C(22)-C(23)-C(24)	108.63(12)
H(23A)-C(23)-H(23B)	108.3
C(24)-C(23)-H(23A)	110.0
C(24)-C(23)-H(23B)	110.0
P(2)-C(24)-H(24)	108.3
C(23)-C(24)-P(2)	105.00(11)
C(23)-C(24)-H(24)	108.3
C(25)-C(24)-P(2)	115.23(9)
C(25)-C(24)-C(23)	111.52(12)
C(25)-C(24)-H(24)	108.3
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
P(1)-C(26)-H(26)	108.8
C(27)-C(26)-P(1)	112.55(8)
C(27)-C(26)-H(26)	108.8
C(27)-C(26)-C(28)	111.36(10)
C(28)-C(26)-P(1)	106.49(8)

C(28)-C(26)-H(26)	108.8
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.8
C(26)-C(28)-H(28B)	109.8
H(28A)-C(28)-H(28B)	108.2
C(29)-C(28)-C(26)	109.50(9)
C(29)-C(28)-H(28A)	109.8
C(29)-C(28)-H(28B)	109.8
C(28)-C(29)-H(29A)	110.3
C(28)-C(29)-H(29B)	110.3
C(28)-C(29)-C(30)	107.19(10)
H(29A)-C(29)-H(29B)	108.5
C(30)-C(29)-H(29A)	110.3
C(30)-C(29)-H(29B)	110.3
P(1)-C(30)-H(30)	107.9
C(29)-C(30)-P(1)	104.18(8)
C(29)-C(30)-H(30)	107.9
C(31)-C(30)-P(1)	114.89(8)
C(31)-C(30)-C(29)	113.86(10)
C(31)-C(30)-H(30)	107.9
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
P(1)-C(32)-Fe(1)	121.65(5)
C(33)-C(32)-Fe(1)	70.15(6)
C(33)-C(32)-P(1)	131.41(8)
C(36)-C(32)-Fe(1)	69.26(6)
C(36)-C(32)-P(1)	121.32(8)

C(36)-C(32)-C(33)	107.08(9)
Fe(1)-C(33)-H(33)	127.1
C(32)-C(33)-Fe(1)	68.59(6)
C(32)-C(33)-H(33)	125.8
C(34)-C(33)-Fe(1)	70.09(7)
C(34)-C(33)-C(32)	108.35(10)
C(34)-C(33)-H(33)	125.8
Fe(1)-C(34)-H(34)	127.0
C(33)-C(34)-Fe(1)	69.35(7)
C(33)-C(34)-H(34)	125.9
C(35)-C(34)-Fe(1)	69.33(8)
C(35)-C(34)-C(33)	108.24(11)
C(35)-C(34)-H(34)	125.9
Fe(1)-C(35)-H(35)	126.7
C(34)-C(35)-Fe(1)	70.17(8)
C(34)-C(35)-H(35)	126.0
C(34)-C(35)-C(36)	108.05(11)
C(36)-C(35)-Fe(1)	68.74(7)
C(36)-C(35)-H(35)	126.0
Fe(1)-C(36)-H(36)	126.2
C(32)-C(36)-Fe(1)	69.29(6)
C(32)-C(36)-H(36)	125.9
C(35)-C(36)-Fe(1)	70.23(8)
C(35)-C(36)-C(32)	108.27(11)
C(35)-C(36)-H(36)	125.9
P(2)-C(37)-Fe(1)	120.29(5)
C(38)-C(37)-Fe(1)	69.63(6)
C(38)-C(37)-P(2)	131.10(8)
C(41)-C(37)-Fe(1)	69.41(6)
C(41)-C(37)-P(2)	121.81(7)
C(41)-C(37)-C(38)	106.71(9)
Fe(1)-C(38)-H(38)	126.7
C(37)-C(38)-Fe(1)	69.07(6)
C(37)-C(38)-H(38)	125.9
C(39)-C(38)-Fe(1)	69.94(6)
C(39)-C(38)-C(37)	108.25(9)

C(39)-C(38)-H(38)	125.9
Fe(1)-C(39)-H(39)	126.6
C(38)-C(39)-Fe(1)	69.14(6)
C(38)-C(39)-H(39)	125.8
C(40)-C(39)-Fe(1)	70.04(7)
C(40)-C(39)-C(38)	108.33(10)
C(40)-C(39)-H(39)	125.8
Fe(1)-C(40)-H(40)	127.1
C(39)-C(40)-Fe(1)	69.55(8)
C(39)-C(40)-H(40)	126.1
C(39)-C(40)-C(41)	107.85(10)
C(41)-C(40)-Fe(1)	68.80(7)
C(41)-C(40)-H(40)	126.1
Fe(1)-C(41)-H(41)	126.3
C(37)-C(41)-Fe(1)	69.24(6)
C(37)-C(41)-H(41)	125.6
C(40)-C(41)-Fe(1)	70.48(8)
C(40)-C(41)-C(37)	108.86(10)
C(40)-C(41)-H(41)	125.6
P(1B)-Pd(1B)-P(2B)	106.013(16)
C(1B)-Pd(1B)-P(1B)	144.11(3)
C(1B)-Pd(1B)-P(2B)	109.84(3)
C(2B)-Pd(1B)-P(1B)	105.28(3)
C(2B)-Pd(1B)-P(2B)	148.31(3)
C(2B)-Pd(1B)-C(1B)	38.86(4)
C(32B)-Fe(1B)-C(33B)	41.50(4)
C(32B)-Fe(1B)-C(34B)	69.43(4)
C(32B)-Fe(1B)-C(35B)	69.53(5)
C(32B)-Fe(1B)-C(36B)	41.50(4)
C(32B)-Fe(1B)-C(37B)	113.38(4)
C(32B)-Fe(1B)-C(38B)	148.40(4)
C(32B)-Fe(1B)-C(39B)	167.59(5)
C(32B)-Fe(1B)-C(40B)	128.04(5)
C(32B)-Fe(1B)-C(41B)	105.17(5)
C(33B)-Fe(1B)-C(34B)	40.80(5)
C(33B)-Fe(1B)-C(35B)	68.59(5)

C(33B)-Fe(1B)-C(38B)	169.42(4)
C(33B)-Fe(1B)-C(39B)	130.50(5)
C(33B)-Fe(1B)-C(40B)	108.35(5)
C(35B)-Fe(1B)-C(34B)	40.32(6)
C(36B)-Fe(1B)-C(33B)	68.96(5)
C(36B)-Fe(1B)-C(34B)	68.33(5)
C(36B)-Fe(1B)-C(35B)	40.72(5)
C(36B)-Fe(1B)-C(38B)	116.45(5)
C(36B)-Fe(1B)-C(39B)	150.76(5)
C(36B)-Fe(1B)-C(40B)	166.81(5)
C(36B)-Fe(1B)-C(41B)	127.73(4)
C(37B)-Fe(1B)-C(33B)	148.16(5)
C(37B)-Fe(1B)-C(34B)	168.09(5)
C(37B)-Fe(1B)-C(35B)	128.59(5)
C(37B)-Fe(1B)-C(36B)	105.62(4)
C(37B)-Fe(1B)-C(38B)	41.41(4)
C(37B)-Fe(1B)-C(39B)	69.39(5)
C(37B)-Fe(1B)-C(40B)	69.47(5)
C(37B)-Fe(1B)-C(41B)	41.44(4)
C(38B)-Fe(1B)-C(34B)	130.91(5)
C(38B)-Fe(1B)-C(35B)	109.02(5)
C(38B)-Fe(1B)-C(39B)	40.77(5)
C(38B)-Fe(1B)-C(40B)	68.52(5)
C(39B)-Fe(1B)-C(34B)	110.52(5)
C(39B)-Fe(1B)-C(35B)	118.98(6)
C(39B)-Fe(1B)-C(40B)	40.36(6)
C(40B)-Fe(1B)-C(34B)	118.68(6)
C(40B)-Fe(1B)-C(35B)	151.56(6)
C(41B)-Fe(1B)-C(33B)	115.85(5)
C(41B)-Fe(1B)-C(34B)	150.32(5)
C(41B)-Fe(1B)-C(35B)	167.01(5)
C(41B)-Fe(1B)-C(38B)	68.89(5)
C(41B)-Fe(1B)-C(39B)	68.41(5)
C(41B)-Fe(1B)-C(40B)	40.77(5)
C(26B)-P(1B)-Pd(1B)	120.02(4)
C(30B)-P(1B)-Pd(1B)	121.68(3)

C(30B)-P(1B)-C(26B)	93.33(5)
C(32B)-P(1B)-Pd(1B)	111.64(3)
C(32B)-P(1B)-C(26B)	104.46(5)
C(32B)-P(1B)-C(30B)	102.71(5)
C(20B)-P(2B)-Pd(1B)	118.70(4)
C(20B)-P(2B)-C(24B)	93.85(6)
C(24B)-P(2B)-Pd(1B)	116.94(4)
C(37B)-P(2B)-Pd(1B)	117.00(3)
C(37B)-P(2B)-C(20B)	102.84(5)
C(37B)-P(2B)-C(24B)	104.05(5)
C(16B)-O(3B)-C(19B)	117.40(11)
C(6B)-O(1B)-C(9B)	117.40(10)
Pd(1B)-C(1B)-H(1B)	116.4
C(2B)-C(1B)-Pd(1B)	69.92(6)
C(2B)-C(1B)-H(1B)	116.4
C(2B)-C(1B)-C(10B)	124.51(10)
C(10B)-C(1B)-Pd(1B)	100.47(7)
C(10B)-C(1B)-H(1B)	116.4
Pd(1B)-C(2B)-H(2B)	114.6
C(1B)-C(2B)-Pd(1B)	71.22(6)
C(1B)-C(2B)-H(2B)	114.6
C(1B)-C(2B)-C(3B)	121.43(9)
C(3B)-C(2B)-Pd(1B)	113.17(7)
C(3B)-C(2B)-H(2B)	114.6
C(4B)-C(3B)-C(2B)	119.63(9)
C(4B)-C(3B)-C(8B)	117.68(9)
C(8B)-C(3B)-C(2B)	122.67(9)
C(3B)-C(4B)-H(4B)	119.1
C(3B)-C(4B)-C(5B)	121.86(9)
C(5B)-C(4B)-H(4B)	119.1
C(4B)-C(5B)-H(5B)	120.3
C(6B)-C(5B)-C(4B)	119.44(9)
C(6B)-C(5B)-H(5B)	120.3
O(1B)-C(6B)-C(5B)	125.03(10)
O(1B)-C(6B)-C(7B)	115.30(9)
C(5B)-C(6B)-C(7B)	119.67(9)

C(6B)-C(7B)-H(7B)	119.8
C(8B)-C(7B)-C(6B)	120.36(9)
C(8B)-C(7B)-H(7B)	119.8
C(3B)-C(8B)-H(8B)	119.5
C(7B)-C(8B)-C(3B)	120.98(10)
C(7B)-C(8B)-H(8B)	119.5
O(1B)-C(9B)-H(9BA)	109.5
O(1B)-C(9B)-H(9BB)	109.5
O(1B)-C(9B)-H(9BC)	109.5
H(9BA)-C(9B)-H(9BB)	109.5
H(9BA)-C(9B)-H(9BC)	109.5
H(9BB)-C(9B)-H(9BC)	109.5
O(2B)-C(10B)-C(1B)	121.63(10)
O(2B)-C(10B)-C(11B)	120.28(10)
C(1B)-C(10B)-C(11B)	118.08(9)
C(10B)-C(11B)-H(11B)	119.5
C(12B)-C(11B)-C(10B)	121.08(10)
C(12B)-C(11B)-H(11B)	119.5
C(11B)-C(12B)-H(12B)	116.6
C(11B)-C(12B)-C(13B)	126.80(10)
C(13B)-C(12B)-H(12B)	116.6
C(14B)-C(13B)-C(12B)	123.35(9)
C(14B)-C(13B)-C(18B)	117.27(10)
C(18B)-C(13B)-C(12B)	119.32(10)
C(13B)-C(14B)-H(14B)	119.2
C(15B)-C(14B)-C(13B)	121.64(10)
C(15B)-C(14B)-H(14B)	119.2
C(14B)-C(15B)-H(15B)	120.2
C(14B)-C(15B)-C(16B)	119.60(11)
C(16B)-C(15B)-H(15B)	120.2
O(3B)-C(16B)-C(15B)	124.82(11)
O(3B)-C(16B)-C(17B)	115.32(10)
C(17B)-C(16B)-C(15B)	119.85(11)
C(16B)-C(17B)-H(17B)	120.2
C(18B)-C(17B)-C(16B)	119.68(10)
C(18B)-C(17B)-H(17B)	120.2

C(13B)-C(18B)-H(18B)	119.1
C(17B)-C(18B)-C(13B)	121.85(11)
C(17B)-C(18B)-H(18B)	119.1
O(3B)-C(19B)-H(19D)	109.5
O(3B)-C(19B)-H(19E)	109.5
O(3B)-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
P(2B)-C(20B)-H(20B)	107.5
C(21B)-C(20B)-P(2B)	113.94(9)
C(21B)-C(20B)-H(20B)	107.5
C(21B)-C(20B)-C(22B)	115.66(12)
C(22B)-C(20B)-P(2B)	104.30(9)
C(22B)-C(20B)-H(20B)	107.5
C(20B)-C(21B)-H(21D)	109.5
C(20B)-C(21B)-H(21E)	109.5
C(20B)-C(21B)-H(21F)	109.5
H(21D)-C(21B)-H(21E)	109.5
H(21D)-C(21B)-H(21F)	109.5
H(21E)-C(21B)-H(21F)	109.5
C(20B)-C(22B)-H(22C)	110.5
C(20B)-C(22B)-H(22D)	110.5
H(22C)-C(22B)-H(22D)	108.7
C(23B)-C(22B)-C(20B)	105.96(12)
C(23B)-C(22B)-H(22C)	110.5
C(23B)-C(22B)-H(22D)	110.5
C(22B)-C(23B)-H(23C)	109.8
C(22B)-C(23B)-H(23D)	109.8
C(22B)-C(23B)-C(24B)	109.24(12)
H(23C)-C(23B)-H(23D)	108.3
C(24B)-C(23B)-H(23C)	109.8
C(24B)-C(23B)-H(23D)	109.8
P(2B)-C(24B)-H(24B)	108.2
C(23B)-C(24B)-P(2B)	105.69(10)
C(23B)-C(24B)-H(24B)	108.2

C(25B)-C(24B)-P(2B)	114.85(9)
C(25B)-C(24B)-C(23B)	111.55(11)
C(25B)-C(24B)-H(24B)	108.2
C(24B)-C(25B)-H(25D)	109.5
C(24B)-C(25B)-H(25E)	109.5
C(24B)-C(25B)-H(25F)	109.5
H(25D)-C(25B)-H(25E)	109.5
H(25D)-C(25B)-H(25F)	109.5
H(25E)-C(25B)-H(25F)	109.5
P(1B)-C(26B)-H(26B)	108.8
C(27B)-C(26B)-P(1B)	112.91(8)
C(27B)-C(26B)-H(26B)	108.8
C(27B)-C(26B)-C(28B)	110.66(10)
C(28B)-C(26B)-P(1B)	106.62(7)
C(28B)-C(26B)-H(26B)	108.8
C(26B)-C(27B)-H(27D)	109.5
C(26B)-C(27B)-H(27E)	109.5
C(26B)-C(27B)-H(27F)	109.5
H(27D)-C(27B)-H(27E)	109.5
H(27D)-C(27B)-H(27F)	109.5
H(27E)-C(27B)-H(27F)	109.5
C(26B)-C(28B)-H(28C)	109.8
C(26B)-C(28B)-H(28D)	109.8
H(28C)-C(28B)-H(28D)	108.3
C(29B)-C(28B)-C(26B)	109.36(9)
C(29B)-C(28B)-H(28C)	109.8
C(29B)-C(28B)-H(28D)	109.8
C(28B)-C(29B)-H(29C)	110.4
C(28B)-C(29B)-H(29D)	110.4
C(28B)-C(29B)-C(30B)	106.49(9)
H(29C)-C(29B)-H(29D)	108.6
C(30B)-C(29B)-H(29C)	110.4
C(30B)-C(29B)-H(29D)	110.4
P(1B)-C(30B)-H(30B)	107.7
C(29B)-C(30B)-P(1B)	104.37(7)
C(29B)-C(30B)-H(30B)	107.7

C(31B)-C(30B)-P(1B)	114.93(7)
C(31B)-C(30B)-C(29B)	114.09(9)
C(31B)-C(30B)-H(30B)	107.7
C(30B)-C(31B)-H(31D)	109.5
C(30B)-C(31B)-H(31E)	109.5
C(30B)-C(31B)-H(31F)	109.5
H(31D)-C(31B)-H(31E)	109.5
H(31D)-C(31B)-H(31F)	109.5
H(31E)-C(31B)-H(31F)	109.5
P(1B)-C(32B)-Fe(1B)	121.00(5)
C(33B)-C(32B)-Fe(1B)	69.81(6)
C(33B)-C(32B)-P(1B)	132.54(8)
C(36B)-C(32B)-Fe(1B)	69.59(6)
C(36B)-C(32B)-P(1B)	120.70(7)
C(36B)-C(32B)-C(33B)	106.52(9)
Fe(1B)-C(33B)-H(33B)	126.6
C(32B)-C(33B)-Fe(1B)	68.69(6)
C(32B)-C(33B)-H(33B)	125.8
C(34B)-C(33B)-Fe(1B)	70.46(7)
C(34B)-C(33B)-C(32B)	108.40(10)
C(34B)-C(33B)-H(33B)	125.8
Fe(1B)-C(34B)-H(34B)	127.1
C(33B)-C(34B)-Fe(1B)	68.74(6)
C(33B)-C(34B)-H(34B)	125.9
C(35B)-C(34B)-Fe(1B)	69.83(7)
C(35B)-C(34B)-C(33B)	108.28(10)
C(35B)-C(34B)-H(34B)	125.9
Fe(1B)-C(35B)-H(35B)	127.1
C(34B)-C(35B)-Fe(1B)	69.85(8)
C(34B)-C(35B)-H(35B)	126.1
C(34B)-C(35B)-C(36B)	107.81(11)
C(36B)-C(35B)-Fe(1B)	68.56(7)
C(36B)-C(35B)-H(35B)	126.1
Fe(1B)-C(36B)-H(36B)	126.4
C(32B)-C(36B)-Fe(1B)	68.92(6)
C(32B)-C(36B)-H(36B)	125.5

C(35B)-C(36B)-Fe(1B)	70.71(7)
C(35B)-C(36B)-C(32B)	108.99(10)
C(35B)-C(36B)-H(36B)	125.5
P(2B)-C(37B)-Fe(1B)	119.62(5)
C(38B)-C(37B)-Fe(1B)	69.91(6)
C(38B)-C(37B)-P(2B)	131.40(8)
C(41B)-C(37B)-Fe(1B)	69.55(6)
C(41B)-C(37B)-P(2B)	121.55(8)
C(41B)-C(37B)-C(38B)	106.64(9)
Fe(1B)-C(38B)-H(38B)	127.0
C(37B)-C(38B)-Fe(1B)	68.69(6)
C(37B)-C(38B)-H(38B)	125.9
C(39B)-C(38B)-Fe(1B)	69.98(6)
C(39B)-C(38B)-C(37B)	108.26(10)
C(39B)-C(38B)-H(38B)	125.9
Fe(1B)-C(39B)-H(39B)	126.6
C(38B)-C(39B)-Fe(1B)	69.25(6)
C(38B)-C(39B)-H(39B)	125.8
C(40B)-C(39B)-Fe(1B)	69.99(7)
C(40B)-C(39B)-C(38B)	108.48(10)
C(40B)-C(39B)-H(39B)	125.8
Fe(1B)-C(40B)-H(40B)	127.1
C(39B)-C(40B)-Fe(1B)	69.65(7)
C(39B)-C(40B)-H(40B)	126.1
C(39B)-C(40B)-C(41B)	107.81(11)
C(41B)-C(40B)-Fe(1B)	68.74(7)
C(41B)-C(40B)-H(40B)	126.1
Fe(1B)-C(41B)-H(41B)	126.5
C(37B)-C(41B)-Fe(1B)	69.01(6)
C(37B)-C(41B)-H(41B)	125.6
C(40B)-C(41B)-Fe(1B)	70.49(8)
C(40B)-C(41B)-C(37B)	108.80(10)
C(40B)-C(41B)-H(41B)	125.6
C(42)-O(4)-C(45)	110.54(15)
C(44)-O(5)-C(43)	108.75(14)
O(4)-C(42)-H(42A)	109.6

O(4)-C(42)-H(42B)	109.6
O(4)-C(42)-C(43)	110.5(2)
H(42A)-C(42)-H(42B)	108.1
C(43)-C(42)-H(42A)	109.6
C(43)-C(42)-H(42B)	109.6
O(5)-C(43)-C(42)	109.21(19)
O(5)-C(43)-H(43A)	109.8
O(5)-C(43)-H(43B)	109.8
C(42)-C(43)-H(43A)	109.8
C(42)-C(43)-H(43B)	109.8
H(43A)-C(43)-H(43B)	108.3
O(5)-C(44)-H(44A)	109.5
O(5)-C(44)-H(44B)	109.5
O(5)-C(44)-C(45)	110.92(14)
H(44A)-C(44)-H(44B)	108.0
C(45)-C(44)-H(44A)	109.5
C(45)-C(44)-H(44B)	109.5
O(4)-C(45)-C(44)	111.17(14)
O(4)-C(45)-H(45A)	109.4
O(4)-C(45)-H(45B)	109.4
C(44)-C(45)-H(45A)	109.4
C(44)-C(45)-H(45B)	109.4
H(45A)-C(45)-H(45B)	108.0
C(42B)-O(4B)-C(45B)	108.74(14)
C(43B)-O(5B)-C(44B)	108.29(16)
O(4B)-C(42B)-H(42C)	109.6
O(4B)-C(42B)-H(42D)	109.6
O(4B)-C(42B)-C(43B)	110.3(2)
H(42C)-C(42B)-H(42D)	108.1
C(43B)-C(42B)-H(42C)	109.6
C(43B)-C(42B)-H(42D)	109.6
O(5B)-C(43B)-C(42B)	109.5(2)
O(5B)-C(43B)-H(43C)	109.8
O(5B)-C(43B)-H(43D)	109.8
C(42B)-C(43B)-H(43C)	109.8
C(42B)-C(43B)-H(43D)	109.8

H(43C)-C(43B)-H(43D)	108.2
O(5B)-C(44B)-H(44C)	109.5
O(5B)-C(44B)-H(44D)	109.5
O(5B)-C(44B)-C(45B)	110.69(15)
H(44C)-C(44B)-H(44D)	108.1
C(45B)-C(44B)-H(44C)	109.5
C(45B)-C(44B)-H(44D)	109.5
O(4B)-C(45B)-C(44B)	111.24(15)
O(4B)-C(45B)-H(45C)	109.4
O(4B)-C(45B)-H(45D)	109.4
C(44B)-C(45B)-H(45C)	109.4
C(44B)-C(45B)-H(45D)	109.4
H(45C)-C(45B)-H(45D)	108.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^4) for v18320. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	89(1)	90(1)	115(1)	22(1)	17(1)	3(1)
Fe(1)	94(1)	107(1)	142(1)	47(1)	3(1)	0(1)
P(1)	101(1)	91(1)	132(1)	31(1)	16(1)	1(1)
P(2)	105(1)	95(1)	142(1)	17(1)	16(1)	8(1)
O(1)	232(4)	193(3)	158(3)	18(2)	69(3)	17(3)
O(2)	198(3)	130(3)	207(3)	4(2)	16(3)	-28(2)
O(3)	326(5)	258(4)	162(3)	74(3)	30(3)	34(4)
C(1)	117(3)	136(3)	167(4)	22(3)	19(3)	-13(2)
C(2)	114(3)	130(3)	152(3)	26(3)	16(3)	12(2)
C(3)	111(3)	131(3)	150(3)	35(2)	26(2)	17(2)
C(4)	157(3)	144(3)	148(3)	36(3)	25(3)	37(3)
C(5)	176(4)	149(3)	162(3)	31(3)	37(3)	43(3)
C(6)	149(3)	153(3)	151(3)	26(3)	39(3)	3(3)
C(7)	175(4)	166(4)	166(3)	60(3)	43(3)	12(3)
C(8)	165(3)	141(3)	176(4)	54(3)	44(3)	31(3)
C(9)	272(6)	191(5)	228(5)	-3(4)	95(4)	24(4)
C(10)	121(3)	129(3)	167(3)	12(3)	5(2)	-9(2)
C(11)	164(4)	148(4)	147(3)	18(3)	8(3)	2(3)
C(12)	167(4)	157(3)	161(3)	6(3)	11(3)	-17(3)
C(13)	173(4)	161(4)	141(3)	6(3)	-1(3)	-8(3)
C(14)	331(6)	171(4)	143(4)	9(3)	17(4)	-52(4)
C(15)	355(7)	178(4)	162(4)	26(3)	23(4)	-43(4)
C(16)	226(4)	194(4)	149(4)	40(3)	-2(3)	28(3)
C(17)	232(5)	253(5)	138(4)	1(3)	-11(3)	-21(4)
C(18)	206(5)	215(5)	152(4)	-11(4)	-1(4)	-43(4)
C(19)	539(11)	239(6)	257(6)	115(5)	139(7)	40(6)
C(20)	146(3)	162(4)	215(4)	-45(3)	17(3)	14(3)
C(21)	257(6)	302(6)	204(5)	-51(4)	54(4)	20(5)
C(22)	403(8)	123(4)	416(9)	-13(5)	139(7)	37(5)
C(23)	475(10)	114(4)	467(10)	35(5)	194(8)	-45(5)
C(24)	159(4)	150(3)	250(5)	90(3)	24(3)	-3(3)

C(25)	311(6)	218(5)	269(6)	97(4)	115(5)	-15(4)
C(26)	144(3)	174(4)	181(4)	84(3)	28(3)	-5(3)
C(27)	260(5)	266(5)	167(4)	87(4)	36(4)	25(4)
C(28)	224(5)	163(4)	281(5)	125(4)	10(4)	-33(3)
C(29)	191(4)	113(3)	275(5)	49(3)	4(4)	-14(3)
C(30)	139(3)	99(3)	202(4)	25(3)	14(3)	15(2)
C(31)	205(4)	179(4)	205(4)	4(3)	46(3)	30(3)
C(32)	117(3)	111(3)	147(3)	32(2)	7(2)	-2(2)
C(33)	140(3)	125(3)	225(4)	30(3)	-17(3)	-21(3)
C(34)	169(4)	205(4)	221(5)	18(4)	-59(3)	-12(3)
C(35)	238(5)	240(5)	144(4)	58(4)	-22(4)	26(4)
C(36)	168(4)	170(4)	140(3)	54(3)	29(3)	13(3)
C(37)	113(3)	117(3)	164(3)	34(2)	18(2)	13(2)
C(38)	123(3)	130(3)	230(4)	69(3)	1(3)	14(2)
C(39)	109(3)	166(4)	285(5)	74(3)	19(3)	23(3)
C(40)	129(4)	194(4)	243(5)	74(4)	62(3)	3(3)
C(41)	144(3)	165(4)	159(3)	56(3)	39(3)	14(3)
Pd(1B)	89(1)	95(1)	113(1)	34(1)	18(1)	10(1)
Fe(1B)	86(1)	105(1)	157(1)	40(1)	15(1)	5(1)
P(1B)	97(1)	91(1)	124(1)	32(1)	17(1)	11(1)
P(2B)	111(1)	111(1)	146(1)	54(1)	19(1)	3(1)
O(3B)	257(4)	220(4)	150(3)	0(3)	15(3)	52(3)
O(1B)	188(3)	197(3)	128(2)	42(2)	40(2)	-1(2)
O(2B)	204(3)	158(3)	181(3)	77(2)	19(2)	42(2)
C(1B)	123(3)	146(3)	145(3)	45(3)	24(3)	32(2)
C(2B)	115(3)	137(3)	129(3)	32(2)	20(2)	2(2)
C(3B)	106(3)	129(3)	131(3)	28(2)	21(2)	2(2)
C(4B)	149(3)	133(3)	132(3)	17(2)	25(2)	-21(2)
C(5B)	164(3)	143(3)	145(3)	27(3)	33(3)	-24(3)
C(6B)	124(3)	149(3)	129(3)	33(2)	25(2)	9(2)
C(7B)	162(3)	134(3)	137(3)	14(2)	34(3)	7(3)
C(8B)	154(3)	123(3)	151(3)	22(3)	38(3)	-3(3)
C(9B)	226(5)	241(5)	202(4)	90(4)	63(4)	-13(4)
C(10B)	120(3)	142(3)	141(3)	47(2)	12(2)	20(2)
C(11B)	151(3)	161(4)	127(3)	41(3)	16(3)	17(3)
C(12B)	167(3)	162(3)	133(3)	52(3)	22(3)	27(3)

C(13B)	154(3)	163(3)	126(3)	48(3)	16(2)	21(3)
C(14B)	267(5)	176(4)	136(3)	56(3)	21(3)	60(3)
C(15B)	281(5)	178(4)	151(4)	46(3)	15(3)	68(4)
C(16B)	181(4)	172(4)	137(3)	20(3)	6(3)	21(3)
C(17B)	204(4)	218(4)	124(3)	49(3)	9(3)	43(3)
C(18B)	188(4)	191(4)	131(4)	61(3)	13(3)	44(3)
C(19B)	315(7)	227(5)	255(6)	-3(4)	42(5)	89(5)
C(20B)	167(4)	216(4)	198(4)	119(4)	13(3)	-6(3)
C(21B)	276(6)	368(7)	198(5)	130(5)	69(4)	17(5)
C(22B)	394(8)	196(5)	337(7)	156(5)	70(6)	-23(5)
C(23B)	394(8)	147(4)	367(7)	122(5)	104(6)	71(5)
C(24B)	161(4)	126(3)	227(4)	34(3)	30(3)	18(3)
C(25B)	283(6)	187(5)	318(6)	27(4)	141(5)	57(4)
C(26B)	140(3)	134(3)	154(3)	20(2)	37(3)	24(2)
C(27B)	260(5)	204(4)	144(4)	21(3)	40(3)	13(4)
C(28B)	217(4)	113(3)	210(4)	19(3)	45(3)	44(3)
C(29B)	184(4)	119(3)	204(4)	60(3)	28(3)	29(3)
C(30B)	126(3)	107(3)	150(3)	37(2)	25(2)	1(2)
C(31B)	191(4)	176(4)	156(3)	50(3)	49(3)	-4(3)
C(32B)	106(3)	113(3)	148(3)	44(2)	8(2)	8(2)
C(33B)	126(3)	141(3)	227(4)	77(3)	1(3)	21(2)
C(34B)	143(3)	200(4)	221(4)	86(3)	-38(3)	-11(3)
C(35B)	165(4)	182(4)	156(4)	34(3)	-11(3)	-26(3)
C(36B)	129(3)	132(3)	143(3)	29(2)	21(2)	4(2)
C(37B)	120(3)	127(3)	169(3)	54(3)	29(2)	1(2)
C(38B)	124(3)	125(3)	229(4)	54(3)	19(3)	-10(2)
C(39B)	113(3)	173(4)	283(5)	73(3)	46(3)	-4(3)
C(40B)	148(4)	184(4)	247(5)	49(4)	91(3)	31(3)
C(41B)	159(3)	155(4)	171(4)	36(3)	57(3)	15(3)
O(4)	670(10)	150(4)	315(6)	39(4)	158(6)	-10(5)
O(5)	367(6)	179(4)	405(7)	-39(4)	94(5)	-10(4)
C(42)	970(20)	268(8)	317(8)	-2(6)	283(11)	-174(10)
C(43)	691(16)	319(9)	256(7)	7(6)	99(9)	2(9)
C(44)	262(6)	189(5)	392(8)	51(5)	77(5)	-18(4)
C(45)	282(6)	227(5)	242(5)	47(4)	34(4)	-8(4)
O(4B)	300(5)	154(4)	418(7)	63(4)	-24(5)	-24(3)

O(5B)	446(7)	170(4)	428(7)	99(4)	157(6)	71(4)
C(42B)	940(20)	322(9)	310(9)	155(7)	178(11)	7(11)
C(43B)	860(20)	285(8)	670(16)	117(9)	564(16)	157(11)
C(44B)	411(9)	318(7)	255(6)	102(5)	-22(6)	0(6)
C(45B)	335(8)	252(6)	369(8)	-11(6)	115(6)	48(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for v18320.

	x	y	z	U(eq)
H(1)	4535	6602	1338	17
H(2)	4622	8493	636	16
H(4)	3893	9984	1652	18
H(5)	3329	10909	3107	19
H(7)	4433	8485	4345	20
H(8)	4940	7551	2882	19
H(9A)	2347	11236	4393	35
H(9B)	3634	11783	4715	35
H(9C)	2878	11535	5507	35
H(11)	5428	7727	-600	19
H(12)	4914	5800	-1919	20
H(14)	6232	8390	-1662	26
H(15)	6863	9079	-2888	28
H(17)	5496	6461	-4844	26
H(18)	4889	5778	-3611	24
H(19A)	7570	9244	-5121	49
H(19B)	7965	9133	-4040	49
H(19C)	6761	9695	-4303	49
H(20)	6891	5138	-12	23
H(21A)	8220	5991	-741	40
H(21B)	8221	4733	-1117	40
H(21C)	9275	5329	-344	40
H(22A)	7683	3550	158	38
H(22B)	8875	4116	779	38
H(23A)	7689	3765	1896	41
H(23B)	6564	4262	1387	41
H(24)	8590	5372	2556	22
H(25A)	7238	6440	3364	38
H(25B)	6823	5236	3268	38
H(25C)	6166	5921	2569	38

H(26)	9284	9712	1055	19
H(27A)	8036	8562	-202	34
H(27B)	8304	9649	-501	34
H(27C)	7061	9449	-160	34
H(28A)	8893	11429	1160	26
H(28B)	7513	11193	799	26
H(29A)	7550	12032	2390	23
H(29B)	8670	11390	2723	23
H(30)	6314	10532	2047	18
H(31A)	6419	9969	3517	30
H(31B)	6523	11231	3697	30
H(31C)	7678	10565	3862	30
H(33)	10440	10081	2625	20
H(34)	11625	9294	3902	25
H(35)	10291	7994	4390	25
H(36)	8270	7966	3410	19
H(38)	10426	5883	2554	19
H(39)	12263	6933	2431	22
H(40)	11729	8034	1190	22
H(41)	9556	7691	555	18
H(1B)	5460	961	8691	16
H(2B)	5342	3196	9364	15
H(4B)	6078	4190	8347	17
H(5B)	6675	4392	6899	18
H(7B)	5675	1330	5692	17
H(8B)	5106	1128	7142	17
H(9BA)	7262	3768	4505	32
H(9BB)	7864	3947	5598	32
H(9BC)	6619	4453	5350	32
H(11B)	4523	3053	10591	17
H(12B)	5036	1789	11925	18
H(14B)	3837	4317	11689	23
H(15B)	3183	5579	12919	24
H(17B)	4376	3811	14834	22
H(18B)	5002	2552	13598	20
H(19D)	1970	6135	14105	41

H(19E)	3179	6821	14337	41
H(19F)	2413	6763	15182	41
H(20B)	3092	-72	9914	22
H(21D)	1936	1214	10758	40
H(21E)	1776	107	11055	40
H(21F)	774	488	10332	40
H(22C)	2081	-1687	9682	35
H(22D)	946	-1278	9098	35
H(23C)	2014	-2218	7922	35
H(23D)	3230	-1635	8466	35
H(24B)	1402	-823	7318	21
H(25D)	2919	-167	6669	39
H(25E)	3227	-1361	6717	39
H(25F)	3886	-395	7501	39
H(26B)	652	4120	8940	17
H(27D)	1933	3622	10206	31
H(27E)	1606	4842	10495	31
H(27F)	2866	4527	10164	31
H(28C)	1010	5790	8830	22
H(28D)	2392	5759	9198	22
H(29C)	2352	5816	7599	20
H(29D)	1257	4979	7265	20
H(30B)	3616	4525	7989	15
H(31D)	3677	3304	6542	25
H(31E)	3379	4438	6316	25
H(31F)	2353	3551	6162	25
H(33B)	-502	3671	7297	19
H(34B)	-1615	2196	6028	22
H(35B)	-220	691	5617	21
H(36B)	1761	1231	6627	16
H(38B)	-480	-431	7525	19
H(39B)	-2281	714	7645	22
H(40B)	-1686	2452	8825	22
H(41B)	496	2403	9427	19
H(42A)	10795	7172	6356	61
H(42B)	10048	7962	5814	61

H(43A)	8467	6694	5345	51
H(43B)	9643	6207	4949	51
H(44A)	8651	5484	7269	34
H(44B)	7858	6234	6713	34
H(45A)	8945	7281	8083	30
H(45B)	10151	6791	7755	30
H(42C)	1528	3229	4508	60
H(42D)	401	2584	4668	60
H(43C)	-850	3533	3704	67
H(43D)	-143	4334	4615	67
H(44C)	927	3953	2068	39
H(44D)	-226	3319	2194	39
H(45C)	1371	2192	2105	39
H(45D)	2117	2988	2996	39

Table 6. Torsion angles [°] for v18320.

Pd(1)-P(1)-C(26)-C(27)	13.50(10)
Pd(1)-P(1)-C(26)-C(28)	135.79(7)
Pd(1)-P(1)-C(30)-C(29)	-157.26(6)
Pd(1)-P(1)-C(30)-C(31)	77.50(9)
Pd(1)-P(1)-C(32)-Fe(1)	54.66(6)
Pd(1)-P(1)-C(32)-C(33)	145.33(9)
Pd(1)-P(1)-C(32)-C(36)	-28.92(10)
Pd(1)-P(2)-C(20)-C(21)	89.36(10)
Pd(1)-P(2)-C(20)-C(22)	-142.60(9)
Pd(1)-P(2)-C(24)-C(23)	114.76(10)
Pd(1)-P(2)-C(24)-C(25)	-8.34(12)
Pd(1)-P(2)-C(37)-Fe(1)	41.00(7)
Pd(1)-P(2)-C(37)-C(38)	129.54(9)
Pd(1)-P(2)-C(37)-C(41)	-42.27(10)
Pd(1)-C(1)-C(2)-C(3)	-105.19(9)
Pd(1)-C(1)-C(10)-O(2)	117.08(10)
Pd(1)-C(1)-C(10)-C(11)	-61.56(10)
Pd(1)-C(2)-C(3)-C(4)	125.75(9)
Pd(1)-C(2)-C(3)-C(8)	-51.89(12)
Fe(1)-C(32)-C(33)-C(34)	-58.97(9)
Fe(1)-C(32)-C(36)-C(35)	59.62(9)
Fe(1)-C(33)-C(34)-C(35)	-58.57(10)
Fe(1)-C(34)-C(35)-C(36)	-58.46(10)
Fe(1)-C(35)-C(36)-C(32)	-59.03(8)
Fe(1)-C(37)-C(38)-C(39)	-59.14(8)
Fe(1)-C(37)-C(41)-C(40)	59.54(9)
Fe(1)-C(38)-C(39)-C(40)	-59.27(9)
Fe(1)-C(39)-C(40)-C(41)	-58.29(9)
Fe(1)-C(40)-C(41)-C(37)	-58.77(8)
P(1)-C(26)-C(28)-C(29)	20.10(12)
P(1)-C(32)-C(33)-Fe(1)	-115.18(9)
P(1)-C(32)-C(33)-C(34)	-174.15(9)
P(1)-C(32)-C(36)-Fe(1)	115.24(8)
P(1)-C(32)-C(36)-C(35)	174.85(9)

P(2)-C(20)-C(22)-C(23)	41.40(16)
P(2)-C(37)-C(38)-Fe(1)	-112.95(9)
P(2)-C(37)-C(38)-C(39)	-172.09(9)
P(2)-C(37)-C(41)-Fe(1)	113.64(8)
P(2)-C(37)-C(41)-C(40)	173.17(9)
O(1)-C(6)-C(7)-C(8)	-179.87(11)
O(2)-C(10)-C(11)-C(12)	7.81(17)
O(3)-C(16)-C(17)-C(18)	176.06(13)
C(1)-C(2)-C(3)-C(4)	-152.82(10)
C(1)-C(2)-C(3)-C(8)	29.53(15)
C(1)-C(10)-C(11)-C(12)	-173.53(11)
C(2)-C(1)-C(10)-O(2)	-169.93(10)
C(2)-C(1)-C(10)-C(11)	11.43(15)
C(2)-C(3)-C(4)-C(5)	-178.16(10)
C(2)-C(3)-C(8)-C(7)	177.07(10)
C(3)-C(4)-C(5)-C(6)	1.28(17)
C(4)-C(3)-C(8)-C(7)	-0.61(16)
C(4)-C(5)-C(6)-O(1)	178.89(11)
C(4)-C(5)-C(6)-C(7)	-1.15(17)
C(5)-C(6)-C(7)-C(8)	0.16(17)
C(6)-C(7)-C(8)-C(3)	0.73(18)
C(8)-C(3)-C(4)-C(5)	-0.40(16)
C(9)-O(1)-C(6)-C(5)	0.68(18)
C(9)-O(1)-C(6)-C(7)	-179.29(11)
C(10)-C(1)-C(2)-Pd(1)	-90.34(10)
C(10)-C(1)-C(2)-C(3)	164.47(9)
C(10)-C(11)-C(12)-C(13)	-176.13(11)
C(11)-C(12)-C(13)-C(14)	10.3(2)
C(11)-C(12)-C(13)-C(18)	-172.00(13)
C(12)-C(13)-C(14)-C(15)	175.87(14)
C(12)-C(13)-C(18)-C(17)	-176.27(13)
C(13)-C(14)-C(15)-C(16)	-0.1(2)
C(14)-C(13)-C(18)-C(17)	1.5(2)
C(14)-C(15)-C(16)-O(3)	-176.27(14)
C(14)-C(15)-C(16)-C(17)	2.4(2)
C(15)-C(16)-C(17)-C(18)	-2.7(2)

C(16)-C(17)-C(18)-C(13)	0.7(2)
C(18)-C(13)-C(14)-C(15)	-1.8(2)
C(19)-O(3)-C(16)-C(15)	-1.7(2)
C(19)-O(3)-C(16)-C(17)	179.58(14)
C(20)-P(2)-C(24)-C(23)	-7.45(11)
C(20)-P(2)-C(24)-C(25)	-130.55(11)
C(20)-P(2)-C(37)-Fe(1)	170.96(6)
C(20)-P(2)-C(37)-C(38)	-100.51(11)
C(20)-P(2)-C(37)-C(41)	87.68(10)
C(20)-C(22)-C(23)-C(24)	-49.7(2)
C(21)-C(20)-C(22)-C(23)	169.22(14)
C(22)-C(23)-C(24)-P(2)	33.22(18)
C(22)-C(23)-C(24)-C(25)	158.68(15)
C(24)-P(2)-C(20)-C(21)	-147.46(11)
C(24)-P(2)-C(20)-C(22)	-19.41(11)
C(24)-P(2)-C(37)-Fe(1)	-91.06(7)
C(24)-P(2)-C(37)-C(38)	-2.53(12)
C(24)-P(2)-C(37)-C(41)	-174.34(9)
C(26)-P(1)-C(30)-C(29)	-28.30(8)
C(26)-P(1)-C(30)-C(31)	-153.54(9)
C(26)-P(1)-C(32)-Fe(1)	-75.89(7)
C(26)-P(1)-C(32)-C(33)	14.78(12)
C(26)-P(1)-C(32)-C(36)	-159.46(9)
C(26)-C(28)-C(29)-C(30)	-42.57(13)
C(27)-C(26)-C(28)-C(29)	143.14(11)
C(28)-C(29)-C(30)-P(1)	44.45(11)
C(28)-C(29)-C(30)-C(31)	170.36(10)
C(30)-P(1)-C(26)-C(27)	-117.12(9)
C(30)-P(1)-C(26)-C(28)	5.17(8)
C(30)-P(1)-C(32)-Fe(1)	-172.97(6)
C(30)-P(1)-C(32)-C(33)	-82.30(11)
C(30)-P(1)-C(32)-C(36)	103.46(9)
C(32)-P(1)-C(26)-C(27)	139.26(9)
C(32)-P(1)-C(26)-C(28)	-98.45(8)
C(32)-P(1)-C(30)-C(29)	76.66(8)
C(32)-P(1)-C(30)-C(31)	-48.58(9)

C(32)-C(33)-C(34)-Fe(1)	58.05(8)
C(32)-C(33)-C(34)-C(35)	-0.52(15)
C(33)-C(32)-C(36)-Fe(1)	-60.25(8)
C(33)-C(32)-C(36)-C(35)	-0.63(13)
C(33)-C(34)-C(35)-Fe(1)	58.59(10)
C(33)-C(34)-C(35)-C(36)	0.12(16)
C(34)-C(35)-C(36)-Fe(1)	59.36(10)
C(34)-C(35)-C(36)-C(32)	0.32(15)
C(36)-C(32)-C(33)-Fe(1)	59.68(7)
C(36)-C(32)-C(33)-C(34)	0.71(13)
C(37)-P(2)-C(20)-C(21)	-41.75(11)
C(37)-P(2)-C(20)-C(22)	86.30(11)
C(37)-P(2)-C(24)-C(23)	-112.78(11)
C(37)-P(2)-C(24)-C(25)	124.11(10)
C(37)-C(38)-C(39)-Fe(1)	58.60(8)
C(37)-C(38)-C(39)-C(40)	-0.66(14)
C(38)-C(37)-C(41)-Fe(1)	-59.93(8)
C(38)-C(37)-C(41)-C(40)	-0.39(13)
C(38)-C(39)-C(40)-Fe(1)	58.71(9)
C(38)-C(39)-C(40)-C(41)	0.42(15)
C(39)-C(40)-C(41)-Fe(1)	58.76(10)
C(39)-C(40)-C(41)-C(37)	-0.01(14)
C(41)-C(37)-C(38)-Fe(1)	59.79(7)
C(41)-C(37)-C(38)-C(39)	0.64(13)
Pd(1B)-P(1B)-C(26B)-C(27B)	13.94(10)
Pd(1B)-P(1B)-C(26B)-C(28B)	135.68(7)
Pd(1B)-P(1B)-C(30B)-C(29B)	-158.20(6)
Pd(1B)-P(1B)-C(30B)-C(31B)	76.08(8)
Pd(1B)-P(1B)-C(32B)-Fe(1B)	56.33(6)
Pd(1B)-P(1B)-C(32B)-C(33B)	146.60(9)
Pd(1B)-P(1B)-C(32B)-C(36B)	-26.98(9)
Pd(1B)-P(2B)-C(20B)-C(21B)	84.54(10)
Pd(1B)-P(2B)-C(20B)-C(22B)	-148.43(9)
Pd(1B)-P(2B)-C(24B)-C(23B)	123.93(9)
Pd(1B)-P(2B)-C(24B)-C(25B)	0.53(11)
Pd(1B)-P(2B)-C(37B)-Fe(1B)	44.77(7)

Pd(1B)-P(2B)-C(37B)-C(38B)	133.30(9)
Pd(1B)-P(2B)-C(37B)-C(41B)	-38.19(10)
Pd(1B)-C(1B)-C(2B)-C(3B)	-106.22(9)
Pd(1B)-C(1B)-C(10B)-O(2B)	115.92(10)
Pd(1B)-C(1B)-C(10B)-C(11B)	-63.29(10)
Pd(1B)-C(2B)-C(3B)-C(4B)	125.76(9)
Pd(1B)-C(2B)-C(3B)-C(8B)	-52.35(11)
Fe(1B)-C(32B)-C(33B)-C(34B)	-59.46(8)
Fe(1B)-C(32B)-C(36B)-C(35B)	59.54(8)
Fe(1B)-C(33B)-C(34B)-C(35B)	-58.79(9)
Fe(1B)-C(34B)-C(35B)-C(36B)	-58.21(9)
Fe(1B)-C(35B)-C(36B)-C(32B)	-58.44(7)
Fe(1B)-C(37B)-C(38B)-C(39B)	-58.96(8)
Fe(1B)-C(37B)-C(41B)-C(40B)	59.44(9)
Fe(1B)-C(38B)-C(39B)-C(40B)	-59.17(9)
Fe(1B)-C(39B)-C(40B)-C(41B)	-58.31(9)
Fe(1B)-C(40B)-C(41B)-C(37B)	-58.53(8)
P(1B)-C(26B)-C(28B)-C(29B)	20.05(11)