10.1071/CH15504_AC
©CSIRO 2015
Australian Journal of Chemistry 2015, 68 (12), 1854-1858

Supplementary Material

Steric and electronic effects in the synthesis and regioselective hydrolysis of unsymmetrical imides

Jing Katherine Shang, Aysa Pourvali, James R. Cochrane and Craig A. Hutton*

School of Chemistry and Bio21 Molecular Science and Biotechnology Institute, The University of Melbourne, VIC 3010, Australia

**E-mail: chutton@unimelb.edu.au*

Table of contents

Experimental procedures for synthesis of amides **10** and thioamides **11**	S2–S8
$^{1}H/^{13}C$ NMR spectra of imides **13a*y*** and **13b*y***	S9–S30
IR spectra of imides **13a*y*** and **13b*y***	S31–S40

***N*-Benzylacetamide (10a)**

To a solution of benzylamine (2.2 mL, 22.0 mmol) in toluene (5.0 mL) at 0°C was added acetic anhydride (2.2 mL, 23.2 mmol) dropwise. The mixture was stirred under nitrogen for 18 h at room temperature to give the title compound **10a**, which was used in the next step without purification. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33–7.24 (5H, m, ArH), 6.12 (1H, brs, NH), 4.38 (2H, d, *J*=5.7 Hz, CH_2), 1.98 (3H, s, Me); ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.0, 138.3, 128.6, 127.8, 127.4, 43.7, 23.2; MS (ESI) *m/z*: 150 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for $C_9H_{11}NO$ 150.0913 found 150.0929; IR ($CHCl_3$): 3282, 3068, 3031, 2971, 1739, 1638, 1548, 1373, 748, 695 cm^{-1}.

***N*-Benzylpivalamide (10b)**

A solution of benzylamine (1.0 g, 9.3 mmol), triethylamine (2.6 mL, 18.7 mmol) and HBTU (3.0 g, 11.2 mol) in acetonitrile (20 mL) was added pivalic acid (1.6 mL, 14.0 mmol) at room temperature. The resulting mixture was stirred for 3 h at room temperature. The reaction mixture was diluted with ethyl acetate (50 mL) and washed with HCl solution (50 mL, 1 M), saturated aqueous sodium carbonate (30 mL), brine (30 mL) and dried with magnesium sulphate. The solution was concentrated in reduced pressure. Purification by column chromatography (1:4 ethyl acetate/ petroleum spirits) afforded the title compound **10b** (1.32 g, 74%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34–7.24 (5H, m, ArH), 6.00 (1H, brs, NH), 4.84 (2H, d, *J*=5.0 Hz, CH_2), 1.22 (9H, s, *t*Bu); ^{13}C NMR (100 MHz, $CDCl_3$): δ 178.3, 138.7, 128.7, 127.6, 127.4, 43.5, 38.7, 27.6; MS (ESI) *m/z*: 192 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for $C_{12}H_{17}NO$ 192.1383 found 192.1443.

***N*-Benzyltrichloroacetamide (10d)**

To a solution of benzylamine (1.0 mL, 9.5 mmol) and triethylamine (2.6 mL, 18.7 mmol) in dichloromethane (30 mL) was added trichloroacetic anhydride (2.0 mL, 11.2 mmol) at 0°C. The resulting mixture was stirred for 12 h at room temperature. Purification by column chromatography (1:4 ethyl acetate/ petroleum spirits) afforded the title compound **10d** (2.4 g, 98%) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37–7.29 (5H, m, ArH), 7.14 (1H, brs, NH), 4.53 (2H, d, *J*=5.8 Hz, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.0, 136.4, 129.0, 128.1, 127.7, 92.6, 45.3; MS (ESI) *m/z*: 251 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for $C_9H_8Cl_3NO$ 251.9744 found 251.9729; IR ($CHCl_3$): 3319, 3020, 1703, 1520, 1216, 818, 699 cm^{-1}.

***N*-Benzylformamide (10e)**

To a solution of benzylamine (428 mg, 4.0 mmol) and triethylamine (0.7 mL, 4.76 mmol), was added ethyl formate (1.6 mL, 19.8 mmol) at 0°C. The mixture was stirred for 12 h at room temperature. Purification by column chromatography (1:3 ethyl acetate/ petroleum spirits) afforded the title compound **10e** (500 mg, 92%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (1H, s, HCO), 7.36–7.23 (5H, m, ArH), 6.07 (1H, brs, NH), 4.46 (2H, d, *J*=5.7 Hz, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.5, 137.7, 128.6, 127.6, 127.0, 42.0; MS (ESI) *m/z*: 136 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for C_8H_9NO 136.0757, found 136.0762; IR ($CHCl_3$): 3868, 3280, 3033, 1654, 1383, 750, 720, 696 cm^{-1}.

***N*-Benzylbenzamide (10f)**

A solution of benzylamine (1.0 mL, 9.3 mmol), triethylamine (2.6 mL, 18.7 mmol) and HBTU (2.8 g, 9.3 mol) in acetonitrile (40 mL) was added benzoic acid (1.7 g, 14.0 mmol) at room temperature. The resulting mixture was stirred for 3 h at room temperature. Purification by column chromatography (1:3 ethyl acetate/ petroleum spirits) afforded the title compound **10f** (1.9 g, 95%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80–7.26 (10H, m, ArH), 6.46 (1H, brs, NH), 4.65 (2H, d, *J*=5.7 Hz, CH_2); ^{13}C NMR (400 MHz, $CDCl_3$): δ 167.3, 138.2, 134.4, 131.5, 128.8, 128.6, 127.9, 127.6, 126.9, 44.1; MS (ESI) *m/z*: 212 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for $C_{14}H_{13}NO$ 212.1070 found 212.1060; IR ($CHCl_3$): 3307, 3063, 3031, 2971, 1722, 1635, 1603, 1577, 1537, 1490, 692 cm^{-1}.

***N*-Benzyl-4-methoxybenzamide (10g)**

To a solution of benzylamine (1.1 mL, 9.3 mmol) and triethylamine (2.0 mL, 14.0 mmol) in acetonitrile (20 mL), was added p-methoxyl benzoyl chloride (1.5 mL, 11.2 mmol) at 0°C. The mixture was stirred for 12 h at room temperature. Purification by column chromatography (1:4 ethyl acetate/ petroleum spirits) afforded the title compound **10g** (2.0 g, 89%) as a colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78–6.90 (9H, m, ArH), 6.32 (1H, brs, NH), 4.64 (2H, d, *J*=5.7 Hz, CH_2), 3.85 (3H, s, OMe); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.2, 138.4, 128.8, 128.7, 127.9, 127.6, 127.5, 126.6, 113.8, 55.4, 44.1; MS (ESI) *m/z*: 242 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for $C_{15}H_{15}NO_2$ 242.1176 found 242.1172; IR ($CHCl_3$): 3307, 3032, 2929, 2840, 1737, 1630, 1606, 1550, 1505, 1251,1179, 1029, 845 cm^{-1}.

***N*-Benzyl-2,4-dimethoxybenzamide (10h)**

To a solution of benzylamine (1.1 mL, 9.3 mmol) and triethylamine (1.9 mL, 14.0 mmol) in acetonitrile (25 mL), was added 2,4-dimethoxylbenzoylchloride (2.3 g, 11.2 mmol) at 0°C. The mixture was stirred for 12 h at room temperature. Purification by column chromatography (1:1 ethyl acetate/ petroleum spirits) afforded the title compound **10h** (2.3 g, 91.6%) as a colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24–6.47 (8H, m, ArH), 8.10 (1H, brs, NH), 4.68 (2H, d, *J*=5.7 Hz, CH_2), 3.88 (3H, s, OMe), 3.85 (3H, s, OMe); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.2, 163.4, 158.8, 139.0, 134.1, 128.6, 127.5, 127.1, 114.4, 105.3, 98.6, 55.9, 55.5, 51.2; MS (ESI) *m/z*: 272 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for $C_{16}H_{17}NO_3$ 272.1281 found 272.1341; IR ($CHCl_3$): 3403, 2942, 2840, 1737, 1642, 1603, 1528, 1496, 1259, 1166, 1115, 1023, 833, 698 cm^{-1}.

***N*-Benzyl-4-nitrobenzamide (10i)**

To a solution of benzylamine (1.1 mL, 9.3 mmol) and triethylamine (1.9 mL, 14.0 mmol) in acetonitrile (25.0 mL), was added p-nitrobenzoylchloride (2.1 g, 11.2 mmol) at 0°C. The mixture was stirred for 12 h at room temperature. The reaction mixture was filtered through a pad of celite,

washed with DCM (20.0 mL) twice. The crude product **10i** (3.2 g) was isolated as an off-white solid which was used in the next step without purification. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28–7.36 (9H, m, ArH), 6.56 (H, brs, NH), 4.66 (2H, d, *J*=5.6 Hz, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.3, 137.4, 129.0, 128.9, 128.2, 128.1, 128.0, 127.9, 123.8, 44.5; MS (ESI) *m/z*: 257 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for $C_{14}H_{12}N_2O_3$ 257.0921 found 257.0915; IR ($CHCl_3$): 3298, 3032, 2926, 1737, 1643, 1599, 1520, 1344, 699 cm^{-1}.

***N*-Benzyl-2,4-dinitrobenzamide (10j)**

To a solution of benzylamine (0.4 mL, 4.0 mmol) and triethylamine (0.6 mL, 4.0 mmol) in acetonitrile (5.0 mL), was added 2,4-dinitrobenzoylchloride (0.5 g, 2.0 mmol) at 0°C. The mixture was stirred for 12 h at room temperature. The reaction mixture was filtered through a pad of celite, washed with H_2O (5.0 mL) twice. The crude product **10j** (0.27 g) was isolated as a pale yellow solid which was used in the next step without purification. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.91(1H, s, ArH), δ 8.51 (1H, d, *J* = 8.3 Hz, ArH), δ 7.75 (1H, d, *J* = 8.3 Hz, ArH), 7.39–7.33 (5H, m, ArH), 6.08 (1H, brs, NH), 4.67 (2H, m, CH_2).

General Procedure B: Synthesis of thioamides 11 using Lawesson's reagent

A solution of the amide **10** and Lawesson's reagent (0.55 equiv) in tetrahydrofuran (3 mL/mmol) was stirred at 80°C for 18 h, then the solvent was removed under reduced pressure. Purification of the residue by chromatography on silica gave the thioamide **11**.

***N*-Benzylthioacetamide (11a)**[1]

The title compound was prepared from *N*-benzylacetamide **10a** (3.3 g, 24.5 mmol) according to General Procedure B, followed by recrystallization (ether/hexanes) to give **11a** as yellow crystals (3.4 g, 92%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.4–7.32 (5H, m, ArH), 7.30 (1H, brs, NH), 4.82 (2H, d, *J*=5.0 Hz, CH_2), 2.59 (3H, s, Me); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.9, 136.0, 129.0, 128.4,

128.2, 50.6, 34.1; MS (ESI) *m/z*: 166 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for $C_9H_{11}NS$ 166.0685 found 166.0686; IR ($CHCl_3$): 3207, 3066, 2921, 2720, 1951, 1869, 1739, 1586, 1548, 1383, 1340, 1162, 938, 735, 693 cm^{-1}.

_N_-Benzylthiopivalamide (11b)[2]

The title compound was prepared from N-benzylpivalamide **10b** (1.0 g, 5.3 mmol) according to General Procedure B to give the product **11b** (510 mg, 47%) as a yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.57 (1H, brs, NH), 7.35–7.28 (5H, m, ArH), 4.84 (2H, d, *J*=5.0 Hz, CH_2), 1.37 (9H, s, *t*Bu); ^{13}C NMR (100 MHz, $CDCl_3$): δ 213.4, 136.4, 129.0, 128.03, 128.01, 50.6, 44.5, 30.2; MS (ESI) *m/z*: 208 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for $C_{12}H_{17}NS$ 208.1154 found 208.1140; IR ($CHCl_3$): 3320, 3030, 2965, 2867, 1738, 1605, 1517, 1228, 1218, 1103, 956, 819, 734, 695 cm^{-1}.

_N_-Benzyltrichlorothioacetamide (11d)

The title compound was prepared from *N*-benzyltrichloroacetamide **10d** (1.8 g, 7.34 mmol) according to General Procedure B to give the product **11d** (1.0 g, 51.4%) as a yellow solid. ^1H NMR (400 MHz, $CDCl_3$) δ 7.37–7.27 (5H, m, ArH), 7.09 (1H, brs, NH), 4.48 (2H, d, *J*=5.8 Hz, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 136.7, 128.9, 127.9, 127.7, 66.4, 44.2; IR ($CHCl_3$): 3292, 3032, 1672, 1522, 1455, 1213, 811, 746cm^{-1}.

_N_-Benzylthioformamide (11e)[3]

The title compound was prepared from N-benzylformamide **10e** (1.0 g, 7.5 mmol) according to General Procedure B to give the thioamide **11e** (741 mg, 66%) as yellow oil. ^1H NMR (400 MHz, $CDCl_3$): δ 9.49 (1H, s, HCS), 7.55 (1H, brs, NH), 7.37–7.33 (5H, m, ArH), 4.86 (2H, d, *J*=5.0 Hz, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.8, 135.7, 128.9, 128.3, 128.2, 47.5; MS (ESI) *m/z*: 152 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for C_8H_9NS 152.0528 found 152.0529; IR ($CHCl_3$): 3210, 2972, 1714, 1532, 1215, 745, 696, 666 cm^{-1}.

***N*-Benzylthiobenzamide (11f)**[1]

The title compound was prepared from *N*-benzylbenzamide **10f** (1.8 g, 8.8 mmol) according to General Procedure B to give the product **11f** (1.0 g, 50.5%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12–7.35 (10H, m, ArH), 6.36 (1H, brs, NH), 4.99 (2H, d, *J*=5.1 Hz, CH_2); ^{13}C NMR (400 MHz, $CDCl_3$): δ 199.2, 131.2, 130.2, 129.0, 128.5, 128.5, 128.4, 128.2, 126.7, 51.0; MS (ESI) *m/z*: 234 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for $C_{14}H_{13}NS$ 228.0841 found 228.0887; IR ($CHCl_3$): 3222, 3029, 2918, 1956, 1738, 1691, 1603, 1584, 1516, 1377, 940, 769, 690 cm^{-1}.

***N*-Benzyl-4-methoxythiobenzamide (11g)**[1]

The title compound was prepared from *N*-benzyl-4-methoxybenzamide **10g** (1.0 g, 4.3 mmol) according to General Procedure B to give the product **11g** (0.9 g, 83%) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79–6.86 (9H, m, ArH), 7.63 (1H, brs, NH), 5.00 (2H, d, *J*=5.1 Hz, CH_2), 3.83 (3H, s, OMe); ^{13}C NMR (100 MHz, $CDCl_3$): δ 198.0, 162.2, 136.4, 133.9, 129.0, 128.5, 128.4, 128.2, 113.7, 55.5, 51.0; MS (ESI) *m/z*: 258 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for $C_{15}H_{15}NOS$ 258.0947 found 258.0980; IR ($CHCl_3$): 3241, 3029, 2931, 2837, 2553, 2050, 1739, 1602, 1575, 1525, 1498, 1249, 1172, 1027, 940, 834, 733, 695 cm^{-1}.

***N*-Benzyl-2,4-dimethoxythiobenzamide (11h)**

The title compound was prepared from *N*-benzyl-2,4-dimethoxybenzamide **10h** (2.0 g, 7.5 mmol) according to General Procedure B to give the product **11h** (2.1 g, 97%) as a yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.60 (1H, brs, NH), 8.66–6.42 (8H, m, ArH), 5.06 (2H, d, *J*=4.9 Hz, CH_2), 3.84 (3H, s, OMe), 3.82 (3H, s, OMe); ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.4, 163.3, 157.0, 137.6, 136.9, 128.8, 127.9, 127.8, 120.0, 105.5, 98.4, 56.0, 55.6, 51.2; MS (ESI) *m/z*: 288 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for $C_{16}H_{17}NO_2S$ 288.1053 found 288.1076; IR ($CHCl_3$): 3325, 3004, 2940, 2837, 1737, 1604, 1568, 1530, 1495, 1453, 1252, 1206, 1140, 1022 cm^{-1}.

***N*-Benzyl-4-nitrothiobenzamide (11i)**[4]

A solution of *N*-Benzyl-4-nitrobenzamide **10i** (2.0 g, 7.8 mmol) and Lawesson's reagent (1.7 g, 4.3 mol) in toluene (20 mL) was heated at 110°C for 16 h. Purification by column chromatography (1:3 ethyl acetate/ petroleum spirits) gave the product **11i** (1.4 g, 62.2%) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24–7.39 (9H, m, ArH), 4.99 (2H, d, *J*=5.04 Hz, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): δ 178.9, 147.4, 129.2, 128.6, 128.5, 127.8, 127.7, 123.8, 120.3, 51.4; MS (ESI) *m/z*: 273 [$(M+H)^+$, 100%); HRMS (ESI) calcd. for $C_{14}H_{12}N_2O_2S$ 273.0692 found 273.0695; IR ($CHCl_3$): 2971, 1739, 1602, 1522, 1347 cm^{-1}.

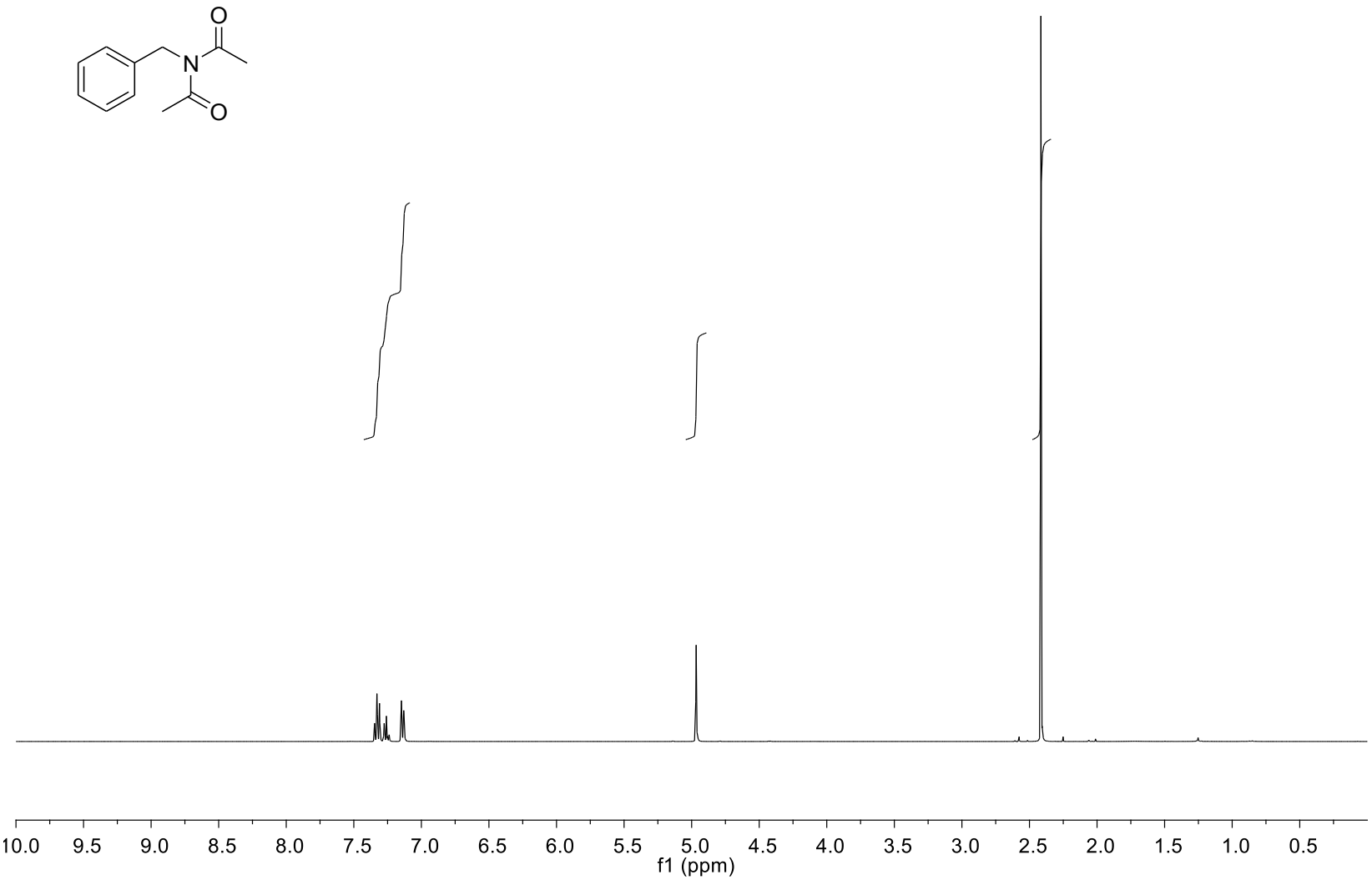
***N*-Benzyl-2,4-dinitrothiobenzamide (11j)**

A solution of *N*-Benzyl-2,4-dinitrobenzamide **10j** (0.27 g, 0.9 mmol) and Lawesson's reagent (0.2 g, 0.5 mol) in toluene (10 mL) was heated at 110°C for 16 h. Purification by column chromatography (1:2 ethyl acetate/ petroleum spirits) gave the product **11j** (0.15 g, 60.0%) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.86(1H, s, ArH), δ 8.50 (1H, d, *J* = 8.3 Hz, ArH), δ 7.70 (1H, d, *J* = 8.3 Hz, ArH), 7.41–7.30 (5H, m, ArH), 4.98 (2H, m, CH_2).

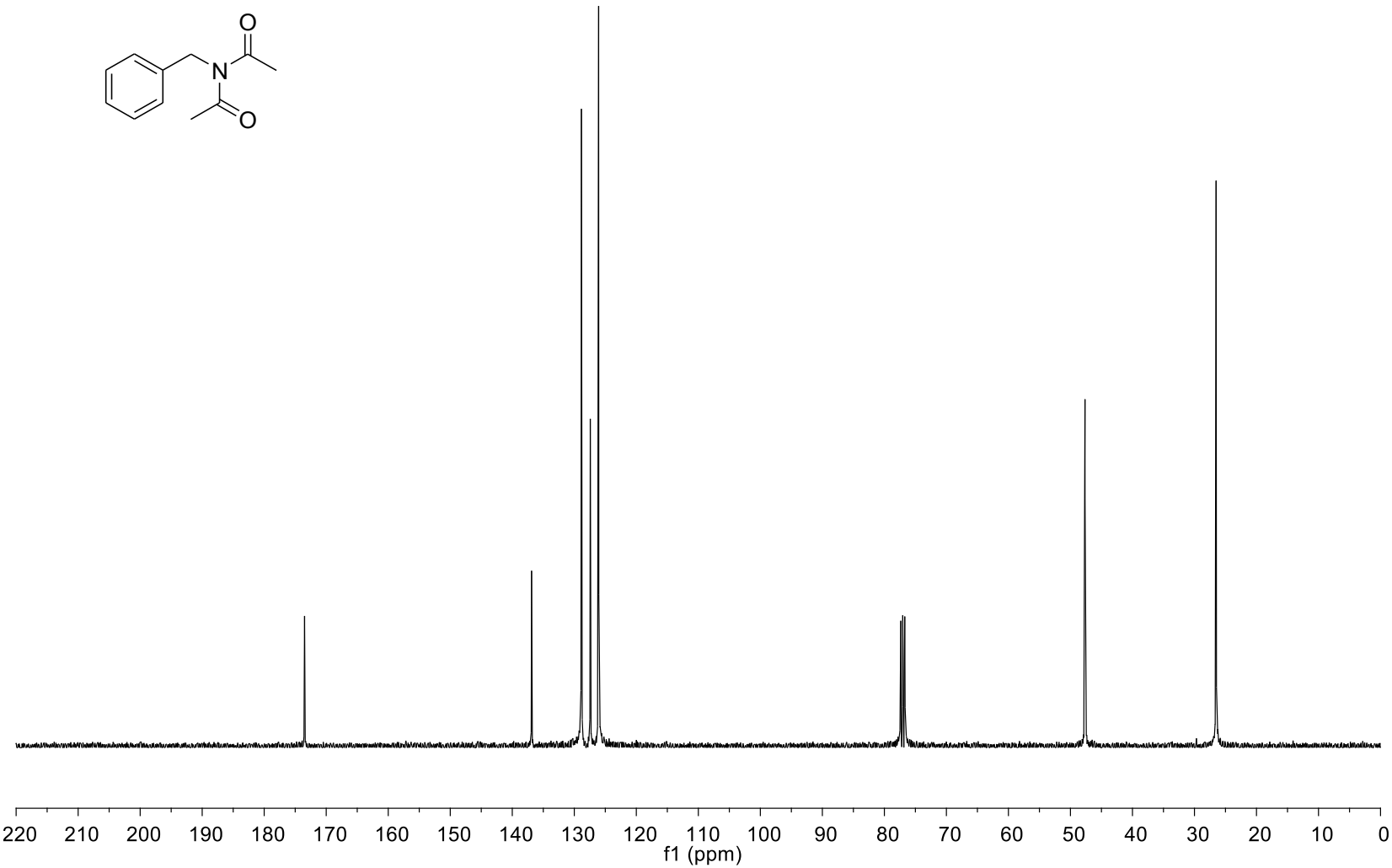
References

(1) Shibahara, F.; Sugiura, R.; Murai, T. *Org. Lett.* **2009**, *11*, 3064.
(2) Gade, T.; Streek, M.; VoB, J. *Chem. Ber.* **1992**, 125, 127.
(3) Ramazani, A.; Joo, S. W.; Nasrabadi, F. Z. *Turk. J. Chem.* **2013**, *37*, 405.
(4) Movassagh, B.; Lakouraj, M. M.; Ghodratl, K. *Synth. Commun.* **2000**, *30*, 2353.

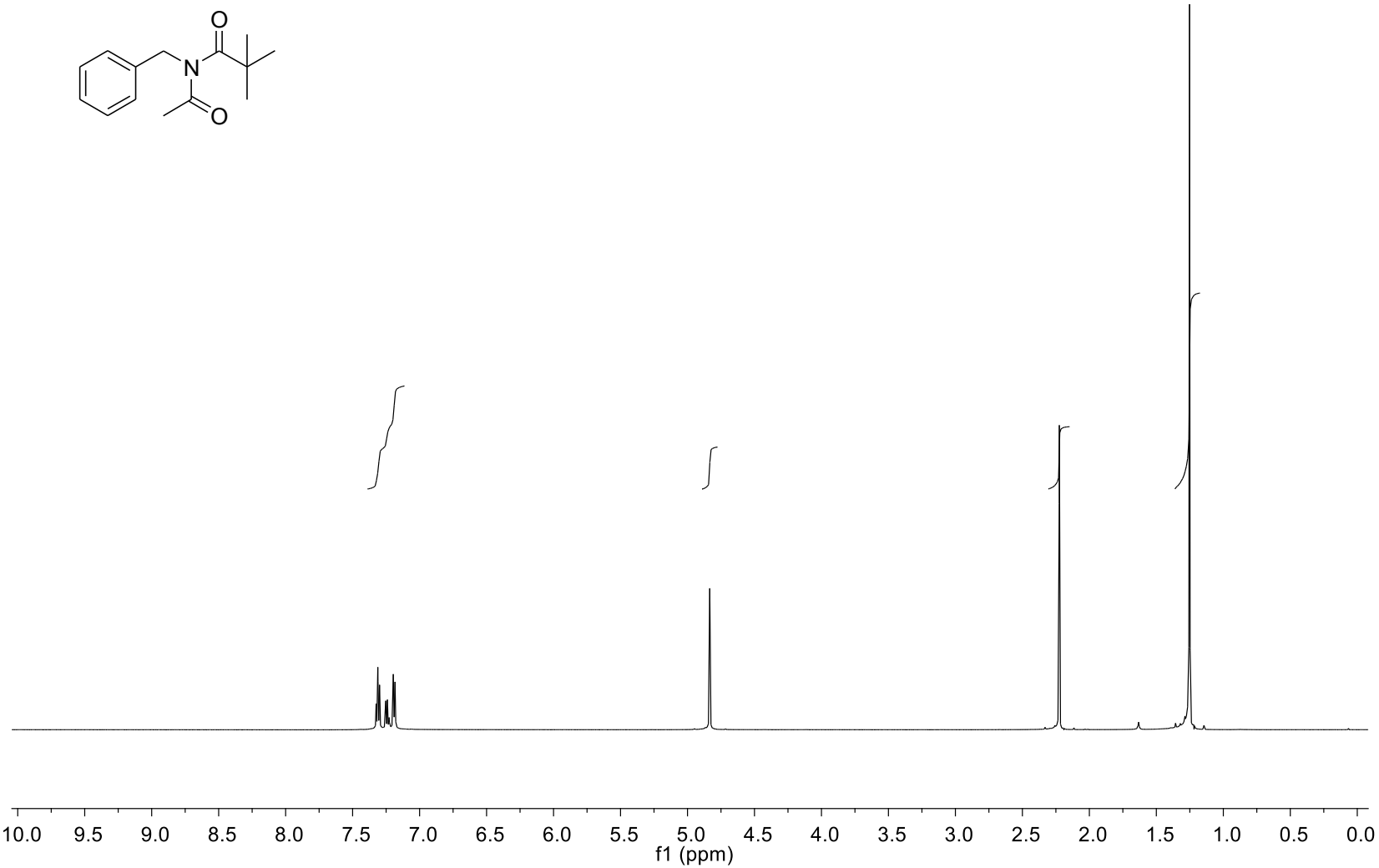
13aa: ^{1}H NMR ($CDCl_3$, 400 MHz)



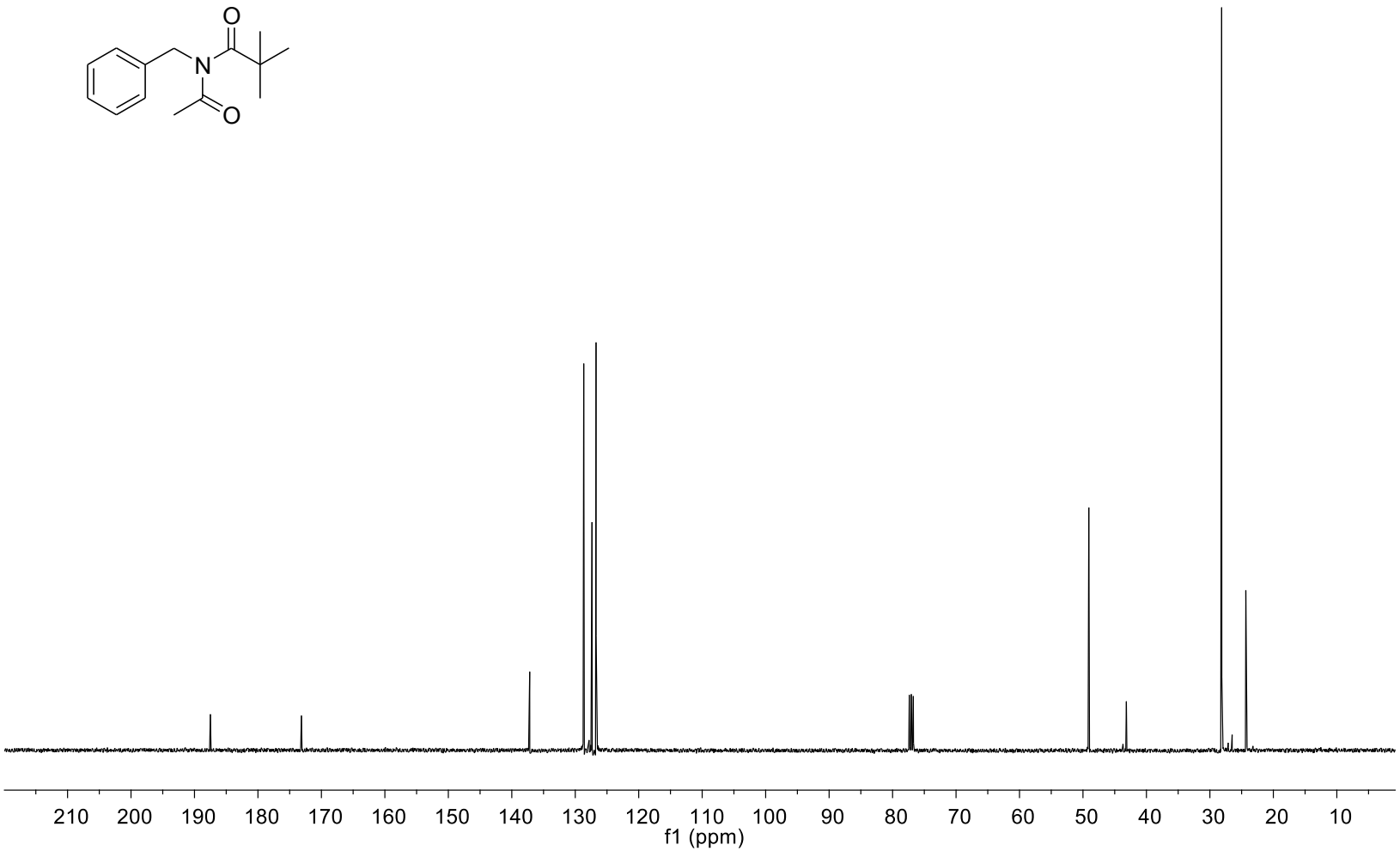
13aa: ^{13}C NMR ($CDCl_3$, 100 MHz)



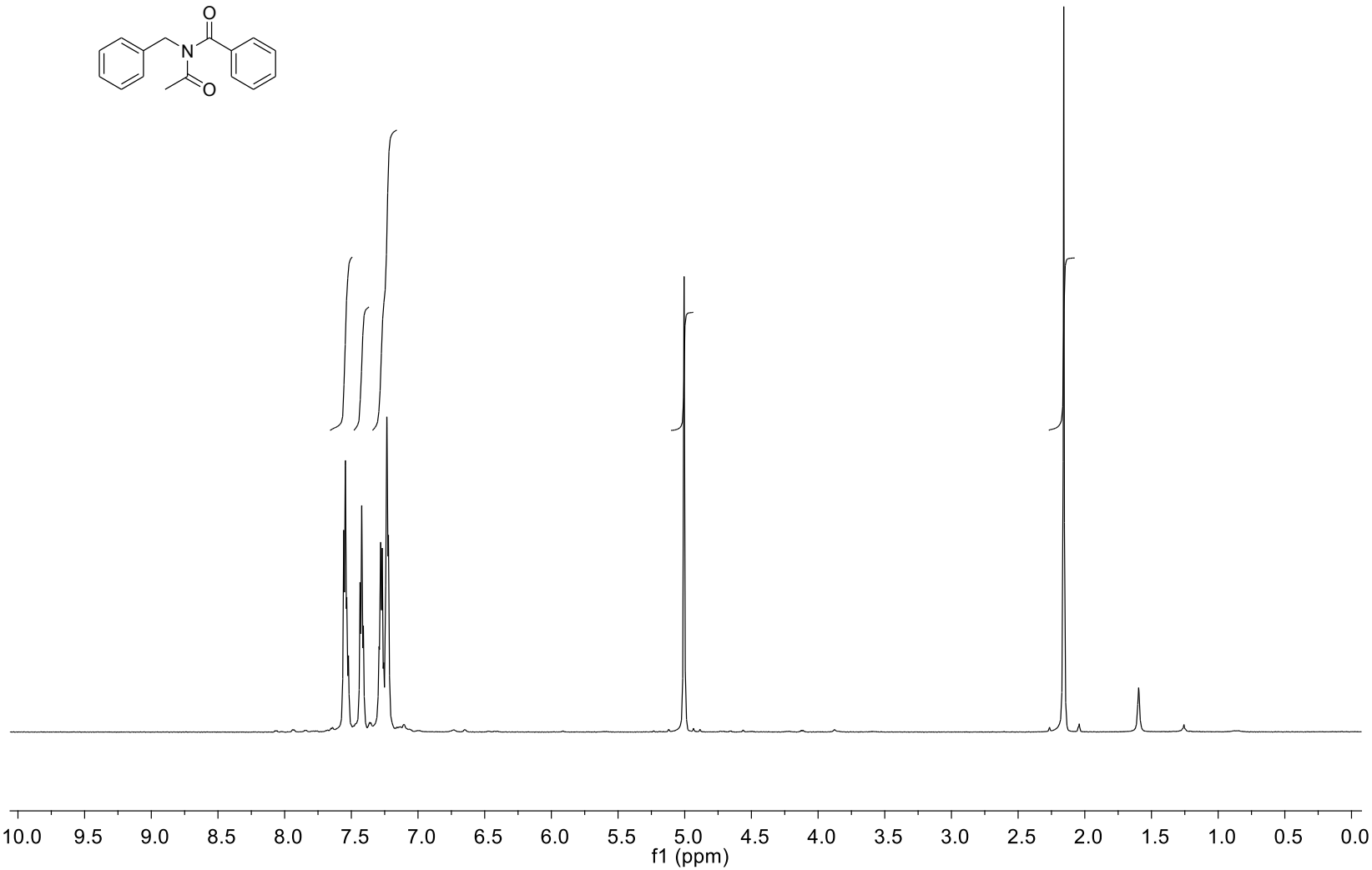
13ab: ^{1}H NMR ($CDCl_3$, 400 MHz)



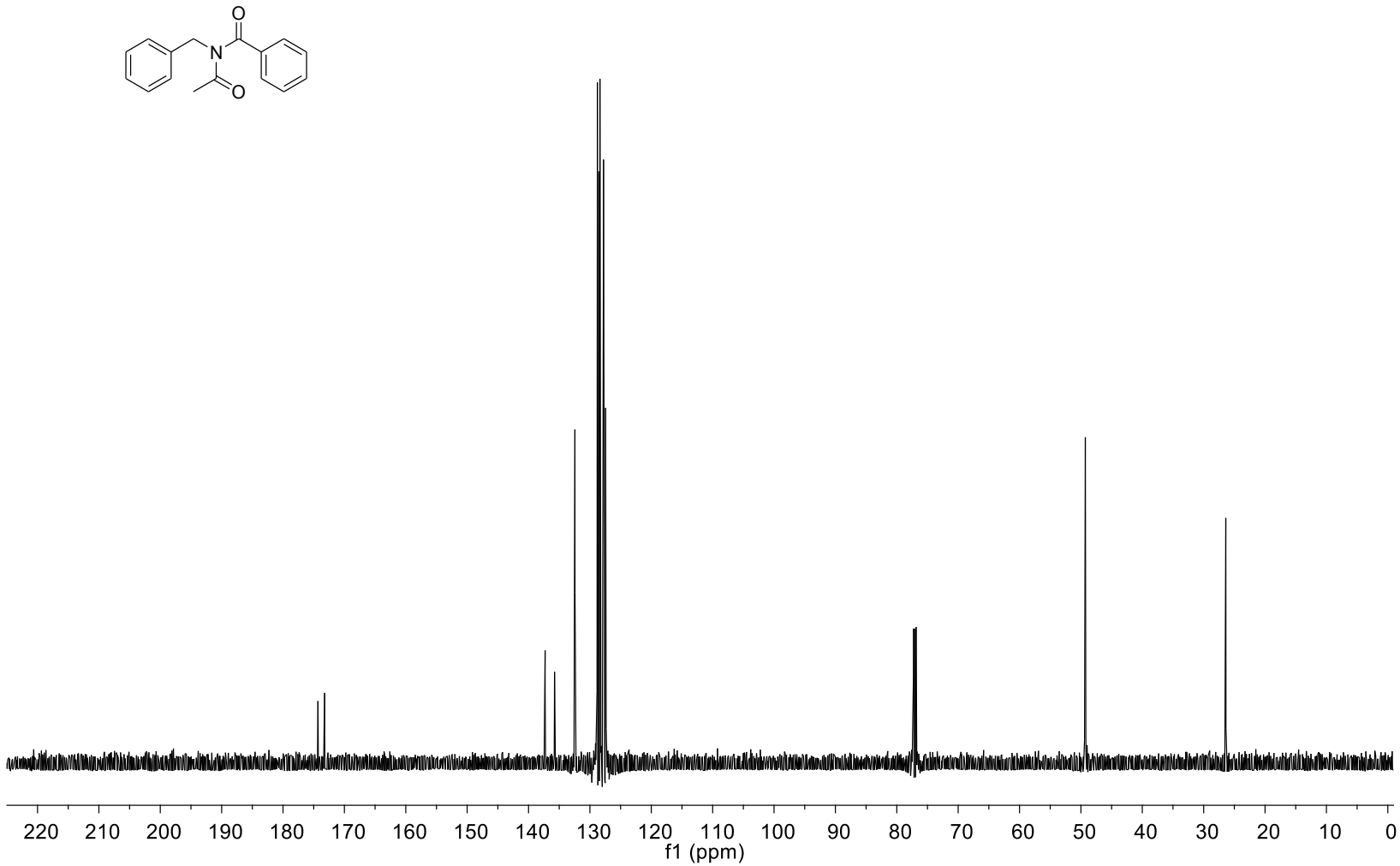
13ab: ^{13}C NMR ($CDCl_3$, 100 MHz)



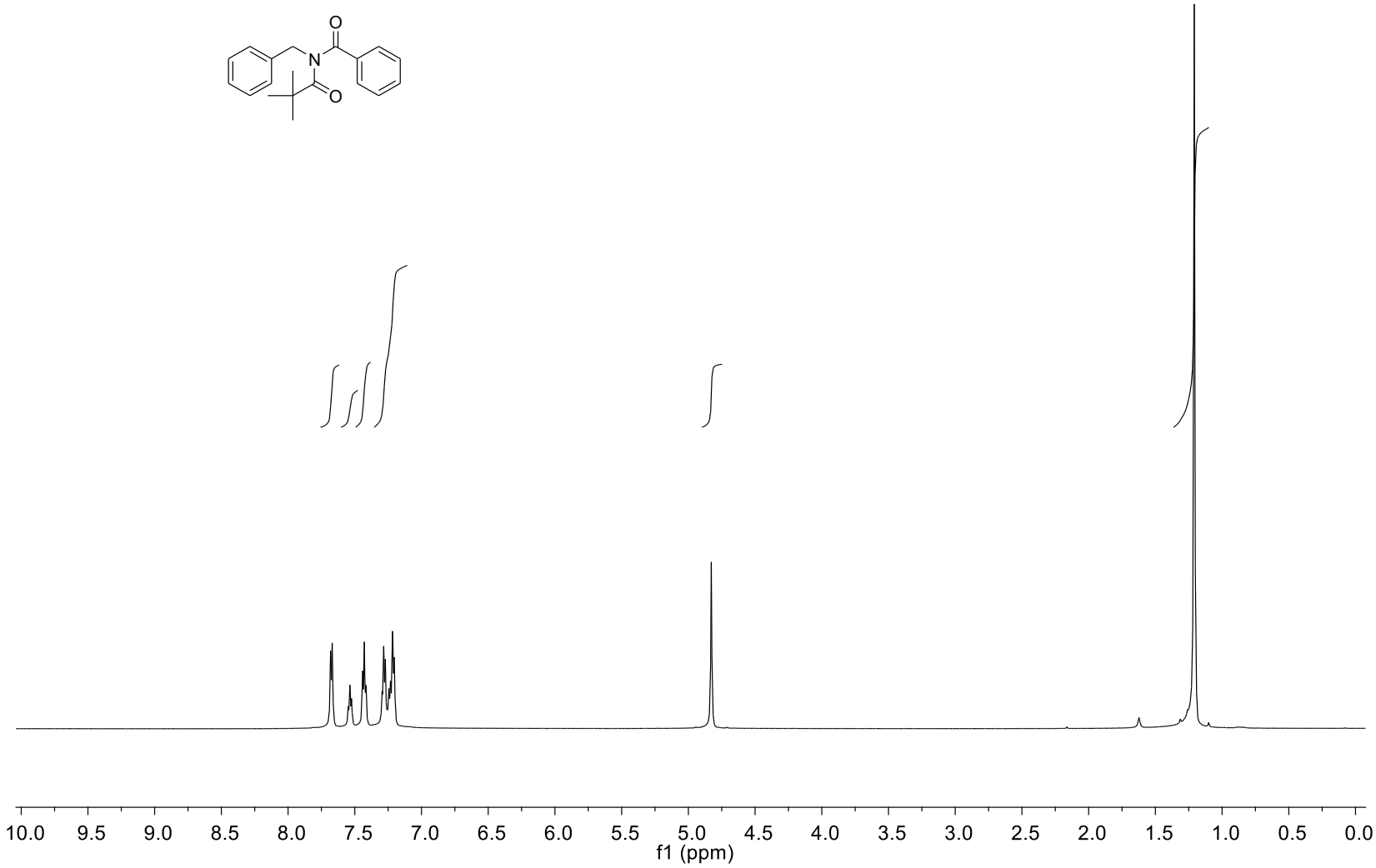
13af: ^{1}H NMR ($CDCl_3$, 400 MHz)



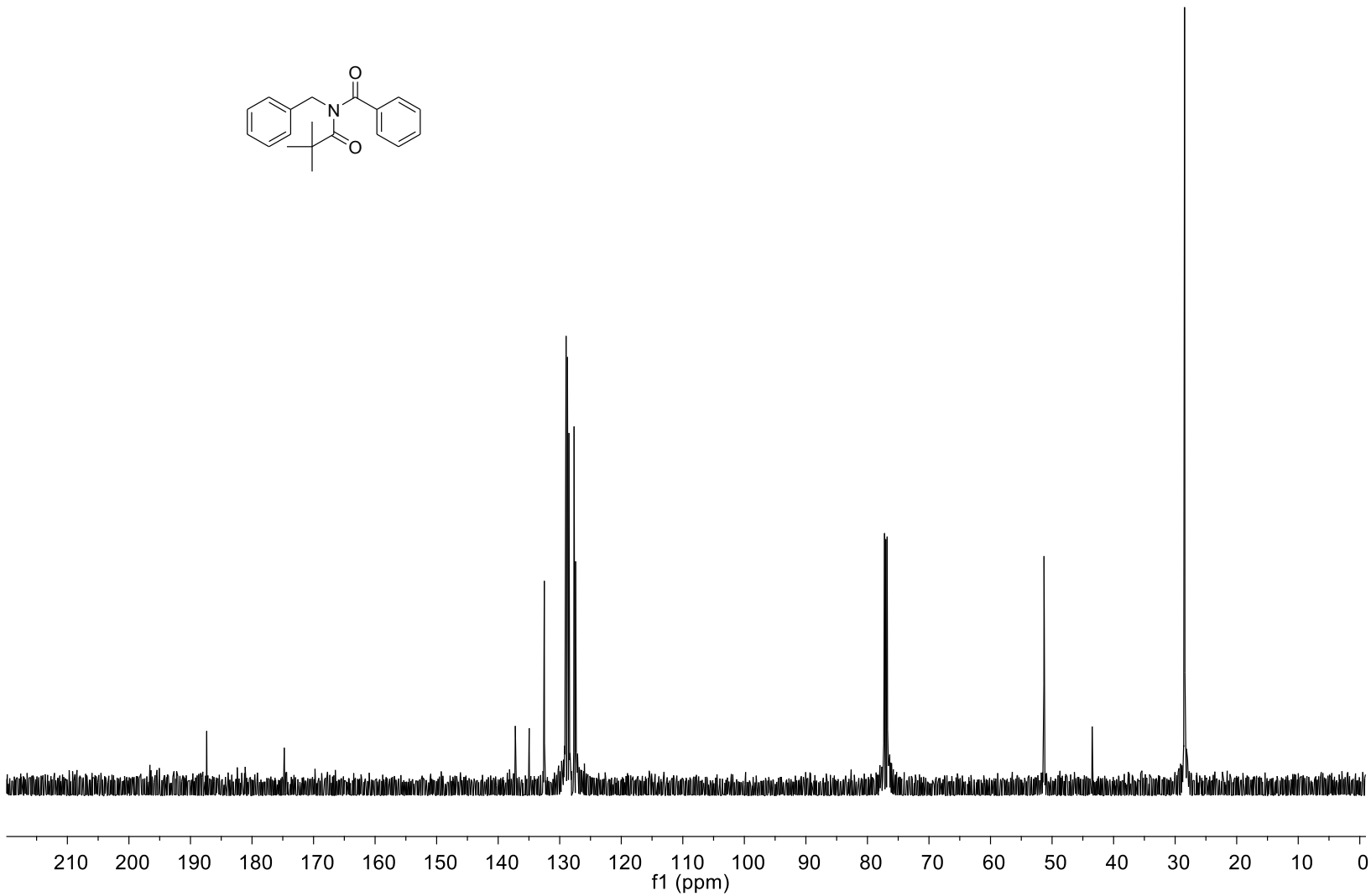
13af: ^{13}C NMR ($CDCl_3$, 100 MHz)



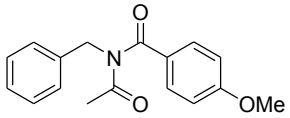
13bf: ^{1}H NMR ($CDCl_3$, 400 MHz)

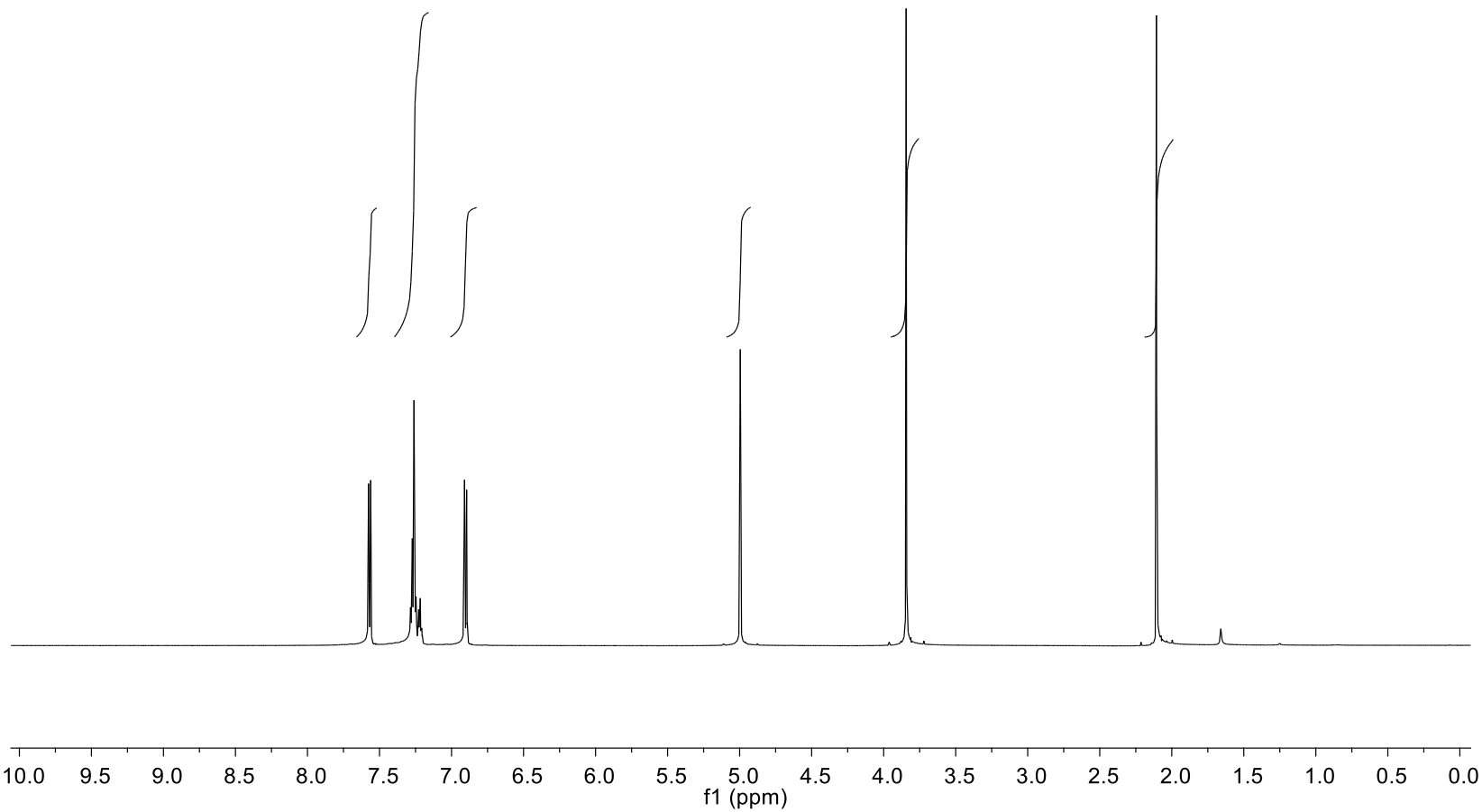


13bf: ^{13}C NMR ($CDCl_3$, 100 MHz)

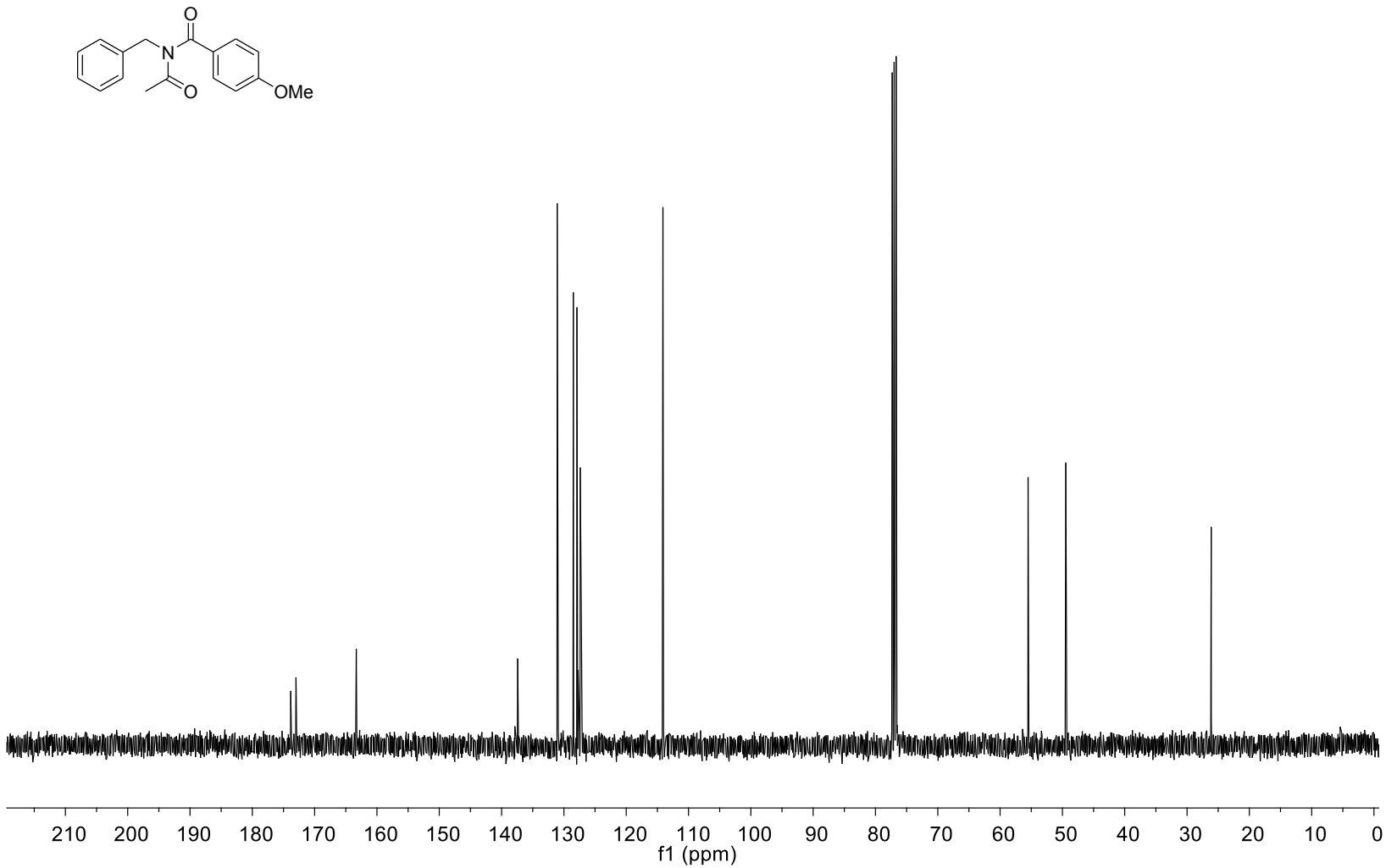


13ag: ^{1}H NMR ($CDCl_3$, 400 MHz)

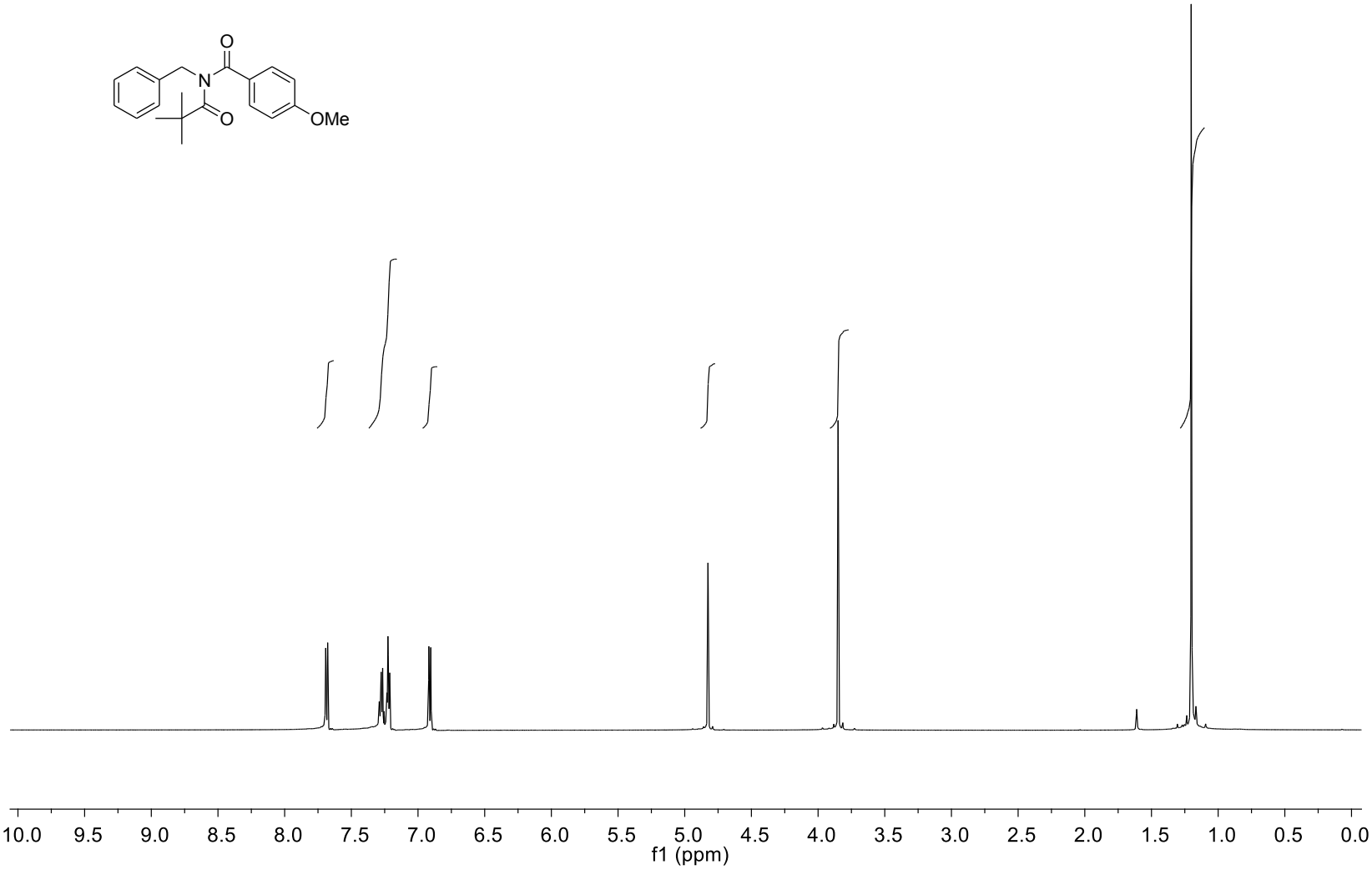




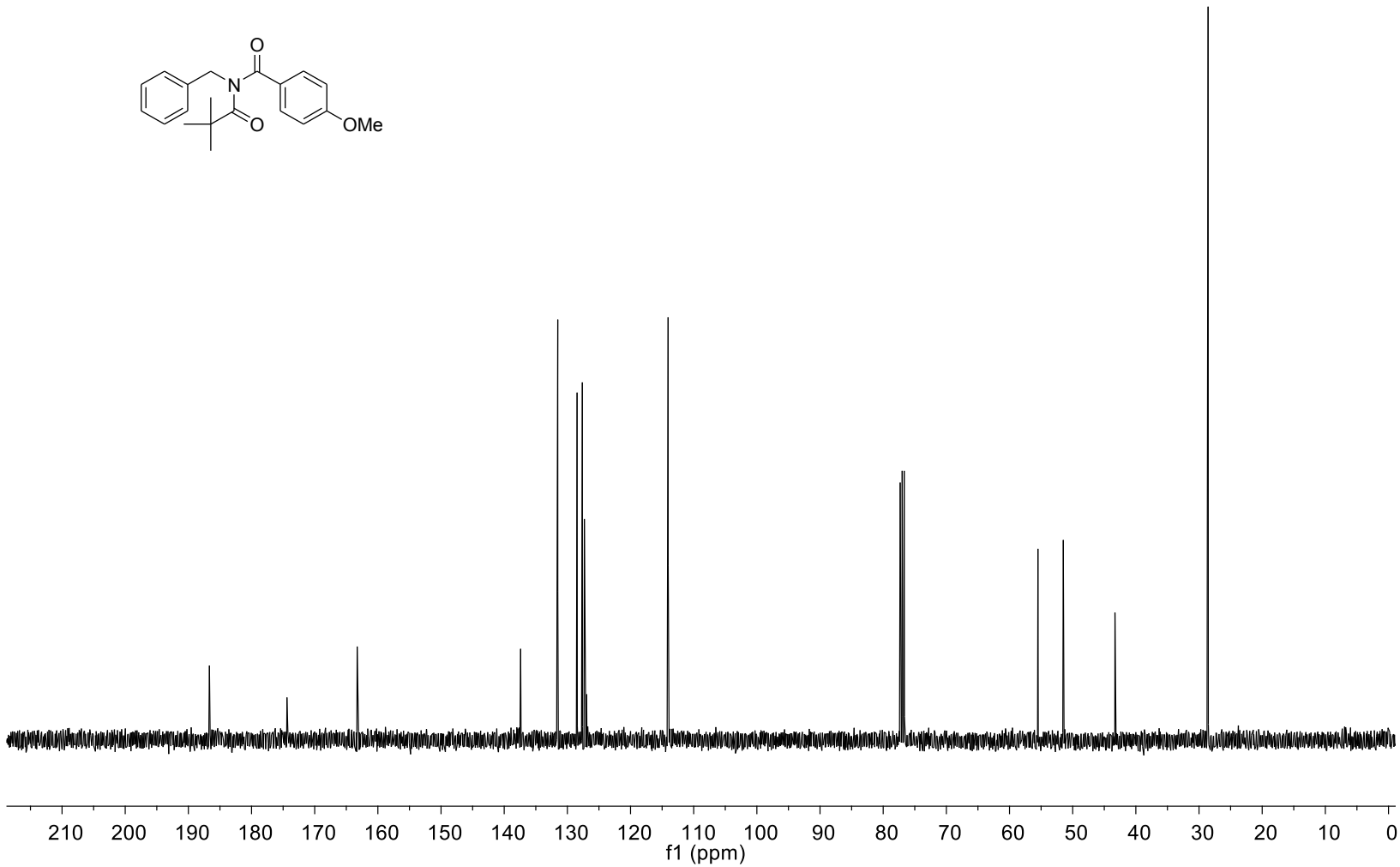
13ag: ^{13}C NMR ($CDCl_3$, 100 MHz)



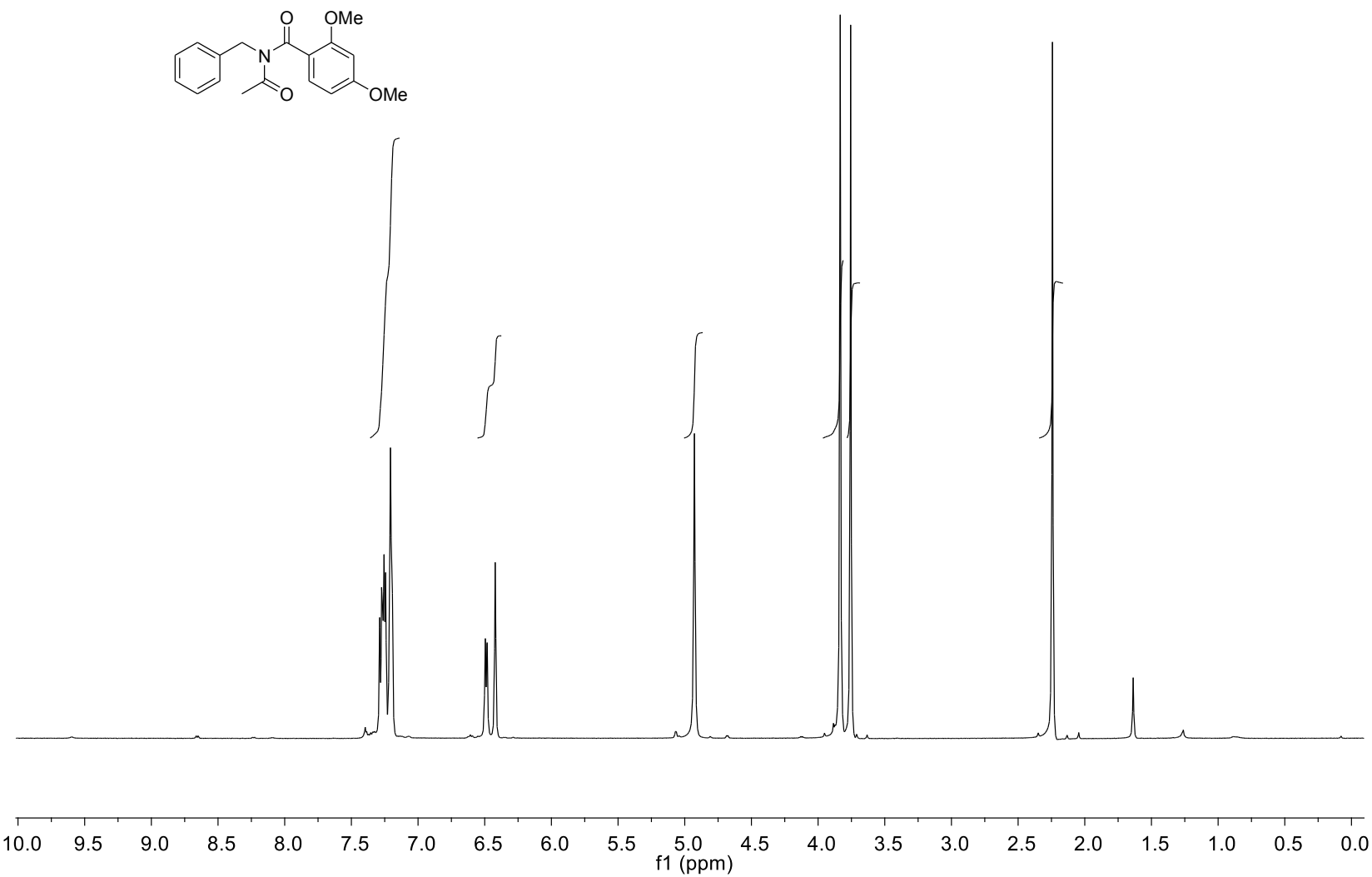
13bg: ^{1}H NMR ($CDCl_3$, 400 MHz)



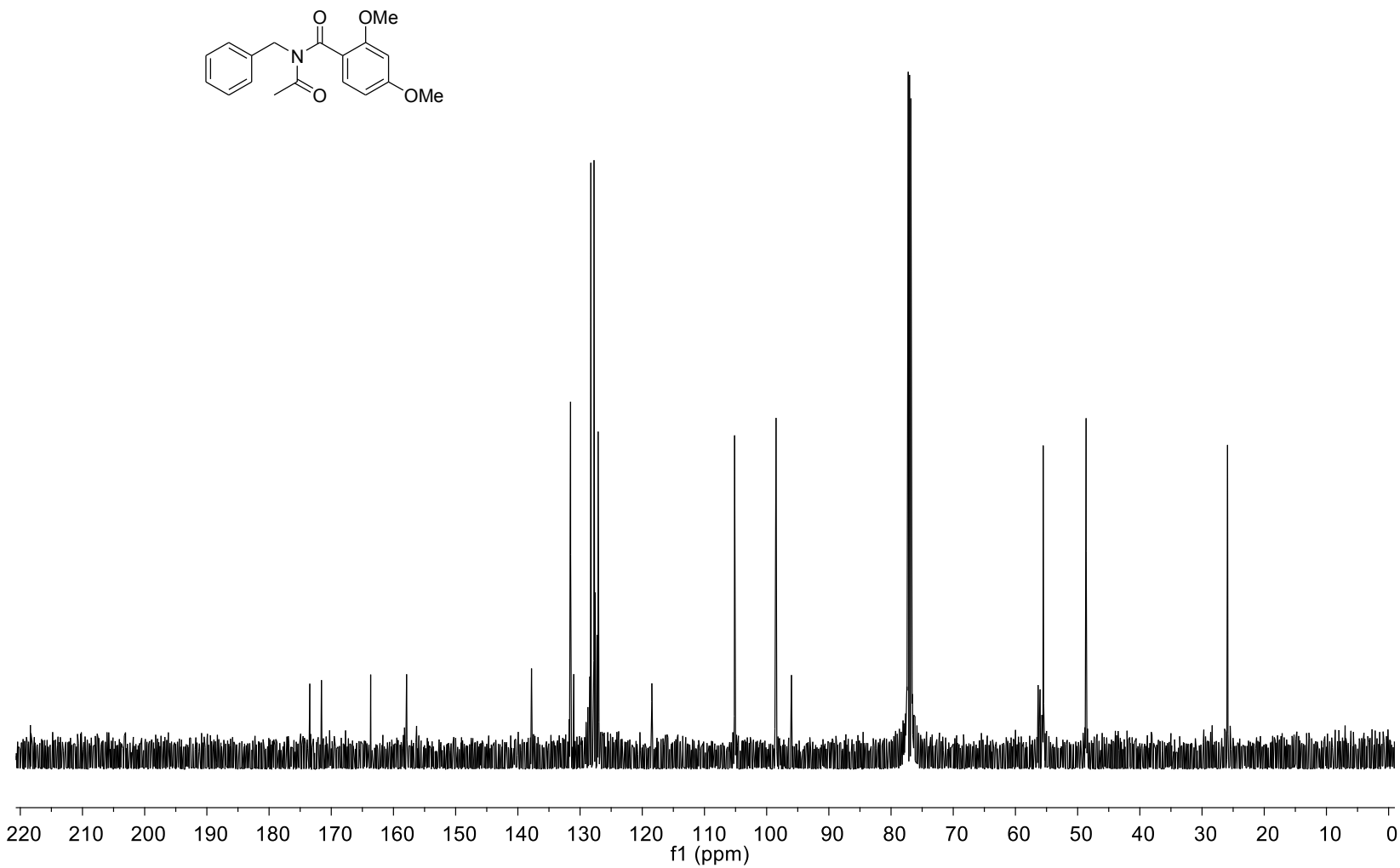
13bg: ^{13}C NMR ($CDCl_3$, 100 MHz)



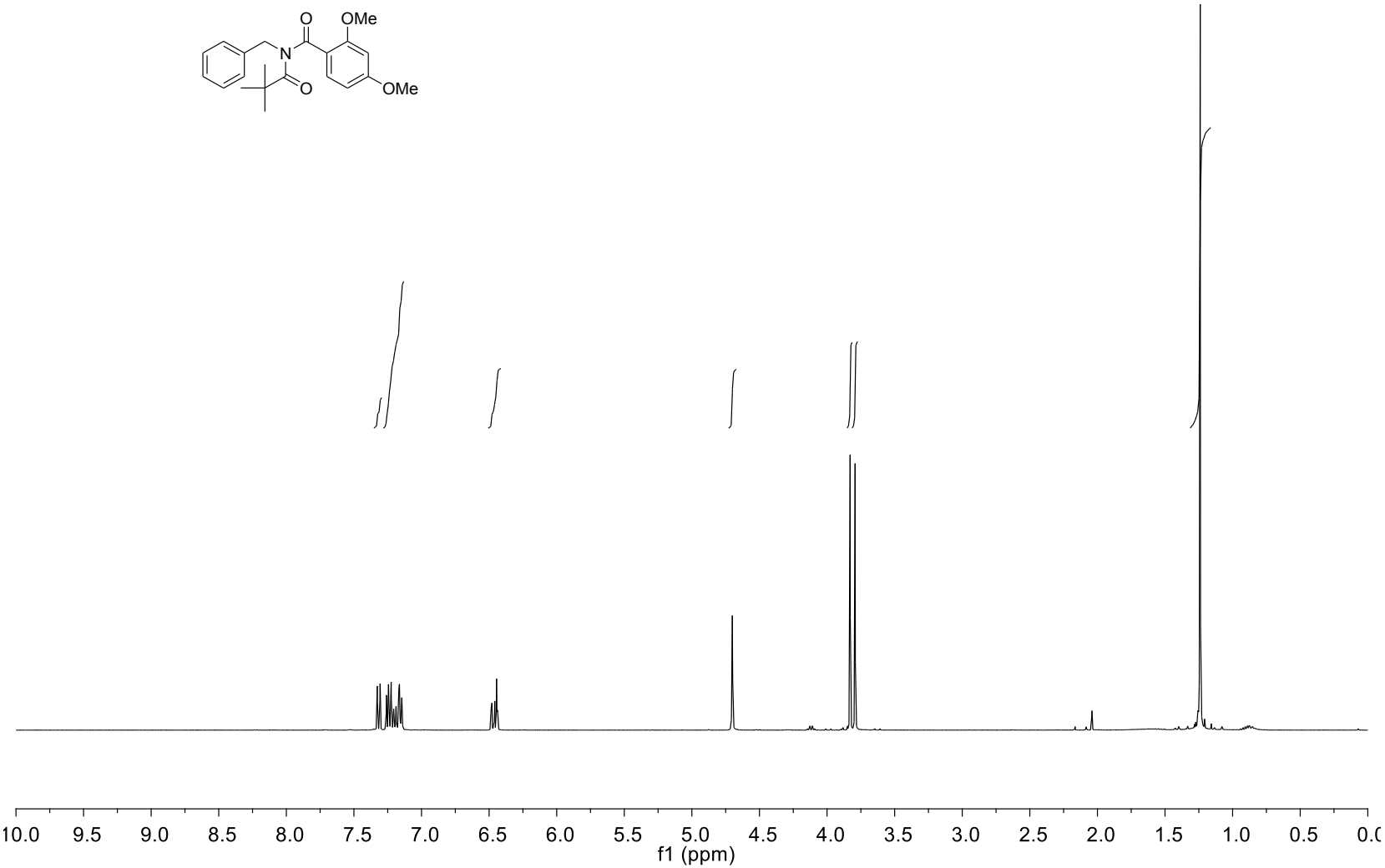
13ah: ^{1}H NMR ($CDCl_3$, 400 MHz)



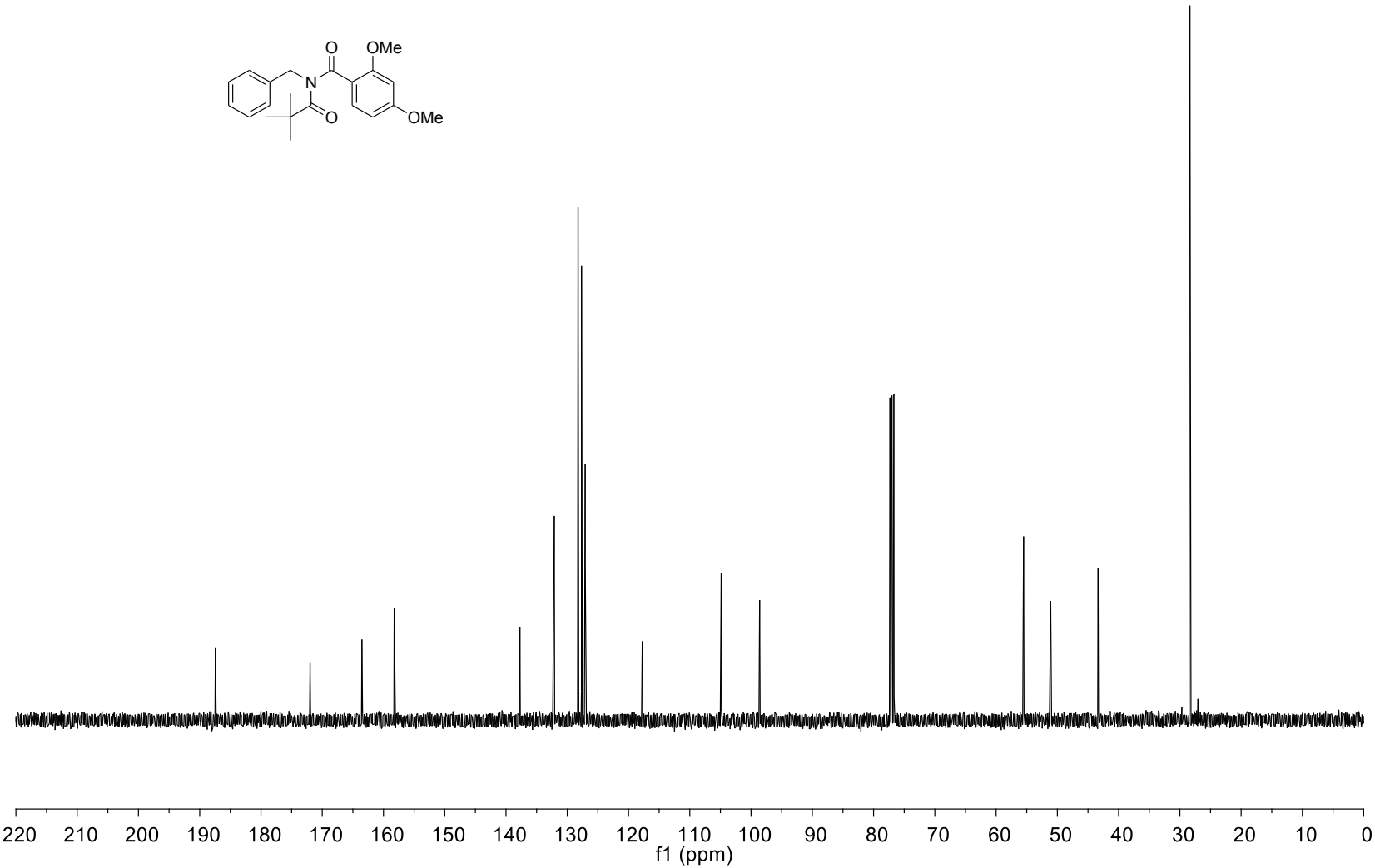
13ah: ^{13}C NMR ($CDCl_3$, 100 MHz)



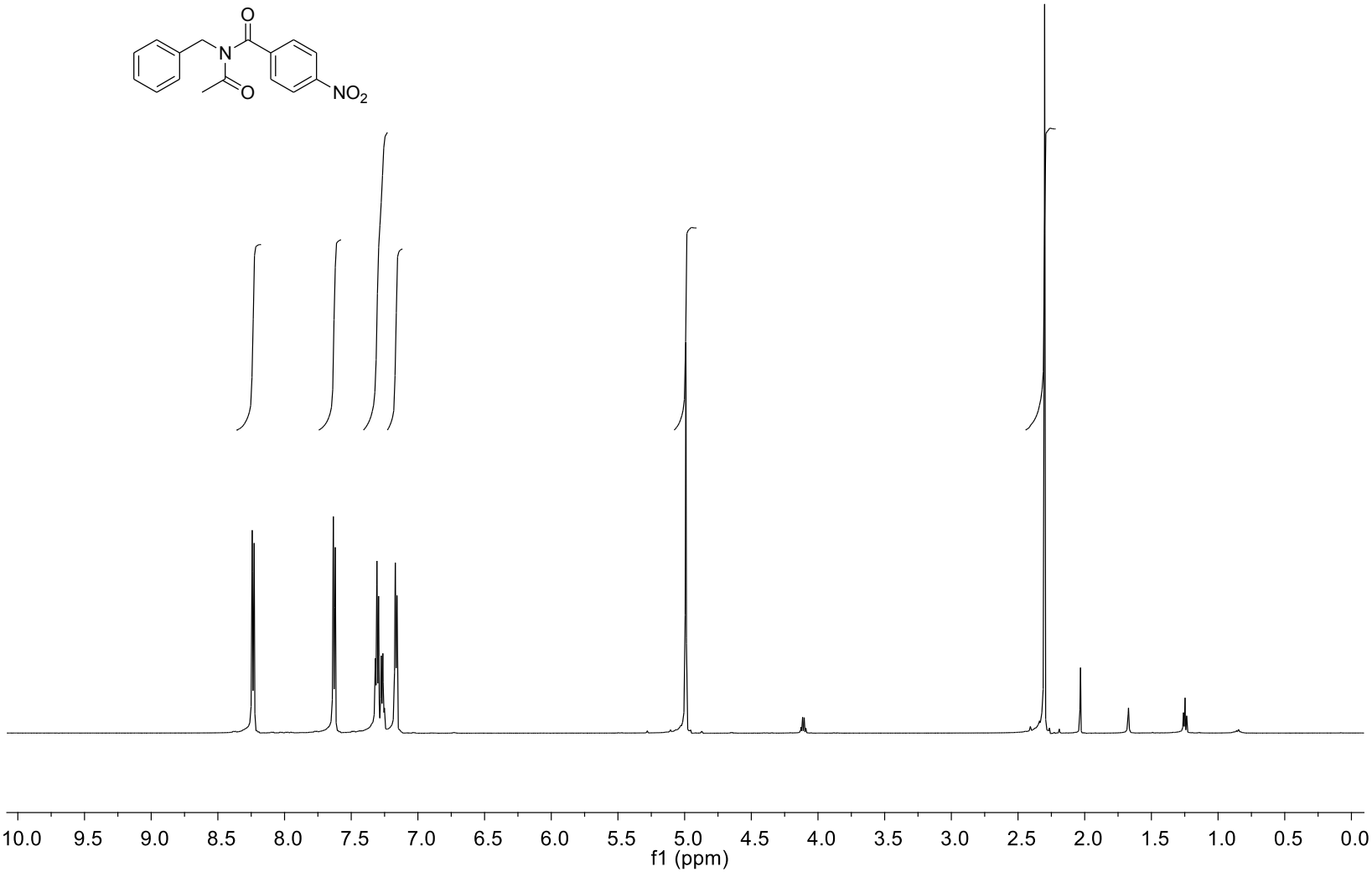
13bh: ^{1}H NMR ($CDCl_3$, 400 MHz)



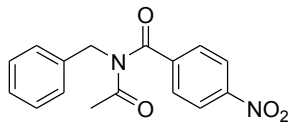
13bh: ^{13}C NMR ($CDCl_3$, 100 MHz)

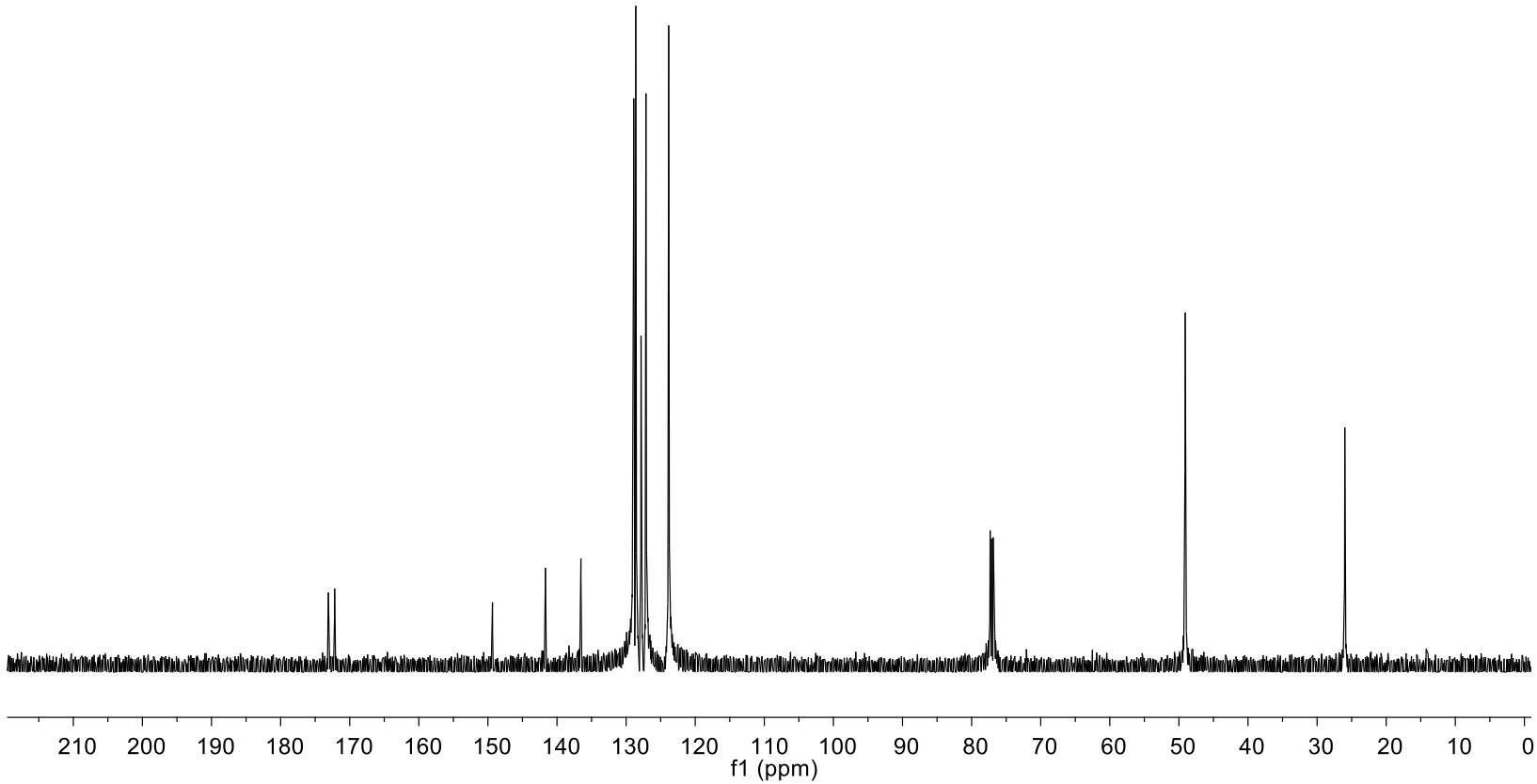


13ai: ^{1}H NMR ($CDCl_3$, 400 MHz)

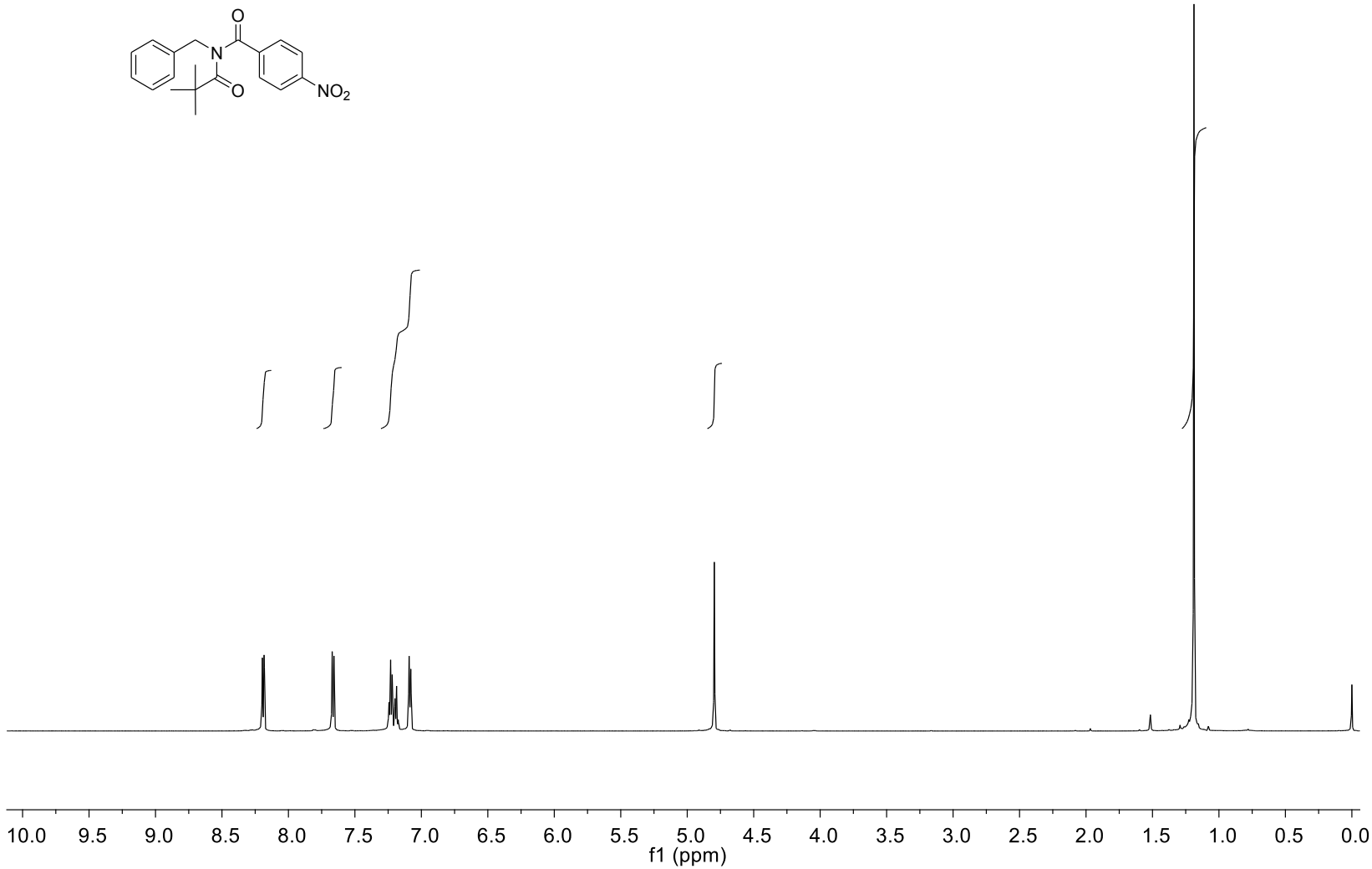


13ai: ^{13}C NMR ($CDCl_3$, 100 MHz)

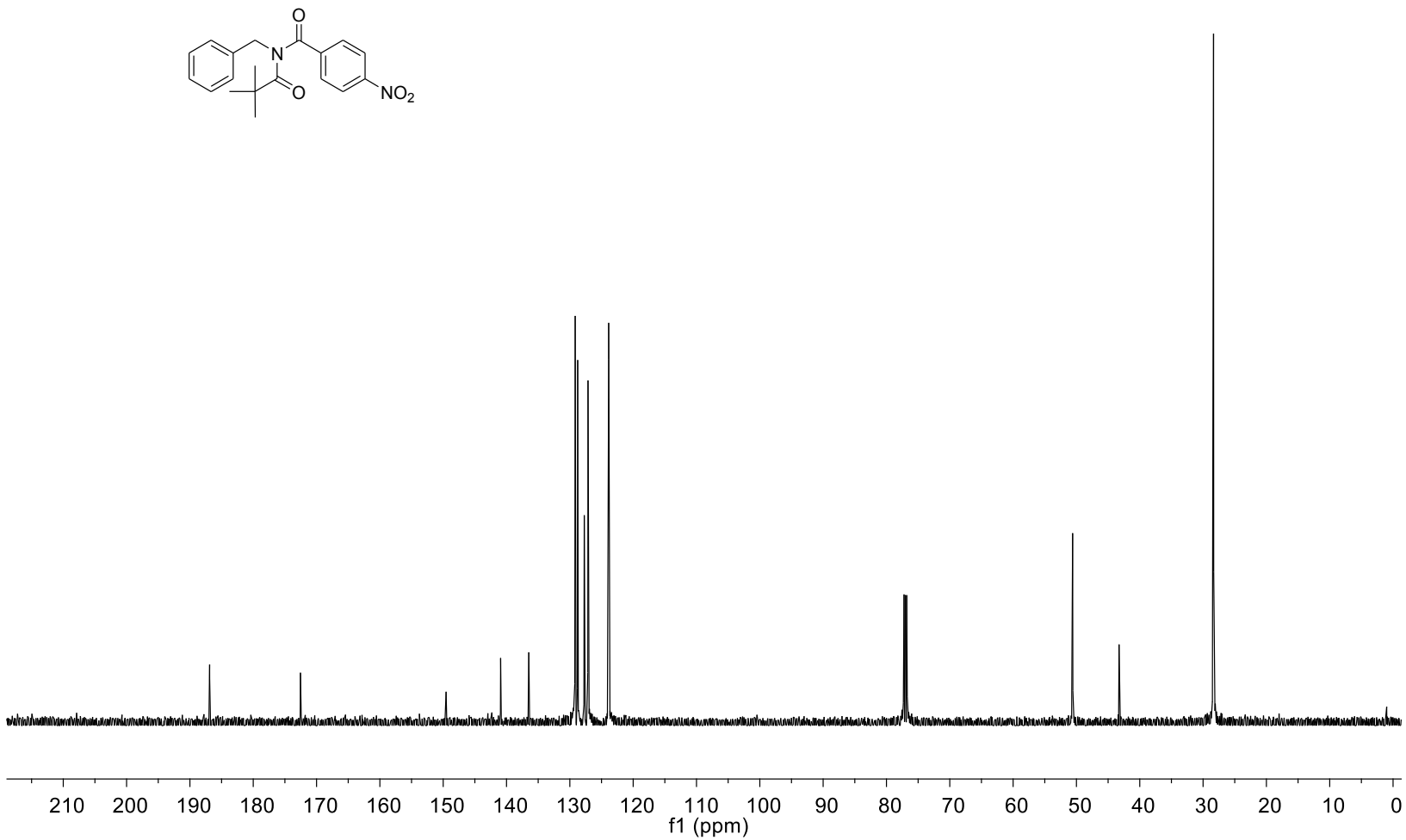




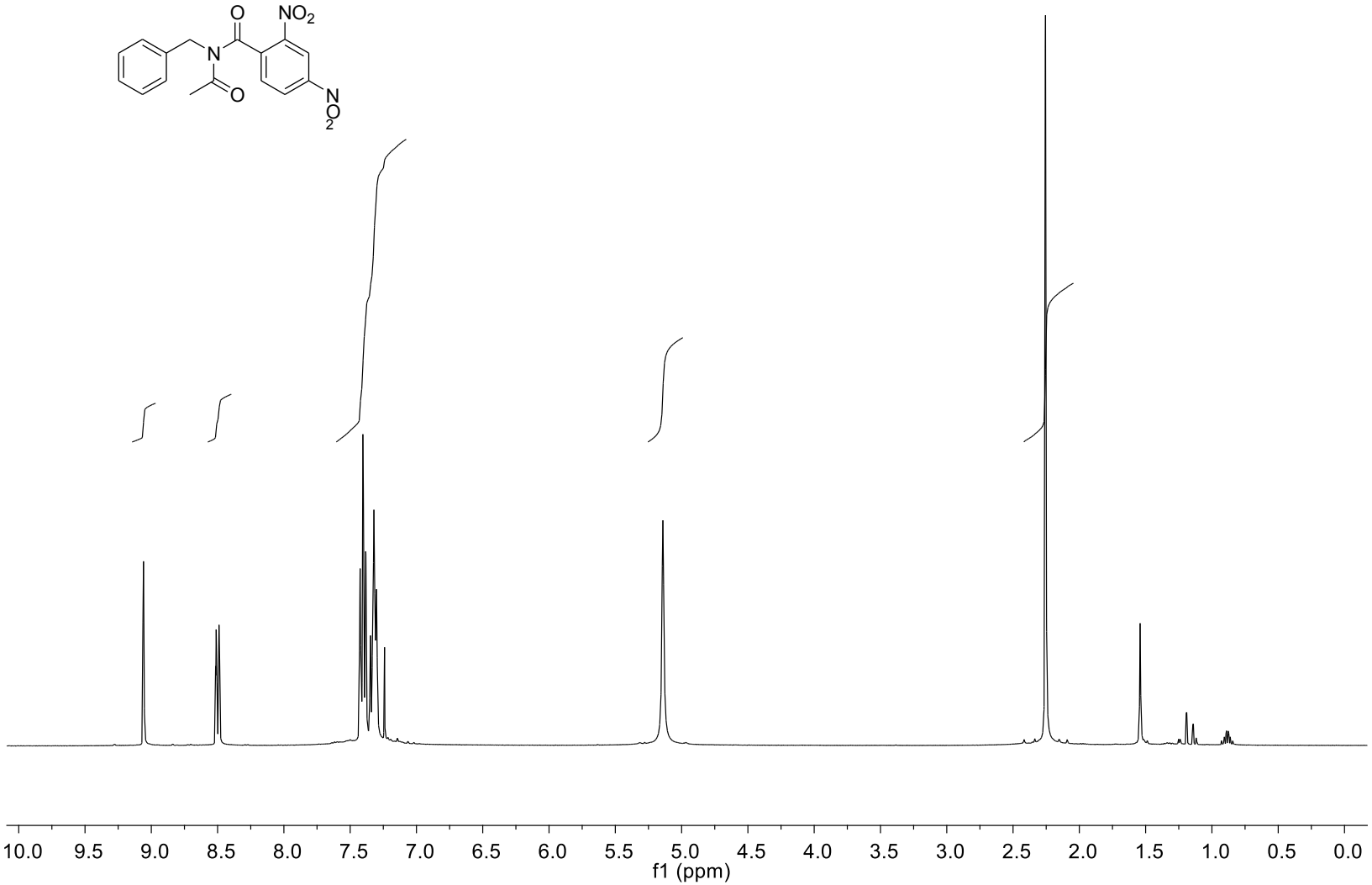
13bi: ^{1}H NMR ($CDCl_3$, 400 MHz)



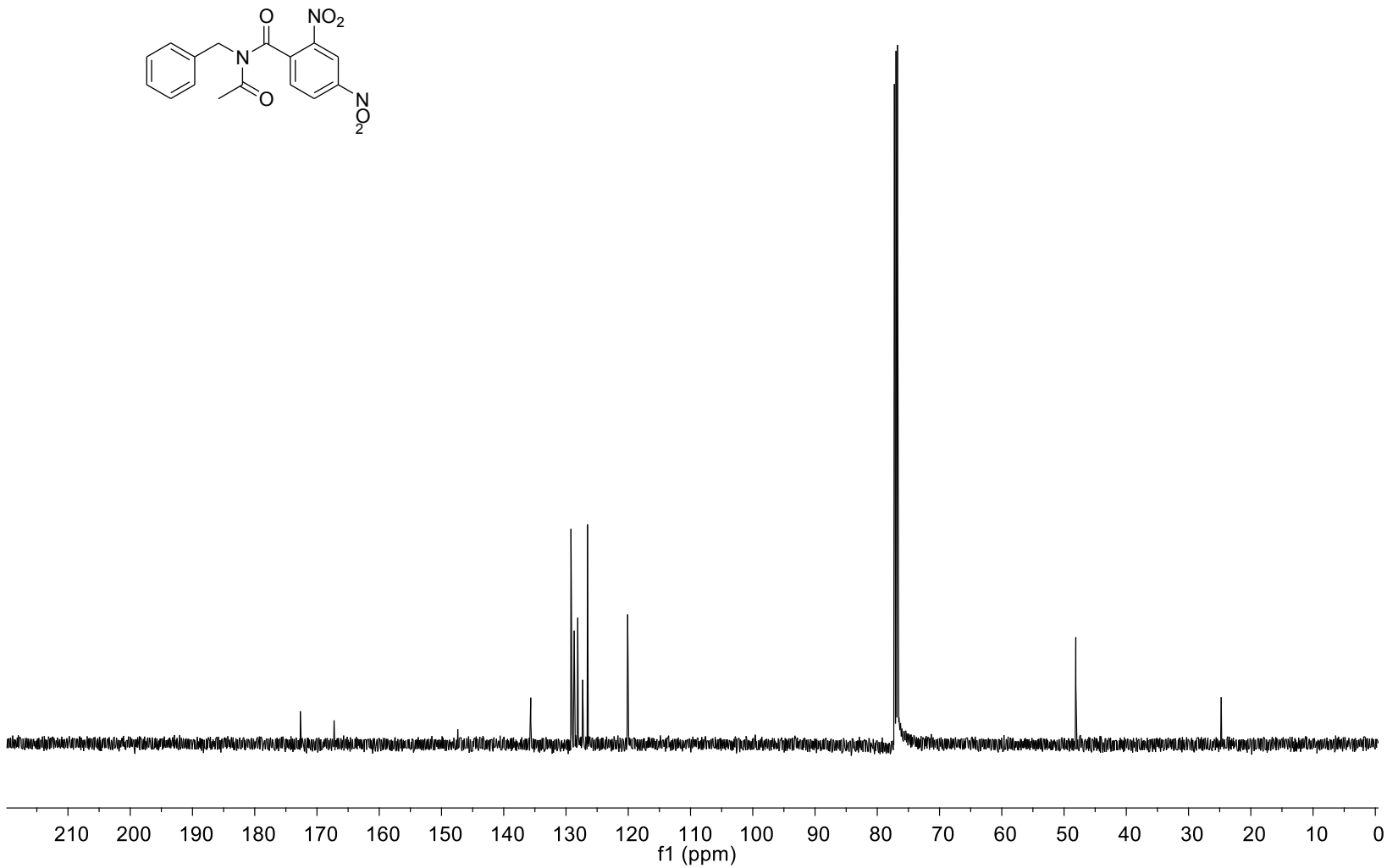
13bi: ^{13}C NMR ($CDCl_3$, 100 MHz)



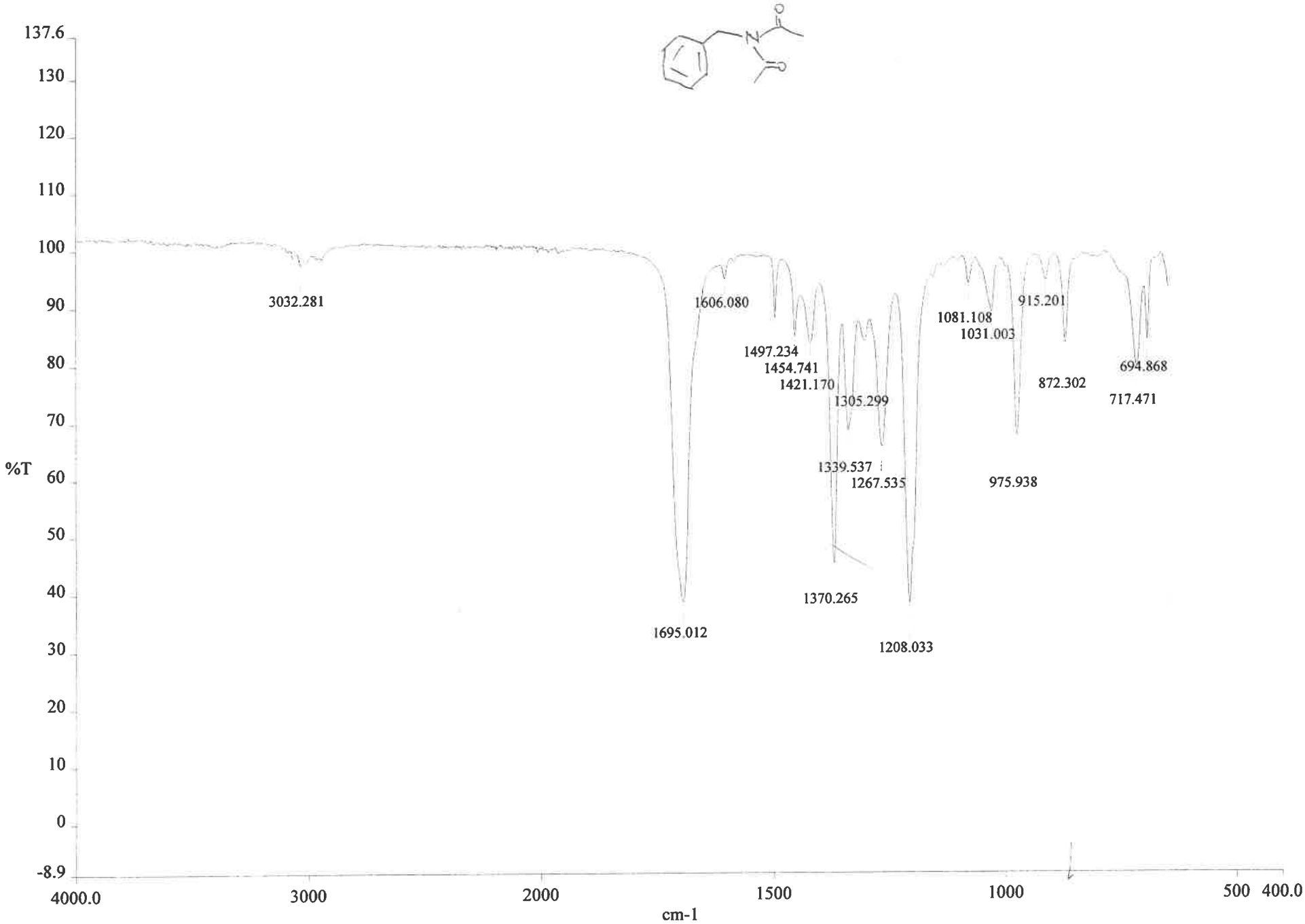
13aj: ^{1}H NMR ($CDCl_3$, 400 MHz)



13aj: ^{13}C NMR ($CDCl_3$, 100 MHz)

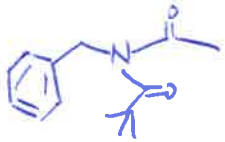


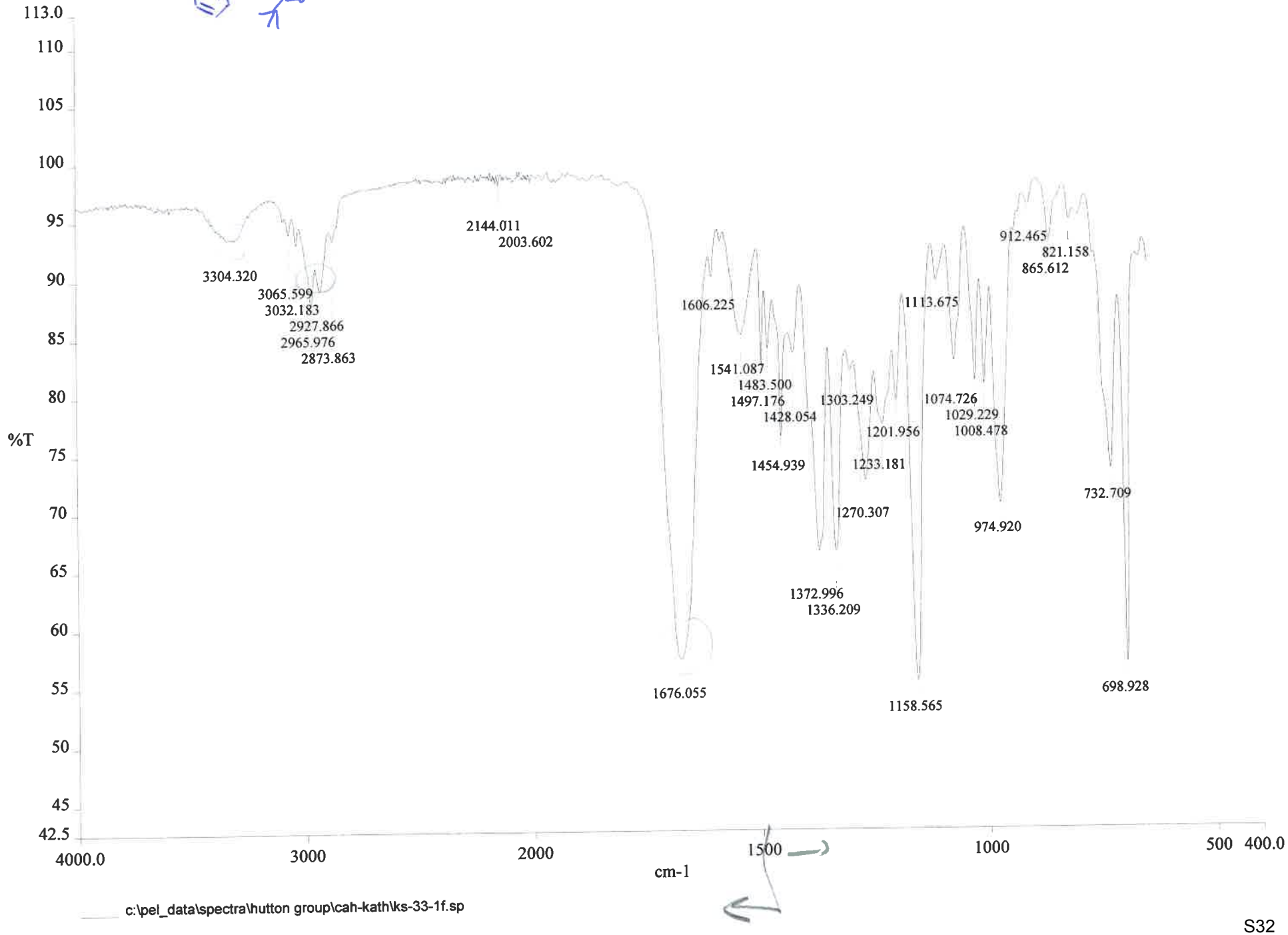
13aa



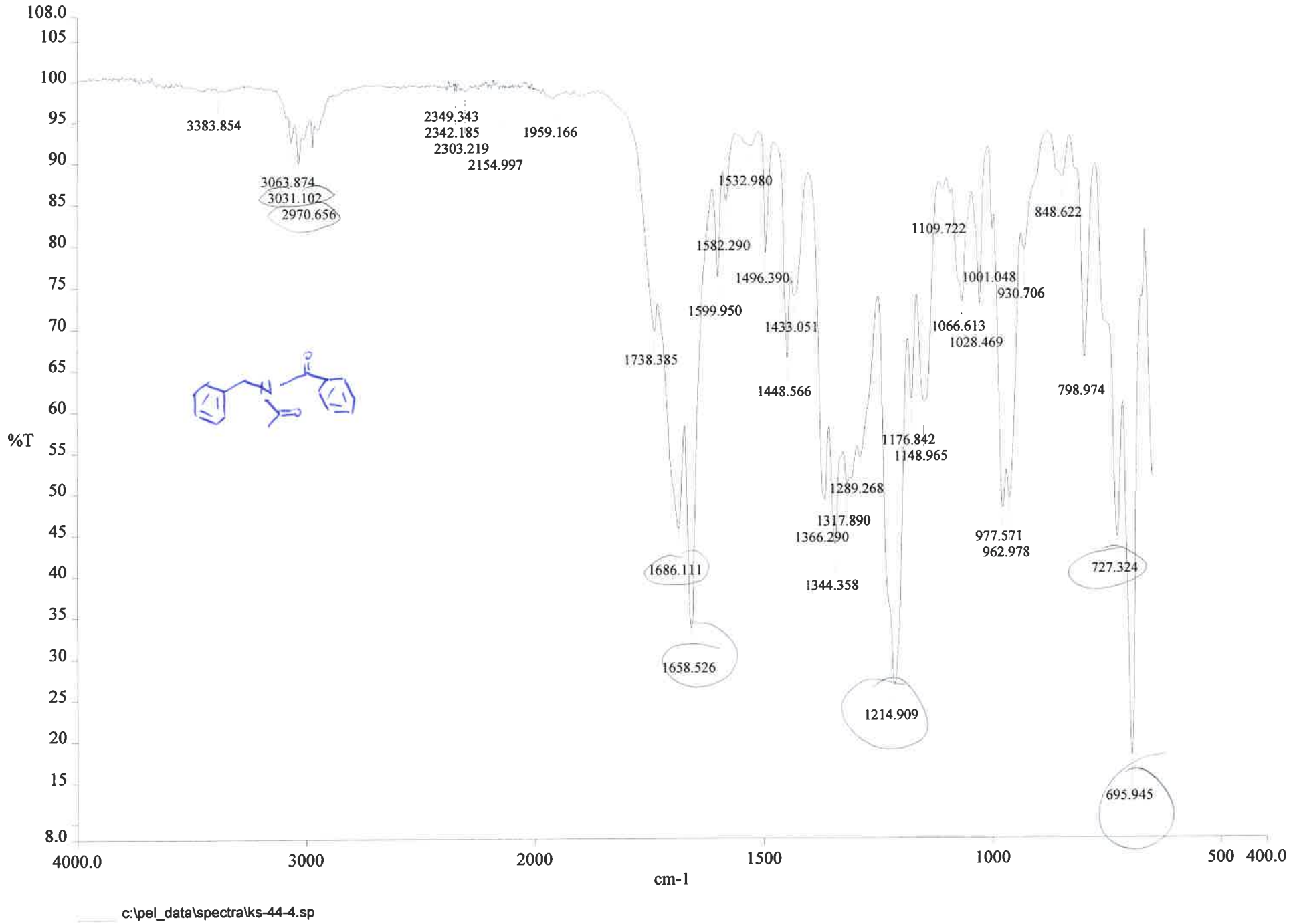
____ c:\pel_data\spectra\page37-f18-20.sp

13ab

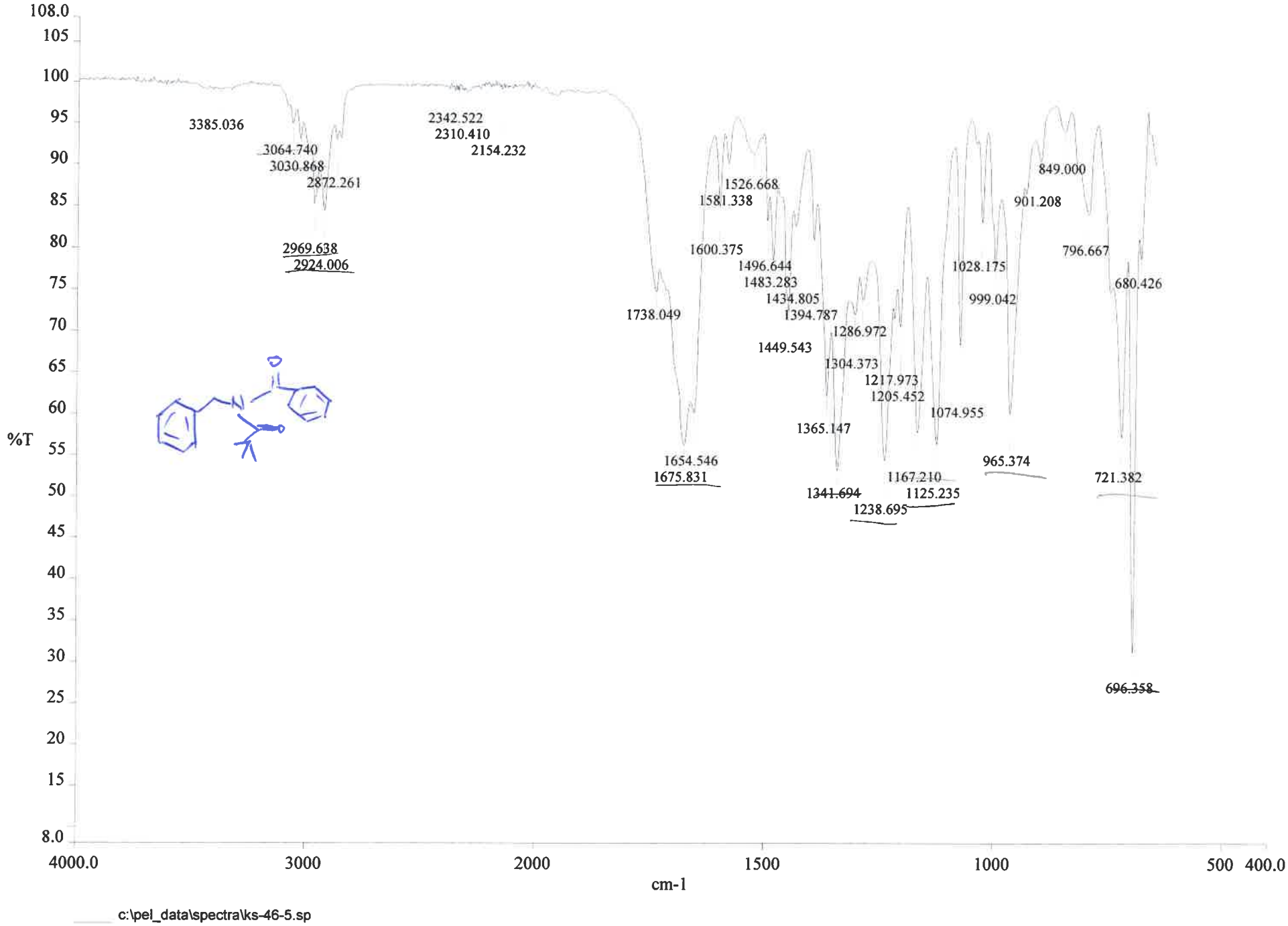



113.0
110
105
100
95
90
85
80
75
70
65
60
55
50
45
42.5
%T
4000.0
3000
2000
1500
1000
500
400.0
cm-1
3304.320
3065.599
3032.183
2927.866
2965.976
2873.863
2144.011
2003.602
1606.225
1541.087
1483.500
1497.176
1428.054
1454.939
1303.249
1270.307
1372.996
1336.209
1676.055
1201.956
1233.181
1113.675
1158.565
1074.726
1029.229
1008.478
974.920
912.465
821.158
865.612
732.709
698.928
c:\pel_data\spectra\hutton group\cah-kath\ks-33-1f.sp

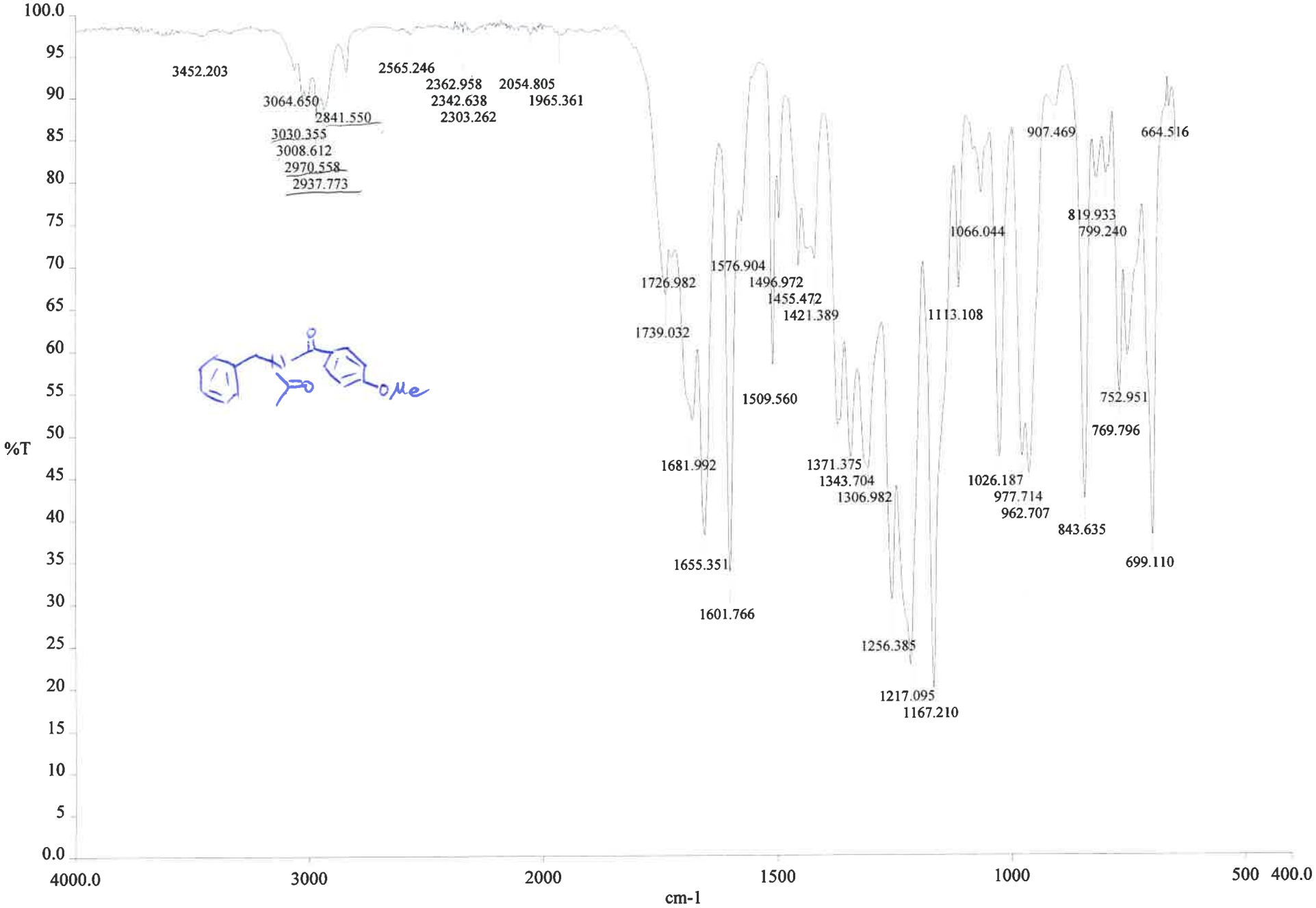
13af


%T
cm-1
3383.854
3063.874
3031.102
2970.656
2349.343
2342.185
2303.219
2154.997
1959.166
1738.385
1686.111
1658.526
1599.950
1582.290
1532.980
1496.390
1448.566
1433.051
1366.290
1344.358
1317.890
1289.268
1214.909
1176.842
1148.965
1109.722
1066.613
1028.469
1001.048
977.571
962.978
930.706
848.622
798.974
727.324
695.945
c:\pel_data\spectra\ks-44-4.sp

13bf

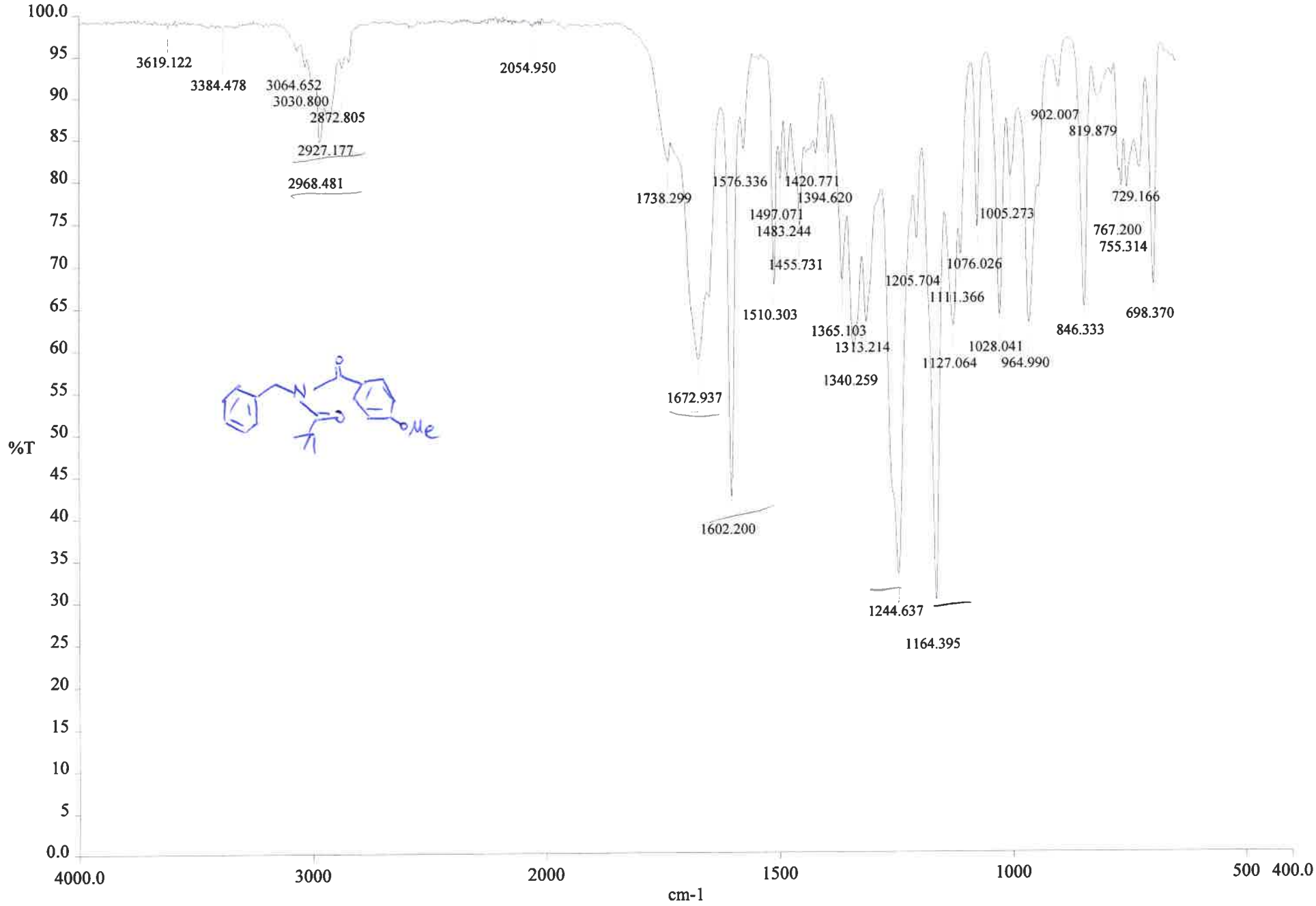

108.0
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
8.0
%T
3385.036
3064.740
3030.868
2872.261
2969.638
2924.006
2342.522
2310.410
2154.232
1738.049
1654.546
1675.831
1600.375
1581.338
1526.668
1496.644
1483.283
1449.543
1434.805
1394.787
1365.147
1341.694
1304.373
1286.972
1238.695
1217.973
1205.452
1167.210
1125.235
1074.955
1028.175
999.042
965.374
901.208
849.000
796.667
721.382
696.358
680.426
4000.0
3000
2000
1500
1000
500
400.0
cm-1
c:\pel_data\spectra\ks-46-5.sp

13ag



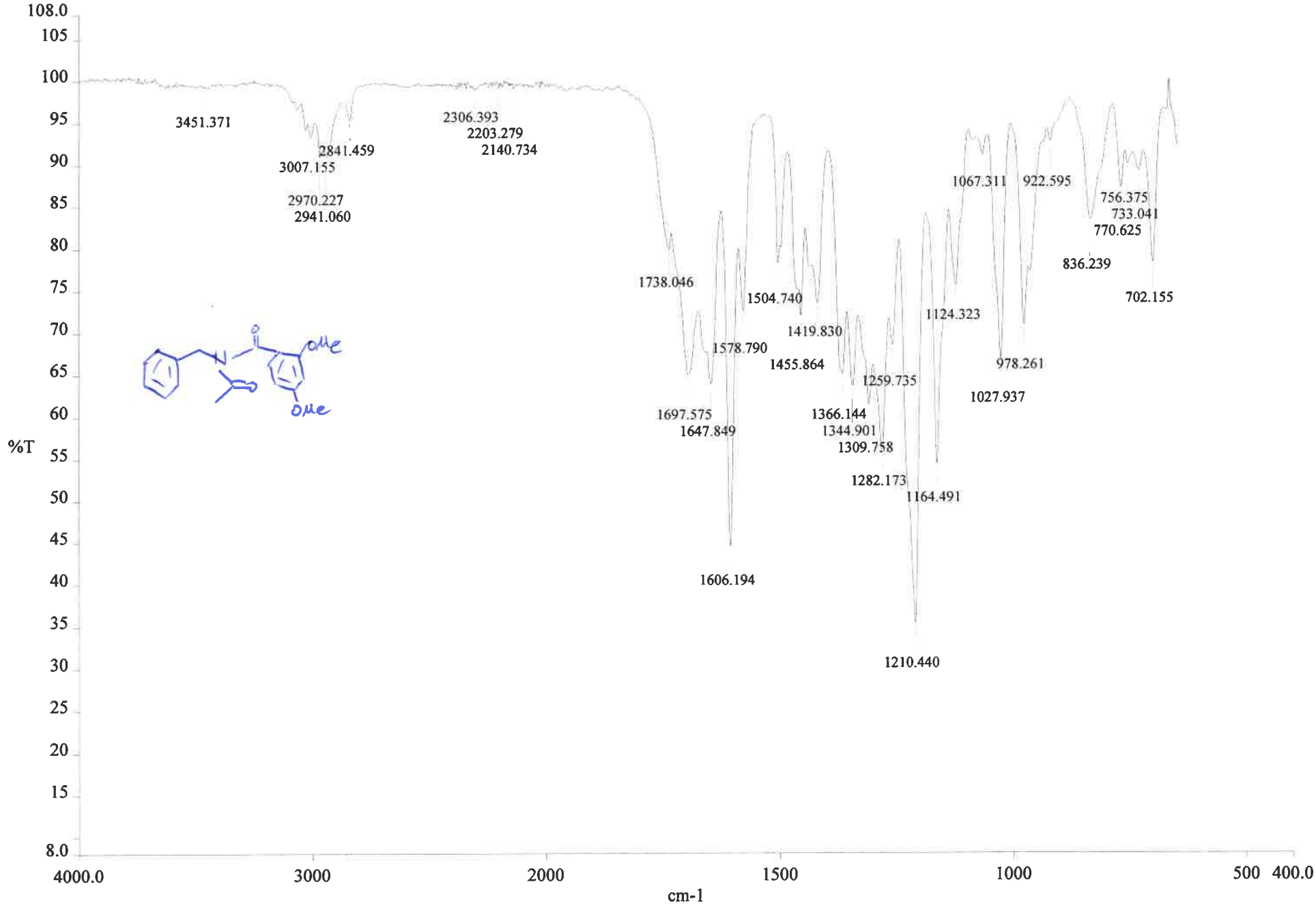
c:\pel_data\spectra\ks-37-2.sp

13bg



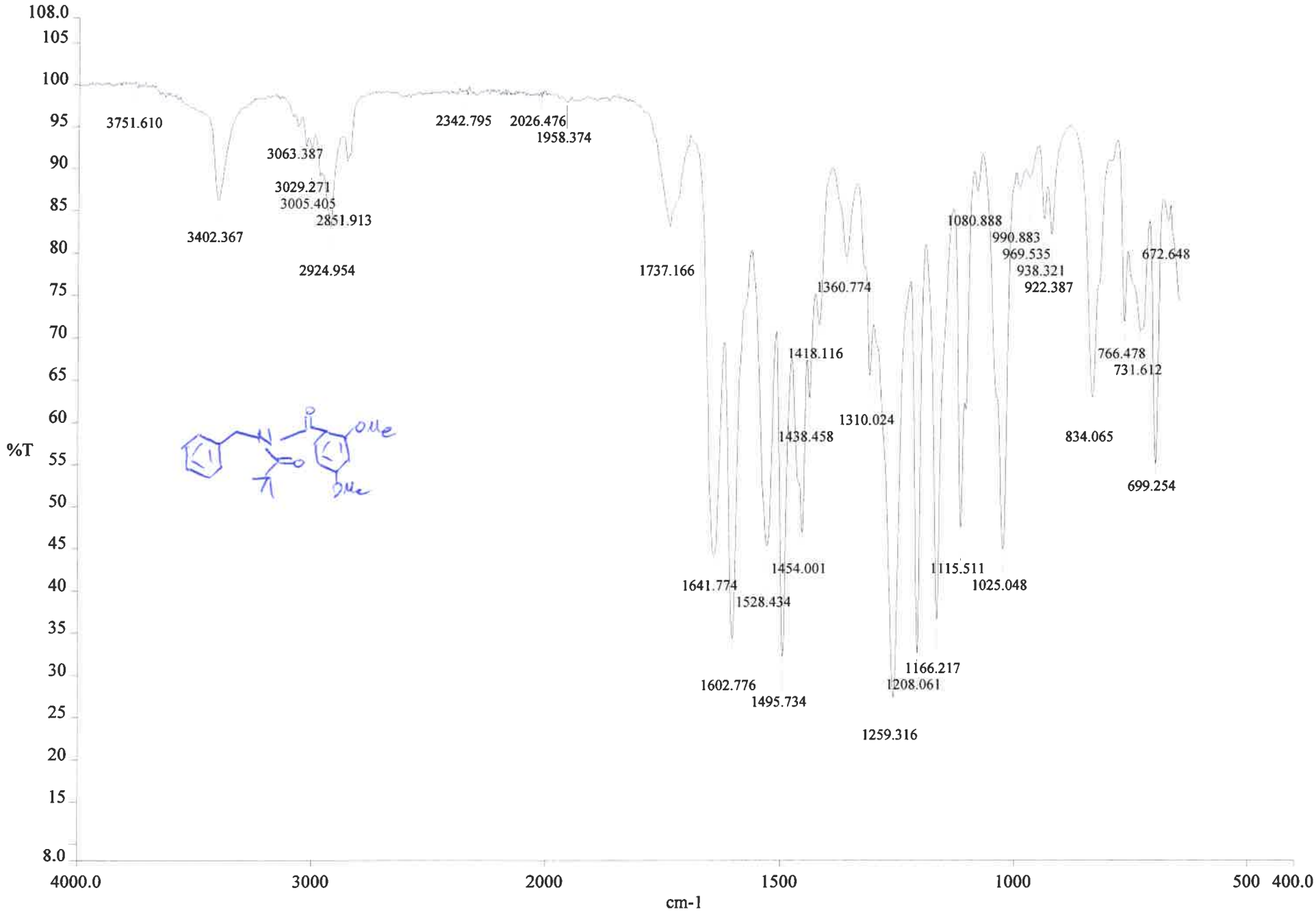
c:\pel_data\spectra\ks-38-3.sp

13ah



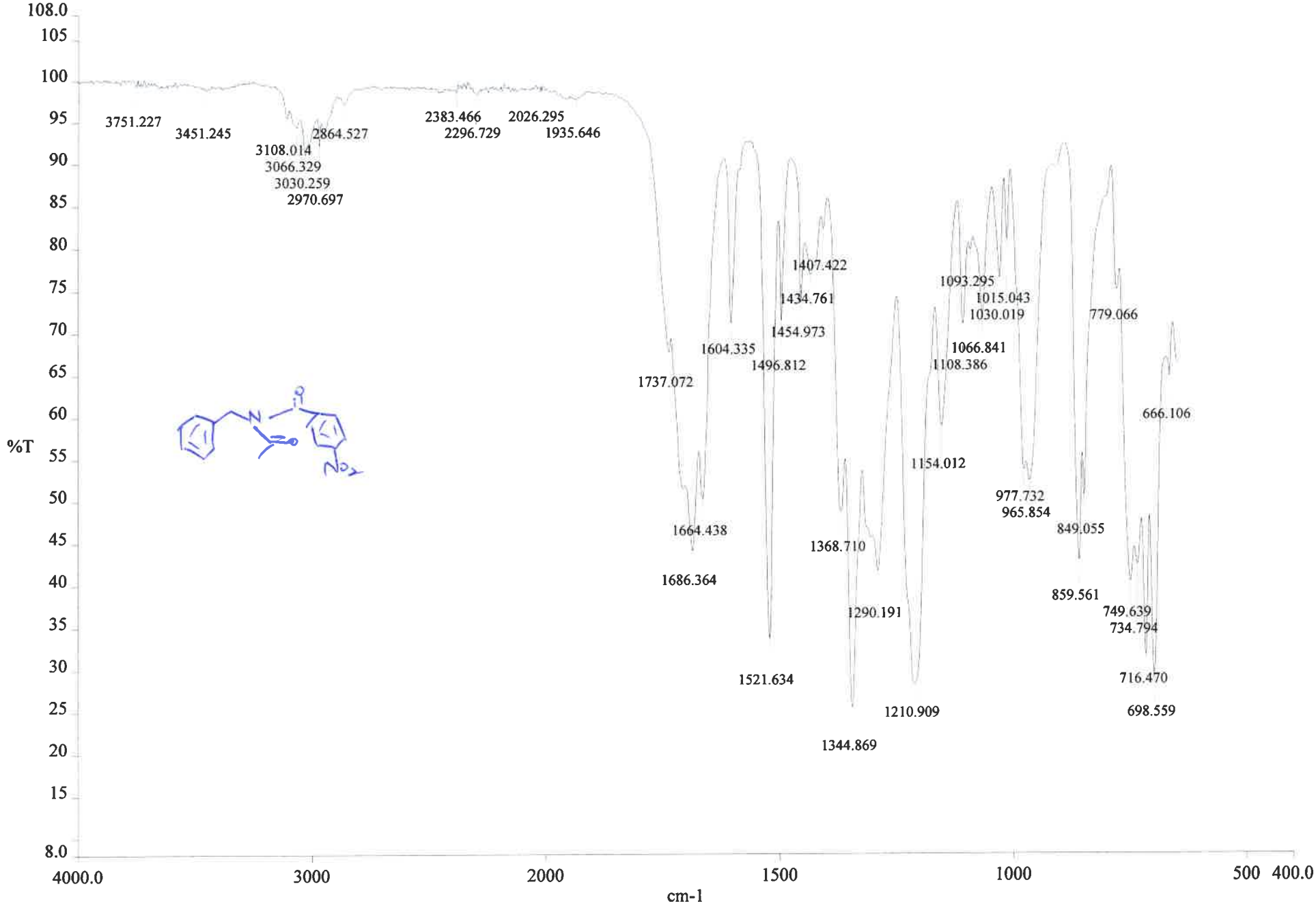
c:\pel_data\spectra\ks-55-7.sp

13bh



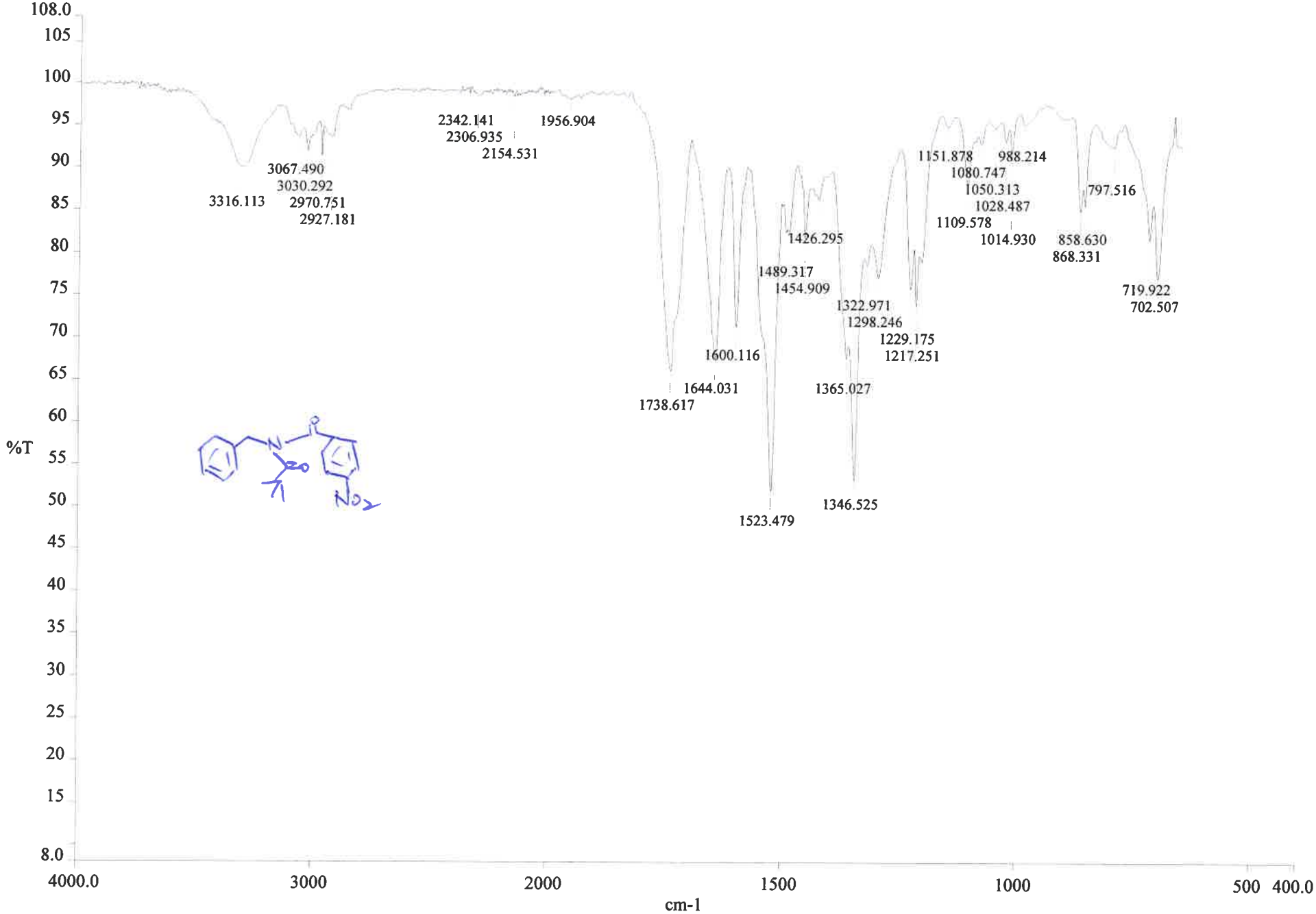
c:\pel_data\spectra\ks-56-8.sp

13ai



c:\pel_data\spectra\ks-58-9.sp

13bi


108.0
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
8.0
%T
3316.113
3067.490
3030.292
2970.751
2927.181
2342.141
2306.935
2154.531
1956.904
1738.617
1644.031
1600.116
1523.479
1489.317
1454.909
1426.295
1365.027
1346.525
1322.971
1298.246
1229.175
1217.251
1151.878
1109.578
1080.747
1050.313
1028.487
1014.930
988.214
858.630
868.331
797.516
719.922
702.507
4000.0
3000
2000
1500
1000
500
400.0
cm-1
c:\pel_data\spectra\ks-59-10.sp