

Copper(I)-catalyzed Carboxylation of Aryl- and Alkenylboronic Esters

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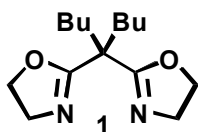
Contents

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| 1) Experimental section and analytical data for new compounds | SI1-SI8 |
| 2) Copies of ^1H NMR, ^{13}C NMR and IR spectra for new compounds
and carboxylation products | SI9-SI98 |

General. ^1H and ^{13}C -NMR spectra were recorded on a JEOL Lambda-400 (400 MHz for ^1H and 100 MHz for ^{13}C), a JEOL AL-400 (400 MHz for ^1H and 100 MHz for ^{13}C), a JEOL Lambda-300 (300 MHz for ^1H and 75 MHz for ^{13}C) or a JEOL AL-300 (300 MHz for ^1H and 75 MHz for ^{13}C) spectrometer using CHCl_3 (^1H , $\delta = 7.26$), CDCl_3 (^{13}C , $\delta = 77.0$), DMSO (^1H , $\delta = 2.49$), DMSO (^{13}C , $\delta = 40.45$) as an internal standard. IR spectra were recorded on an FT/IR-460 plus (JASCO Co., Ltd.) or a Spectrum 100 with universal ATR sampling accessory (Perkim Elmer instruments). Flash column chromatography was conducted on silica gel 60N (Kanto Chemical Co., Inc.). THF was purified by solvent purification system of Glass Contour. Dehydrated *N,N*-dimethylformamide, diethyl ether and dichloromethane were purchased from Kanto Chemicals. Recycling preparative GPC-HPLC was carried out on LC-918 (Japan Analytical Industry Co., Ltd.) using JAIGEL-2H. Cesium fluoride (Wako Pure Chemical Industries, Ltd.) was dried by heating at 150 °C for 2 days in vacuo.

preparation of bisoxazoline ligand 1:

5,5-Bis(4,5-dihydrooxazol-2-yl)nonan 1



Under an argon atmosphere, *N,N'*-bis(2-chloroethyl)-2,2-di-*n*-butylpropan-1,3-diamide¹ (2.92 g, 8.61 mmol) was

added to 5% NaOH / MeOH (NaOH 1.31 g, MeOH 24 ml) and the mixture was refluxed for 2 hours. The reaction mixture was cooled to room temperature and the solvent was removed under reduced pressure. The resulting solids were dissolved in water (20 ml), followed by extraction 6 times with methylene chloride. After the combined organic layer was dried over MgSO₄, the solvent was removed under reduced pressure to give crude product (2.05 g). The crude product was purified by recrystallization from hexane to give **1** (1.59 g, 5.97 mmol, 62% from **6**) as colorless crystal.

IR (KBr): 2957, 2925, 2902, 2871, 1652 cm⁻¹.

¹H-NMR (400 MHz, CDCl₃): δ = 0.88 (6H, t, *J* = 7.2 Hz), 1.08-1.22 (4H, m), 1.22-1.39 (4H, m), 1.85-1.98 (4H, m), 3.87 (4H, t, *J* = 9.2 Hz), 4.23 (4H, t, *J* = 9.2 Hz).

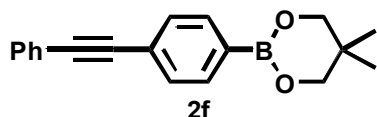
¹³C-NMR (100 MHz, CDCl₃): δ = 14.0, 22.9, 26.1, 32.7, 45.9, 54.2, 67.5, 168.5.

Anal. Calcd. For C₁₅H₂₆N₂O₂: C 67.63; H 9.84; N 10.52; Found: C 67.34; H 9.67; N 10.29.

preparation of aryl- or alkenylboronic esters:

2a², **2b**², **2c**², **2d**³, **2e**³, **2l**³ and **4a**⁴ were prepared according to the literature procedures. **2f**, **2g**, **2h**, **2j** and **4e** were prepared from the corresponding bromobenzene or bromostyrene derivatives according to the literature procedure using 2,2-dimethylpropan-1,3-diol instead of ethylene glycol.⁵

5,5-Dimethyl-2-[4-(phenylethynyl)phenyl]-1,3,2-dioxaborinane (2f**)**



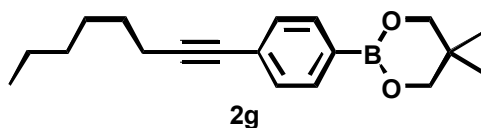
IR (KBr) 3076, 3033, 2956, 2937, 2900, 2211, 1604, 1478, 1421 cm⁻¹;

¹H NMR (CDCl₃) (400 MHz): δ = 1.04 (6H, s), 3.78 (4H, s), 7.30-7.39 (3H, m), 7.50-7.58 (4H, m), 7.80 (2H, d, *J* = 8.4 Hz);

¹³C NMR (CDCl₃) (100 MHz): δ = 22.0, 31.9, 72.3, 89.7, 90.3, 123.2, 125.2, 128.18, 128.25, 130.6, 131.5, 133.6 (1C_{C-B} missing);

Anal. Calcd for C₁₉H₁₉BO₂: C 78.65, H 6.60. Found: C 78.54, H 6.70.

5,5-Dimethyl-2-(4-(oct-1-yn-1-yl)phenyl)-1,3,2-dioxaborinane (2g**)**



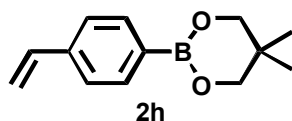
IR (KBr) 3072, 3030, 2958, 2932, 2871, 2857, 2223, 1603, 1477, 1421 cm^{-1} ;

^1H NMR (CDCl_3) (400 MHz): δ = 0.91 (3H, t, J = 7.2 Hz), 1.02 (6H, s), 1.26-1.40 (4H, m), 1.41-1.52 (2H, m), 1.61 (2H, tt, J = 7.6, 7.2 Hz), 2.41 (2H, t, J = 7.2 Hz), 3.76 (4H, s), 7.38 (2H, d, J = 8.0 Hz), 7.72 (2H, d, J = 8.0 Hz);

^{13}C NMR (CDCl_3) (100 MHz): δ = 14.1, 19.6, 21.9, 22.6, 28.7, 28.8, 31.4, 31.9, 72.3, 80.9, 91.5, 126.2, 130.5, 133.5 ($1\text{C}_{\text{C-B}}$ missing);

Anal. Calcd for $\text{C}_{19}\text{H}_{27}\text{BO}_2$: C 76.52, H 9.13. Found: C 76.32, H 9.20.

5,5-Dimethyl-2-(4-ethenylphenyl)-1,3,2-dioxaborinane (2h)



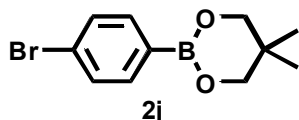
IR (KBr) 2960, 2928, 2873, 1605, 1479, 1423 cm^{-1} ;

^1H NMR (CDCl_3) (400 MHz): δ = 1.03 (6H, s), 3.78 (4H, s), 5.28 (1H, d, J = 11.0 Hz), 5.81 (1H, d, J = 17.8 Hz), 6.74 (1H, dd, J = 17.8, 11.0 Hz), 7.41 (2H, d, J = 8.0 Hz), 7.77 (2H, d, J = 8.0 Hz);

^{13}C NMR (CDCl_3) (100 MHz): δ = 21.9, 31.9, 72.3, 114.4, 125.4, 134.1, 137.0, 139.6 ($1\text{C}_{\text{C-B}}$ missing);

Anal. Calcd for $\text{C}_{13}\text{H}_{17}\text{BO}_2$: C 72.26, H 7.93. Found: C 72.50, H 8.13.

5,5-Dimethyl-2-(4-bromophenyl)-1,3,2-dioxaborinane (2j)



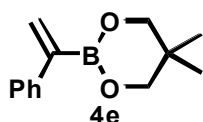
IR (KBr) 3050, 2958, 2939, 2903, 1584, 1480, 1422 cm^{-1} ;

^1H NMR (CDCl_3) (400 MHz): δ = 1.02 (6H, s), 3.76 (4H, s), 7.48 (2H, d, J = 8.3 Hz), 7.65 (2H, d, J = 8.3 Hz);

^{13}C NMR (CDCl_3) (100 MHz): δ = 21.9, 31.9, 72.3, 125.6, 130.7, 135.5 ($1\text{C}_{\text{C-B}}$ missing);

Anal. Calcd for $\text{C}_{11}\text{H}_{14}\text{BBrO}_2$: C 49.12, H 5.25. Found: C 49.35, H 5.53.

5,5-Dimethyl-2-(1-phenylethen-1-yl)-1,3,2-dioxaborinane (4e)



IR (neat) 3056, 3025, 2962, 2933, 2890, 1597, 1476, 1415, 1340, 1251, 1230, 1197, 1104, 1001, 943, 912, 781, 731, 699, 644 cm^{-1} ;

^1H NMR (CDCl_3) (400 MHz): δ = 1.05 (6H, s), 3.75 (4H, s), 5.97 (1H, d, J = 3.4 Hz),

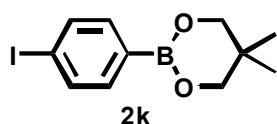
6.07 (1H, d, $J = 3.4$ Hz), 7.27 (1H, t, $J = 7.3$ Hz), 7.35 (2H, t, $J = 7.3$ Hz), 7.45 (2H, d, $J = 7.3$ Hz);

^{13}C NMR (CDCl_3) (100 MHz): $\delta = 21.8, 31.6, 72.3, 126.6, 127.5, 127.9, 129.5, 142.4$ ($1\text{C}_{\text{C-B}}$ missing);

Anal. Calcd for $\text{C}_{13}\text{H}_{17}\text{BO}_2$: C 72.26, H 7.93. Found: C 72.05, H 7.63.

Arylboronic esters **2k** and **4b** were prepared by esterification of the corresponding commercially available arylboronic acids: To a mixture of arylboronic acid (3.0 mmol) and 2,2-dimethylpropan-1,3-diol (3.3 mmol) in CH_2Cl_2 (6.0 ml) was added MgSO_4 (4.0 g) and the mixture was stirred at room temperature overnight. After filtration, the solvent was evaporated and the crude product was purified by silica gel chromatography (5~10% ethyl acetate in hexanes) or by recrystallization from hexane and ethyl acetate.

5,5-Dimethyl-2-(4-iodophenyl)-1,3,2-dioxaborinane (**2k**)



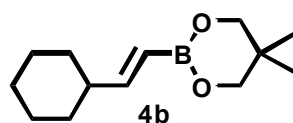
IR (KBr) 2955, 1579, 1479, 1421 cm^{-1} ;

^1H NMR (CDCl_3) (300 MHz): $\delta = 1.02(6\text{H}, \text{s}), 3.75(4\text{H}, \text{s}), 7.51(2\text{H}, \text{d}, J = 6.6 \text{ Hz}), 7.70(2\text{H}, \text{d}, J = 6.6 \text{ Hz})$;

^{13}C NMR (CDCl_3) (75 MHz): $\delta = 21.9, 31.9, 72.3, 98.1, 135.5, 136.7$ ($1\text{C}_{\text{C-B}}$ missing);

Anal. Calcd for $\text{C}_{11}\text{H}_{14}\text{BIO}_2$: C 41.82, H 4.47. Found: C 41.92, H 4.54.

5,5-Dimethyl-2-(2-cyclohexylethen-1-yl)-1,3,2-dioxaborinane (**4b**)



IR (KBr) 2925, 2851, 1634, 1476, 1413 cm^{-1} ;

^1H NMR (CDCl_3) (300 MHz): $\delta = 0.97(6\text{H}, \text{s}), 1.03-1.35(5\text{H}, \text{m}), 1.52-1.78(5\text{H}, \text{m}), 1.92-2.08(1\text{H}, \text{m}), 3.63(4\text{H}, \text{s}), 5.29(1\text{H}, \text{dd}, J = 18.0, 1.2 \text{ Hz}), 6.49(1\text{H}, \text{dd}, J = 18.0, 6.6 \text{ Hz})$;

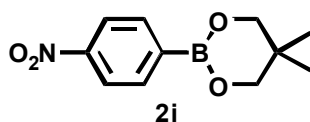
^{13}C NMR (CDCl_3) (75 MHz): $\delta = 21.9, 26.0, 26.2, 31.8, 32.2, 43.0, 72.1, 157.2$ ($1\text{C}_{\text{C-B}}$ missing);

Anal. Calcd for $\text{C}_{13}\text{H}_{23}\text{BO}_2$: C 70.29, H 10.44. Found: C 70.30, H 10.15.

Preparation of **2i**⁶:

A mixture of 4-bromonitrobenzene (202 mg, 1.00 mmol), bis(neopentyl glycolato)diboron (247 mg, 1.09 mmol), PdCl₂(dppf) (21.8 mg, 0.03 mmol) and potassium acetate (290 mg, 3.04 mmol) in DMSO (6 ml) was heated at 80 °C for 5 hours. The reaction was quenched by adding water and the mixture was filtered through a short pad of Celite. The filtrate was extracted four times with ether and combined organic layer was washed with brine, and dried over MgSO₄. Solvent was removed under reduced pressure to give crude product. This crude product was purified by silica gel chromatography (10% ethyl acetate in hexanes) to afford **2i** (125 mg, 0.53 mmol, 53%).

5,5-Dimethyl-2-(4-nitrophenyl)-1,3,2-dioxaborinane (**2i**)



IR (KBr) 2963, 1514, 1478, 1425, 1348, 1333, 1309, 1255, 1125, 851, 729, 700, 633 cm⁻¹;

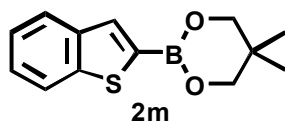
¹H NMR (CDCl₃) (300 MHz): δ = 1.04 (6H, s), 3.80 (4H, s), 7.98 (2H, d, *J* = 8.8 Hz), 8.17 (2H, d, *J* = 8.8 Hz);

¹³C NMR (CDCl₃) (100 MHz): δ = 21.8, 31.9, 72.4, 122.2, 134.7, 149.6 (1C_{C-B} missing);
Anal. Calcd for C₁₁H₁₄BNO₄: C 56.21, H 6.00, N 5.96. Found: C 56.19, H 6.16, N 5.86.

Preparation of **2m**:

To a stirred solution of benzothiophene (1.75 ml, 15.0 mmol) in THF (75 ml) was added *n*-butyllithium (9.6 ml, 1.56 M) at -40 °C. After 2 h, triethylborate (2.80 ml, 16.5 mmol) was added dropwise over 5 min at -40 °C and the mixture was stirred overnight at the same temperature. The mixture was treated with 1 M HCl and then extracted with AcOEt three times. To the combined organic layer was added Na₂SO₄ and 2,2-dimethyl-1,3-propanediol (1.58 g, 15.2 mmol), and the mixture was stirred overnight. Removal of the solvent under reduced pressure afforded white solids, which were recrystallized to give **2m** (2.42 g, 9.8 mmol) in 66% yield.

5,5-Dimethyl-2-(benzothiophen-2-yl)-1,3,2-dioxaborinane (**2m**)



IR (KBr) 3055, 3022, 2954, 2906, 2867, 1518, 1493, 1480, 1455 cm^{-1} ;

^1H NMR (CDCl_3) (300 MHz): δ = 1.05 (6H, s), 3.80 (4H, s), 7.32-7.37 (2H, m), 7.81-7.97 (3H, m);

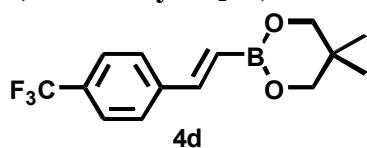
^{13}C NMR (CDCl_3) (75 MHz): δ = 21.8, 32.0, 72.5, 122.5, 123.9, 124.2, 124.9, 132.8, 140.6, 143.4 (1 $\text{C}_{\text{C-B}}$ missing);

Anal. Calcd for $\text{C}_{13}\text{H}_{15}\text{BO}_2\text{S}$: C 63.44, H 6.14, S 13.03. Found: C 63.74, H 6.34, S 13.01.

Preparation of 4d⁷:

A mixture of *p*-trifluoromethylphenylacetylene (2.57 g, 15.1 mmol) and catecholborane (2.5 ml, 23.5 mmol) was heated at 70 °C for 4 hours. The reaction was quenched by adding water and the mixture was stirred for 9 hours at room temperature. The mixture was extracted with AcOEt three times, and the combined organic layer was washed with water (2 times) and brine, and dried over MgSO_4 . After removal of solvent under reduced pressure, 2,2-dimethylpropan-1,3-diol (1.76g, 16.9 mmol) and toluene (40 ml) were added and the mixture was heated to reflux with the azeotropic removal of water. Organic layer was extracted with ether and the combined ether extract was washed with water three times, dried over MgSO_4 . After removal of solvent under reduced pressure, the residue was purified by silica gel chromatography (10% ethyl acetate in hexanes) and recrystallization from hexane to give the alkenylboronic ester **4d** (860 mg, 20 %, 2 steps).

5,5-Dimethyl-2-[2-(4-trifluoromethylphenyl)ethen-1-yl]-1,3,2-dioxaborinane (**4d**)



IR (KBr) 3055, 3016, 2962, 2905, 1631, 1615, 1577, 1477, 1415, 1378, 1314, 1282, 1259, 1172, 1111, 1066, 1014, 990, 819, 679, 588, 498 cm^{-1} ;

^1H NMR (CDCl_3) (400 MHz): δ = 1.01 (6H, s), 3.71 (4H, s), 6.20 (1H, d, J = 18.4 Hz), 7.33 (1H, d, J = 18.4 Hz), 7.53-7.61 (4H, m);

^{13}C NMR (CDCl_3) (100 MHz): δ = 21.9, 31.9, 72.2, 124.1(1C, q, J_{CF} = 270.6 Hz), 125.4 (1C, q, J_{CF} = 3.3 Hz), 127.0, 130.0 (1C, q, J_{CF} = 32 Hz), 141.0, 145.3 (1 $\text{C}_{\text{C-B}}$ missing);

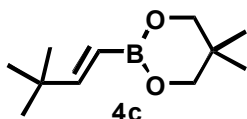
Anal. Calcd for $\text{C}_{14}\text{H}_{16}\text{BF}_3\text{O}_2$: C 59.19, H 5.68. Found: C 59.44, H 5.85.

Preparation of 4c:

A mixture of 3,3-dimethyl-1-butyne (1.0 ml, 8.2 mmol) and dibromoborane dimethylsulfide complex (1 M CH₂Cl₂ sol., 8.2 ml, 8.2 mmol) in methylene chloride (8 ml) was stirred overnight at room temperature. After removal of solvent, 1 M aq. NaOH (8.0 ml) was slowly added to give precipitates, which were collected by suction filtration. The filtrate was extracted with methylene chloride and the solvent was removed under reduced pressure. To the residue was added a small amount of 1M aq. NaOH to give precipitates, which were collected again by suction filtration. The combined precipitates (609 mg) were used for the next esterification.

To a solution of the above precipitates and 2,2-dimethylpropan-1,3-diol (850 mg 8.16 mmol) in ether was added Na₂CO₃, and the mixture was stirred overnight at room temperature. Filtration and evaporation gave crude product (white solid, 1.12 g). A part of this crude product (ca. 700 mg) was purified by GPC to give **4c** (423 mg, 2.2 mmol) in 27 % yield (2 steps).

5,5-Dimethyl-2-(2-*t*-butylethen-1-yl)-1,3,2-dioxaborinane (**4c**)



IR (KBr) 2960, 2869, 1634, 1477, 1414 cm⁻¹;

¹H NMR (CDCl₃) (300 MHz): δ = 0.97 (6H, s), 1.01 (9H, s), 3.64 (4H, s) 5.26 (1H, d, *J* = 18.3 Hz), 6.55 (1H, d, *J* = 18.3 Hz);

¹³C NMR (CDCl₃) (75 MHz): δ = 21.9, 29.0, 31.8, 34.6, 72.1, 161.8 (1C_{C-B} missing);

Anal. Calcd for C₁₁H₂₁BO₂: C 67.37, H 10.79. Found: C 67.08, H 10.59.

General procedure for copper-catalyzed carboxylation of arylboronic esters with carbon dioxide (in the presence of bis(oxazoline)):

A DMF suspension (2.5 ml) of CuI (1.9 mg, 0.01 mmol), bisoxazoline ligand **1** (2.9 mg, 0.01 mmol), arylboronic ester (0.2 mmol) and CsF (0.60 mmol, 91 mg) was stirred in a glass tube (ϕ = 1.7 cm, 18 cm) under an atmospheric pressure of CO₂ and then the system was closed. The mixture was heated at 90 °C for 10 hours, and then the reaction was quenched with 1 M HCl aq. Organic layer was extracted with Et₂O four times and the combined extract was dried over MgSO₄. After removal of the solvent under reduced pressure, the residue was purified by silica gel chromatography (hexane : CH₂Cl₂ = 7:1 – 0:1, followed by CH₂Cl₂: ethyl acetate = 9:1) or by reverse extraction (Et₂O/aq. NaHCO₃ then Et₂O/ aq. HCl) followed by filtration through silica gel to afford corresponding carboxylic acids.

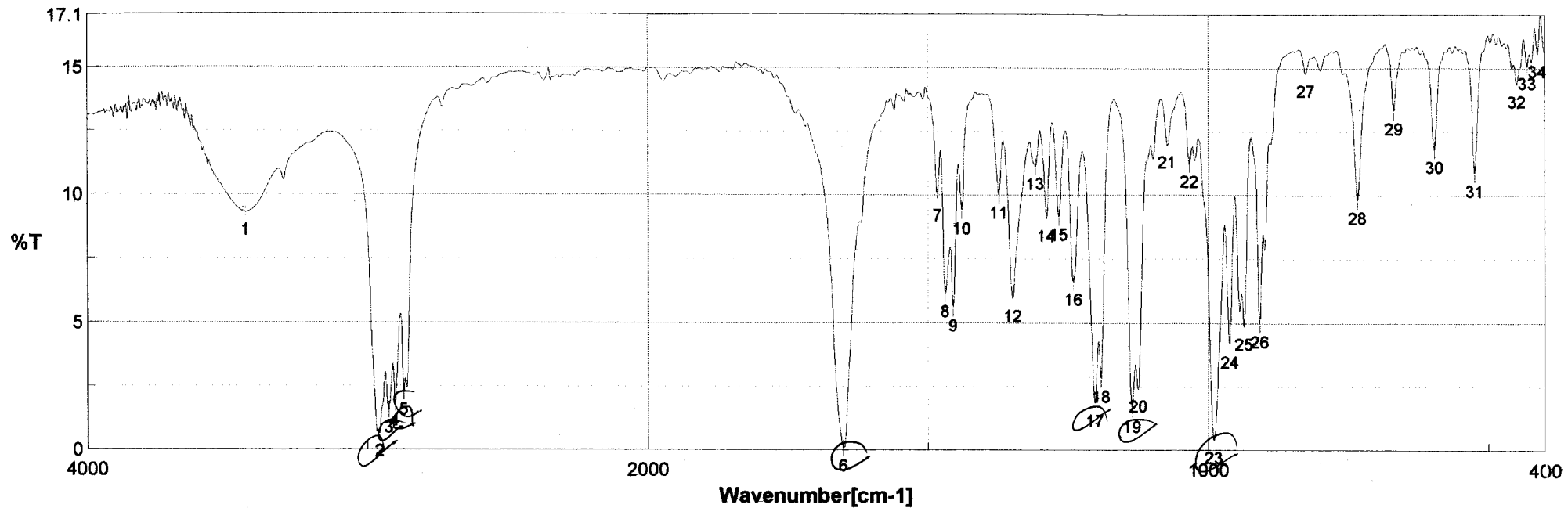
General procedure for copper-catalyzed carboxylation of alkenylboronic esters with carbon dioxide (in the absence of bis(oxazoline)):

A DMF suspension (2.5 ml) of CuI (1.9 mg, 0.01 mmol), alkenylboronic ester (0.2 mmol) and CsF (0.60 mmol, 91 mg) was stirred in a glass tube ($\phi = 1.7$ cm, 18 cm) under an atmospheric pressure of CO₂ and then the system was closed. The mixture was heated at 90 °C for 10 hours, and then the reaction was quenched with 1 M HCl aq. Organic layer was extracted with Et₂O four times and the combined extract was dried over MgSO₄. After removal of the solvent under reduced pressure, the residue was purified by silica gel chromatography (hexane : CH₂Cl₂ = 7:1 – 0:1, followed by CH₂Cl₂ : ethyl acetate = 9:1) or by reverse extraction (Et₂O/aq. NaHCO₃ then Et₂O/ aq. HCl) followed by filtration through silica gel to afford corresponding carboxylic acids.

Spectroscopic data of carboxylic acids **3f**⁸, **3g**⁹, **5b**¹⁰, **5c**¹¹ and **5e**¹² were reported in the literature. Other carboxylic acids were commercially available.

References

- (1) *N,N'*-Bis(2-chloroethyl)-2,2-di-*n*-butylpropan-1,3-diamide was prepared according to the literature procedure for the synthesis of analogous diamide, which was an intermediate for the synthesis of well established chiral bis(oxazoline) ligand, see; Evans, D. A.; Woerpel, K. A.; Hinman, M. M.; Faul, M. M. *J. Am. Chem. Soc.* **1991**, *113*, 726-728.
- (2) Kabalka, G. W.; Akula, M. R.; Zhang, J. *Nuclear Medicine and Biology* **2002**, *29*, 841.
- (3) Ukai, K.; Aoki, M.; Takaya, J.; Iwasawa, N. *J. Am. Chem. Soc.* **2006**, *128*, 8706.
- (4) Kobayashi, Y.; Nakayama, Y.; Mizojiri, R. *Tetrahedron* **1998**, *54*, 1053.
- (5) Wong, K. -T.; Chien, Y.-Y.; Liao, Y.-L.; Lin, C.-C.; Chou, M.-Y.; Leung, M.-k. *J. Org. Chem.* **2002**, *67*, 1041.
- (6) (a) Ishiyama, T.; Murata, M.; Miyaura, N. *J. Org. Chem.* **1995**, *60*, 7508. (b) Ishiyama, T.; Itoh, Y.; Kitano, T.; Miyaura, N. *Tetrahedron Lett.* **1997**, *38*, 3447.
- (7) Brown, H. C.; Gupta, S. K. *J. Am. Chem. Soc.* **1975**, *97*, 5249.
- (8) Moore, L. R.; Western, E. C.; Craciun, R.; Spruell, J. M. Dixon, D. A.; O'Halloran, K. P.; Shaughnessy, K. H. *Organometallics* **2008**, *27*, 576.
- (9) Gavrin, A. J.; Douglas, E. P. *Macromolecules* **2001**, *34*, 5876.
- (10) Concellón, J. M.; Concellón, C. *J. Org. Chem* **2006**, *71*, 1728.
- (11) Freeman, F.; Kappos, J. C. *J. Org. Chem* **1986**, *51*, 1654.
- (12) Zhao, X.; Alper, H.; Yu, Z. *J. Org. Chem* **2006**, *71*, 3988.



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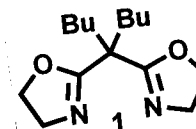
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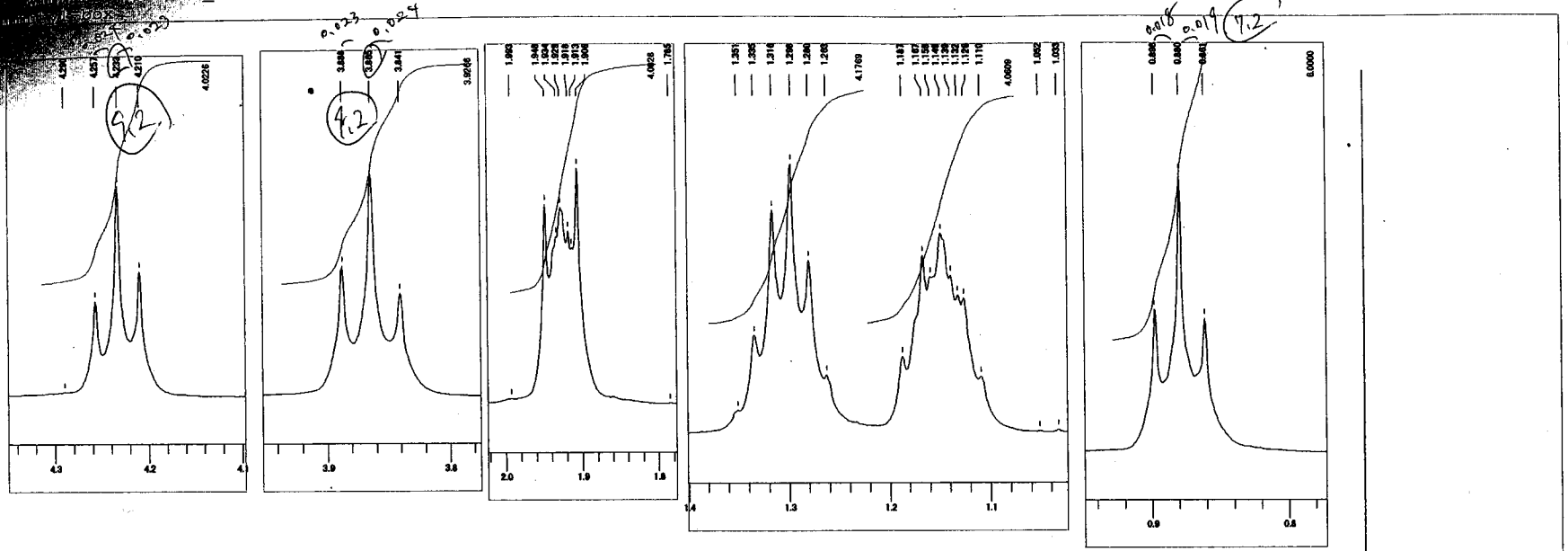
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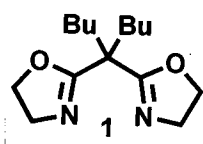
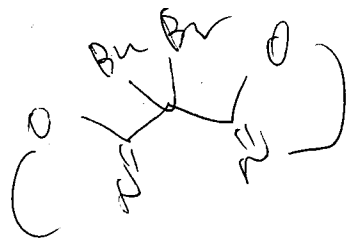
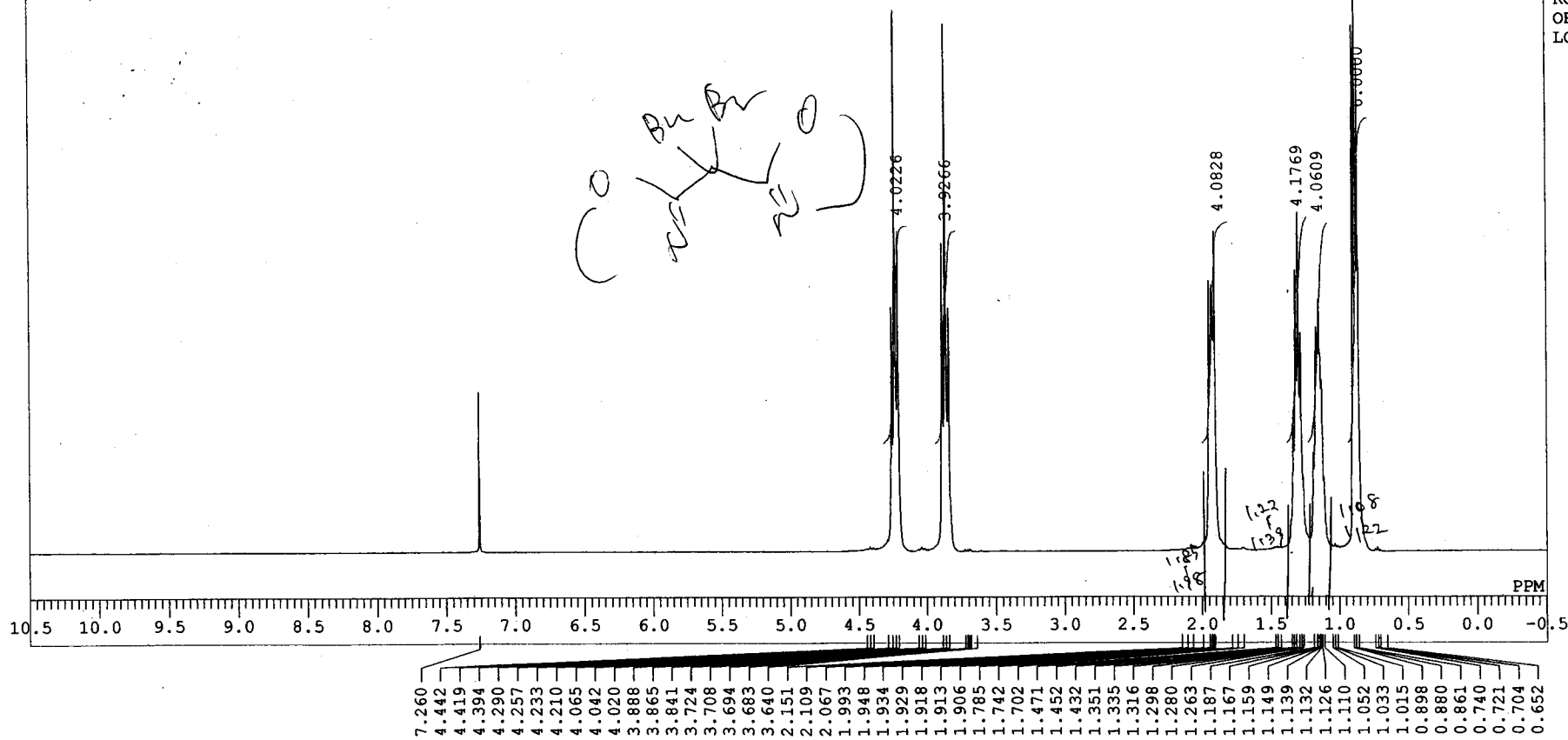


KBr

No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3434.6	9.30336	2	2957.3	0.644323	3	2925.48	1.5638	4	2902.34	1.84656
6	1651.73	0.0884961	7	1482.99	9.89013	8	1469.49	6.12949	9	1455.03	5.57555
11	1374.03	9.98835	12	1348.96	5.94129	13	1308.46	11.1259	14	1289.18	9.07627
16	1240.97	6.59655	17	1202.4	1.84133	18	1191.79	2.79966	19	1135.87	1.61584
21	1073.19	11.9587	22	1033.66	11.1954	23	990.268	0.396422	24	962.305	4.1444
26	908.308	4.94581	27	826.348	14.792	28	733.782	9.79478	29	669.178	13.2945
31	524.543	10.8477	32	449.333	14.3615	33	431.012	15.0836	34	412.692	15.5631



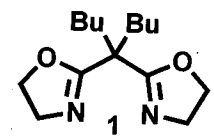
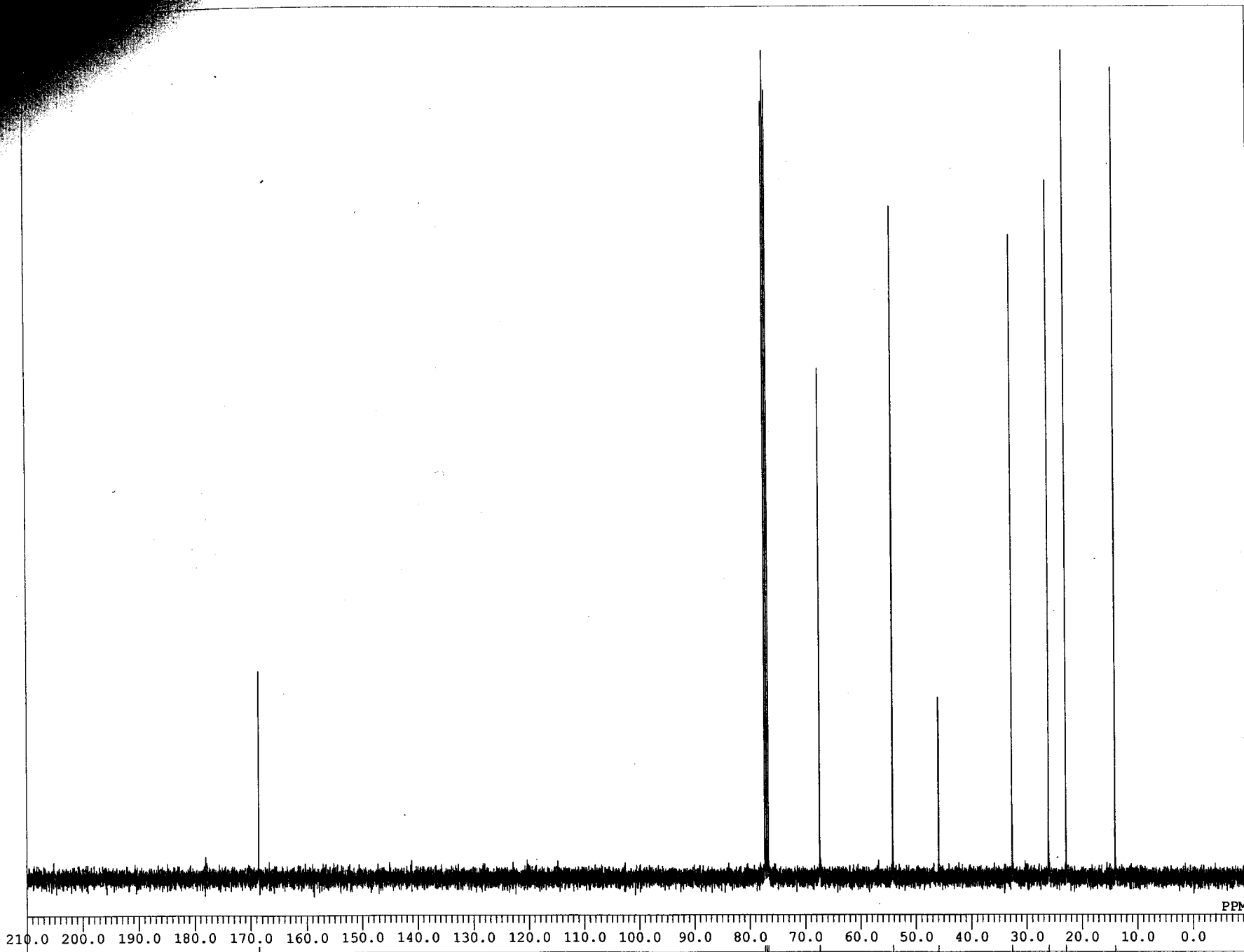
DFILE C:\WINNMR98\COMMON\
 COMNT dubutyl-box
 DATIM Sat Jan 27 22:39:46
 EXMOD NON
 OBNUC 1H
 OBFRQ 399.65 MHz
 OBSET 124.00 KHz
 OBFIN 10500.0 Hz
 POINT 32768
 FREQU 8000.0 Hz
 CLPNT 256
 TODAT 1
 CLFRQ 500.0 Hz
 SCANS 16
 ACQTM 4.096 sec
 PD 2.904 sec
 PW1 6.2 us
 PW2 10.0 us
 PW3 10.0 us
 PI1 1.000 ms
 PI2 1.000 ms
 PI3 1.00 ms
 IRNUC 1H
 CTEMP 24.7 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 CLEXR 0.00
 RGAIN 13
 OBATN 511
 LOOP1 1



in CDCl₃

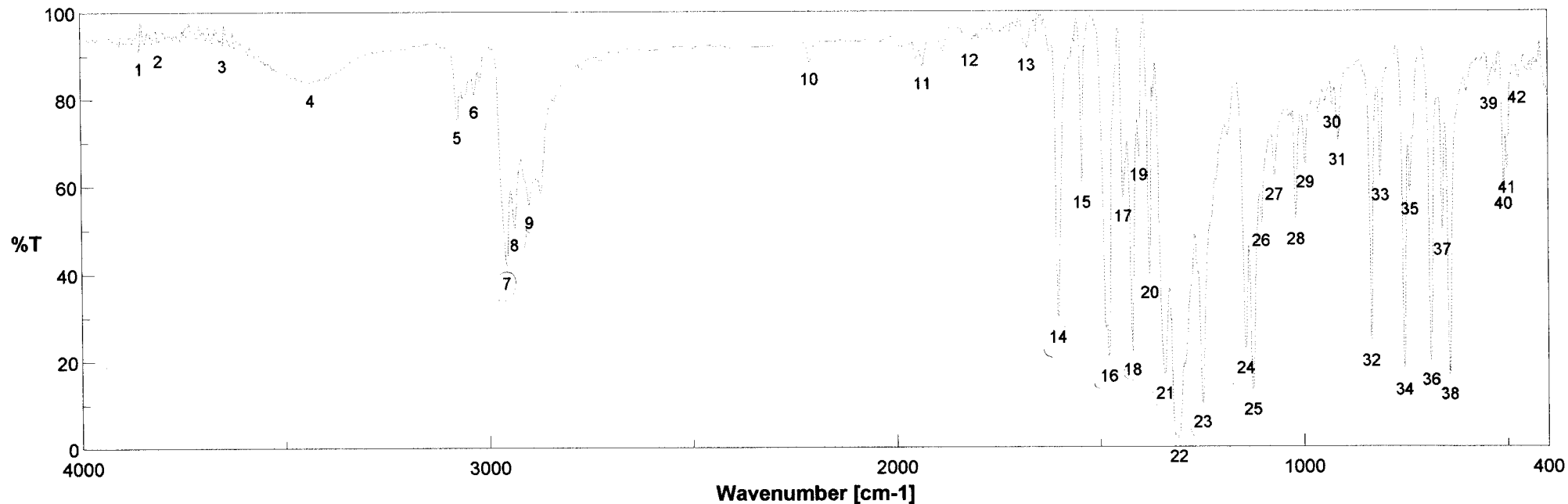
7.260
 4.442
 4.419
 4.394
 4.290
 4.257
 4.233
 4.210
 4.065
 4.042
 4.020
 3.888
 3.865
 3.841
 3.724
 3.708
 3.694
 3.683
 3.640
 2.151
 2.109
 2.067
 1.993
 1.948
 1.934
 1.929
 1.918
 1.913
 1.906
 1.785
 1.742
 1.702
 1.471
 1.452
 1.432
 1.351
 1.335
 1.316
 1.298
 1.280
 1.263
 1.187
 1.167
 1.159
 1.149
 1.139
 1.132
 1.126
 1.110
 1.052
 1.033
 1.015
 0.898
 0.880
 0.861
 0.740
 0.721
 0.704
 0.652

DFILE C:\WINNMR98\COMMON\
 COMNT dubutyl-box
 DATIM Sat Jan 27 23:22:58
 EXMOD BCM
 OBNUC 13C
 OBFRQ 100.40 MHz
 OBSET 125.00 KHz
 OBFIN 10500.0 Hz
 POINT 32768
 FREQU 27173.9 Hz
 CLPNT 256
 TODAT 1
 CLFRQ 500.0 Hz
 SCANS 818
 ACQTM 1.206 sec
 PD 1.794 sec
 PW1 5.9 us
 PW2 10.0 us
 PW3 10.0 us
 PI1 1.000 ms
 PI2 1.000 ms
 PI3 1.00 ms
 IRNUC 1H
 CTEMP 24.3 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 CLEXR 0.00
 RGAIN 25
 OBATN 511
 LOOP1 1



in CDCl₃

68.536
 77.322
 77.000
 76.687
 SI 11
 57.472
 54.248
 45.924
 32.676
 26.092
 22.941
 14.040

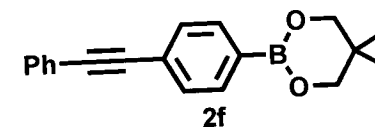


number of scan
zero filling
gain
date of scan
sample name

16
ON
Auto (8)
2007/02/20 21:29
NO. 2-2-20

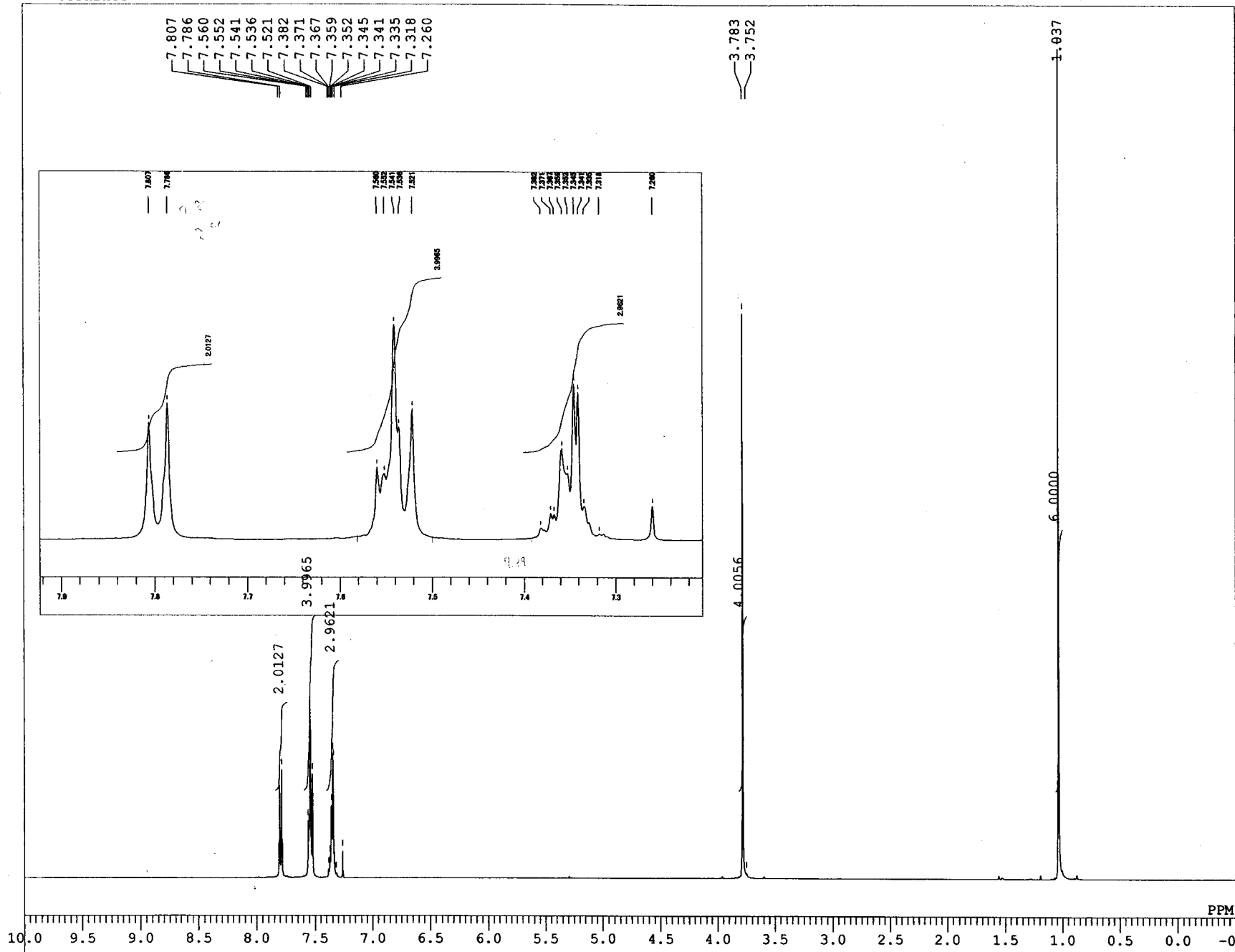
resolution
apodization
scan speed
date of data processing

4 cm-1
Cosine
Auto (2 mm/sec)
2007/02/20 21:30



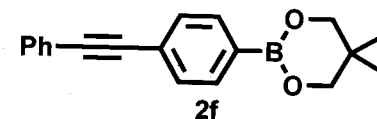
KBr

No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3855.01	91.1013	2	3807.76	92.8935	3	3650.59	91.6271	4	3434.6	83.631
6	3033.48	81.0022	7	2956.34	41.774	8	2937.06	50.5001	9	2900.41	55.6262
11	1932.32	87.3045	12	1816.62	92.7239	13	1677.77	91.5581	14	1603.52	29.2498
16	1478.17	20.2883	17	1442.49	56.8353	18	1421.28	21.6623	19	1403.92	66.2783
21	1341.25	16.2837	22	1308.46	1.85978	23	1249.65	9.67323	24	1142.62	22.1147
26	1103.08	51.2216	27	1070.3	61.7868	28	1018.23	51.6274	29	995.089	64.5191
31	914.093	69.614	32	834.062	23.6986	33	810.92	61.615	34	753.066	17.0829
36	687.498	19.3045	37	659.536	49.0449	38	642.179	16.0254	39	543.828	82.49
41	499.473	63.2658	42	473.439	83.9786				5	3075.9	75.1079
									10	2210.99	88.356
									15	1542.77	60.0363
									20	1377.89	39.3488
									25	1125.26	12.5859
									30	927.593	78.1489
									35	738.603	58.3344
									40	509.115	59.6203

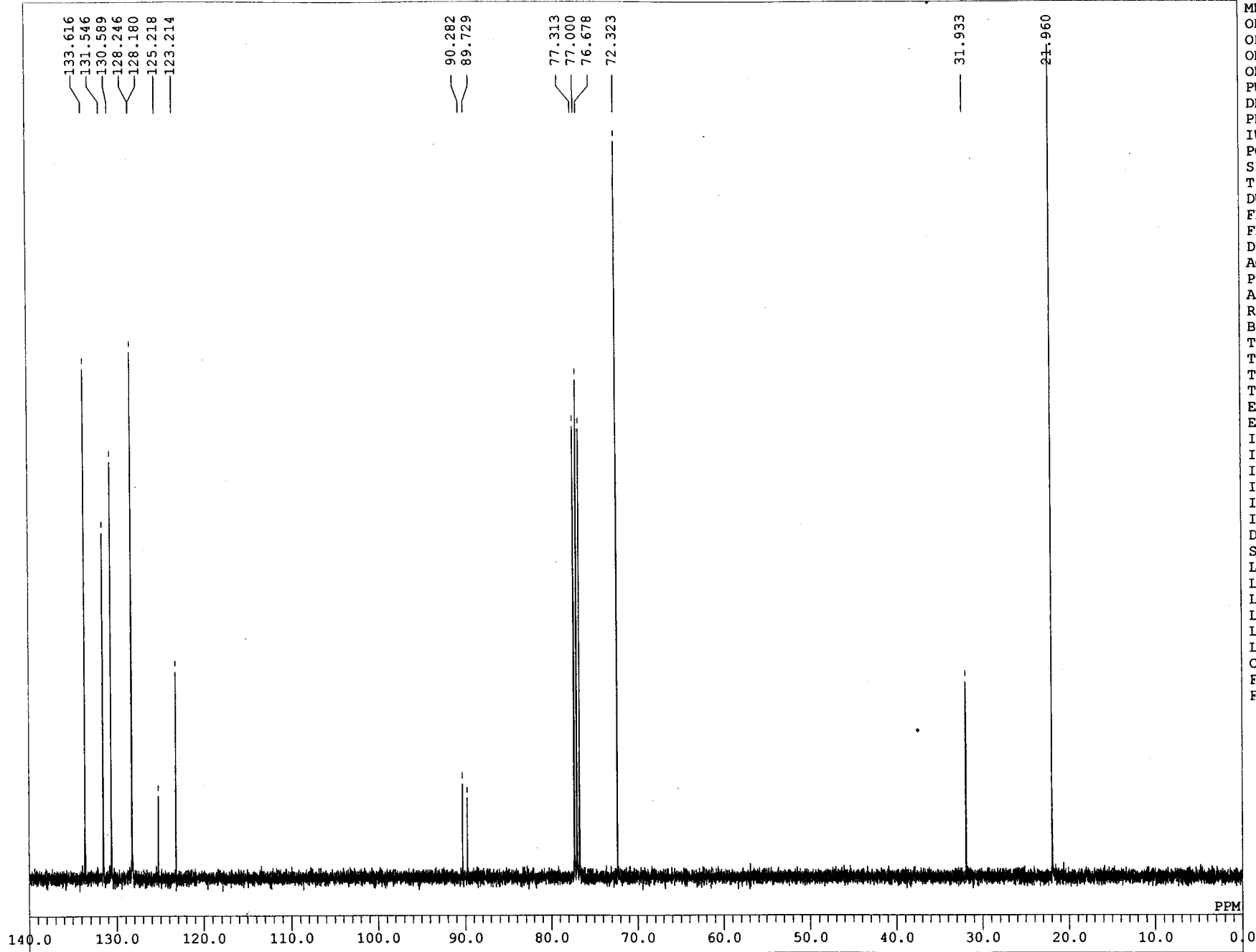


```

MENUF  NON
OBNUC  1H
OFR    399.65 MHz
OBSET  124.00 KHz
OBFIN  10500.0 Hz
PW1    6.2 us
DEADT  71.9 us
PREDL  0.2000 ms
IWT    1.0 sec
POINT  32768
SPO    32768
TIMES  16
DUMMY  0
FREQU  8000.0 Hz
FLT    4000 Hz
DELAY  50.0 us
ACQTM  4.096 sec
PD     1.500 sec
ABBIT  16.00
RGAIN  14
BF     0.10 Hz
T1    0.00
T2    0.00
T3    90.00
T4    100.00
EXMOD  NON
EXPCM  NON:Single.coupled:PW1_F
IRNUC  1H
IFR    399.65 MHz
IRSET  124.00 KHz
IRFIN  10500.0 Hz
IRRPW  50 us
IRATN  511
DFILE  C:\WINNMR98\COMMON\DATA\
SF     TH5
LKSET  61.60 KHz
LKFIN  79.0 Hz
LKLEV  200
LGAIN  22
LKPHS  77
LKSIG  402
CSPED  12 Hz
FILDC
FILDF
    
```

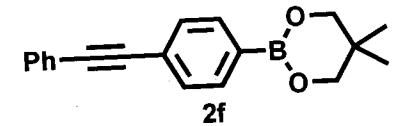


in CDCl₃

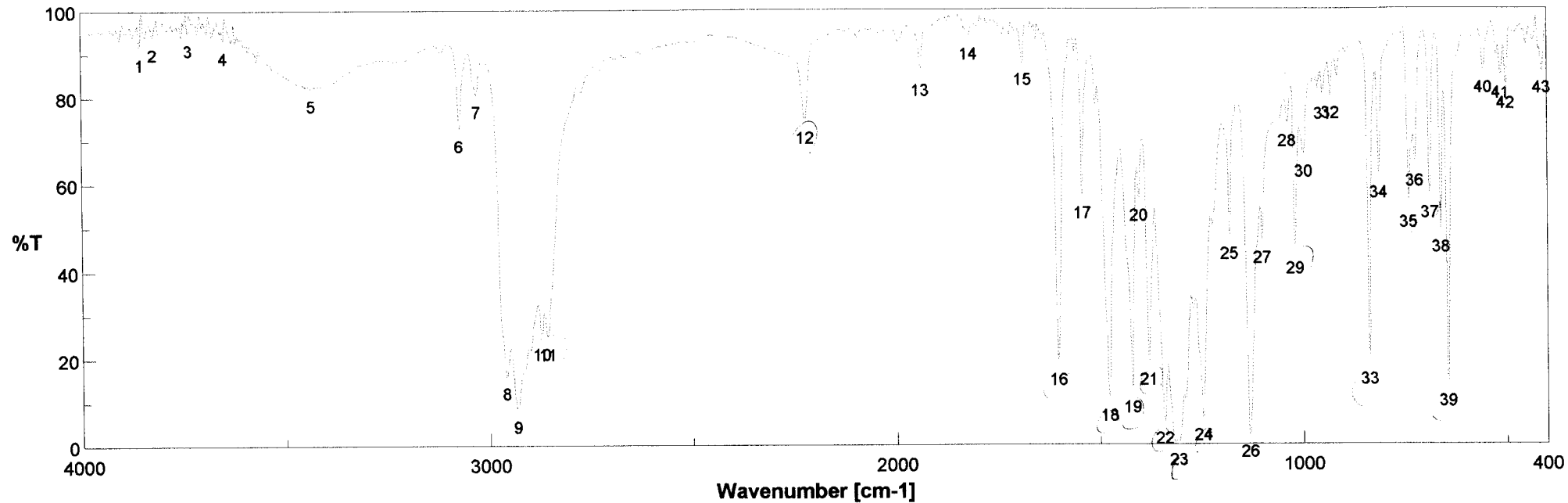


```

MENUF BCM
OBNUC 13C
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.0 Hz
PW1 5.9 us
DEADT 19.1 us
PREDL 0.2000 ms
IWT 1.0 sec
POINT 32768
SPO 32768
TIMES 1000
DUMMY 1
FREQU 27173.9 Hz
FLT 13600 Hz
DELAY 14.7 us
ACQTM 1.206 sec
PD 2.000 sec
ADBIT 16.00
RGAIN 24
BF 0.10 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD BCM
EXPCM Bilevel.complete.decoupl
IRNUC 1H
IFR 399.65 MHz
IRSET 124.00 KHz
IRFIN 10500.0 Hz
IRRPW 60 us
IRATN 511
DFILE C:\WINNMR98\COMMON\DATA\
SF TH5
LKSET 61.60 KHz
LKFIN 79.0 Hz
LKLEV 200
LGAIN 22
LKPHS 77
LKSIG 409
CSPED 13 Hz
FILDC
FILDF
  
```



in CDCl₃



number of scan
zero filling
gain
date of scan

16
ON
Auto (8)
2007/02/20 21:41

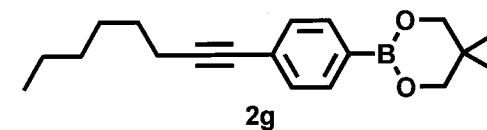
sample name

NO. 3-2-20

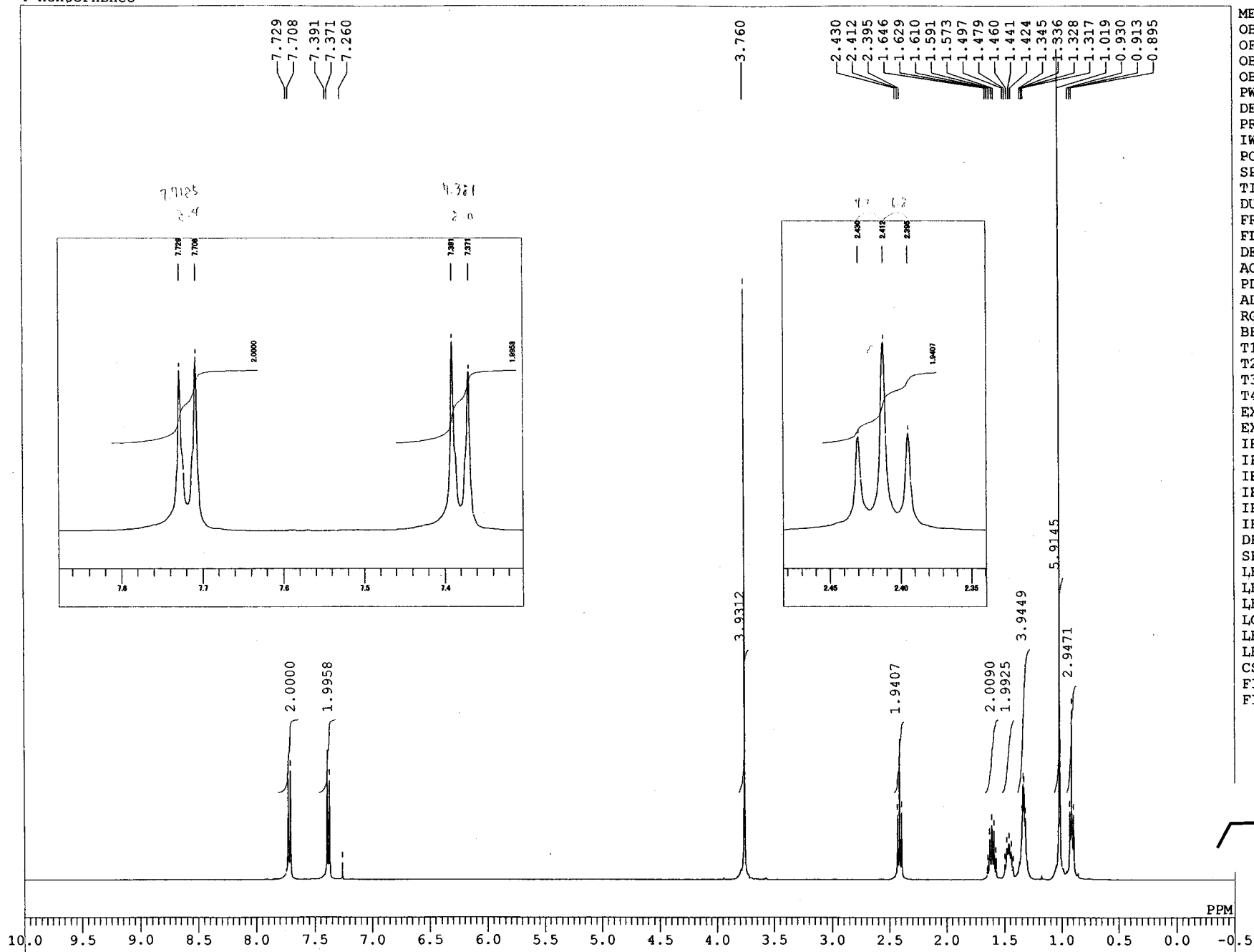
resolution
apodization
scan speed
date of data processing

4 cm-1
Cosine
Auto (2 mm/sec)
2007/02/20 21:42

KBr

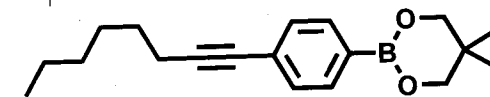


No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3855.01	91.5947	2	3823.19	93.9744	3	3736.4	94.8937	4	3650.59	93.0593
6	3072.05	72.5614	7	3029.62	80.431	8	2958.27	15.9149	9	2932.23	8.24167
11	2857.02	24.8694	12	2222.56	74.4286	13	1938.11	85.2948	14	1819.51	93.6314
16	1602.56	18.9313	17	1541.81	57.0555	18	1477.21	10.7108	19	1421.28	12.5496
21	1380.78	18.9522	22	1342.21	5.42476	23	1308.46	0.477955	24	1247.72	6.14621
26	1132.01	2.31796	27	1100.19	46.6867	28	1037.52	73.3644	29	1019.19	44.2533
31	949.77	79.5985	32	931.45	79.8181	33	837.919	18.8909	34	813.813	61.5733
36	725.104	64.2977	37	688.463	57.1031	38	661.464	49.2047	39	645.072	13.9688
41	512.972	84.5394	42	500.437	82.1799	43	412.692	85.7136	5	3434.6	81.865
									10	2871.49	25.0067
									15	1687.41	87.6778
									20	1403.92	56.4848
									25	1181.19	47.68
									30	997.982	66.3839
									35	740.531	54.8949
									40	556.363	85.7839



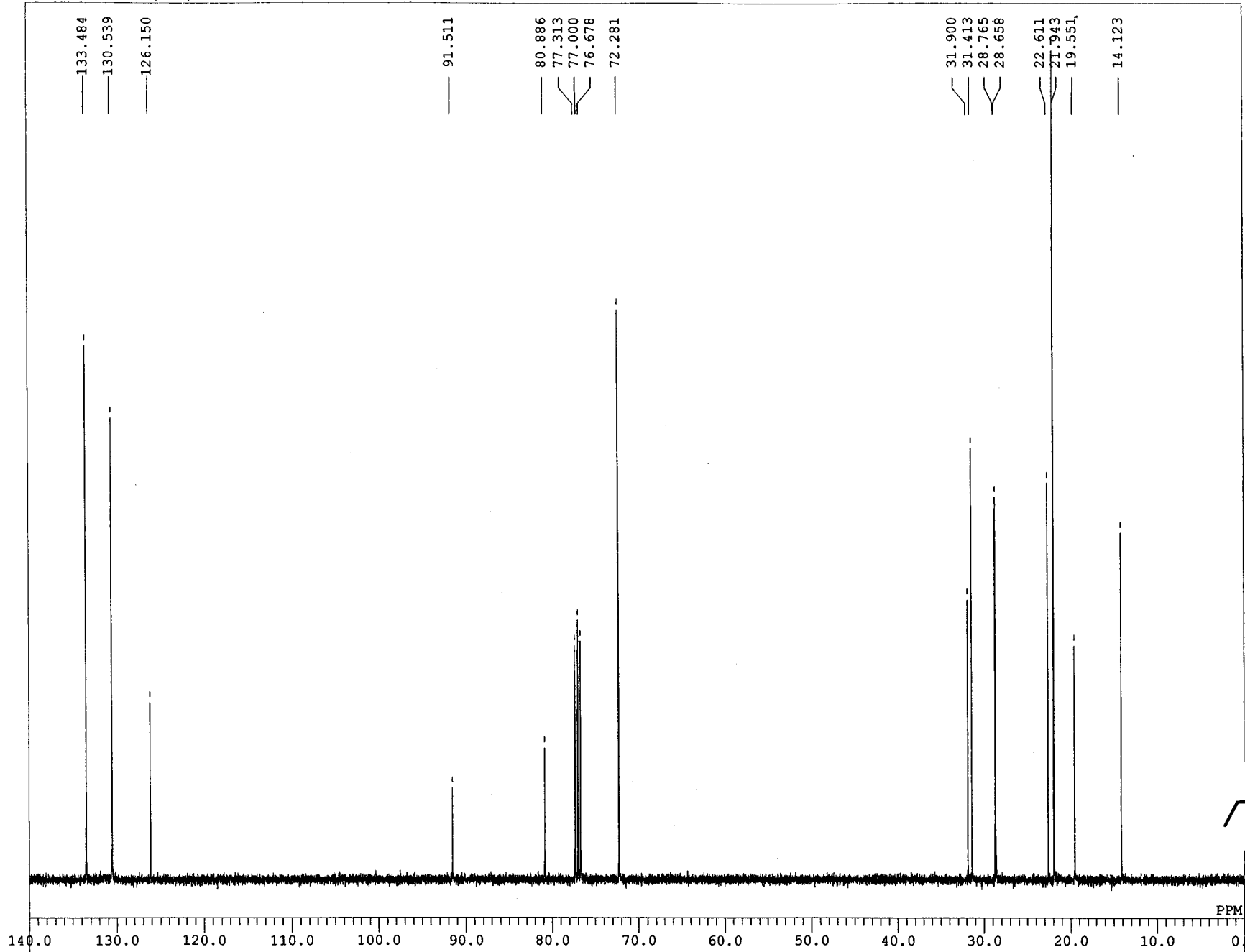
```

MENUF  NON
OBNUC  1H
OFR    399.65 MHz
OBSET  124.00 KHz
OBFIN  10500.0 Hz
PW1    6.2 us
DEADT  71.9 us
PREDL  0.2000 ms
IWT    1.0 sec
POINT  32768
SPO    32768
TIMES  16
DUMMY  0
FREQU  8000.0 Hz
FLT    4000 Hz
DELAY  50.0 us
ACQTM  4.096 sec
PD     1.500 sec
ADBIT  16.00
RGAIN  11
BF     0.10 Hz
T1    0.00
T2    0.00
T3    90.00
T4    100.00
EXMOD  NON
EXPCM  NON:Single.coupled:PW1_f
IRNUC  1H
IFR    399.65 MHz
IRSET  124.00 KHz
IRFIN  10500.0 Hz
IRRPW  50 us
IRATN  511
DFILE  C:\WINNMR98\COMMON\_DEF
SF     TH5
LKSET  61.60 KHz
LKFIN  79.0 Hz
LKLEV  200
LGAIN  22
LKPHS  77
LKSIG  433
CSPED  13 Hz
FILDC
FILDF
  
```



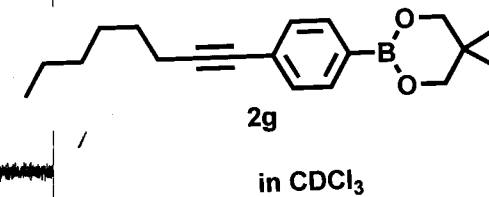
2g

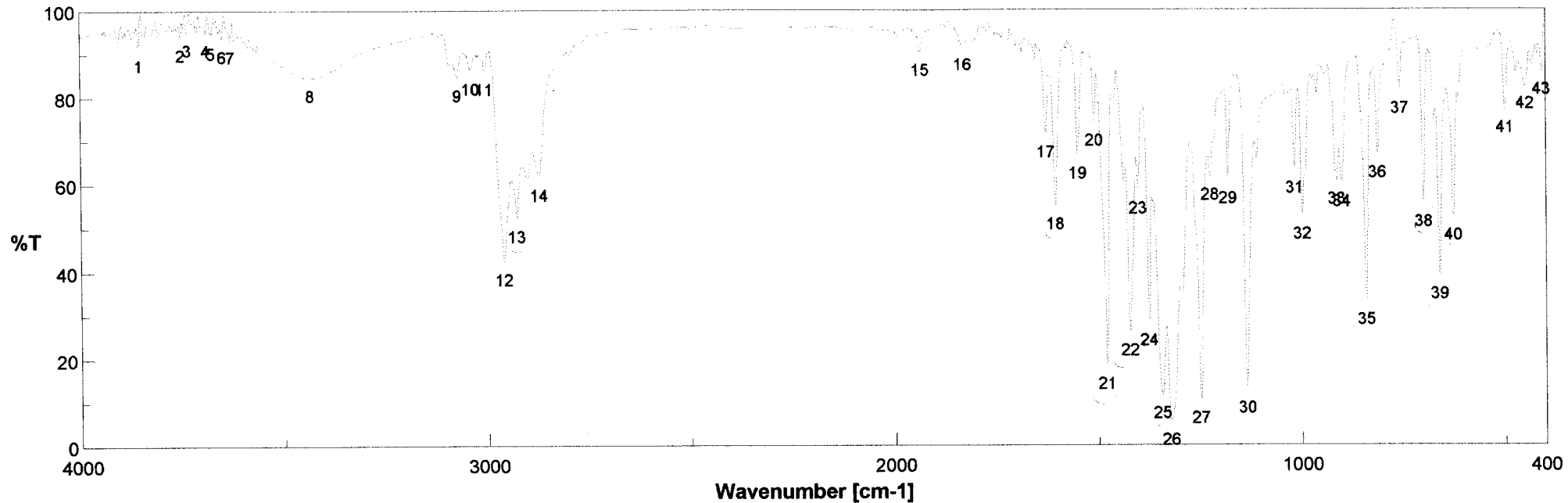
in CDCl₃



```

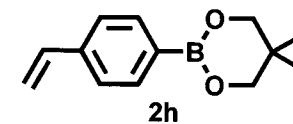
MENUF BCM
OBNUC 13C
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.0 Hz
PW1 5.9 us
DEADT 19.1 us
PREDL 0.2000 ms
IWT 1.0 sec
POINT 32768
SPO 32768
TIMES 1000
DUMMY 1
FREQU 27173.9 Hz
FLT 13600 Hz
DELAY 14.7 us
ACQTM 1.206 sec
PD 2.000 sec
ADBIT 16.00
RGAIN 25
BF 0.10 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD BCM
EXPCM Bilevel.complete.decoupl
IRNUC 1H
IFR 399.65 MHz
IRSET 124.00 KHz
IRFIN 10500.0 Hz
IRRPW 60 us
IRATN 511
DFILE C:\WINNMR98\COMMON\_DEF
SF TH5
LKSET 61.60 KHz
LKFIN 79.0 Hz
LKLEV 200
LGAIN 22
LKPHS 77
LKSIG 434
CSPED 13 Hz
FILDC
FILDF
    
```





number of scan 16
 zero filling ON
 gain Auto (8)
 date of scan 2007/02/20 21:16
 sample name NO. 1-2-20

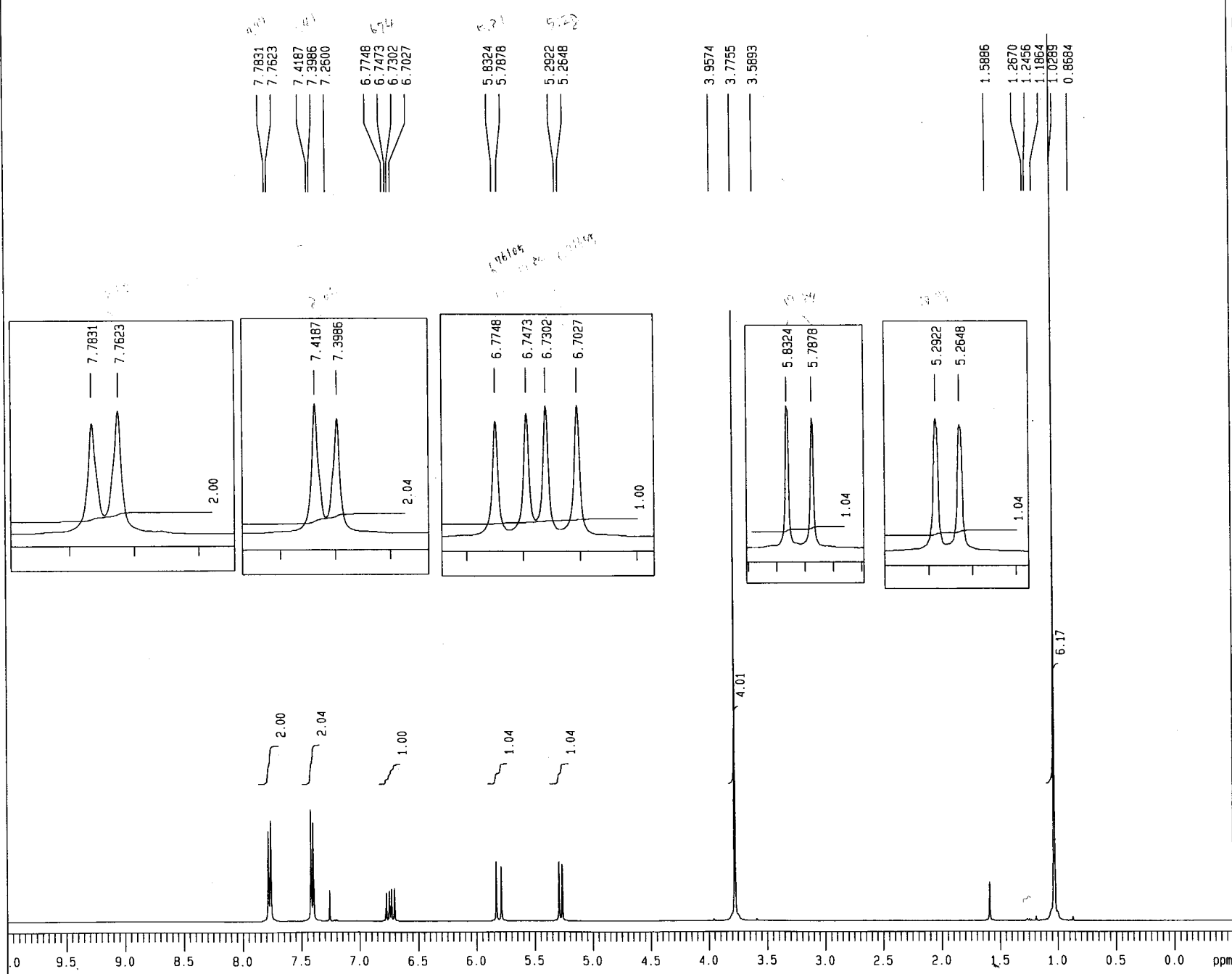
resolution 4 cm-1
 apodization Cosine
 scan speed Auto (2 mm/sec)
 date of data processing 2007/02/20 21:18



KBr

No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3855.01	91.4717	2	3752.8	93.8778	3	3736.4	94.9612	4	3691.09	94.8611
6	3650.59	93.4394	7	3630.34	93.3671	8	3434.6	84.4313	9	3073.98	84.4126
11	3006.48	85.8975	12	2960.2	42.2095	13	2928.38	52.0438	14	2873.42	61.5234
16	1831.08	91.3291	17	1628.59	71.1353	18	1605.45	54.8026	19	1550.49	66.3106
21	1479.13	18.1768	22	1423.21	25.8698	23	1402.96	58.3249	24	1375.96	28.1924
26	1321.96	5.28914	27	1249.65	10.2446	28	1225.54	61.4059	29	1181.19	60.6499
31	1017.27	62.9169	32	998.946	52.441	33	913.129	60.4658	34	901.558	59.8236
36	813.813	66.4201	37	758.852	81.1916	38	700.998	55.2665	39	661.464	38.7255
41	499.473	76.7273	42	450.297	82.29	43	409.799	85.6178			
									5	3677.59	94.2052
									10	3040.23	85.9796
									15	1935.22	90.0719
									20	1509.03	73.8859
									25	1344.14	11.3914
									30	1135.87	12.5815
									35	841.776	32.8188
									40	627.716	52.1901

p-vinyl-C6H4Bneo

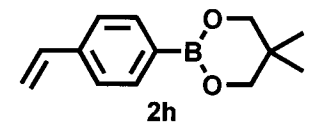


Date : Thu Jul 27 01:57:38 2006

FileName : .LoadingFID.nmdata
 Comment : p-vinyl-C6H4Bneo
 SliceHistory :
 EXMODE : non

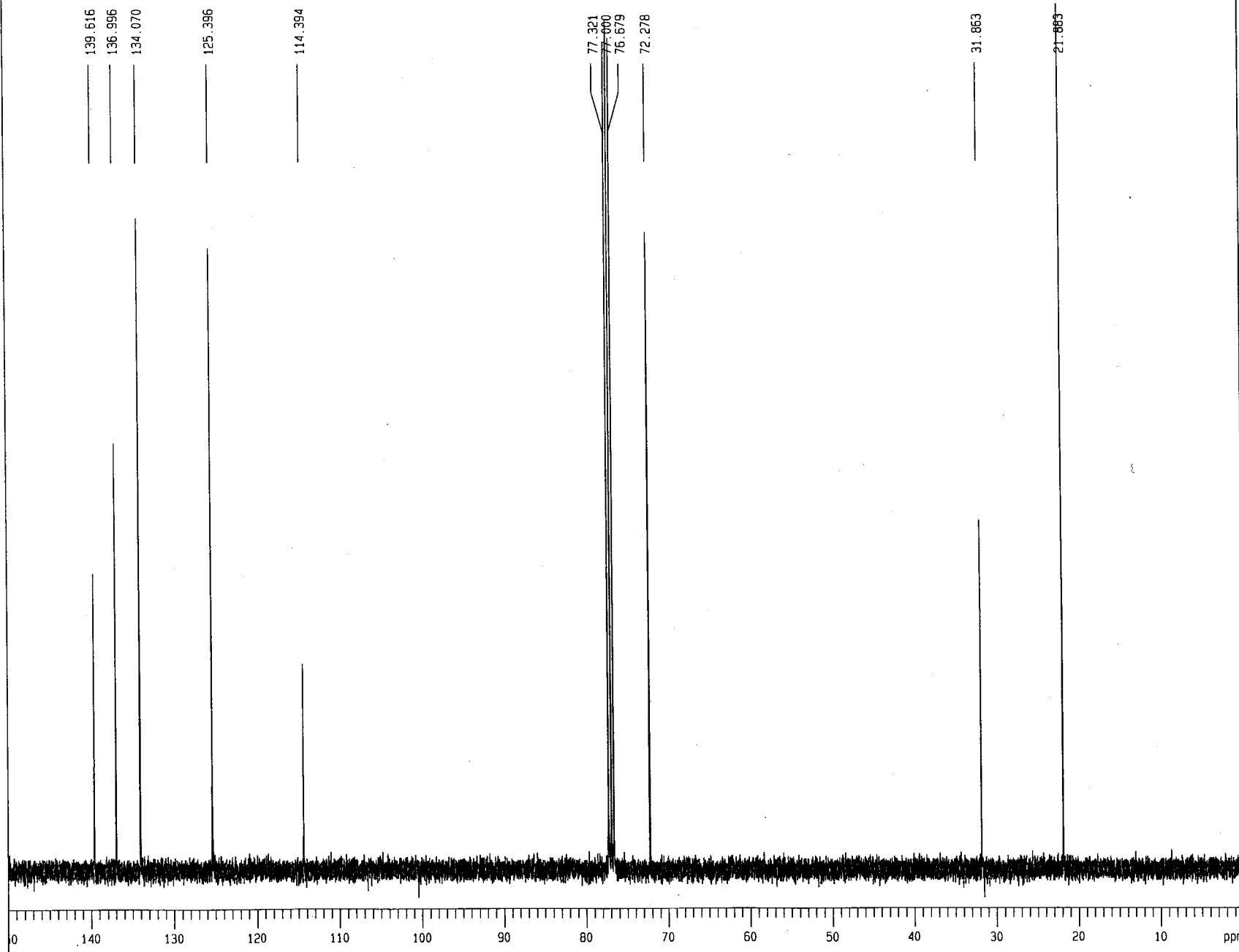
POINT : 32768 points
 SAMPO : 32768 points
 FREQU : 7917.7 Hz
 FILTR : 3950 Hz
 DELAY : 50.6 usec
 DEADT : 72.4 usec
 INTVL : 126.3 usec
 TIMES : 16 times
 DUMMY : 1 times
 PD : 1.5000 sec
 ACQTM : 4138.5986 msec
 PREDL : 0.01000 msec
 INIWT : 1000.0000 msec
 RESOL : 0.24 Hz
 PW1 : 7.00 usec
 OBNUC : 1H
 OBFRO : 395.75 MHz
 OBSET : 134498.00 Hz
 RBAIN : 20

SCANS : 16 times
 SLVNT : CDCL3
 SPINNING : 12 Hz
 TEMP : 24.0 C

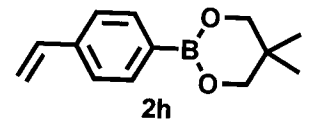


in CDCl₃

p-vinylC6H4Bneo

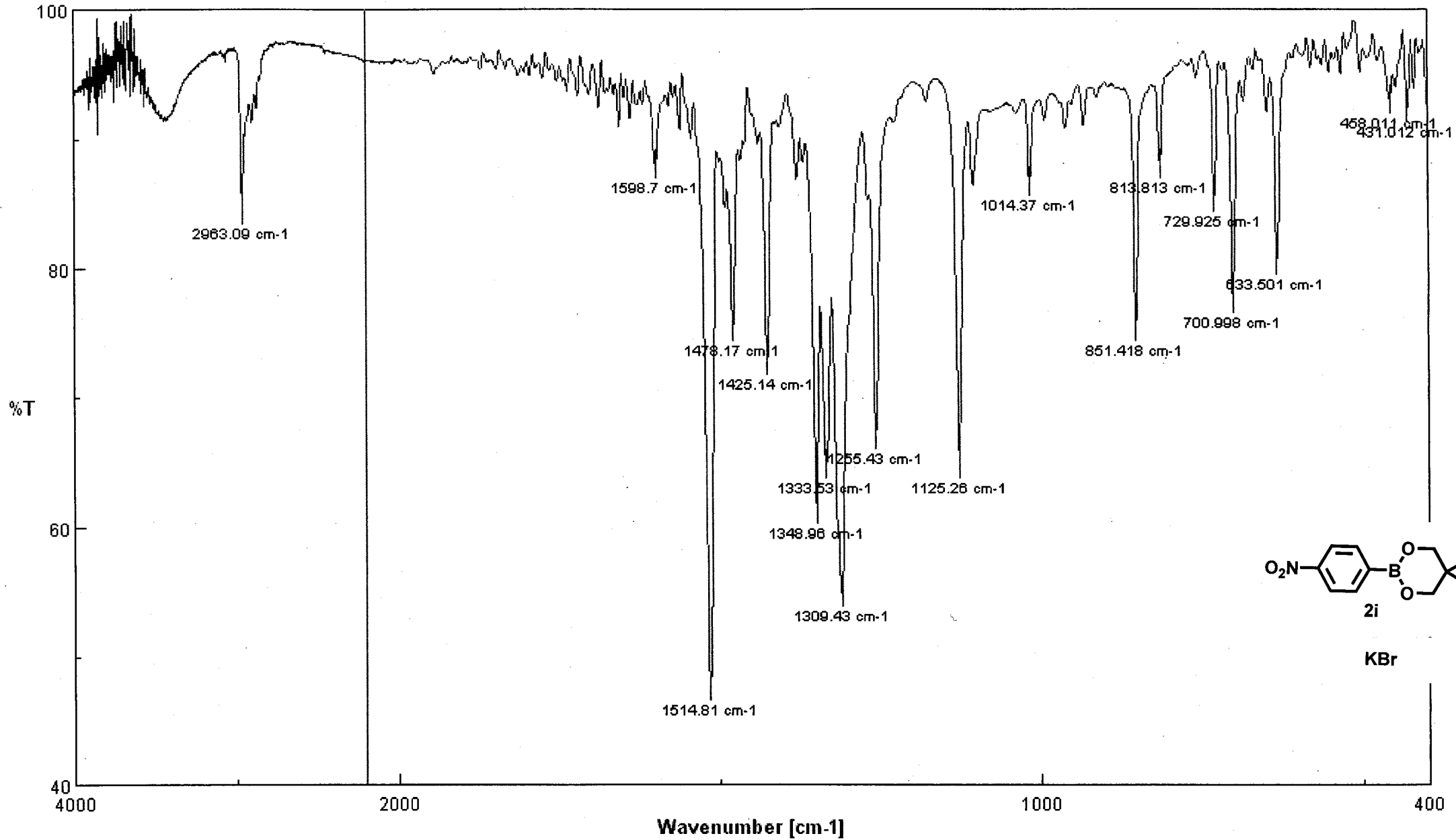


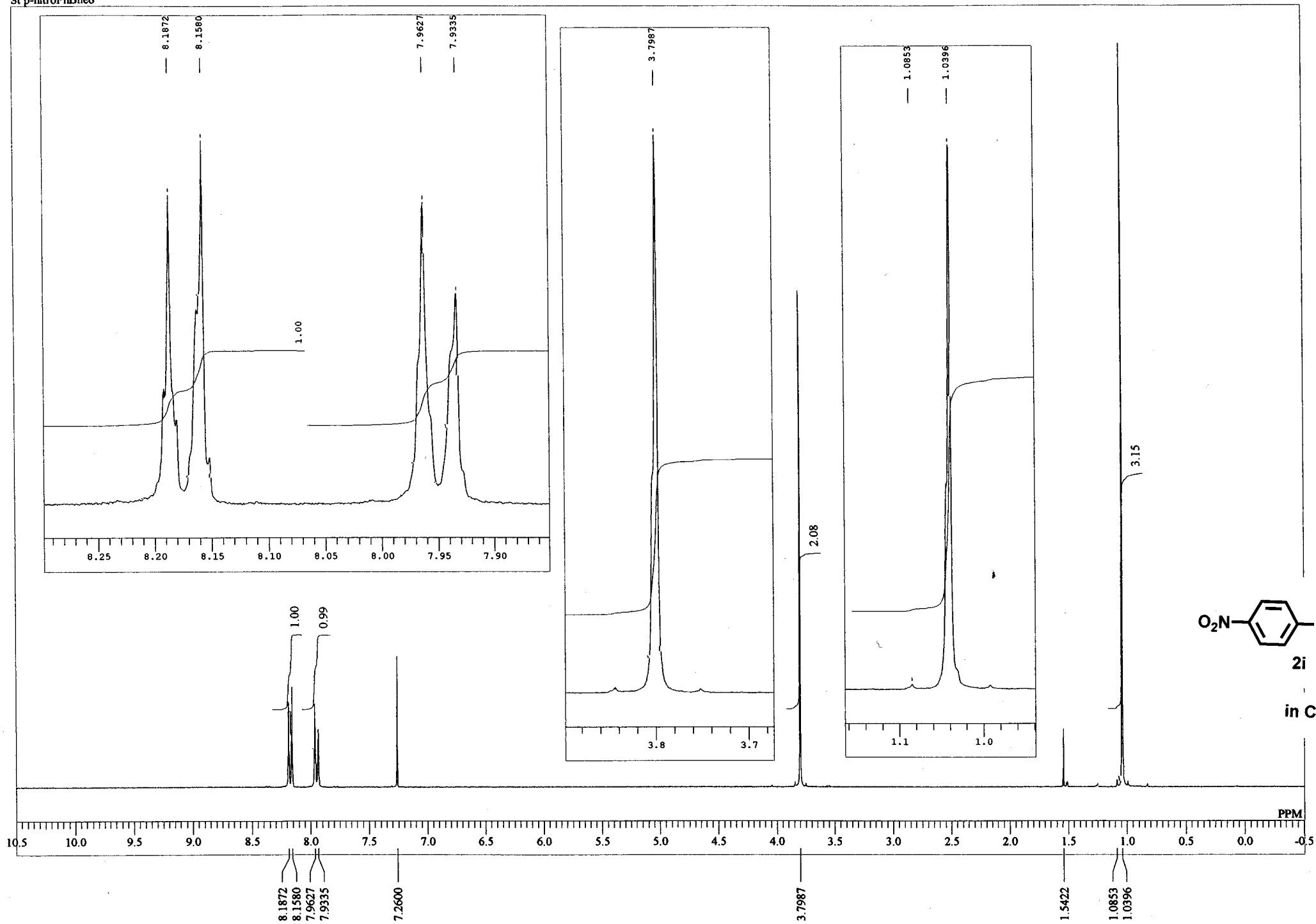
Date : Thu Jul 27 02: 46: 44 2006
FileName : .LoadingFID.nmdata
Comment : p-vinylC6H4Bneo
SliceHistory :
EXMODE : bcm
POINT : 65536 points
SAMPO : 65536 points
FREQU : 26881.7 Hz
FILTR : 13450 Hz
DELAY : 14.9 usec
DEADT : 19.9 usec
INTVL : 37.2 usec
TIMES : 1000 times
DUMMY : 4 times
PD : 2.0000 sec
ACQTM : 2437.9392 msec
PREDL : 0.01000 msec
INIWT : 1000.0000 msec
RESOL : 0.41 Hz
PW1 : 4.90 usec
QBNUC : 13C
QBFRQ : 99.45 MHz
OBSET : 104750.00 Hz
RGAIN : 35
IRNUC : 1H
IRFRQ : 395.75 MHz
IRSET : 134498.00 Hz
IRRPW : 46.0 usec
IRRNS : 0
SCANS : 645 times
SLVNT : CDCL3
SPINNING : 13 Hz
TEMP : 24.8 C



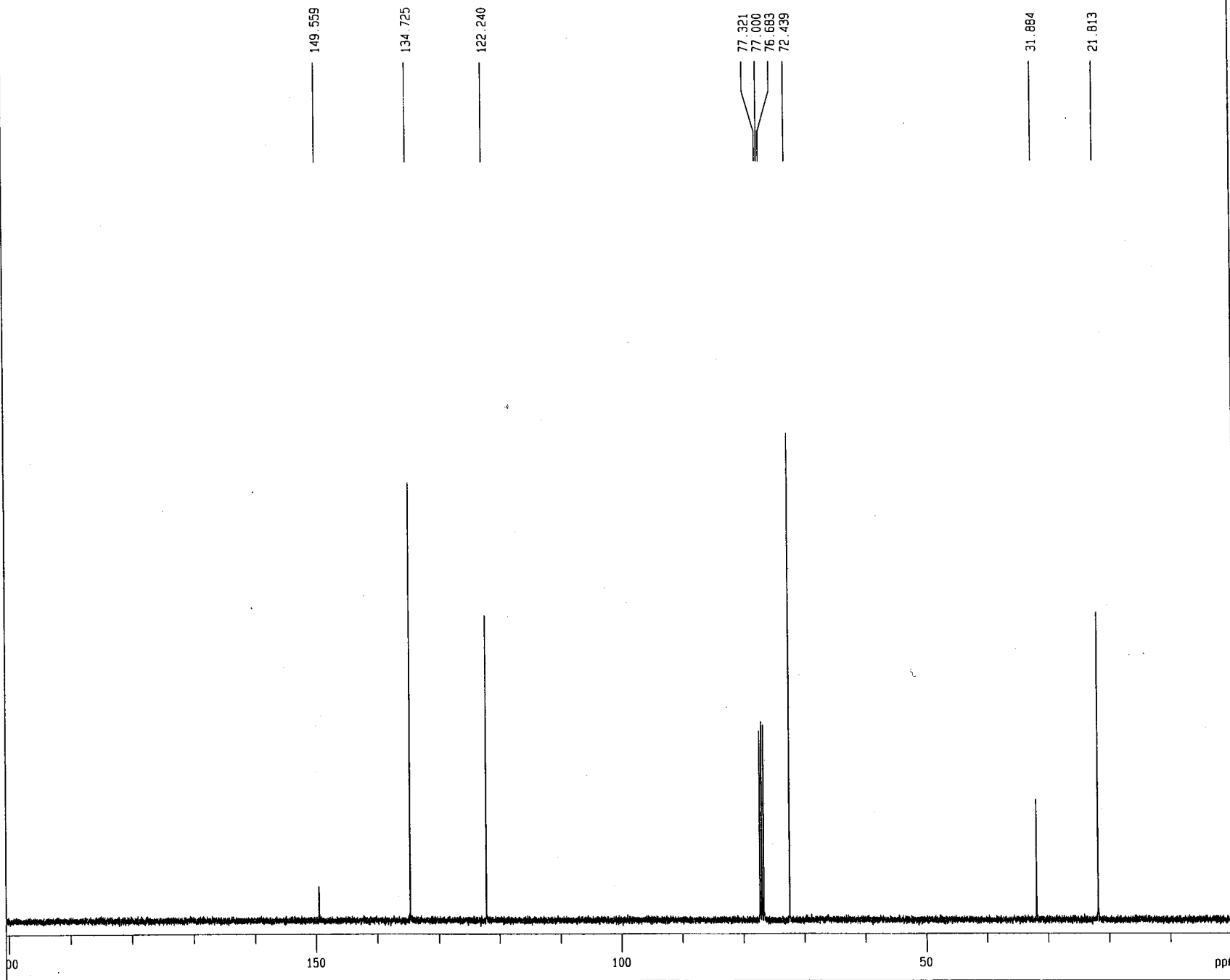
in CDCl₃

p-Nitro ph Bneo





T-02NC6H4Bneo



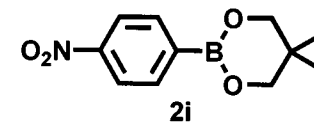
Date : Thu Jun 14 14:29:53 2007

FileName : .LoadingFID.nmdat
 Comment : T-02NC6H4Bneo
 SliceHistory :
 EXMODE : bcm

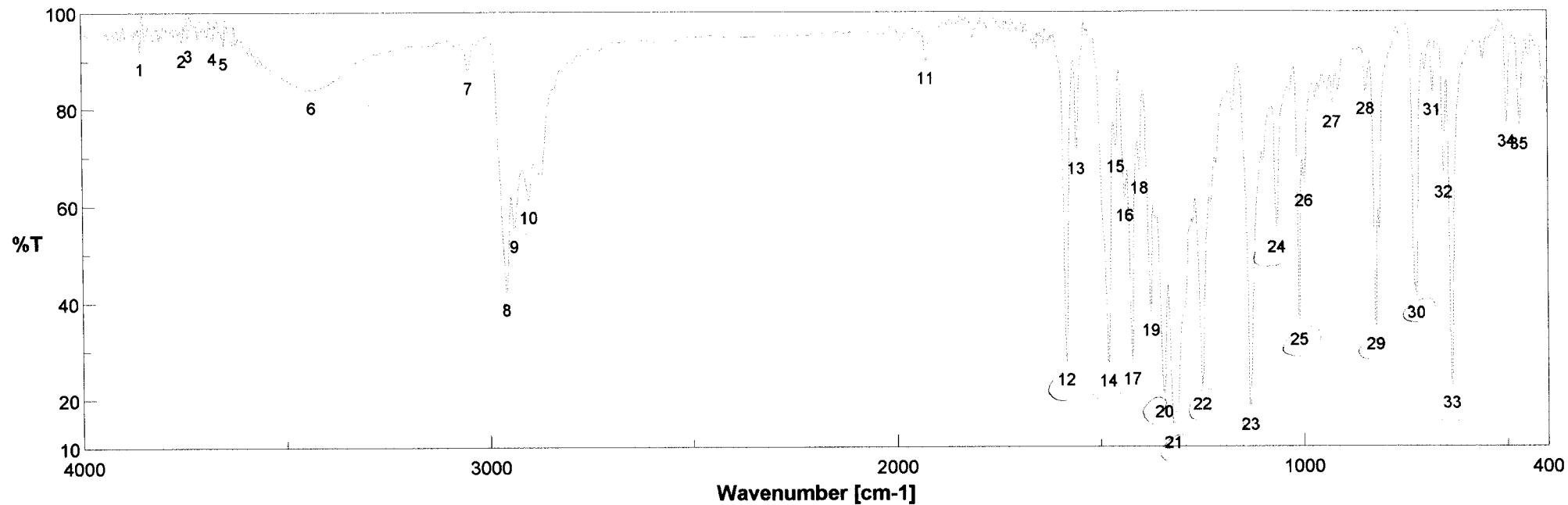
POINT : 65536 points
 SAMPO : 65536 points
 FREQU : 26881.7 Hz
 FILTR : 13450 Hz
 DELAY : 14.9 usec
 DEADT : 19.9 usec
 INTVL : 37.2 usec
 TIMES : 2000 times
 DUMMY : 0 times
 PD : 1.0000 sec
 ACQTM : 2437.9392 msec
 PREOL : 0.01000 msec
 INIWT : 1000.0000 msec
 RESOL : 0.41 Hz
 PW1 : 4.90 usec
 OBNUC : 13C
 OBFRO : 99.45 MHz
 OBSET : 104750.00 Hz
 RGAIN : 23
 IRNUC : 1H
 IRFRO : 395.75 MHz
 IRSET : 134498.00 Hz
 IRRPW : 46.0 usec
 IRRNS : 0

SCANS : 1220 times

SLVNT : CDCL3
 SPINNING : 12 Hz
 TEMP : 26.7 C

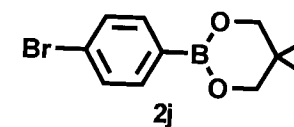


in CDCl₃



number of scan 16
 zero filling ON
 gain Auto (8)
 date of scan 2007/02/20 21:54
 sample name NO. 4-2-20

resolution 4 cm-1
 apodization Cosine
 scan speed Auto (2 mm/sec)
 date of data processing 2007/02/20 21:55



KBr

No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3855.01	91.9697	2	3752.8	93.7262	3	3736.4	94.6935	4	3677.59	94.0935
6	3434.6	83.8105	7	3049.87	87.8194	8	2958.27	42.068	9	2938.98	55.151
11	1925.57	89.7682	12	1584.24	27.4431	13	1557.24	70.9663	14	1480.1	27.2381
16	1438.64	61.38	17	1422.24	27.6141	18	1402.96	67.0011	19	1375.96	37.643
21	1321	14.4083	22	1250.61	22.3306	23	1132.01	18.1111	24	1065.48	54.8068
26	997.982	64.2599	27	927.593	80.5866	28	845.633	83.2929	29	823.455	34.7555
31	682.677	83.046	32	655.679	66.0056	33	637.358	22.5933	34	499.473	76.5797
									5	3650.59	93.0547
									10	2903.31	61.0797
									15	1459.85	71.3526
									20	1344.14	20.7815
									25	1011.48	35.6355
									30	723.175	41.205
									35	468.617	75.9739

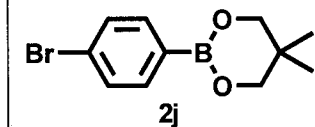
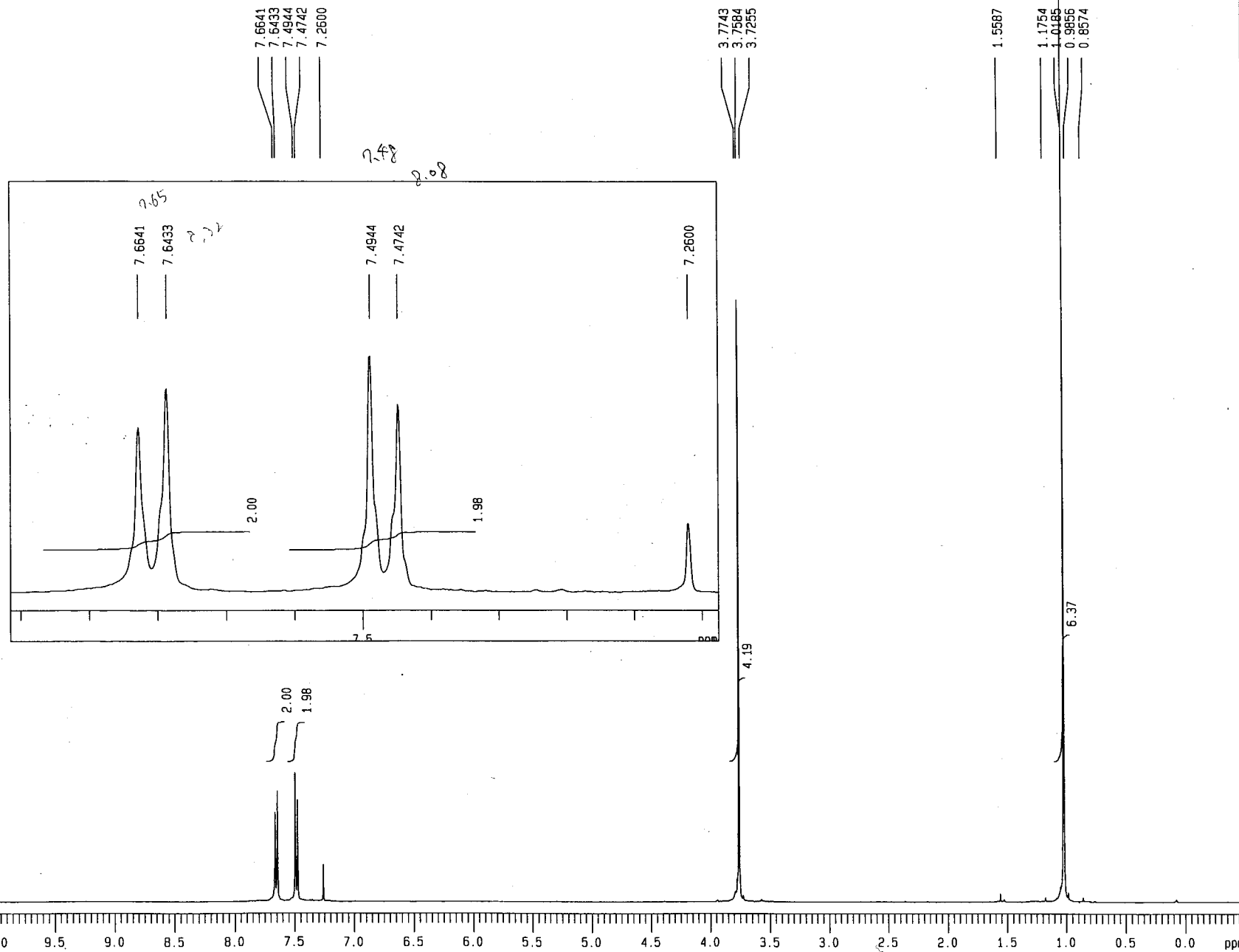
Date : Sat Feb 24 21:15:23 2007

FileName : .LoadingFID.nmdata
 Comment : 4-Br-PhBneo
 SliceHistory :
 EXMODE : non

POINT : 32768 points
 SAMPO : 32768 points
 FREQU : 7917.7 Hz
 FILTR : 3950 Hz
 DELAY : 50.6 usec
 DEADT : 72.4 usec
 INTVL : 126.3 usec
 TIMES : 16 times
 DUMMY : 1 times
 PD : 1.5000 sec
 ACQTM : 4138.5986 msec
 PREDL : 0.01000 msec
 INIWT : 1000.0000 msec
 RESOL : 0.24 Hz
 PW1 : 7.00 usec
 OBNUC : 1H
 OBFREQ : 395.75 MHz
 OBSSET : 134498.00 Hz
 RGAIN : 22

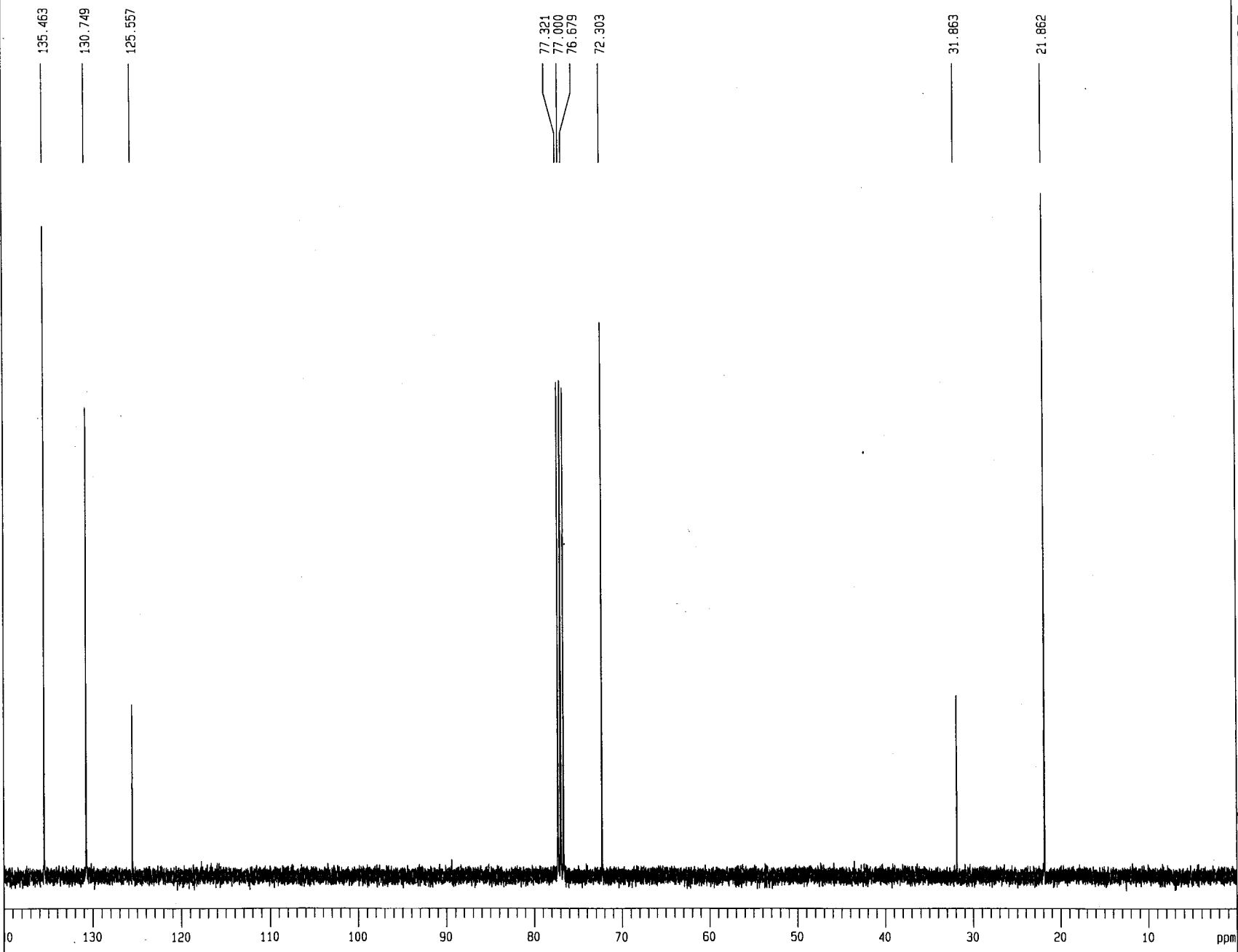
SCANS : 16 times

SLVNT : CDCL3
 SPINNING : 12 Hz
 TEMP : 23.6 C



in CDCl₃

4-Br-PhBneo (13C)



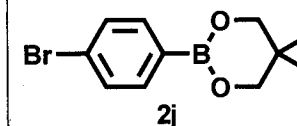
Date : Sat Feb 24 21:55:56 2007

FileName : .LoadingFID.nmdata
 Comment : 4-Br-PhBneo (13C)
 SliceHistory :
 EXMODE : bcm

POINT : 65536 points
 SAMPO : 65536 points
 FREQU : 26881.7 Hz
 FILTR : 13450 Hz
 DELAY : 14.9 usec
 DEADT : 19.9 usec
 INTVL : 37.2 usec
 TIMES : 1000 times
 DUMMY : 4 times
 PD : 2.0000 sec
 ACQTM : 2437.9392 msec
 PREDL : 0.01000 msec
 INIWT : 1000.0000 msec
 RESOL : 0.41 Hz
 PW1 : 4.90 usec
 OBNUC : 13C
 OBFREQ : 99.45 MHz
 OBSET : 104750.00 Hz
 RGAIN : 35
 IRNUC : 1H
 IRFREQ : 395.75 MHz
 IRSET : 134498.00 Hz
 IRRPW : 46.0 usec
 IRRNS : 0

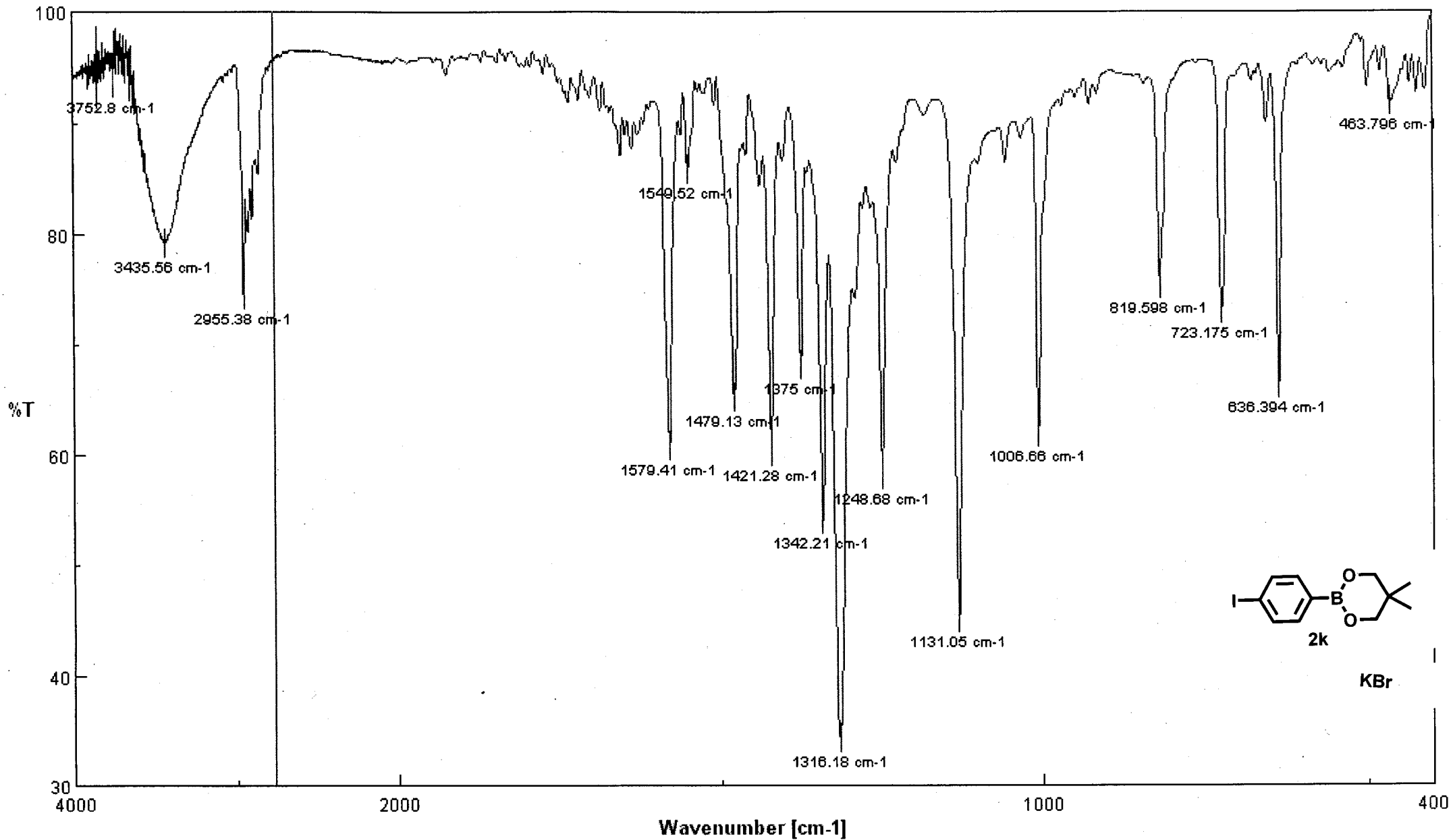
SCANS : 531 times

SLVNT : CDCL3
 SPINNING : 10 Hz
 TEMP : 25.2 C

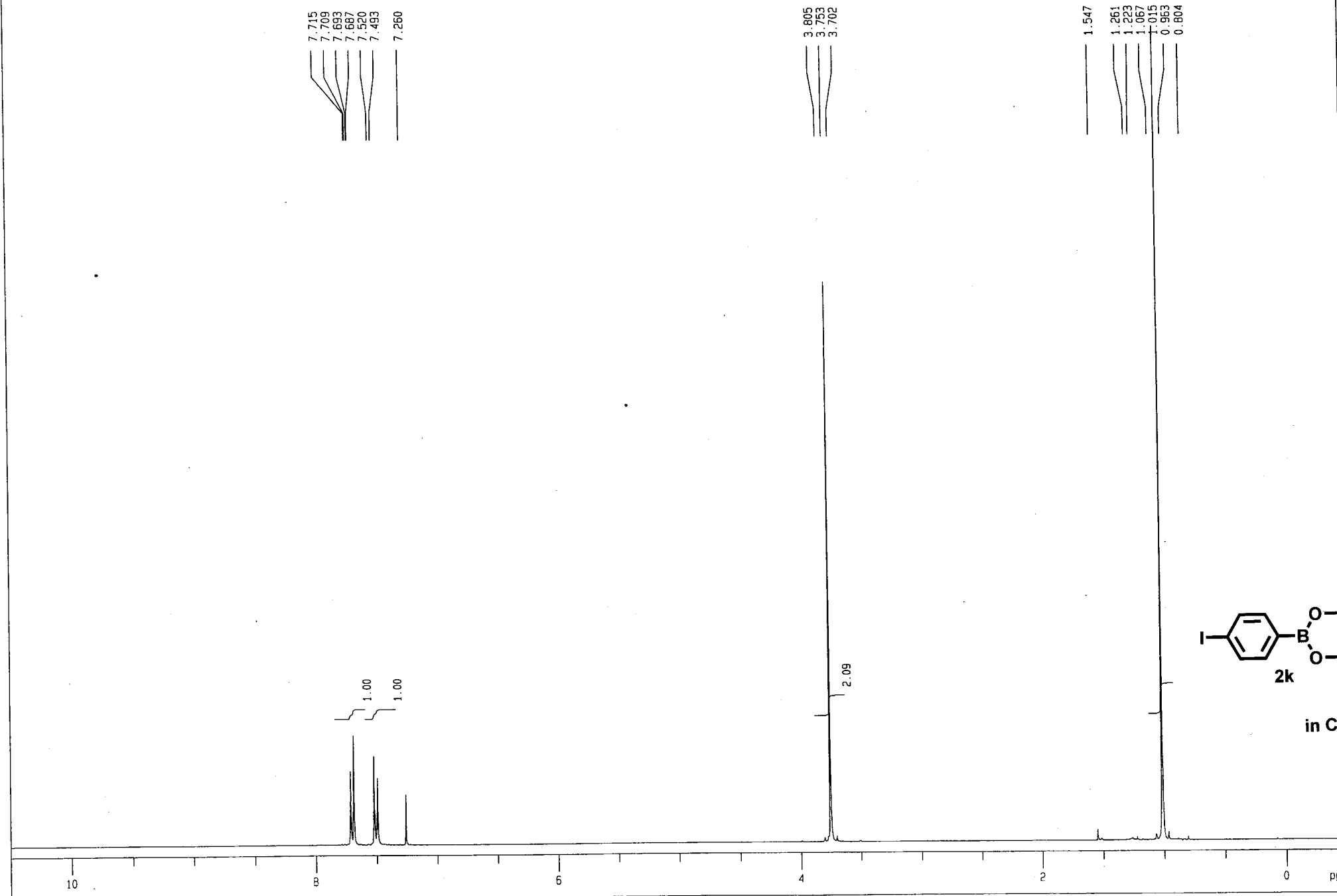


in CDCl₃

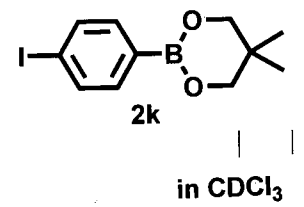
p-Iodo phenyl Bneo



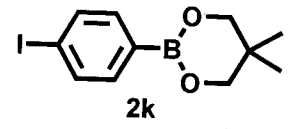
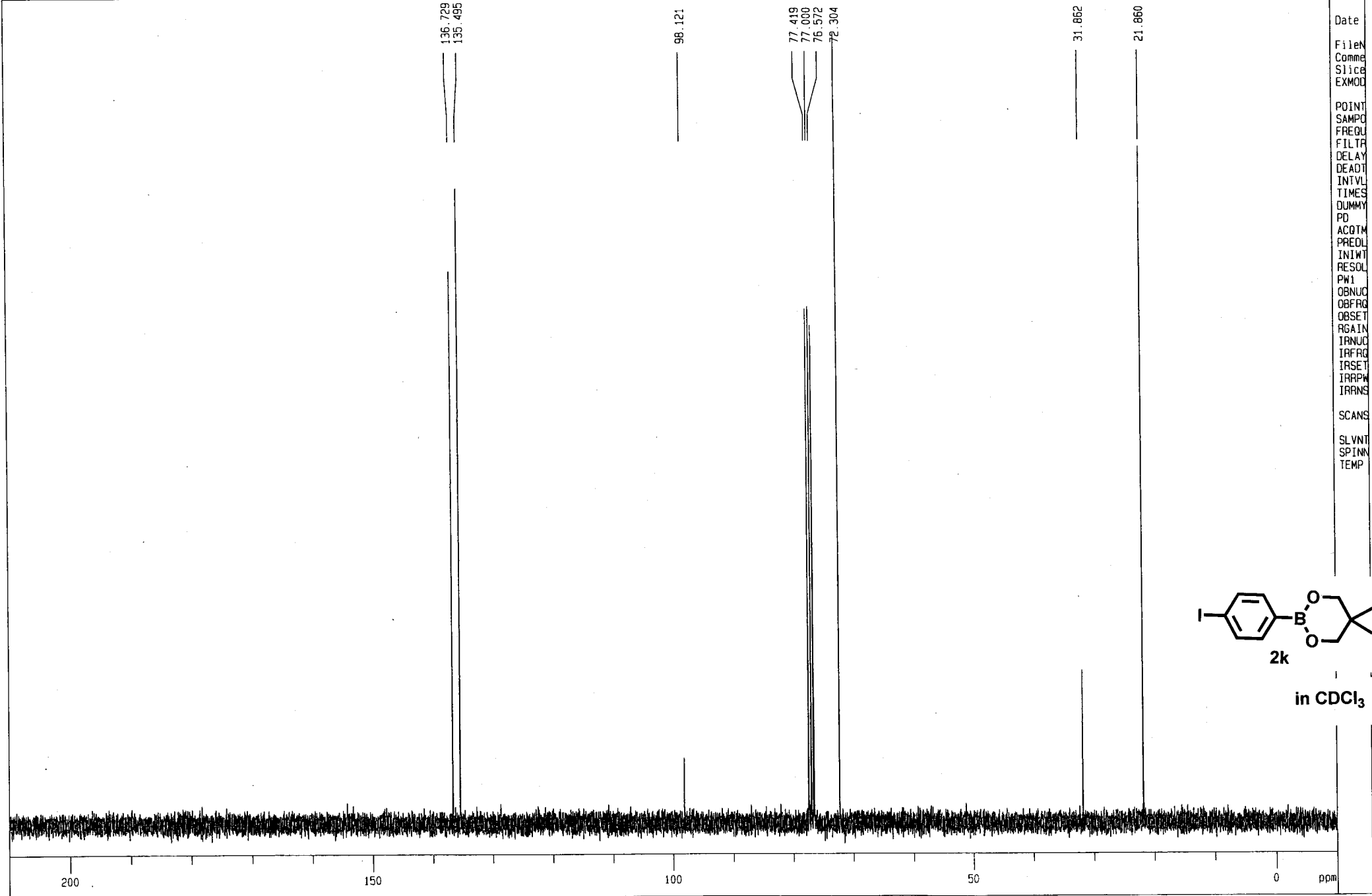
St SM p-iodophenyl Bneo



Date
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POINT
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FILTR
DELAY
DEADT
INTVL
TIMES
DUMMY
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ACQTM
PREDL
INIWT
RESOL
PW1
OBNUC
OBFRQ
OBSET
RGAIN
SCANS
SLVNT
SPINN
TEMP

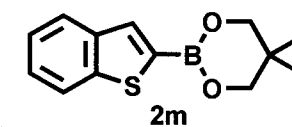
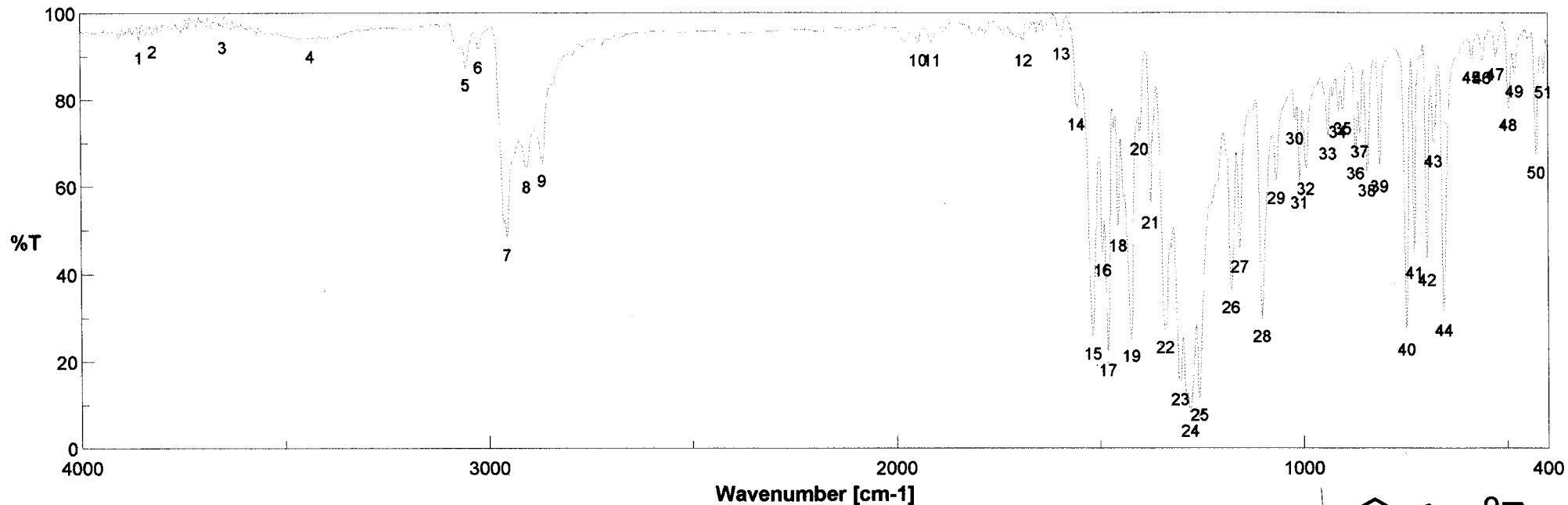


St SM p-iodophenyl Bneo



in CDCl₃

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RESOL
PW1
OBNUC
OBFRO
OBSET
RGAIN
IRNUC
IRFRQ
IRSET
IRRPW
IRRS
SCANS
SLVNT
SPINN
TEMP



KBr

number of scan 16
 zero filling ON
 gain Auto (8)
 date of scan 2007/03/08 17:49
 sample name Memory#1

resolution 4 cm-1
 apodization Cosine
 scan speed Auto (2 mm/sec)
 date of data processing 2007/03/08 17:50

2-thiophene-Benzo
 benzo

No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3855.01	93.7038	2	3822.22	95.054	3	3650.59	96.032	4	3434.6	93.8789
6	3022.87	91.4007	7	2954.41	48.3417	8	2906.2	63.9041	9	2867.63	65.3499
11	1909.18	92.9609	12	1686.44	93.0112	13	1592.91	94.5623	14	1556.27	78.1759
16	1492.63	44.788	17	1480.1	21.9394	18	1455.03	50.4446	19	1423.21	25.2009
21	1375	55.7446	22	1339.32	27.2019	23	1303.64	15.1934	24	1279.54	7.95172
26	1178.29	36.3515	27	1157.08	45.6259	28	1102.12	29.6766	29	1066.44	61.3218
31	1009.55	60.2239	32	993.16	63.4415	33	939.163	71.4838	34	914.093	76.4812
36	871.667	66.9798	37	861.06	71.9906	38	843.704	63.0469	39	812.849	63.9936
41	727.996	44.1592	42	697.141	42.5453	43	680.749	69.7786	44	655.679	31.0037
46	560.22	88.9287	47	527.436	89.8178	48	496.58	78.1181	49	481.152	85.8886
51	410.763	85.6892							50	429.084	67.1595
									5	3054.69	87.3062
									10	1943.89	92.966
									15	1517.7	25.6286
									20	1401.03	72.4995
									25	1256.4	11.6172
									30	1020.16	74.9635
									35	902.523	77.2267
									40	747.281	26.6535
									45	587.218	89.0266

St 2-benzothiophenylCOOH

7.909
7.897
7.879
7.853
7.836
7.823
7.813
7.356
7.352
7.345
7.333
7.327
7.260

3.808

1.539

1.255

1.056

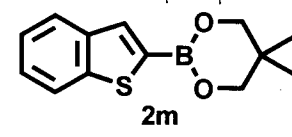
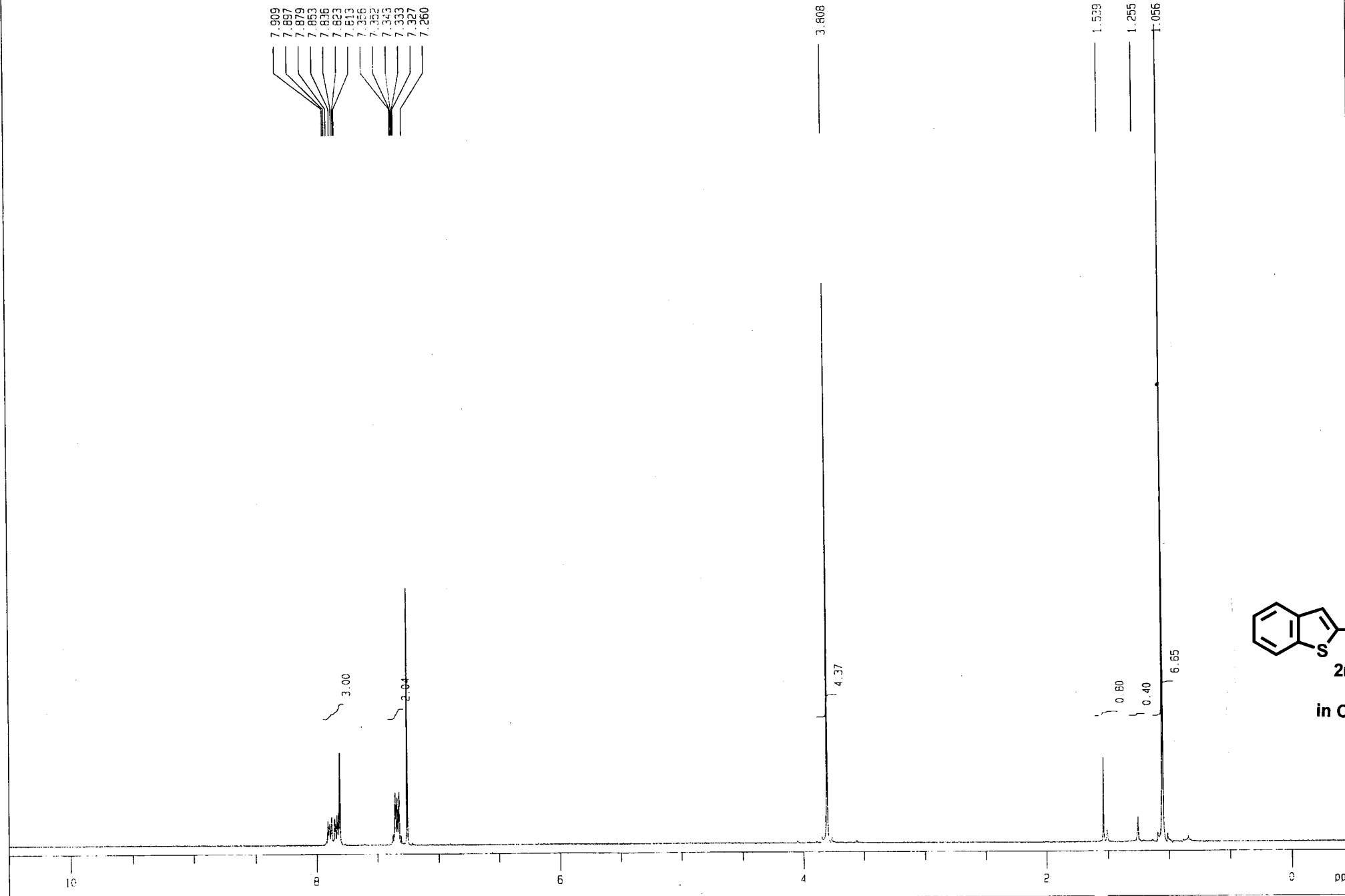
Date

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TIMES
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RESOL
PW1
OBNUC
OBFRO
OBSET
PGAIN

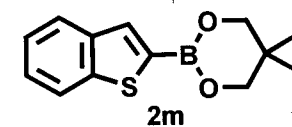
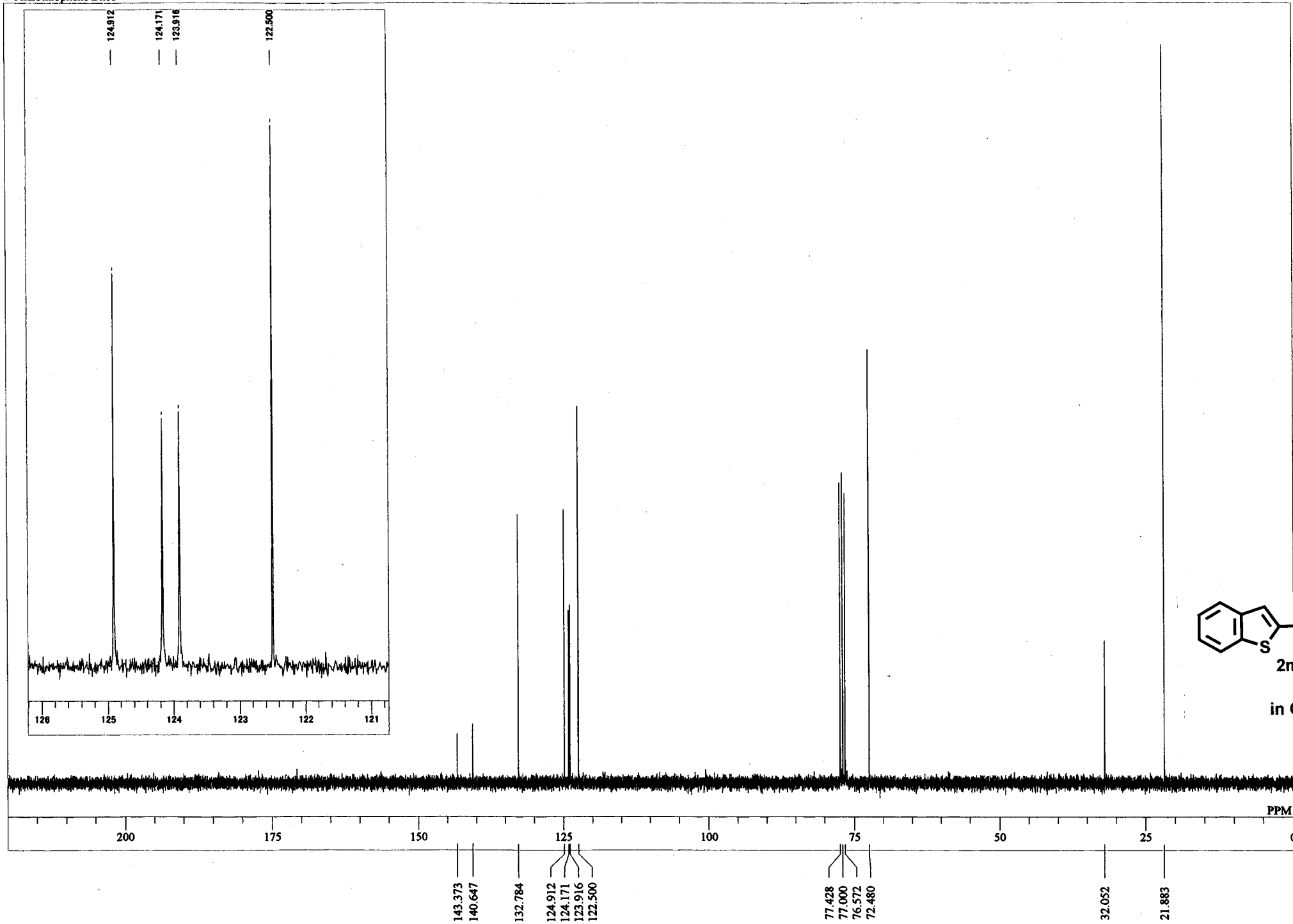
SCANS

SLVNT
SPINN
TEMP

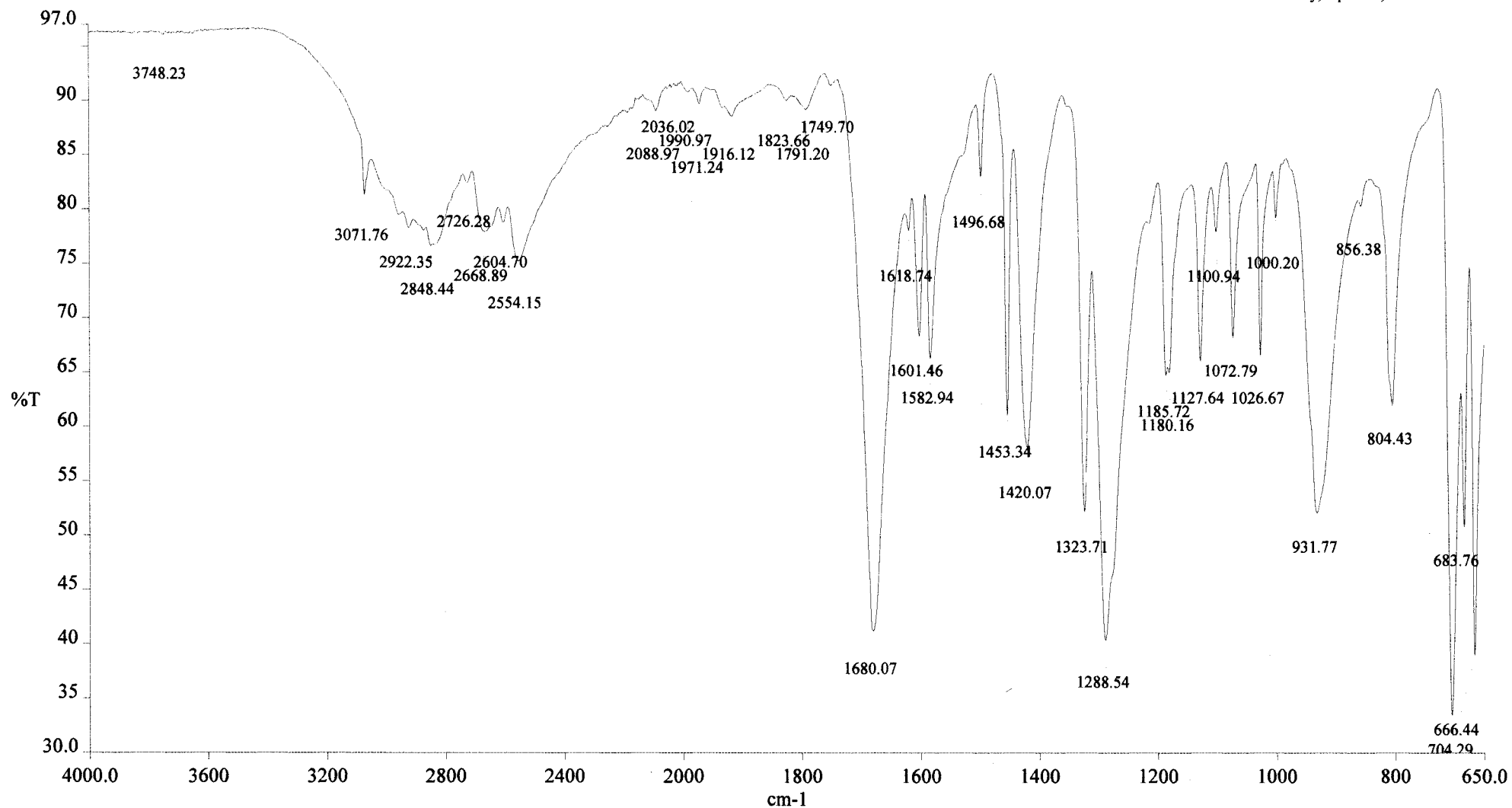


in CDCl₃

2-benzothiophene Bneo



in CDCl₃



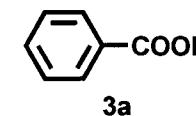
Spectrum Pathname: C:\pel_data\spectra\guest\216-1.sp

St PhCOOH

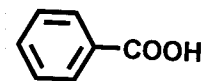
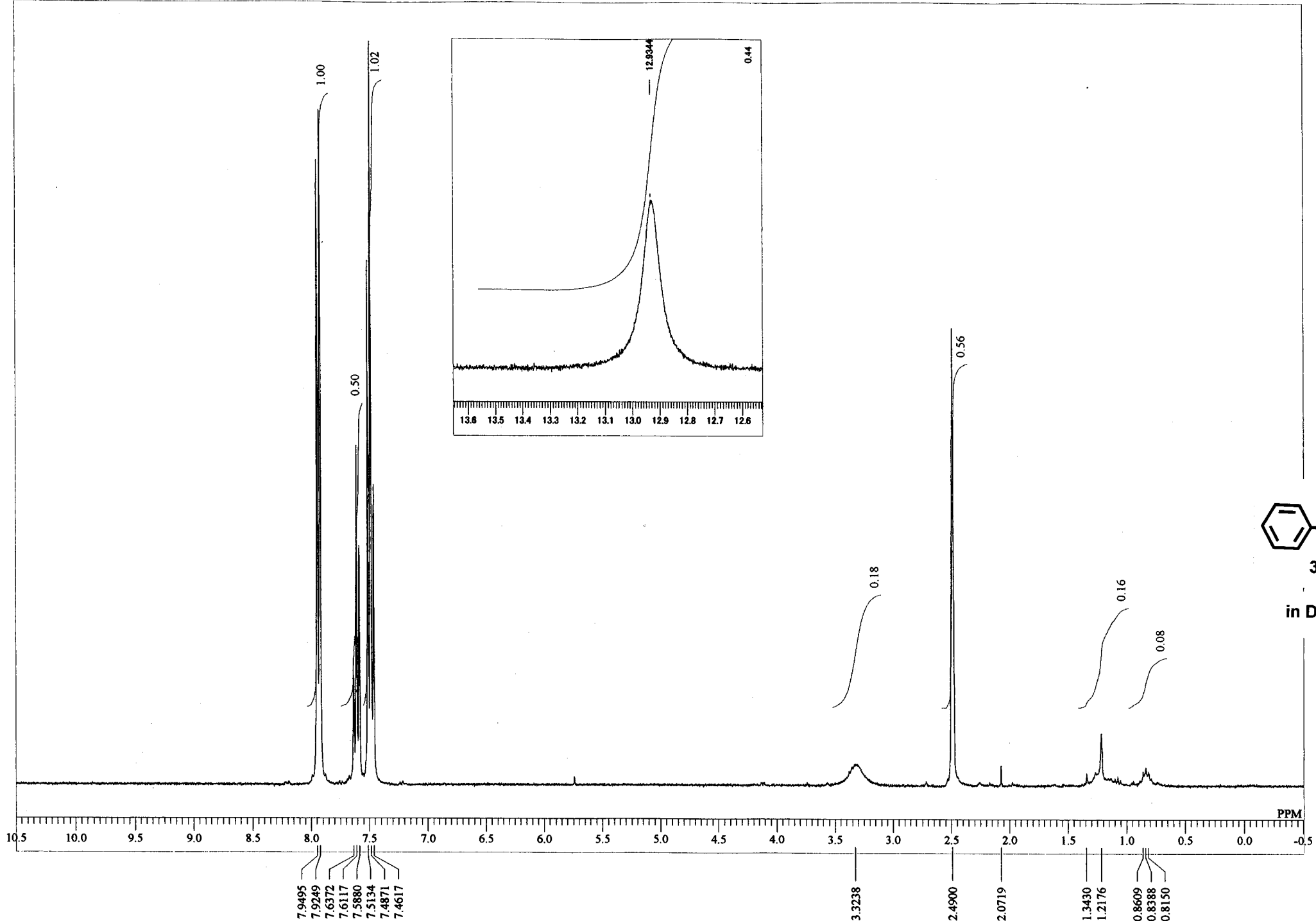
Date Created: Thursday, April 10, 2008 6:20 PM

Analyst: guest

Description:



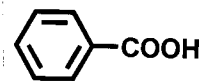
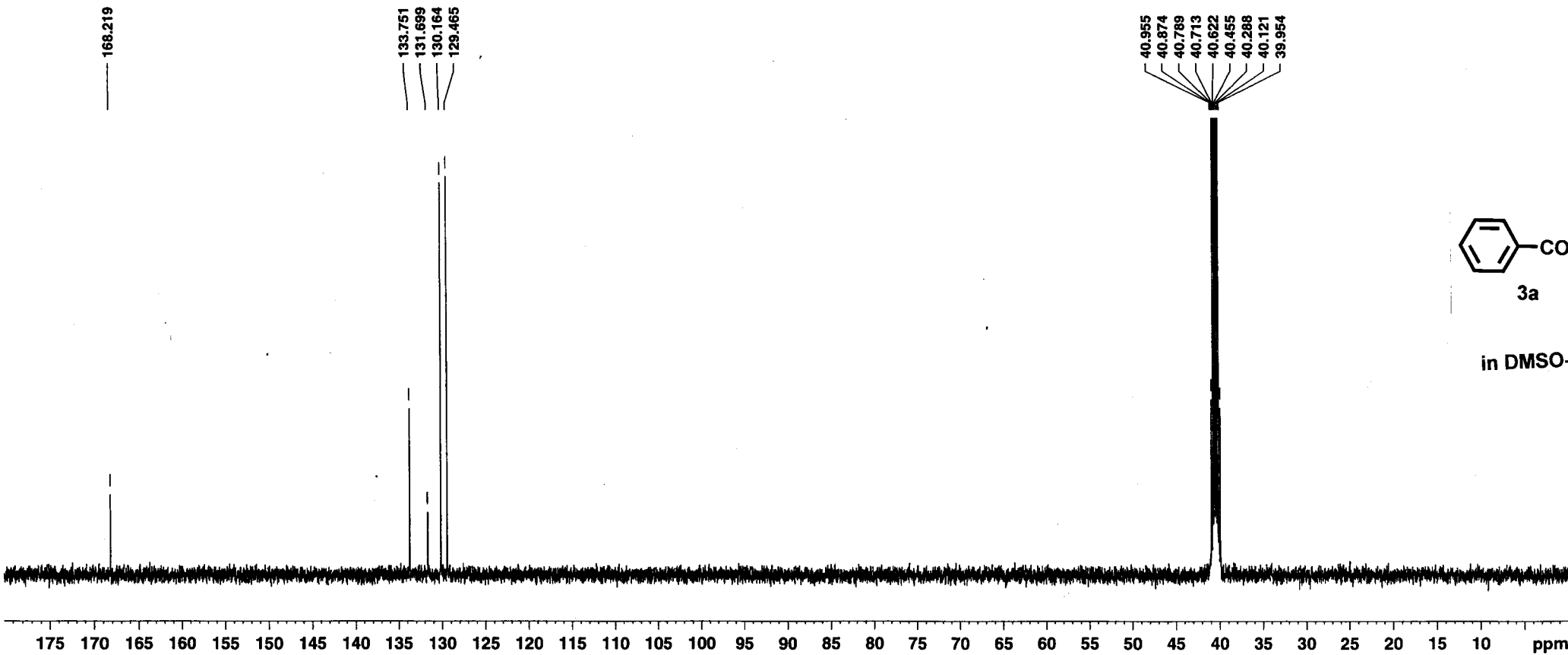
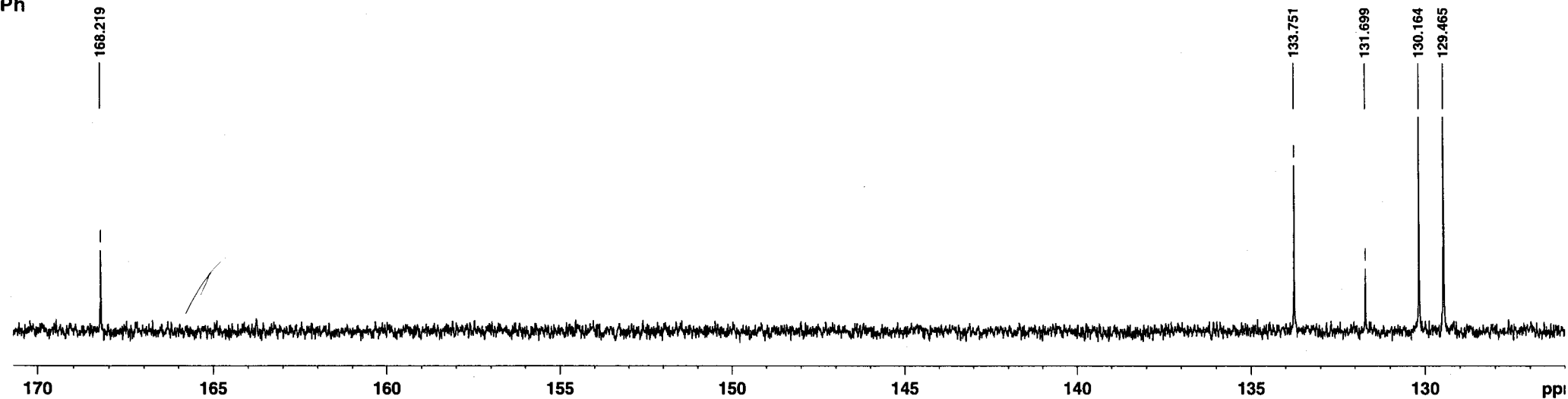
ATR



3a

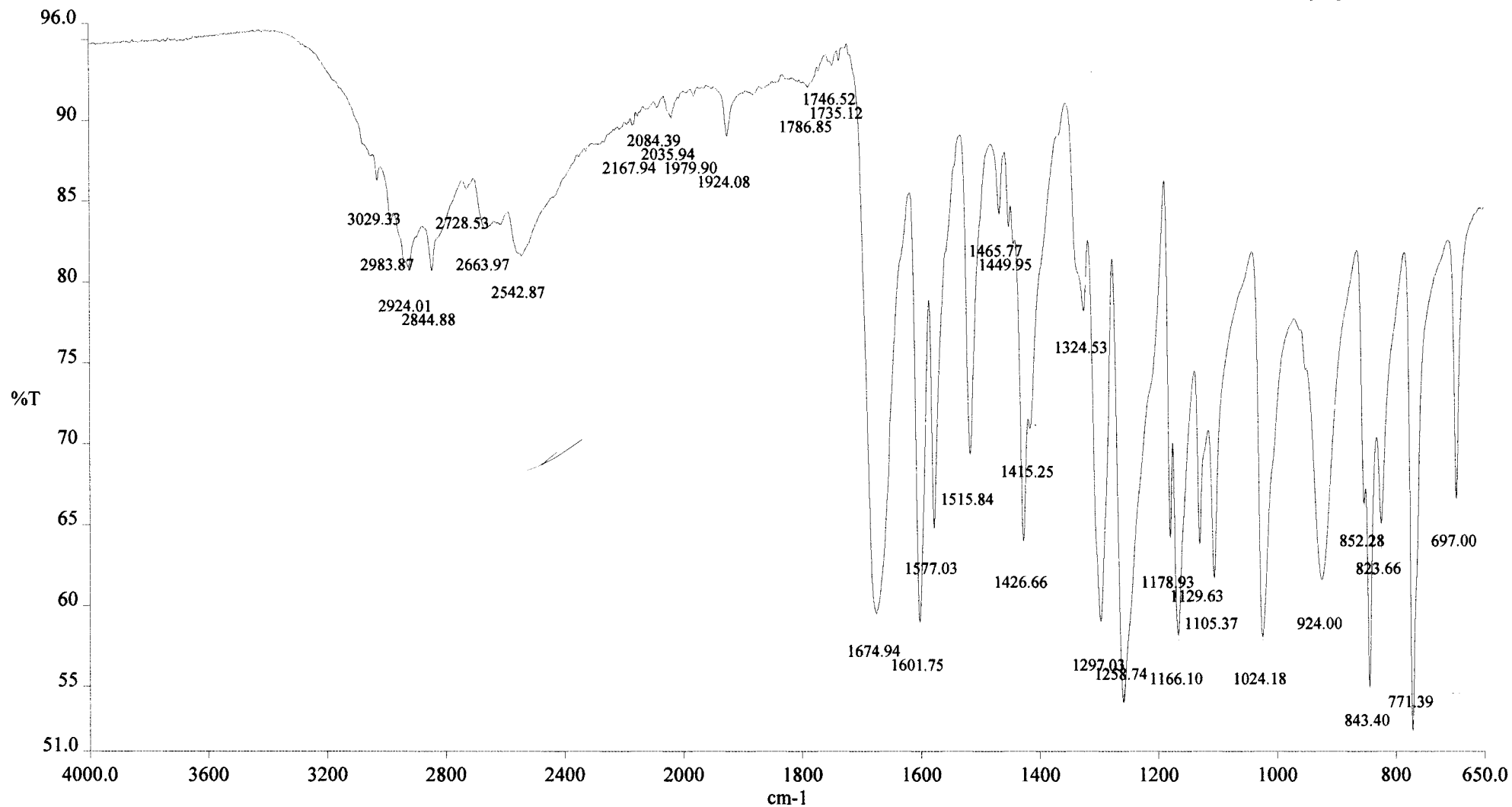
in DMSO-d⁶

Ph



3a

in DMSO-d₆

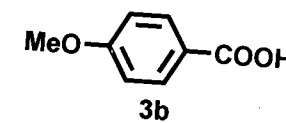


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\STp-MeOPhCOOH.sp

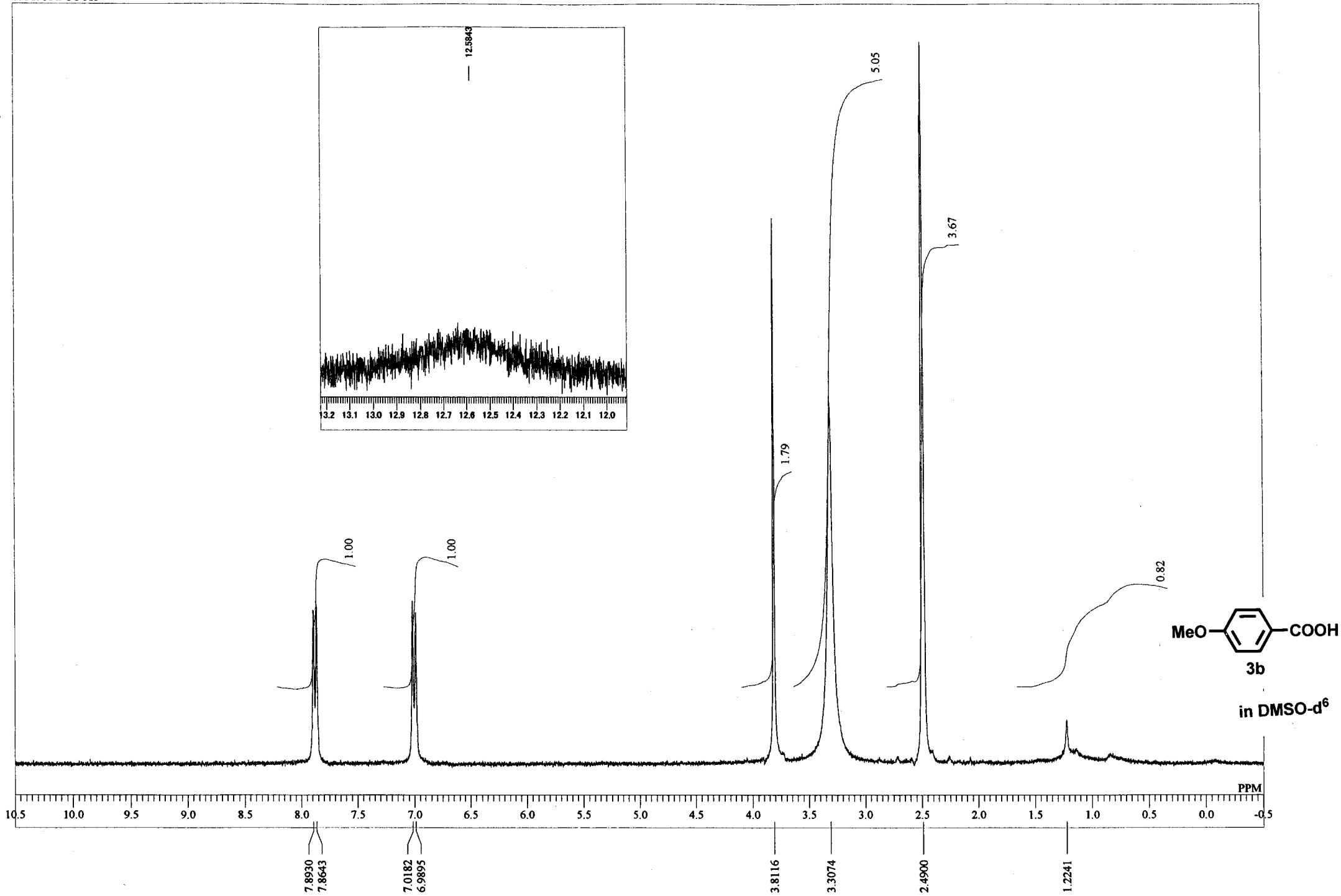
Date Created: Thursday, April 03, 2008 1:05 PM "Ež (•WlčŽž)

Analyst: guest

Description:

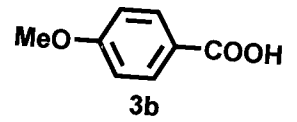
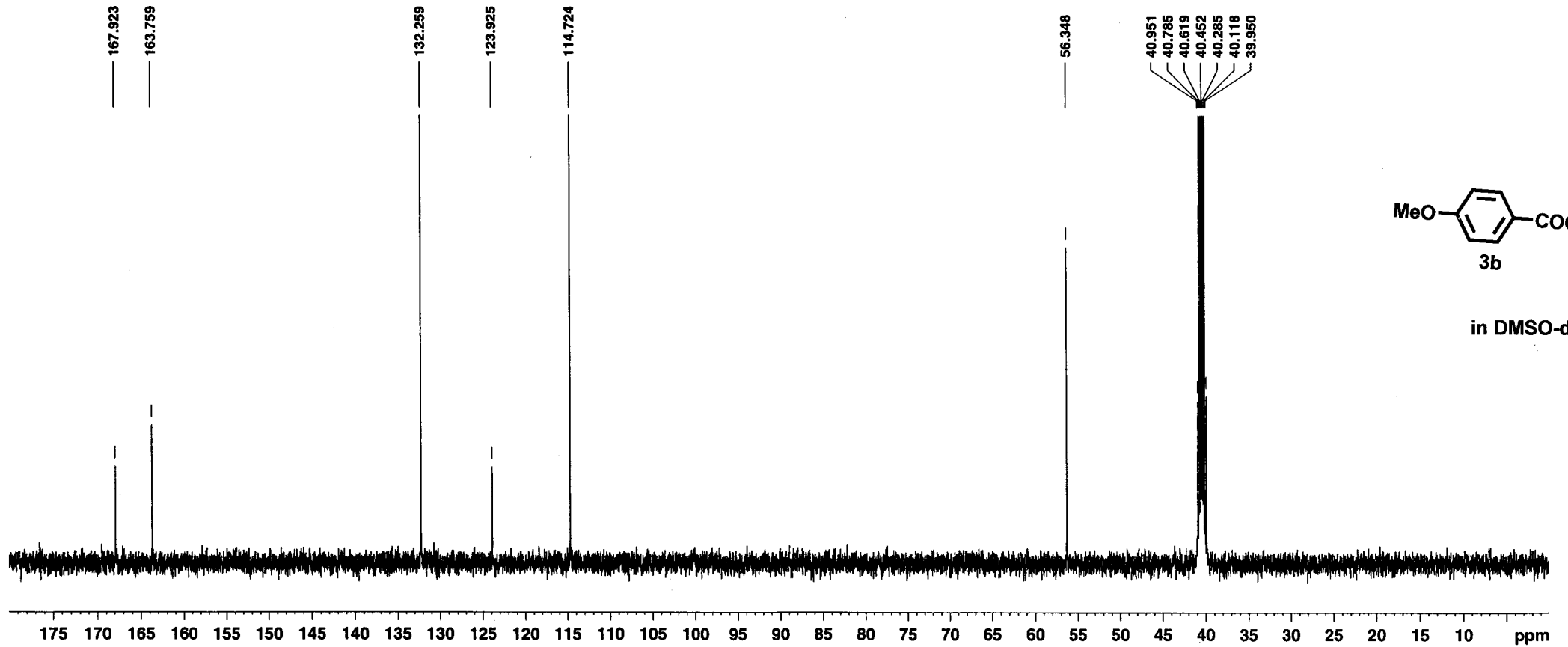


ATR

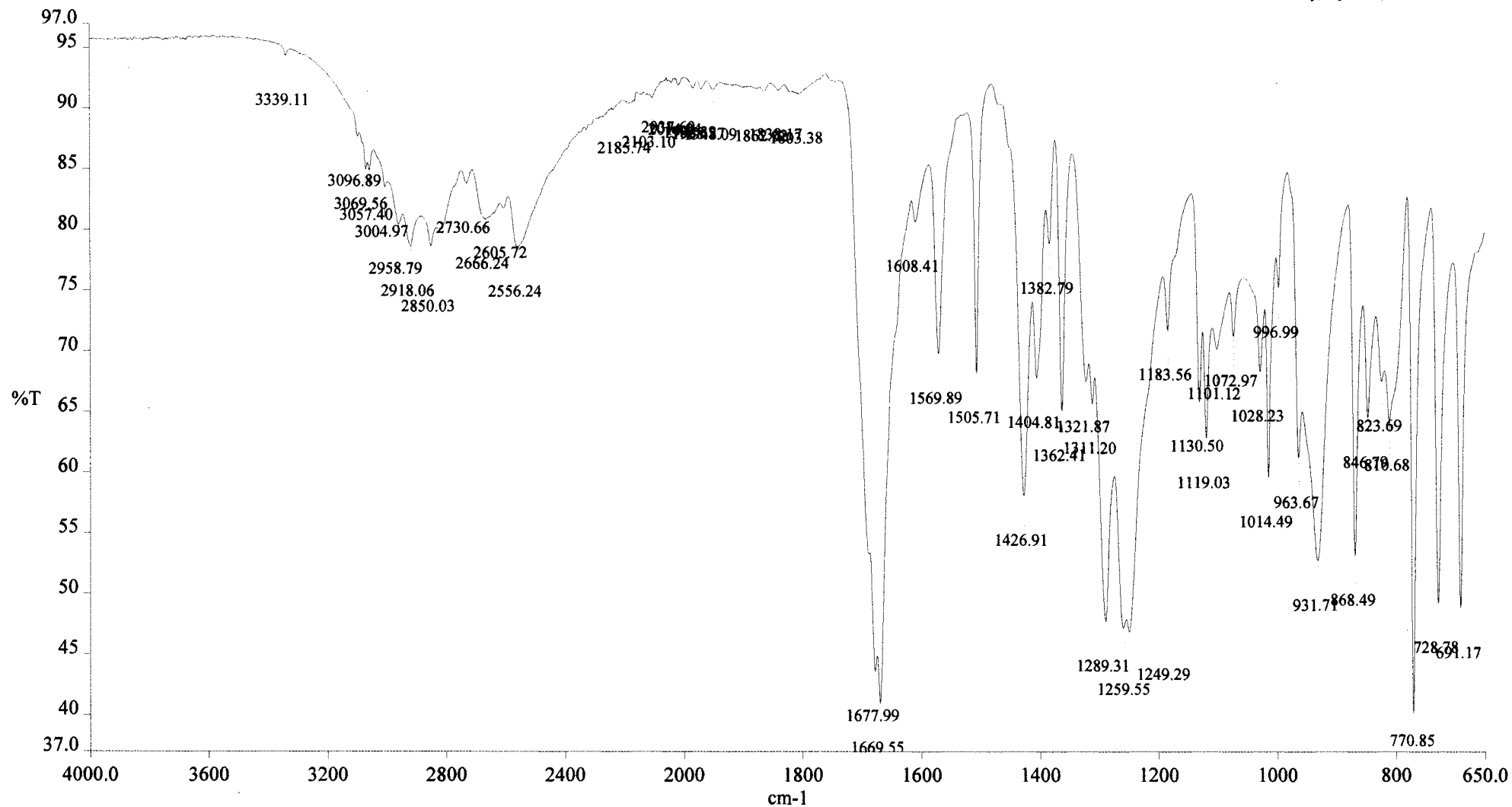


No title

MeO



in DMSO-d⁶

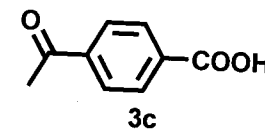


Spectrum Pathname: C:\pel_data\spectra\guest\iwawasa\STp-AcPhCOOH.sp

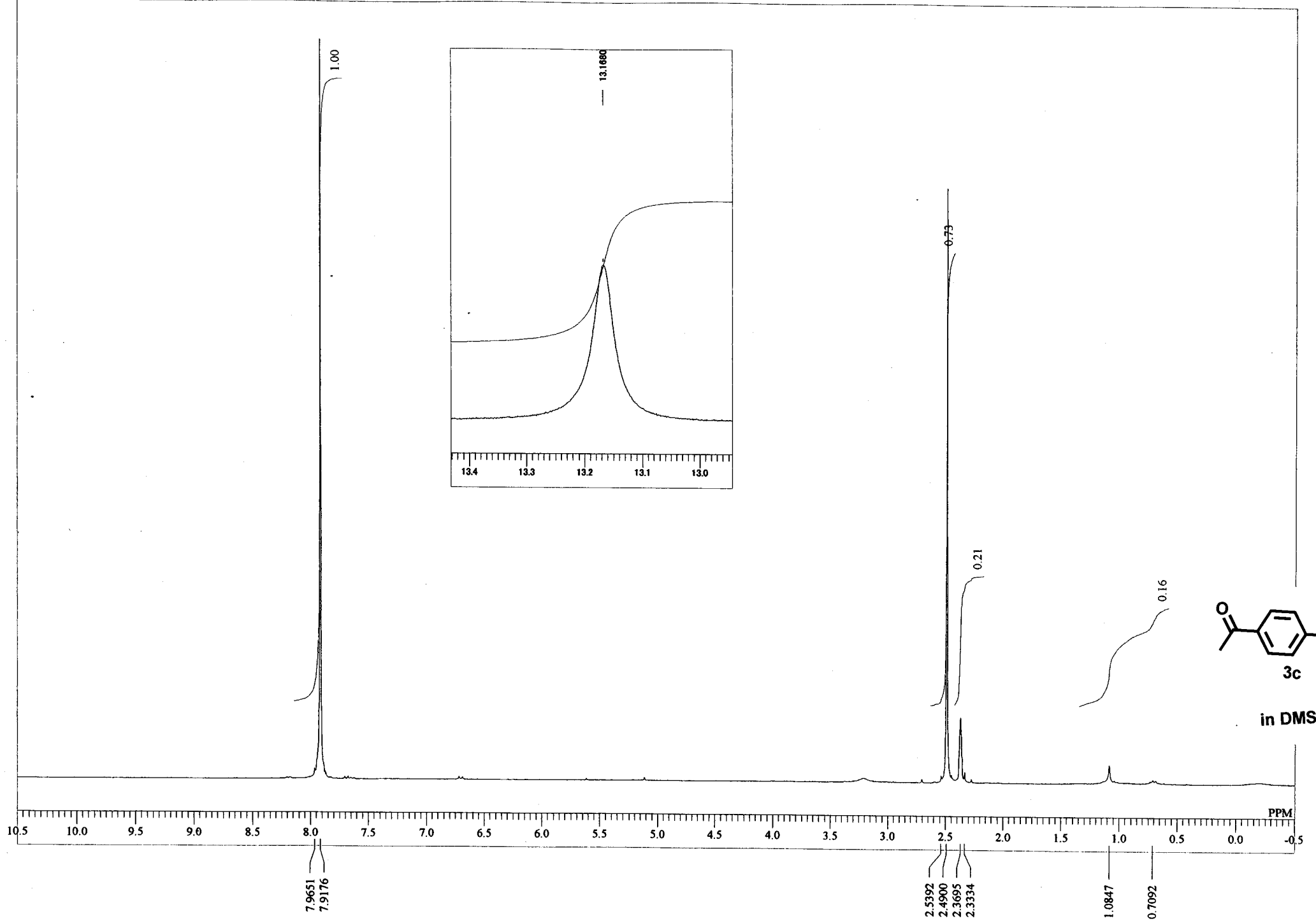
Date Created: Thursday, April 03, 2008 1:25 PM "Cēž (•Wlēžž)

Analyst: guest

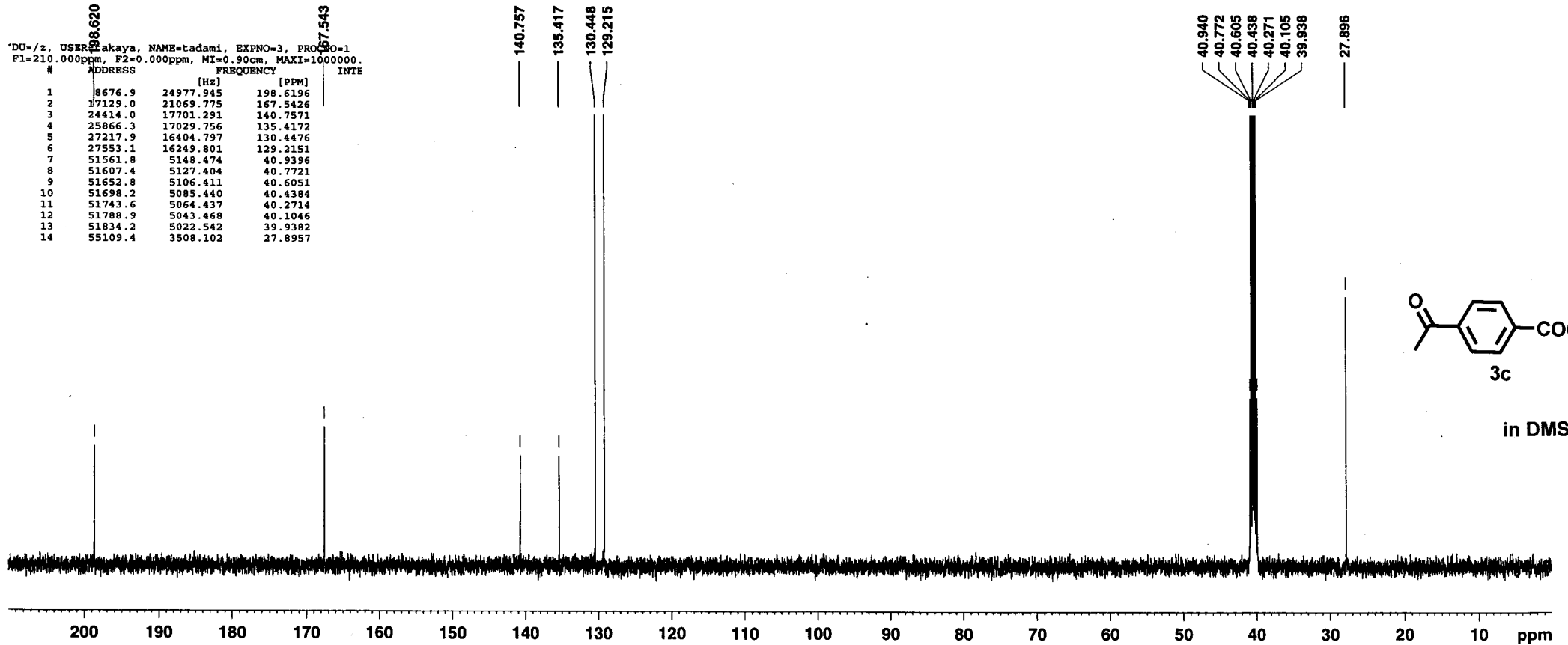
Description:

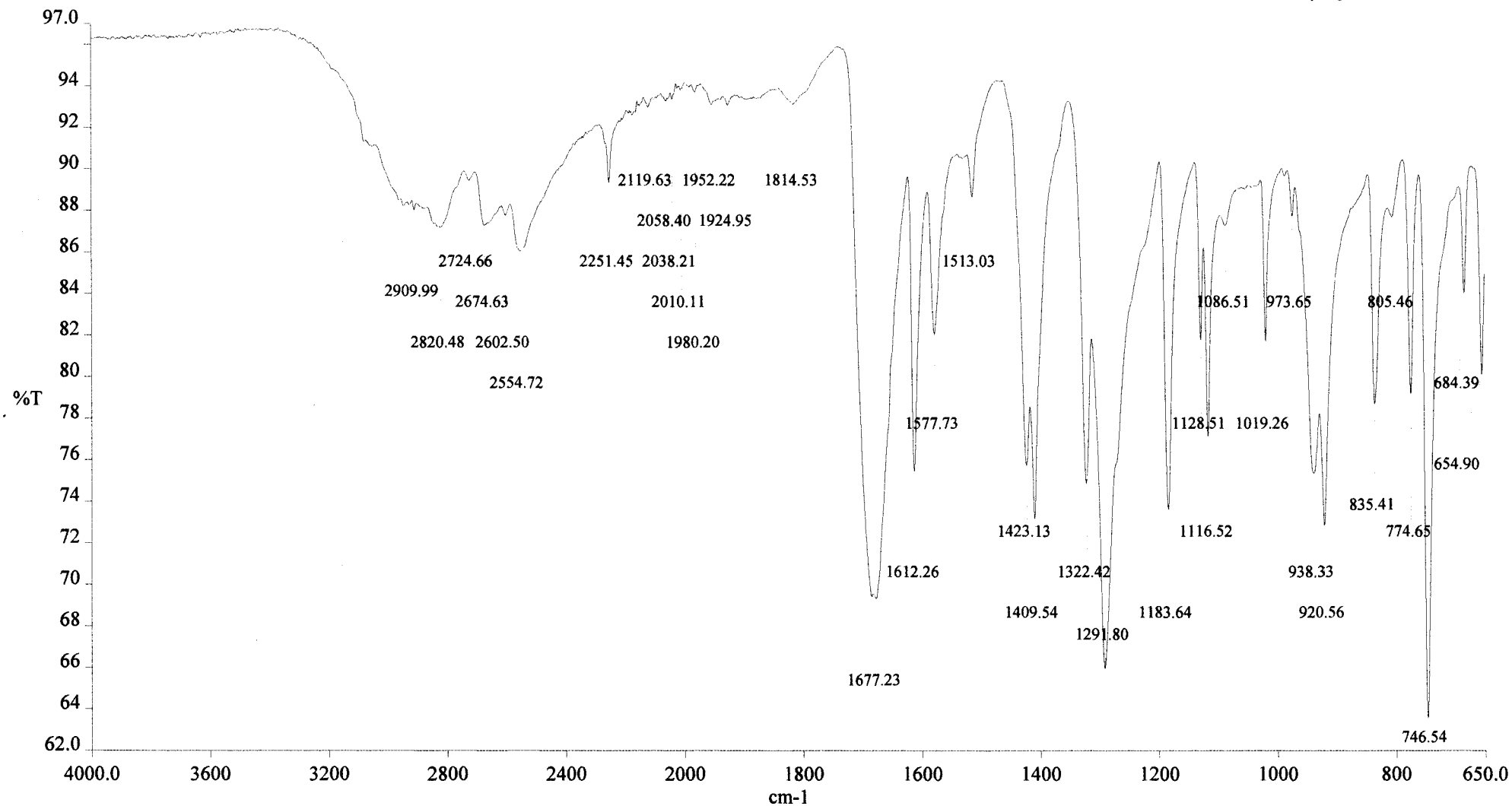


ATR



Ac



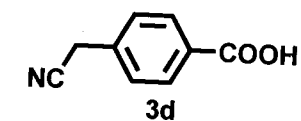


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\STp-cyanomethylPhCOOH.sp

Date Created: Thursday, April 03, 2008 12:50 PM "Cz (•Wlčžž)

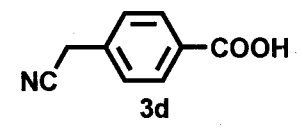
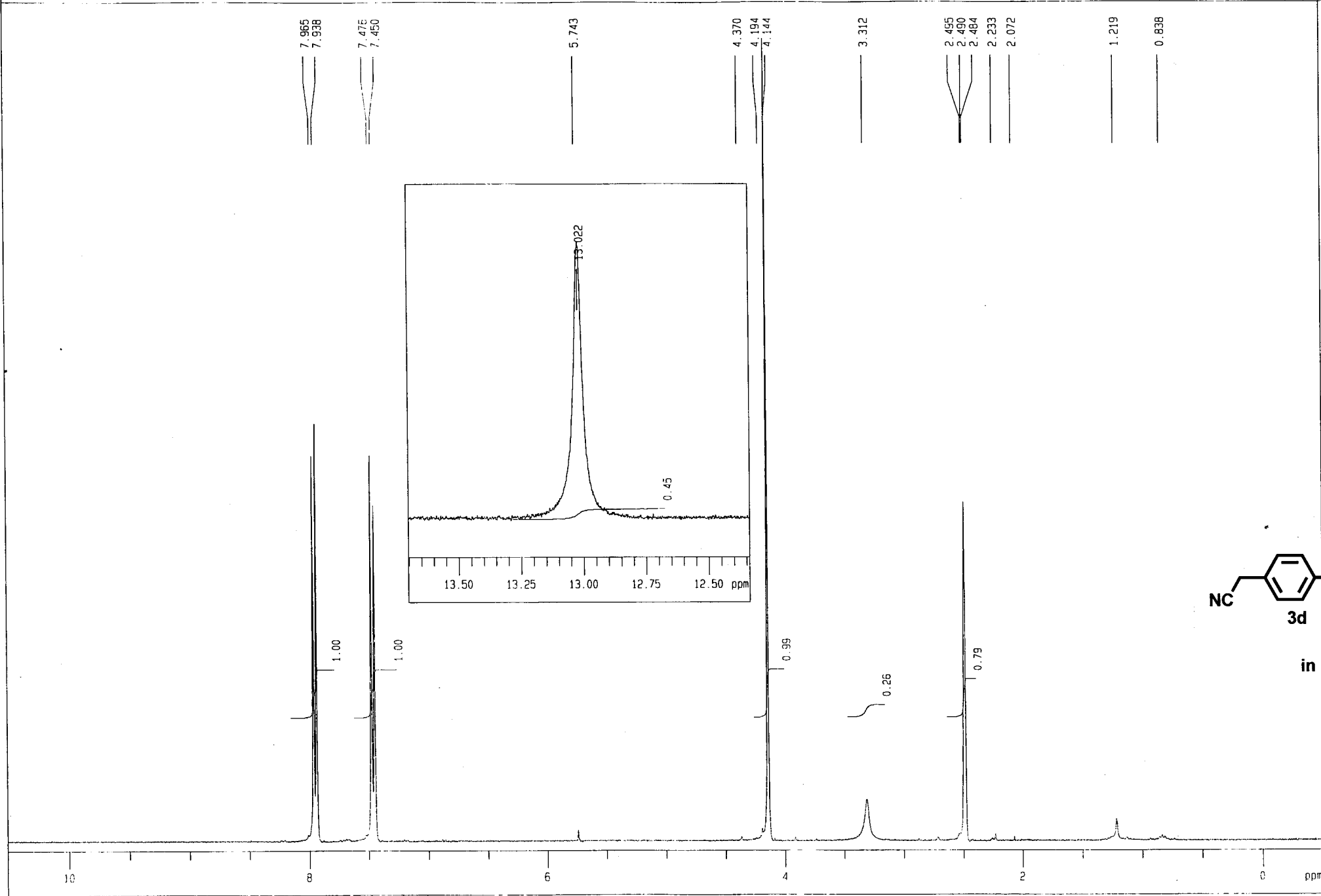
Analyst: guest

Description:



ATR

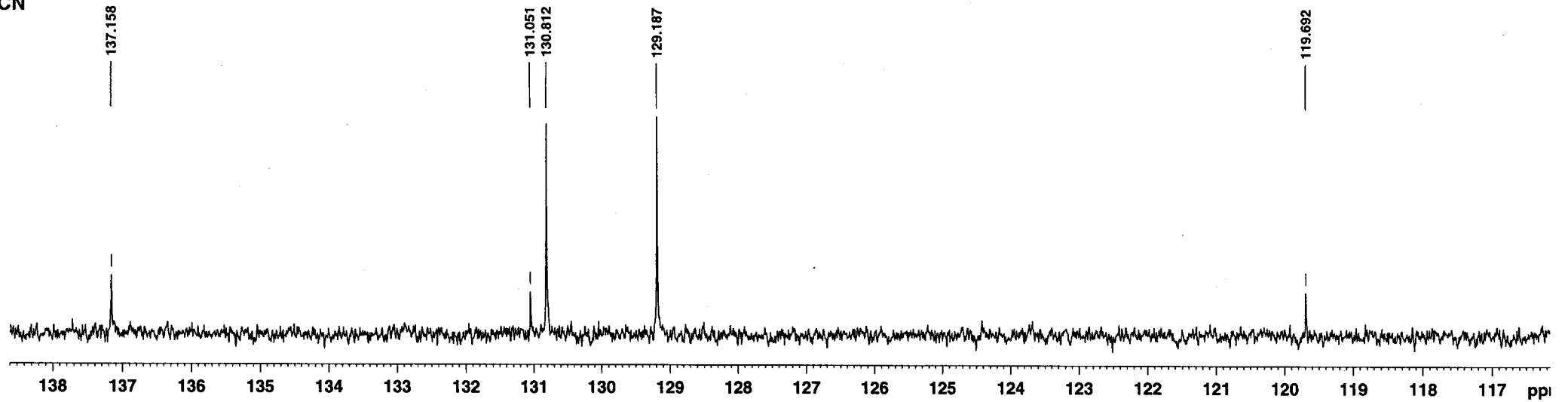
St p-(cyanomethyl)PhCOOH



in DMSO-d⁶

Date
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DELAY
DEAD1
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PREDL
INTWT
RESOL
PW1
OBNUC
OBFRG
OBSE T
RGAIN
SCANG
SLVNT
SPINN
TEMP

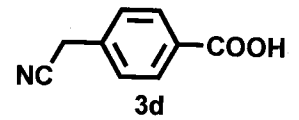
CN



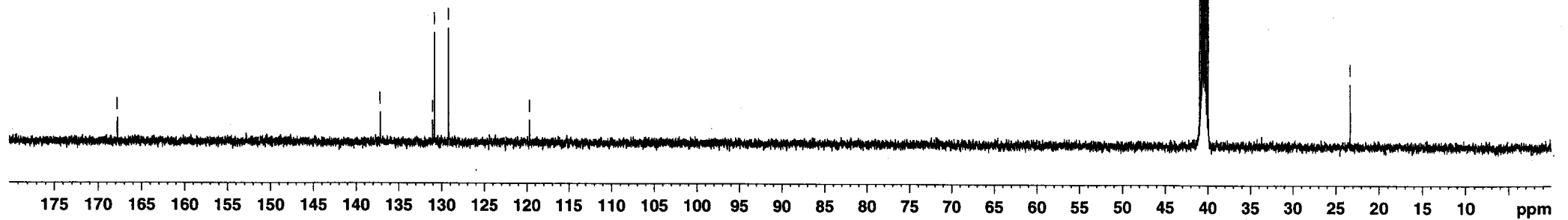
DU=/z, USER=tadami, NAME=tadami, EXPNO=9, PROCNO=1
 F1=180.000ppm, F2=0.000ppm, MI=0.28cm, MAXI=1000000

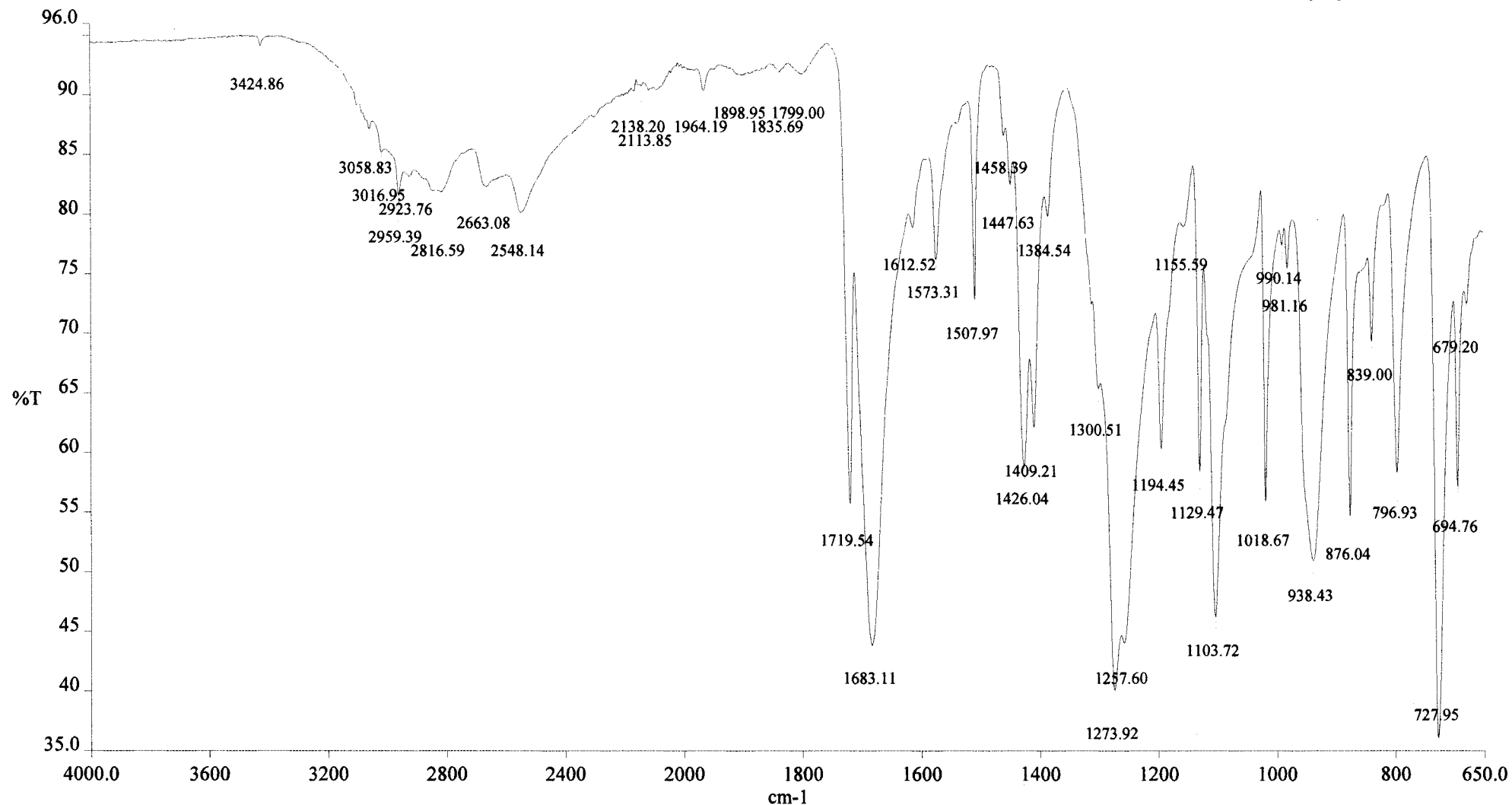
#	ADDRESS	FREQUENCY [Hz]	[PPM]	INTE
1	17060.9	21100.365	167.7858	
2	25390.8	17248.693	137.1581	
3	27051.9	16480.650	131.0508	
4	27116.9	16450.576	130.8116	
5	27558.8	16246.260	129.1870	
6	30141.3	15052.147	119.6916	
7	51557.0	5149.792	40.9501	
8	51578.3	5139.928	40.8717	
9	51602.3	5128.831	40.7834	
10	51623.4	5119.077	40.7059	
11	51647.7	5107.843	40.6165	
12	51693.1	5086.844	40.4496	
13	51738.5	5065.851	40.2826	
14	51783.9	5044.882	40.1159	
15	51829.2	5023.932	39.9493	
16	56350.1	2933.512	23.3267	

40.950
 40.872
 40.783
 40.706
 40.617
 40.450
 40.283
 40.116
 39.949



in DMSO-d⁶



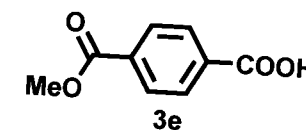


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\STp-COOMePhCOOH.sp

Date Created: Thursday, April 03, 2008 1:14 PM "Ež (•WlEžž)

Analyst: guest

Description:



ATR

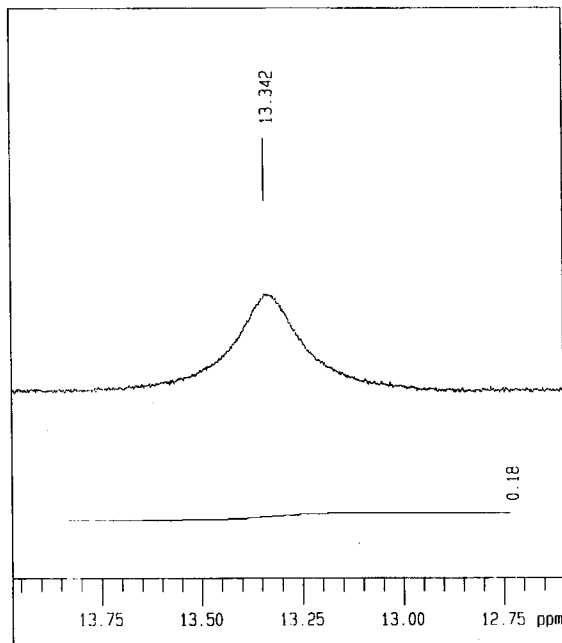
St p-COOMePhCOOH

8.305
8.095
8.043
7.998
7.895
7.780

4.113
3.921
3.869
3.839
3.822
3.757
3.621
3.518
3.330

2.714
2.495
2.490
2.484

1.319
1.206
0.942
0.864
0.826
0.752



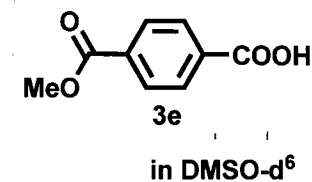
1.00

0.73

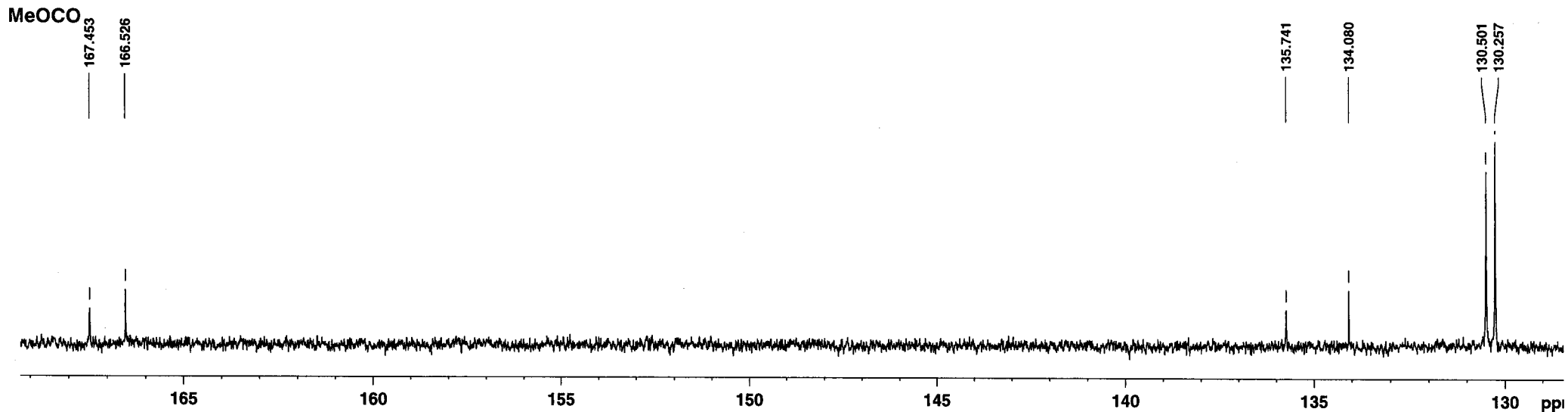
0.39

0.24

10 8 6 4 2 0 ppm

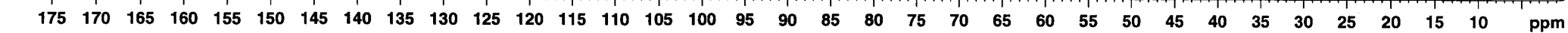
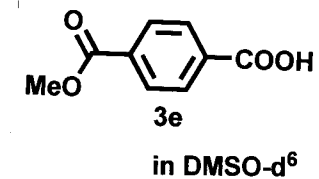


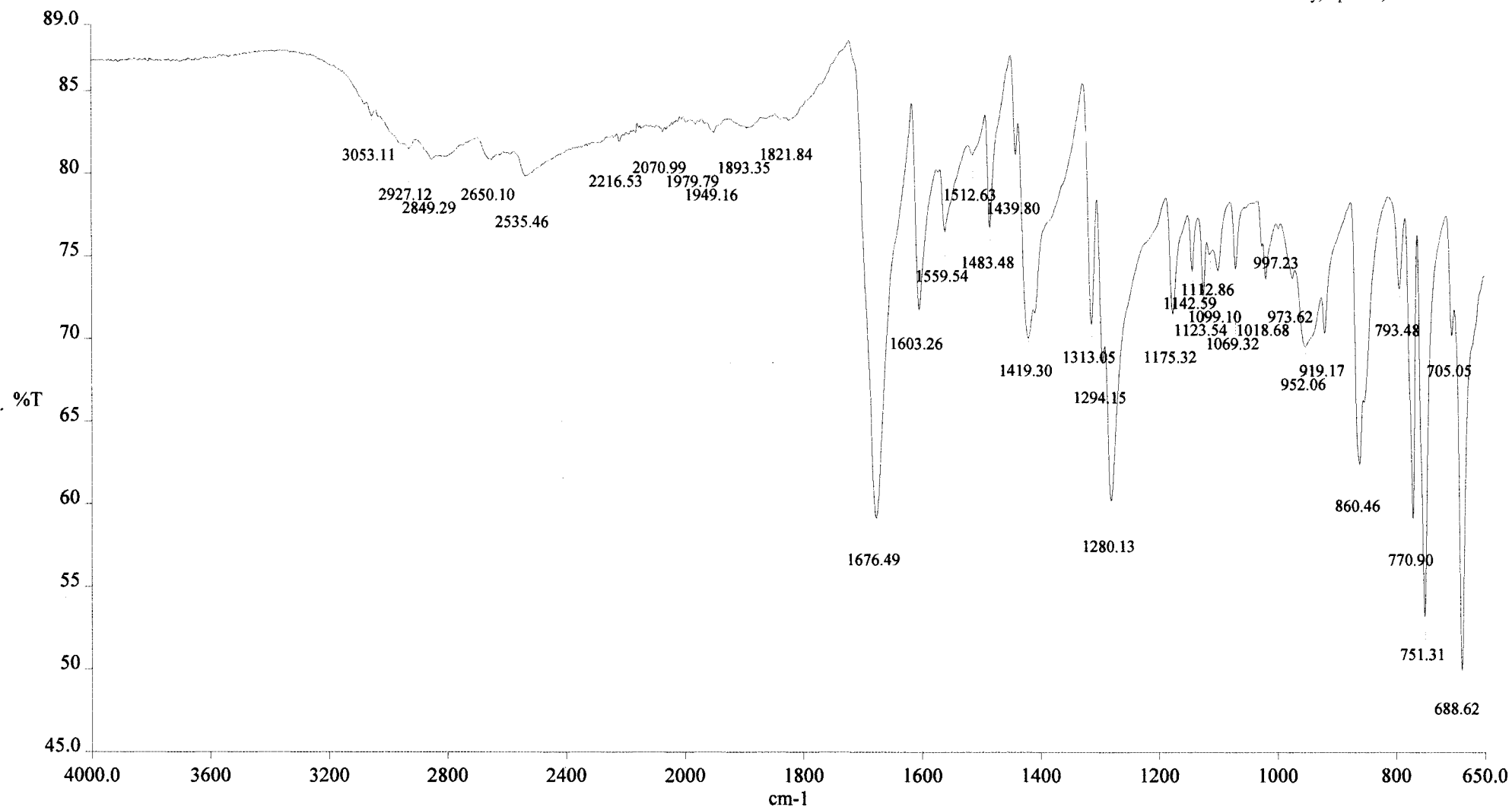
Date
FileN
Comme
Slice
EXMOD
POINT
SAMPO
FREQU
FILTR
DELAY
DEADT
INTVL
TIMES
DUMMY
PD
ACQTM
PREDL
INIWT
RESOL
PW1
OBNUC
OBFRQ
OBSET
RGAIN
SCANS
SLVNT
SPINN
TEMP



DU=/z, USER=tadami, NAME=tadami, EXPNO=7, PROCNO=1
F1=180.000ppm, F2=0.000ppm, M1=0.36cm, MAXI=1000000.

#	ADDRESS	[Hz]	[PPM]	INTE
1	17154.4	21058.482	167.4528	
2	17406.15	20941.922	166.5259	
3	25779.1	17070.520	135.7413	
4	26231.0	16861.607	134.0801	
5	27204.3	16411.545	130.5013	
6	27270.9	16380.770	130.2566	
7	48182.9	6711.285	53.3668	
8	51559.3	5150.077	40.9524	
9	51604.7	5129.102	40.7856	
10	51626.3	5119.124	40.7062	
11	51650.1	5108.113	40.6187	
12	51695.5	5087.129	40.4518	
13	51740.9	5066.116	40.2847	
14	51786.4	5045.097	40.1176	
15	51831.6	5024.208	39.9515	



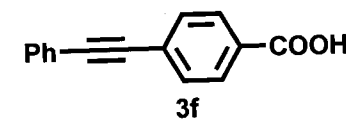


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\Tadami\STp-(Phenylacetynyl)PhCOOH.sp

Date Created: Thursday, April 10, 2008 10:04 PM "Cēž (•WlčŽž)

Analyst: guest

Description:



ATR

SI p-(phenylacetynyl)PhCOOH

7.978
7.951
7.868
7.840
7.837
7.867
7.875
7.869
7.864
7.851
7.458
7.445
7.436
7.424

5.736

3.804
3.744

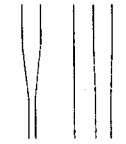
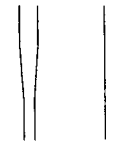
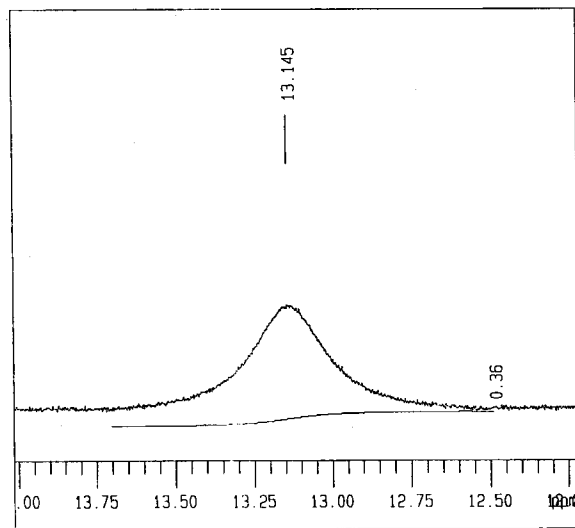
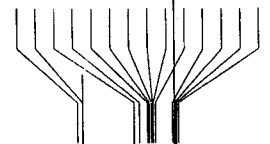
3.354

2.501
2.495
2.490
2.484

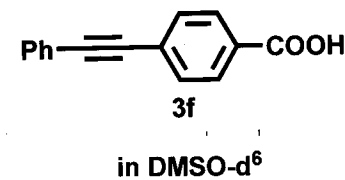
1.968

1.189
1.153

0.937
0.821
0.739

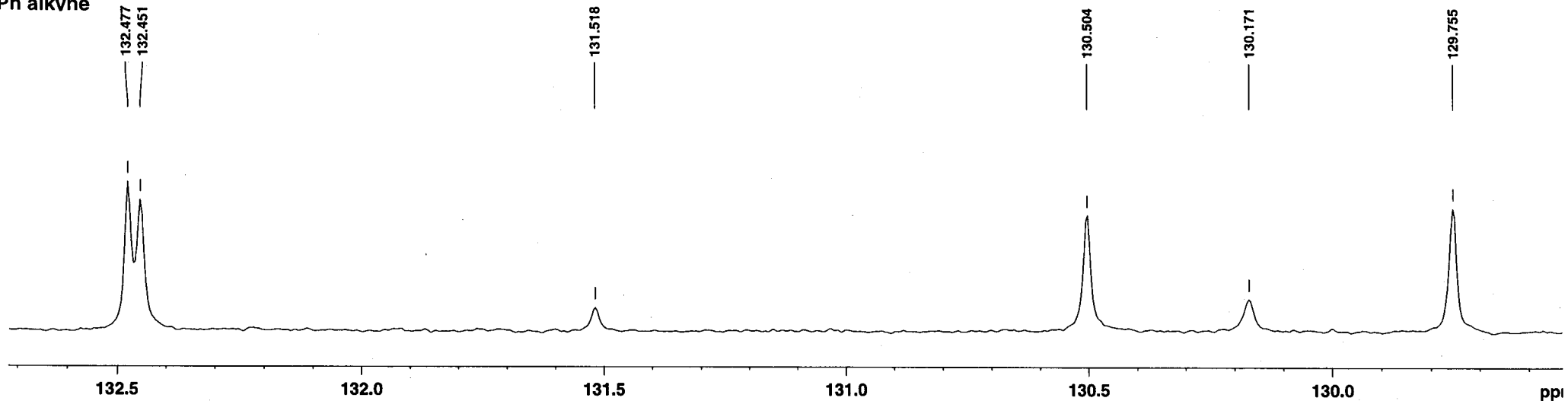


Date
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PW1
OBNUC
OBFRG
OBSET
RGAIN
SCANS
SLVNT
SPINN
TEMP



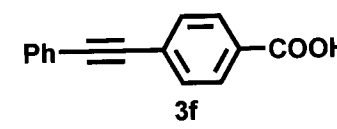
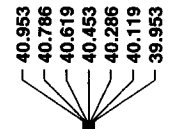
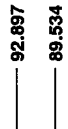
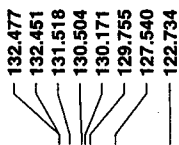
10 8 6 4 2 0 ppm

Ph alkyne

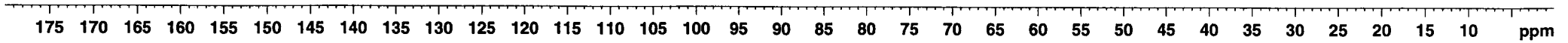


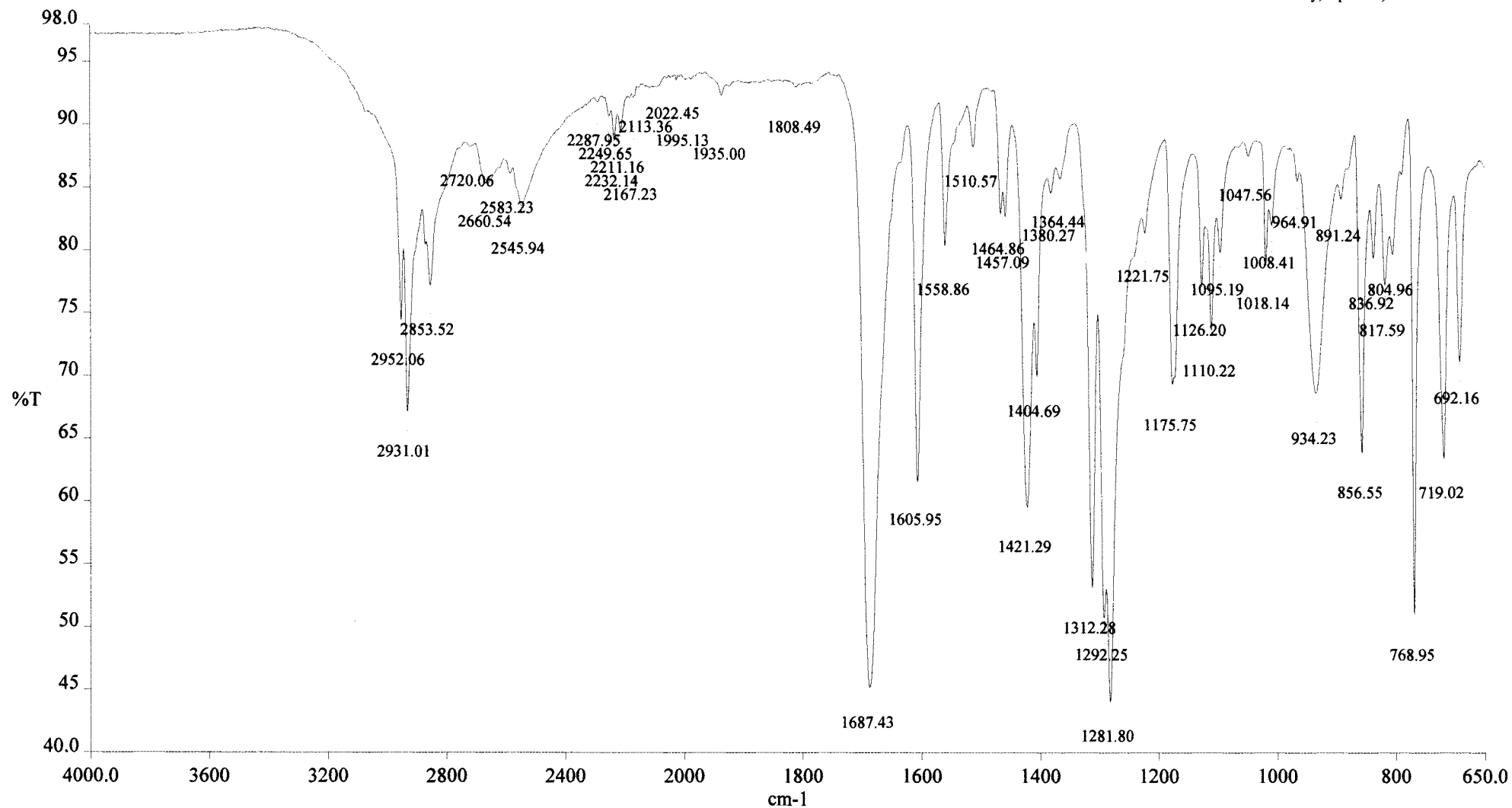
DU=/z, USER=tadami, NAME=tadami, EXPNO=19, PROCNO=1
 F1=180.000ppm, F2=0.000ppm, MI=0.70cm, MAXI=1000000.

#	ADDRESS	FREQUENCY [Hz]	[PPM]	INTE
1	17112.9	21081.412	167.6351	
2	26675.1	16659.951	132.4766	
3	26682.1	16656.727	132.4509	
4	26935.9	16539.354	131.5176	
5	27211.6	16411.857	130.5038	
6	27302.2	16369.987	130.1708	
7	27415.2	16317.716	129.7552	
8	28017.6	16039.179	127.5403	
9	29324.9	15434.714	122.7337	
10	37439.8	11682.468	92.8966	
11	38354.4	11259.581	89.5339	
12	51567.3	5150.097	40.9525	
13	51612.5	5129.190	40.7863	
14	51657.9	5108.204	40.6194	
15	51703.3	5087.227	40.4526	
16	51748.7	5066.250	40.2858	
17	51794.1	5045.234	40.1187	
18	51839.2	5024.364	39.9527	



in DMSO-d⁶



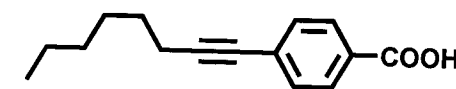


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\Tadami\STp-(Hexylacetynyl)PhCOOH.sp

Date Created: Thursday, April 10, 2008 10:00 PM "Cz (•Wlčžž)

Analyst: guest

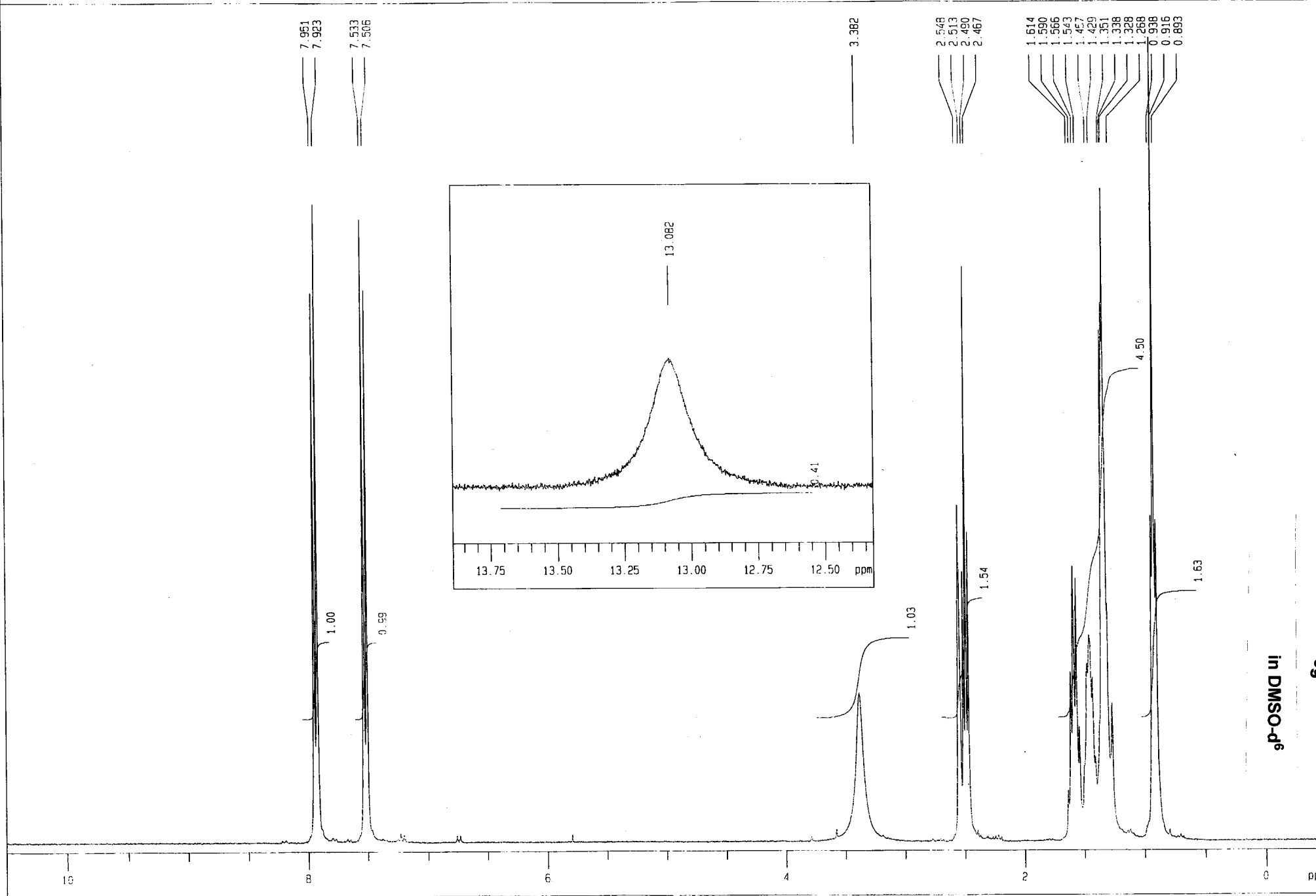
Description:



3g

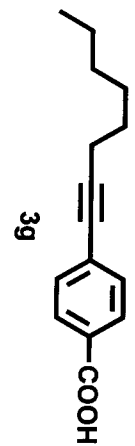
ATR

St p-(hexylacetynyl)PhCOOH

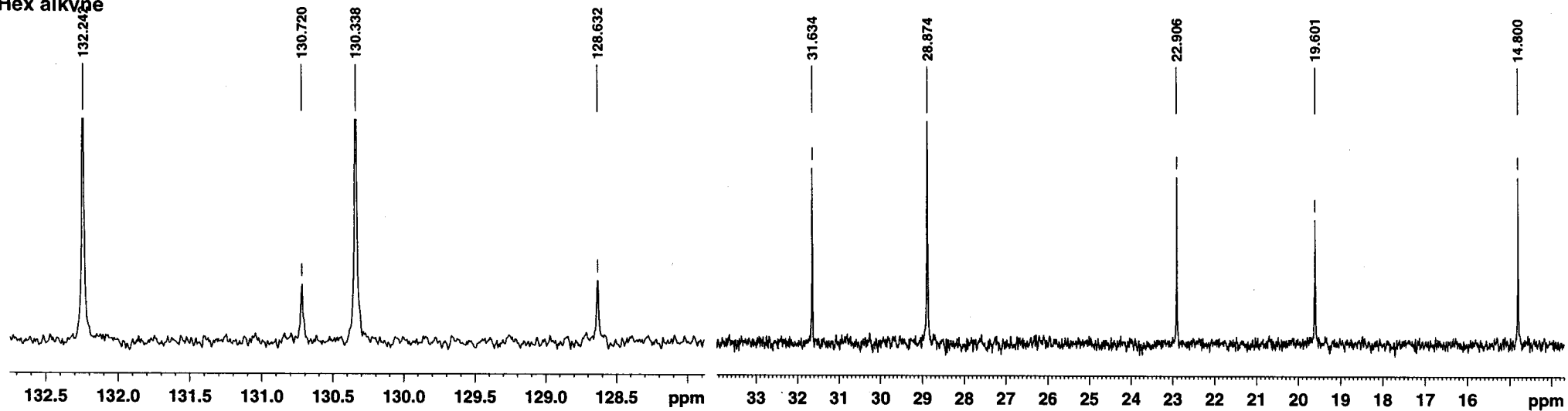


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RESOL
PW1
OBNUC
OBFRQ
OBSET
RGAIN
SCANS
SLVNT
SPINN
TEMP

in DMSO-d₆



Hex alkyl



DU=/z, USER=tadami, NAME=tadami, EXPNO=18, PROCNO=1
 F1=180.000ppm, F2=0.000ppm, MI=0.39cm, MAXI=1000000.

#	ADDRESS	FREQUENCY [Hz]	INTE
1	17099.3	21083.986	167.6556
2	26730.9	16630.471	132.2421
3	27144.8	16439.082	130.7202
4	27248.8	16390.967	130.3376
5	27712.8	16176.425	128.6317
6	36891.9	11932.124	94.8818
7	40676.3	10182.260	80.9673
8	51560.3	5149.643	40.9489
9	51605.5	5128.749	40.7828
10	51651.0	5107.729	40.6156
11	51696.4	5086.738	40.4487
12	51741.8	5065.733	40.2817
13	51787.1	5044.769	40.1150
14	51832.7	5023.683	39.9473
15	54093.8	3978.209	31.6339
16	54844.5	3631.086	28.8737
17	56467.6	2880.577	22.9058
18	57366.5	2464.948	19.6008
19	58672.1	1861.236	14.8002

132.242
130.720
130.338
128.632

94.882

80.967

40.949
40.783
40.616
40.449
40.282
40.115
39.947

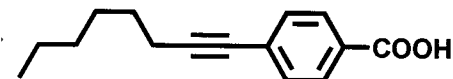
31.634

28.874

22.906

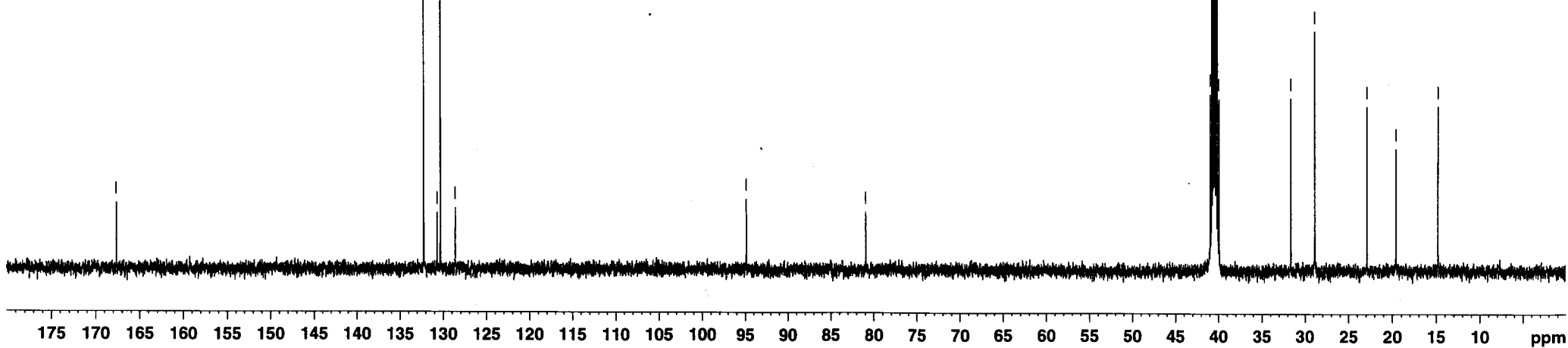
19.601

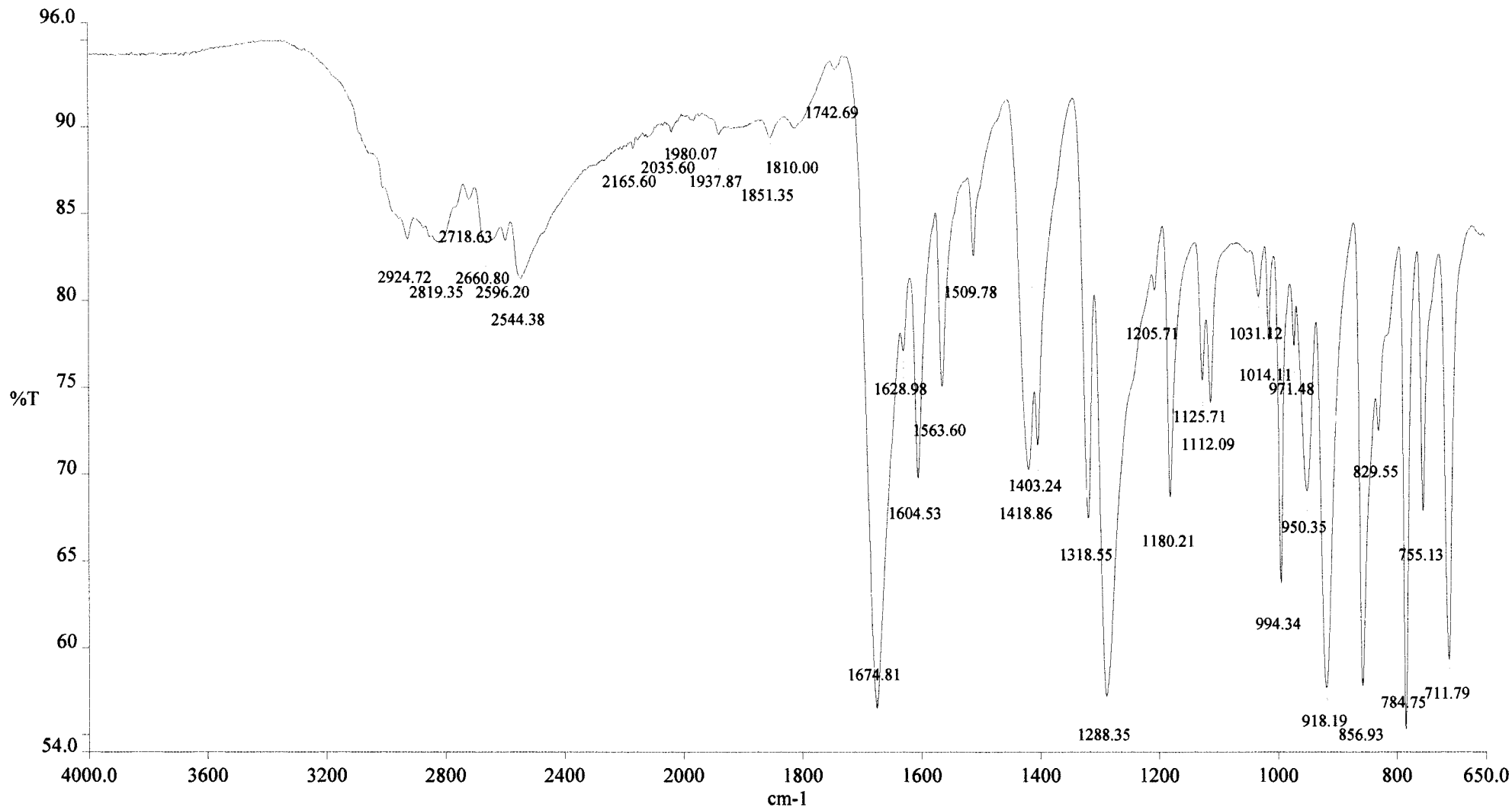
14.800



3g

in DMSO-d⁶



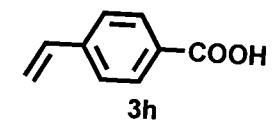


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\STp-vinylPhCOOH.sp

Date Created: Thursday, April 03, 2008 1:17 PM "C<ž (•WlEžž)

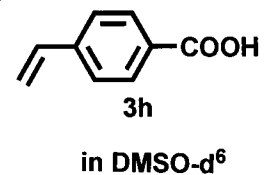
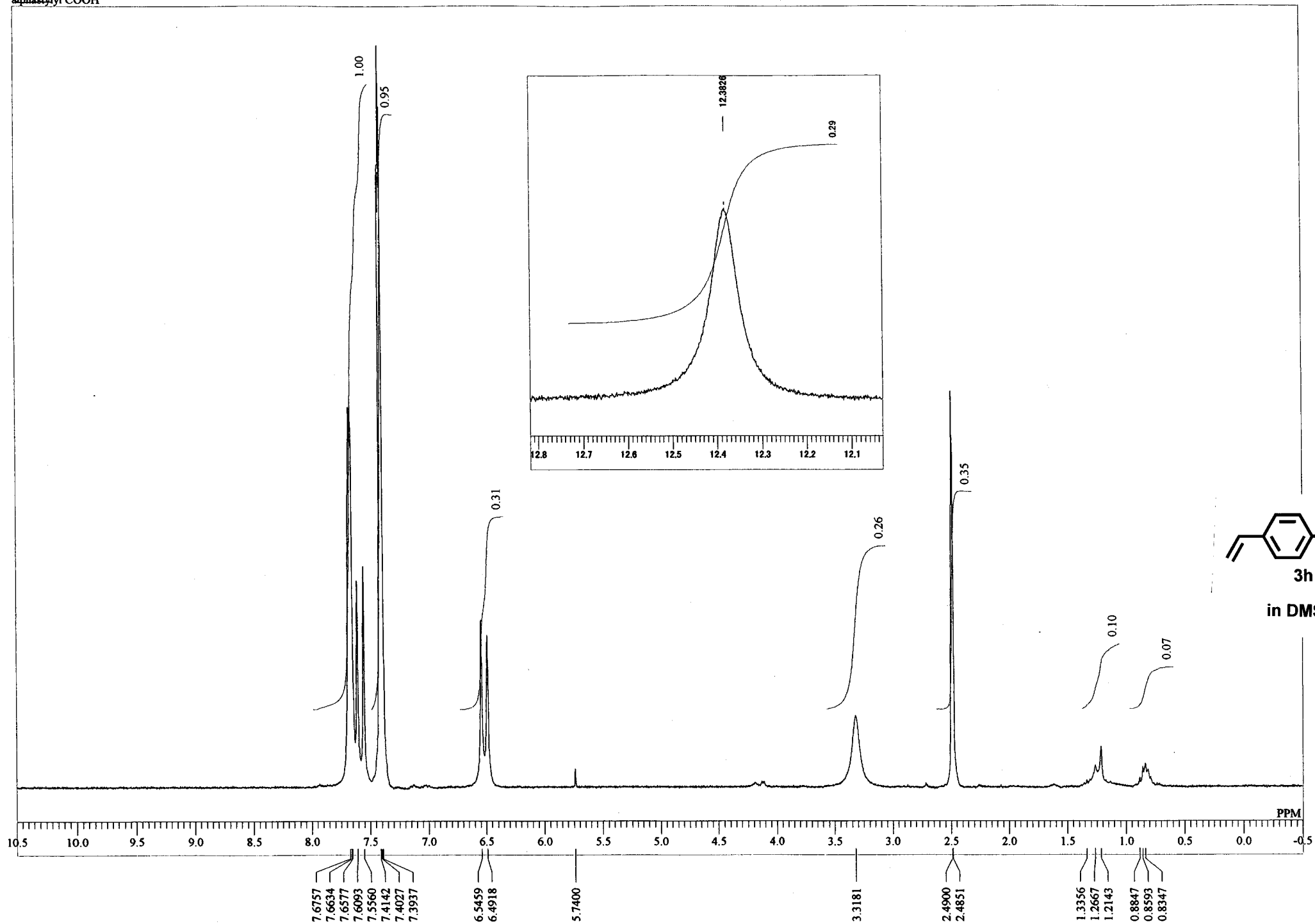
Analyst: guest

Description:

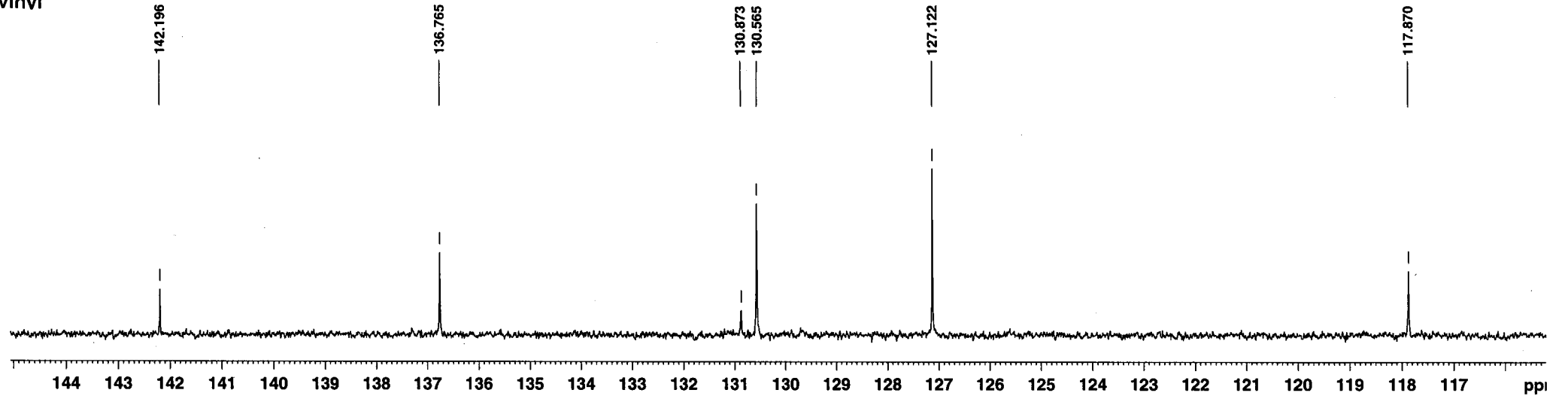


ATR

Vinyl
alpha-styryl COOH



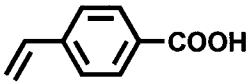
vinyl



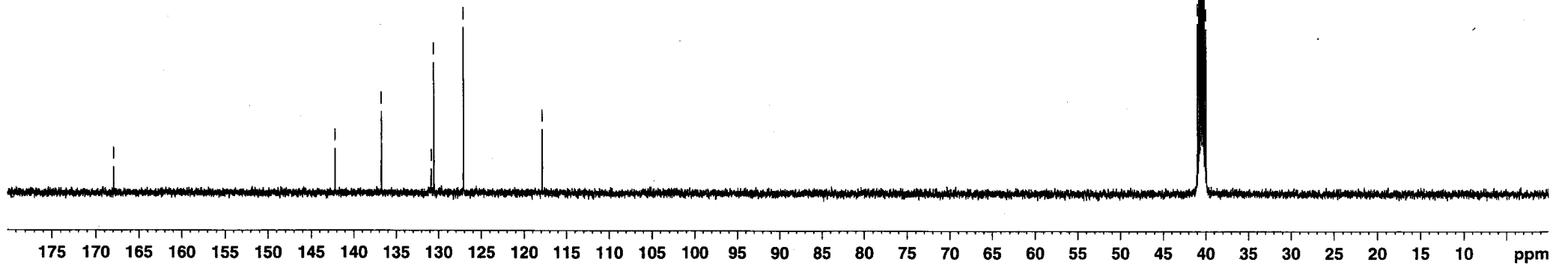
DU=/z, USER=ta, NAME=tadami, EXPNO=2, PROCNO=1
F1=180.000ppm, F2=0.000ppm, MI=0.27cm, MAXI=1000000.

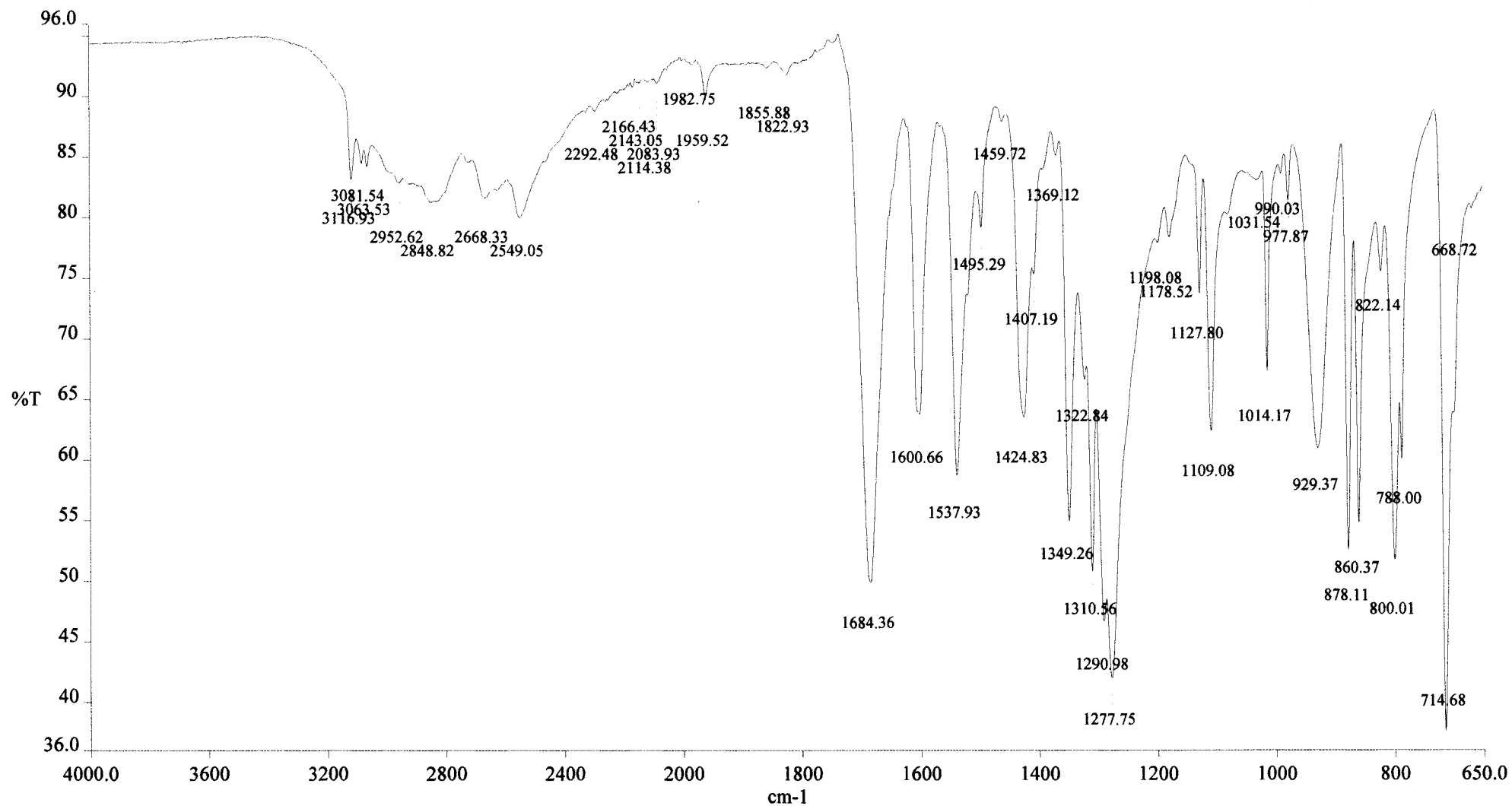
#	ADDRESS	FREQUENCY [Hz]	[PPM]	INTE
1	17021.4	21118.588	167.9307	
2	24020.6	17882.254	142.1961	
3	25497.7	17199.279	136.7652	
4	27100.3	16458.273	130.8728	
5	27184.1	16419.506	130.5646	
6	28120.4	15986.567	127.1219	
7	30636.6	14823.104	117.8703	
8	51531.7	5161.471	41.0430	
9	51557.0	5149.792	40.9501	
10	51577.4	5140.351	40.8750	
11	51602.4	5128.794	40.7831	
12	51622.6	5119.446	40.7088	
13	51647.8	5107.796	40.6162	
14	51693.2	5086.806	40.4492	
15	51738.6	5065.822	40.2824	
16	51784.0	5044.813	40.1153	
17	51829.4	5023.810	39.9483	

41.043
40.950
40.875
40.783
40.708
40.616
40.449
40.282
40.115
39.948



3h
in DMSO-d⁶



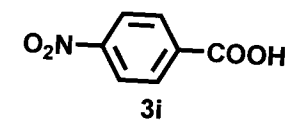


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\STp-NO2PhCOOH.sp

Date Created: Thursday, April 03, 2008 1:09 PM "C<ž (•WlEŽž)

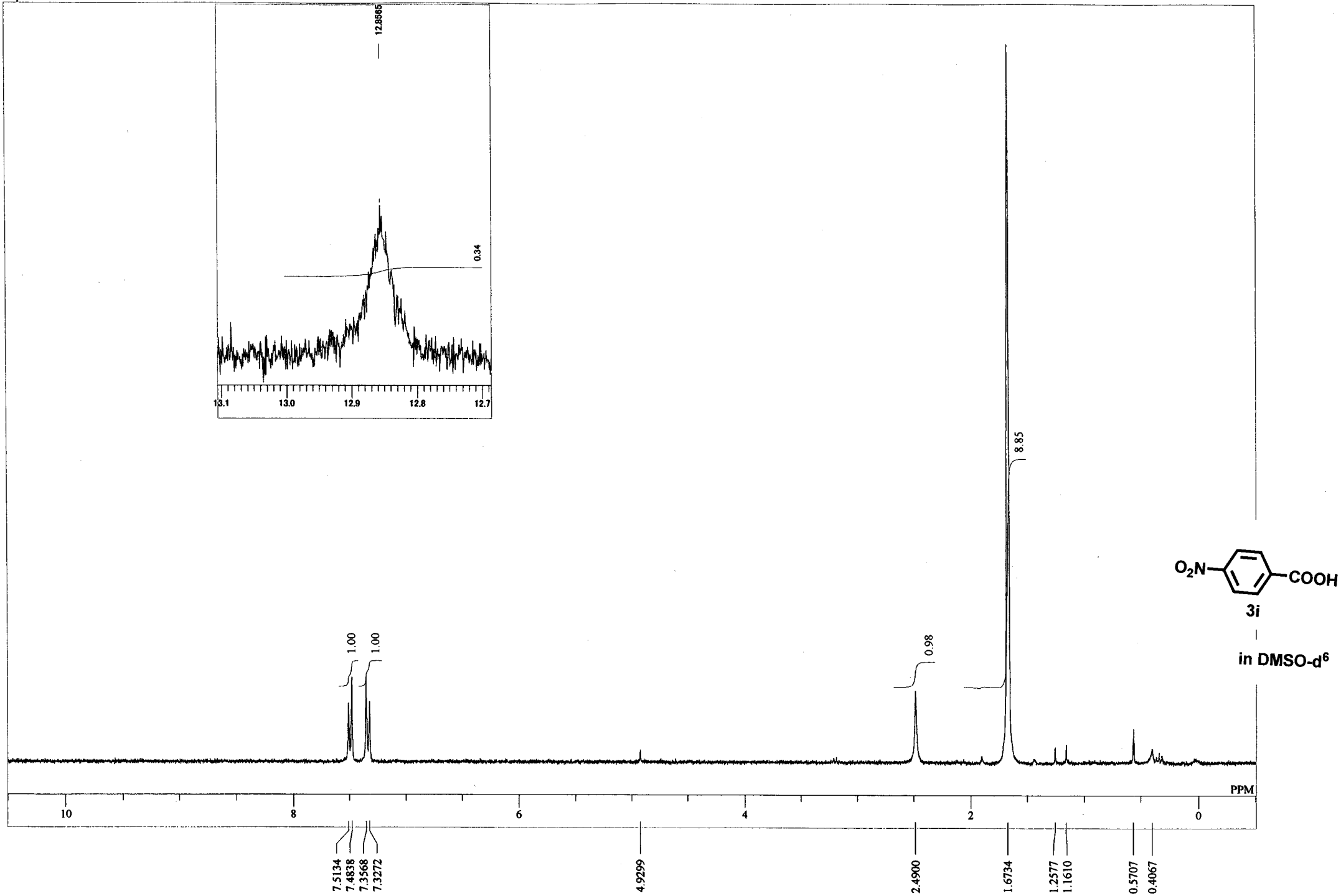
Analyst: guest

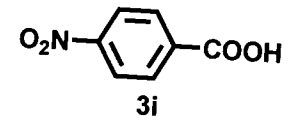
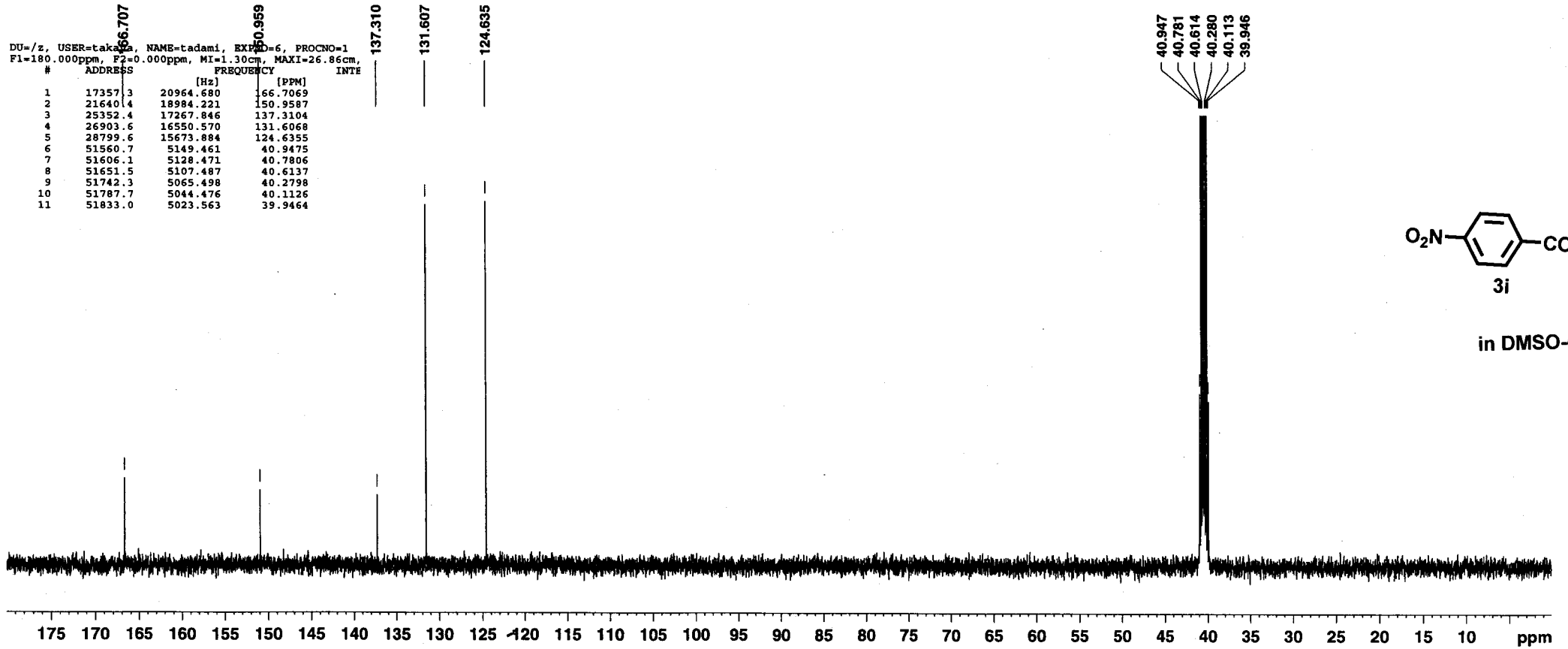
Description:



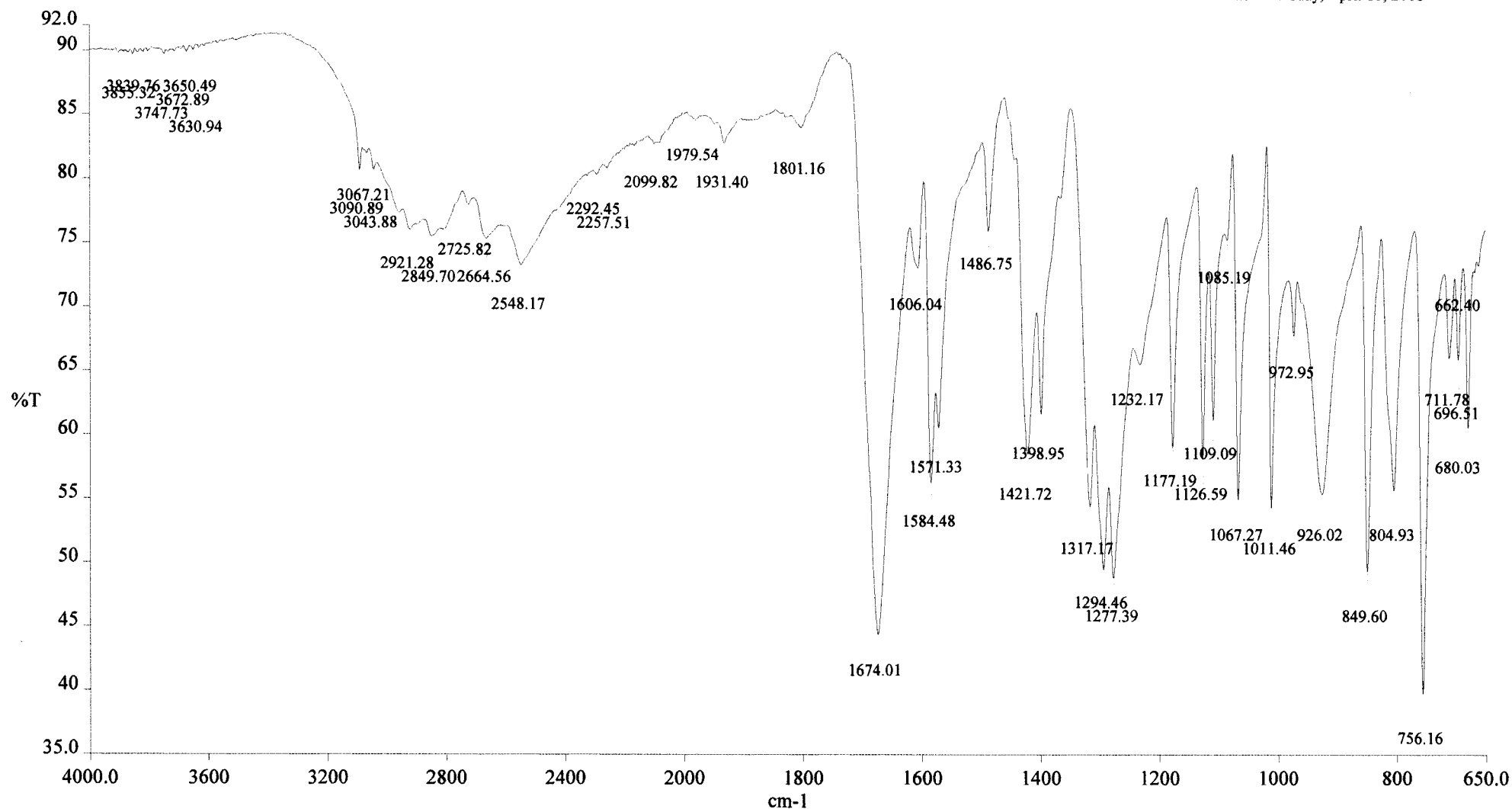
ATR

St p-nitroPhCOOH





in DMSO-d⁶

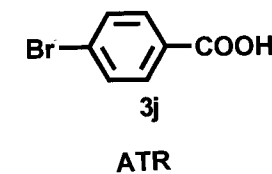


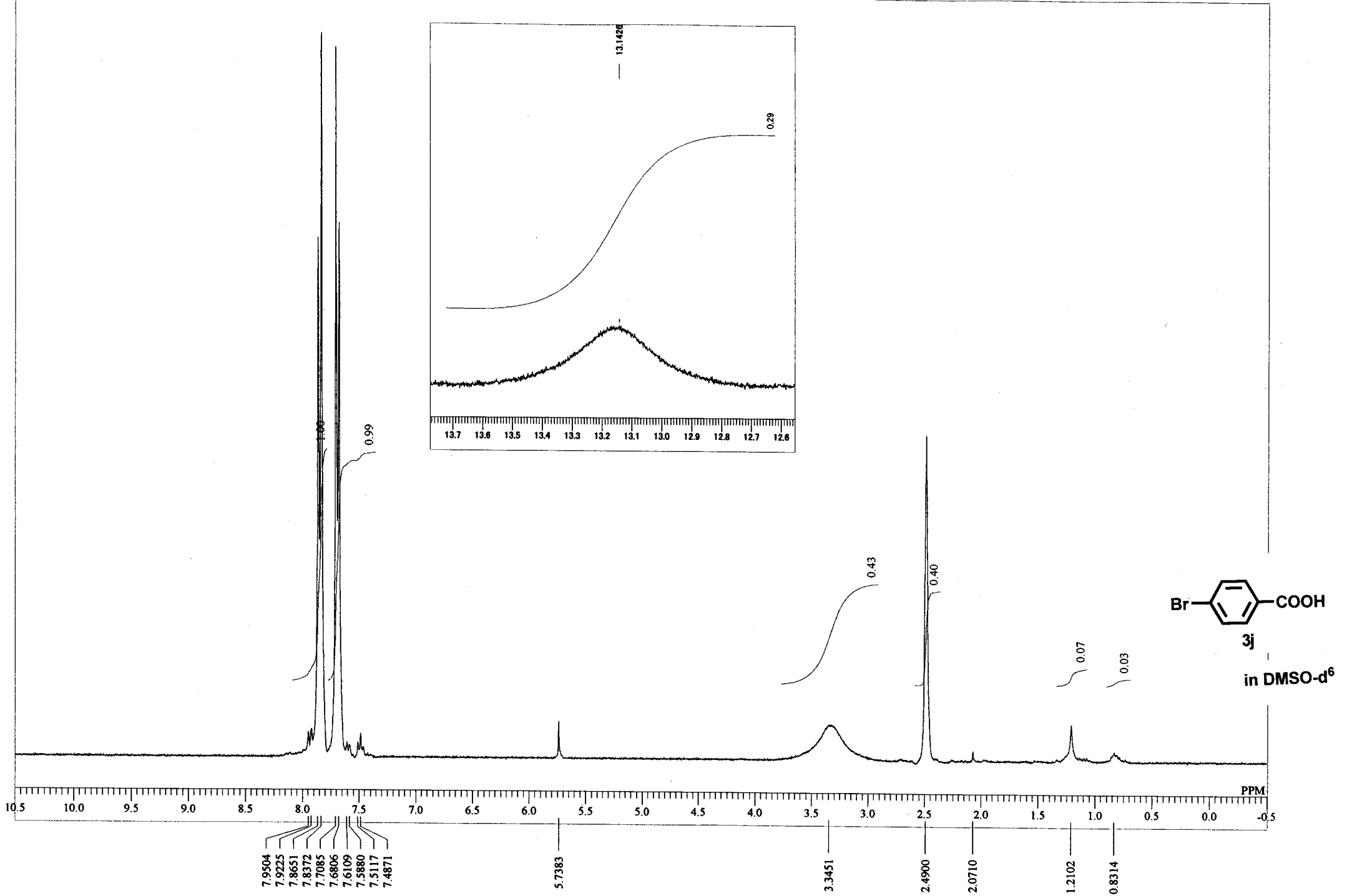
Spectrum Pathname: C:\pel_data\spectra\guest\216-1.sp *St p-Br Ph COOH*

Date Created: Thursday, April 10, 2008 6:25 PM "C.ž (•Wležž)

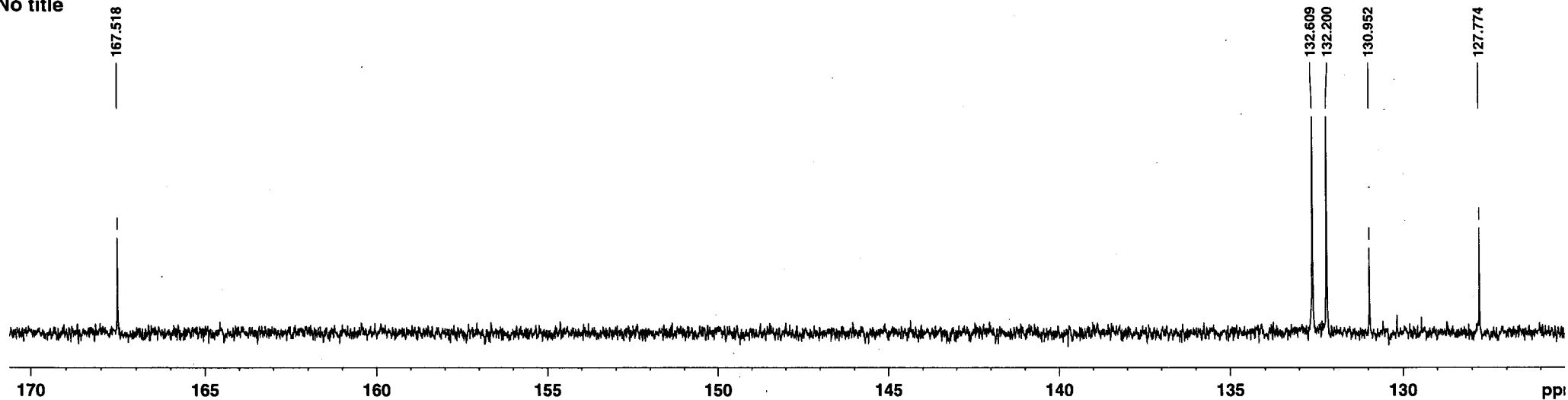
Analyst: guest

Description:



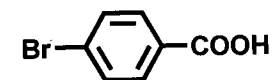
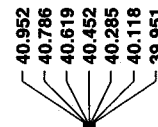


Br
No title



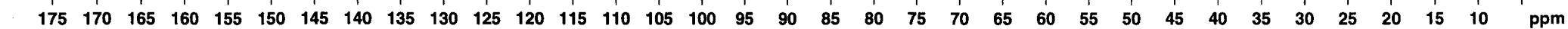
DU=/z, USER=takaya, NAME=tadami, EXPNO=16, PROCNO=1
F1=180.000ppm, F2=0.000ppm, MI=0.64cm, MAXI=1000000.

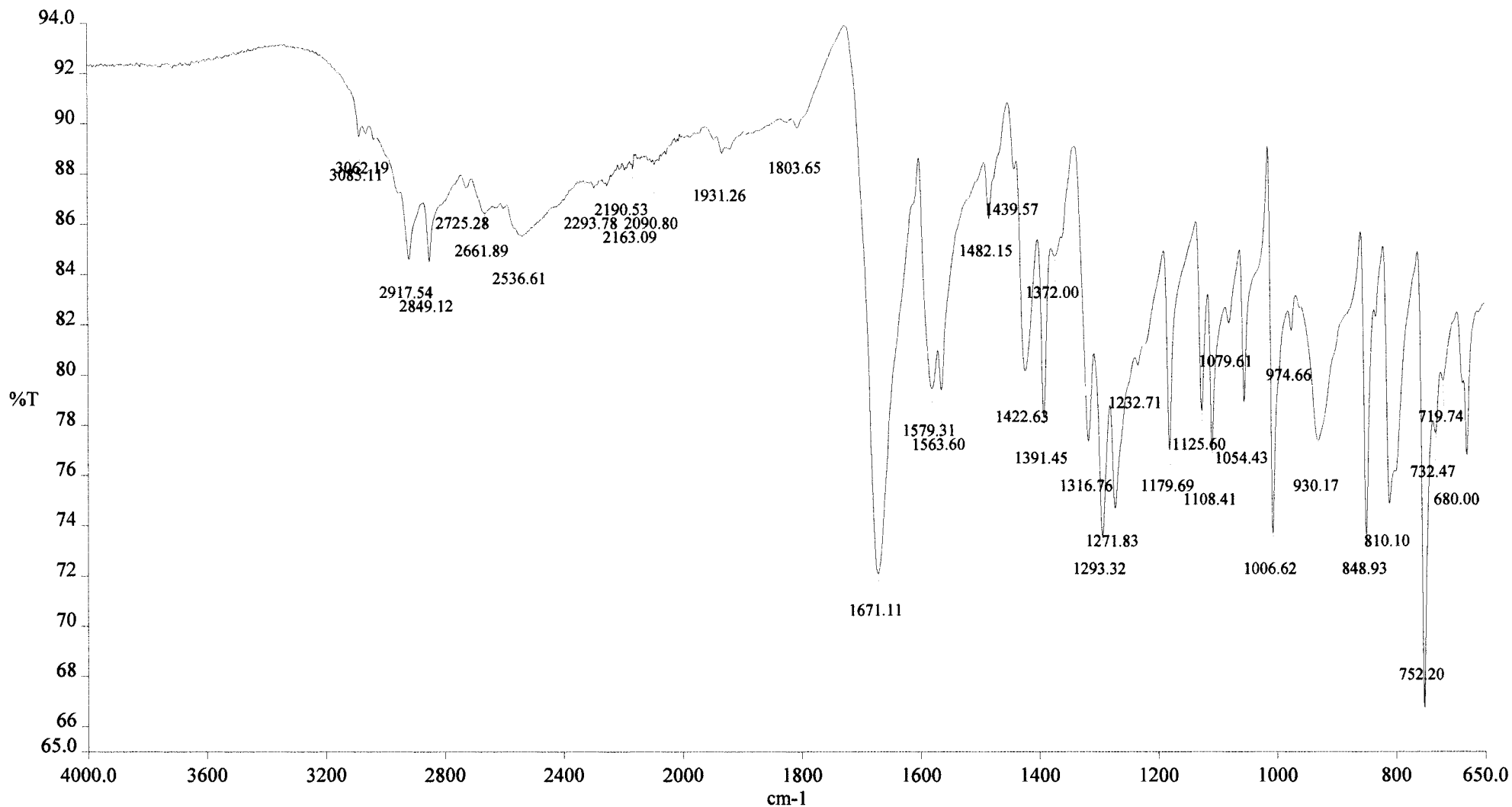
#	ADDRESS	FREQUENCY [Hz]	[PPM]	INTE
1	17137.6	21066.742	167.5185	
2	26632.0	16676.666	132.6095	
3	26743.4	16625.137	132.1997	
4	27082.7	16468.271	130.9524	
5	27947.2	16068.540	127.7738	
6	51560.4	5150.085	40.9524	
7	51605.7	5129.117	40.7857	
8	51651.2	5108.102	40.6186	
9	51696.5	5087.123	40.4518	
10	51742.0	5066.120	40.2848	
11	51787.3	5045.143	40.1180	
12	51832.8	5024.124	39.9508	



3j

in DMSO-d⁶



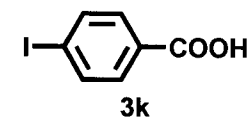


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\STp-iodoPhCOOH.sp

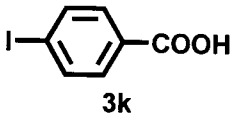
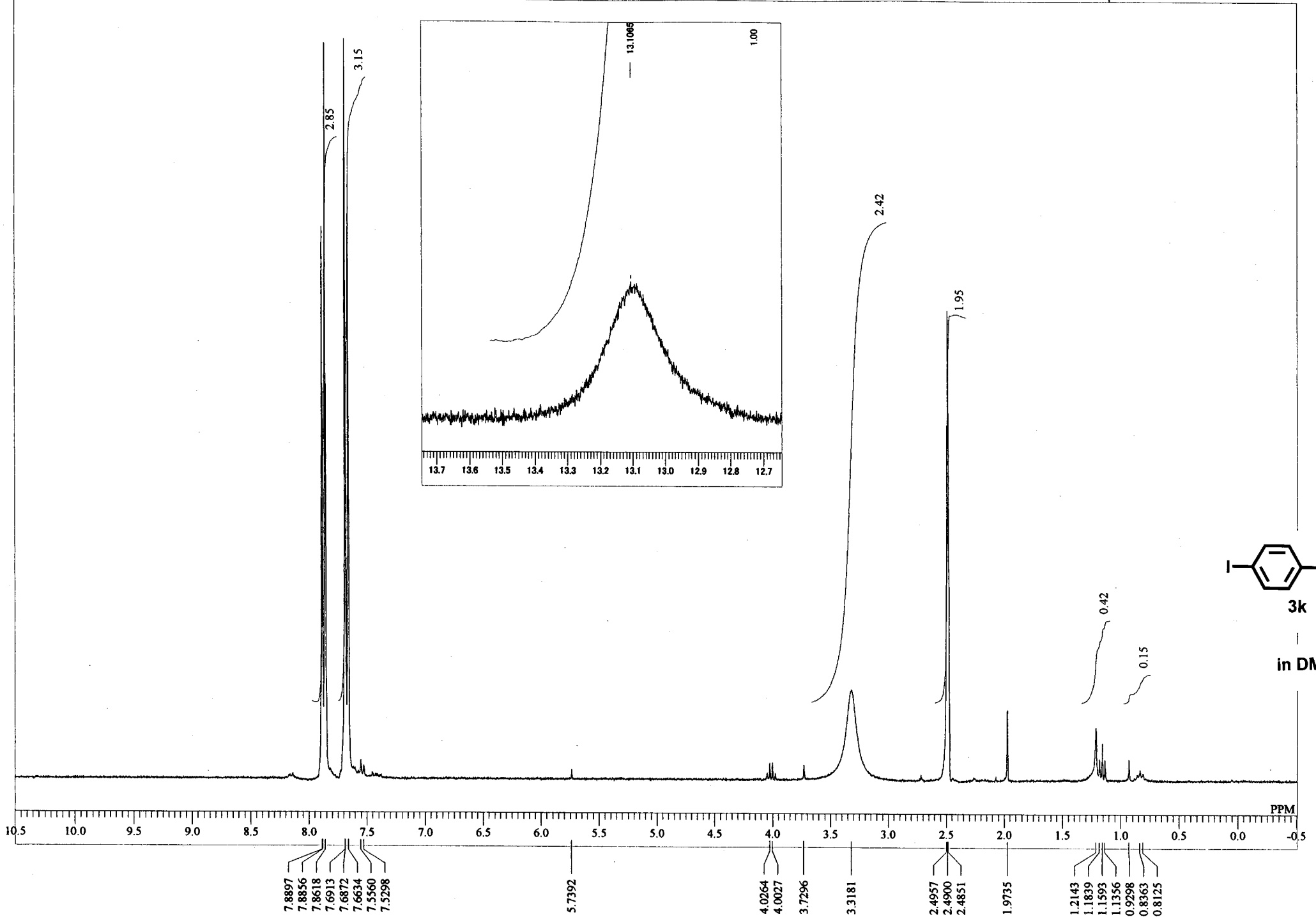
Date Created: Thursday, April 03, 2008 1:21 PM

Analyst: guest

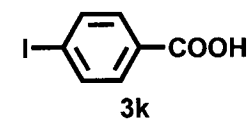
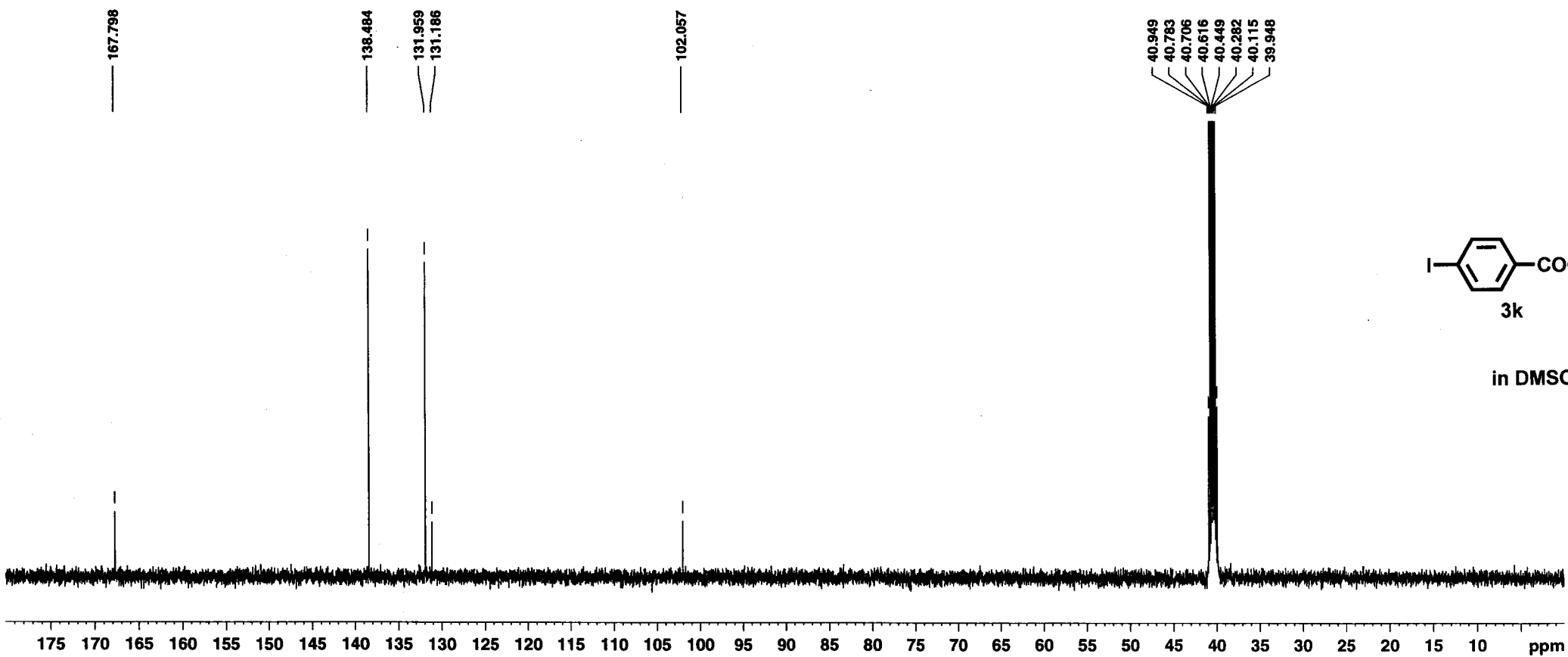
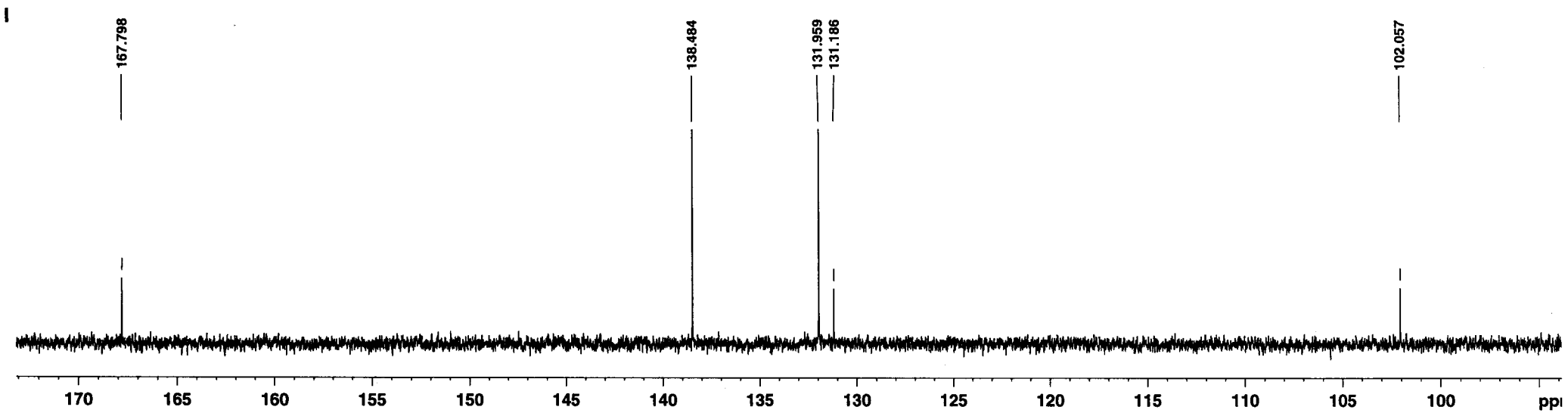
Description:



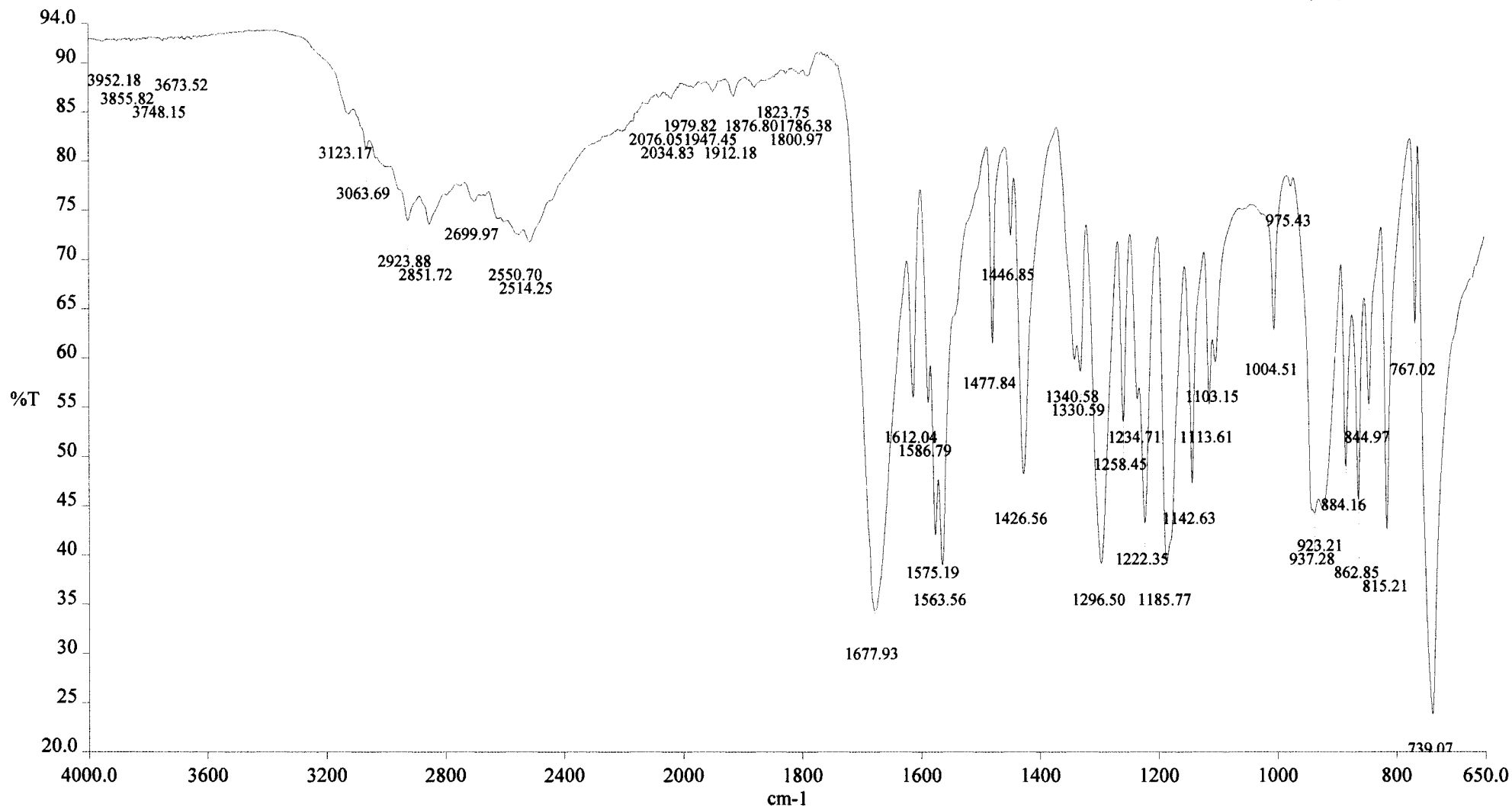
ATR



in DMSO-d⁶



in DMSO-d⁶



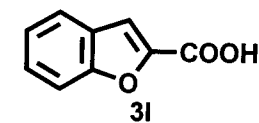
Spectrum Pathname: C:\pel_data\spectra\guest\216-1.sp

st benzofuranyl COOH

Date Created: Thursday, April 10, 2008 6:15 PM "Cez (•Wležž)"

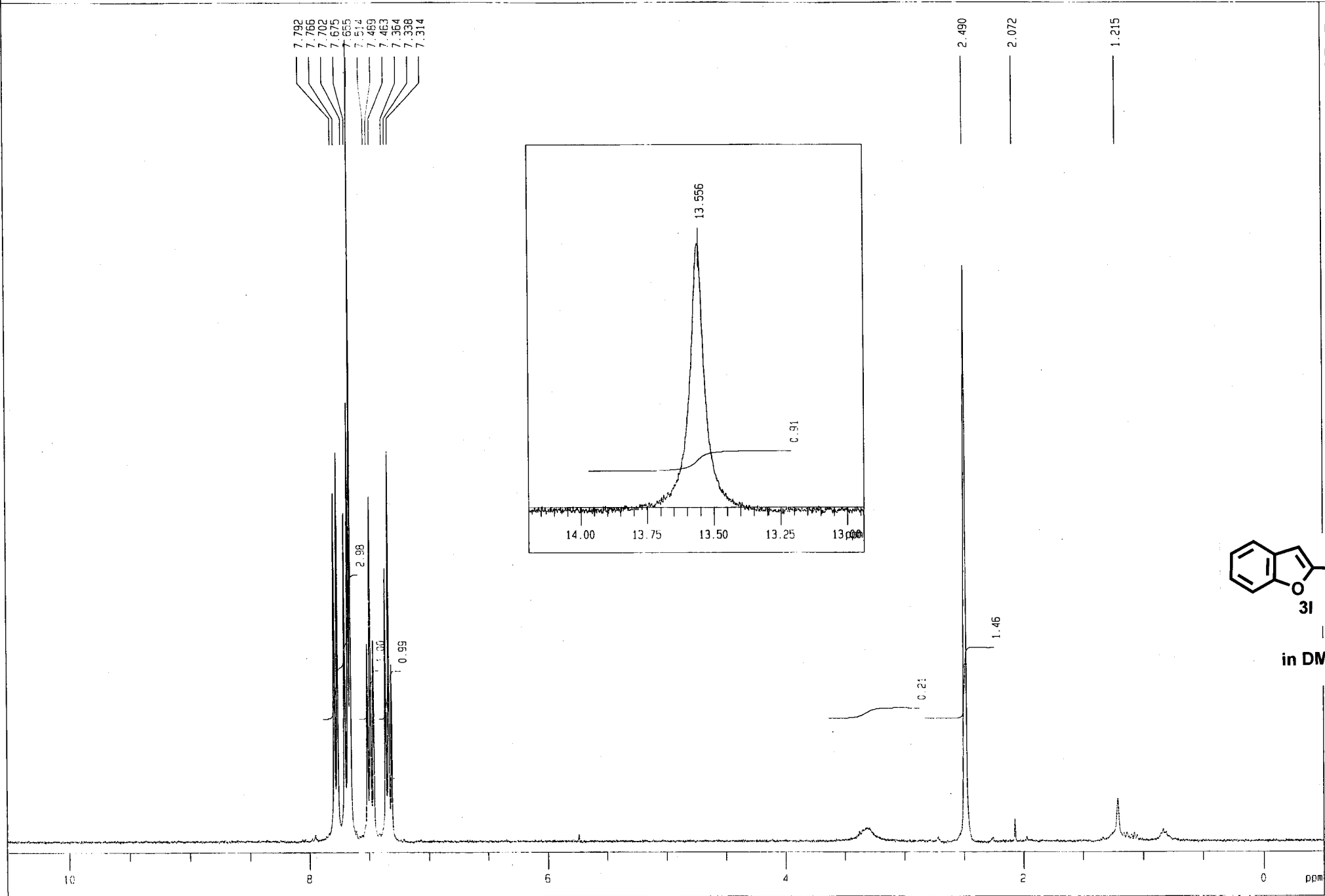
Analyst: guest

Description:



ATR

St. benzofuranylCOOH



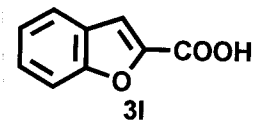
Date

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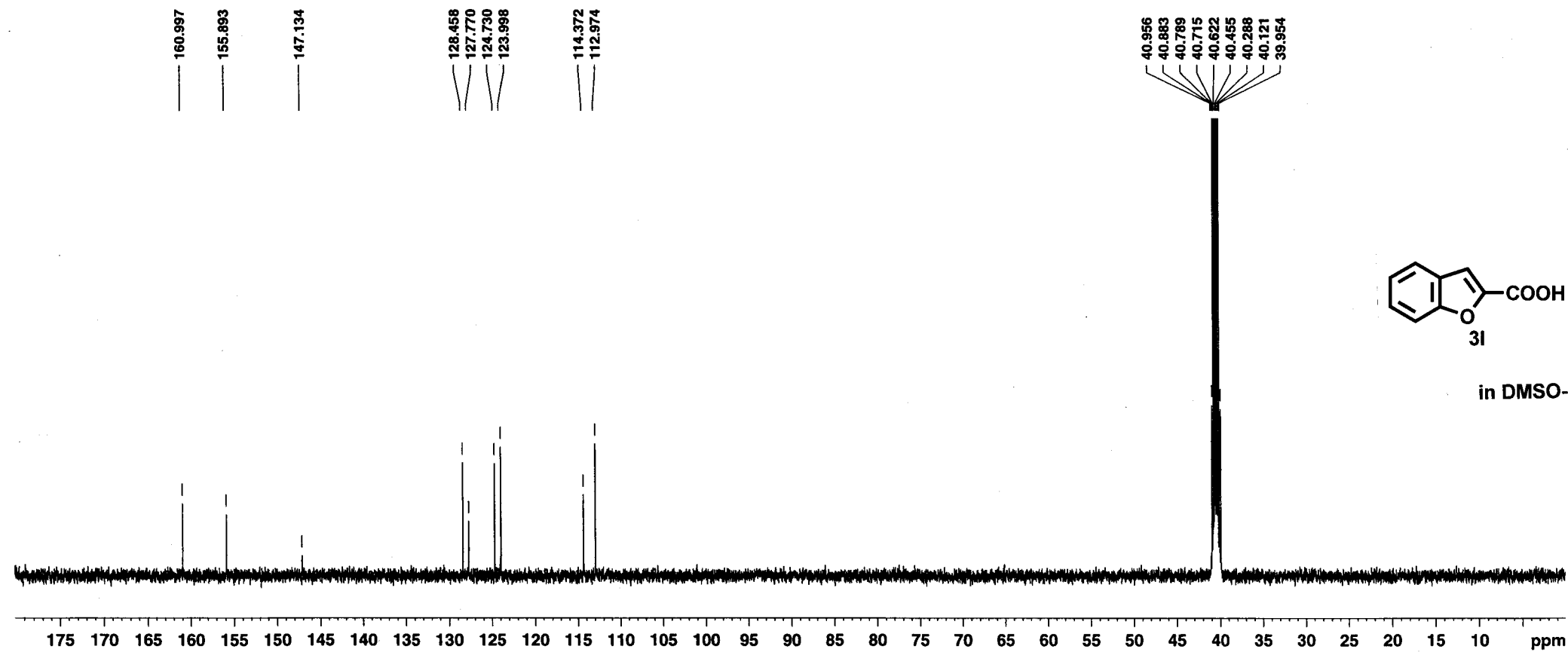
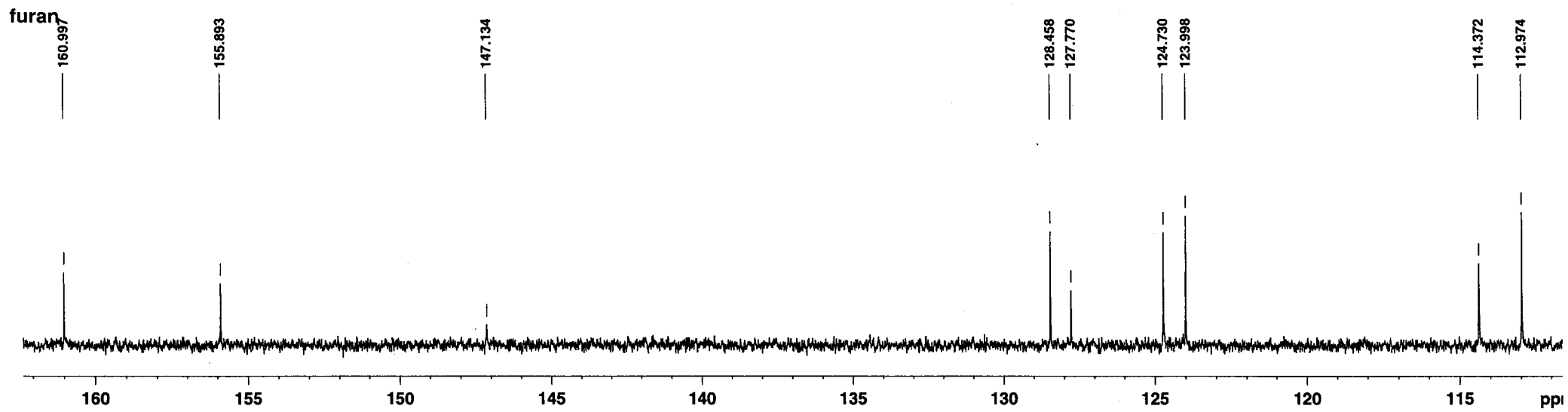
POINT
SAMPQ
FREQ
FILTR
DELAY
DEADT
INTVL
TIMES
DUMMY
PD
ACQTM
PREDL
INIWT
RESOL
PW1
OBNUC
OBFRQ
OBSEI
RGAIN

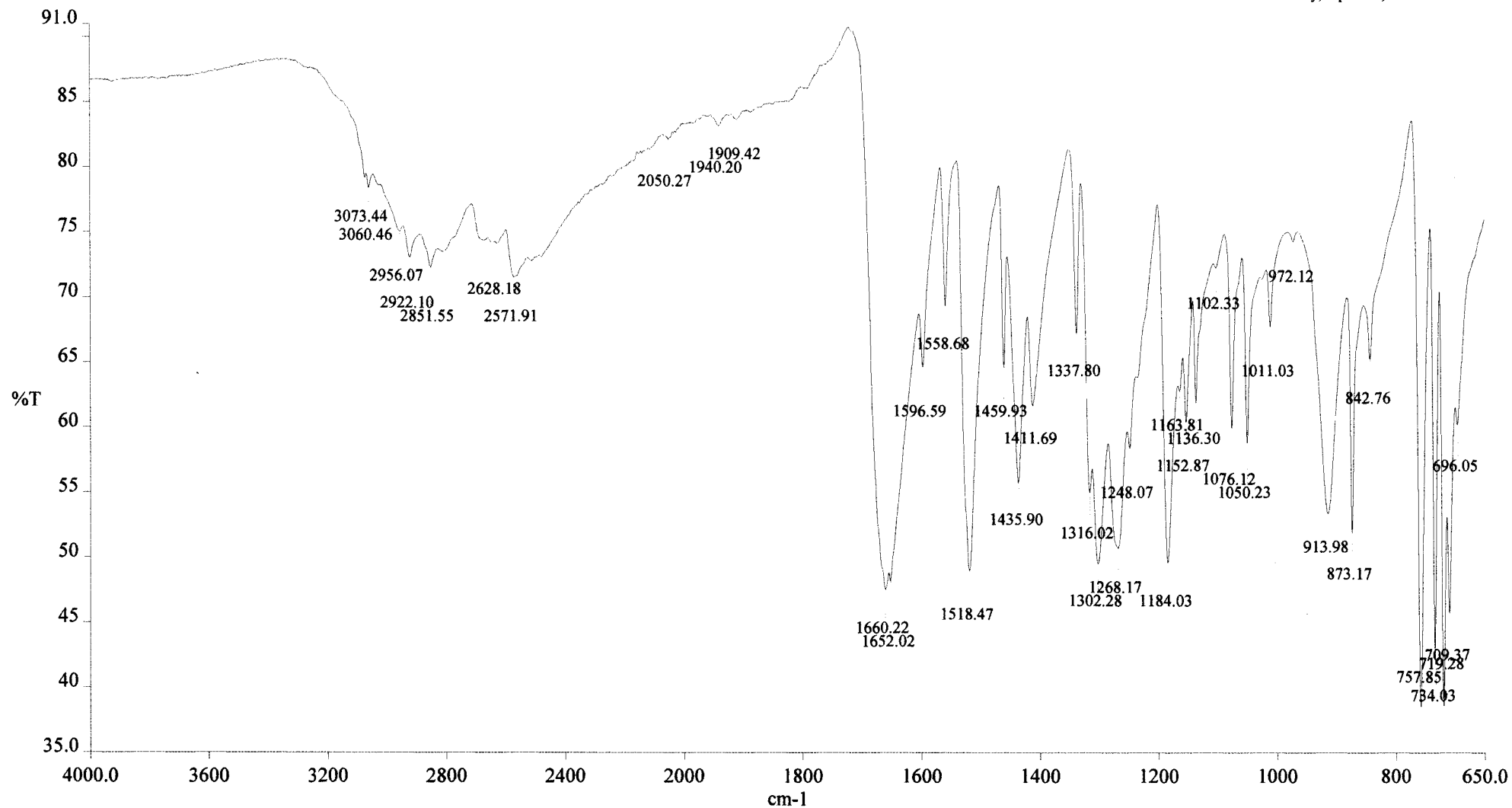
SCANS

SLVNT
SPINN
TEMP



in DMSO-d⁶



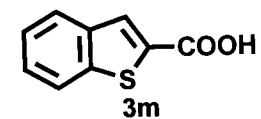


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\Tadami\ST2-benzothiophenylCOOH.sp

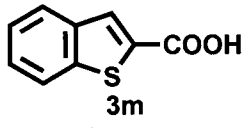
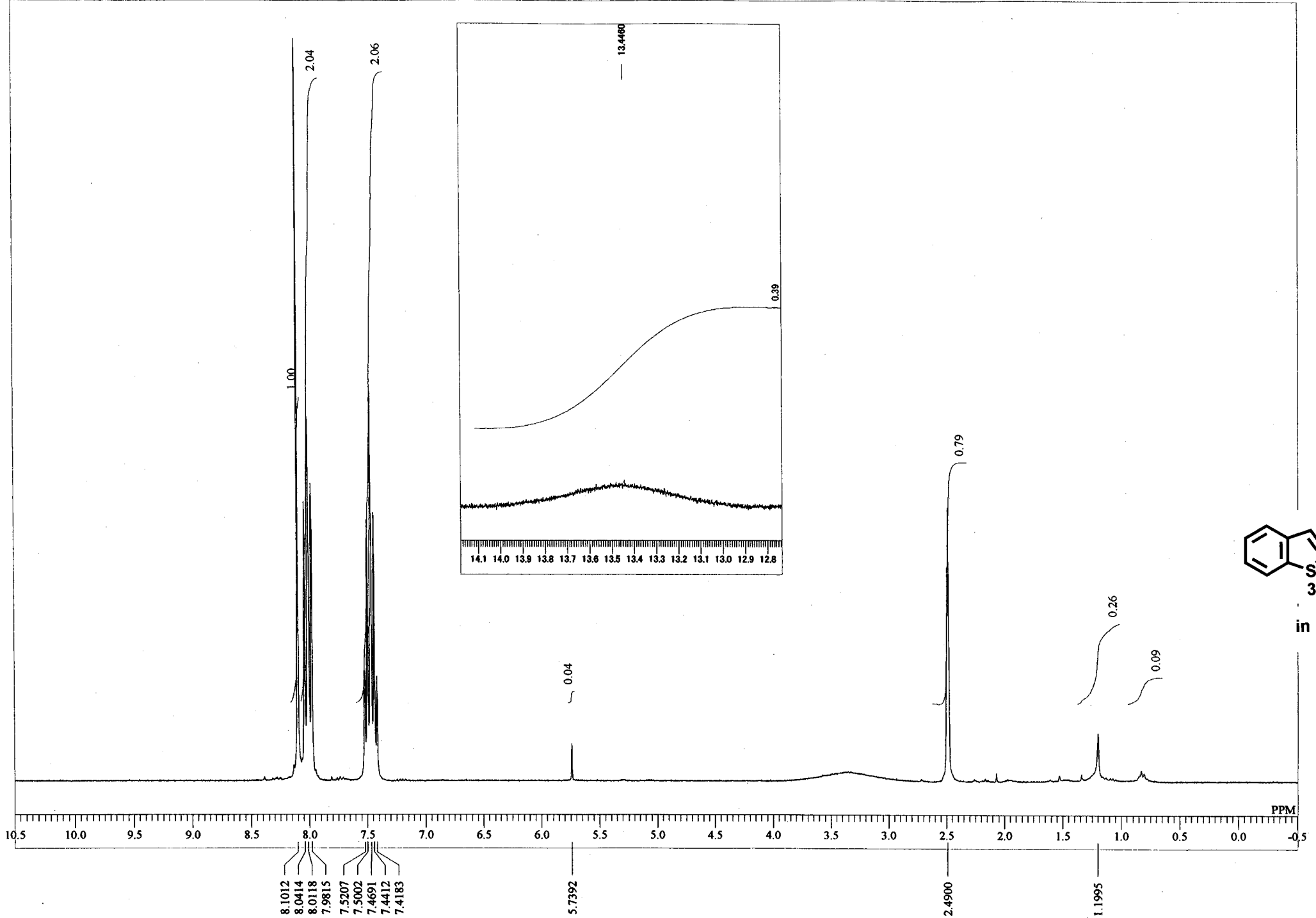
Date Created: Thursday, April 10, 2008 6:29 PM

Analyst: guest

Description:

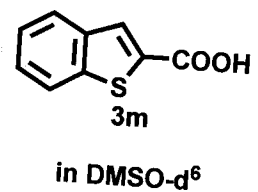
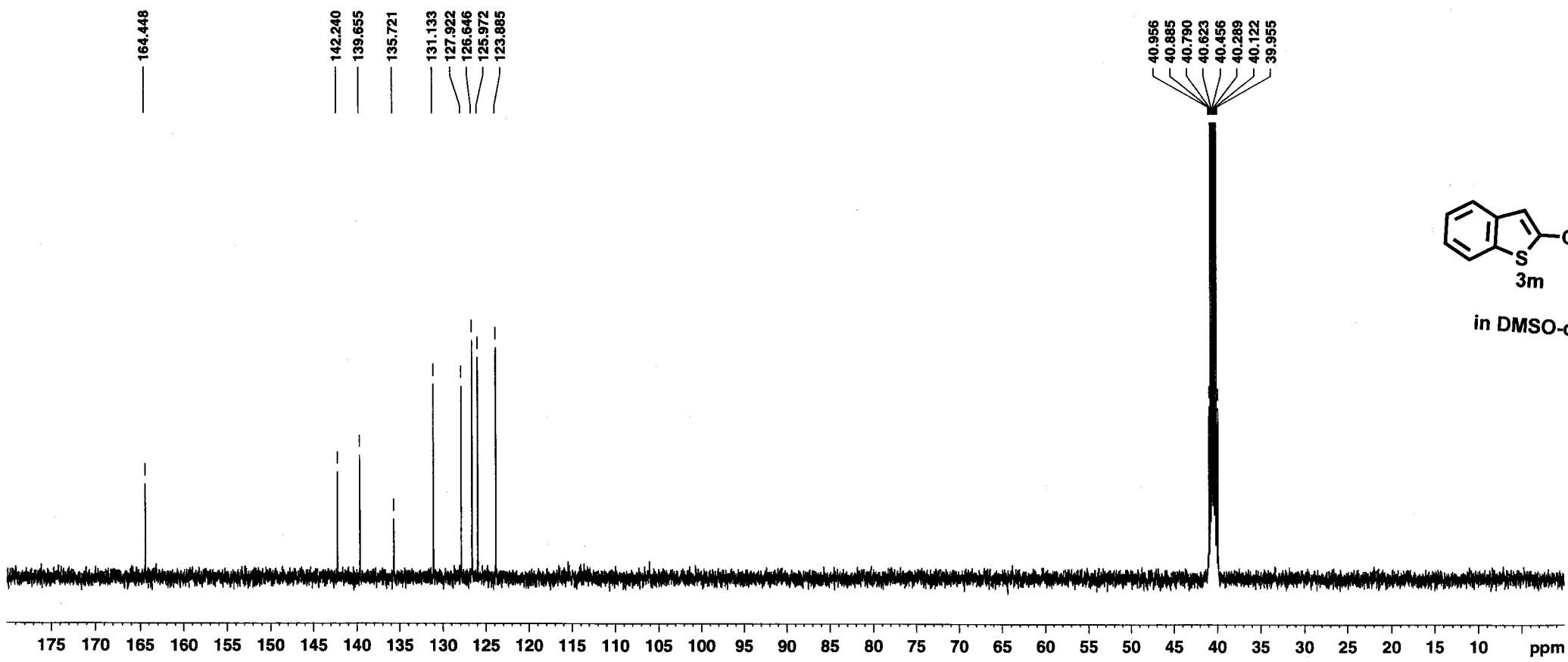
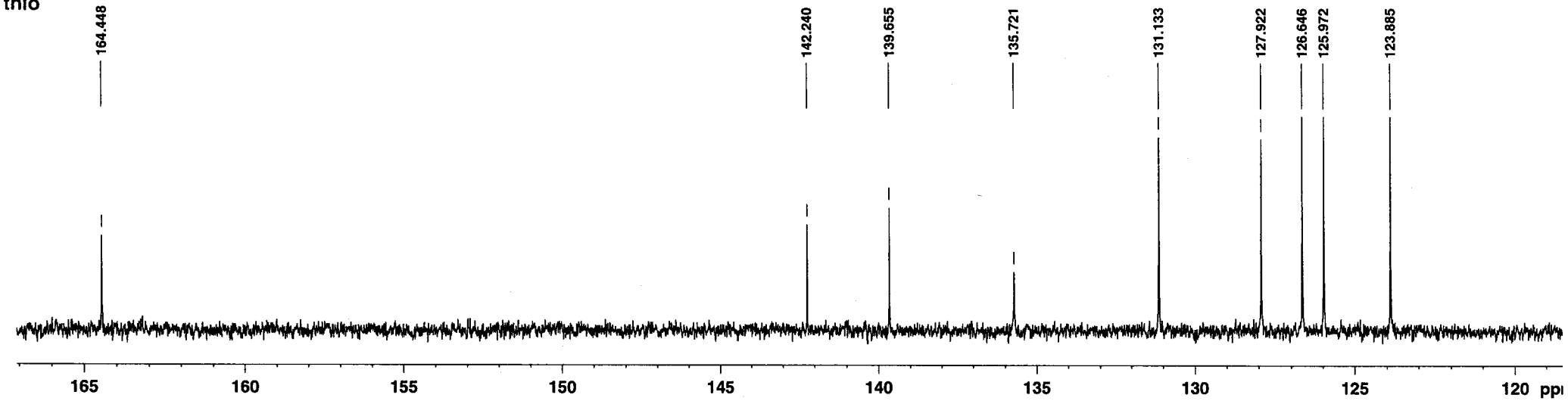


ATR

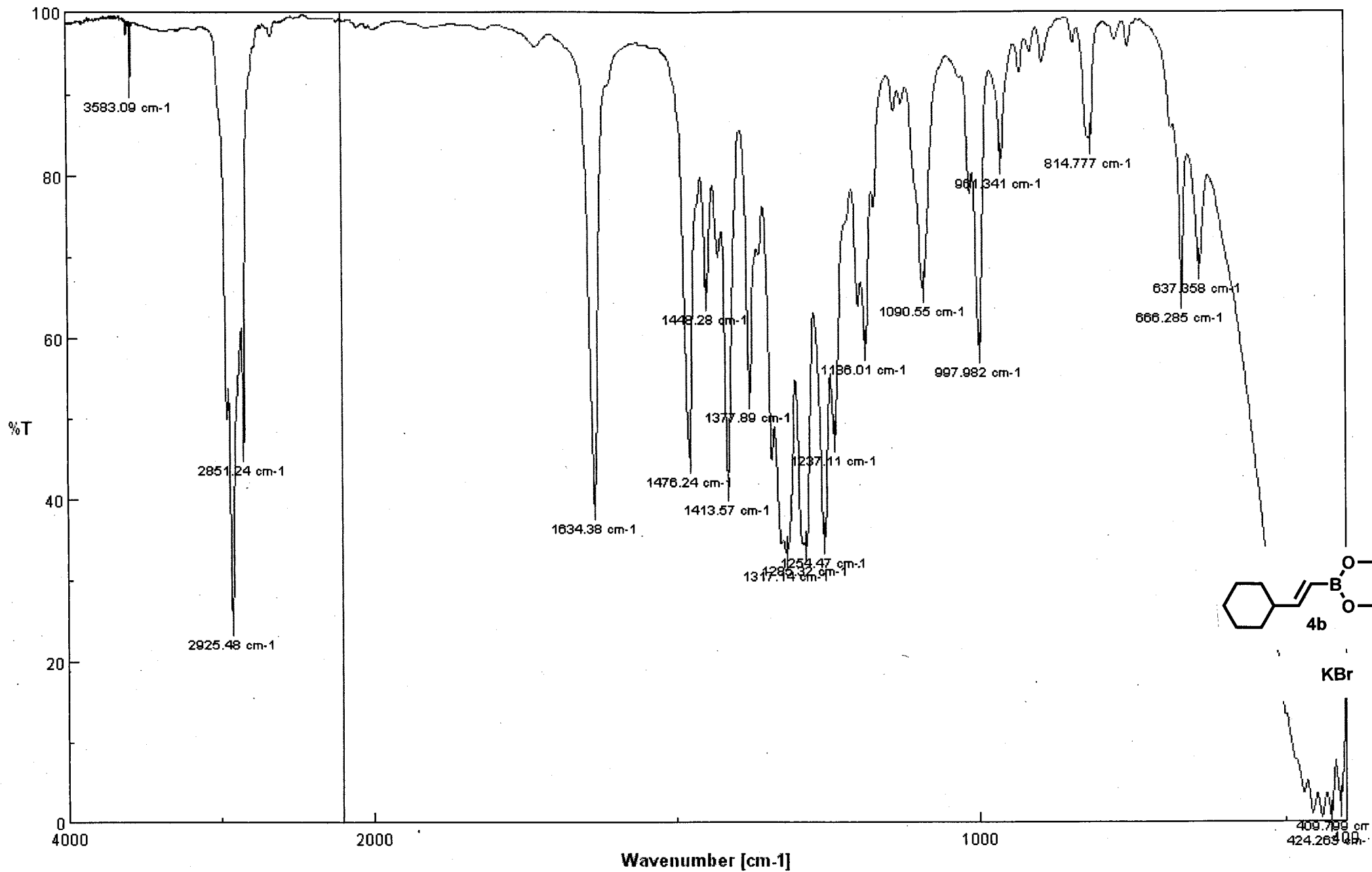


in DMSO-d₆

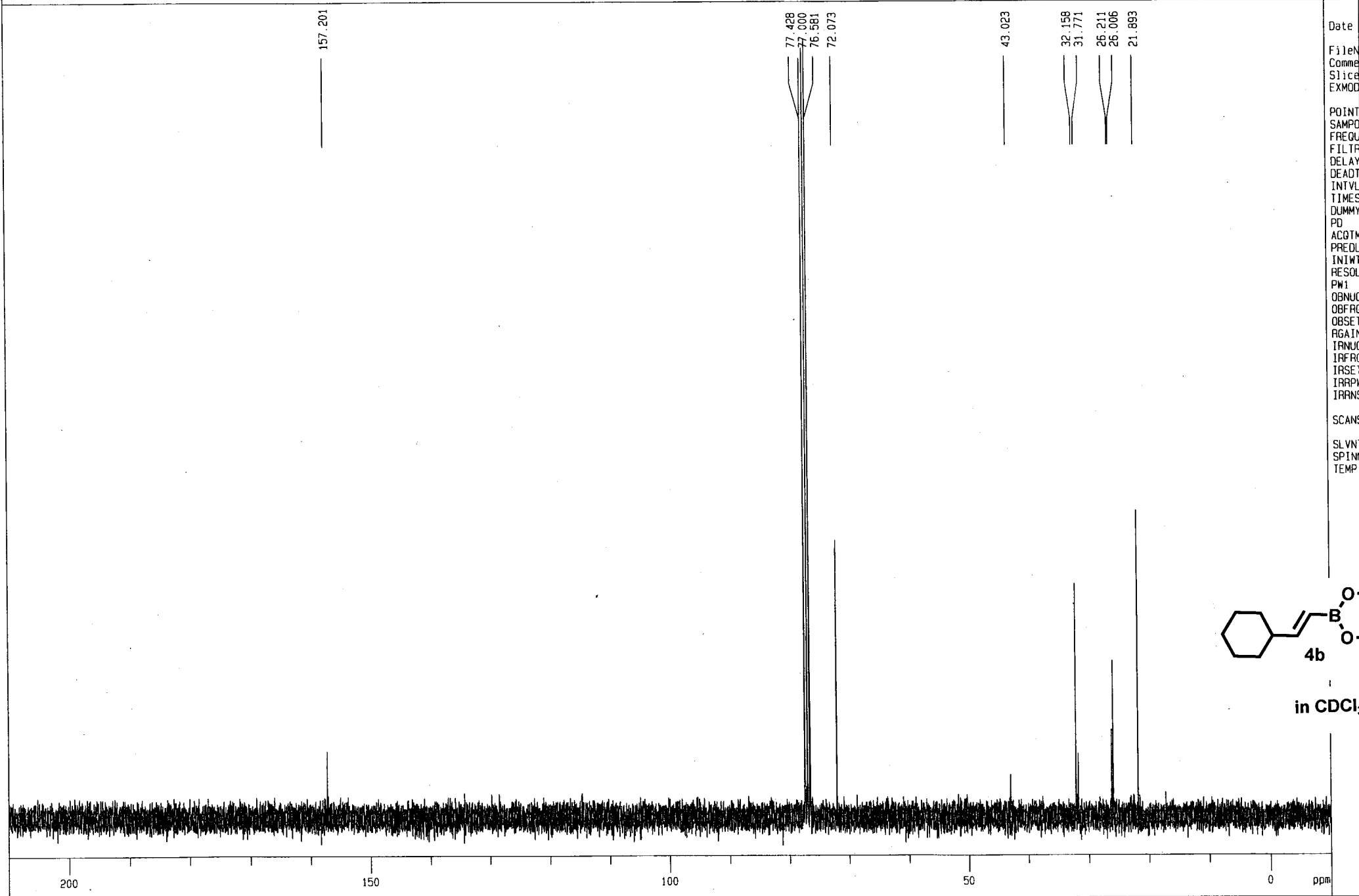
thio



C-Hex \approx Bneo



St SM c-hex alkenyl Bneo



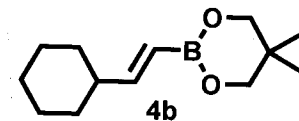
Date

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OBFRQ
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RGAIN
IRNUC
IRFRQ
IRSET
IRRPW
IRRNS

SCANS

SLVNT
SPINN
TEMP

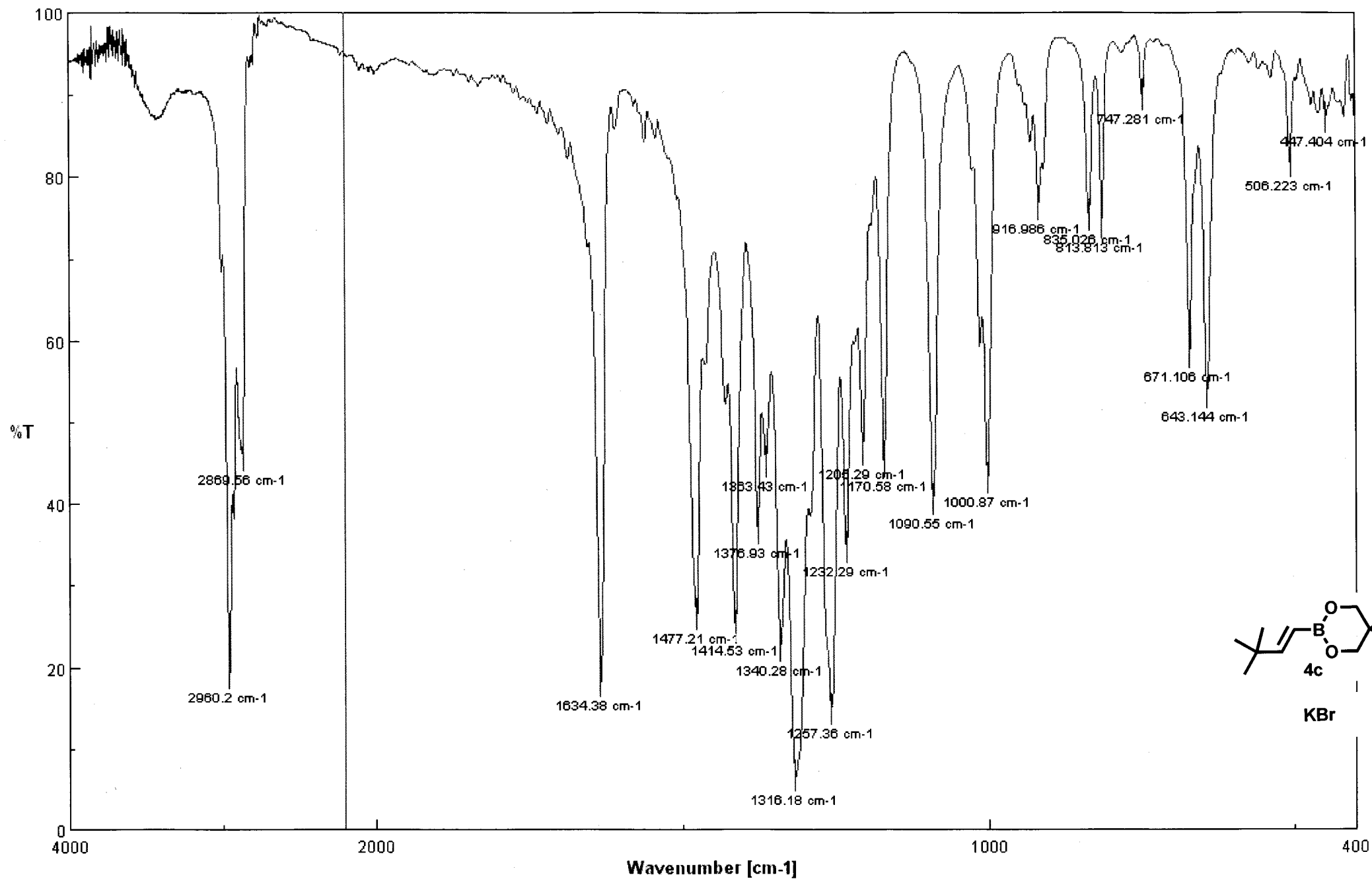


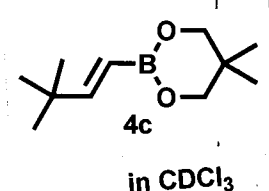
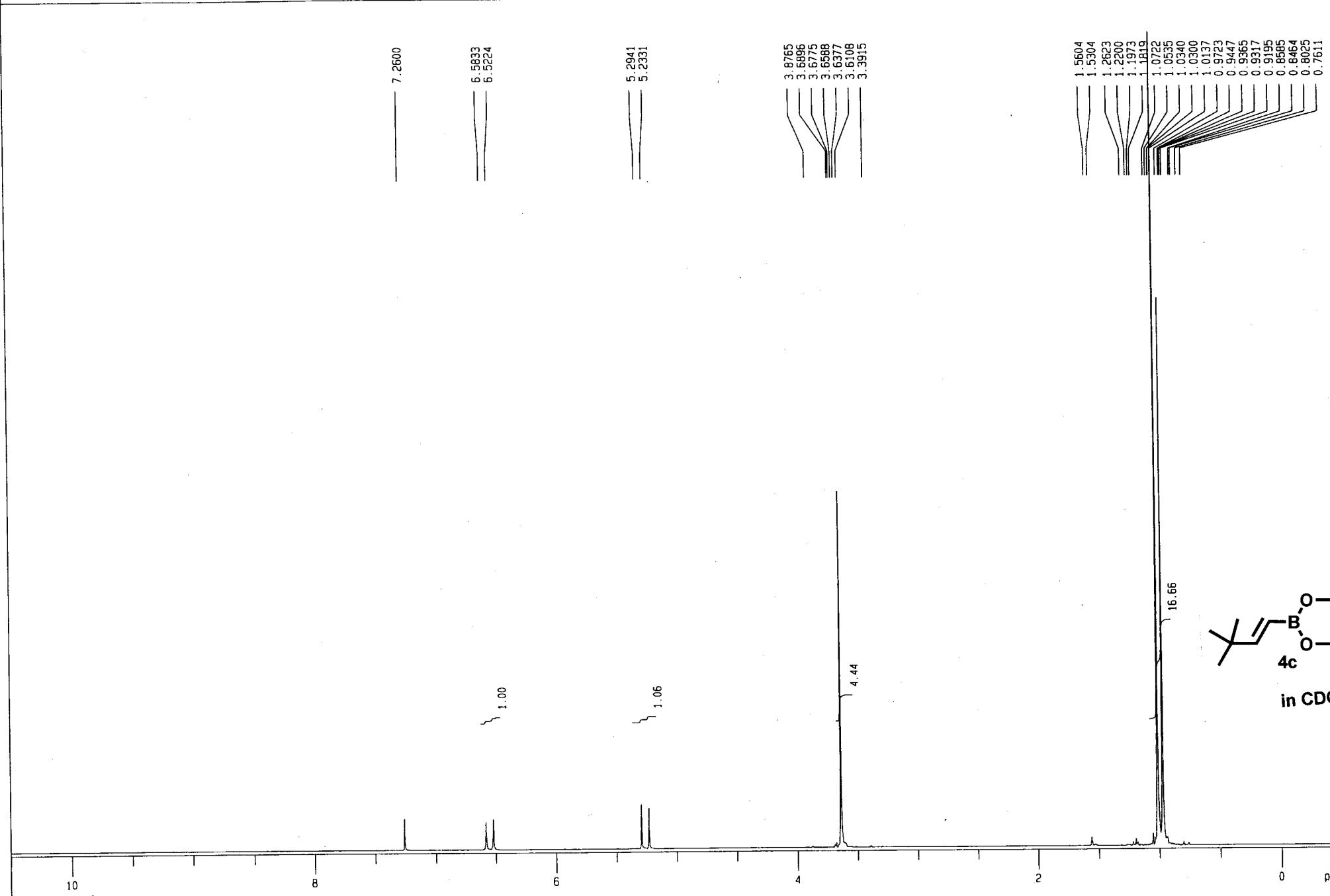
in CDCl₃



Date
 FileN
 Comme
 Slice
 EXMOD
 POINT
 SAMPO
 FREQU
 FILTR
 DELAY
 DEADT
 INTVL
 TIMES
 DUMMY
 PD
 ACQTM
 PREDL
 INIWT
 RESOL
 PW1
 OBNUC
 OBFRG
 OBSET
 RGAIN
 SCANS
 SLVNT
 SPINN
 TEMP

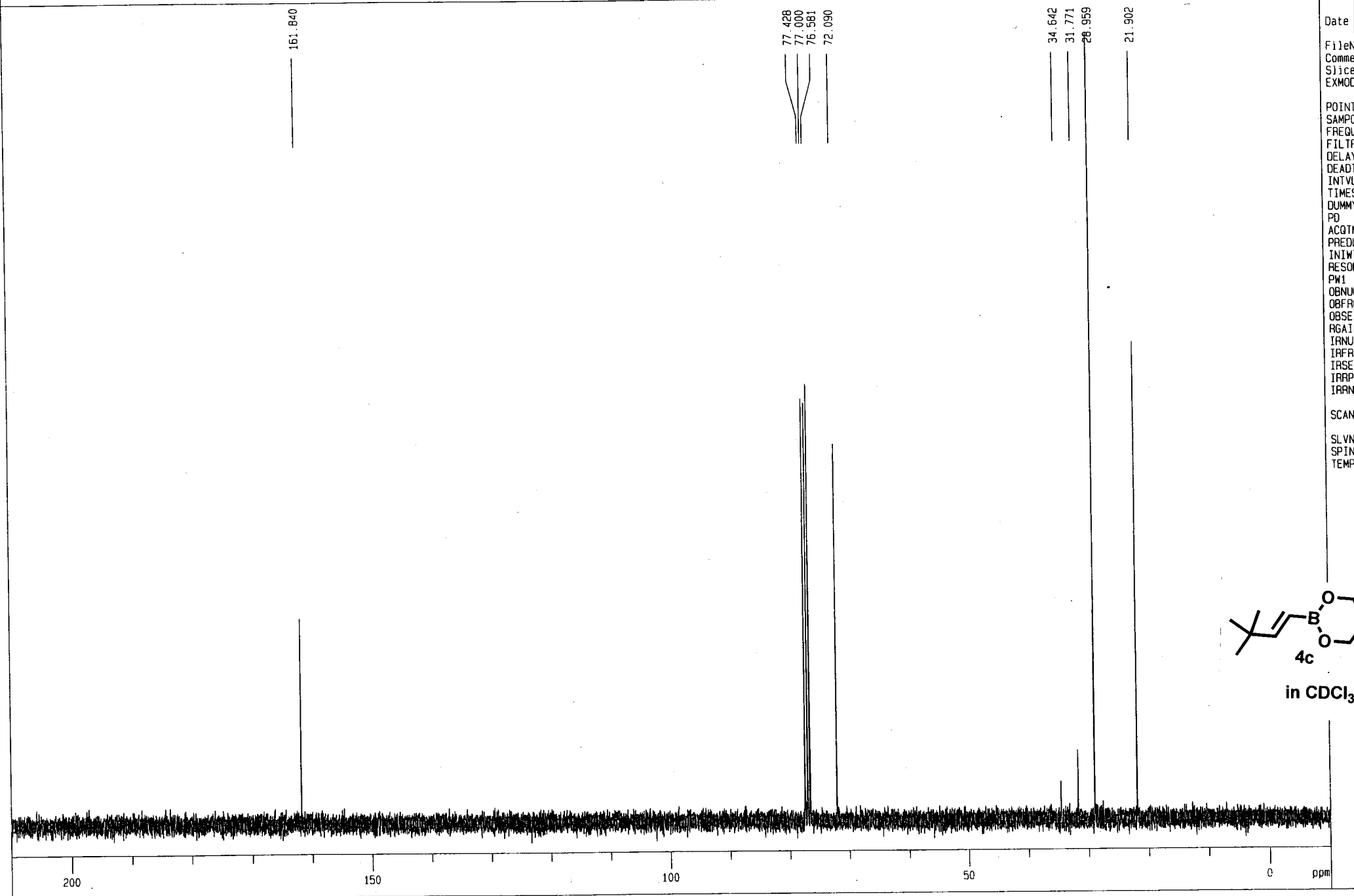
tBu \approx Bneo





Date
 FileN
 Comme
 Slice
 EXMOD
 POINT
 SAMPO
 FREQU
 FILTR
 DELAY
 DEADT
 INTVL
 TIMES
 DUMMY
 PD
 ACQTM
 PREDL
 INIWT
 RESOL
 PW1
 OBNUC
 OBFRO
 OBSET
 RGAIN
 SCANS
 SLVNT
 SPINN
 TEMP

St SM trans t-Bu alkenyl Bneo



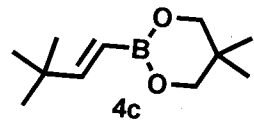
Date

FileN
Comme
Slice
EXMOD

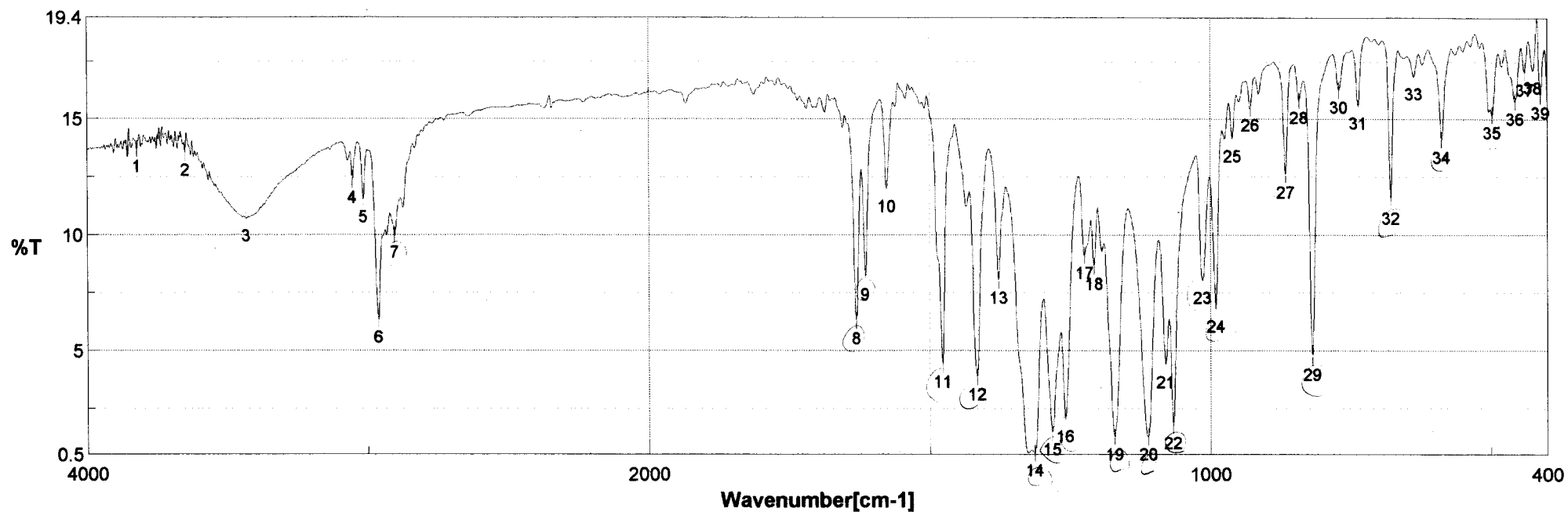
POINT
SAMPD
FREQU
FILTR
DELAY
DEADT
INTVL
TIMES
DUMMY
PD
ACGTM
PREDL
INIWT
RESOL
PW1
OBNUC
OBFRC
OBSET
RGAIN
IRNUC
IRFRQ
IRSET
IRRPW
IRANS

SCANS

SLVNT
SPINN
TEMP



in CDCl₃

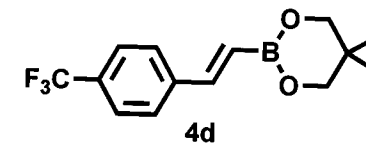


number of scan
zero filling
gain
date of scan
sample name

16
ON
Auto (8)
06/02/18 22:29
No. 4

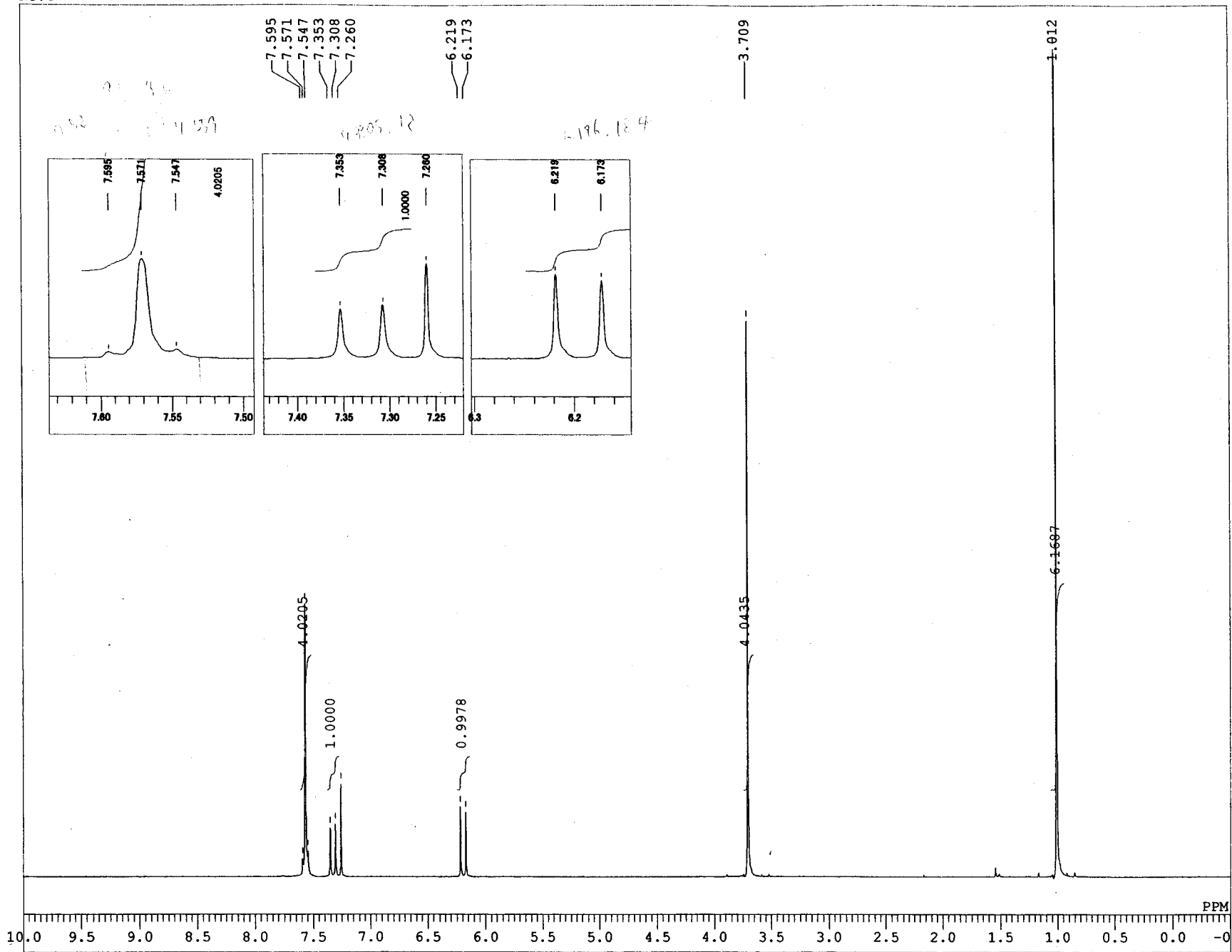
resolution
apodization
scan speed
date of data processing

4 cm-1
Cosine
Auto (2 mm/sec)
06/02/18 22:30



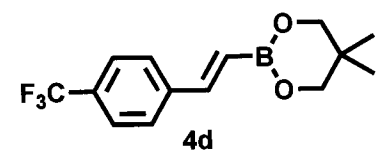
KBr

No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3822.22	13.6999	2	3650.59	13.5441	3	3434.6	10.7054	4	3054.69	12.3631	5	3016.12	11.5184
6	2962.13	6.33464	7	2905.24	9.9882	8	1630.52	6.27737	9	1615.09	8.17188	10	1576.52	11.9689
11	1477.21	4.4123	12	1415.49	3.85937	13	1377.89	8.03145	14	1314.25	0.566949	15	1282.43	1.47838
16	1259.29	2.04588	17	1224.58	9.1018	18	1207.22	8.62847	19	1171.54	1.26191	20	1110.8	1.25901
21	1079.94	4.38564	22	1066.44	1.75094	23	1014.37	8.03999	24	990.268	6.80216	25	960.377	14.1288
26	928.557	15.4757	27	865.882	12.5773	28	841.776	15.7981	29	818.634	4.7124	30	770.423	16.2666
31	736.674	15.5669	32	678.82	11.4613	33	637.358	16.8565	34	588.182	14.1008	35	497.544	15.1736
36	457.047	15.7642	37	439.69	17.0359	38	425.227	17.1265	39	411.728	16.0347			

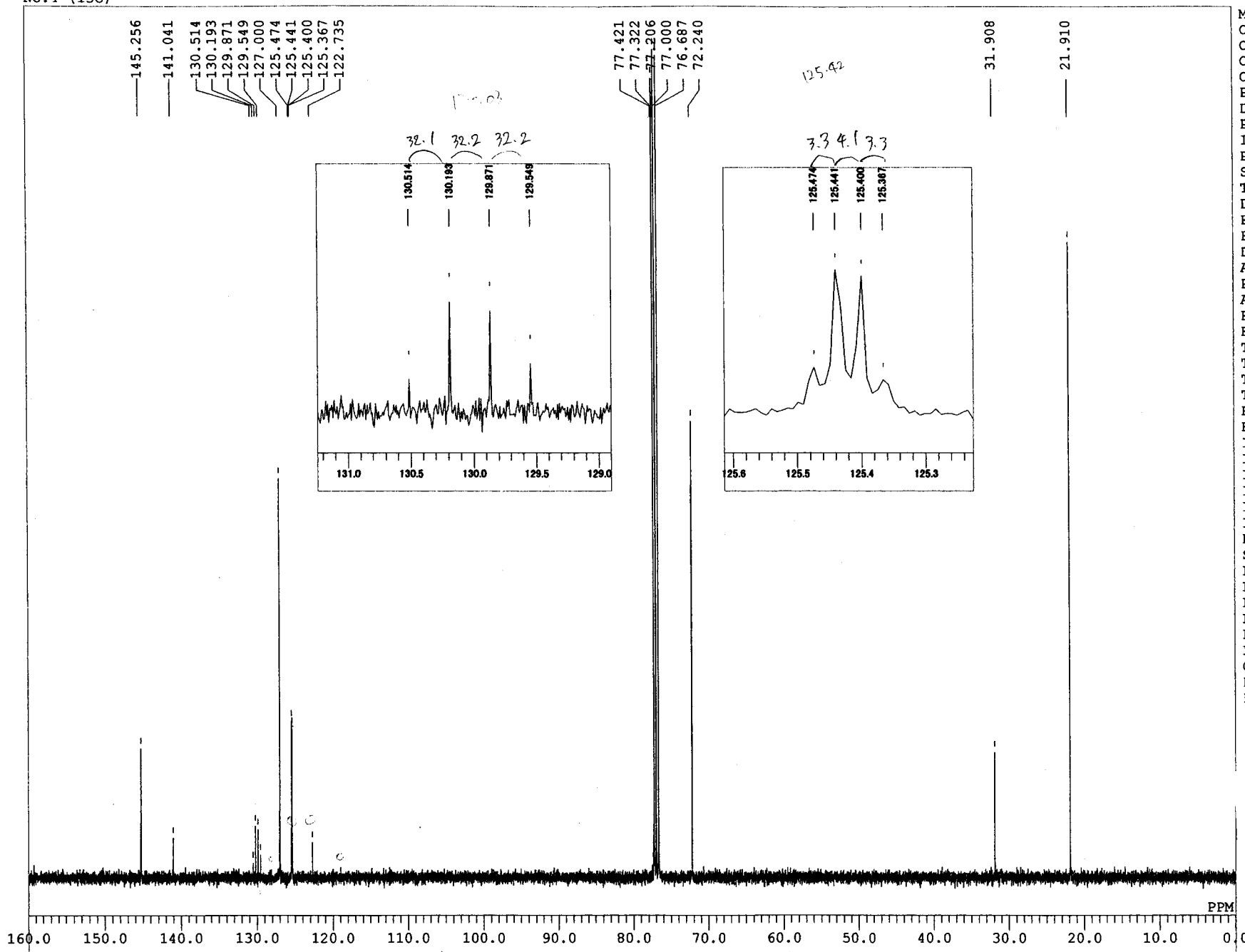


```

MENUF NON
OBNUC 1H
OFR 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.0 Hz
PW1 5.8 us
DEADT 72.1 us
PREDL 0.2000 ms
IWT 1.0 sec
POINT 32768
SPO 32768
TIMES 8
DUMMY 1
FREQU 8000.0 Hz
FLT 4000 Hz
DELAY 50.0 us
ACQTM 4.096 sec
PD 1.500 sec
ADBIT 16.00
RGAIN 18
BF 0.10 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD NON
EXPCM NON:Single.coupled:PW1_F
IRNUC 1H
IFR 399.65 MHz
IRSET 124.00 KHz
IRFIN 10500.0 Hz
IRRPW 50 us
IRATN 511
DFILE C:\WINNMR98\COMMON\_DEF
SF TH5
LKSET 61.60 KHz
LKFIN 79.0 Hz
LKLEV 200
LGAIN 20
LKPHS 58
LKSIG 518
CSPED 12 Hz
FILDC
FILDF
    
```

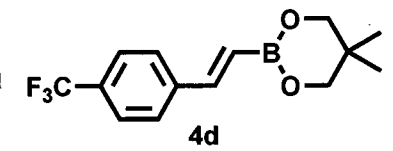


in CDCl₃

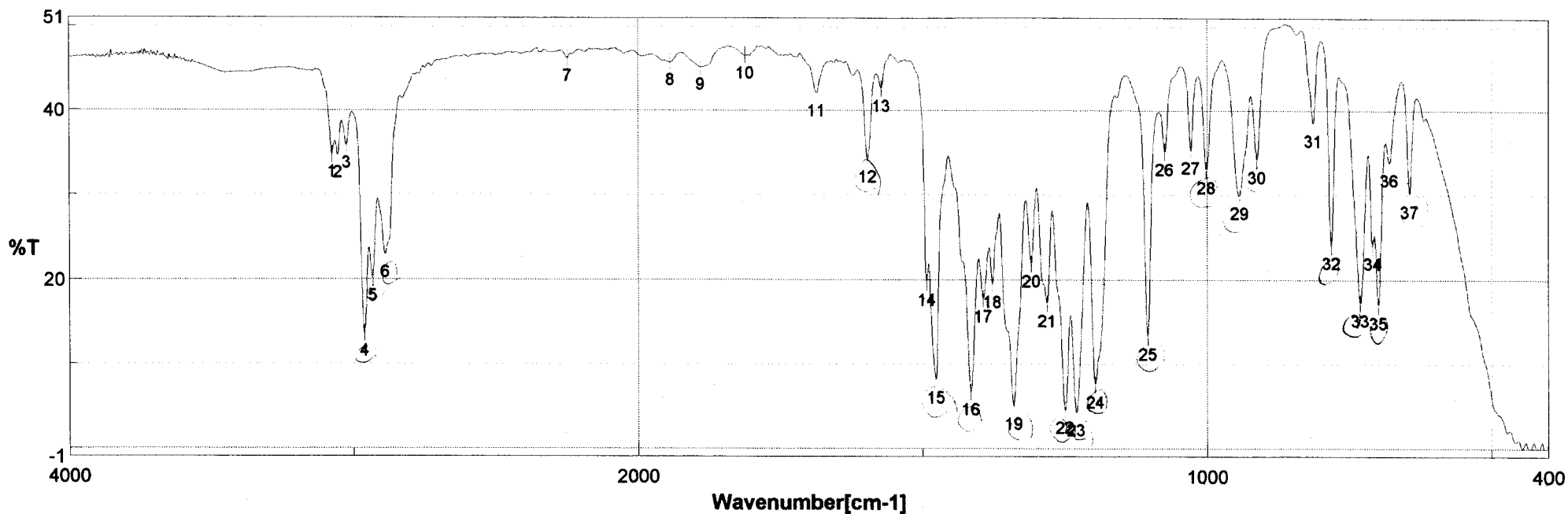


```

MENUF BCM
OBNUC 13C
OFR 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.0 Hz
PW1 5.0 us
DEADT 19.6 us
PREDL 0.2000 ms
IWT 1.0 sec
POINT 32768
SPO 32768
TIMES 1000
DUMMY 1
FREQU 27173.9 Hz
FLT 13600 Hz
DELAY 14.7 us
ACQTM 1.206 sec
PD 2.000 sec
ADBIT 16.00
RGAIN 25
BF 0.10 Hz
T1 0.00
T2 0.00
T3 90.00
T4 100.00
EXMOD BCM
EXPCM Bilevel.complete.decoupl
IRNUC 1H
IFR 399.65 MHz
IRSET 124.00 KHz
IRFIN 10500.0 Hz
IRRPW 50 us
IRATN 511
DFILE C:\WINNMR98\COMMON\_DEFF
SF TH5
LKSET 61.60 KHz
LKFIN 79.0 Hz
LKLEV 200
LGAIN 20
LKPHS 58
LKSIG 655
CSPED 13 Hz
FILDC
FILDF
    
```



in CDCl₃

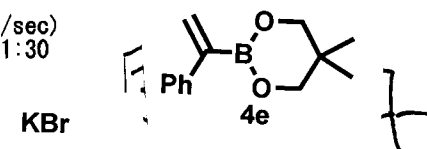


number of scan
zero filling
gain
date of scan
sample name

16
ON
Auto (2)
06/02/18 21:30
No. 19

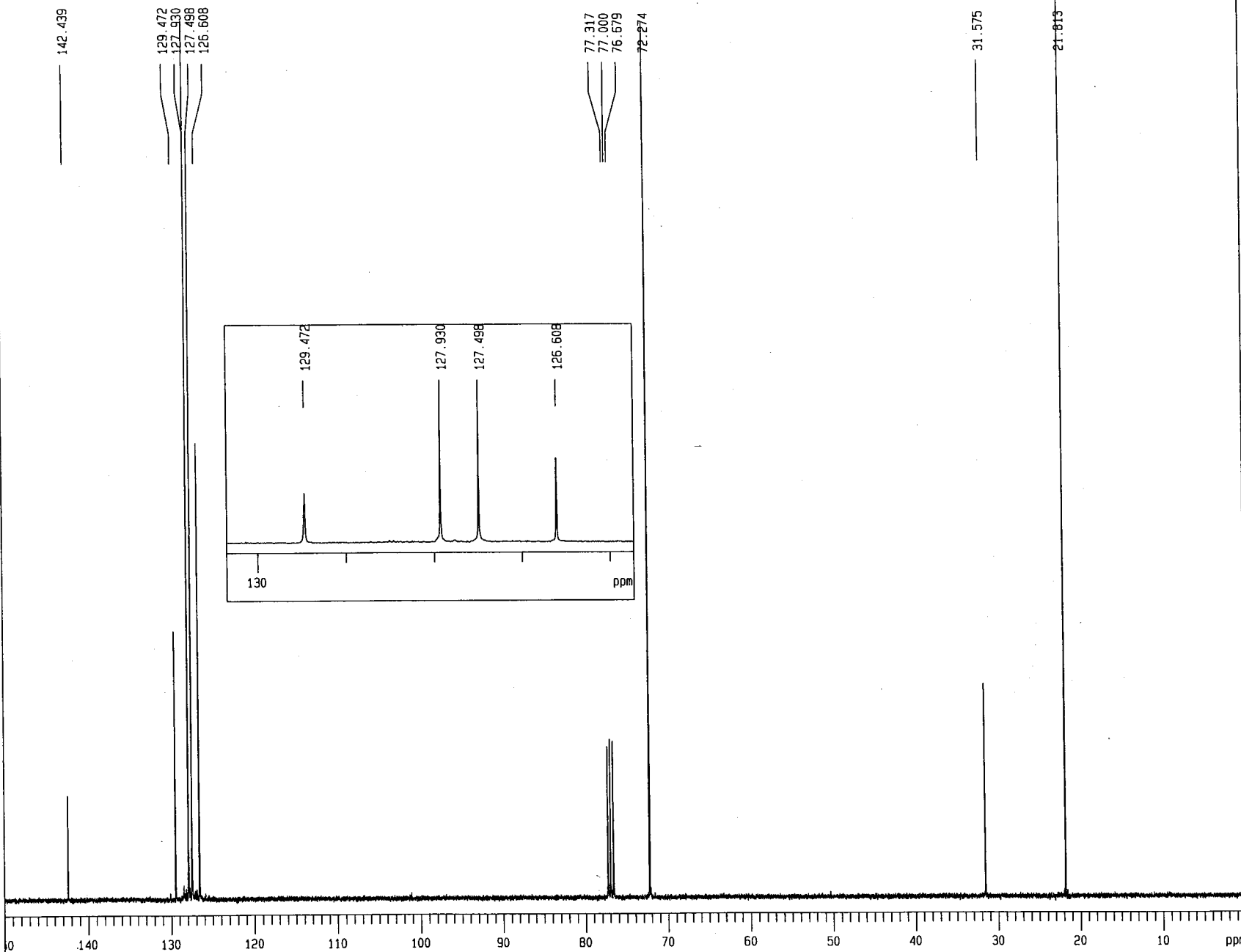
resolution
apodization
scan speed
date of data processing

4 cm-1
Cosine
Auto (2 mm/sec)
06/02/18 21:30



No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T	No.	cm-1	%T
1	3075.9	34.828	2	3055.66	34.6997	3	3024.8	35.8738	4	2962.13	13.6419
5	2889.81	22.9167	7	2248.59	46.2523	8	1943.89	45.749	9	1889.9	45.2019
11	1686.44	42.0574	12	1596.77	34.2085	13	1572.66	42.6088	14	1492.63	19.677
16	1415.49	6.69466	17	1394.28	17.7475	18	1377.89	19.4537	19	1340.28	5.00197
21	1281.47	17.1762	22	1250.61	4.52371	23	1230.36	4.2502	24	1196.61	7.51706
26	1074.16	35.0479	27	1028.84	35.2668	28	1000.87	32.9026	29	943.02	29.935
31	812.849	38.4789	32	781.029	24.032	33	730.889	17.2186	34	708.712	23.9716
36	679.785	33.8215	37	644.108	30.1124				35	699.069	16.9357

(Ph) (Bneo) CCH2



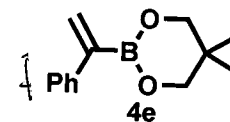
Date : Fri Feb 10 23:15:45 2006

FileName : .LoadingFID.nmdata
Comment : (Ph) (Bneo) CCH2
SliceHistory :
EXMODE : bcn

POINT : 65536 points
SAMPO : 65536 points
FREQU : 26881.7 Hz
FILTR : 13450 Hz
DELAY : 14.9 usec
DEADT : 19.9 usec
INTVL : 37.2 usec
TIMES : 800 times
DUMMY : 4 times
PD : 2.0000 sec
ACQTM : 2437.9392 msec
PREDL : 0.01000 msec
INIWT : 1000.0000 msec
RESOL : 0.41 Hz
PW1 : 4.90 usec
OBNUC : 13C
OBFRQ : 99.45 MHz
OBSET : 104750.00 Hz
RGAIN : 35
IRNUC : 1H
IRFRQ : 395.75 MHz
IRSET : 134498.00 Hz
IRRPW : 46.0 usec
IRRNS : 0

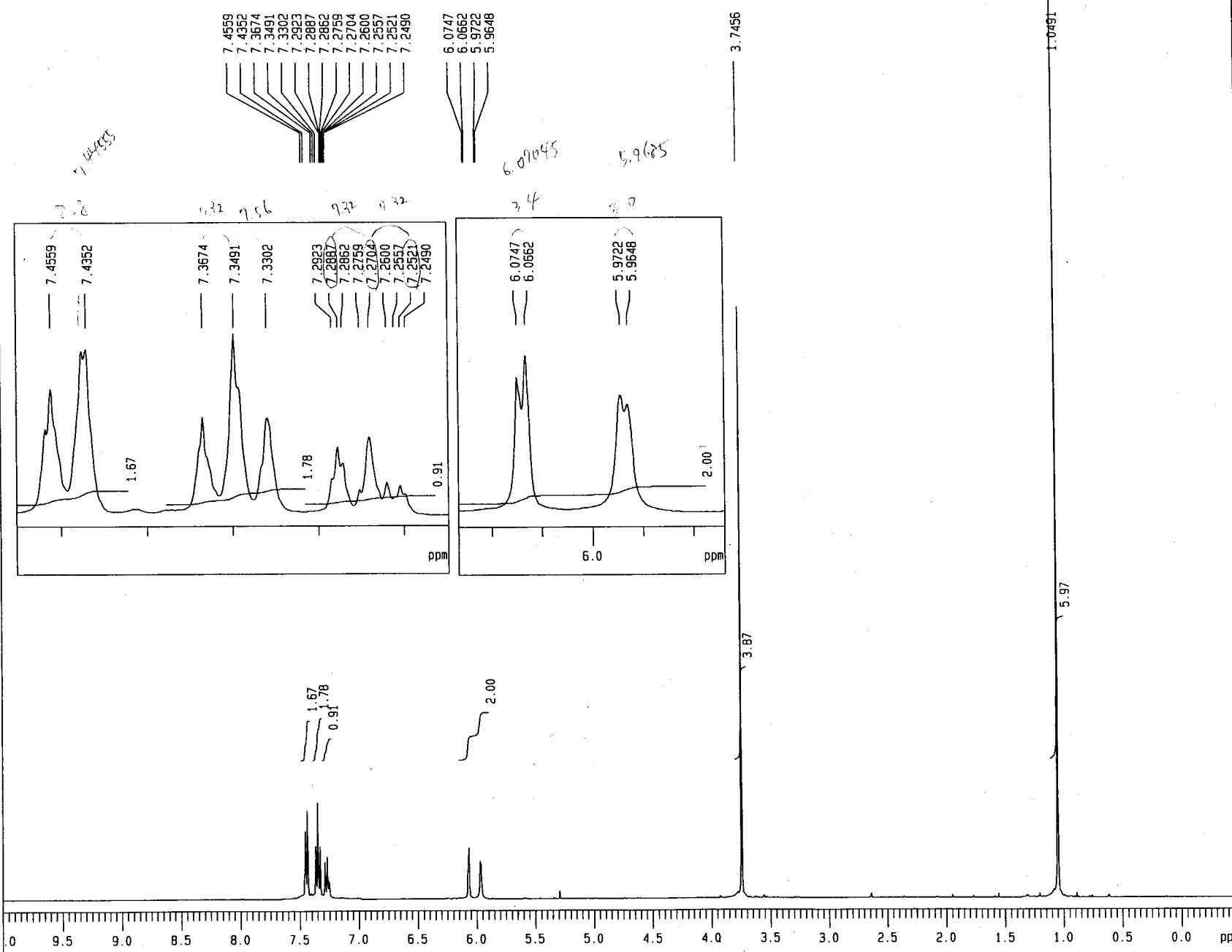
SCANS : 727 times

SLVNT : CDCL3
SPINNING : 14 Hz
TEMP : 26.6 C



in CDCl₃

(Ph) (Bneo) CH2



Date : Fri Feb 10 22:12:34 2006

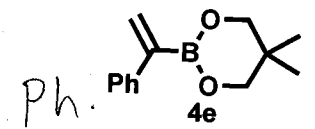
FileName : LoadingFID.nmdata
Comment : (Ph) (Bneo) CH2
SliceHistory :
EXMODE : non

POINT : 32768 points
SAMPO : 32768 points
FREQU : 7917.7 Hz
FILTR : 3950 Hz
DELAY : 50.6 usec
DEADT : 72.4 usec
INTVL : 126.3 usec
TIMES : 16 times
DUMMY : 1 times
PD : 1.5000 sec
ACQTM : 4138.5986 msec
PREDL : 0.01000 msec
INTWT : 1000.0000 msec
RESOL : 0.24 Hz
PW1 : 7.00 usec

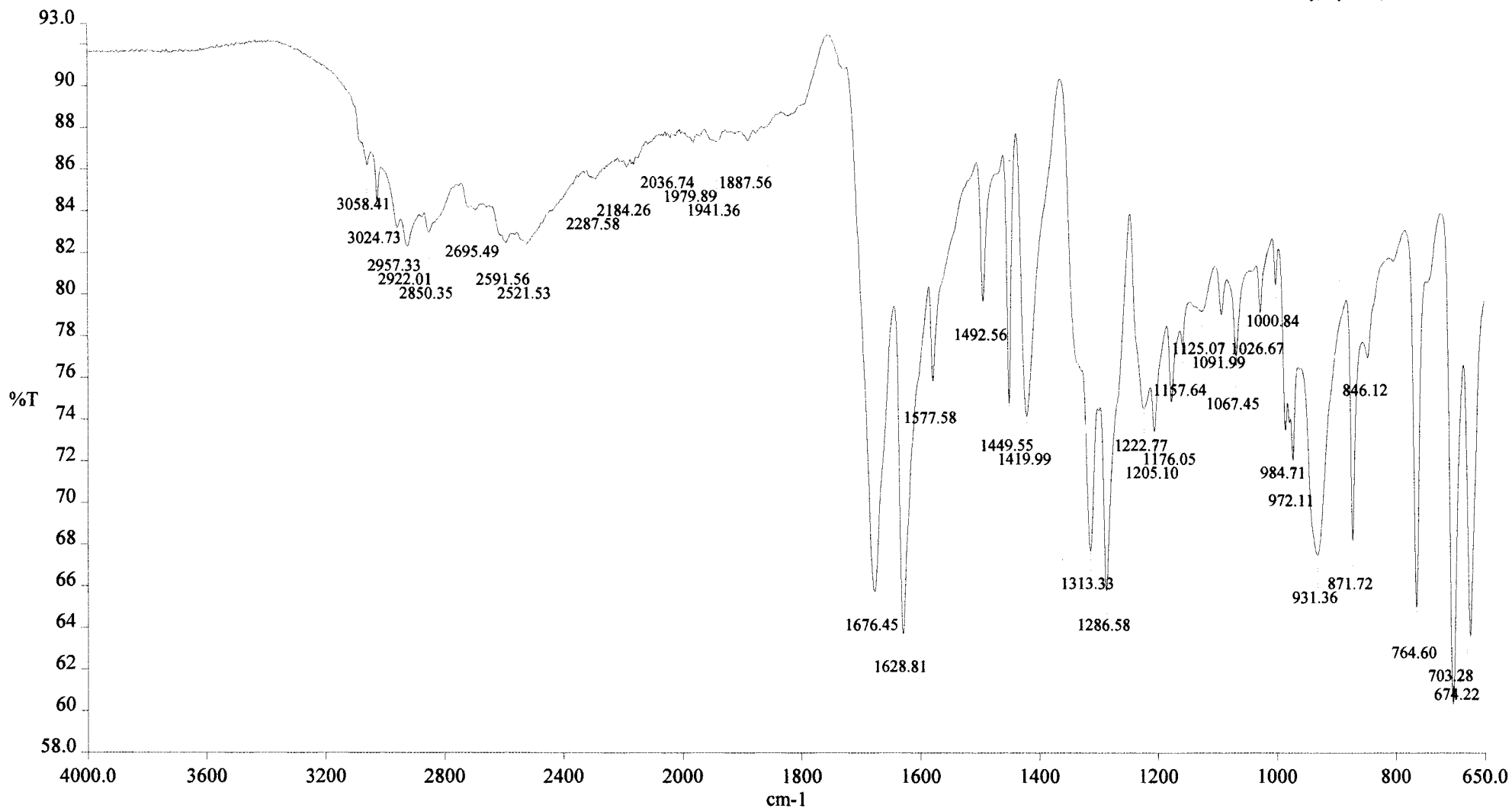
OBNUC : 1H
OBFRQ : 395.75 MHz
OBSET : 134498.00 Hz
RGAIN : 16

SCANS : 16 times

SLVNT : CDCL3
SPINNING : 14 Hz
TEMP : 25.5 C



in CDCl₃

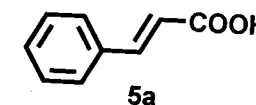


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\STStyCOOH.sp

Date Created: Thursday, April 03, 2008 1:28 PM "Cz (•WleŽž)

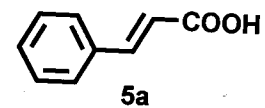
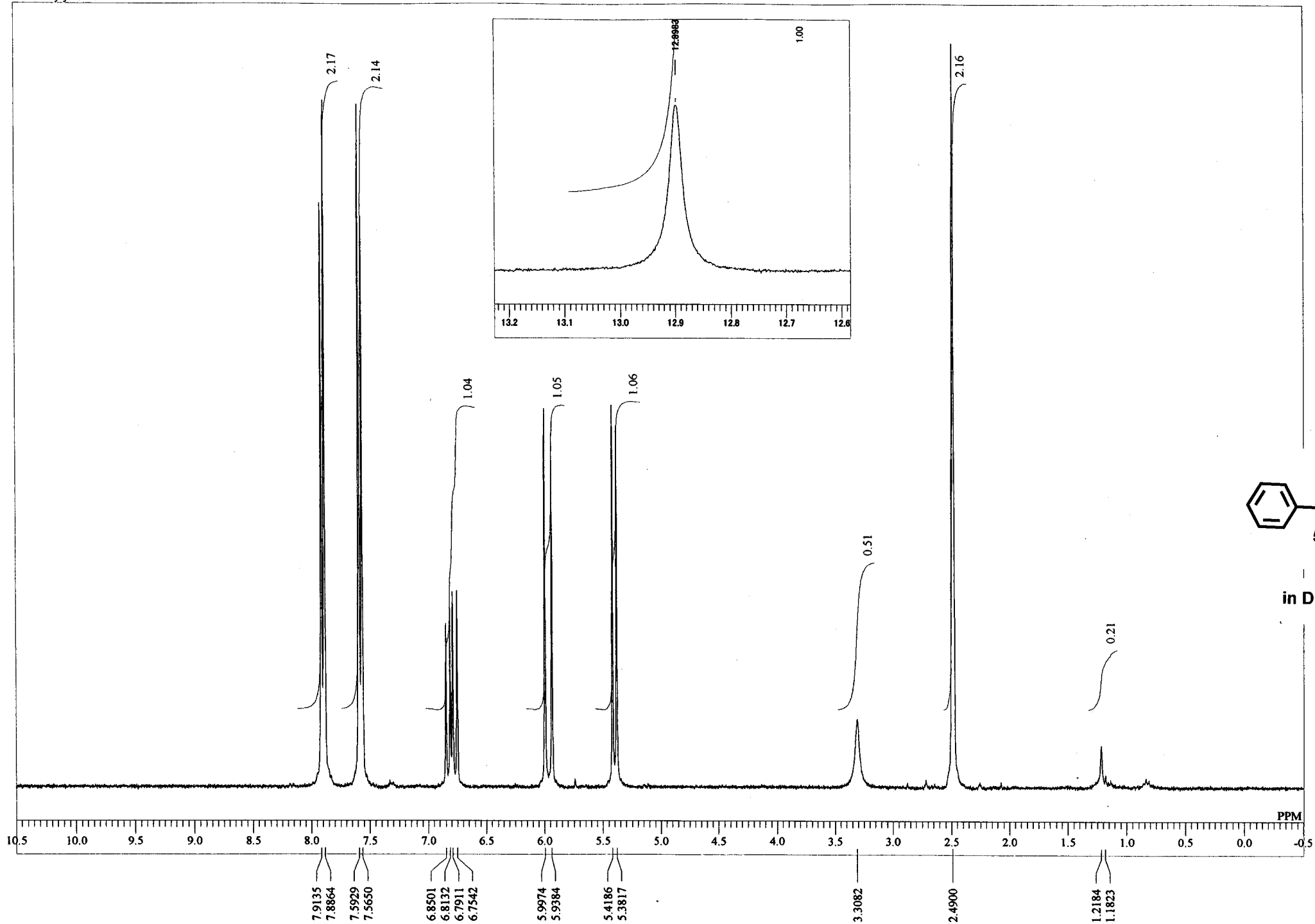
Analyst: guest

Description:



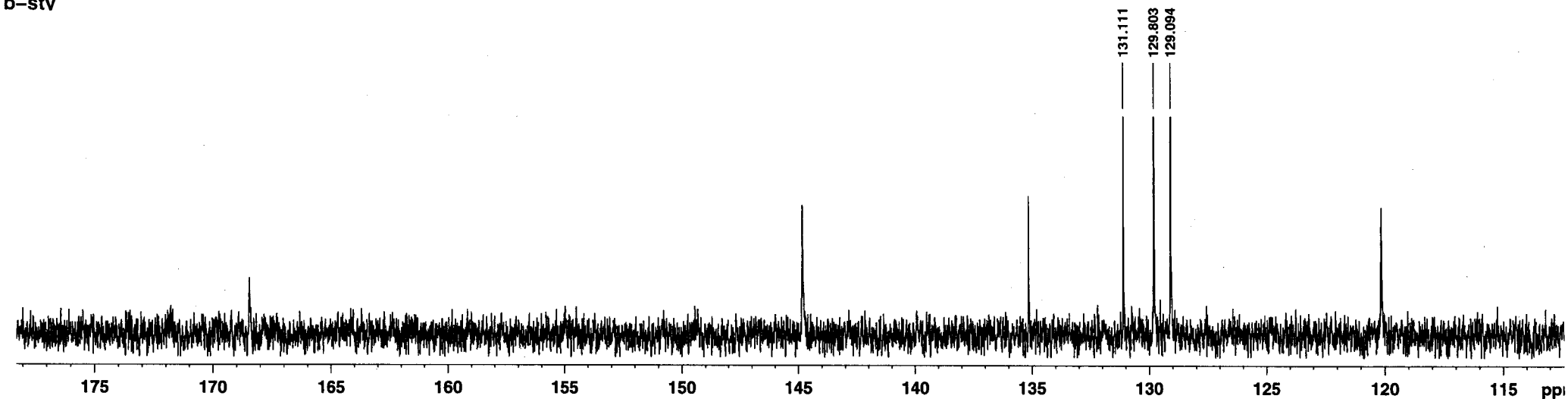
ATR

St betastylyl COOH



in DMSO-d₆

b-stv

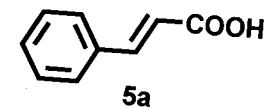


DU=/z, USER=takaya, NAME=tadami, EXPNO=4, PROCNO=1
F1=180.000ppm, F2=0.000ppm, MI=1.30cm, MAXI=26.86cm,

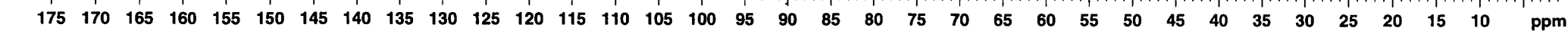
#	ADDRESS	FREQUENCY [Hz]	[PPM]	INTE
1	27036.4	16488.256	131.1113	
2	27392.2	16323.725	129.8029	
3	27585.2	16234.515	129.0936	
4	51558.3	5149.624	40.9488	
5	51603.7	5128.630	40.7818	
6	51624.3	5119.148	40.7064	
7	51649.2	5107.632	40.6149	
8	51740.0	5065.645	40.2810	
9	51785.3	5044.671	40.1142	
10	51830.6	5023.721	39.9476	

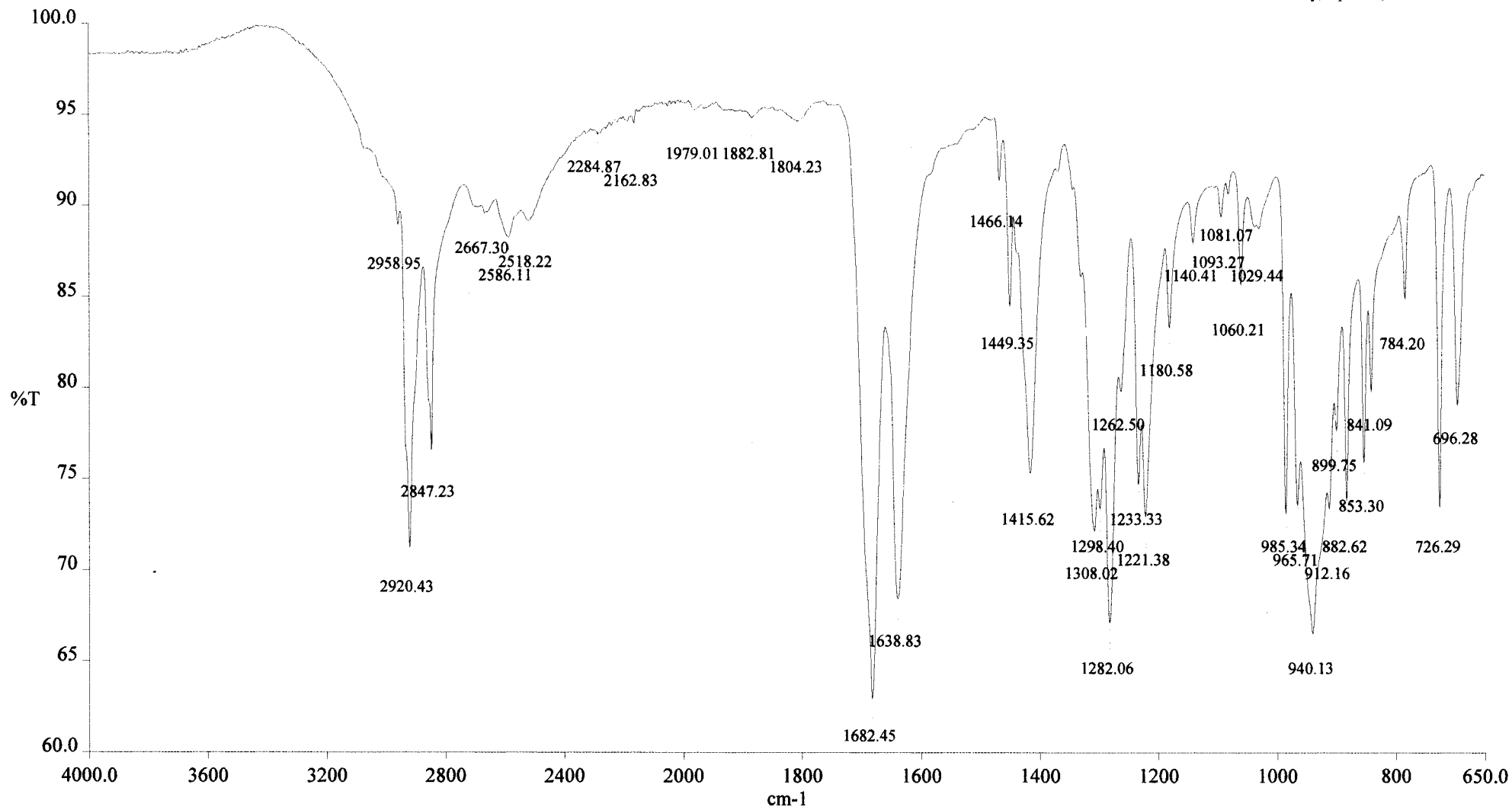
131.111
129.803
129.094

40.949
40.782
40.706
40.615
40.281
40.114
39.948



in DMSO-d⁶



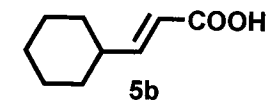


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\Tadami\STCyalkenylCOOH.sp

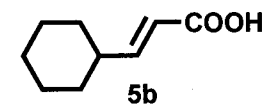
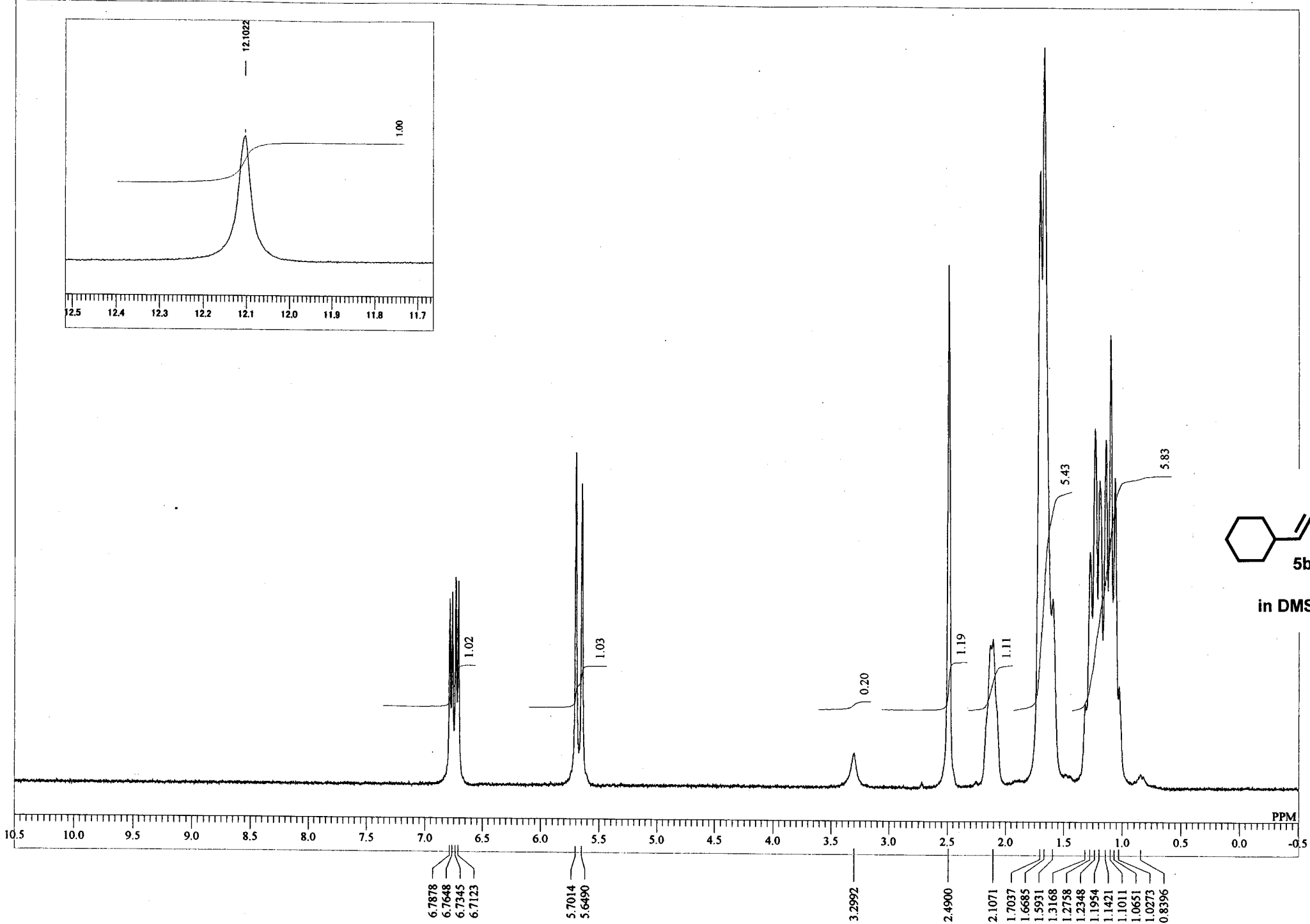
Date Created: Thursday, April 10, 2008 9:57 PM “Āč (•Wlĕžž)

Analyst: guest

Description:

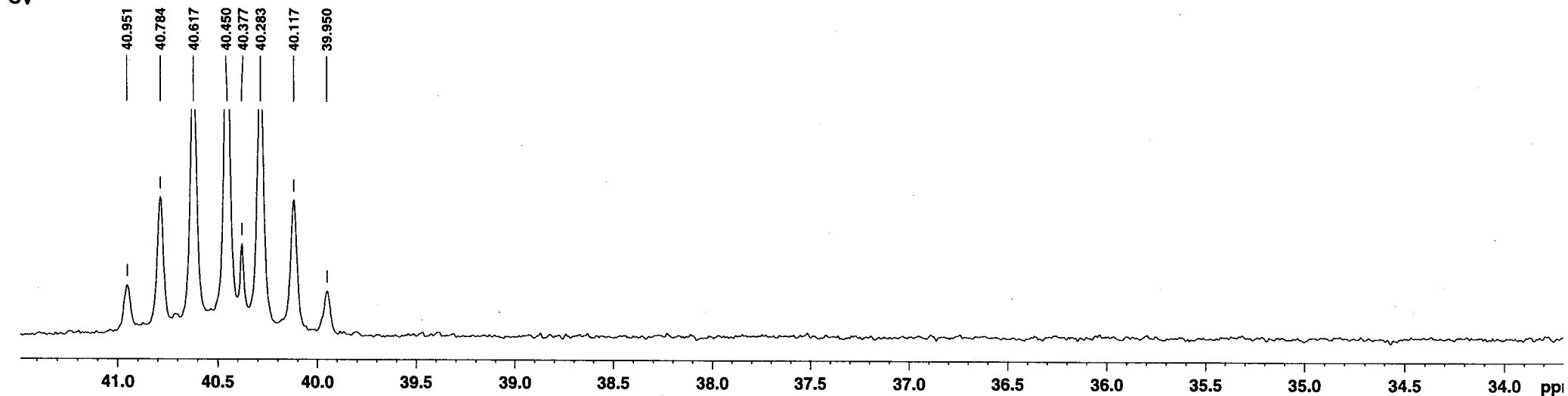


ATR



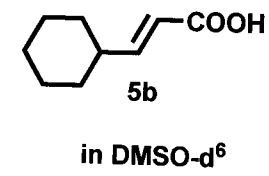
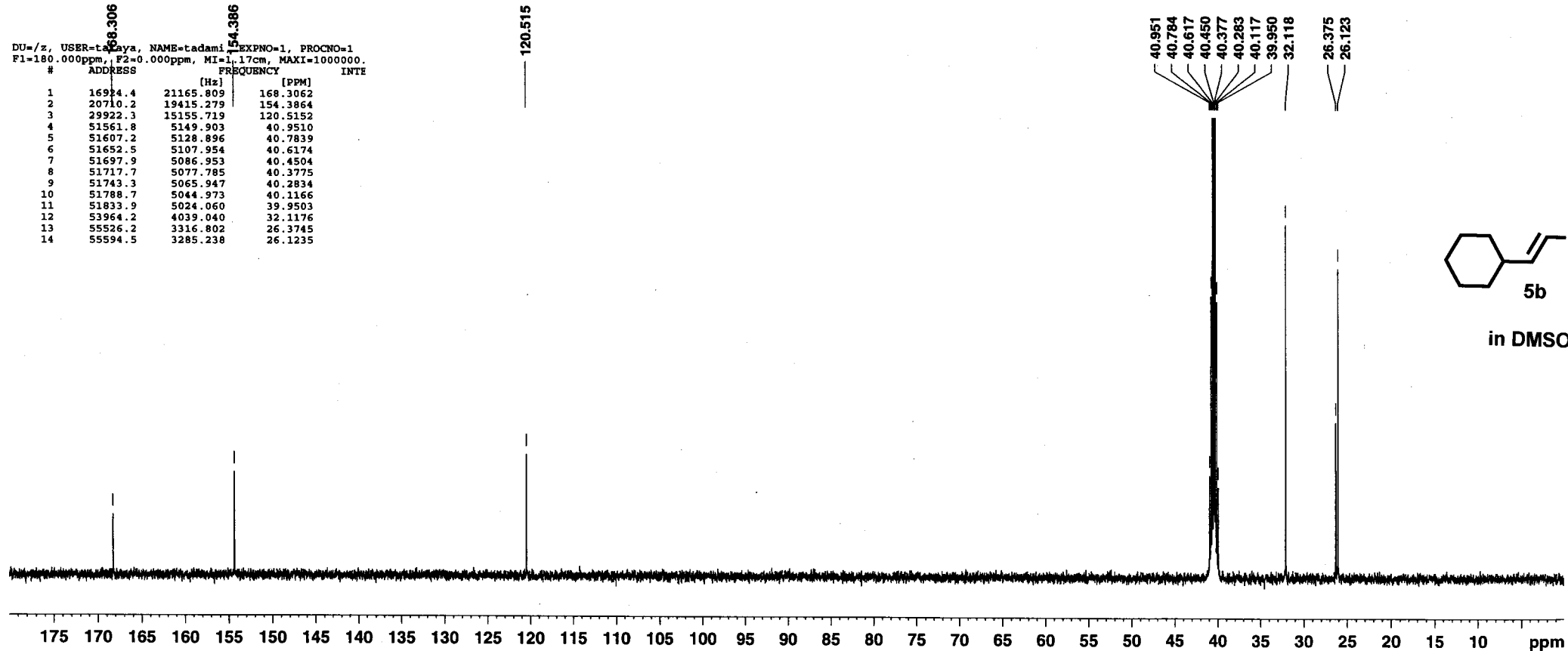
in DMSO-d⁶

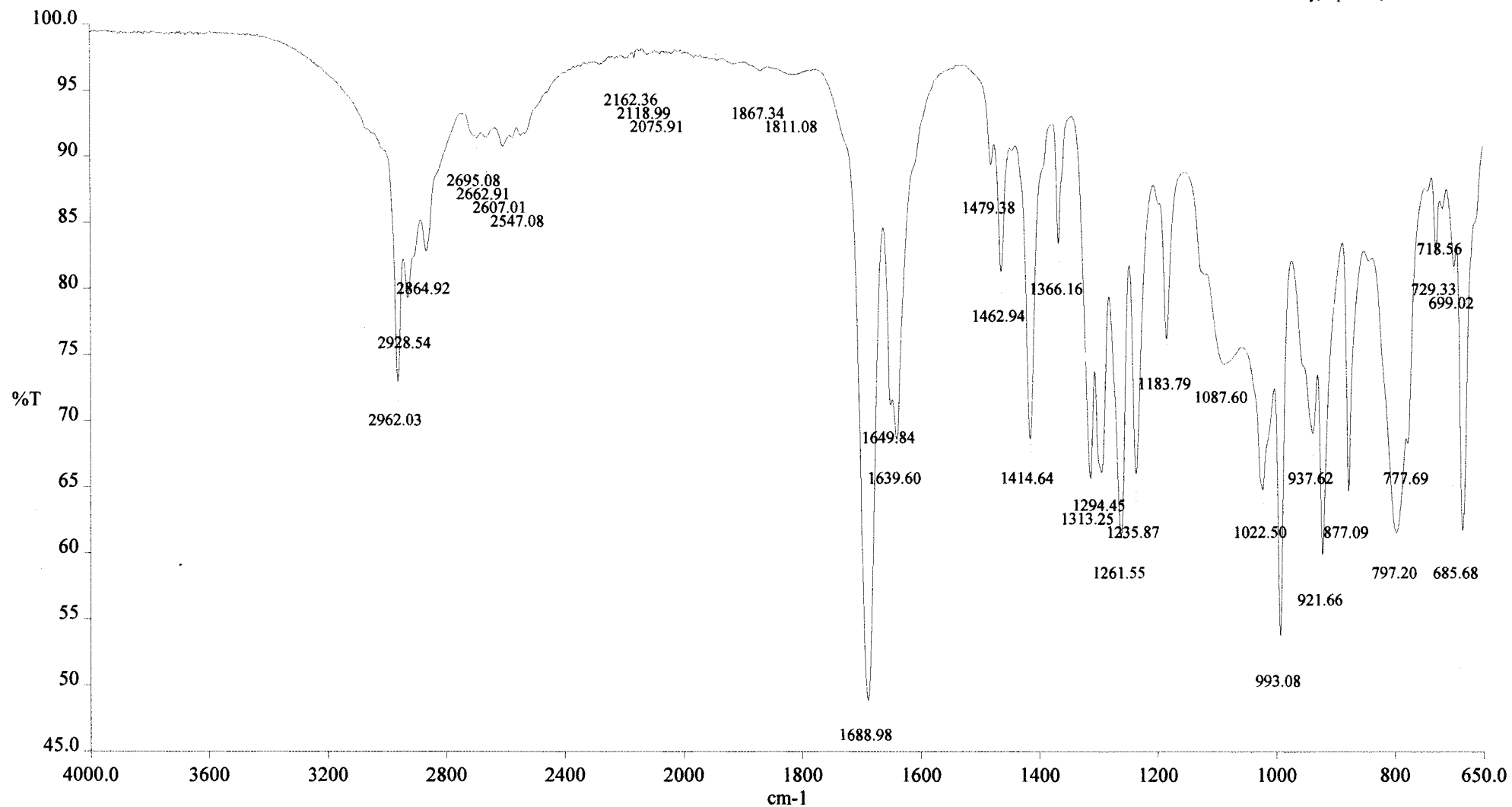
Cv



DU=/z, USER=tadaya, NAME=tadami, EXPNO=1, PROCNO=1
F1=180.000ppm, F2=0.000ppm, MI=1.17cm, MAXI=1000000.

#	ADDRESS	FREQUENCY [Hz]	PPM	INTE
1	16924.4	21165.809	168.3062	
2	20710.2	19415.279	154.3864	
3	29922.3	15155.719	120.5152	
4	51561.8	5149.903	40.9510	
5	51607.2	5128.896	40.7839	
6	51652.5	5107.954	40.6174	
7	51697.9	5086.953	40.4504	
8	51717.7	5077.785	40.3775	
9	51743.3	5065.947	40.2834	
10	51788.7	5044.973	40.1166	
11	51833.9	5024.060	39.9503	
12	53964.2	4039.040	32.1176	
13	55526.2	3316.802	26.3745	
14	55594.5	3285.238	26.1235	



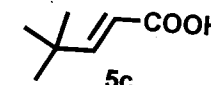


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\Tadami\STt-BualkenylCOOH.sp

Date Created: Thursday, April 10, 2008 9:53 PM “Āč (•WleŽž)

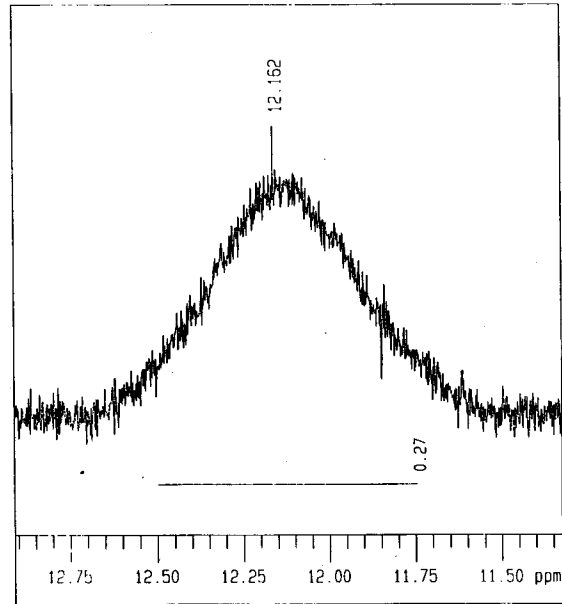
Analyst: guest

Description:



ATR

St t-BualkenylCOOH



6.844
6.791

5.647
5.593

3.333
3.129

2.501
2.495
2.480
2.464

1.234
1.221
1.128
1.078
1.028
0.976
0.883
0.864
0.838
0.815
0.734

1.00

1.07

4.21

0.93

9.20

10

8

6

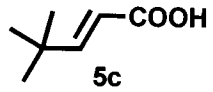
4

2

0

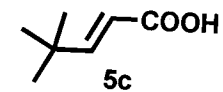
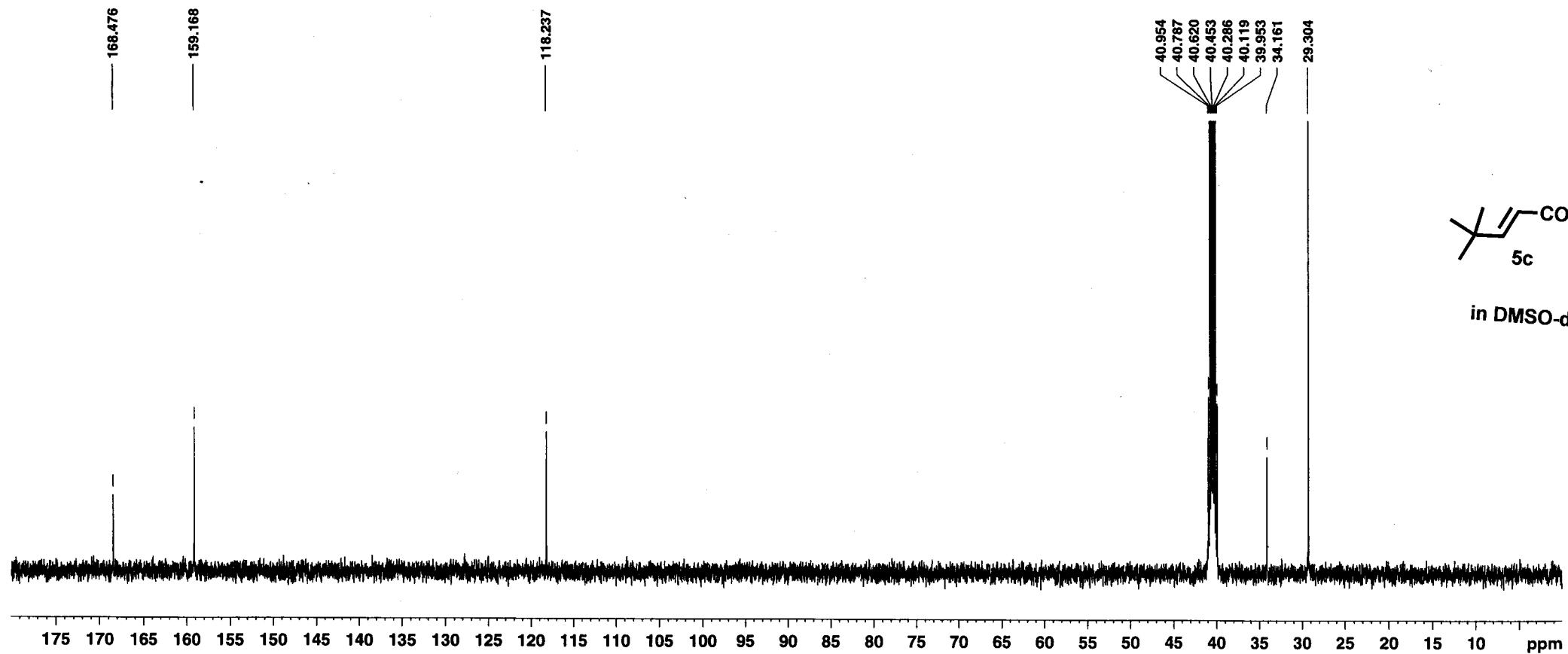
ppm

Date
FileN
Comme
Slice
EXMOD
POINT
SAMPO
FREQU
FILTR
DELAY
DEADT
INTVL
TIMES
DUMMY
PD
ACQTM
PREDL
INIWT
RESOL
PW1
OBNUC
OBFRQ
OBSET
RGAIN
SCANS
SLVNT
SPINN
TEMP

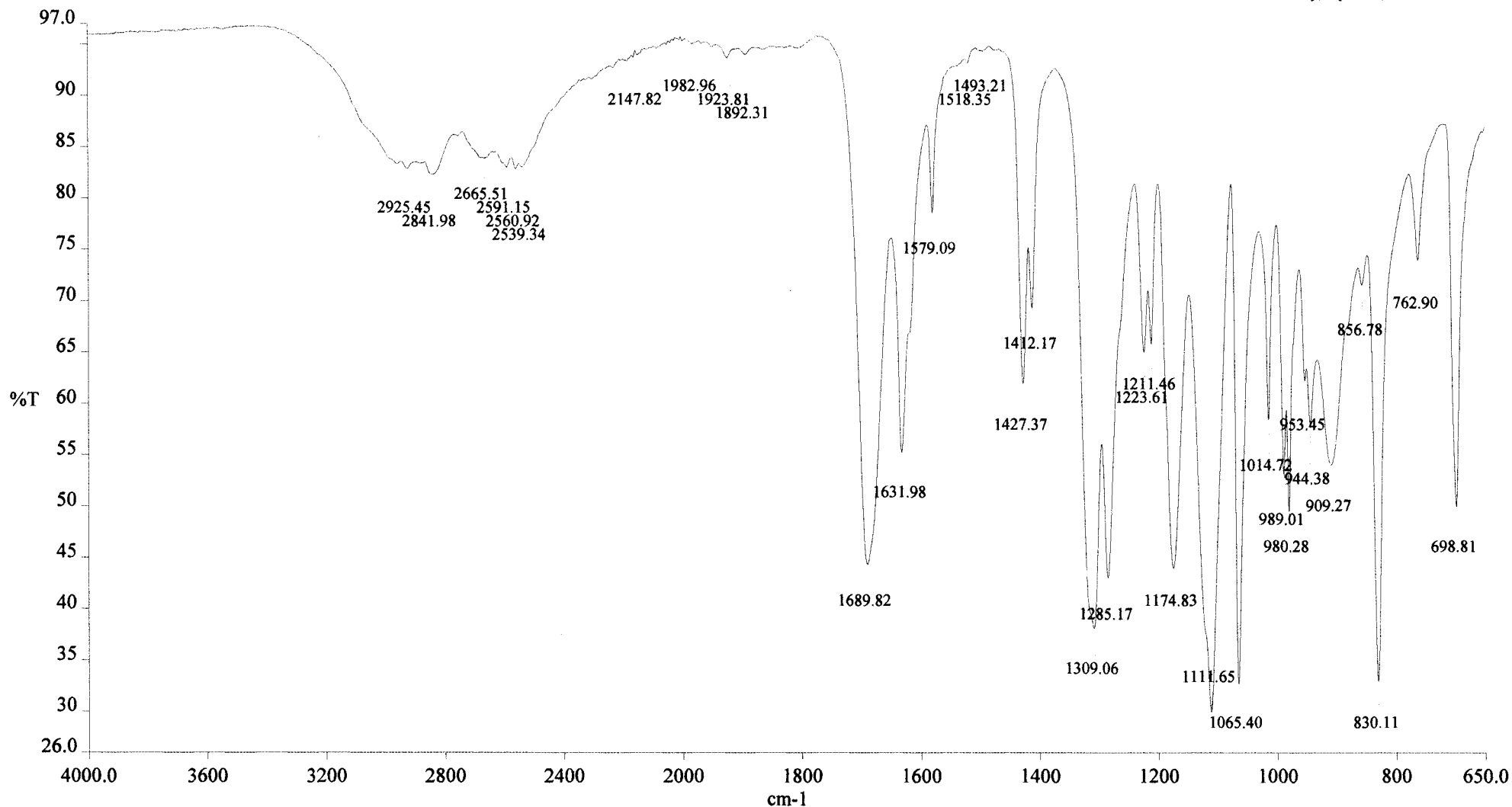


in DMSO-d⁶

t-Bu



in DMSO-d⁶

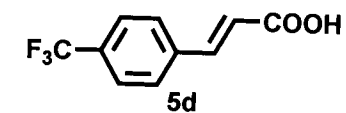


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\STp-CF3StyCOOH.sp

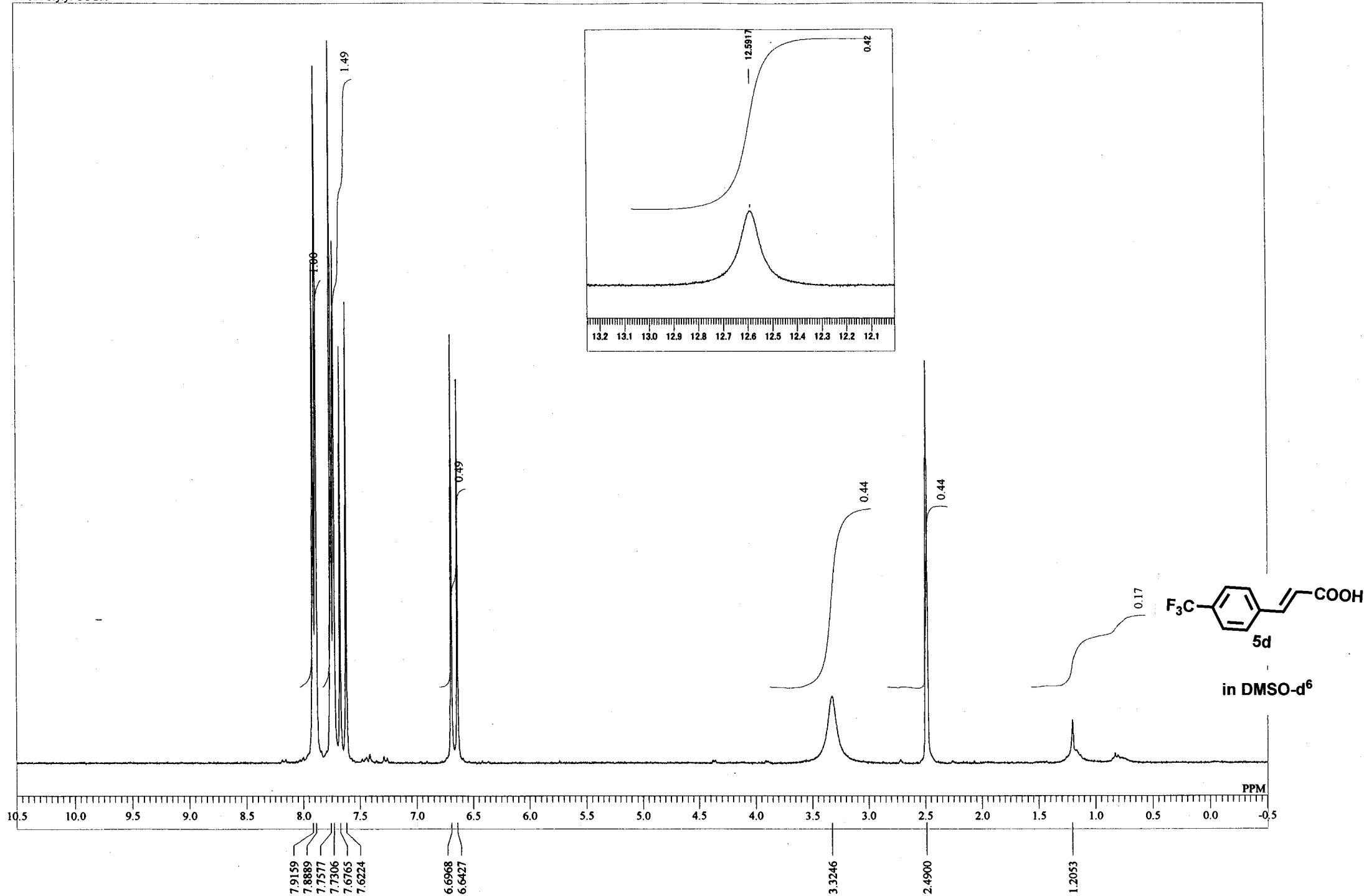
Date Created: Thursday, April 03, 2008 1:36 PM

Analyst: guest

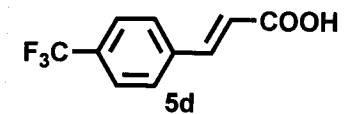
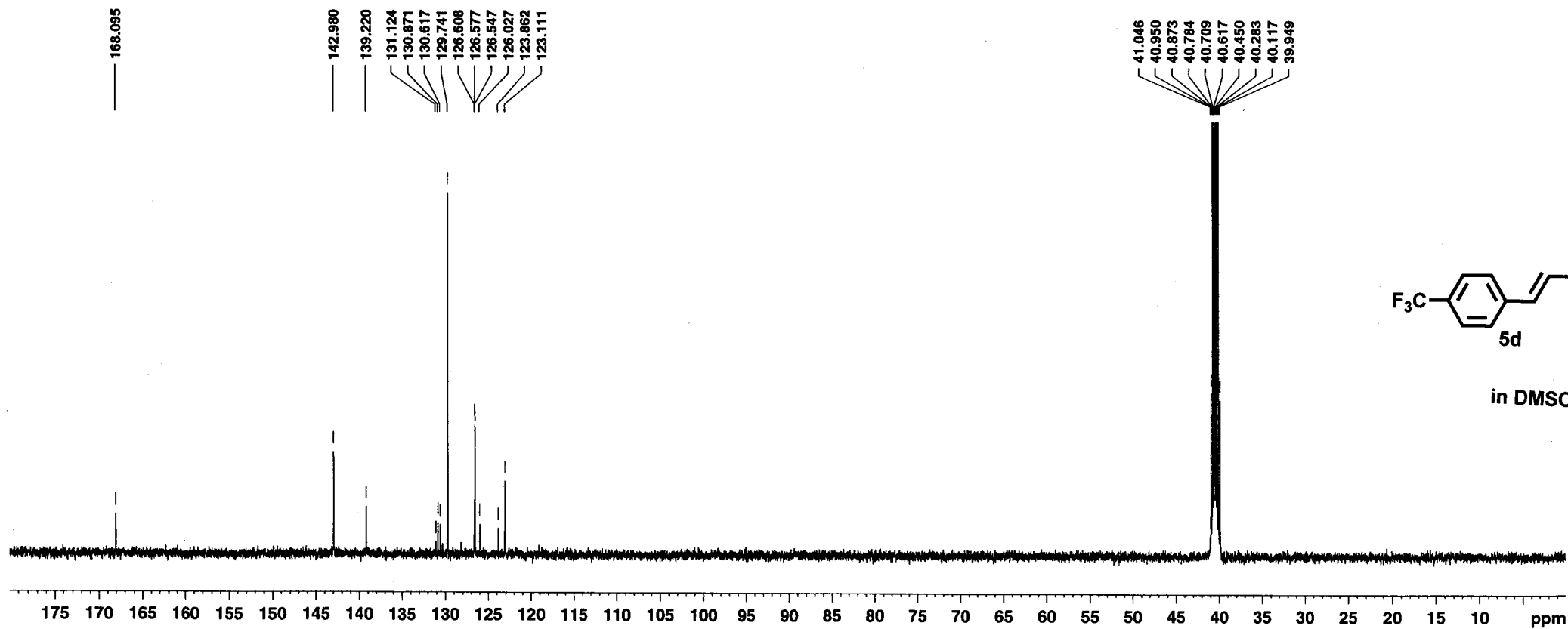
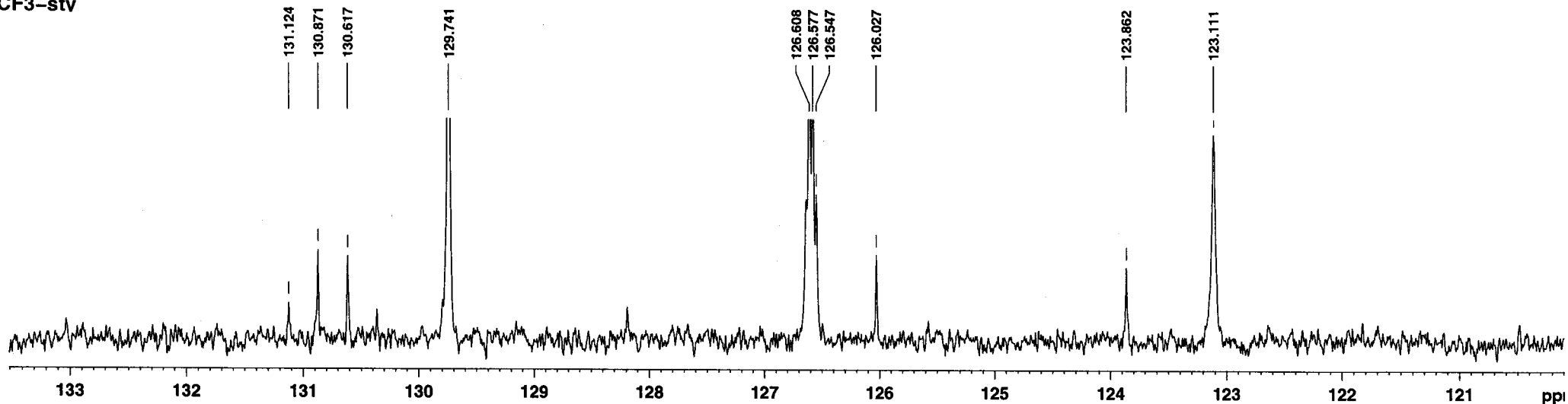
Description:



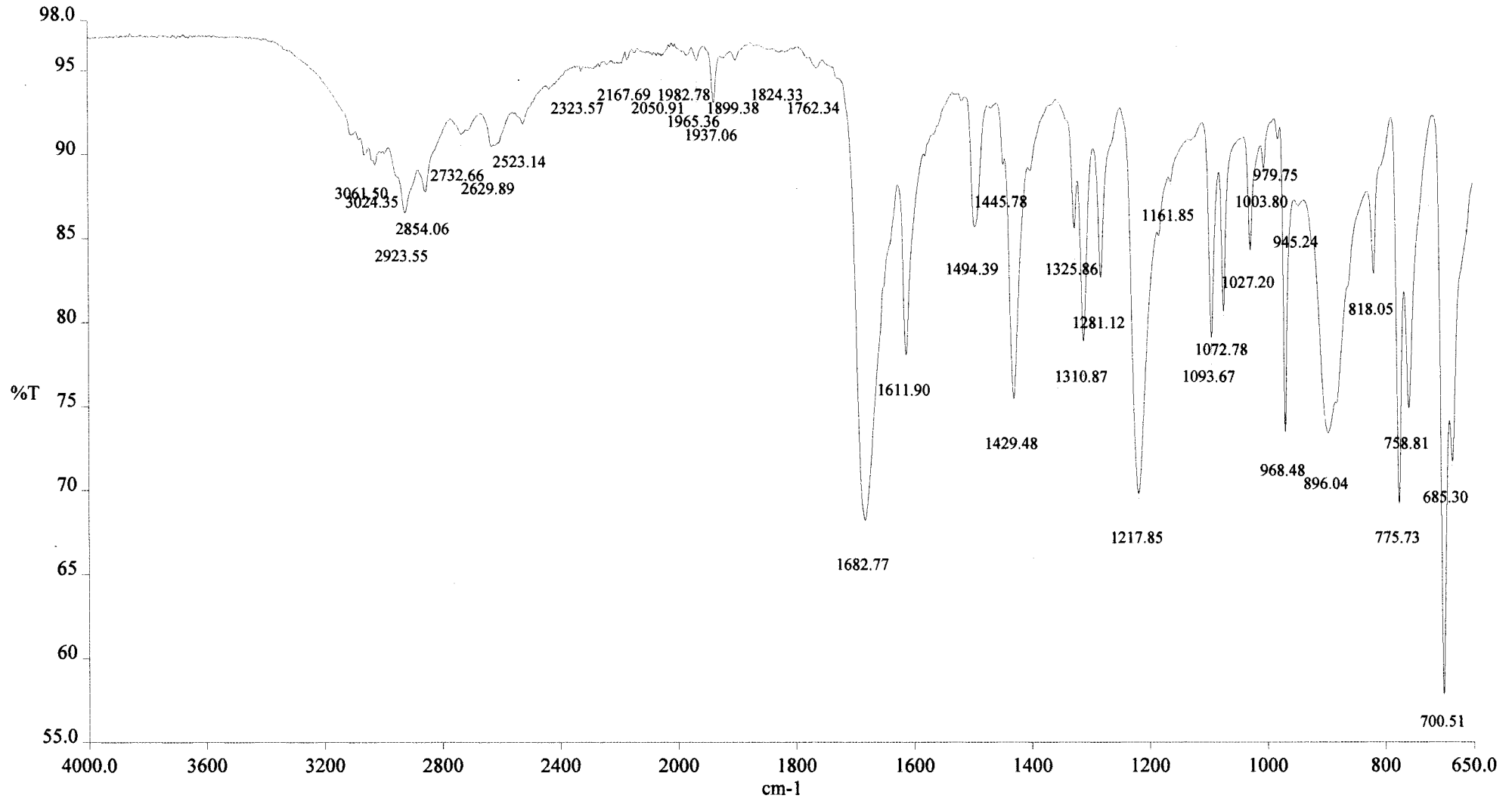
ATR



CF3-stv



in DMSO-d⁶

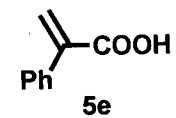


Spectrum Pathname: C:\pel_data\spectra\guest\iwasawa\Tadami\STalphaStyCOOH.sp

Date Created: Thursday, April 10, 2008 11:13 PM "Cz (•WleŽž)

Analyst: guest

Description:



ATR

St alphastyllylCOOH

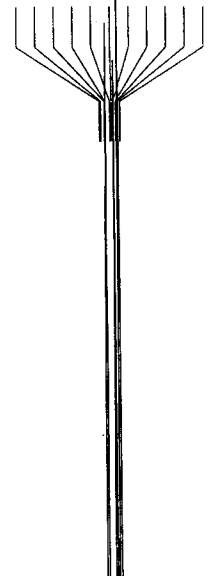
7.431
7.423
7.403
7.398
7.374
7.366
7.356
7.343
7.337
7.332
7.319

6.216
5.943
5.741

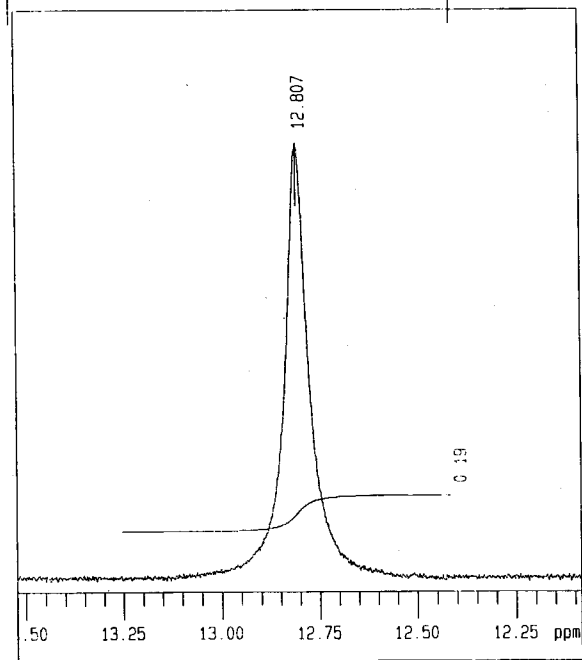
3.323

2.490

1.221



1.00



12.807

0.19

13.50 13.25 13.00 12.75 12.50 12.25 ppm

0.21

0.21

0.18

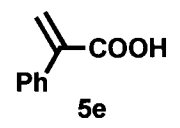
0.17

0.04

0.02

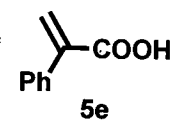
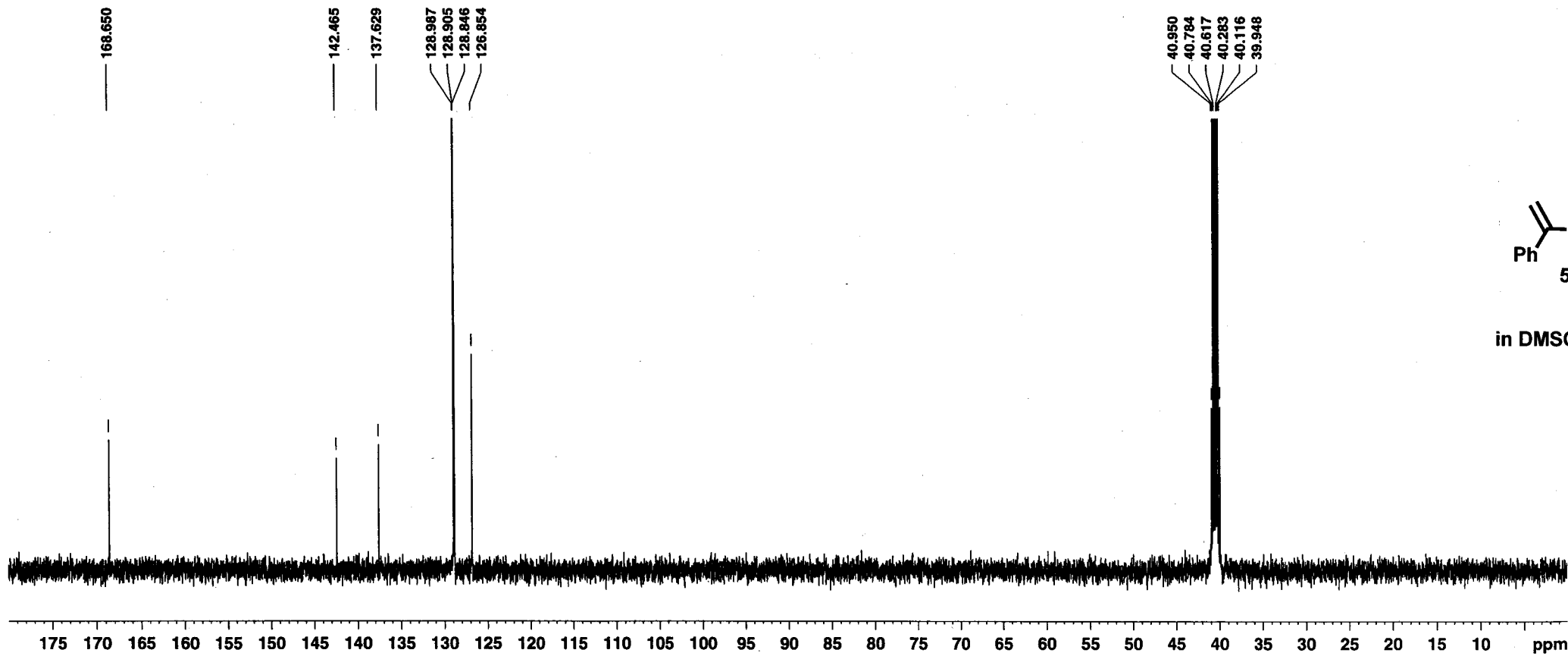
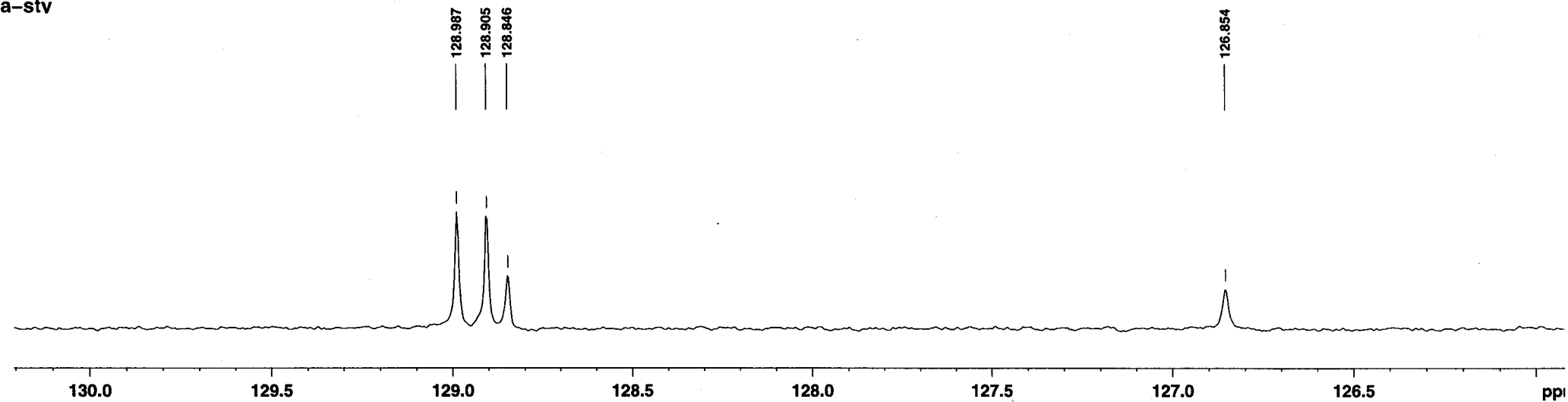
10 8 6 4 2 0 ppm

Date
FileN
Comme
Slice
EXMOD
POINT
SAMPO
FREQU
FILTR
DELAY
DEACT
INTVL
TIMES
DUMMY
PD
ACQTM
PREDL
INIWT
RESOL
PH1
OBNUC
OBFRC
OBSET
RGAIN
SCANS
SLVNT
SPINN
TEMP



in DMSO-d⁶

a-stv



in DMSO-d⁶