Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

(*R*)-(+)-*N*-Methylbenzoguanidine ((*R*)-NMBG) Catalyzed Kinetic Resolution of Racemic Secondary Benzylic Alcohols with Free Carboxylic Acids by Asymmetric Esterification

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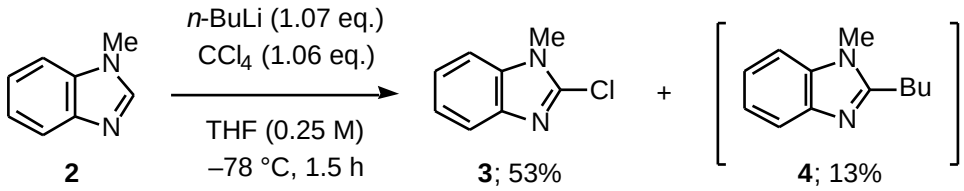
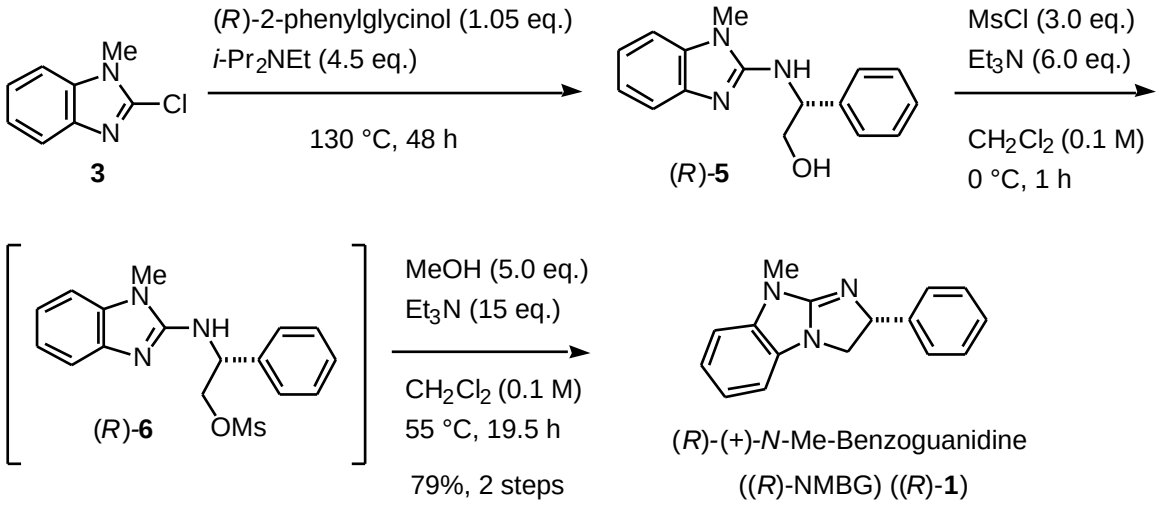
Electronic Supplementary Information (ESI)

General Information. All melting points are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded with tetramethylsilane (TMS) or chloroform (in chloroform-*d*) as internal standard. Thin layer chromatography was performed on Wakogel B5F. All reactions were carried out under argon atmosphere in dried glassware. Dichloromethane was distilled from diphosphorus pentoxide, then calcium hydride, and dried over MS 4Å, benzene and toluene were distilled from diphosphorus pentoxide, and dried over MS 4 Å, and THF and diethyl ether were distilled from sodium/benzophenone immediately prior to use. All reagents were purchased from Tokyo Kasei Kogyo Co., Ltd., Kanto Chemical Co., Inc. or Aldrich Chemical Co., Inc., and used without further purification unless otherwise noted.

Procedure for the Synthesis of (*R*)-NMBG ((*R*)-1)



To a solution of *N*-methylbenzimidazole(**2**) (655.3 mg, 4.96 mmol) in THF (20.0 mL) at –78 °C was slowly added *n*-BuLi in hexane (1.66 M, 3.20 mL, 5.31 mmol). The reaction mixture was stirred for 1 h at the same temperature and then CCl_4 (507 μL, 5.25 mmol) was slowly added. After the reaction mixture had been stirred for 1.5 h, the reactant was quenched with H_2O and diluted with CH_2Cl_2 at –78 °C. The organic layer was separated and the aqueous layer was extracted with ethyl acetate. The combined organic layer was dried over Na_2SO_4. After filtration of the mixture and evaporation of the solvent, the crude product was purified by column chromatography on silica (eluant; CH_2Cl_2) to afford the mixture of **3** and **4** (581.2 mg). The mixture was separated by thin layer chromatography (eluant; CH_2Cl_2) to afford **3** (435.4 mg, 53%) as a pale ocher solid and **4** (123.6 mg, 13%) as a brown solid, respectively.



A 20 mL autoclave was charged with 2-chloro-*N*-methylbenzimidazole(**3**) (1.45 g, 8.70 mmol), (*R*)-phenylglycinol (1.25 g, 9.11 mmol), and *i*-Pr_2NEt (6.80 mL, 39.0 mmol). The vessel was sealed and then the whole mixture was stirred for 48 h at 130 °C. After cooling to room temperature, the reactant was diluted with MeOH and CH_2Cl_2, and it was transferred into a 300 mL two-necked flask. The mixture was concentrated in vacuo at 50 °C to afford the crude intermediate (*R*)-**5**, which was used for the next reaction

without purification.

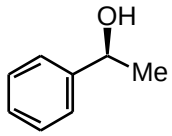
To a mixture of the above product (*R*)-**5** and Et_3N (7.28 mL, 52.2 mmol) in CH_2Cl_2 (87.0 mL) at 0 °C was added MsCl (2.02 mL, 26.1 mmol). After stirring for 1 h at 0 °C, MeOH (1.76 mL, 43.4 mmol) and Et_3N (18.2 mL, 130.6 mmol) were successively added at room temperature and the reaction mixture was stirred for 19.5 h at 55 °C. After cooling to 0 °C, it was quenched with 1.0 M NaOH. The organic layer was separated and the aqueous layer was extracted with diethyl ether. The combined organic layer was dried over Na_2SO_4. After filtration of the mixture and evaporation of the solvent, the crude product was purified by column chromatography on silica (first eluant; ethyl acetate/hexane/formic acid = 20/80/2, second eluant; ethyl acetate, and third eluant; $CHCl_3$/MeOH = 9/1 (saturated with 35% NH_3)) to afford (*R*)-NMBG ((*R*)-**1**) (1.72 g, 79%) as a pale brown amorphous solid.

The product was re-purified for analysis by thin layer chromatography (eluant; acetate/hexane = 4/1 (saturated with 35% NH_3)) to provide a white precipitate and it was filtrated with diethyl ether to afford (*R*)-NMBG ((*R*)-**1**) (843.7 mg, 39%) as a white solid: $[\alpha]_D^{22}$ = +116.1 (c 1.00, benzene); Mp. 101–102 °C; IR (KBr): 1653, 1604, 1496, 763, 737, 704 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.42–7.39 (m, 2H, Ph), 7.37–7.32 (m, 2H, Ph), 7.26 (dt, *J* = 7.3, 1.5 Hz, 1H, Ph), 6.96 (ddd, *J* = 8.3, 7.5, 2.0 Hz, 2H, Ar), 6.85–6.79 (m, 1H, Ar), 6.74–6.68 (m, 1H, Ar), 5.57 (dd, *J* = 9.0, 8.0 Hz, 1H, 2-H), 4.26 (dd, *J* = 9.0, 9.0 Hz, 1H, 3-H), 3.70 (dd, *J* = 9.0, 8.0 Hz, 1H, 3-H), 3.43 (s, 3H, Me); ^{13}C NMR ($CDCl_3$): δ 162.3, 144.2, 138.0, 130.7, 128.5, 127.2, 126.6, 120.9, 120.3, 107.0, 106.7, 73.4, 53.3, 28.6; HR MS: calcd for $C_{16}H_{16}N_3$ ($M+H^+$) 250.1339, found 250.1328.

Typical Procedure for the Asymmetric Esterification

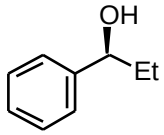
Typical procedure for the NMBG-catalyzed asymmetric esterification of racemic 1-phenyl-1-propanol ((±)-**9b**) with diphenylacetic acid using Piv_2O was described (**Table 3**, Entry 2): To a solution of diphenylacetic acid (47.8 mg, 0.225 mmol) in diethyl ether (1.5 mL) at room temperature were successively added Piv_2O (54.8 μL, 0.269 mmol), (*R*)-MNBG (**1**) (3.7 mg, 0.015 mmol), and racemic 1-phenyl-1-propanol ((±)-**9b**) (40.8 μL, 0.300 mmol). The reaction mixture was stirred for 12 h at room temperature and then it was quenched with saturated aqueous $NaHCO_3$ and diluted with CH_2Cl_2. The organic layer was separated and the aqueous layer was extracted with diethyl ether. The combined organic layer was dried over Na_2SO_4. After filtration of the mixture and evaporation of the solvent, the crude product was purified by preparative thin layer chromatography on silica (eluant; ethyl acetate/hexane = 1/4) to afford the corresponding optically active ester (*R*)-**10b** (49.6 mg, 50% yield, 92% ee) and the recovered optically active alcohol (*S*)-**9b** (20.4 mg, 50% yield, 87% ee). [s = 67.8]

(Optically Active Secondary Alcohols)



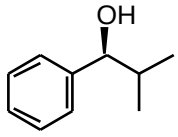
(*S*)–**9a**

(*S*)-1-Phenyl-1-ethanol ((*S*)-9a) [Table 3, Entry 1, 80% ee]: HPLC (CHIRALCEL OD-H, *i*-PrOH/hexane = 1/50, flow rate = 1.0 mL/min): t_R = 18.8 min (10.2%), t_R = 23.3 min (89.8%); ^{1}H NMR ($CDCl_3$): δ 7.41–7.23 (m, 5H, Ar), 4.88 (q, *J* = 6.5 Hz, 1H, 1-H), 1.90 (br s, 1H, OH), 1.48 (d, *J* = 6.5 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 145.8, 128.5, 127.4, 125.3, 70.4, 25.1.



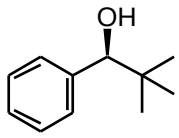
(*S*)–**9b** (= (*S*)–**7**)

(*S*)-1-Phenyl-1-propanol ((*S*)-9b) (= **(*S*)-7**) [Table 3, Entry 2, 87% ee]: HPLC (CHIRALCEL OD-H, *i*-PrOH/hexane = 1/100, flow rate = 0.75 mL/min): t_R = 26.3 min (6.5%), t_R = 31.8 min (93.5%); ^{1}H NMR ($CDCl_3$): δ 7.12–6.96 (m, 5H, Ph), 4.31 (dt, *J* = 3.0, 6.6 Hz, 1H, 1-H), 1.79 (d, *J* = 3.0 Hz, 1H, OH), 1.64–1.38 (m, 2H, 2-H), 0.65 (t, *J* = 7.5 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 144.5, 128.3, 127.4, 125.9, 75.9, 31.8, 10.1.



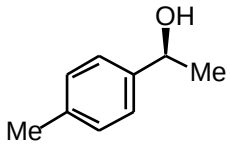
(*S*)–**9c**

(*S*)-2-Methyl-1-phenyl-1-propanol ((*S*)-9c) [Table 3, Entry 5, 97% ee]: HPLC (CHIRALCEL OD-Hx2, *i*-PrOH/hexane = 1/9, flow rate = 0.5 mL/min): t_R = 21.9 min (98.6%), t_R = 24.5 min (1.4%); IR (neat): 3398, 3029, 1604, 1492, 760, 701 cm^{-1}; ^{1}H NMR ($CDCl_3$): δ 7.31–7.15 (m, 5H, Ph), 4.27 (dd, *J* = 6.6, 3.0 Hz, 1H, 1-H), 1.95–1.79 (m, 2H, 2-H, OH), 0.92 (d, *J* = 6.6 Hz, 3H, Me), 0.72 (d, *J* = 6.6 Hz, 3H, Me); ^{13}C NMR ($CDCl_3$): δ 143.6, 128.1, 127.4, 126.5, 80.0, 35.2, 19.0, 18.2; HR MS: calcd for $C_{10}H_{14}ONa$ ($M+Na^+$) 173.0937, found 173.0930.



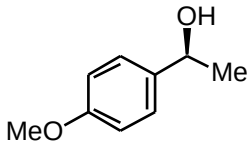
(*S*)–**9d**

(*S*)-2,2-Dimethyl-1-phenyl-1-propanol ((*S*)-9d) [Table 3, Entry 6, 72% ee]: HPLC (CHIRALCEL OD-H, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min): t_R = 19.4 min (86.1%), t_R = 29.6 min (13.9%); ^{1}H NMR ($CDCl_3$): δ 7.26–7.13 (m, 5H, Ph), 4.30 (d, *J* = 2.7 Hz, 1H, 1-H), 1.78 (br s, 1H, OH), 0.83 (s, 9H, *t*-Bu); ^{13}C NMR ($CDCl_3$): δ 142.1, 127.6, 127.5, 127.2, 82.4, 35.6, 25.9.



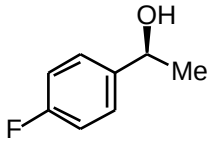
(*S*)–**12Aa**

(*S*)-1-(4-Methylphenyl)-1-ethanol ((*S*)-12Aa) [Table 4, Entry 1, 78% ee]: HPLC (CHIRALPAK AS-H, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min): t_R = 25.4 min (11.1%), t_R = 28.0 min (88.9%); ^{1}H NMR ($CDCl_3$): δ 7.25 (d, *J* = 8.0 Hz, 2H, Ar), 7.15 (d, *J* = 8.0 Hz, 2H, Ar), 4.84 (q, *J* = 6.5 Hz, 1H, 1-H), 2.34 (s, 3H, *p*-Me), 2.00 (br s, 1H, OH), 1.47 (d, *J* = 6.5 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 142.8, 137.1, 129.1, 125.3, 70.2, 25.0, 21.1.



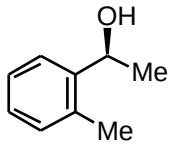
(*S*)–**12Ab**

(*S*)-1-(4-Methoxyphenyl)-1-ethanol ((*S*)-12Ab) [Table 4, Entry 2, 85% ee]: HPLC (CHIRALCEL OD-H, *i*-PrOH/hexane = 1/50, flow rate = 0.75 mL/min): t_R = 31.8 min (7.5%), t_R = 35.9 min (92.5%); ^{1}H NMR ($CDCl_3$): δ 7.34–7.26 (m, 2H, Ar), 6.92–6.84 (m, 2H, Ar), 4.86 (q, *J* = 6.3 Hz, 1H, 1-H), 3.81 (s, 3H, *p*-MeO), 1.81 (br s, 1H, OH), 1.48 (d, *J* = 6.3 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 158.9, 138.0, 126.6, 113.8, 70.0, 55.3, 25.0.



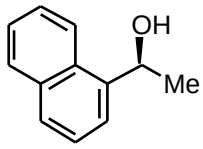
(*S*)–**12Ac**

(*S*)-1-(4-Fluorophenyl)-1-ethanol ((*S*)-12Ac) [Table 4, Entry 3, 75% ee]: HPLC (CHIRALPAK AS-H, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min): t_R = 35.7 min (12.7%), t_R = 40.0 min (87.3%); ^{1}H NMR ($CDCl_3$): δ 7.36–7.27 (m, 2H, Ar), 7.05–6.96 (m, 2H, Ar), 4.86 (q, *J* = 6.3 Hz, 1H, 1-H), 2.13 (br s, 1H, OH), 1.46 (d, *J* = 6.3 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 162.0 (d, *J* = 244.4 Hz), 141.5 (d, *J* = 3.1 Hz), 127.0 (d, *J* = 8.1 Hz), 115.2 (d, *J* = 21.1 Hz), 69.7, 25.2.



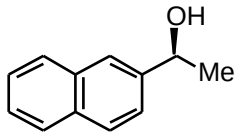
(*S*)–**12Ad**

(*S*)-1-(2-Methylphenyl)-1-ethanol ((*S*)-12Ad) [Table 4, Entry 4, 87% ee]: HPLC (CHIRALPAK IA, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min): t_R = 25.7 min (6.6%), t_R = 29.0 min (93.4%); ^{1}H NMR ($CDCl_3$): δ 7.53–7.46 (m, 1H, Ar), 7.27–7.08 (m, 3H, Ar), 5.10 (q, *J* = 6.5 Hz, 1H, 1-H), 2.33 (s, 3H, *o*-Me), 1.88 (br s, 1H, OH), 1.45 (d, *J* = 6.5 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 143.8, 134.2, 130.3, 127.1, 126.3, 124.4, 66.7, 23.9, 18.9.



(*S*)–**12Ae**

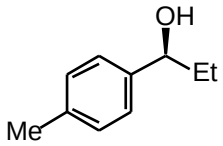
(*S*)-1-(1-Naphthyl)-1-ethanol ((*S*)-12Ae) [Table 4, Entry 5, 87% ee]: HPLC (CHIRALCEL OB-H, *i*-PrOH/hexane = 1/9, flow rate = 0.5 mL/min): t_R = 18.1 min (93.5%), t_R = 21.9 min (6.5%); ^{1}H NMR ($CDCl_3$): δ 8.12–8.04 (m, 1H, Ar), 7.89–7.82 (m, 1H, Ar), 7.76 (d, *J* = 8.4 Hz, 1H, Ar), 7.65 (d, *J* = 6.9 Hz, 1H, Ar), 7.54–7.42 (m, 3H, Ar), 5.64 (dq, *J* = 2.3, 6.5 Hz, 1H, 1-H), 2.06 (d, *J* = 2.3 Hz, OH), 1.64 (d, *J* = 6.5 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 141.3, 133.7, 130.2, 128.8, 127.9, 126.0, 125.5, 125.5, 123.1, 121.9, 67.0, 24.3.



(*S*)–**12Af**

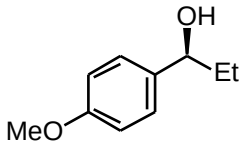
(*S*)-1-(2-Naphthyl)-1-ethanol ((*S*)-12Af) [Table 4, Entry 6, 83% ee]: HPLC (CHIRALCEL OB-H, *i*-PrOH/hexane = 1/9, flow rate = 0.5 mL/min): t_R = 17.6 min

(91.5%), t_R = 20.1 min (8.5%); ^{1}H NMR ($CDCl_3$): δ 7.84–7.72 (m, 4H, Ar), 7.50–7.40 (m, 3H, Ar), 5.00 (q, *J* = 6.3 Hz, 1H, 1-H), 2.17 (br s, 1H, OH), 1.54 (d, *J* = 6.3 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 143.1, 133.2, 132.8, 128.2, 127.9, 127.6, 126.1, 125.7, 123.8, 123.7, 70.4, 25.1.



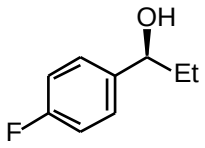
(*S*)–**13Ba**

(*S*)-1-(4-Methylphenyl)-1-propanol ((*S*)-13Ba) [Table 4, Entry 7, 80% ee]: HPLC (CHIRALPAK AS-H, *i*-PrOH/hexane = 1/50, flow rate = 0.75 mL/min): t_R = 7.5 min (9.9%), t_R = 18.2 min (90.1%); ^{1}H NMR ($CDCl_3$): δ 7.17 (d, *J* = 8.3 Hz, 2H, Ar), 7.10 (d, *J* = 8.3 Hz, 2H, Ar), 4.52–4.47 (m, 1H, 1-H), 2.29 (s, 3H, *p*-Me), 1.85–1.62 (m, 3H, 2-H, OH), 0.85 (dd, *J* = 7.5, 7.0 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 141.6, 137.1, 129.0, 125.9, 75.9, 31.8, 21.1, 10.2.



(*S*)–**13Bb**

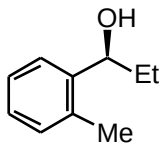
(*S*)-1-(4-Methoxyphenyl)-1-propanol ((*S*)-13Bb) [Table 4, Entry 8, 86% ee]: HPLC (CHIRALCEL OD-H, *i*-PrOH/hexane = 1/50, flow rate = 0.75 mL/min): t_R = 30.3 min (6.9%), t_R = 34.1 min (93.1%); ^{1}H NMR ($CDCl_3$): δ 7.10 (dt, *J* = 9.5, 2.3 Hz, 2H, Ar), 6.73 (dt, *J* = 9.5, 2.3 Hz, 2H, Ar), 4.35 (t, *J* = 6.5 Hz, 1H, 1-H), 3.65 (s, 3H, *p*-MeO), 2.58 (br s, 1H, OH), 1.71–1.51 (m, 2H, 2-H), 0.75 (dd *J* = 7.5, 7.0 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 158.7, 136.7, 127.1, 113.5, 75.3, 55.0, 31.6, 10.0.



(*S*)–**13Bc**

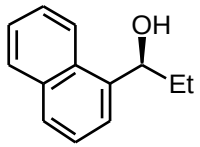
(*S*)-1-(4-Fluorophenyl)-1-propanol ((*S*)-13Bc) [Table 4, Entry 9, 78% ee]: HPLC (CHIRALCEL OB-H, *i*-PrOH/hexane = 1/50, flow rate = 0.35 mL/min): t_R = 29.1 min (89.2%), t_R = 31.4 min (10.8%); ^{1}H NMR ($CDCl_3$): δ 7.32–7.28 (m, 2H, Ar), 7.05–7.00 (m, 2H, Ar), 4.58 (t, *J* = 6.5 Hz, 1H, 1-H), 2.10 (br s, 1H, OH), 1.80

(ddq, *J* = 14.3, 6.5, 7.5 Hz, 1H, 2-H), 1.71 (ddq, *J* = 14.3, 6.5, 7.0 Hz, 1H, 2-H), 0.90 (dd, *J* = 7.5, 7.0 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 162.1 (d, *J* = 244.9 Hz), 140.3 (d, *J* = 3.1 Hz), 127.5 (d, *J* = 8.3 Hz), 115.1 (d, *J* = 20.6 Hz), 75.3, 32.0, 10.0.



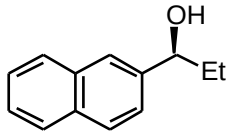
(*S*)–**13Bd**

(*S*)-1-(2-Methylphenyl)-1-propanol ((*S*)-13Bd) [Table 4, Entry 10, 83% ee]: HPLC (CHIRALCEL OB-H, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min): t_R = 16.4 min (91.7%), t_R = 22.8 min (8.3%); ^{1}H NMR ($CDCl_3$): δ 7.29 (d, *J* = 7.5 Hz, 1H, Ar), 7.09–6.96 (m, 3H, Ar), 4.65 (dt, *J* = 2.5, 6.3 Hz, 1H, 1-H), 2.41 (br s, 1H, OH), 2.18 (s, 3H, *o*-Me), 1.62–1.56 (m, 2H, 2-H), 0.82 (t, *J* = 7.5 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 142.7, 134.4, 130.1, 126.8, 126.0, 125.2, 71.7, 30.7, 18.9, 10.2.



(*S*)–**13Be**

(*S*)-1-(1-Naphthyl)-1-propanol ((*S*)-13Be) [Table 4, Entry 11, 82% ee]: HPLC (CHIRALCEL OB-H, *i*-PrOH/hexane = 1/50, flow rate = 0.75 mL/min): t_R = 23.1 min (90.9%), t_R = 27.2 min (9.1%); ^{1}H NMR ($CDCl_3$): δ 8.05 (d, *J* = 8.5 Hz, 1H, Ar), 7.82–7.78 (m, 1H, Ar), 7.71 (d, *J* = 8.0 hz, 1H, Ar), 7.56 (d, *J* = 7.0 Hz, 1H, Ar), 7.47–7.37 (m, 3H, Ar), 5.36–5.31 (m, 1H, 1-H), 2.00–1.81 (m, 3H, 2-H, OH), 0.96 (dd, *J* = 8.0, 7.0 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 140.2, 133.8, 130.5, 128.9, 127.9, 125.9, 125.5, 125.4, 123.2, 122.9, 72.6, 31.1, 10.5.

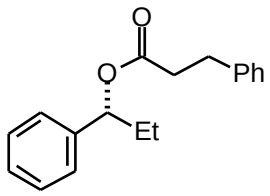


(*S*)–**13Bf**

(*S*)-1-(2-Naphthyl)-1-propanol ((*S*)-13Bf) [Table 4, Entry 12, 91% ee]: HPLC (CHILALPAK IC, *i*-PrOH/hexane = 1/9, flow rate = 0.5 mL/min): t_R = 10.3 min (4.6%), t_R = 15.5 min (95.4%); ^{1}H NMR ($CDCl_3$): δ 7.89–7.74 (m, 4H, Ar), 7.53–7.43 (m, 3H, Ar), 4.81–4.70 (m, 1H, 1-H), 2.19 (br s, 1H, OH), 1.92 (ddq, *J* = 14.0, 7.1, 7.5 Hz, 1H, 2-H), 1.85 (ddq, *J* = 14.0, 7.1, 7.5 Hz, 1H, 2-H), 0.95 (t, *J* = 7.5

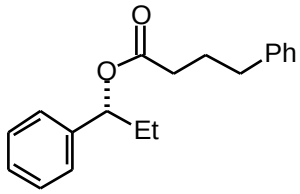
Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 141.9, 133.2, 132.9, 128.2, 127.9, 127.6, 126.0, 125.7, 124.7, 124.1, 76.1, 31.7, 10.1.

(Optically Active Esters)



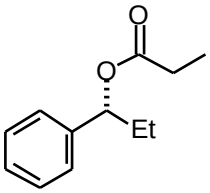
(*R*)–**8a**

(*R*)-1-Phenylpropyl 3-phenylpropanoate ((*R*)-8a) [Table 2, Entry 1, 87% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min); t_R = 11.9 min (93.6%), t_R = 16.4 min (6.4%); IR (neat): 3031, 1741, 1604, 1496, 752, 700 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.27–7.14 (m, 7H, Ph), 7.13–7.07 (m, 3H, Ph), 5.59 (t, *J* = 7.0 Hz, 1H, 1-H), 2.87 (t, *J* = 8.0 Hz, 2H, 2'-H), 2.61 (ddd, *J* = 16.0, 9.0, 9.0 Hz, 1H, 3'-H), 2.57 (ddd, *J* = 16.0, 9.6, 9.0 Hz, 1H, 3'-H), 1.86–1.66 (m, 2H, 2-H), 0.76 (t, *J* = 7.5 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 172.2, 140.48, 140.46, 128.4, 128.3, 128.2, 127.7, 126.5, 126.2, 77.4, 36.1, 30.9, 29.3, 9.8; HR MS: calcd for $C_{18}H_{20}O_2Na$ ($M+Na^+$) 291.1356, found 291.1344.



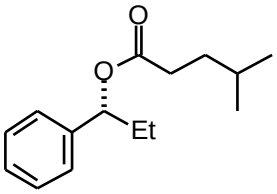
(*R*)–**8b**

(*R*)-1-Phenylpropyl 4-phenylbutanoate ((*R*)-8b) [Table 2, Entry 2, 90% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min); t_R = 12.6 min (95.0%), t_R = 16.6 min (5.0%); IR (neat): 3030, 1734, 1603, 1496, 749, 700 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.23–6.99 (m, 10H, Ph), 5.60 (t, *J* = 7.0 Hz, 1H, 1-H), 2.53 (t, *J* = 7.5 Hz, 2H, 2'-H), 2.29 (dt, *J* = 16.2, 7.5 Hz, 1H, 4'-H), 2.24 (dt, *J* = 16.2, 6.6 Hz, 1H, 4'-H), 1.93–1.65 (m, 4H, 2-H, 3'-H), 0.80 (t, *J* = 7.5 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 172.7, 141.4, 140.6, 128.4, 128.3, 128.3, 127.7, 126.5, 125.9, 77.2, 35.0, 33.8, 29.3, 26.5, 9.9; HR MS: calcd for $C_{19}H_{22}O_2Na$ ($M+Na^+$) 305.1512, found 305.1507.



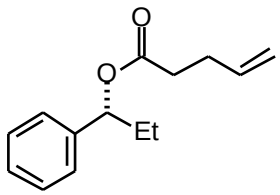
(*R*)–**8c**

(*R*)-1-Phenylpropyl propanoate ((*R*)-8c) [Table 2, Entry 3, 92% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/50, flow rate = 0.35 mL/min); t_R = 13.5 min (96.1%), t_R = 15.7 min (3.9%); IR (neat): 3034, 1734, 1604, 1495, 756, 700 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.30–7.16 (m, 5H, Ph), 5.60 (dd, *J* = 7.5, 6.6 Hz, 1H, 1-H), 2.34–2.22 (m, 2H, 2'-H), 1.93 –1.65 (m, 2H, 2-H), 1.06 (t, *J* = 7.5 Hz, 3H, 3'-H), 0.81 (t, *J* = 7.5 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 173.8, 140.7, 128.3, 127.7, 126.5, 77.1, 29.4, 27.8, 9.9, 9.1; HR MS: calcd for $C_{12}H_{16}O_2Na$ ($M+Na^+$) 215.1043, found 215.1049.



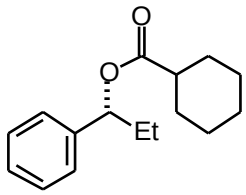
(*R*)–**8d**

(*R*)-1-Phenylpropyl 4-methylpentanoate ((*R*)-8d) [Table 2, Entry 4, 92% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min); t_R = 9.7 min (96.0%), t_R = 11.6 min (4.0%); IR (neat): 3033, 1742, 1604, 1495, 757, 700 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.31–7.13 (m, 5H, Ph), 5.59 (t, *J* = 7.5 Hz, 1H, 1-H), 2.33–2.17 (m, 2H, 2'-H), 1.93–1.63 (m, 2H, 2-H), 1.52–1.36 (m, 3H, 3'-H, 4'-H), 0.88–0.73 (m, 9H, 3-H, Me, Me); ^{13}C NMR ($CDCl_3$): δ 173.3, 140.7, 128.3, 127.7, 126.5, 77.0, 33.7, 32.6, 29.3, 27.6, 22.19, 22.15, 9.9; HR MS: calcd for $C_{15}H_{22}O_2Na$ ($M+Na^+$) 257.1512, found 257.1509.



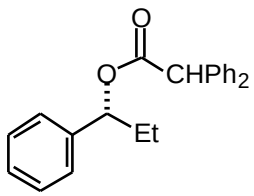
(*R*)–**8e**

(*R*)-1-Phenylpropyl 4-pentenoate ((*R*)-8e) [Table 2, Entry 5, 84% ee]: Enantiomeric excess of (*R*)-**8e** has been determined after cleaving the ester moiety; HPLC (CHIRALCEL OD-H, *i*-PrOH/hexane = 1/100, flow rate = 0.75 mL/min); t_R = 26.2 min (91.8%), t_R = 29.7 min (8.2%); IR (neat): 3033, 1735, 1642, 1495, 755, 700 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.27–7.15 (m, 5H, Ph), 5.76–5.67 (m, 1H, 4'-H), 5.60 (t, *J* = 7.5 Hz, 1-H), 4.98–4.86 (m, 2H, 5'-H), 2.39–2.25 (m, 4H, 2'-H, 3'-H), 1.89–1.68 (m, 2H, 2-H), 0.80 (t, *J* = 7.5 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 172.3, 140.5, 136.6, 128.3, 127.7, 126.5, 115.4, 77.2, 33.7, 29.3, 28.8, 9.9; HR MS: calcd for $C_{14}H_{18}O_2Na$ ($M+Na^+$) 241.1199, found 241.1207.



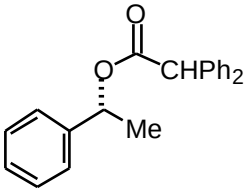
(*R*)–**8f**

(*R*)-1-Phenylpropyl cyclohexanecarboxylate ((*R*)-8f) [Table 2, Entry 6, 90% ee]: Enantiomeric excess of (*R*)-**8f** has been determined after cleaving the ester moiety; HPLC (CHIRALCEL OD-H, *i*-PrOH/hexane = 1/100, flow rate = 0.75 mL/min): t_R = 31.6 min (94.8%), t_R = 35.8 min (5.2%); IR (neat): 3032, 1736, 1450, 756, 702 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.36–7.22 (m, 5H, Ar), 5.66 (dd, *J* = 7.2, 6.2 Hz, 1H, 1-H), 2.33 (tt, *J* = 11.3, 3.6 Hz, 1H, 2'-H), 1.99–1.15 (m, 12H, 2-H, *c*-Hex), 0.88 (t, *J* = 7.6 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 175.3, 140.9, 128.3, 127.6, 126.3, 76.7, 43.3, 29.5, 29.0, 28.9, 25.7, 25.42, 25.39, 9.9; HR MS: calcd for $C_{16}H_{22}O_2Na$ ($M+Na^+$) 269.1512, found 269.1525.



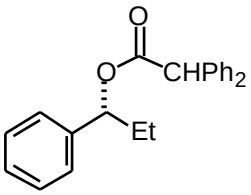
(*R*)–**8g**

(*R*)-1-Phenylpropyl diphenylacetate ((*R*)-8g) [Table 2, Entry 7, 87% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/9, flow rate = 0.5 mL/min): t_R = 10.9 min (93.4%), t_R = 18.0 min (6.6%); IR (neat): 3031, 1736, 1601, 1495, 1453, 748, 699 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.32–7.15 (m, 15H, Ar), 5.71 (dd, *J* = 6.9, 6.6 Hz, 1H, 1-H), 5.06 (s, 1H, 2'-H), 1.88 (ddq, *J* = 14.1, 7.2, 6.9 Hz, 1H, 2-H), 1.77 (ddq, *J* = 14.1, 7.2, 6.6 Hz, 1H, 2-H), 0.79 (t, *J* = 7.2 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 171.7, 140.1, 138.7, 138.5, 128.7, 128.6, 128.5, 128.4, 128.2, 127.7, 127.13, 127.07, 126.5, 78.2, 57.2, 29.2, 9.8; HR MS: calcd for $C_{23}H_{22}O_2Na$ ($M+Na^+$) 353.1512, found 353.1512.



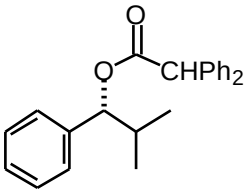
(*R*)–**10a**

(*R*)-1-Phenylethyl diphenylacetate ((*R*)-10a) [Table 3, Entry 1, 89% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/50, flow rate = 1.0 mL/min): t_R = 11.5 min (94.7%), t_R = 27.4 min (5.3%); IR (neat): 3032, 1735, 1603, 1496, 745, 700 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.24–7.11 (m, 15H, Ar), 5.86 (q, *J* = 6.5 Hz, 1H, 1-H), 4.97 (s, 1H, 2'-H), 1.43 (d, *J* = 6.5 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 171.6, 141.3, 138.7, 138.5, 128.6, 128.6, 128.48, 128.45, 128.3, 127.8, 127.2, 127.1, 126.0, 73.1, 57.2, 22.0; HR MS: calcd for $C_{22}H_{20}O_2Na$ ($M+Na^+$) 339.1356, found 339.1367.



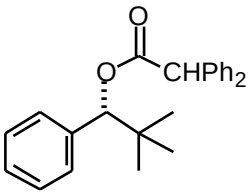
(*R*)–**10b** (= (*R*)-**8g**)

(*R*)-1-Phenylpropyl diphenylacetate ((*R*)-10b) (= **(*R*)-8g**) [Table 3, Entry 2, 92% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/9, flow rate = 0.5 mL/min): t_R = 10.8 min (96.0%), t_R = 27.4 min (4.0%).



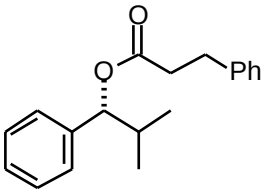
(*R*)–**10c**

(*R*)-2-Methyl-1-phenylpropyl diphenylacetate ((*R*)-10c) [Table 3, Entry 3, 88% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/50, flow rate = 1.0 mL/min): t_R = 9.7 min (93.9%), t_R = 21.8 min (6.1%); IR (neat): 3032, 1736, 1599, 1496, 742, 696 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.25–7.03 (m, 15H, Ar), 5.42 (d, *J* = 7.5 Hz, 1H, 1-H), 4.99 (s, 1H, 2'-H), 1.97 (dqq, *J* = 7.5, 6.6, 6.6 Hz, 1H, 2-H), 0.77 (d, *J* = 6.6 Hz, 3H, 3-H), 0.65 (d, *J* = 6.6 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 171.6, 139.2, 138.7, 138.5, 128.73, 128.68, 128.44, 128.40, 128.0, 127.6, 127.2, 127.1, 127.0, 81.8, 57.4, 33.5, 18.6, 18.3; HR MS: calcd for $C_{24}H_{24}O_2Na$ ($M+Na^+$) 367.1669, found 367.1651.



(*R*)–**10d**

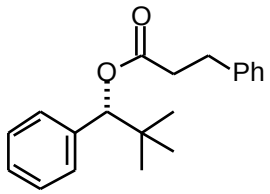
(*R*)-2,2-Dimethyl-1-phenylpropyl diphenylacetate ((*R*)-10d) [Table 3, Entry 4, 87% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/9, flow rate = 0.5 mL/min): t_R = 11.0 min (93.4%), t_R = 18.8 min (6.6%); IR (KBr): 3031, 1737, 1599, 1491, 741, 701 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.29–7.15 (m, 13H, Ar), 7.08–7.06 (m, 2H, Ar), 5.48 (s, 1H, 1-H), 5.07 (s, 1H, 2'-H), 0.79 (s, 9H, 3-H); ^{13}C NMR ($CDCl_3$): δ 171.3, 138.7, 138.5, 138.0, 128.82, 128.79, 128.4, 128.4, 127.7, 127.4, 127.4, 127.2, 127.1, 83.8, 57.6, 35.0, 25.9; HR MS: calcd for $C_{25}H_{26}O_2Na$ ($M+Na^+$) 381.1825, found 381.1824.



(*R*)–**11c**

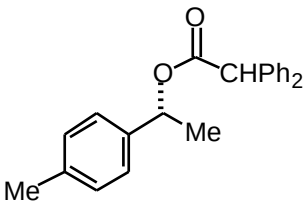
(*R*)-2-Methyl-1-phenylpropyl 3-phenylpropanoate ((*R*)-11c) [Table 3, Entry

5, 90% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min): t_R = 11.4 min (95.2%), t_R = 16.5 min (4.8%); IR (neat): 3030, 1734, 1604, 1496, 751, 699 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.28–7.02 (m, 10H, Ph), 5.41 (d, *J* = 7.5 Hz, 1H, 1-H), 2.88 (t, *J* = 7.5 Hz, 2H, 2'-H), 2.65–2.53 (m, 2H, 3'-H), 2.07–1.83 (m, 1H, 2-H), 0.85 (d, *J* = 7.0 Hz, 3H, Me), 0.70 (d, *J* = 7.0 Hz, 3H, Me); ^{13}C NMR ($CDCl_3$): δ 172.1, 140.4, 139.6, 128.4, 128.2, 128.1, 127.6, 127.0, 126.2, 81.0, 36.0, 33.4, 30.9, 18.6, 18.4; HR MS: calcd for $C_{19}H_{22}O_2Na$ ($M+Na^+$) 305.1512, found 305.1520.



(*R*)–**11d**

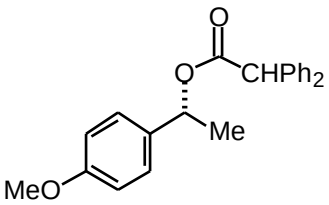
(*R*)-2,2-Dimethyl-1-phenylpropyl 3-phenylpropanoate ((*R*)-11d) [Table 3, Entry 6, 94% ee]: HPLC (CHIRALPAK IC, *i*-PrOH/hexane = 1/100, flow rate = 0.5 mL/min): t_R = 16.0 min (96.9%), t_R = 21.9 min (3.1%); IR (neat): 3030, 1737, 1604, 1496, 740, 702 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.40–7.17 (m, 10H, Ph), 5.53 (s, 1H, 1-H), 3.00 (t, *J* = 7.5 Hz, 2H, 2'-H), 2.79–2.68 (m, 2H, 3'-H), 0.93 (s, 9H, *t*-Bu); ^{13}C NMR ($CDCl_3$): δ 172.0, 140.4, 138.4, 128.5, 128.2, 127.7, 127.6, 127.4, 126.2, 82.9, 36.0, 35.0, 30.9, 26.0; HR MS: calcd for $C_{20}H_{24}O_2Na$ ($M+Na^+$) 319.1669, found 319.1660.



(*R*)–**13Aa**

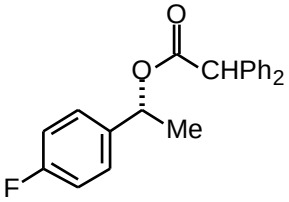
(*R*)-1-(4-Methylphenyl)ethyl diphenylacetate ((*R*)-13Aa) [Table 4, Entry 1, 89% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/9, flow rate = 0.5 mL/min): t_R = 10.1 min (94.7%), t_R = 18.7 min (5.3%); IR (neat): 3029, 1734, 1596, 1517, 818, 749, 697 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.26–7.10 (m, 10H, Ar), 7.06–6.98 (m, 4H, Ar), 5.83 (q, *J* = 6.6 Hz, 1H, 1-H), 4.95 (s, 1H, 2'-H), 2.24 (s, 3H, *p*-Me), 1.42 (d, *J* = 6.6 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 171.6, 138.7, 138.6, 138.3, 137.5, 129.0, 128.6, 128.6, 128.5, 128.4, 127.13, 127.08, 126.0, 73.1, 57.2, 22.0, 21.1; HR MS:

calcd for $C_{23}H_{22}O_2Na$ ($M+Na^+$) 353.1512, found 353.1497.



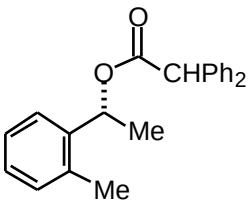
(*R*)–**13Ab**

(*R*)-1-(4-Methoxyphenyl)ethyl diphenylacetate ((*R*)-13Ab) [Table 4, Entry 2, 86% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/9, flow rate = 0.5 mL/min): t_R = 13.5 min (93.2%), t_R = 26.2 min (6.8%); IR (neat): 2979, 1656, 1608, 829, 742, 698 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.25–7.08 (m, 12H, Ar), 6.74 (dt, *J* = 9.5, 2.5 Hz, 2H, Ar), 5.83 (q, *J* = 6.5 Hz, 1H, 1-H), 4.94 (s, 1H, 2'-H), 3.70 (s, 3H, *p*-MeO), 1.42 (d, *J* = 6.5 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 171.6, 159.2, 138.8, 138.6, 133.4, 128.6, 128.6, 128.5, 128.4, 127.6, 127.13, 127.07, 113.7, 72.9, 57.2, 55.2, 21.8; HR MS: calcd for $C_{23}H_{22}O_3Na$ ($M+Na^+$) 369.1461, found 369.1460.



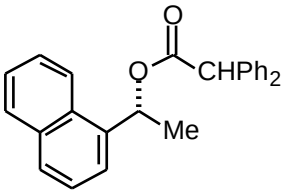
(*R*)–**13Ac**

(*R*)-1-(4-Fluorophenyl)ethyl diphenylacetate ((*R*)-13Ac) [Table 4, Entry 3, 81% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/9, flow rate = 0.5 mL/min): t_R = 10.2 min (90.6%), t_R = 17.6 min (9.4%); IR (neat): 3033, 1735, 1606, 1514, 841, 743, 697 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.25–7.08 (m, 12H, Ar), 6.91–6.85 (m, 2H, Ar), 5.84 (q, *J* = 6.5 Hz, 1H, 1-H), 4.95 (s, 1H, 2'-H), 1.42 (d, *J* = 6.5 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 171.5, 162.3 (d, *J* = 245.9 Hz), 138.6, 138.4, 137.1 (d, *J* = 3.1 Hz), 128.62, 128.58, 128.51, 128.51, 127.9 (d, *J* = 7.2 Hz), 127.21, 127.18, 115.2 (d, *J* = 21.7 Hz), 72.5, 57.2, 22.0; HR MS: calcd for $C_{22}H_{19}FO_2Na$ ($M+Na^+$) 357.1261, found 357.1254.



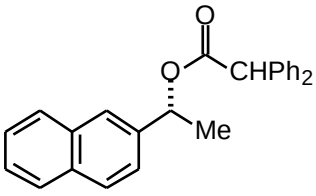
(*R*)–**13Ad**

(*R*)-1-(2-Methylphenyl)ethyl diphenylacetate ((*R*)-13Ad) [Table 4, Entry 4, 90% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min): t_R = 14.7 min (95.1%), t_R = 23.1 min (4.9%); IR (neat): 3030, 1733, 1596, 1496, 753, 697 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.26–7.12 (m, 10H, Ar), 7.11–7.00 (m, 4H, Ar), 6.04 (q, *J* = 6.5 Hz, 1H, 1-H), 4.98 (s, 1H, 2'-H), 2.24 (s, 3H, *o*-Me), 1.41 (d, *J* = 6.5 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 171.6, 139.7, 138.7, 138.4, 134.7, 130.3, 128.7, 128.6, 128.50, 128.48, 127.6, 127.2, 127.1, 126.1, 125.3, 70.2, 57.2, 21.2, 18.9; HR MS: calcd for $C_{23}H_{22}O_2Na$ ($M+Na^+$) 353.1512, found 353.1498.



(*R*)–**13Ae**

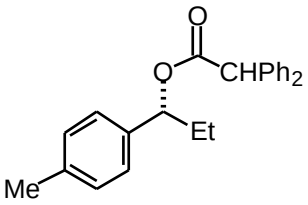
(*R*)-1-Naphthylethyl diphenylacetate ((*R*)-13Ae) [Table 4, Entry 5, 88% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/9, flow rate = 0.35 mL/min): t_R = 16.9 min (93.9%), t_R = 26.5 min (6.1%); IR (neat): 3058, 1734, 1600, 1496, 777, 748, 698 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.92–7.82 (m, 1H, Ar), 7.78–7.61 (m, 2H, Ar), 7.37–7.10 (m, 14H, Ar), 6.40 (q, *J* = 6.6 Hz, 1H, 1-H), 5.01 (s, 1H, 2'-H), 1.58 (d, *J* = 6.6 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 171.6, 138.6, 138.4, 137.0, 133.7, 130.1, 128.8, 128.7, 128.7, 128.52, 128.47, 128.37, 127.19, 127.16, 126.2, 125.6, 125.2, 123.2, 123.1, 70.3, 57.2, 21.5; HR MS: calcd for $C_{26}H_{22}O_2Na$ ($M+Na^+$) 389.1512, found 389.1511.



(*R*)–**13Af**

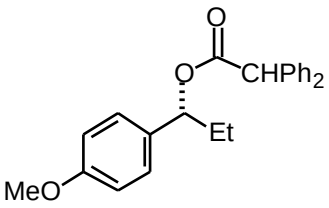
(*R*)-2-Naphthylethyl diphenylacetate ((*R*)-13Af) [Table 4, Entry 6, 85% ee]:

HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/9, flow rate = 0.75 mL/min): t_R = 8.5 min (92.6%), t_R = 22.6 min (7.4%); IR (neat): 3057, 1734, 1602, 1495, 821, 746, 698 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.72–7.64 (m, 2H, Ar), 7.63–7.58 (m, 1H, Ar), 7.53 (s, 1H, Ar), 7.37–7.32 (m, 2H, Ar), 7.25–7.11 (m, 11H, Ar), 6.02 (q, *J* = 6.8 Hz, 1H, 1-H), 5.00 (s, 1H, 2'-H), 1.50 (d, *J* = 6.8 Hz, 3H, 2-H); ^{13}C NMR ($CDCl_3$): δ 171.6, 138.7, 138.7, 138.4, 133.0, 132.9, 128.7, 128.6, 128.5, 128.5, 128.1, 128.0, 127.6, 127.2, 127.1, 126.1, 125.9, 124.8, 124.0, 73.2, 57.2, 22.1; HR MS: calcd for $C_{26}H_{22}O_2Na$ ($M+Na^+$) 389.1512, found 389.1510.



(*R*)–**13Ba**

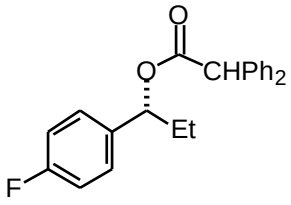
(*R*)-1-(4-Methylphenyl)propyl diphenylacetate ((*R*)-13Ba) [Table 4, Entry 7, 93% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/9, flow rate = 0.5 mL/min): t_R = 13.1 min (93.2%), t_R = 25.4 min (6.8%); IR (neat): 3029, 1734, 1600, 1496, 815, 741, 697 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.23–7.09 (m, 10H, Ar), 7.03–6.96 (m, 4H, Ar), 5.60 (dd, *J* = 6.9, 6.6 Hz, 1H, 1-H), 4.96 (s, 1H, 2'-H), 2.22 (s, 3H, *p*-Me), 1.87–1.59 (m, 2H, 2-H), 0.70 (dd, *J* = 7.5, 7.2 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 171.7, 138.8, 138.5, 137.4, 137.1, 128.9, 128.7, 128.7, 128.44, 128.38, 127.1, 127.0, 126.5, 78.2, 57.3, 29.2, 21.1, 9.8; HR MS: calcd for $C_{24}H_{24}O_2Na$ ($M+Na^+$) 367.1669, found 367.1684.



(*R*)–**13Bb**

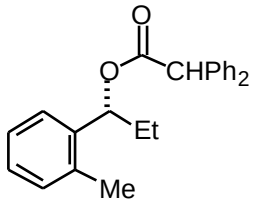
(*R*)-1-(4-Methoxyphenyl)propyl diphenylacetate ((*R*)-13Bb) [Table 4, Entry 8, 89% ee]: HPLC (CHIRALPAK IC, *i*-PrOH/hexane = 1/9, flow rate = 0.5 mL/min): t_R = 9.5 min (94.7%), t_R = 13.3 min (5.3%); IR (neat): 3030, 1733, 1615, 1517, 829, 744, 697 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.24–7.02 (m, 12H, Ar), 6.75–6.68 (m, 2H, Ar), 5.58 (dd, *J* = 7.0, 6.9 Hz, 1H, 1-H), 4.95 (s, 1H, 2'-H), 3.68 (s, 3H, *p*-MeO), 1.87–1.58 (m, 2H, 2-H), 0.70 (dd, *J* = 7.5, 7.2 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 171.7, 159.1, 138.8, 138.5, 132.2, 128.64, 128.62, 128.44, 128.39, 128.0, 127.1, 127.0,

113.6, 78.0, 57.2, 55.2, 29.0, 9.9; HR MS: calcd for $C_{24}H_{24}O_3Na$ ($M+Na^+$) 383.1618, found 383.1599.



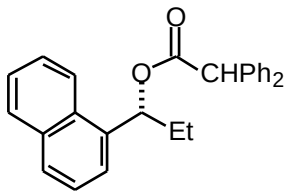
(*R*)–**13Bc**

(*R*)-1-(4-Fluorophenyl)propyl diphenylacetate ((*R*)-13Bc) [Table 4, Entry 9, 84% ee]: HPLC (CHIRALPAK IC, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min): t_R = 10.9 min (91.8%), t_R = 14.2 min (8.2%); IR (neat): 3033, 1735, 1607, 1504, 833, 742, 703 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.25–7.03 (m, 12H, Ar), 6.90–6.81 (m, 2H, Ar), 5.59 (t, *J* = 6.9 Hz, 1H, 1-H), 4.96 (s, 1H, 2'-H), 1.79 (ddq, *J* = 14.1, 6.9, 7.5 Hz, 1H, 2-H), 1.66 (ddq, *J* = 14.1, 6.9, 7.2 Hz, 1H, 2-H), 0.71 (dd, *J* = 7.5, 7.2 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 171.7, 162.3 (d, *J* = 245.6 Hz), 138.6, 138.3, 135.9 (d, *J* = 3.2 Hz), 128.63, 128.58, 128.47, 128.45, 128.3 (d, *J* = 8.1 Hz), 127.2, 127.1, 115.1 (d, *J* = 21.1 Hz), 77.5, 57.2, 29.2, 9.8; HR MS: calcd for $C_{23}H_{21}FO_2Na$ ($M+Na^+$) 371.1418, found 371.1423.



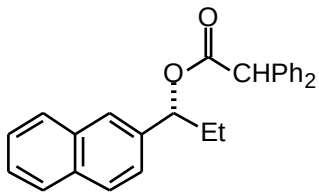
(*R*)–**13Bd**

(*R*)-1-(2-Methylphenyl)propyl diphenylacetate ((*R*)-13Bd) [Table 4, Entry 10, 92% ee]: HPLC (CHIRALPAK AD-H, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min): t_R = 12.4 min (96.2%), t_R = 20.9 min (3.8%); IR (neat): 3029, 1733, 1603, 1496, 751, 697 cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.33–7.04 (m, 14H, Ar), 5.91 (dd, *J* = 7.8, 6.0 Hz, 1H, 1-H), 5.06 (s, 1H, 2'-H), 2.35 (s, 3H, *o*-Me), 1.93–1.66 (m, 2H, 2-H), 0.83 (dd, *J* = 7.5, 7.2 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 171.8, 138.8, 138.7, 138.4, 135.0, 130.2, 128.7, 128.7, 128.5, 128.4, 127.4, 127.13, 127.08, 125.9, 125.7, 75.0, 57.2, 28.8, 19.1, 10.0; HR MS: calcd for $C_{24}H_{24}O_2Na$ ($M+Na^+$) 367.1669, found 367.1669.



(*R*)–**13Be**

(*R*)-1-Naphthylpropyl diphenylacetate ((*R*)-13Be) [Table 4, Entry 11, 95% ee]: HPLC (CHIRALPAK IC, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min): t_R = 13.1 min (97.5%), t_R = 24.6 min (2.5%); IR (neat): 3029, 1737, 1599, 1495, 799, 778, 744, 701 cm^{-1}; ^1H NMR ($CDCl_3$): δ 8.08–8.02 (m, 1H, Ar), 7.87–7.82 (m, 1H, Ar), 7.76 (d, *J* = 8.0 Hz, 1H, Ar), 7.49–7.43 (m, 2H, Ar), 7.36–7.20 (m, 12H, Ar), 6.51 (t, *J* = 6.5 Hz, 1H, 1-H), 5.13 (s, 1H, 2'-H), 2.02 (dq, *J* = 6.5, 7.5 Hz, 1H, 2-H), 2.01 (dq, *J* = 6.5, 7.0 Hz, 1H, 2-H), 0.88 (dd, *J* = 7.5, 7.0 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 171.7, 138.7, 138.4, 136.0, 133.7, 130.3, 128.8, 128.71, 128.69, 128.5, 128.4, 128.2, 127.2, 127.1, 126.1, 125.5, 125.1, 123.8, 123.2, 75.4, 57.3, 29.0, 10.2; HR MS: calcd for $C_{27}H_{24}O_2Na$ ($M+Na^+$) 403.1669, found 403.1663.

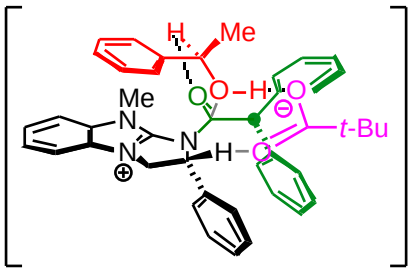


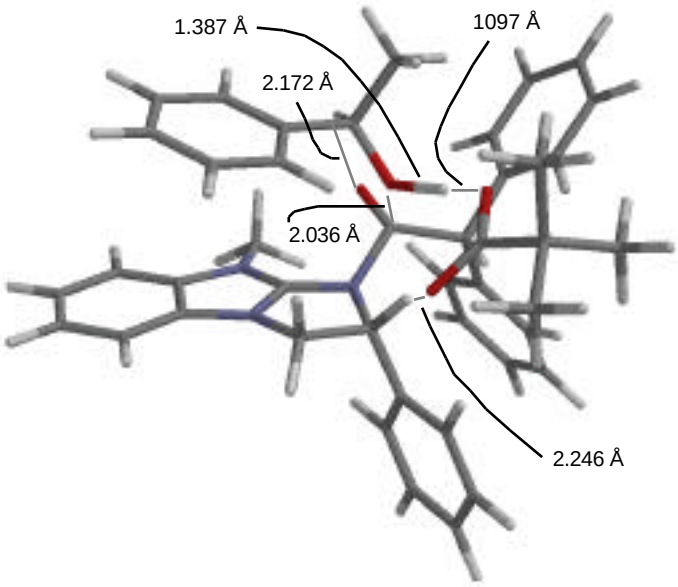
(*R*)–**13Bf**

(*R*)-2-Naphthylpropyl diphenylacetate ((*R*)-13Bf) [Table 4, Entry 12, 90% ee]: HPLC (CHIRAKPAK IC, *i*-PrOH/hexane = 1/50, flow rate = 0.5 mL/min): t_R = 15.4 min (92.0%), t_R = 29.3 min (8.0%); IR (neat): 3057, 1734, 1602, 822, 743, 697, cm^{-1}; ^1H NMR ($CDCl_3$): δ 7.73–7.57 (m, 3H, Ar), 7.50 (s, 1H, Ar), 7.38–7.31 (m, 2H, Ar), 7.25–7.09 (m, 11H, Ar), 5.79 (dd, *J* = 6.9, 6.6 Hz, 1H, 1-H), 5.01 (s, 1H, 2'-H), 1.96–1.68 (m, 2H, 2-H), 0.75 (dd, *J* = 7.5, 7.2 Hz, 3H, 3-H); ^{13}C NMR ($CDCl_3$): δ 171.7, 138.7, 138.4, 137.5, 133.0, 132.9, 128.71, 128.66, 128.5, 128.5, 128.03, 127.98, 127.6, 127.2, 127.1, 126.0, 125.9, 125.5, 124.3, 78.3, 57.3, 29.2, 9.8; HR MS: calcd for $C_{27}H_{24}O_2Na$ ($M+Na^+$) 403.1669, found 403.1659.

Cartesian Coordinates of (*R*)-ts-1, (*S*)-ts-2a, and (*S*)-ts-2b

All calculations were performed with the program package *Spartan '08* 1.2.0 of Wavefunction Inc. (http://www.wavefun.com). All structures were optimized and subjected to frequency analysis with the B3LYP/6-31G* method, followed by single point B3LYP/6-31G* calculation.





Transition Structure (*R*)-**ts-1**

E(B3LYP/6-31G*) = -2130.849673 au

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
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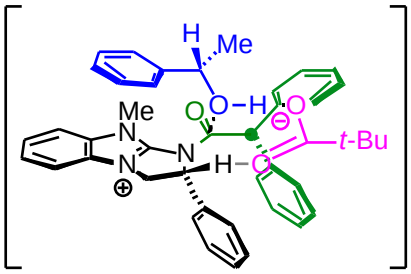
6	1.778256498	0.982956279	0.954376064
1	2.050542248	0.443947329	0.044502145

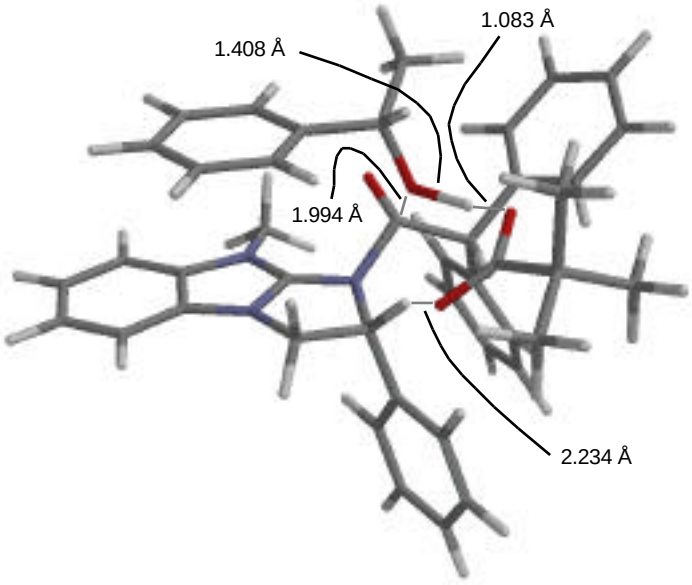
8	-0.288086340	1.033391980	2.245181486
7	-0.542656461	1.123203054	-0.046923500
6	-1.888360557	1.204332767	0.057302302
7	-2.544667833	0.593670500	-0.949410426
6	-1.617724781	-0.100142143	-1.843681138
6	-0.249617977	0.499983416	-1.381172608
6	0.326566610	1.474018882	-2.393116144
6	1.116083612	0.952114997	-3.428021835
6	1.620046704	1.791428348	-4.421596103
6	1.345358755	3.160258326	-4.390807157
6	0.563672038	3.684824183	-3.360705599
6	0.054879624	2.845693398	-2.368507085
1	-0.530242233	3.266975017	-1.556568695
1	0.354728351	4.750607193	-3.322329207
1	1.743514599	3.814719833	-5.161765922
1	2.233503026	1.376287087	-5.217135404
1	1.323940157	-0.115146216	-3.447565030
1	0.422784535	-0.337999479	-1.230865702
1	-1.662643759	-1.177256791	-1.676982022
1	-1.833058280	0.136667316	-2.887111341
8	0.210177092	-1.195418410	0.872221970
6	-0.493024739	-1.822533267	1.911570419
6	-1.814985721	-2.425314395	1.429986117
6	-2.964096804	-2.349540482	2.227394312
6	-4.170809757	-2.919012194	1.813865400
6	-4.247990222	-3.576428890	0.585299025
6	-3.109662020	-3.658365598	-0.221453748
6	-1.906320824	-3.086968052	0.196633442
1	-1.029389550	-3.139698794	-0.441589369
1	-3.158392077	-4.171753067	-1.179384876
1	-5.185098870	-4.020506608	0.258606154
1	-5.050881591	-2.844284093	2.448588023
1	-2.910640878	-1.834805146	3.185229448
1	-0.745998650	-1.049532884	2.657203567
6	0.368454621	-2.881422264	2.625964767
1	1.280804188	-2.412821161	3.007976902
1	-0.176509158	-3.330862980	3.464998025
1	0.657184705	-3.683424246	1.937665301
1	1.137720654	-1.978847390	0.202595150
8	1.897445574	-2.607803518	-0.276902343
6	1.691671287	-2.838463729	-1.554192161
6	2.696726315	-3.832924844	-2.167014529
8	0.790160111	-2.320820406	-2.218864085
7	-2.772851813	1.796382609	0.889659781
6	-3.911245581	0.735187617	-0.771989866
6	-4.061227836	1.498056853	0.404293027
6	-5.320109333	1.842525468	0.884674669
1	-5.445463903	2.419514351	1.794926526
6	-6.424500197	1.403181026	0.150746176
1	-7.422188181	1.652622046	0.498513257
6	-6.272024671	0.642702506	-1.018435903
1	-7.154361859	0.311869459	-1.557559208
6	-5.010022618	0.294844407	-1.502428966
1	-4.888868073	-0.300403358	-2.401112062

6	2.585821928	-5.173619592	-1.408699496
1	3.304372379	-5.895924078	-1.814968787
1	1.582365280	-5.604422270	-1.508837406
1	2.791941873	-5.036528300	-0.343899273
6	2.384898237	-4.038916199	-3.656203010
1	3.088688724	-4.758054830	-4.092437902
1	2.462600630	-3.100177422	-4.214278313
1	1.368301912	-4.418033207	-3.798836797
6	4.123644475	-3.268121956	-1.994995755
1	4.855530028	-3.958372073	-2.432207931
1	4.365768194	-3.131914071	-0.937328151
1	4.234728464	-2.300048409	-2.499307839
6	2.601319935	0.383710106	2.095414129
6	4.225259636	-0.695057955	4.126987022
6	3.531009310	-0.623465969	1.811367420
6	2.496679999	0.844934429	3.415179027
6	3.298616786	0.307047916	4.421579858
6	4.337278469	-1.159543226	2.816729106
1	3.603654094	-1.013710617	0.800980246
1	1.777319220	1.616738236	3.661094299
1	3.198971804	0.674573355	5.439967923
1	5.048854526	-1.944558149	2.573356423
1	4.851484258	-1.111120673	4.912112120
6	2.134386745	2.457544767	0.725151405
6	2.904110252	5.135044759	0.290420169
6	1.556895832	3.500005306	1.463688236
6	3.105326631	2.782013507	-0.231291836
6	3.489080076	4.105208001	-0.447724118
6	1.936292986	4.825754190	1.247125512
1	0.807765460	3.268459676	2.214568067
1	3.564272001	1.988632137	-0.816098939
1	4.242545996	4.329893592	-1.198184630
1	1.475160158	5.618508115	1.831470431
1	3.199573055	6.167324567	0.122270315
6	-2.503309952	2.698181869	2.007878834
1	-1.567221187	3.223305479	1.827727827
1	-2.421463098	2.143315972	2.942255129
1	-3.321818075	3.420726813	2.054215212

Requested basis set is 6-31G(d)

There are 290 shells and 840 basis functions.





Transition Structure (*S*)-**ts-2a**

E(B3LYP/6-31G*) = -2130.839790 au

Cartesian Coordinates (Angstroms)

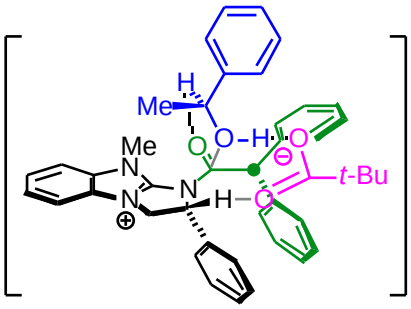
Atom	X	Y	Z
6	-0.065713517	-0.844708523	1.040304407
7	0.768416757	-0.709046802	-0.204484629
6	2.105324556	-0.555220711	-0.114132260
7	2.607450186	0.323106903	-1.008094303
7	3.113586661	-1.114484863	0.591633327
6	1.540248770	0.962381665	-1.777204811
6	0.326273710	0.038235525	-1.431966879
1	-0.503070582	0.684214113	-1.161526052
6	-0.044822879	-0.867804241	-2.592698478
6	0.596803968	-2.087133356	-2.837858932
6	0.268198069	-2.846926698	-3.961057805
6	-0.704600869	-2.395114740	-4.854302284
6	-1.349468767	-1.179977184	-4.616646142
6	-1.022718321	-0.419756902	-3.492650698

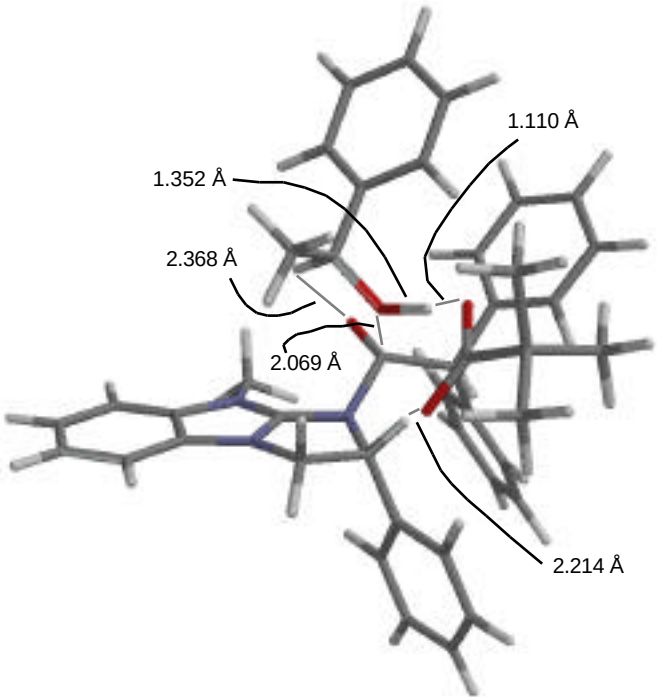
1	-1.513773198	0.532531294	-3.307421973
1	-2.111339076	-0.823119689	-5.305012072
1	-0.961615153	-2.988677393	-5.727840423
1	0.768610754	-3.796076715	-4.133945964
1	1.338445640	-2.461812579	-2.138219309
1	1.385946472	1.987212514	-1.433101170
1	1.768344748	0.948905115	-2.844450043
6	-1.439015676	-1.476839872	0.739177664
1	-1.849185848	-0.978931411	-0.143140685
8	0.567258958	-1.059186025	2.070323889
8	-0.736917391	1.032890849	1.020363960
6	-0.343630822	1.966312139	2.013075299
6	1.104504796	2.428327317	1.815665872
6	2.185611872	1.908733872	2.539583712
6	3.486410696	2.373309208	2.323527993
6	3.732296335	3.369981014	1.377950714
6	2.664876898	3.894812518	0.644684591
6	1.368882789	3.425169359	0.863711004
1	0.539230305	3.834682559	0.290310683
1	2.839708035	4.680199982	-0.087508043
1	4.742995458	3.735594483	1.216114311
1	4.309552505	1.959561587	2.901758484
1	2.008262381	1.136016122	3.280724306
6	-0.665511305	1.509867184	3.442648605
1	-1.734964739	1.292887680	3.513638599
1	-0.422361247	2.301338966	4.163118010
1	-0.126814199	0.601344519	3.716933109
1	-0.957102278	2.866783059	1.833879827
1	-1.893472724	1.554163162	0.409044719
8	-2.780691517	2.043139802	0.027120745
6	-2.580961649	2.646580285	-1.125841266
6	-3.784961776	3.490127424	-1.586300981
8	-1.543844052	2.560130385	-1.785639470
6	4.310346535	-0.518550755	0.148869714
6	3.984767210	0.388817563	-0.880160419
6	4.963271417	1.118982020	-1.545766076
1	4.708597419	1.816649453	-2.336516272
6	6.285888526	0.919792707	-1.145761393
1	7.076944005	1.476062616	-1.639424742
6	6.612942190	0.020653196	-0.120069944
1	7.652210416	-0.107867175	0.166243230
6	5.628523108	-0.713647414	0.546594649
1	5.887736281	-1.401397753	1.344686436
6	-4.017680168	4.607426238	-0.545087183
1	-4.879154553	5.222224129	-0.834497947
1	-3.145396972	5.268316451	-0.470223031
1	-4.209353580	4.184806012	0.445216666
6	-3.495225303	4.101213773	-2.964332817
1	-4.341509451	4.718387193	-3.289146158
1	-3.329859396	3.322106265	-3.715675150
1	-2.597483614	4.725912408	-2.939455783
6	-5.034838320	2.587366014	-1.655858493
1	-5.903886921	3.172169095	-1.981680074
1	-5.257401170	2.149917032	-0.678856355

1	-4.895290324	1.769494068	-2.373660105
6	-1.274646261	-2.959713208	0.373403431
6	-1.110264888	-5.692138967	-0.308969040
6	-0.492271138	-3.844607697	1.131187012
6	-1.972770215	-3.471710582	-0.727707647
6	-1.895232397	-4.823042105	-1.066858192
6	-0.409036358	-5.195907734	0.791499405
1	0.049900068	-3.470723085	1.993188245
1	-2.585222212	-2.803695212	-1.327828338
1	-2.447553641	-5.193354137	-1.926630426
1	0.200676089	-5.864561873	1.394771875
1	-1.047345795	-6.745285178	-0.570294265
6	-2.456148586	-1.307445869	1.866830303
6	-4.430314612	-1.063073042	3.861748534
6	-3.700035270	-0.732230576	1.580237406
6	-2.217266605	-1.764294321	3.170140336
6	-3.193294158	-1.638427297	4.158490939
6	-4.679266725	-0.608454700	2.566826485
1	-3.895675235	-0.351400146	0.582185030
1	-1.256010235	-2.196796716	3.419656393
1	-2.984347244	-1.991252410	5.165511331
1	-5.634502543	-0.151461200	2.321031759
1	-5.190572518	-0.967909237	4.632929870
6	3.050805578	-2.231691812	1.530841961
1	3.984002761	-2.792550692	1.438582544
1	2.214464084	-2.877019406	1.268070602
1	2.912957351	-1.873679864	2.551204122

Requested basis set is 6-31G(d)

There are 290 shells and 840 basis functions.





Transition Structure (*S*)-**ts-2b**

E(B3LYP/6-31G*) = -2130.843832 au

Cartesian Coordinates (Angstroms)

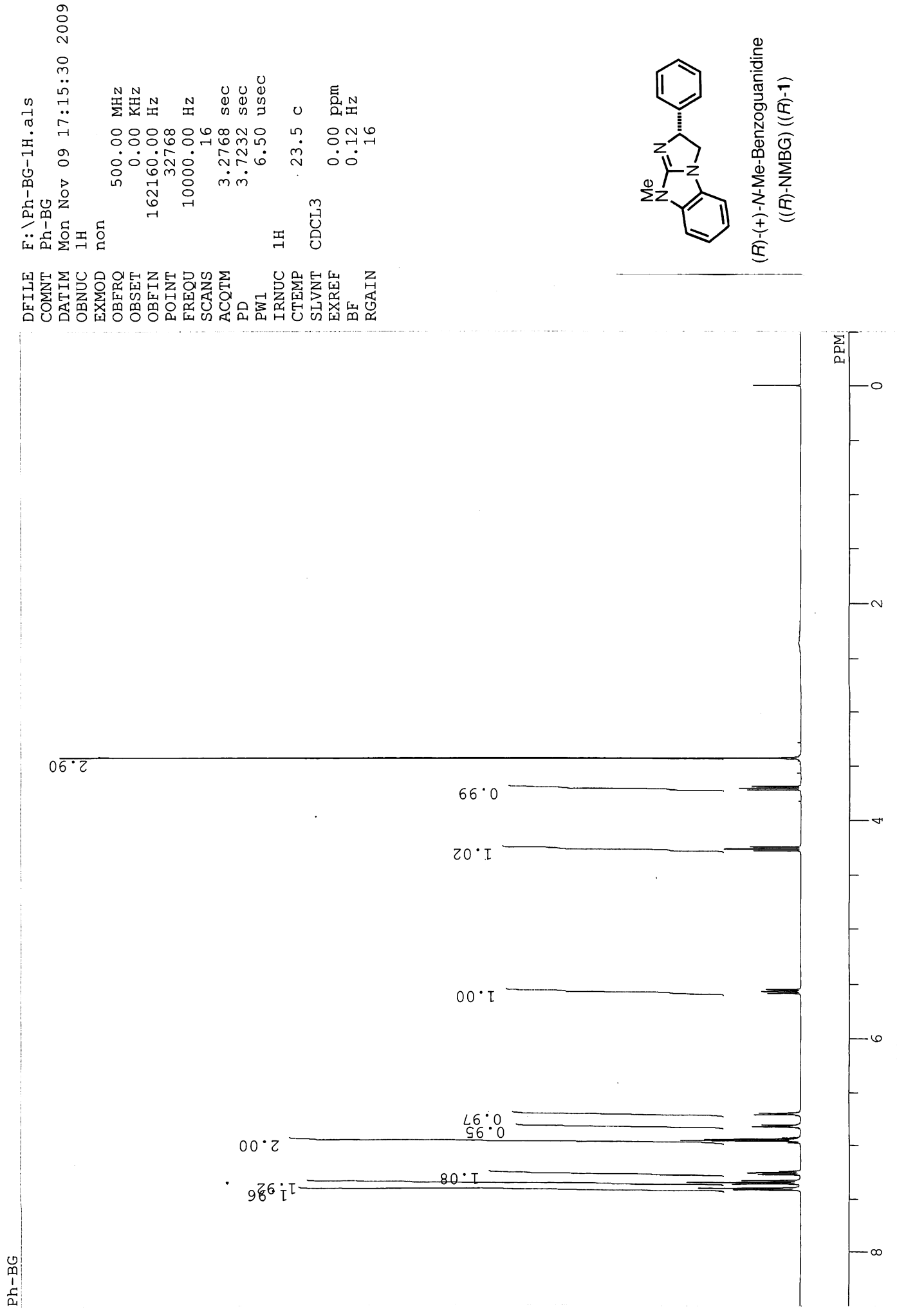
Atom	X	Y	Z
6	-0.264118908	0.158263664	-1.168509813
6	0.568147235	-1.112070016	-1.375512001
1	0.604687965	-1.649796876	-0.425982669
8	-0.363459296	1.061324112	-1.988645261
7	-1.472422673	-0.081081188	-0.316638456
6	-2.365835747	0.921265671	-0.167481557
7	-2.776234524	1.097475315	1.105143036
6	-3.700790194	2.128558866	1.159133484
7	-3.016415476	1.777609209	-0.984782204
6	-2.076581831	0.191671137	2.018206781

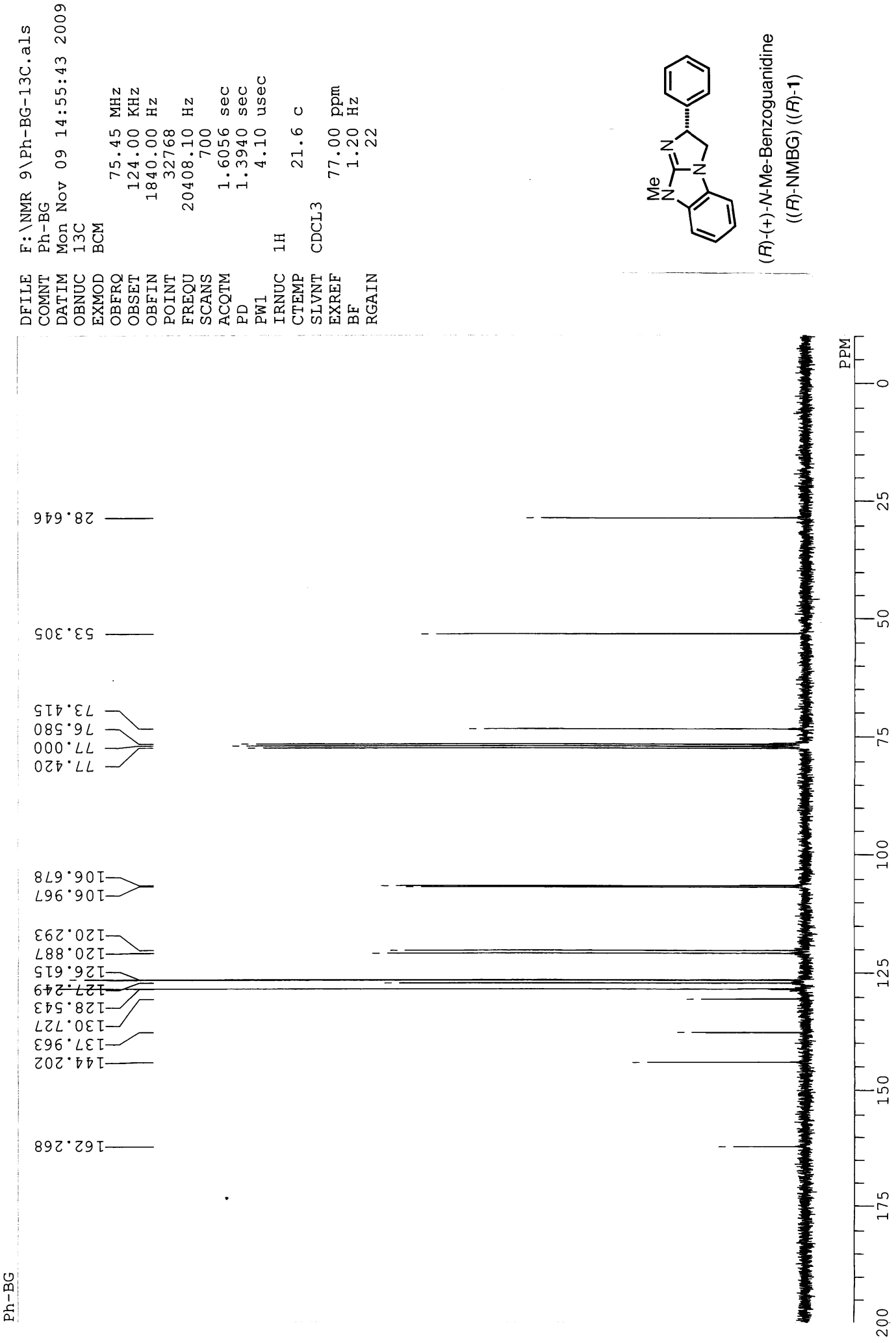
6	-1.393967631	-0.785988238	1.007007850
6	-2.034535755	-2.161550035	0.998448941
6	-3.083447967	-2.509168894	0.141033714
6	-3.664487858	-3.776401915	0.213078781
6	-3.204313264	-4.708580908	1.143976267
6	-2.157782454	-4.367277195	2.003920854
6	-1.575476718	-3.101477345	1.933071463
1	-0.763886103	-2.826907085	2.603290855
1	-1.789453460	-5.088993501	2.728346493
1	-3.654362691	-5.696474885	1.195513292
1	-4.471830188	-4.036825368	-0.466460000
1	-3.426925274	-1.802920062	-0.609185281
1	-0.353635548	-0.855458860	1.305648837
1	-1.330266257	0.723794489	2.610959212
1	-2.784253037	-0.323551306	2.669874339
8	0.830048415	0.923787041	0.411242338
6	0.945329995	2.317571312	0.302035340
6	2.225334544	2.800827708	-0.384909485
6	3.476180011	2.243516748	-0.090067619
6	4.633720620	2.738166960	-0.691723399
6	4.565673220	3.802998086	-1.593285958
6	3.324809989	4.365619284	-1.895620442
6	2.168269525	3.862549284	-1.296670026
1	1.201468385	4.297069219	-1.546040401
1	3.254868135	5.189661805	-2.602796127
1	5.470113867	4.186664111	-2.059532277
1	5.594152797	2.284860130	-0.458540655
1	3.543670240	1.408978213	0.600034964
6	0.810277516	2.981726019	1.688643707
1	0.861236361	4.074305546	1.611340102
1	1.616106769	2.650389460	2.352405235
1	-0.146164561	2.710473116	2.151358616
1	0.111355933	2.678212476	-0.325236047
1	1.641554733	0.315738220	1.304978105
8	2.371285529	-0.165175880	1.989825908
6	1.855543645	-0.731574026	3.053200104
6	2.914422271	-1.311852537	4.012429885
8	0.645363949	-0.826624852	3.280742404
6	-3.847607125	2.572608114	-0.172123551
6	-4.411359545	2.707723195	2.205791878
1	-4.291963825	2.364937787	3.228201636
6	-5.275823938	3.754277183	1.879963947
1	-5.843571115	4.236180579	2.670063573
6	-5.422363157	4.199193700	0.557356734
1	-6.101567393	5.018514638	0.343256482
6	-4.708662031	3.616472295	-0.492971398
1	-4.817528187	3.971944881	-1.512104280
6	3.894834479	-0.191823593	4.420137586
1	3.376407392	0.614028839	4.953677862
1	4.383397938	0.240828770	3.543153499
1	4.668987568	-0.592222195	5.086526266
6	2.229086144	-1.894644216	5.257113033
1	1.683169265	-1.121637431	5.807723289
1	2.976296239	-2.335125542	5.928543183

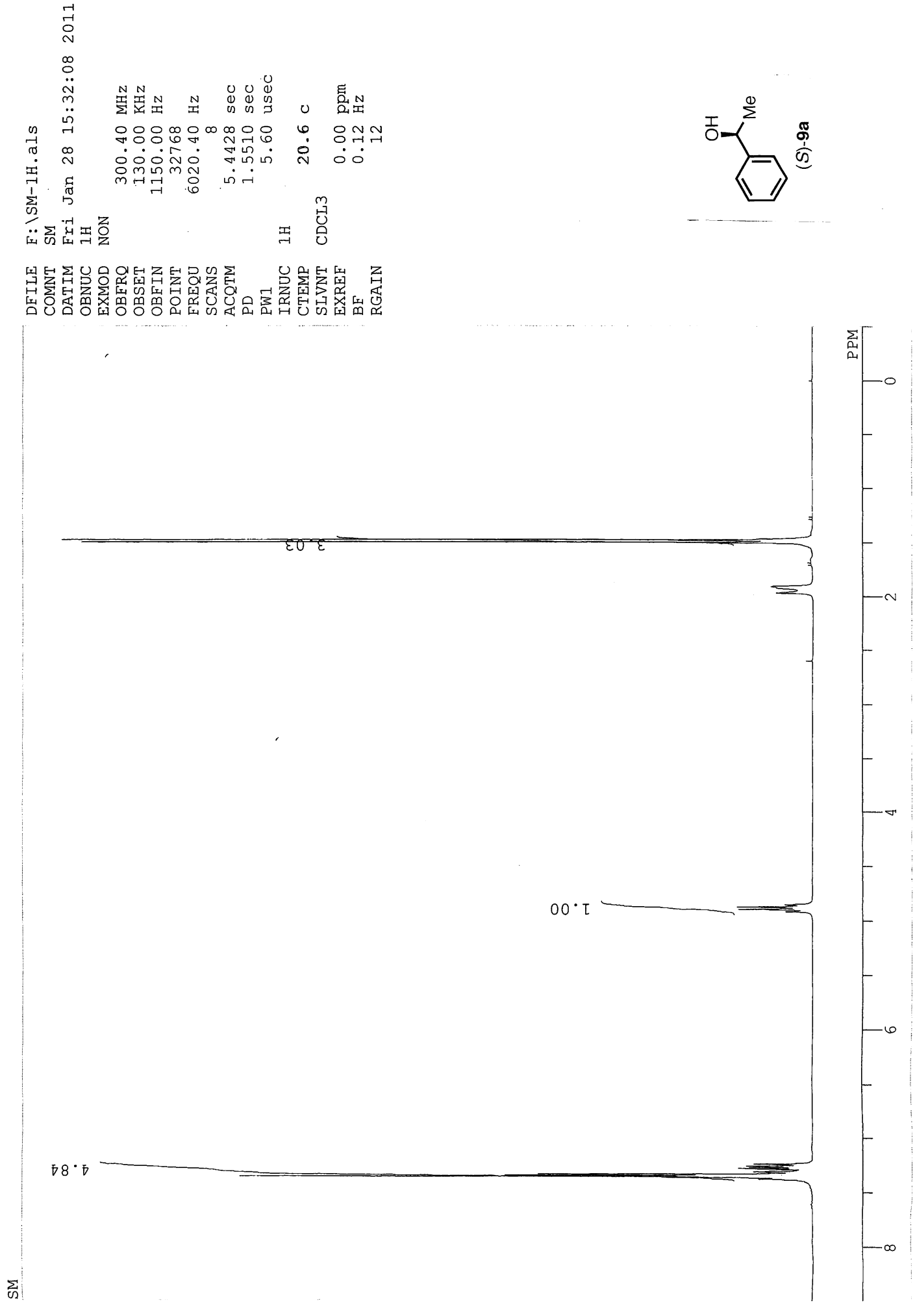
1	1.508263090	-2.673050830	4.987516455
6	3.686516015	-2.420735956	3.262889983
1	3.015820152	-3.233036039	2.955017291
1	4.455906987	-2.850716293	3.915572396
1	4.172038400	-2.021542925	2.367557424
6	-0.155364462	-2.025109313	-2.379069935
6	-1.389322304	-3.767179947	-4.218663444
6	-0.529169168	-1.573866380	-3.653781020
6	-0.414144662	-3.359416154	-2.043070321
6	-1.022371869	-4.225502951	-2.953849662
6	-1.142370109	-2.436119290	-4.562710623
1	-0.337766694	-0.543162460	-3.933988867
1	-0.144905226	-3.725805079	-1.055665675
1	-1.210200599	-5.257424772	-2.668781483
1	-1.420578461	-2.067551531	-5.547167224
1	-1.861888160	-4.438876219	-4.930613100
6	2.014229963	-0.872854548	-1.802689235
6	4.698884110	-0.659523349	-2.624701991
6	2.383250539	0.032625244	-2.805916803
6	3.011641506	-1.662548507	-1.216734559
6	4.342143775	-1.561020026	-1.621949201
6	3.714543663	0.138409155	-3.208188956
1	1.636403247	0.681440749	-3.246718651
1	2.746052491	-2.364046970	-0.429456981
1	5.097483458	-2.183420550	-1.148777966
1	3.983423947	0.860569069	-3.974455562
1	5.734823443	-0.573589608	-2.942259204
6	-3.004571436	1.818597830	-2.446244033
1	-2.693359638	0.849312680	-2.829710241
1	-2.306019272	2.575329248	-2.805332327
1	-4.021479023	2.040873284	-2.780950073

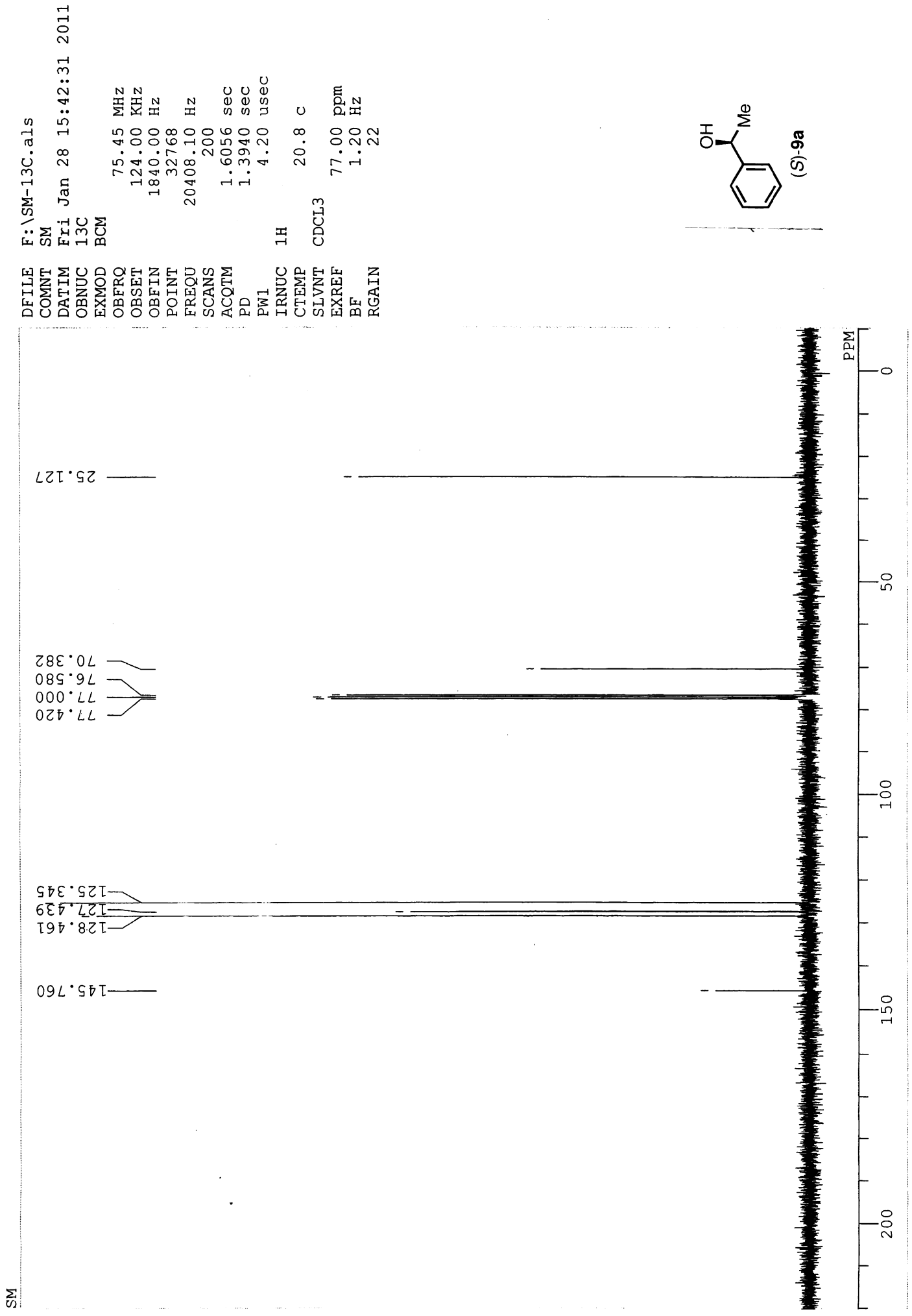
Requested basis set is 6-31G(d)

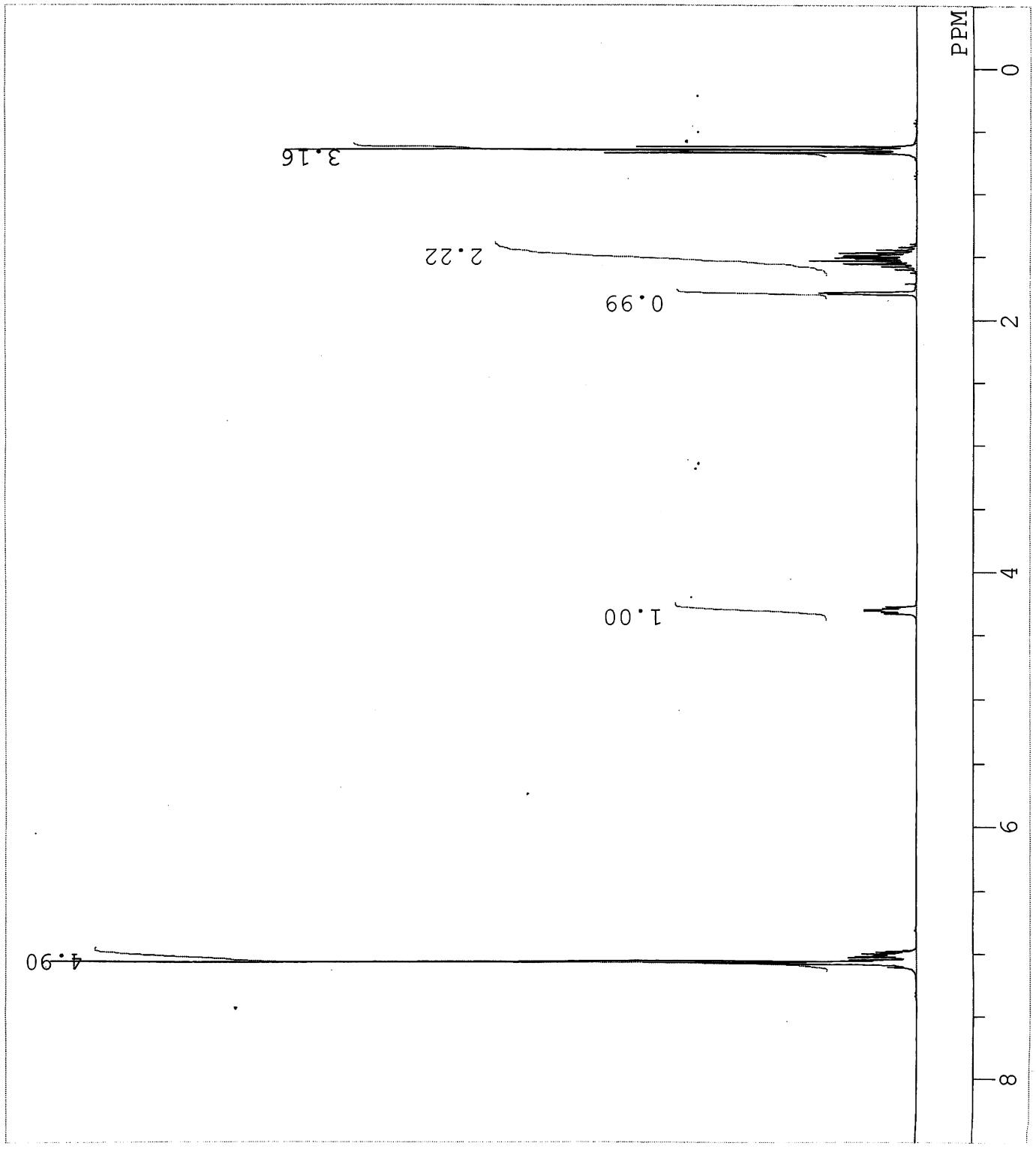
There are 290 shells and 840 basis functions.

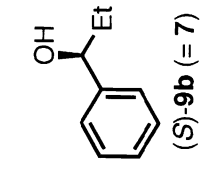




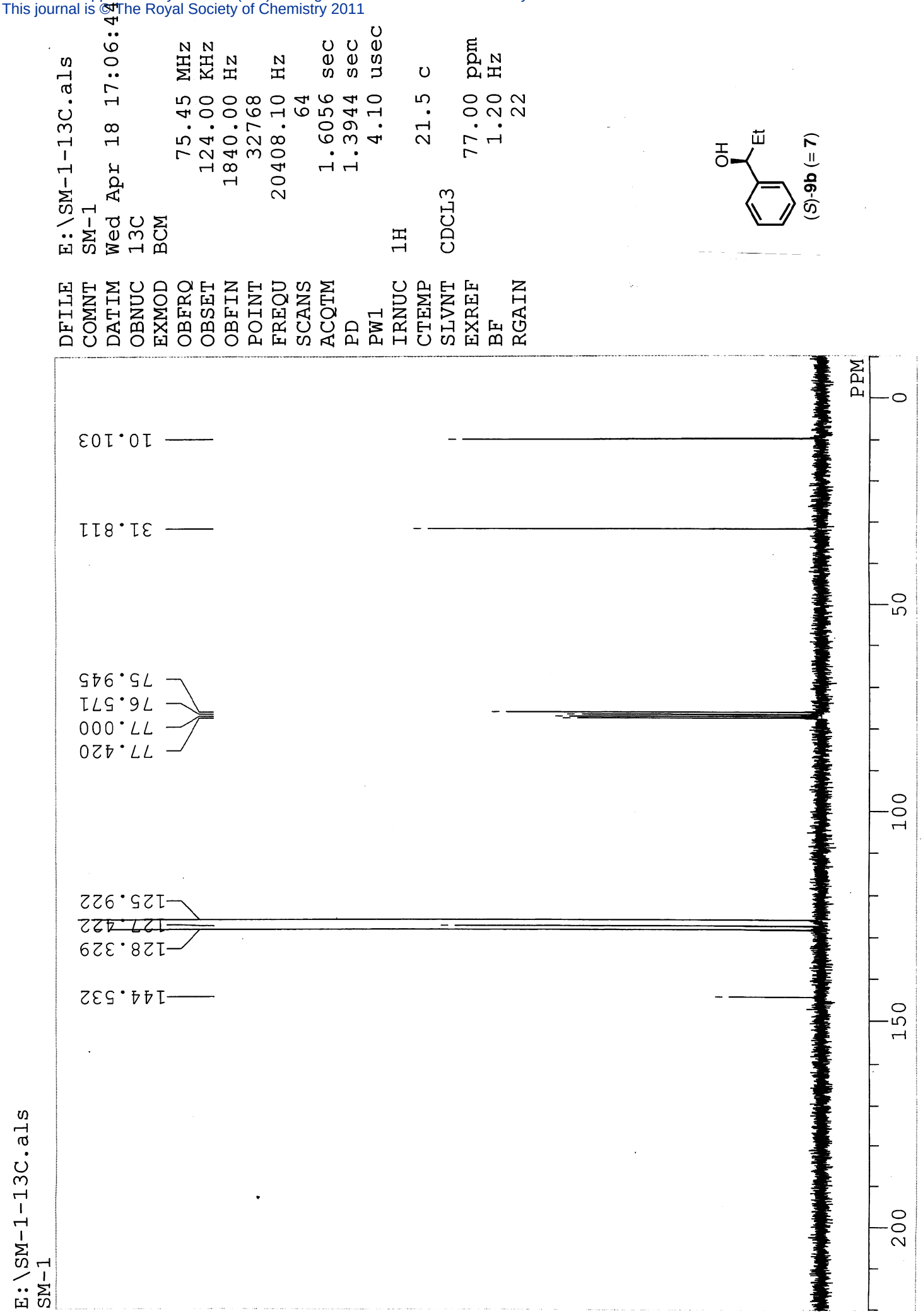


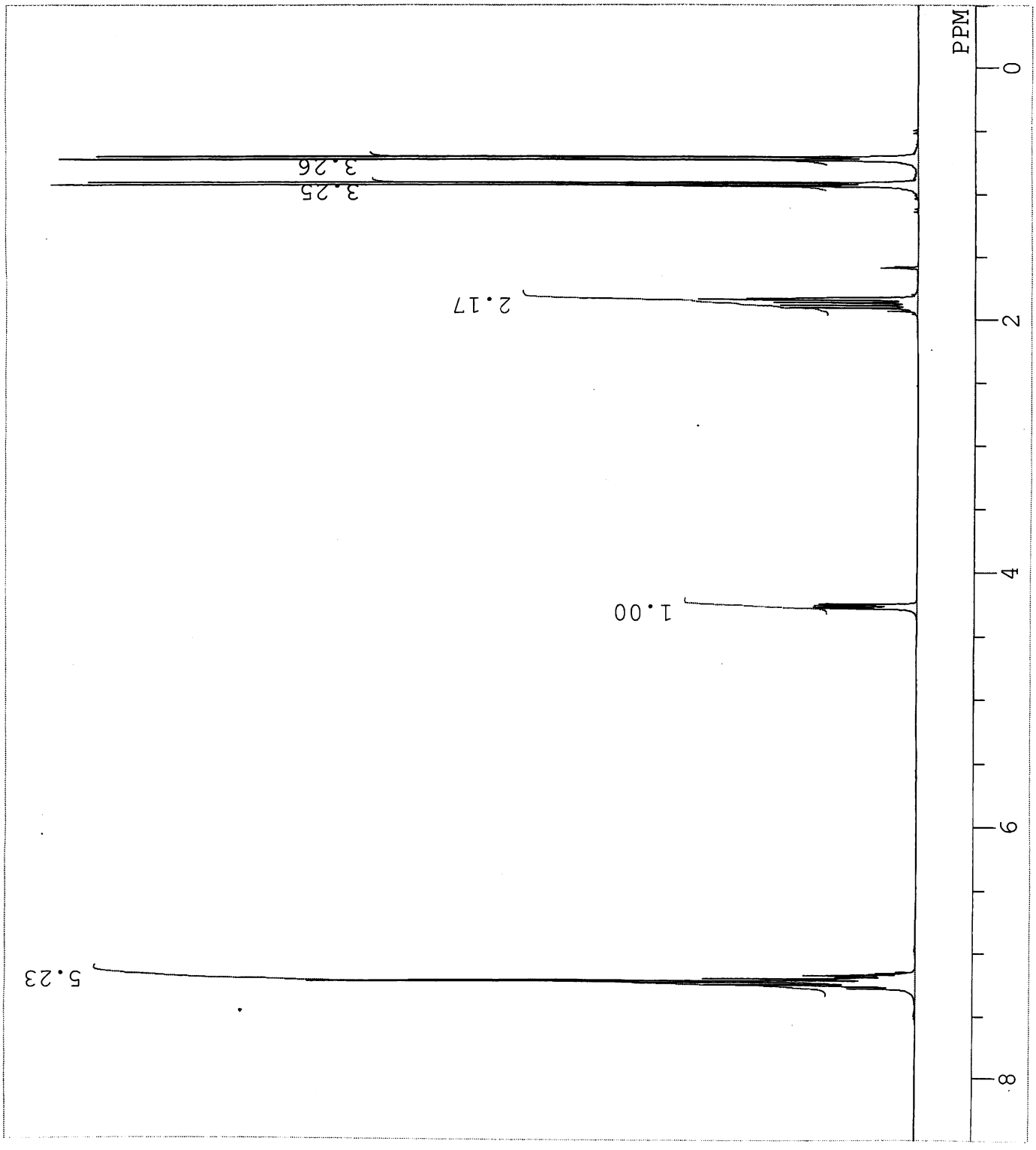


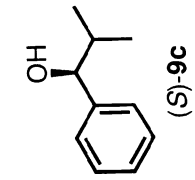




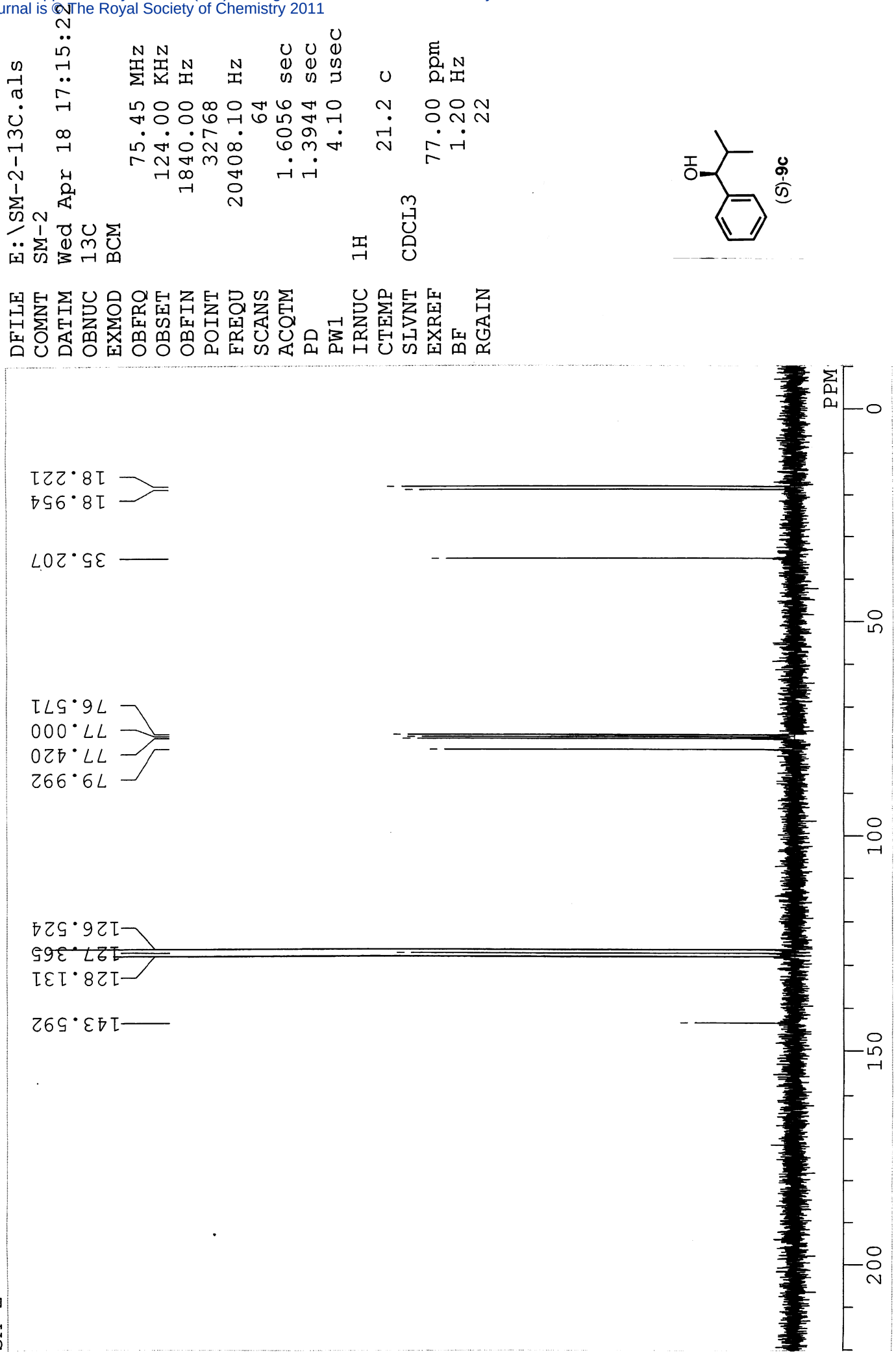
(S)-**9b** (= **7**)







(S)-**9c**



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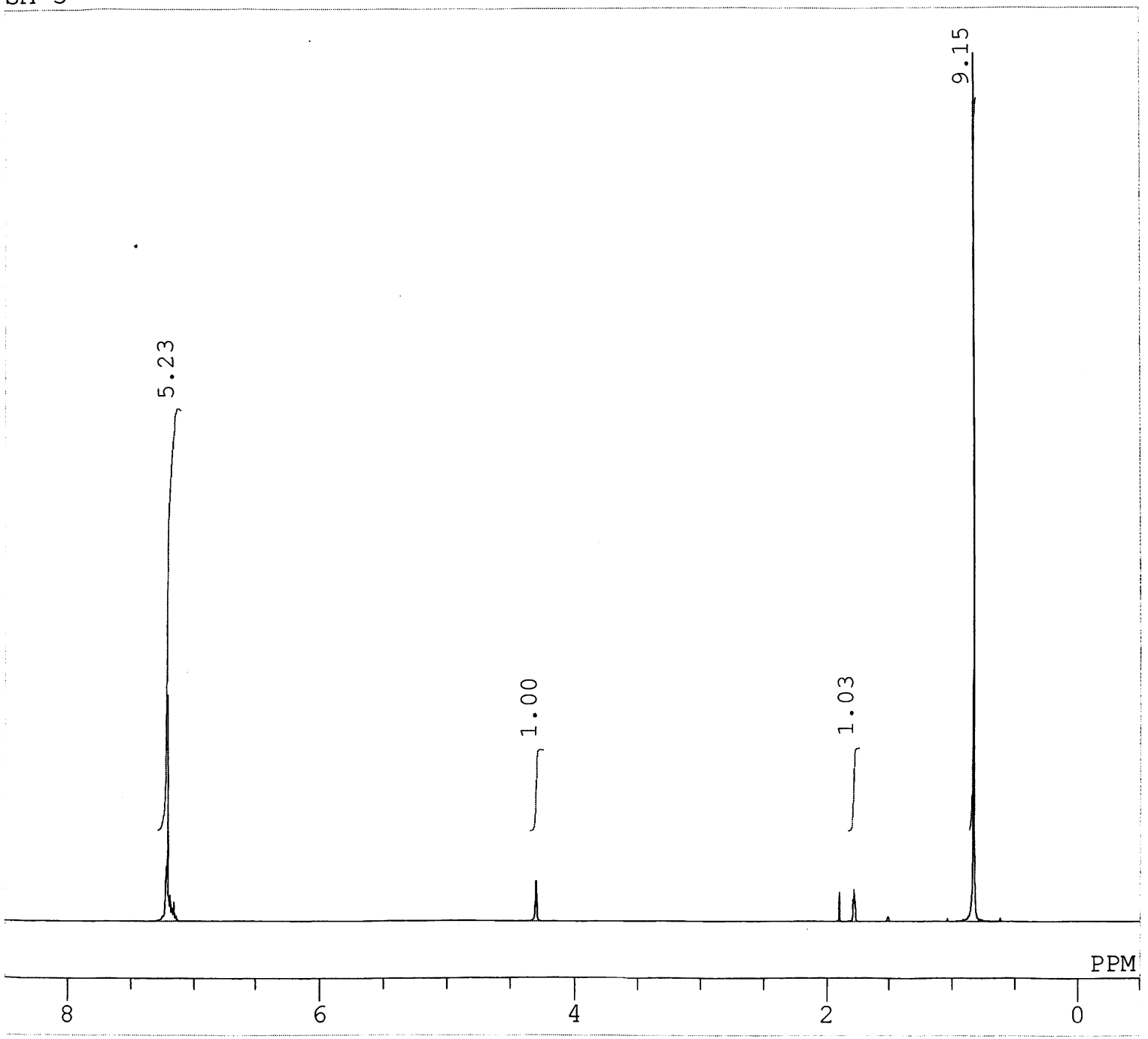
SM-3



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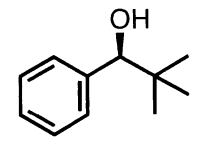
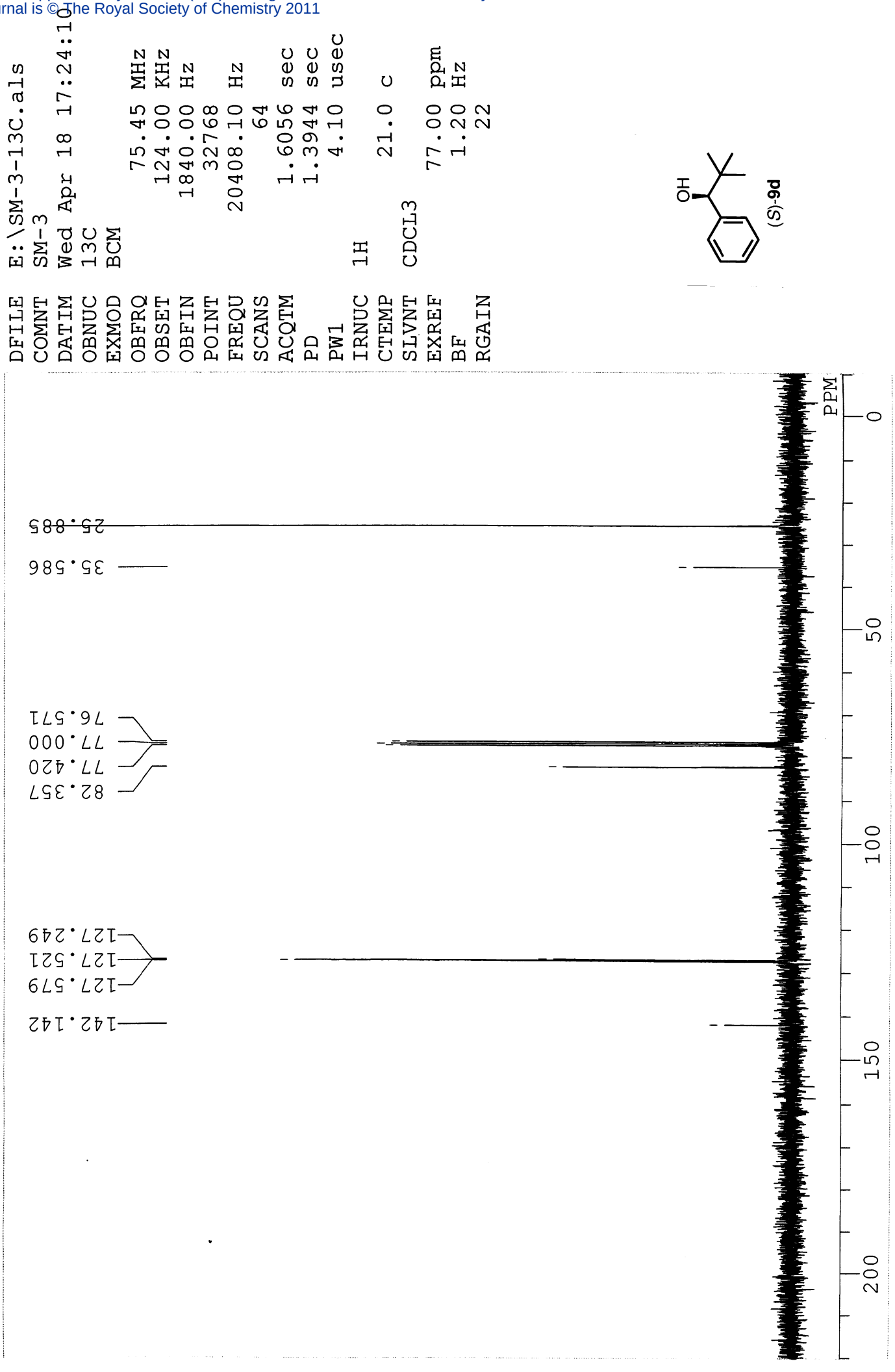
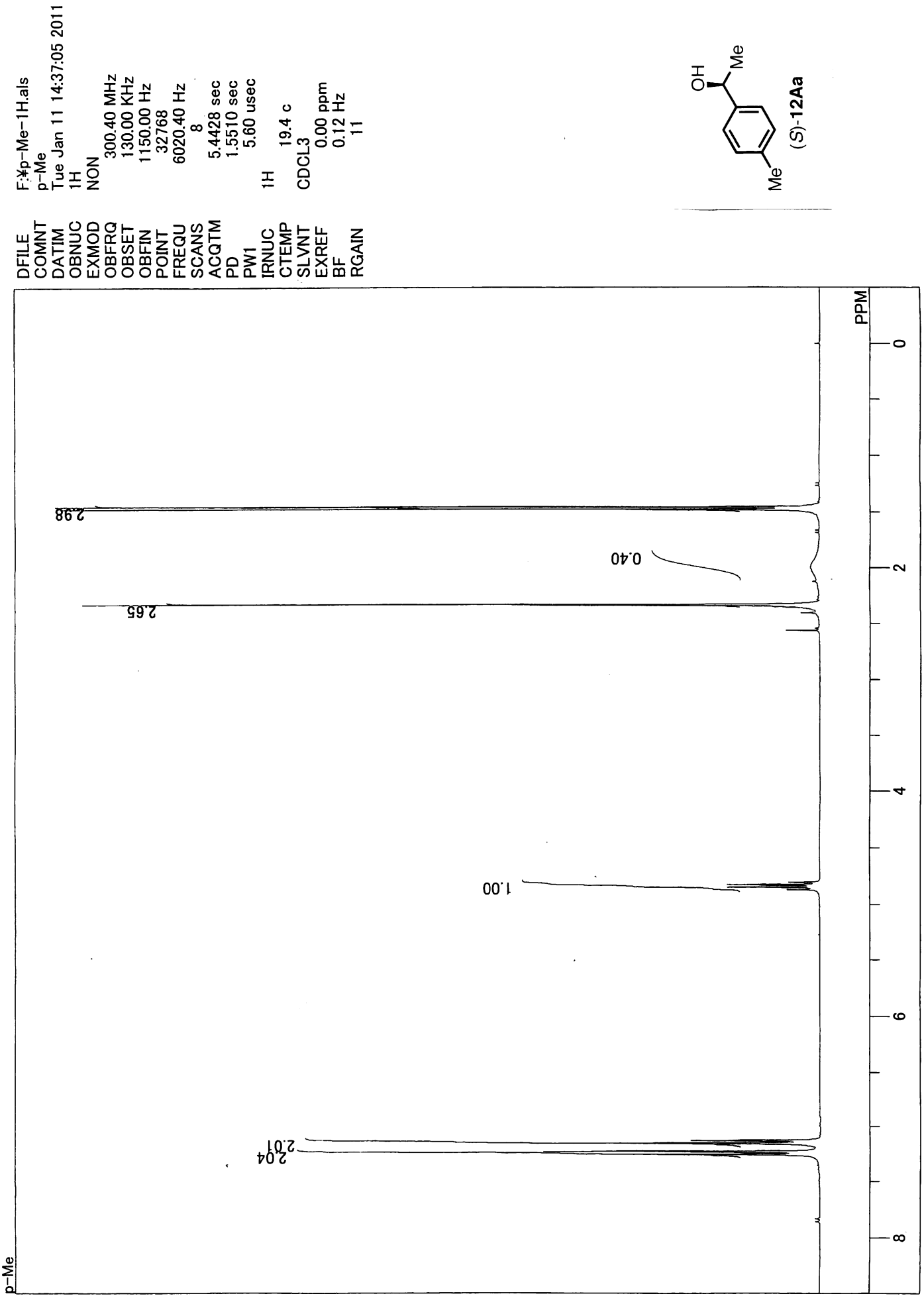
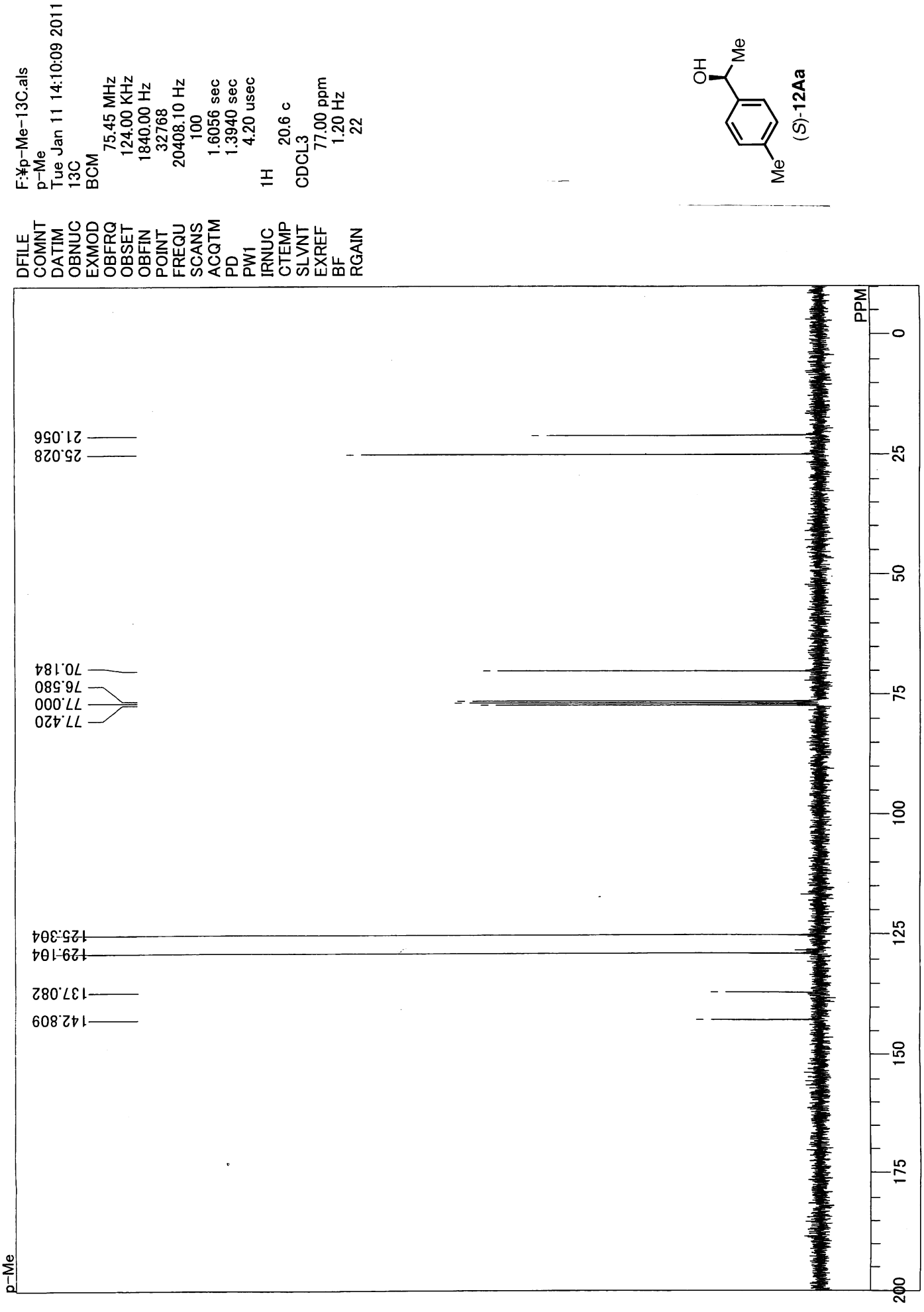
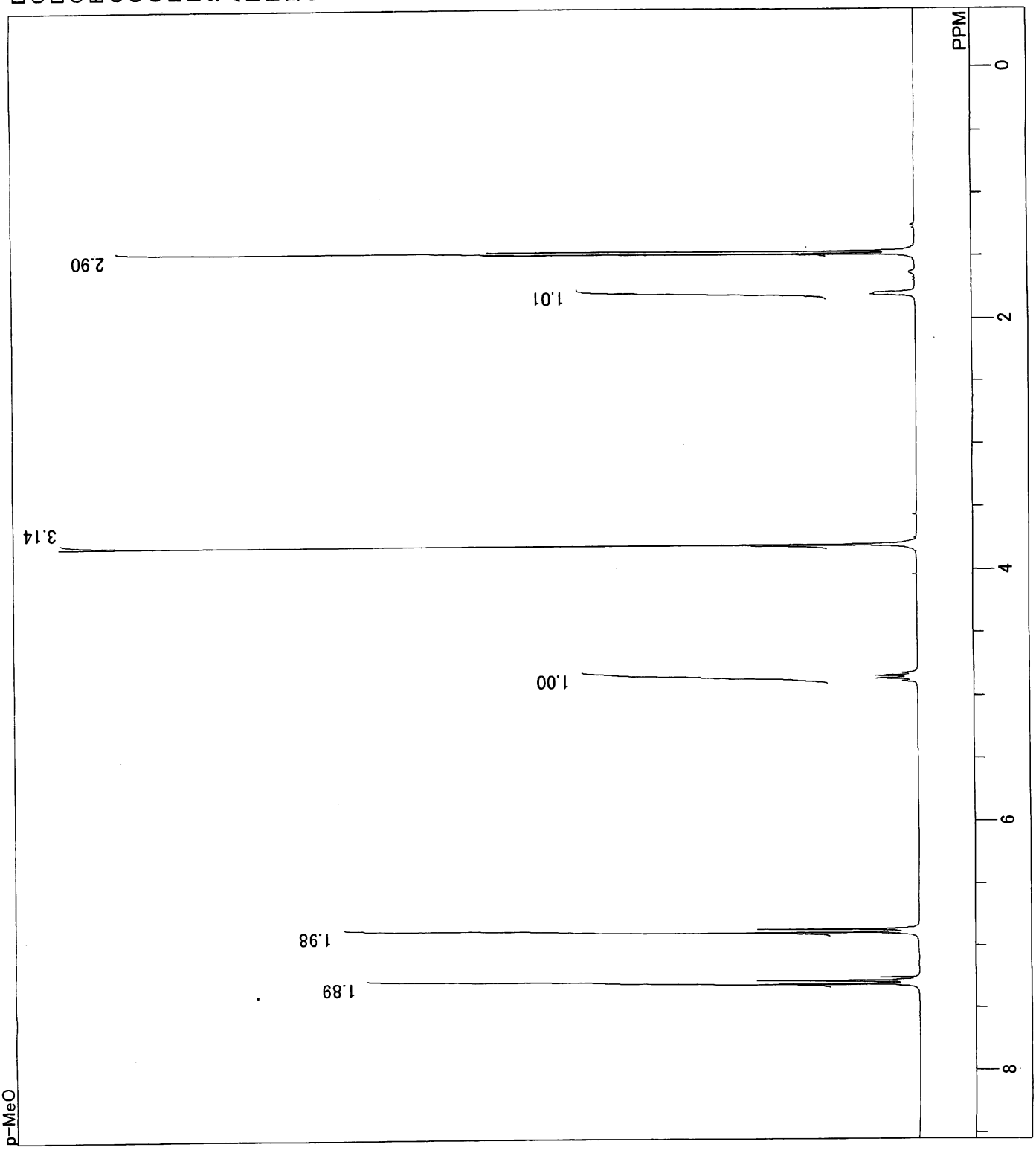


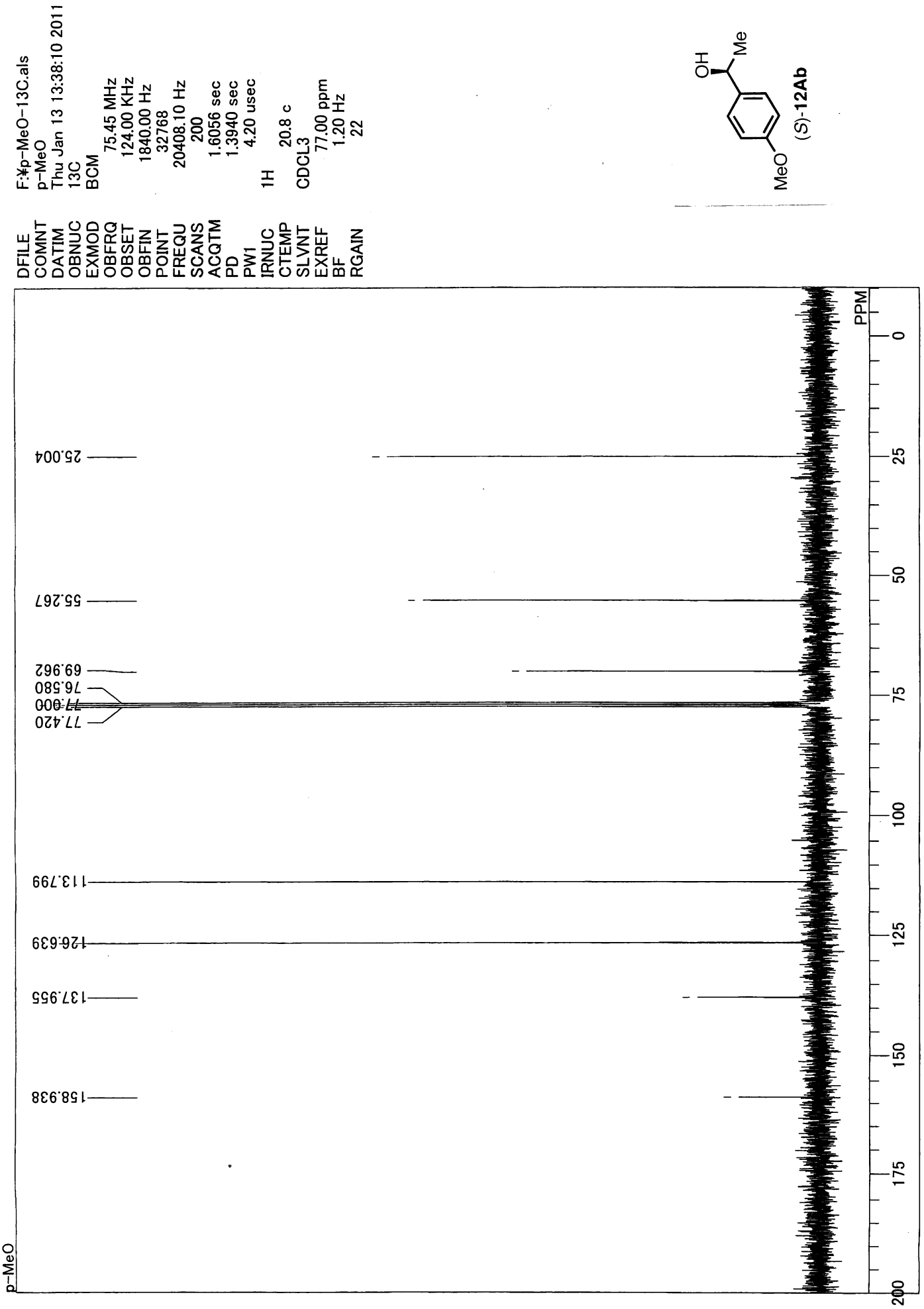
(*S*)-**9d**

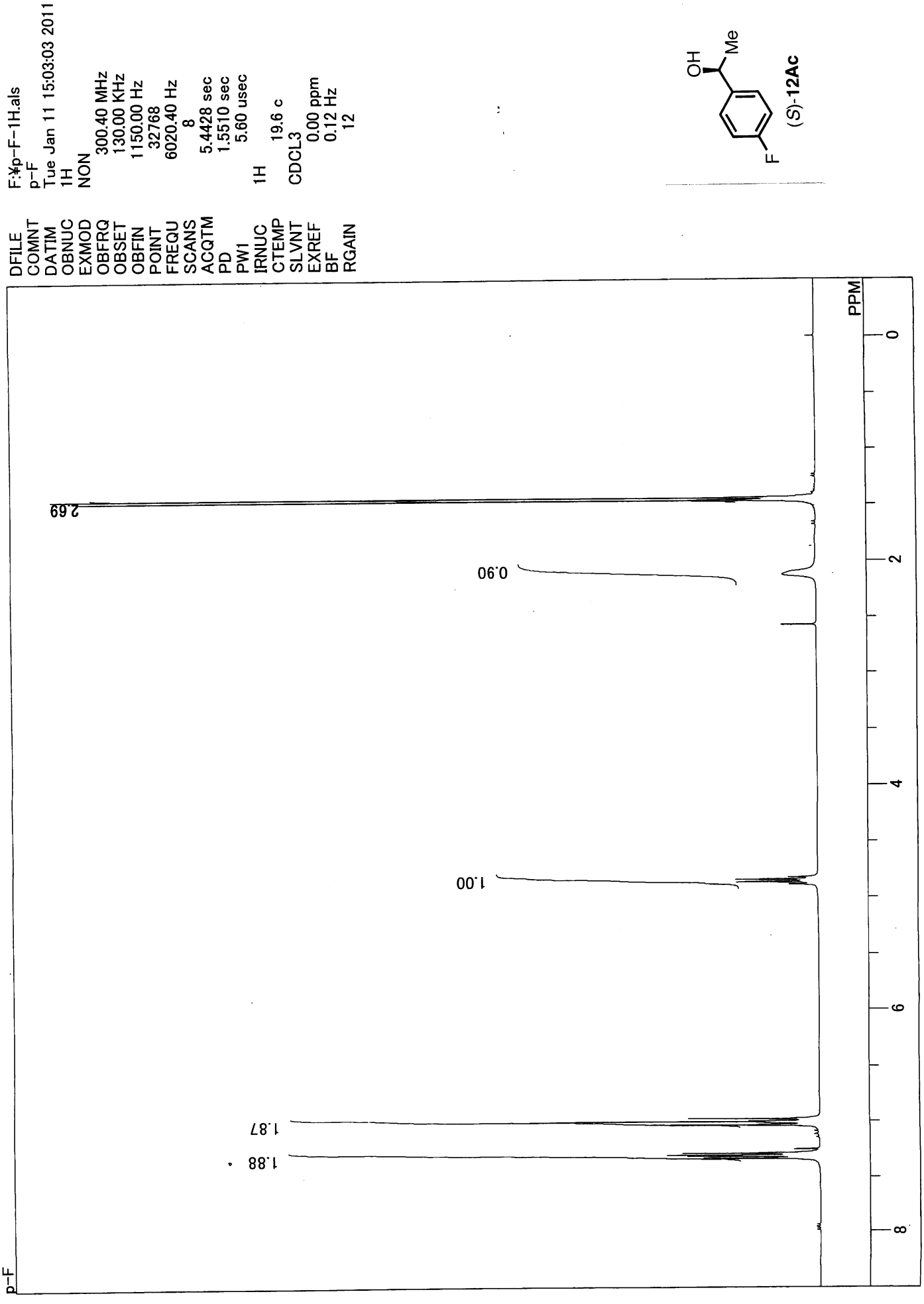


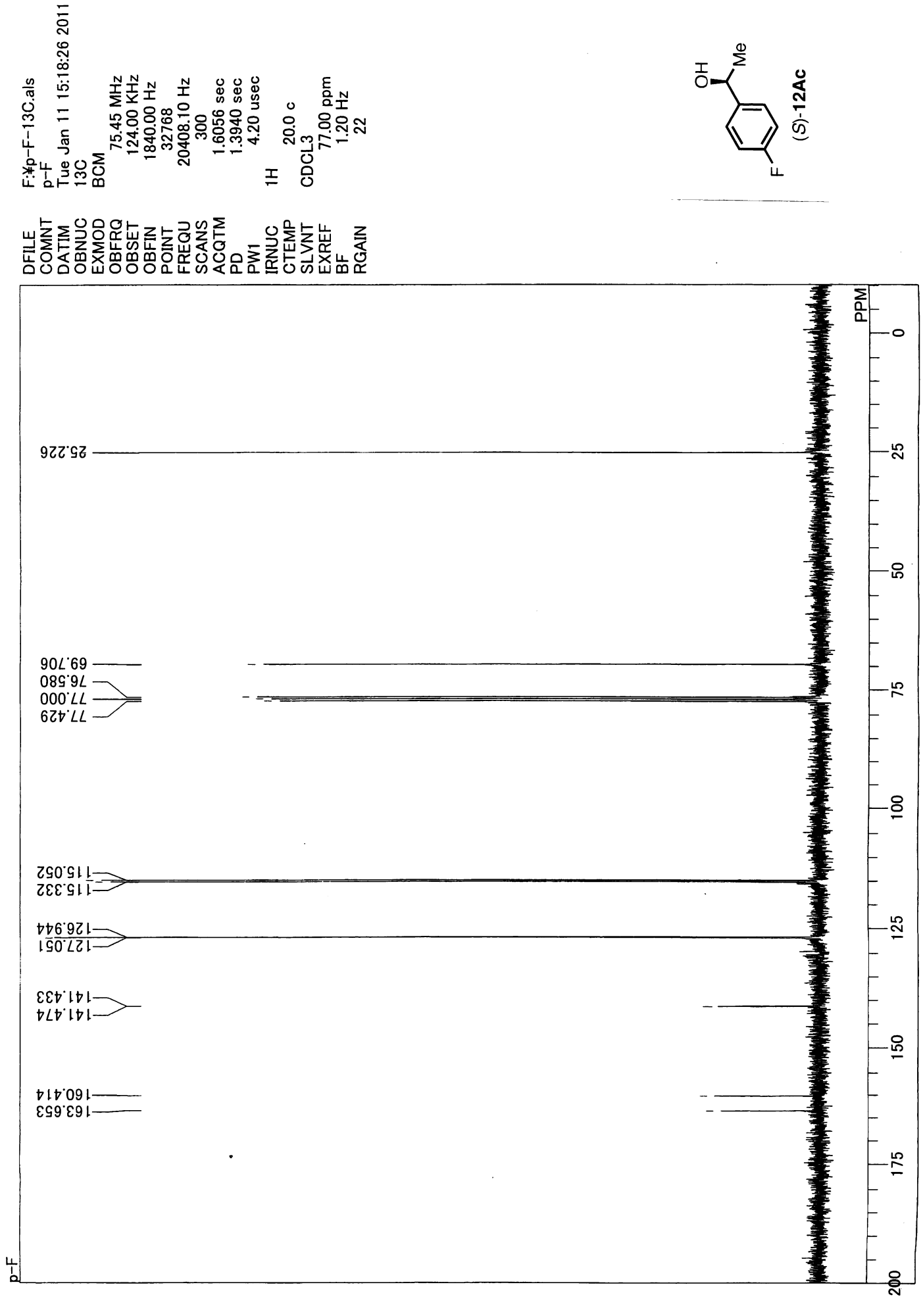


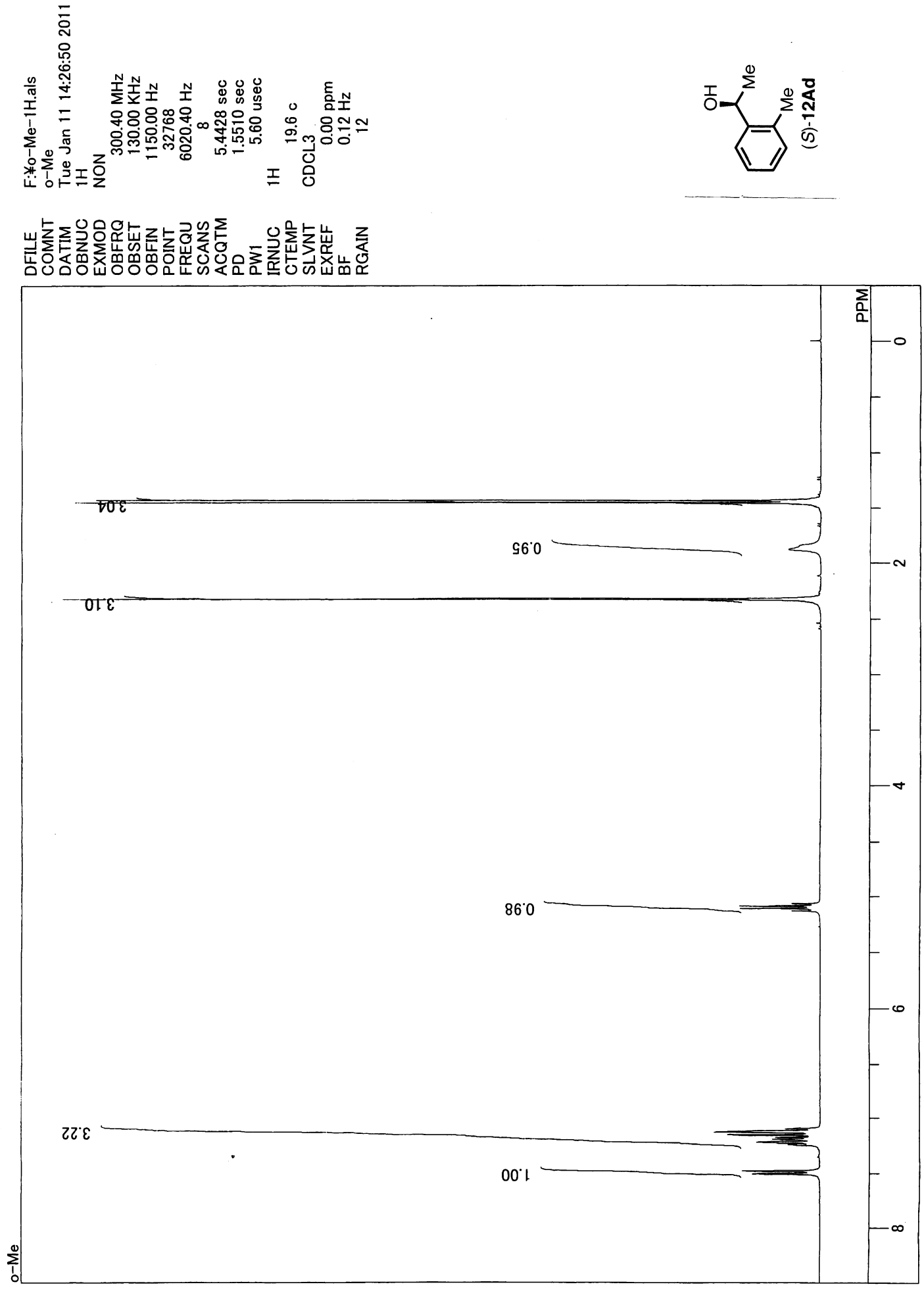


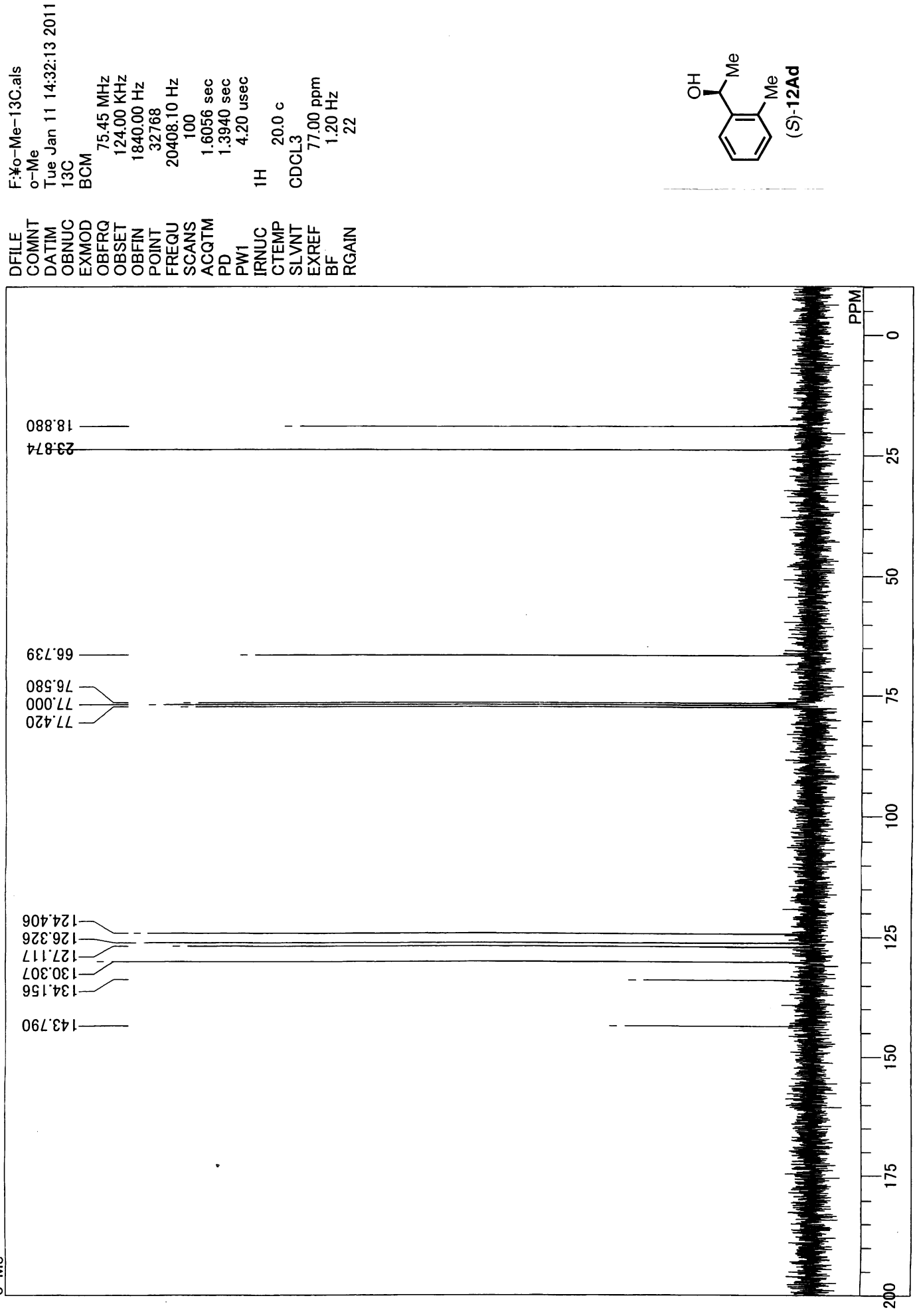


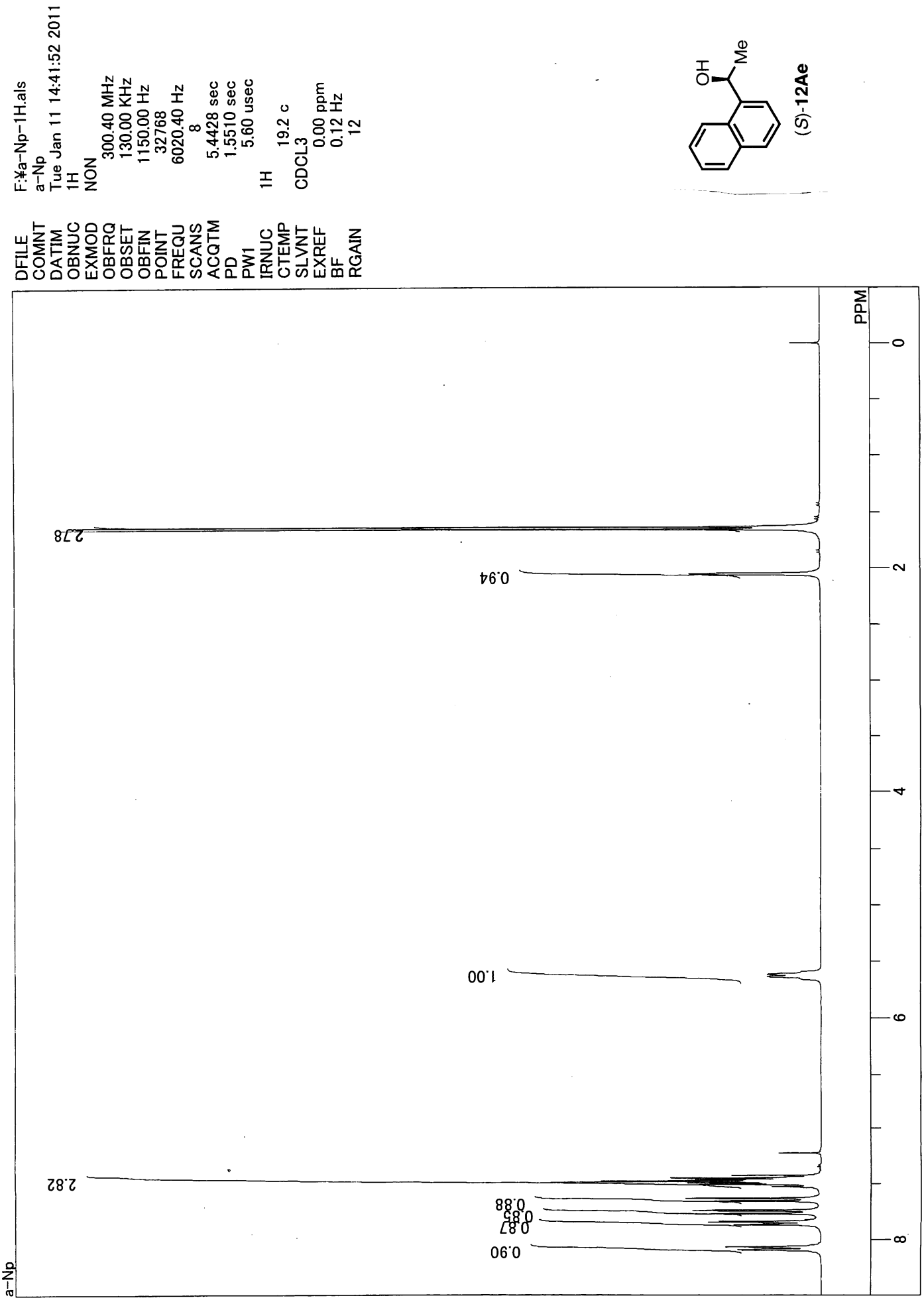


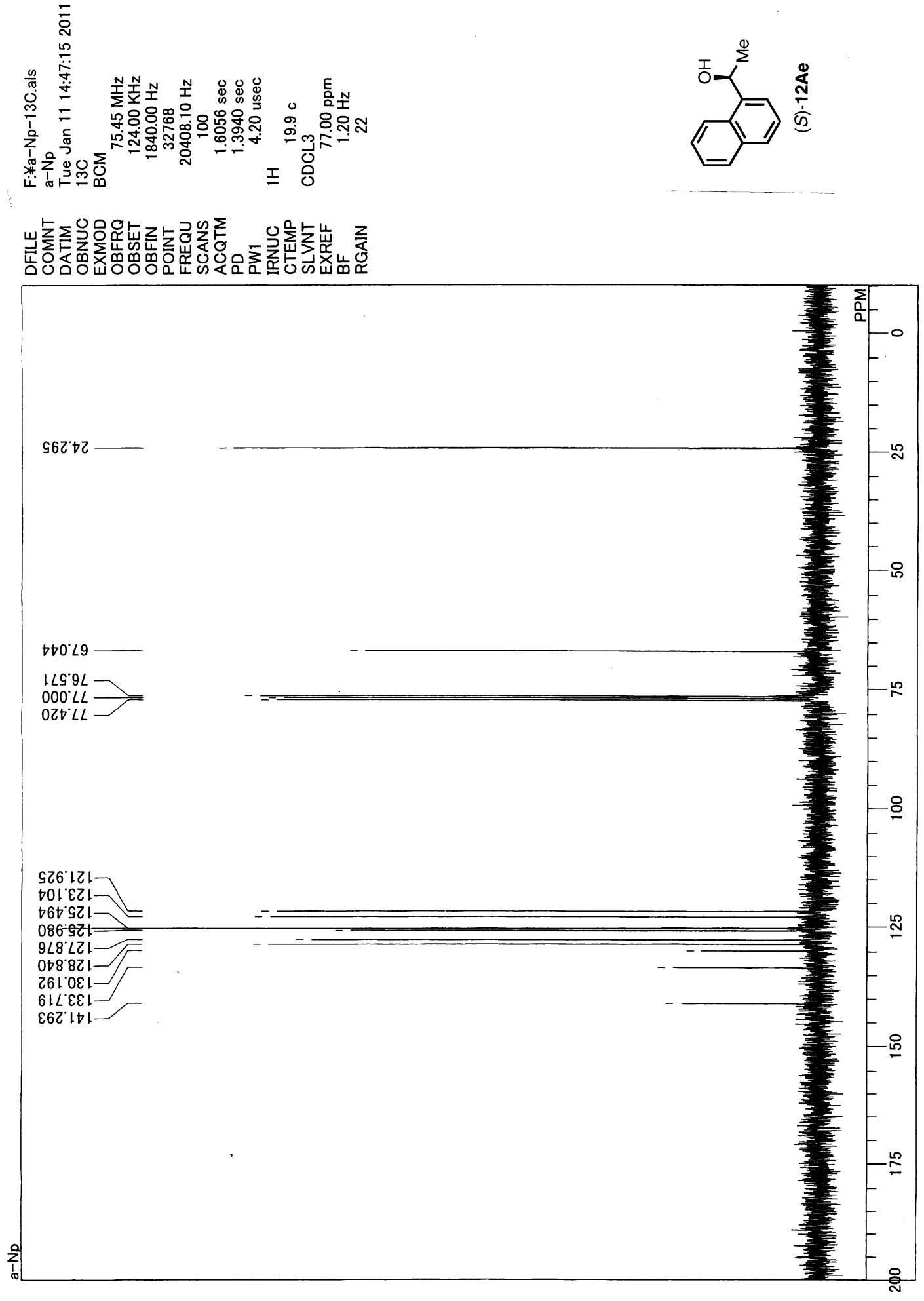


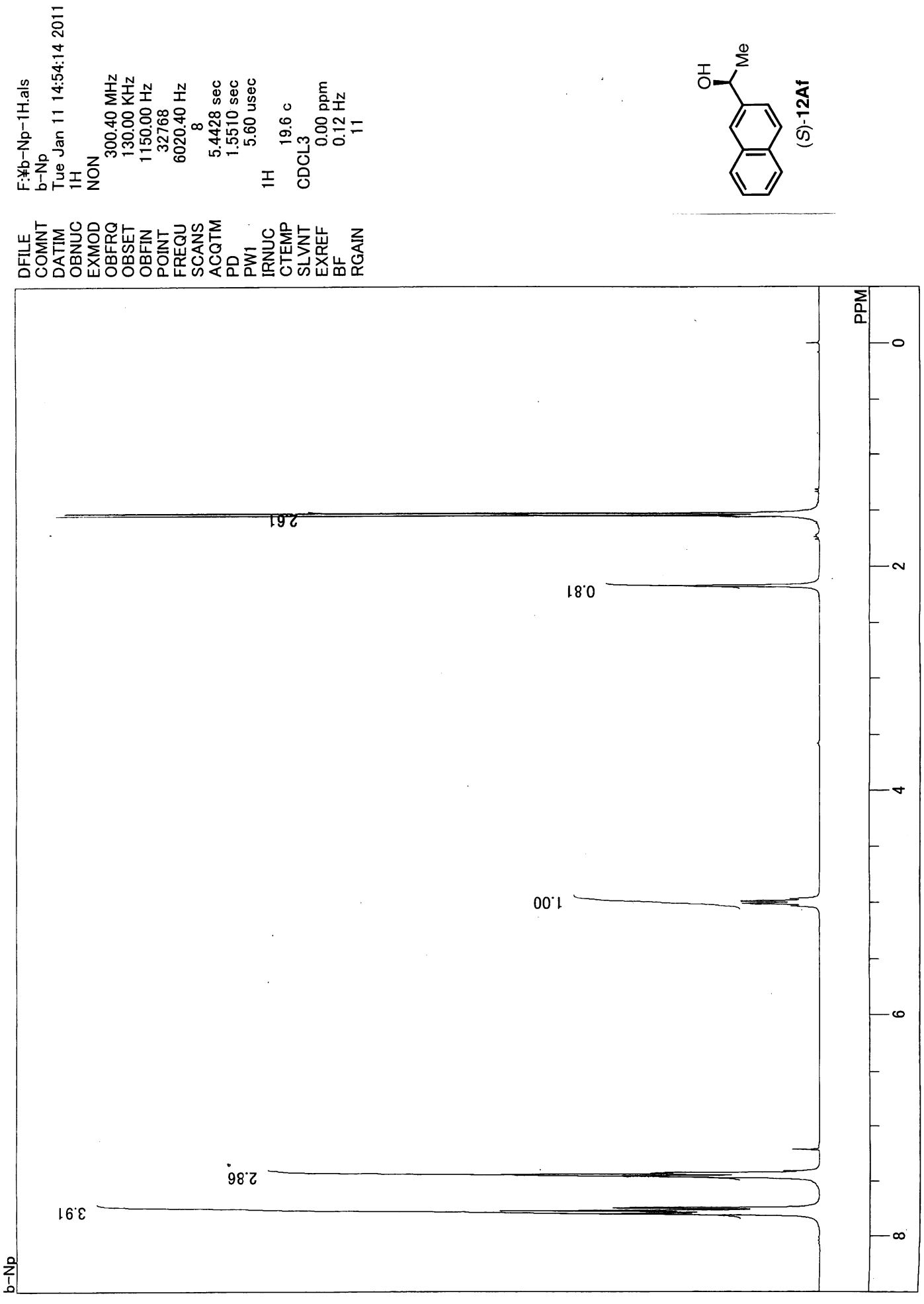


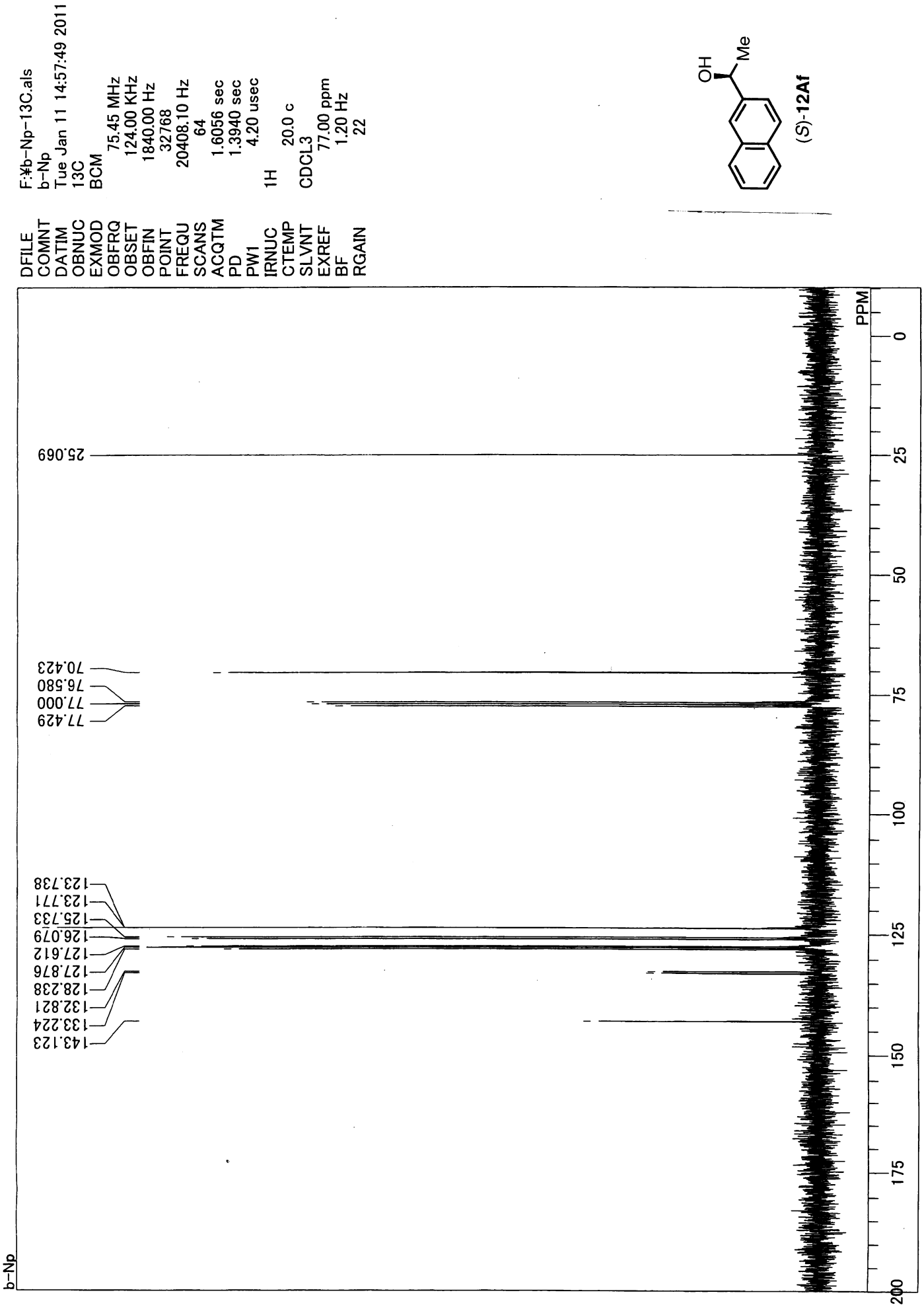


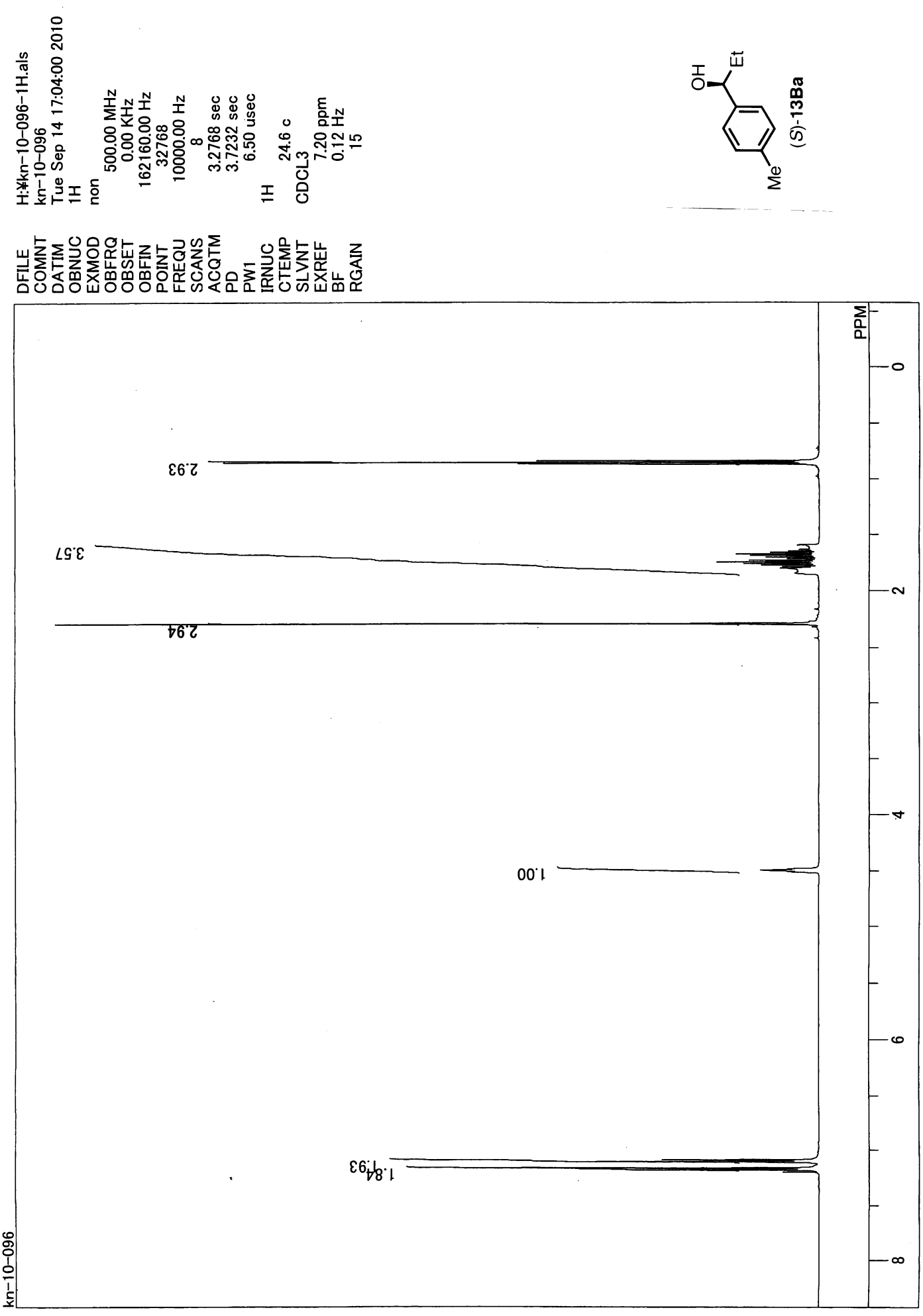


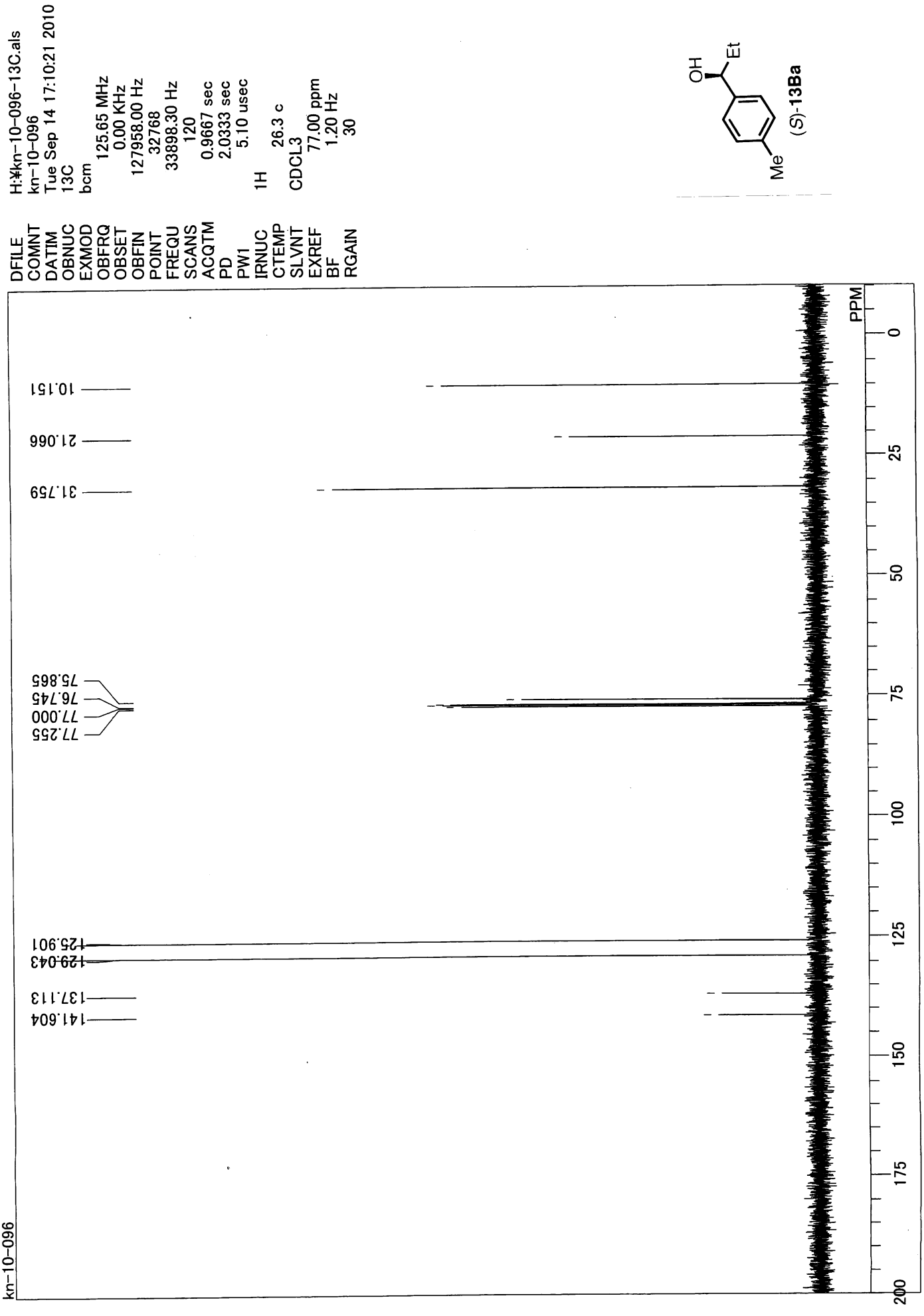


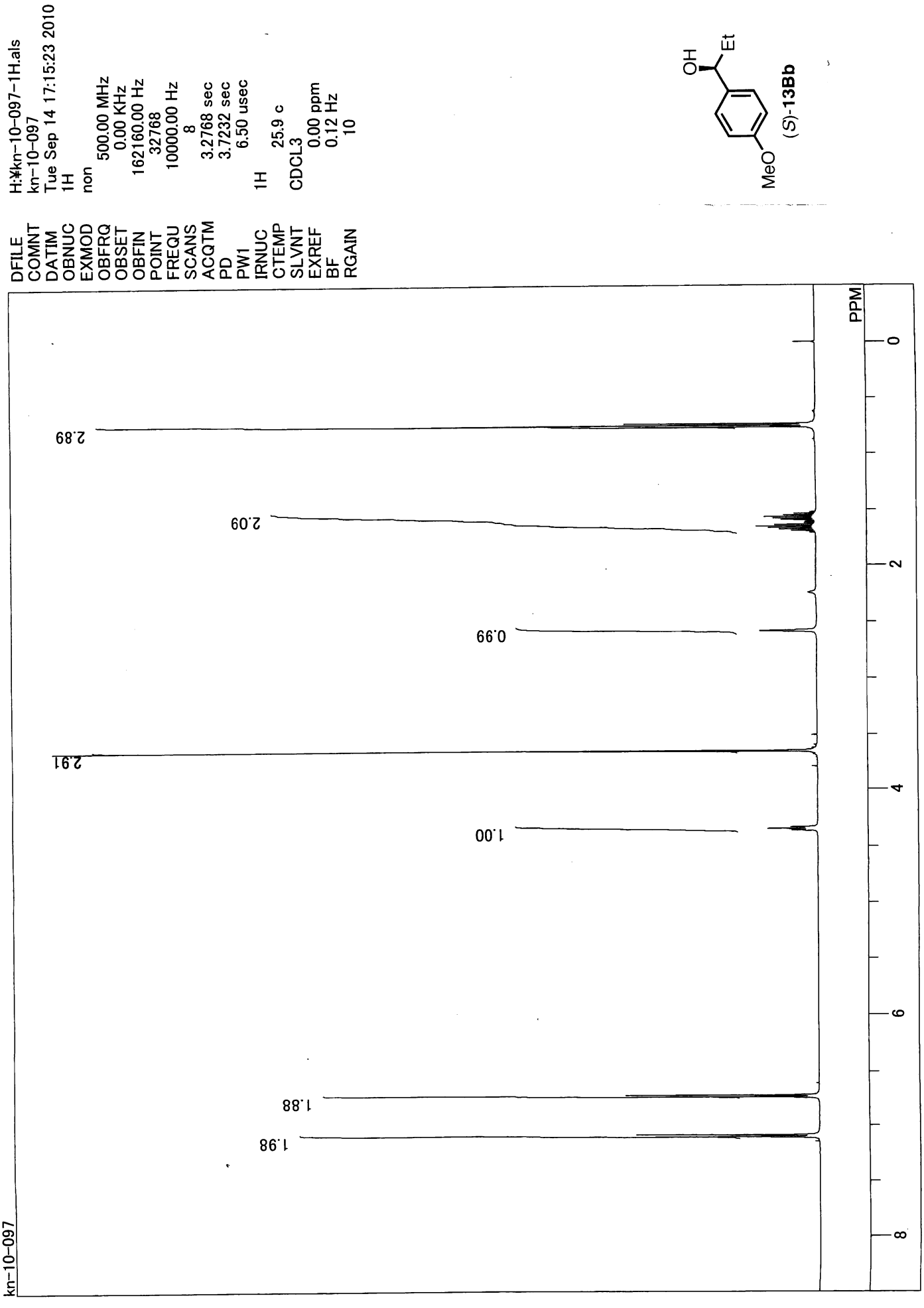


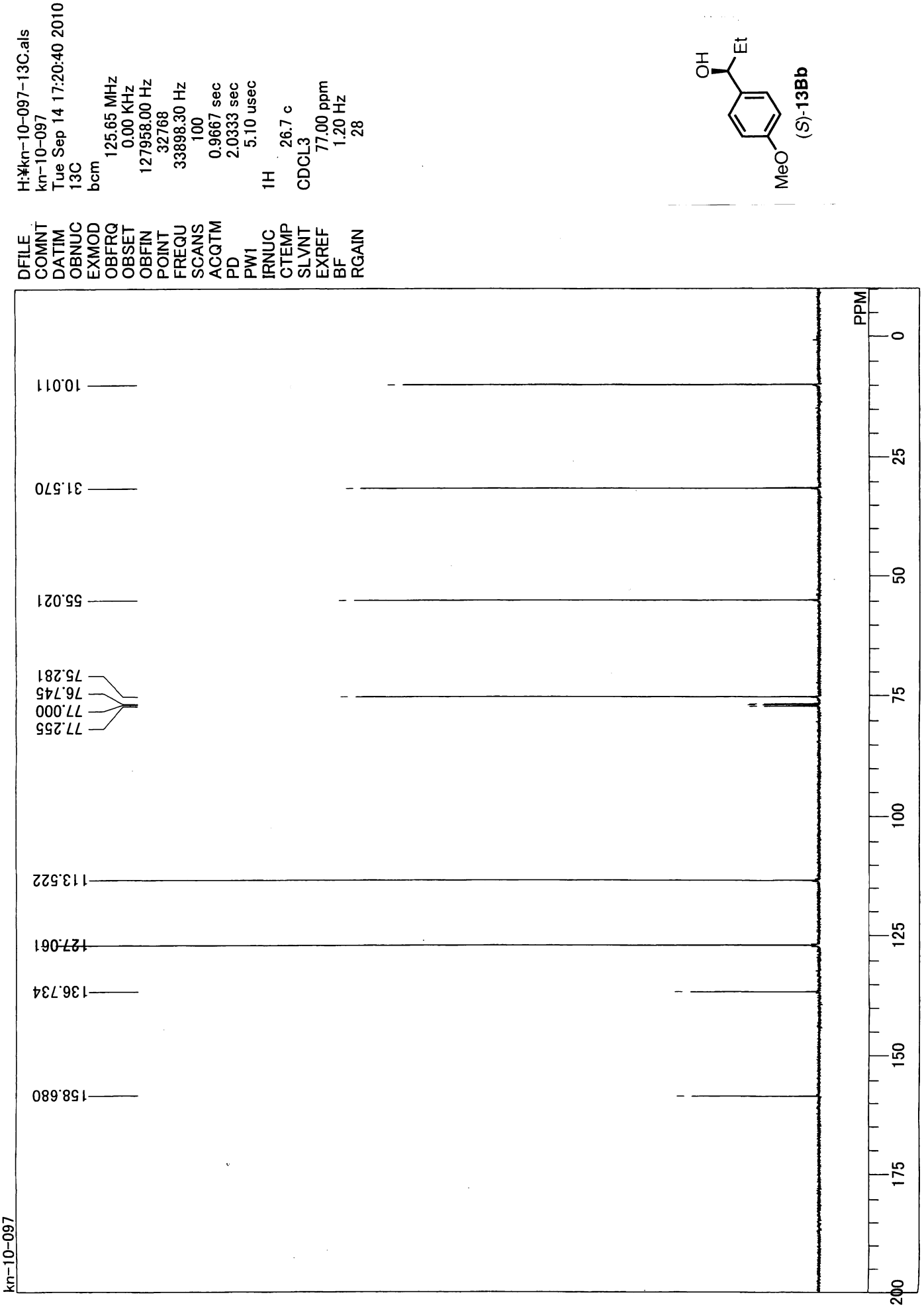


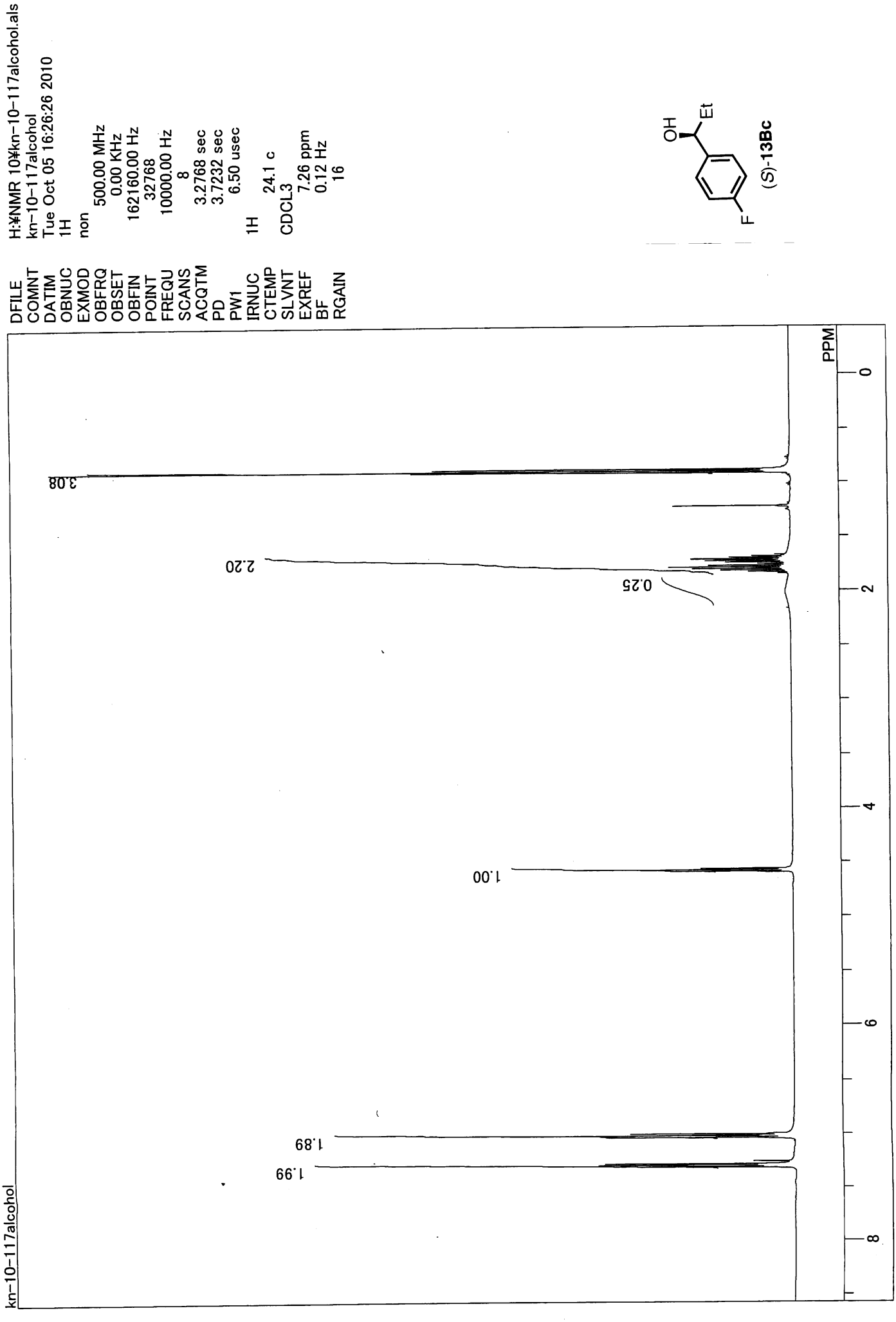

F:¥b-Np-13C.als
b-Np
Tue Jan 11 14:57:49 2011
13C
BCM
75.45 MHz
124.00 KHz
1840.00 Hz
32768
20408.10 Hz
64
1.6056 sec
1.3940 sec
4.20 usec
1H
20.0 c
CDCL3
77.00 ppm
1.20 Hz
22
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN
OH
Me
(S)-12Af
25.069
70.423
76.580
77.000
77.429
123.738
123.771
125.733
126.079
127.612
127.876
128.238
132.821
133.224
143.123
b-Np
PPM
0
25
50
75
100
125
150
175
200

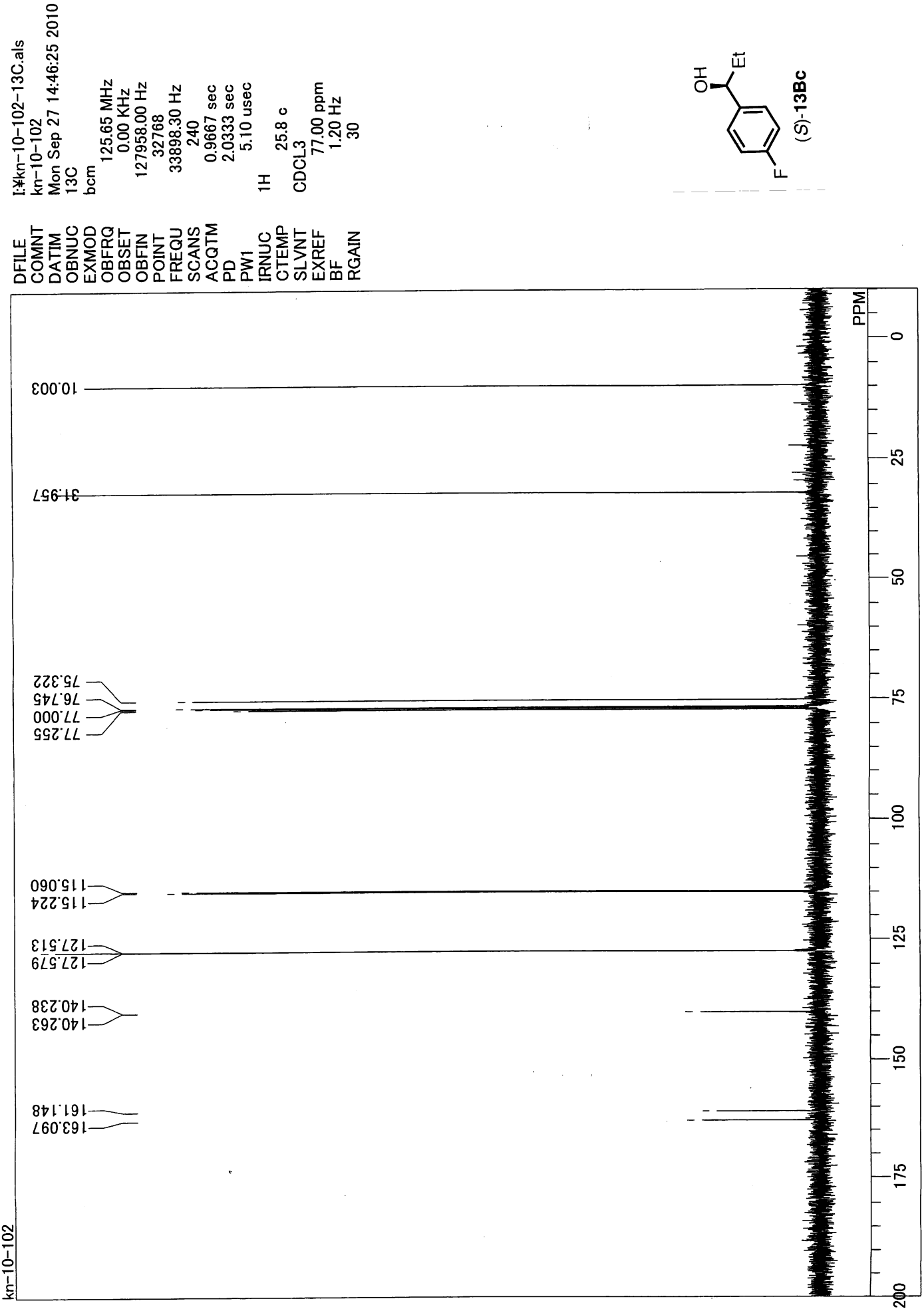


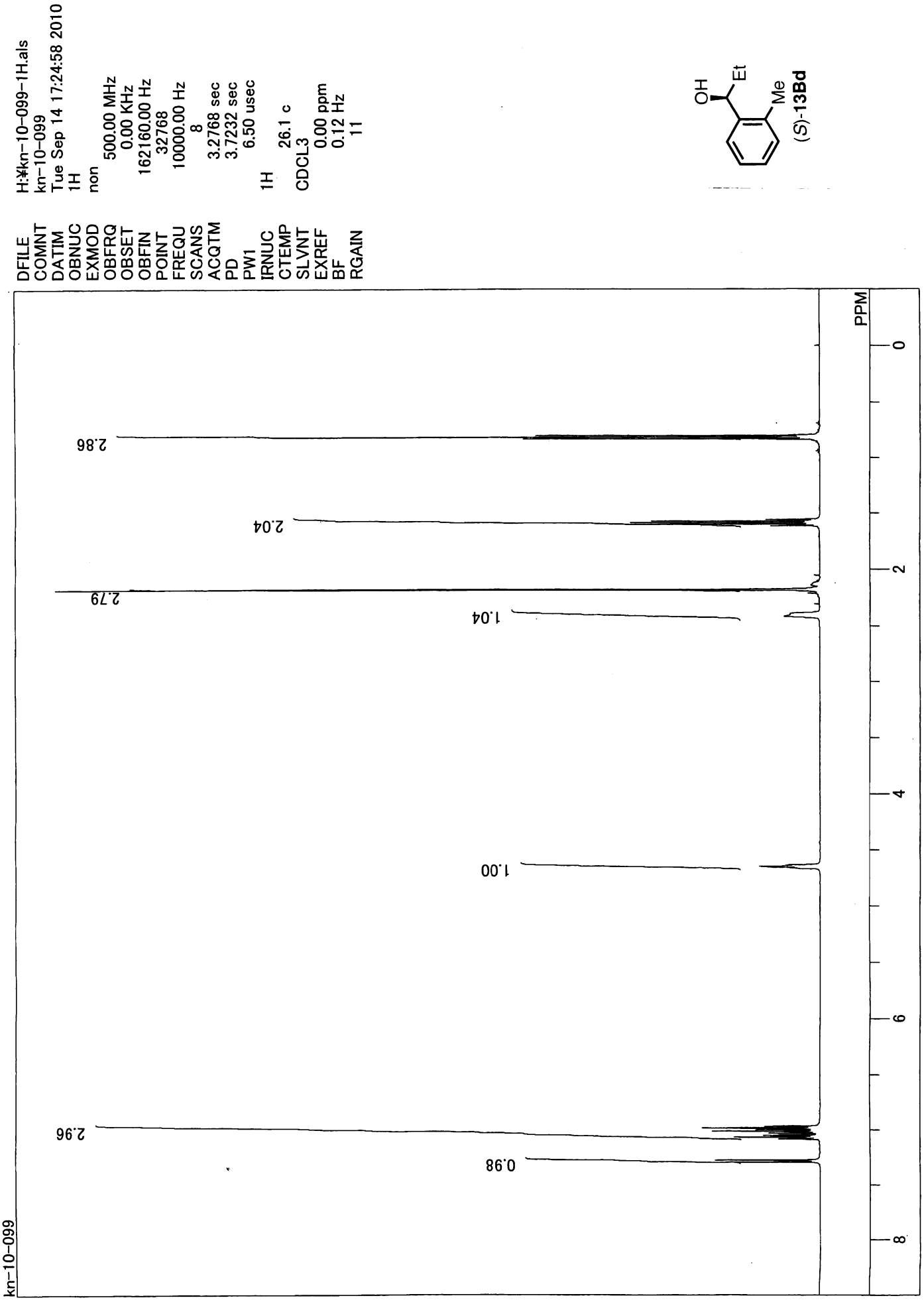

H:¥kn-10-096-13C.als
kn-10-096
Tue Sep 14 17:10:21 2010
13C
bcm
125.65 MHz
0.00 KHz
127958.00 Hz
32768
33898.30 Hz
120
0.9667 sec
2.0333 sec
5.10 usec
1H
26.3 c
CDCL3
77.00 ppm
1.20 Hz
30
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN
OH
Et
Me
(S)-13Ba
10.151
21.066
31.759
75.865
76.745
77.000
77.255
125.901
129.043
137.113
141.604
PPM
0
25
50
75
100
125
150
175
200
kn-10-096

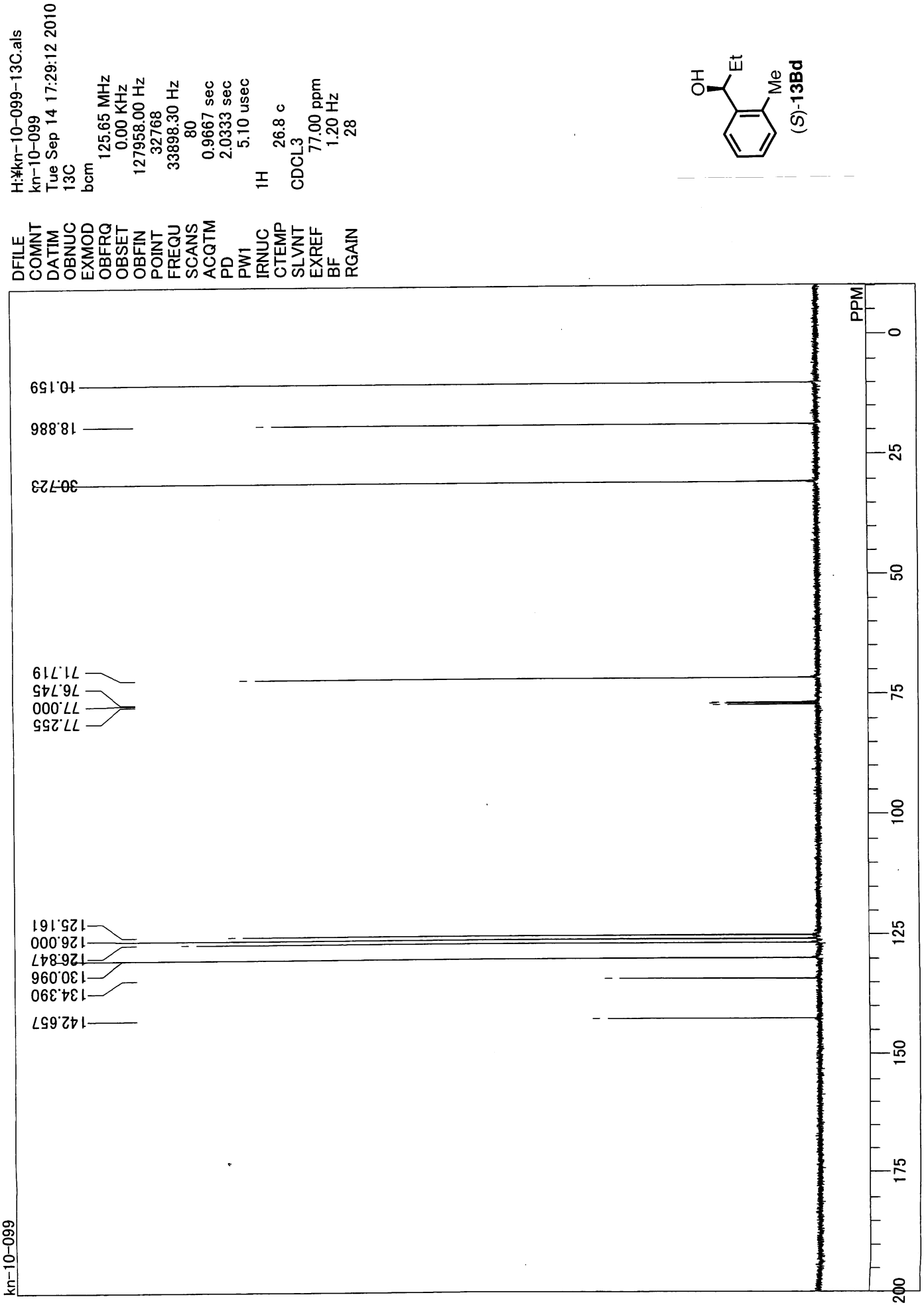


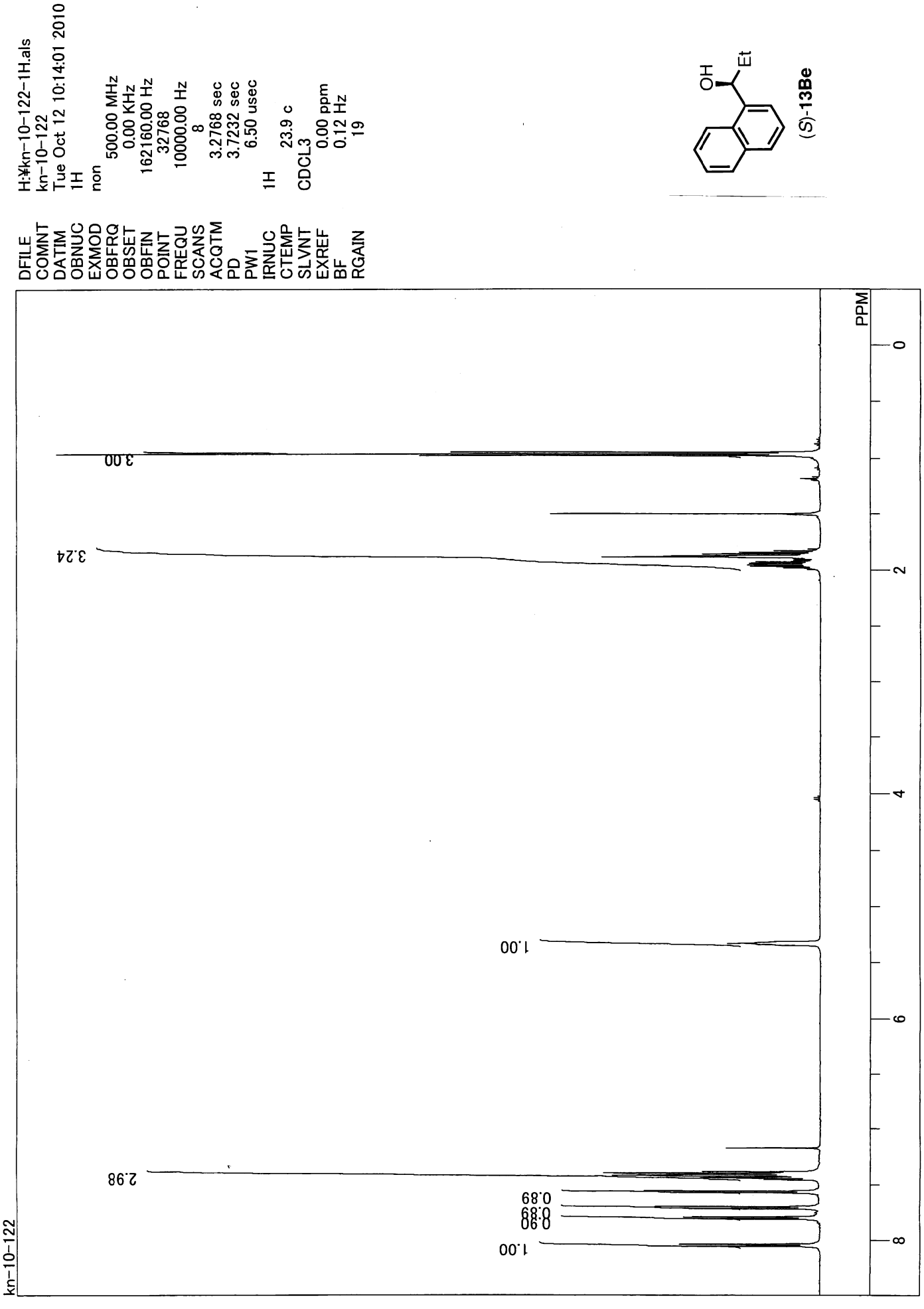


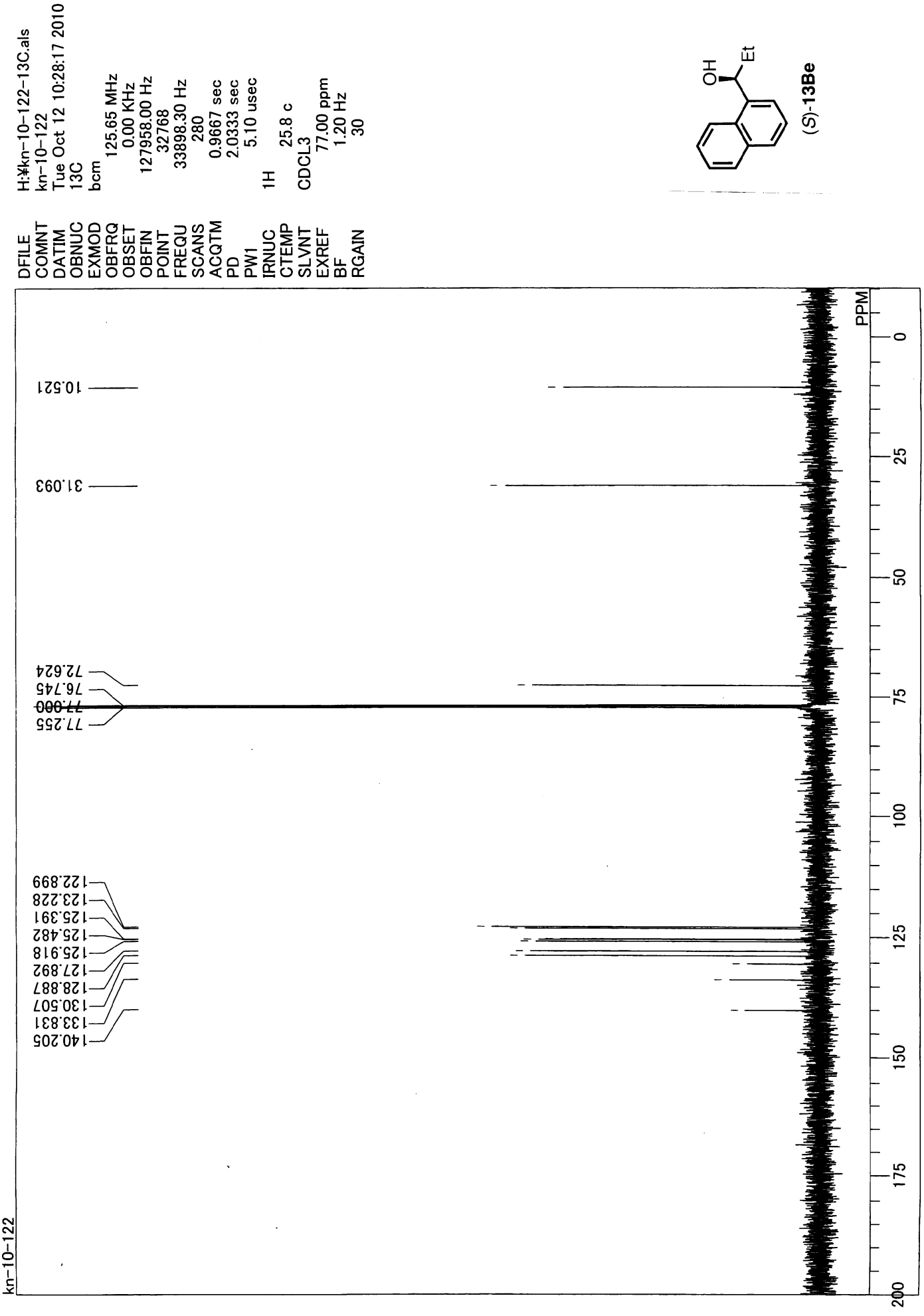


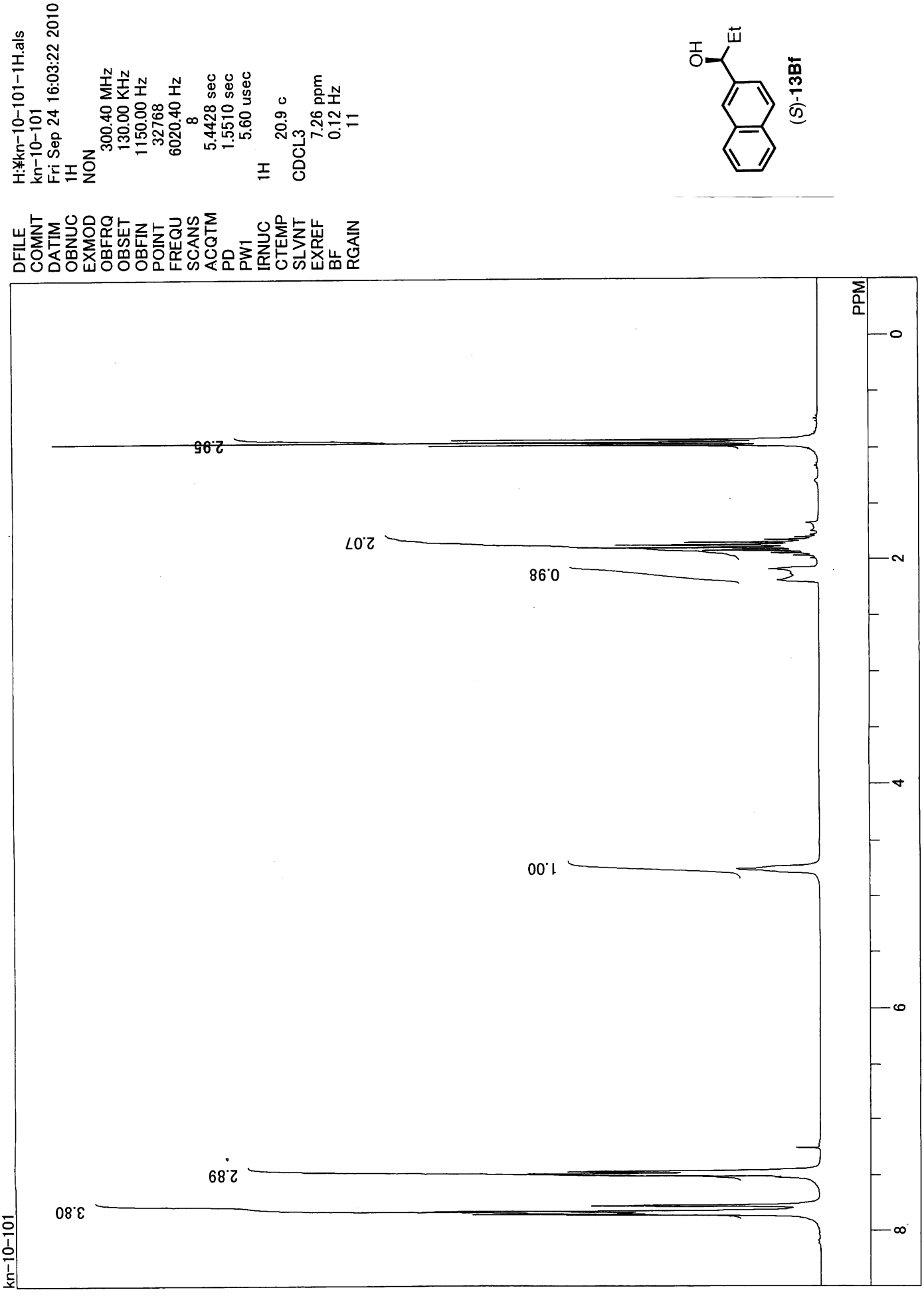


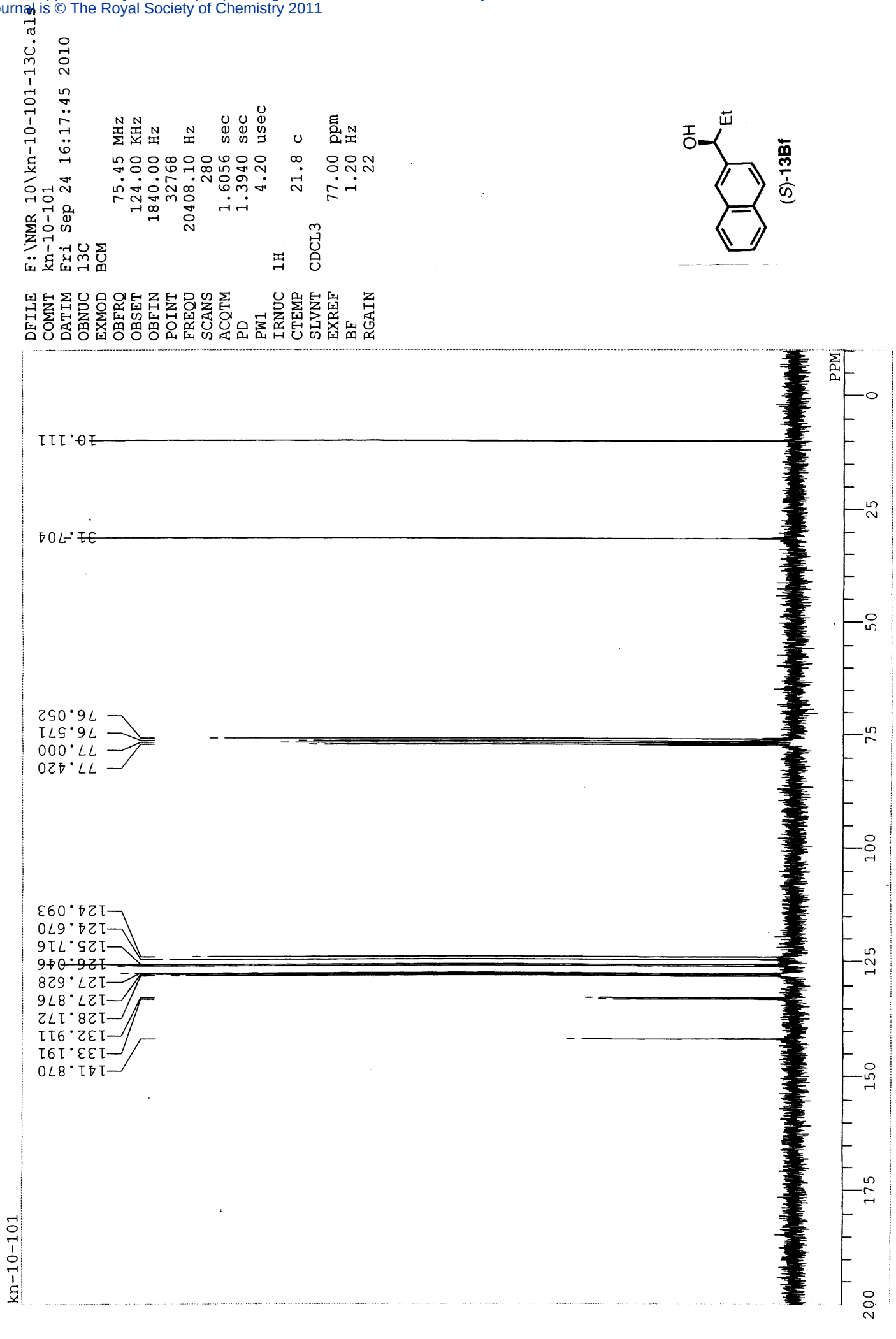




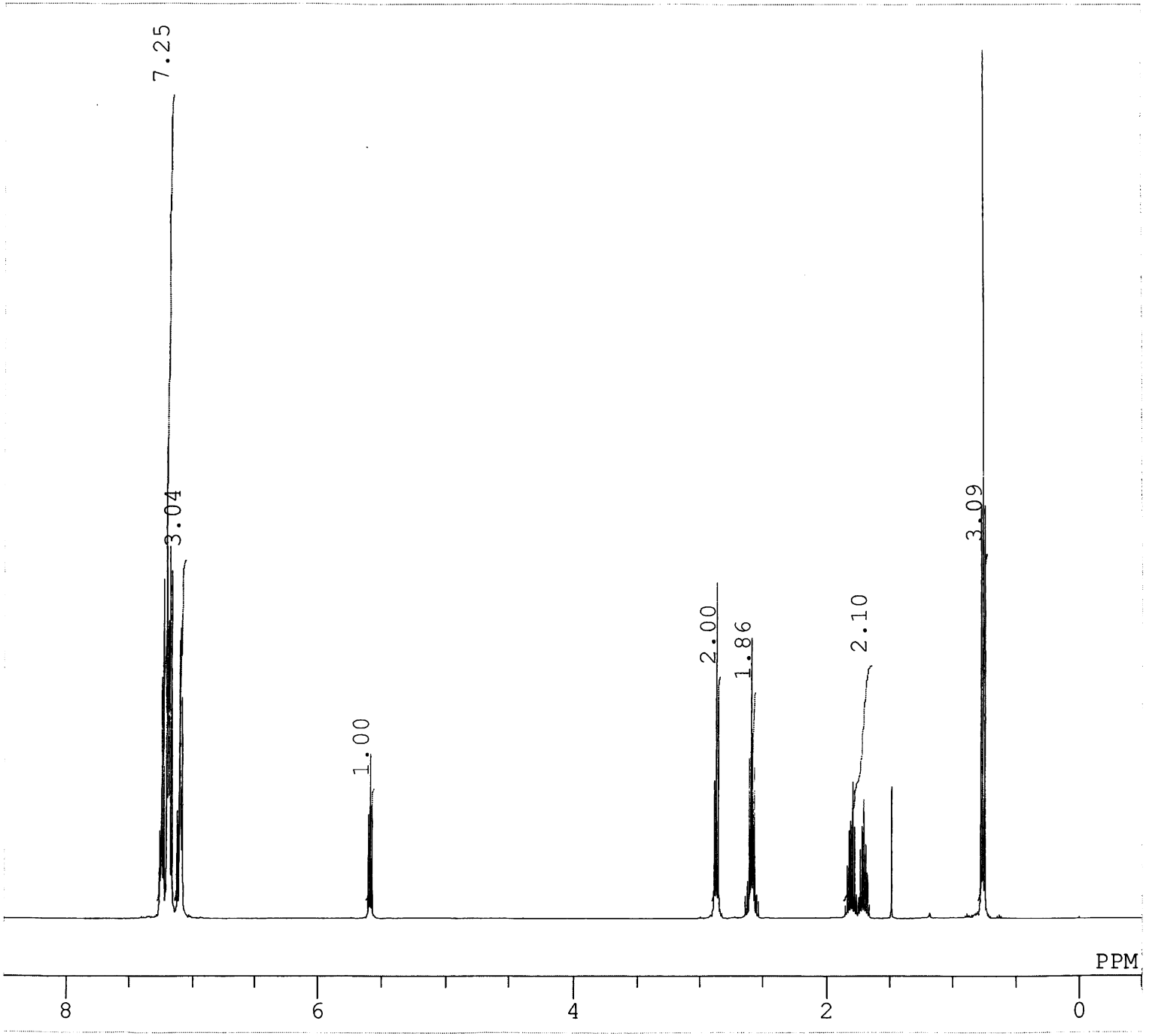




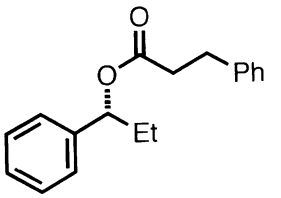




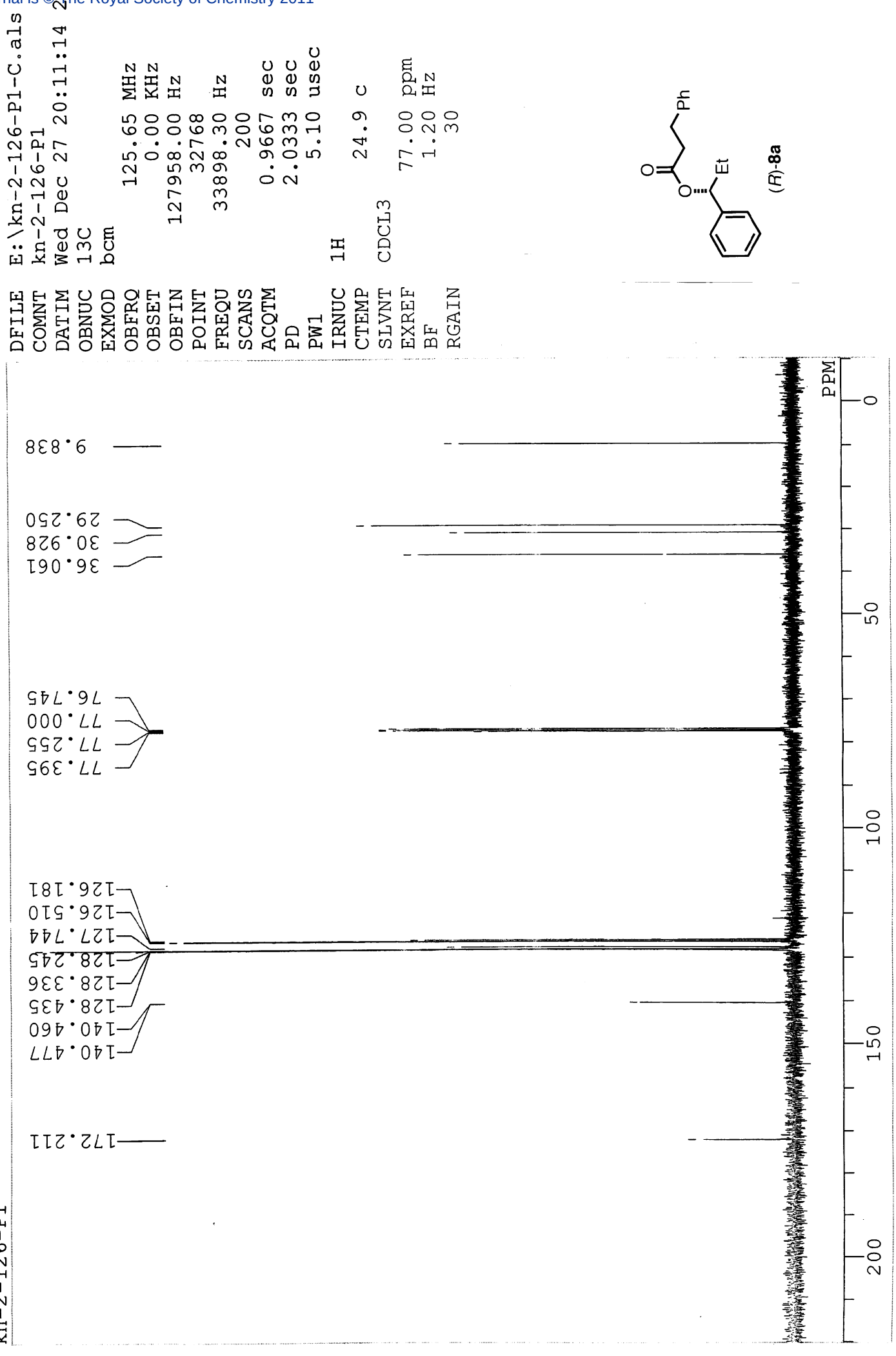
E:\kn-2-126-P1-H.als
kn-2-126-P1



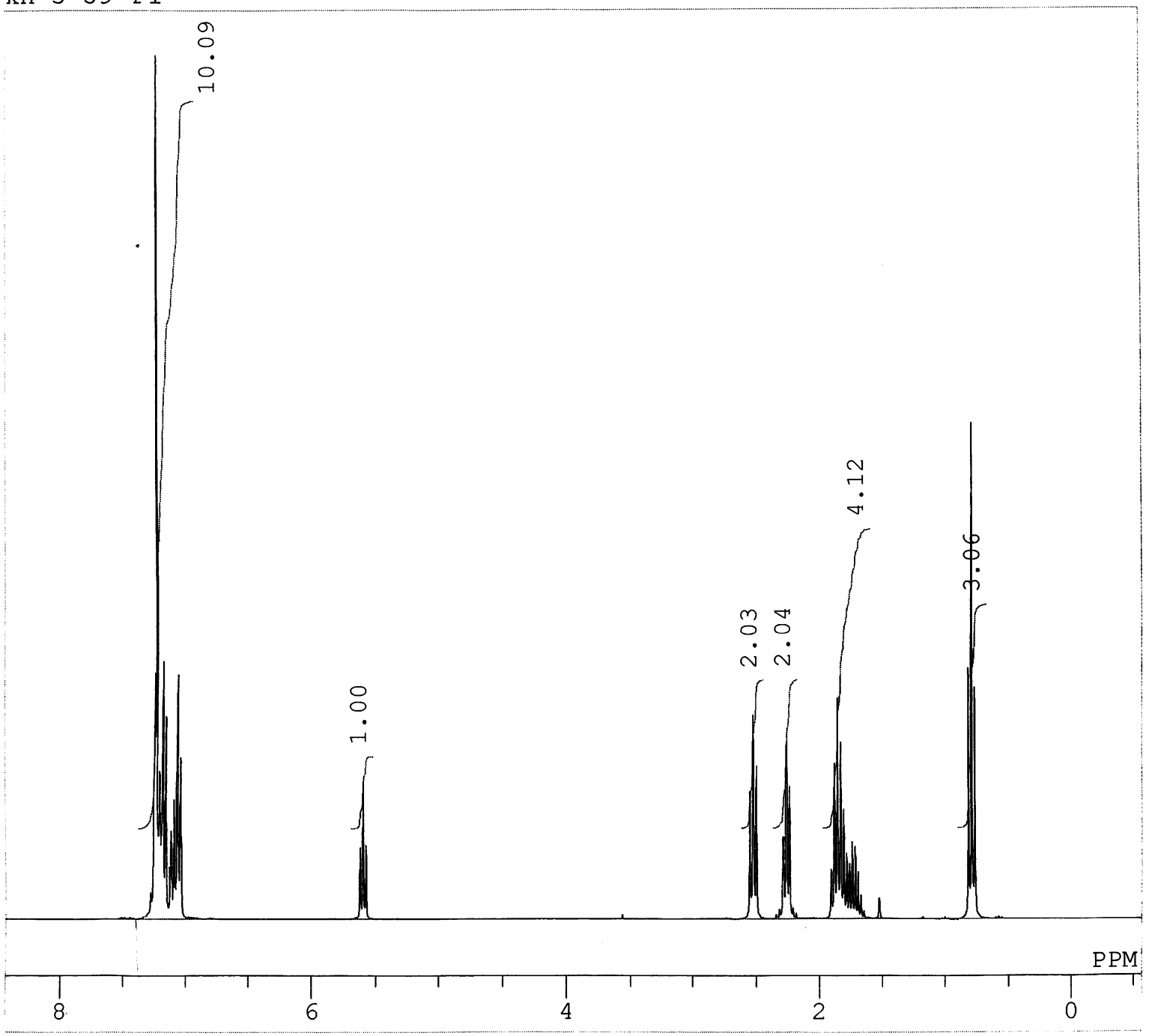
DFILE	E:\kn-2-126-P1-H.als
COMNT	kn-2-126-P1
DATIM	Wed Dec 27 20:00:53 2
OBNUC	1H
EXMOD	non
OBFRQ	500.00 MHz
OBSET	0.00 KHz
OBFIN	162160.00 Hz
POINT	32768
FREQU	10000.00 Hz
SCANS	8
ACQTM	3.2768 sec
PD	3.7232 sec
PW1	5.95 usec
IRNUC	1H
CTEMP	23.9 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	15



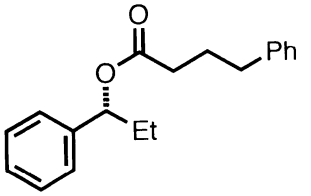
(*R*)-**8a**



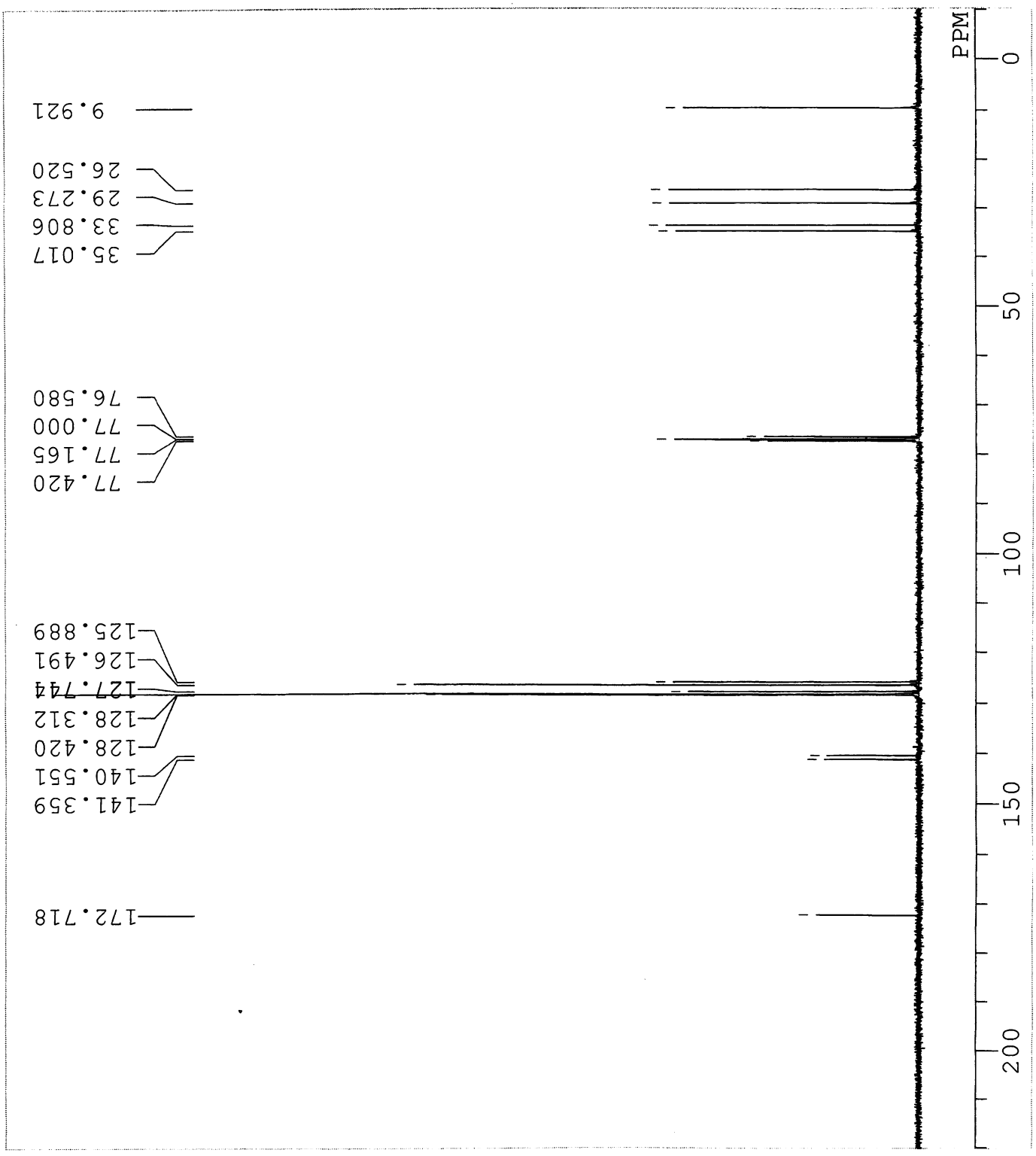
F:\kn-3-59-1H.als
kn-3-59-P1

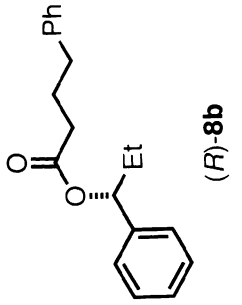


DFILE	F:\kn-3-59-1H.als	
COMNT	kn-3-59-P1	
DATIM	Fri Mar 16 19:28:48	
OBNUC	1H	
EXMOD	NON	
OBFRQ	300.40	MHz
OBSET	130.00	KHz
OBFIN	1150.00	Hz
POINT	32768	
FREQU	6020.40	Hz
SCANS	8	
ACQTM	5.4428	sec
PD	1.5539	sec
PW1	5.40	usec
IRNUC	1H	
CTEMP	20.2	c
SLVNT	CDCL3	
EXREF	0.00	ppm
BF	0.12	Hz
RGAIN	10	



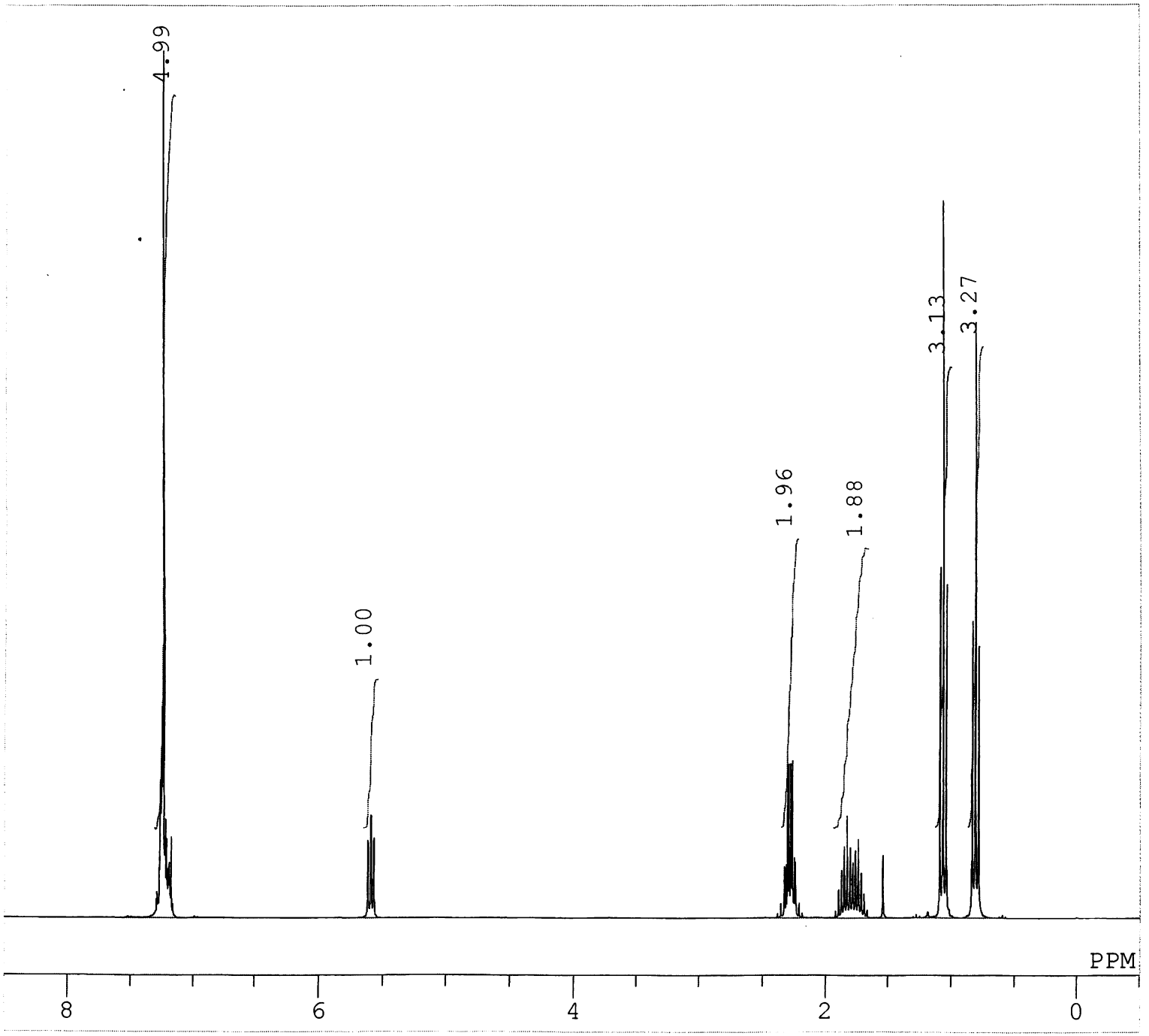
(*R*)-**8b**



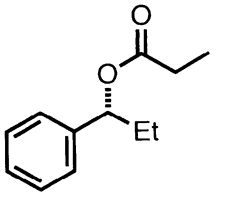


(*R*)-**8b**

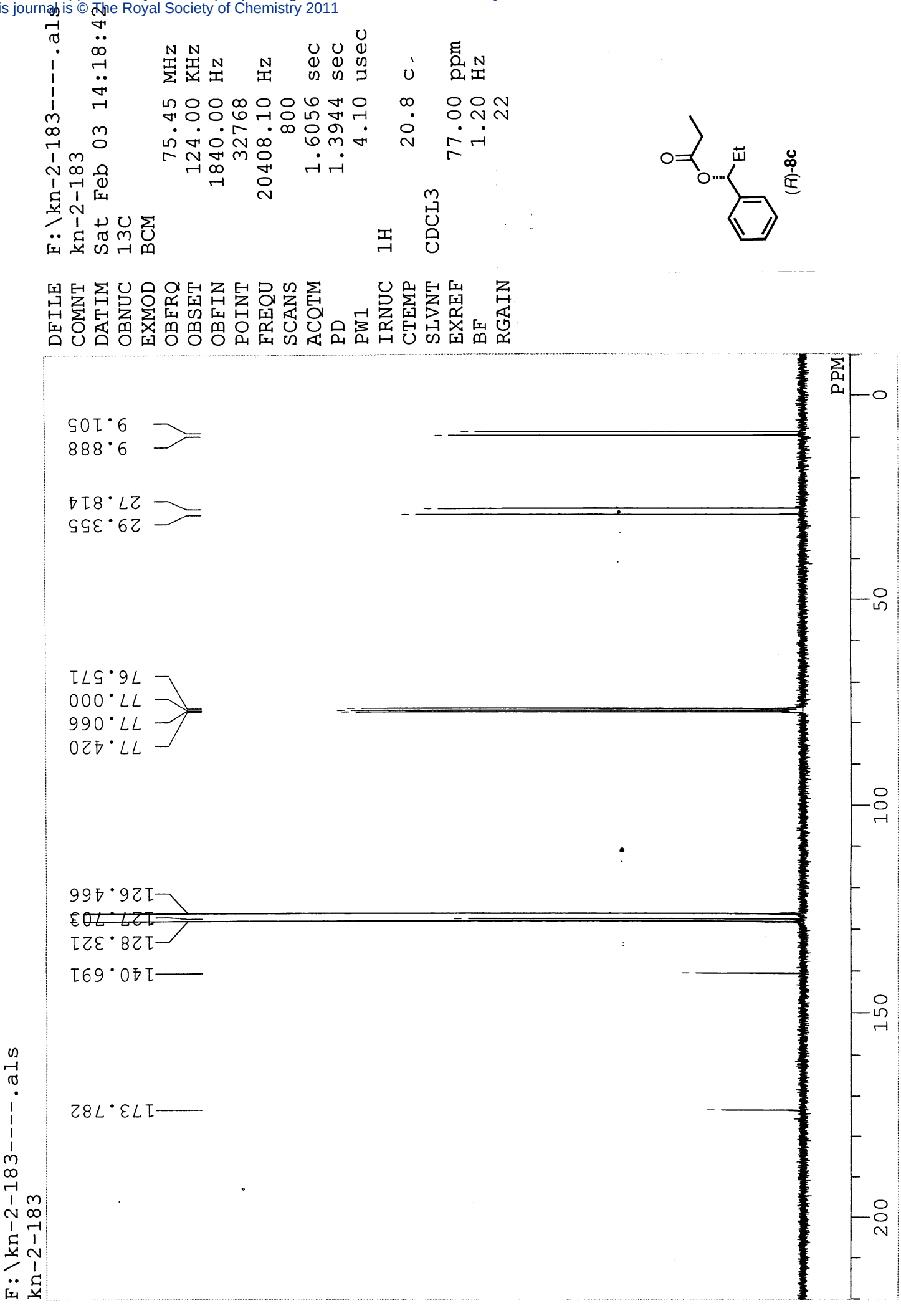
F:\kn-2-182-.als
kn-2-183



DFILE	F:\kn-2-182-.als	
COMNT	kn-2-183	
DATIM	Sat Feb 03 13:38:12	
OBNUC	1H	
EXMOD	NON	
OBFRQ	300.40	MHz
OBSET	130.00	KHz
OBFIN	1150.00	Hz
POINT	32768	
FREQU	6020.40	Hz
SCANS	8	
ACQTM	5.4428	sec
PD	1.5539	sec
PW1	5.40	usec
IRNUC	1H	
CTEMP	20.8	c
SLVNT	CDCL3	
EXREF	0.00	ppm
BF	0.12	Hz
RGAIN	12	

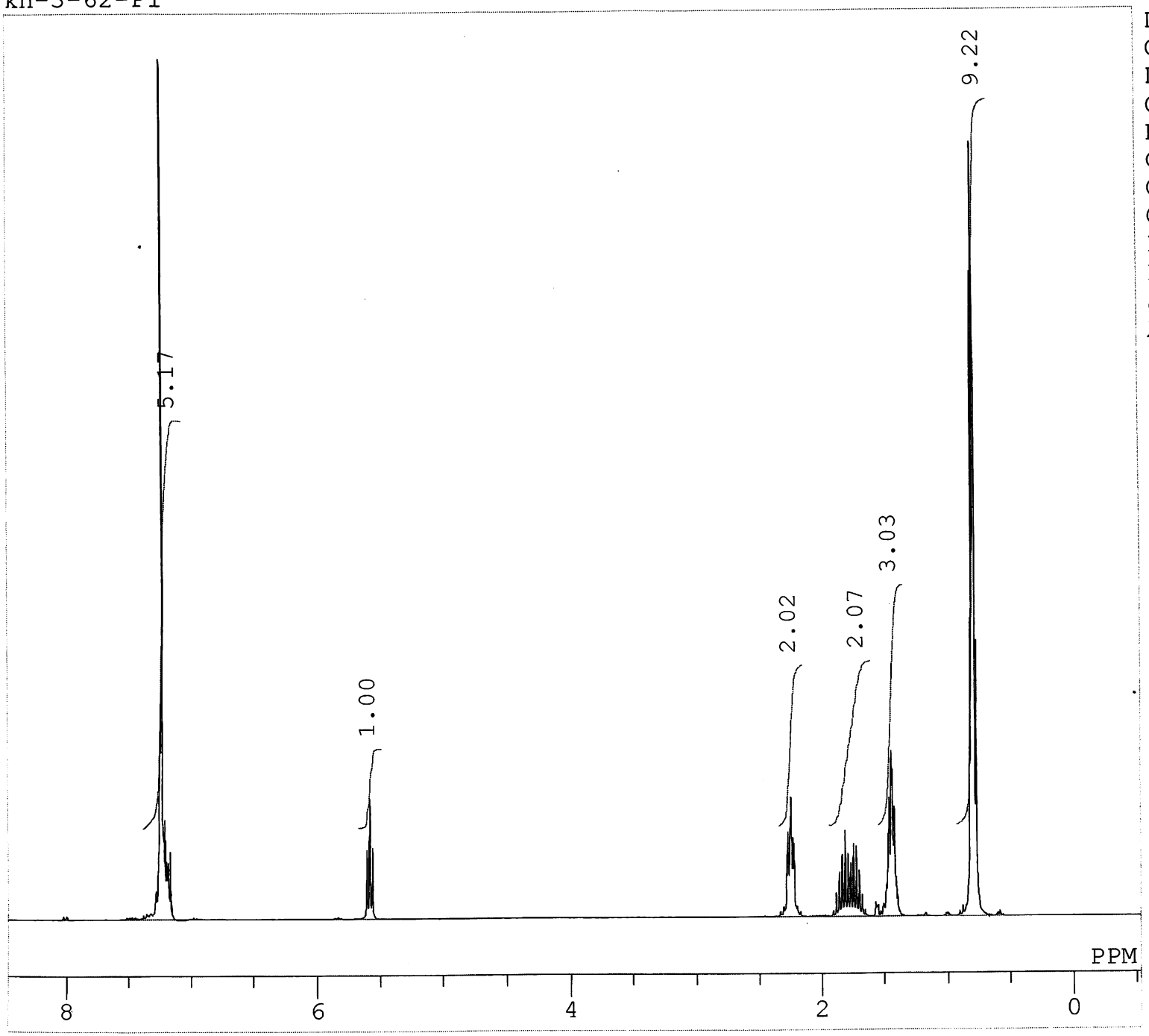


(*R*)-**8c**

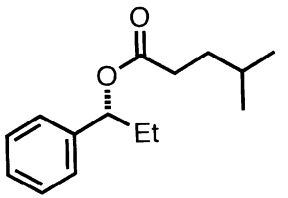


(*R*)-**8c**

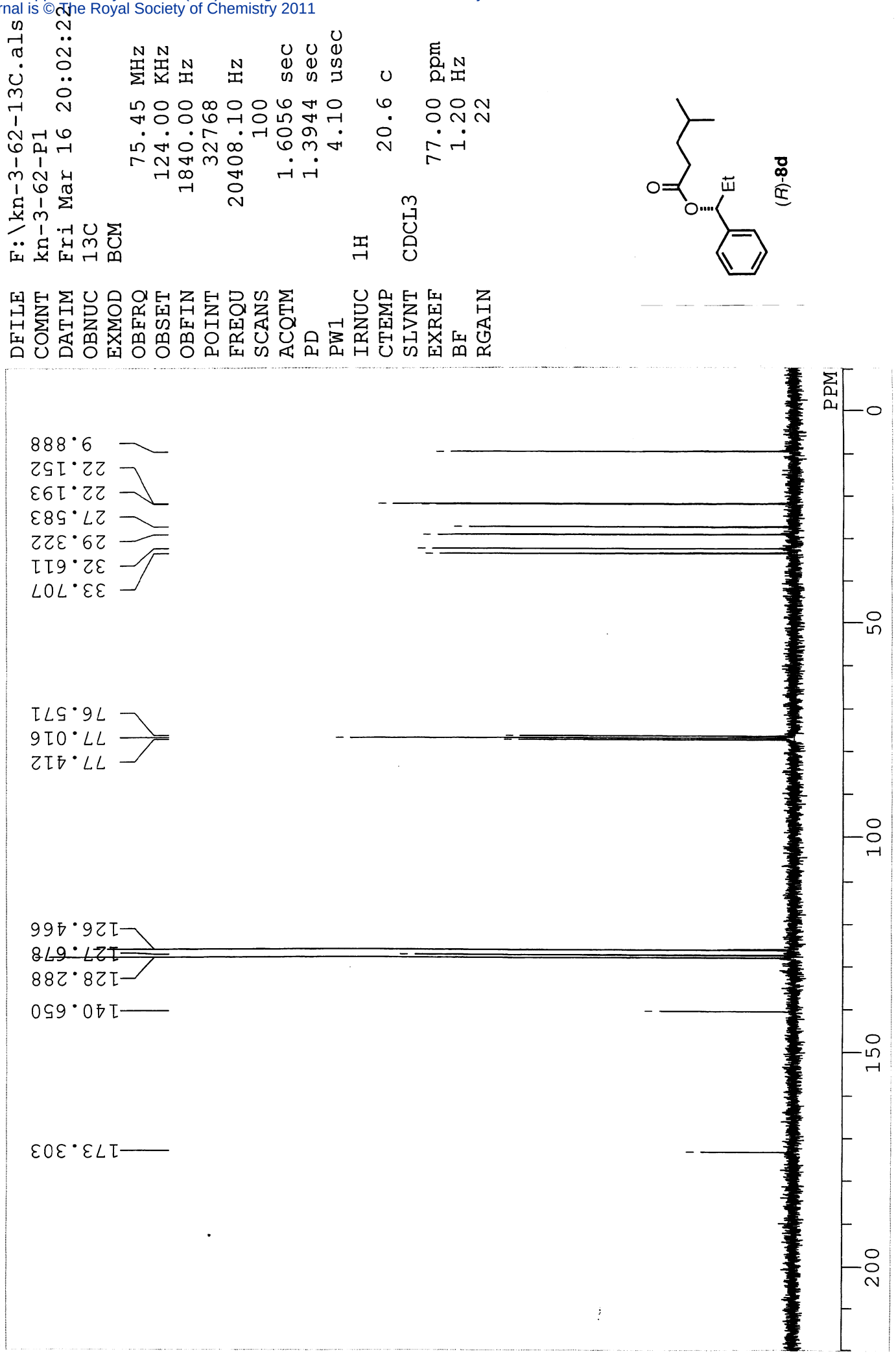
F:\kn-3-62-1H.als
kn-3-62-P1



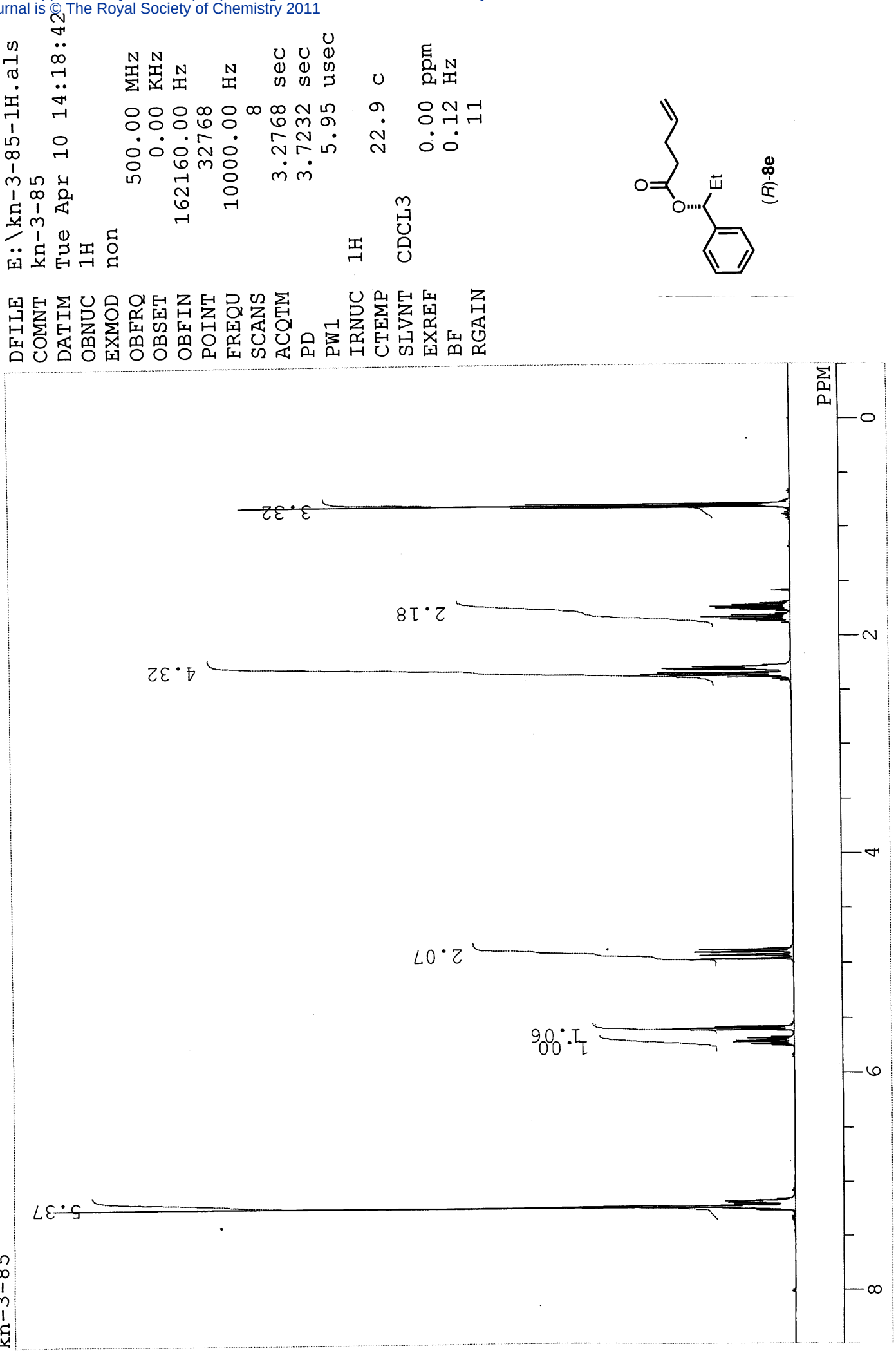
DFILE	F:\kn-3-62-1H.als	
COMNT	kn-3-62-P1	
DATIM	Fri Mar 16 19:56:56	
OBNUC	1H	
EXMOD	NON	
OBFRQ	300.40	MHz
OBSET	130.00	KHz
OBFIN	1150.00	Hz
POINT	32768	
FREQU	6020.40	Hz
SCANS	8	
ACQTM	5.4428	sec
PD	1.5539	sec
PW1	5.40	usec
IRNUC	1H	
CTEMP	20.4	c
SLVNT	CDCL3	
EXREF	0.00	ppm
BF	0.12	Hz
RGAIN	11	



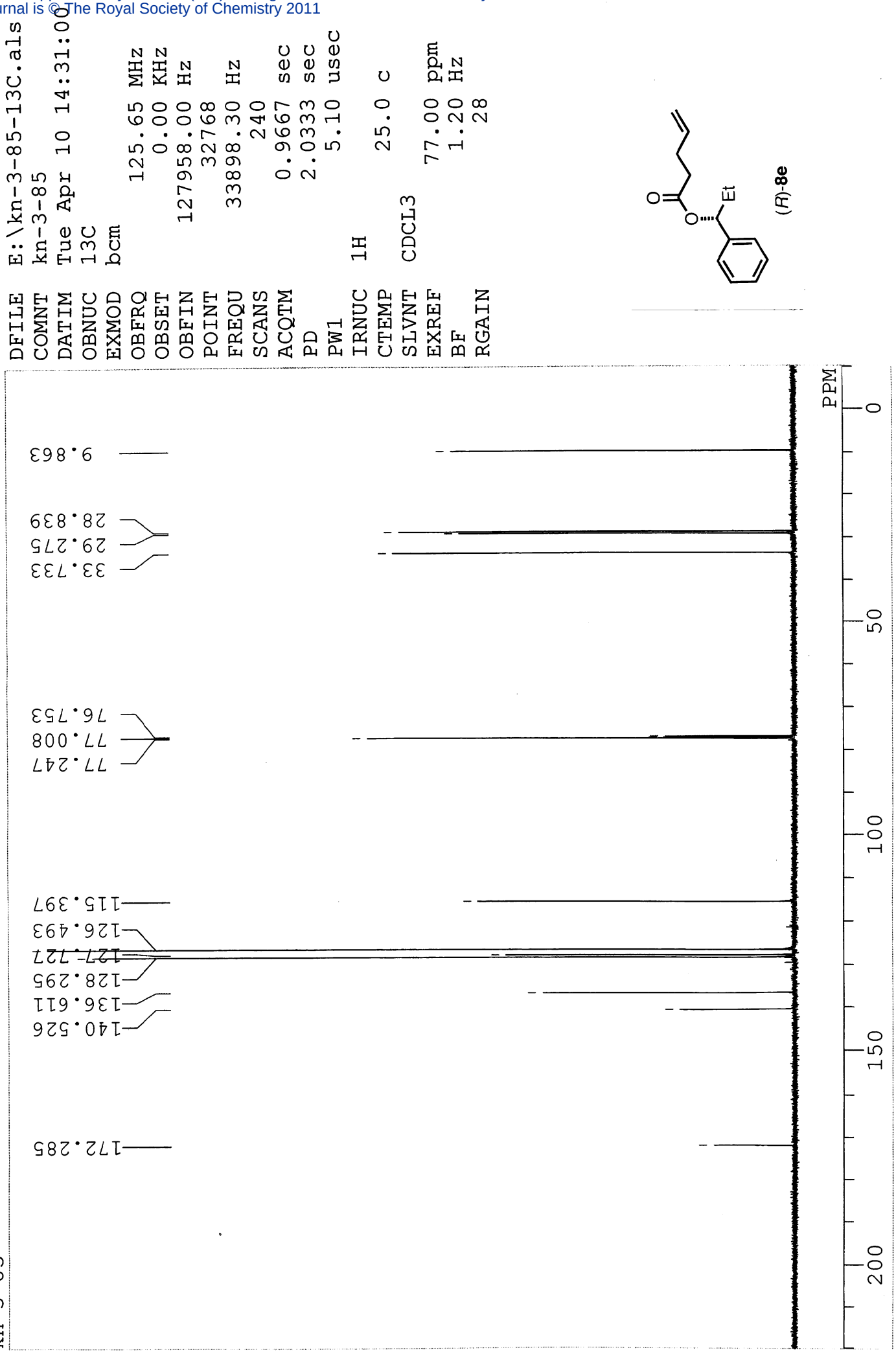
(*R*)-**8d**



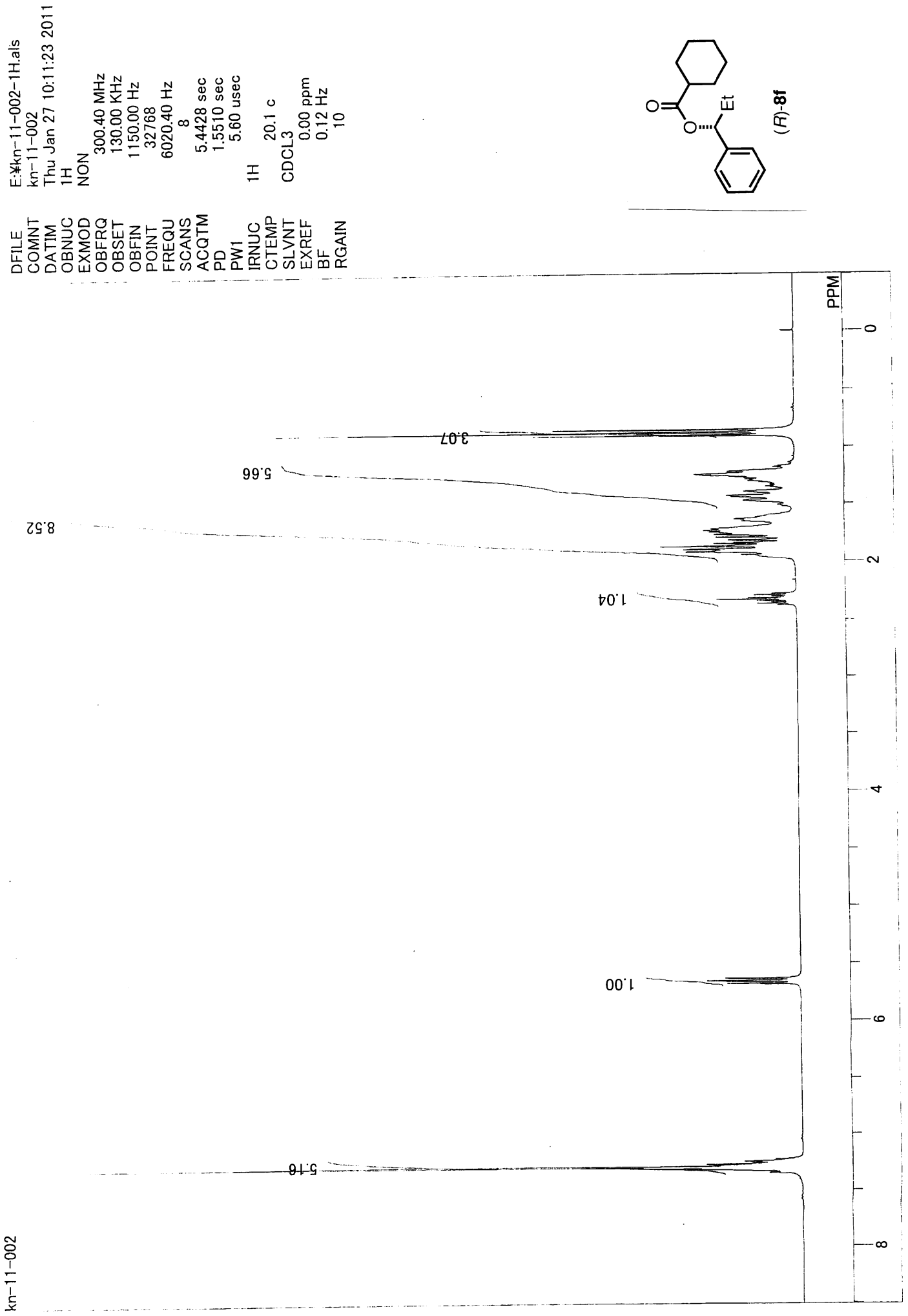
(*R*)-**8d**

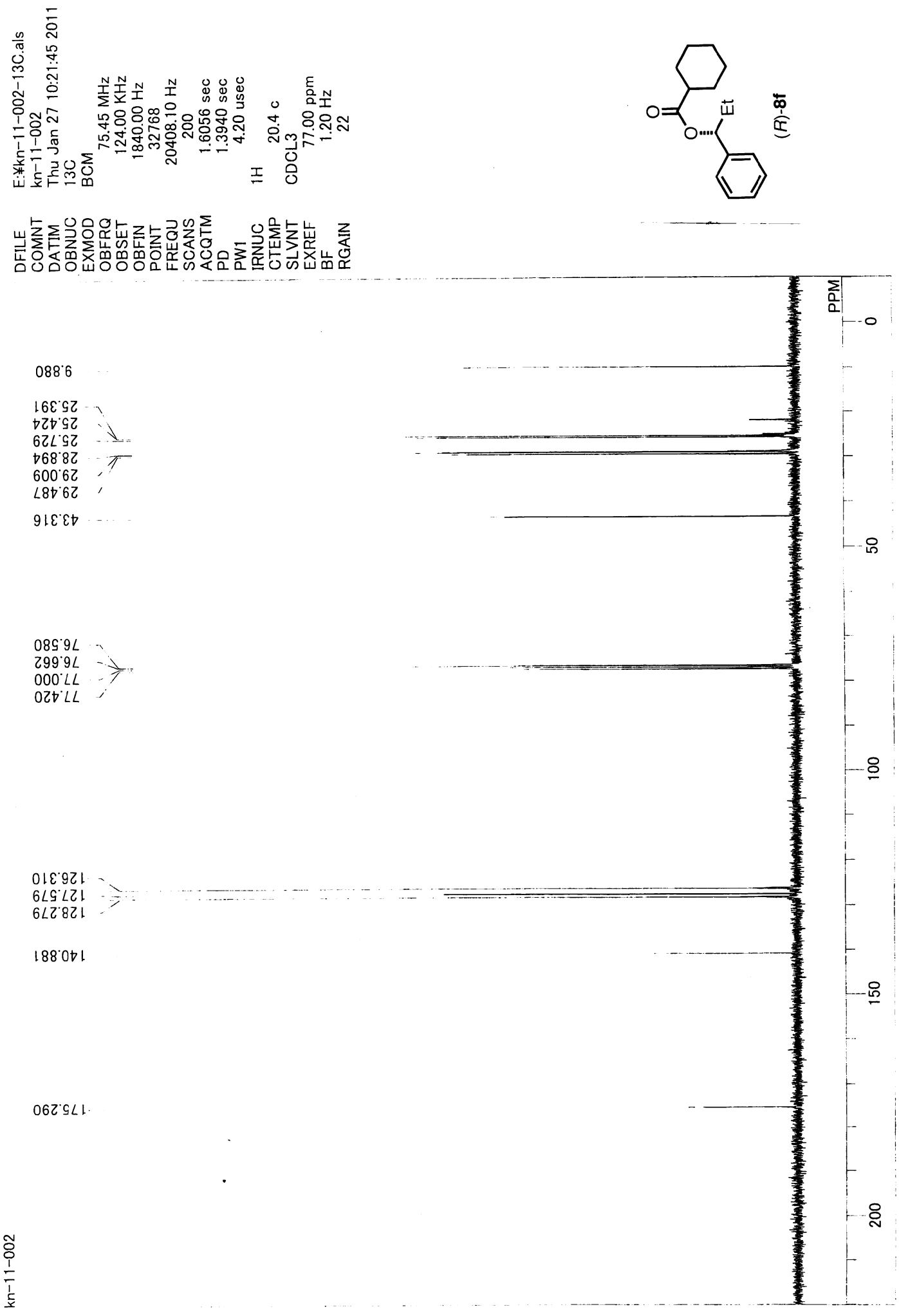


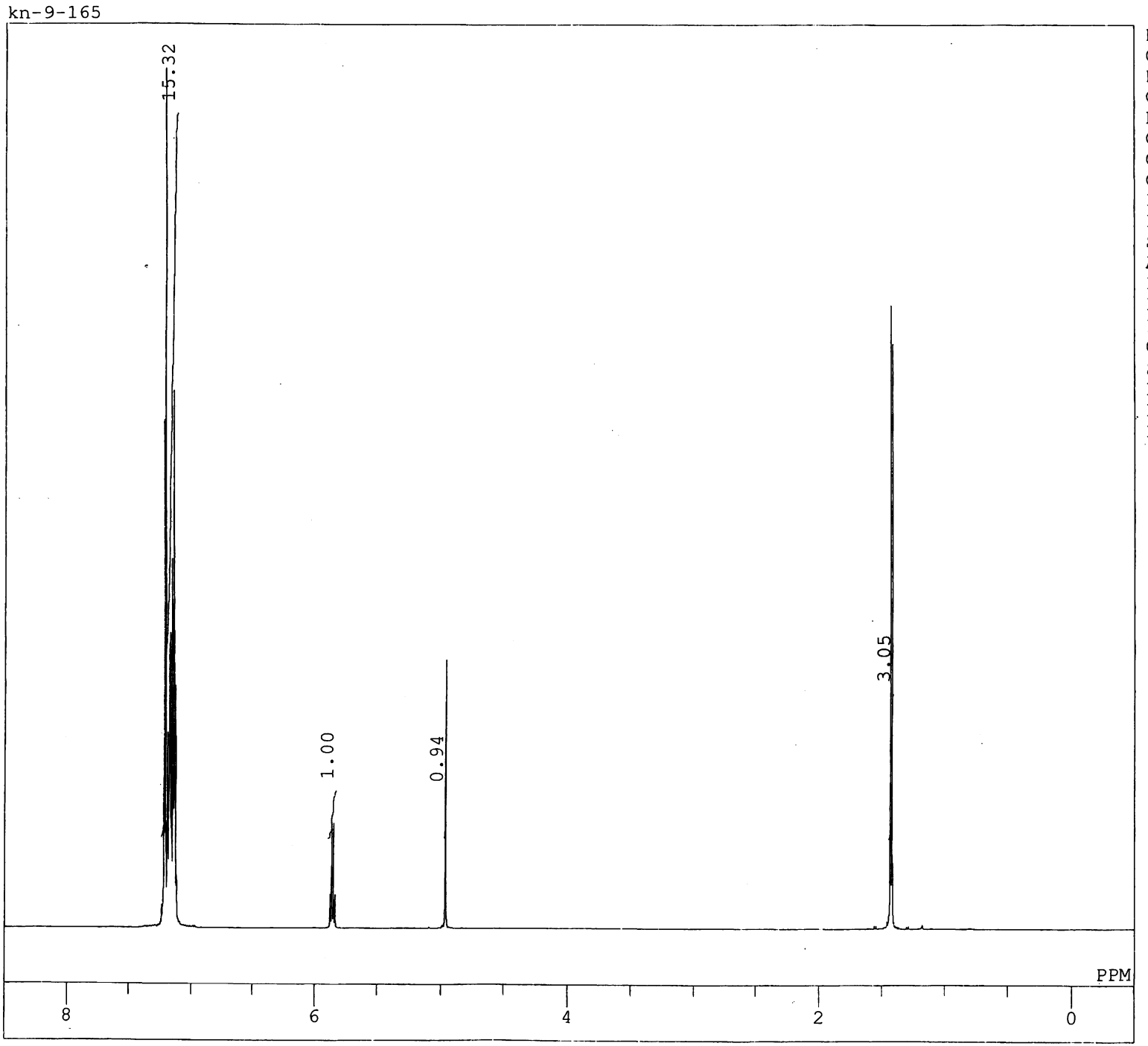
(*R*)-**8e**



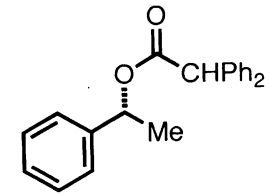
(*R*)-**8e**


DFILE E:¥kn-11-002-1H.als
COMNT kn-11-002
DATIM Thu Jan 27 10:11:23 2011
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.00 Hz
POINT 32768
FREQU 6020.40 Hz
SCANS 8
ACQTM 5.4428 sec
PD 1.5510 sec
PW1 5.60 usec
IRNUC 1H
CTEMP 20.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 10
O
O
Et
(R)-8f
kn-11-002
5.16
1.00
1.04
8.52
5.66
3.07
PPM
0
2
4
6
8

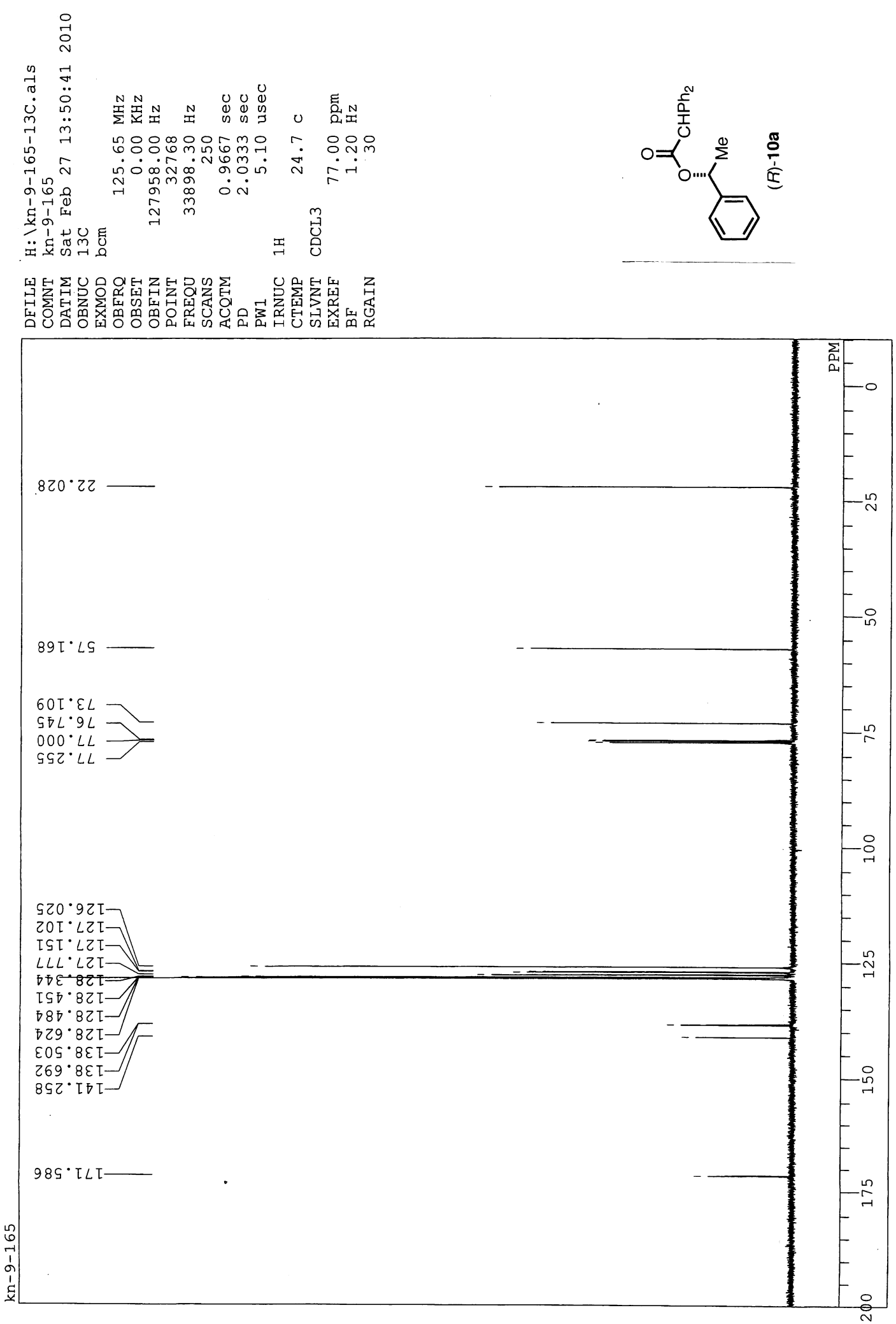


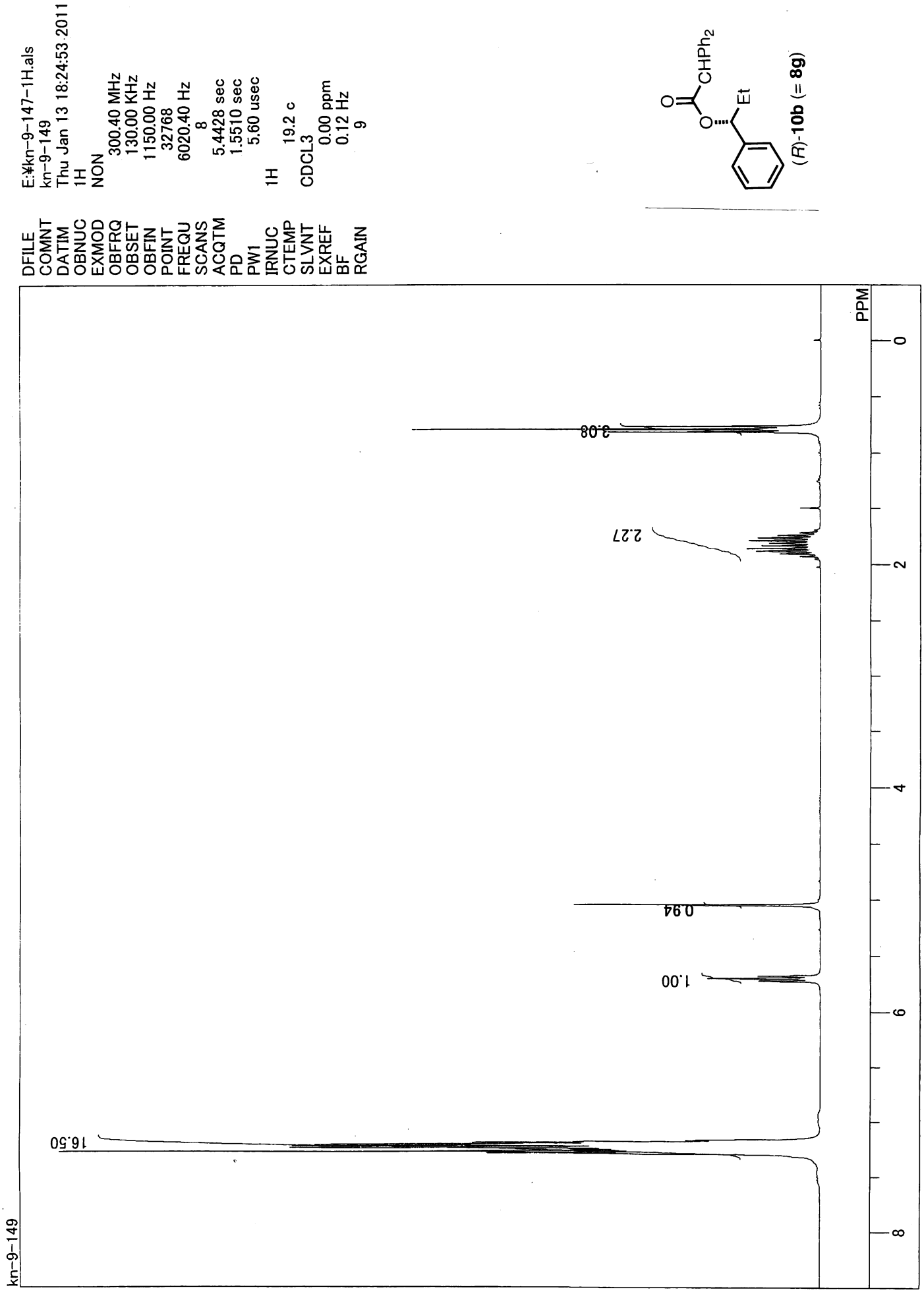


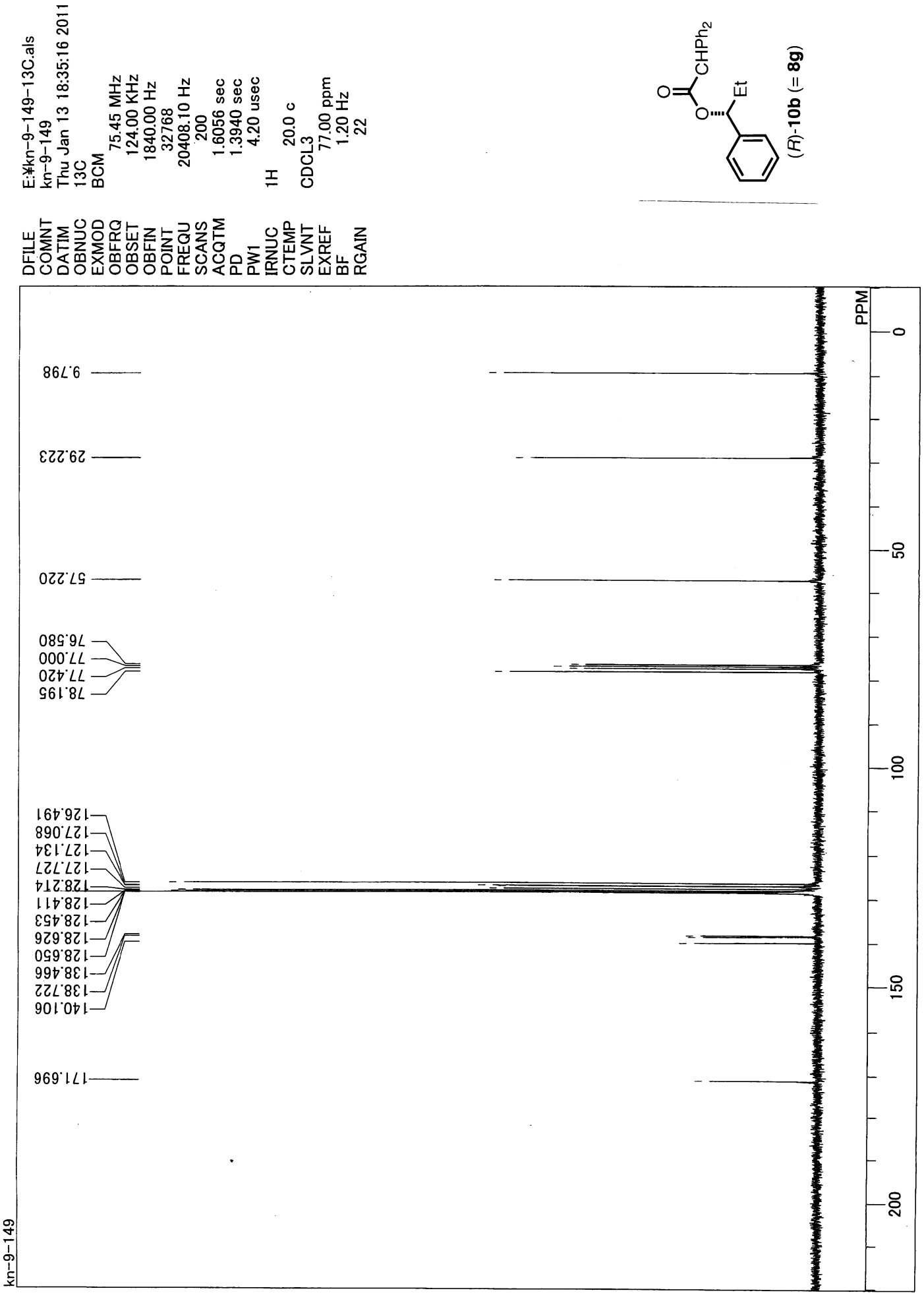
DFILE	H:\kn-9-165-1H.als
COMNT	kn-9-165
DATIM	Sat Feb 27 13:37:48 2010
OBNUC	1H
EXMOD	non
OBFRQ	500.00 MHz
OBSET	0.00 KHz
OBFIN	162160.00 Hz
POINT	32768
FREQU	10000.00 Hz
SCANS	8
ACQTM	3.2768 sec
PD	3.7232 sec
PW1	6.50 usec
IRNUC	1H
CTEMP	23.3 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	13



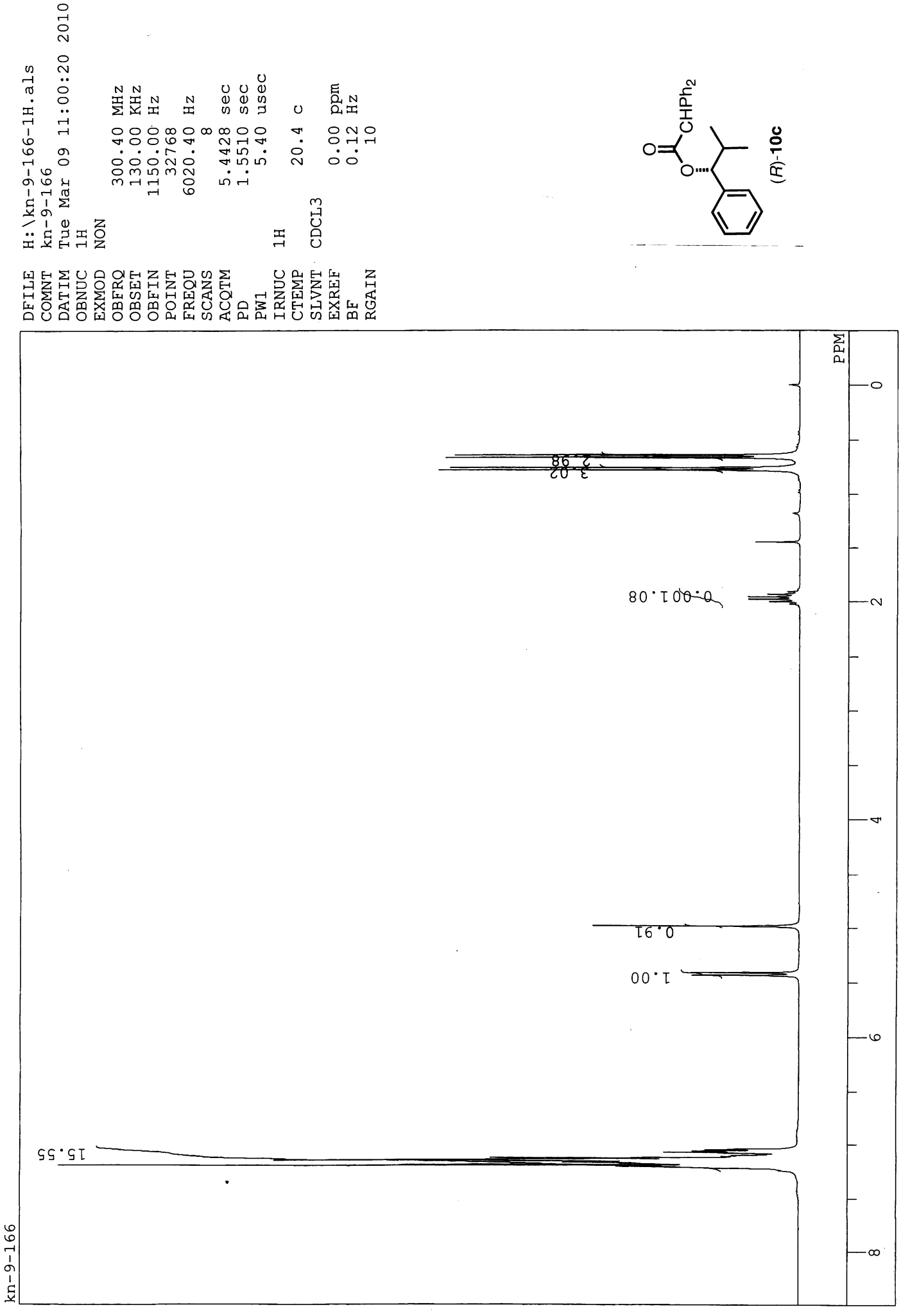
(*R*)-**10a**

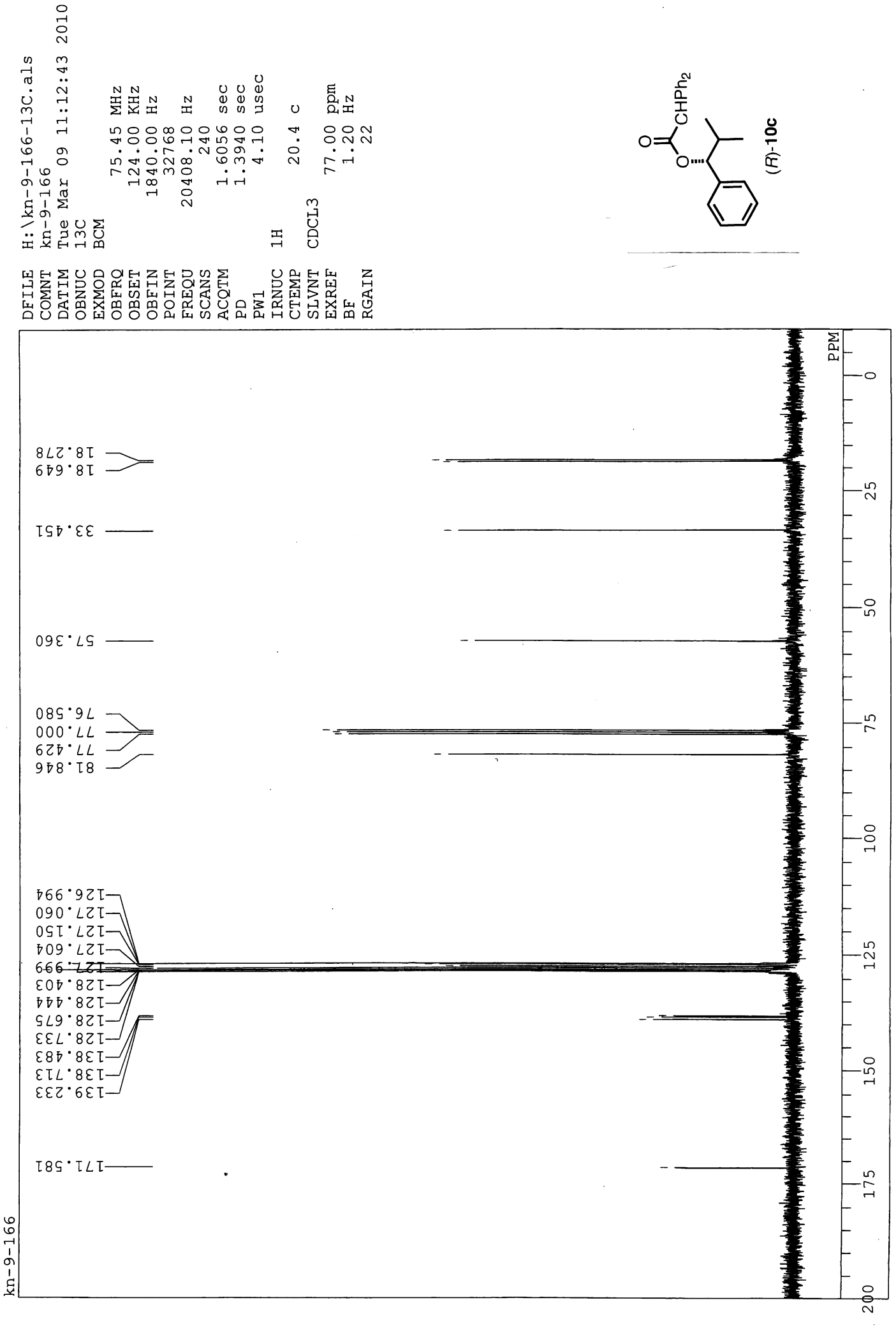


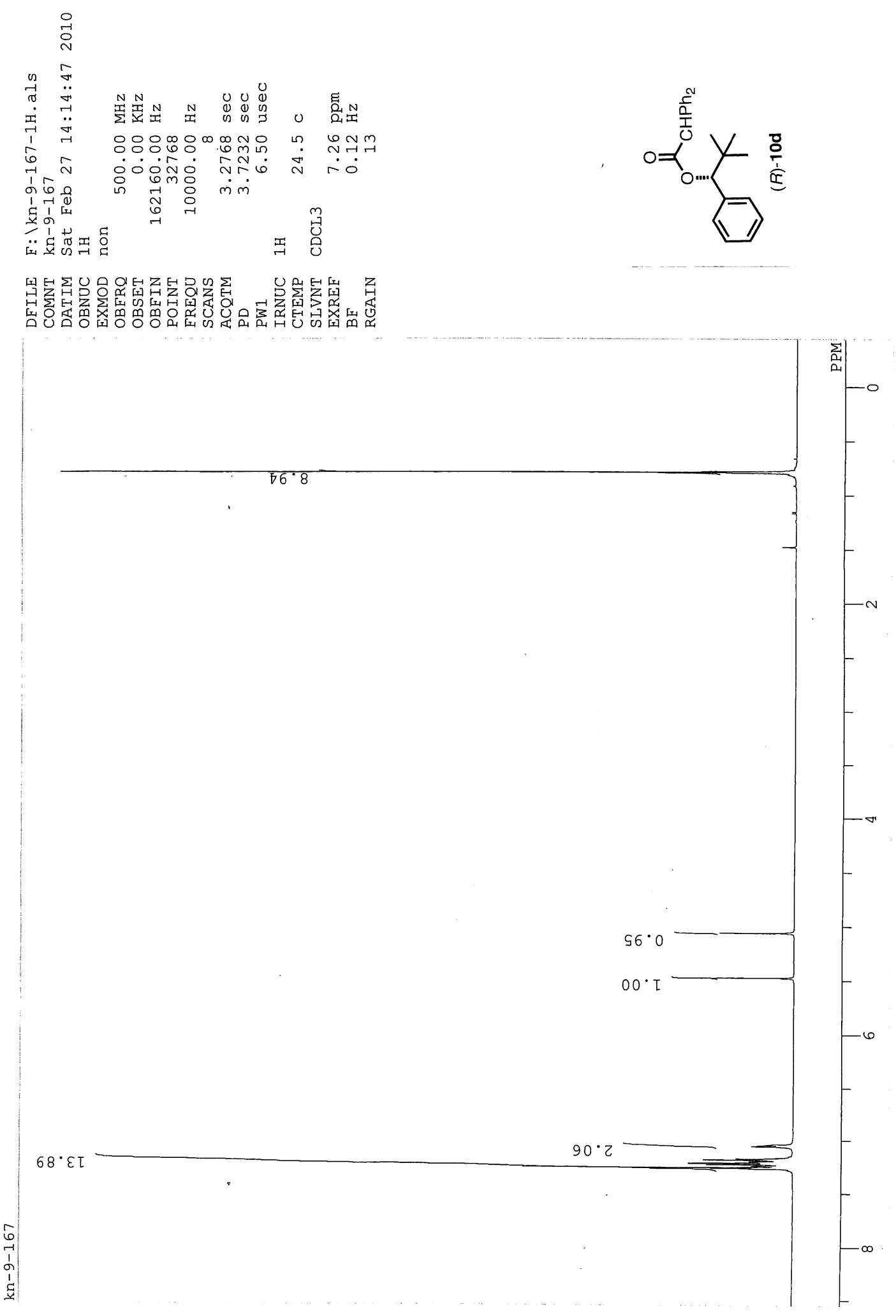


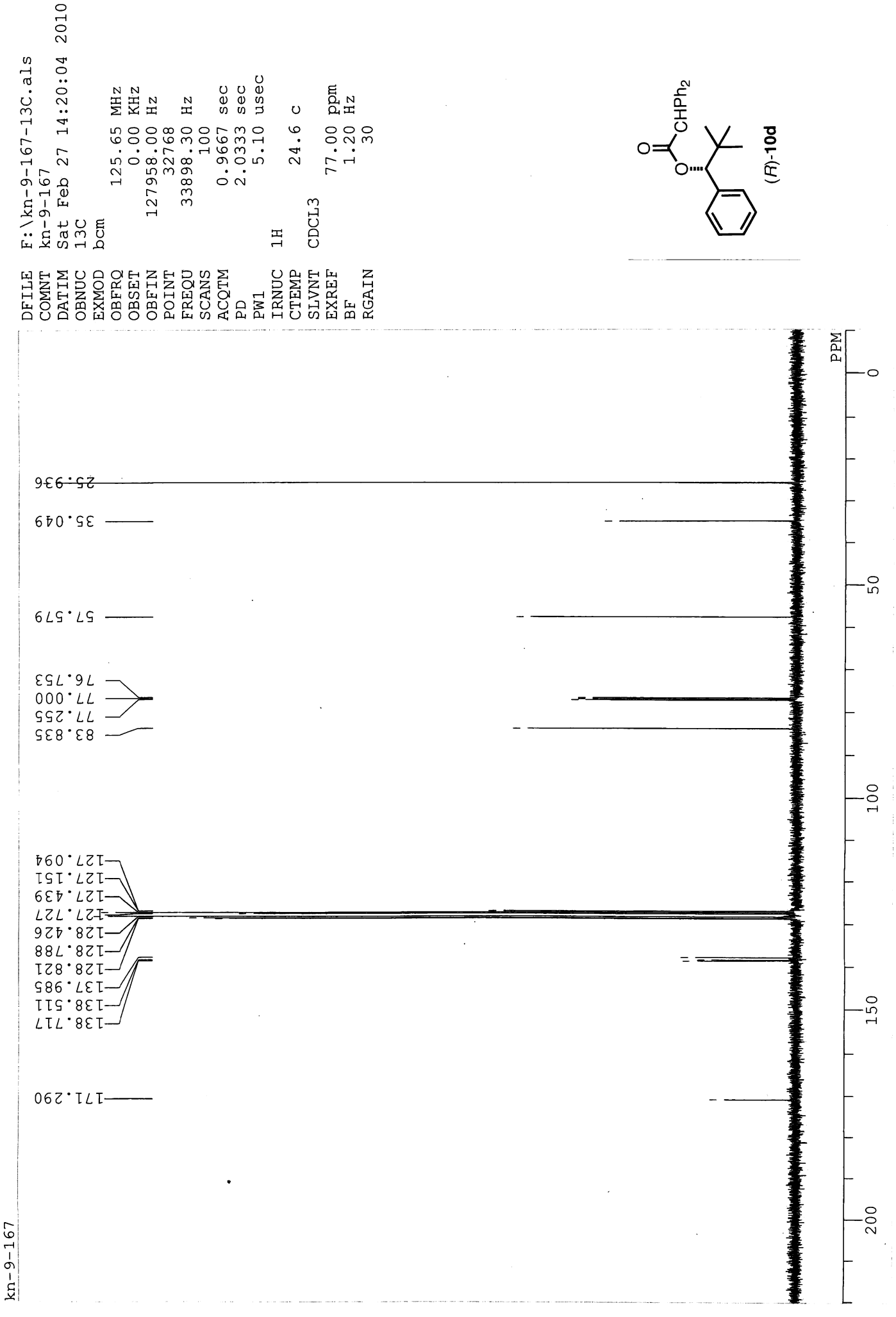


(*R*)-**10b** (= **8g**)

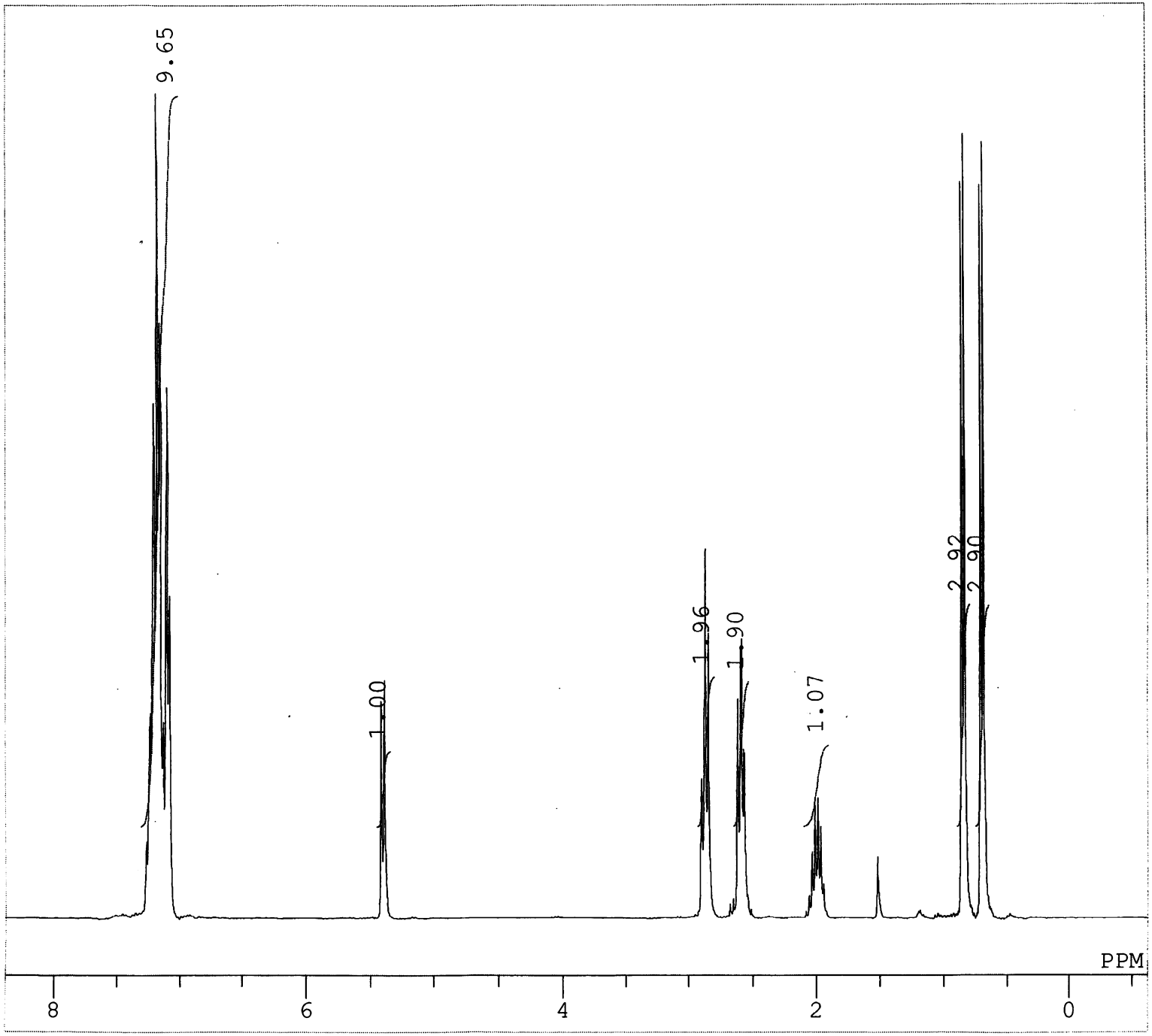




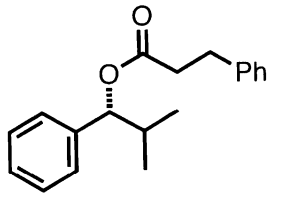




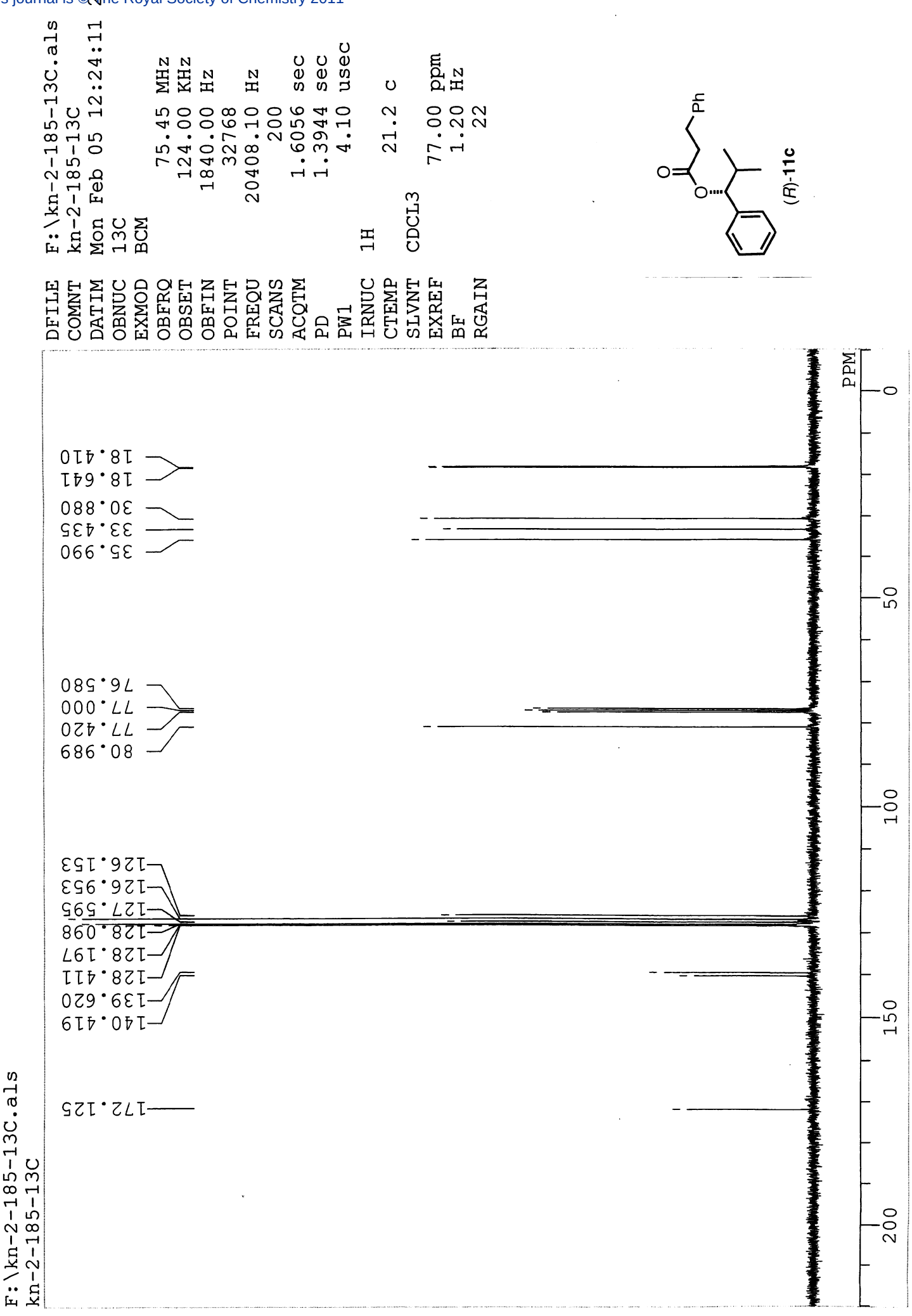
E:\KN-2-185-1H.als
JCAMP-DX Data file

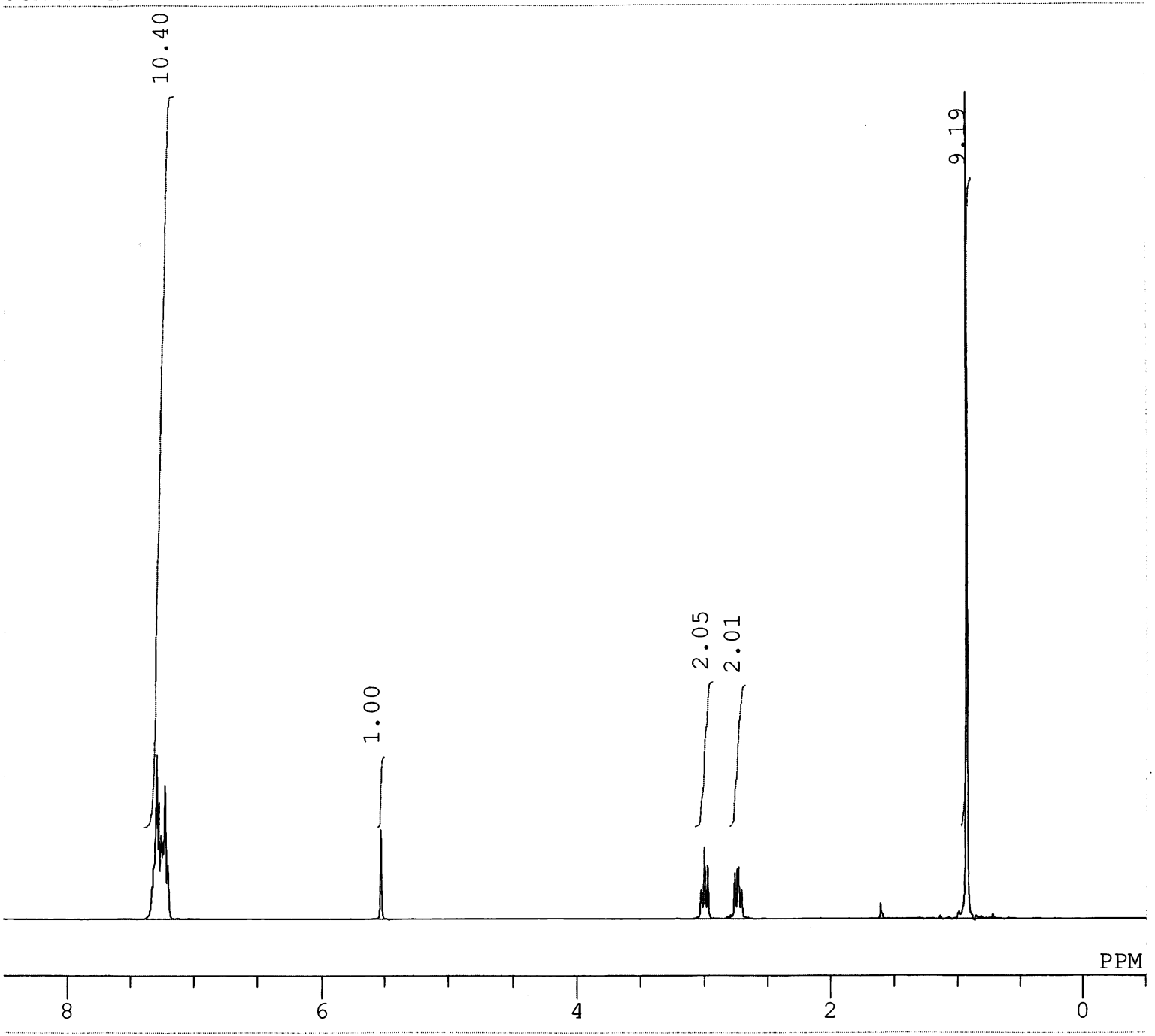


DFILE	E:\KN-2-185-1H.als
COMNT	JCAMP-DX Data file
DATIM	2007/Feb/05 01:18:57
OBNUC	1H
EXMOD	ZG30
OBFRQ	300.01 MHz
OBSET	0.00 KHz
OBFIN	1842.92 Hz
POINT	32768
FREQU	6172.84 Hz
SCANS	8
ACQTM	0.0000 sec
PD	0.0000 sec
PW1	11.70 usec
IRNUC	OFF
CTEMP	22.9 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.25 Hz
RGAIN	81

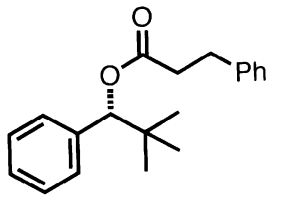


(*R*)-**11c**

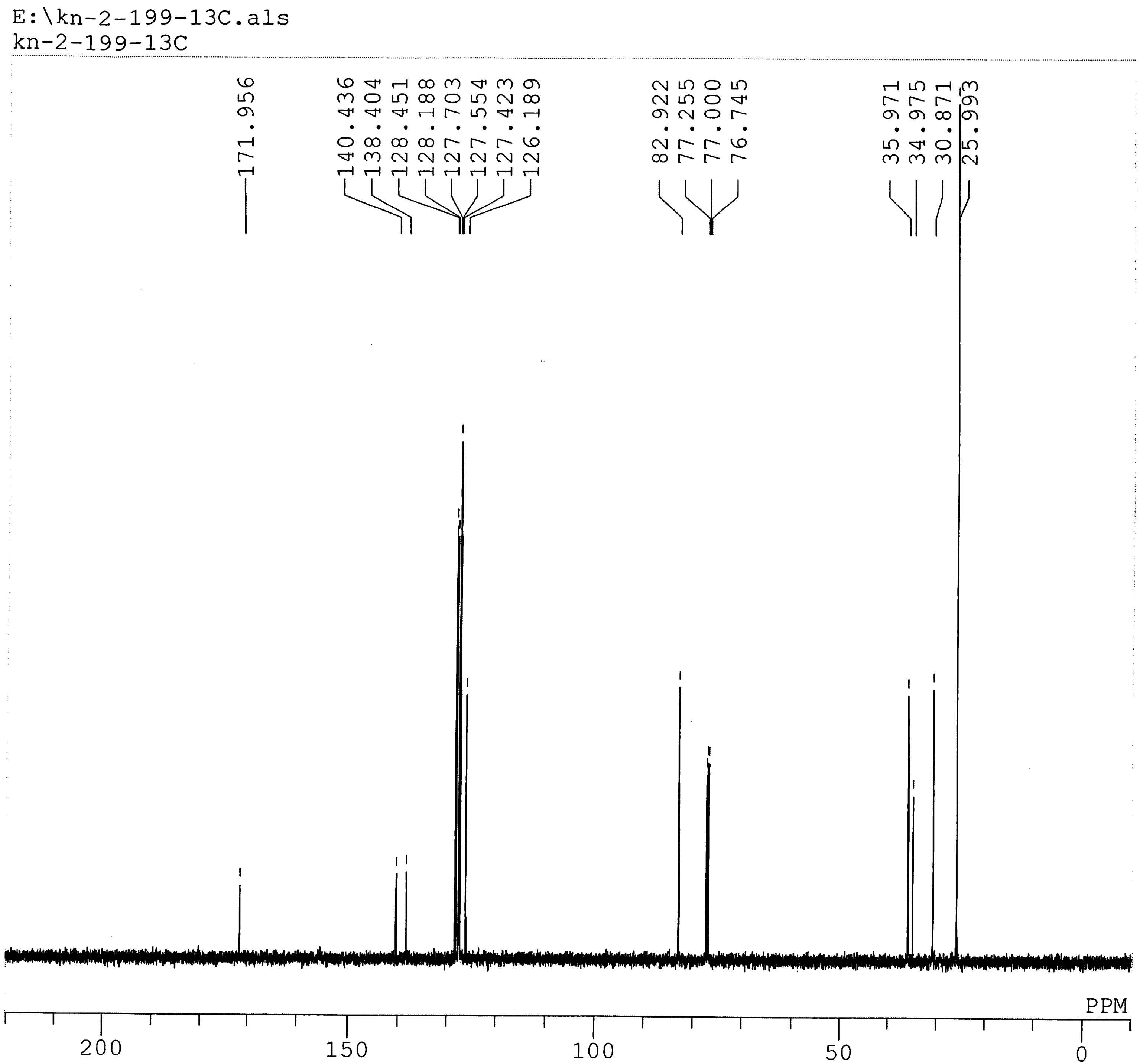

DFILE F:\kn-2-185-13C.als
COMNT kn-2-185-13C
DATIM Mon Feb 05 12:24:11
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.00 Hz
POINT 32768
FREQU 20408.10 Hz
SCANS 200
ACQTM 1.6056 sec
PD 1.3944 sec
PW1 4.10 usec
IRNUC 1H
CTEMP 21.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 22
Ph
(R)-11c
18.410
18.641
30.880
33.435
35.990
76.580
77.000
77.420
80.989
126.153
126.953
127.595
128.098
128.197
128.411
139.620
140.419
172.125
PPM
0
50
100
150
200
F:\kn-2-185-13C.als
kn-2-185-13C



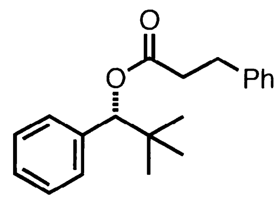
DFILE E:\KN-2-199-1H.als
COMNT JCAMP-DX Data file
DATIM 2007/Feb/15 10:02:57
OBNUC 1H
EXMOD ZG30
OBFRQ 300.01 MHz
OBSET 0.00 KHz
OBFIN 1842.92 Hz
POINT 32768
FREQU 6172.84 Hz
SCANS 8
ACQTM 0.0000 sec
PD 0.0000 sec
PW1 11.70 usec
IRNUC OFF
CTEMP 22.9 c
SLVNT CDCL3
EXREF -4.11 ppm
BF 0.25 Hz
RGAIN 114



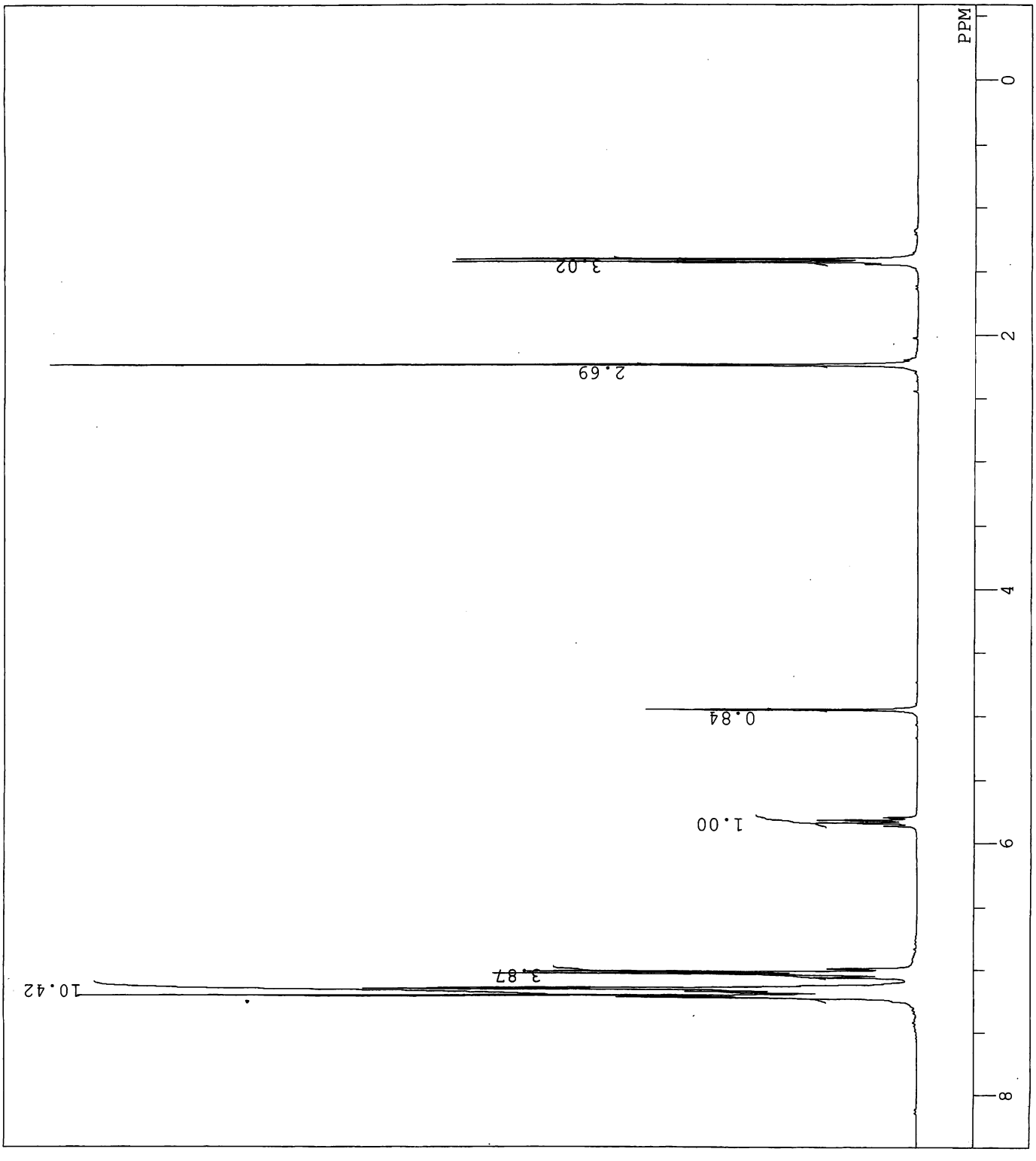
(*R*)-**11d**

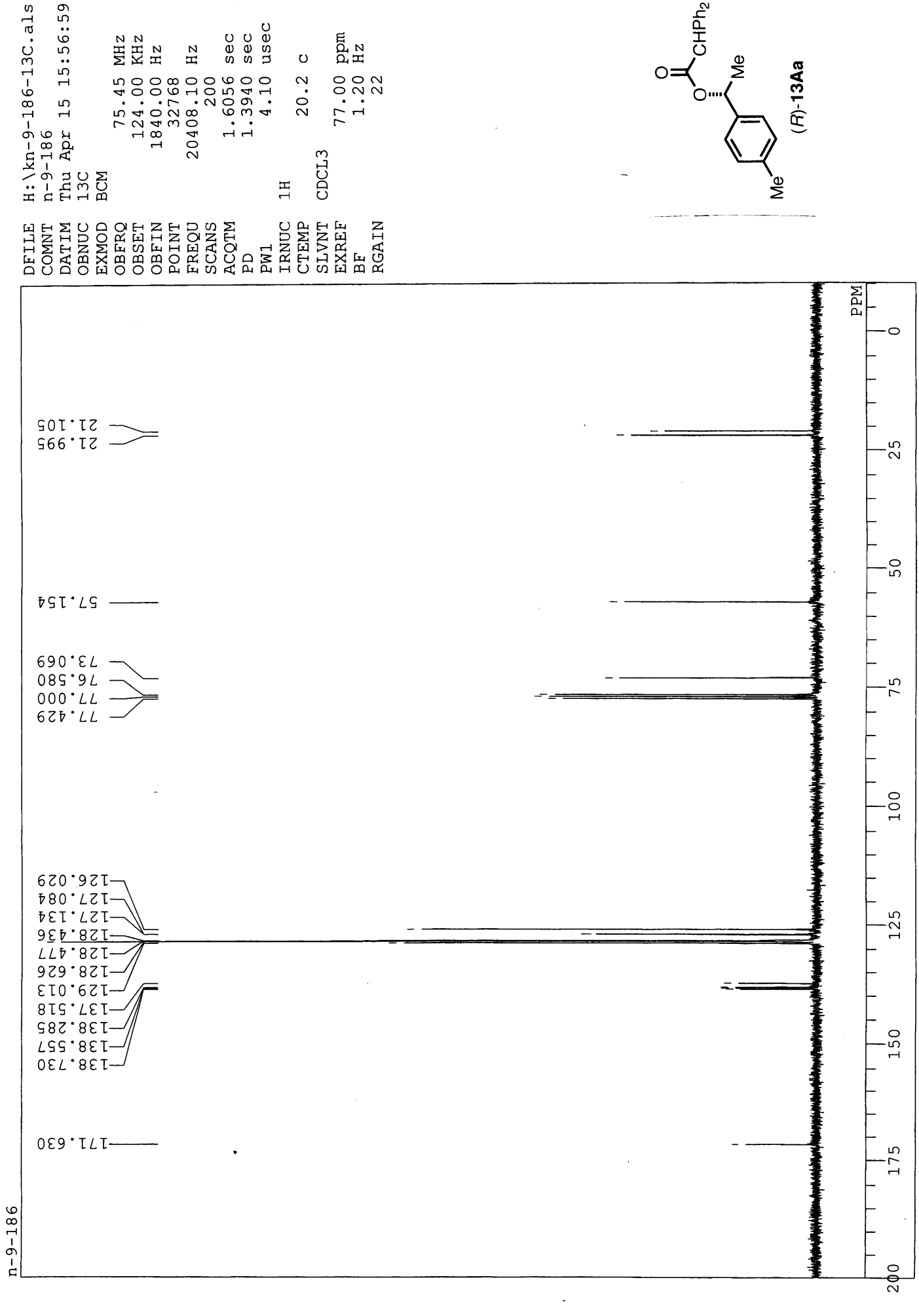


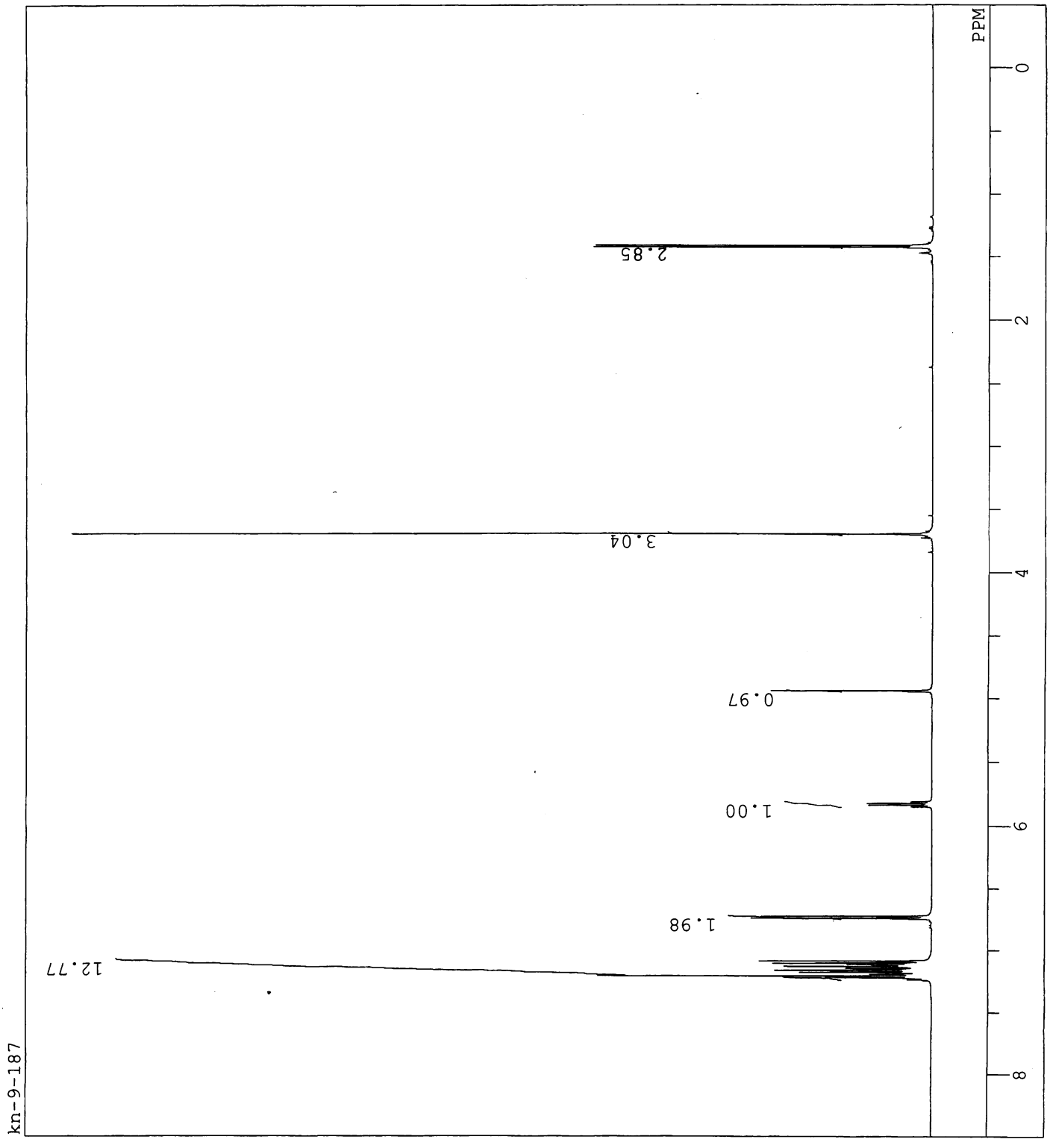
DFILE	E:\kn-2-199-13C.als
COMNT	kn-2-199-13C
DATIM	Thu Feb 15 20:18:12
OBNUC	13C
EXMOD	bcm
OBFRQ	125.65 MHz
OBSET	0.00 KHz
OBFIN	127958.00 Hz
POINT	32768
FREQU	33898.30 Hz
SCANS	100
ACQTM	0.9667 sec
PD	2.0333 sec
PW1	5.10 usec
IRNUC	1H
CTEMP	25.0 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	30

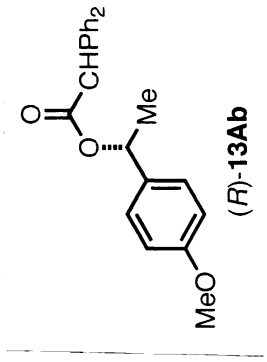


(*R*)-**11d**

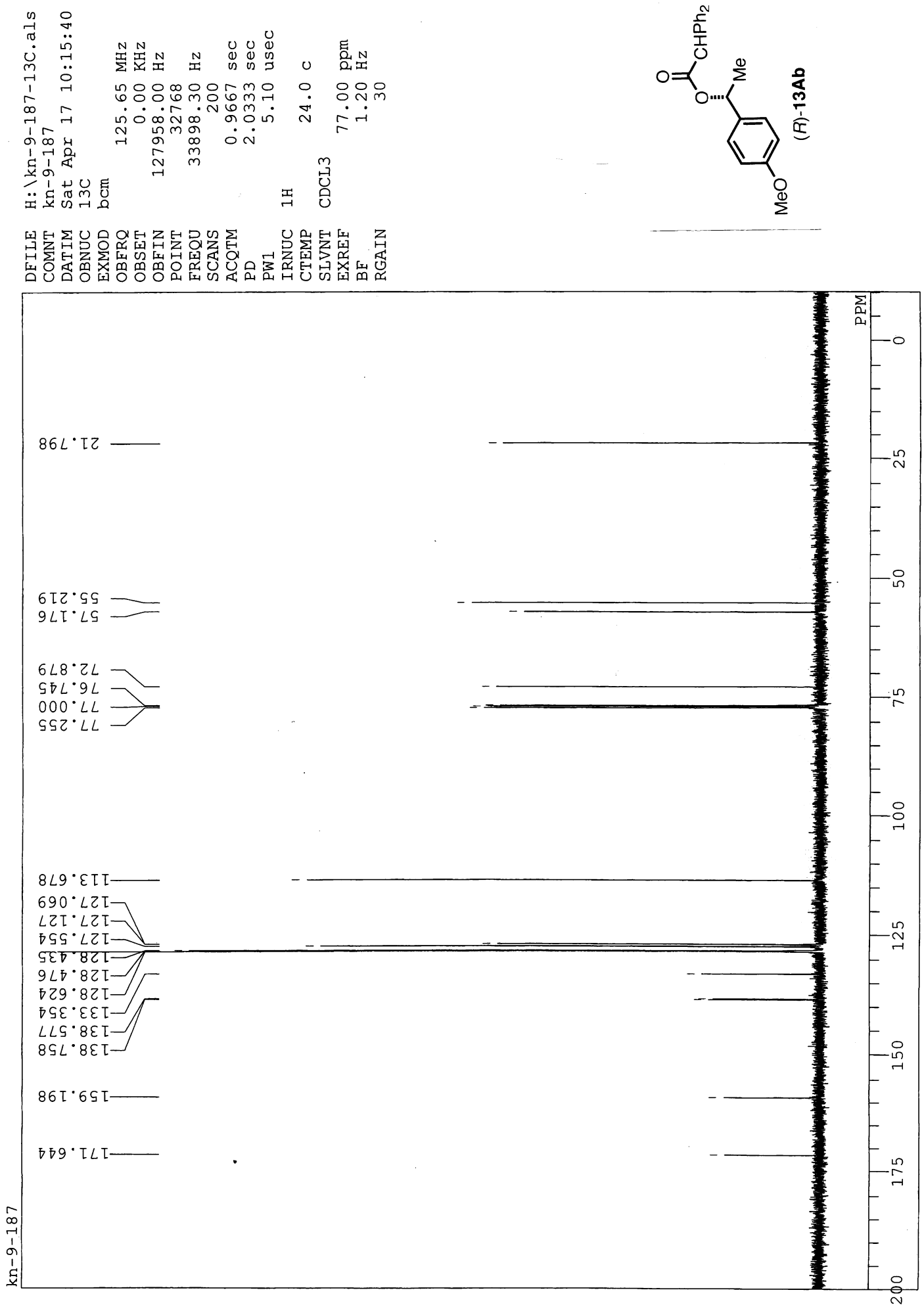


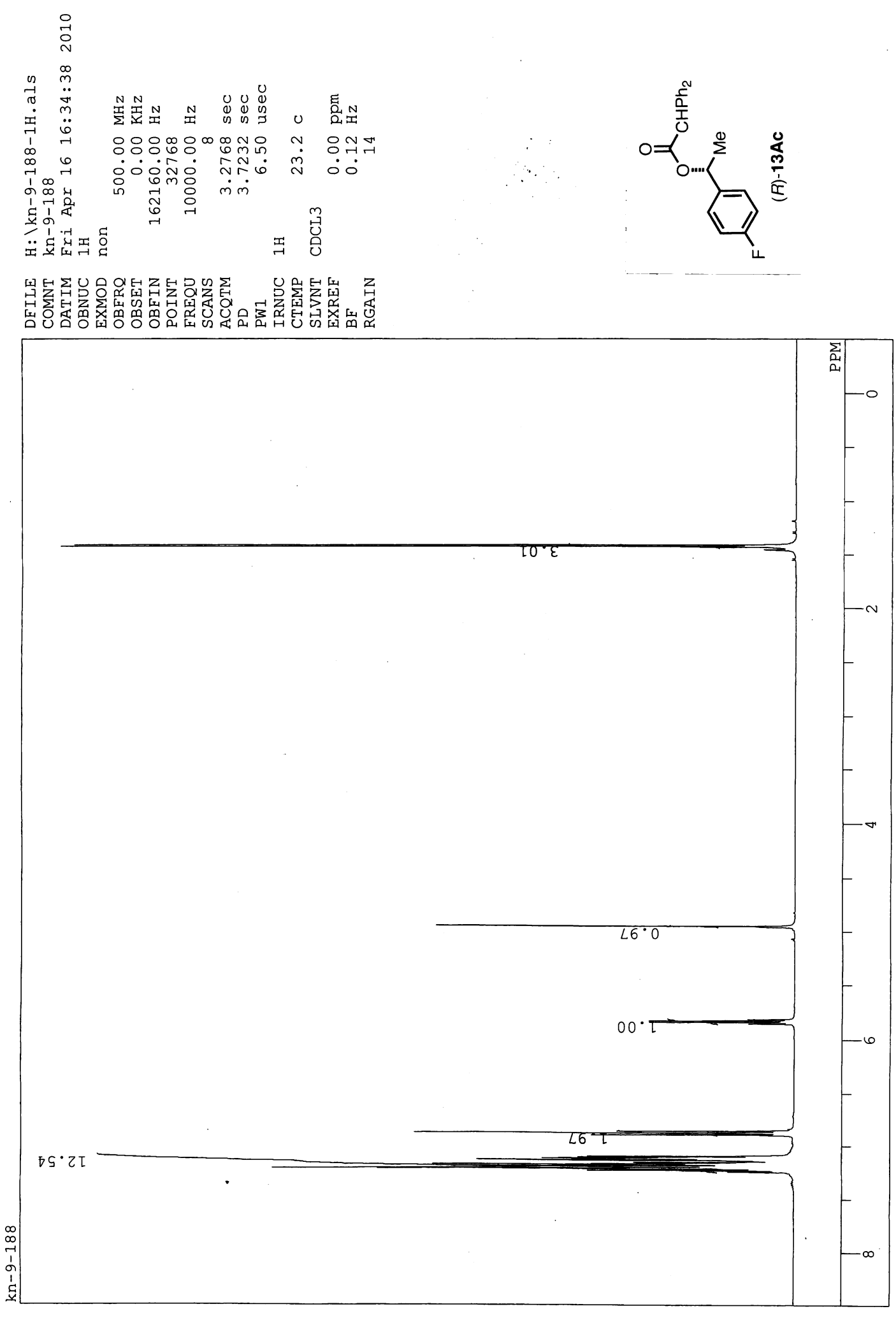


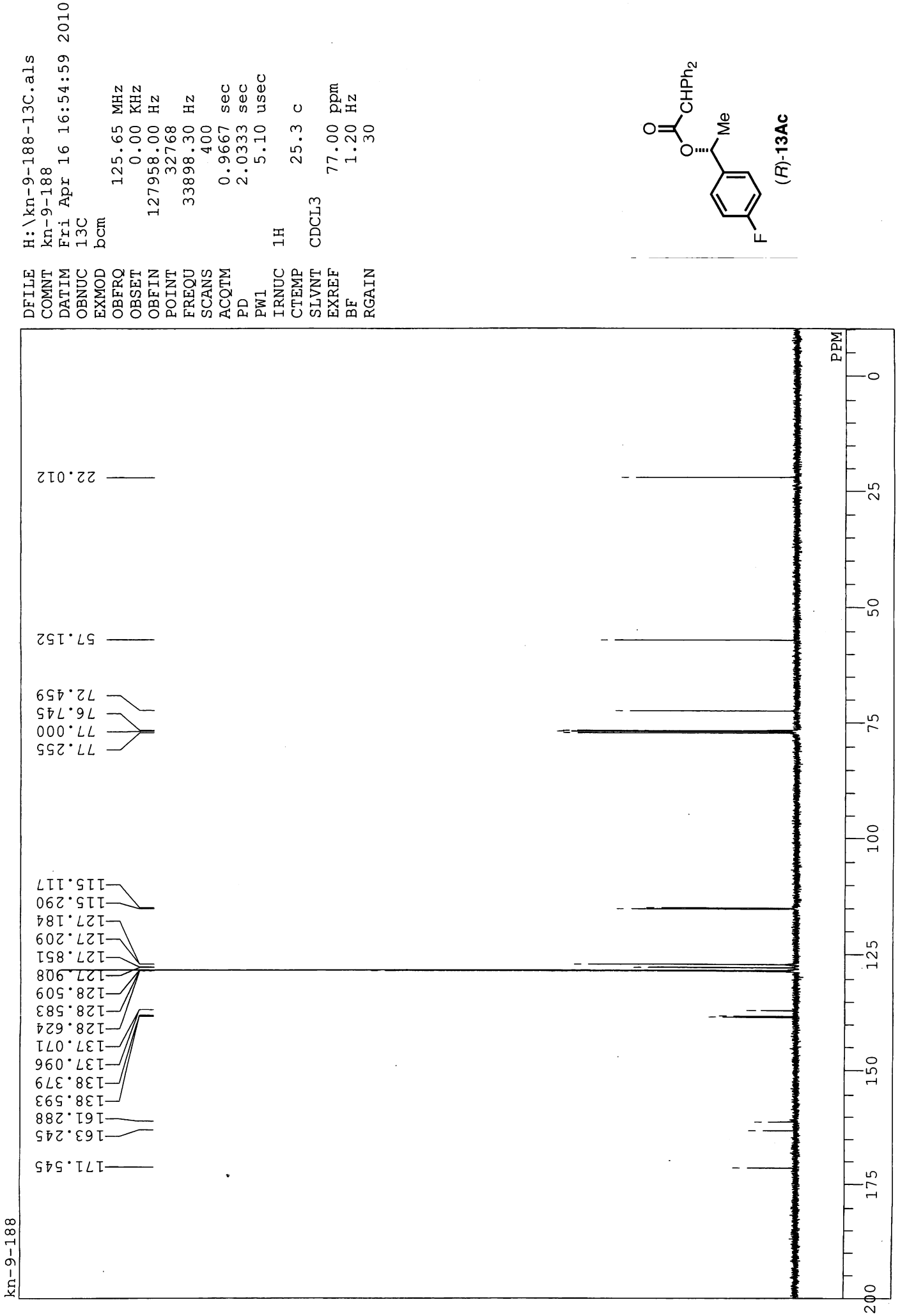


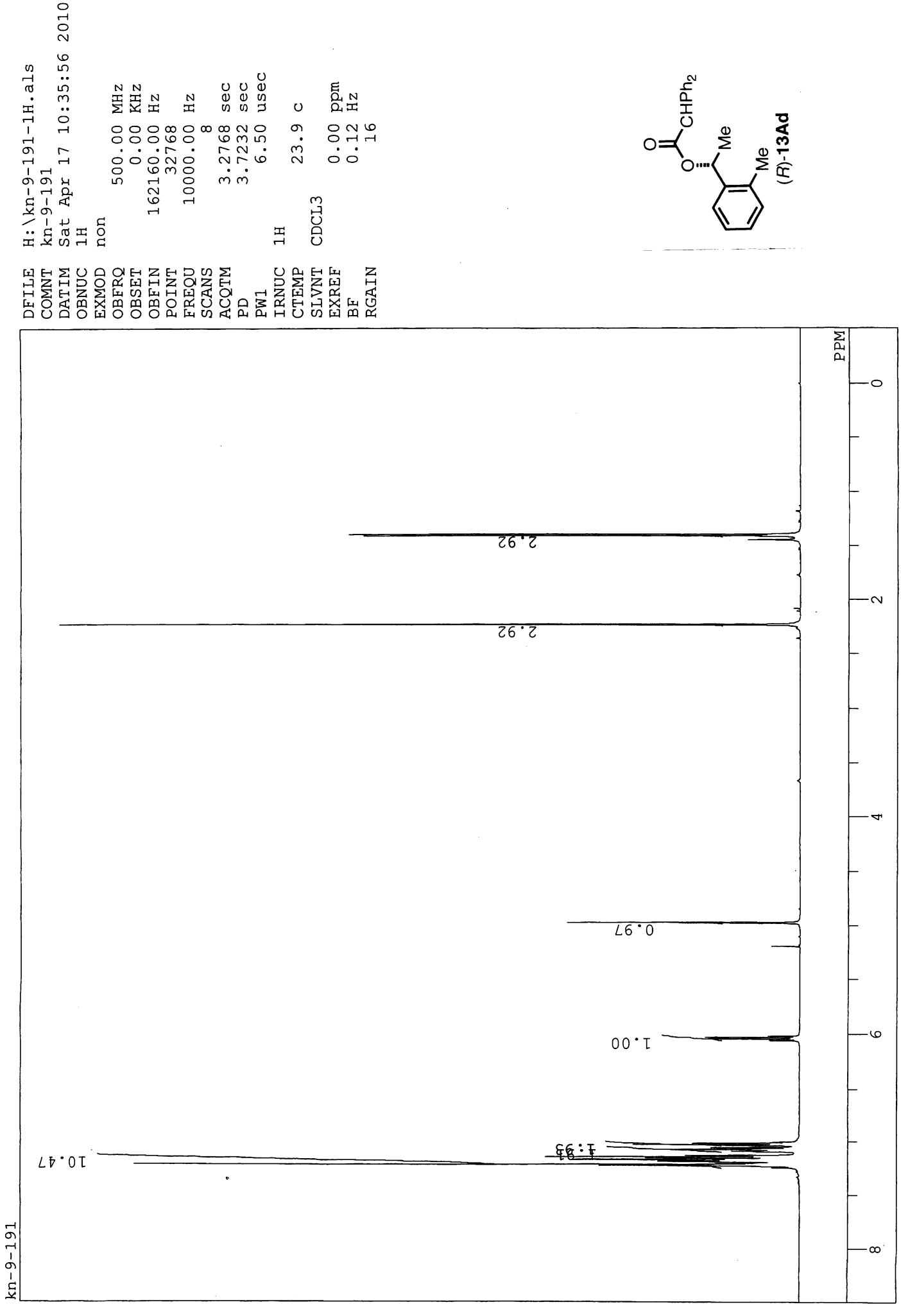


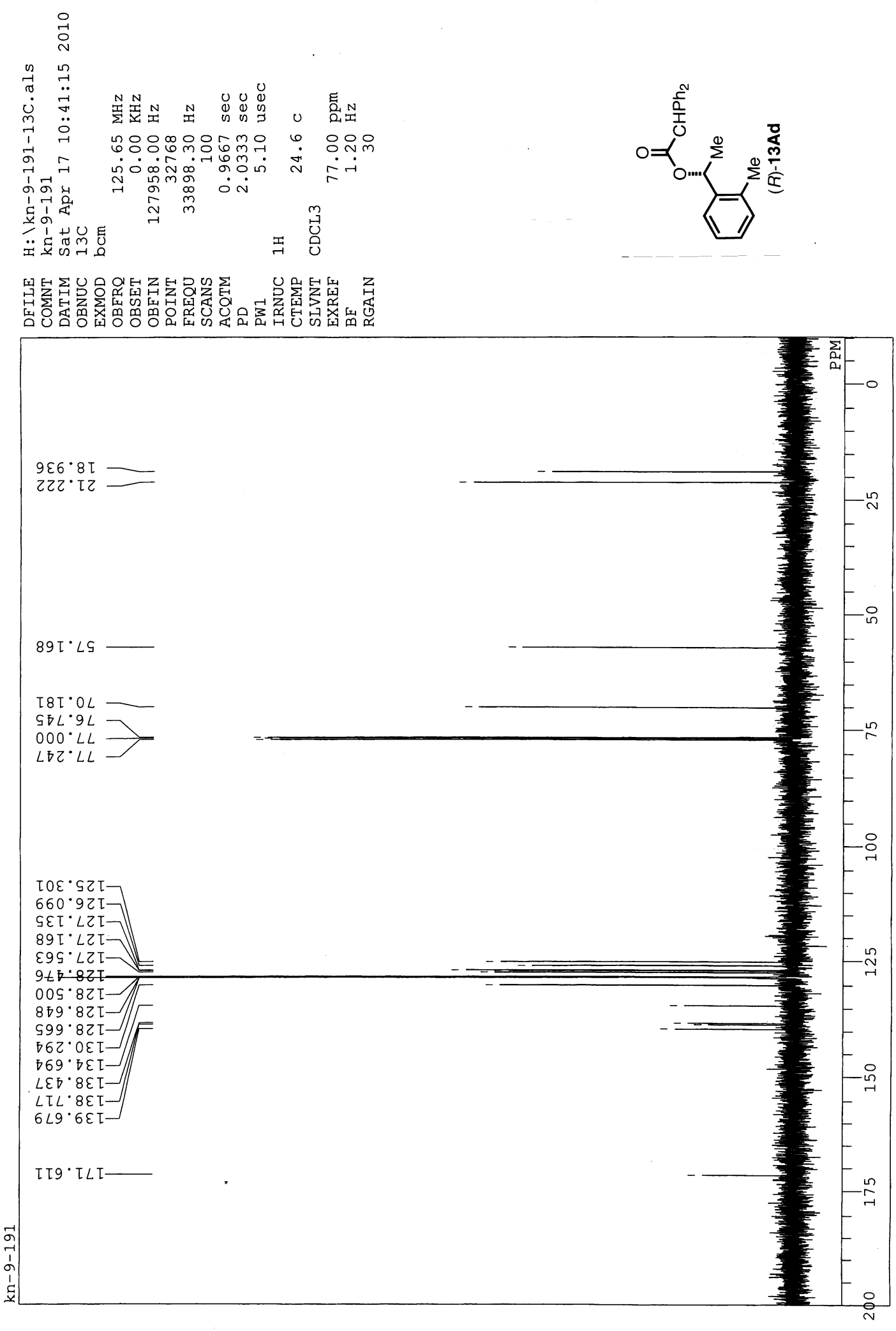
(*R*)-**13Ab**



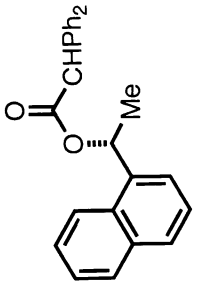




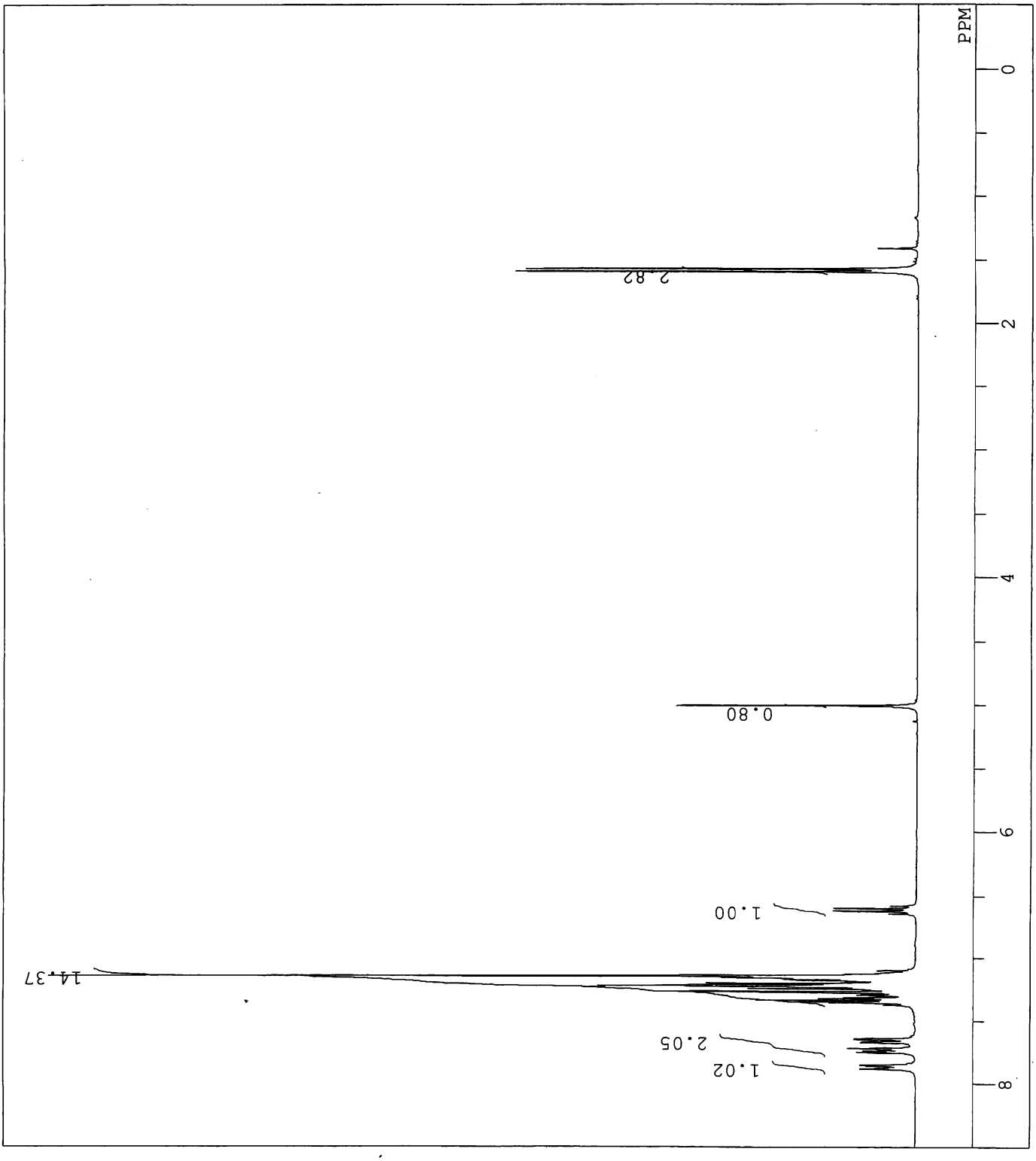


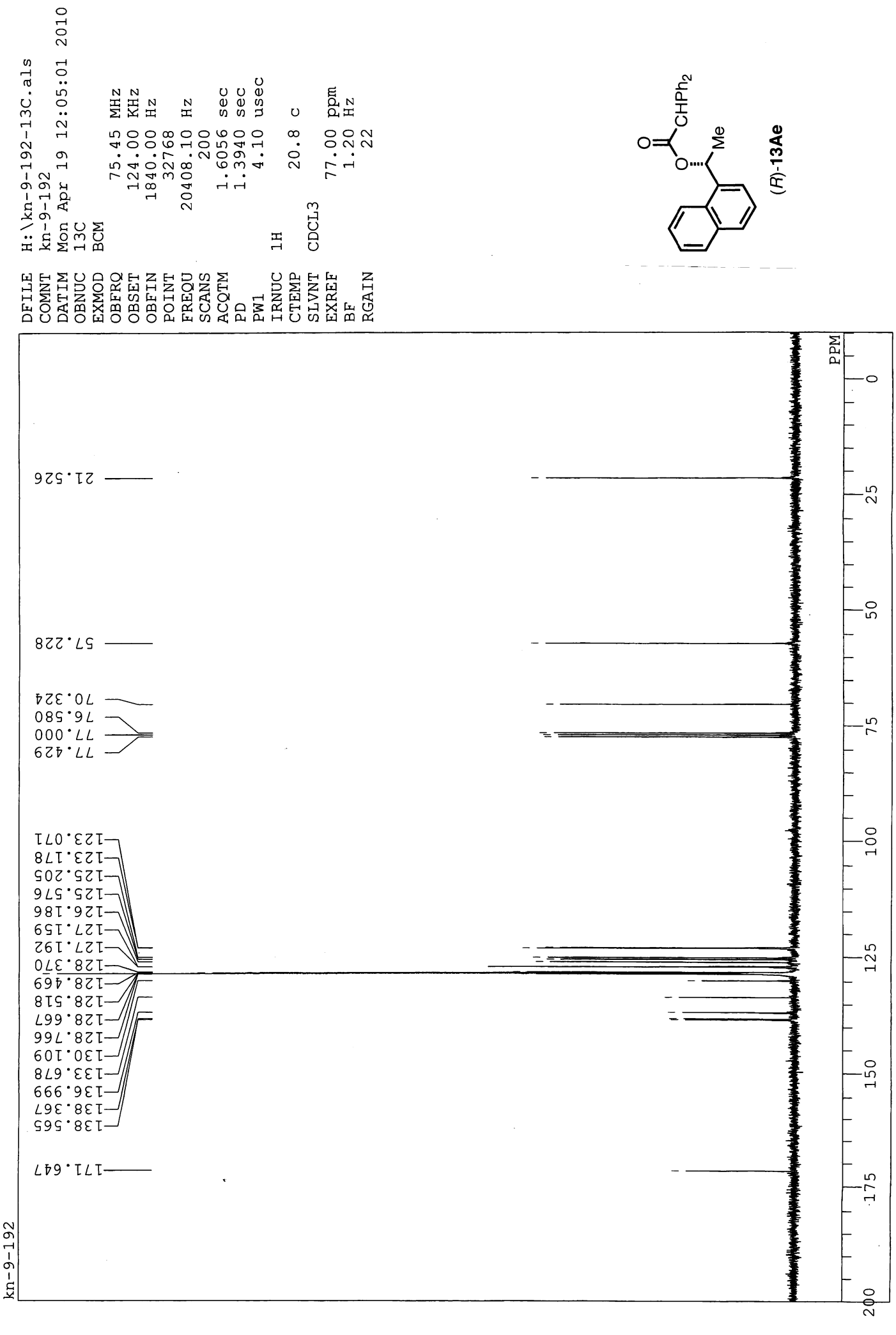


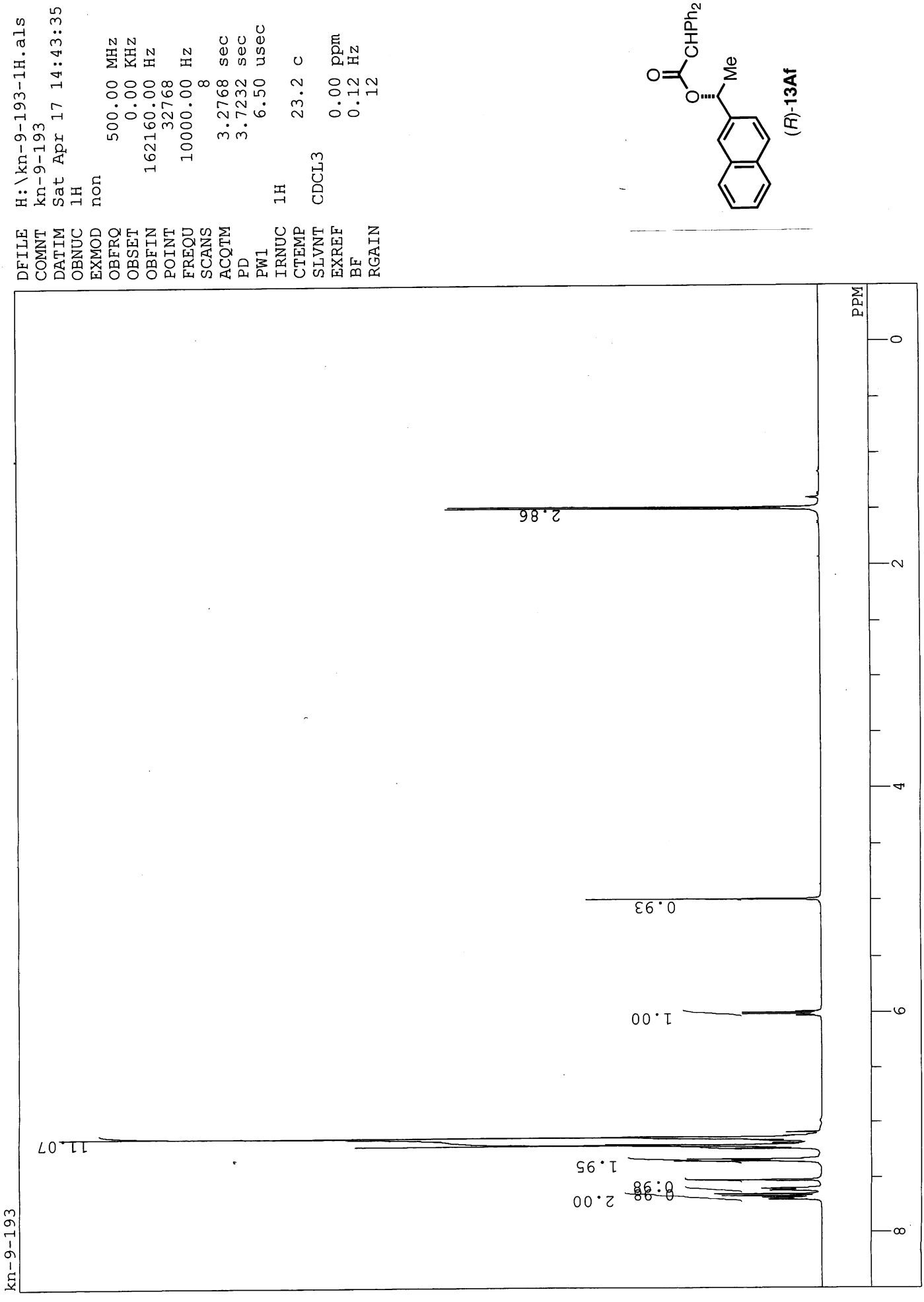
```
DFILE  H:\kn-9-192-1H.als
COMNT  kn-9-192
DATIM  Mon Apr 19 11:54:38 2010
OBNUC  1H
EXMOD  NON
OBFRQ      300.40 MHz
OBSET      130.00 KHz
OBFIN     1150.00 Hz
POINT       32768
FREQU     6020.40 Hz
SCANS            8
ACQTM      5.4428 sec
PD         1.5510 sec
PW1           5.40 usec
IRNUC  1H
CTEMP      20.6 c
SLVNT  CDCL3
EXREF         0.00 ppm
BF            0.12 Hz
RGAIN            9
```

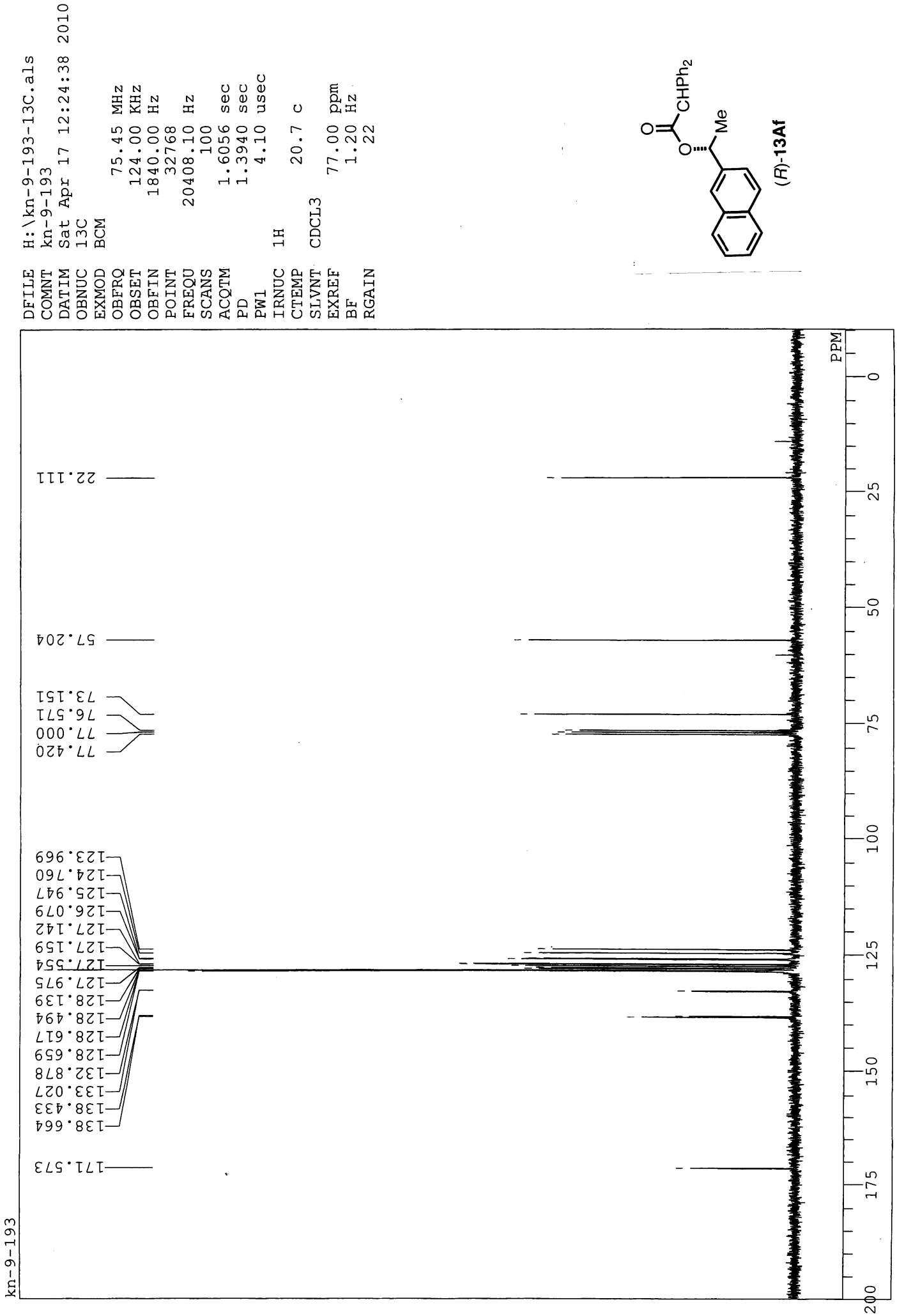


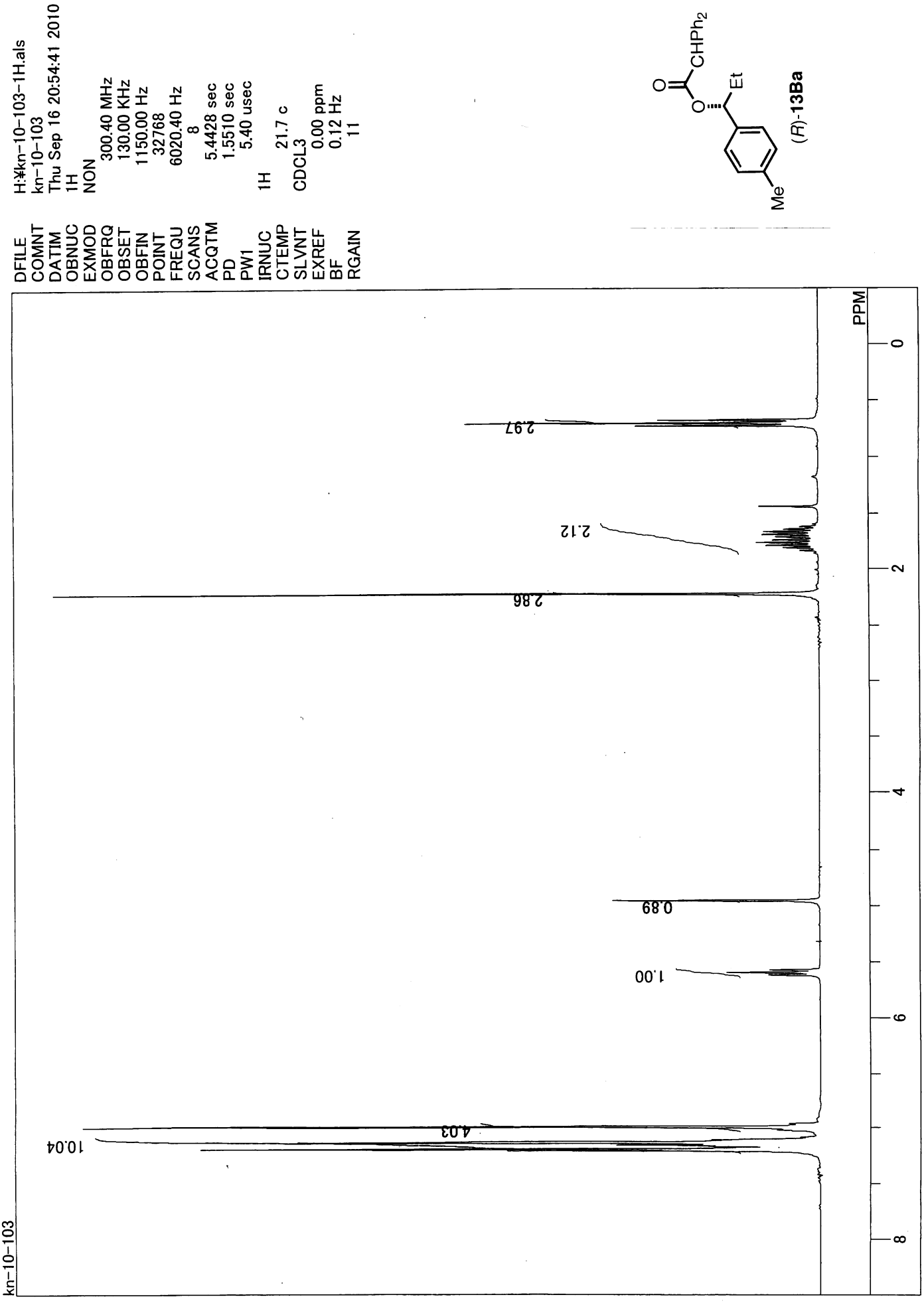
(*R*)-**13Ae**

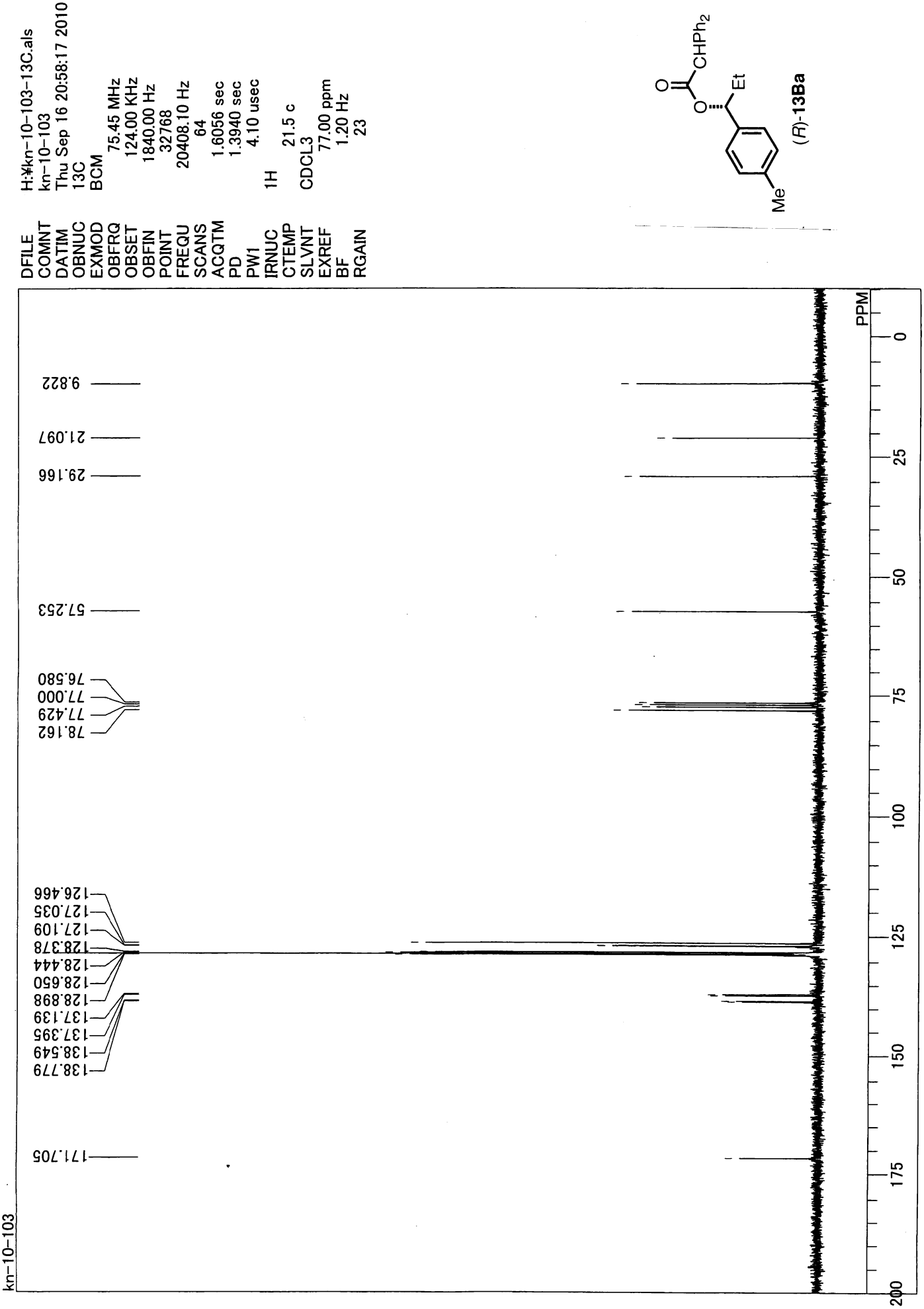


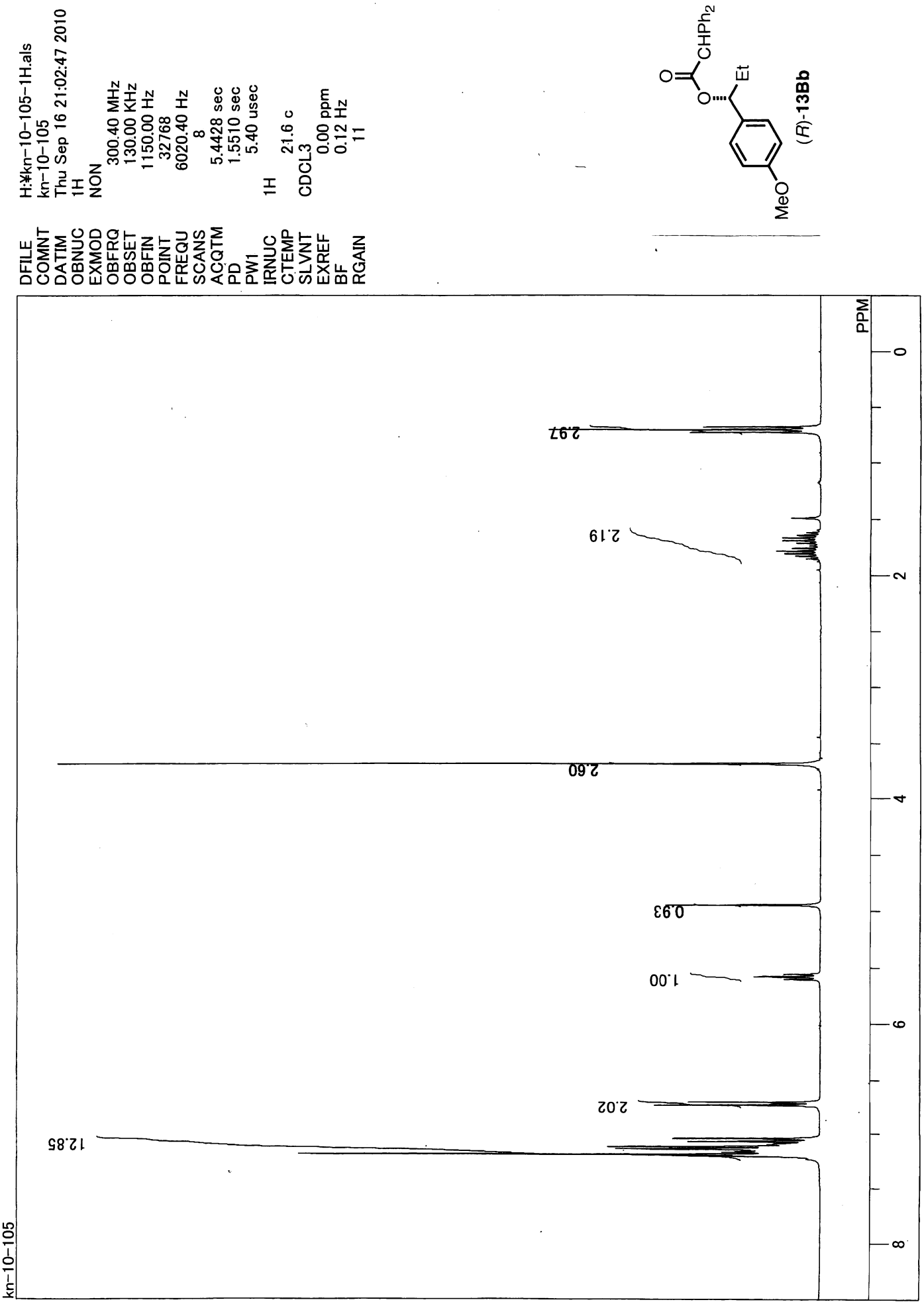


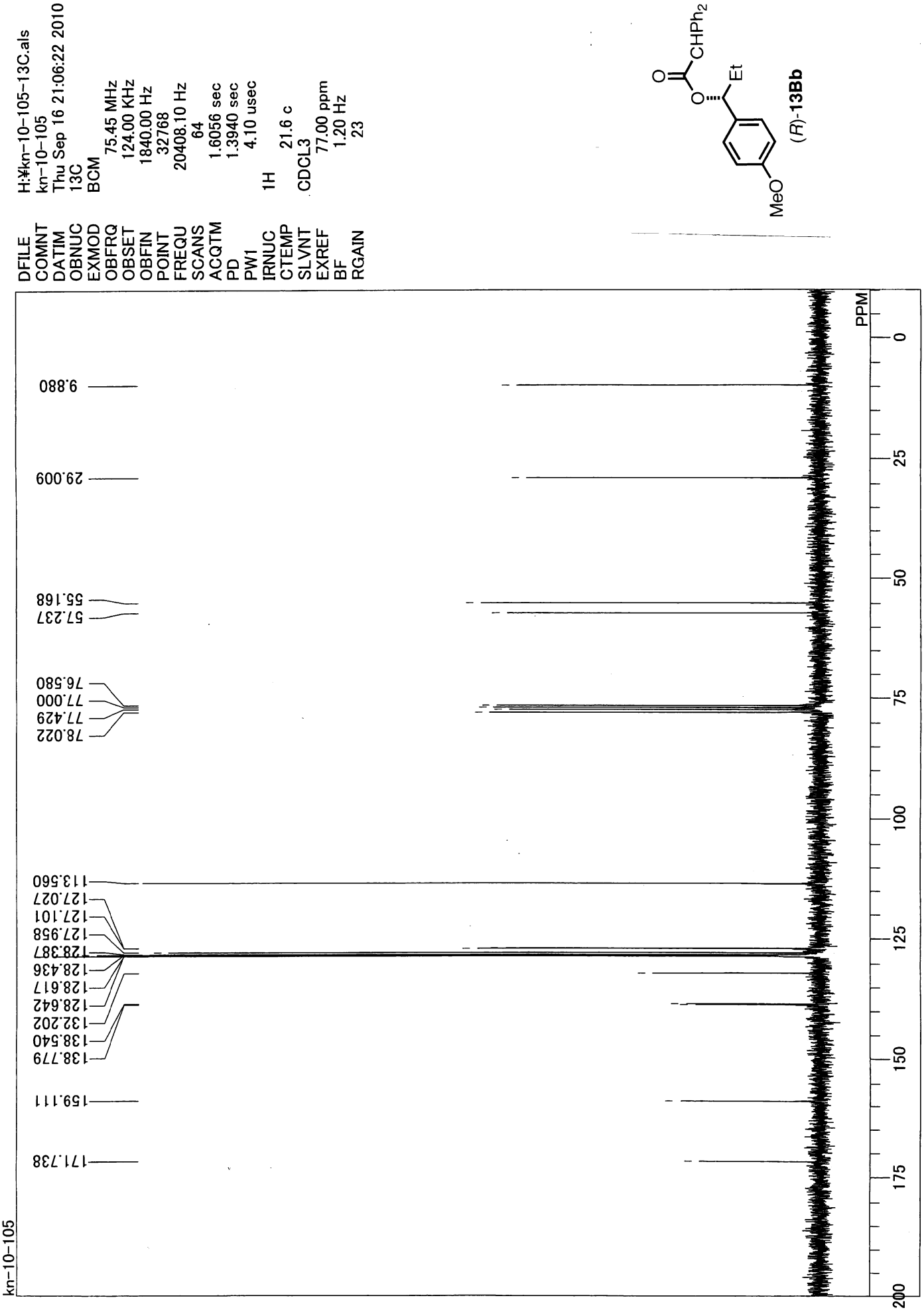

DFILE H:\kn-9-193-1H.als
COMNT kn-9-193
DATIM Sat Apr 17 14:43:35 2010
OBNUC 1H
EXMOD non
OBFRQ 500.00 MHz
OBSET 0.00 KHz
OBFIN 162160.00 Hz
POINT 32768
FREQU 10000.00 Hz
SCANS 8
ACQTM 3.2768 sec
PD 3.7232 sec
PW1 6.50 usec
IRNUC 1H
CTEMP 23.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 12
O
CHPh2
O
Me
(R)-13Af
kn-9-193
11.07
2.00
0.98
0.98
1.95
1.00
0.93
2.86
PPM
0
2
4
6
8

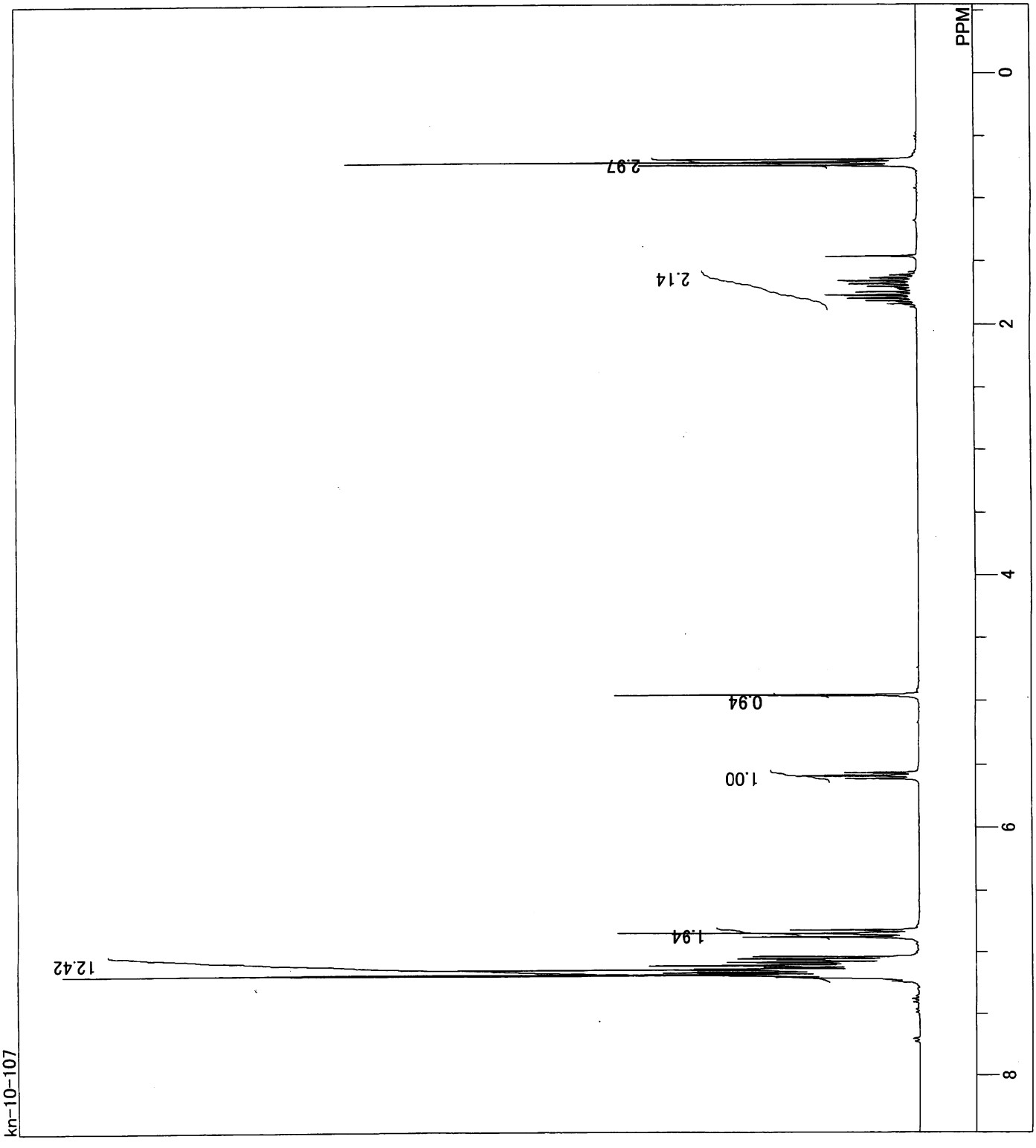




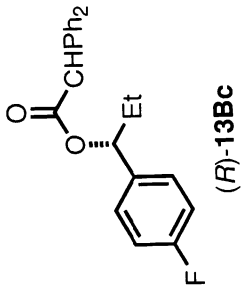




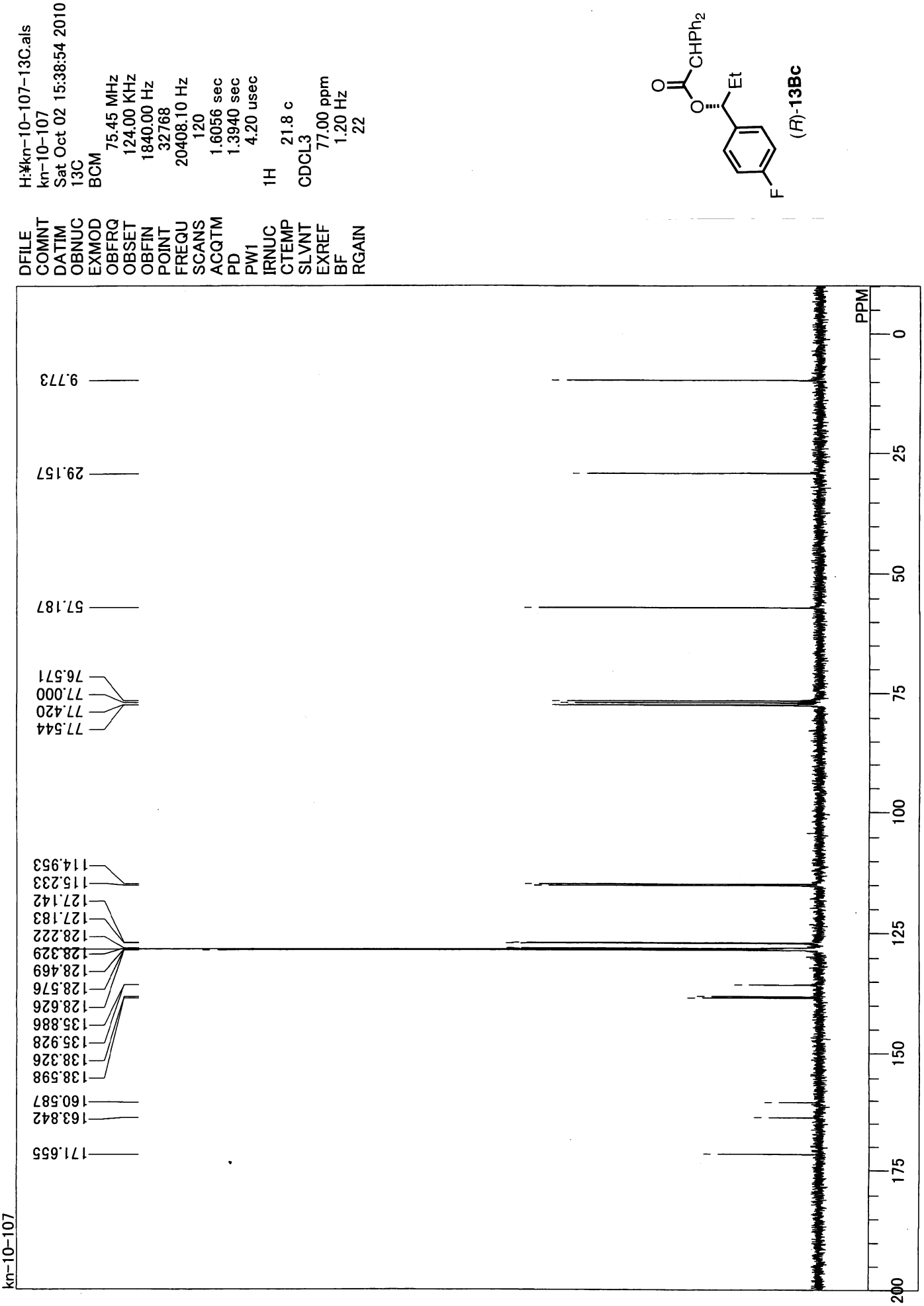


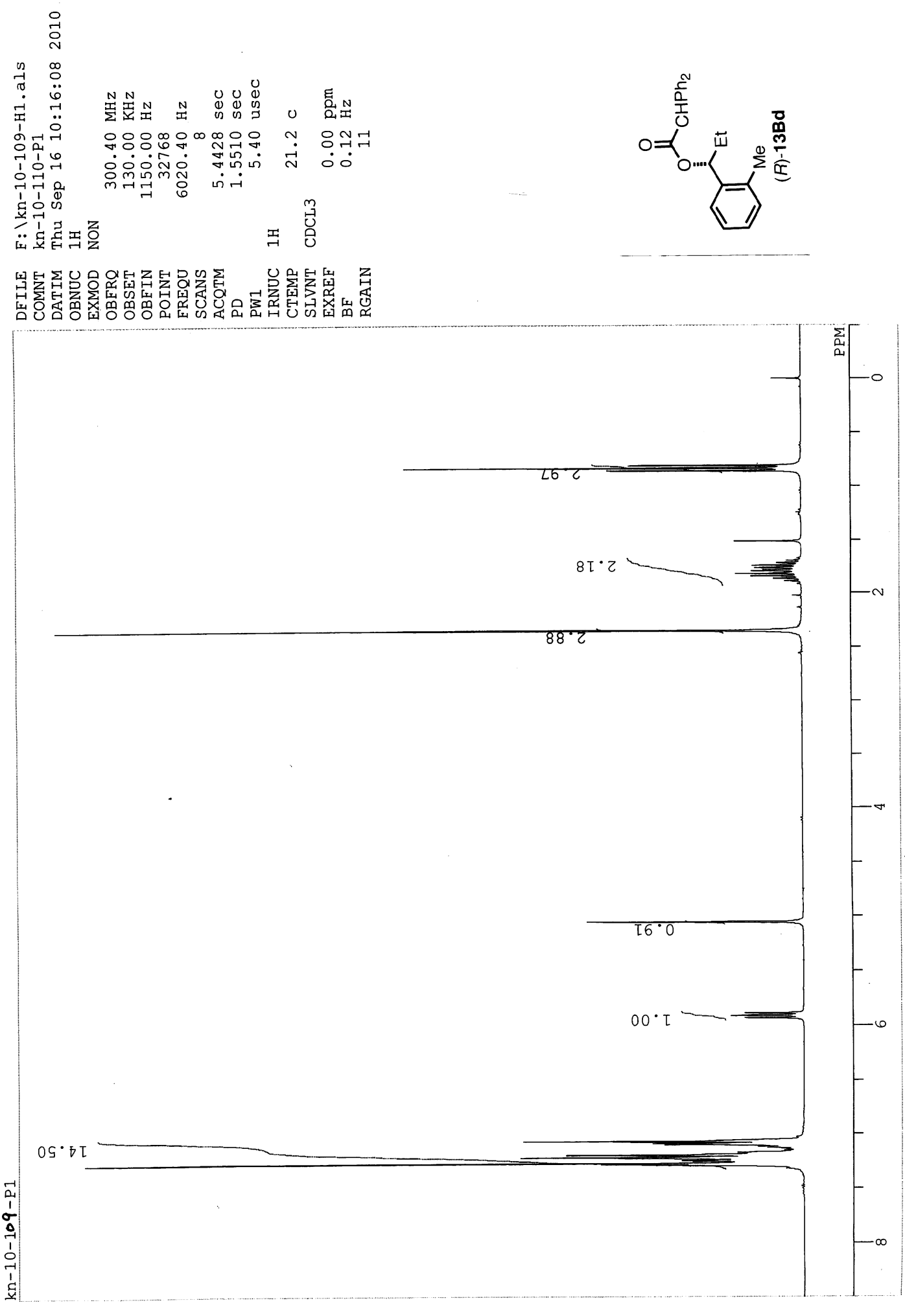


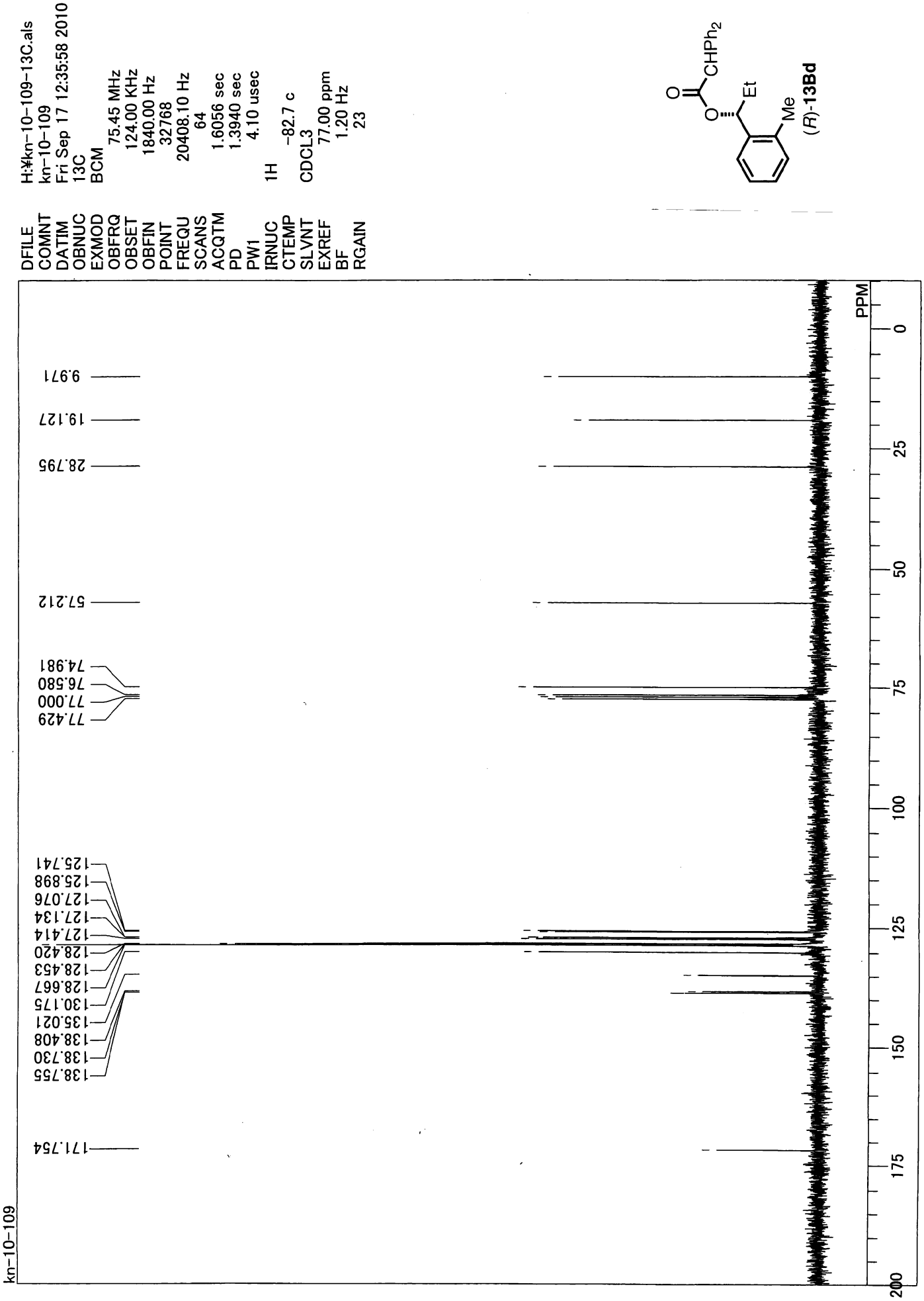
DFILE H:¥kn-10-107-1H.als
COMNT kn-10-107
DATIM Sat Oct 02 15:32:31 2010
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.00 Hz
POINT 32768
FREQU 6020.40 Hz
SCANS 8
ACQTM 5.4428 sec
PD 1.5510 sec
PW1 5.60 usec
IRNUC 1H
CTEMP 21.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 10



(*R*)-**13Bc**






H:¥kn-10-109-13C.als
kn-10-109
Fri Sep 17 12:35:58 2010
13C
BCM
75.45 MHz
124.00 KHz
1840.00 Hz
32768
20408.10 Hz
64
1.6056 sec
1.3940 sec
4.10 usec
1H
-82.7 c
CDCL3
77.00 ppm
1.20 Hz
23
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN
O
CHPh2
O
Et
Me
(R)-13Bd
9.971
19.127
28.795
57.212
74.981
76.580
77.000
77.429
125.741
125.898
127.076
127.134
127.414
128.420
128.453
128.667
130.175
135.021
138.408
138.730
138.755
171.754
kn-10-109
PPM
0
25
50
75
100
125
150
175
200