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Supporting Information

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Supporting Information I

Enantioselective Ene Reaction of Cyclopentadiene and α,β-Enals Catalyzed by Diphenylprolinol Silyl Ether

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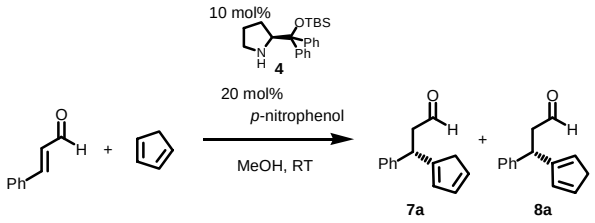
Contents

I. General Procedure. All reactions were carried out under argon and monitored by thin-layer chromatography using Merck 60 F_{254} precoated silica gel plates (0.25 mm thickness). Specific rotations were measured using a JASCO P-1020 polarimeter. FTIR spectra were recorded on a Horiba FT-720 spectrometer. ^{1}H and ^{13}C NMR spectra were recorded on Brucker DPX 400 and Brucker AV 600 instruments. High-resolution mass spectral analyses (HRMS) were carried out using JEOL JMS-SX 102A. Preparative thin layer chromatography was performed using Wakogel B-5F purchased from Wako Pure Chemical Industries, Tokyo, Japan. Flash chromatography was performed using silica gel 60N (spherical, neutral) or 60N (crused, neutral) of Kanto Chemical Co. Int., Tokyo, Japan.

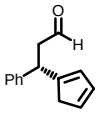
Typical procedure of enantioselective Ene reaction of cyclopentadiene and α,β-enal catalyzed by compound 4.(Table 1, entry 12)



To a solution of catalyst **4** (146.3 mg, 0.40 mmol) and *p*-nitrophenol (110.7 mg, 0.80 mmol) in MeOH (8.0 ml) was added (*E*)-cinnamaldehyde (500 μl, 4.0 mmol) at room temperature. The solution was stirred for 1 minute before the addition of cyclopentadiene (0.98 ml, 12 mmol). After stirring the reaction mixture for 20 h at room temperature, excess cyclopentadiene was azeotropically removed with benzene from the reaction mixture. The residue was purified by silica gel column chromatography (AcOEt/hexane=1/20) to afford ene products **7a** and **8a** (667.2 mg, 84%). The ratio of **7a** and **8**a was determined by 400 MHz ^{1}H-NMR

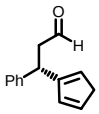
As isomers **7a** and **8a** were separated by HPLC with a OJ-H column (at 254 nm 2-propanol:hexane = 1:200, 1.0 mL/min; **7a** tr = 15.7 min, **8a** tr = 18.0 min), small amount of **7a** and **8a** was isolated and analyzed.

(*R*)-3-(cyclopenta-1,3-dienyl)-3-phenylpropanal (7a)



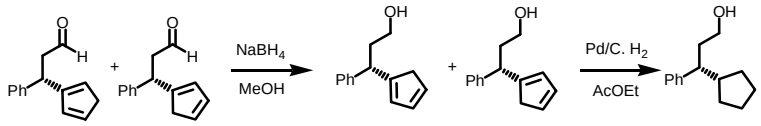
^{1}H NMR ($CDCl_3$) δ 2.77 (1H, dd, *J*=15.6, 0.8 Hz), 2.83 (1H, dd, *J*=15.6, 0.8 Hz), 2.93 (1H, ddd, *J*=10.8, 5.2, 1.2 Hz), 3.06 (*J*=10.8, 5.2, 1.2 Hz), 4.45 (1H, t, *J*=5.2 Hz), 6.26-6.29 (2H, m), 6.40-6.42 (1H, m), 7.17-.7.23 (3H, m), 7.27-7.32 (2H, m), 9.72 (1H, t, *J*=1.2 Hz); ^{13}C NMR ($CDCl_3$) δ 41.4, 42.5, 49.2, 126.8, 127.5, 128.7, 131.9, 132.2, 143.3, 150.3, 201.5.

(*R*)-3-(cyclopenta-1,4-dienyl)-3-phenylpropanal (8a)



^{1}H NMR ($CDCl_3$) δ 2.93 (1H, ddd, *J*=11.2, 4.8, 1.2 Hz), 3.00 (2H, s), 3.06 (1H, ddd, *J*= 11.2, 5.2, 1.6 Hz), 4.32 (1H, t, *J*=5.2 Hz), 6.09-6.12 (1H, m), 6.30-6.33 (1H, m), 6.40-6.42 (1H, m), 7.20-7.23 (3H, m), 7.28-7.32 (2H, m), 9.73 (1H, t, *J*=1.2 Hz); ^{13}C NMR ($CDCl_3$) δ 40.5, 41.3, 48.8, 126.7, 126.8, 127.9, 128.7, 133.6, 134.6, 142.4, 148.2, 201.7.

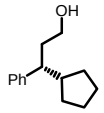
Typical procedure of the determination of enantiomeric excess of Ene product 7 and 8 (Table 1, entry 5)



To a MeOH solution (0.65 ml) of the **7a** and **8a** (12.8 mg, 0.065 mmol) was added $NaBH_4$ (7.3 mg, 0.194 mmol) at 0 °C and stirred for 20 min at that temperature. The reaction mixture was quenched with pH 7.0 phosphate buffer solution. The organic materials were extracted with AcOEt and dried over anhydrous Na_2SO_4, the extracts were concentrated under reduced pressure which was used in the next reaction without further purification.

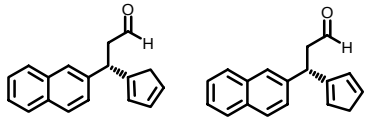
To a solution of this crude mixture in AcOEt (0.65 ml) was added 10% Pd/C (3.2 mg) at room temperature and stirred for overnight under H_2 atmosphere. The reaction mixture was filtered through a pad of Celite and concentrated in vacuo. The residue was purified by preparative thin-layer chromatography (AcOEt/hexane=1/3) to afford (*R*)-3-cyclopentyl-3-phenylpropan-1-ol (13.2 mg, quant).

(*R*)-3-cyclopentyl-3-phenylpropan-1-ol



^{1}H NMR ($CDCl_3$) δ 0.98-1.11 (1H, m), 1.24-1.77 (1H, m), 1.86 (1H, quint, *J*=5.6 Hz), 1.95-2.20 (3H, m), 2.44-2.53 (1H, m), 3.39-3.56 (2H, m), 7.19-7.26 (3H, m), 7.34 (2H, t, *J*=7.2 Hz); ^{13}C NMR ($CDCl_3$) δ 24.9, 25.2, 31.5, 31.7, 38.1, 46.6, 48.8, 61.3, 126.0, 127.9, 128.2, 144.5; IR (neat) ν 3325, 2950, 2868, 1495, 1451, 1046, 764, 701 cm^{-1}; HRMS (ESI): $[M+Na]^+$ calculated for $C_{14}H_{20}ONa$: 227.1406, found 227.1411; $[\alpha]_D^{31}$ 17.1 (*c*=0.82, $CHCl_3$), 92% *ee*; The enantiomeric excess was determined by HPLC with a AS-H column at 254 nm (2-propanol:hexane = 1:200), 1.0 mL/min; major enantiomer tr = 13.4 min, minor enantiomer tr = 11.5 min.

(*R*)-3-(cyclopenta-1,3-dienyl)-3-(naphthalen-2-yl)propanal (7b) and (*R*)-3-(cyclopenta-1,4-dienyl)-3-(naphthalen-2-yl)propanal (8b)

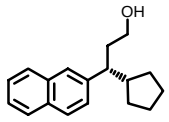


7b:8b=1:1

^{1}H NMR ($CDCl_3$) δ 2.74-2.91 (1H, m), 2.99-3.08 (2H, m), 3.13 (1H, ddd, *J*=16.8, 7.6, 2.0 Hz), 4.46-4.55 (1H, m), 6.14-6.19 (0.5H, m), 6.26-6.31 (0.5H, m), 6.31-6.36 (1H,

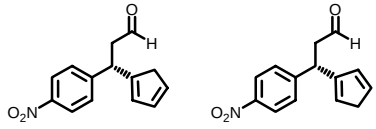
m), 6.39-6.46 (1H, m), 7.28-7.36 (1H, m), 7.40-7.50 (2H, m), 7.65 (1H, d, *J*=10.8 Hz), 7.74-7.84 (3H, m), 9.74-9,79 (1H, m); ^{13}C NMR ($CDCl_3$) δ 40.7, 41.3, 41.6, 42.6, 48.7, 49.1, 125.70, 125.71, 125.9, 126.0, 126.14, 126.16, 126.19, 126.32, 127.6, 127.7, 128.46, 128.53, 201.2, 201.4; IR (neat) ν 3056, 1722, 1362, 897, 821, 749 cm^{-1}.

(*R*)-3-cyclopentyl-3-(naphthalen-2-yl)propan-1-ol



^{1}H NMR ($CDCl_3$) δ 0.93-1.15 (2H, m), 1.17-1.74 (4H, m), 1.82-2.24 (4H, m), 2.50-2.68 (1H, m), 3.30-3.55 (2H, m), 7.30-7.37 (1H, m), 7.38-7.49 (2H, m), 7.56 (1H, bs), 7.71-7.85 (3H, m); ^{13}C NMR ($CDCl_3$) δ 24.9, 25.3, 31.6, 31.8, 38.0, 46.6, 48.9, 61.4, 125.2, 125.9, 126.0, 126.6, 127.5, 127.6, 128.0, 132.3, 133.5, 142.5; IR (neat) ν 3331, 2949, 2867, 1507, 1450, 1046, 853, 818, 746, 477 cm^{-1}; HRMS (ESI): $[M+Na]^+$calculated for $C_{18}H_{22}O_1Na_1$: 277.1563, found 277.1555. ; $[\alpha]_D^{20}$ 6.8 (c=0.78, MeOH), 93% *ee*; The enantiomeric excess was determined by HPLC with a AS-H column at 279 nm (2-propanol:hexane = 1:200), 1.0 mL/min; major enantiomer tr = 17.1 min, minor enantiomer tr = 19.9 min.

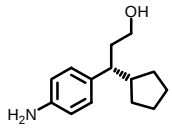
(*R*)-3-(cyclopenta-1,3-dienyl)-3-(4-nitrophenyl)propanal (7c) and **(*R*)-3-(cyclopenta-1,4-dienyl)-3-(4-nitrophenyl)propanal (8c)**



7c:8c=4:6

^{1}H NMR ($CDCl_3$) δ 2.68-2.89 (0.8H, m), 2.94-3.05 (2.2H, m), 3.15 (1H, dd, *J*=17.2, 7.2 Hz), 4.42-4.51 (1H, m), 6.24-6.29 (0.6H, m), 6.29-6.35 (0.8H, m), 6.40-6.48 (1H, m), 7.39 (2H, d, *J*=8.8 Hz), 8.16 (2H, d, *J*=8.4 Hz), 9.73-9.77 (1H, m); ^{13}C NMR ($CDCl_3$) δ 40.0, 40.8, 41.4, 42.5, 48.5, 48.9, 125.70, 123.88, 123.95, 127.6, 128.49, 128.55, 128.8, 131.9, 132.6, 132.8, 135.3, 146.8, 148.3, 150.1, 150.9, 199.7, 199.8; IR (neat) ν 2849, 2729, 1724, 1596, 1518, 1518, 1347 cm^{-1}.

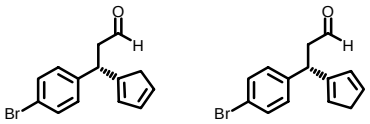
(*R*)-3-(4-aminophenyl)-3-cyclopentylpropan-1-ol



^{1}H NMR ($CDCl_3$) δ 0.91-1.08 (1H, m), 1.12-1.30 (2H, m), 1.31-1.79 (5H, m), 1.82-2.10 (3H, m), 2.24-2.37 (1H, m), 3.33-3.54 (2H, m), 6.62 (2H, d, *J*=8.4 Hz), 6.94 (2H, d, *J*=8.4 Hz); ^{13}C NMR ($CDCl_3$) δ 24.9, 25.3, 29.7, 31.5, 31.6, 38.2, 46.8, 48.0, 61.6,

115.3, 128.7, 135.1, 144.3; IR (neat) ν 3347, 2949, 2867, 1621, 1515, 1265, 1045, 828, 757, 533 cm^{-1}; HRMS (ESI): $[M+Na]^+$calculated for $C_{14}H_{21}O_1N_1Na_1$: 242.1515, found 242.1511. ;$[\alpha]_D^{20}$ 13.5 (c=1.17, MeOH), 90% *ee*; The enantiomeric excess was determined by HPLC with a AS-H column at 261 nm (2-propanol:hexane=1:100), 1.0 mL/min; major enantiomer tr = 9.4 min, minor enantiomer tr = 13.8 min.

(*R*)-3-(4-bromophenyl)-3-(cyclopenta-1,3-dienyl)propanal (7d) and **(*R*)-3-(4-bromophenyl)-3-(cyclopenta-1,4-dienyl)propanal (8d)**

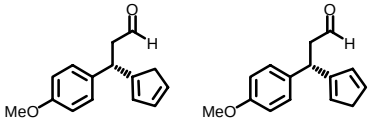


7d:8d=1:1

^1H NMR ($CDCl_3$) δ 2.69-2.86 (1H, m), 2.90 (1H, ddt, J_d=16.8, 7.2 Hz, *J*t=2.0 Hz), 2.98-3.02 (1H, m), 3.05 (1H, dd, *J*=16.8, 7.6 Hz), 4.25-4.35 (1H, m), 6.08-6.11 (0.5H, m), 6.24-6.31 (1.5H, m), 6.39-6.45 (1H, m), 7.08 (2H, t, *J*=8.8 Hz), 7.41 (2H, d, *J*=8.4 Hz), 9.70-9.75 (1H, m); ^{13}C NMR ($CDCl_3$) δ 39.9, 40.7, 41.3, 42.5, 48.7, 49.1, 120.5, 120.6, 127.0, 127.8, 129.4, 129.6, 131.77, 131.81, 131.85, 132.3, 134.8, 141.5, 142.4, 147.7, 149.6, 200.7, 200.9; IR (neat) ν 1723, 1488, 1403, 1366, 1010, 897, 827, 684 cm^{-1}.

Enantiomeric excess of compounds 7d and 8e were determined by HPLC analysis after the conversion to 3-cyclopentyl-3-phenylpropan-1-ol.

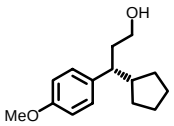
(*R*)-3-(cyclopenta-1,3-dienyl)-3-(4-methoxyphenyl)propanal (7e) and **(*R*)-3-(cyclopenta-1,4-dienyl)-3-(4-methoxyphenyl)propanal (8e)**



7e:8e=6:4

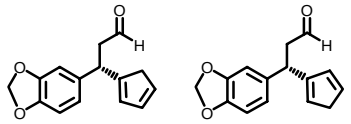
^1H NMR ($CDCl_3$) δ 2.74-2.87 (1.2H, m), 2.85-2.94 (1H, m), 2.98-3.02 (0.8H, m), 2.98-3.07 (1H, m), 3.78 (3H, s), 4.24-4.33 (1H, m), 6.07-6.10 (0.4H, m), 6.23-6.29 (1.2H, m), 6.30-6.34 (0.4H, m), 6.38-6.43 (1H, m), 6.81-6.87 (2H, m), 7.08-7.16 (2H, m), 9.69-9.73 (1H, m); ^{13}C NMR ($CDCl_3$) δ 39.8, 40.7, 41.2, 42.5, 49.0, 49.4, 55.2, 114.1, 126.4, 127.2, 128.5, 128.8, 131.86, 131.95, 133.6, 134.4, 135.4, 148.6, 150.7, 158.4, 201.5, 201.7; IR (neat) ν 1722, 1610, 1512, 1250, 118, 1035, 834 cm^{-1}.

(*R*)-3-cyclopentyl-3-(4-methoxyphenyl)propan-1-ol



^{1}H NMR ($CDCl_3$) δ 0.90-1.05 (1H, m), 1.08-1.81 (7H, m), 1.86-2.12 (3H, m), 2.32-2.42 (1H, m), 3.33-3.51 (2H, m), 3.79 (3H, s), 6.82 (2H, d, *J* = 8.4 Hz), 7.07 (2H, d, *J* = 8.4 Hz);^{13}C NMR ($CDCl_3$) δ 24.9, 25.3, 31.5, 31.7, 38.2, 46.8, 47.9, 55.2, 61.4, 113.7, 128.8, 137.1, 157.8; IR (neat) ν 3347, 2950, 2867, 1610, 1513, 1455, 1301, 1246, 1178, 828 cm^{-1}; HRMS (ESI): [M+Na]$^+$calculated for $C_{15}H_{22}O_2Na_1$: 257.1512, found 257.1508.; $[\alpha]_D^{20}$ 10.6 (c=1.49, CH_3OH), 94% *ee*; The enantiomeric excess was determined by HPLC with a AS-H column at 220 nm (2-propanol:hexane = 1:100), 1.0 mL/min; major enantiomer tr = 18.0 min, minor enantiomer tr = 23.4 min.

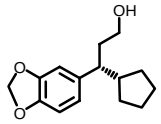
(*R*)-3-(benzo[d][1,3]dioxol-5-yl)-3-(cyclopenta-1,3-dienyl)propanal (7f) and **(*R*)-3-(benzo[d][1,3]dioxol-5-yl)-3-(cyclopenta-1,4-dienyl)propanal (8f)**



7f:8f=6:4

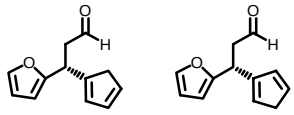
^{1}H NMR ($CDCl_3$) δ 2.78-2.82 (1.2H, m), 2.83-2.92 (1H, m), 2.96-3.05 (1H, m), 2.99-3.01 (0.8H, m), 4.20-4.30 (1H, m), 5.92 (2H, s), 6.08-6.11 (0.4H, m), 6.24-6.27 (0.6H, m), 6.26-6.33 (1H, m), 6.39-6.43 (1H, m), 6.64-6.75 (3H, m), 9.70-9.73 (1H, m); ^{13}C NMR ($CDCl_3$) δ 40.2, 41.1, 41.2, 42.5, 48.9, 49.3, 100.9, 107.9, 108.15, 108.26, 120.6, 120.9, 126.5, 127.3, 128.3, 131.8, 132.0, 133.5, 134.5, 136.3, 137.2, 146.26, 146.30, 147.9, 148.3, 150.3, 201.2, 201.4; IR (neat) ν 2894, 1716, 1505, 1440, 1363, 1247, 1038, 932, 813 cm^{-1}.

(*R*)-3-(benzo[d][1,3]dioxol-5-yl)-3-cyclopentylpropan-1-ol



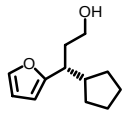
^{1}H NMR ($CDCl_3$) δ 0.90–1.06 (1H, m), 1.10-1.80 (7H, m), 1.82-2.12 (3H, m), 2.29-2.40 (1H, m), 3.32-3.52 (2H, m), 5.91 (2H, s), 6.59 (1H, dd, *J* = 7.6, 1.6 Hz), 6.66 (1H, d, *J*=1.2 Hz), 6.70 (1H, d, *J*=7.6 Hz); ^{13}C NMR ($CDCl_3$) δ 24.9, 25.3, 31.5, 31.7, 38.2, 46.8, 48.5, 61.3, 100.8, 107.7, 108.0, 121.0, 139.0, 145.5, 147.6; IR (neat) ν 3336, 2950, 2869, 1504, 1488, 1440, 1244, 1040, 938, 810 cm^{-1}; HRMS (ESI): [M+Na]$^+$calculated for $C_{15}H_{20}O_3Na_1$: 271.1305 found 271.1295. ; $[\alpha]_D^{20}$ 9.4 (c=1.75, MeOH), 93% *ee*; The enantiomeric excess was determined by HPLC with a AS-H column at 285 nm (2-propanol:hexane = 1:50), 1.0 mL/min; major enantiomer tr = 15.0 min, minor enantiomer tr = 20.8 min.

(*R*)-3-(cyclopenta-1,3-dienyl)-3-(furan-2-yl)propanal (7g) and **(*R*)-3-(cyclopenta-1,4-dienyl)-3-(furan-2-yl)propanal (8g)**

 **7g:8g**=1:1

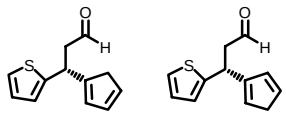
^{1}H NMR ($CDCl_3$) δ 2.89-2.97 (2H, m), 2.99-3.07 (2H, m), 4.41-4.51 (1H, m), 6.03 (1H, dd, *J*=5.2, 4.0 Hz), 6.12-6.16 (0.5H, m), 6.26-6.34 (2H, m), 6.39-6.44 (0.5H, m), 6.44-6.47 (1H, m), 9.72-9.77 (1H, m); ^{13}C NMR ($CDCl_3$) δ 34.2, 34.8, 41.3, 42.1, 46.5, 47.1, 105.5, 105.9, 110.2, 127.8, 128.4, 131.9, 132.1, 132.9, 134.5, 141.5, 141.6, 145.7, 147.3, 155.3, 155.8, 200.7, 200.8; IR (neat) ν 2898, 2830, 2728, 1725, 1505, 1363, 1011, 898, 736 cm^{-1}.

(*R*)-3-cyclopentyl-3-(furan-2-yl)propan-1-ol



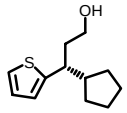
^{1}H NMR ($CDCl_3$) δ 1.08-1.70 (7H, m), 1.78-2.12 (4H, m), 2.61-2.71 (1H, m), 3.41-3.50 (1H, m), 3.52-3.61 (1H, m), 6.00 (1H, d, *J* = 2.8 Hz), 6.25-6.29 (1H, m), 7.29-7.32 (1H, m); ^{13}C NMR ($CDCl_3$) δ 25.0, 25.3, 30.8, 31.2, 36.1, 41.2, 44.4, 61.3, 105.6, 109.8, 140.8, 158.0; IR (neat) ν 3336, 2951, 2869, 1506, 1148, 1046, 1007, 729, 600 cm^{-1}; HRMS (ESI): $[M+Na]^+$calculated for $C_{12}H_{18}O_2Na_1$: 217.1199 found 217.1193.; $[\alpha]_D^{20}$ 10.3 (c=1.08, MeOH), 90% *ee*; The enantiomeric excess was determined by HPLC with a AS-H column at 211 nm (2-propanol:hexane = 1:100), 1.0 mL/min; major enantiomer tr= 11.1 min, minor enantiomer tr = 12.0 min.

(*R*)-3-(cyclopenta-1,3-dienyl)-3-(thiophen-2-yl)propanal (7h) and **(*R*)-3-(cyclopenta-1,4-dienyl)-3-(thiophen-2-yl)propanal (8h)**

 **7h:8h**=4:6

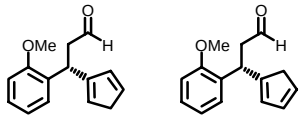
^{1}H NMR ($CDCl_3$) δ 2.90-2.93 (0.8H, m), 2.99-3.06 (3.2H, m), 4.61-4.71 (1H, m), 6.14-6.18 (0.6H, m), 6.29-6.33 (0.8H, m), 6.39-6.47 (1.6H, m), 6.84 (1H, dd, *J*=8.0, 3.2 Hz), 6.92 (1H, dt, J_d=5.2 Hz, *J*t=3.2 Hz), 7.13-7.18 (1H, m), 9.73-9.76 (1H, m); ^{13}C NMR ($CDCl_3$) δ 35.7, 36.4, 41.3, 50.0, 123.95, 124.0, 124.1, 124.4, 126.8, 127.1, 127.9, 128.3, 131.8, 132.2, 132.9, 134.7, 146.2, 147.3, 147.8, 149.5, 200.6, 200.8; IR (neat) ν 2924, 2726, 1724, 1363, 898, 698 cm^{-1}.

(*R*)-3-cyclopentyl-3-(thiophen-2-yl)propan-1-ol



^{1}H NMR ($CDCl_3$) δ 1.08-1.30 (3H, m), 1.41-1.66 (4H, m), 1.69-1.81 (1H, m), 1.85-1.95 (1H, m), 1.95-2.05 (1H, m), 1.95-2.05 (1H, m), 2.06-2.16 (1H, m), 2.79-2.88 (1H, m), 3.42-3.52 (1H, m), 3.53-3.62 (1H, m), 6.79 (1H, d, *J*=2.8 Hz), 6.91 (1H, dd, *J*=4.8, 3.6 Hz), 7.14 (1H, d, *J*=5.2 Hz); ^{13}C NMR ($CDCl_3$) δ 24.9, 25.4, 31.35, 31.38, 39.2, 43.7, 47.6, 61.1, 122.9, 124.1, 126.3, 148.9; IR (neat) ν 3333, 2950, 2862, 1044, 691 cm^{-1}; HRMS (ESI): $[M+Na]^+$ calculated for $C_{12}H_{18}OSNa$: 233.0971, found 233.0977; $[\alpha]_D^{20}$ 3.9 (*c*=1.3, MeOH), 78% *ee*; The enantiomeric excess was determined by HPLC with a AS-H column at 244 nm (2-propanol:hexane = 1:100), 1.0 mL/min; major enantiomer tr = 11.7 min, minor enantiomer tr = 13.7 min.

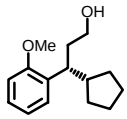
(*R*)-3-(cyclopenta-1,4-dienyl)-3-(2-methoxyphenyl)propanal (7i) and **(*R*)-3-(cyclopenta-1,3-dienyl)-3-(2-methoxyphenyl)propanal (8i)**



7i:8i=4:6

^{1}H NMR ($CDCl_3$) δ 2.82-2.86 (0.8H, m), 2.82-2.90 (1H, m), 2.91-3.01 (1H, m), 3.00-3.03 (1.2H, m), 3.85 (1.2H, s), 3.86 (1.8H, s), 4.73-4.84 (1H, m), 6.09-6.13 (0.6H, m), 6.25-6.29 (0.8H, m), 6.30-6.34 (0.6H, m), 6.39-6.44 (1H, m), 6.85-6.91 (2H, m), 6.98-7.03 (1H, m), 7.16-7.23 (1H, m), 9.68-9.72 (1H, m); ^{13}C NMR ($CDCl_3$) δ 33.4, 34.1, 41.2, 42.8, 47.8, 48.3, 55.3, 110.56, 110.62, 120.68, 120.74, 127.1, 127.65, 127.72, 127.8, 128.2, 128.4, 130.5, 131.5, 131.6, 131.9, 134.0, 134.1, 147.9, 150.0, 156.4, 156.6, 202.1, 202.4; IR (neat) ν 2935, 1723, 1493, 1464, 1245, 1028, 755 cm^{-1}.

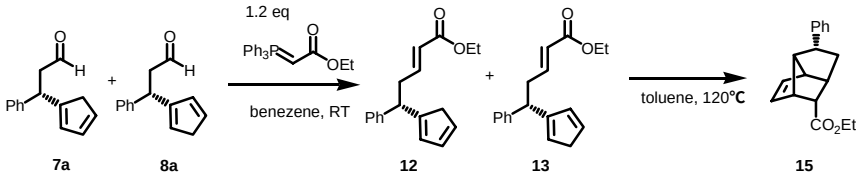
(*R*)-3-cyclopentyl-3-(2-methoxyphenyl)propan-1-ol



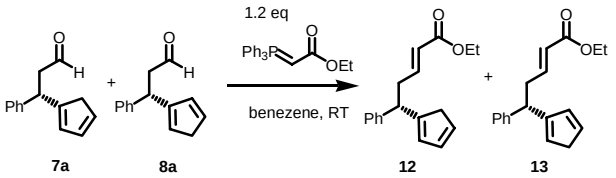
^{1}H NMR ($CDCl_3$) δ 0.88-1.01 (1H, m), 1.20-1.33 (1H, m), 1.35-1.73 (5H, m), 1.90-2.05 (2H, m), 2.06-2.22 (2H, m), 3.01 (1H, t, *J*=10.0 Hz), 3.25 (1H, dt, J_d=4.8 Hz, J_t=10.0 Hz), 3.39-3.47 (1H, m), 3.82 (3H, s), 6.87 (1H, d, *J*=8.4 Hz), 6.94 (1H, t, *J*=7.6 Hz), 7.12-7.19 (2H, m); ^{13}C NMR ($CDCl_3$) δ 24.9, 25.4, 31.72, 31.79, 38.2, 39.7, 38.2, 39.7, 45.4, 55.6, 61.0, 110.6, 121.1, 126.7, 128.0, 133.2, 157.3; IR (neat) ν 3359, 2950, 1492, 1241, 1031, 753 cm^{-1} HRMS (ESI): $[M+Na]^+$ calculated for $C_{15}H_{22}O_2Na$: 257.1521, found 257.1504; $[\alpha]_D^{21}$ 5.9 (*c*=0.67, MeOH), 95% *ee*; The enantiomeric excess was

determined by HPLC with a OD-H column at 220 nm (2-propanol:hexane = 1:200), 1.0 mL/min; major enantiomer tr = 34.4 min, minor enantiomer tr = 26.1 min.

The procedure of intramolecular Diels-Alder reaction of compound 12 and 13 derived from 7a and 8a.

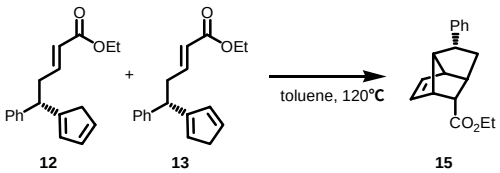


(*R*,2*E*)-ethyl-5-(cyclopenta-1,4-dienyl)-5-phenylpent-2-enoate (12) and (*R*,2*E*)-ethyl 5-(cyclopenta-1,3-dienyl)-5-phenylpent-2-enoate (13)



To a solution benzene solution (1.6 ml) of aldehyde **7**a and **8**a (110.9 mg, 0.56 mmol) was added ethyl (triphenylphosphoranylidene) acetate (234 mg, 0.67 mmol) at room temperature and the reaction mixture was stirred for 1 h. The reaction mixture was concentrated under reduced pressure. The residue was purified by preparative thin-layer chromatography (AcOEt/hexane=1/6) to afford **12** and **13** (106.6 mg, 71%). **12**:**13**=1:1 ^{1}H NMR ($CDCl_3$) δ 1.30 (3H, t, *J*=7.2 Hz), 2.74-2.83 (1H, m), 2.84 (1H, s), 2.88-2.99 (1H, m), 3.04 (1H, s), 5.85 (1H, d, *J*=15.6 Hz), 6.18 (0.5H, s), 6.31-6.41 (1.5 H, s), 6.42-6.50 (1H, m), 6.93 (1H, dt, J_d=7.2 Hz, J_t= 14.7 Hz), 7.17-7.28 (3H, m), 7.29-7.37 (2H, m); ^{13}C NMR ($CDCl_3$) δ 14.1, 37.7, 38.1, 41.1, 42.3, 45.5, 46.4, 60.0, 122.5, 122.6, 126.40, 122.41, 127.1, 127.5, 127.7, 127.8, 128.38, 128.4, 131.6, 131.9, 133.6, 134.0, 142.8, 143.7, 147.0, 148.6, 150.7, 166.2, 166.3; IR (neat) ν 2980, 1717, 1654, 1494, 1453, 1367, 1270, 1202, 1039, 702 cm^{-1}; HRMS (ESI): $[M+Na]^+$ calculated for $C_{18}H_{20}O_2Na$: 291.1356, found 291.1356.

Compound of 15

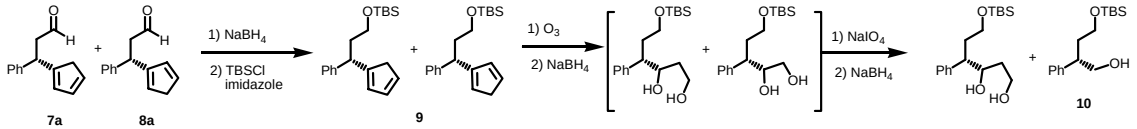


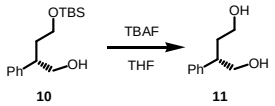
A mixture of **12** and **13** (88.0 mg, 0.328 mmol) and catalytic amount of hydroquinone (3.6 mg, 0.0328 mmol) were dissolved in anhydrous toluene (0.66 ml). The solution was refluxed at 120 °C for 5h. The reaction mixture was concentrated under reduced

pressure. The residue was purified by preparative thin-layer chromatography (AcOEt/hexane=1/6) to afford compound **15** (60.1 mg, 68%).

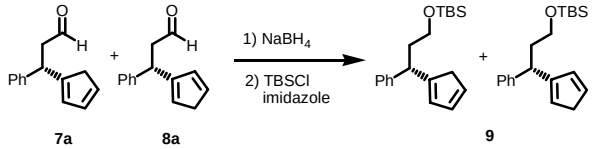
^{1}H NMR ($CDCl_3$) δ 1.24 (3H, t, *J*=7.2 Hz), 1.83 (1H, ddd, *J*=11.2, 7.6, 2.8 Hz), 2.34 (1H, dd, *J*=12.0, 8.0 Hz), 2.39 (1H, d, *J*=2.0 Hz), 2.43 (1H, s), 2.64 (1H, d, *J*=4.8 Hz), 2.76 (1H, t, *J*=8.0 Hz), 3.00-3.09 (2H, m), 4.08 (2H, q, *J*=7.2 Hz), 5.92 (1H, dd, *J*=5.6, 2.8 Hz), 6.11 (1H, dd, *J*=5.6, 3.2 Hz), 7.14-7.22 (3H, m), 7.26-7.31 (2H, m); ^{13}C NMR ($CDCl_3$) δ 14.3, 39.1, 41.0, 44.6, 49.3, 49.9, 51.9, 60.0, 69.5, 125.8, 126.9, 128.4, 133.2, 133.9, 146.3, 173.5; IR (neat) ν 3027, 1734, 1495, 1449, 1205, 1043, 700 cm^{-1}; HRMS (ESI): $[M+Na]^+$ calculated for $C_{18}H_{20}O_2Na$: 291.1356, found 227.1362; $[\alpha]_D^{21}$ -112.3 (*c*=0.81, $CHCl_3$).

Determination of the absolute stereochemistry of 7a and 8a:





Compound of 9



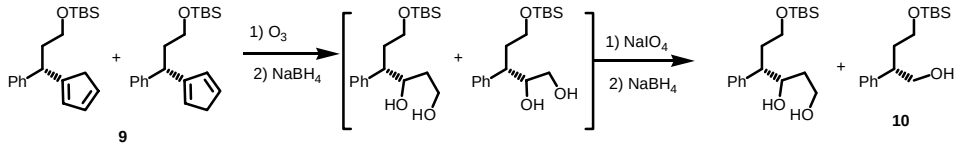
To a solution MeOH (1.7 ml) of the **7a** and **8a** (165.8 mg, 0.84 mmol) was added $NaBH_4$ (378.3 mg, 2.5 mmol) at 0 °C. After stirring for 20 min at that temperature, the reaction mixture was quenched with pH 7.0 phosphate buffer. The organic materials were extracted with AcOEt and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure which was used in the next reaction without further purification.

To a DMF solution (1.7 ml) of alchol and imidazole (284.6 mg, 4.2 mmol) was added TBSCl (378.3 mg, 4.2 mmol) at 0 °C and stirred for 2 h. The reaction mixture was quenched with pH 7.0 phosphate buffer and diluted with AcOEt. The organic phase was washed with saturated aqueous NaCl and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The residue was purified by silica gel column chromatography (AcOEt/hexane=1/20) to afford **9** (208.3 mg, 79%, 2 steps).

^{1}H NMR ($CDCl_3$) δ 0.01 (6H, s), 0.91 (9H, s), 1.99-2.10 (1H, m), 2.18-2.30 (1H, m), 3.46-3.62 (2H, m), 3.85-3.93 (1H, m), 6.09-6.12 (6H, m), 6.23-6.30 (0.8H, m),

6.36-6.40 (1.2H, m), 6.41-6.45 (0.4H, m), 7.15-7.31 (6H, m); ^{13}C NMR ($CDCl_3$) δ -5.4, 18.3, 26.0, 37.8, 38.3, 41.1, 42.3, 42.4, 43.3, 61.0, 125.9, 126.07, 126.10, 126.41, 127.9, 128.1, 128.29, 128.32, 131.3, 132.0, 133.7, 134.1, 143.9, 144.7, 149.8, 152.4 ; IR (neat) ν 3061, 3028, 2928, 2857, 1471, 1254, 1102, 834, 834, 775 cm^{-1}

Compound of 10



To a MeOH solution (2.0 ml) of diene (26.1 mg, 0.083 mmol) was treated with a oxygen-ozone stream for 10 minutes at -78 °C. An argon stream was then bubbled through the cold solution and $NaBH_4$ (62.9 mg, 1.65 mmol) was added. The mixture was allowed to warm slowly to room temperature and stirred overnight. The reaction was quenched with pH 7.0 phosphate buffer solution and the organic materials were extracted with AcOEt and the combined organic extracts were dried over anhydrous Na_2SO_4, then concentrated under reduced pressure which was used in the next reaction without further purification.

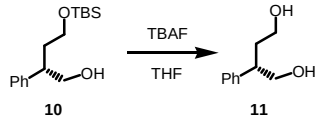
To a CH_2Cl_2 solution (0.5 ml) of the diol and silica gel (20 mg) was added $NaIO_4$ at 0 °C and the reaction mixture was stirred for 1 h at that temperature. The reaction mixture was quenched with saturated aqueous $Na_2S_2O_3$ and the organic materials were extracted with AcOEt and the combined organic extracts were dried over anhydrous Na_2SO_4, then concentrated under reduced pressure which was used in the next reaction without further purification.

To a MeOH solution (1.7 ml) of aldehyde and diol was added $NaBH_4$ (9.4 mg, 0.25 mmol) at 0 °C and the reaction mixture was stirred for 20 min at that temperature. The reaction mixture was quenched with pH 7.0 phosphate buffer. The organic materials were extracted with AcOEt and dried over anhydrous Na_2SO_4. The residue was purified by silica gel column chromatography (AcOEt/hexane=1/3) to afford alchol **10** (2.6 mg, 11%, 4 steps) and 1,3-diol (4.2 mg, 16%, 4 steps).

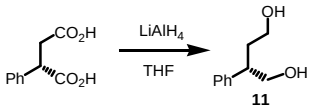
^{1}H NMR ($CDCl_3$) δ 0.02 (3H, s), 0.03 (3H, s), 0.89 (9H, s), 1.80-1.90 (1H, m), 1.91-2.01 (1H, m), 2.27 (1H, t, *J*=6.4 Hz), 2.96 (1H, quint, *J*=6.8 Hz), 3.55 (1H, ddd, *J*=10.0, 8.4, 5.2 Hz), 3.67 (1H, quint, *J*=5.2 Hz), 3.76 (1H, sex, *J*=3.2 Hz), 7.20-7.25 (3H, m), 7.30-7.36 (2H, m); ^{13}C NMR ($CDCl_3$) δ -5.47, -5.44, 18.2, 25.9, 36.1, 46.1, 61.5, 67.6, 126.7, 127.9, 128.6, 142.7; IR (neat) ν 3373, 2928, 2852, 1464, 1255, 1095, 835, 775, 700 cm^{-1}; HRMS (ESI): $[M+Na]^+$ calculated for $C_{18}H_{20}O_2Na$: 291.1356,

found 227.1362.

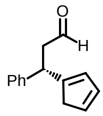
(*S*)-2-phenylbutane-1,4-diol (11)

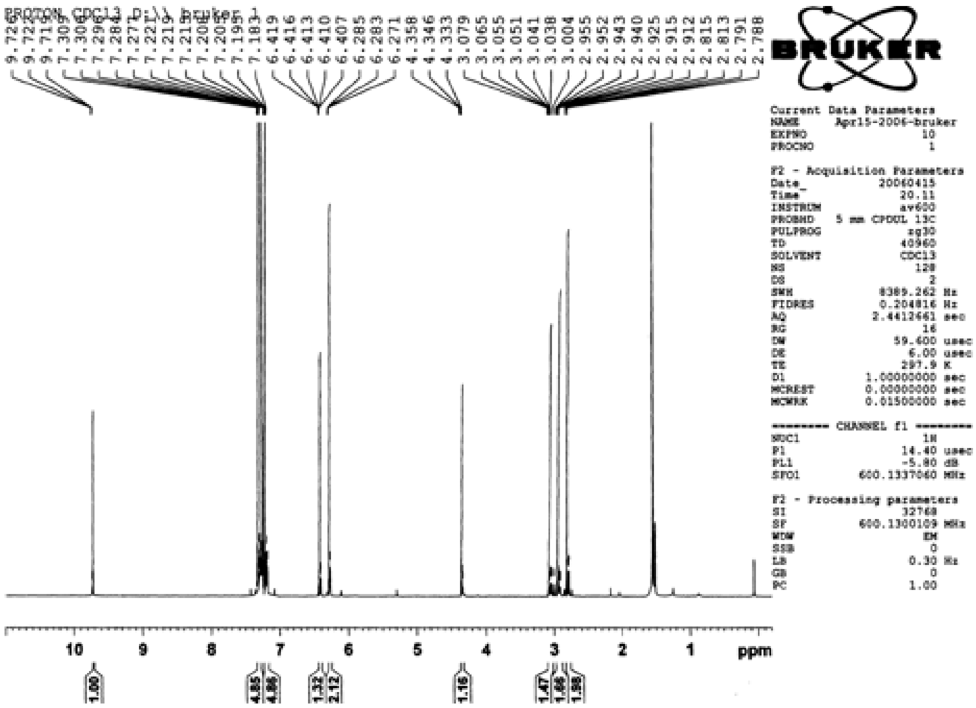


To a THF solution (200 μl) of alcohol **10** (2.6 mg, 0.093 mmol) was added 1.0M THF solution of TBAF (18.5 μl, 0.0185 mmol) at 0 °C and the reaction mixture was stirred for 1 h at that temperature. The reaction mixture was quenched with pH 7.0 phosphate buffer. The organic materials were extracted with $CHCl_3$ and dried over anhydrous Na_2SO_4, then concentrated under reduced pressure. The residue was purified by preparative thin-layer chromatography (AcOEt) to afford (*S*)-2-phenylbutane-1,4-diol **11** (1.5 mg, quant).



To a THF solution (0.27 ml) of $LiAlH_4$ (30.8 mg, 0.81 mmol) was added THF solution (0.81 ml) of (*S*)-phenylsuccinic acid (52.6 mg, 0.27 mmol) at 0 °C and the temperature of the reaction mixture was raised to room temperature gradually. After refluxing the reaction mixture for 5h, saturated Na_2SO_4 solution was added to the reaction mixture at 0 °C. After filtration of the inorganic materials, volatile materials were removed under reduced pressure and the residue was purified by thin-layer chromatography (AcOEt) to afford (*S*)-2-phenylbutane-1,4-diol **11** (33.8 mg, 75%).
^{1}H NMR ($CDCl_3$) δ 1.85-1.95 (1H, m), 1.98-2.08 (1H, m), 2.97 (1H, quint, *J*=7.2 Hz), 3.55-3.64 (1H, m), 3.70 (1H, quint, *J*=5.6 Hz), 3.79 (2H, d, *J*=6.4 Hz), 7.21-7.27 (3H, m), 7.34 (2H, t, *J*=7.6 Hz); ^{13}C NMR ($CDCl_3$) δ 35.8, 45.9, 60.9, 67.4, 126.7, 127.8, 128.7, 142.4; IR (neat) ν 3349, 2935, 2880, 1495, 1454, 1050, 762, 702cm^{-1}; HRMS (ESI): $[M+Na]^+$ calculated for $C_{18}H_{20}O_2Na$: 291.1356, found 227.1362; $[\alpha]_D^{31}$ 27.5 (*c*=0.225, $CHCl_3$), prepared by the reduction of (*S*)-phenylsuccinic acid; The enantiomeric excess was determined by HPLC with a IA column at 220 nm (2-propanol:hexane = 1:40), 1.0 mL/min; major enantiomer tr = 51.6 min, minor enantiomer tr = 53.6 min.


O
H
Ph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BRUKER
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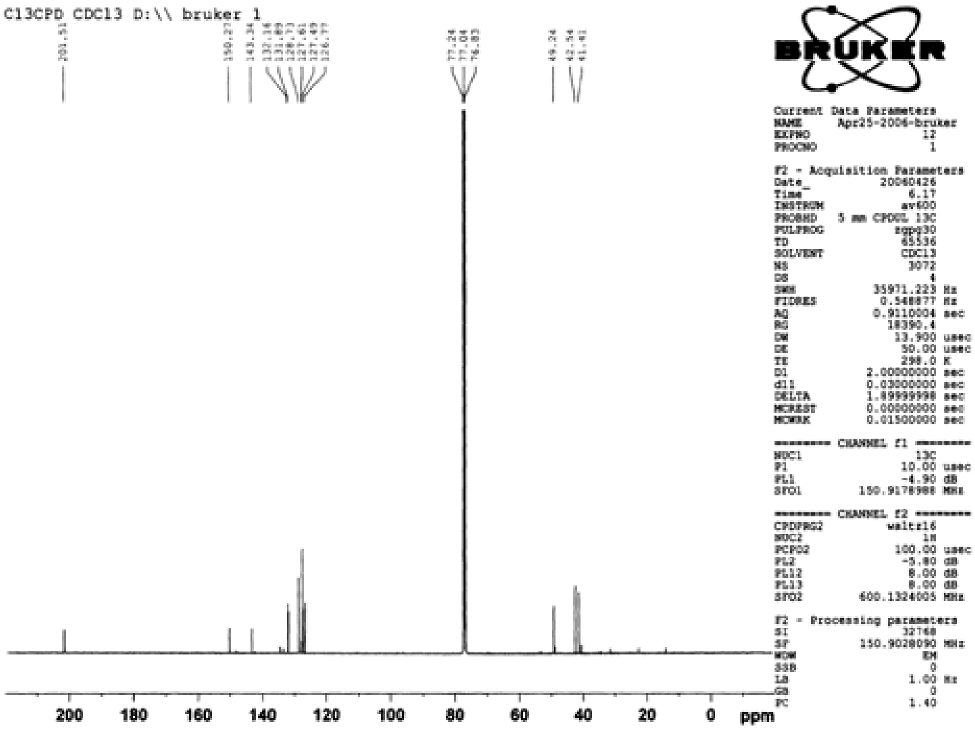
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PL12 8.00 dB
PL13 8.00 dB
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F2 - Processing parameters
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SF 150.9028090 MHz
WDW EM
SSB 0
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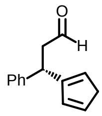
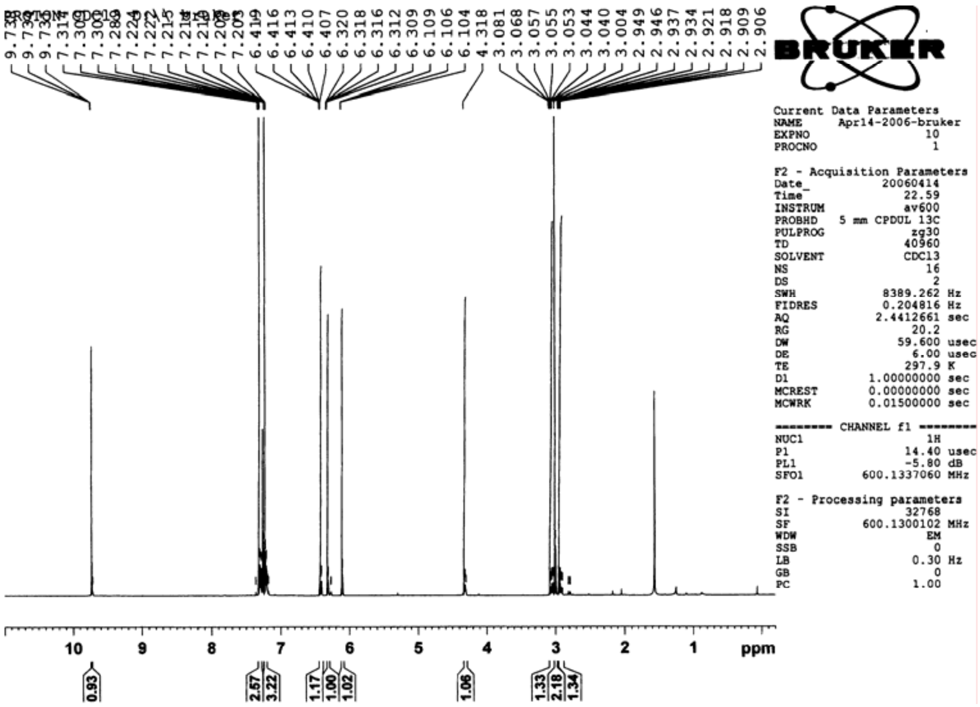
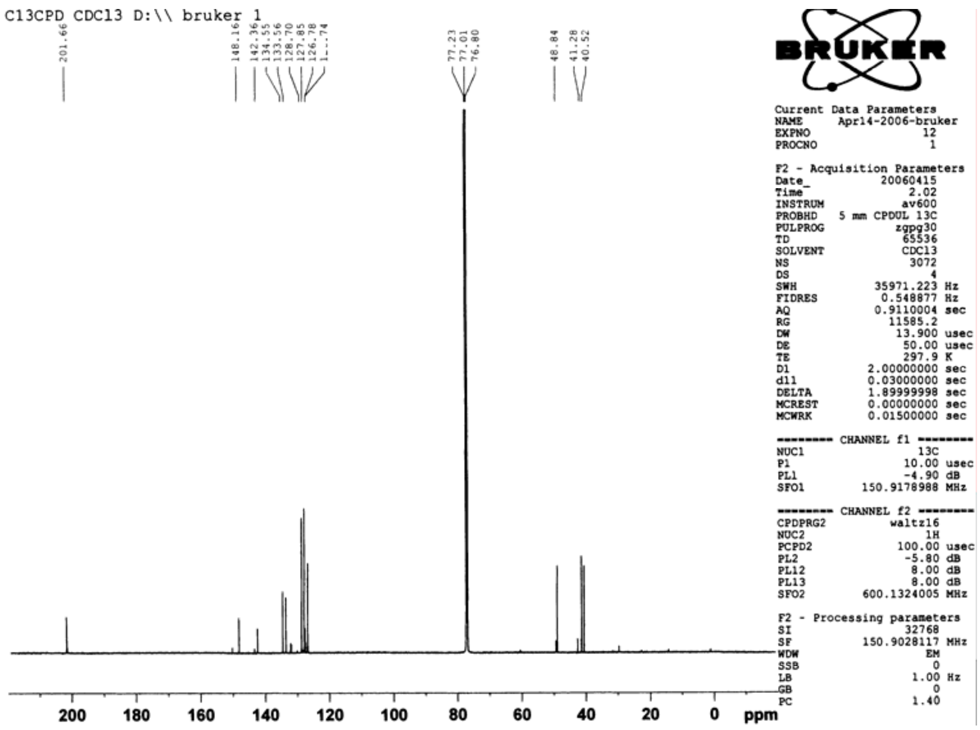
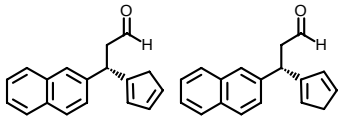
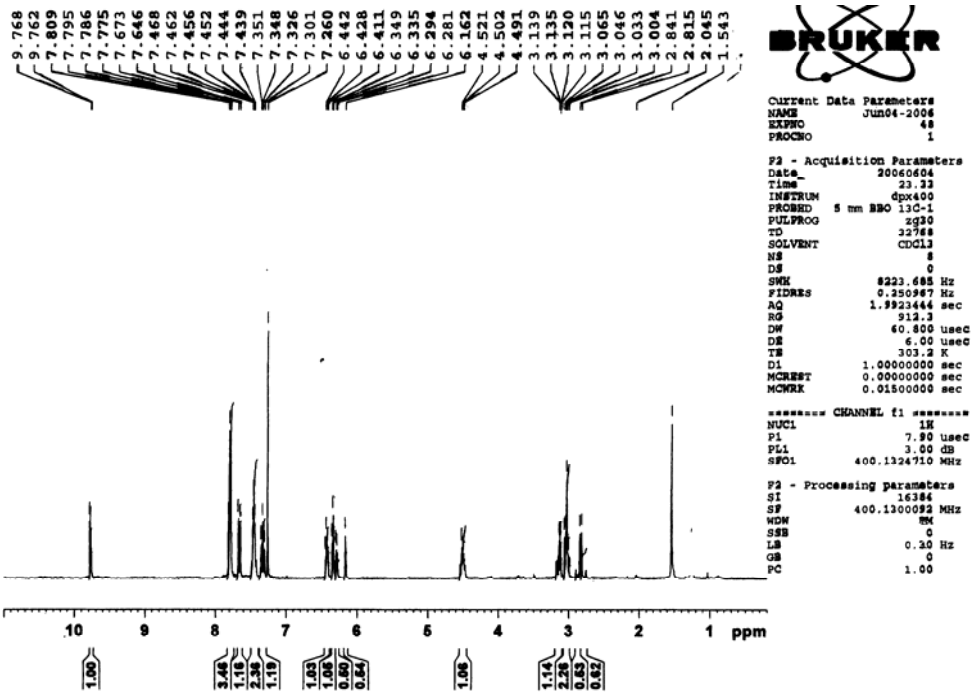
GB 0
PC 1.40
ppm


O
H
Ph


PROTON CDCl3
Current Data Parameters
NAME Apr14-2006-bruker
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060414
Time 22.59
INSTRUM av600
PROBHD 5 mm CPDUL 13C
PULPROG zg30
TD 40960
SOLVENT CDCl3
NS 16
DS 2
SWH 8389.262 Hz
FIDRES 0.204816 Hz
AQ 2.4412661 sec
RG 20.2
DW 59.600 usec
DE 6.00 usec
TE 297.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 14.40 usec
PL1 -5.80 dB
SFO1 600.1337060 MHz
F2 - Processing parameters
SI 32768
SF 600.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
0.93 2.57 3.22 1.17 1.00 1.02 1.06 1.33 2.18 1.34

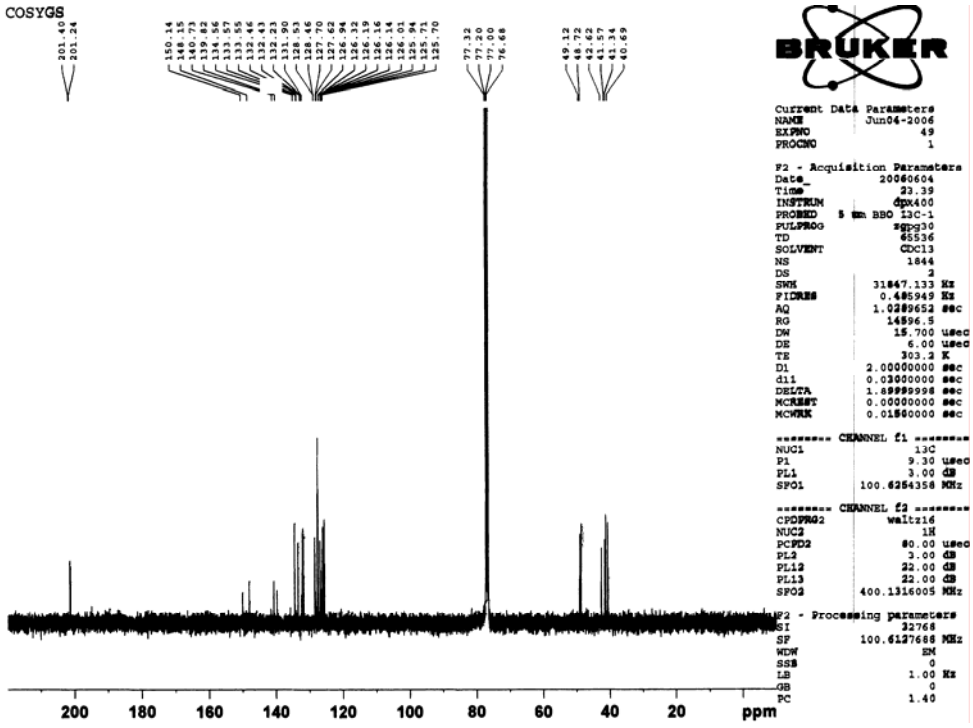

C13CPD CDCl3 D:\\ bruker 1
201.66
148.16
142.36
134.55
133.56
128.70
127.85
126.78
77.23
77.01
76.80
48.84
41.28
40.52
Current Data Parameters
NAME Apr14-2006-bruker
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060415
Time 2.02
INSTRUM av600
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 35971.223 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 11585.2
DW 13.900 usec
DE 50.00 usec
TE 297.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -4.90 dB
SFO1 150.9178988 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -5.80 dB
PL12 8.00 dB
PL13 8.00 dB
SFO2 600.1324005 MHz
F2 - Processing parameters
SI 32768
SF 150.9028117 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm





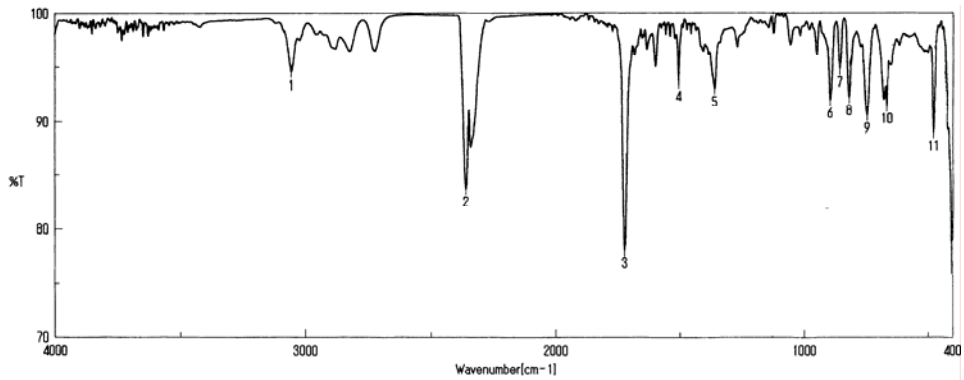
BRUKER

```
Current Data Parameters
NAME                Jun04-2006
EXPNO                       48
PROCNO                       1

F2 - Acquisition Parameters
Date_               20060604
Time                    23.33
INSTRUM                 dpx400
PROBHD     5 mm BBO 13C-1
PULPROG                 zg30
TD                      32768
SOLVENT                 CDCl3
NS                          8
DS                          0
SWH                  8223.685 Hz
FIDRES               0.250967 Hz
AQ                   1.9923444 sec
RG                       912.3
DW                      60.800 usec
DE                       6.00 usec
TE                      303.2 K
D1                   1.00000000 sec
MCREST               0.00000000 sec
MCWRK                0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                       7.90 usec
PL1                      3.00 dB
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                       16384
SF              400.1300092 MHz
WDW                         EM
SSB                          0
LB                        0.20 Hz
GB                           0
PC                        1.00
```



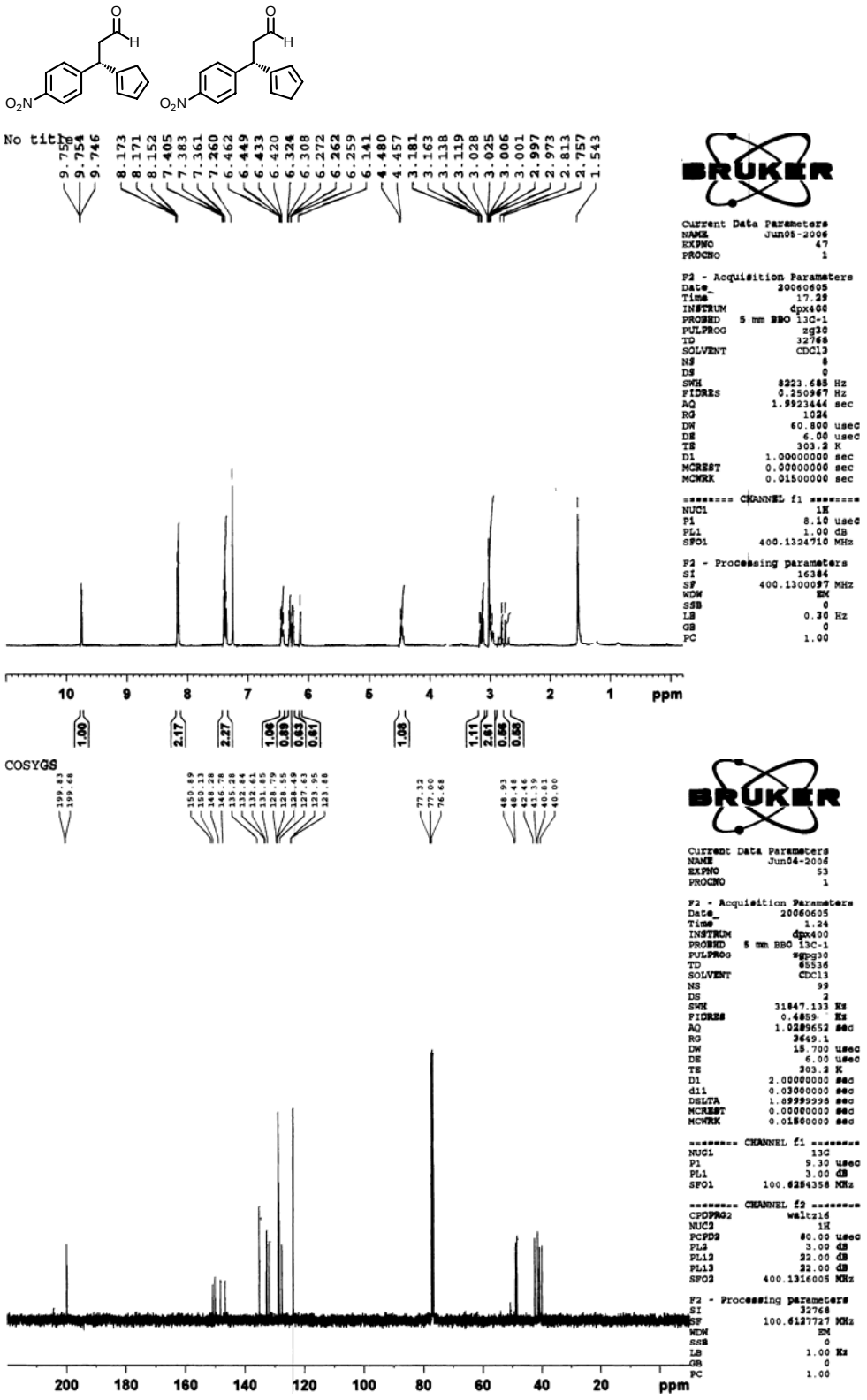
BRUKER

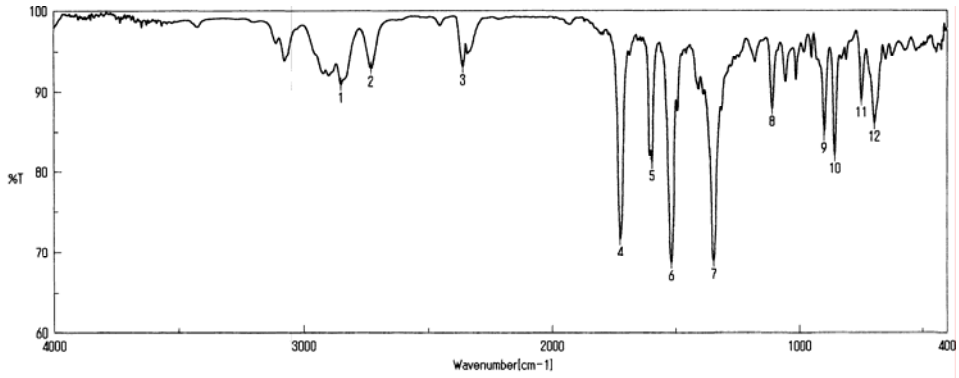
```
Current Data Parameters
NAME                Jun04-2006
EXPNO                       49
PROCNO                       1

F2 - Acquisition Parameters
Date_               20060604
Time                    23.39
INSTRUM                 dpx400
PROBHD     5 mm BBO 13C-1
PULPROG                 zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1844
DS                          2
SWH                 31847.133 Hz
FIDRES               0.485949 Hz
AQ                   1.0289652 sec
RG                     14596.5
DW                      15.700 usec
DE                       6.00 usec
TE                      303.2 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
MCREST               0.00000000 sec
MCWRK                0.01500000 sec

======== CHANNEL f1 ========
NUC1                       13C
P1                       9.30 usec
PL1                      3.00 dB
SFO1            100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      3.00 dB
PL12                    22.00 dB
PL13                    22.00 dB
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF              100.6127688 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```



積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/06/05 17:45		
測定者			
ファイル名	Memory#7		
サンプル名			
コメント	コメント		

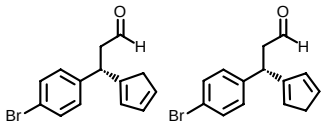
1:	3055.66, 94.5863	2:	2360.44, 83.7662	3:	1722.12, 78.0472	4:	1507.10, 93.6061
5:	1362.46, 93.0823	6:	896.74, 92.0330	7:	858.17, 94.8593	8:	820.56, 92.2810
9:	749.21, 90.6279	10:	669.18, 91.5156	11:	478.26, 89.0013		

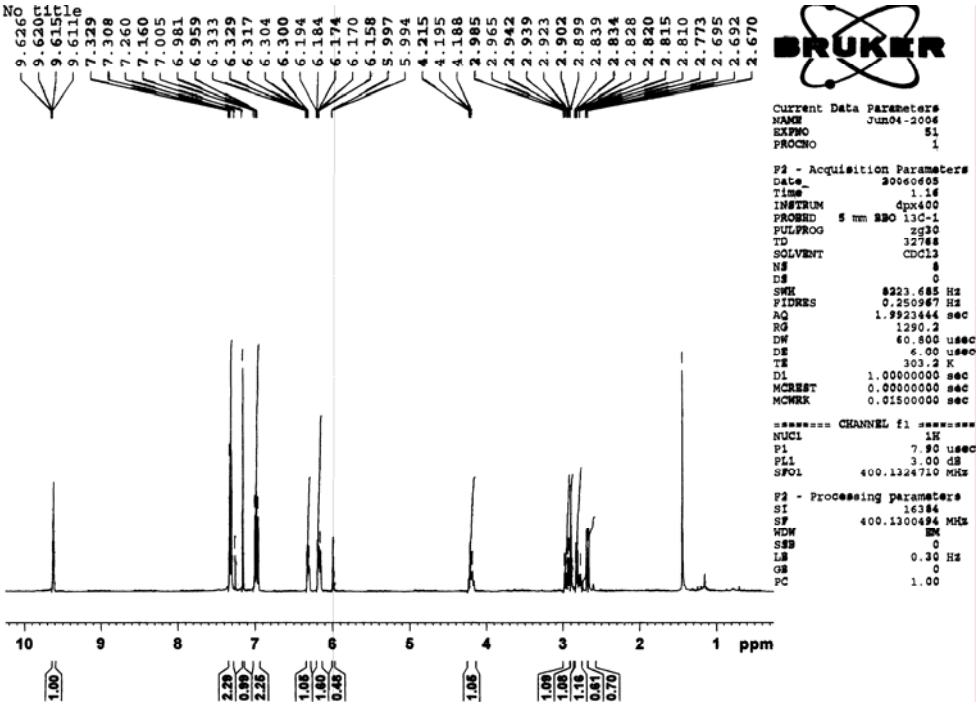

No title
9.754
9.746
8.173
8.171
8.152
7.405
7.383
7.361
7.260
6.462
6.449
6.433
6.420
6.324
6.308
6.272
6.262
6.259
6.141
4.480
4.457
3.181
3.163
3.138
3.119
3.028
3.025
3.006
3.001
2.997
2.973
2.813
2.757
1.543
BRUKER
Current Data Parameters
NAME Jun05-2006
EXPNO 47
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060605
Time 17.29
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 1024
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.10 usec
PL1 1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
1.00 2.17 2.27 1.04 0.89 0.63 0.61 1.08 1.11 2.61 0.56 0.58
COSYGS
199.83
199.68
150.89
150.13
148.28
146.78
135.28
132.84
132.61
131.85
128.79
128.55
128.49
127.63
123.95
123.88
77.32
77.00
76.68
48.93
48.48
42.46
41.39
40.81
40.00
BRUKER
Current Data Parameters
NAME Jun04-2006
EXPNO 53
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060605
Time 1.24
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 99
DS 2
SWH 31847.133 Hz
FIDRES 0.4859 Hz
AQ 1.0289652 sec
RG 3649.1
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127727 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
200 180 160 140 120 100 80 60 40 20 ppm

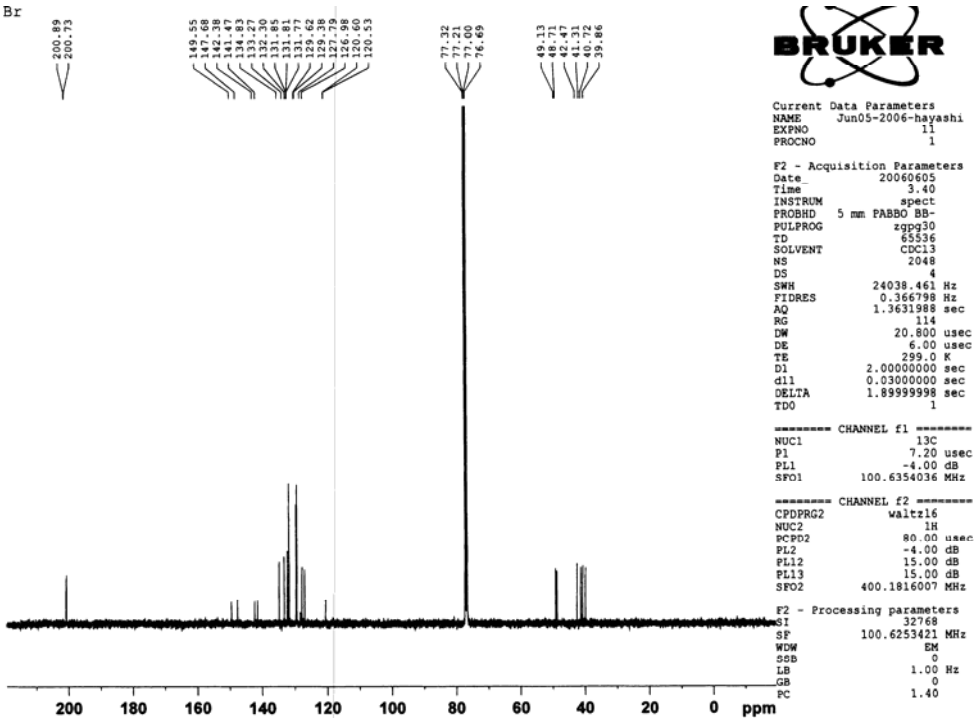


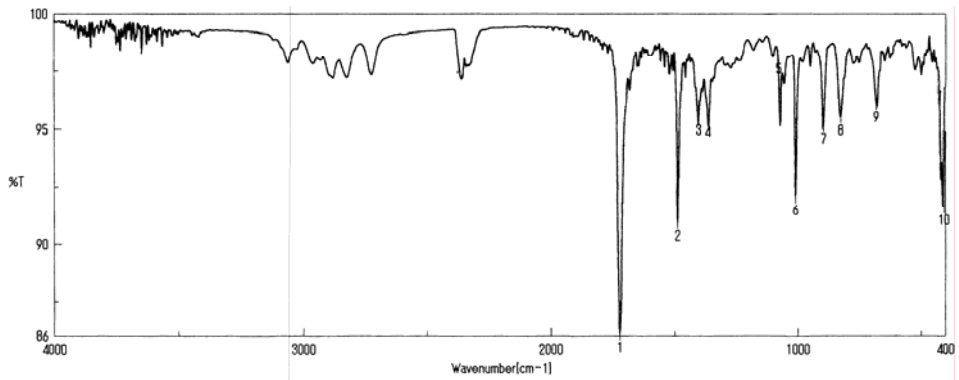
積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/06/05 17:50		
測定者			
ファイル名	Memory#9		
サンプル名			
コメント	コメント		

1:	2849.31,	90.9183	2:	2728.78,	92.8622	3:	2360.44,	93.0537	4:	1724.05,	71.7288
5:	1595.81,	81.1228	6:	1517.70,	68.7247	7:	1347.03,	68.9244	8:	1110.80,	87.8479
9:	899.63,	84.5857	10:	857.20,	82.0383	11:	748.25,	88.9763	12:	696.18,	86.0036


O
H
Br
O
H
Br

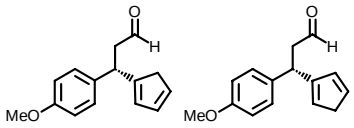

NO title
9.626 9.620 9.615 9.611 7.329 7.308 7.260 7.160 7.005 6.981 6.959 6.333 6.329 6.317 6.304 6.300 6.194 6.184 6.174 6.170 6.158 5.997 5.994 4.215 4.195 4.188 2.985 2.965 2.942 2.939 2.923 2.902 2.899 2.839 2.834 2.828 2.820 2.815 2.810 2.773 2.695 2.692 2.670
BRUKER
Current Data Parameters
NAME Jun04-2006
EXPNO 51
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060605
Time 1.16
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 1290.2
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.90 usec
PL1 3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300494 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
1.00 2.29 0.99 2.26 1.08 1.00 0.48 1.06 1.09 1.08 1.16 0.61 0.70

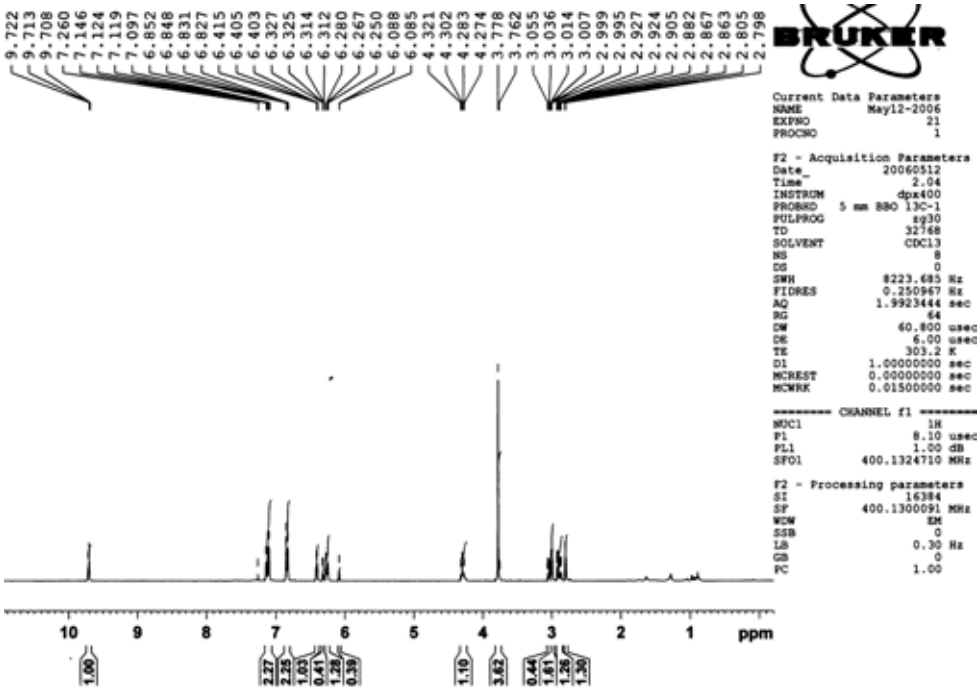

Br
200.89 200.73 149.55 147.68 142.38 141.47 134.83 133.20 132.30 131.85 131.81 131.77 129.62 128.79 127.79 126.98 120.60 120.53 77.32 77.21 77.00 76.69 49.13 48.71 42.47 41.31 40.72 39.86
BRUKER
Current Data Parameters
NAME Jun05-2006-hayashi
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060605
Time 3.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 114
DW 20.800 usec
DE 6.00 usec
TE 299.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.20 usec
PL1 -4.00 dB
SFO1 100.6354036 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1816007 MHz
F2 - Processing parameters
SI 32768
SF 100.6253421 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

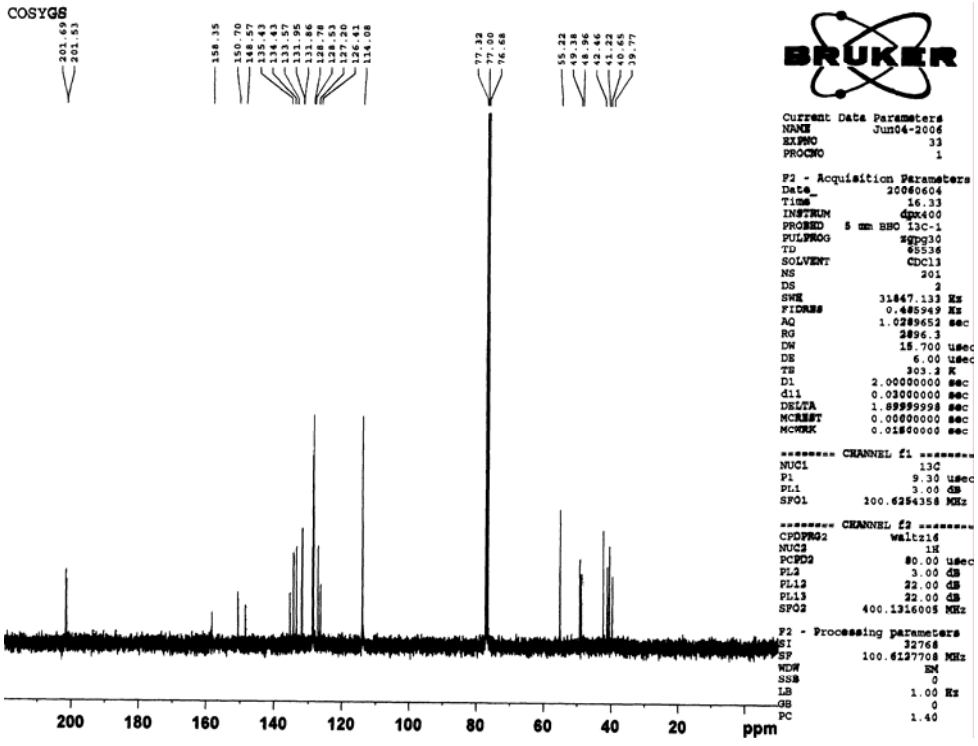


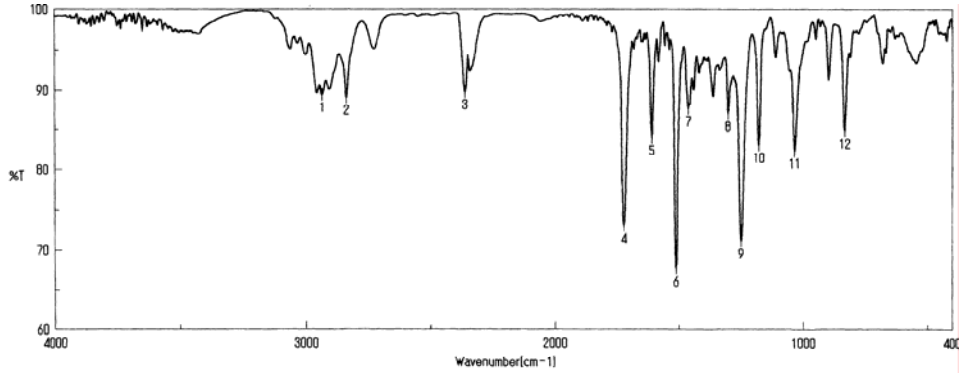
積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/06/05 17:55		
測定者			
ファイル名	Memory#11		
サンプル名			
コメント	コメント		

1:	1723.09,	86.0880	2:	1487.81,	90.9402	3:	1402.96,	95.5349	4:	1366.32,	95.4616
5:	1078.01,	97.0294	6:	1009.55,	92.0582	7:	896.74,	95.1587	8:	827.31,	95.5325
9:	683.64,	96.0882	10:	405.94,	91.6145						


O
H
MeO
O
H
MeO

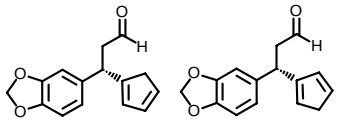

9.722
9.713
9.708
7.260
7.146
7.124
7.119
7.097
6.852
6.848
6.831
6.827
6.415
6.405
6.403
6.327
6.325
6.314
6.312
6.280
6.267
6.250
6.088
6.085
4.321
4.302
4.283
4.274
3.778
3.762
3.055
3.036
3.014
3.007
2.999
2.995
2.927
2.924
2.905
2.882
2.867
2.663
2.805
2.798
BRUKER
Current Data Parameters
NAME May12-2006
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060512
Time 2.04
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 64
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 8.10 usec
PL1 1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.27
2.25
1.03
0.41
1.28
0.39
1.10
3.62
0.44
1.61
1.36
1.30

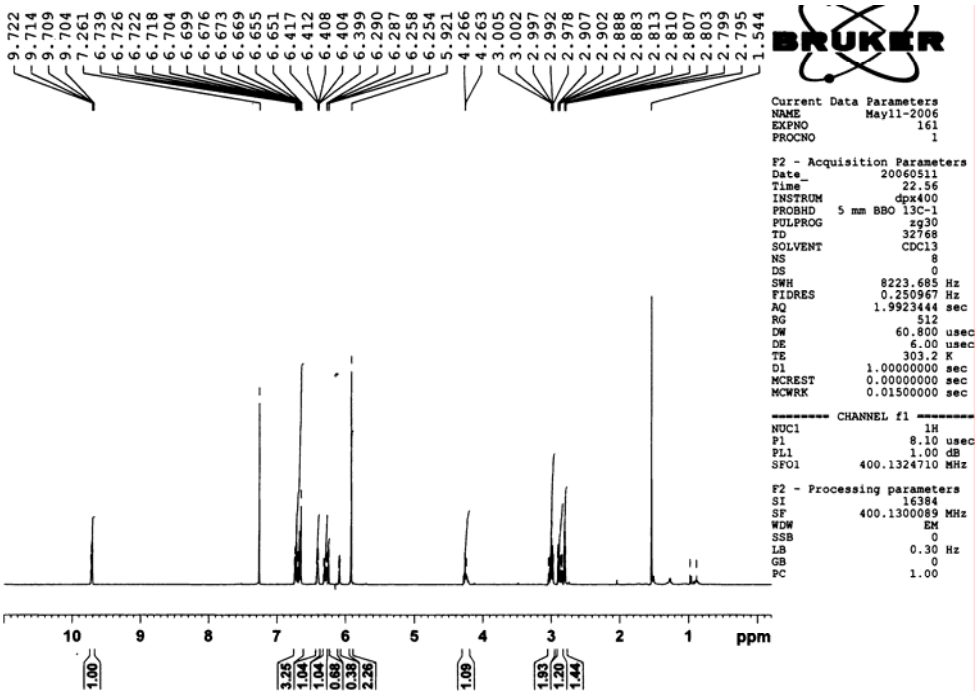

COSYGS
201.69
201.53
158.35
150.70
140.57
135.43
134.43
133.57
131.95
131.86
128.78
128.53
127.20
126.41
114.08
77.32
77.00
76.68
55.22
49.38
48.96
42.46
41.22
40.65
39.77
BRUKER
Current Data Parameters
NAME Jun04-2006
EXPNO 33
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060604
Time 16.33
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 201
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 2896.3
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6254358 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127708 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
ppm

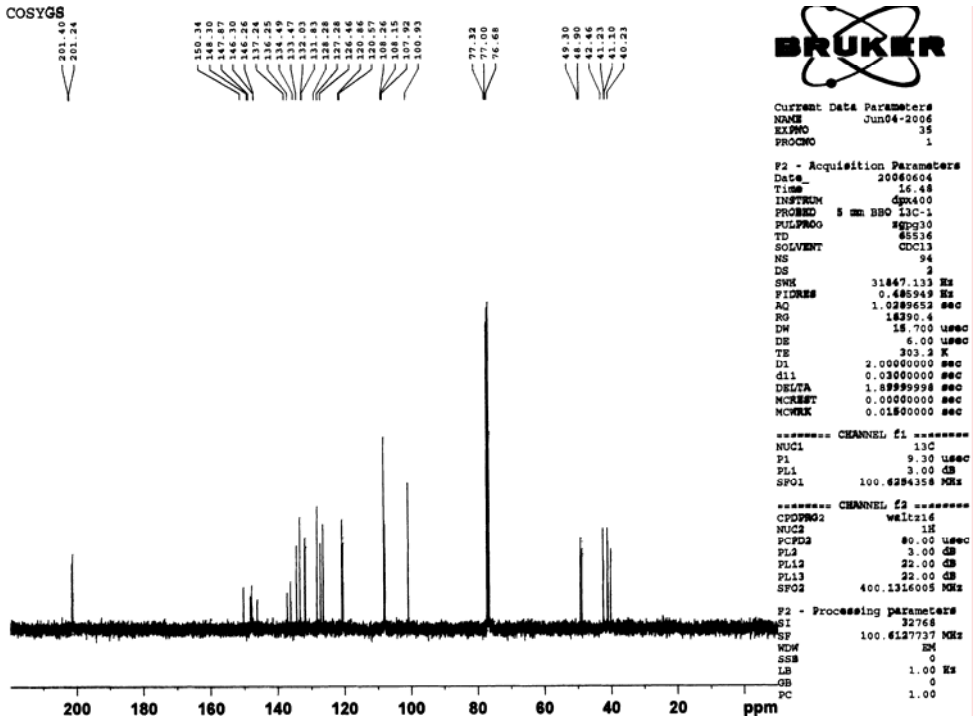


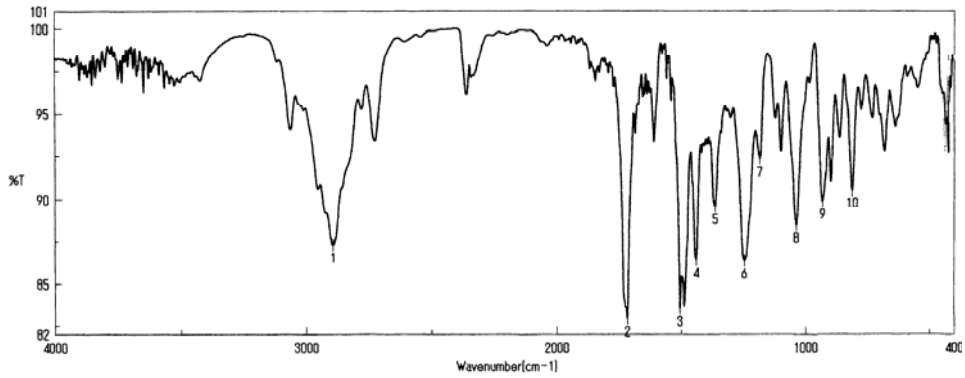
積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/06/04 18:04		
測定者			
ファイル名	Memory#7		
サンプル名			
コメント	コメント		

1:	2933.20,	89.4142	2:	2835.81,	89.0515	3:	2360.44,	89.8009	4:	1722.12,	73.0924
5:	1610.27,	84.0748	6:	1511.92,	67.6439	7:	1463.71,	87.6429	8:	1302.68,	87.0627
9:	1249.65,	71.1996	10:	1178.29,	83.1631	11:	1034.62,	82.4139	12:	834.06,	84.9379



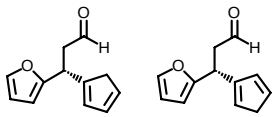

9.722
9.714
9.709
9.704
7.261
6.739
6.726
6.722
6.718
6.704
6.699
6.676
6.673
6.669
6.655
6.651
6.417
6.412
6.408
6.404
6.399
6.290
6.287
6.258
6.254
5.921
4.266
4.263
3.005
3.002
2.997
2.992
2.978
2.907
2.902
2.888
2.883
2.813
2.810
2.807
2.803
2.799
2.795
1.544
BRUKER
Current Data Parameters
NAME May11-2006
EXPNO 161
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060511
Time 22.56
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 512
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.10 usec
PL1 1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
1.00 3.25 1.04 1.04 0.68 0.38 2.26 1.09 1.83 1.20 1.44

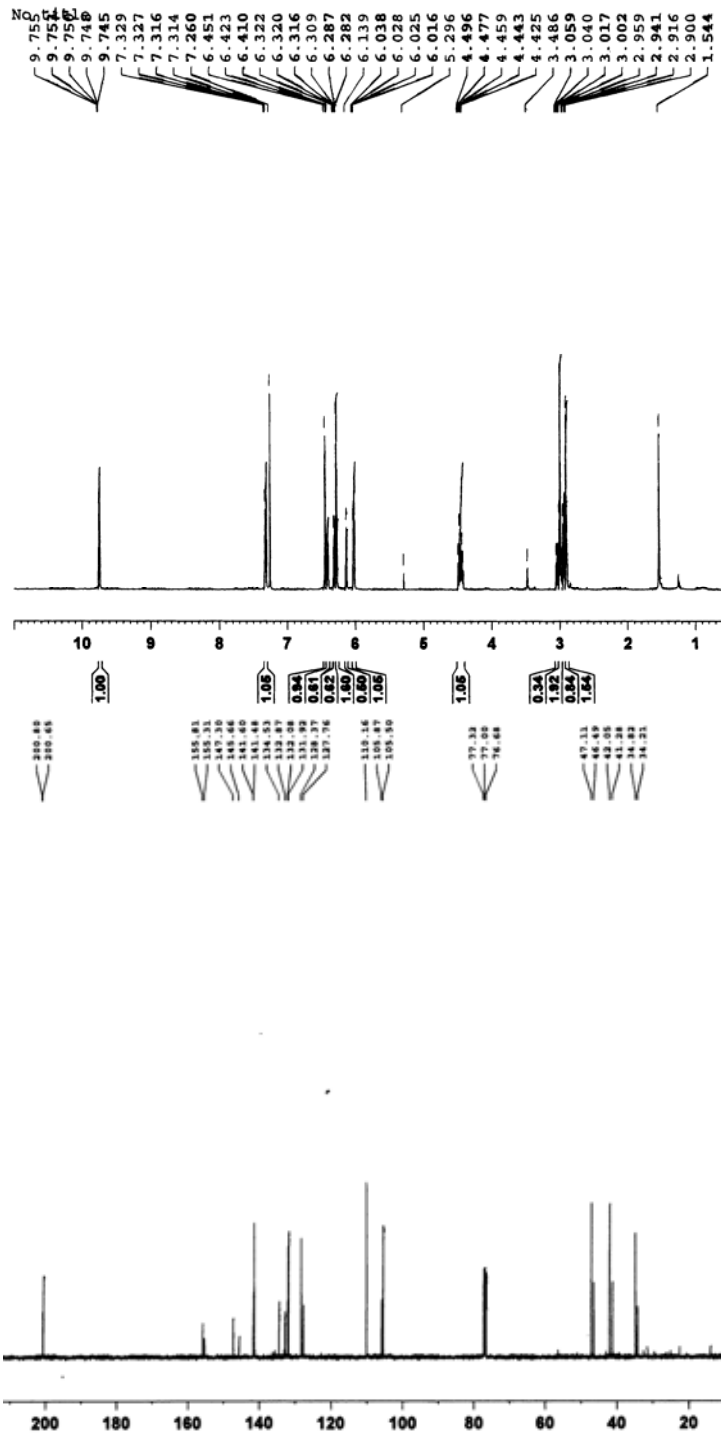

COSYGS
201.40
201.24
150.34
148.30
147.87
146.30
146.26
137.24
136.25
134.49
131.47
132.03
131.83
128.28
127.28
126.46
120.86
120.57
108.26
108.15
107.92
100.93
77.32
77.00
76.68
49.30
48.90
42.46
41.93
41.10
40.23
BRUKER
Current Data Parameters
NAME Jun04-2006
EXPNO 35
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060604
Time 16.48
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 94
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 16390.4
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6284358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
200 180 160 140 120 100 80 60 40 20 ppm



積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/06/04 18:13		
測定者			
ファイル名	Memory#9		
サンプル名			
コメント	コメント		

1:	2893.66,	87.2858	2:	1716.34,	82.9289	3:	1505.17,	83.5287	4:	1439.60,	86.3940
5:	1363.43,	89.5735	6:	1246.75,	86.3675	7:	1185.04,	92.3393	8:	1038.48,	88.4689
9:	932.41,	89.8966	10:	812.85,	90.5461						



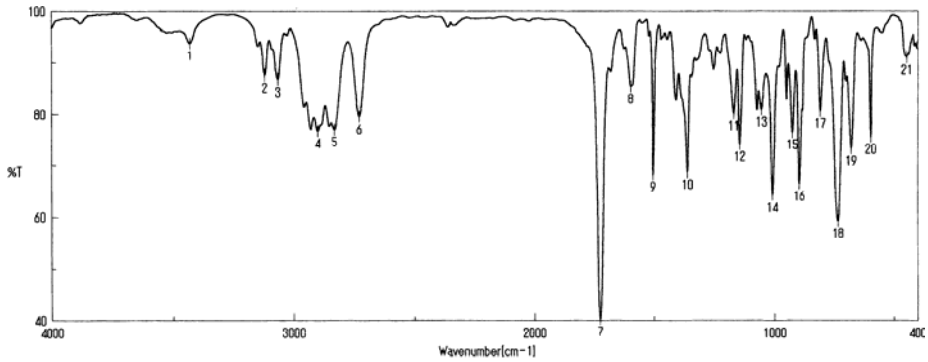


BRUKER

```
Current Data Parameters
NAME          Jun04-2006
EXPNO                 44
PROCNO                 1

F2 - Acquisition Parameters
Date_           20060604
Time              21.57
INSTRUM           dpx400
PROBHD   5 mm BBO 13C-1
PULPROG           zg30
TD               32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            8223.685 Hz
FIDRES         0.250967 Hz
AQ             1.9923444 sec
RG                  512
DW              60.800 usec
DE               6.00 usec
TE              303.2 K
D1          1.00000000 sec
MCREST      0.00000000 sec
MCWRK       0.01500000 sec

======== CHANNEL f1 ========
NUC1                1H
P1               8.10 usec
PL1              1.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI               16384
SF          400.1300097 MHz
WDW                  EM
SSB                   0
LB               0.30 Hz
GB                    0
PC               1.00
```

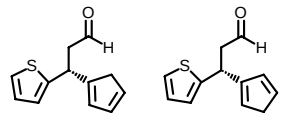
BRUKER

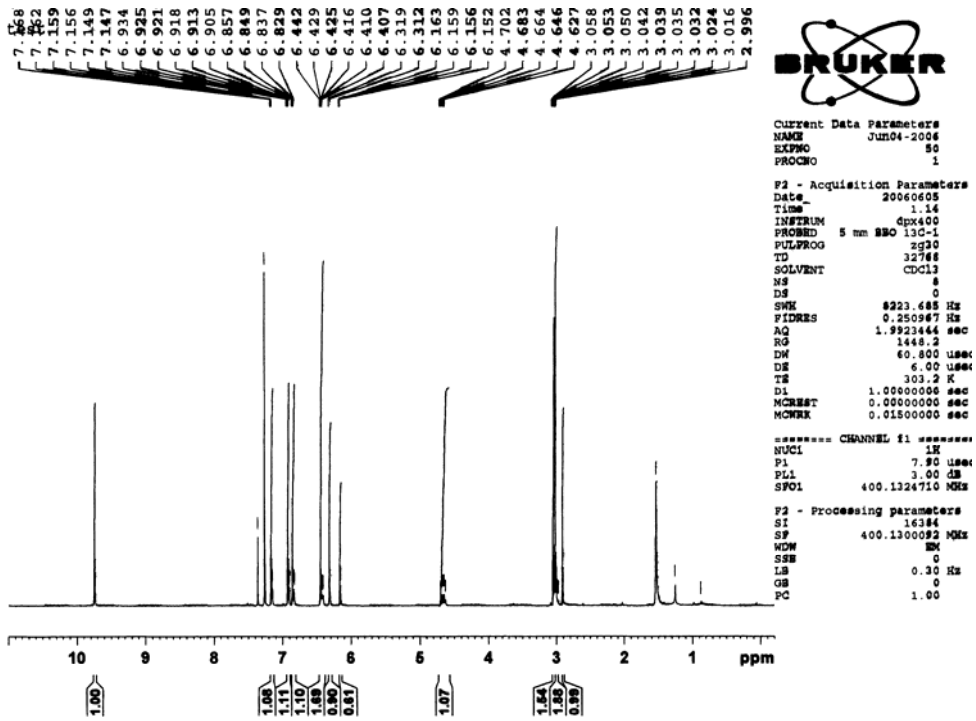
```
Current Data Parameters
NAME          Jun01-2006
EXPNO                 24
PROCNO                 1

F2 - Acquisition Parameters
Date_           20060601
Time              2.07
INSTRUM           dpx400
PROBHD   5 mm BBO 13C-1
PULPROG           zgpg30
TD               65536
SOLVENT           CDCl3
NS                  135
DS                    2
SWH           31847.133 Hz
FIDRES         0.485949 Hz
AQ             1.0289653 sec
RG                2560.3
DW              15.700 usec
DE               6.00 usec
TE              303.2 K
D1          2.00000000 sec
d11         0.03000000 sec
DELTA       1.89999998 sec
MCREST      0.00000000 sec
MCWRK       0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1              10.00 usec
PL1              2.20 dB
SFO1        100.6284358 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2           80.00 usec
PL2              3.00 dB
PL12            20.00 dB
PL13            21.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI               32768
SF          100.6127747 MHz
WDW                  EM
SSB                   0
LB               1.00 Hz
GB                    0
PC               1.40
```

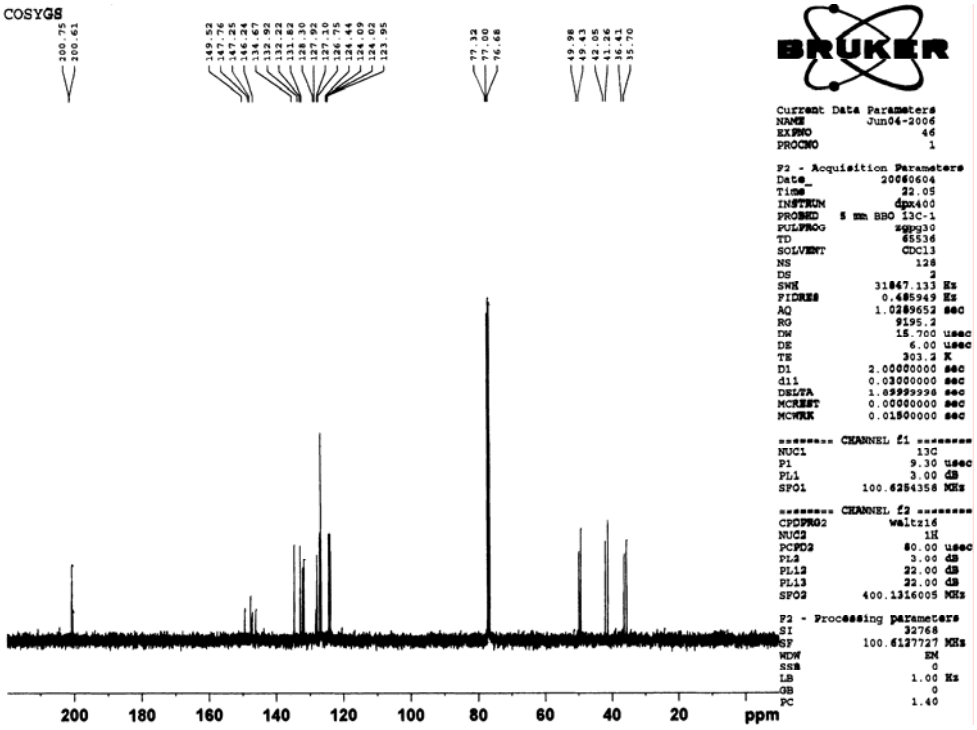


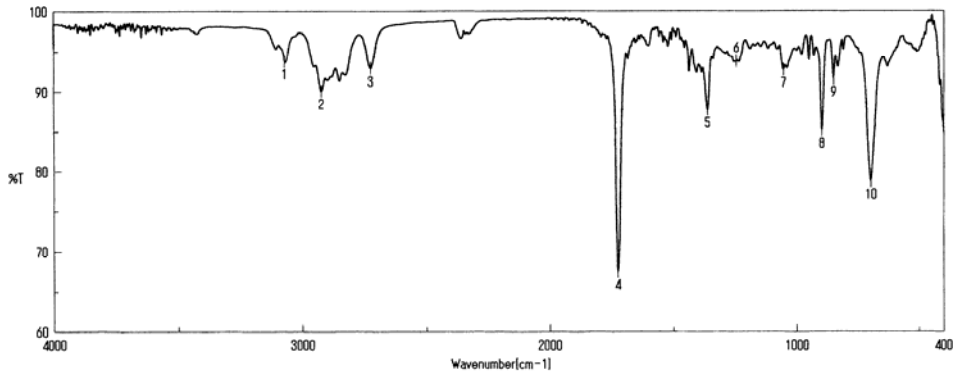
積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	2	スキャンスピード	2 mm/sec
日時	106/06/04 17:41		
測定者			
ファイル名	Memory#3		
サンプル名			
コメント	コメント		

1:	3428.81,	93.8049	2:	3118.33,	87.6964	3:	3063.37,	86.8861	4:	2898.49,	76.7982
5:	2830.03,	77.1467	6:	2727.82,	79.5958	7:	1725.01,	40.2654	8:	1597.73,	85.5471
9:	1505.17,	68.4271	10:	1363.43,	68.9081	11:	1171.54,	80.2374	12:	1146.47,	74.2316
13:	1056.80,	81.0338	14:	1010.52,	64.3482	15:	926.63,	76.5870	16:	897.70,	66.6319
17:	810.92,	80.7484	18:	735.71,	59.3070	19:	680.75,	73.3646	20:	598.79,	75.7114



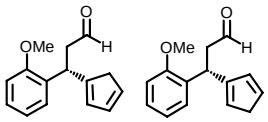

7.668
7.662
7.159
7.156
7.149
7.147
6.934
6.925
6.921
6.918
6.913
6.905
6.857
6.849
6.837
6.829
6.442
6.429
6.425
6.416
6.410
6.407
6.319
6.312
6.163
6.159
6.156
6.152
4.702
4.683
4.664
4.646
4.627
3.058
3.053
3.050
3.042
3.039
3.035
3.032
3.024
3.016
2.996
BRUKER
Current Data Parameters
NAME Jun04-2006
EXPNO 50
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060605
Time 1.14
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 1448.2
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
1.00 1.08 1.11 1.10 1.69 0.90 0.81 1.07 1.64 1.88 0.99

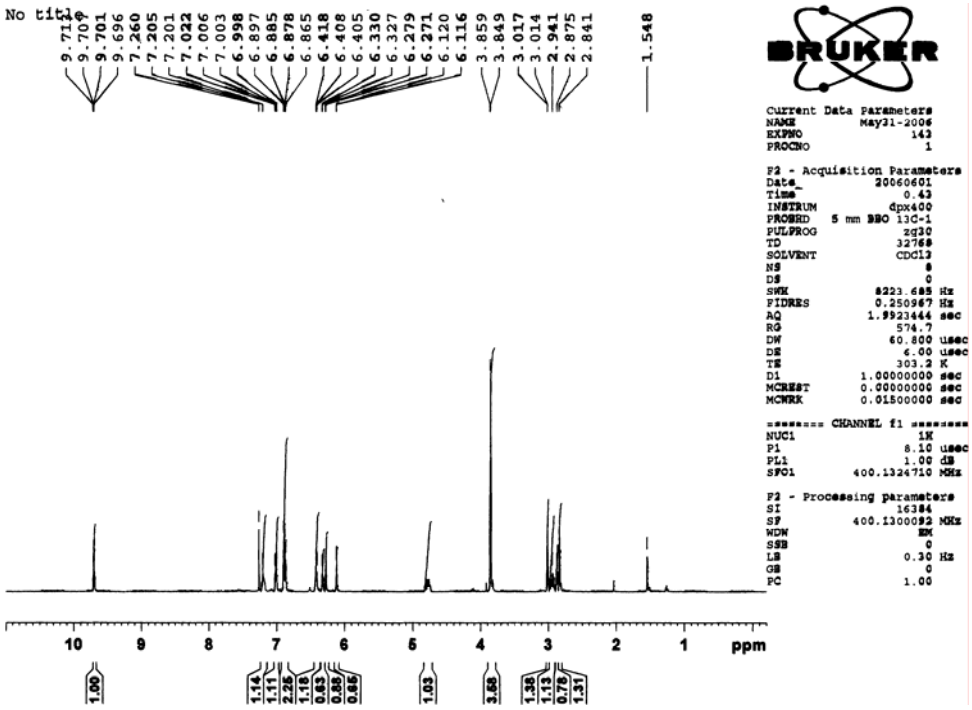

COSYGS
200.75
200.61
149.52
147.76
147.25
146.24
134.67
132.93
132.22
131.82
128.30
127.92
127.30
126.75
126.44
124.09
124.02
123.95
77.32
77.00
76.68
49.98
49.43
42.05
41.26
16.41
15.70
BRUKER
Current Data Parameters
NAME Jun04-2006
EXPNO 46
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060604
Time 22.05
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 9195.2
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127727 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm

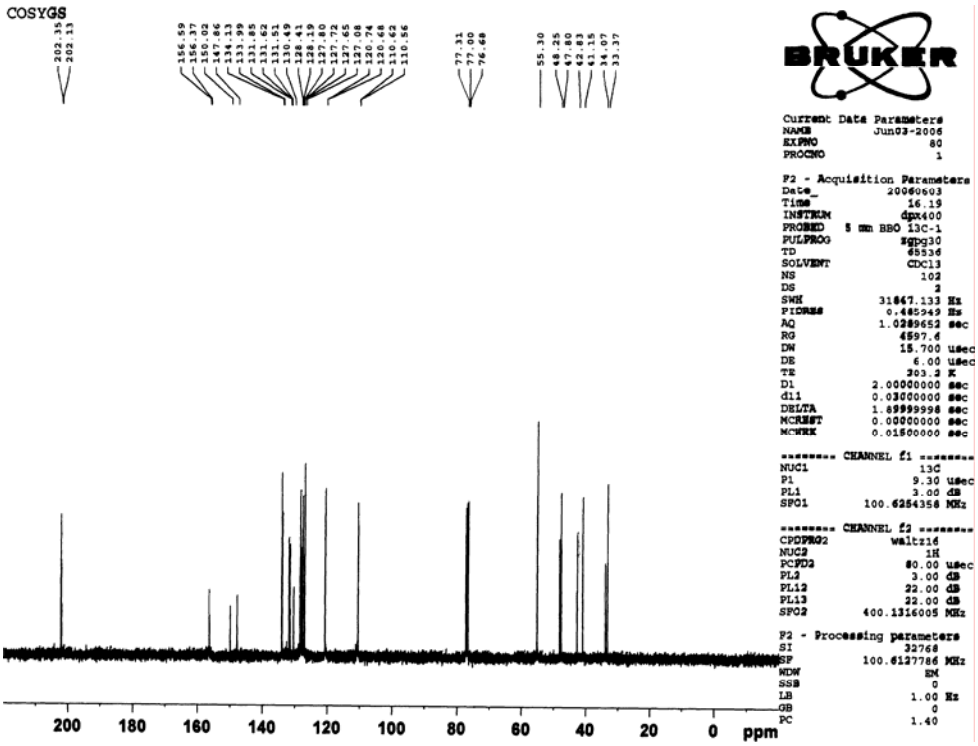


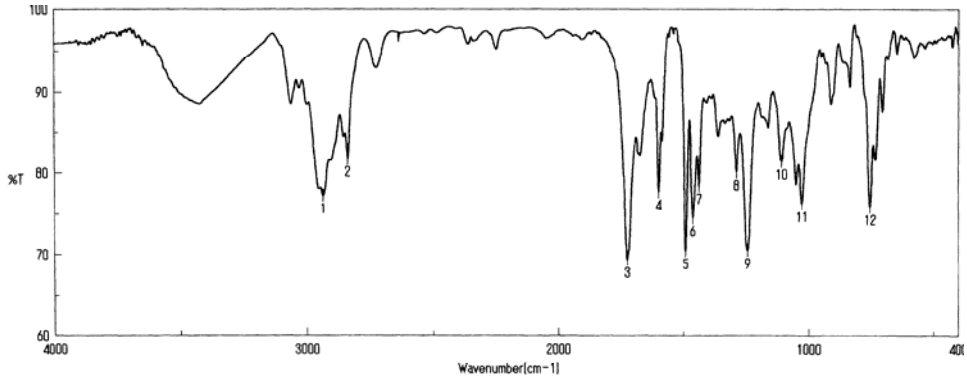
積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/06/05 18:04		
測定者			
ファイル名	Memory#14		
サンプル名			
コメント	コメント		

1:	3071.08,	93.7764	2:	2923.56,	90.0950	3:	2725.89,	92.8870	4:	1724.05,	67.5877
5:	1383.43,	87.7724	6:	1245.79,	93.8000	7:	1054.87,	92.7518	8:	897.70,	85.2231
9:	850.45,	91.6369	10:	698.11,	78.8559						


OMe
H
OMe
H

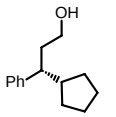

No title
9.716
9.709
9.701
9.696
7.260
7.205
7.201
7.022
7.006
7.003
6.998
6.897
6.885
6.878
6.865
6.418
6.408
6.405
6.330
6.327
6.279
6.271
6.120
6.116
3.859
3.849
3.017
3.014
2.941
2.875
2.841
1.548
BRUKER
Current Data Parameters
NAME May31-2006
EXPNO 143
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060601
Time 0.43
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 574.7
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.10 usec
PL1 1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
1.00 1.14 1.11 2.26 1.18 0.83 0.88 0.86 1.03 3.68 1.38 1.13 0.76 1.31

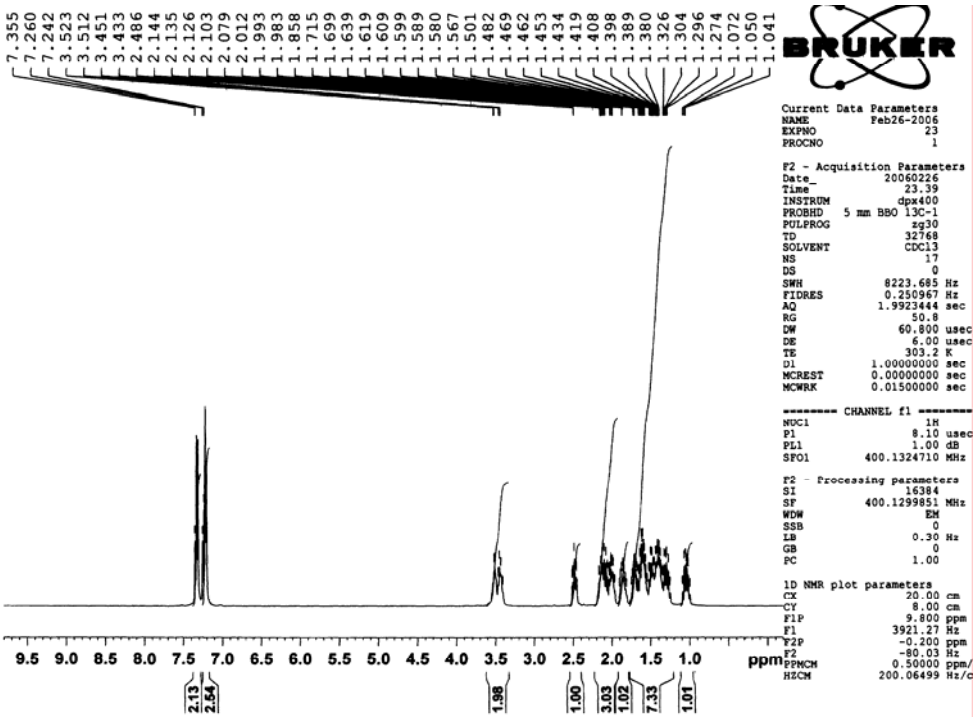

COSYGS
202.35
202.13
156.59
156.37
150.02
147.86
134.13
133.99
131.85
131.62
131.51
130.49
128.41
128.19
127.70
127.52
127.65
127.08
120.74
120.68
110.62
110.56
77.31
77.00
76.68
55.30
48.25
47.80
42.83
41.15
34.07
33.37
BRUKER
Current Data Parameters
NAME Jun03-2006
EXPNO 80
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060603
Time 16.19
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 102
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 4597.6
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6254356 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127786 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

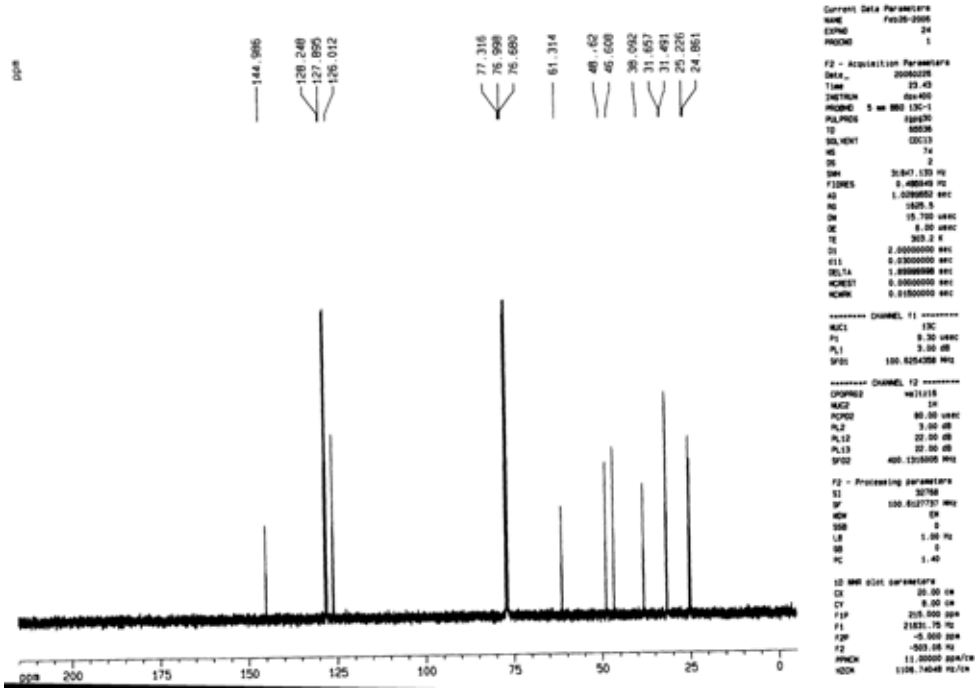


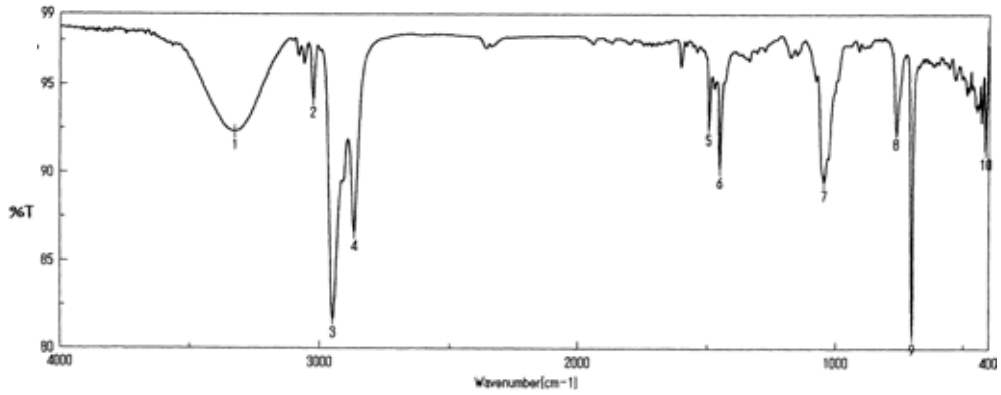
積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	2	スキャンスピード	2 mm/sec
日時	106/06/04 17:51		
測定者			
ファイル名	Memory#6		
サンプル名			
コメント	コメント		

1:	2935.13, 77.2679	2:	2837.74, 81.7965	3:	1723.09, 69.4235	4:	1599.66, 77.7602
5:	1492.63, 70.4966	6:	1463.71, 74.5607	7:	1438.64, 78.4804	8:	1290.14, 80.1883
9:	1244.83, 70.5501	10:	1109.83, 81.5259	11:	1027.87, 76.3142	12:	754.99, 75.9544


OH
Ph

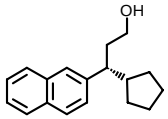

7.355
7.260
7.242
3.523
3.512
3.451
3.433
2.486
2.144
2.135
2.126
2.103
2.079
2.012
1.993
1.983
1.858
1.715
1.699
1.639
1.619
1.609
1.599
1.589
1.580
1.567
1.501
1.482
1.469
1.462
1.453
1.434
1.419
1.408
1.398
1.389
1.380
1.326
1.304
1.296
1.274
1.072
1.050
1.041
BRUKER
Current Data Parameters
NAME Feb26-2006
EXPNO 23
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060226
Time 23.39
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 17
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 50.8
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 8.10 usec
PL1 1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1299851 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 9.800 ppm
F1 3921.27 Hz
F2P -0.200 ppm
F2 -80.03 Hz
PPMCM 0.50000 ppm/
HZCM 200.06499 Hz/c
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.13
2.54
1.98
1.00
3.03
1.02
7.33
1.01


ppm
144.986
128.248
127.895
126.012
77.316
76.998
76.680
61.314
48.162
46.608
39.092
31.657
31.491
25.226
24.861
Current Data Parameters
F2 - Acquisition Parameters
-------- CHANNEL f1 --------
-------- CHANNEL f2 --------
F2 - Processing parameters
1D NMR plot parameters
200 175 150 125 100 75 50 25 0 ppm

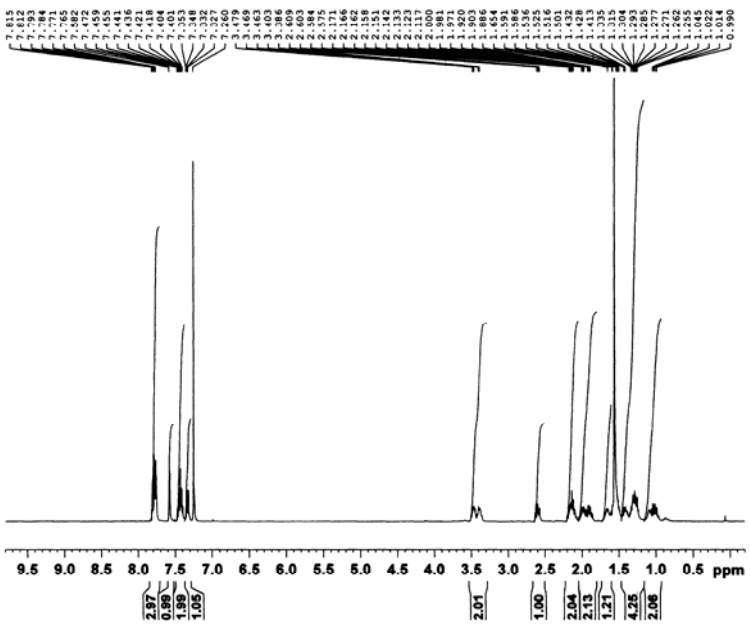


積算回数	16	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/02/27 19:59		
測定者			
ファイル名	060227.jws		
サンプル名			
コメント	コメント		

1:	3324.68,	92.3137	2:	3025.76,	94.1611	3:	2949.59,	81.6935	4:	2867.63,	86.6293
5:	1494.56,	92.6645	6:	1451.17,	90.2589	7:	1046.19,	89.4997	8:	763.67,	92.4321
9:	701.00,	80.7626	10:	411.73,	91.3079						

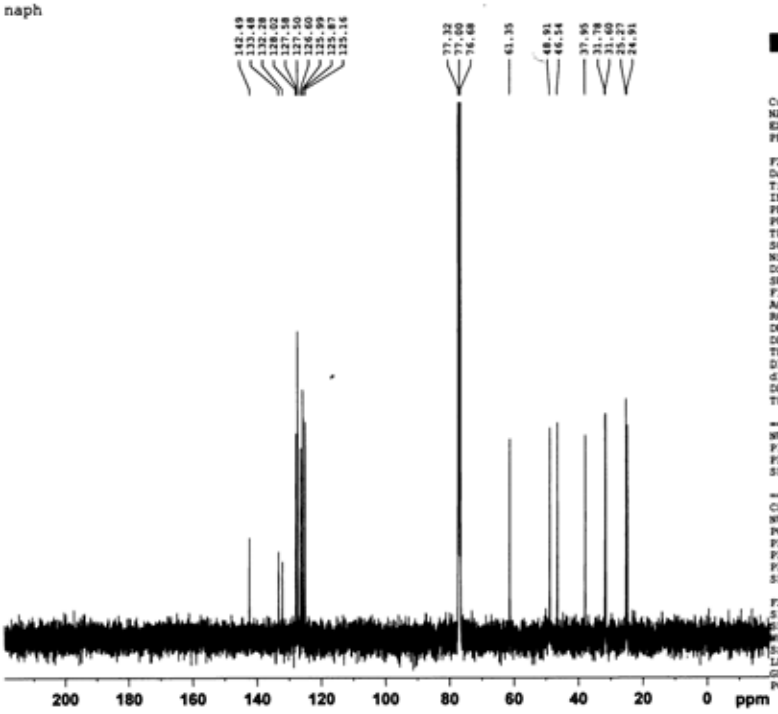


naph

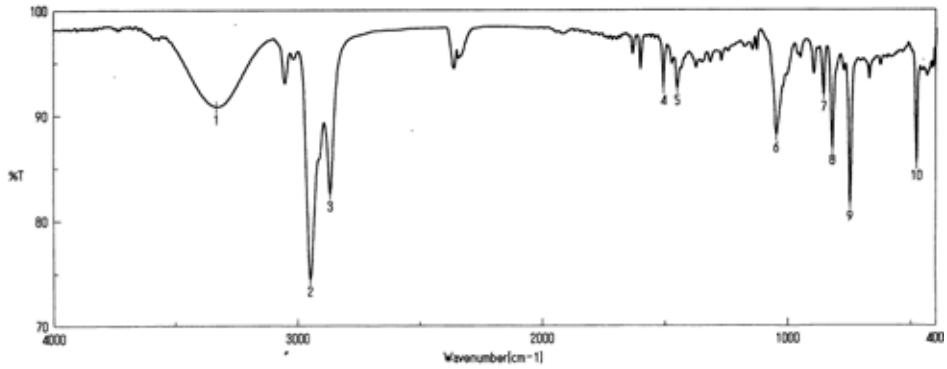



```
Current Data Parameters
NAME        Jun03-2006-hayashi
EXPNO                       20
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20060603
Time_                     3.13
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9846387 sec
RG                        256
DW                     60.800 usec
DE                      6.00 usec
TE                     297.3 K
D1                   1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                        1H
P1                      12.00 usec
PL1                     -4.00 dB
SFO1           400.1824713 MHz

F2 - Processing parameters
SI                      32768
SF                 400.1800078 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```

naph



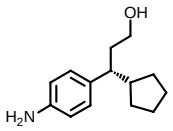

```
Current Data Parameters
NAME        Jun09-2006-hayashi
EXPNO                       10
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20060609
Time                      3.07
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                 zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1024
DS                          4
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631988 sec
RG                         32
DW                     20.800 usec
DE                      6.00 usec
TE                     298.8 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       13C
P1                      7.20 usec
PL1                     -4.00 dB
SFO1           100.6354036 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                  80.00 usec
PL2                     -4.00 dB
PL12                    15.00 dB
PL13                    15.00 dB
SFO2           400.1816007 MHz

F2 - Processing parameters
SI                      32768
SF                 100.6253442 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

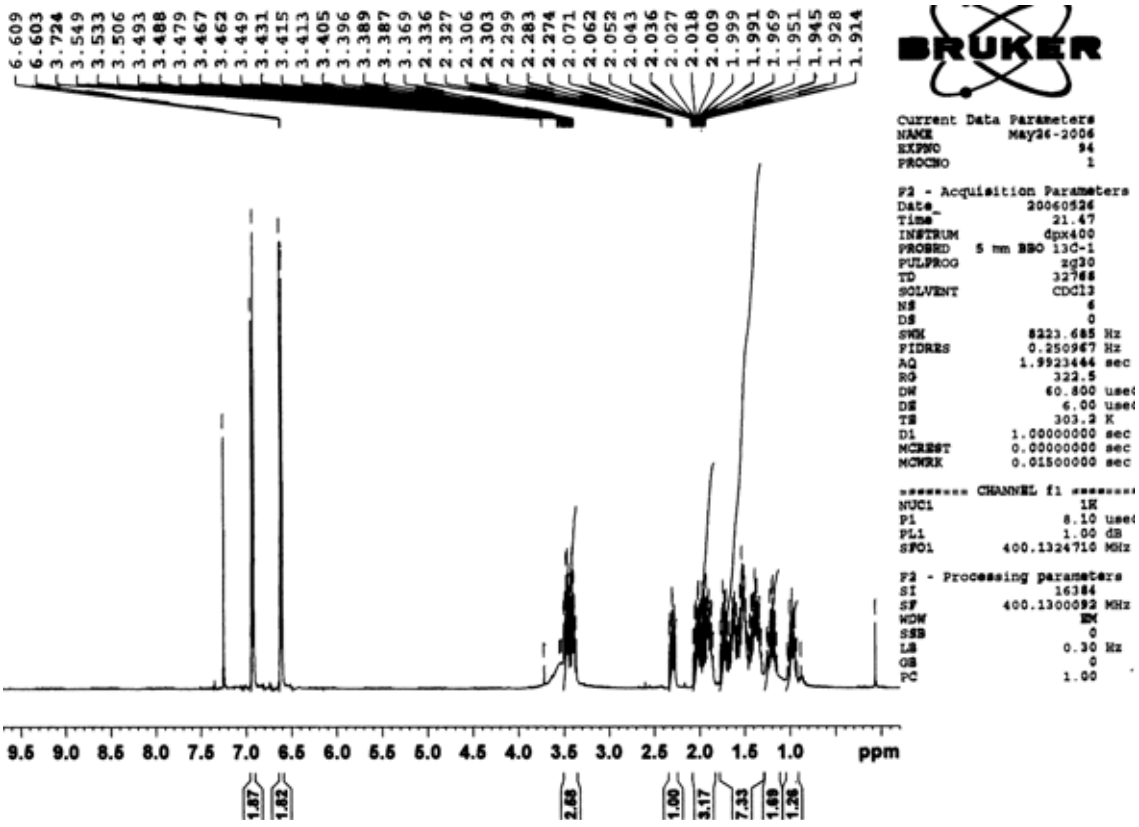


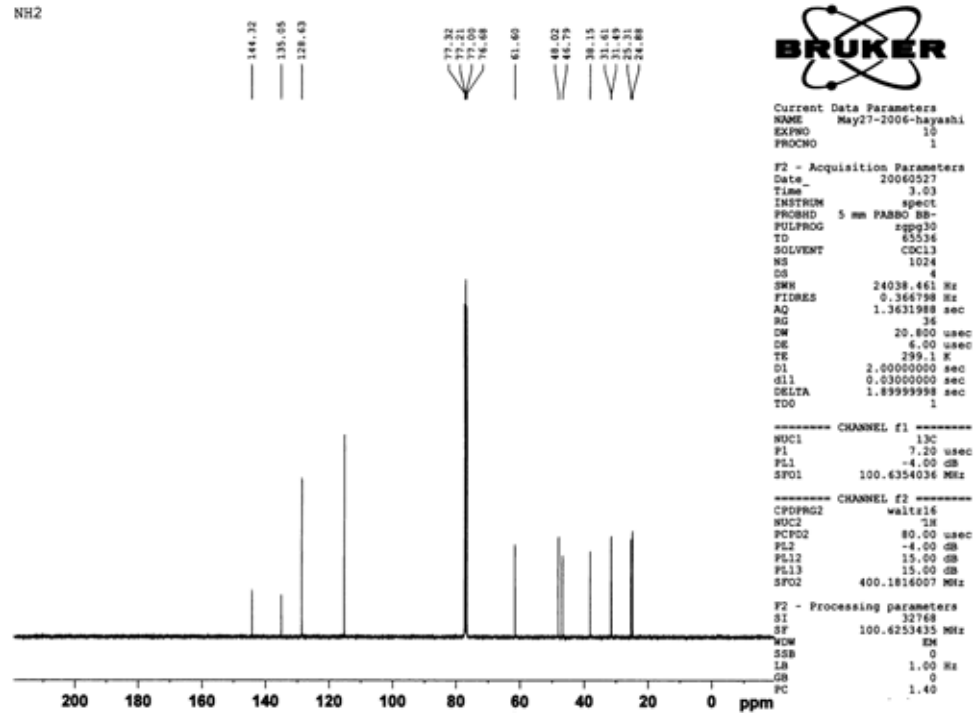
積算回数 64
ゼロフィリング ON
ゲイン 1
日時 106/06/08 18:50
測定者
ファイル名 Memory#7
サンプル名
コメント コメント

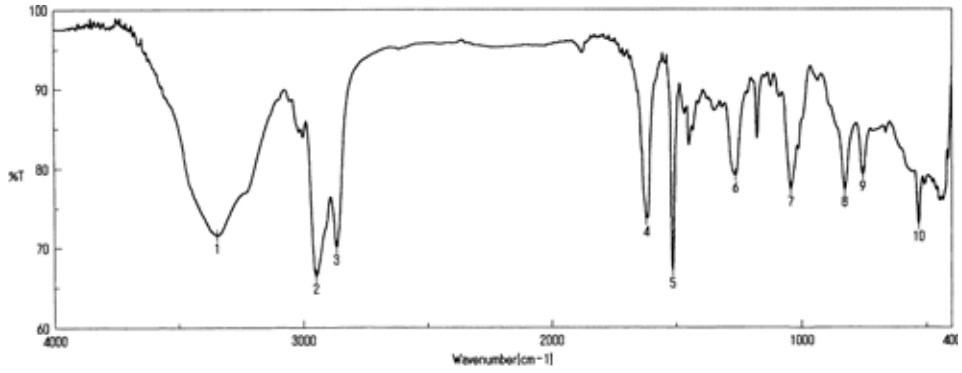
分解 4 cm-1
アポダイゼーション Cosine
スキャンスピード 2 mm/sec

1: 3331.43, 90.8236 2: 2948.63, 74.4865 3: 2866.67, 82.6093 4: 1507.10, 92.6255
5: 1450.21, 92.6310 6: 1046.19, 88.1499 7: 853.35, 92.0060 8: 817.67, 86.9653
9: 746.32, 81.6580 10: 477.30, 85.4647


OH
H_2N

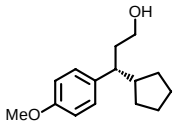

6.609 6.603 3.724 3.549 3.533 3.506 3.493 3.488 3.479 3.467 3.462 3.449 3.431 3.415 3.413 3.405 3.396 3.389 3.387 3.369 2.336 2.327 2.306 2.303 2.299 2.283 2.274 2.071 2.062 2.052 2.043 2.036 2.027 2.018 2.009 1.999 1.991 1.969 1.951 1.945 1.928 1.914
BRUKER
Current Data Parameters
NAME May26-2006
EXPNO 94
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060526
Time 21.47
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 322.5
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.10 usec
PL1 1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.87 1.82 2.68 1.00 3.17 7.33 1.69 1.26

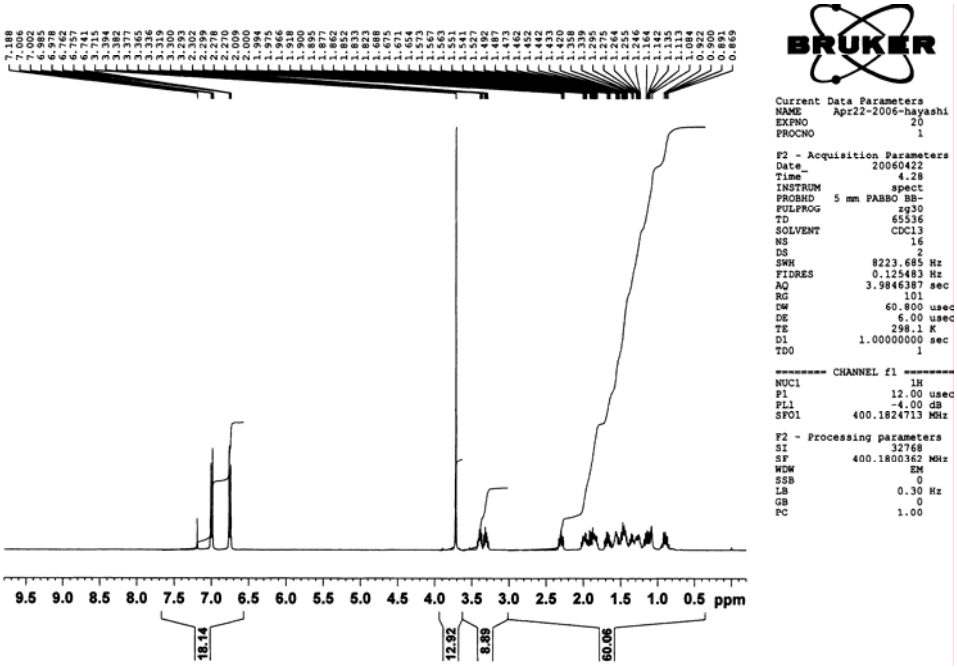

NH2
144.32 135.05 128.63 77.32 77.21 77.00 76.68 61.60 48.02 46.79 38.15 31.61 31.49 25.31 24.88
BRUKER
Current Data Parameters
NAME May27-2006-hayashi
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060527
Time 3.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 36
DW 20.800 usec
DE 6.00 usec
TE 299.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.20 usec
PL1 -4.00 dB
SFO1 100.6354036 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1816007 MHz
F2 - Processing parameters
SI 32768
SF 100.6253435 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm



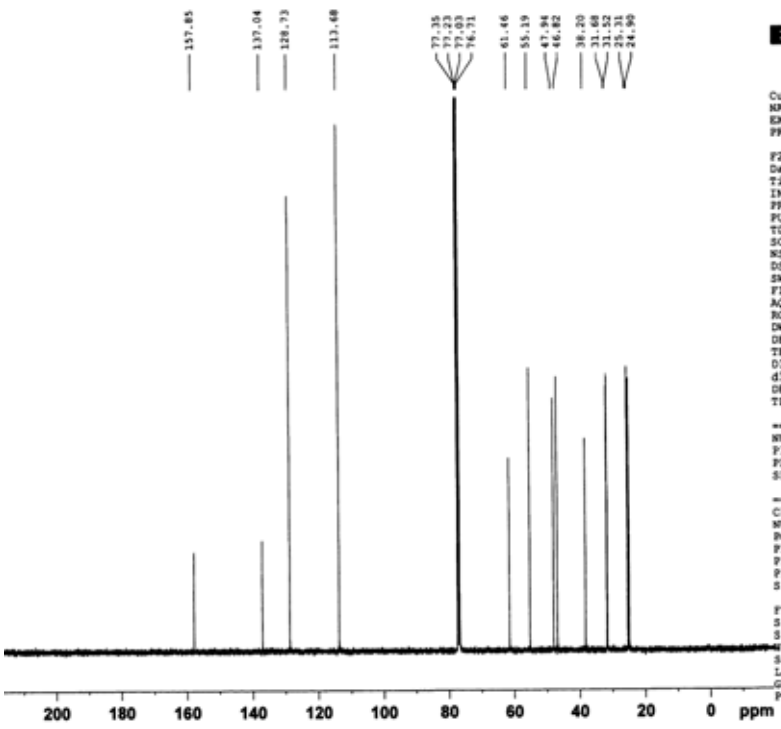
積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/06/06 21:33		
測定者			
ファイル名	Memory03		
サンプル名			
コメント	コメント		

1:	3346.85,	71.5485	2:	2948.63,	66.4421	3:	2866.67,	70.0667	4:	1620.88,	73.6116
5:	1514.81,	67.1321	6:	1265.07,	79.1264	7:	1045.23,	77.3456	8:	828.28,	77.3457
9:	756.92,	79.2563	10:	533.22,	72.9660						

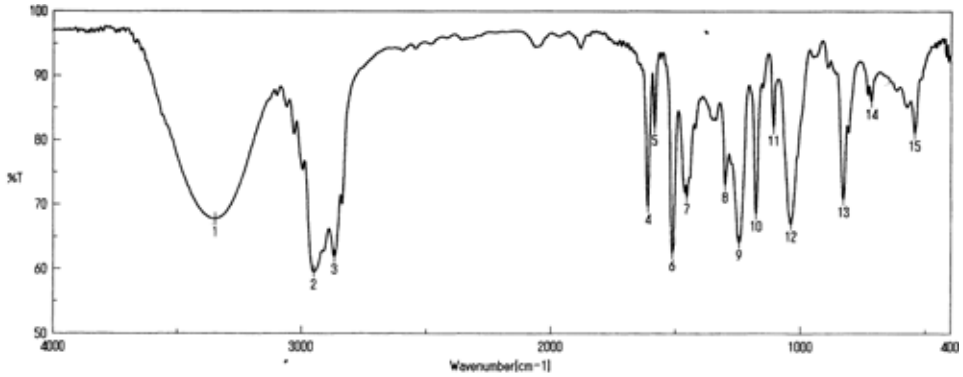





```
Current Data Parameters
NAME      Apr22-2006-hayashi
EXPNO                     20
PROCNO                     1

F2 - Acquisition Parameters
Date_              20060422
Time                   4.28
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                       101
DW                    60.800 usec
DE                     6.00 usec
TE                   298.1 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     12.00 usec
PL1                    -4.00 dB
SFO1           400.1824713 MHz

F2 - Processing parameters
SI                    32768
SF             400.1800362 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

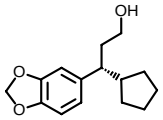


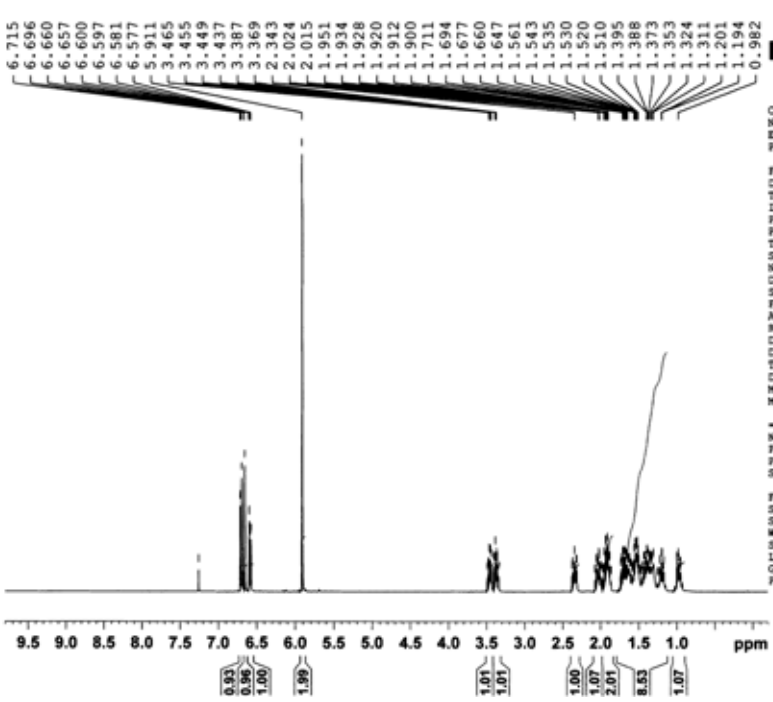

```
Current Data Parameters
NAME      Apr22-2006-hayashi
EXPNO                     30
PROCNO                     1

F2 - Acquisition Parameters
Date_              20060422
Time                   4.25
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                      80.6
DW                    20.800 usec
DE                     6.00 usec
TE                   299.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     13C
P1                     7.20 usec
PL1                    -4.00 dB
SFO1           100.6354036 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                    -4.00 dB
PL12                   15.00 dB
PL13                   15.00 dB
SFO2           400.1816007 MHz

F2 - Processing parameters
SI                    32768
SF             100.6253410 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/06/06 11:21		
測定者			
ファイル名	p-methoxy-alchol.JWS		
サンプル名			
コメント	コメント		

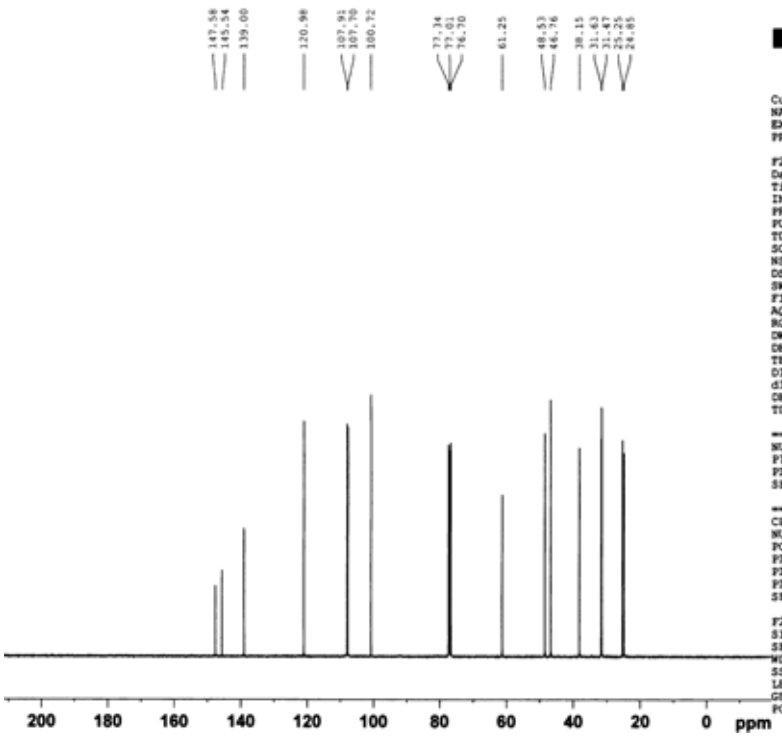
1:	3348.85,	67.7183	2:	2949.59,	59.5339	3:	2866.67,	61.9228
4:	1610.27,	69.7818	5:	1583.27,	82.0163	6:	1512.88,	62.5209
7:	1455.03,	71.3403	8:	1301.72,	73.1381	9:	1245.79,	64.1867
10:	1178.29,	68.7188	11:	1108.87,	81.9926	12:	1038.48,	67.0484
13:	828.28,	70.9132	14:	717.39,	86.0783	15:	543.83,	81.1705





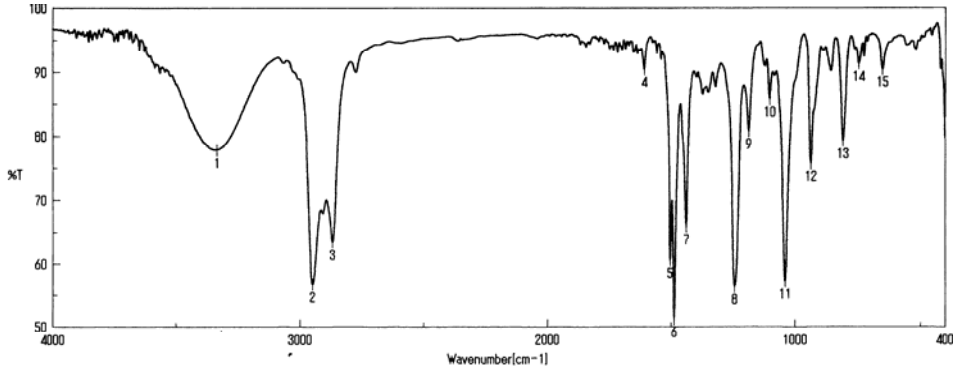
BRUKER

```
Current Data Parameters
NAME          May16-2006
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20060516
Time                3.29
INSTRUM          dpx400
PROBHD   5 mm BBO 13C-1
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                 101.6
DW                60.800 usec
DE                 6.00 usec
TE                303.2 K
D1             1.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 8.10 usec
PL1                1.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300088 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



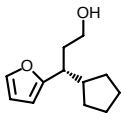
BRUKER

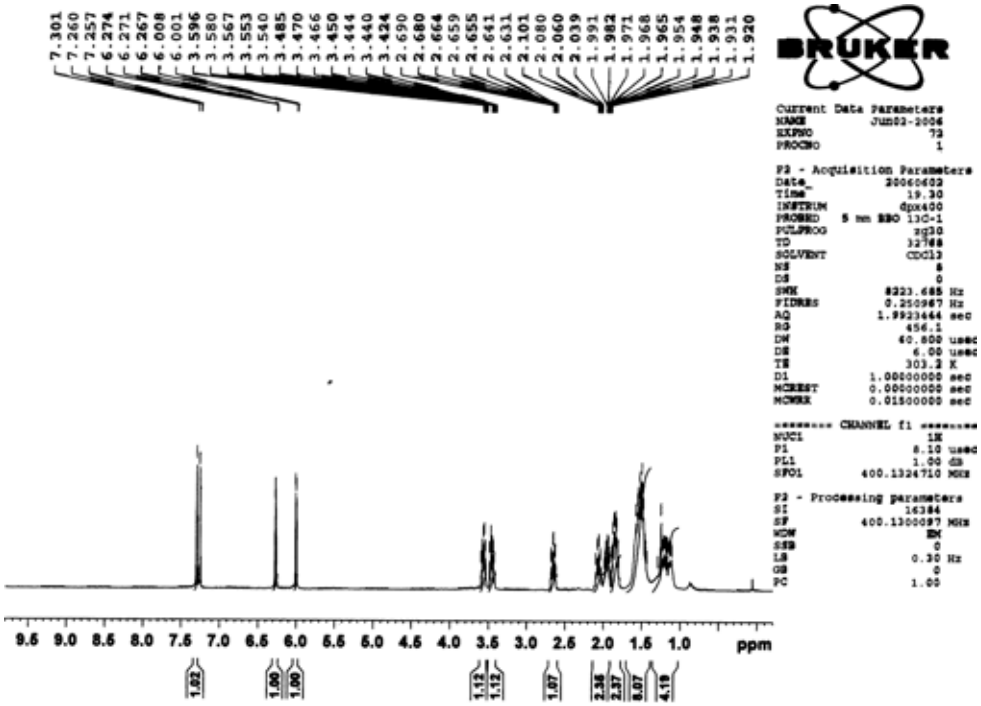
```
Current Data Parameters
NAME      May16-2006-hayashi
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20060516
Time                4.33
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                  80.6
DW                20.800 usec
DE                 6.00 usec
TE                299.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 7.20 usec
PL1                -4.00 dB
SFO1         100.6354036 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2             80.00 usec
PL2                -4.00 dB
PL12               15.00 dB
PL13               15.00 dB
SFO2         400.1816007 MHz

F2 - Processing parameters
SI                 32768
SF          100.6253461 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

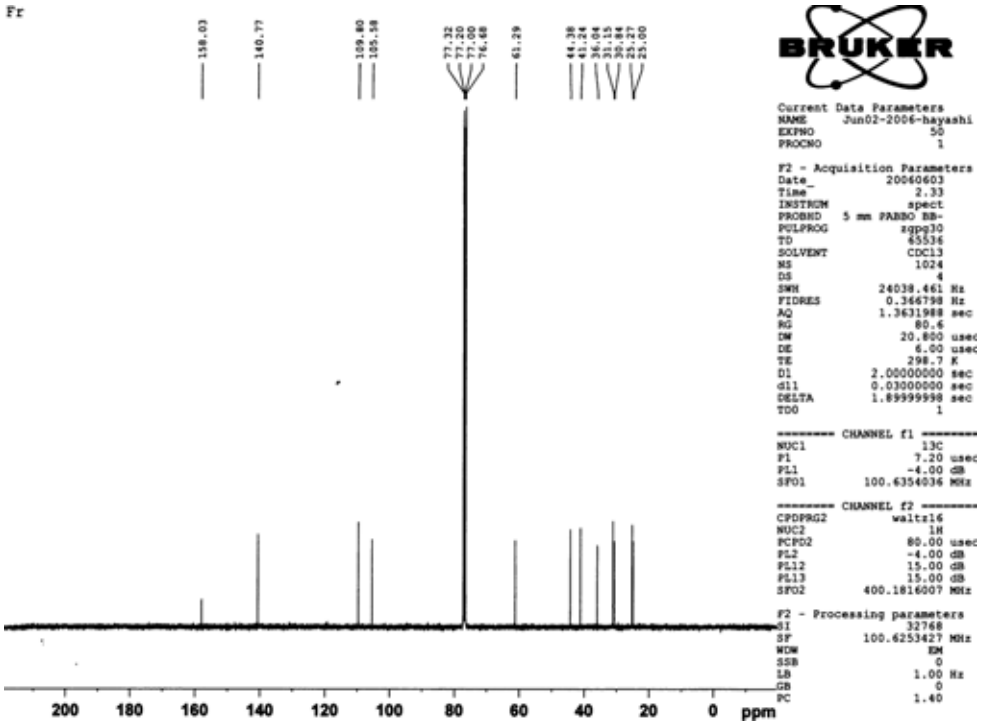


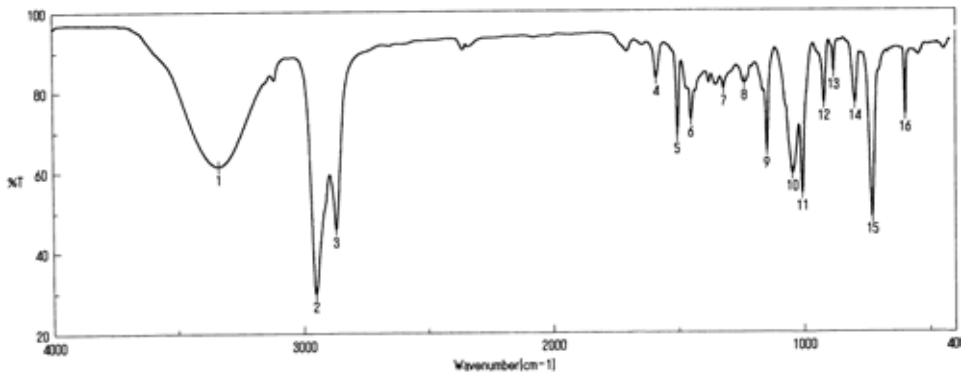
積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/06/06 11:28		
測定者			
ファイル名	acetal-alchol.JWS		
サンプル名			
コメント	コメント		

1:	3336.25,	77.8507	2:	2949.59,	59.6799	3:	2868.59,	63.4192	4:	1608.34,	90.5055
5:	1504.20,	60.5530	6:	1467.81,	51.2385	7:	1439.60,	65.8965	8:	1243.86,	56.3838
9:	1187.94,	80.8198	10:	1104.05,	85.8007	11:	1040.41,	57.2000	12:	938.20,	75.8035
13:	809.96,	79.3509	14:	748.25,	91.3845	15:	653.75,	90.5115			


OH
O

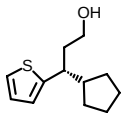

7.301
7.260
7.257
6.274
6.271
6.267
6.008
6.001
3.596
3.580
3.567
3.553
3.540
3.485
3.470
3.466
3.450
3.444
3.440
3.424
2.690
2.680
2.664
2.659
2.655
2.641
2.631
2.101
2.080
2.060
2.039
1.991
1.982
1.971
1.968
1.965
1.954
1.948
1.938
1.931
1.920
BRUKER
Current Data Parameters
NAME Jun02-2006
EXPNO 73
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060602
Time 19.30
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923464 sec
RG 456.1
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.10 usec
PL1 1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.02
1.00
1.00
1.12
1.12
1.07
2.36
2.37
8.07
4.19

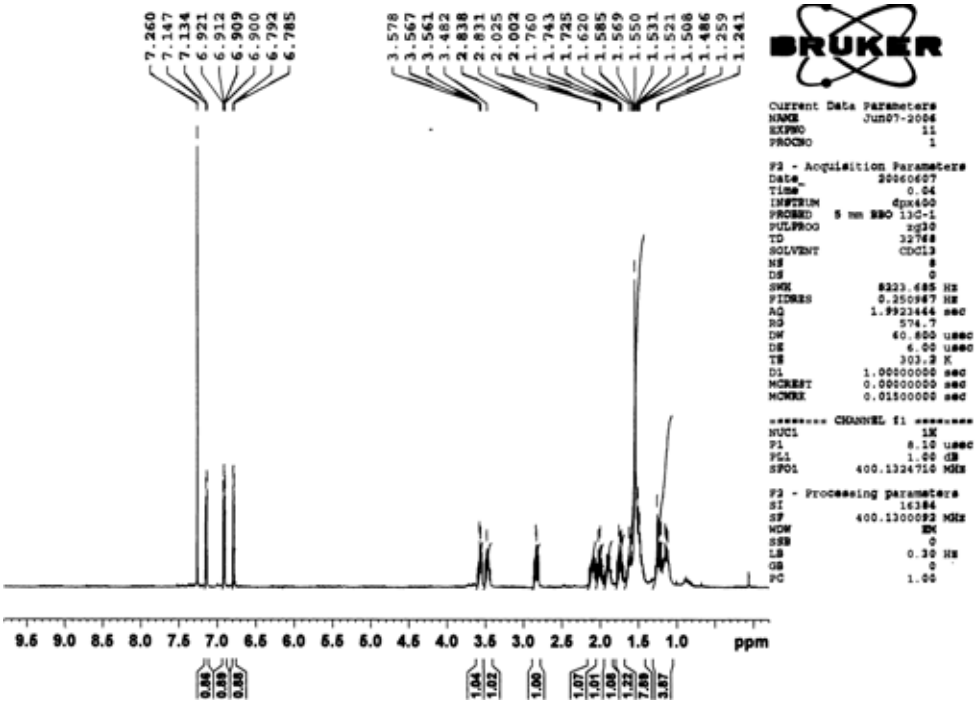

Fr
158.03
140.77
109.80
105.58
77.32
77.20
77.00
76.68
61.29
44.38
41.24
36.04
31.15
29.84
25.37
23.00
BRUKER
Current Data Parameters
NAME Jun02-2006-hayashi
EXPNO 50
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060603
Time 2.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 80.6
DW 20.800 usec
DE 6.00 usec
TE 298.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.20 usec
PL1 -4.00 dB
SFO1 100.6354036 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1816007 MHz
F2 - Processing parameters
SI 32768
SF 100.6253427 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm



積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	2	スキャンスピード	2 mm/sec
日時	106/06/08 18:45		
測定者			
ファイル名	Memory#5		
サンプル名			
コメント	コメント		

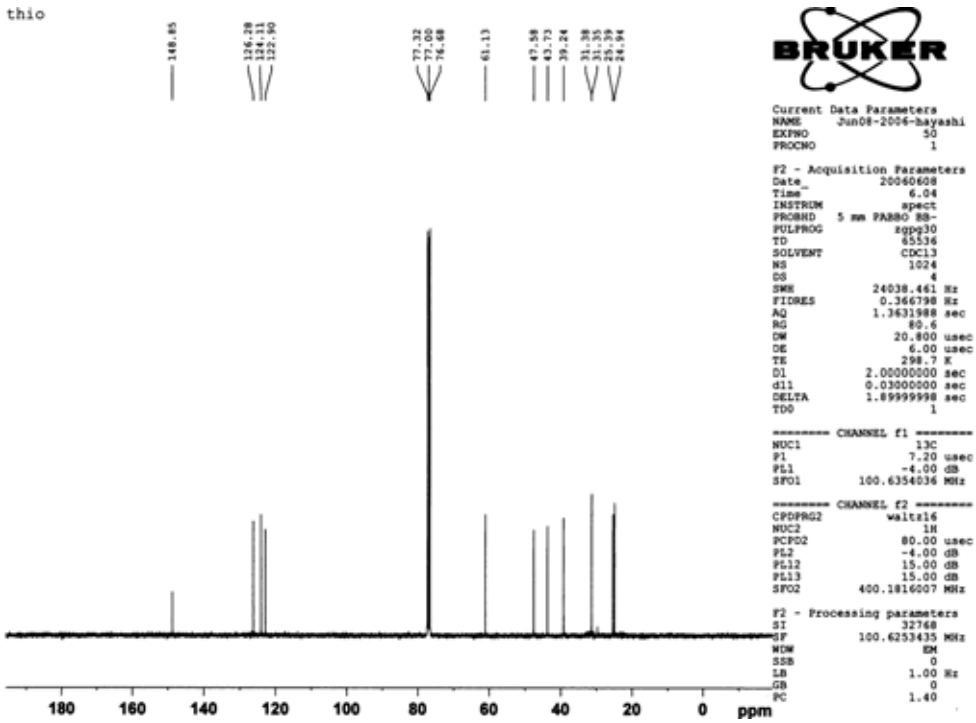
1:	3336.25,	61.4962	2:	2950.55,	29.6914	3:	2868.59,	45.7573	4:	1591.95,	83.1248
5:	1506.13,	68.7658	6:	1451.17,	72.6584	7:	1321.96,	80.5411	8:	1239.04,	81.9923
9:	1148.40,	65.1142	10:	1046.19,	59.3493	11:	1006.66,	54.4198	12:	921.81,	76.8394
13:	884.20,	84.6250	14:	798.39,	76.8660	15:	728.96,	48.5778	16:	599.75,	74.0091



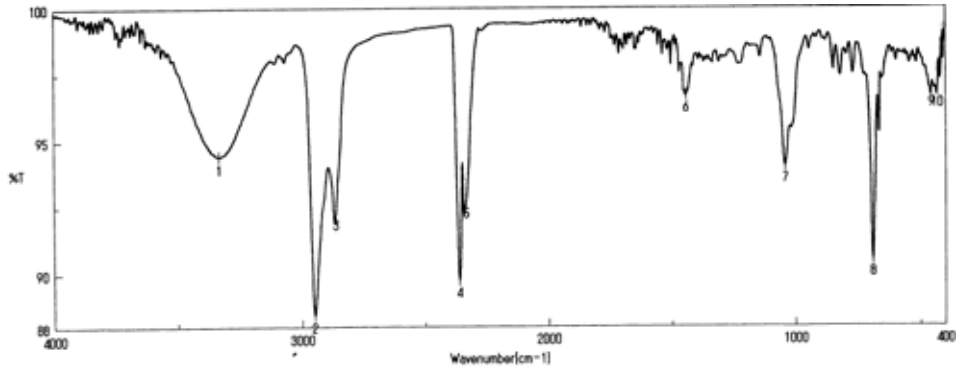



```
Current Data Parameters
NAME            Jun07-2006
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_             20060607
Time                  0.04
INSTRUM             dpx400
PROBHD   5 mm BBO 13C-1
PULPROG              zg30
TD                  32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH              8223.685 Hz
FIDRES           0.250967 Hz
AQ               1.9923444 sec
RG                   574.7
DW                  60.800 usec
DE                   6.00 usec
TE                  303.2 K
D1               1.00000000 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                    8.10 usec
PL1                   1.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                      16384
SF            400.1300092 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

thio

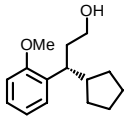


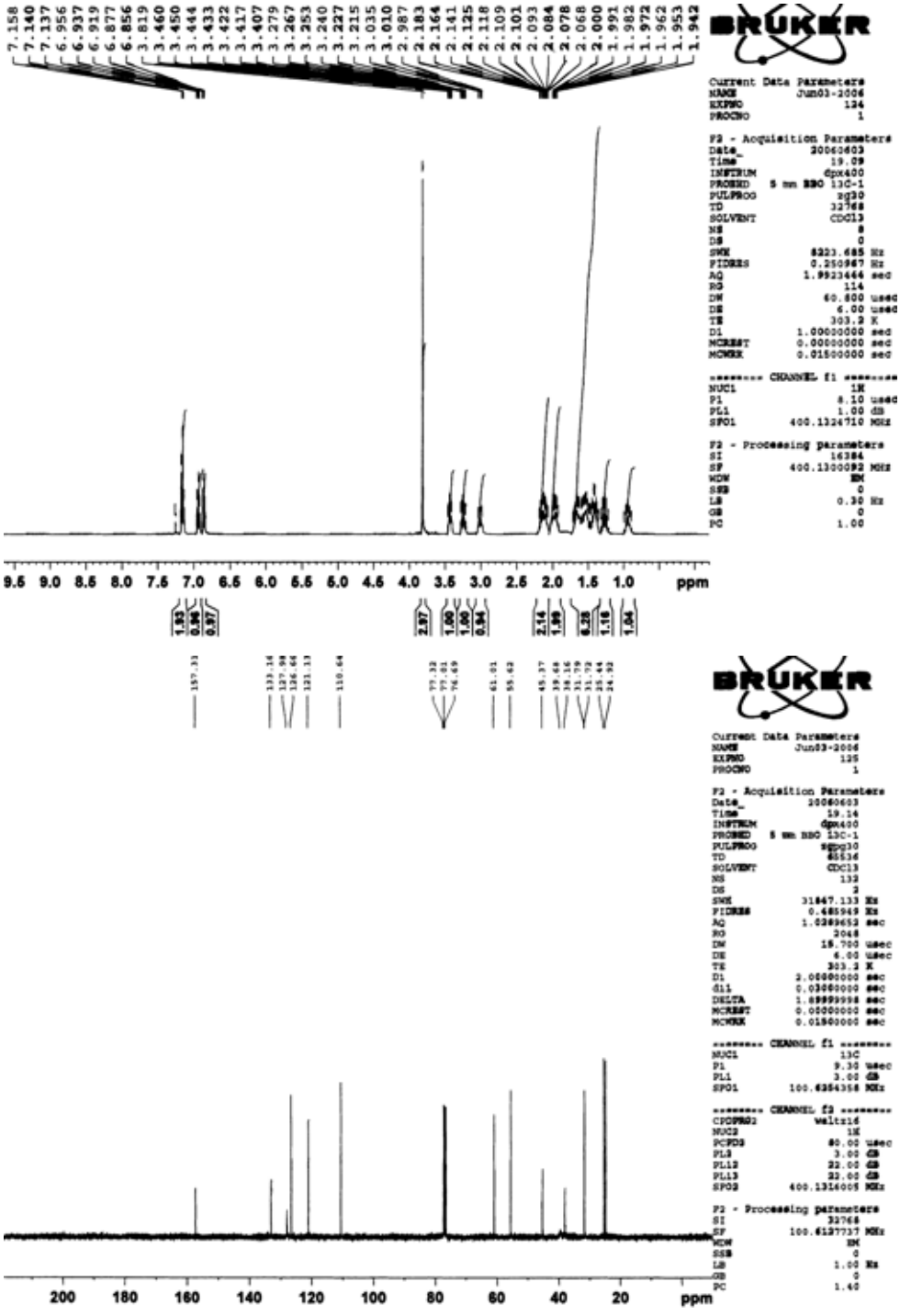

```
Current Data Parameters
NAME      Jun08-2006-hayashi
EXPNO                   50
PROCNO                   1

F2 - Acquisition Parameters
Date_             20060608
Time                  6.04
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    80.6
DW                  20.800 usec
DE                   6.00 usec
TE                  298.7 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   7.20 usec
PL1                  -4.00 dB
SFO1          100.6354036 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -4.00 dB
PL12                 15.00 dB
PL13                 15.00 dB
SFO2          400.1816007 MHz

F2 - Processing parameters
SI                      32768
SF            100.6253435 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

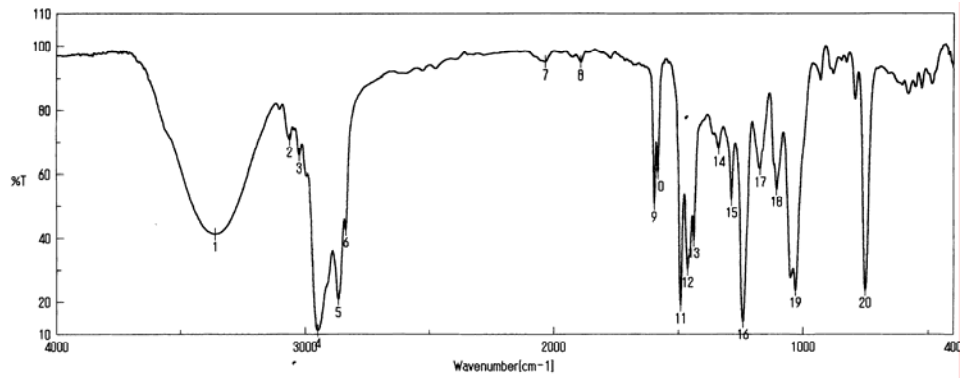


積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/06/08 18:38		
測定者			
ファイル名	Memory03		
サンプル名			
コメント	コメント		

1:	3333.35,	94.4149	2:	2949.59,	88.4557	3:	2861.84,	92.3260	4:	2360.44,	89.7489
5:	2332.48,	92.7525	6:	1445.39,	96.7155	7:	1044.26,	94.0439	8:	691.36,	90.5190
9:	456.06,	98.8768	10:	432.94,	96.8578						

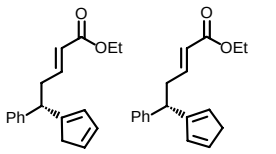

OH
OMe

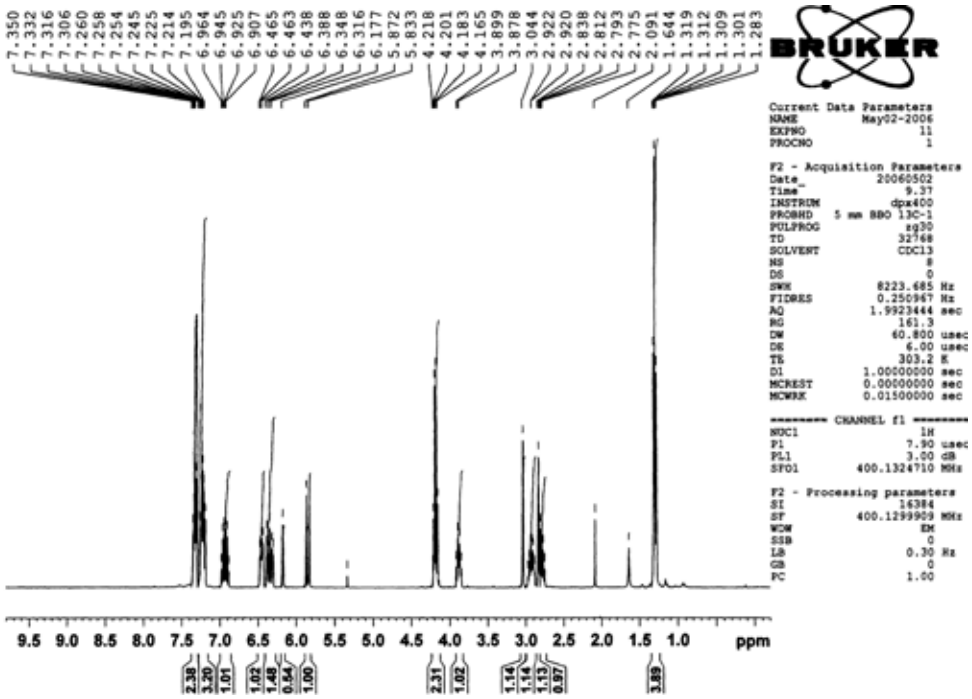

7.158
7.140
7.137
6.956
6.937
6.919
6.877
6.856
3.819
3.460
3.450
3.444
3.433
3.422
3.417
3.407
3.279
3.267
3.253
3.240
3.227
3.215
3.035
3.010
2.987
2.183
2.164
2.141
2.125
2.118
2.109
2.101
2.093
2.084
2.078
2.068
2.000
1.991
1.982
1.972
1.962
1.953
1.942
BRUKER
Current Data Parameters
NAME Jun03-2006
EXPNO 134
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060603
Time 19.09
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 114
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 8.10 usec
PL1 1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.83 0.96 0.87 2.97 1.00 1.05 0.84 2.14 1.99 6.28 1.16 1.04
157.31 133.14 127.98 126.64 121.33 110.64 77.32 77.01 76.69 61.01 55.62 45.37 39.66 31.76 31.72 25.84 24.92
BRUKER
Current Data Parameters
NAME Jun03-2006
EXPNO 135
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060603
Time 19.14
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 132
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289653 sec
RG 2048
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6354358 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1314005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm

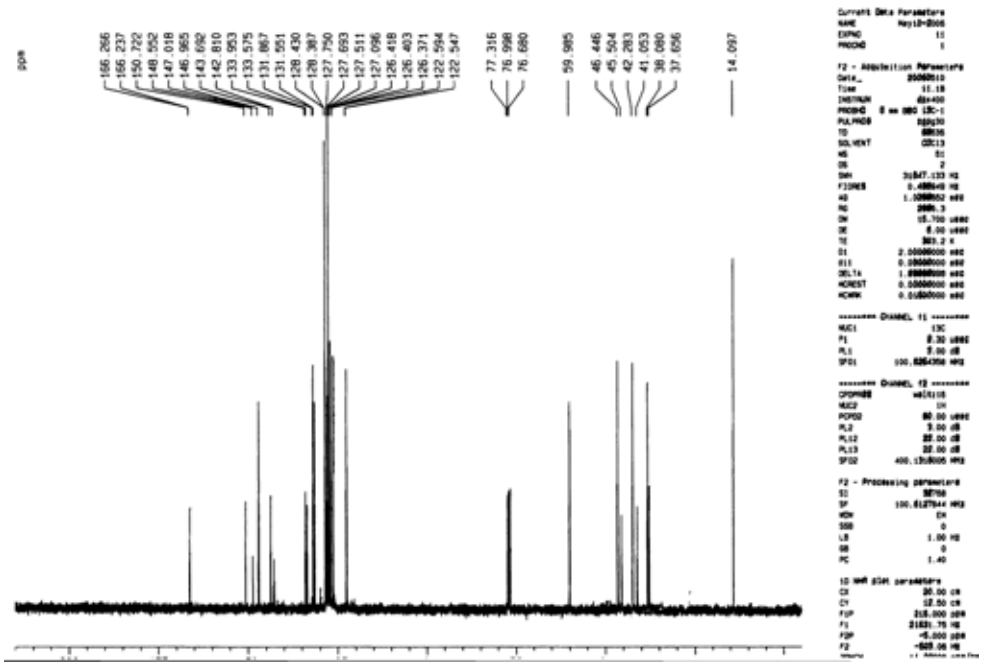


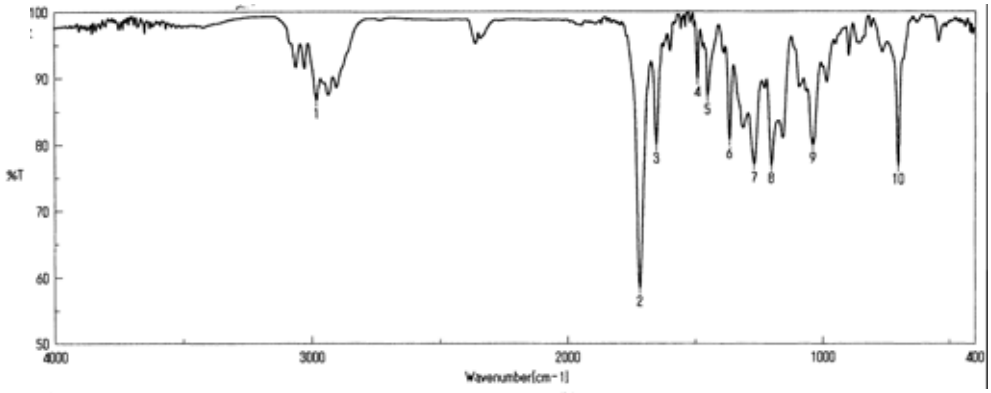
積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/06/03 21:22		
測定者			
ファイル名	Memory#3		
サンプル名			
コメント	コメント		

1:	3359.39, 41.2141	2:	3063.37, 70.7495	3:	3024.80, 65.8531	4:	2949.59, 11.1838
5:	2866.67, 20.7983	6:	2835.81, 42.6232	7:	2035.50, 95.1167	8:	1893.75, 95.0614
9:	1598.70, 50.6321	10:	1584.24, 60.4474	11:	1491.67, 18.9517	12:	1463.71, 30.3044
13:	1438.64, 39.2689	14:	1339.32, 67.9604	15:	1288.22, 52.0222	16:	1240.97, 14.0086
17:	1172.51, 61.7338	18:	1106.94, 55.4650	19:	1030.77, 23.7958	20:	753.07, 23.8334


O
OEt
Ph
O
OEt
Ph

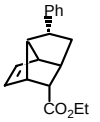

7.350
7.332
7.316
7.306
7.260
7.258
7.254
7.245
7.225
7.214
7.195
6.964
6.945
6.925
6.907
6.465
6.463
6.438
6.388
6.348
6.316
6.177
5.872
5.833
4.218
4.201
4.183
4.165
3.899
3.878
3.044
2.922
2.920
2.838
2.812
2.793
2.775
2.091
1.644
1.319
1.312
1.309
1.301
1.283
BRUKER
Current Data Parameters
NAME May02-2006
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060502
Time 9.37
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 161.3
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.90 usec
PL1 3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1299909 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
ppm
2.38
3.20
1.01
1.02
1.48
0.54
1.00
2.31
1.02
1.14
1.14
1.13
0.97
3.89

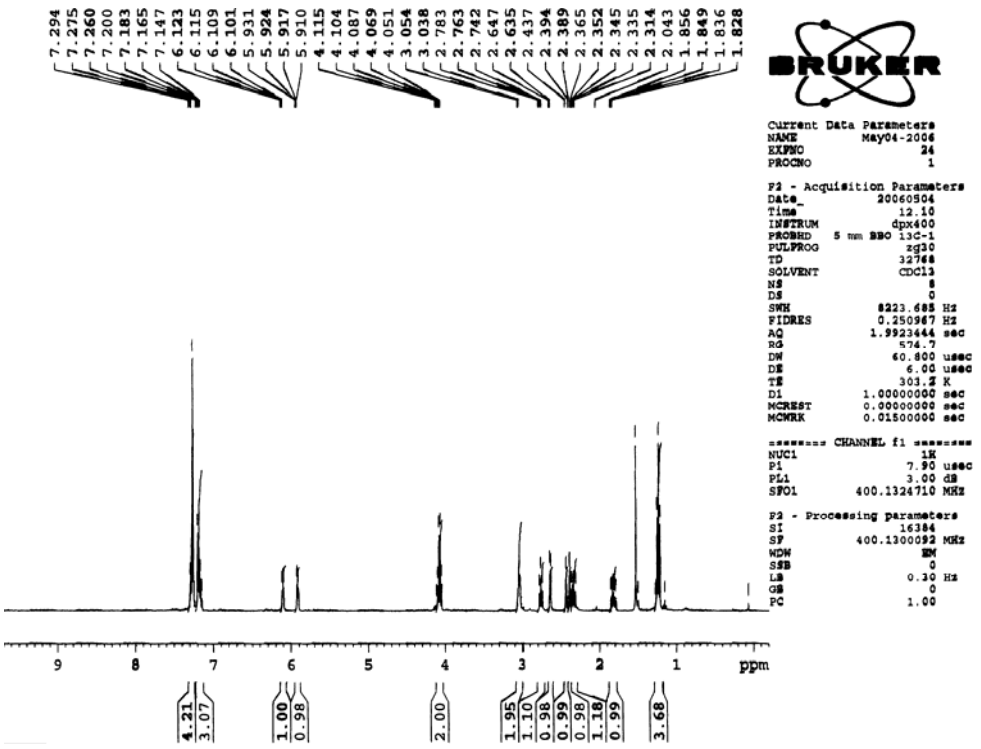

ppm
166.266
166.237
150.722
148.552
147.018
146.985
143.692
142.810
133.953
133.575
131.867
131.551
128.430
128.387
127.750
127.693
127.511
127.096
126.418
126.403
126.371
122.594
122.547
77.316
76.998
76.680
59.985
46.446
45.504
42.283
41.053
38.080
37.656
14.097

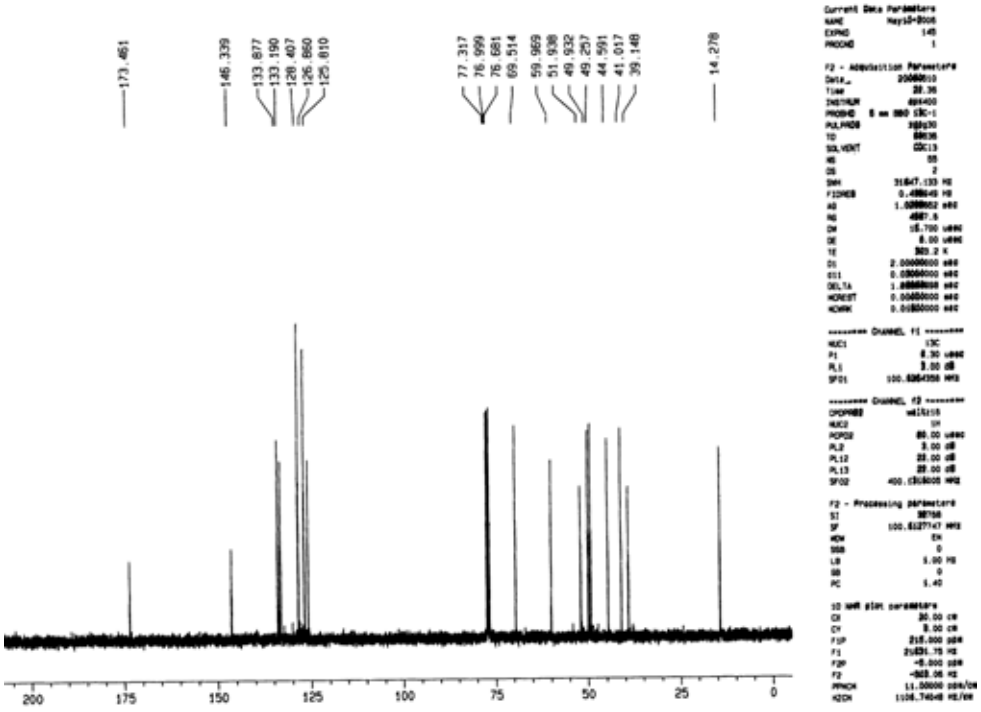


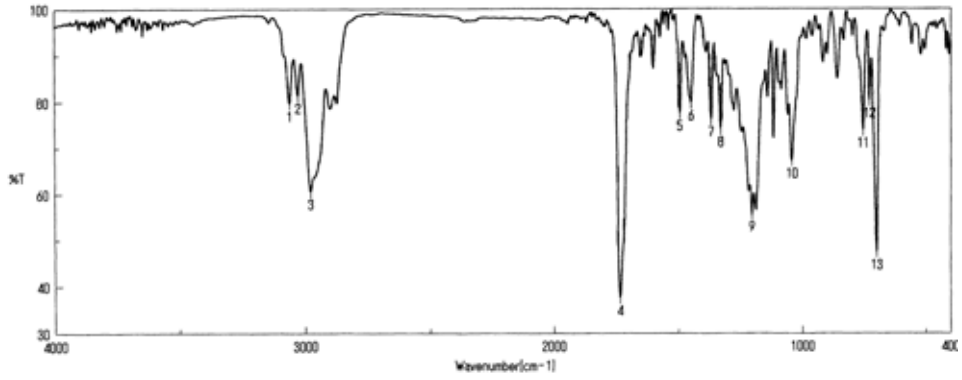
積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/05/11 17:18		
測定者			
ファイル名	Memory#3		
サンプル名			
コメント	コメント		

1:	2980.45,	86.7556	2:	1717.30,	58.4681	3:	1653.66,	80.0203	4:	1493.60,	89.9690
5:	1453.10,	87.3342	6:	1367.28,	80.7208	7:	1269.90,	77.1021	8:	1202.40,	76.9490
9:	1039.44,	80.0829	10:	701.96,	76.8674						


Ph
CO2Et

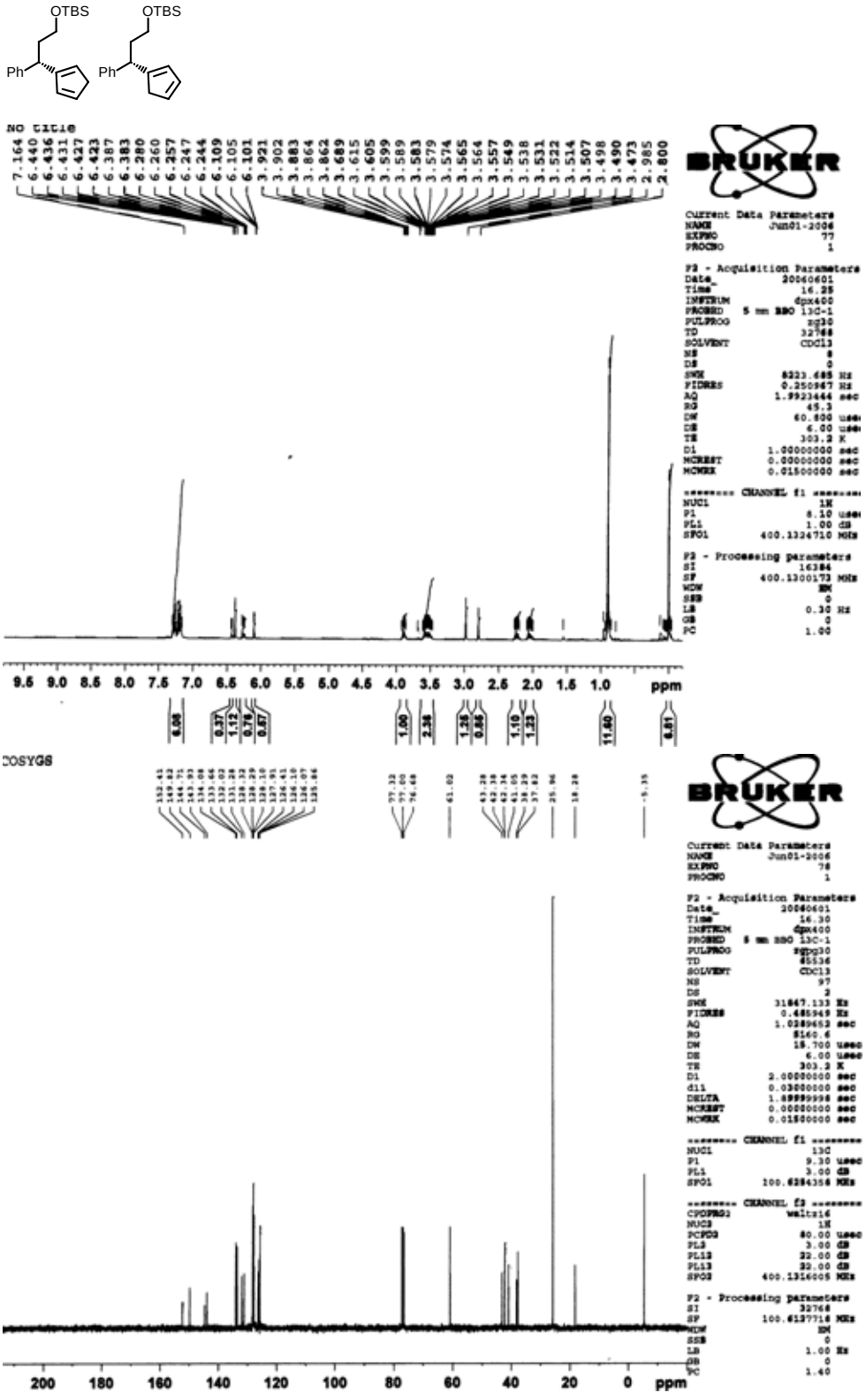

7.294
7.275
7.260
7.200
7.183
7.165
7.147
6.123
6.115
6.109
6.101
5.931
5.924
5.917
5.910
4.115
4.104
4.087
4.069
4.051
3.054
3.038
2.783
2.763
2.742
2.647
2.635
2.437
2.394
2.389
2.365
2.352
2.345
2.335
2.314
2.043
1.856
1.849
1.836
1.828
BRUKER
Current Data Parameters
NAME May04-2006
EXPNO 24
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060504
Time 12.10
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 574.7
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.90 usec
PL1 3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 ppm
4.21 3.07 1.00 0.98 2.00 1.95 1.10 0.98 0.99 0.98 1.18 0.99 3.68

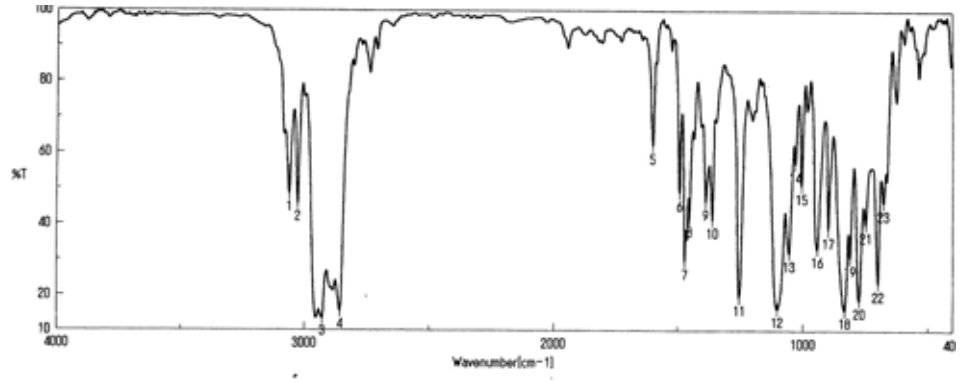

173.461
146.339
133.877
133.190
128.407
126.860
125.810
77.317
76.999
76.681
69.514
59.969
51.938
49.932
49.257
44.591
41.017
39.148
14.278
200 175 150 125 100 75 50 25 0



積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/05/11 17:33		
測定者			
ファイル名	Memory#7		
サンプル名			
コメント	コメント		

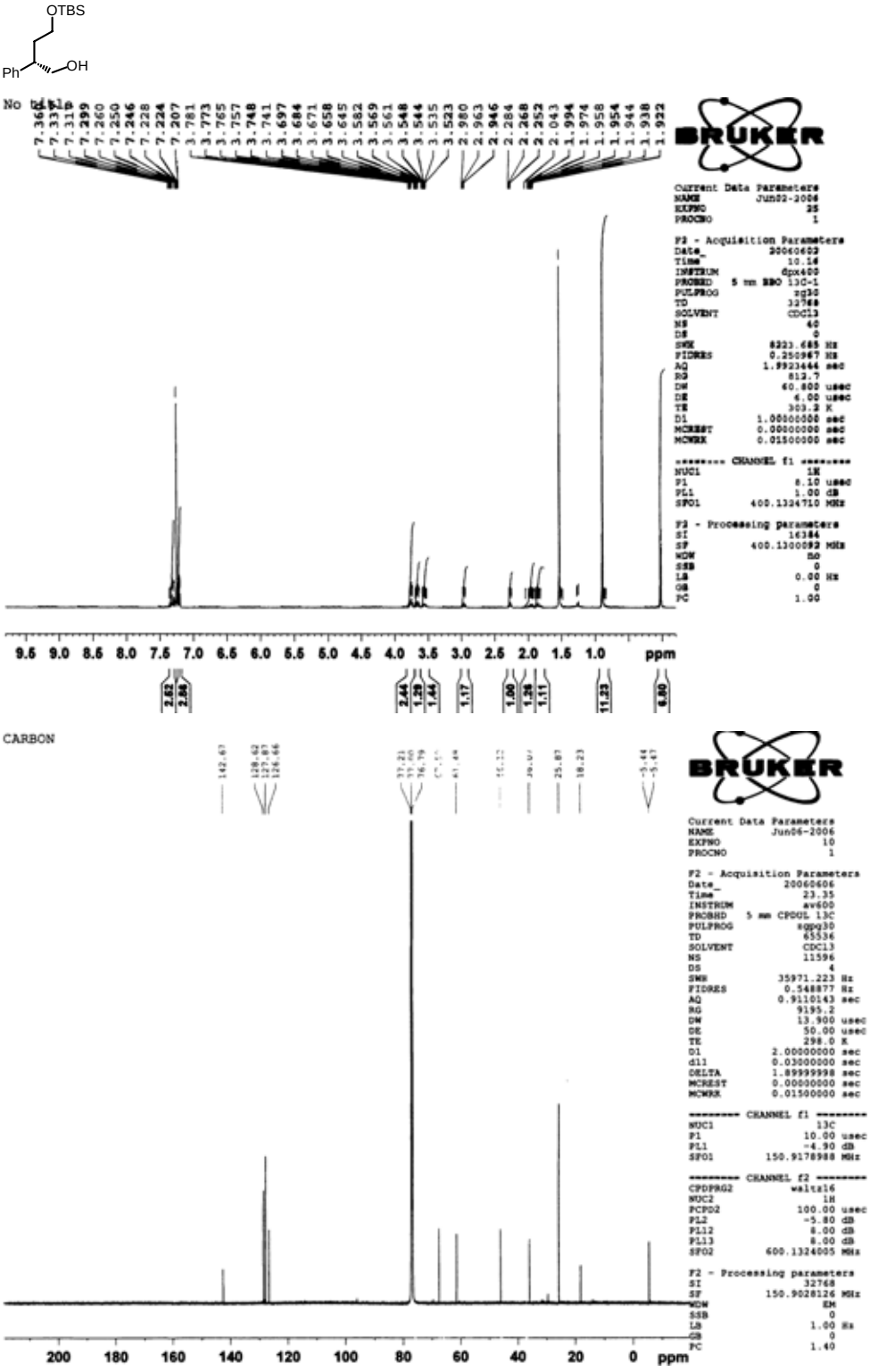
1:	3061.44,	79.6934	2:	3026.73,	81.4000	3:	2977.55,	60.6357	4:	1733.69,	37.5992
5:	1494.56,	77.5150	6:	1449.24,	79.6809	7:	1368.25,	76.2405	8:	1329.68,	74.0545
9:	1205.29,	55.6758	10:	1043.30,	67.2801	11:	754.99,	73.8201	12:	728.00,	80.2211
13:	700.03,	47.4988									

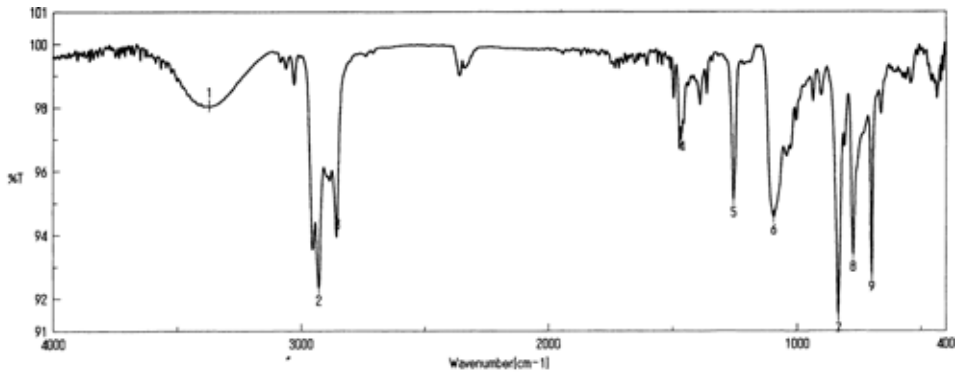

OTBS
OTBS
Ph
Ph
NO title
7.164
6.440
6.436
6.431
6.427
6.423
6.387
6.383
6.280
6.260
6.257
6.247
6.244
6.109
6.105
6.101
3.921
3.902
3.883
3.864
3.862
3.689
3.615
3.605
3.599
3.589
3.583
3.579
3.574
3.565
3.564
3.557
3.549
3.538
3.531
3.522
3.514
3.507
3.498
3.490
3.473
2.985
2.800
BRUKER
Current Data Parameters
NAME Jun01-2006
EXPNO 77
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060601
Time 16.25
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250947 Hz
AQ 1.9923444 sec
RG 45.3
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.10 usec
PL1 1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
6.68
0.37
1.12
0.76
0.87
1.00
2.58
1.35
0.86
1.10
1.23
11.60
6.01
COSYGS
BRUKER
Current Data Parameters
NAME Jun01-2006
EXPNO 76
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060601
Time 16.30
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 97
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289653 sec
RG 8160.6
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 3.00 dB
SFO1 100.6284356 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127716 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm



積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	2	スキャンスピード	2 mm/sec
日時	106/06/09 13:01		
測定者			
ファイル名	Memory03		
サンプル名			
コメント	コメント		

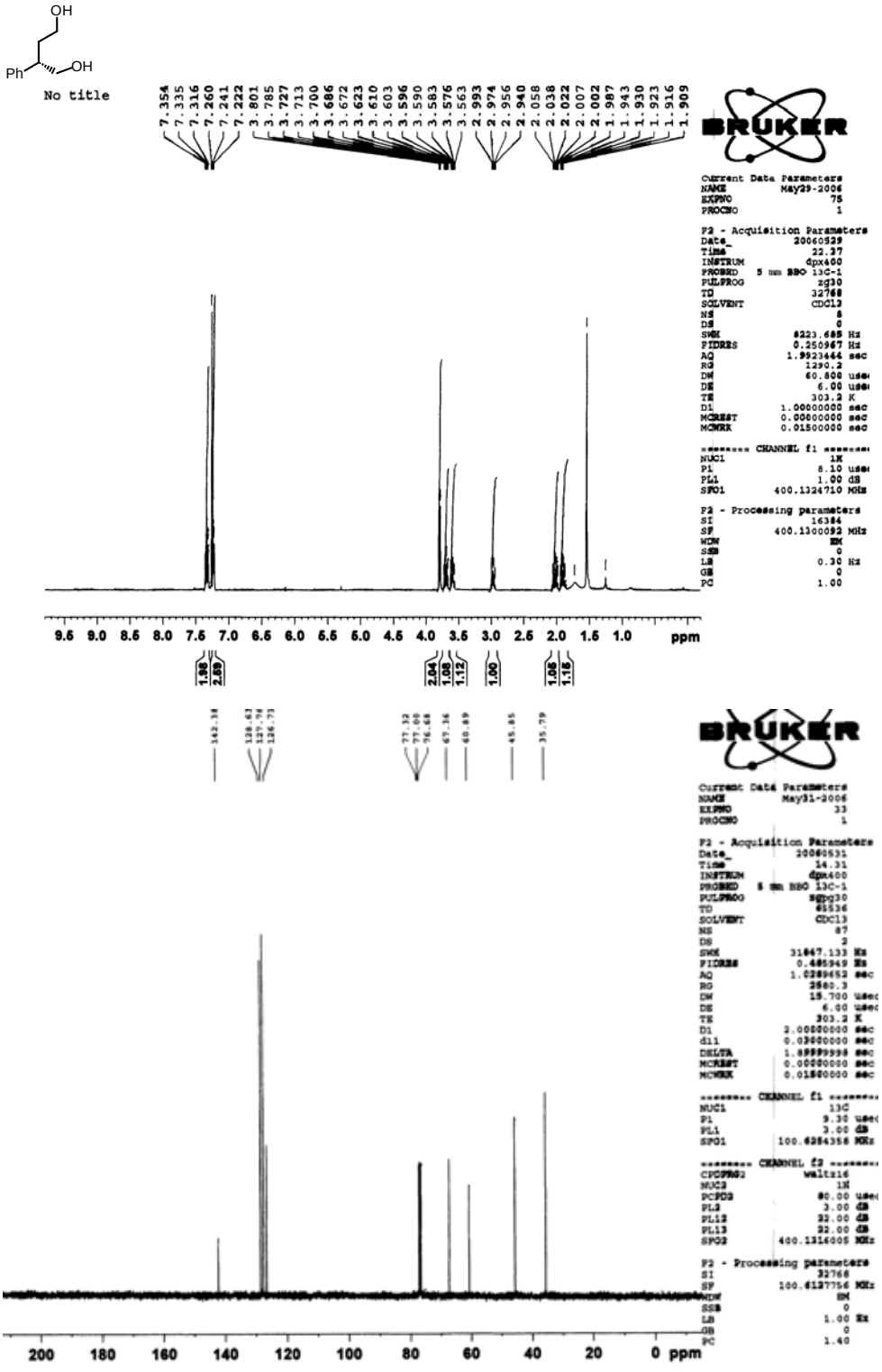
1:	3061.44, 48.4905	2:	3027.69, 45.7574	3:	2928.38, 13.4594	4:	2857.02, 15.5034
5:	1600.63, 61.9727	6:	1492.63, 46.8873	7:	1471.42, 29.5783	8:	1453.10, 41.6645
9:	1387.53, 46.3923	10:	1361.50, 41.2039	11:	1254.47, 19.5002	12:	1102.12, 16.2121
13:	1054.87, 31.8316	14:	1030.77, 57.0724	15:	1005.70, 50.9246	16:	943.02, 33.2457
17:	898.67, 38.5098	18:	834.06, 15.9336	19:	811.88, 30.6844	20:	775.24, 18.6666

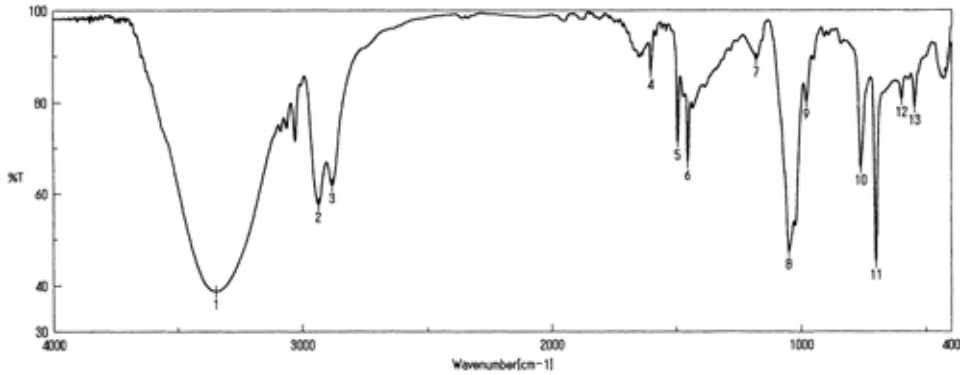

OTBS
Ph
OH
BRUKER
Current Data Parameters
NAME Jun02-2006
EXPNO 25
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060602
Time 10.16
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 40
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 812.7
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.10 usec
PL1 1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.63 2.66 2.44 1.29 1.44 1.17 1.00 1.26 1.11 11.23 6.80
CARBON
142.63
128.62
127.83
126.66
77.21
77.00
76.79
61.44
25.87
18.23
-5.44
-5.47
BRUKER
Current Data Parameters
NAME Jun06-2006
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060606
Time 23.35
INSTRUM av600
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 11596
DS 4
SWH 35971.223 Hz
FIDRES 0.548877 Hz
AQ 0.9110143 sec
RG 9195.2
DW 13.900 usec
DE 50.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -4.90 dB
SFO1 150.9178988 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -5.80 dB
PL12 8.00 dB
PL13 8.00 dB
SFO2 600.1324005 MHz
F2 - Processing parameters
SI 32768
SF 150.9028126 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm



積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	2	スキャンスピード	2 mm/sec
日時	106/06/07 10:01		
測定者			
ファイル名	Memory03		
サンプル名			
コメント	コメント		

1:	3372.89,	98.0510	2:	2928.38,	92.3399	3:	2852.20,	94.7578	4:	1463.71,	97.1895
5:	1255.43,	95.1266	6:	1095.37,	94.5620	7:	835.03,	91.4998	8:	775.24,	93.4104
9:	700.03,	92.7750									


OH
Ph
OH
No title
7.354
7.335
7.316
7.260
7.241
7.222
3.801
3.785
3.727
3.713
3.700
3.686
3.672
3.623
3.610
3.603
3.596
3.590
3.583
3.576
3.563
2.993
2.974
2.956
2.940
2.058
2.038
2.022
2.007
2.002
1.987
1.943
1.930
1.923
1.916
1.909
BRUKER
Current Data Parameters
NAME May29-2006
EXPNO 75
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060529
Time 22.37
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923464 sec
RG 1290.2
DW 60.800 use
DE 6.00 use
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 8.10 use
PL1 1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.06
2.89
2.04
1.08
1.12
1.00
1.06
1.16
142.34
128.63
127.94
126.73
77.33
77.00
76.68
67.36
60.89
45.85
35.79
BRUKER
Current Data Parameters
NAME May31-2006
EXPNO 33
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060531
Time 14.31
INSTRUM dpx400
PROBHD 5 mm BBO 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 87
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289653 sec
RG 2580.3
DW 15.700 usec
DE 6.00 usec
TE 303.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 13C
P1 9.30 use
PL1 3.00 dB
SFO1 100.6284356 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 use
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127754 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm



積算回数	64	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/05/30 15:25		
測定者			
ファイル名	Memory03		
サンプル名			
コメント	コメント		

1:	3348.76,	38.6738	2:	2935.13,	57.6422	3:	2880.17,	61.8405	4:	1602.56,	86.7387
5:	1494.56,	71.3257	6:	1454.06,	66.9060	7:	1182.15,	89.4288	8:	1050.05,	47.4565
9:	980.63,	80.2070	10:	761.74,	65.7836	11:	701.98,	45.1391	12:	599.75,	80.7290
13:	547.68,	78.9904									