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Supporting Information

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Proline-Surfactant Combined Organocatalyst for the Highly Diastereo- and Enantio-Selective Aqueous Direct Cross-Aldol Reaction of Aldehydes

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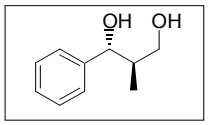
Typical procedure of asymmetric cross-aldol reaction of two aldehydes in water (Table 2, entry 4)

To a mixture of (2*S,* 4*R*)-4-decanoyloxypyrrolidine-2-carboxylic acid (11 mg, 0.04 mmol), water (130 μL) and benzaldehyde (41μl, 0.4 mmol) added propanal (144 μL, 2.0 mmol) successively at 0 °C. After stirring the reaction mixture for 72 hours at that temperature, MeOH (2 mL) and $NaBH_4$ (151 mg, 4 mmol) was added. The reaction mixture was stirred for 1 hour at 0 °C. The reaction was quenched with pH 7.0 phosphate buffer solution and the organic materials were extracted with chloroform three times and the combined organic extracts were dried over anhydrous Na_2SO_4, and concentrated in vacuo after filtration. Purification by preparative thin layer chromatography (diethyl ether : benzene = 2 : 1) gave (1*R*,2*R*)-1-phenyl-2-methylpropane-1,3-diol (59 mg, 0.35 mmol) in 88% yield as the diastereomeric mixture (*anti* : *syn* =>20:1).

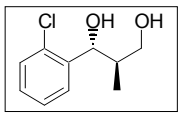
(1*R*, 2*R*)-1-Phenyl-2-methylpropane-1,3-diol[1, 2] **(Table 2, entry 4)**



was known compound.
Enantiometric excess was determined by HPLC with a Chiralpak AD-H column (30 : 1 hexane : 2-propanol, λ= 230 nm), 1.0 mL / min; major enantiomer tr = 27.2 min, minor enantiomer tr = 38.6 min, after conversion to the monobenzoyl ester.

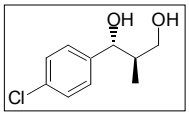
The absolute stereochemistry of the *anti* aldol adduct was determined by the chiral HPLC analysis by comparing the retention time of present aldol product with that synthesized by L-proline in DMF by MacMillan's procedure[3].

(1*R*, 2*R*)-1-(*o*-Chlorophenyl)-2-methylpropane-1,3-diol (Table 2, entry 1)



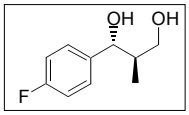
^{1}H NMR (400 MHz, $CDCl_3$): δ 0.81 (3H, d, *J*= 7.2 Hz), 2.02-2.05 (1H, m), 2.80 (1H, br s), 3.30 (1H, br s), 3.61-3.70 (2H, m), 5.05 (1H, d, *J*= 6.8 Hz), 7.14 (1H, t, *J*= 7.6 Hz), 7.22-7.27 (2H, m), 7.50 (1H, d, *J*= 7.6 Hz);
^{13}C NMR (100 MHz, $CDCl_3$): δ 13.7, 40.7, 67.1, 76.1, 127.2, 128.1, 128.7, 129.4, 132.5, 140.9;
IR (neat): ν 3357, 2966, 2932, 1572, 1471, 1438, 1034, 754, 703 cm^{-1};
HRMS (FAB): [M+Na] calcd for [$C_{10}H_{13}ClNaO_2$]: 223.0504, found: 223.0496;
Enantiomeric excess was determined by HPLC with a Chiralpak AS-H column (100 : 1 hexane:2-propanol, λ=254 nm), 1.2 mL/min; major enantiomer tr =15.2 min, minor enantiomer tr =17.2 min, after conversion to the monobenzoyl ester.

(1*R*, 2*R*)-1-(*p*-Chlorophenyl)-2-methylpropane-1,3-diol (Table 2, entry 2)



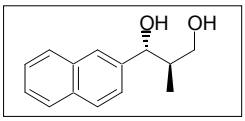
^{1}H NMR (400 MHz, $CDCl_3$): δ 0.62 (3H, d, *J*= 7.2Hz), 1.88-1.95 (1H, m), 2.79 (1H, br s), 3.29 (1H, br s), 3.58-3.70 (2H, m), 4.45 (1H, d, *J*= 8.4 Hz), 7.12-7.21 (2H, m), 7.25-7.26 (2H, m);
^{13}C NMR (100 MHz, $CDCl_3$): δ 13.7, 41.7, 67.8, 76.7, 128.1, 128.6, 133.5, 141.9;
IR (neat): ν 3342, 2927, 2359, 1490, 1456, 1089, 1013, 830 cm^{-1};
HRMS (FAB): [M+Na] calced for [$C_{10}H_{13}ClNaO_2$]: 223.0496, found: 223.0487;
Enantiomeric excess was determined by HPLC with a Chiralcel OD-H column (100 : 1 hexane : 2-propanol, λ= 254 nm), 1.0 mL / min; major enantiomer tr = 9.6 min, minor enantiomer tr = 13.0 min, after conversion to the dibenzoyl ester.

(1*R*, 2*R*)-1-(*p*-Fluorophenyl)-2-methylpropane-1,3-diol (Table 2, entry 3)



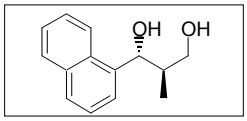
^{1}H NMR (400 MHz, $CDCl_3$): 0.65 (3H, d, *J*= 4.0 Hz), 1.94-2.01 (1H, m), 3.00 (1H, br s), 3.37 (1H, br s), 3.63-3.75 (2H, m), 4.49 (1H, d, *J*= 8.0 Hz), 6.98-7.03 (2H, m), 7.25-7.30 (2H, m);
^{13}C NMR (100 MHz, $CDCl_3$): 13.7, 41.7, 67.9, 76.7, 115.3, 128.3, 139.1, 162.3;
IR (KBr): 3341, 2925, 1604, 1510, 1224, 1025, 834 cm^{-1};
HRMS (FAB): [M+Na] calced for [$C_{10}H_{13}FNaO_2$]: 207.0792, found: 207.0787;
Enantiomeric excess was determined by HPLC with a Chiralpak AS-H column (100 : 1 hexane : 2-propanol, = 254 nm), 1.0 mL / min; major enantiomer tr = 20.2 min, minor enantiomer tr = 26.9 min, after conversion to the monobenzoyl ester.

(1*R*, 2*R*)-1-(Naphthalen-2-yl)-2-methylpropane-1,3-diol (Table 2, entry 5)



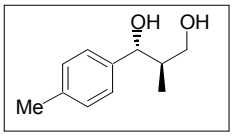
^{1}H NMR (400 MHz, $CDCl_3$): 0.72 (3H, d, *J*=7.2 Hz), 2.22-2.10 (1H, m), 3.01 (1H, br d, *J*=2.4 Hz), 3.46 (1H, br s), 3.66-3.84 (2H, m), 4.71 (1H, d, *J*= 8.4 Hz), 7.43-7.51 (3H, m), 7.76 (1H, s), 7.78-7.86 (3H, m);
^{13}C NMR (100 MHz, $CDCl_3$): 13.9, 41.4, 68.0, 80.9, 124.5, 125.8, 126.0, 126.2, 127.7, 128.0, 128.3, 133.1, 133.2, 140.7;
IR (neat): 3308, 2964, 2925, 2878, 1389, 1357, 1030, 867, 821, 750 cm^{-1};
HRMS (FAB): [M+Na] calcd for [$C_{14}H_{16}NaO_2$]: 239.1043, found: 239.1043;
Enantiomeric excess was determined by HPLC with a Chiralcel OD-H column, (50 : 1 hexane : 2-propanol), = 254 nm, 1.0 mL / min; major enantiomer tr =9.0 min, minor enantiomer tr =10.3 min after, conversion to the dibenzoyl ester.

(1*R*, 2*R*)-1-(Naphthalen-1-yl)-2-methylpropane-1,3-diol (Table 2, entry 6)



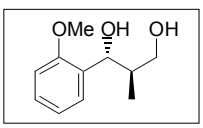
^{1}H NMR (400 MHz, $CDCl_3$): 0.79 (3H, d, *J*=4.5 Hz), 2.30-2.41 (1H, m), 3.04 (1H, br s), 3.15 (1H, br s), 3.67-3.84 (2H, m), 5.31 (1H, d, *J*=7.6 Hz), 7.43-7.53 (3H, m), 7.59 (1H, d, *J*=7.2 Hz), 7.78 (1H, d, *J*=8.0 Hz), 7.83-7.89 (1H, m), 8.15-8.22 (1H, m);
^{13}C NMR (100 MHz, $CDCl_3$): 14.4, 40.8, 67.6, 78.0, 123.6, 124.6, 125.3, 125.6, 126.0, 128.3, 128.9, 130.8, 134.0, 139.0;
IR (KBr): 3347, 2927, 2360, 1509, 1457, 1167, 1086, 1025, 799, 778 cm^{-1};
HRMS (FAB): [M+Na] calcd for [$C_{14}H_{16}NaO_2$]: 239.1043, found: 239.1029;
Enantiomeric excess was determined by HPLC with a Chiralcel OD-H column (100:1 hexane:2-propanol), 1.0 mL/min; major enantiomer tr = 15.5 min, minor enantiomer tr =18.6 min, after conversion to the dibenzoyl ester.

(1*R*, 2*R*)-1-(*p*-Tolyl)-2-methylpropane-1,3-diol(Table 2, entry 7)



^{1}H NMR (400 MHz, $CDCl_3$): 0.68 (3H, d, *J*=6.8 Hz), 2.01-2.07 (1H, m), 2.33 (3H, s), 2.60 (1H, br s), 2.77 (1H, br s), 3.68-3.80 (2H, m), 4.50 (1H, d, *J*=8.4 Hz), 7.15 (2H, d, *J*=8.0 Hz), 7.21 (2H, d, *J*=8.0 Hz);
^{13}C NMR (150 MHz, $CDCl_3$): 13.9, 21.2, 41.7, 68.2, 80.9, 126.6, 129.2, 137.7, 140.4;
IR (neat): 3358, 2924, 2386, 1558, 1541, 1508, 1457, 1027, 812, 560 cm^{-1};
HRMS (FAB): [M+Na] calcd for [$C_{11}H_{16}NaO_2$]: 203.1043, found: 203.1046;
Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (30 : 1 hexane:2-propanol), 1.0 mL/min; major enantiomer tr = 19.2 min, minor enantiomer tr =28.3 min, after conversion to the dibenzoyl ester.

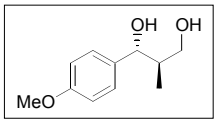
(1*R*, 2*R*)-1-(*o*-Methoxyphenyl)-2-methylpropane-1,3-diol(Table 2, entry 8)



^{1}H NMR (400 MHz, $CDCl_3$): 0.72(3H, d, *J*=6.8 Hz), 1.64 (1H, br s), 2.15-2.27 (1H, m), 3.04 (1H, br s), 3.65-3.76 (2H, m), 3.84 (3H, s), 4.80 (1H, d, *J*=8.4 Hz), 6.88 (1H,

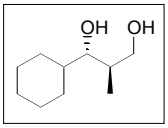
d, *J*= 8.0 Hz), 6.96 (1H, t, *J*=7.6), 7.22-7.31 (2H, m);
^{13}C NMR (100 MHz, $CDCl_3$): 13.8, 40.4, 55.3, 67.9, 76.2, 110.6, 120.8, 128.1, 128.6, 130,9, 156.6;
IR (KBr): 3367, 2931, 2360, 1602, 1491, 1458, 1287, 1241, 1028, 934, 755, 418cm^{-1};
HRMS (FAB): [M+Na] calcd for [$C_{11}H_{16}NaO_3$]: 219.0992, found: 219.1015;
Enantiomeric excess was determined by HPLC with a Chiralpak AS-H column (10 : 1 hexane:2-propanol), 1.0 mL/min; major enantiomer tr =6.8 min, minor enantiomer tr =7.2 min, after conversion to the dibenzoyl ester.

(1*R*, 2*R*)-1-(*p*-Methoxyphenyl)-2-methylpropane-1,3-diol[4] **(Table 2, entry 9)**



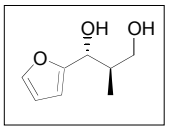
was known compound.
^{1}H NMR (400 MHz, $CDCl_3$): 0.66 (3H, d, *J*= 7.2 Hz), 1.98-2.09 (1H, m), 2.66 (1H, br s), 2.87 (1H, br s), 3.61-3.77 (2H, m), 3.79 (3H, s), 4.48 (1H, d, *J*= 8.6 Hz), 6.87 (2H, br d, *J*= 8.7 Hz), 7.26 (2H, br d, *J*= 8.7 Hz);
^{13}C NMR (100 MHz, $CDCl_3$): 13.8, 41.7, 55.3, 68.1, 80.6, 113.8, 127.9, 135.7, 159.2;
IR (neat): 3366, 2959, 2927, 2360, 1612, 1513, 1247, 1032, 834 cm^{-1};
HRMS (FAB): [M+Na] calced for [$C_{11}H_{16}NaO_3$]: 219.0992, found: 219.0992;
Enantiomeric excess was determined by HPLC with a Chiralcel OD-H column (100 : 1 hexane:2-propanol), 1.2 mL/min; minor enantiomer tr =145.1 min, major enantiomer tr =149.4 min

(1*R*, 2*R*)-1-Cyclohexyl-2-methylpropane-1,3-diol[2, 5] **(Table 2, entry 10)**



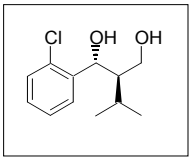
was known compound.
Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (100 : 1 hexane:2-propanol), 0.5 mL/min; major enantiomer tr =11.8 min, minor enantiomer tr =13.6 min after conversion to the dibenzoyl ester.

(1*R*, 2*R*)-1-(Furan-2-yl)-2-methylpropane-1,3-diol[2] **(Table 2, entry 11)**



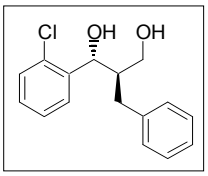
was known compound.
Enantiomeric excess was determined by HPLC with a Chiralpak AS-H column (100 : 1 hexane:2-propanol), 0.5 mL/min; major enantiomer tr =42.4 min, minor enantiomer tr =47.8 min, after conversion to the monobenzoyl ester.

(1*R*, 2*R*)-1-(*o*-Chlorophenyl)-2-isopropylpropane-1,3-diol (Table 2, entry 12)



^{1}H NMR (400 MHz, $CDCl_3$): 1.01 (3H, dd, *J*= 1.2, 6.8 Hz), 1.13 (3H, dd, *J*= 1.2, 6.8 Hz), 1.97-2.08 (1H, m), 2.41-2.47 (1H, m), 3.20-3.27 (1H, m), 3.66-3.82 (2H, m), 5.45 (1H, t, *J*= 4.9 Hz), 7.17-7.27 (1H, m), 7.28-7.36 (2H, m), 7.61-7.66 (1H, m);
^{13}C NMR (100 MHz, $CDCl_3$): 20.0, 21.1, 25.8, 49.6, 61.2, 73.4, 126.9, 128.0, 128.4, 129.5, 131.8, 141.4;
IR (neat): 3324, 2960, 1469, 1439, 1194, 1048, 1036, 998, 757, 705 cm^{-1};
HRMS (FAB): [M+Na] calcd for [$C_{12}H_{17}ClNaO_2$]: 251.0809, found: 251.0815;
Enantiomeric excess was determined by HPLC with a Chiralpak IA column (150 : 1 hexane:2-propanol), 1.0 mL/min; major enantiomer tr = 21.9 min, minor enantiomer tr =25.2 min.

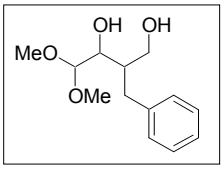
(1*R*, 2*R*)-1-(*o*-Chlorophenyl)-2-benzylpropane-1,3-diol (Table 2, entry 13)



^{1}H NMR (400 MHz, $CDCl_3$): 2.15-2.23 (1H, m), 2.82-2.96 (2H, m), 3.50-3.56 (1H, m), 3.68-3.72 (1H, m), 5.21 (1H, t, *J*= 4.8 Hz), 7.15-7.38 (8H, m), 7.65 (1H, dd, *J*= 1.2, 7.6 Hz);
^{13}C NMR (100 MHz, $CDCl_3$): 34.9, 45.8, 62.4, 74.5, 126.2, 127.0, 127.8, 128.4, 128.6, 128.8, 129.0, 129.2, 129.5, 131.9, 140.0, 140.9;
IR (neat): 3336, 2924, 1440, 1192, 1127, 1073, 1031, 911, 753, 701 cm^{-1};
HRMS (FAB): [M+Na] calcd for [$C_{16}H_{17}ClNaO_2$]: 299.0809, found: 299.0810;
Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column (30 : 1 hexane:2-propanol), 1.0

mL/min; major enantiomer tr = 17.6 min, minor enantiomer tr =22.5 min.

4,4-Dimethoxy-2-benzylbutane-1,3-diol (diastereomeric mixture (ratio=4 : 1), Table 2, entry 14)

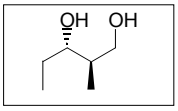


The relative stereochemistry of this compound was not determined.
^{1}H NMR (400 MHz, $CDCl_3$): □2.07-2.17 (0.8H, m), 2.45-2.48 (0.2H, m), 2.67 (0.2H, d, *J*= 2.4 Hz), 2.72 (0.8H, d, *J*= 3.2 Hz), 2.80-2.92 (3H, m), 3.34 (2.4H, s), 3.40 (0.6H, s), 3.45 (2.4H, s), 3.49 (0.6H, s), 3.62-3.73 (2H, m), 3.90 (0.8H, dt, *J*= 11.6, 3.2 Hz), 3.95 (0.2H, dt, *J*= 2.4, 6.8 Hz), 4.41 (0.2H, d, *J*= 6.8 Hz), 4.49 (0.8H, d, *J*= 6.8 Hz), 7.22-7.36 (5H, m);
^{13}C NMR (100 MHz, $CDCl_3$): □31.7, 35.6, 42.6, 43.6, 54.8, 55.1, 55.3, 55.5, 62.8, 64.3, 73.4, 73.7, 105.2, 105.6, 126.4, 126.5, 128.8, 129.6, 140.6, 141.1;
IR (neat): □3423, 3061, 3027, 2936, 2832, 2360, 1496, 1454, 1193, 1133, 1064, 971, 746, 701 cm^{-1};
HRMS (FAB): [M+Na] calcd for [$C_{13}H_{20}NaO_4$]: 263.1254, found: 263.1248;
Enantiomeric excess of major diastereomer was determined by HPLC with a Chiralpak IA column (50 : 1 hexane:2-propanol), 1.0 mL/min; major enantiomer tr = 21.2 min, minor enantiomer tr =19.6 min after conversion to the monobenzoyl ester.

Procedure of asymmetric self-aldol reaction of propanal in water (Table 2, entry 15)

To a mixture of (2*S,* 4*R*)-4-Decanoyloxypyrrolidine-2-carboxylic acid (29 mg, 0.1 mmol) and water (54 □L) added propanal (144 □L, 2.0 mmol) successively at room tempreture. After stirring the reaction mixture for 96 hours at that temperature, the reaction mixture was cooled at 0 °C and MeOH (2 mL) and $NaBH_4$ (151 mg, 4 mmol) was added. The reaction mixture was stirred for 1 hour at 0 °C. The reaction was quenched with pH 7.0 phosphate buffer solution and the organic materials were extracted with ethyl acetate three times and the combined organic extracts were dried over anhydrous Na_2SO_4, and concentrated in vacuo after filtration. Purification by silica gel column chromatography (ethyl acetate:hexane=1:2 ~ 1:1) gave (2*R*,3*R*)-2-methylpentane-1,3-diol and (2*R*, 3*S*)-2-methylpentane-1,3-diol (41 mg, 0.35 mmol) in 35% yield as the diastereomeric mixture (*anti* : *syn* =10:1).

(2*R*, 3*S*)-2-Methylpentane-1,3-diol [1]



was known compound.
Enantiomeric excess was determined by HPLC with a Chiralpak IA column (100 : 1 hexane:2-propanol, □=254 nm), 1.0 mL/min; major enantiomer(*anti*) tr =31.5 min, minor enantiomer(*anti*) tr =34.4 min, after conversion to the monobenzoyl ester.

The absolute stereochemistry of the *anti* aldol adduct was determined by the chiral HPLC analysis by comparing the retention time of the monobenzoyl ester of present aldol product with that synthesized by L-proline in DMF by MacMillan's procedure[3].

References

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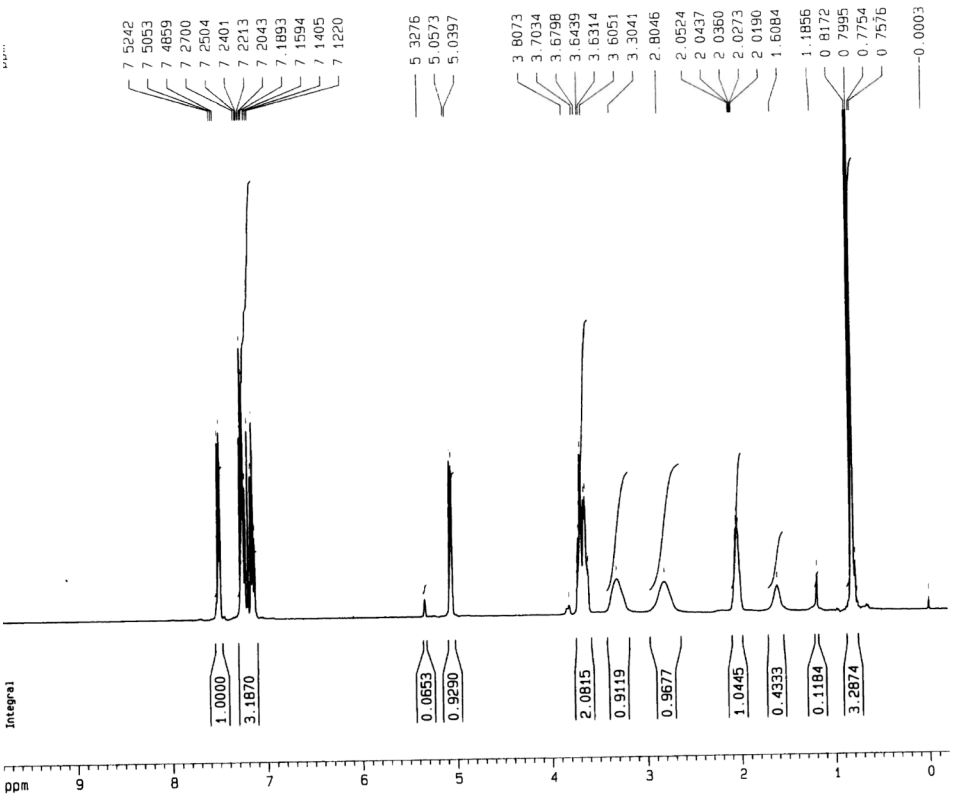
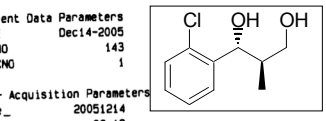
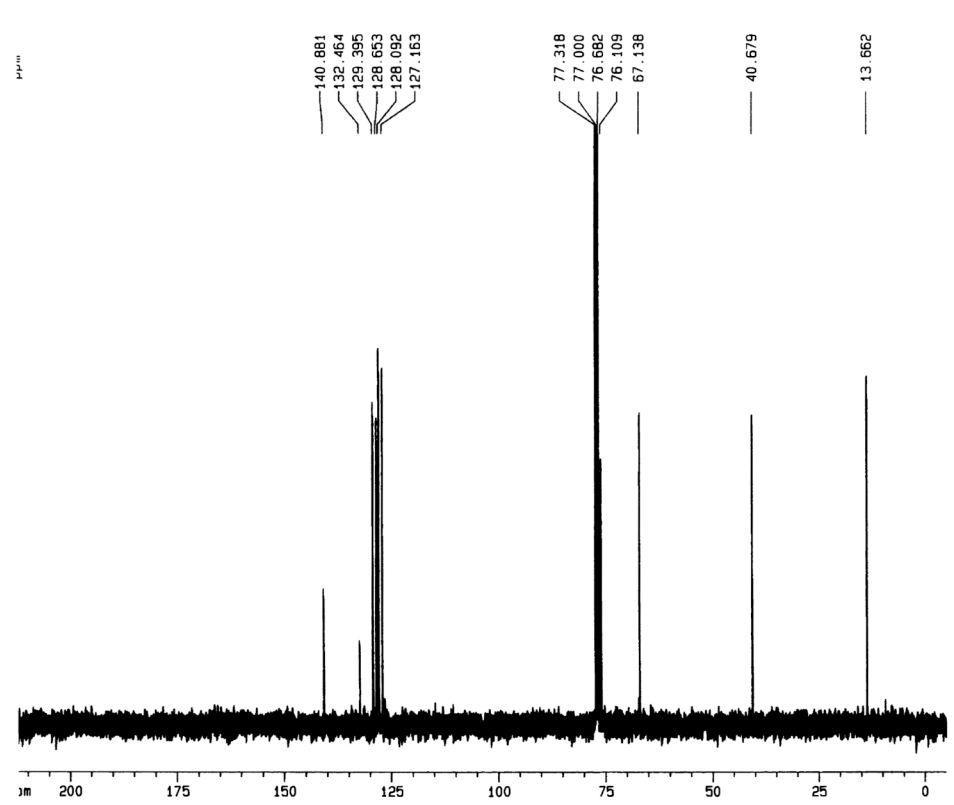
(5) Roush W. R.; Ando K.; Powers D. B.; Palkowitz A. D.; Halterman R. L. *J. Am. Chem. Soc.* **1990**, *112*, 6339.

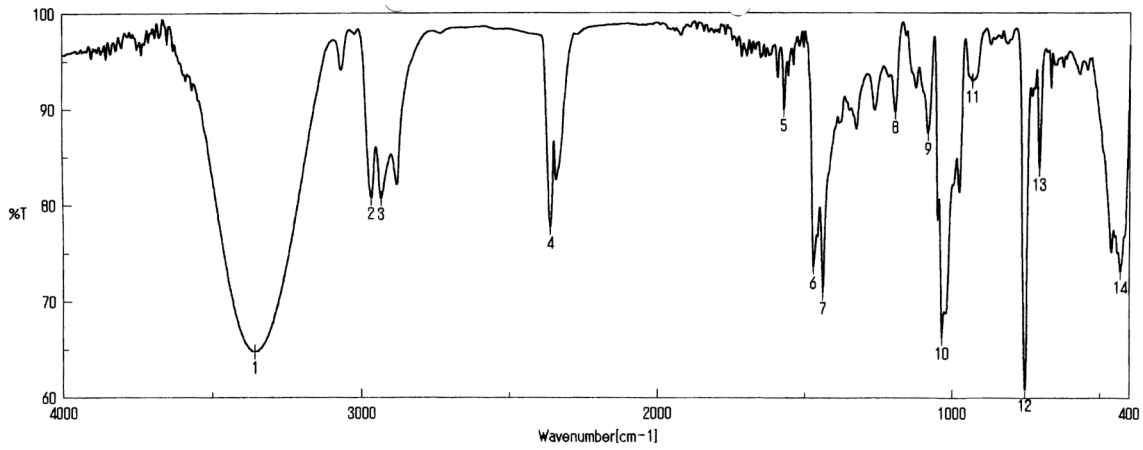





```
Current Data Parameters
NAME                  Dec14-2005
EXPNO                        143
PROCNO                         1

F2 - Acquisition Parameters
Date_                 20051214
Time                      22.19
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                         203.2
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                       8.10 usec
PL1                      1.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                           16384
SF                  400.1300375 MHz
WDW                            EM
SSB                            0
LB                       0.30 Hz
GB                             0
PC                       1.00

1D NMR plot parameters
CX                      20.00 cm
CY                      12.50 cm
F1P                      9.800 ppm
F1                    3921.27 Hz
F2P                     -0.200 ppm
F2                     -80.03 Hz
PPMCM                0.50000 ppm/cm
HZCM                200.06502 Hz/cm
```

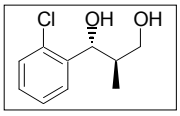


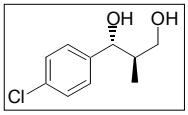

```
Current Data Parameters
NAME                  Dec14-2005
EXPNO                        144
PROCNO                         1

F2 - Acquisition Parameters
Date_                 20051214
Time                      22.20
INSTRUM                  dpx400
PROBHD     5 mm BBO 13C-1
PULPROG                zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                           172
DS                             2
SWH                31847.133 Hz
FIDRES              0.485949 Hz
AQ                  1.0289852 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 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                  100.6127698 MHz
WDW                            EM
SSB                            0
LB                       1.00 Hz
GB                             0
PC                       1.40

1D NMR plot parameters
CX                      20.00 cm
CY                       8.00 cm
F1P                    215.000 ppm
F1                    21631.75 Hz
F2P                     -5.000 ppm
F2                     -503.06 Hz
PPMCM               11.00000 ppm/cm
HZCM                1106.74048 Hz/cm
```

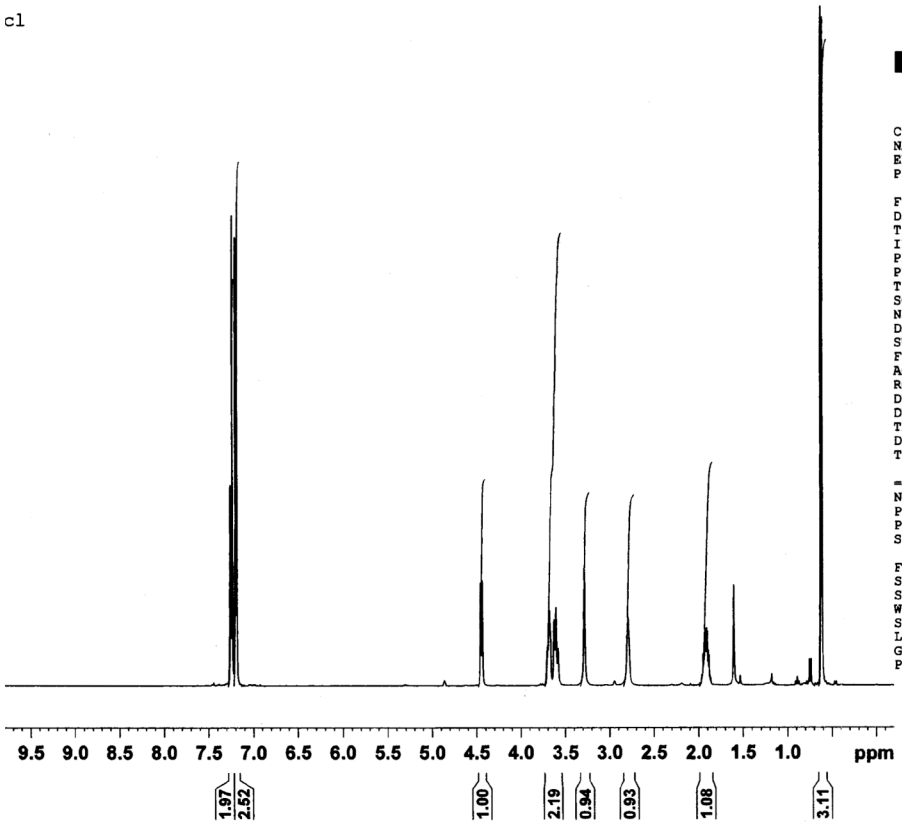


積算回数	16	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/01/25 21:13		
測定者			
ファイル名	Memory#6		
サンプル名			
コメント	コメント		

1:	3357.46,	64.7432	2:	2965.98,	80.7845	3:	2932.23,	80.7236	4:	2360.44,	77.7355
5:	1572.66,	89.9476	6:	1471.42,	73.6355	7:	1438.64,	70.9591	8:	1194.69,	89.7558
9:	1082.83,	87.5273	10:	1034.62,	66.2728	11:	934.34,	92.9301	12:	754.03,	60.8449
13:	705.82,	83.8262	14:	431.01,	73.1540						

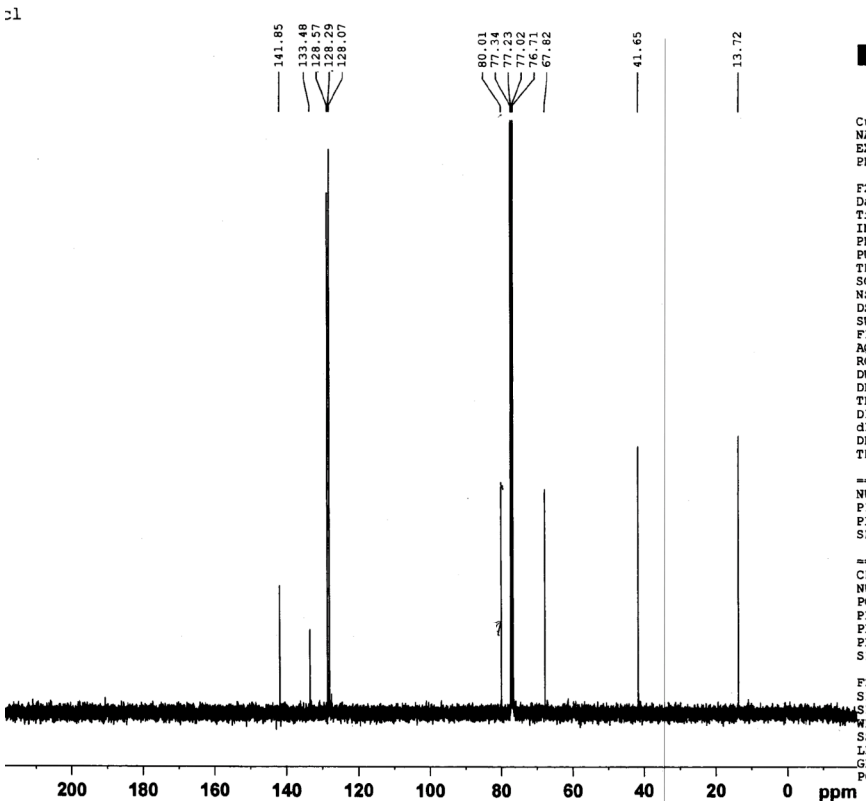






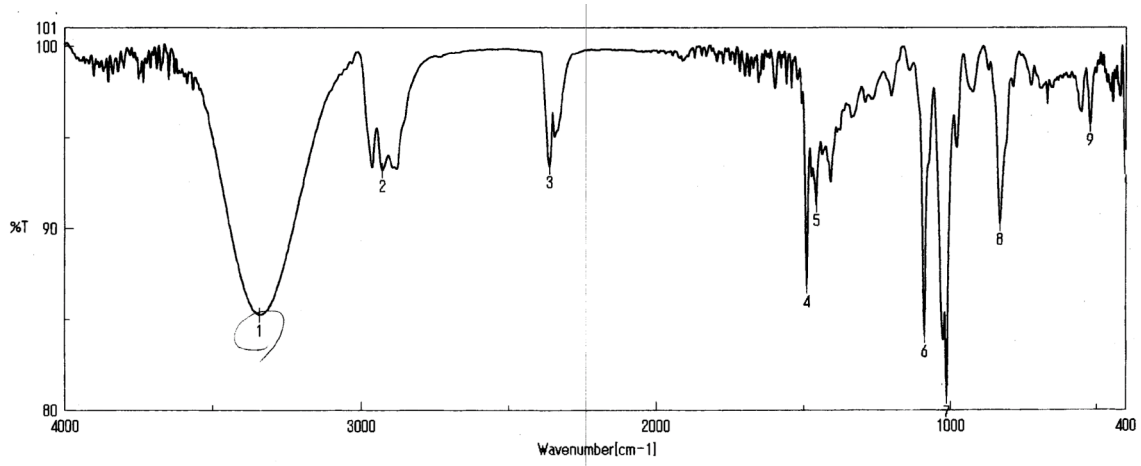
BRUKER

```
Current Data Parameters
NAME      Dec22-2005-hayashi
EXPNO                     40
PROCNO                     1

F2 - Acquisition Parameters
Date_              20051222
Time                  18.45
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                       181
DW                  60.800 usec
DE                   6.00 usec
TE                   297.7 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             400.1800368 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



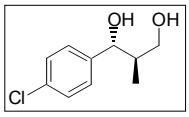
BRUKER

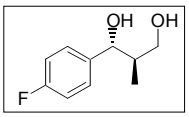
```
Current Data Parameters
NAME      Dec22-2005-hayashi
EXPNO                     30
PROCNO                     1

F2 - Acquisition Parameters
Date_              20051222
Time                  23.21
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      256
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                      128
DW                  20.800 usec
DE                   6.00 usec
TE                   299.3 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
```

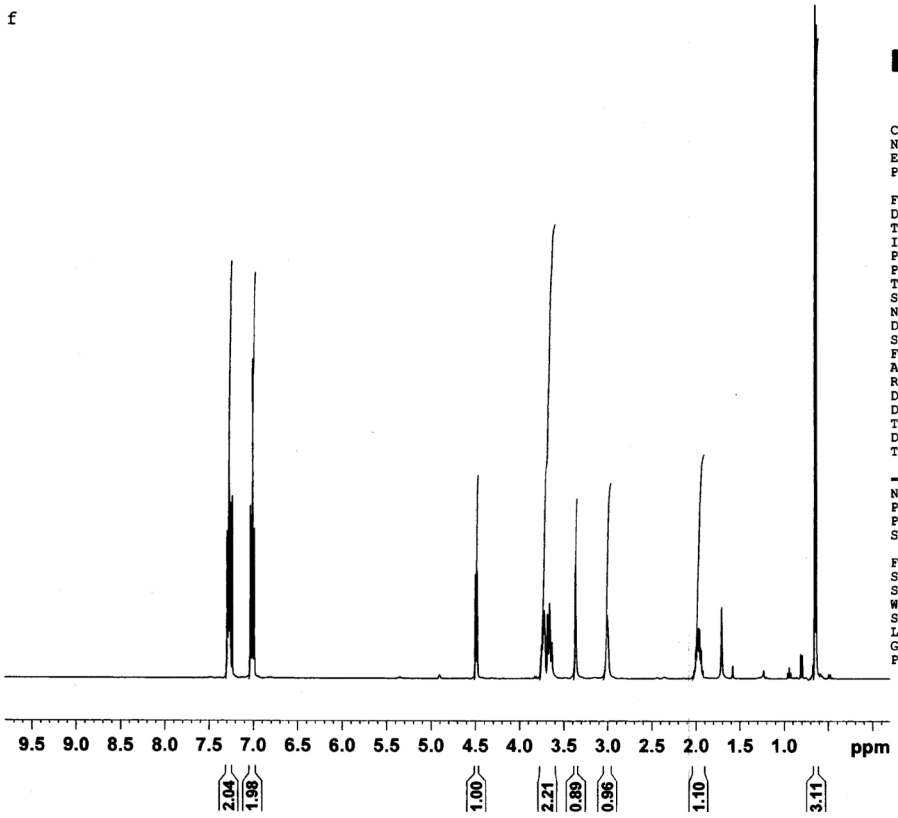


積算回数	16	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/02/10 9:52		
測定者			
ファイル名	Memory#6		
サンプル名			
コメント	コメント		

1:	3342.03, 85.2281	2:	2927.41, 93.1859	3:	2359.48, 93.3831	4:	1489.74, 86.8246
5:	1456.96, 91.3057	6:	1089.58, 84.0947	7:	1013.41, 80.7654	8:	830.21, 90.2420
9:	522.61, 95.6961						



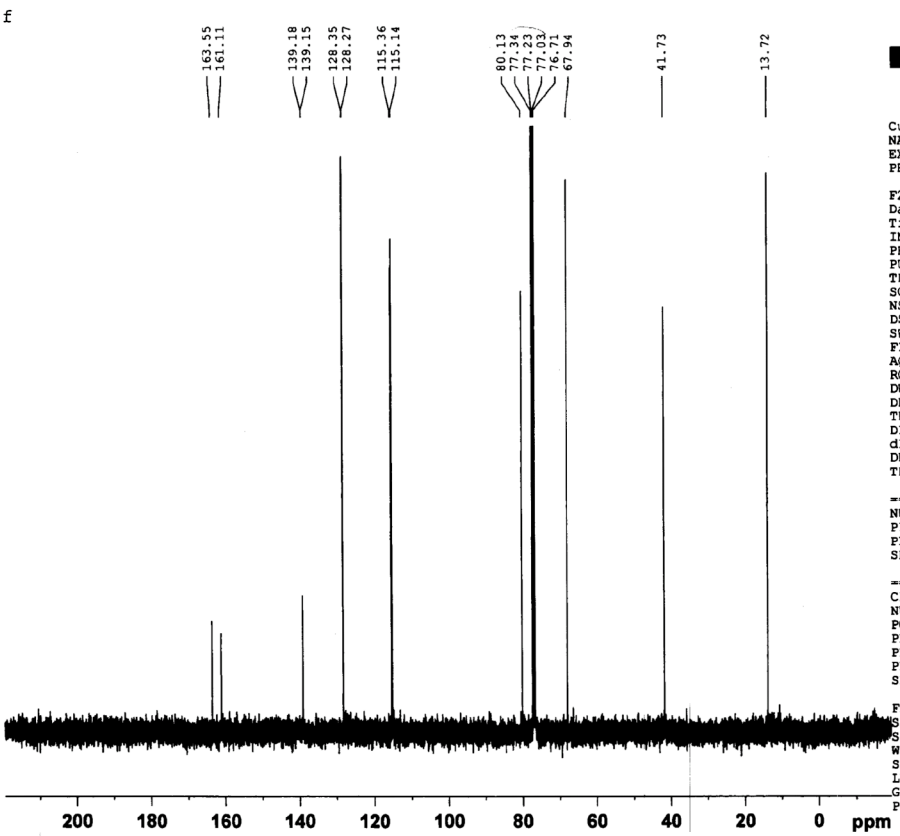




BRUKER

```
Current Data Parameters
NAME      Dec22-2005-hayashi
EXPNO                 50
PROCNO                 1

F2 - Acquisition Parameters
Date_           20051222
Time              18.56
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                  161
DW               60.800 usec
DE                6.00 usec
TE               297.7 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         400.1800157 MHz
WDW                EM
SSB                 0
LB              0.30 Hz
GB                  0
PC               1.00
```

f



BRUKER

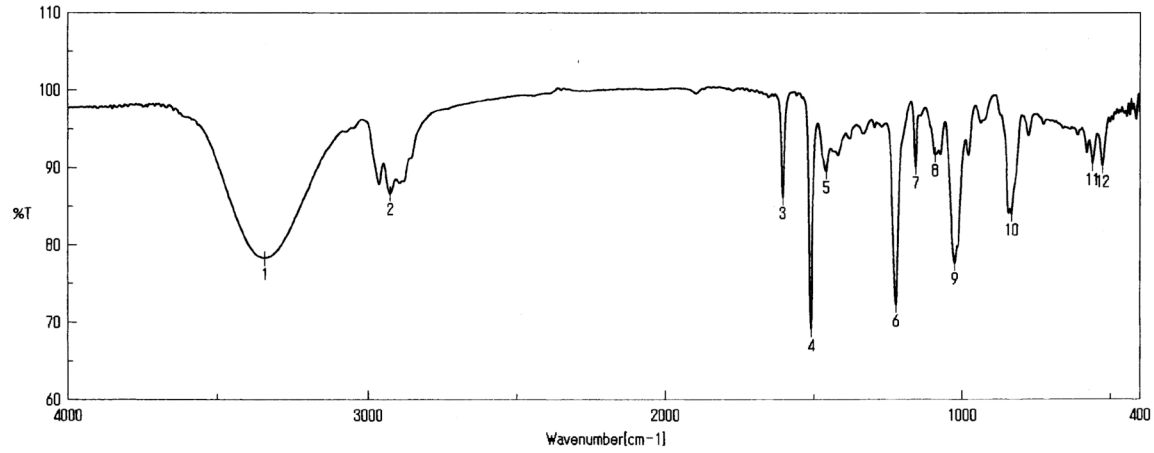
Current Data Parameters
NAME Dec22-2005-hayashi
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051222
Time 23.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 128
DW 20.800 usec
DE 6.00 usec
TE 299.3 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

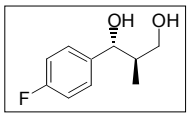
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1816007 MHz

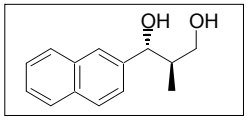
F2 - Processing parameters
SI 32768
SF 100.6253410 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

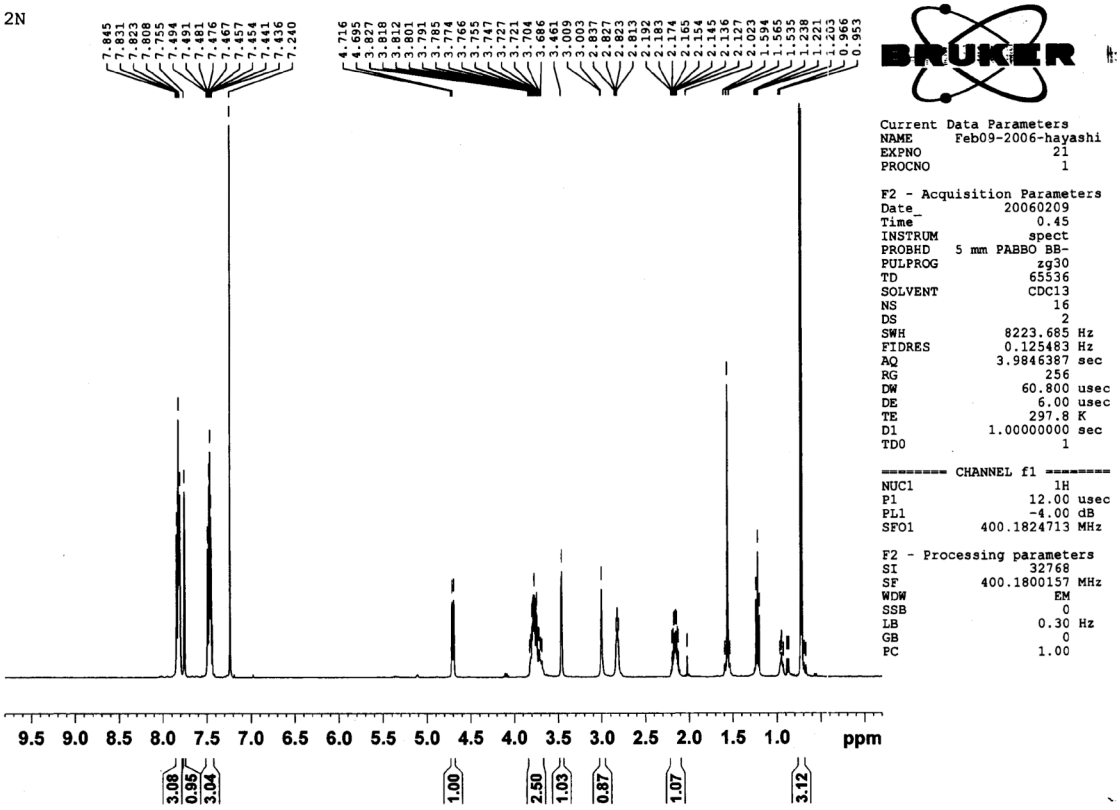


積算回数	16	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/02/10 9:34		
測定者			
ファイル名	Memory#3		
サンプル名			
コメント	コメント		

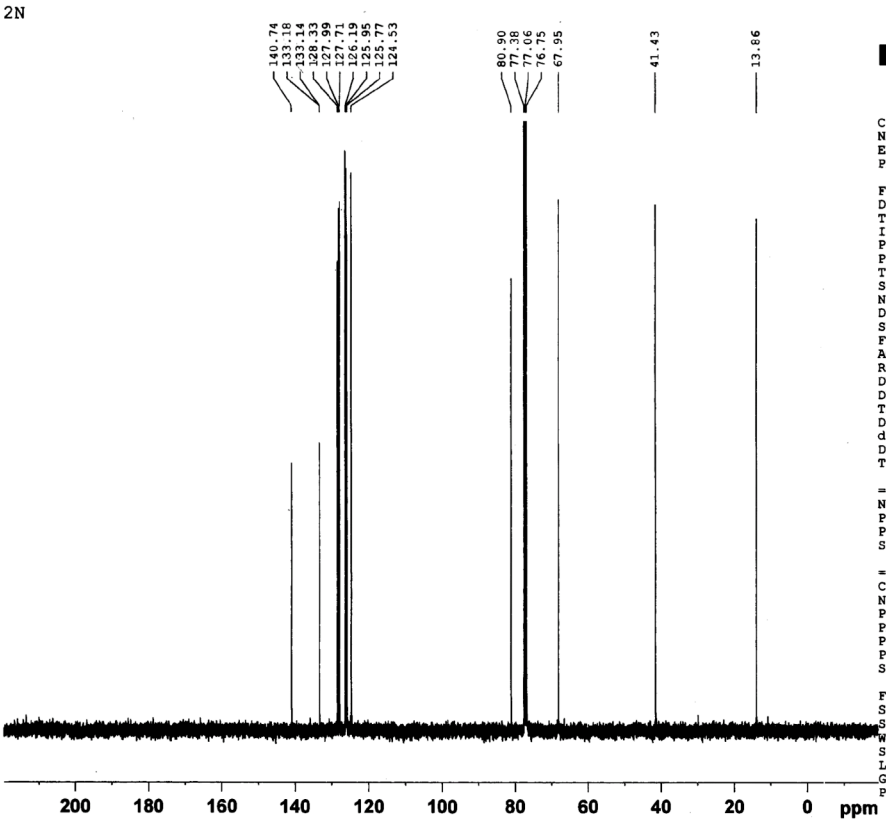
1:	3341.07,	78.2135	2:	2925.48,	86.6147	3:	1604.48,	86.1127	4:	1509.99,	69.0552
5:	1458.89,	89.4813	6:	1223.61,	72.2172	7:	1157.08,	90.0552	8:	1091.51,	91.6565
9:	1024.98,	77.6477	10:	834.06,	83.9744	11:	560.22,	90.4821	12:	526.47,	90.2066



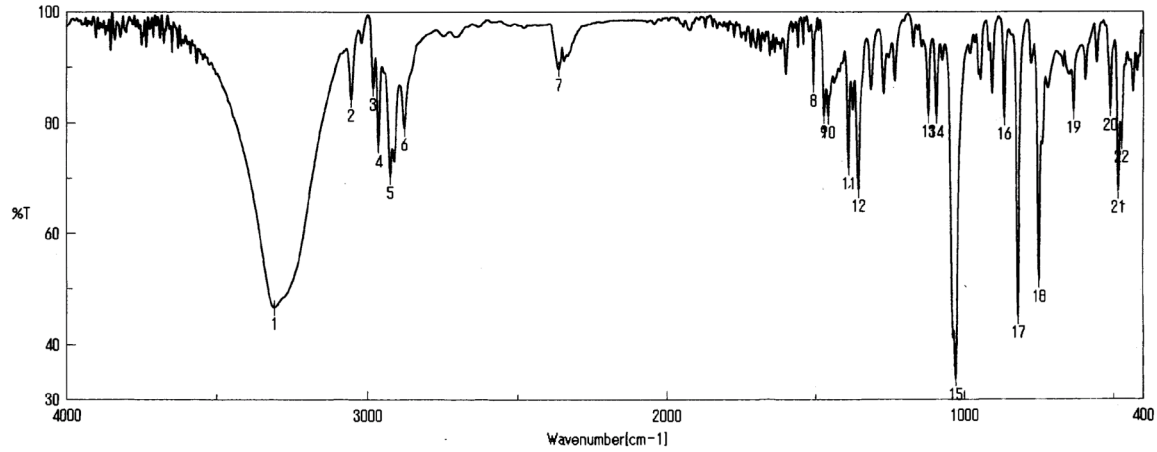

OH
OH


2N
7.845
7.831
7.823
7.808
7.755
7.494
7.481
7.476
7.467
7.457
7.454
7.441
7.436
7.240
4.716
4.695
3.827
3.818
3.812
3.801
3.791
3.785
3.774
3.766
3.755
3.747
3.727
3.721
3.704
3.686
3.461
3.009
3.003
2.837
2.827
2.823
2.813
2.192
2.183
2.174
2.165
2.154
2.145
2.136
2.127
2.023
1.594
1.565
1.535
1.238
1.221
1.213
0.966
0.953
BRUKER
Current Data Parameters
NAME Feb09-2006-hayashi
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060209
Time 0.45
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 297.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
SF01 400.1824713 MHz
F2 - Processing parameters
SI 32768
SF 400.1800157 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
3.08
0.95
3.04
1.00
2.50
1.03
0.87
1.07
3.12

2N

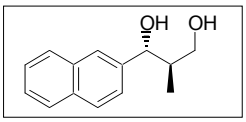


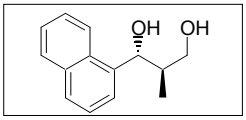

```
Current Data Parameters
NAME      Dec15-2005-hayashi
EXPNO                     40
PROCNO                     1

F2 - Acquisition Parameters
Date_              20051215
Time                  23.23
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      256
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                  299.4 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
```

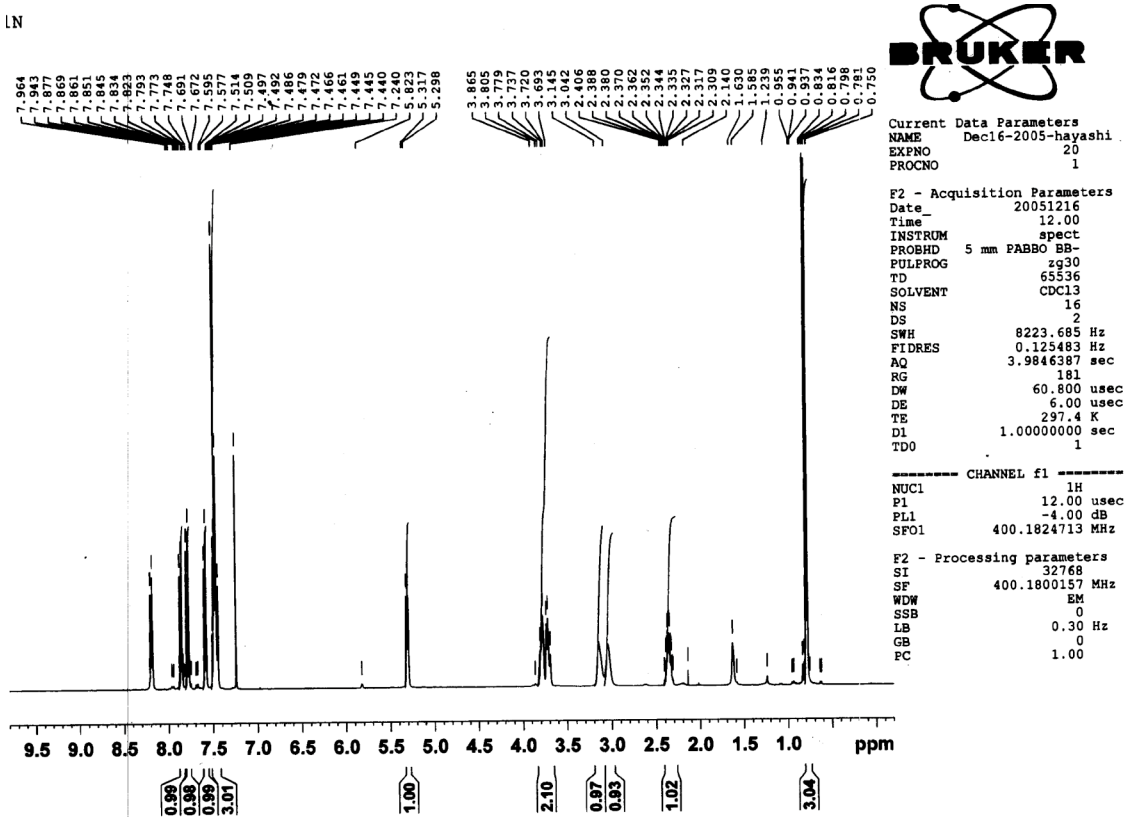


積算回数	16	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	2	スキャンスピード	2 mm/sec
日時	105/12/16 18:12		
測定者			
ファイル名	Memory#10		
サンプル名	2naph		
コメント	コメント		

1:	3308.28,	46.5624	2:	3054.69,	84.2359	3:	2982.37,	86.1997	4:	2964.05,	75.9463
5:	2925.48,	70.2465	6:	2878.24,	78.9654	7:	2361.41,	89.6916	8:	1507.10,	86.8050
9:	1471.42,	81.2031	10:	1457.92,	81.0947	11:	1389.46,	71.8899	12:	1356.68,	67.8209
13:	1121.40,	81.2575	14:	1094.41,	81.1844	15:	1029.80,	33.8087	16:	866.85,	80.8590
17:	820.56,	44.9918	18:	750.17,	51.4468	19:	634.47,	81.9844	20:	510.08,	82.4424







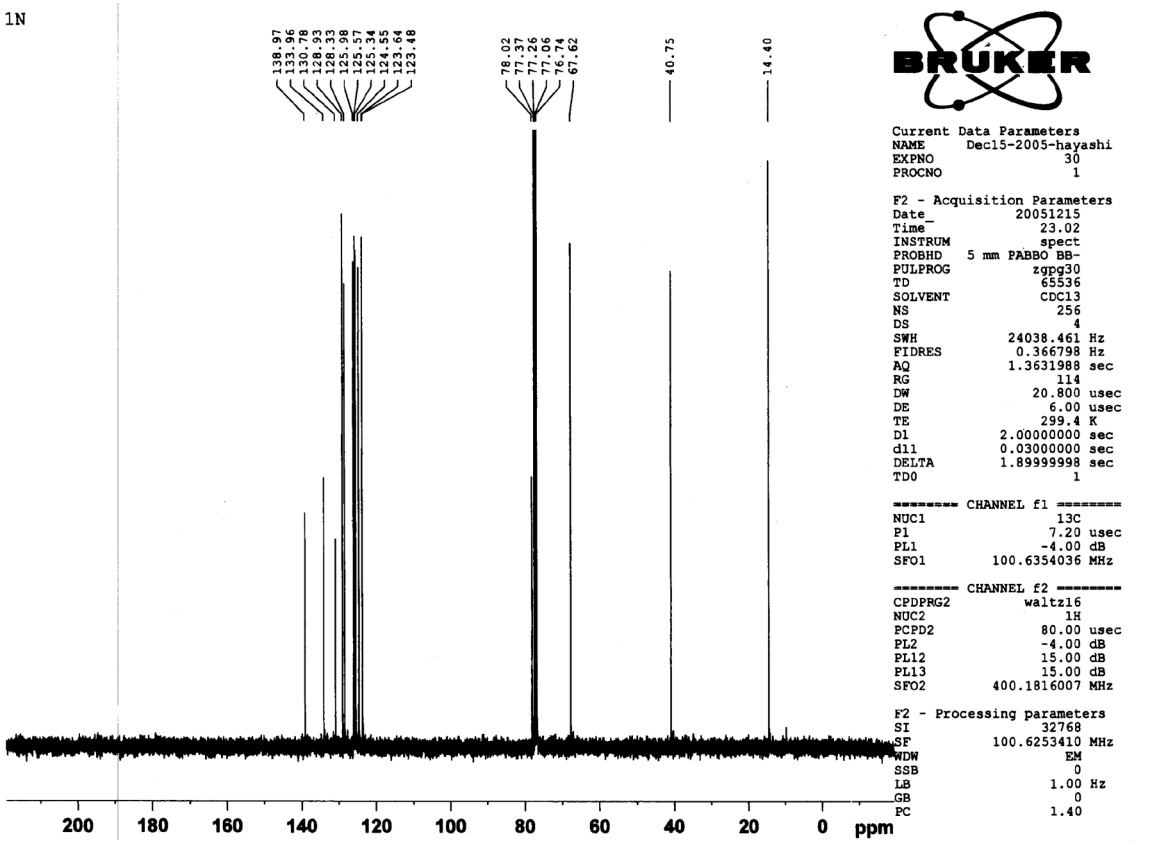
BRUKER

Current Data Parameters
NAME Dec16-2005-hayashi
EXPNO 20
PROCNO 1

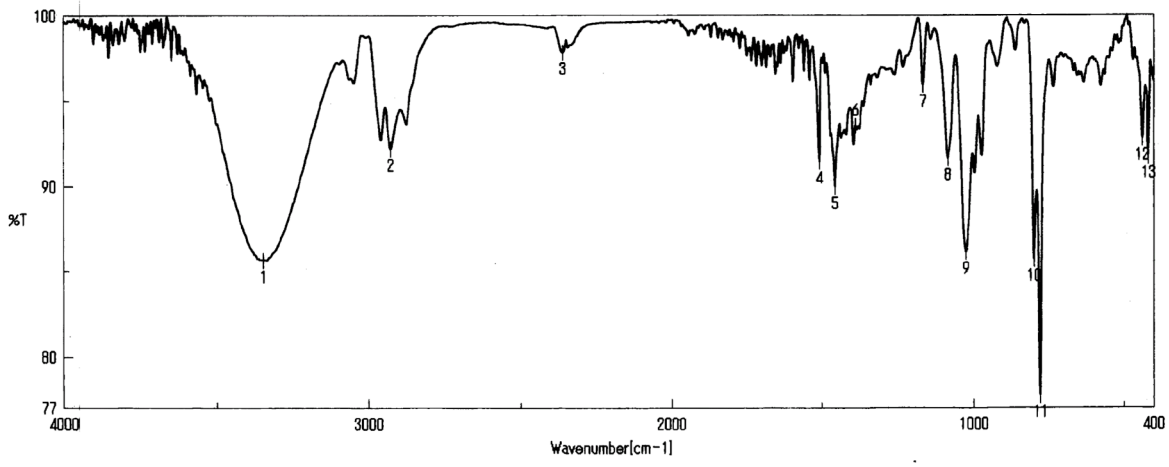
F2 - Acquisition Parameters
Date_ 20051216
Time 12.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 400.1800157 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

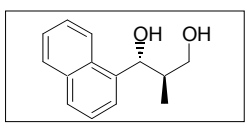


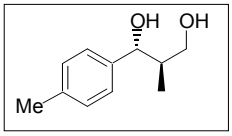

```
Current Data Parameters
NAME      Dec15-2005-hayashi
EXPNO                     30
PROCNO                     1

F2 - Acquisition Parameters
Date_              20051215
Time                  23.02
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     256
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                  299.4 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
```

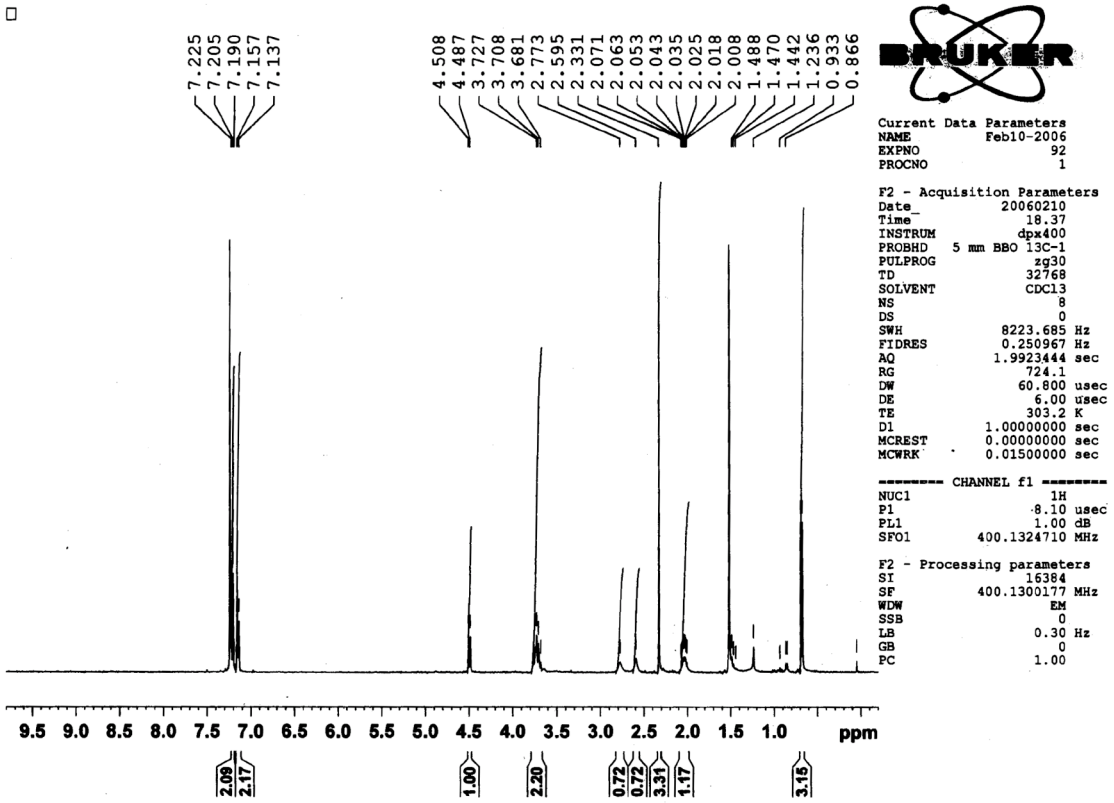


積算回数	16	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	105/12/16 17:29		
測定者			
ファイル名	Memory#5		
サンプル名			
コメント	コメント 1naph		

1:	3346.85,	85.6135	2:	2927.41,	92.1661	3:	2360.44,	97.8168
4:	1509.03,	91.4414	5:	1456.96,	89.9480	6:	1389.46,	93.5154
7:	1166.72,	95.8991	8:	1085.73,	91.5950	9:	1024.98,	86.1191
10:	799.35,	85.6940	11:	778.14,	77.7154	12:	437.76,	92.7438
13:	417.51,	91.6860						







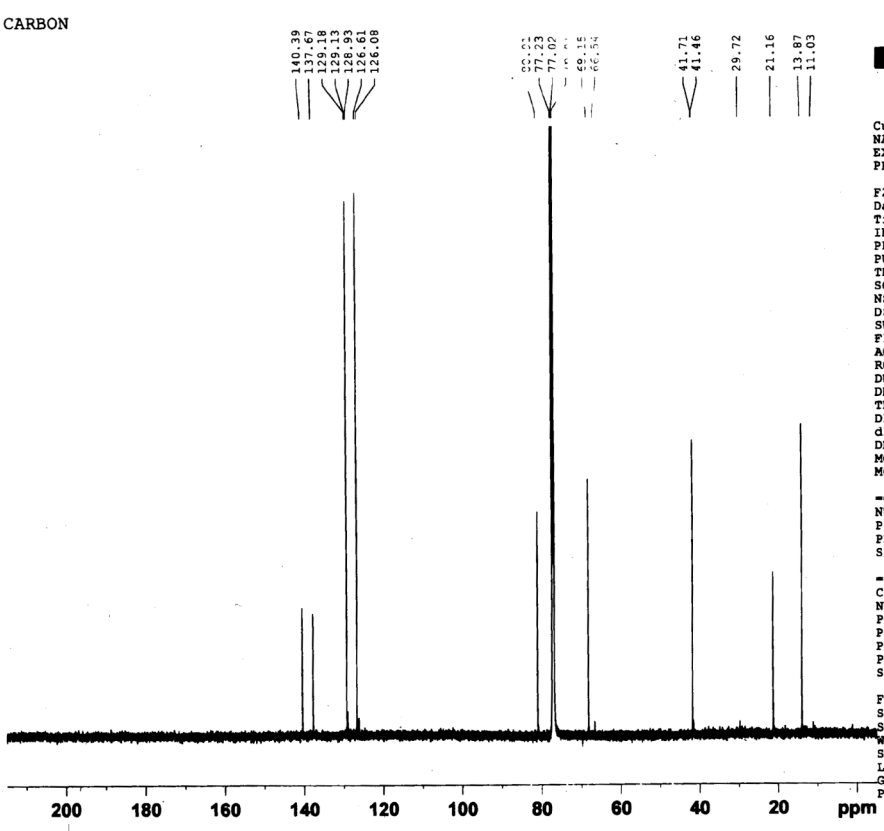
Current Data Parameters
NAME Feb10-2006
EXPNO 92
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060210
Time 18.37
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 724.1
DW 60.800 usec
DE 6.00 usec
TE 303.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

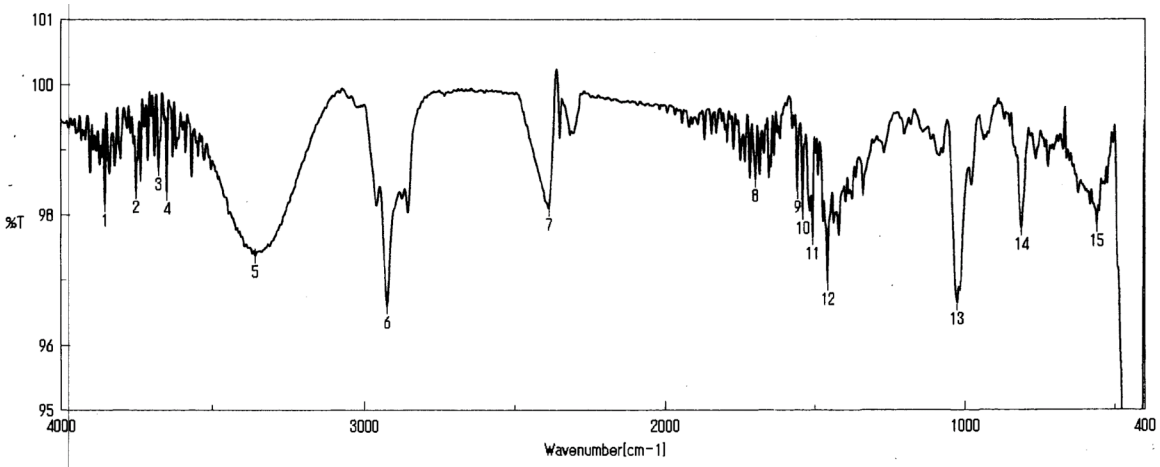
-------- CHANNEL f1 --------
NUC1 1H
P1 8.10 usec
PL1 1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300177 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CARBON

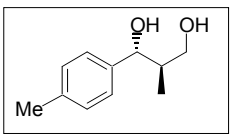


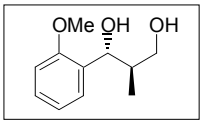

```
Current Data Parameters
NAME            Feb11-2006
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_             20060211
Time                 19.08
INSTRUM              av600
PROBHD   5 mm CPDUL 13C
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2417
DS                     4
SWH            35971.223 Hz
FIDRES          0.548877 Hz
AQ              0.9110143 sec
RG                14596.5
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           150.9028090 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

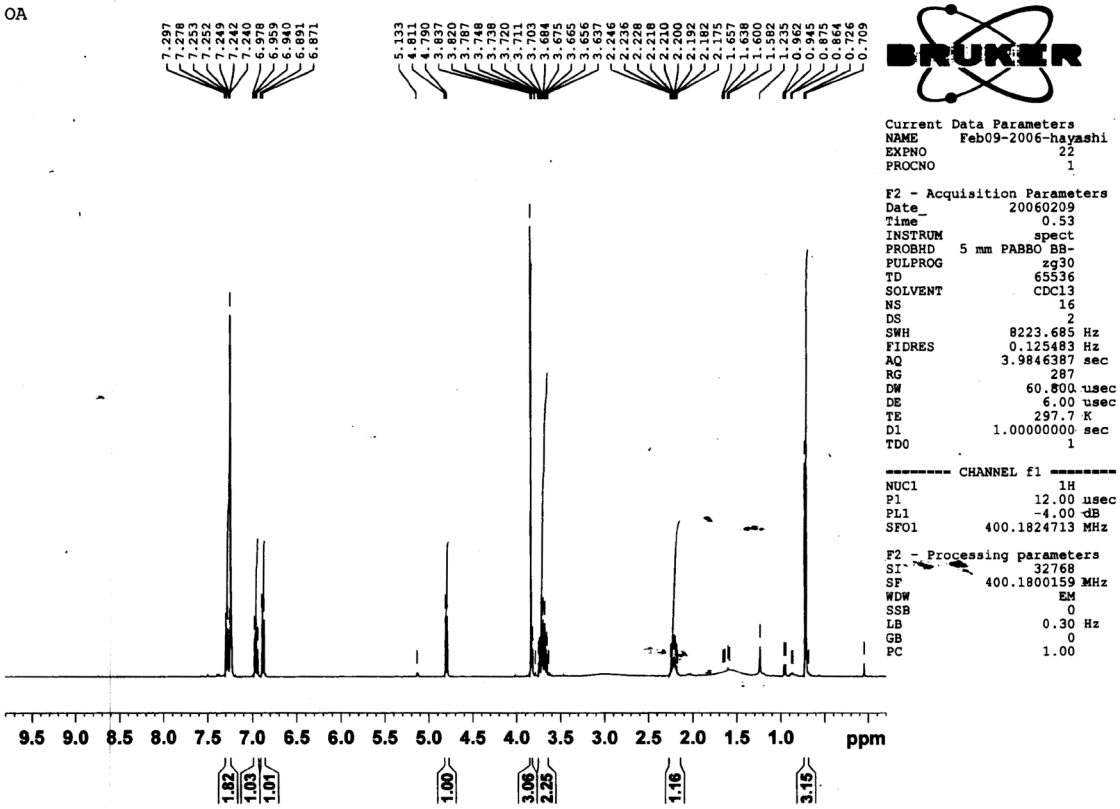


積算回数	16	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/02/10 13:39		
測定者			
ファイル名	Memory#3		
サンプル名			
コメント	コメント		

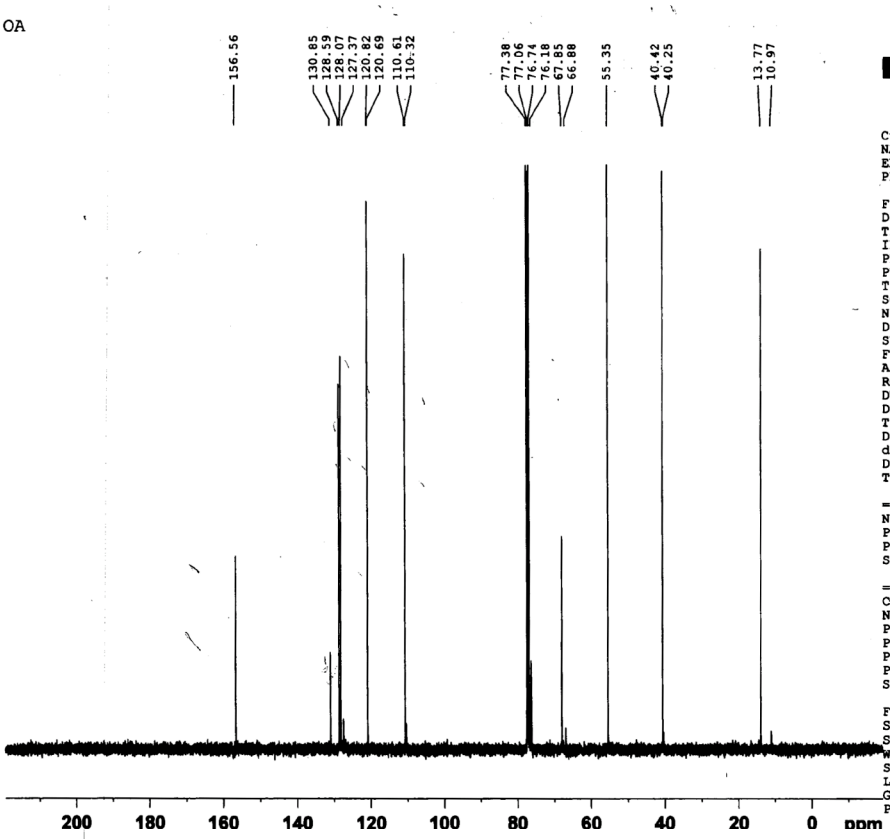
1:	3854.04,	98.1565	2:	3750.87,	98.3648	3:	3675.66,	98.7179	4:	3648.66,	98.3406
5:	3358.43,	97.3746	6:	2923.56,	96.5935	7:	2385.51,	98.0939	8:	1698.98,	98.5419
9:	1558.20,	98.3680	10:	1540.85,	98.0434	11:	1508.06,	97.6544	12:	1456.96,	96.9498
13:	1026.91,	96.6443	14:	811.88,	97.7933	15:	560.22,	97.8415	16:	420.41,	87.7287




OMe
OH
OH


OA
7.297
7.278
7.253
7.252
7.249
7.242
7.240
6.978
6.959
6.940
6.891
6.871
5.133
4.811
4.790
3.837
3.820
3.787
3.748
3.738
3.720
3.711
3.703
3.684
3.675
3.665
3.656
3.637
2.246
2.236
2.228
2.218
2.210
2.200
2.192
2.182
2.175
1.657
1.638
1.600
1.582
1.235
0.962
0.945
0.875
0.864
0.726
0.709
BRUKER
Current Data Parameters
NAME Feb09-2006-hayashi
EXPNO 22
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060209
Time 0.53
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 287
DW 60.800 usec
DE 6.00 usec
TE 297.7 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 400.1800159 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
1.82
1.03
1.01
1.00
3.06
2.25
1.16
3.15

OA



BRUKER

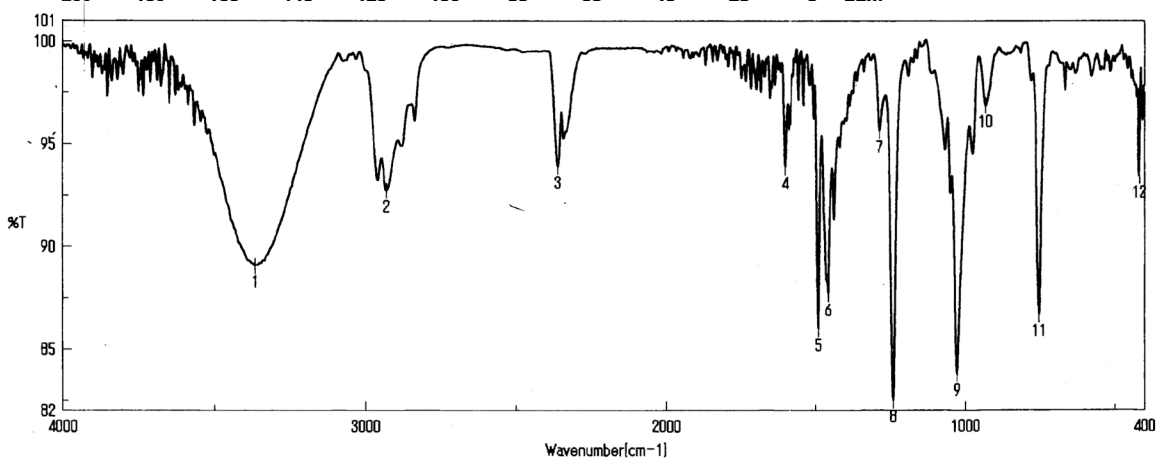
Current Data Parameters
NAME Dec15-2005-hayashi
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051215
Time 23.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
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 299.4 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

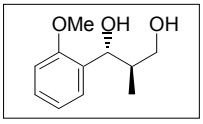
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -4.00 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.1816007 MHz

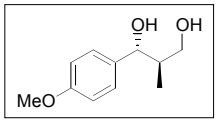
F2 - Processing parameters
SI 32768
SF 100.6253410 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

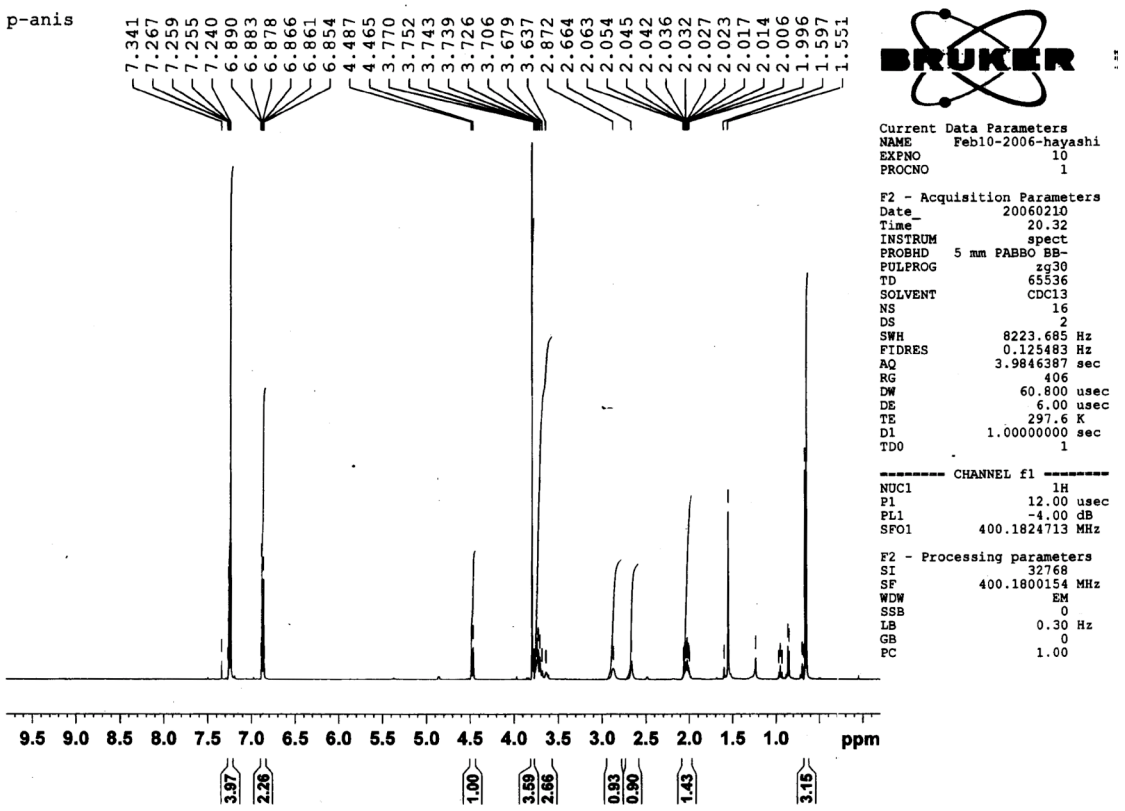


積算回数	16	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	105/12/16 17:36		
測定者			
ファイル名	Memory#7		
サンプル名	o anis		
コメント	コメント		

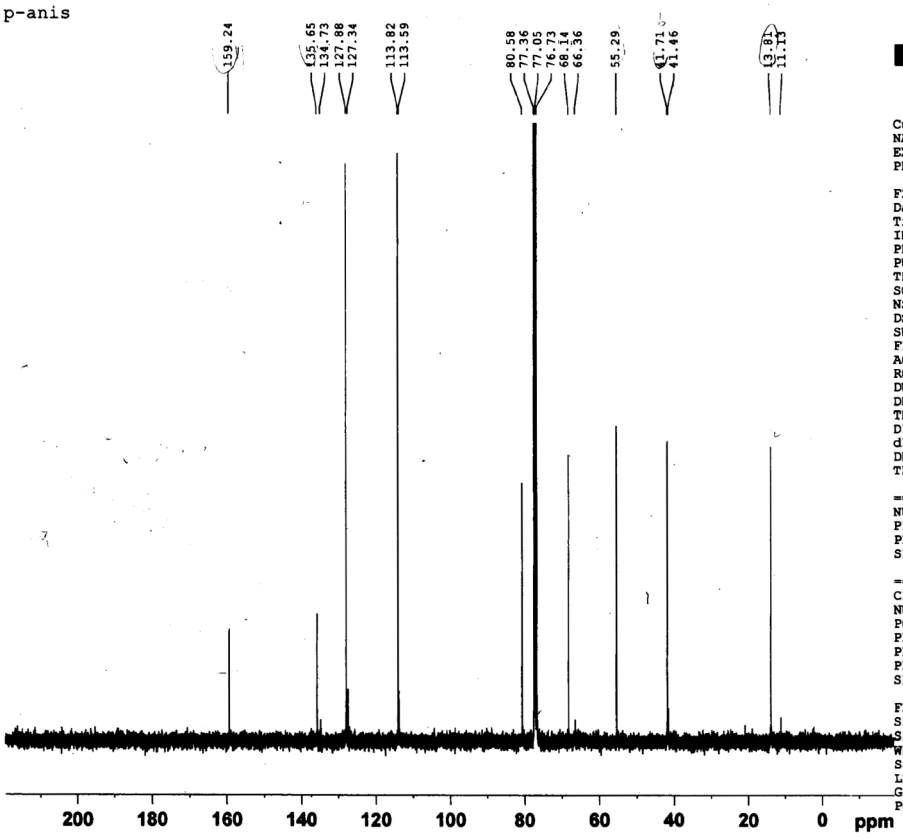
1:	3367.10,	89.0478	2:	2931.27,	92.7195	3:	2360.44,	93.8817
4:	1601.59,	93.8678	5:	1490.70,	85.9626	6:	1457.92,	87.6688
7:	1287.25,	95.6284	8:	1240.97,	82.4882	9:	1027.87,	83.7649
10:	934.34,	96.8755	11:	754.99,	86.6723	12:	417.51,	93.3933




OH
OH
MeO


p-anis
7.341
7.267
7.259
7.255
7.240
6.890
6.883
6.878
6.866
6.861
6.854
4.487
4.465
3.770
3.752
3.743
3.739
3.726
3.706
3.679
3.637
2.872
2.664
2.063
2.054
2.045
2.042
2.036
2.032
2.027
2.023
2.017
2.014
2.006
1.996
1.597
1.551
BRUKER
Current Data Parameters
NAME Feb10-2006-hayashi
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060210
Time 20.32
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 406
DW 60.800 usec
DE 6.00 usec
TE 297.6 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 400.1800154 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
3.97
2.26
1.00
3.59
2.66
0.93
0.90
1.43
3.15

p-anis



BRUKER

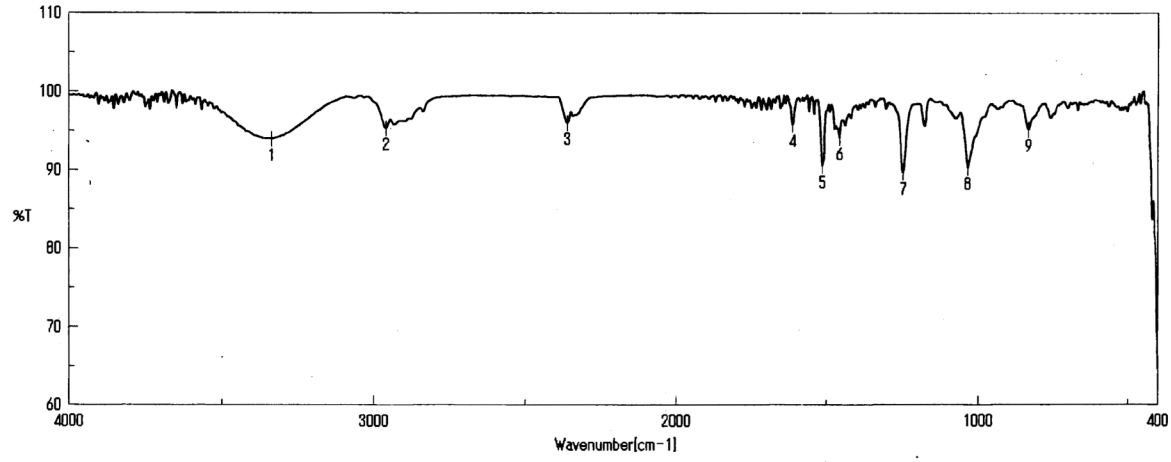
Current Data Parameters
NAME Feb09-2006-hayashi
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060209
Time 2.38
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 299.3 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

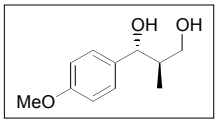
F2 - Processing parameters
SI 32768
SF 100.6253410 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

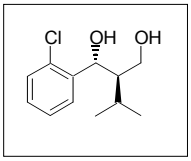


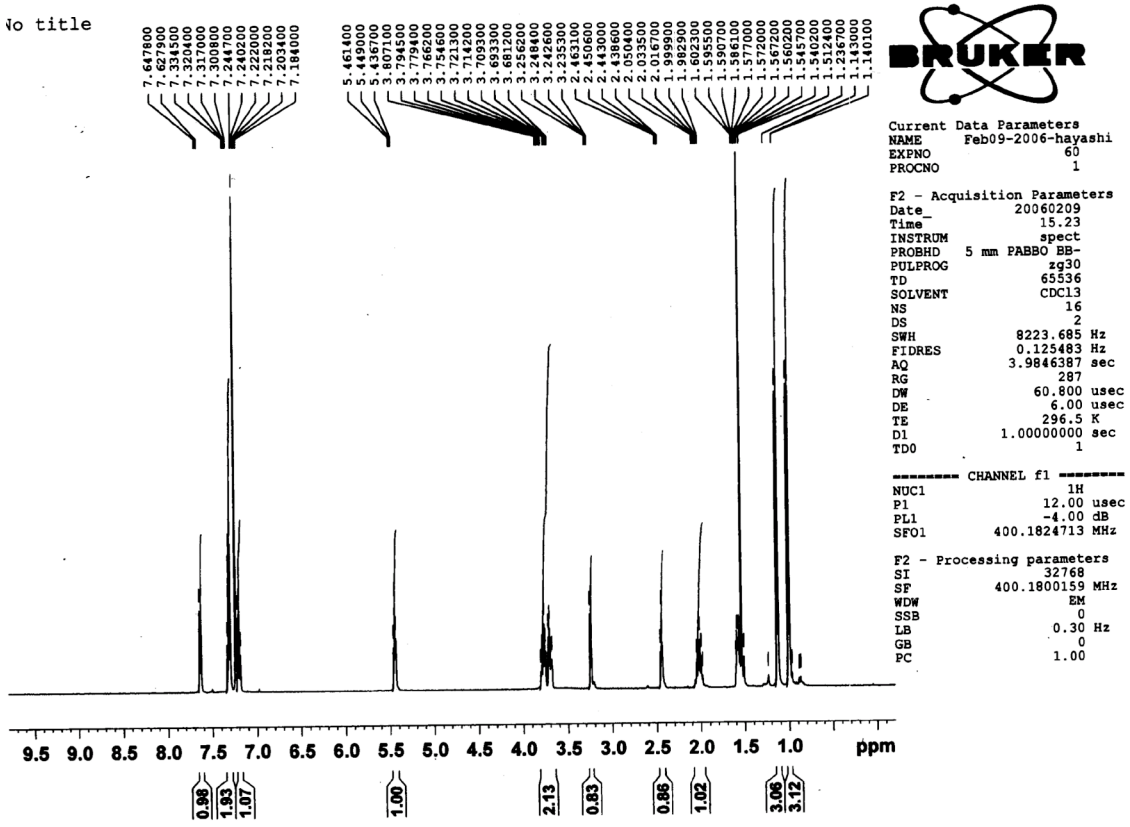
積算回数 16
ゼロフィリング ON
ゲイン 1
日時 06/02/10 14:27
測定者
ファイル名 Memory#5
サンプル名
コメント コメント

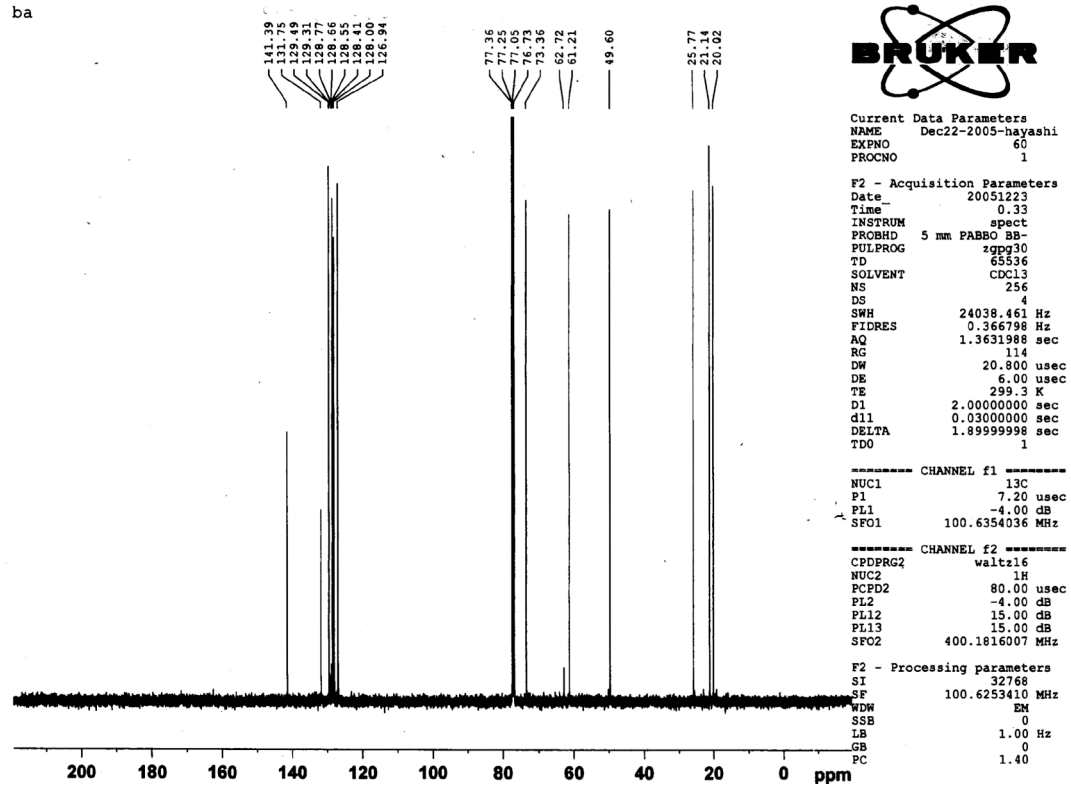
分解 4 cm-1
アポダイゼーション Cosine
スキャンスピード 2 mm/sec

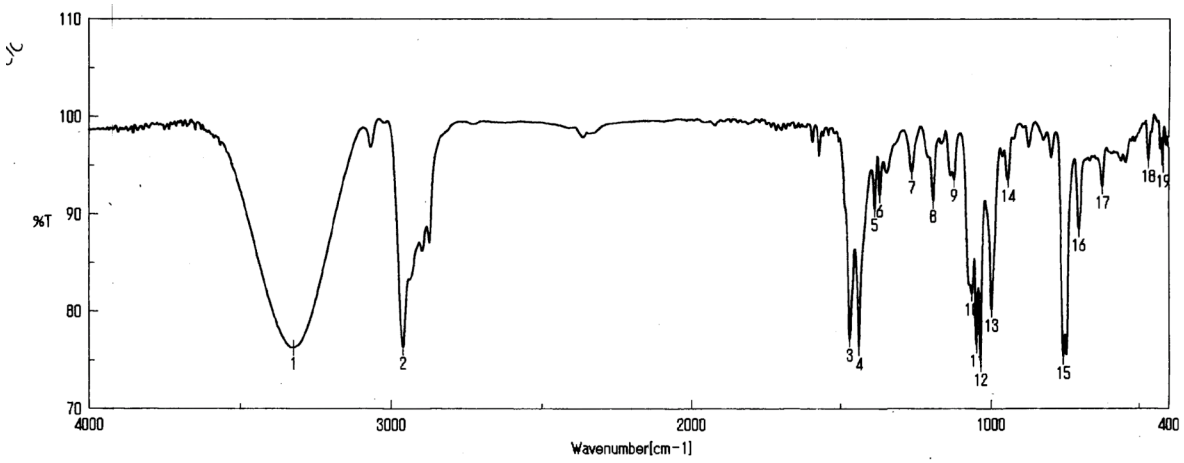
1: 3336.25, 93.9145 2: 2959.23, 95.2844 3: 2360.44, 95.9888 4: 1613.16, 95.7904
5: 1513.85, 90.5187 6: 1456.96, 94.1221 7: 1246.75, 89.6747 8: 1033.66, 90.3071
9: 833.10, 95.1297




Cl
OH
OH

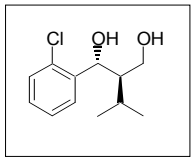

No title
7.647800
7.627900
7.334500
7.320400
7.317000
7.306900
7.247700
7.240200
7.222000
7.218200
7.203400
7.184000
5.461400
5.449000
5.436700
3.807100
3.794500
3.779400
3.766200
3.754600
3.721300
3.714200
3.709300
3.683200
3.651300
3.256200
3.248400
3.242600
3.235300
3.463100
2.450600
2.443000
2.438600
2.050400
2.033500
2.016700
1.999900
1.982900
1.602300
1.595500
1.590700
1.586100
1.577000
1.572000
1.567200
1.545700
1.540200
1.512400
1.236700
1.143000
1.140100
BRUKER
Current Data Parameters
NAME Feb09-2006-hayashi
EXPNO 60
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060209
Time 15.23
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 287
DW 60.800 usec
DE 6.00 usec
TE 296.5 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 400.1800159 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
0.98
1.93
1.07
1.00
2.13
0.83
0.86
1.02
3.06
3.12

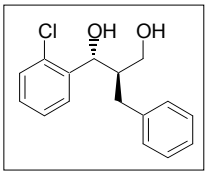

ba
141.39
131.75
129.49
129.31
128.77
128.66
128.55
128.41
128.00
126.94
77.36
77.25
77.05
76.73
73.36
62.72
61.21
49.60
25.77
21.14
20.02
BRUKER
Current Data Parameters
NAME Dec22-2005-hayashi
EXPNO 60
PROCNO 1
F2 - Acquisition Parameters
Date_ 20051223
Time 0.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
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 299.3 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
200 180 160 140 120 100 80 60 40 20 0 ppm

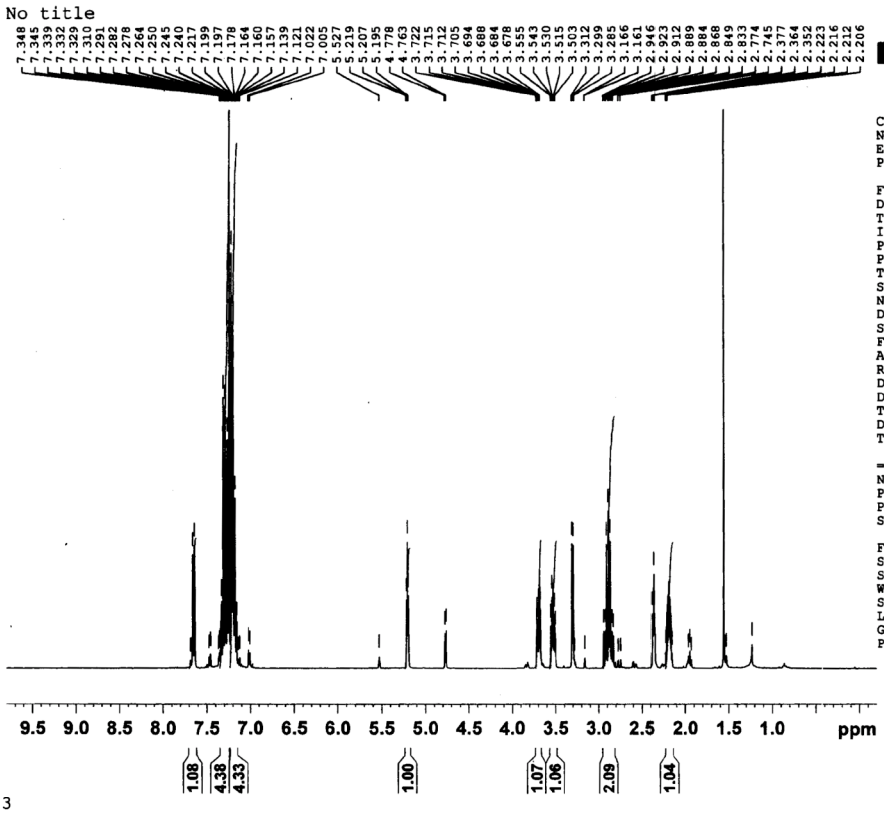


積算回数	16	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/02/10 14:07		
測定者			
ファイル名	Memory#6		
サンプル名			
コメント	コメント		

1:	3323.71,	76.2701	2:	2960.20,	76.3046	3:	1469.49,	77.1449	4:	1438.64,	76.2451
5:	1386.57,	90.4917	6:	1369.21,	91.8887	7:	1264.11,	94.3444	8:	1193.72,	91.3642
9:	1124.30,	93.5199	10:	1064.51,	81.8303	11:	1048.12,	76.5740	12:	1035.59,	74.5961
13:	997.98,	80.1303	14:	943.98,	93.5012	15:	756.92,	75.3215	16:	704.85,	88.4228
17:	625.79,	92.7805	18:	469.58,	95.4395	19:	419.44,	94.9444			

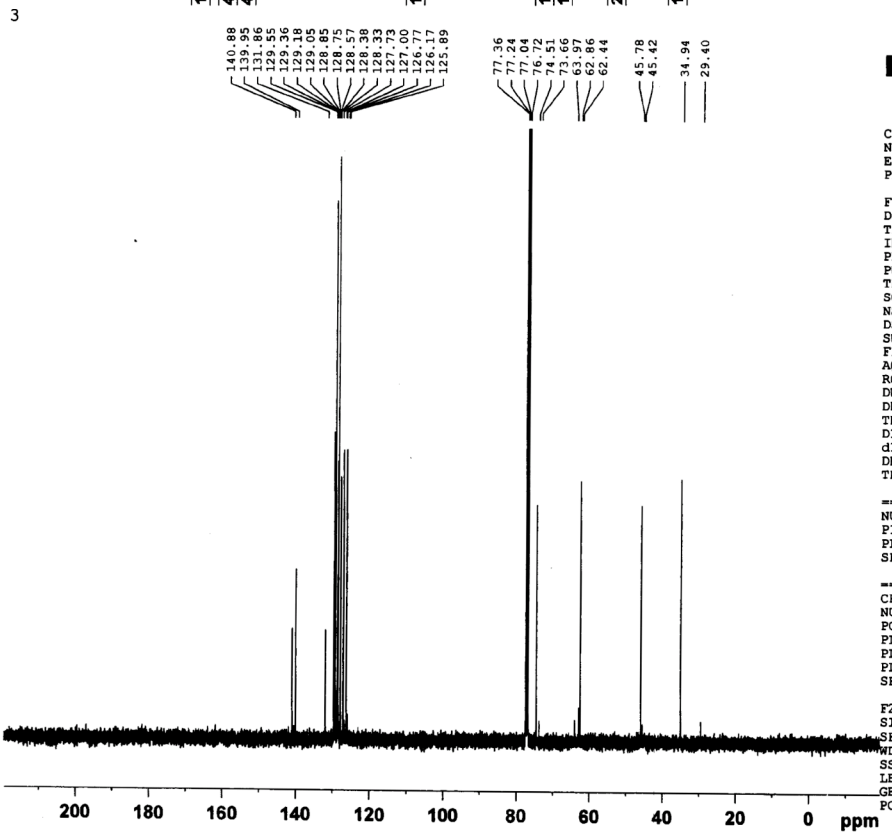






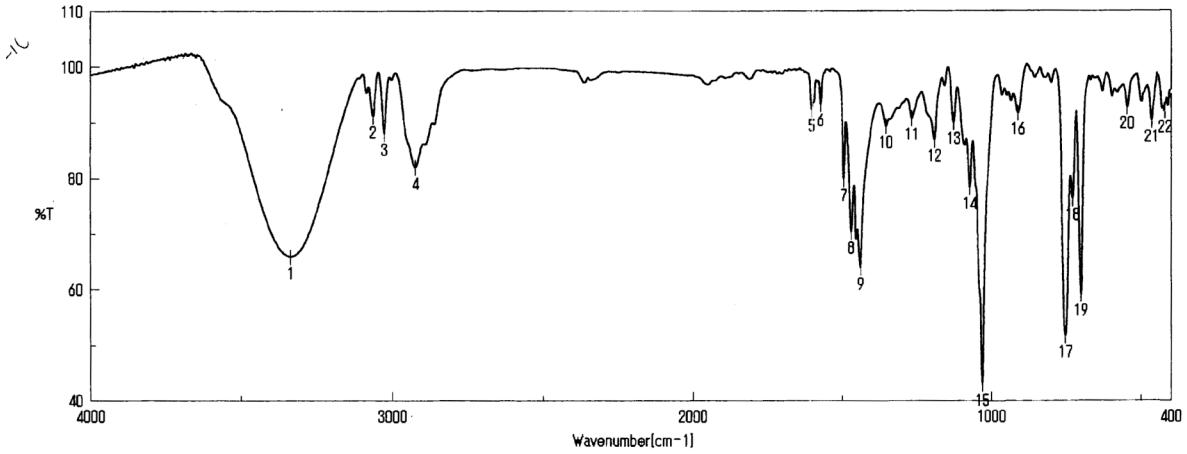
BRUKER

```
Current Data Parameters
NAME      Feb09-2006-hayashi
EXPNO                     50
PROCNO                     1

F2 - Acquisition Parameters
Date_           20060209
Time              15.15
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                  228
DW               60.800 usec
DE                6.00 usec
TE               296.5 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          400.1800157 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



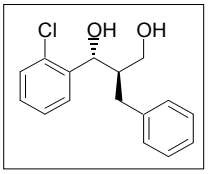
BRUKER

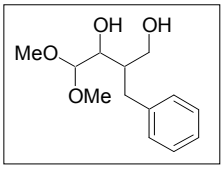
```
Current Data Parameters
NAME      Dec22-2005-hayashi
EXPNO                     50
PROCNO                     1

F2 - Acquisition Parameters
Date_           20051223
Time                 0.09
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                  144
DW               20.800 usec
DE                6.00 usec
TE               299.3 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
```

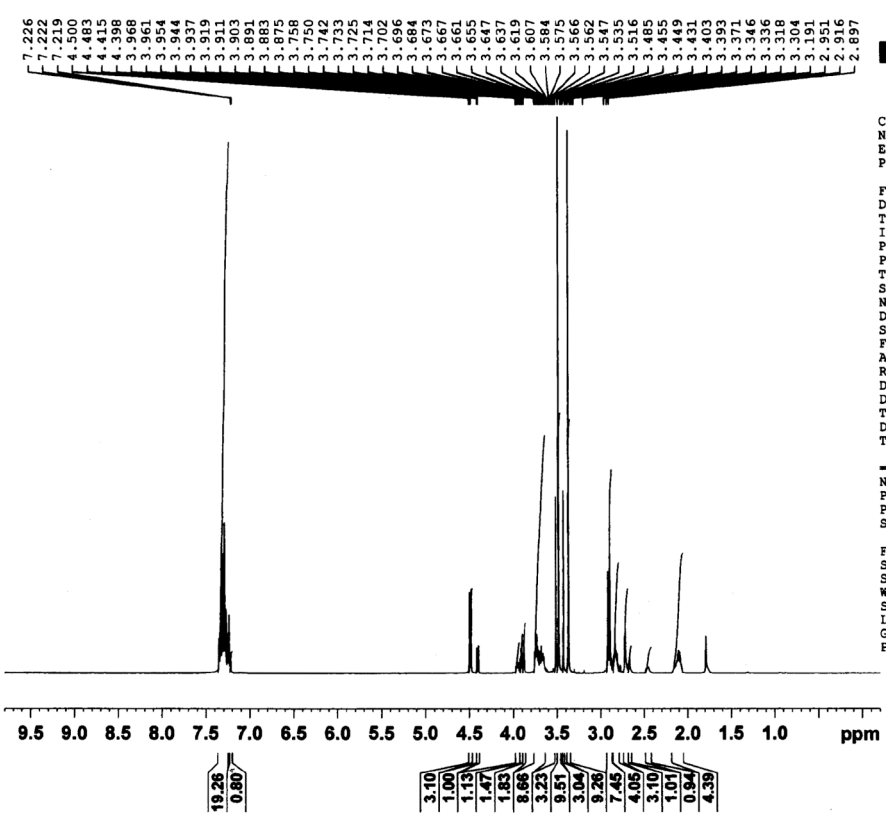


積算回数	16	分解	4 cm-1
ゼロフィリング	ON	アポダイゼーション	Cosine
ゲイン	1	スキャンスピード	2 mm/sec
日時	106/02/10 13:57		
測定者			
ファイル名	Memory#4		
サンプル名			
コメント	コメント		

1:	3336.25,	65.7928	2:	3063.37,	91.0649	3:	3025.76,	87.9958	4:	2923.56,	81.9092
5:	1602.56,	92.2757	6:	1572.66,	93.2486	7:	1495.53,	79.7522	8:	1470.46,	70.3393
9:	1439.60,	63.8327	10:	1353.78,	89.2770	11:	1267.00,	90.7028	12:	1191.79,	86.8061
13:	1127.19,	89.9391	14:	1073.19,	78.3189	15:	1030.77,	42.9604	16:	911.20,	91.6380
17:	753.07,	51.6752	18:	728.00,	76.3015	19:	701.00,	59.0891	20:	545.76,	92.6847

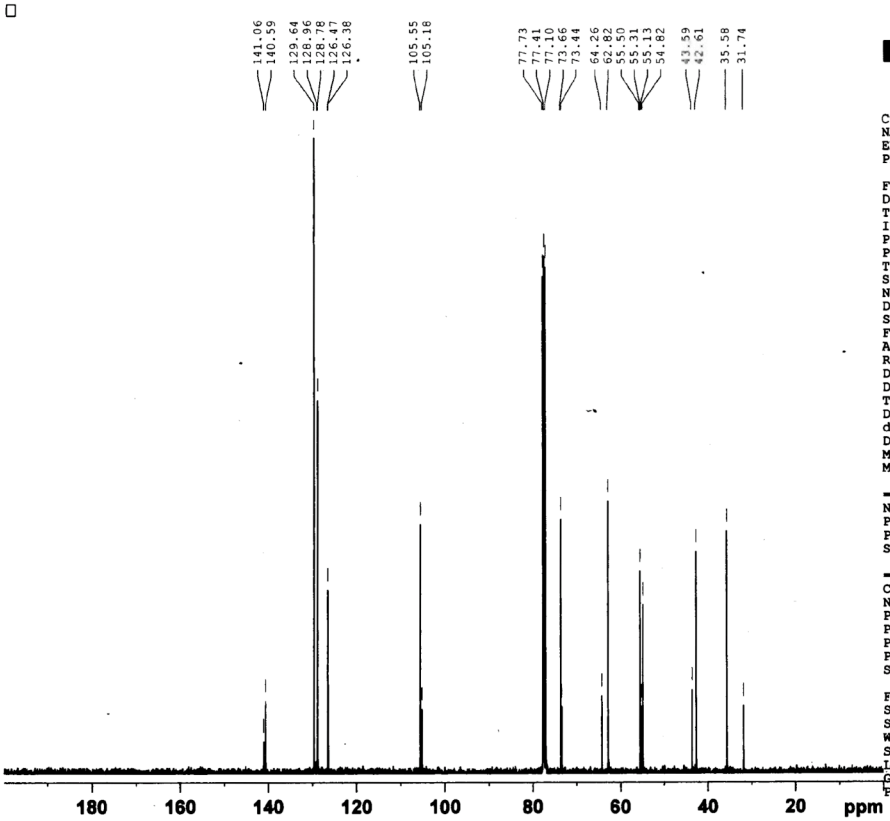






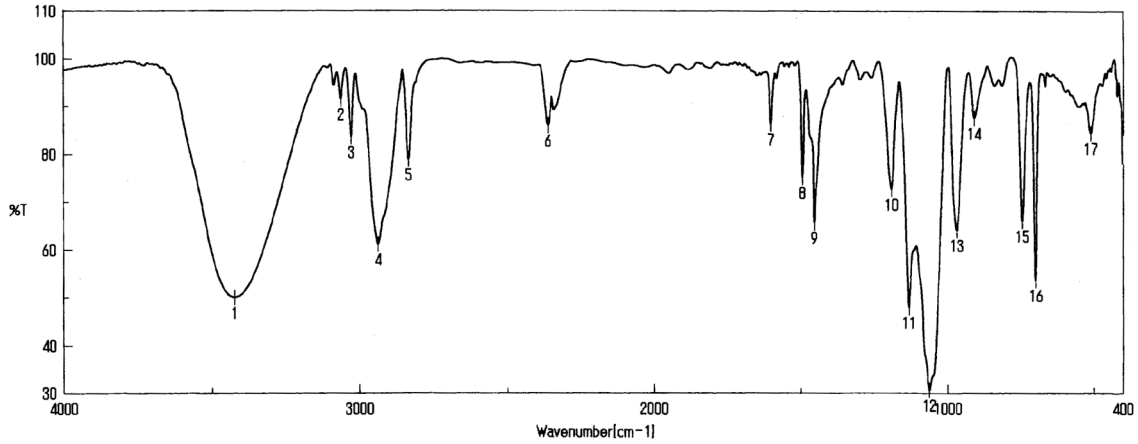
BRUKER

```
Current Data Parameters
NAME      Feb23-2006-hayashi
EXPNO                     41
PROCNO                     1

F2 - Acquisition Parameters
Date_              20060223
Time                  23.27
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                   298.0 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             400.1799873 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```



BRUKER

```
Current Data Parameters
NAME          Feb24-2006
EXPNO                 81
PROCNO                 1

F2 - Acquisition Parameters
Date_          20060224
Time              19.18
INSTRUM          dpx400
PROBHD    5 mm BBO 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  555
DS                    2
SWH            31847.133 Hz
FIDRES          0.485949 Hz
AQ              1.0289652 sec
RG                 3251
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          100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                    3.00 dB
PL12                  20.00 dB
PL13                  22.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF            100.6127290 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```



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	106/02/24 19:21		
測定者			
ファイル名	Memory#3		
サンプル名			
コメント	コメント		

1:	3423.03,	50.0156	2:	3061.44,	91.4794	3:	3026.73,	83.6091	4:	2936.09,	61.1712
5:	2831.95,	78.9846	6:	2360.44,	85.9987	7:	1602.56,	86.3100	8:	1495.53,	75.1662
9:	1454.06,	65.7203	10:	1192.76,	72.7447	11:	1132.97,	48.0437	12:	1063.55,	30.7035
13:	970.98,	64.1610	14:	911.20,	87.6000	15:	746.32,	66.1189	16:	701.00,	53.7279
17:	511.04,	84.5132