

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications
MOST TRUSTED. MOST CITED. MOST READ.

61 2966-1

¹H and ¹³C NMR Data with Peak Assignments

Benzyl acetate spectrum was compared with Aldrich NMR 2(2), 269A.

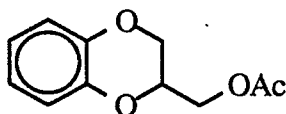
Benzyl benzoate spectrum was compared with Aldrich NMR 2(2), 281D.

Bornyl acetate spectrum was compared with Aldrich NMR 2(1) 533B.

Bornyl benzoate: ¹H NMR (CDCl₃): 0.90 (s, 6 H), 0.95 (s, 3 H), 1.11 (dd, 1 H, J_{HH} = 3 Hz, 12 Hz), 1.33 (m, 2 H), 1.73 (m, 2 H), 2.13 (m, 1 H), 2.47 (m, 1 H), 5.10 (m, 1 H), 7.43 (t, 2 H, J_{HH} = 9 Hz), 7.53 (t, 1 H, J = 9 Hz), 8.05 (d, 2 H, J = 9 Hz); ¹³C NMR (CDCl₃): 12.47 (CH₃), 13.59 (CH₃), 18.89, 19.70, 27.37, 28.07, 36.89, 44.96, 47.85, 49.06, 80.48 (CH), 128.30, 129.48, 130.86, 132.71 (CH), 166.78 (O-C=O).

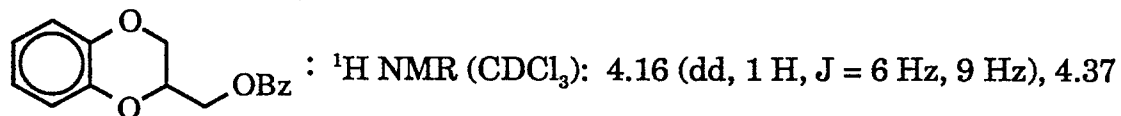
(±)Menthyl acetate: ¹H NMR (CDCl₃): 0.71 (d, 3 H, J = 9 Hz), 0.75 to 1.94 overlapping region (15 H), 1.97 (s, 3 H), 4.61 (dt, 1 H, J = 3 Hz, 9 Hz); ¹³C NMR (CDCl₃): 16.05, 16.34, 20.69, 20.98, 21.28, 21.97, 22.18, 23.10, 23.45, 25.78, 26.15, 26.27, 31.33, 31.56, 31.61, 34.52, 40.89, 40.95, 45.03, 46.96, 50.10, 71.46, 73.99, 74.12; 170.67 (S, O-C=O).

(±)Menthyl benzoate: ¹H NMR (CDCl₃): 0.78 (d, 3 H, J = 6 Hz), 0.91 (dd, 6 H, J = 3 Hz, 6 Hz), 1.09 (m, 1 H), 1.55 (m, 2 H), 1.72 (m, 2 H), 1.96 (dq, J = 3 Hz, 6 Hz), 2.12 (m, 1 H), 4.90 (dt, 1 H, J = 3 Hz, 9 Hz), 7.42 (t, 2 H, J = 9 Hz), 7.53 (t, 1 H, J = 9 Hz), 8.07 (d, 2 H, J = 9 Hz); ¹³C NMR (CDCl₃): 12.46, 16.49, 20.76, 22.03, 23.60, 26.46, 31.42, 34.30, 40.95, 47.25, 74.79, 128.26, 130.84, 132.66, 166.06 (s, O-C=O).



: ¹H NMR (CDCl₃): 2.09 (s, 3 H), 4.04 (dd, 1 H, J = 6 Hz, 9 Hz), 4.30 (m, 4 H), 6.82 (m, 4 H); ¹³C NMR (CDCl₃): 20.67 (s, CH₃), 62.51 (s, OCH₂), 64.97 (s, CH), 70.82 (s, CH₂), 117.14, 113.6, 121.55, 121.74, 142.68, 142.90 (CH), 170.57 (s, O-C=O).

612966-2



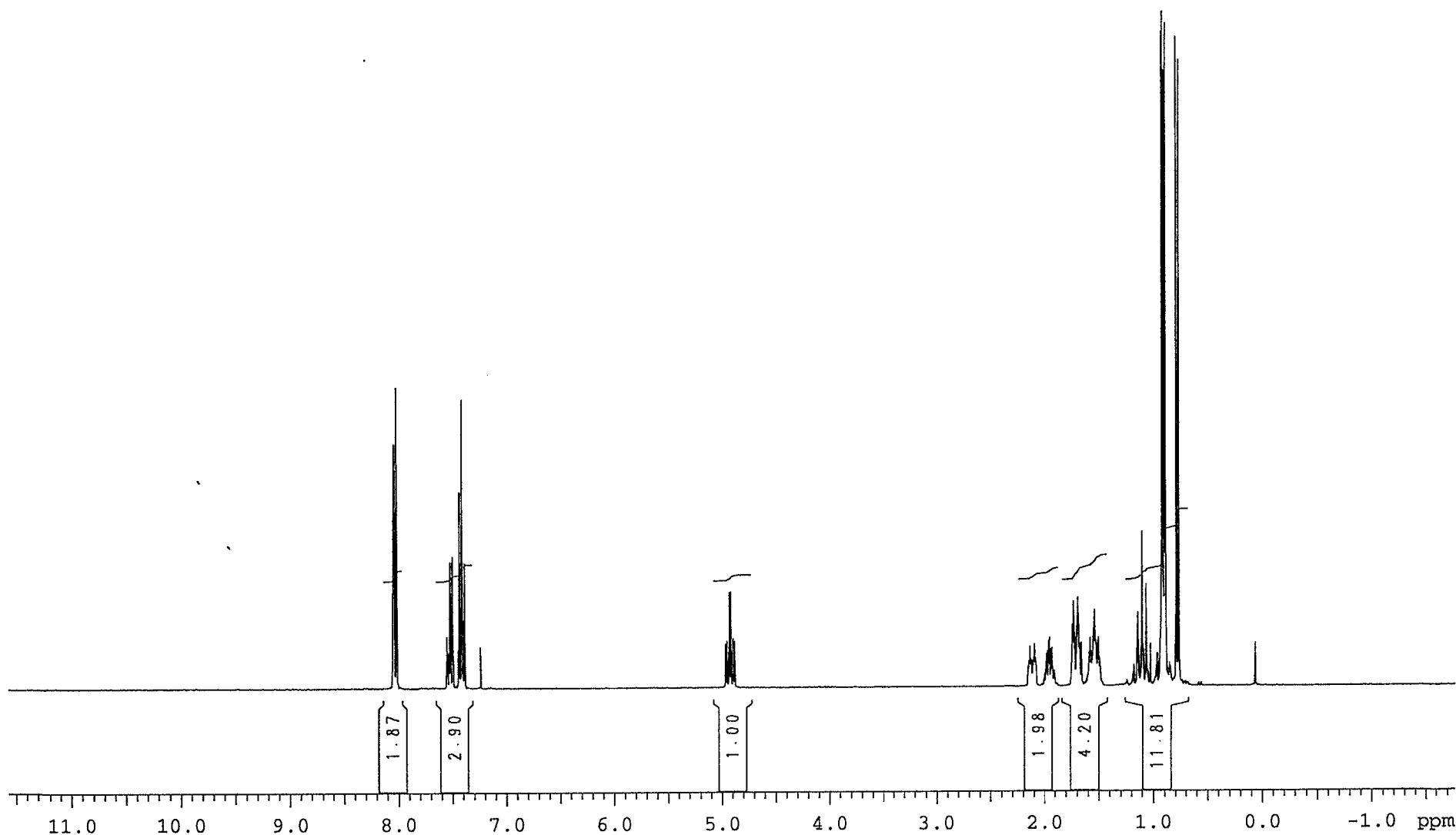
(dd, 1 H, $J = 3$ Hz, 12 Hz), 4.54 (m, 3 H), 6.88 (m, 4 H), 7.44 (t, 2 H, $J = 9$ Hz), 7.58 (t, 1 H, $J = 9$ Hz), 8.05 (d, 2 H, $J = 9$ Hz); ^{13}C NMR (CDCl_3): 62.99 (s, OCH_2), 65.13 (s, CH), 70.93 (s, CH_2), 117.20, 117.43, 121.58, 121.79, 128.44, 129.46, 129.72, 133.31, 142.81, 142.97 (CH), 166.16 (s, $\text{O}-\text{C}=\text{O}$).

menthyl benzoate

8.05
8.04
8.04
8.03
8.02
8.02
7.56
7.55
7.55
7.54
7.53
7.52
7.51
7.50
7.50
7.45
7.44
7.44
7.44
7.42
7.42
7.41
7.40
7.39
7.39
7.24

4.96
4.95
4.93
4.91
4.89
4.88

2.15
2.15
2.14
2.13
2.13
2.12
2.11
2.11
2.10
2.09
2.09
2.08
1.98
1.97
1.96
1.95
1.95
1.93
1.93
1.75
1.74
1.73
1.73
1.71
1.70
1.69
1.69
1.69
1.66
1.66
1.59
1.58
1.57
1.56
1.55
1.54
1.53
1.53

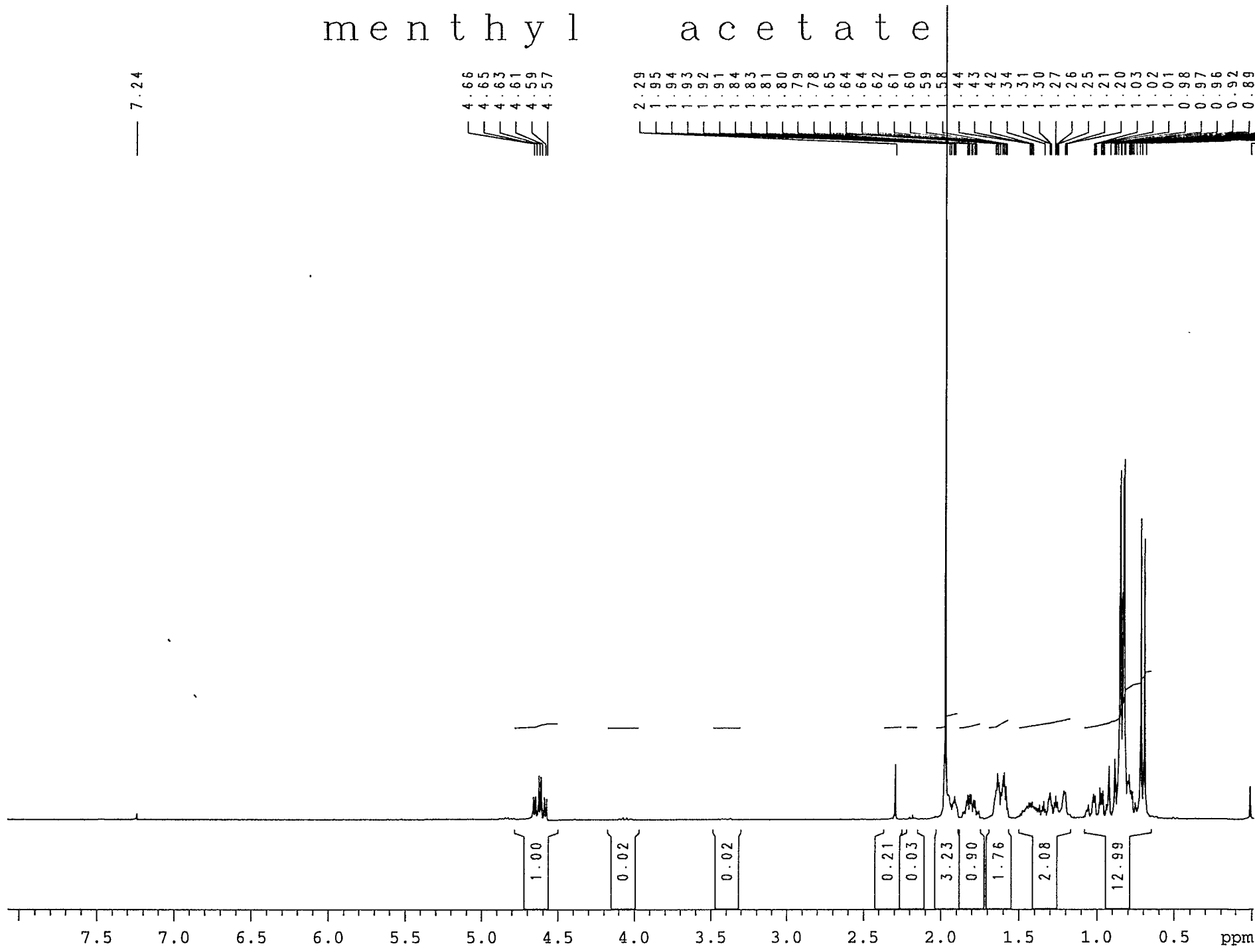


file:/giga/data/bkdsa/nmr/bos.081.fid/1/pdata/1/plotfile.16 user:unknown date:Fri Jun 2 14:46:32 1995

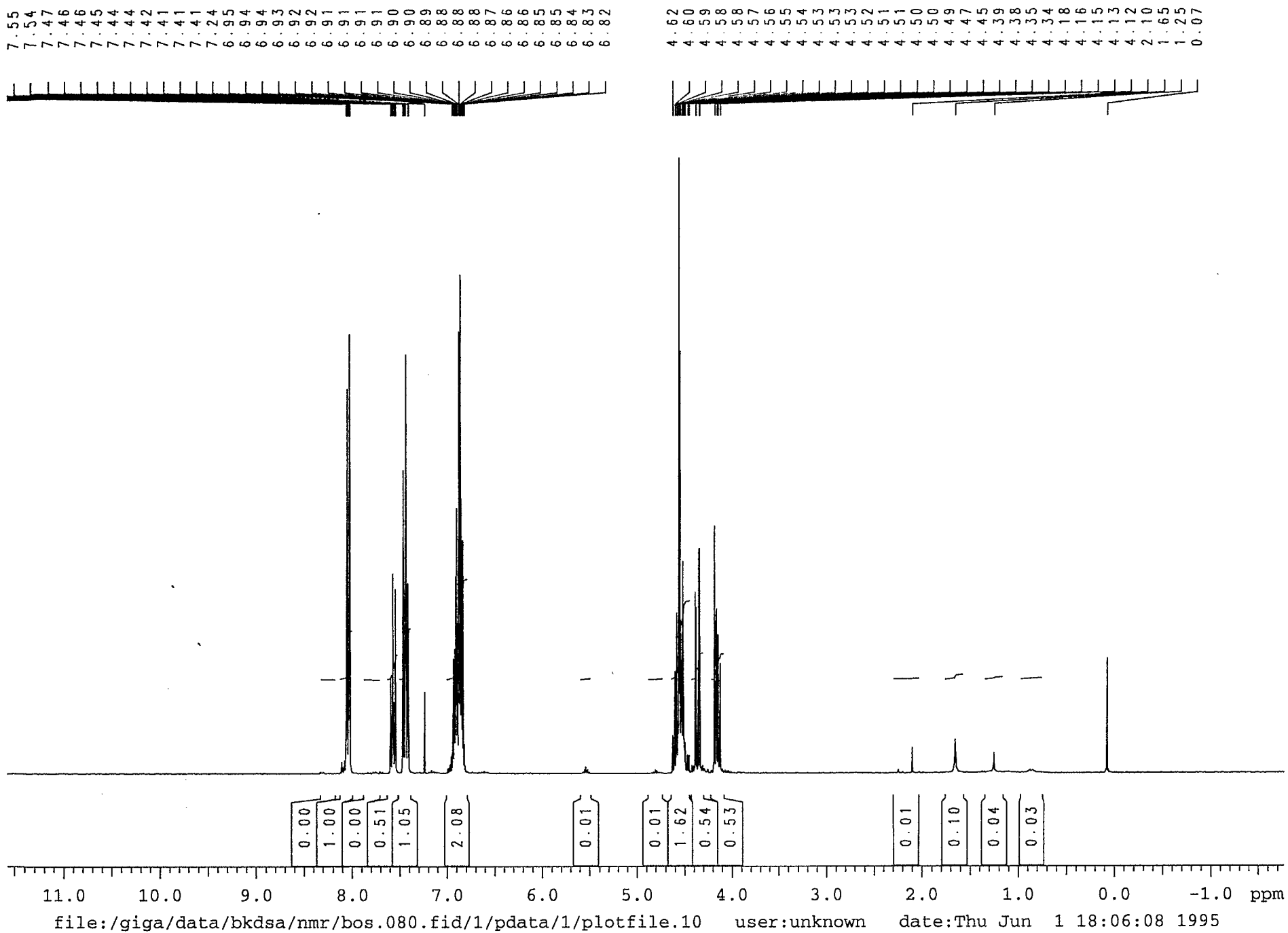
572966-3

Gr 2964-4

menthyl acetate

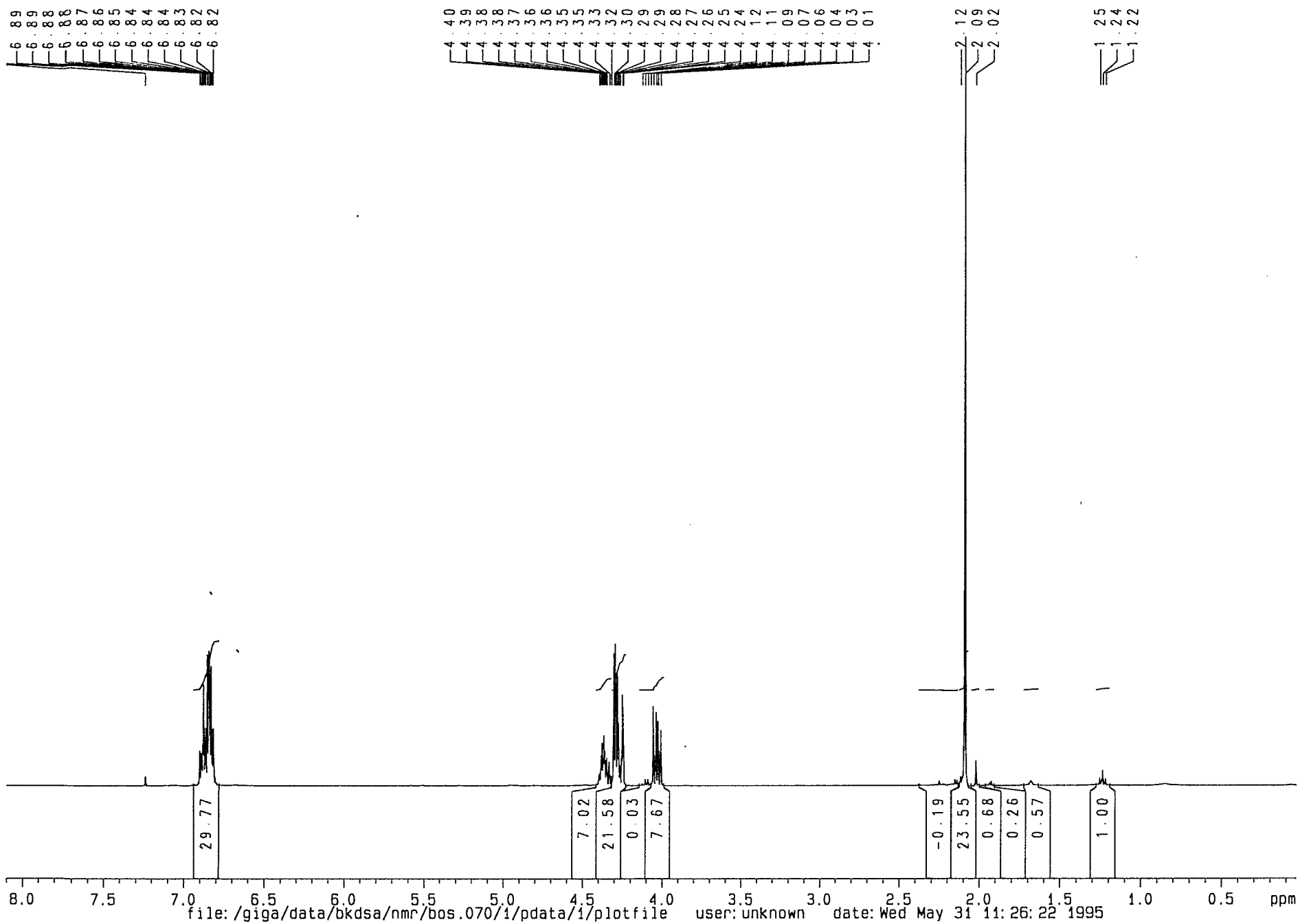


62966-5



file:/giga/data/bkdsa/nmr/bos.080.fid/1/pdata/1/plotfile.10 user:unknown date:Thu Jun 1 18:06:08 1995

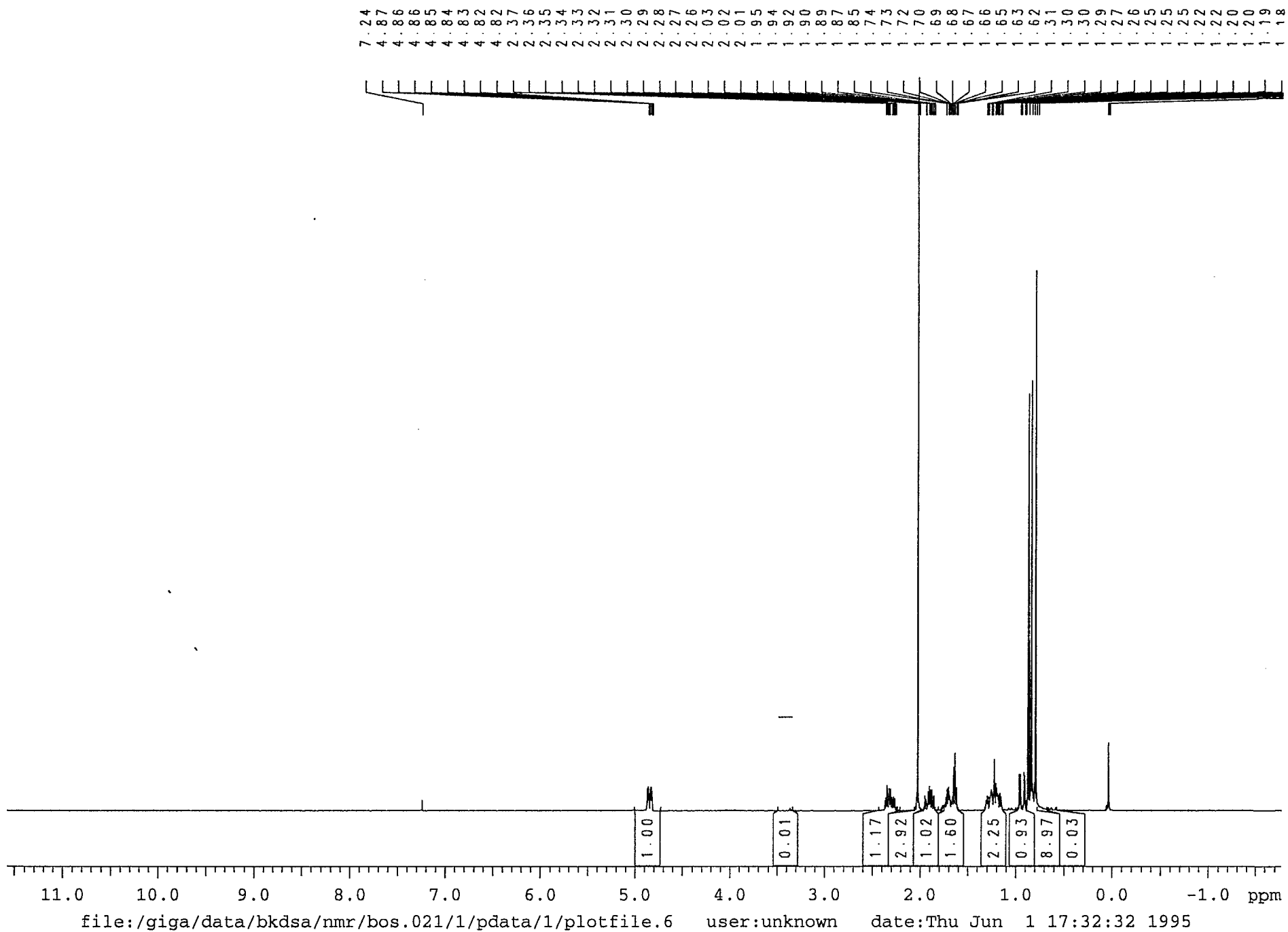
612466-6



sample A

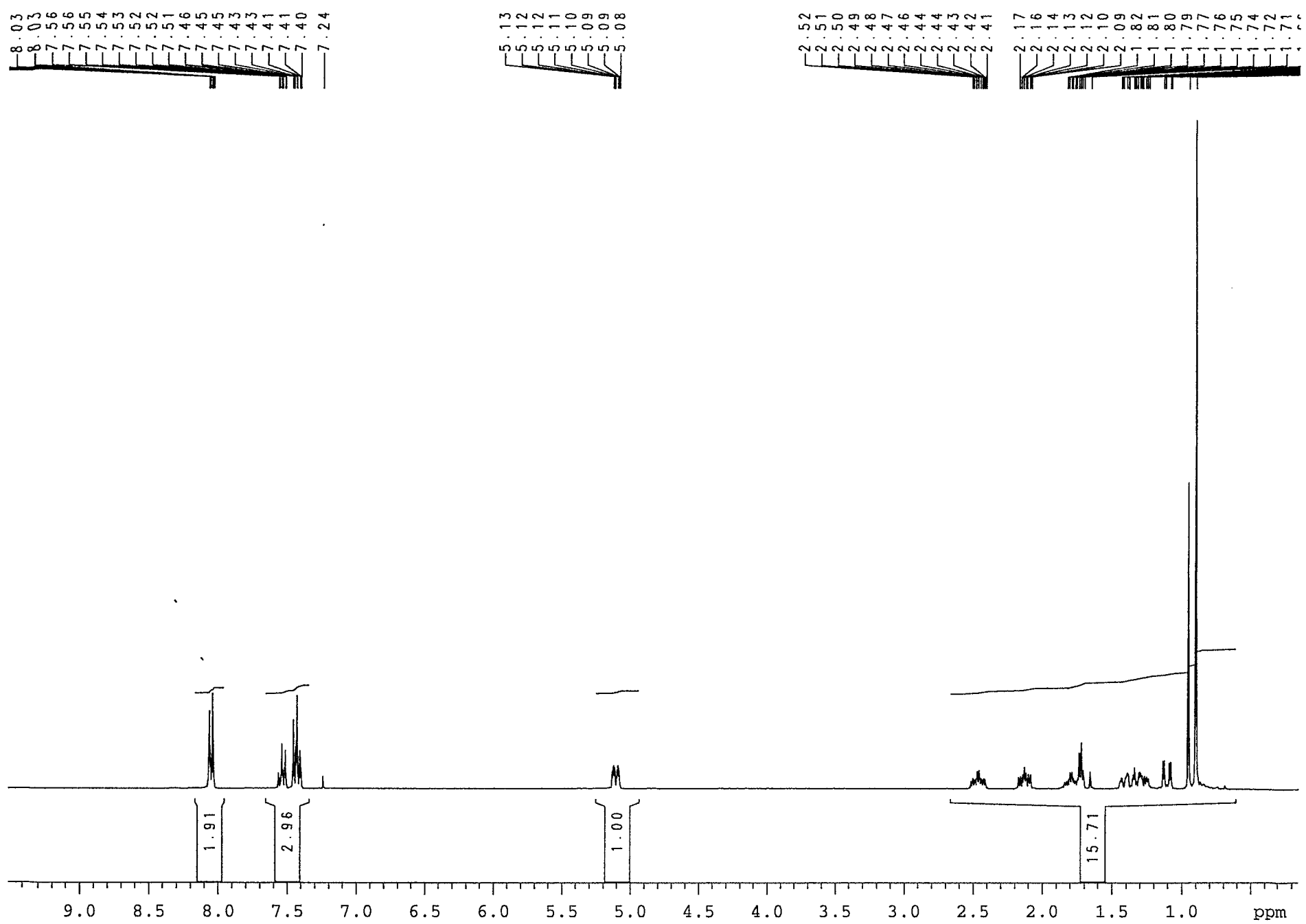
672946-7

bornyl acetate

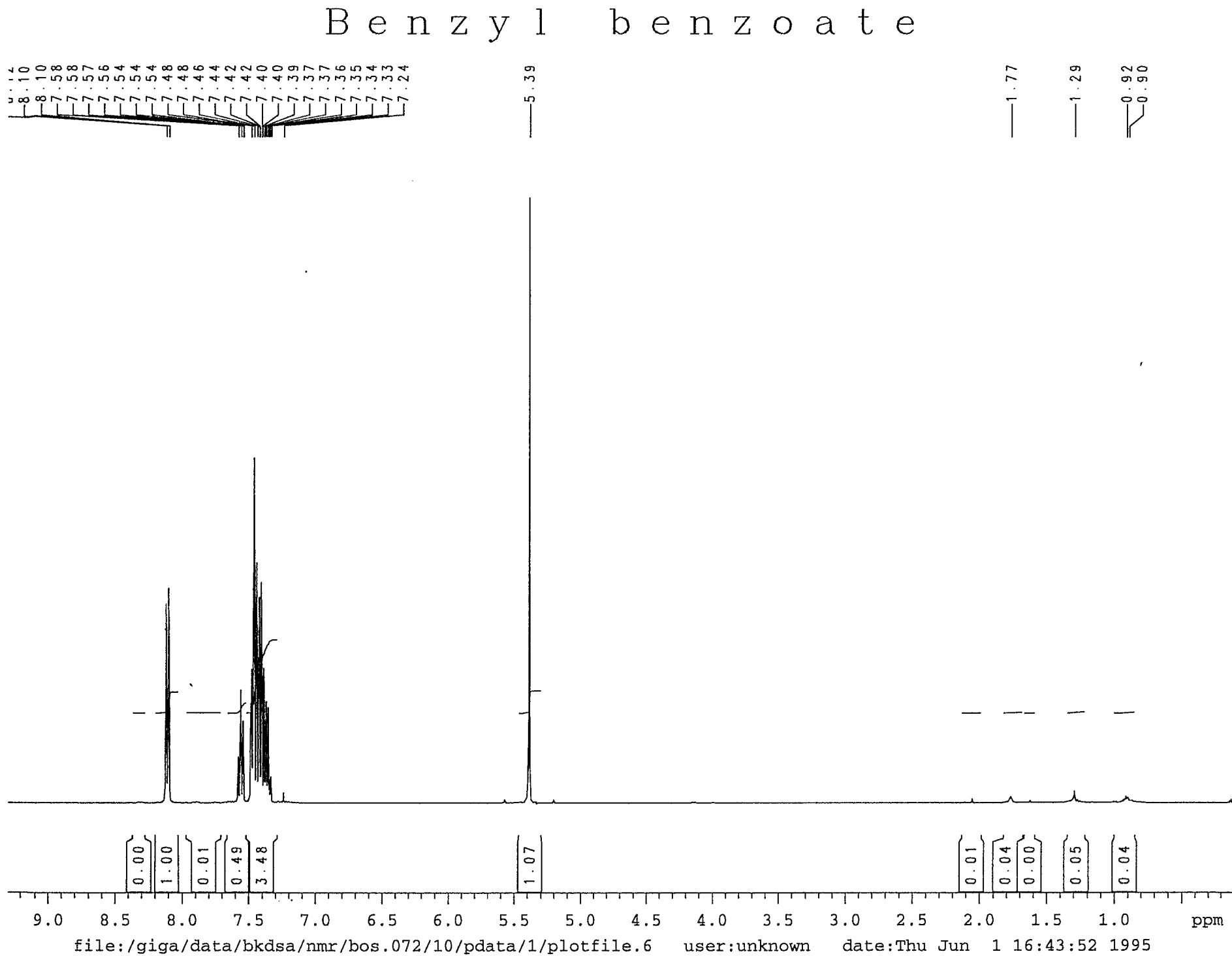


572966-8

bornyl benzoate

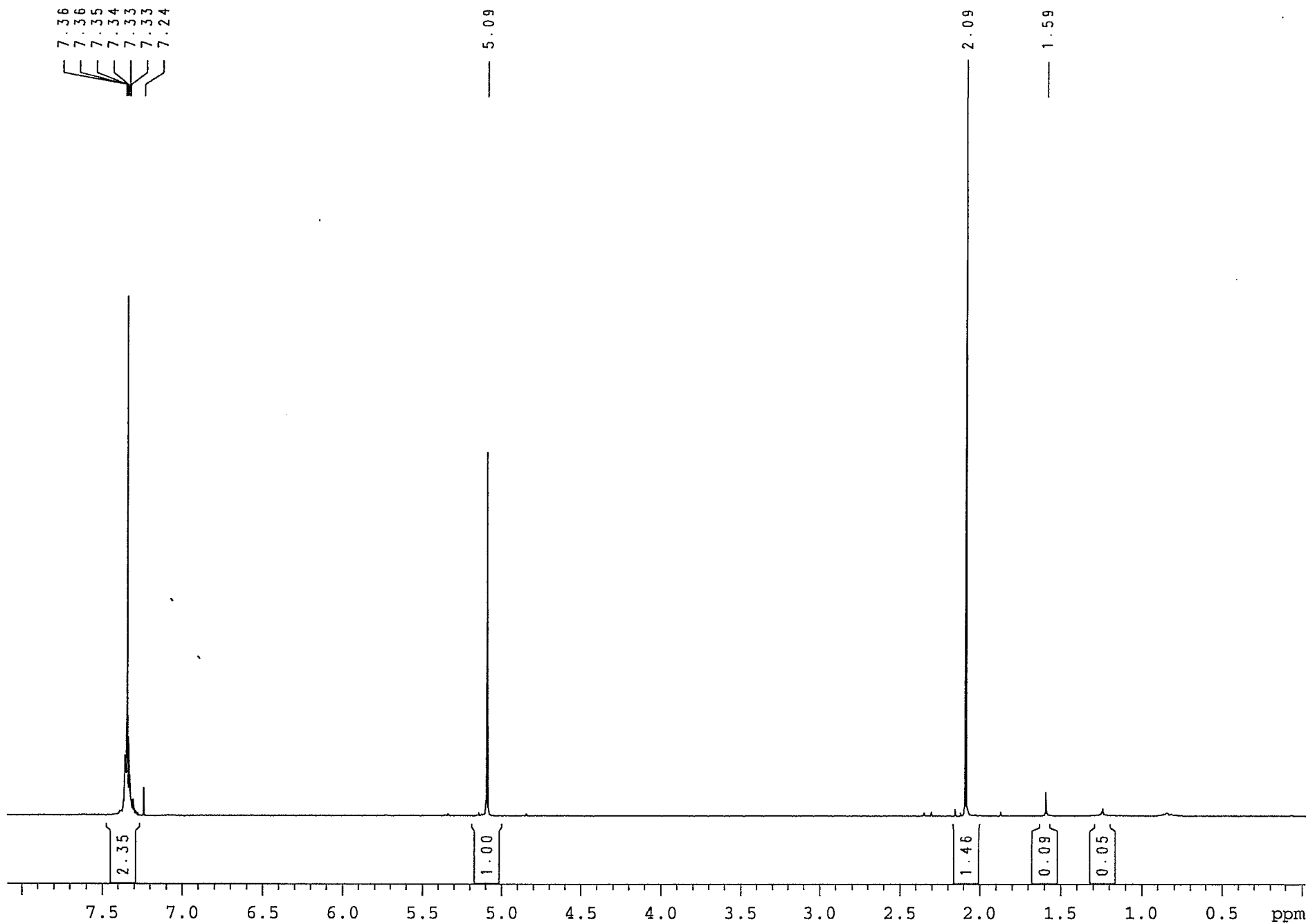


file:/giga/data/bkdsa/nmr/bos.083.fid/1/pdata/1/plotfile.21 user:unknown date:Fri Jun 2 14:58:45 1995



572966-9

benzyl acetate



file:/giga/data/bkdsa/nmr/bos.010/1/pdata/1/plotfile.13 user:unknown date:Thu Jun 1 18:20:06 1995

672946-10