

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>

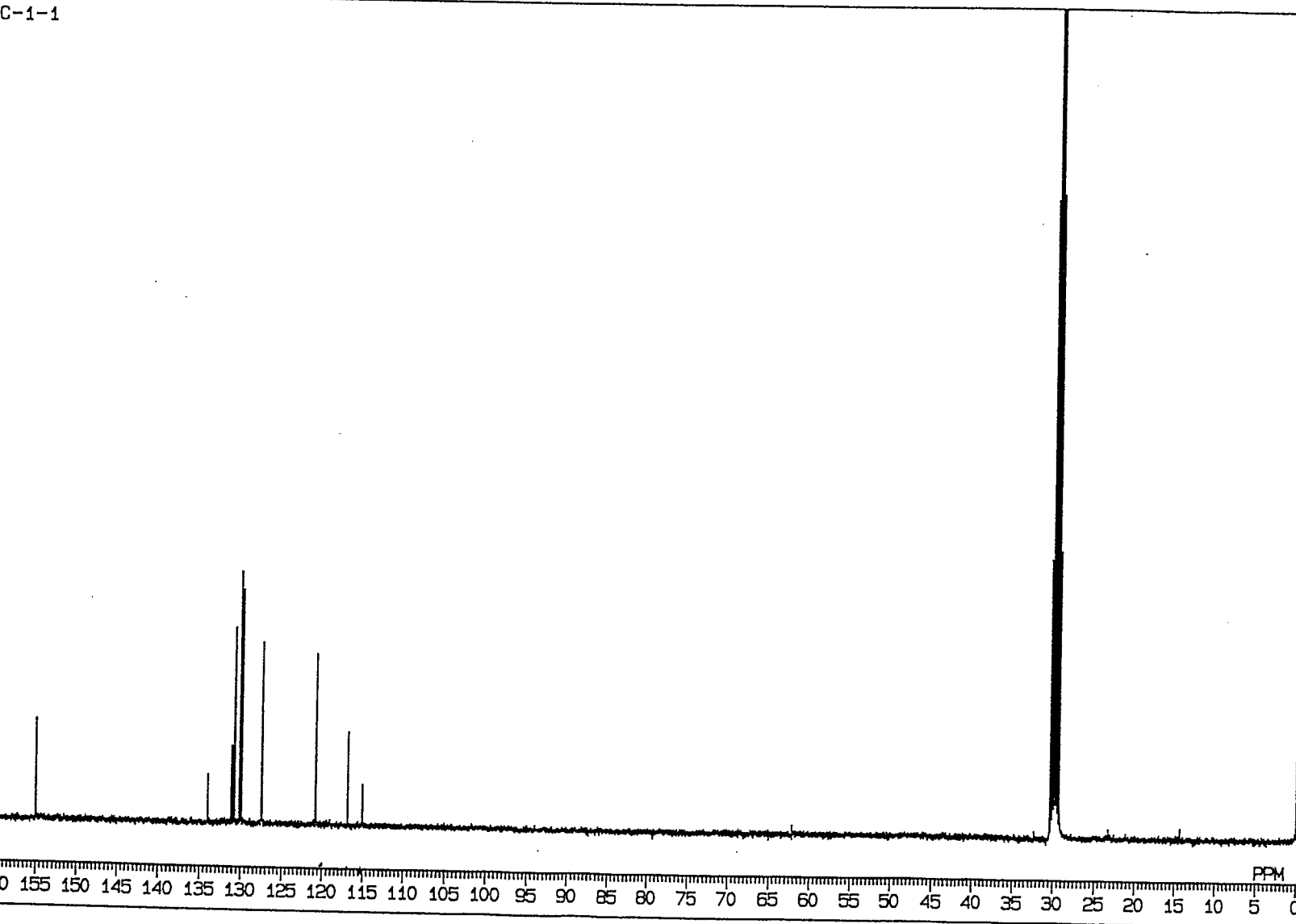


ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1997 American Chemical Society

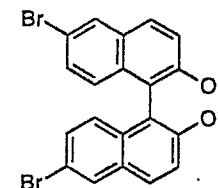
C-1-1



19-JAN-94 13:31:22

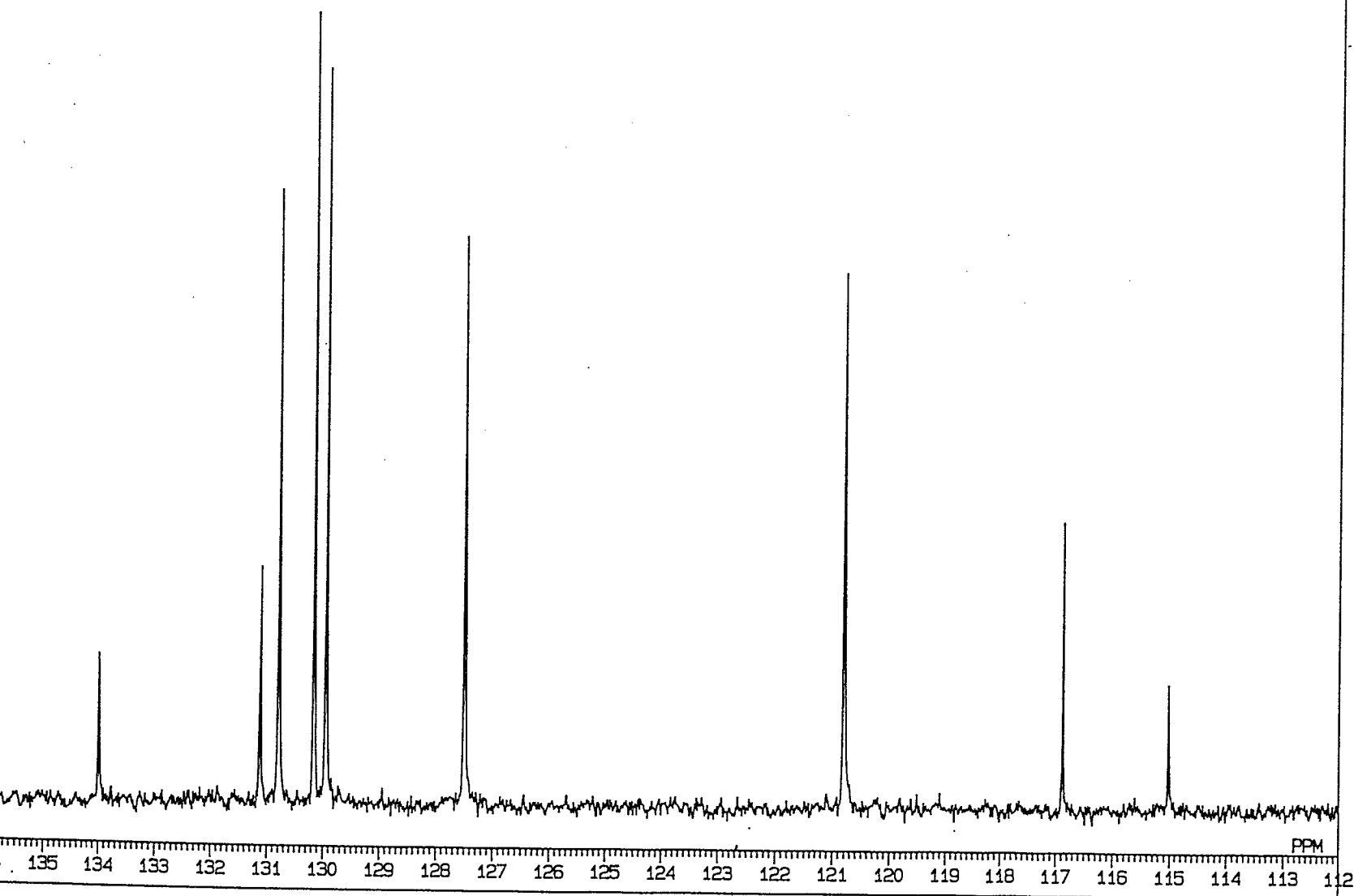
DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100, 100] 13C11
COMNT 13C-1-1
EXMOD SGBCM
QBNUC 13C
OBFIN 10244.0 Hz
POINT 32768
FREQU 25000.0 Hz
SCANS 4000
ACQTM 0.655 sec
PD 1.345 sec
PW1 4.4 us
IRFIN 10300.0 Hz
IRATN 15
IRRPW 50 us
TEMP. 27.0 c
SLVNT ACETN
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 27
XE 16636.9500 Hz
XS 1590.4900 Hz



4 b

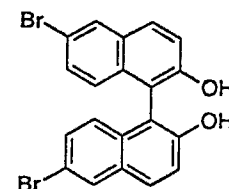
13C-1-1



19-JAN-94 13:35:00

DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100, 100] 13C11
COMNT 13C-1-1
EXMOD SGBCM
OBNUC 13C
OBFIN 10244.0 Hz
POINT 32768
FREQU 25000.0 Hz
SCANS 4000
ACQTM 0.655 sec
PD 1.345 sec
PW1 4.4 us
IRFIN 10300.0 Hz
IRATN 15
IRRPW 50 us
TEMP. 27.0 c
SLVNT ACETN
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 27
XE 2412.6100 Hz
XS -2506.4450 Hz



4b

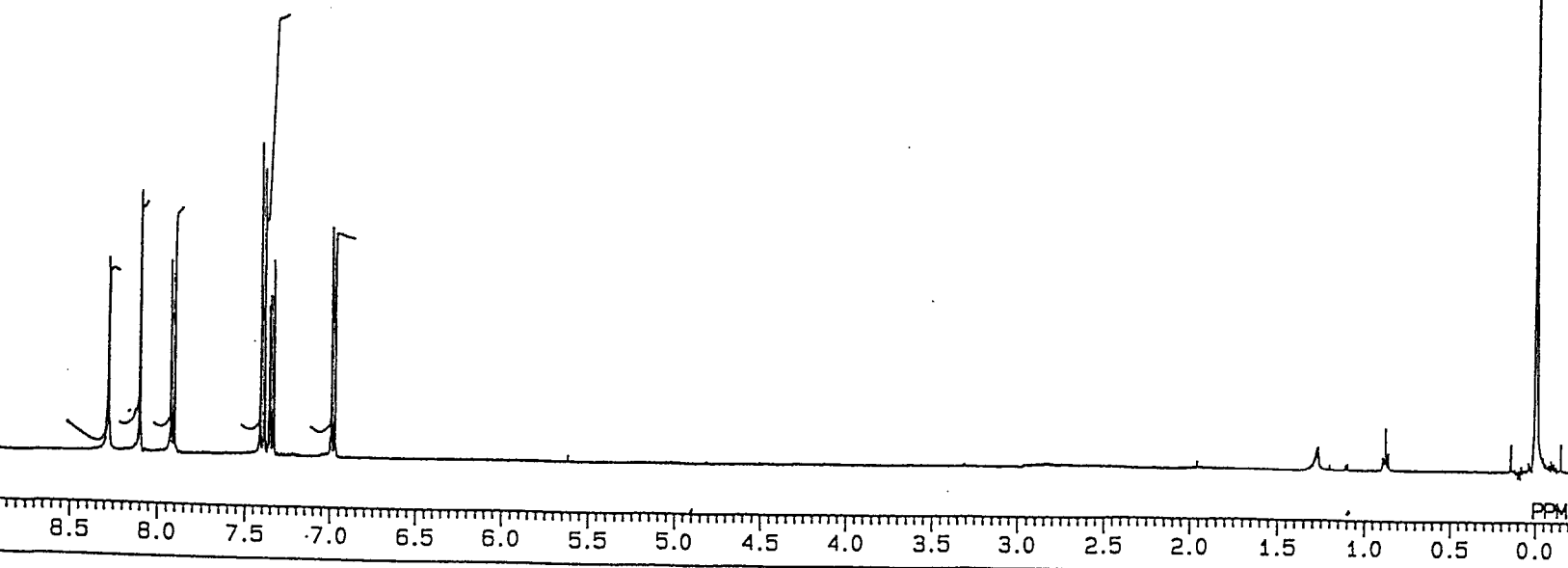
1H-1-1

4.042
1.177
1.148

2.163
1.000

↓
↓
↓

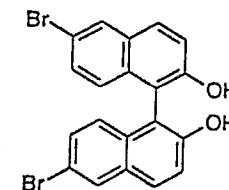
↓
↓



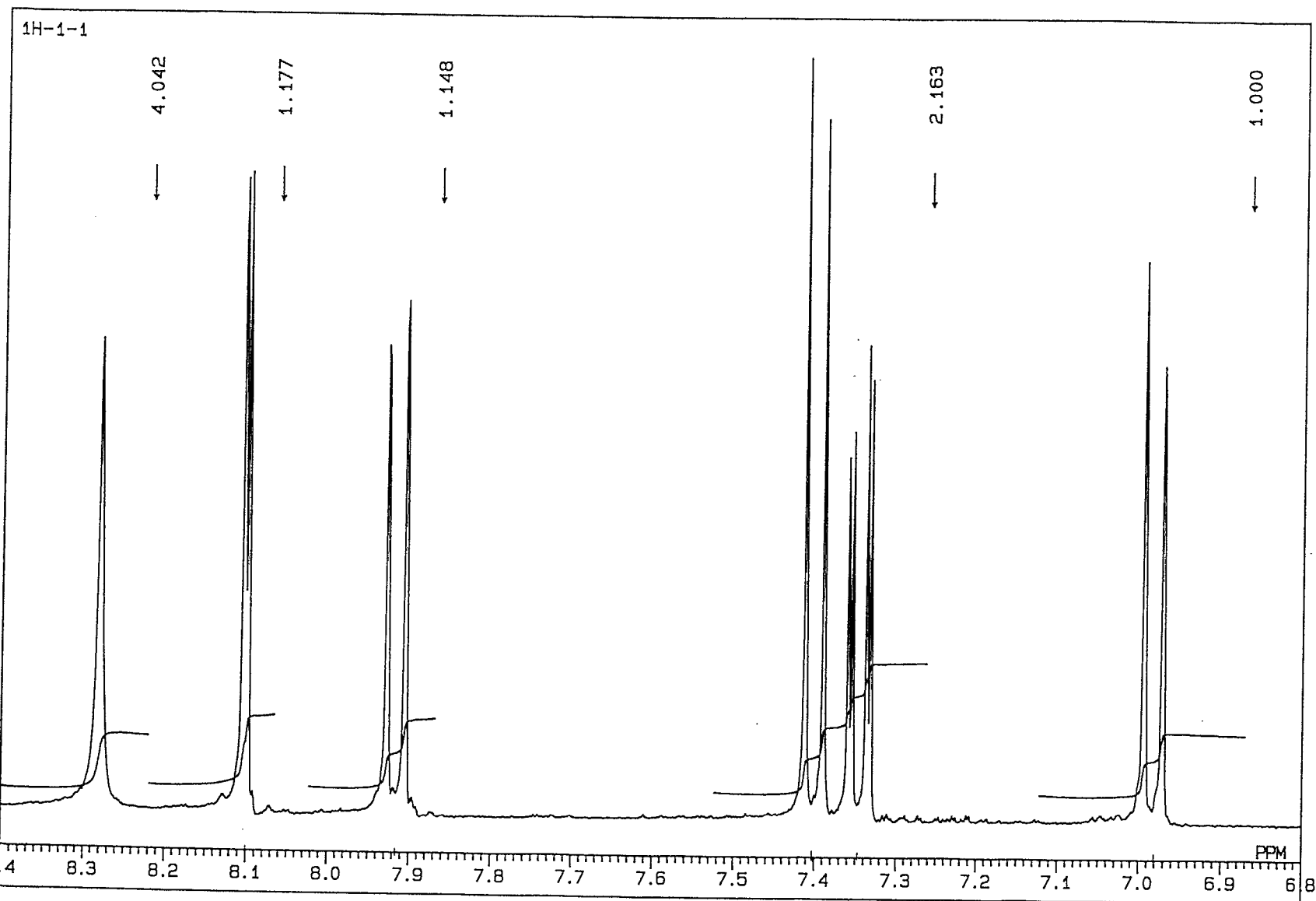
19-JAN-94 13:54:45

DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100, 100] 1H11
COMNT 1H-1-1
EXMOD SGNON
OBNUC 1H
OBFIN 11323.4 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 2.048 sec
PD 10.000 sec
PW1 6.4 us
IRFIN 10300.0 Hz
IRATN 0
IRRPW 30 us
TEMP. 27.0 c
SLVNT ACETN
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 17
XE 3717.9810 Hz
XS 741.9015 Hz



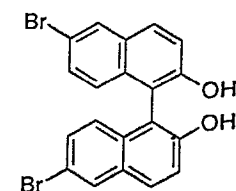
4b



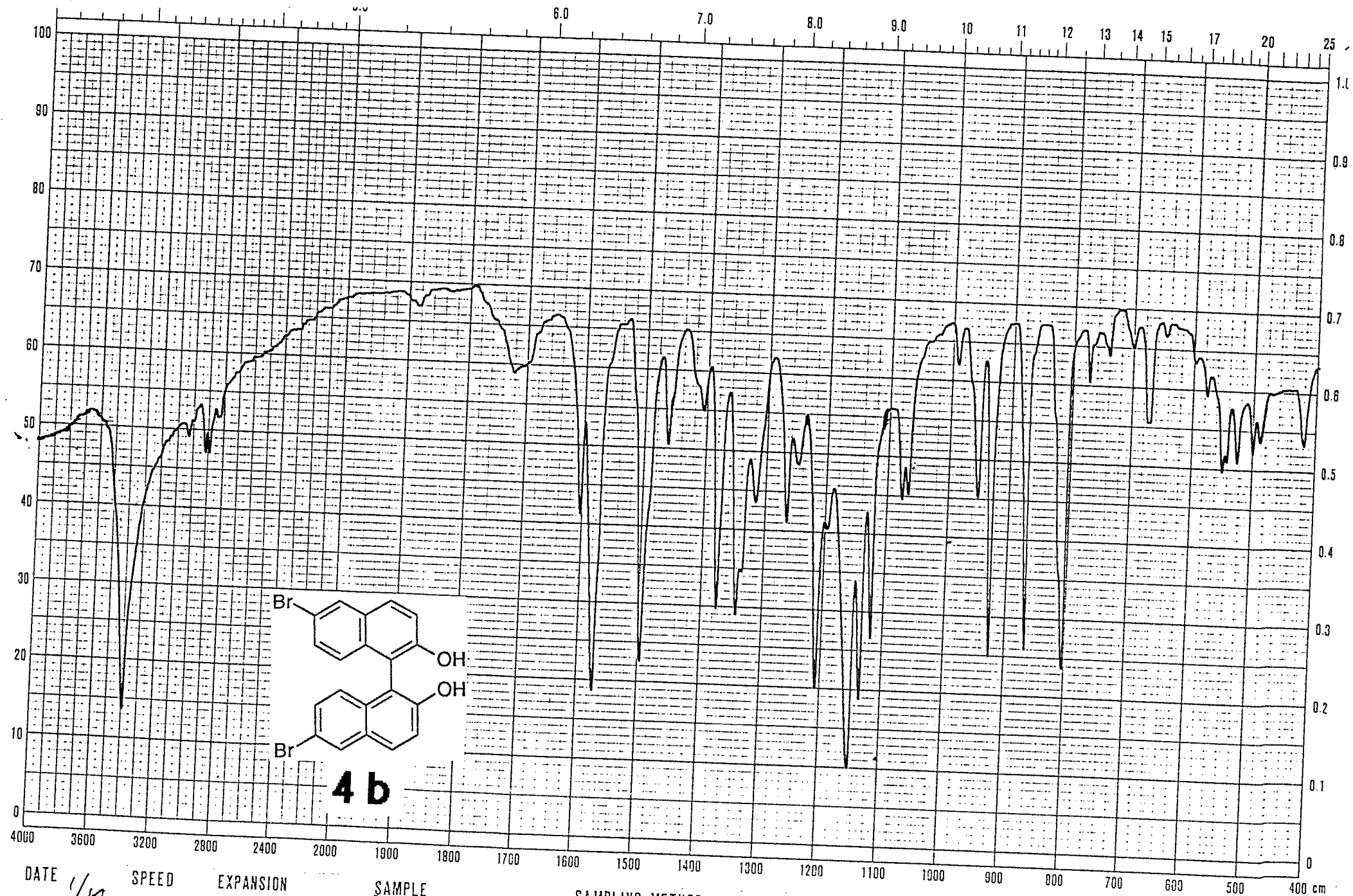
19-JAN-94 13:58:33

DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

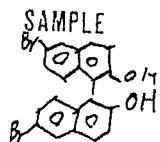
DFILE [100,100] 1H11
COMNT 1H-1-1
EXMOD SGNON
OBNUC 1H
OBFIN 11323.4 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 2.048 sec
PD 10.000 sec
PW1 6.4 us
IRFIN 10300.0 Hz
IRATN 0
IRRPW 30 us
TEMP. 27.0 c
SLVNT ACETN
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 17
XE 639.6523 Hz
XS -557.3926 Hz



4 b



DATE *1/14* SPEED
 OPERATOR GAIN EXPANSION
 T%
 ABS
 ν



SAMPLING-METHOD
KBr
 CELL-LENGTH

CONCENTRATION
 SOLVENT

REMARKS

Jasco

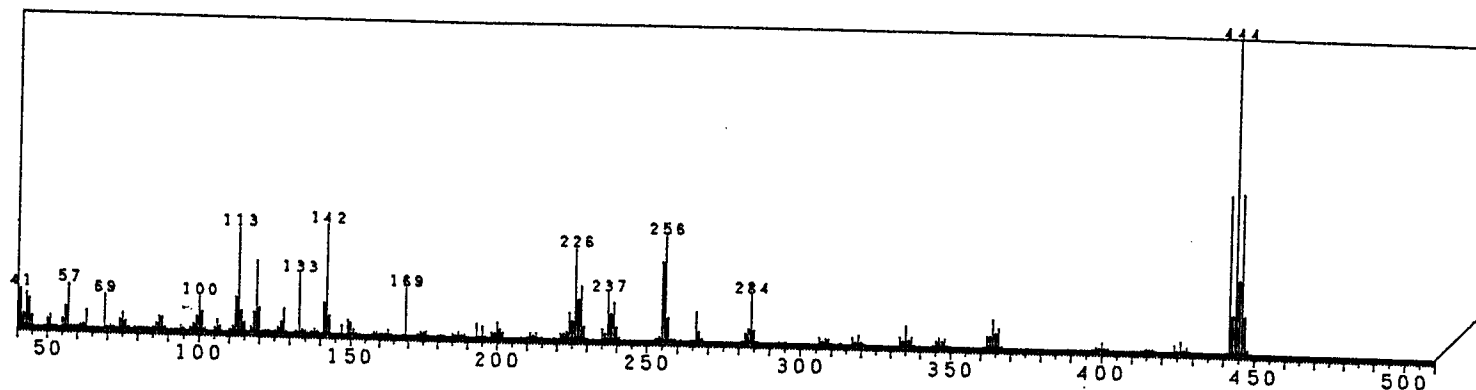
JAPAN SPECTROSCOPIC CO., LTD.

東京科学工業株式会社

xxxxx Mass Spectrum Data Bargraph xxxxx

Sample No. : 205
 Sample Name : Sakamoto 1-1 (EIMS)
 Data Type : Process-1
 Date : 13-JAN-94 18:03
 Comment :

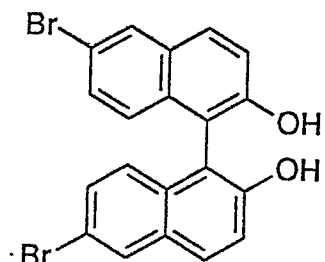
Scan No. : -5
 Total : 2360119
 Average Data No.: 9-13
 R.Time : 3.7
 Base/Total : 0.093
 Base Peak : 219500. (444.0).



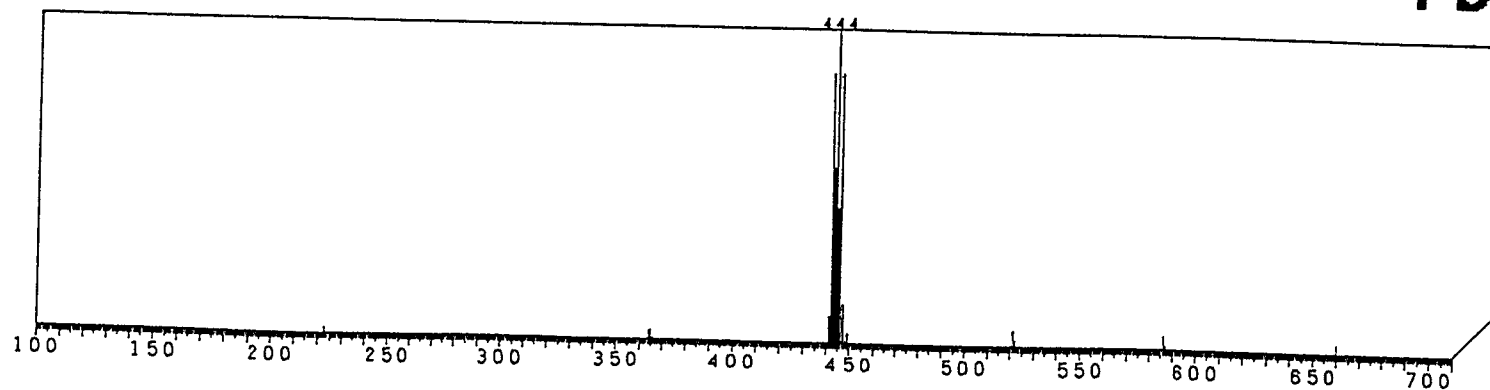
xxxxx Mass Spectrum Data Bargraph xxxxx

Sample No. : 222
 Sample Name : Sakamoto 1-1 FDMS
 Data Type : Process-1
 Date : 17-JAN-94 18:04
 Comment :

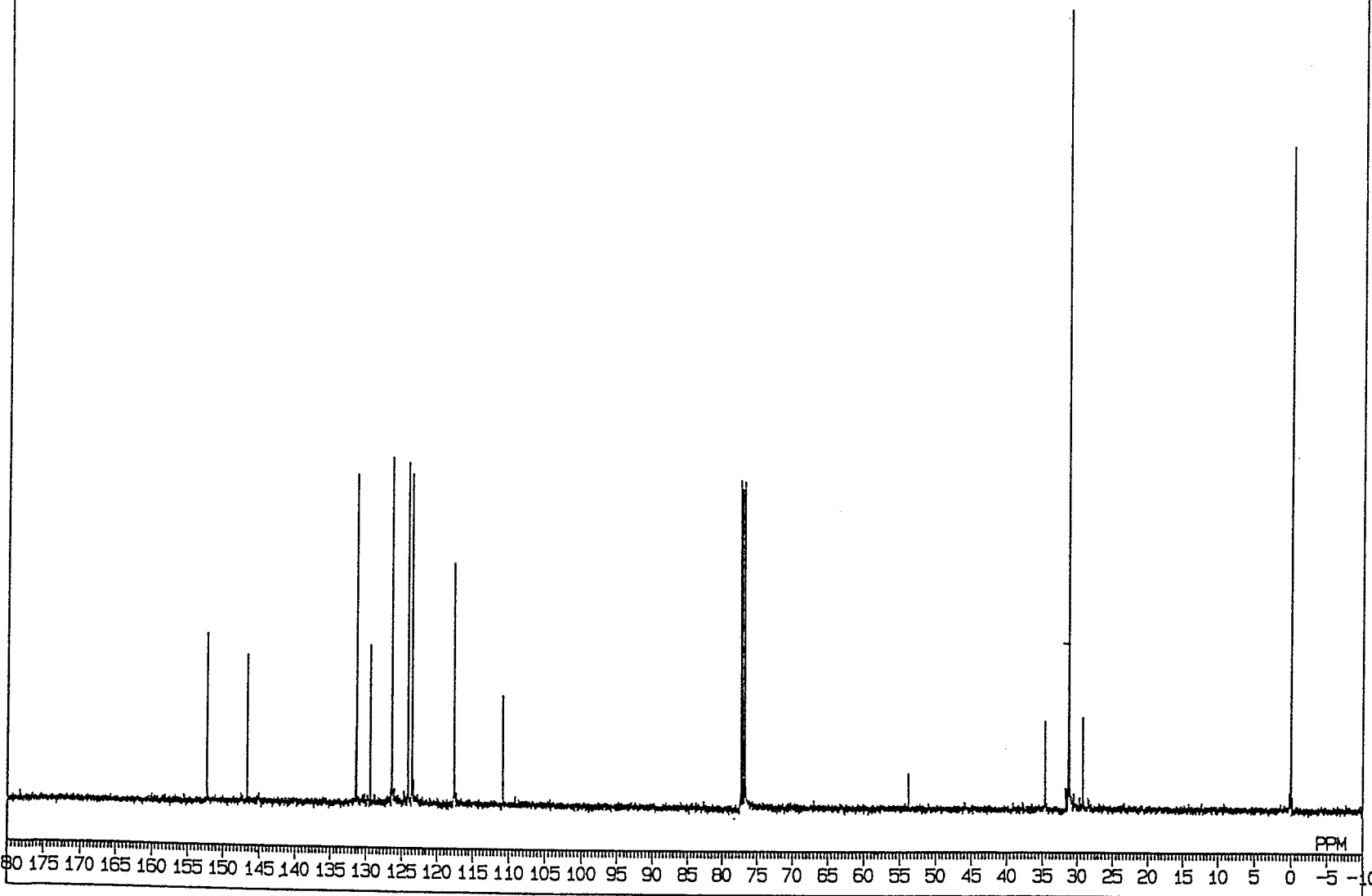
Scan No. : -11
 Total : 99526
 Average Data No.: 10-20
 R.Time : 1.4
 Base/Total : 0.236
 Base Peak : 23460. (444.0)



4 b



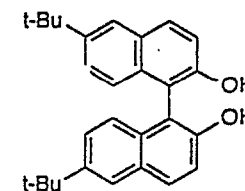
13C-No.600



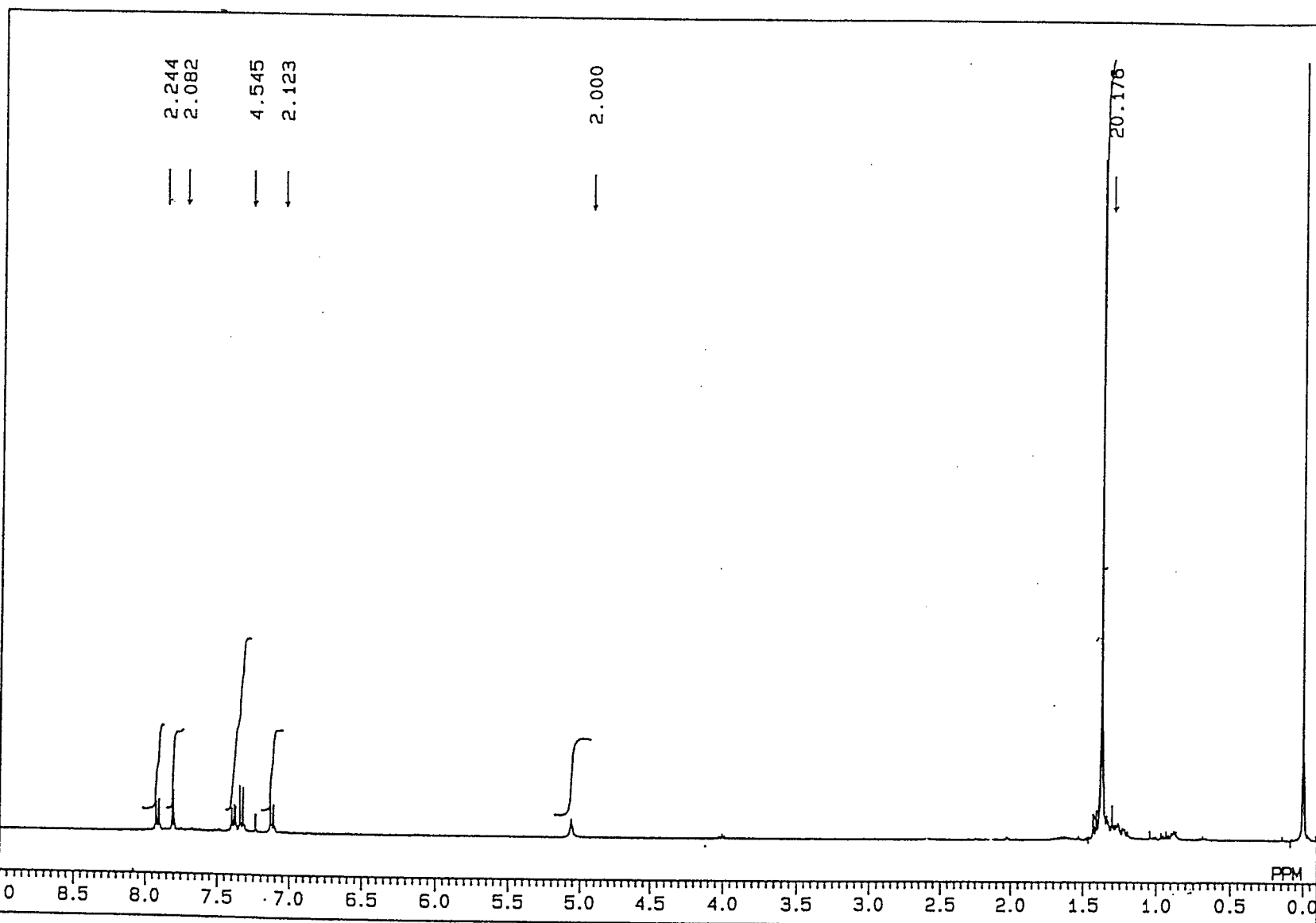
28-SEP-94 09:43:02

DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100, 100] 13C600
CQNT 13C-No.600
EXMOD S6BCM
OBNUC 13C
OBFIN 10244.0 Hz
POINT 32768
FREQU 25000.0 Hz
SCANS 1600
ACQTM 0.655 sec
PD 1.345 sec
PW1 4.4 us
IRFIN 10300.0 Hz
IRATN 15
IRRPW 50 us
TEMP. 27.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 28
XE 19099.8300 Hz
XS 1309.4680 Hz



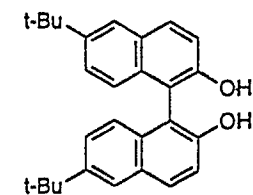
4 c



28-SEP-94 09:32:27

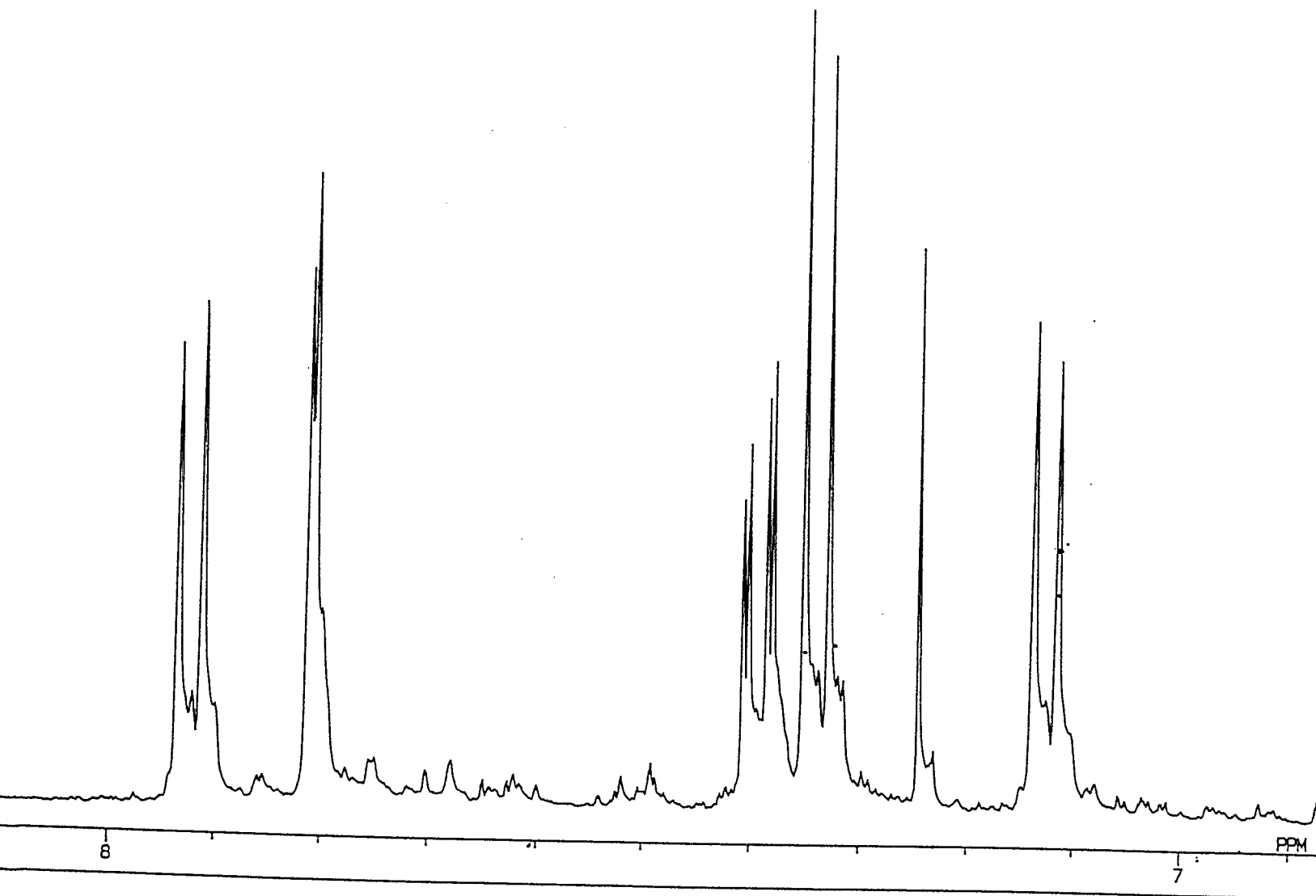
 DAINIPPON INK
 AND CHEMICALS, INC.
 CENTRAL RES. LAB.

 DFILE [100, 100] 1H600
 COMNT 1H-No.600
 EXMOD SGNON
 OBNUC 1H
 OBFIN 11323.4 Hz
 POINT 32768
 FREQU 8000.0 Hz
 SCANS 16
 ACQTM 2.048 sec
 PD 10.000 sec
 PW1 6.4 us
 IRFIN 10300.0 Hz
 IRATN 0
 IRRPW 30 us
 TEMP. 27.0 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 14
 XE 4037.8030 Hz
 XS 831.1350 Hz



4 c

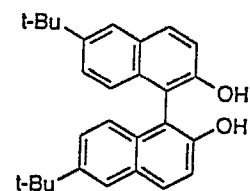
1H-No.600



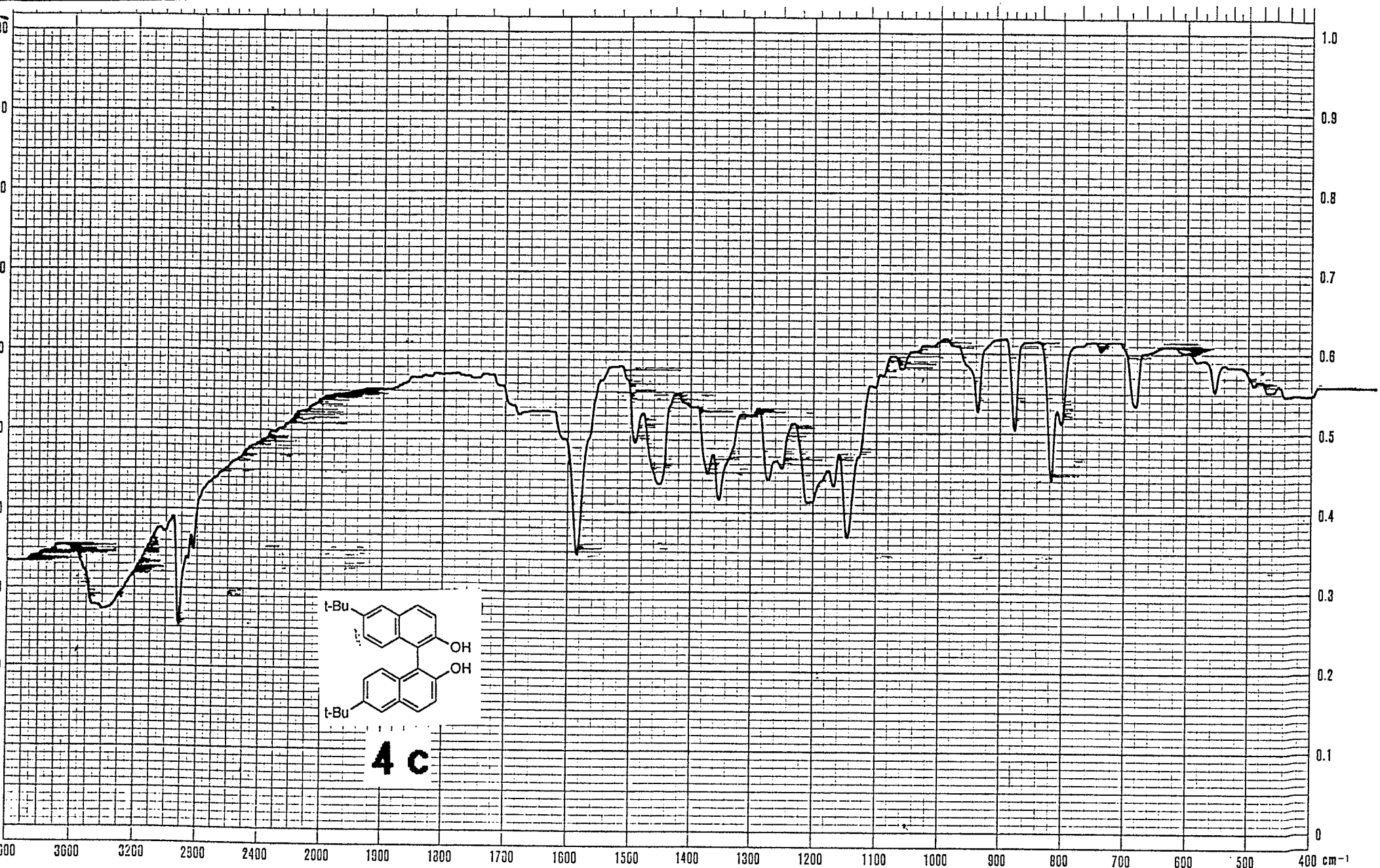
28-SEP-94 09:34:56

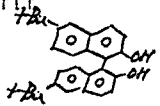
DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100, 100] 1H600
COMNT 1H-No.600
EXMOD SGNON
OBNUC 1H
OBFIN 11323.4 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 2.048 sec
PD 10.000 sec
PW1 6.4 us
IRFIN 10300.0 Hz
IRATN 0
IRRPW 30 us
TEMP. 27.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 14
XE 500.0000 Hz
XS -185.0543 Hz



4 c



DATE	SPEED	EXPANSION	SAMPLE	SAMPLING-METHOD	CONCENTRATION	REMARKS
98 th 9-16		T%		KBr		
OPERATOR	GAIN	ABS	CELL-LENGTH	SOLVENT		
T. Sakamoto		ν				

JASCO

JAPAN SPECTROSCOPIC CO., LTD.

日本分光工業株式会社

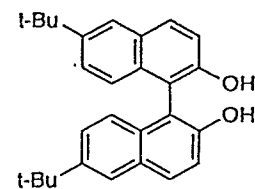
J-0033

***** Output of Mass Chromatogram *****

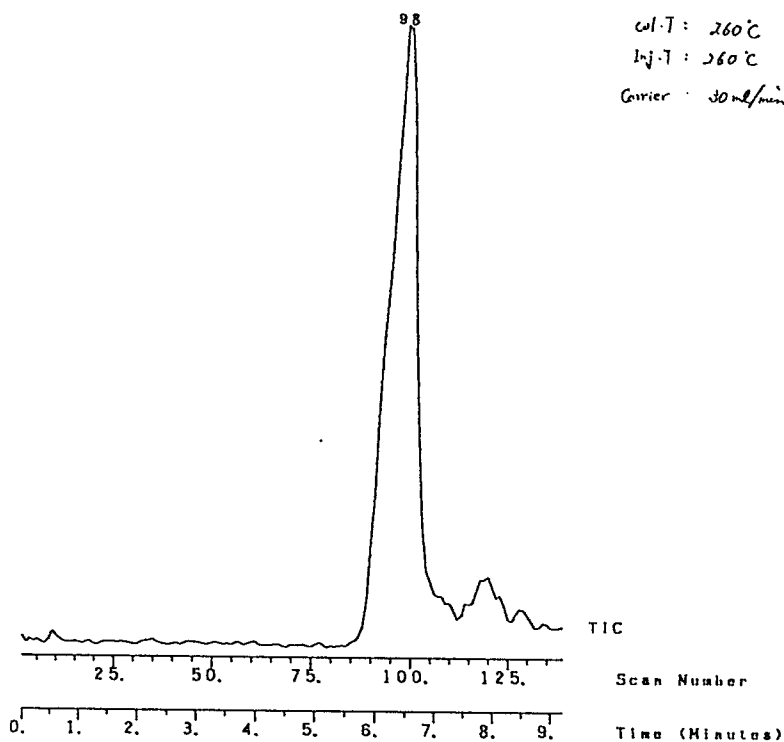
Sample No. : 222
 Sample Name : Sakamoto No.595 GC-EI-MS Col.T:260
 Data Type : Measure
 Date : 19-SEP-94 17:32
 Comment :

TIC = 649430.

GC条件
 Col : 2% Silicone OV-17(11)
 Col-T : 260°C
 Inj-T : 260°C
 Carrier : 30 ml/min



4c



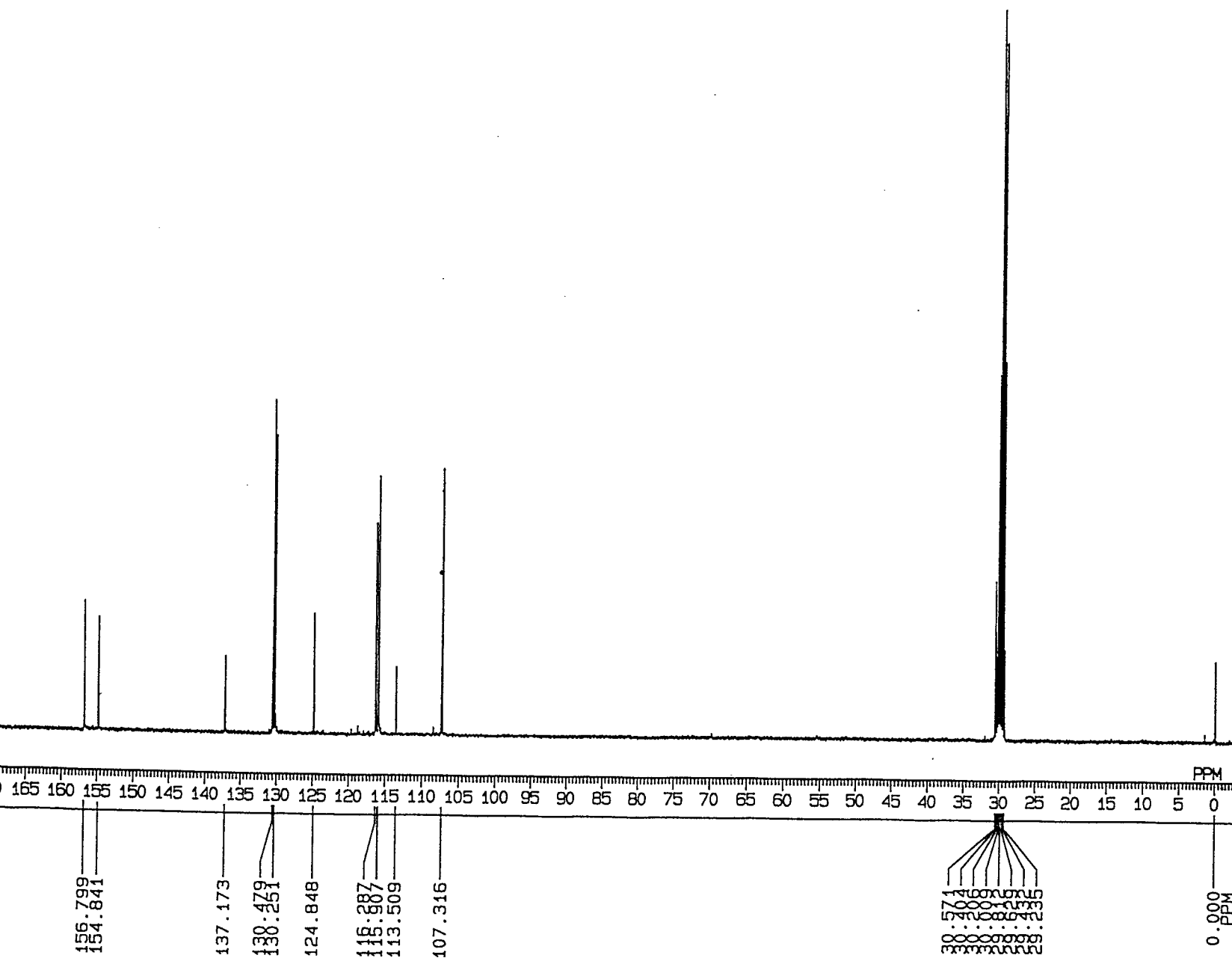
***** Mass Spectrum Data Diagram *****

Sample No. : 222
 Sample Name : Sakamoto No.595 GC-EI-MS Col.T:260
 Data Type : Process-1
 Date : 19-SEP-94 17:49
 Comment :

Scan No. : -13 R.Time : 6.3 Base Peak : 34840. (383.0)
 Total : 377416 Base/Total : 0.092
 Average Data No.: 90-102



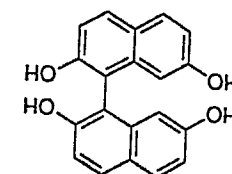
13C-11-2



31-JAN-94 09: 45: 49

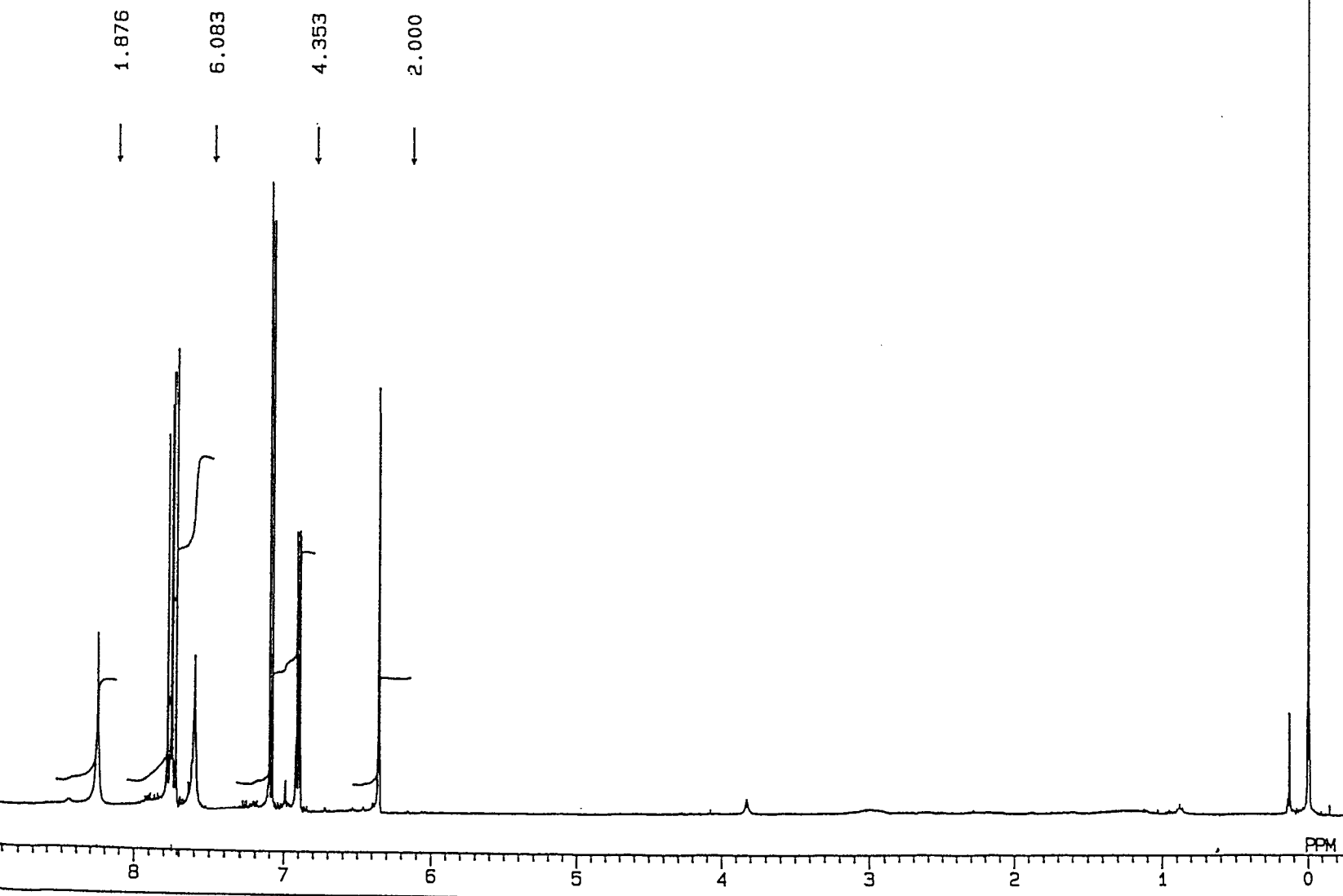
DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100, 100] 13C112
COMNT 13C-11-2
EXMOD SGBCM
OBNUC 13C
OBFIN 10244.0 Hz
POINT 32768
FREQU 25000.0 Hz
SCANS 3200
ACQTM 0.655 sec
PD 1.345 sec
PW1 4.4 us
IRFIN 10300.0 Hz
IRATN 15
IRRPW 50 us
TEMP 27.0 c
SLVNT ACETN
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 27
XE 17390.8900 Hz
XS 1461.7820 Hz



4 d

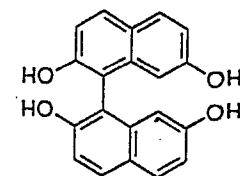
1H-11-2



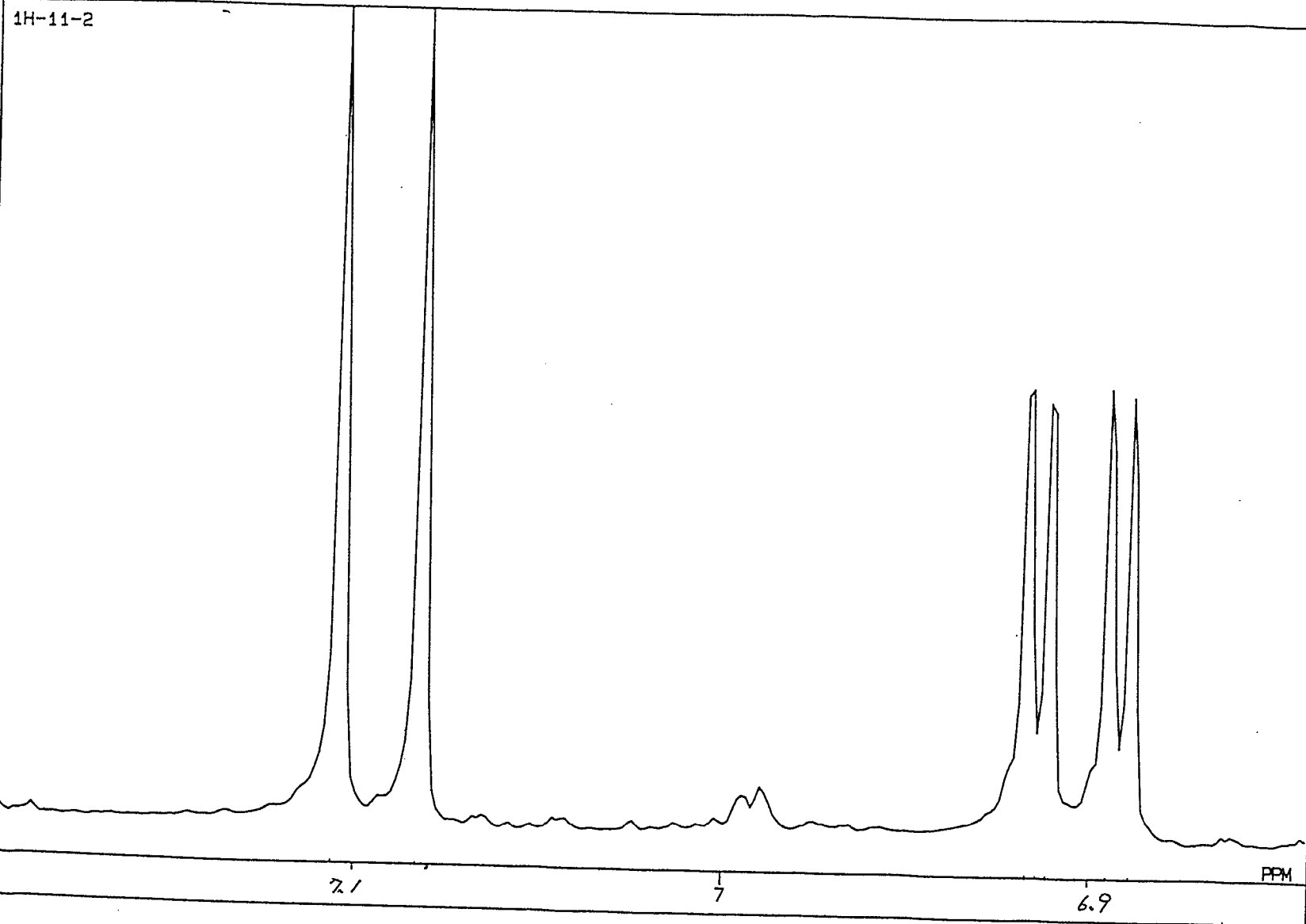
31-JAN-94 09:32:26

DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100, 100] 1H112
COMNT 1H-11-2
EXMOD SGNON
OBNUC 1H
OBFIN 11323.4 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 2.048 sec
PD 10.000 sec
PW1 6.4 us
IRFIN 10300.0 Hz
IRATN 0
IRRPW 30 us
TEMP. 27.0 c
SLVNT ACETN
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 14
XE 3717.9810 Hz
XS 736.5304 Hz



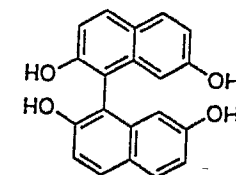
4d



31-JAN-94 09:36:59

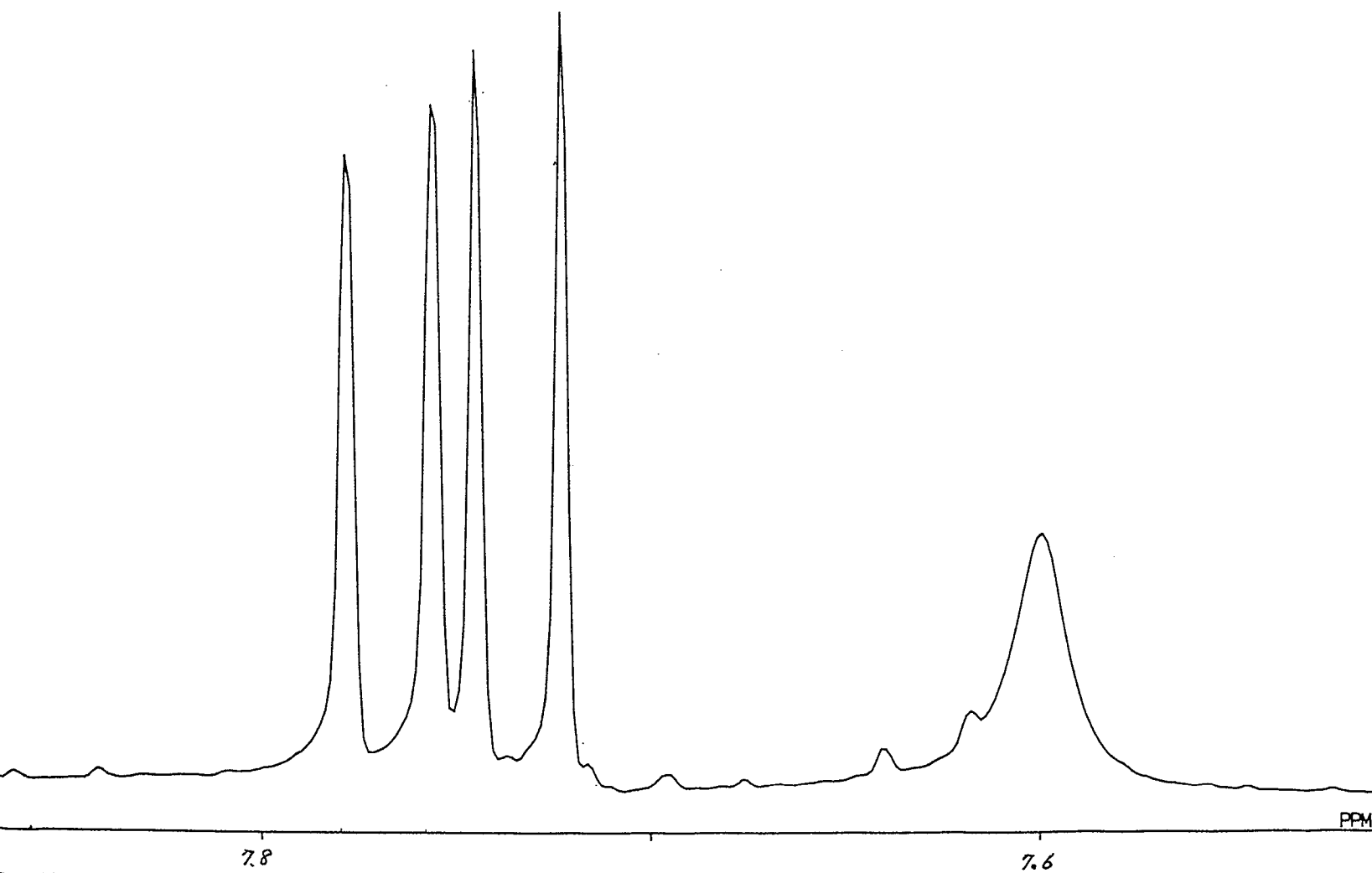
DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100,100] 1H112
COMNT 1H-11-2
EXMOD SGNON
OBNUC 1H
OBFIN 11323.4 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 2.048 sec
PD 10.000 sec
PW1 6.4 us
IRFIN 10300.0 Hz
IRATN 0
IRRPW 30 us
TEMP. 27.0 c
SLVNT ACETN
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 14
XE 143.9216 Hz
XS -330.8898 Hz



4 d

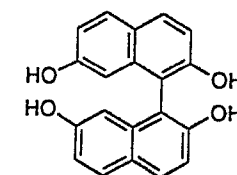
1H-11-2



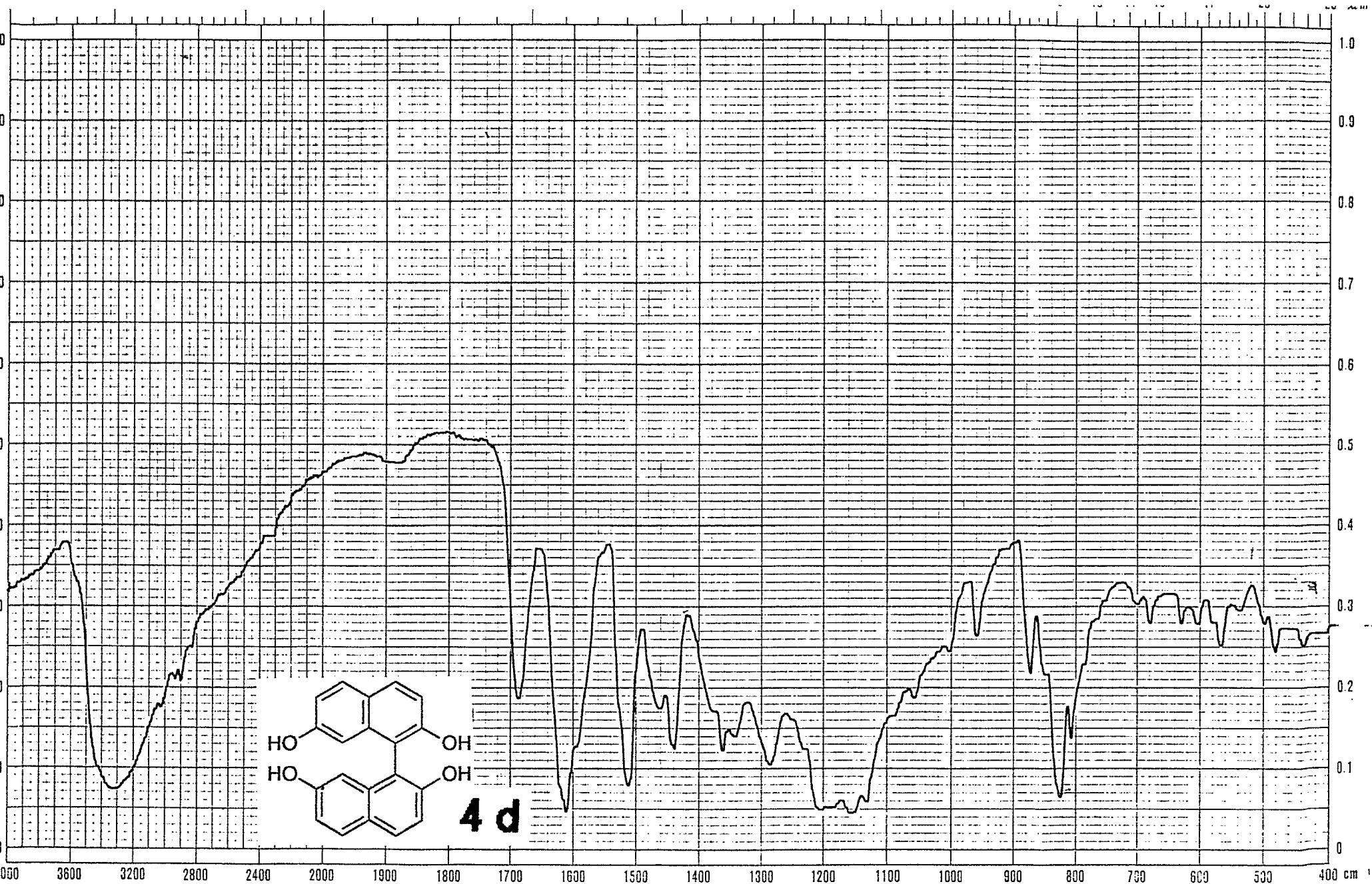
31-JAN-94 09:34:50

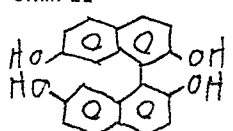
DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100, 100] 1H112
COMNT 1H-11-2
EXMOD SGNON
OBNUC 1H
OBFIN 11323.4 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 2.048 sec
PD 10.000 sec
PW1 6.4 us
IRFIN 10300.0 Hz
IRATN 0
IRRPW 30 us
TEMP. 27.0 c
SLVNT ACETN
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 14
XE 143.9216 Hz
XS -598.7443 Hz



4 d



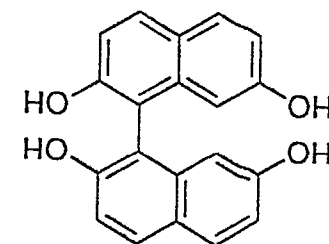
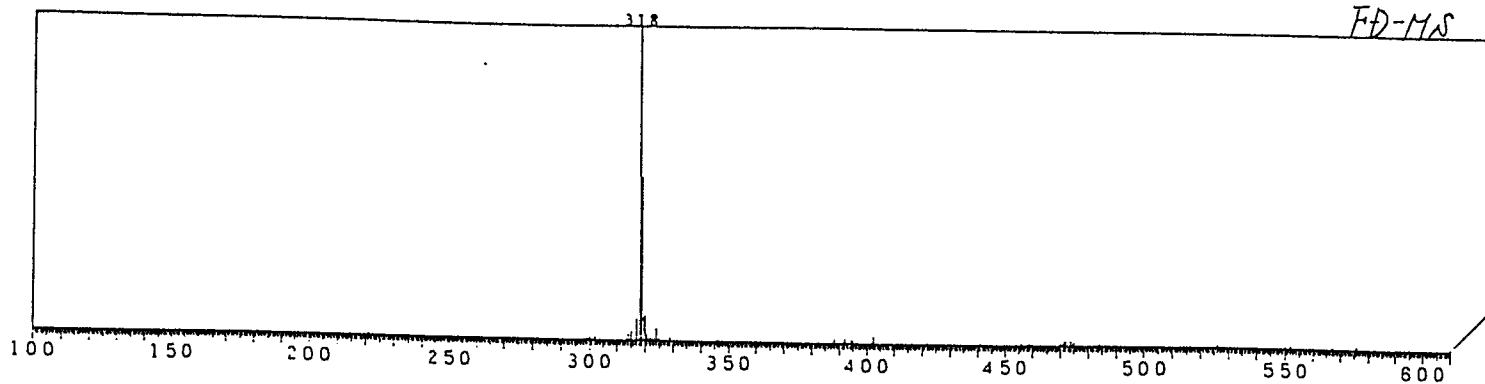
DATE <u>2/2</u>	SPEED	EXPANSION	SAMPLE	SAMPLING-METHOD	CONCENTRATION	REMARKS
OPERATOR <u>APF</u>	GAIN	T% ASS v		<u>KBr</u>		
				CELL-LENGTH	SOLVENT	


 JAPAN SPECTROSCOPIC CO., LTD.
 三本分光工業株式会社
 J-0033

xxxxx Mass Spectrum Data Bargraph xxxxx

Sample No. : 330
 Sample Name : Sakamoto 11-2 FD-MS
 Data Type : Progress-1
 Date : 2-FEB-94 14:13
 Comment :

Scan No. : -39 R.Time : 1.9 Base Peak : 26570. (318.0)
 Total : 72445. Base/Total : 0.367
 Average Data No.: 1-39



4 d

18-APR-94 11:37:51

DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100,100]13C358

COMNT 13C-NMR/No.358

EXMOD SG8CM

OBNUC 13C

OBFIN 10244.0 Hz

POINT 32768

FREQU 25000.0 Hz

SCANS 8000

ACQTM 0.655 sec

PD 1.345 sec

PW1 4.4 us

IRFIN 10300.0 Hz

IRATN 15

IRRPW 50 us

TEMP. 27.0 c

SLVNT CDCL3

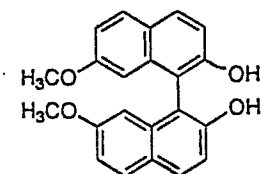
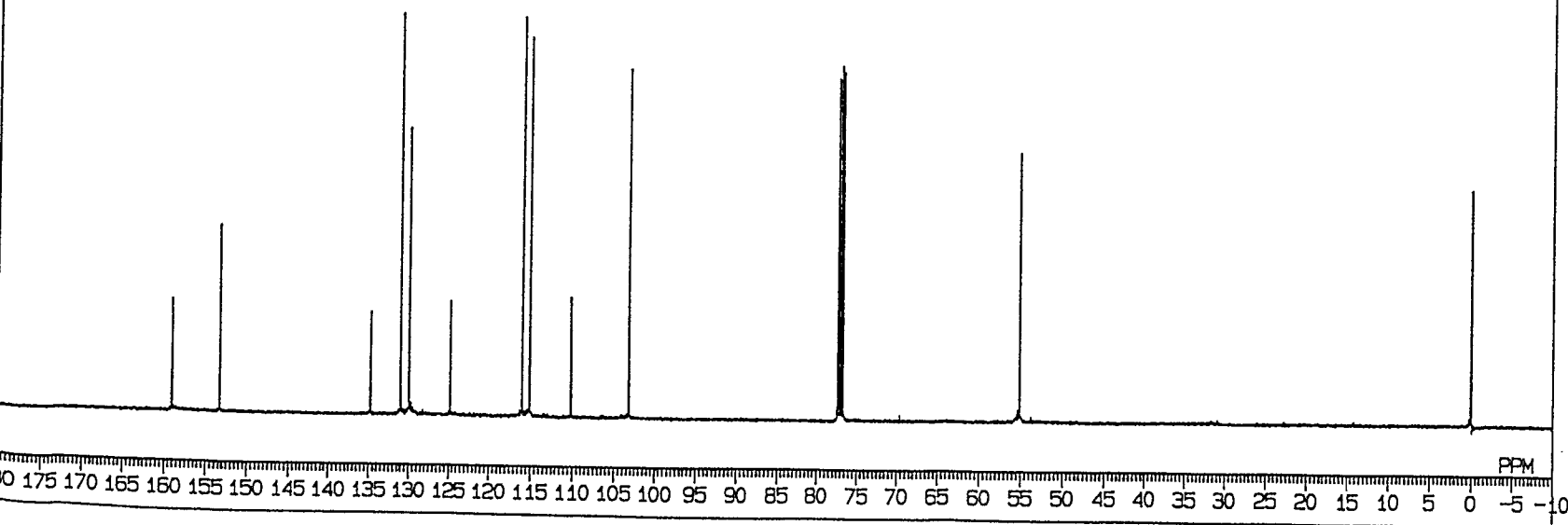
EXREF 0.00 ppm

BF 1.00 Hz

RGAIN 28

XE 19099.8300 Hz

XS 1309.4680 Hz



4 e

18-APR-94 11:26:40

DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100, 100] 1H358

COMNT 1H-NMR/No.358

EXMOD SGNON

OBNUC 1H

OBFIN 11323.4 Hz

POINT 32768

FREQU 8000.0 Hz

SCANS 15

ACQTM 2.048 sec

PD 10.000 sec

PW1 6.4 us

IRFIN 10300.0 Hz

IRATN 0

IRRPW 30 us

TEMP. 27.0 c

SLVNT CDCL3

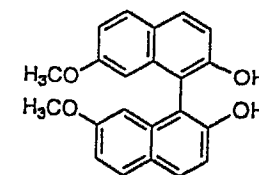
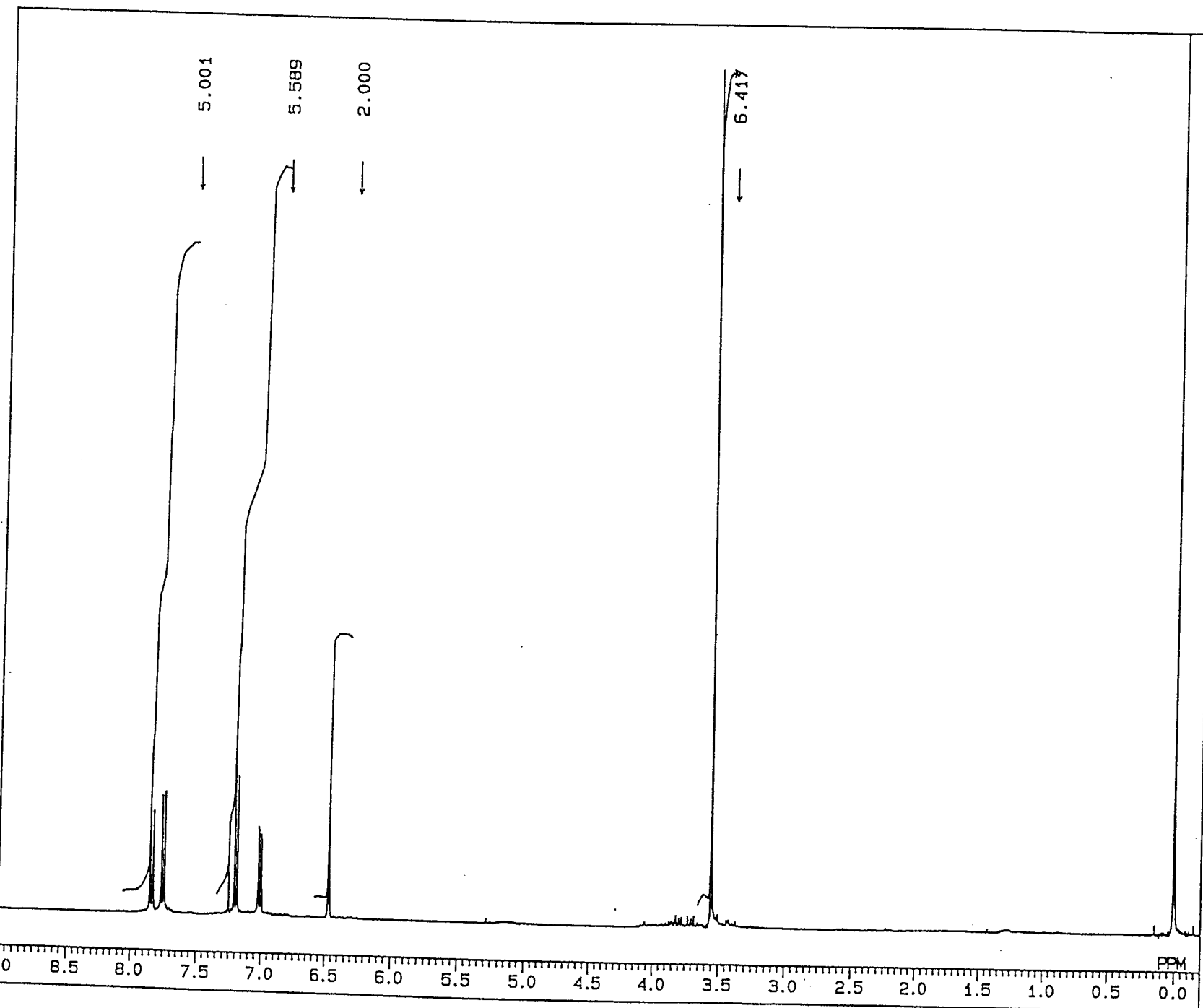
EXREF 0.00 ppm

BF 0.10 Hz

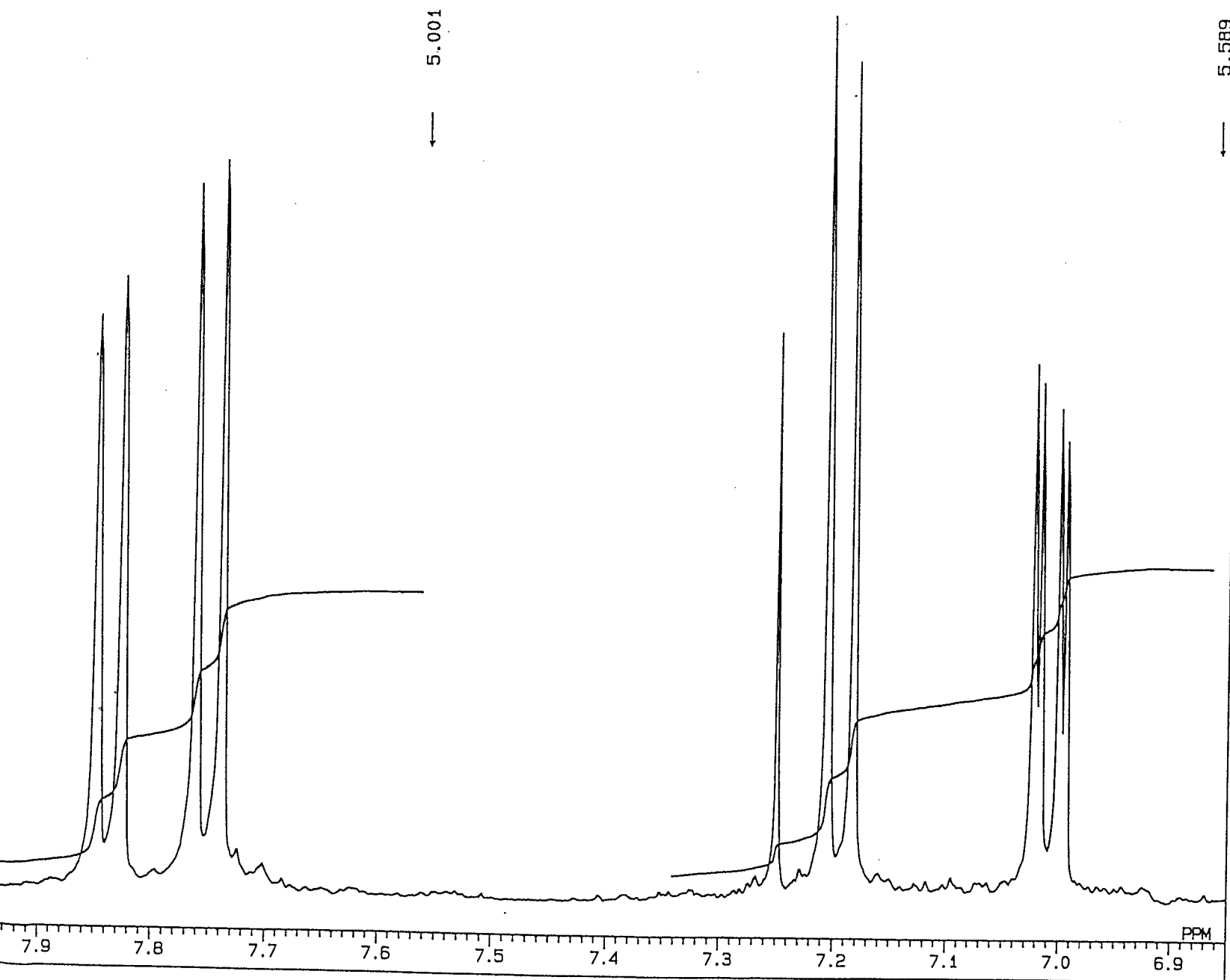
RGAIN 15

XE 3677.9990 Hz

XS 1052.9690 Hz



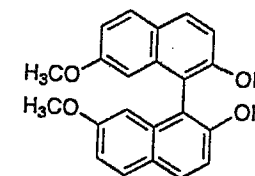
4e



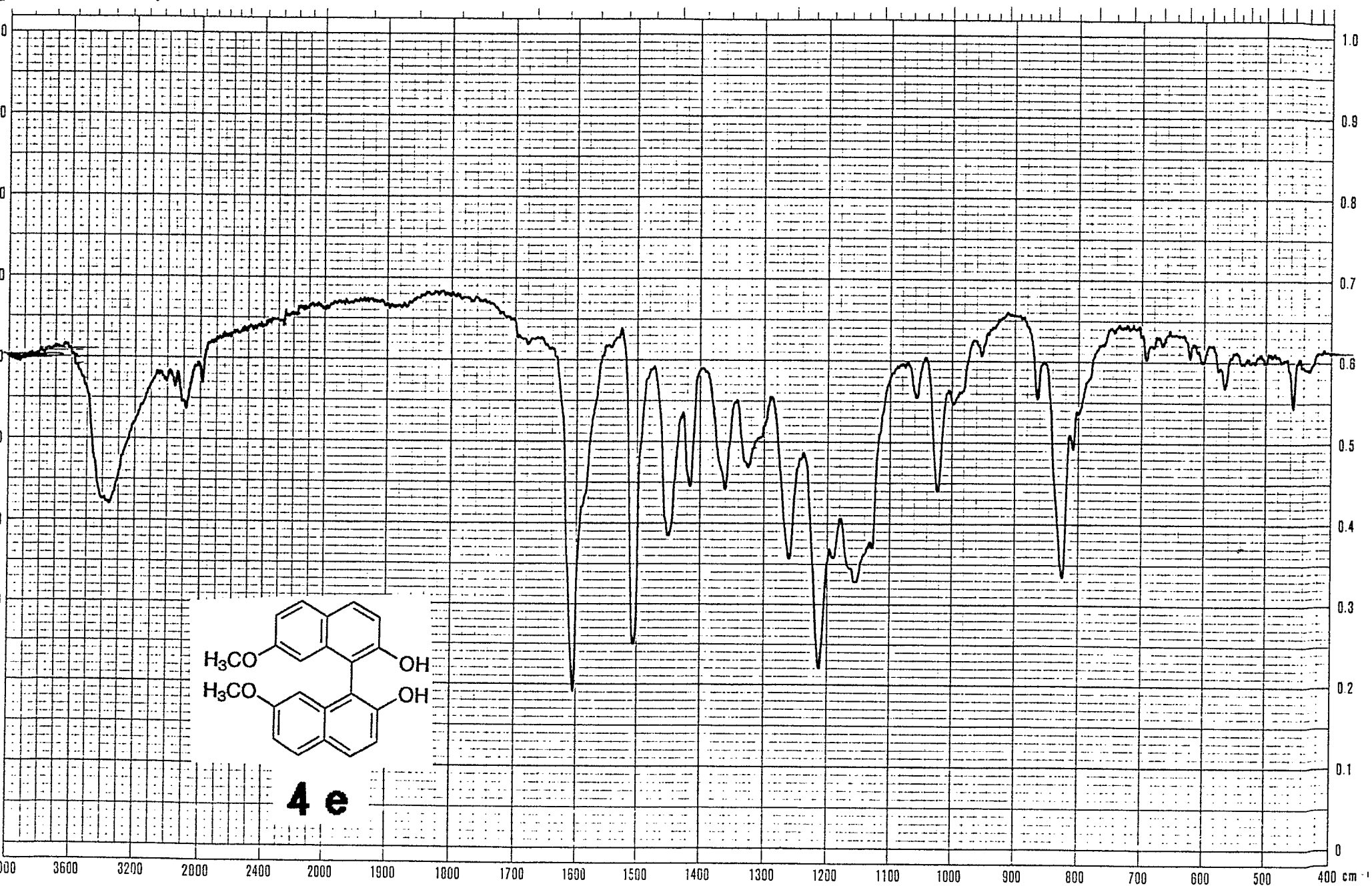
18-APR-94 11:30:09

 DAINIPPON INK
 AND CHEMICALS, INC.
 CENTRAL RES. LAB.

 DFILE [100, 100] 1H358
 COMNT 1H-NMR/No.358
 EXMOD SGNON
 OBNUC 1H
 OBFIN 11323.4 Hz
 POINT 32768
 FREQU 8000.0 Hz
 SCANS 16
 ACQTM 2.048 sec
 PD 10.000 sec
 PW1 6.4 us
 IRFIN 10300.0 Hz
 IRATN 0
 IRRPW 30 us
 TEMP. 27.0 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 15
 XE 439.7612 Hz
 XS -146.3787 Hz



4e

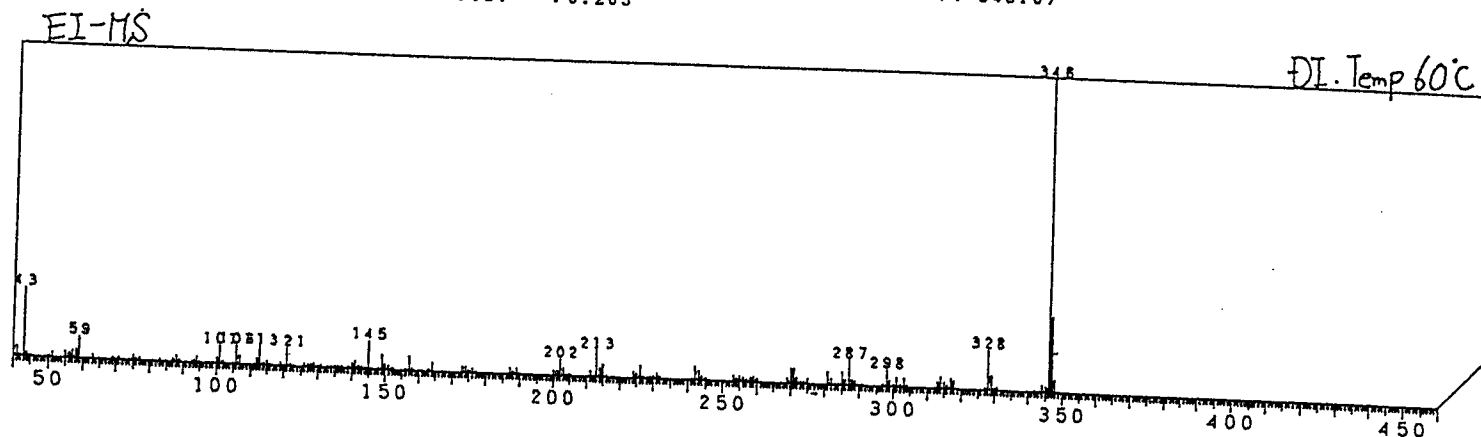


DATE 94-4-12	SPEED GAIN	EXPANSION 1%	SAMPLE CH ₂ Cl ₂	SAMPLING-METHOD KBr	CONCENTRATION	REMARKS	 JAPAN SPECTROSCOPIC CO., LTD. 日本分光工業株式会社 J-0033
OPERATOR T. Sakamoto		ABS ν	 C ₁₃ H ₁₀ O ₄	CELL-LENGTH	SOLVENT		

xxxxx Mass Spectrum Data Bargraph xxxxx

Sample No. : 87
 Sample Name : No.358(Sakamoto) EI-MS
 Data Type : Measure
 Date : 15-APR-94 10:05
 Comment :

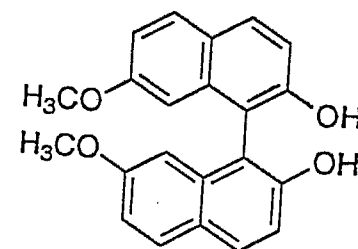
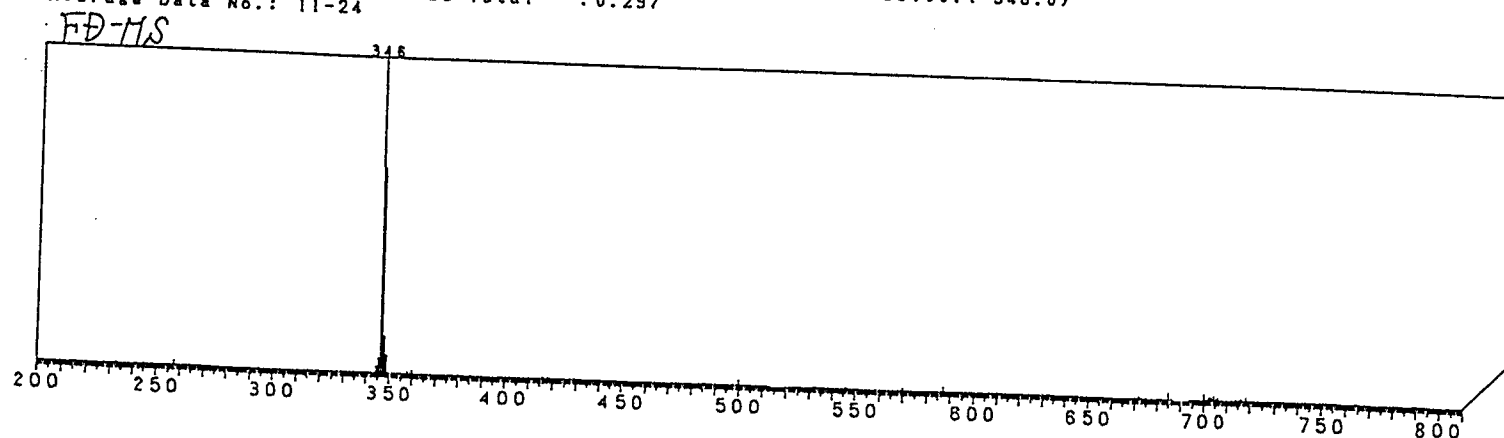
Scan No. : 18
 Total : 2012804. R.Time : 3.8
 Base/Peak : 0.203 Base Peak : 409500.(346.0)



xxxxx Mass Spectrum Data Bargraph xxxxx

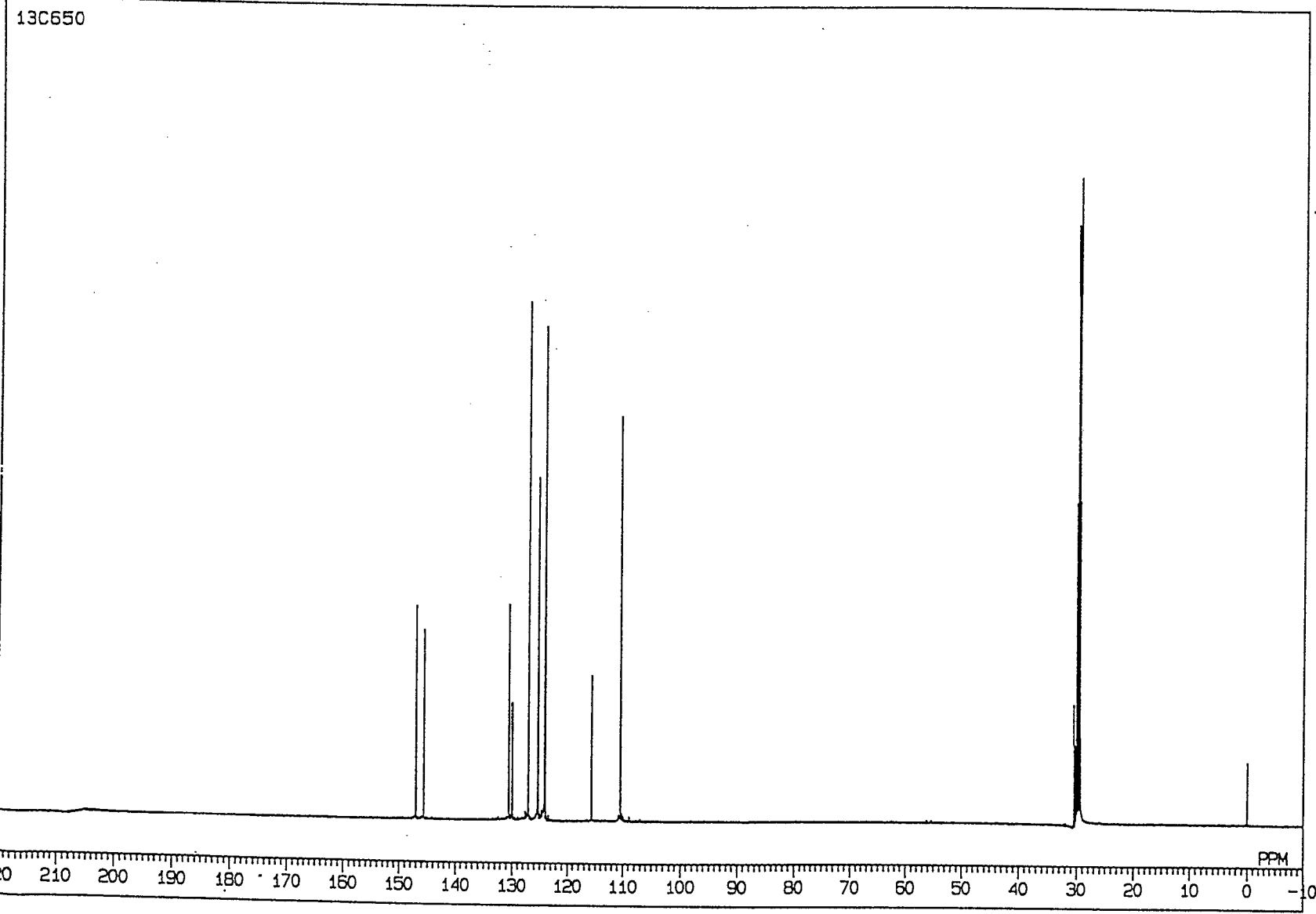
Sample No. : 101
 Sample Name : No.358(Sakamoto) FD-MS
 Data Type : Process-1
 Date : 19-APR-94 09:45
 Comment :

Scan No. : -14
 Total : 313312. R.Time : 1.6
 Average Data No. : 11-24 Base/Peak : 0.297 Base Peak : 93100.(346.0)



4e

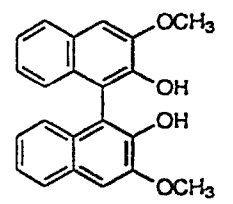
13C650



11-JAN-95 13: 17: 20.

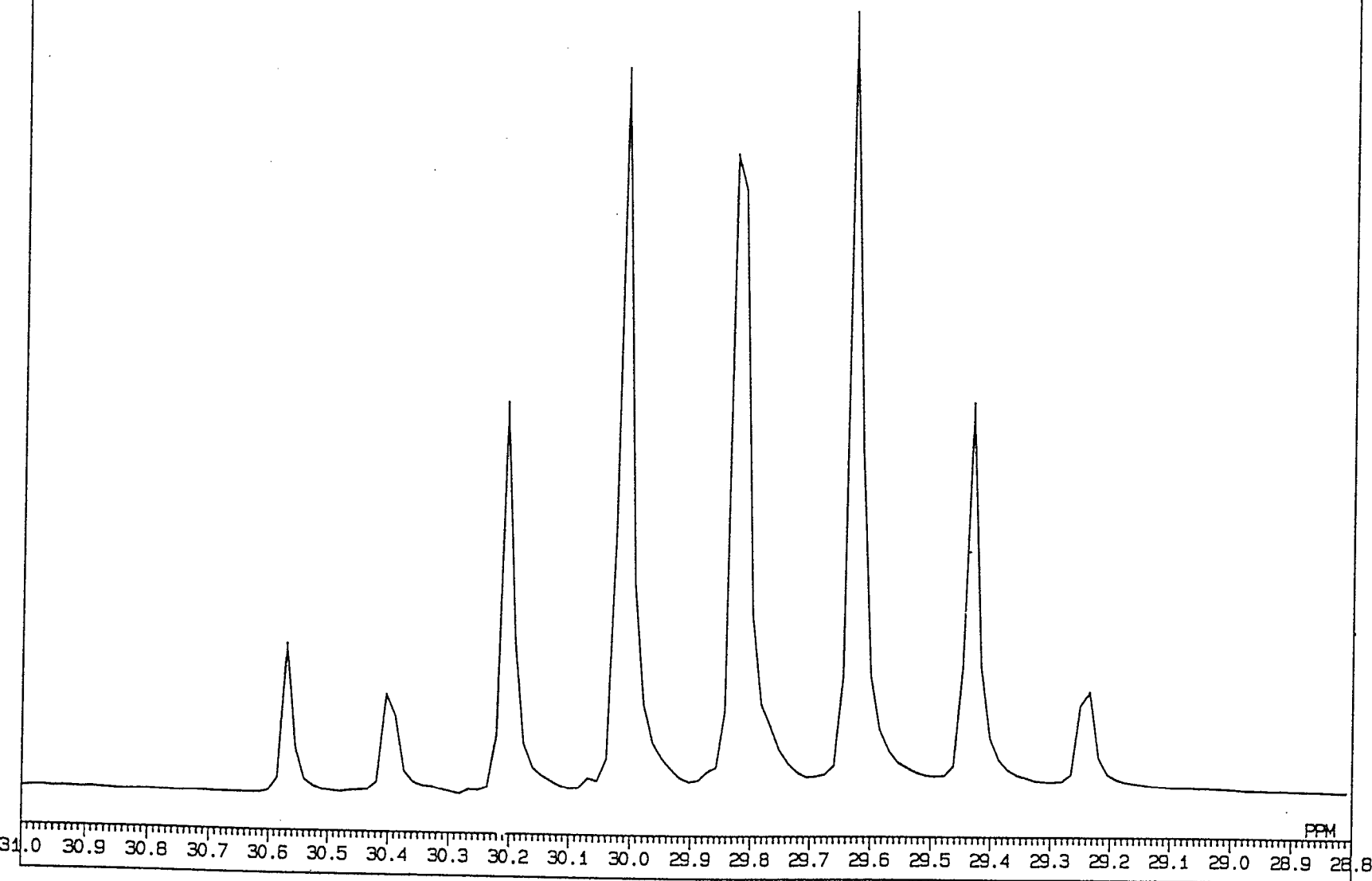
DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100. 100] 13CSA6
COMNT 13C650
EXMOD SGBCM
OBNUC 13C
OBFIN 10244.0 Hz
POINT 32768
FREQU 25000.0 Hz
SCANS 8000
ACQTM 0.655 sec
PD 1.345 sec
PW1 4.4 us
IRFIN 10300.0 Hz
IRATN 15
IRRPW 50 us
TEMP. 27.0 c
SLVNT ACETN
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 27
XE 23120.8400 Hz
XS -704.0918 Hz



4 f

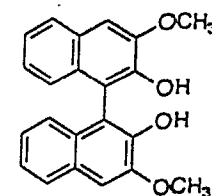
13C650



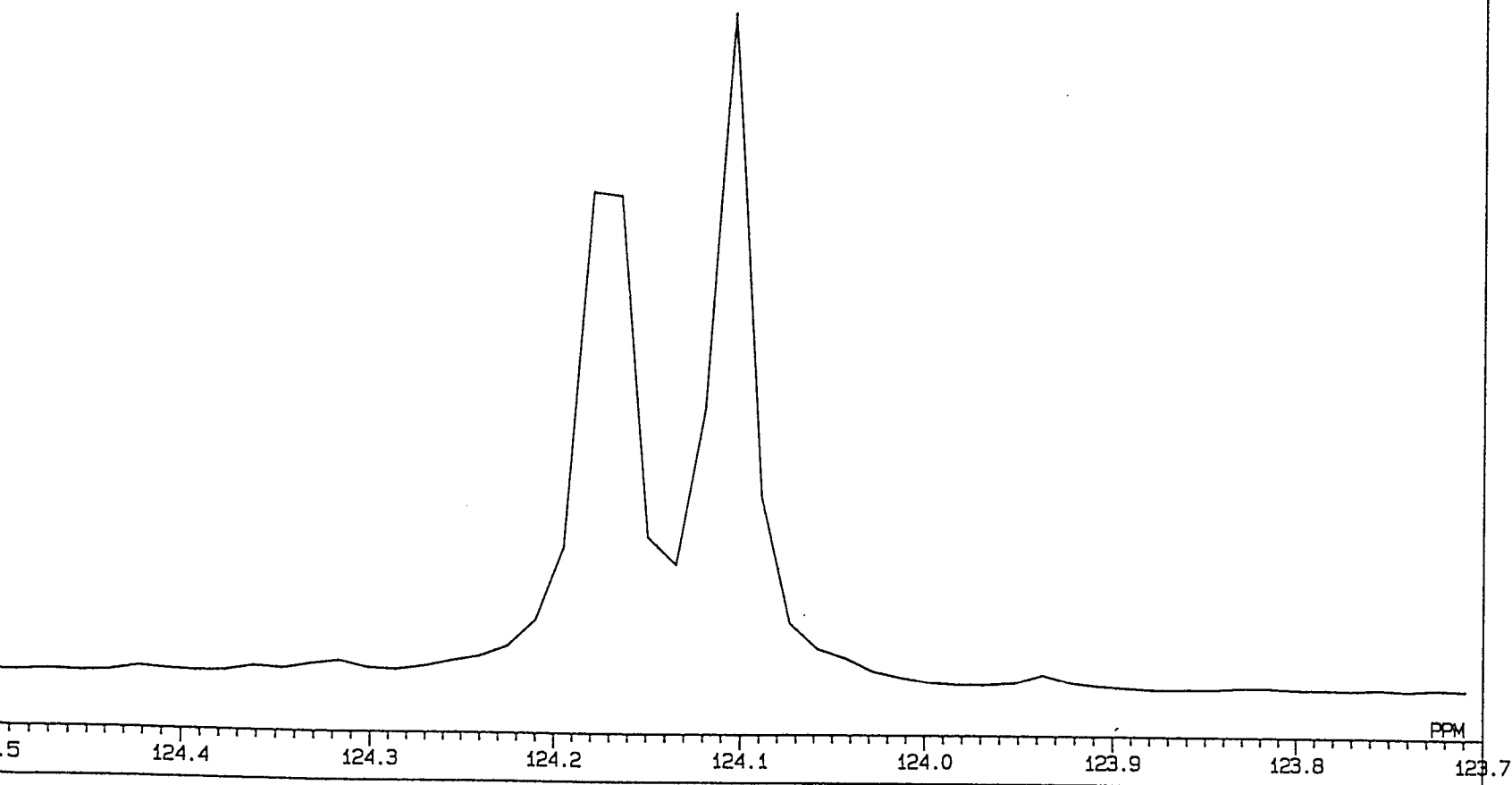
11-JAN-95 13: 22: 52

DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100, 100] 13CSA6
COMNT 13C650
EXMOD SGBCM
OBNUC 13C
OBFIN 10244.0 Hz
POINT 32768
FREQU 25000.0 Hz
SCANS 8000
ACQTM 0.655 sec
PD 1.345 sec
PW1 4.4 us
IRFIN 10300.0 Hz
IRATN 15
IRRPW 50 us
TEMP. 27.0 c
SLVNT ACETN
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 27
XE 221.1556 Hz
XS 6845.3650 Hz

**4 f**

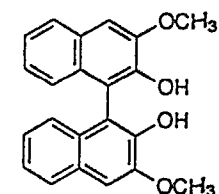
13C650



11-JAN-95 13:20:03

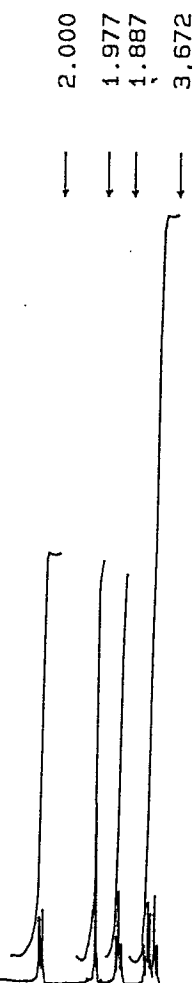
 DAINIPPON INK
 AND CHEMICALS, INC.
 CENTRAL RES. LAB.

 DFILE [100, 100] 13CSA6
 COMNT 13C650
 EXMOD SGBCM
 OBNUC 13C
 OBFIN 10244.0 Hz
 POINT 32768
 FREQU 25000.0 Hz
 SCANS 8000
 ACQTM 0.655 sec
 PD 1.345 sec
 PW1 4.4 us
 IRFIN 10300.0 Hz
 IRATN 15
 IRRPW 50 us
 TEMP. 27.0 c
 SLVNT ACETN
 EXREF 0.00 ppm
 BF 1.00 Hz
 RGAIN 27
 XE 80.4208 Hz
 XS -2624.1270 Hz

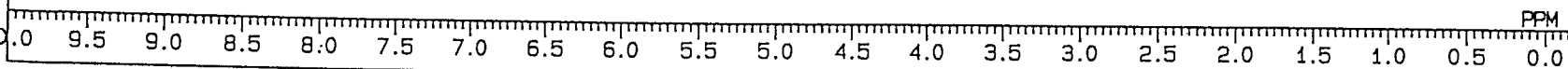


4 f

1H650



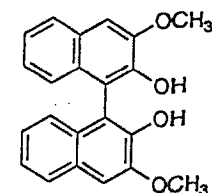
4.708



11-JAN-95 13:05:32

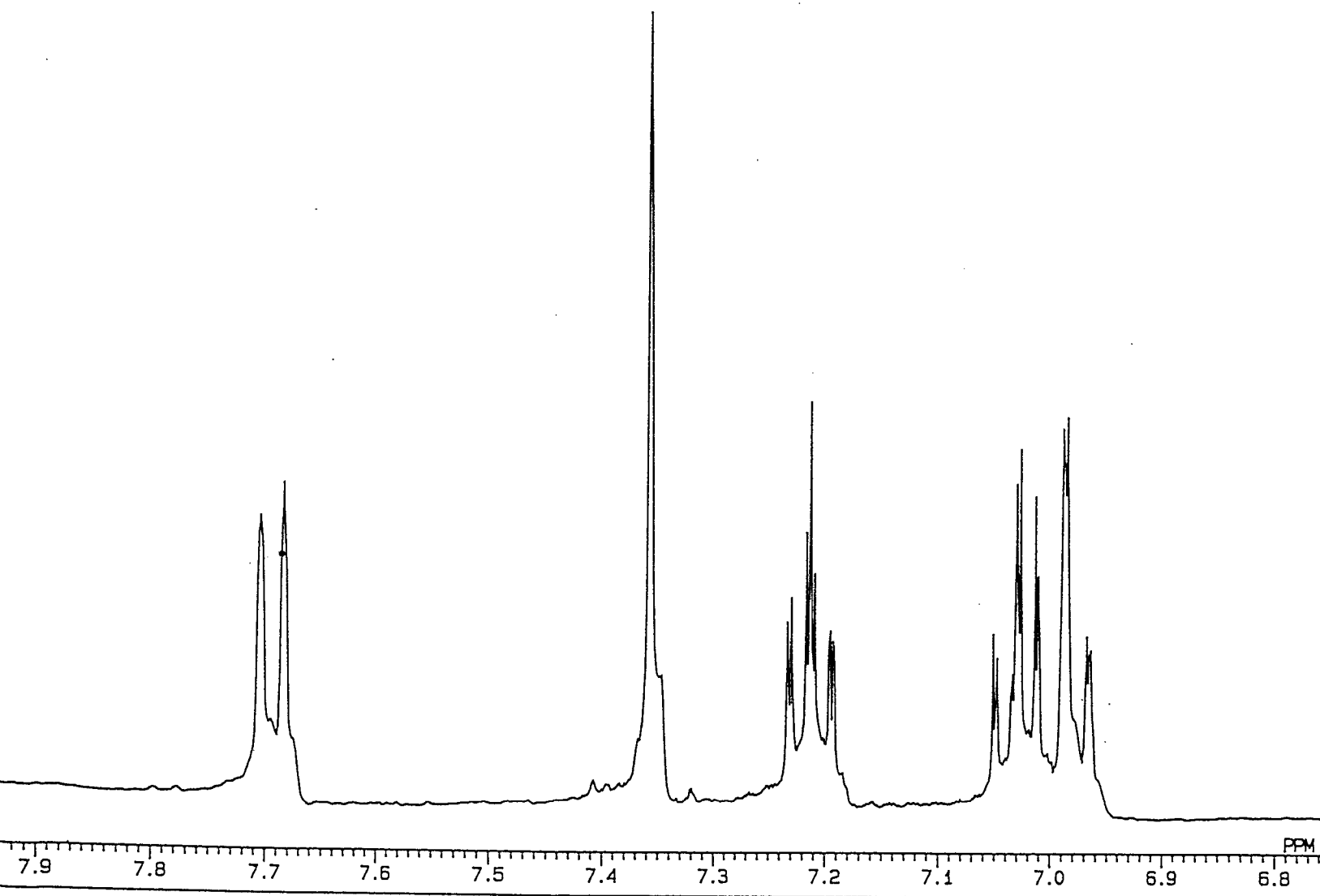
 DAINIPPON INK
 AND CHEMICALS, INC.
 CENTRAL RES. LAB.

 DFILE [100, 100] 1HSA65
 COMNT 1H650
 EXMOD SGNON
 OBNUC 1H
 OBFIN 11323.4 Hz
 POINT 32768
 FREQU 8000.0 Hz
 SCANS 16
 ACQTM 2.048 sec
 PD 10.000 sec
 PW1 6.4 us
 IRFIN 10300.0 Hz
 IRATN 0
 IRRPW 30 us
 TEMP. 27.0 c
 SLVNT ACETN
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 13
 XE 4077.7850 Hz
 XS 512.7435 Hz



4 f

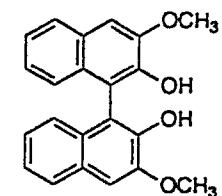
H650

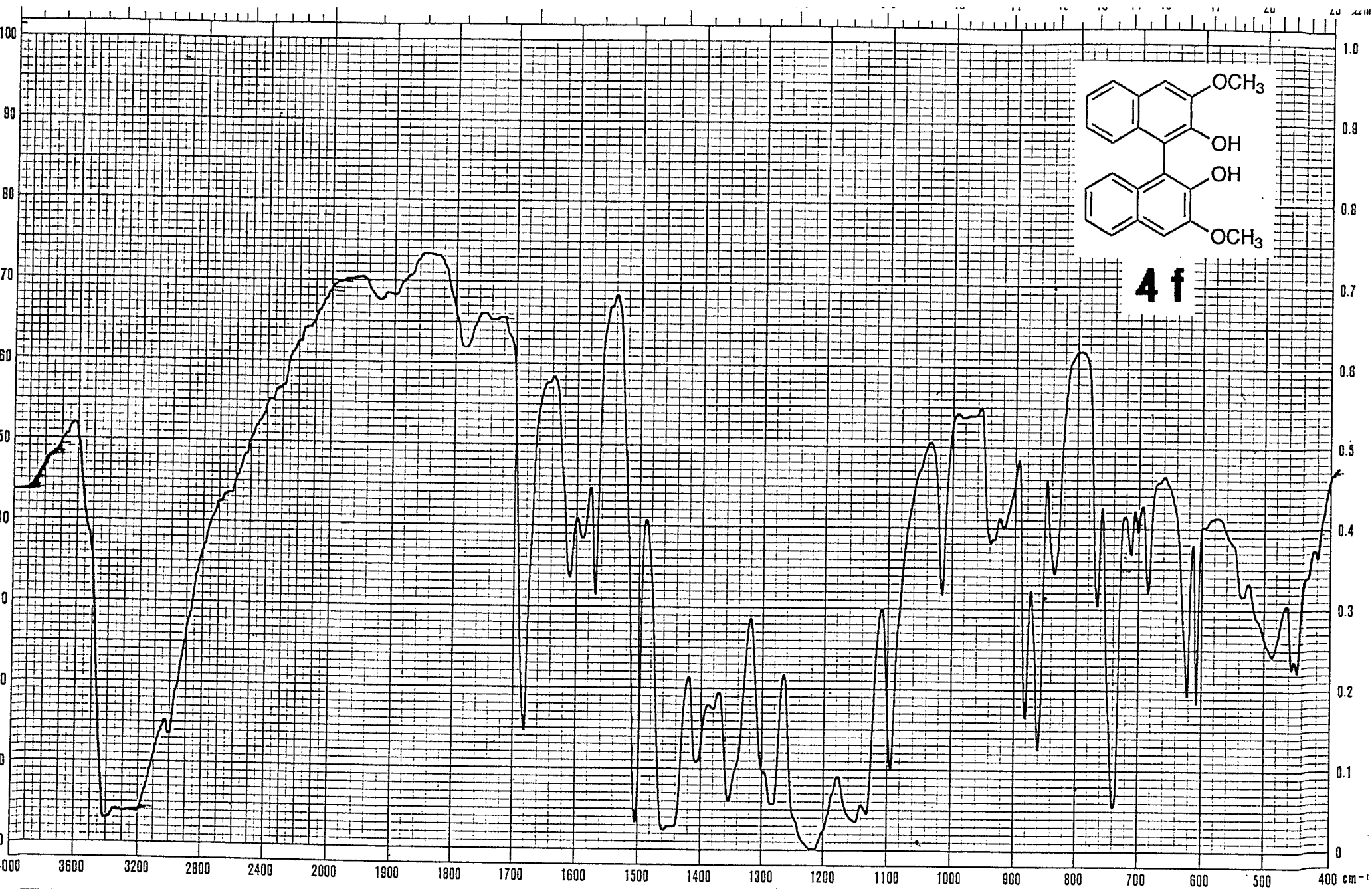


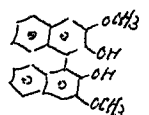
11-JAN-95 13: 08: 21

DAINIPPON INK
AND CHEMICALS, INC.
CENTRAL RES. LAB.

DFILE [100, 100] 1HSA65
COMNT 1H650
EXMOD SGNON
OBNUC 1H
OBFIN 11323.4 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 2.048 sec
PD 10.000 sec
PW1 6.4 us
IRFIN 10300.0 Hz
IRATN 0
IRRPW 30 us
TEMP. 27.0 c
SLVNT ACETN
EXREF 0.00 ppm
BF 0.10 Hz
RGAIN 13
XE 479.7392 Hz
XS -466.7242 Hz

**4 f**



DATE 94-12-20	SPEED GAIN	EXPANSION T% ABS v	SAMPLE 	SAMPLING-METHOD KBr	CONCENTRATION	REMARKS
OPERATOR Sakamoto				CELL-LENGTH	SOLVENT	