Crystal data and structure refinement for **2a-c** and **1a**.

	2a	**2b**	**2c**	**1a**
Formula	$C_{24}H_{16}O_4$	$C_{24}H_{16}O_4$	$C_{24}H_{16}O_4$	$C_{20}H_{16}O_4$
M	368.37	368.37	368.37	320.33
T (K)	143 (2)	143 (2)	173 (2)	143 (2)
λ (pm)	71.073	71.073	71.073	71.073
Crystal system	triclinic	monoclinic	monoclinic	monoclinic
Space group	P-1	C2/c	$P2_1/c$	$P2_1/n$
a (pm)	691.84 (18)	3119.4 (6)	1126.9 (2)	674.11 (10)
b (pm)	886.7 (2)	419.46 (12)	812.94 (16)	423.95 (6)
c(pm)	1540.4 (3)	1606.0 (3)	1076.7 (2)	(2714.2 (4)
α (degrees)	77.045 (6)	90	90	90
β (degrees)	89.105 (6)	117.646 (6)	108.870 (14)	93.947 (3)
γ (degrees)	81.874 (6)	90	90	90
Volume (nm^3)	0.9115 (4)	1.8615 (7)	0.9334 (3)	0.7739 (2)
Z	2	4	2	2
Density (Mg/m^3)	1.342	1.314	1.311	1.375
μ (mm^{-1})	0.091	0.089	0.089	0.096
F(000)	384	768	384	336
θ range (degrees)	1.36-28.55	1.47-28.53	3.15-25.0	1.50-28.58
Reflections measured	9897	6140	2022	12590
Independent reflections	4594	2347	1647	1968
R_{int}	0.1489	0.0911	0.0271	0.0770
R [$I > 2\sigma(I)$]	0.0538	0.0424	0.0381	0.1309
R_w	0.1362	0.1114	0.0793	0.3085

Refinement method: Full-matrix least-squares on F^2 in all the cases

Compounds **4a**,[1] **4b**,[1b] **4c**,[2] **5a**,[1a] **7b**,[3] **7c**[4] are literature known and in this present study they were characterized by IR, high resolution ^{1}H and ^{13}C-NMR and mass spectral data. The spectroscopic and analytical data for the other compounds are reported here.

General procedure for the synthesis of propargyloxyphenol (**5a-c**): To a solution of the benzenediol (**3a-c**) (10.0 g, 90.8 mmol) in dry acetone (250 mL) was added excess anhydrous K_2CO_3 (75.0 g) and the mixture was refluxed for 0.5 h. To the mixture, propargyl bromide (10.1g, 90.8 mmol) was added dropwise over a period of 5 h. The resulting mixture was refluxed for an additional period of 17 h and then cooled, filtered and the filtrate was evaporated . The brown oily residue was dissolved in CH_2Cl_2 (250 mL) and the solution was washed with water (2 x 100 mL) followed by saturated brine solution (100 mL). The organic layer was dried over anhydrous Na_2SO_4 and then the solvent was removed. The crude product consisted of a mixture of unreacted benzenediol (**3a-c**), propargyloxyphenol (**5a-c**) and bispropargyloxybenzene (**4a-c**) which were separated by column chromatography on silica gel using hexane/ethyl acetate (19:1 v/v) as the eluant. From **3a** (10 g) was obtained **4a** (3.65 g, 29%), **5a** (6.62 g, 65%) and unreacted **3a** (2.47 g). Similarly from **3b** (25.0 g) was obtained **4b** (12.55 g, 40%), **5b** (14.6 g, 58%) and unreacted **3b** (6.24 g) and from **3c** (25.0 g) was obtained **4c** (16.05 g, 47%), **5c** (18.2 g, 68%) and unreacted **3c** (4.9 g).

General procedure for the synthesis of bispropargyloxybenzene (4a-c): The above procedure for the synthesis of **5a-c** was adopted using 2 equivalents of propargyl bromide (23.8 g, 200 mmol). Yield: **4a** (15.05 g, 89%), **4b** (14.97 g, 89%) and **4c** (13.35 g, 79%).

General procedure for the synthesis of bis(2-hydroxyphenoxy)hexa-2,4-diyne (6a-c) from bis(2-acetoxyphenoxy)hexa-2,4-diyne (8a-c): To a solution of 8a (0.48 g, 1.27 mmol) in methanol (20 mL) was added Na_2CO_3 (0.48 g, 4.57 mmol) at rt. The resulting mixture was stirred for 24 h and then poured into water (200 mL), extracted with ethyl acetate (2 x 50 mL). The organic phase was separated and washed with water (100 mL) followed by saturated brine (100 mL). It was dried over anhydrous Na_2SO_4 and then solvent was removed. The crude product was purified by column chromatography on

silica gel and eluted with hexane/ethyl acetate (2.3:1 v/v). Yield: **6a** (0.178 g, 48%), **6b** (0.37 g, 68%) from **8b** (0.7 g, 1.84 mmol), **6c** (0.54 g, 56%) from **8c** (1.25 g, 3.31 mmol).

General procedure for the synthesis of propargyloxyphenyl acetate (7a-c) from propargyloxyphenol (5a-c): To a solution of **5a-c** (5.0 g, 33.78 mmol) in dry CH_2Cl_2 (50 mL) was added dry pyridine (5.35 g, 67.57 mmol) followed by acetic anhydride (3.79 g, 37.2 mmol) at rt. After 5h, the mixture was poured into ice cold HCl (2%, 100 mL) and extracted with CH_2Cl_2 (2 x 100 mL). The organic phase was separated, washed with saturated $NaHCO_3$ solution (100 mL), followed by water (2 x 100 mL) and saturated brine solution (100 mL) and dried over anhydrous Na_2SO_4. Removal solvent yielded the crude product which was purified by column chromatography on silica gel using hexane/ethyl acetate (4:1 v/v) as the eluant. Yield: **7a** (4.88 g, 76%), **7b** (4.68 g, 73%), **7c** (4.75 g, 74%).

Syntheses of **6a-c** from **5a-c**, **8a-c** from **7a-c** and **2a-c** from **9a-c,** respectively, were accomplished using the Glaser-Eglington coupling procedure described for the syntheses of **2a-c** from **4a-c**.

Spectroscopic characterization of intermediates:

3-Propargyloxyphenol (5b): Pale yellow liquid, IR ($CHCl_3$): 3600 (br), 1600, 1484 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 300 MHz): δ 7.13 (t, 1H, *J* = 7.8 Hz), 6.55 (s, 1H), 6.54 (dd, 1H, *J* = 7.5 and 1.8 Hz), 6.47 (dd, 1H, *J* = 7.8 and 2.1 Hz), 5.30 (br, s, 1H), 4.64 (d, 2H, *J* = 2.1 Hz), 2.50 (t, 1H, *J* = 2.1 Hz); ^{13}C-NMR($CDCl_3$, 75 MHz): δ 157.0 (s), 156.59 (s), 129. 72 (d), 108.26 (d), 106.58 (d), 102.09 (d), 78.00 (s), 74.87 (d), 55.47 (t); MS (EI, 70 eV) 148 (M^+, 10), 147 (100), 91 (50); HRMS: calcd. for $C_9H_8O_2$ 148.05243 found 148.05515. Anal. calcd. C = 72.95, H = 5.45, found C = 72.70, H = 6.10.

4-Propargyloxyphenol (5c): Pale yellow liquid, IR ($CHCl_3$): 3584 (br), 1600, 1468 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 300 MHz): δ 6.88 and 6.99 (AA'BB', 4H, *J* = 9.0 Hz), 4.61 (d, 2H, *J* = 2.44 Hz), 2.48 (t, 1H, *J* = 2.44 Hz); ^{13}C-NMR($CDCl_3$, 75 MHz): δ 151.14 (s), 150.10 (s),

115.93 (d), 115.59 (d), 78.52 (d), 74.77 (s), 56.28 (t); MS (EI, 70 eV) 148 (M^+, 60), 109 (100); Anal. calcd. C = 72.95, H = 5.45, found C = 72.08, H = 5.38.

2-Propargyloxyphenyl acetate (7a): Colorless solid, m. p 60-61 ^oC, IR ($CHCl_3$): 1760, 1596, 1456 cm^{-1}; ^1H-NMR ($CDCl_3$, 200 MHz): δ 7.22 – 6.99 (m, 4H), 4.70 (d, 2H, *J* = 2.4 Hz), 2.52 (t, 1H, *J* = 2.4 Hz), 2.32 (s, 3H); ^{13}C-NMR($CDCl_3$, 50 MHz): δ 168.94 (s), 149.04 (s), 140.04 (s), 126.69 (d), 123.09 (d), 121.94 (d), 114.43 (d), 78.18 (s), 75.85 (d), 56.67 (t), 20.66 (q); MS (EI, 70 eV) 190 (M^+, 12), 148 (100), 109 (85), 81 (25).

1,6-Bis(2-hydroxyphenoxy)hexa-2,4-diyne (6a): Pale yellow solid, m.p. 136-137 ^oC, IR (KBr): 3440 (br), 1651, 1596 cm^{-1}; ^1H-NMR (CD_3COCD_3, 200 MHz): δ 6.93-6.78 (m, 8H), 5.84 (s, 2H), 4.55 (s, 4H); ^{13}C-NMR(CD_3COCD_3, 50 MHz): δ 144.36 (s), 143.39 (s), 122.24 (d), 122.98 (d), 118.05 (d), 117.17 (d), 100.35 (s), 79.0 (s), 65.56 (t); MS (EI, 70 eV) 294 (M^+, 100), 185 (55), 157 (25), 147 (25), 121 (25); HRMS: calcd. for $C_{18}H_{14}O_4$ 294.08921 found 294.0887. Anal. calcd. C = 73.45, H = 4.80, found C = 73.41, H = 4.91.

1,6-Bis(3-hydroxyphenoxy)hexa-2,4-diyne (6b): Colorless solid, m.p. 135-136 ^oC, IR (KBr): 3440 (br), 1254 cm^{-1}; ^1H-NMR (CD_3COCD_3, 200 MHz): δ 8.41 (br, s, 2H), 6.97-6.03 (m, 2H), 6.38-6.31 (m, 6H), 4.72 (s, 4H); ^{13}C-NMR(CD_3COCD_3, 50 MHz): δ 159.59 (s), 159.44 (s), 130.72 (d), 109.56 (d), 106.53 (d), 103.03 (d), 76.23 (s), 70.74 (s), 56.37 (t); MS (EI, 70 eV) 294 (M^+, 10), 185 (100), 184 (80), 157 (25), 128 (65).

1,6-Bis(4-hydroxyphenoxy)hexa-2,4-diyne (6c): Pale yellow solid, m. p. 161-162 ^oC; IR (KBr): 3536 (br), 1504, 1446 cm^{-1}; ^1H-NMR (CD_3COCD_3, 200 MHz): δ 7.95 (br, s, 2H), 6.74-6.61 (m, 8H), 4.67 (s, 4H); ^{13}C-NMR(CD_3COCD_3, 50 MHz): 152.98 (s), 151.55 (s), 116.96 (d), 116.56 (d), 76.46 (s), 70.66 (s), 57.29 (t); MS (EI, 70 eV): 294 (M^+, 25), 185 (40), 110 (100), 76 (65); HRMS: calcd. for $C_{18}H_{14}O_4$ 294.08921 found 294.0887. Anal. calcd. C = 73.45, H = 4.80, found C = 73.29, H = 4.80.

1,6-Bis(2-acetoxyphenoxy)hexa-2,4-diyne (8a): Colorless solid, m. p. 119-120 ^{o}C; IR (KBr): 1756, 1596, 1497, 1435 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 200 MHz): δ 7.16-7.00 (m, 8H), 4.76 (s, 4H), 2.31 (s, 3H); ^{13}C-NMR ($CDCl_3$, 50 MHz): δ 164.0 (s), 149.0 (s), 140.0 (s), 126.81 (d), 123.18 (d), 122.21 (d), 114.46 (d), 74.39 (s), 71.0 (s), 57.20 (t), 20.65 (q); MS (EI, 70 eV): 378 (M^+, 5), 336 (50), 227 (75), 185 (100).

1,6-Bis(3-acetoxyphenoxy)hexa-2,4-diyne (8b): Colorless solid, m.p. 75-76 ^{o}C; IR (KBr): 1760, 1587, 1164 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 7.25 (t, 2H, *J* = 8.30 Hz), 6.80 (dd, 2H, *J* = 2.44 and 8.30 Hz), 6.72 (dd, 2H, *J* = 1.95 and 8.30 Hz), 6.67 (t, 2H, *J* = 2.44 Hz), 4.68 (s, 4H), 2.24 (s, 6H); ^{13}C-NMR ($CDCl_3$, 100 MHz): δ 169.06 (s), 158.0 (s), 151.41 (s), 129.76 (d), 114.77 (d), 111.97 (d), 108.60 (d), 74.30 (s), 70.96 (s), 56.13 (s), 20.85 (q); MS (EI, 70 eV): 378 (M^+, 5), 336 (50), 294 (30), 165 (100).

1,6-Bis(4-acetoxyphenoxy)hexa-2,4-diyne (8c): Colorless solid, m.p. 146-147 ^{o}C; IR (KBr): 1753, 1593 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 200 MHz): δ 7.03 and 6.92 (AA'BB', 8H, *J* = 9.0 Hz), 4.73 (s, 4H), 2.28 (6H); ^{13}C-NMR ($CDCl_3$, 50 MHz): δ 170.0 (s), 155.00 (s), 154.0 (s), 122.43 (d), 115.57 (d), 75.0 (s), 71.0 (s), 56.59 (t), 21.04 (q); MS (EI, 70 eV): 378 (M^+, 10), 336 (55), 227 (45), 185 (80), 110 (100).

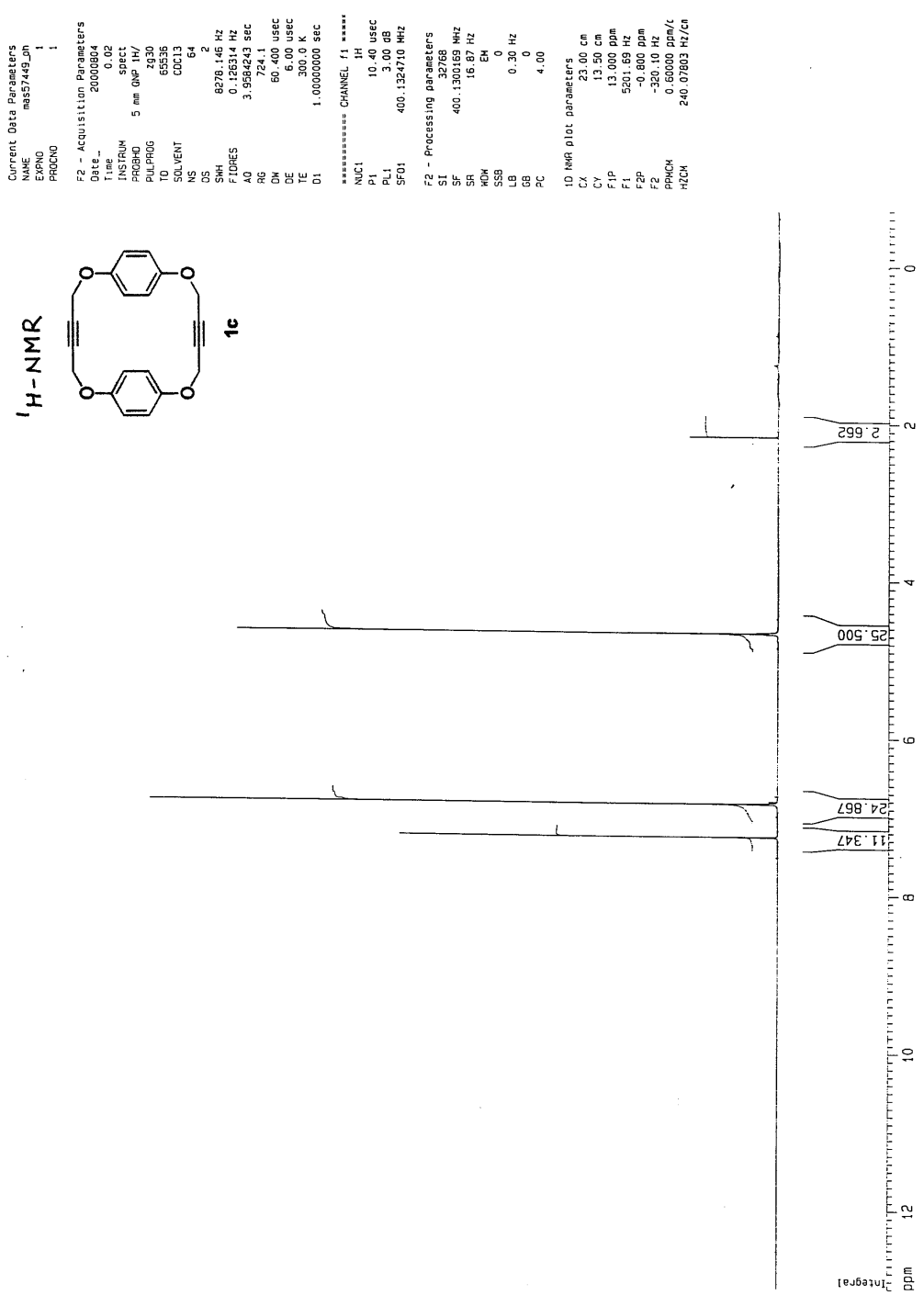
1,6-Bis(3-propargyloxyphenoxy)hexa-2,4-diyne (9b): Colorless solid, m.p. 55-56 ^{o}C; IR ($CHCl_3$): 1600, 1148, 1043 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 7.25 (t, 2H, *J* = 8.72 Hz), 6.64-6.56 (m, 6H), 4.73 (s, 4H), 4.66 (d, 4H, *J* = 2.4 Hz), 2.52 (t, 2H, *J* = 2.42 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz): δ 158.75 (s), 158.54 (s), 130.02 (d), 108.18 (d), 107. 84 (d), 102.39 (d), 78.37 (s), 75.66 (d), 74.50 (s), 71.12 (s), 56.26 (t), 55.88 (t); MS (EI, 70 eV) 370 (M^+, 5), 331 (45), 223 (100), 184 (70); HRMS: calcd. for $C_{28}H_{18}O_4$ 370.12051 found 370.11982.

1,6-Bis(4-propargyloxyphenoxy)hexa-2,4-diyne (9c): Colorless solid, m. p. 99-100 ^{o}C; ^{1}H-NMR ($CDCl_3$, 400 MHz): δ 6.93-6.87 (AA'BB' pattern, 8H), 4.69 (s, 4H), 4.64 (d, 4H, *J* = 2.44 Hz), 2.51 (t, 2H, *J* = 2.44 Hz); ^{13}C-NMR ($CDCl_3$, 50 MHz): δ 152.51 (s),

152.22 (s), 116.05 (d), 79.0 (s), 75.42 (d), 74.79 (s), 71.0 (s), 56.96 (t), 56.46 (t); MS (EI, 70 eV), 370 (M^+, 75), 183 (35), 147 (100); Anal. calcd. C = 77.81, H = 4.90, found C = 76.74, H = 4.78.

References:

1. (a) Yamamoto, M. *J. Chem. Soc. Perkin Trans 1,* **1979,** 3161-3165, (b) Simon D. Z.; Brookman, S.; Beliveau, J.; Salvador, L. L. *J. Pharm. Sci*., **1977**, *66*, 431-432.
2. (a) Whitlock, B. J.; Whitlock, H. W, Jr. *J. Am. Chem. Soc*. **1983**, *105*, 838-844, (b) Balasubramanian, K. K.; Venugopalan, B. *Tetrahedron Lett*. **1973**, 2707-2710.
3. Anderson, W. K.; Lavoie, E. J.; Whitkop, P. G. *J. Org. Chem*. **1974**, *39*, 881-884.
4. Vartanya, R. S.; Kazaryan, Zh. V.; Kucherov, V. F. *Arm. Khim. Zh*, **1974**, *27*, 295-303.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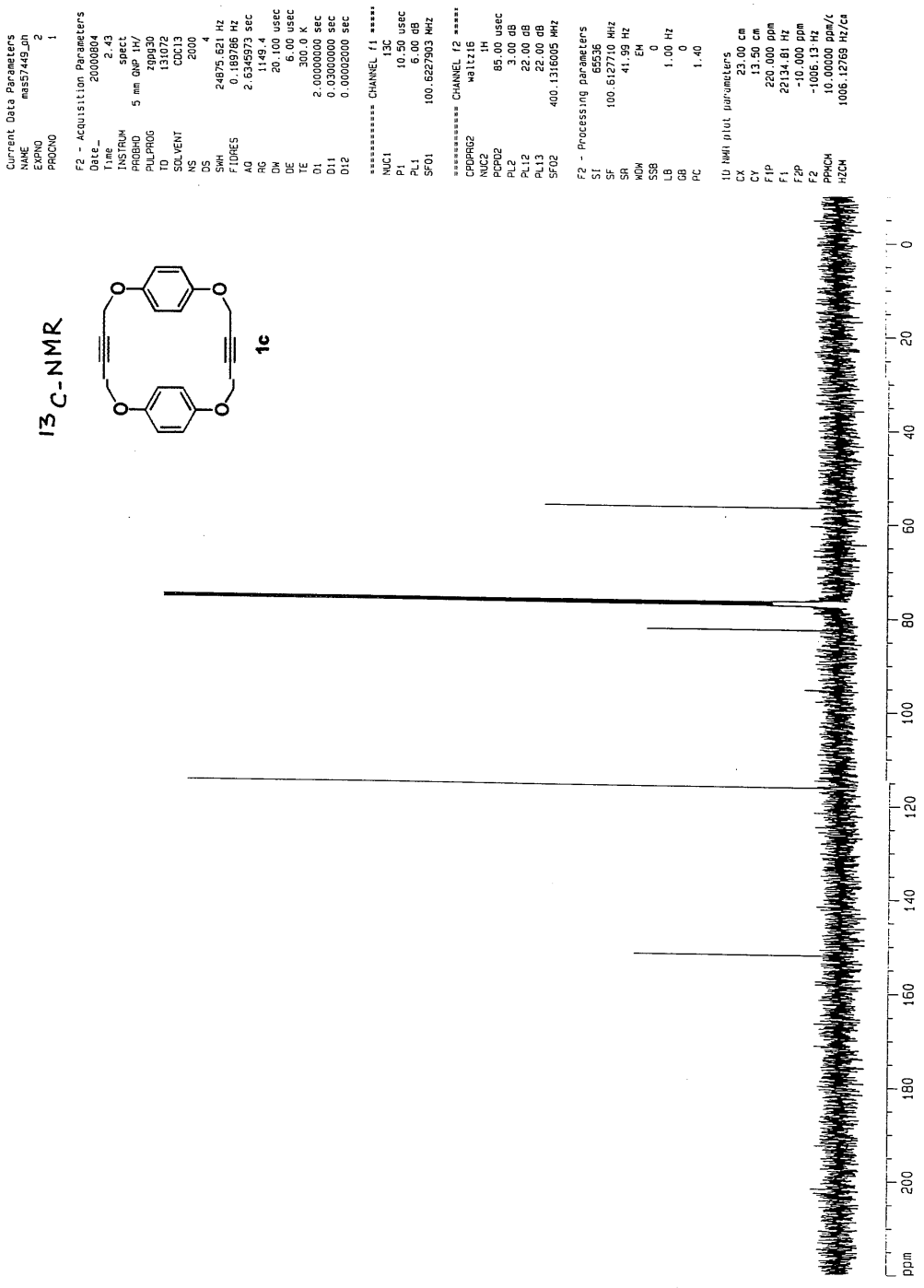
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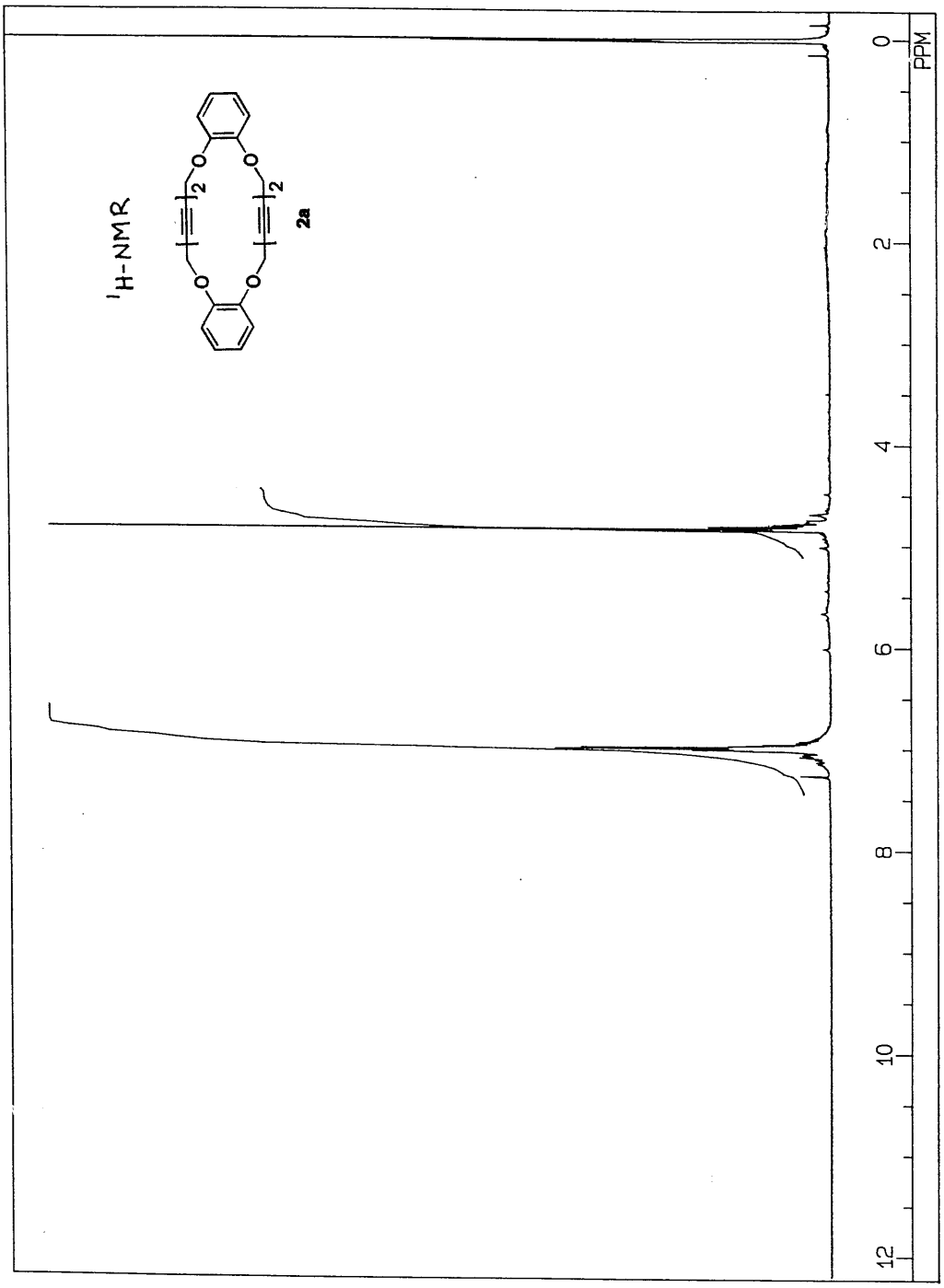
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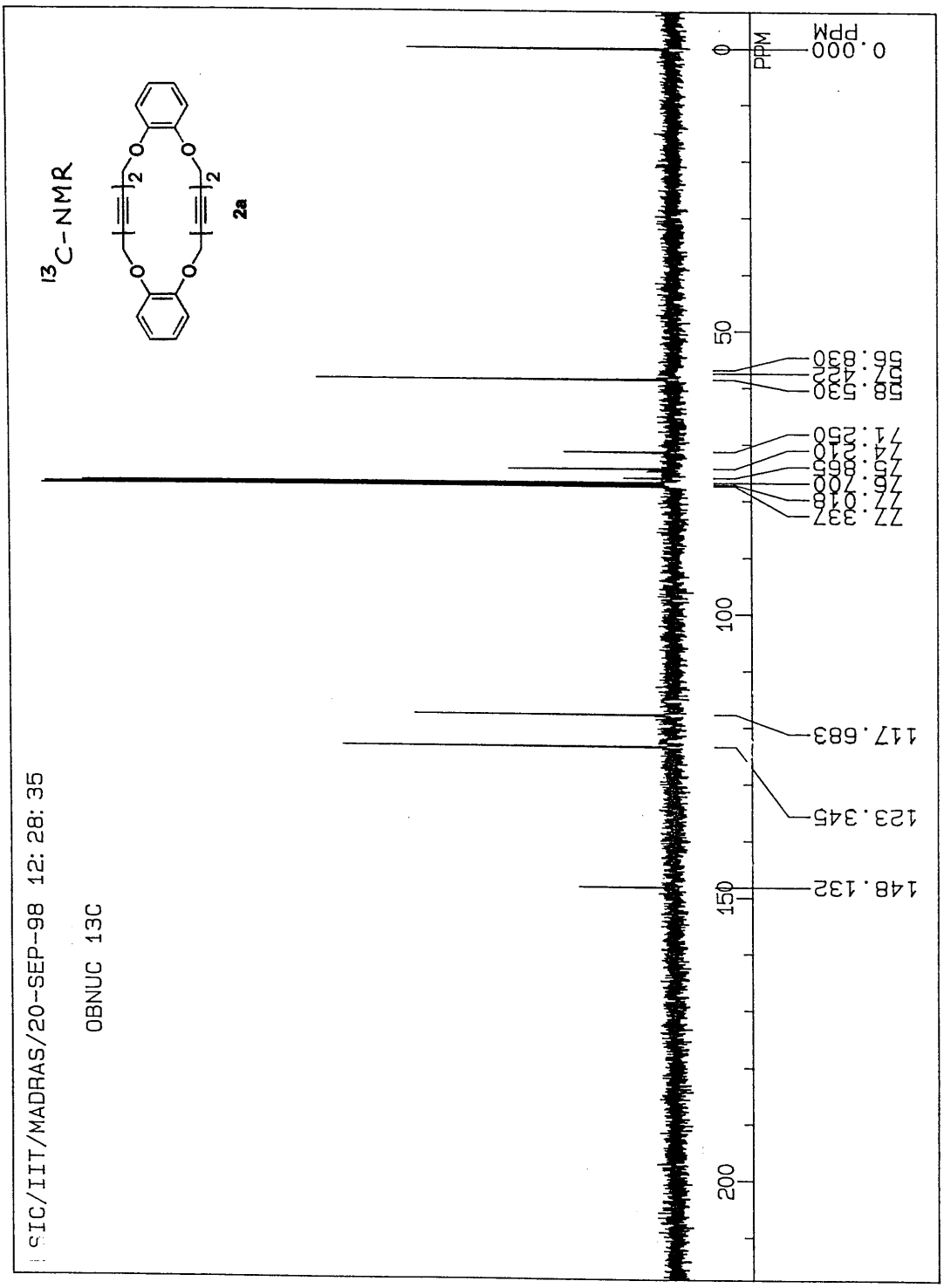
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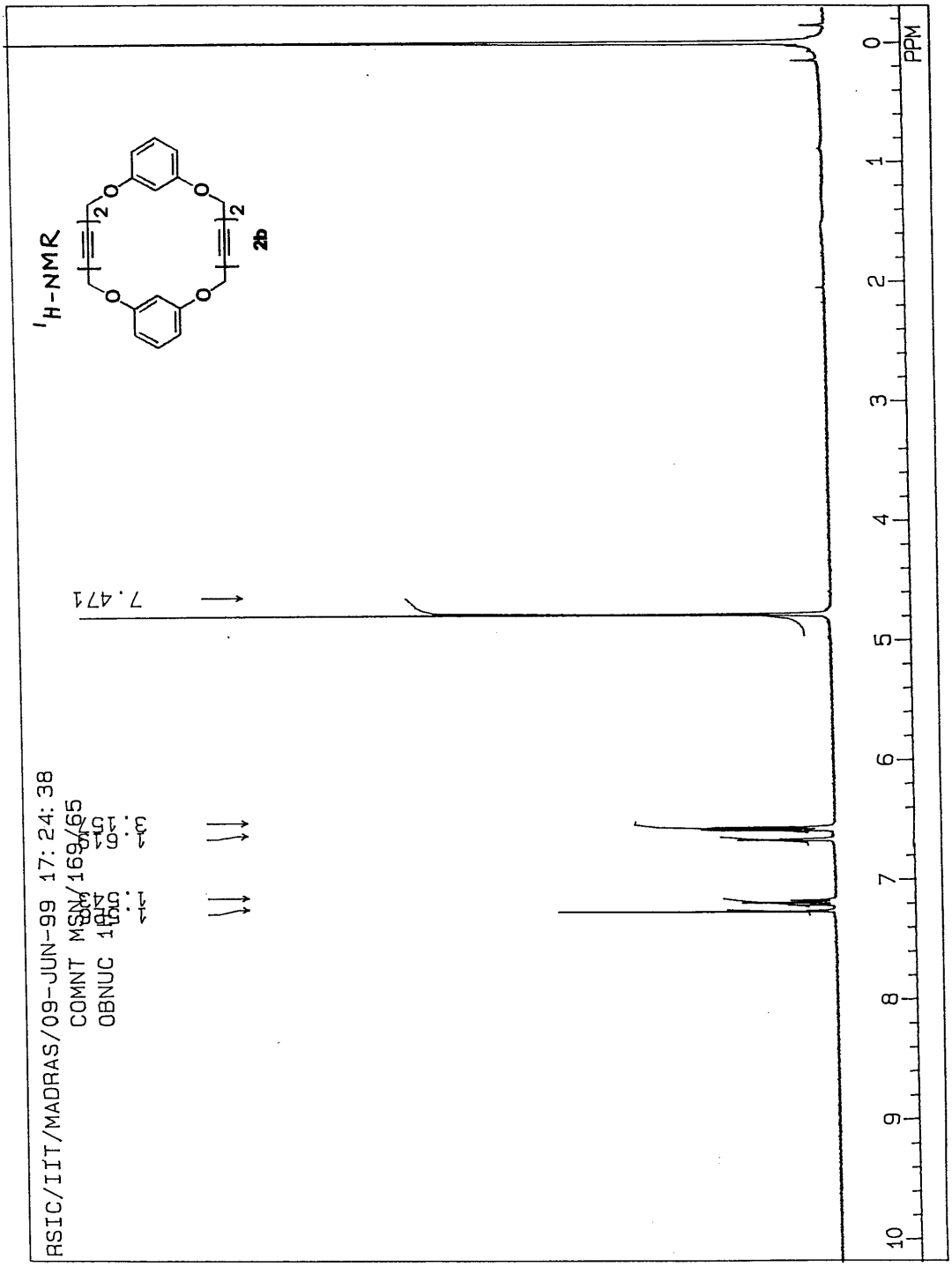
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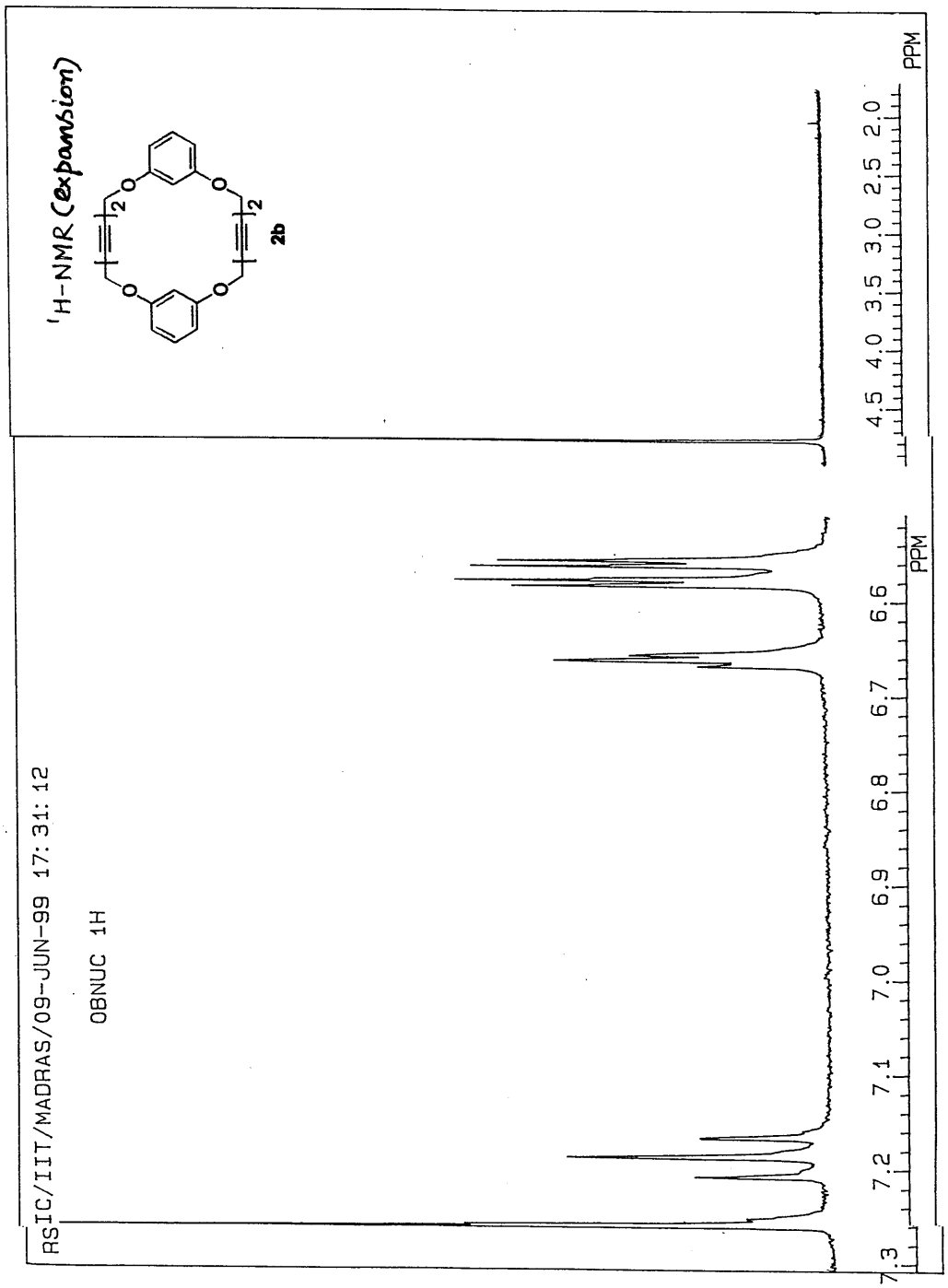
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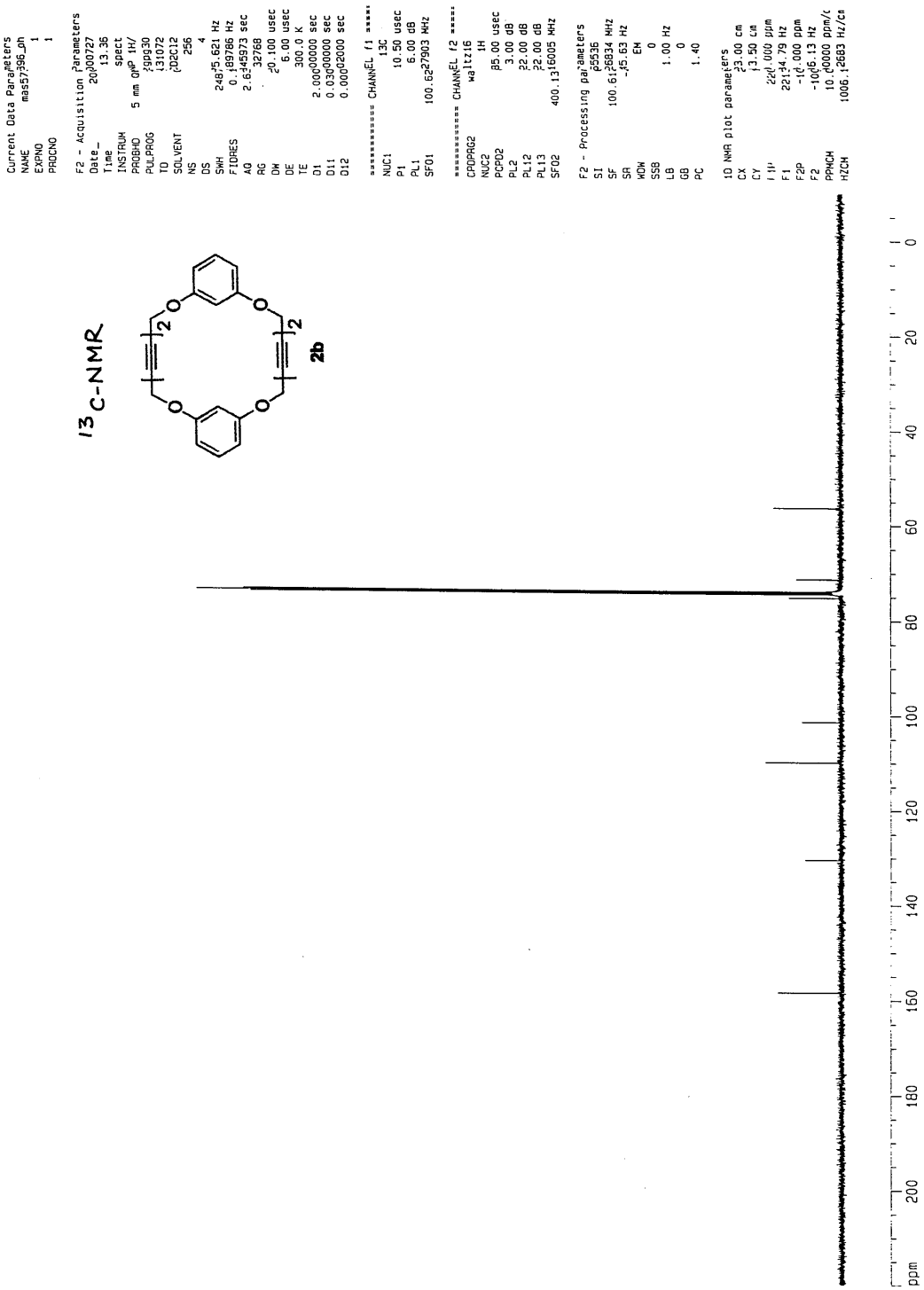
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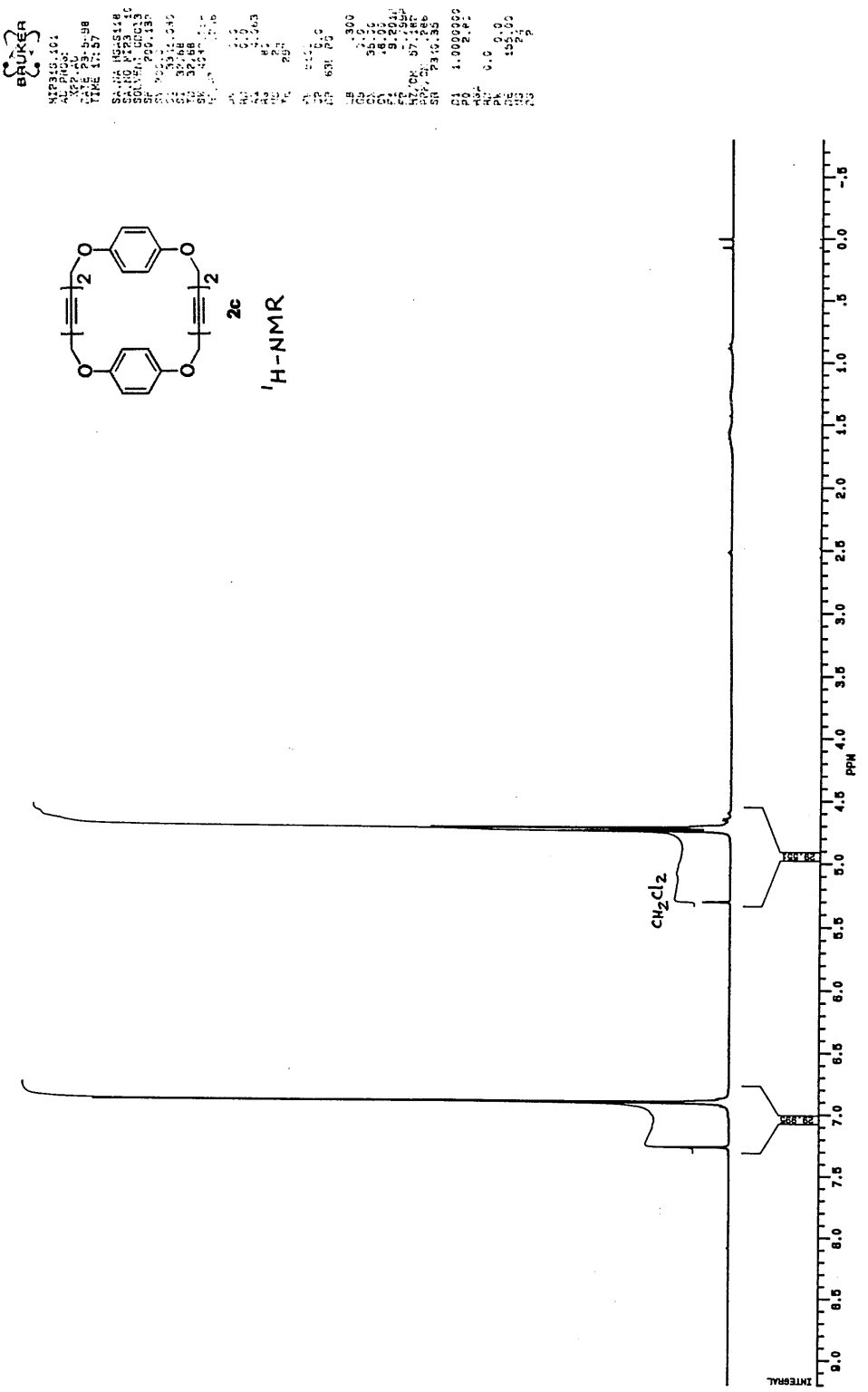
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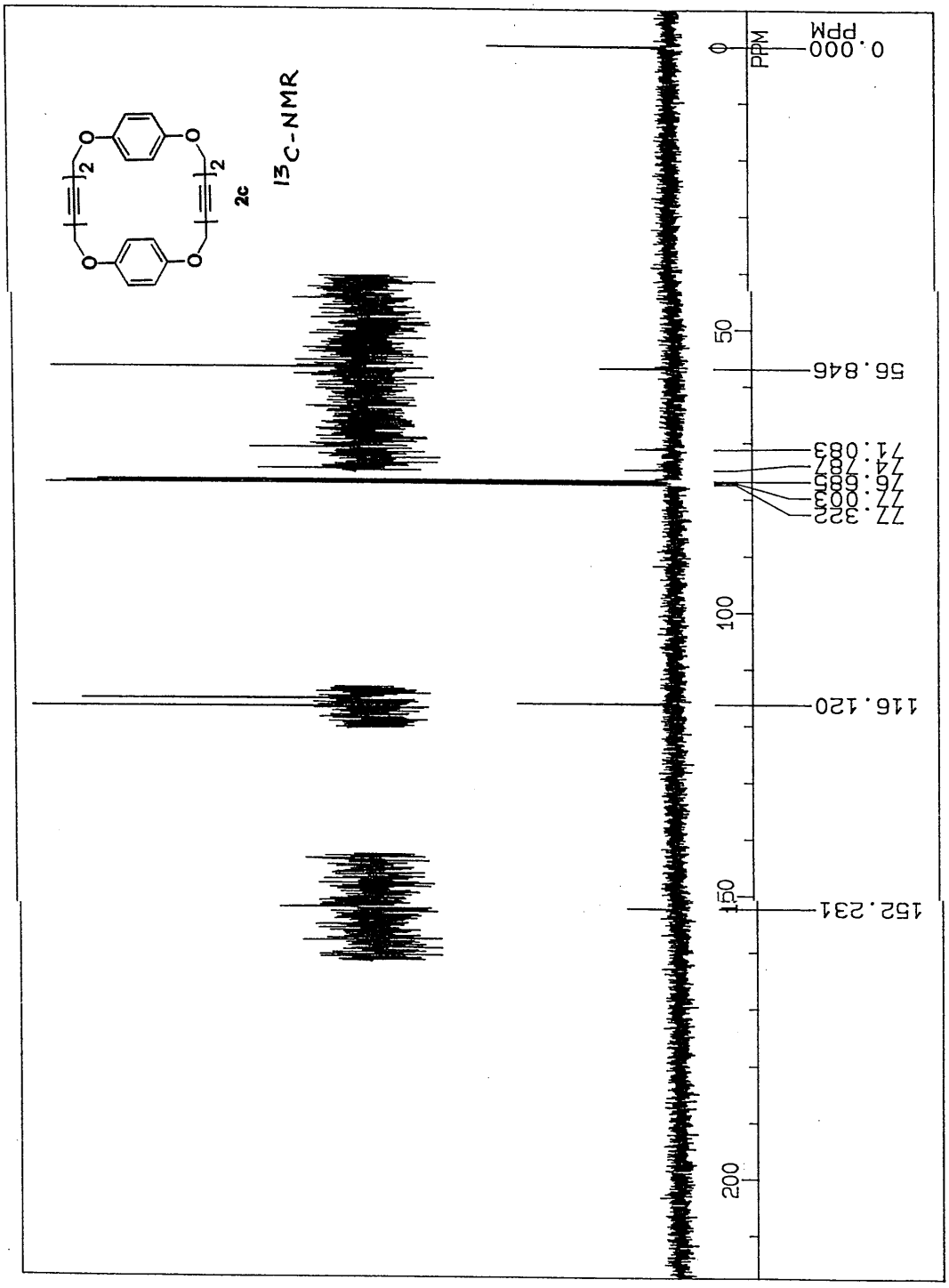
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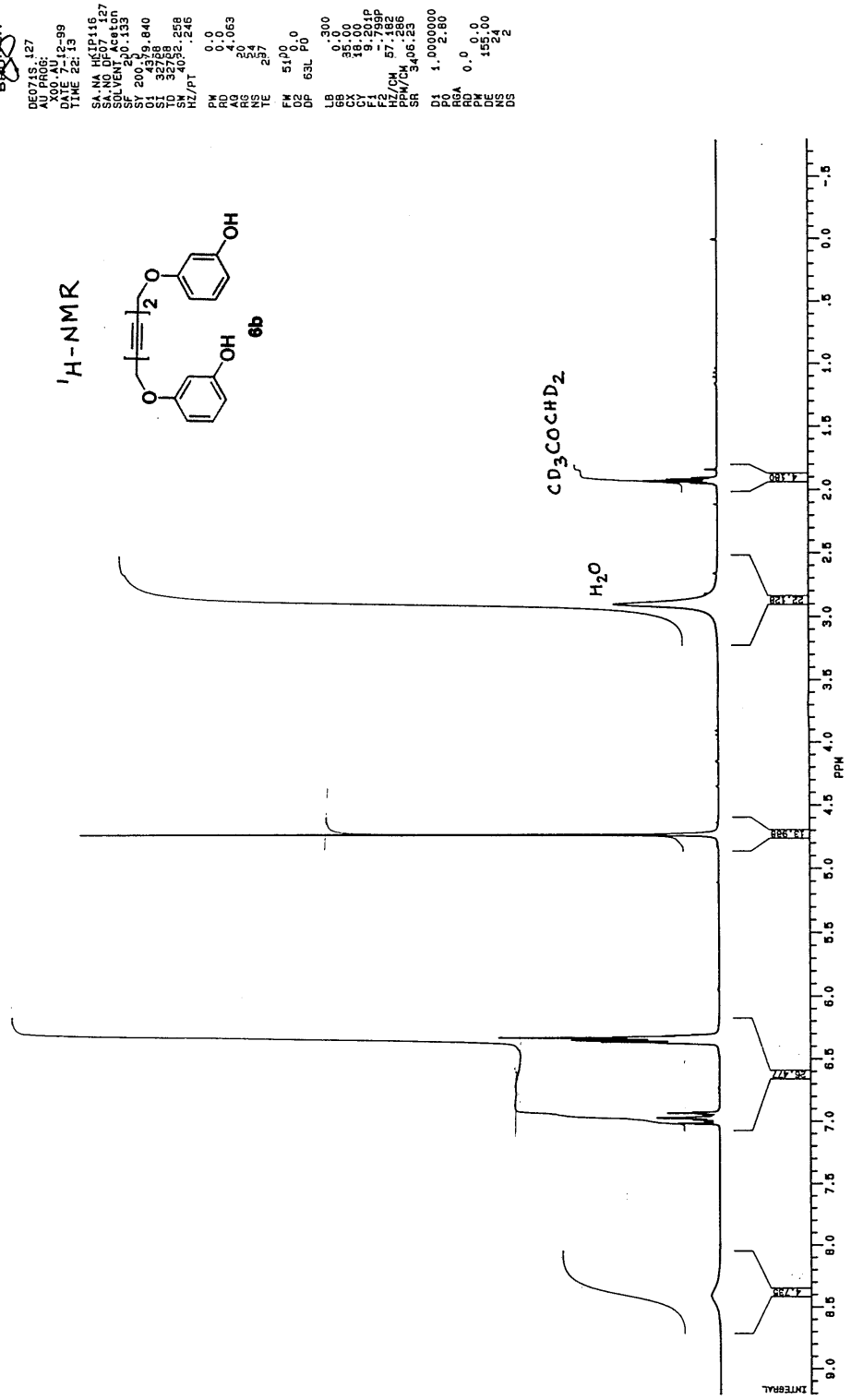
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PPM/CM 286
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6b
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H_2O
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22.128
13.988
25.471
4.784
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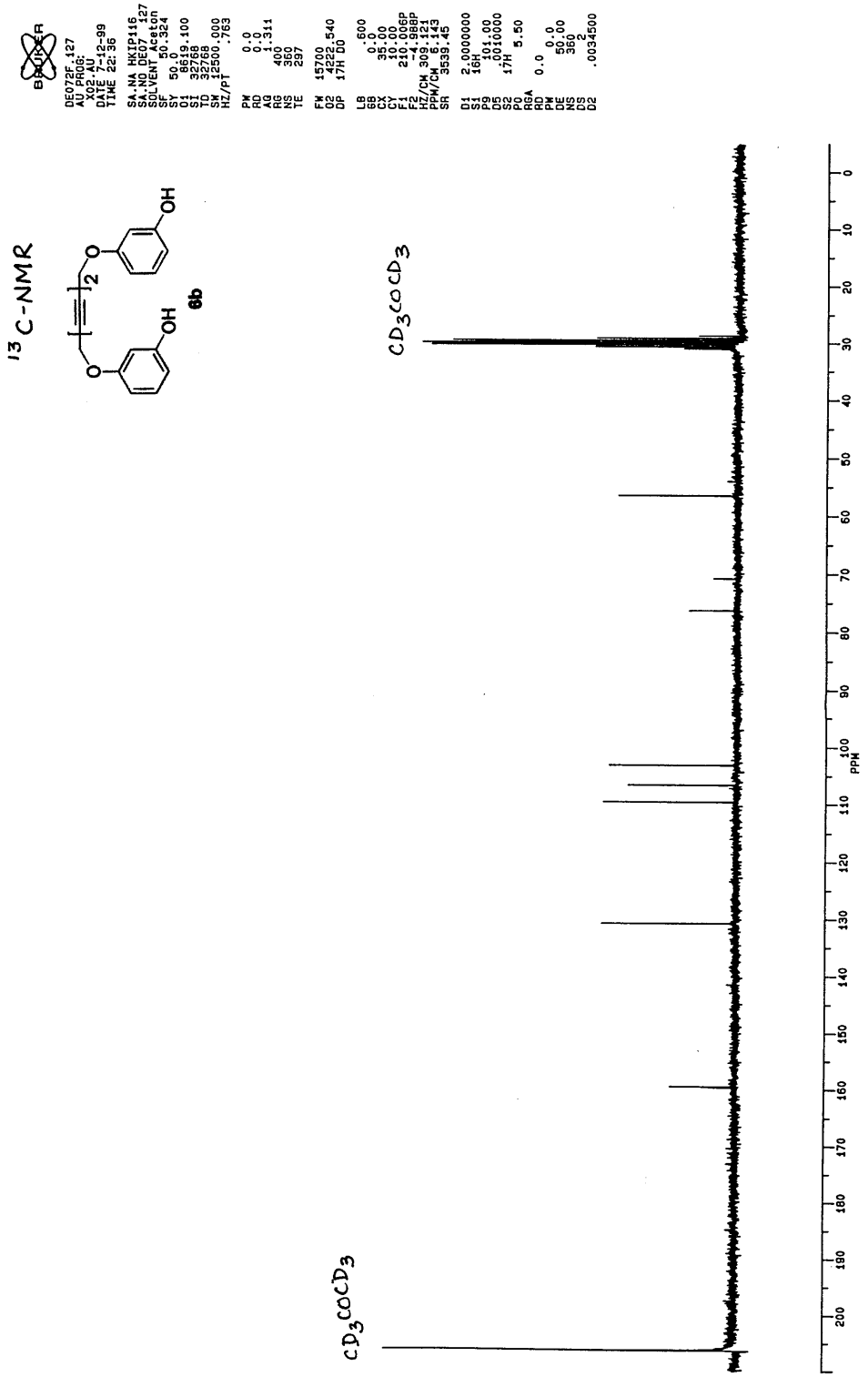
PPM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6b
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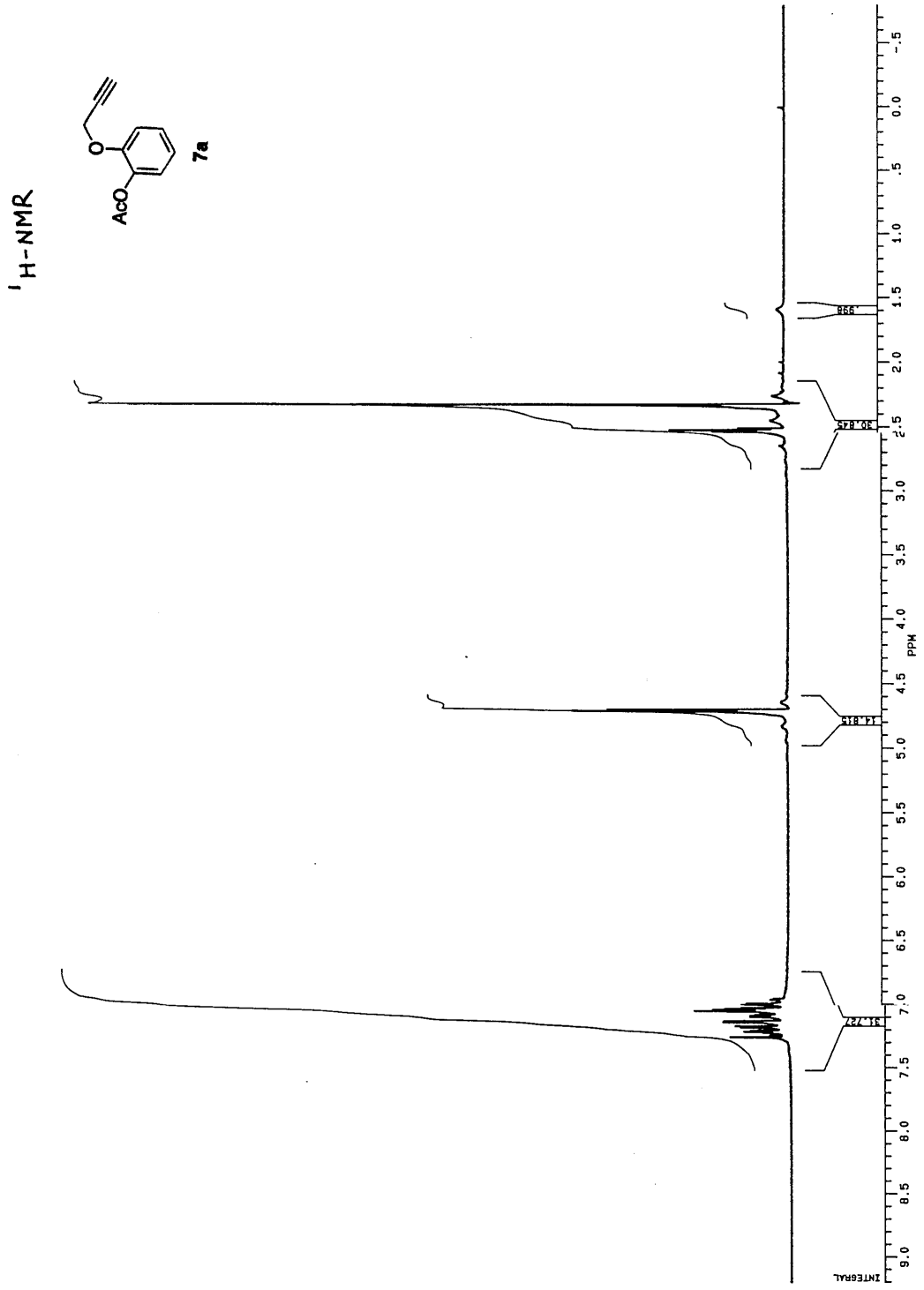
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O
7a
998
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31.727
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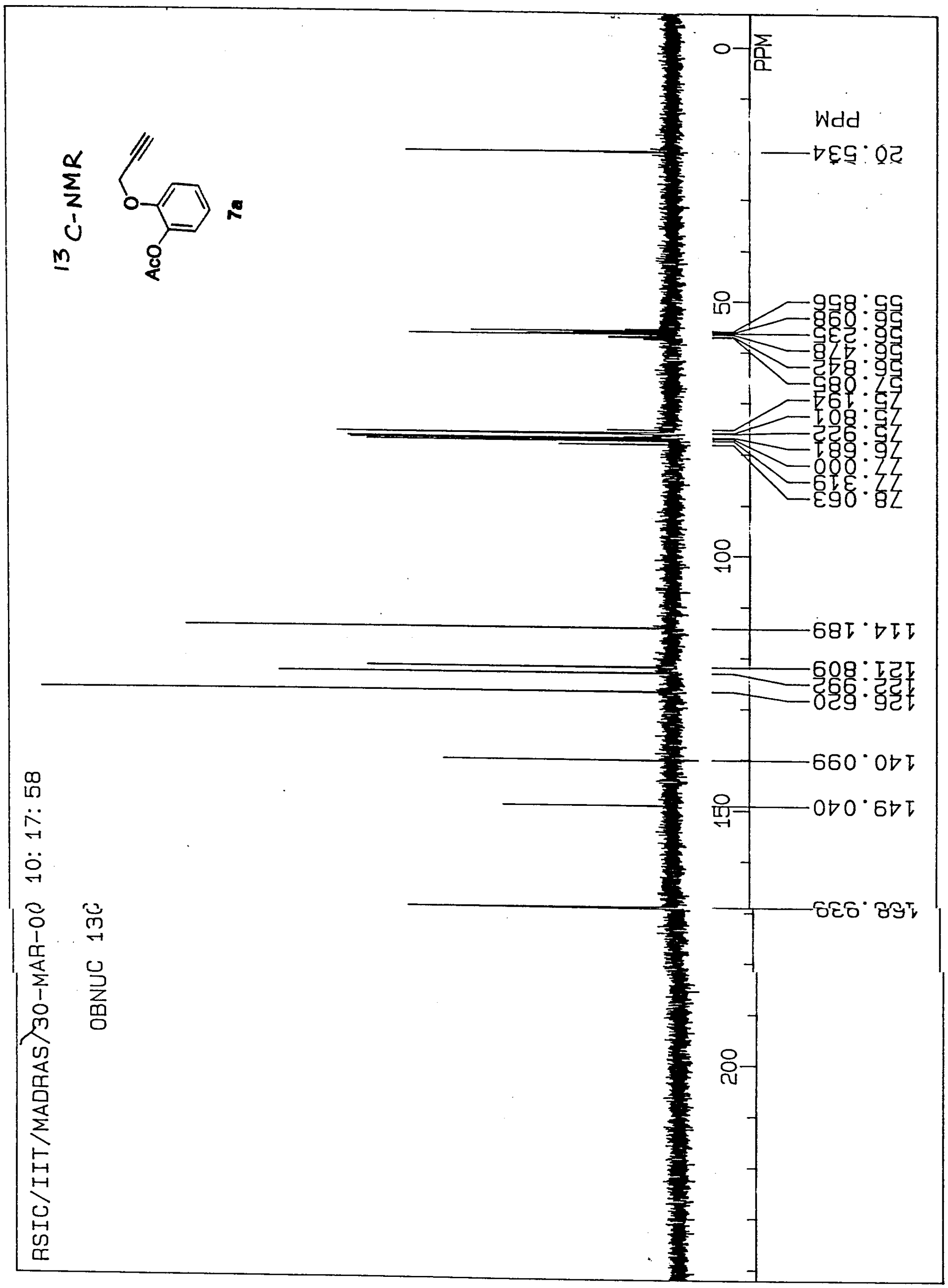

13C-NMR
AcO
7a
RSIC/IIT/MADRAS/30-MAR-00 10: 17: 58
OBNUC 13C
PPM
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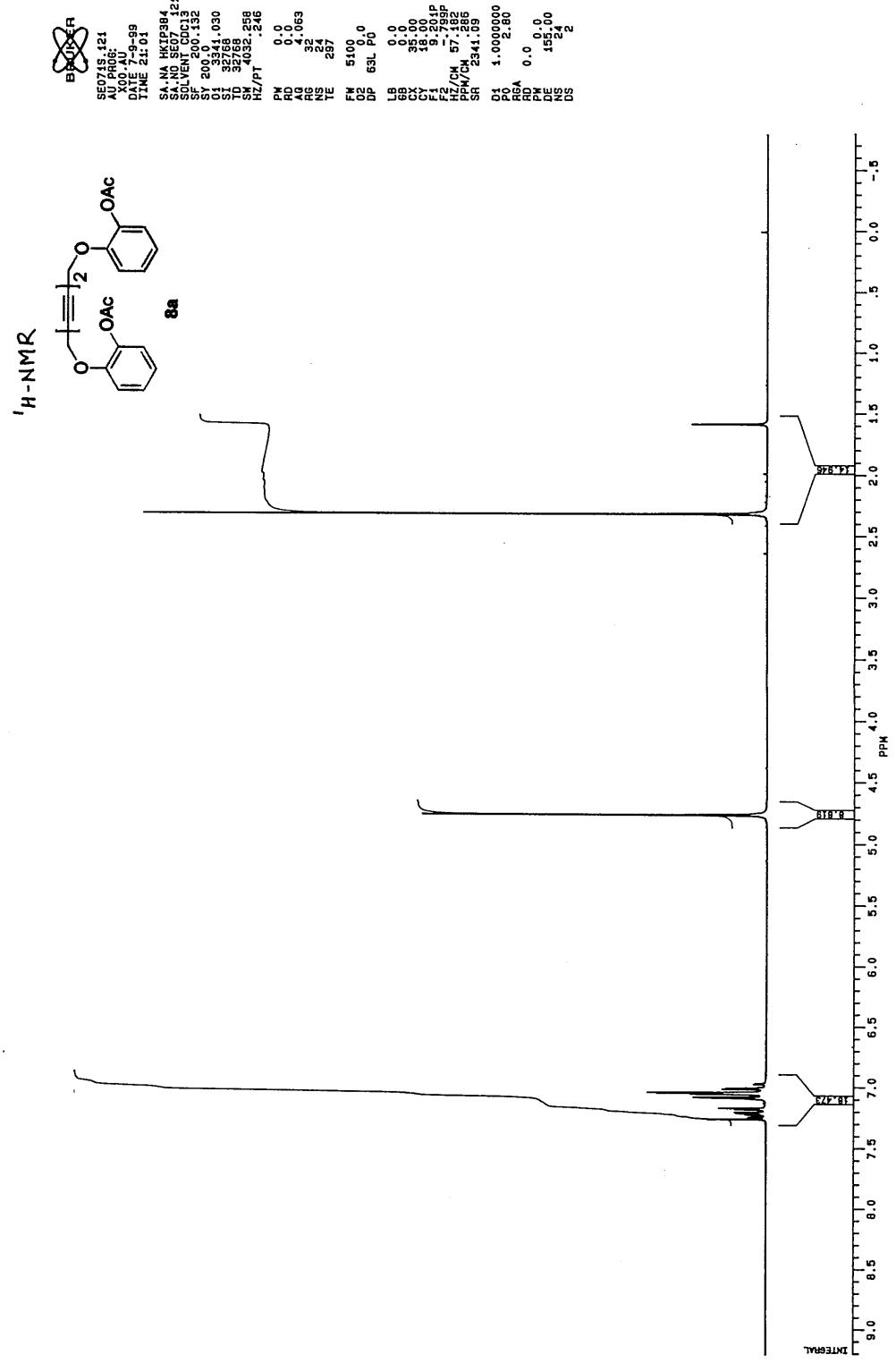
149.040
168.939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OAc
OAc
BRUKER
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DATE 7-9-99
TIME 21:01
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SI 32768
TD 32768
SW 4032.258
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AQ 4.063
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FW 5100
O2 0.0
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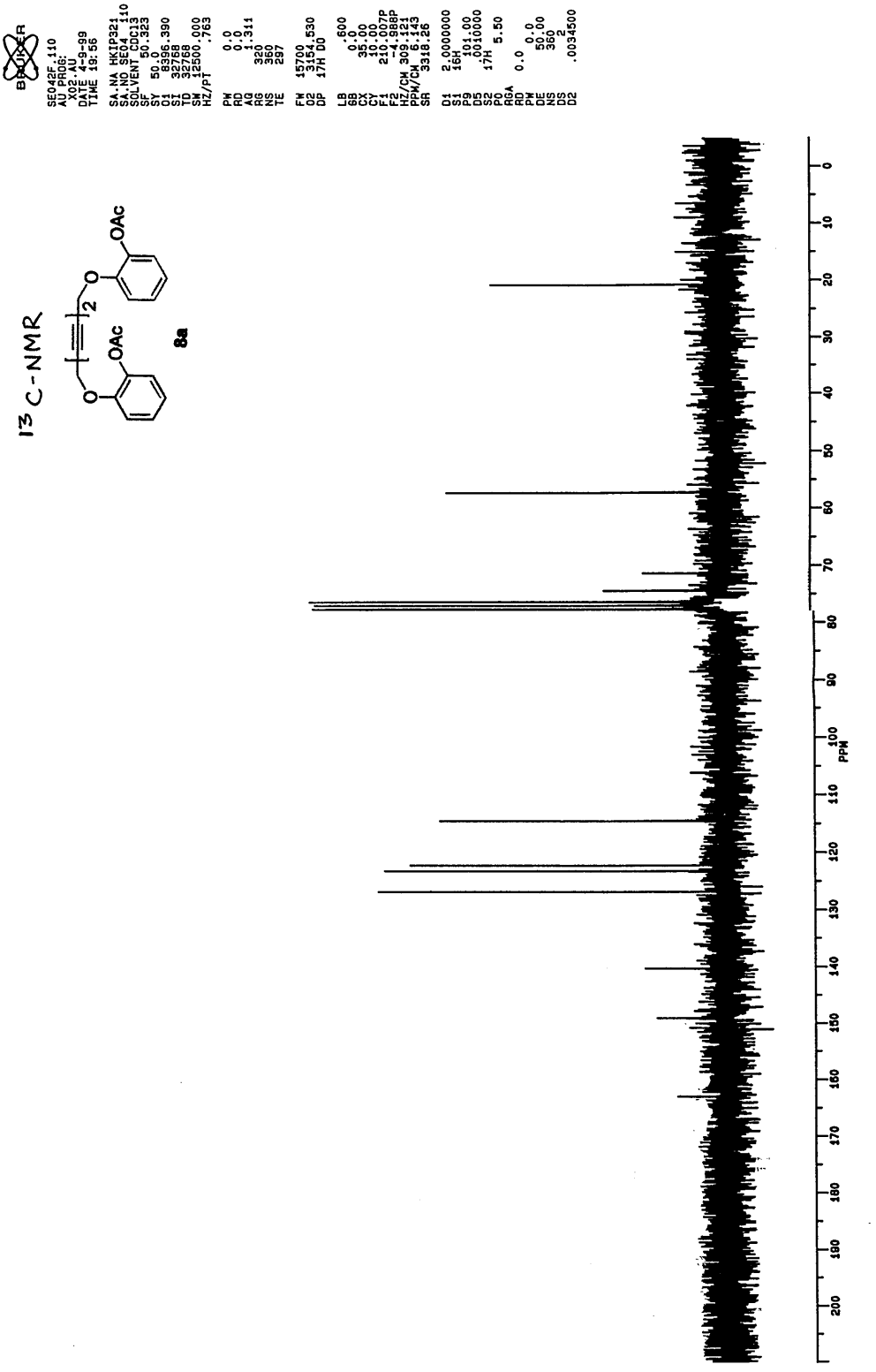
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8a
OAc
OAc
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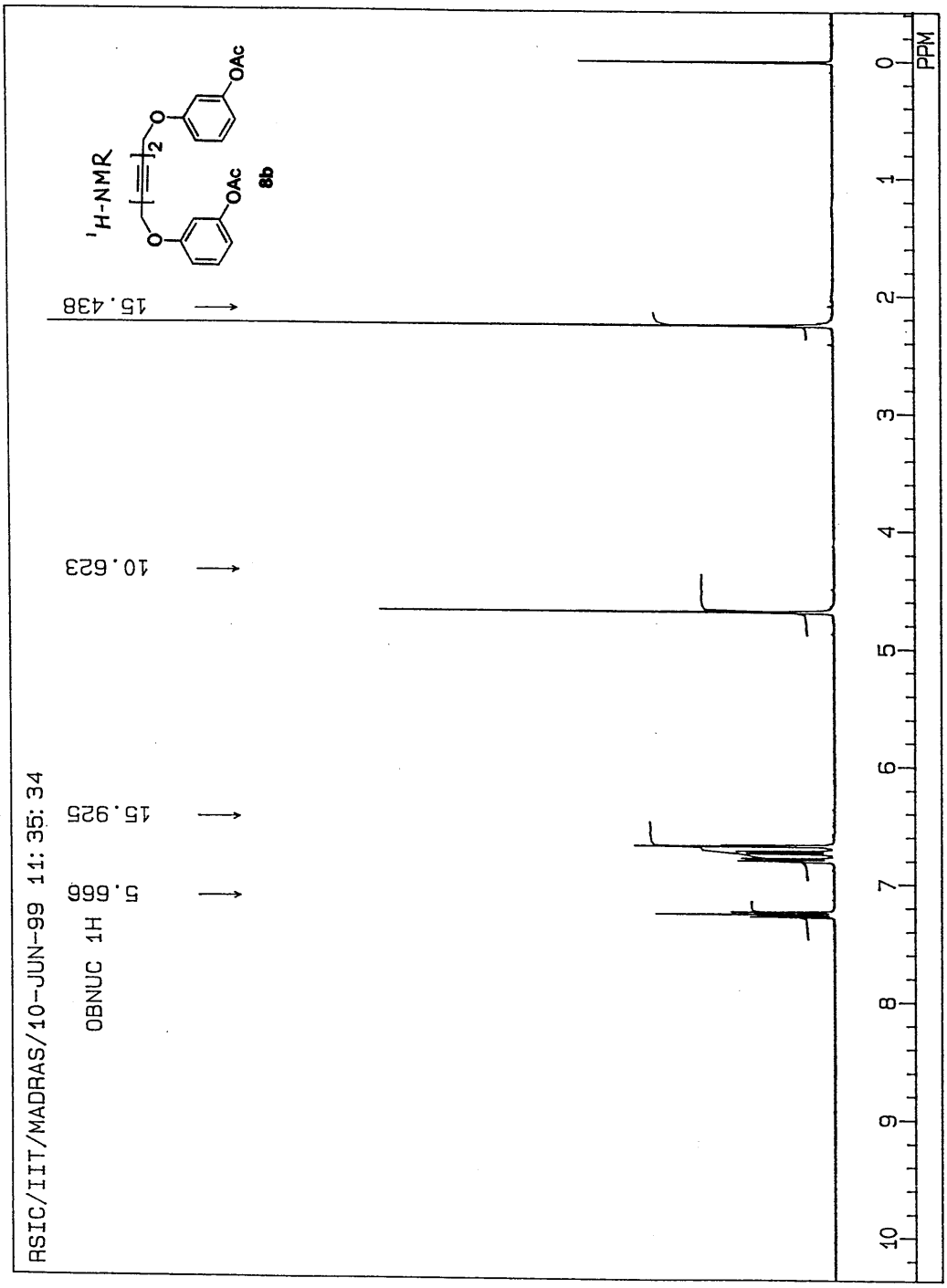
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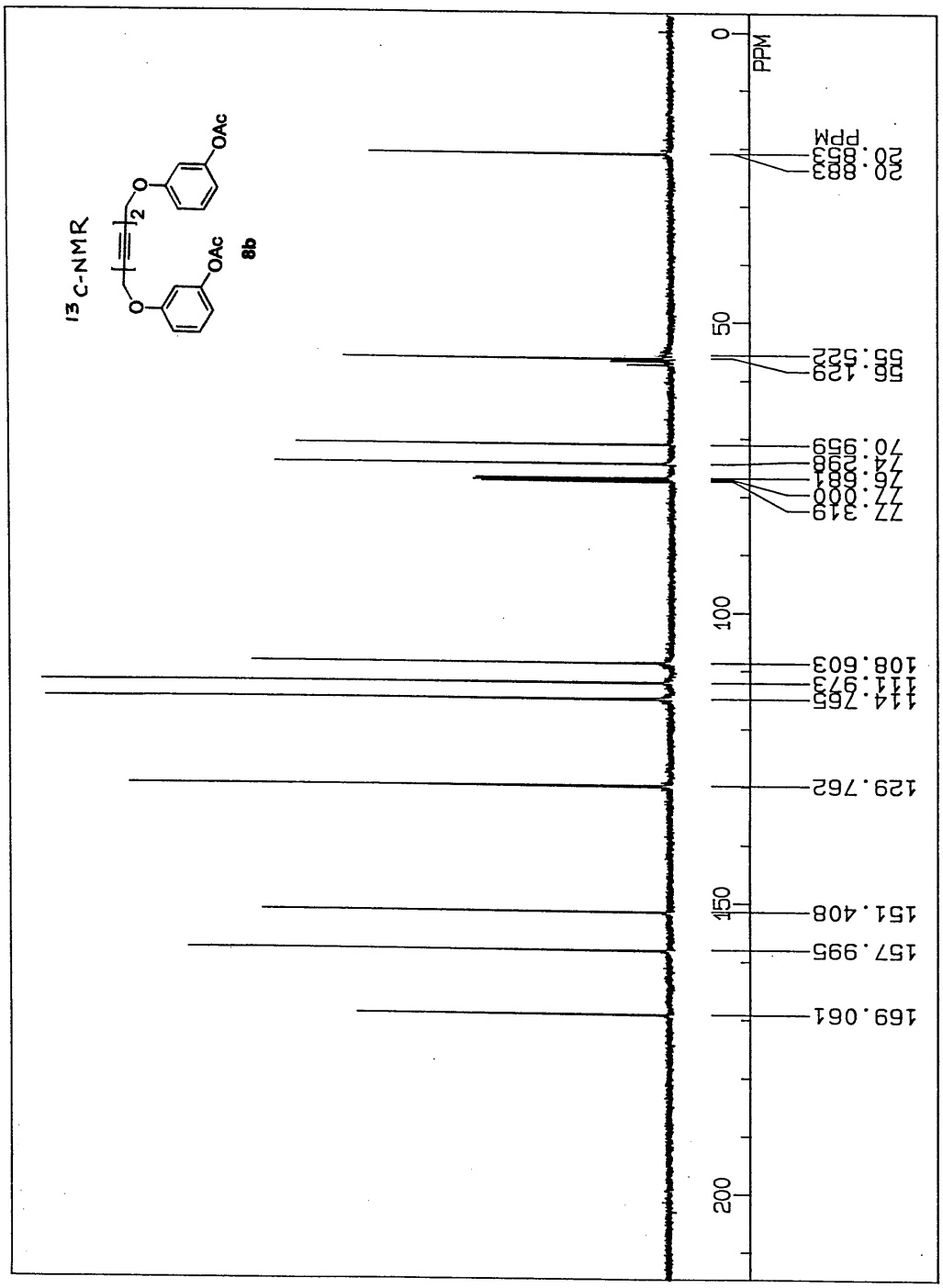
OAc
OAc
8b
PPM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OAc
8b
PPM
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50
100
150
200
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55.529
55.429
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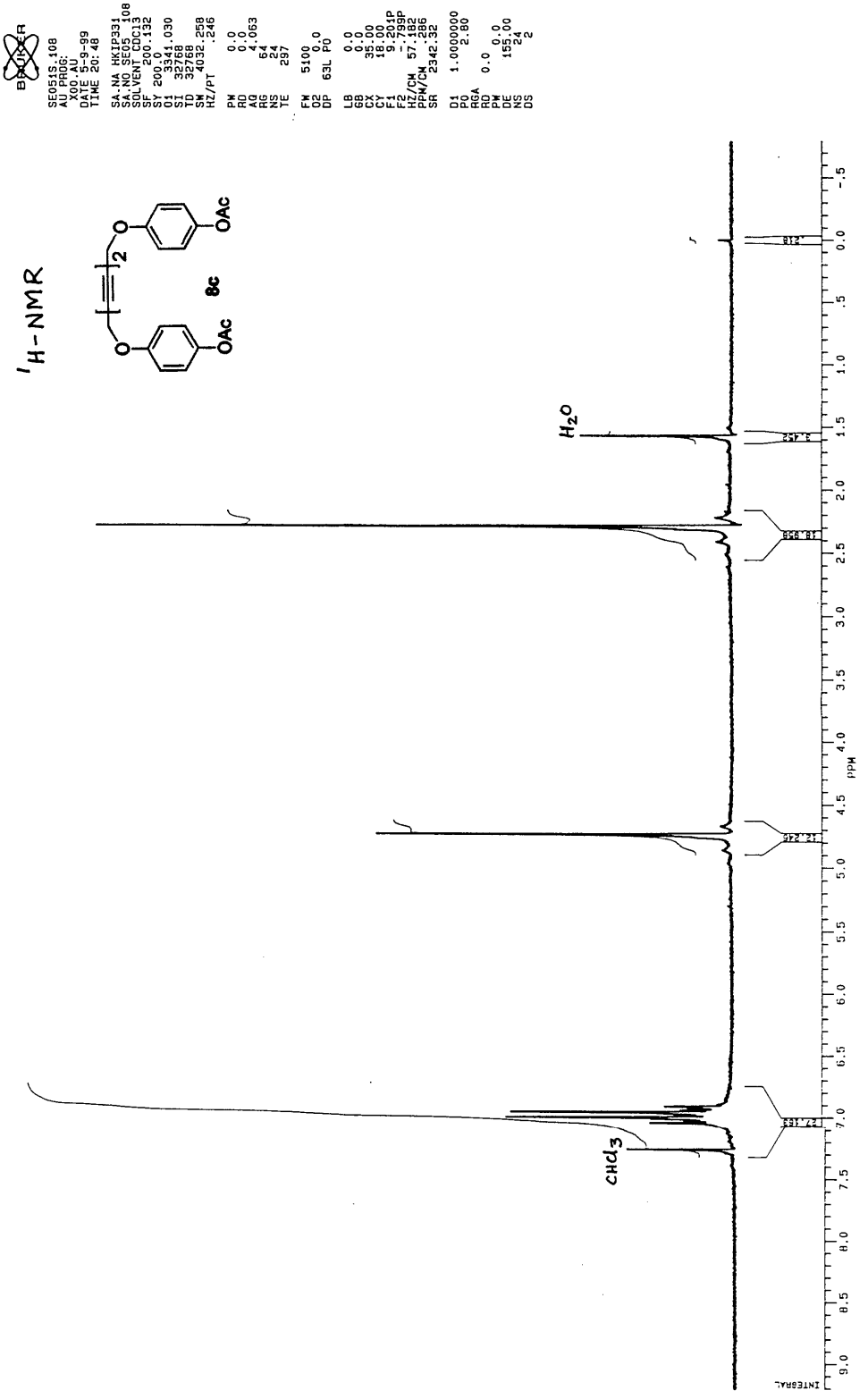
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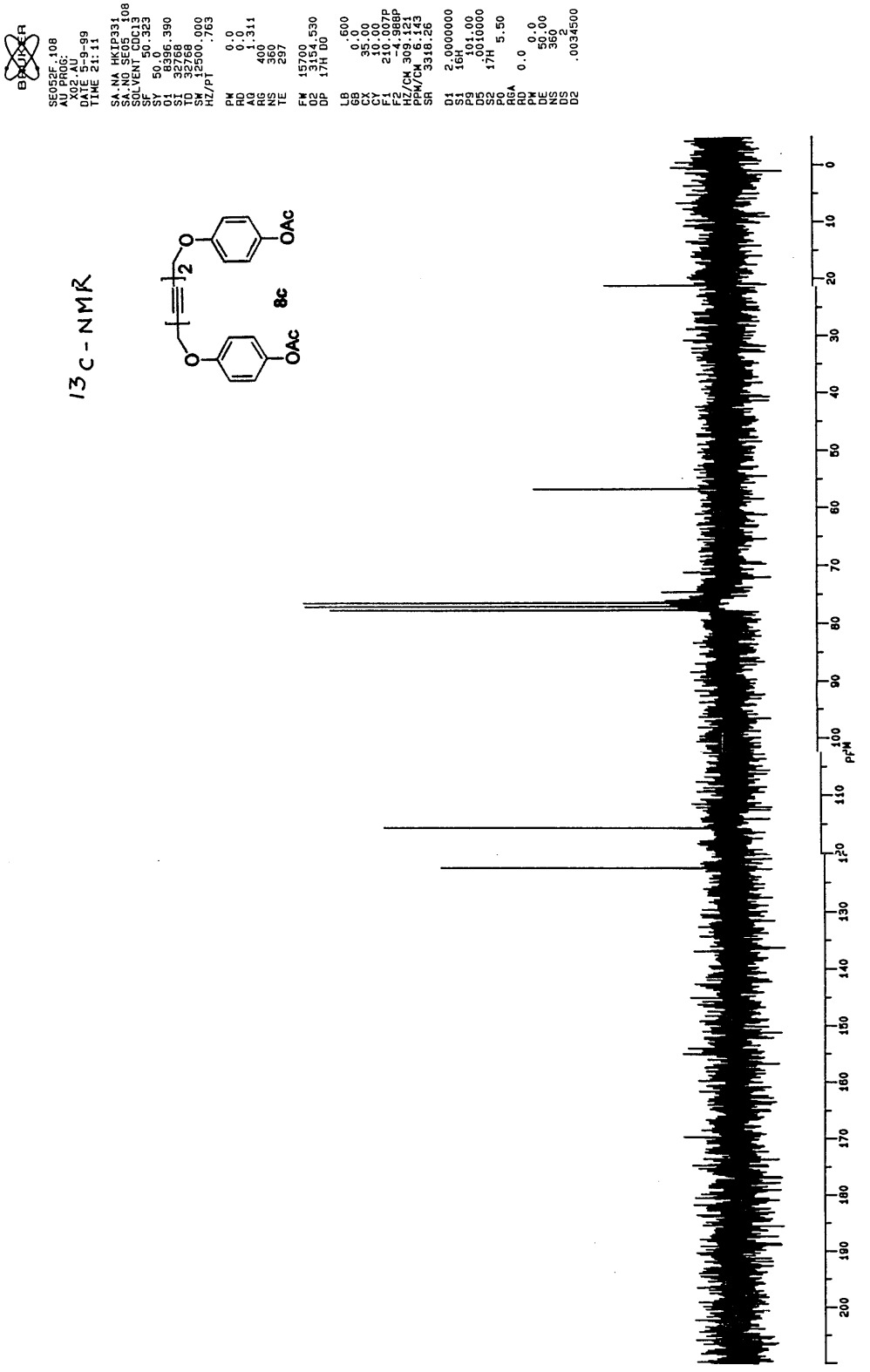
8c
OAc
OAc
H_2O
$CHCl_3$
ppm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TD 32768
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CY 210.007P
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PPM/CM 6.143
SR 3318.26
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P9 101.00
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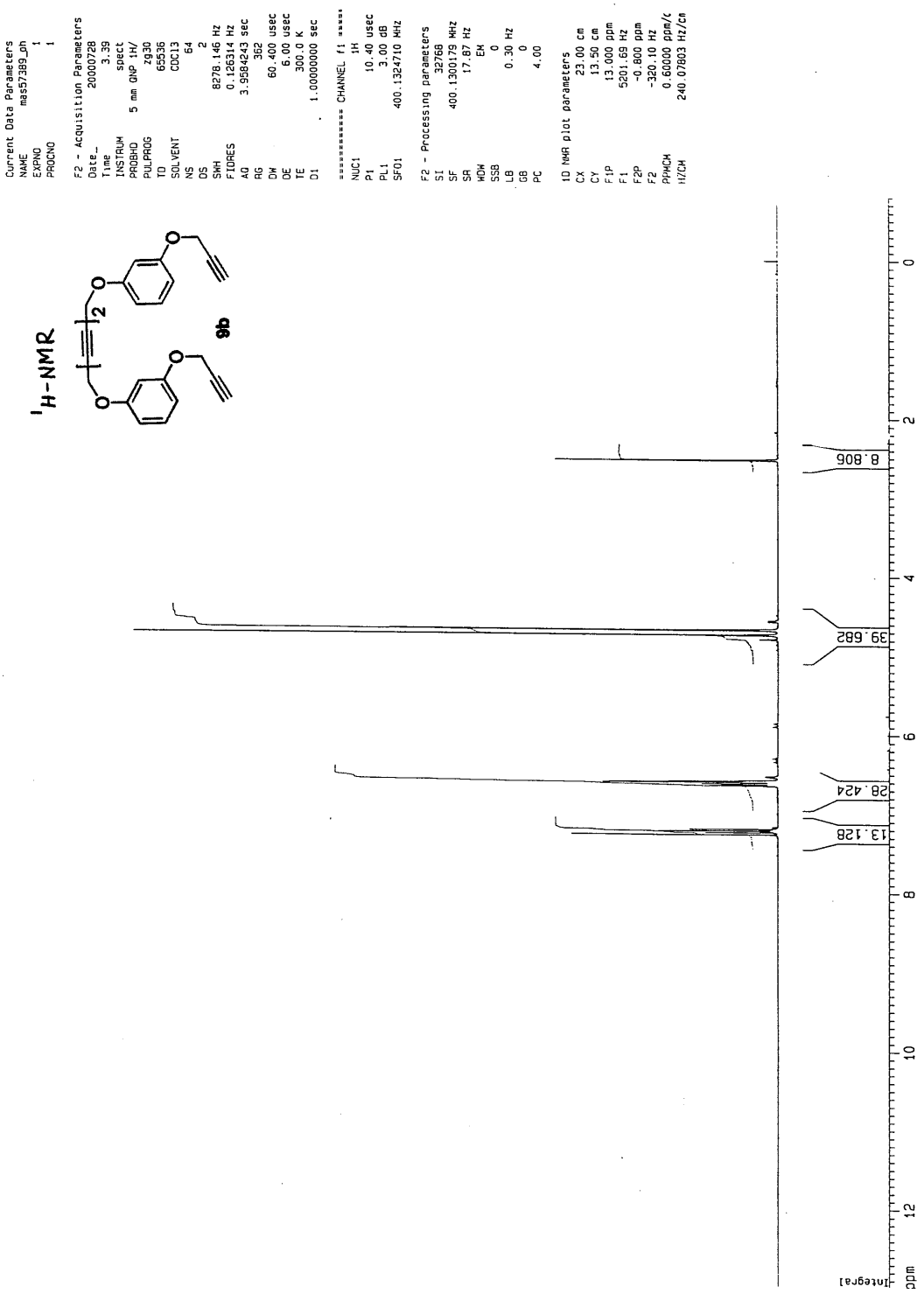
D2
PPM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PROCNO 1
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
========== CHANNEL f1 =====
NUC1 1H
P1 10.40 usec
PL1 3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300179 MHz
SR 17.87 Hz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
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CY 13.50 cm
F1P 13.000 ppm
F1 5201.69 Hz
F2P -0.800 ppm
F2 -320.10 Hz
PPMCM 0.60000 ppm/c
HZCM 240.07803 Hz/cm
1H-NMR
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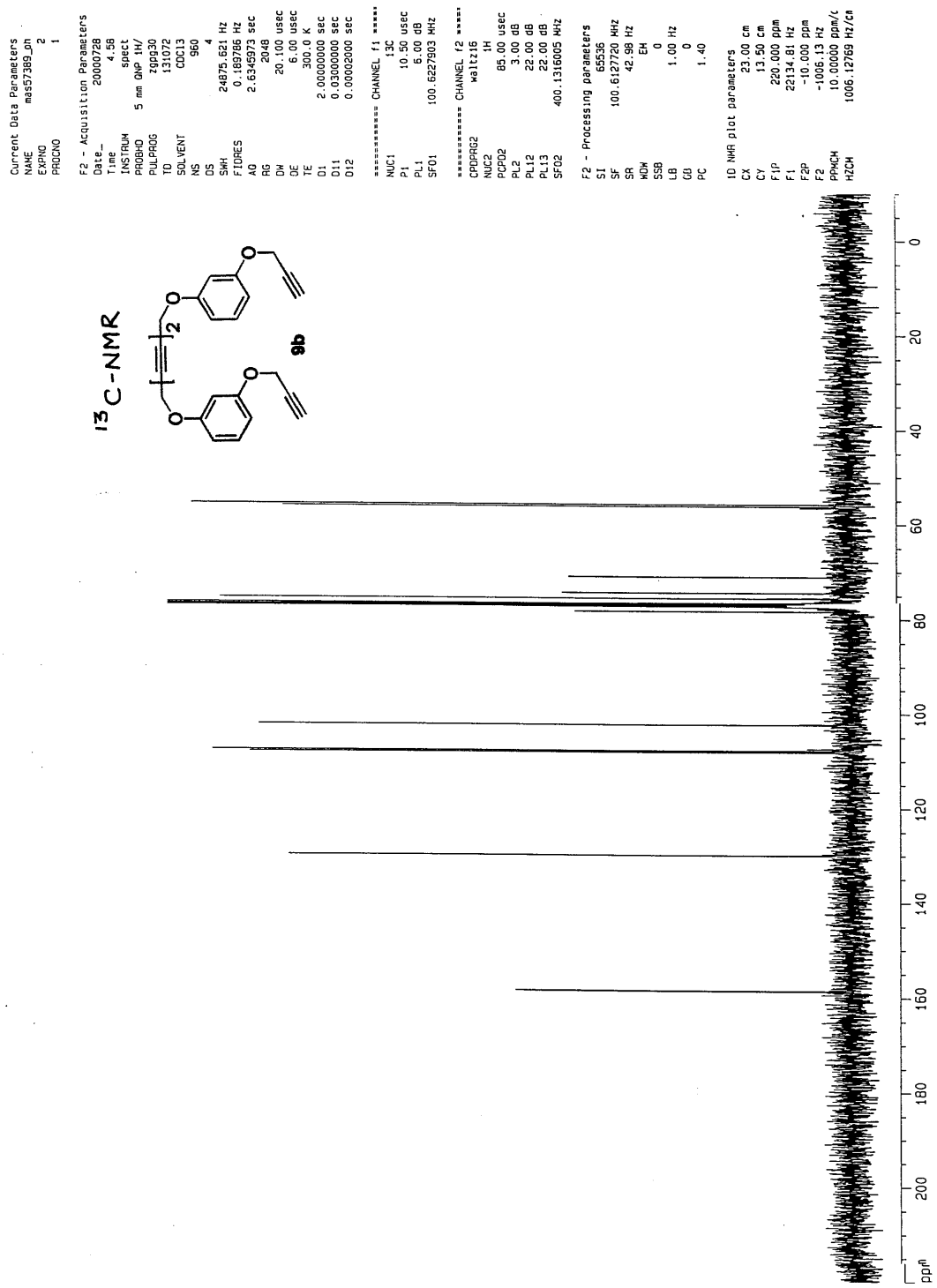
39.682
28.424
13.128
Integral
ppm
0
2
4
6
8
10
12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PROCNO 1
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Time 4.58
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PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 960
DS 4
SWH 24875.621 Hz
FIDRES 0.189766 Hz
AQ 2.6345973 sec
RG 2048
DW 20.100 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
========== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 6.00 dB
SFO1 100.6227903 MHz
========== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 85.00 usec
PL2 3.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
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SR 42.98 Hz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
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CY 13.50 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P -10.000 ppm
F2 -1006.13 Hz
PPMCM 10.00000 ppm/c
HZCM 1006.12769 Hz/cm
13C-NMR
9b
ppm
0
20
40
60
80
100
120
140
160
180
200