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Lewis Acid-Promoted Reactions of 3-Methoxy-*N*-phenylsulfonyl-1,4-benzoquinone**Monoimide with Propenylbenzenes**

Thomas A. Engler and Cynthia M. Scheibe

Department of Chemistry, University of Kansas
Lawrence, KS 66045**Supporting Information**

Complete IR and mass spectral data for all new compounds.

***N*-(2,4-dimethoxyphenyl)benzenesulfonamide:** IR (CHCl₃) 3343, 2948, 2840, 1607, 1506, 1456, 1395, 1342, 1308, 1162, 1123, 1092, 1037, 940, 893. EIMS *m/z* (relative intensity) 294 (3), 293 (M⁺, 16), 153 (12), 152 (100), 124 (23), 122 (22), 109 (17), 93 (27), 92 (16), 79 (13), 77 (41), 52 (21), 51 (35).

5: IR (CHCl₃) 1650, 1630, 1588, 1451, 1324, 1158, 1119, 1090, 1002, 864, 640. EIMS *m/z* (relative intensity) 278 (M⁺+1), 2), 136 (99), 80 (30), 77 (100), 69 (34), 52 (27), 51 (53).

6a: IR (CH₂Cl₂) 3332, 3012, 2912, 2839, 1616, 1514, 1492, 1392, 1336, 1169, 1109, 1091, 1030, 994, 943, 875, 829, 631. EIMS (relative intensity) *m/z* 425 (M⁺, 31), 285 (28), 284 (100), 253 (26), 252 (20), 121 (36), 91 (11), 84 (13), 77 (44), 69 (11), 49 (23).

6b: IR (CH₂Cl₂) 3331, 3013, 2901, 1613, 1515, 1491, 1465, 1392, 1334, 1164, 1141, 1114, 1091, 1026, 995, 927, 864, 827, 622. EIMS (relative intensity) *m/z* 455 (M⁺, 10), 314 (11), 283 (12), 282 (14), 86 (28), 84 (44), 77 (10), 51 (35), 49 (100), 47 (15).

6c: IR (CH₂Cl₂) 3331, 3013, 2896, 1619, 1494, 1392, 1336, 1170, 1100, 1039, 995, 944, 867, 824, 621. EIMS (relative intensity) *m/z* 439 (M⁺, 14), 299 (100), 298 (42), 268 (19), 267 (77), 266 (63), 240 (11), 239 (21), 238 (14), 237 (10), 236 (38), 208 (10), 135 (31), 91 (16), 78 (18), 77 (100), 69 (23), 65 (12), 51 (38).

6d: IR (CH₂Cl₂) 3332, 2900, 1620, 1491, 1337, 1167, 1091, 1025, 995, 927, 873. EIMS (relative intensity) *m/z* 409 (M⁺, 10), 269 (17), 268 (80), 237 (28), 236 (25), 221 (12), 119 (10), 117 (13), 115 (13), 105 (37), 91 (24), 86 (25), 85 (11), 84 (47), 79 (10), 78 (13), 77 (65), 69 (31), 57 (40), 56 (12), 55 (36), 53 (10), 51 (52), 50 (10), 59 (100), 48 (10), 47 (18), 43 (49).

6e: IR (CH₂Cl₂) 3332, 2901, 1621, 1492, 1393, 1335, 1164, 1091, 1025, 996, 957, 875, 827, 629. EIMS (relative intensity) *m/z* 395 (M⁺, 16), 388 (20), 255 (25), 254 (100), 223 (21), 222 (21), 117 (13), 115 (14), 105 (19), 103 (15), 91 (51), 78 (13), 77 (77), 69 (21), 57 (16), 55 (17), 51 (29), 49 (10), 43 (20).

6f: IR (CH₂Cl₂) 3332, 2902, 1616, 1491, 1392, 1336, 1164, 1106, 1091, 1024, 995, 952, 827. EIMS (relative intensity) *m/z* 409 (M⁺, 10), 269 (20), 268 (100), 237 (26), 236 (26), 221 (12), 105 (28), 91 (15), 77 (39), 69 (12), 51 (15).

7d: IR (CH₂Cl₂) 3053, 2934, 2869, 1748, 1692, 1608, 1514, 1452, 1380, 1340, 1162, 1089, 1069, 1043, 988, 890, 817, 696, 612. EIMS (relative intensity) *m/z* 541 (M⁺, 3), 401 (42), 400 (100), 268 (17), 145 (11), 132 (15), 131 (10), 119 (17), 117 (25), 115 (16), 112 (15), 105 (56), 91 (19), 84 (15), 78 (10), 77 (45), 51 (23).

7e: IR (CH₂Cl₂) 3064, 2959, 2829, 1750, 1693, 1494, 1453, 1345, 1255, 1162, 1090, 1045, 989, 910, 885, 696, 613. EIMS (relative intensity) *m/z* 513 (M⁺, 5), 373 (21), 372 (100), 254 (20), 131 (12), 129 (10), 118 (17), 117 (23), 115 (15), 105 (20), 103 (12), 91 (61), 78 (11), 77 (54), 51 (13).

7f: IR (CH₂Cl₂) 3018, 2925, 1746, 1490, 1460, 1338, 1159, 1105, 1089, 1042, 988, 925, 880. EIMS (relative intensity) *m/z* 541 (M⁺, 1), 401 (41), 400 (100), 119 (11), 117 (22), 115 (19), 112 (11), 105 (47), 91 (22), 78 (18), 77 (29), 51 (12).

7g: IR (CH₂Cl₂) 2940, 2841, 1750, 1597, 1491, 1456, 1380, 1341, 1163, 1090, 1068, 1044, 1013, 989, 919, 881, 827. EIMS (relative intensity) *m/z* 581 [M⁺ (C₃₁H₂₉³⁵Cl₂NO₄S) 0.5], 444 (15), 443 (23), 442 (71), 441 (33), 440 (100), 288 (13), 165 (12), 152 (11), 141 (15), 139 (23), 127 (24), 125 (64), 117 (16), 115 (18), 112 (16), 84 (11), 77 (58), 69 (19), 57 (14), 55 (13), 51 (18), 49 (15), 43 (16).

8d: IR (CH₂Cl₂) 2915, 1747, 1711, 1515, 1347, 1161, 1091, 979. EIMS (relative intensity) *m/z* 541 (M⁺, 0.1), 401 (32), 400 (100), 268 (18), 145 (10), 141 (10), 132 (30), 131 (18), 129 (13), 128 (12), 119 (19), 117 (50), 115 (35), 112 (22), 110 (47), 105 (88), 103 (11), 91

(39), 84 (16), 79 (13), 78 (29), 77 (88), 69 (27), 66 (25), 65 (28), 64 (15), 63 (13), 57 (19), 55 (21), 53 (12), 51 (50), 50 (23).

8e: IR (CH₂Cl₂) 3028, 2933, 2871, 2837, 1746, 1694, 1603, 1492, 1455, 1341, 1161, 1116, 1090, 1053, 1031, 1002, 978, 944, 920, 881, 830, 615. EIMS (relative intensity) *m/z* 513 (M^+ , 0.5), 373 (30), 372 (100), 254 (25), 117 (20), 115 (16), 112 (11), 105 (21), 103 (12), 91 (56), 77 (49), 51 (19).

8f: IR (CH₂Cl₂) 2954, 1746, 1604, 1440, 1344, 1160, 1091, 1056, 978, 895, 728, 617. EIMS (relative intensity) *m/z* 542 ($M^+ + 1$, 2), 401 (39), 400 (100), 268 (15), 119 (10), 117 (16), 115 (16), 105 (48), 91 (30), 84 (10), 78 (20), 77 (77), 69 (15), 65 (12), 57 (11), 55 (14), 51 (28), 43 (18).

8g: IR (CH₂Cl₂) 2909, 1749, 1604, 1491, 1343, 1264, 1162, 1091, 1013, 738. IR (CHCl₃) 2914, 1743, 1604, 1492, 1344, 1158, 1092, 980, 857. EIMS (relative intensity) *m/z* 581 [M^+ (C₃₁H₂₉³⁵Cl₂NO₄S), <1], 441 (13), 440 (43), 288 (12), 149 (11), 125 (25), 117 (10), 115 (10), 86 (22), 85 (10), 84 (36), 77 (33), 71 (14), 69 (14), 57 (36), 55 (21), 51 (41), 49 (100), 47 (18), 43 (22).

9g: IR (CH₂Cl₂) 2900, 1751, 1655, 1492, 1327, 1091, 1014, 856, 636. FABMS *m/z* 582.3 ($M^+ + 1$, C₃₁H₃₀³⁵Cl₂NO₄S).

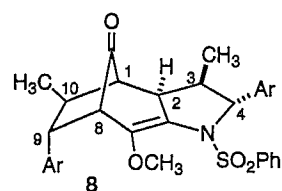
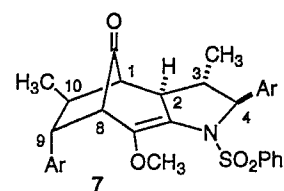
15: IR (CHCl₃) 2930, 1744, 1600, 1457, 1332, 1155, 991, 880. EIMS (relative intensity) *m/z* 543 (M^+ , 2), 403 (33), 402 (100), 121 (20), 112 (19), 105 (14), 91 (47), 86 (14), 84 (23), 77 (30), 69 (13), 58 (10), 56 (11), 52 (13), 50 (11), 45 (17), 43 (14).

16: IR (thin film on NaCl) 2944, 1747, 1611, 1512, 1451, 1344, 1248, 1126, 1095, 1033, 976, 907, 840, 727, 694. EIMS (relative intensity) *m/z* 543 (M^+ , 1), 403 (34), 402 (100), 121 (18), 117 (13), 115 (11), 112 (24), 91 (55), 86 (12), 84 (20), 78 (10), 77 (34), 69 (14), 56 (16), 52 (15), 50 (10), 45 (32), 43 (18).

17: IR (CH₂Cl₂) 3305, 2962, 1770, 1678, 1621, 1493, 1451, 1361, 1304, 1171, 1141, 1088, 1026, 927, 867. EIMS (relative intensity) *m/z* 381 (M^+ , 6), 325 (10), 240 (29), 212 (37),

184 (23), 141 (12), 131 (30), 118 (30), 117 (33), 115 (20), 105 (10), 103 (37), 91 (33), 84 (11), 81 (12), 80 (16), 78 (18), 77 (100), 65 (11), 54 (17), 53 (17), 51 (45), 50 (10), 49 (25).

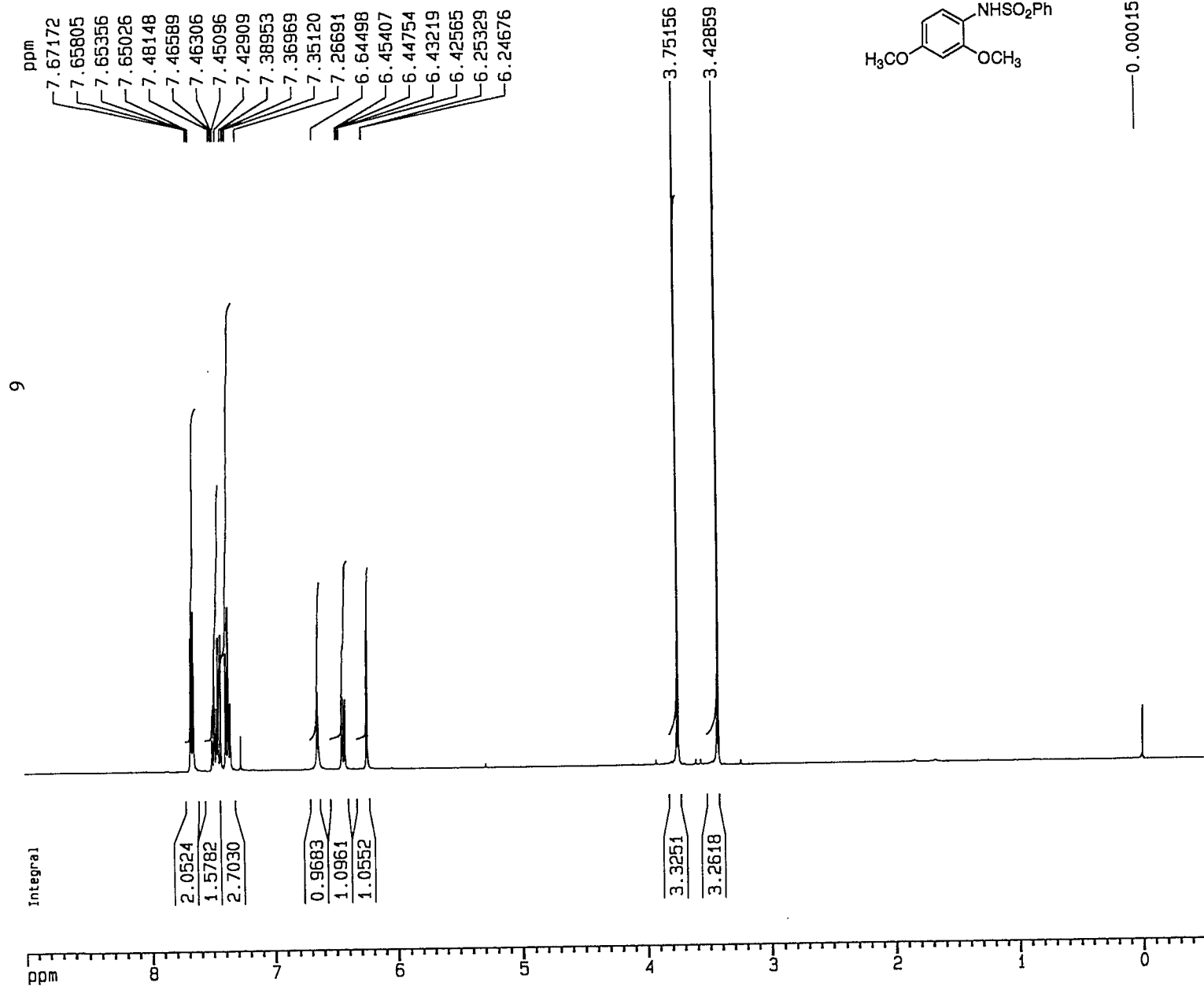
21: IR (CH₂Cl₂) 3327, 2940, 1621, 1491, 1338, 1162, 1114, 1034, 925, 845. EIMS: *m/z* (relative intensity) 439 (M⁺, 38), 299 (30), 298 (100), 283 (27), 77 (59), 51 (32), 49 (30).



d, Ar=C₆H₄-4-CH₃
e, Ar=C₆H₅
f, Ar=C₆H₄-2-CH₃
g, Ar=C₆H₄-4-Cl

Table. Selected ¹H Resonances and Coupling Constants for **7e-g** and **8e-g**.

	H-1	H-2	<i>J</i> H ₁ /H ₂	H-3	<i>J</i> H ₂ /H ₃	H-4	<i>J</i> H ₃ /H ₄	C-3 Me	<i>J</i> H ₃ /Me	H-8	<i>J</i> H ₈ /H ₁	H-9	<i>J</i> H ₉ /H ₉	H-10	<i>J</i> H ₉ /H ₁₀	C-10 Me	<i>J</i> H ₁₀ /Me	<i>J</i> H ₁₀ /H ₁
	ppm	ppm	Hz	ppm	Hz	ppm	Hz	ppm	Hz	ppm	Hz	ppm	Hz	ppm	Hz	ppm	Hz	Hz
7e	2.11	2.66	0	1.86	11.3	4.72	9.1	1.13	6.4	2.97	1.4	3.19	6.6	2.48	6.7	1.18	6.9	0
7d	2.06	2.59	0	1.80	11.4	4.63	9.1	1.06	6.4	2.91	1.5	3.12	6.7	2.41	6.6	1.13	6.9	0
7f	2.13	2.84	0	1.94	11.4	5.12	9.1	1.13	6.3	2.94	1.5	3.47	6.6	2.58	6.3	1.14	6.8	0
7g	2.12	2.70	0	1.78	10.8	4.71	9.2	1.11	6.4	2.95	1.3	3.15	6.6	2.41	6.7	1.16	6.9	0
8e	1.92	3.35	0	2.35	5.6	5.16	0	1.10	6.9	2.76	1.5	3.12	7.2	2.22	5.2	1.00	6.9	0
8d	1.90	3.35	0	2.31	5.4	5.13	0	1.07	7.0	2.74	1.5	3.07	7.2	2.18	5.0	0.98	7.0	0
8f	1.93	3.43	0	2.30	5.5	5.25	0	1.12	7.0	2.82	1.4	3.39	7.1	2.23	4.8	1.00	6.9	0
8g	1.93	3.25	0	2.30	5.4	5.12	0	1.10	7.0	2.78	1.4	3.09	7.2	2.15	5.0	1.00	7.0	0



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 PROCNO 1

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 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 90.5
 DW 104.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 7.70 usec
 DE 4.50 usec
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 NUC1 1H
 PL1 -6.00 dB

F2 - Processing parameters
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 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
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 HZCM 190.06175 Hz/cm

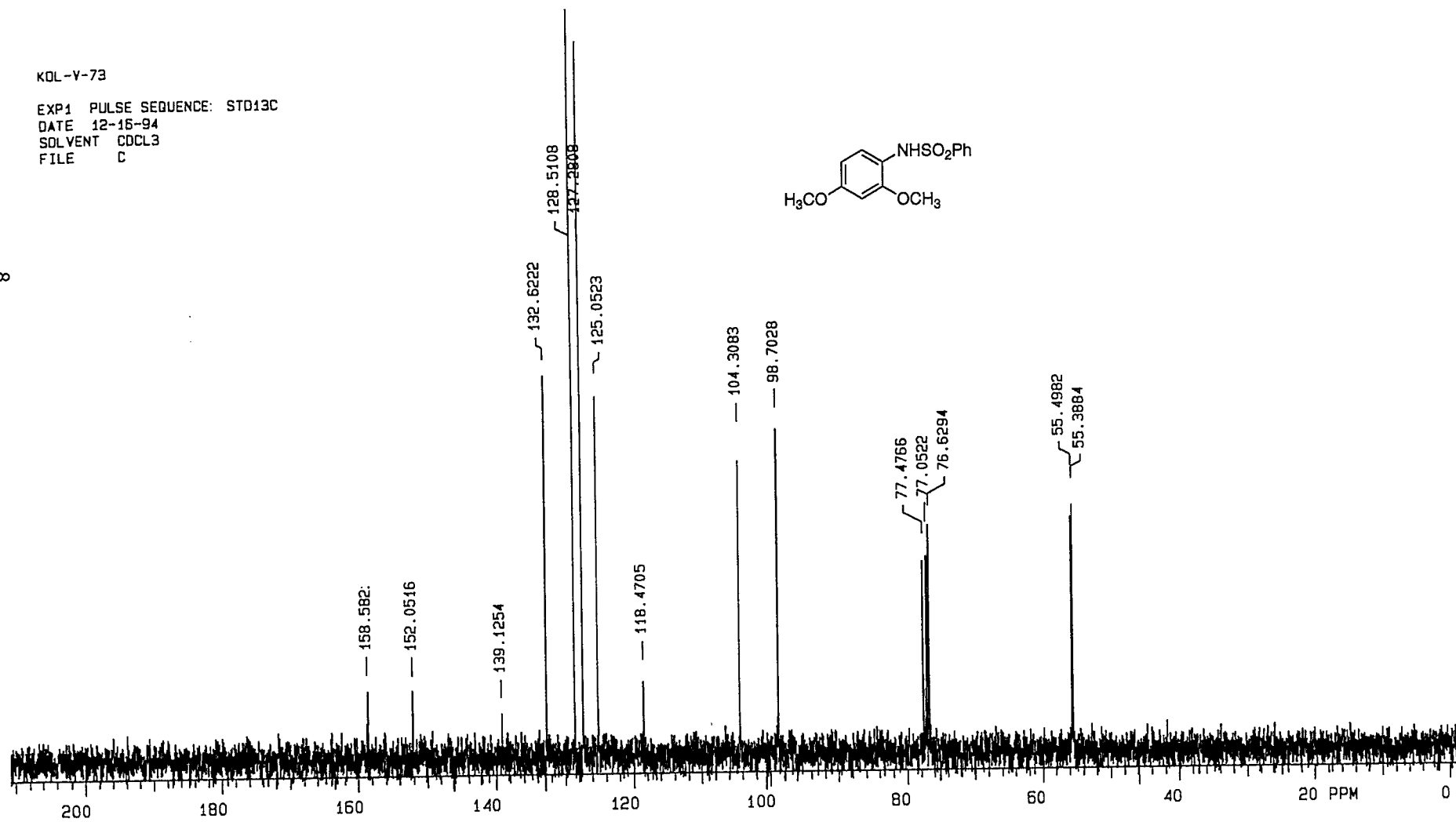


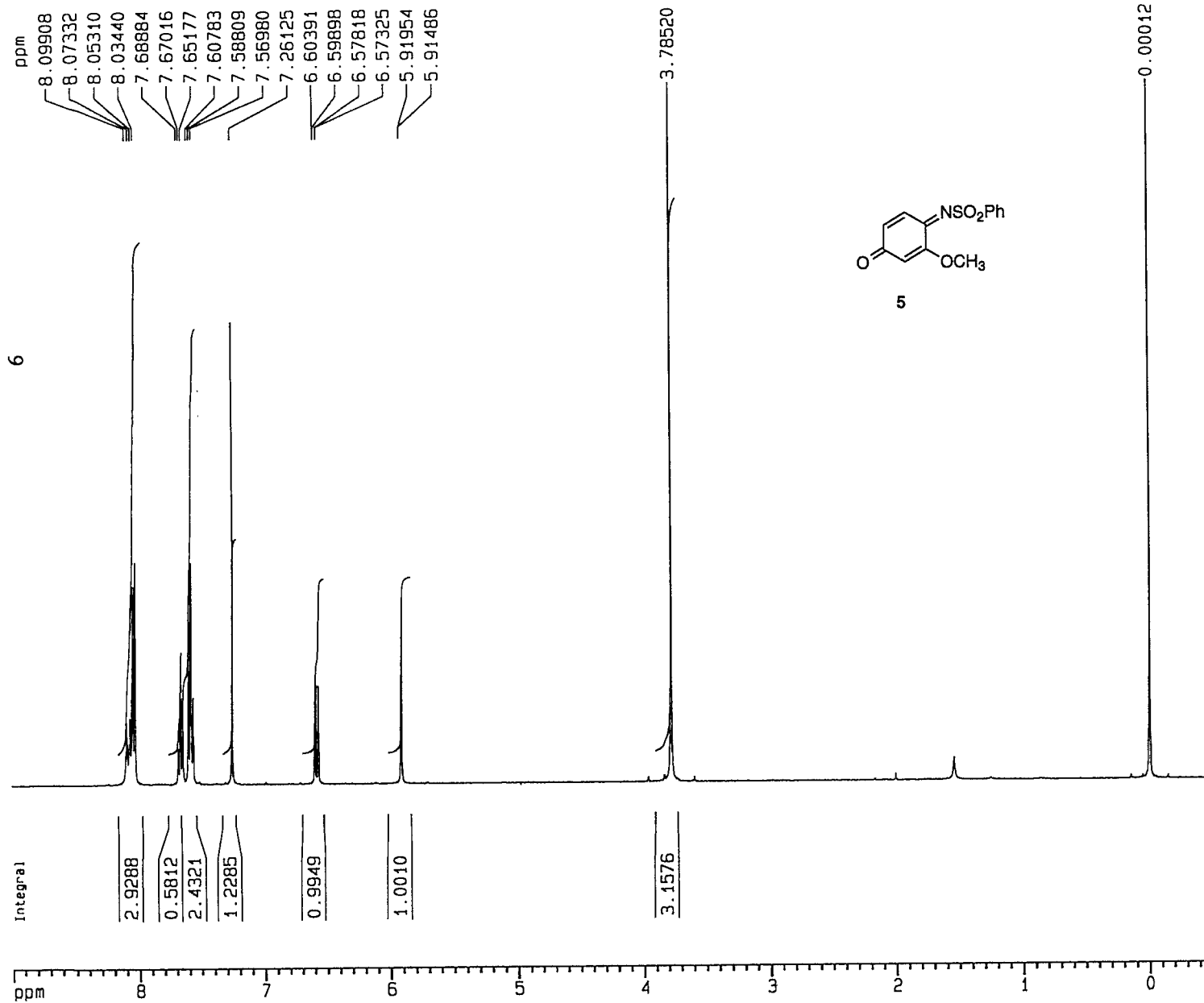
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DATE 11-07-94
SOLVENT DMSO
FILE H



KOL-V-73

EXP1 PULSE SEQUENCE: STD13C
DATE 12-15-94
SOLVENT CDCL3
FILE C





Current Data Parameters

NAME cms-1-225
EXPNO 1
PROCNO 1

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FIDRES 0.146157 Hz
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NUC1 1H
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F2 - Processing parameters

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GB 0
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1D NMR plot parameters

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HZCM 190.06175 Hz/cm

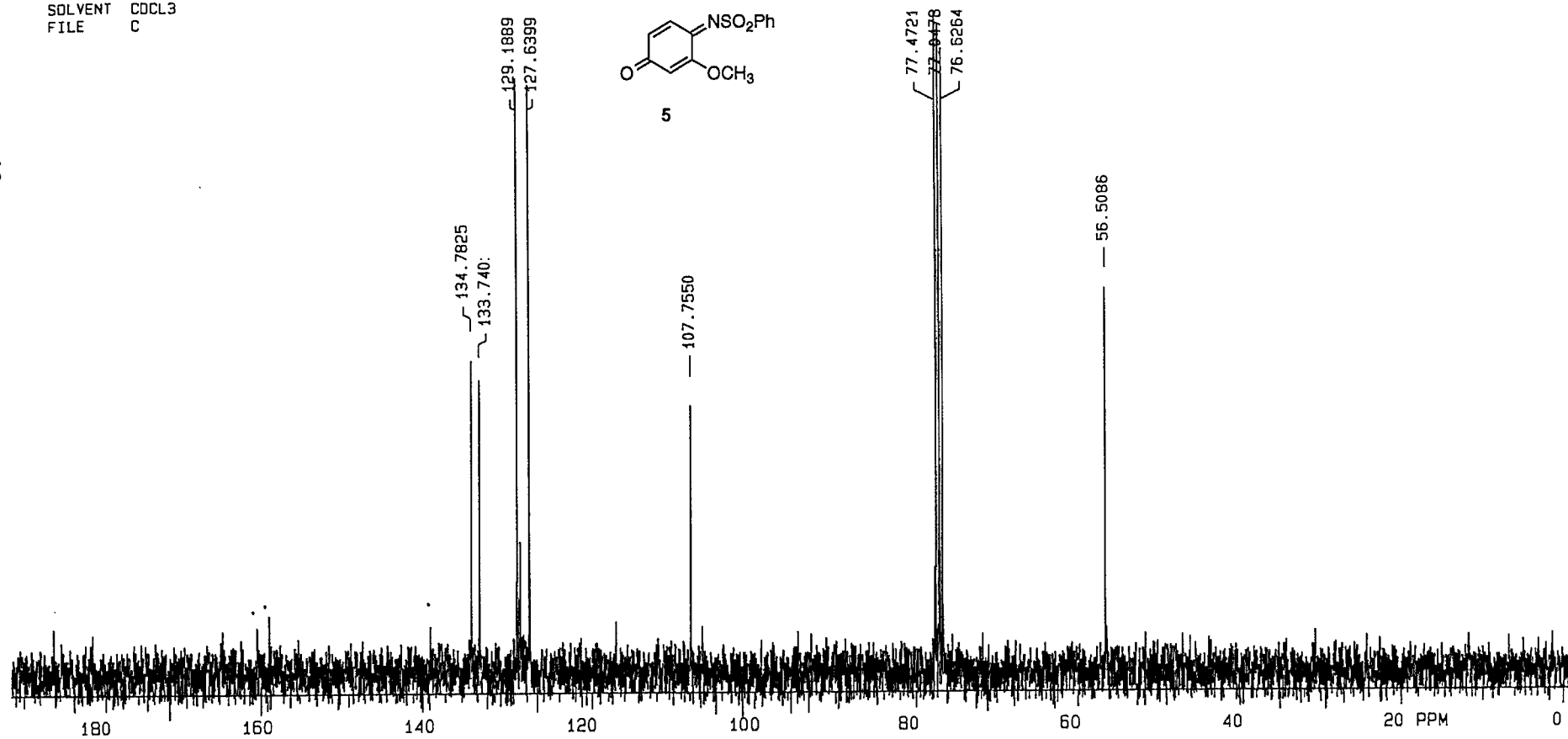
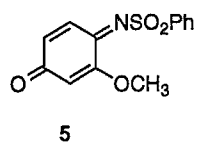
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DATE 02-11-94

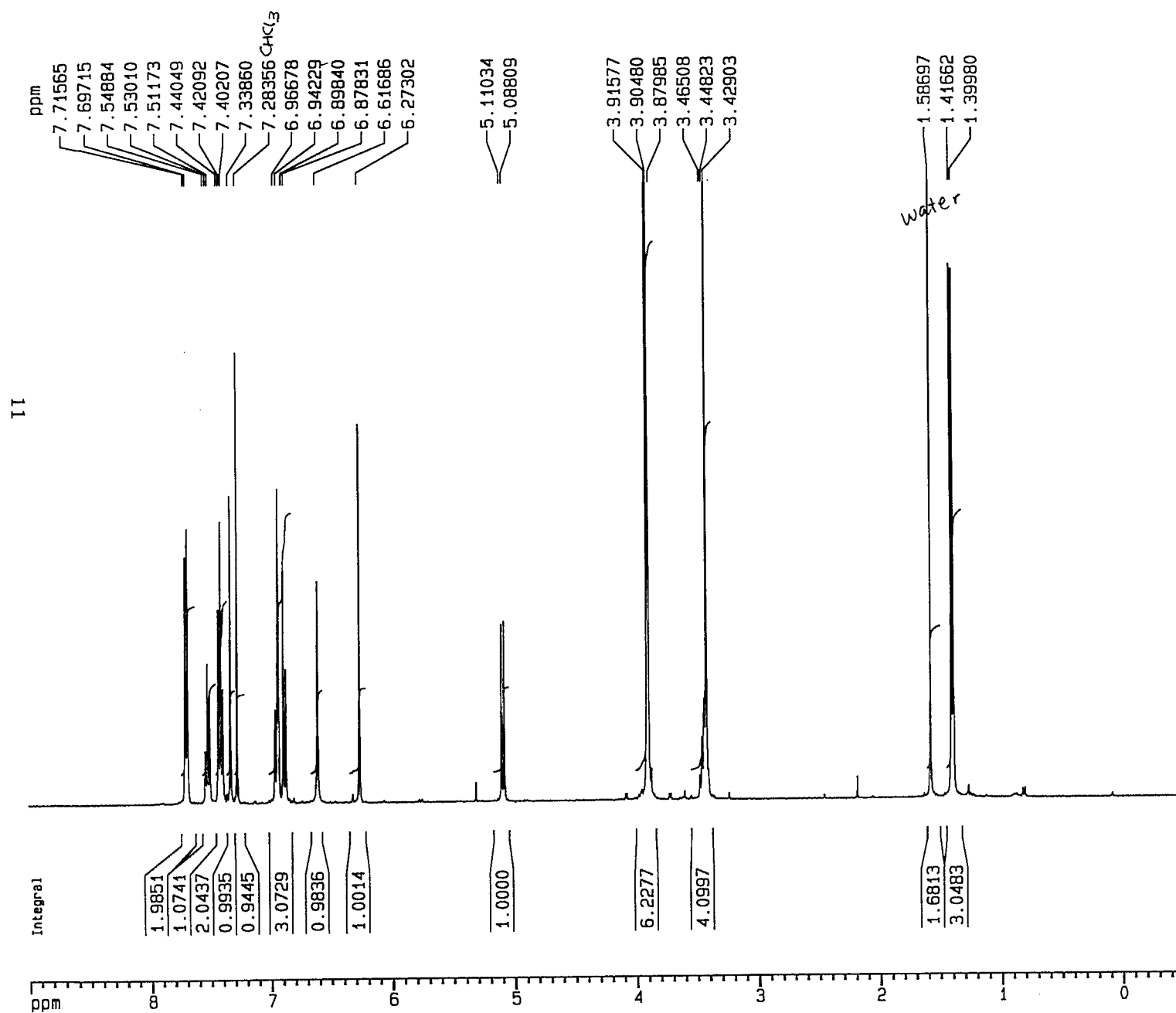
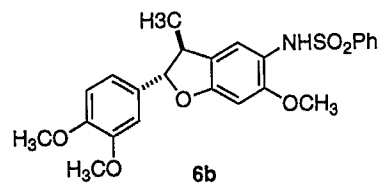
SOLVENT CDCL3

FILE C



CMS-I-151 for CHN.

in CDCl₃



Current Data Parameters

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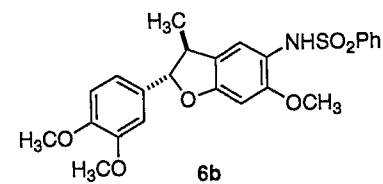
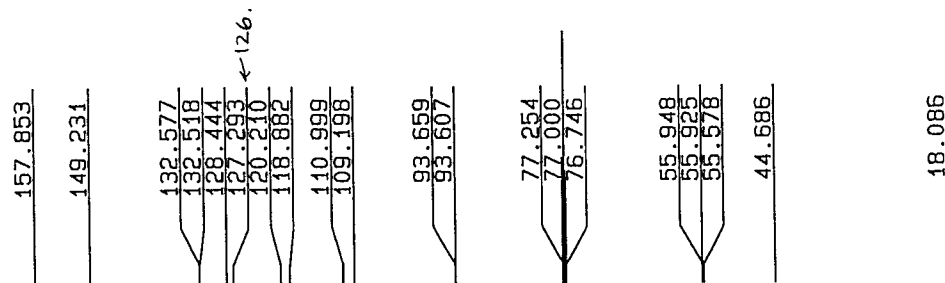
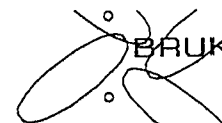
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HZCM 190.06175 Hz/cm

CMS-I-151

PPM

12

CDCl₃CMSI151.002
DATE 3-3-97

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93.0

I 2500.000

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TD 65536

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RD 0.0

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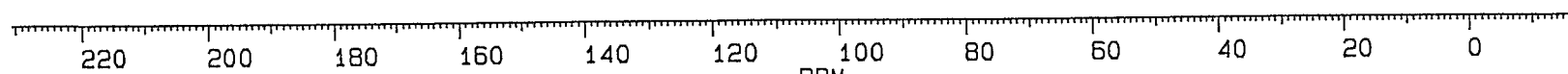
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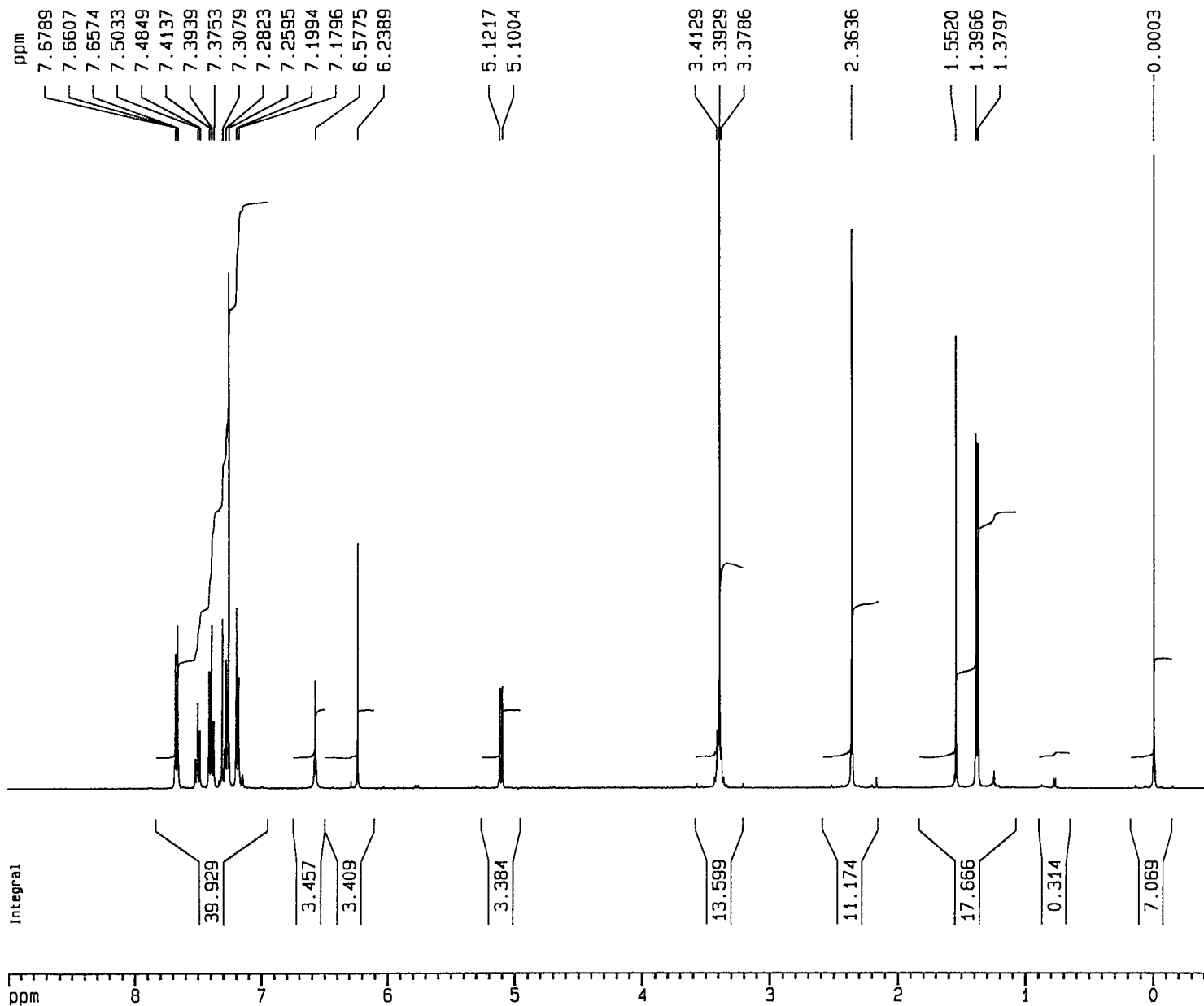
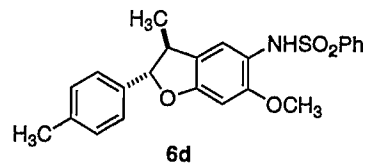
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PPM/CM 11.295

SR -10846.52



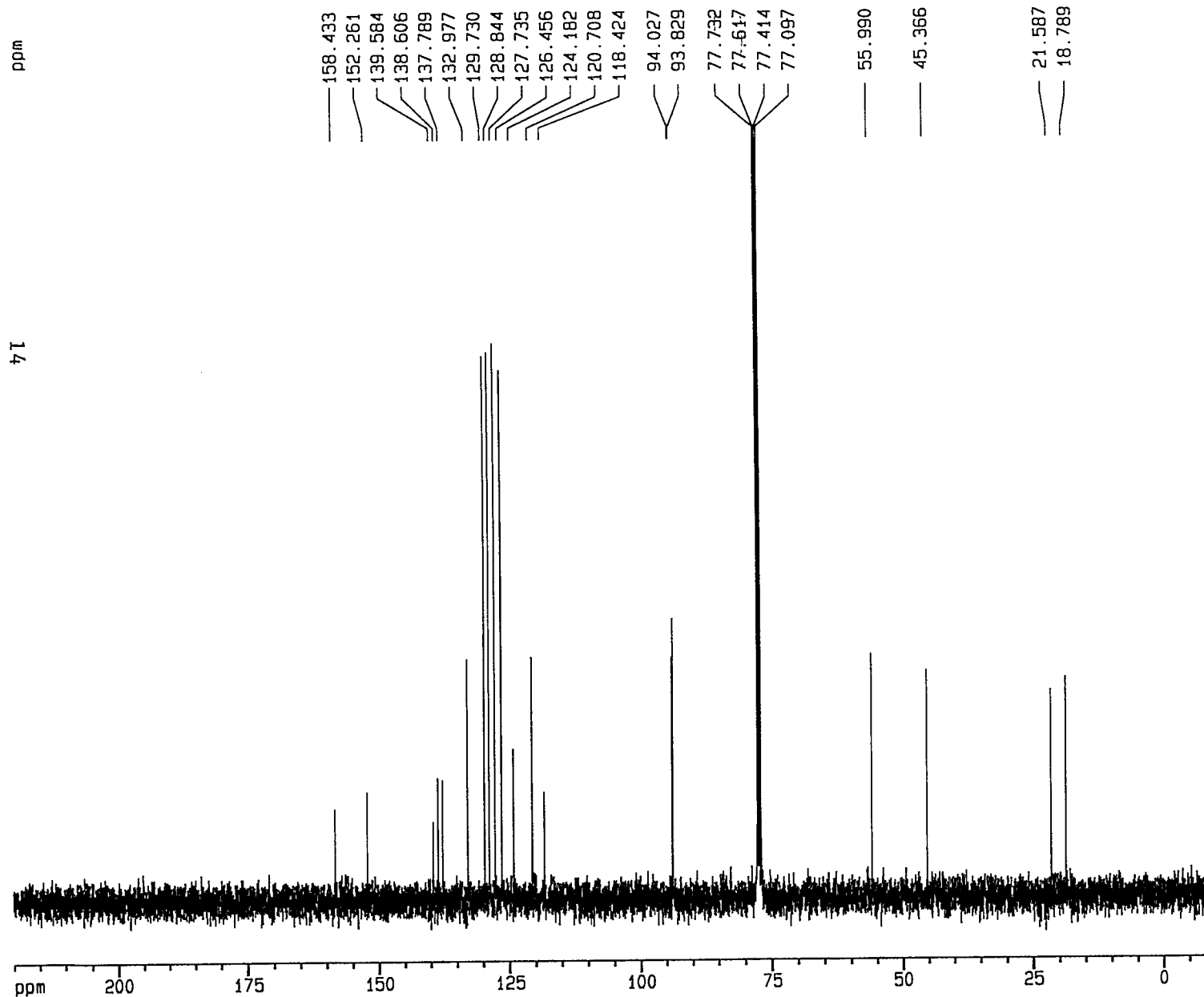
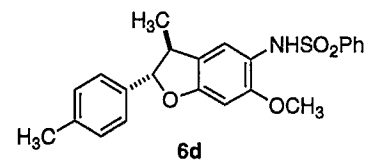


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1D NMR plot parameters
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Current Data Parameters

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EXPNO 2
PROCNO 1

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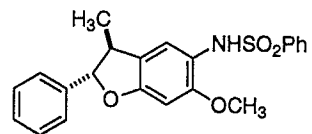
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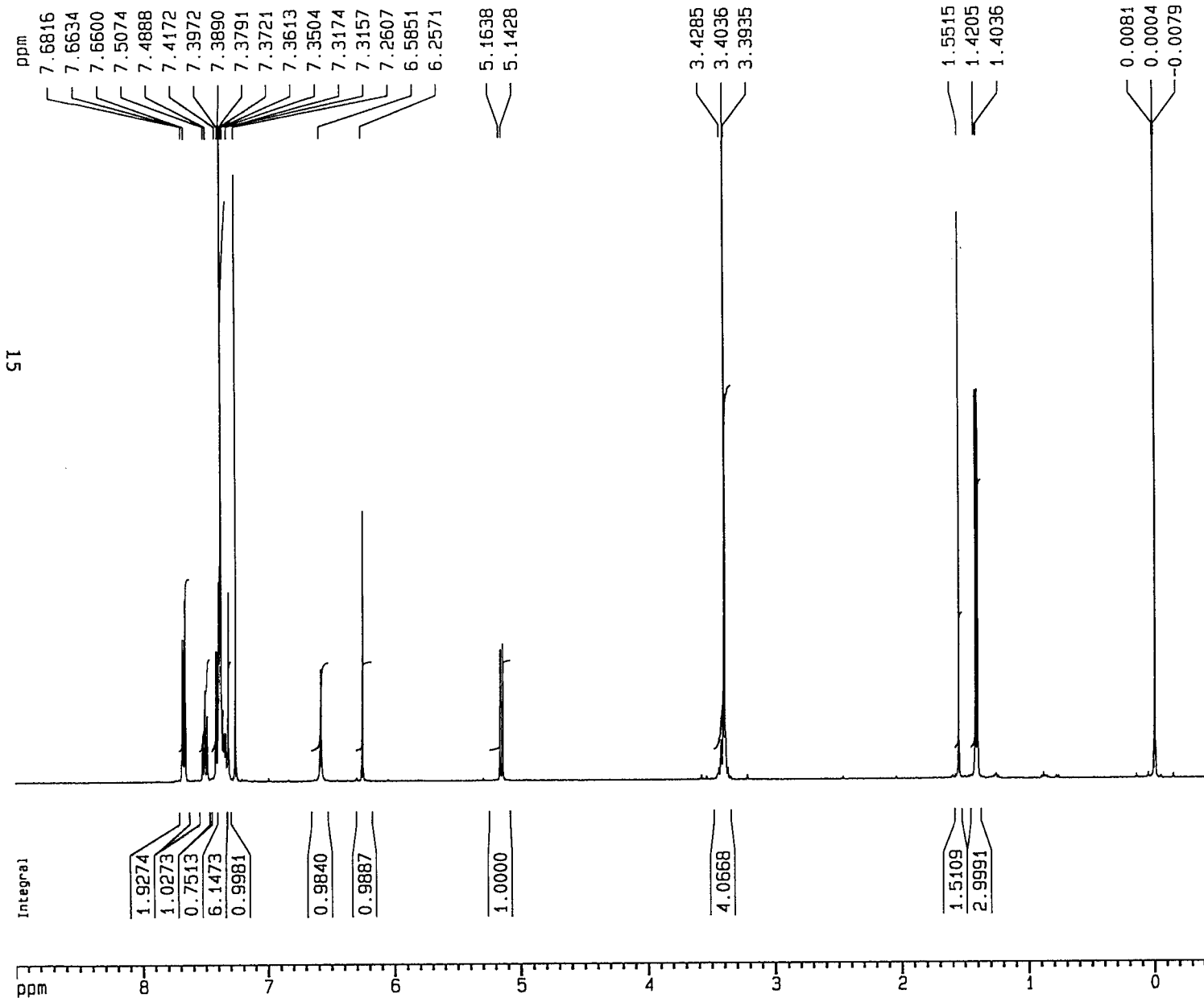
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F2 -1009.74 Hz
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6e



Current Data Parameters

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PROCNO 1

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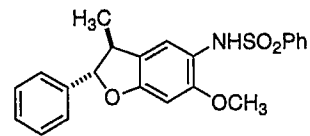
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FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 574.7
DM 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec
P1 7.70 usec
DE 4.50 usec
SFO1 400.1320007 MHz
NUC1 1H
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F2 - Processing parameters

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PC 1.00

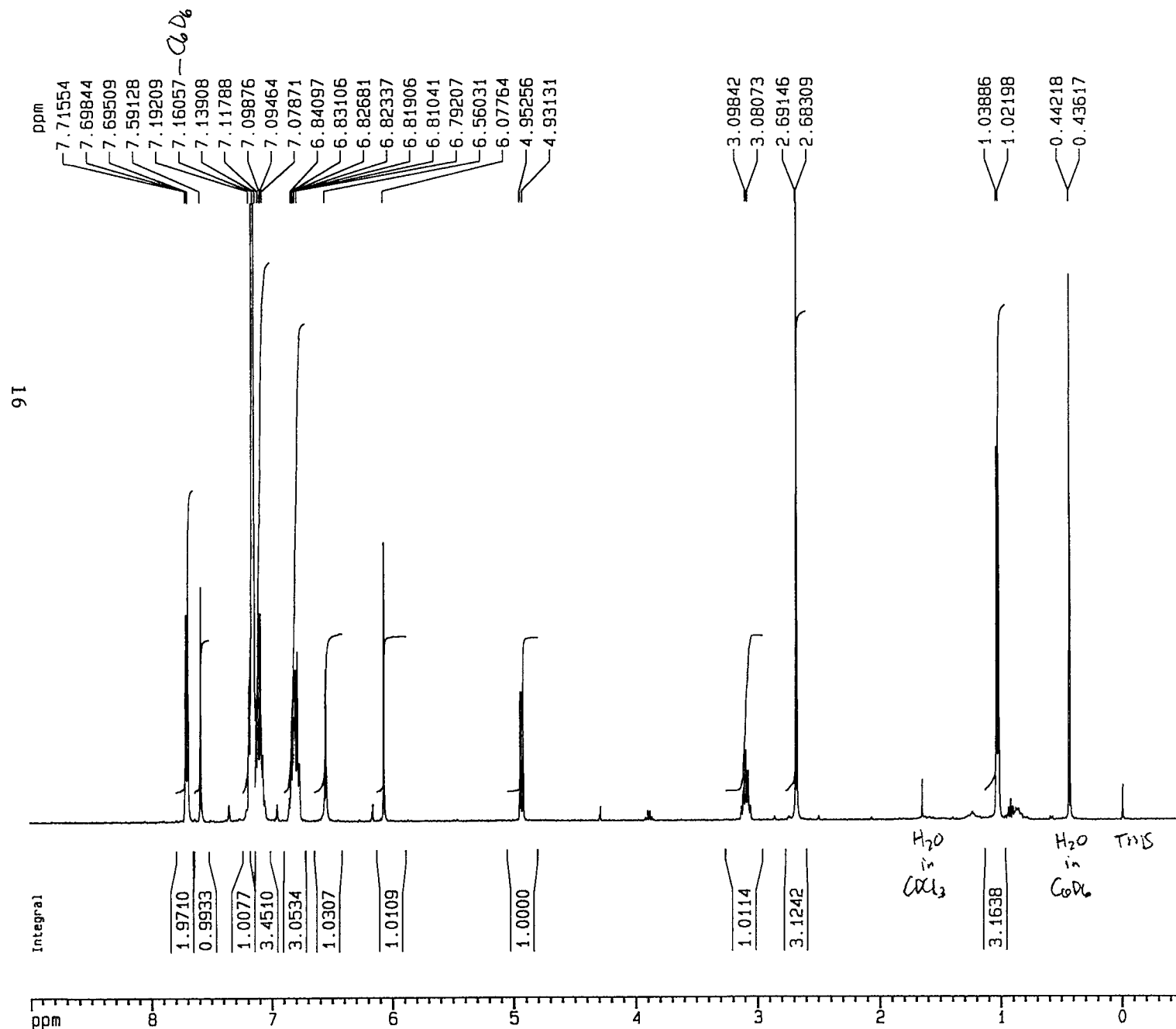
1D NMR plot parameters

CX 20.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.47500 ppm/cm
HZCM 190.06175 Hz/cm



6e

C₆D₆



Current Data Parameters
NAME cms-1-281-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

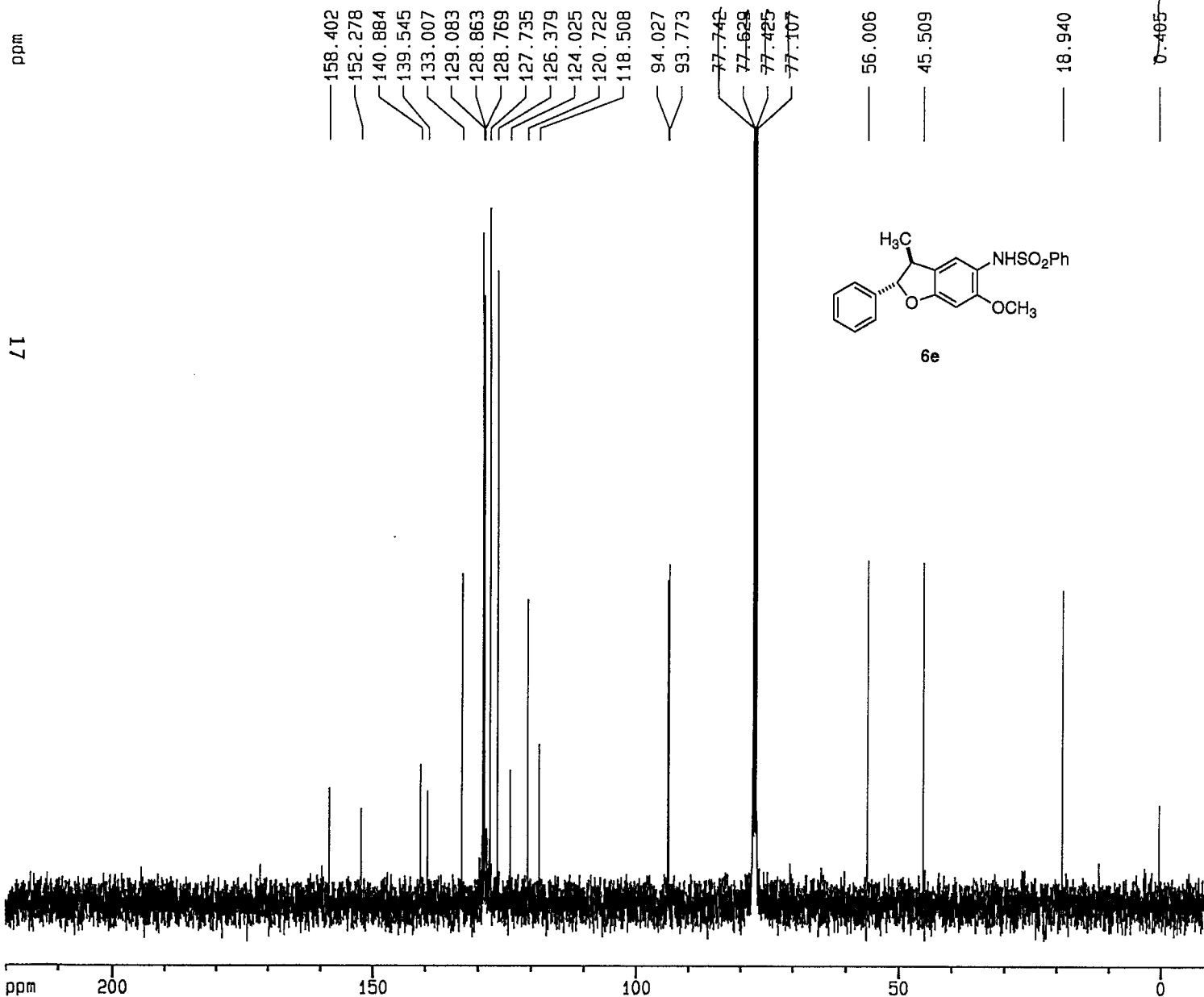
Date_ 970617
Time 20.44
INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT ~~CDC13~~ C₆D₆
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 456.1
DM 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec
P1 7.70 usec
DE 4.50 usec
SF01 400.1320007 MHz
NUC1 1H
PL1 -6.00 dB

F2 - Processing parameters

SI 16384
SF 400.1300439 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.47500 ppm/cm
HZCM 190.06177 Hz/cm

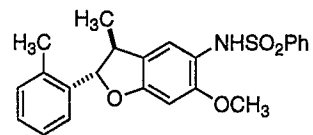


Current Data Parameters
 NAME cms-1-165cc
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 970608
 Time 8.32
 INSTRUM drx400
 PROBHD 5 mm Multinu
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2016
 DS 2
 SWH 23148.148 Hz
 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
 RG 32768
 DW 21.600 usec
 DE 4.50 usec
 TE 300.0 K
 d11 0.0300000 sec
 d12 0.0000200 sec
 PL13 18.00 dB
 D1 0.05000000 sec
 CPOPRG2 waltz16
 PCPD2 100.00 usec
 SF02 400.1316005 MHz
 NUC2 1H
 PL2 -6.00 dB
 PL12 18.00 dB
 P1 6.90 usec
 DE 4.50 usec
 SF01 100.6232933 MHz
 NUC1 13C
 PL1 -6.00 dB

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

1D NMR plot parameters
 CX 20.00 cm
 F1P 220.036 ppm
 F1 22138.42 Hz
 F2P -10.036 ppm
 F2 -1009.73 Hz
 PPMCM 11.50359 ppm/cm
 HZCM 1157.40747 Hz/cm



6f

21 diff C's

Current Data Parameters

NAME cms-1-207c2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

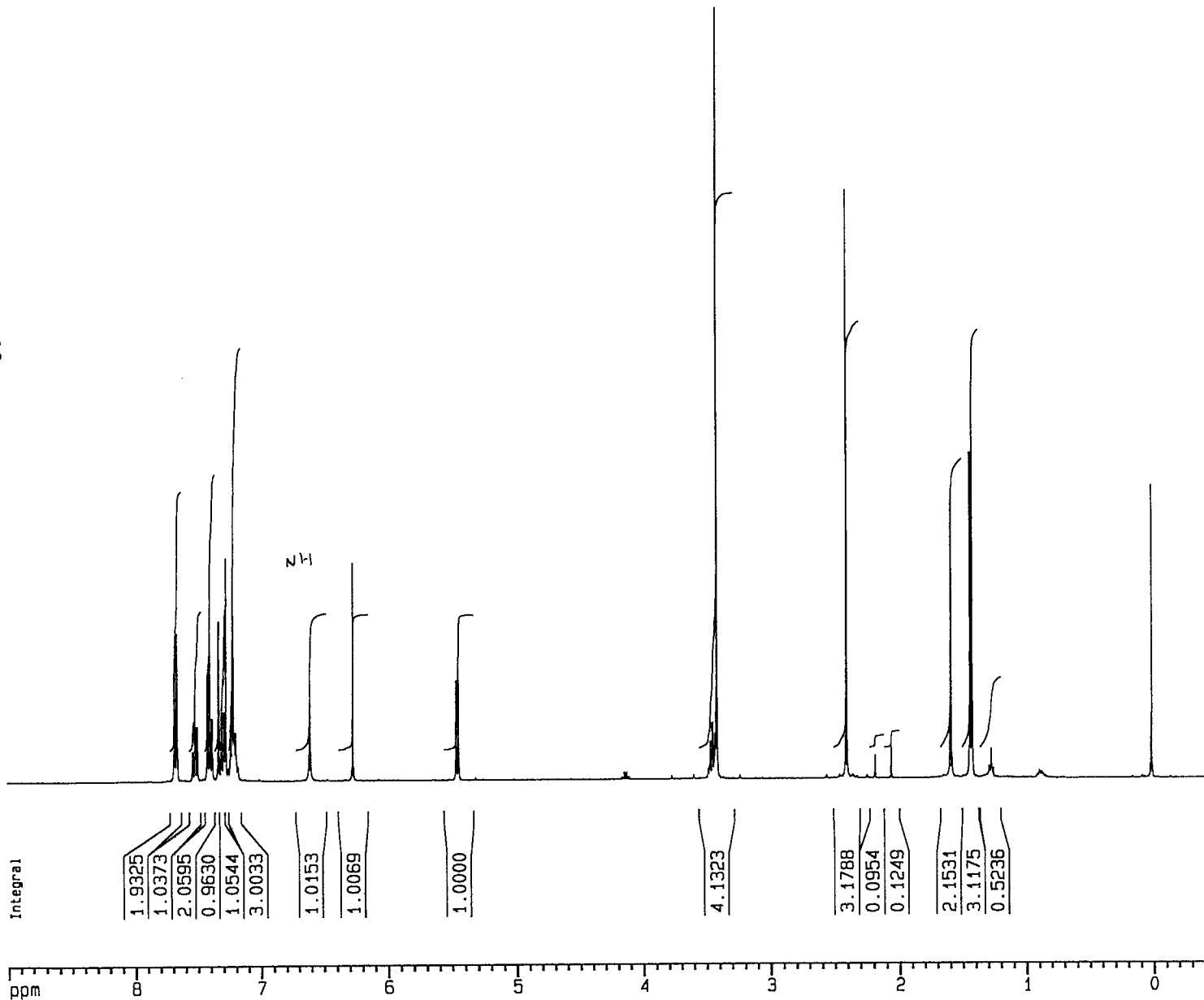
Date_ 970526
Time 17.10
INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 352
OW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec
P1 7.70 usec
DE 4.50 usec
SF01 400.1320007 MHz
NUC1 1H
PL1 -6.00 dB

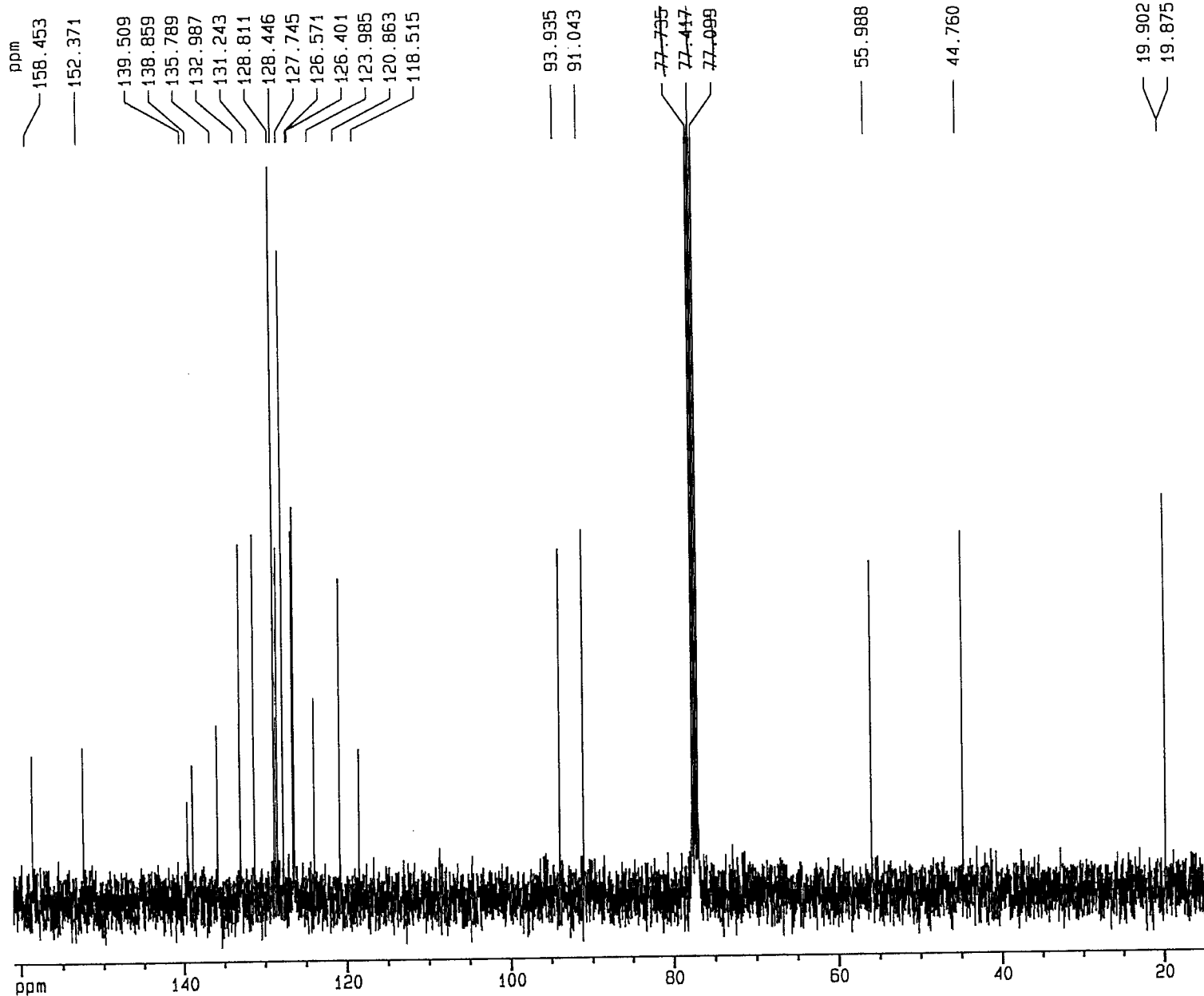
F2 - Processing parameters

SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.47500 ppm/cm
HZCM 190.06175 Hz/cm





Current Data Parameters

NAME cms-1-207c2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

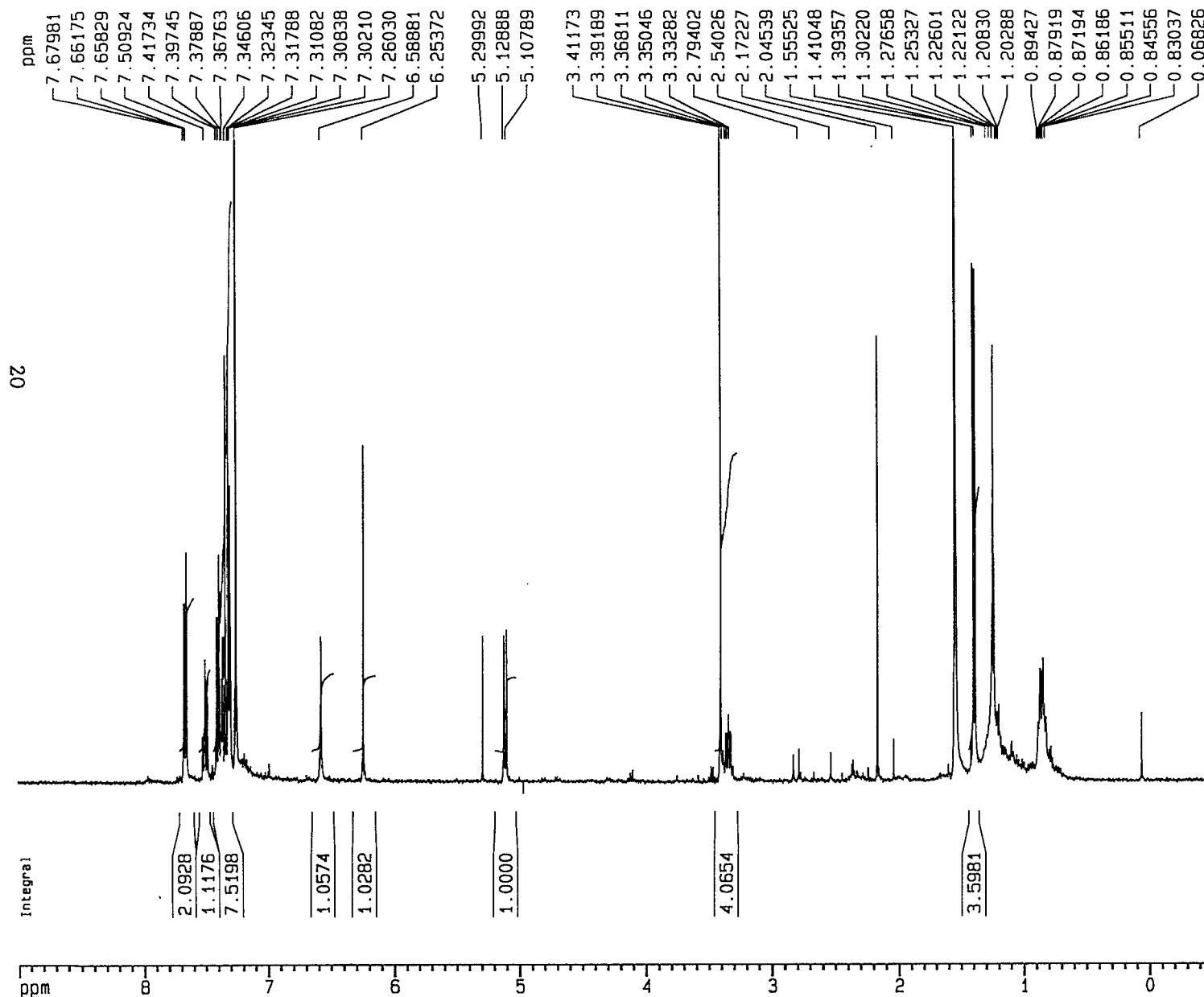
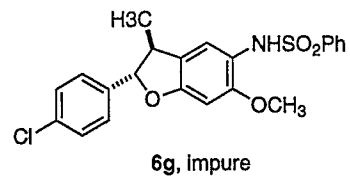
Date_ 970526
Time 17.24
INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 638
DS 2
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 32768
DW 21.600 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
d12 0.0000200 sec
PL13 18.00 dB
D1 0.05000000 sec
CPDPRG2 waltz16
PCPD2 100.00 usec
SF02 400.1316005 MHz
NUC2 1H
PL2 -6.00 dB
PL12 18.00 dB
P1 6.90 usec
DE 4.50 usec
SF01 100.6232933 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters

SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
F1P 160.868 ppm
F1 16185.36 Hz
F2P 14.480 ppm
F2 1456.87 Hz
PPNCH 7.31939 ppm/cm
HZCM 736.42419 Hz/cm



Current Data Parameters

NAME cms1215ye11.2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

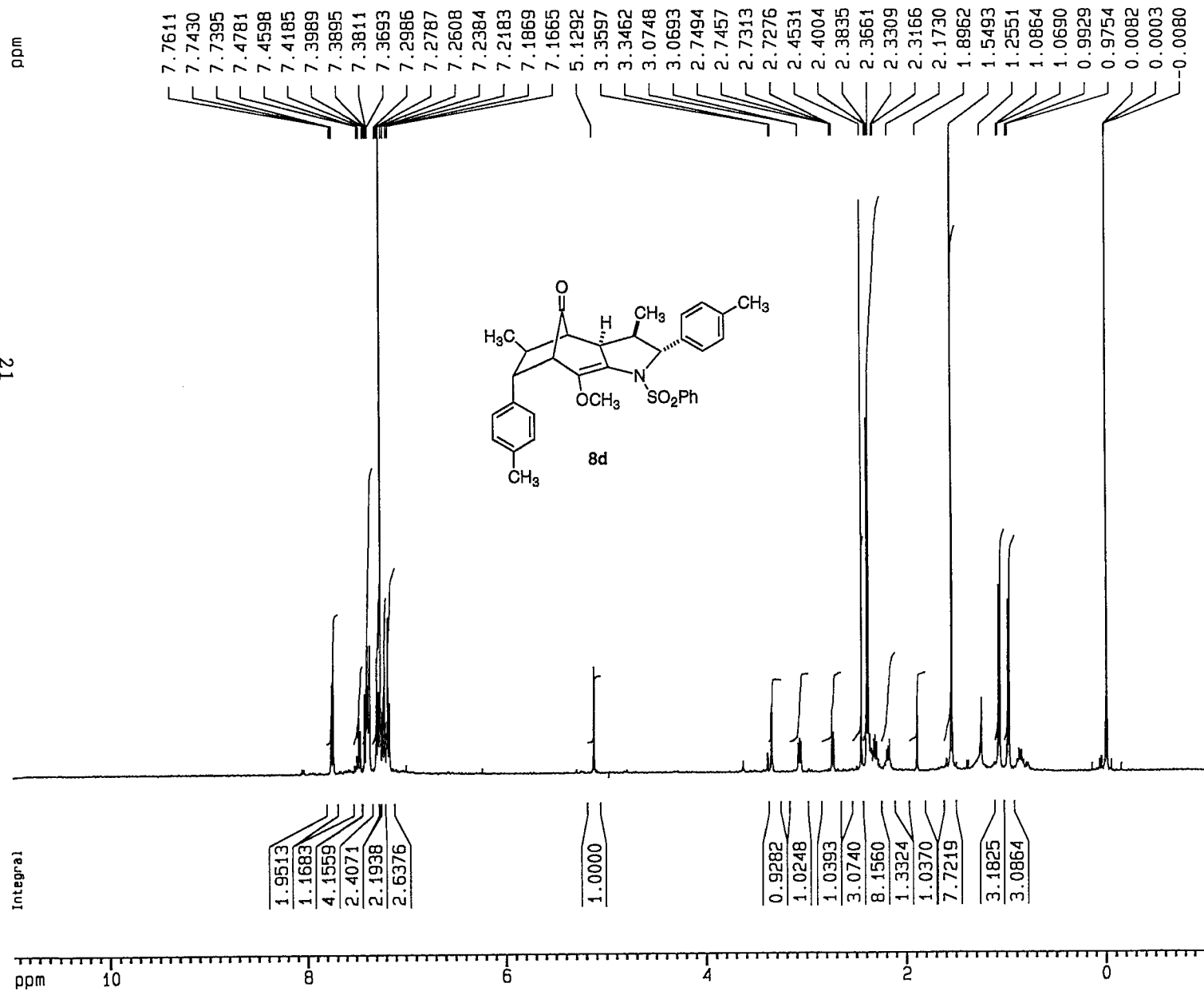
Date_ 970316
Time 14.01
INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 1024
DM 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec
P1 7.70 usec
DE 4.50 usec
SF01 400.1320007 MHz
NUC1 1H
PL1 -6.00 dB

F2 - Processing parameters

SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.47500 ppm/cm
HZCM 190.06175 Hz/cm



Current Data Parameters

NAME cms-1-221Bb
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 970617
Time 1.10
INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zg30
TO 32768
SOLVENT CDC13
NS 16
DS 2
SMH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 812.7
DW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec
P1 7.70 usec
DE 4.50 usec
SF01 400.1320007 MHz
NUC1 1H
PL1 -6.00 dB

F2 - Processing parameters

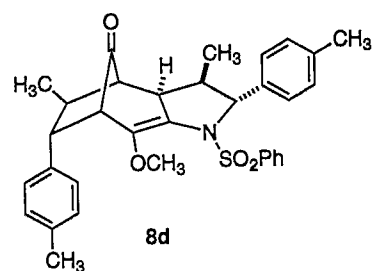
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 11.000 ppm
F1 4401.43 Hz
F2P -1.000 ppm
F2 -400.13 Hz
PPMCM 0.60000 ppm/cm
HZCM 240.07800 Hz/cm

YOURS HERE

209.461



8d

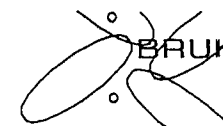
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137.675
136.997
132.029
130.992
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129.180
128.460
126.581
125.218
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77.254
77.000
76.746
75.094

54.902
54.233
53.271
50.895
49.630
44.789
43.133

22.053
21.086
21.046
14.413

-.017



CMS1221B.002

DATE 16-6-97

SF 125.759

3Y 93.0

J1 2500.000

3I 65536

TD 65536

SW 31250.000

HZ/PT .954

PW 2.0

RD 1.000

AQ 1.049

RG 200

NS 34596

TE 297

FW 39100

O2 7500.000

DP 15H CPD

LB 2.000

GB 0.0

CX 22.00

CY 0.0

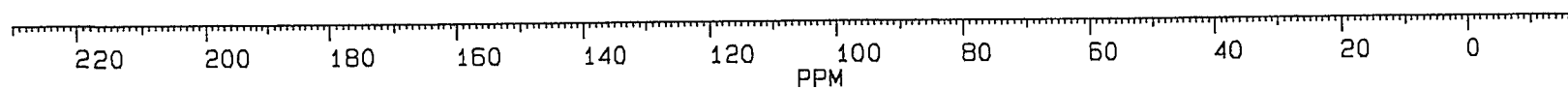
F1 230.146

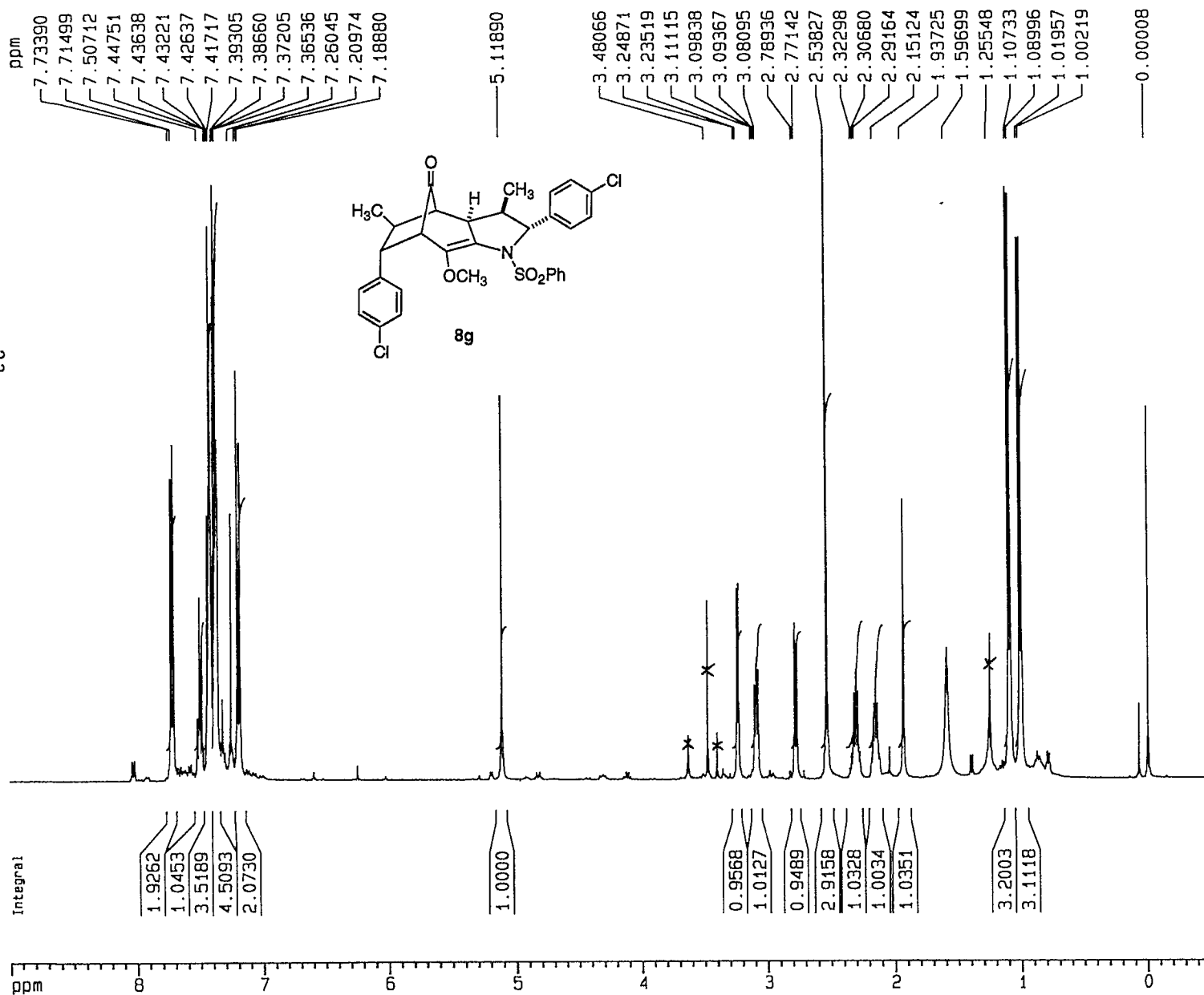
F2 -18.095

HZ/CM 1.419E3

PPM/CM 11.284

SR -10848.43





Current Data Parameters

NAME cms-i-197-C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

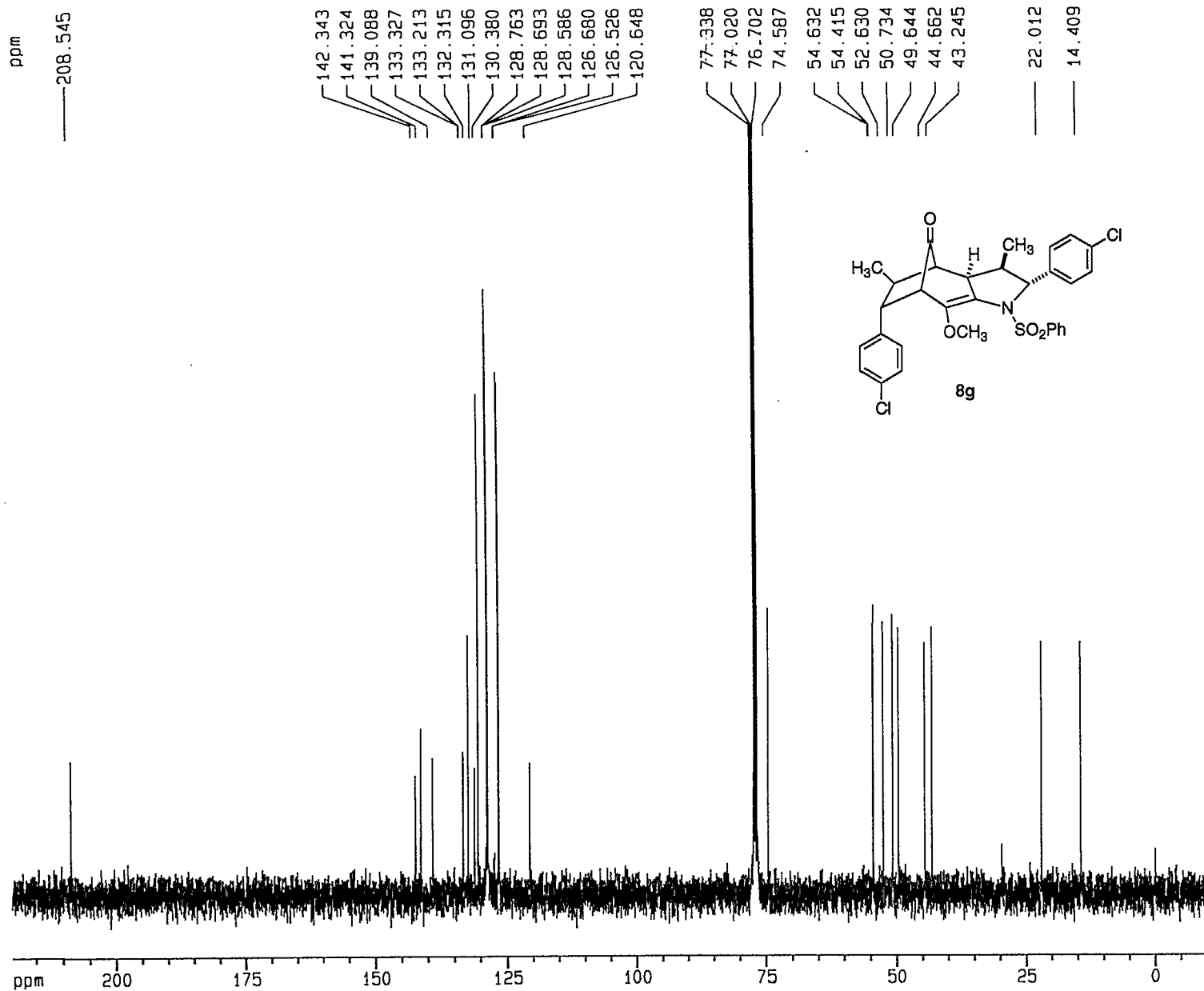
Date_ 970627
Time 2.22
INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SMH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 181
DM 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec
P1 7.70 usec
DE 4.50 usec
SF01 400.1320007 MHz
NUC1 1H
PL1 -6.00 dB

F2 - Processing parameters

SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.47500 ppm/cm
HZCM 190.06175 Hz/cm



Current Data Parameters

NAME cms-1-197-c
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

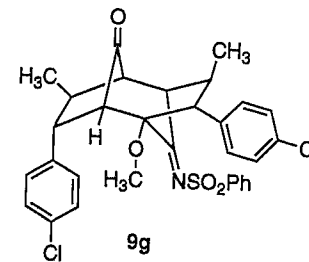
Date_ 970622
Time 1.11
INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SOLVENT CDC13/*in MS*
NS 1078
DS 2
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 32768
DM 21.600 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
d12 0.0000200 sec
PL13 18.00 dB
D1 0.05000000 sec
CPOPRG2 waltz16
PCPD2 100.00 usec
SF02 400.1316005 MHz
NUC2 1H
PL2 -6.00 dB
PL12 18.00 dB
P1 6.90 usec
DE 4.50 usec
SF01 100.6232933 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters

SI 32768
SF 100.6127697 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
F1P 219.631 ppm
F1 22097.69 Hz
F2P -10.441 ppm
F2 -1050.46 Hz
PPMCM 11.50358 ppm/cm
HZCM 1157.40747 Hz/cm



Current Data Parameters
 NAME cms-i-215CR
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

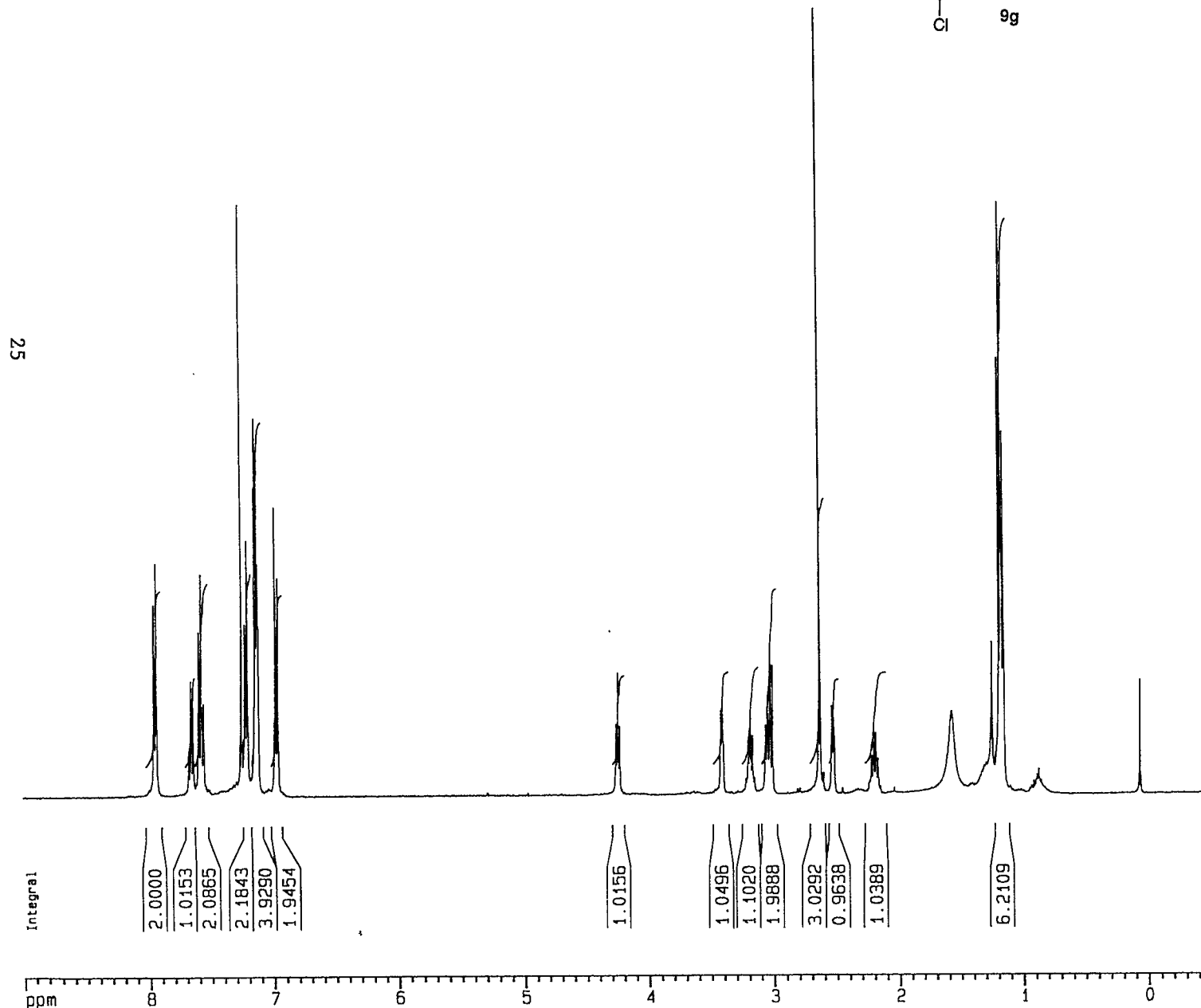
Date_ 970619
 Time 18.03
 INSTRUM drx400
 PROBHD 5 mm Multinu
 PULPROG zg30
 TO 32768
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 512
 DW 104.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 7.70 usec
 DE 4.50 usec
 SF01 400.1320007 MHz
 MJC1 1H
 PL1 -6.00 dB

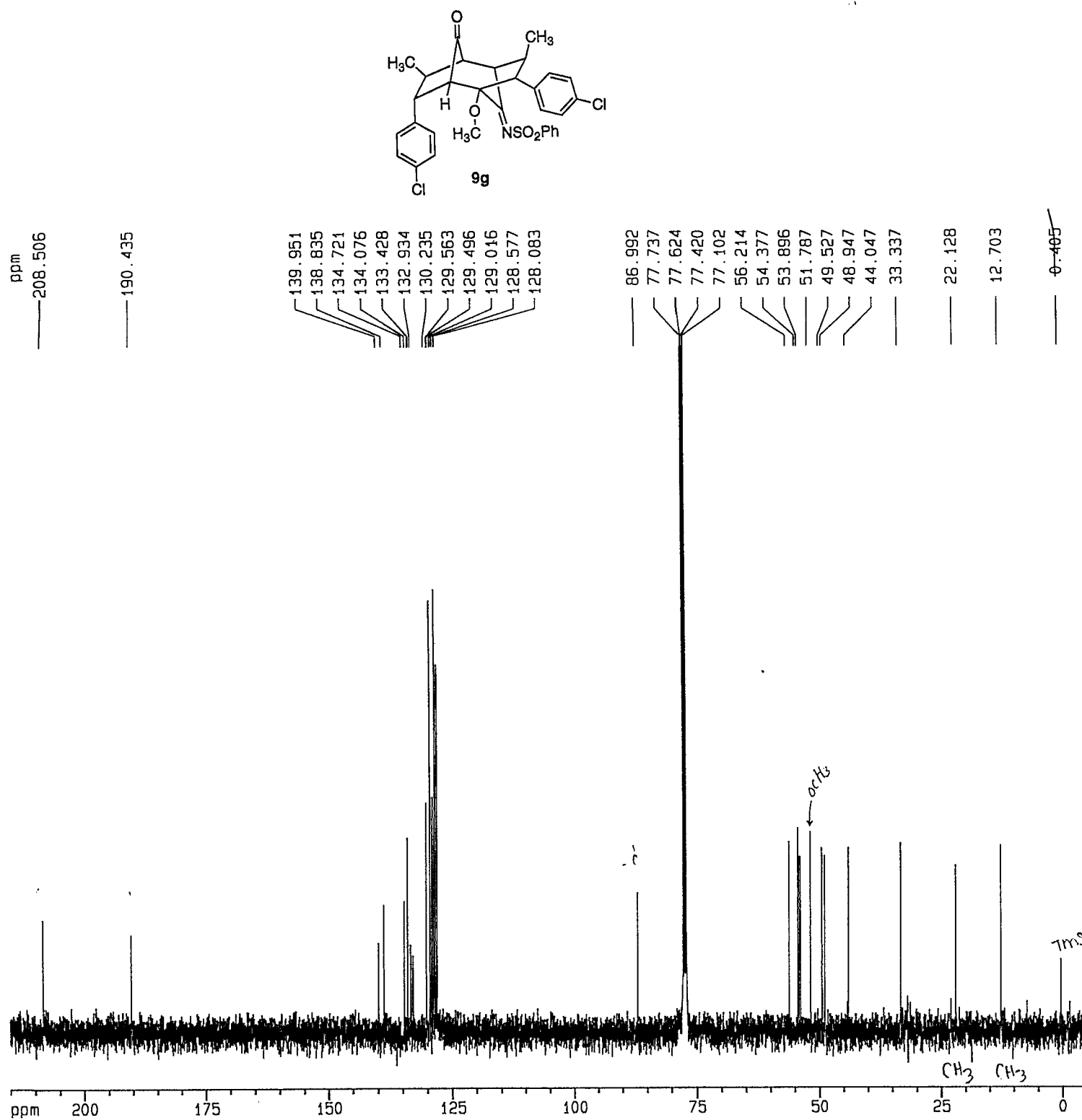
F2 - Processing parameters

SI 16384
 SF 400.1300092 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 20.00 cm
 F1P 9.000 ppm
 F1 3601.17 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 PPMCM 0.47500 ppm/cm
 HZCM 190.06175 Hz/cm





Current Data Parameters

NAME cms-i-215pr
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

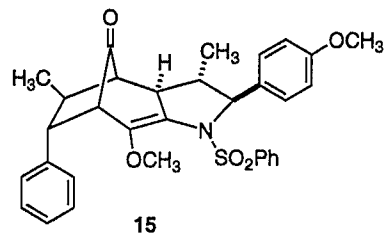
Date_ 970416
Time 22.15
INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4016
DS 2
SMH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156276 sec
RG 32768
DM 21.600 usec
DE 4.50 usec
TE 300.0 K
d11 0.0300000 sec
d12 0.0000200 sec
PL13 18.00 dB
D1 0.05000000 sec
CPOPRG2 waltz16
PCPD2 100.00 usec
SF02 400.1316005 MHz
NUC2 1H
PL2 -6.00 dB
PL12 18.00 dB
P1 6.90 usec
DE 4.50 usec
SF01 100.6232933 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters

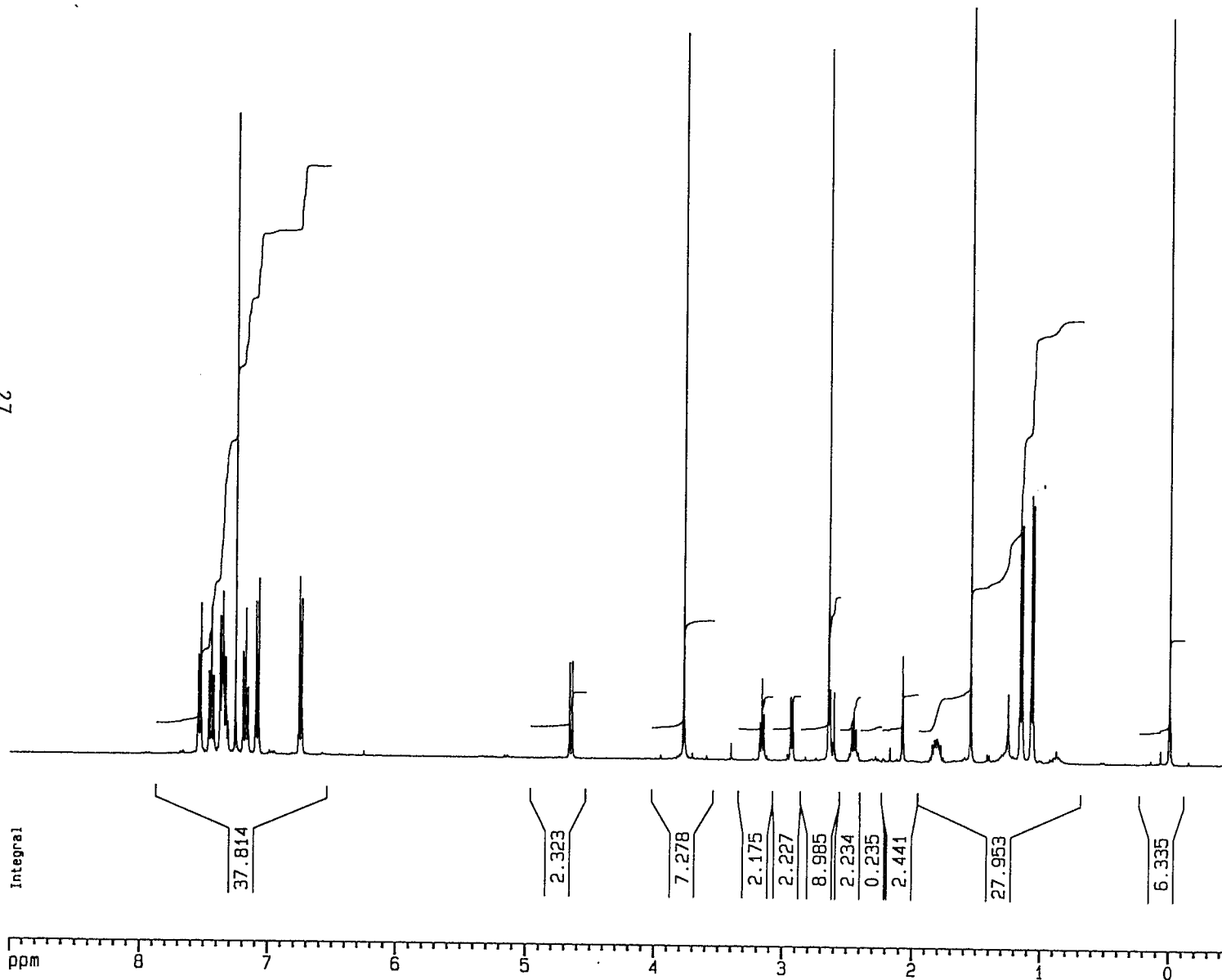
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
F1P 215.000 ppm
F1 21631.74 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 11.00000 ppm/cm
HZCM 1106.73999 Hz/cm



15



Current Data Parameters
 NAME cms-1-287-Ta
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 970628
 Time 16.46
 INSTRUM drx400
 PROBHD 5 mm Multinu
 PULPROG zg30
 TO 32768
 SOLVENT CDCl₃
 NS 64
 DS 2
 SMH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 574.7
 DW 104.400 usec
 DE 4.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 7.70 usec
 DE 4.50 usec
 SFO1 400.1320007 MHz
 NUC1 1H
 PL1 -6.00 dB

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

1D NMR plot parameters
 CX 20.00 cm
 F1P 9.000 ppm
 F1 3601.17 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 PPMCM 0.47500 ppm/cm
 HZCM 190.06175 Hz/cm

209.805

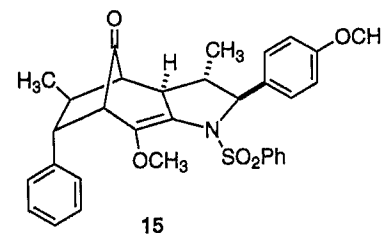
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77.257	56.898
77.002	56.053
76.749	55.291
72.789	54.387
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	51.815
	44.716
	43.221

21.838

14.569

-014


$$\text{CDCl}_3 + \text{TMS}$$

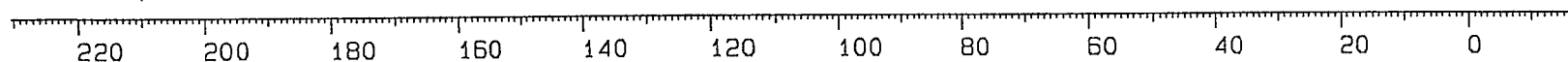

CMS2179T.002
DATE 29-6-97

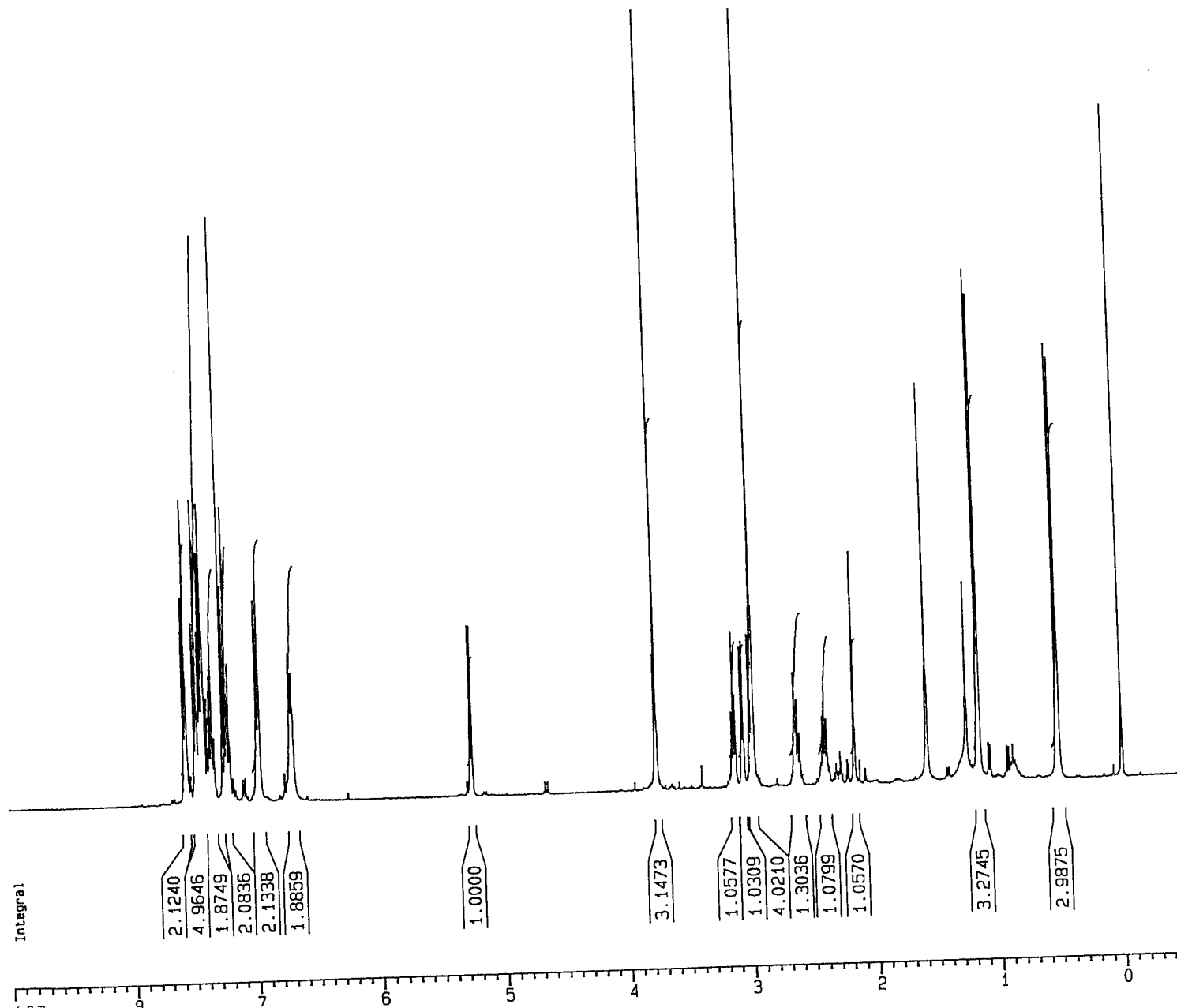
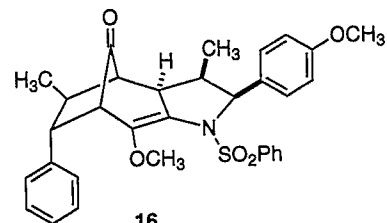
SF	125.759
SY	93.0
O1	2500.000
SI	65536
TD	65536
SW	31250.000
HZ/PT	.954

PW	2.0
RD	0.0
AQ	1.049
RG	200
NS	15000
TE	297

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FW 39100
02 7500.000
DP 15H D0
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LB	1.000
GB	0.0
CX	22.00
CY	0.0
F1	230.547
F2	-17.936
HZ/CM	1.420E3
PPM/CM	11.295
SR	-10849.38





Data Parameters

NAME cms-1-287-c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 970629
Time 13.36
INSTRUM drx400
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SMH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 322.5
DW 104.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec
P1 7.70 usec
DE 4.50 usec
SFO1 400.1320007 MHz
NUC1 1H
PL1 -6.00 dB

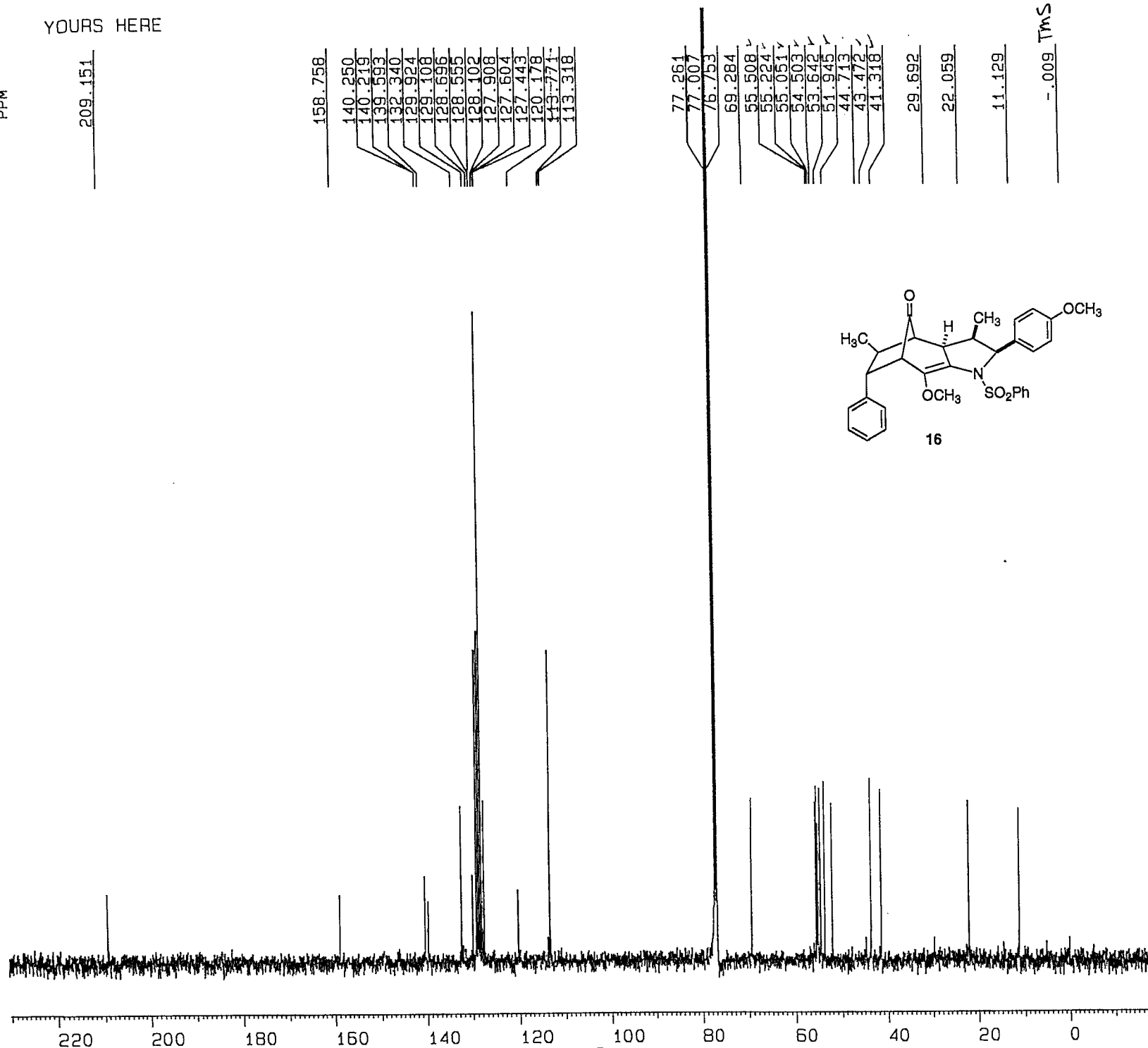
F2 - Processing parameters

SI 16384
SF 400.1300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.47500 ppm/cm
HZCM 190.06175 Hz/cm

YOURS HERE



CMS-1287-C

CDCl₃/TMS
BRUKCMS1282C.002
DATE 30-6-97

SF 125.768
 SY 93.0
 O1 2500.000
 SI 65536
 TD 65536
 SW 31250.000
 HZ/PT .954

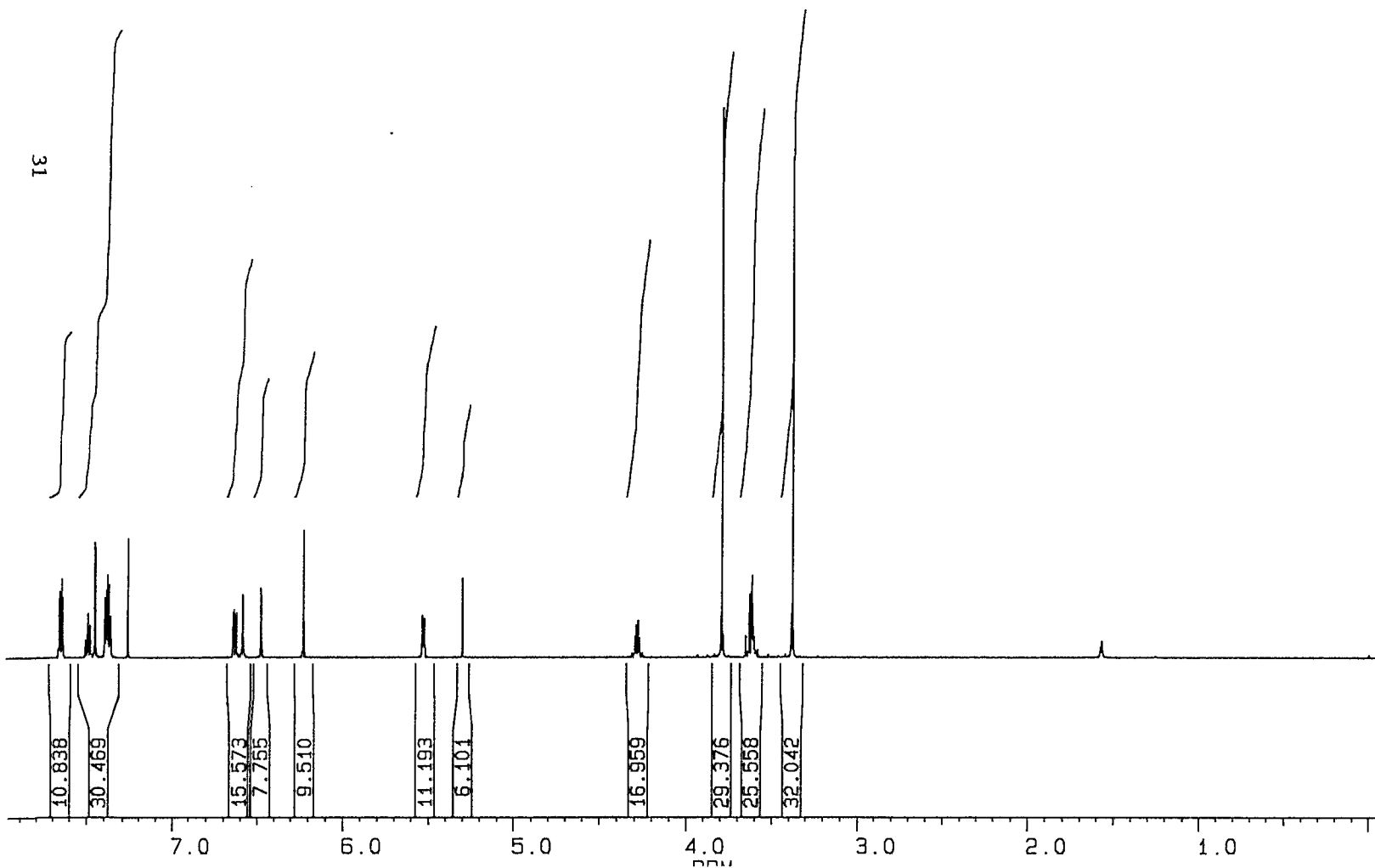
PW 2.0
 RD 0.0
 AQ 1.049
 RG 200
 NS 3210
 TE 297

FW 39100
 O2 7500.000
 DP 15H CPD

LB 3.000
 GB 0.0
 CX 22.00
 CY 0.0
 F1 230.380
 F2 -18.329
 HZ/CM 1.421E3
 PPM/CM 11.305
 SR -10849.38

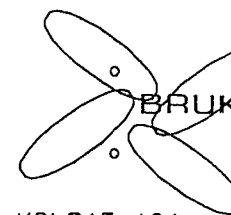
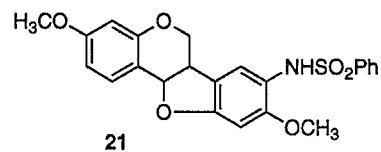
KOL-VI-15

PPM



3.78855

3.37615



KOL615.101
DATE 30-11-94

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SY 165.0
O1 7490.000
SI 32768
TD 32768
SW 6024.096
HZ/PT .368

PW 5.0
RD 0.0
AQ 2.720
RG 100
NS 16
TE 297

FW 7600
O2 0.0
DP 63L P0

LB .100
GB 0.0
CX 22.00
CY 0.0
F1 8.000
F2 -.100
HZ/CM 184.142
PPM/CM .368
SR 5421.30

KOL-VI-15

PPM

23

132.646
131.638
128.451
127.248

109.307

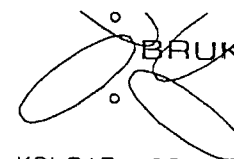
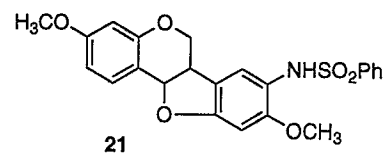
101.601

94.191

78.759
77.251
76.997
76.743

55.563

39.790



KOL615.102
DATE 30-11-94

SF 125.759
SY 93.0
O1 2500.000
SI 65536
TD 65536
SW 31250.000
HZ/PT .954

PW 2.0
RD 0.0
AQ 1.049
RG 200
NS 256
TE 297

FW 39100
O2 7500.000
DP 15H CPD

LB 1.000
GB 0.0
CX 22.00
CY 0.0
F1 170.002
F2 -.995
HZ/CM 977.473
PPM/CM 7.773
SR -10846.52

