

Lewis Acid Promoted Preparation of Isomerically Pure Fullerol from Fullerene Peroxides



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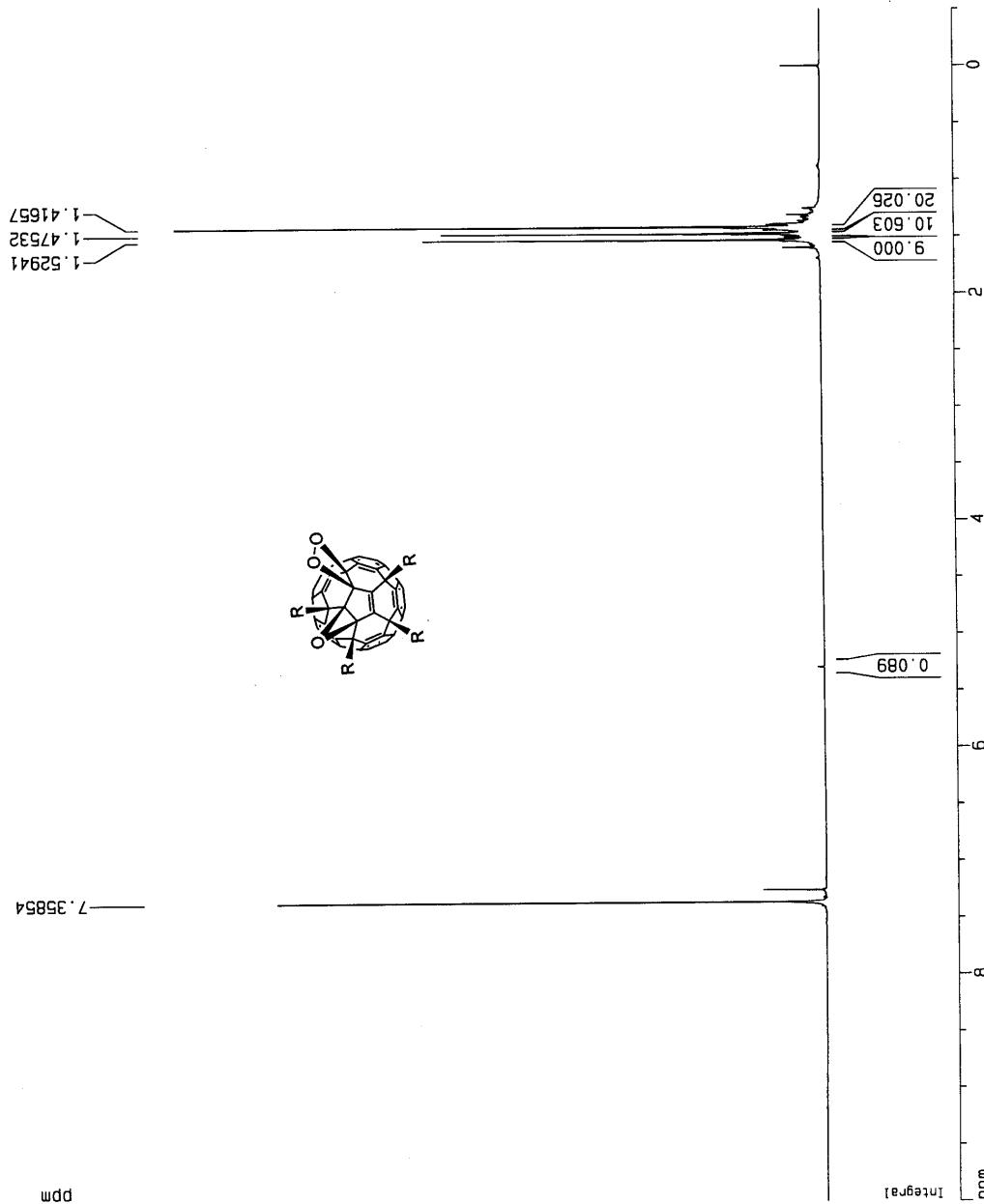
Note common impurities in NMR spectra: benzene (7.36 ppm in ¹H NMR, 128 ppm in ¹³C NMR), toluene (2.3, 7.1-7.4 ppm in ¹H NMR, 125, 128, 129, 137 ppm in ¹³C NMR), water (1.5-1.6 ppm in ¹H NMR) and grease (1.25 ppm in ¹H NMR, 14.1, 22.7, 29.9 ppm in ¹³C NMR).

Current Data Parameters
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 EXPNO 1
 PROCNO 1

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 PULPROG PULPROG
 TD 32768
 SOLVENT CDCl3
 NS 45
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.198625 Hz
 AQ 2.5555540 sec
 RG 715
 DW 78.000 usec
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 NUCLEUS 1H

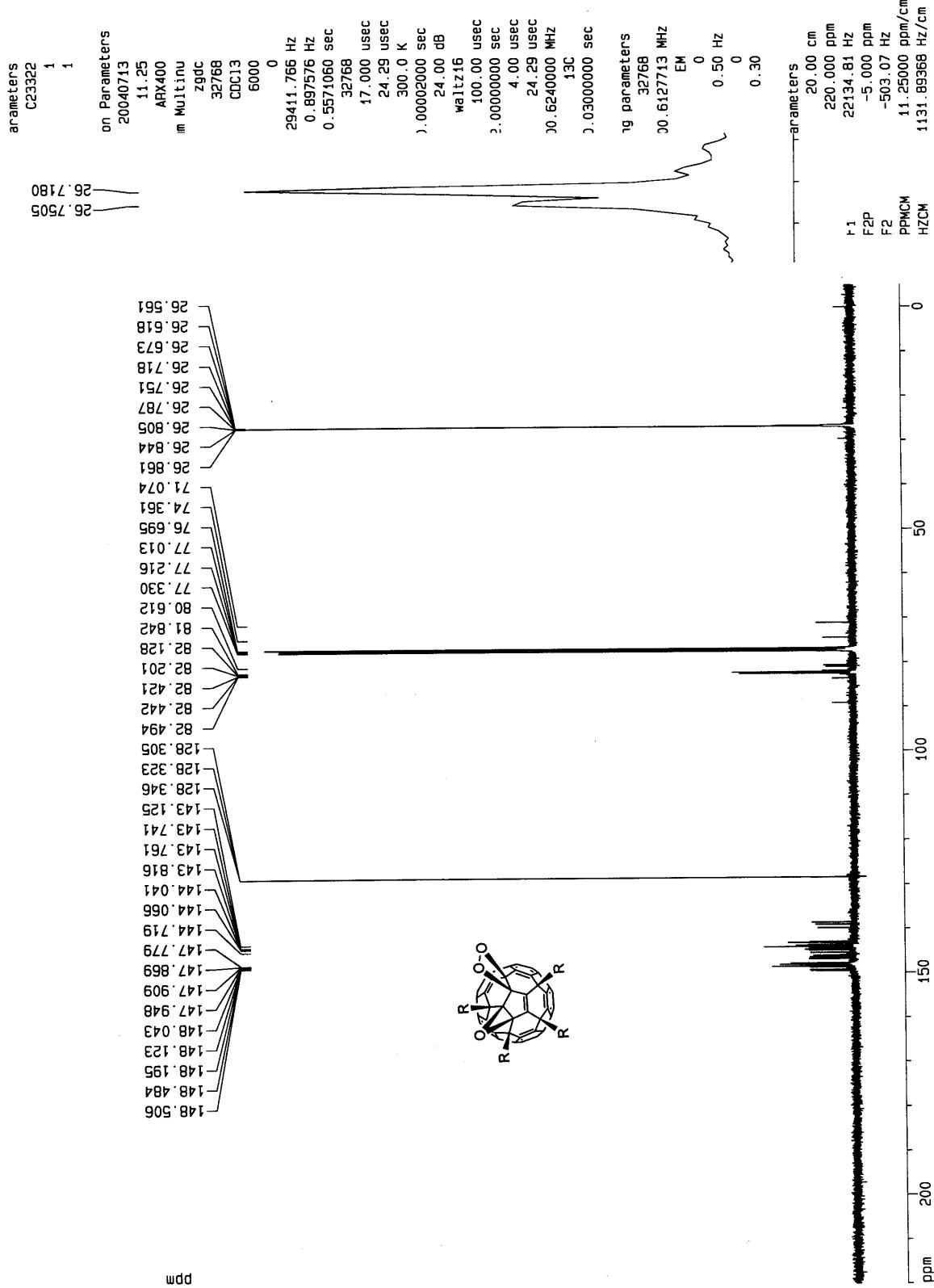
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 F1 4001.30 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 210.06825 Hz/cm



ppm

Integral



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	13C	
	NUCLEUS	
D11	0.03000000	sec

E3 - Processing Diameters

String pair, $\text{c.c.}, \frac{1}{2}$

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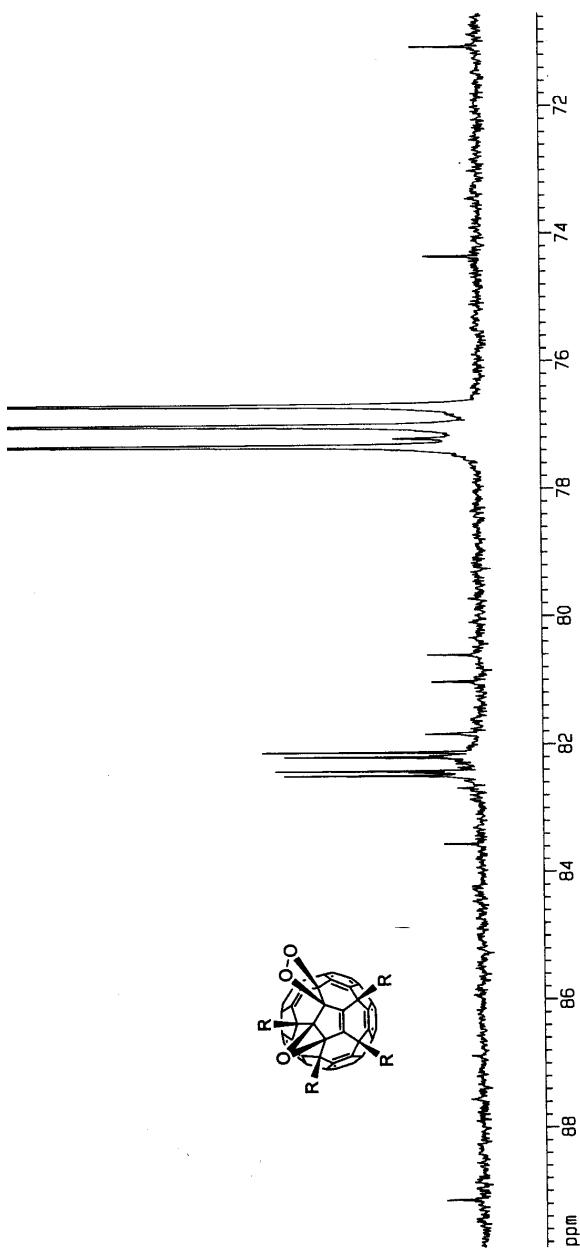
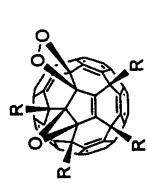
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1D NMB plot parameters

cx 110 NMR Blue pearl/gemstone 20.00 cm

F1P 89.884 ppm
E1 9043.50 Hz

F1	3045.30 Hz
F2P	70.541 ppm
F2	7097.33 Hz
PPMCM	0.96715 ppm
HZCM	97.30811 Hz/°



EM 100

Ergonomics

0.50 Hz 0

0.30

110 NMR plot parameters

20.00 cm
145.108 ppm

F1 F2P 14599.71 Hz 138.395 ppm

13924.35 Hz

PPPMCM 0.33563 ppm/
Hz/C
HZCM 33.76821 Hz/C

卷之三

868

0.50 Hz

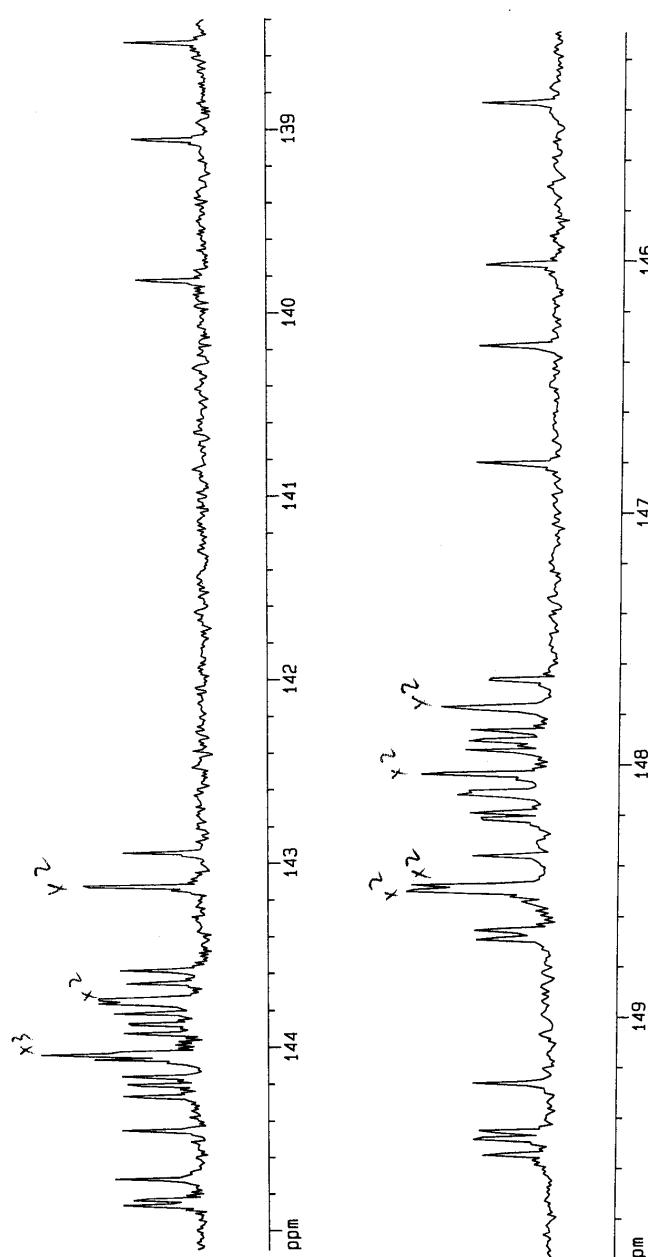
0.30

D NMR pilot parameters

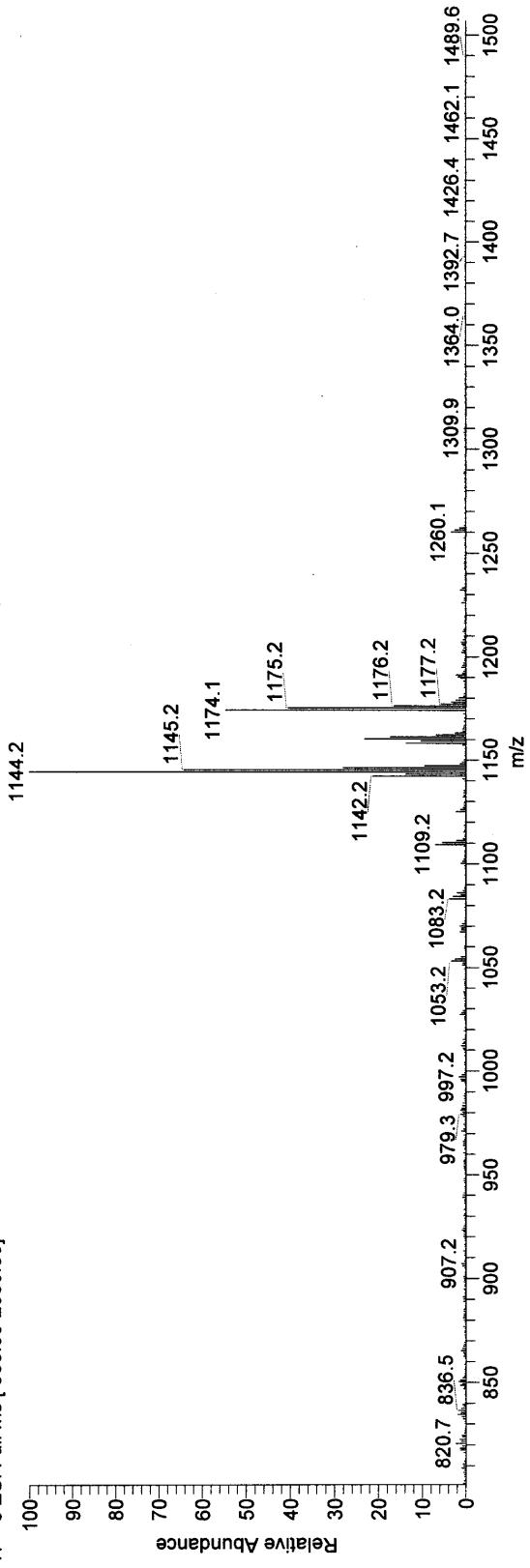
20.00 cm
149.007 mm

149.99/ ppm
15091.64 Hz

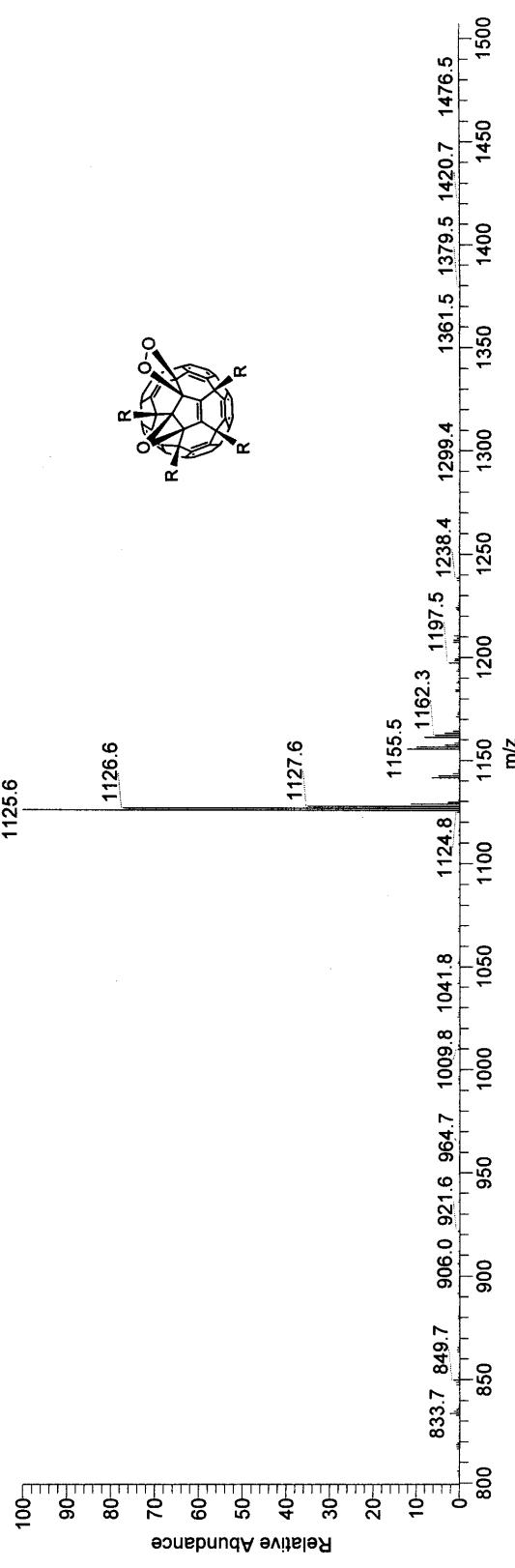
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145.98 Hz

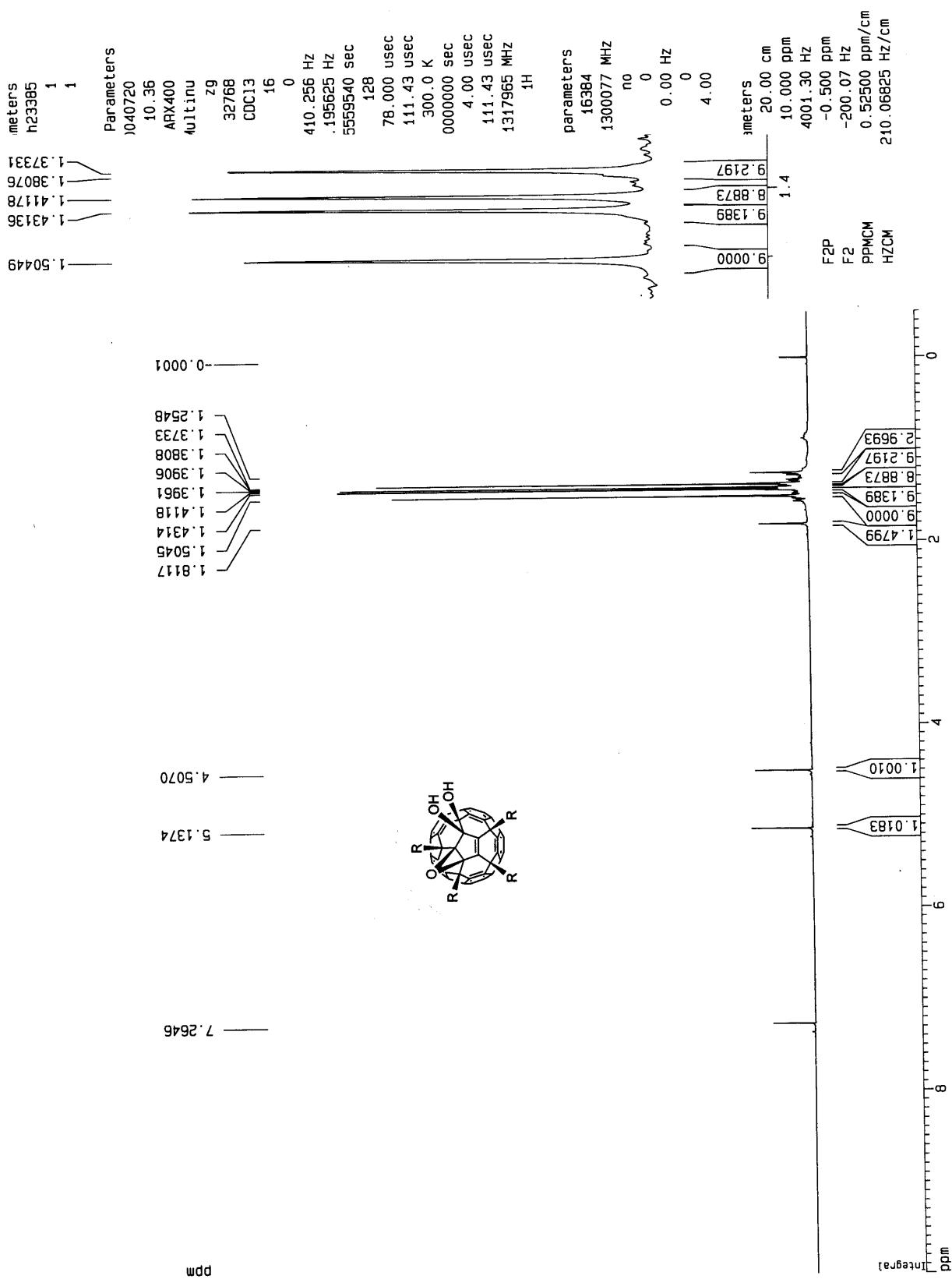


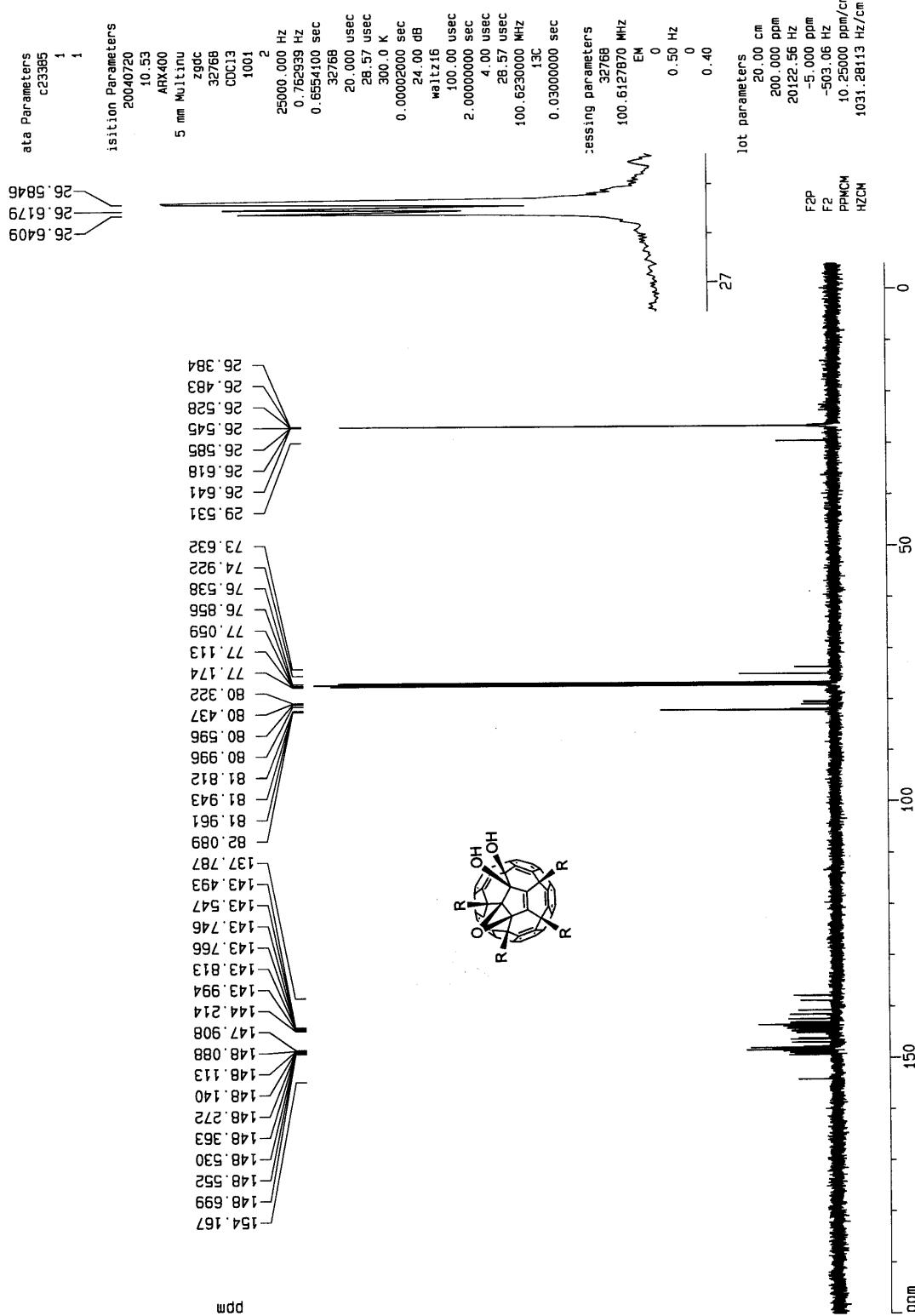
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GAN092901 #29-33 RT: 0.79-0.88 AV: 5 NL: 2.72E7
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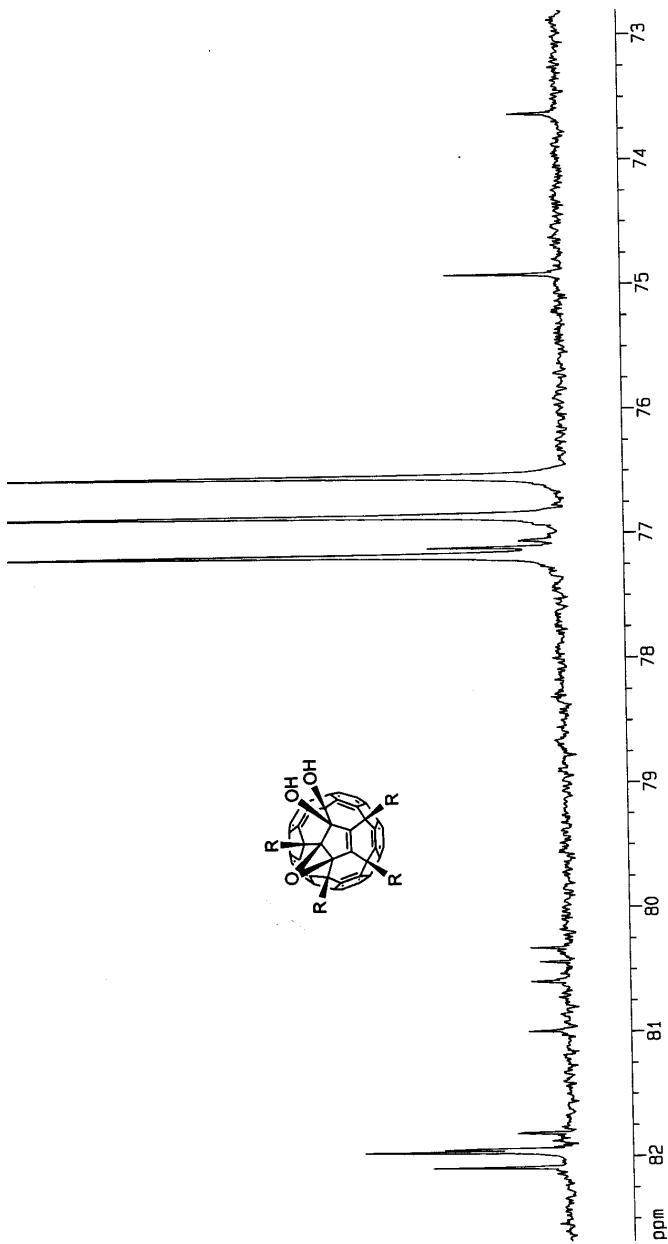


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 TE 300.0 K
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 CPDPG
 P1 100.00 usec
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 P1 28.57 usec
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 SF01 13C
 NUCLEUS D11 0.0300000 sec

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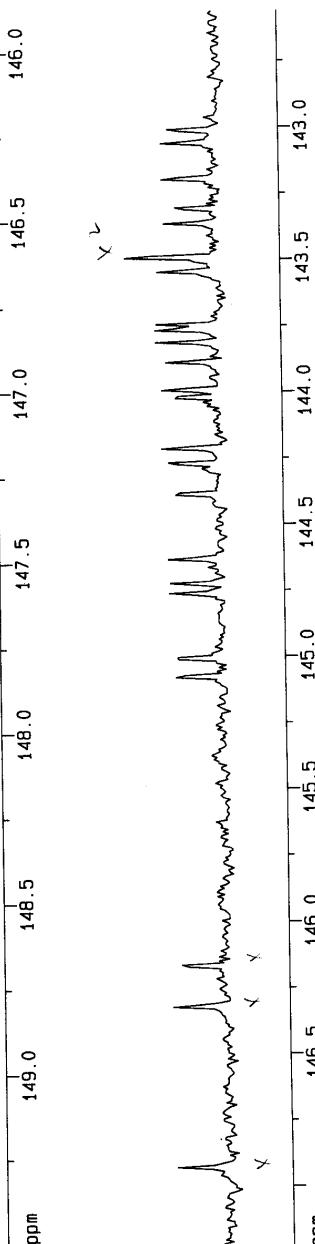
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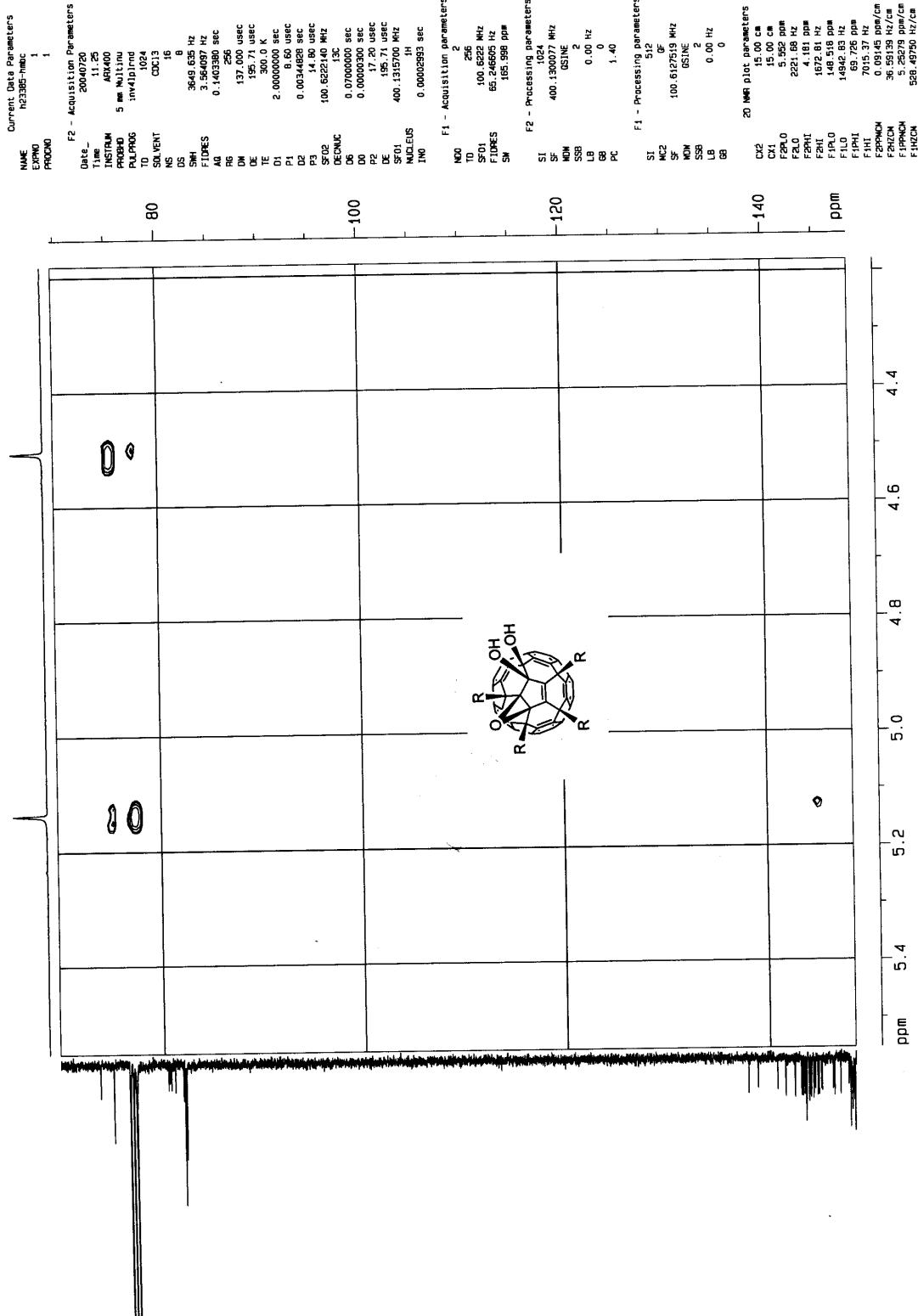


EB 0.40
 PC

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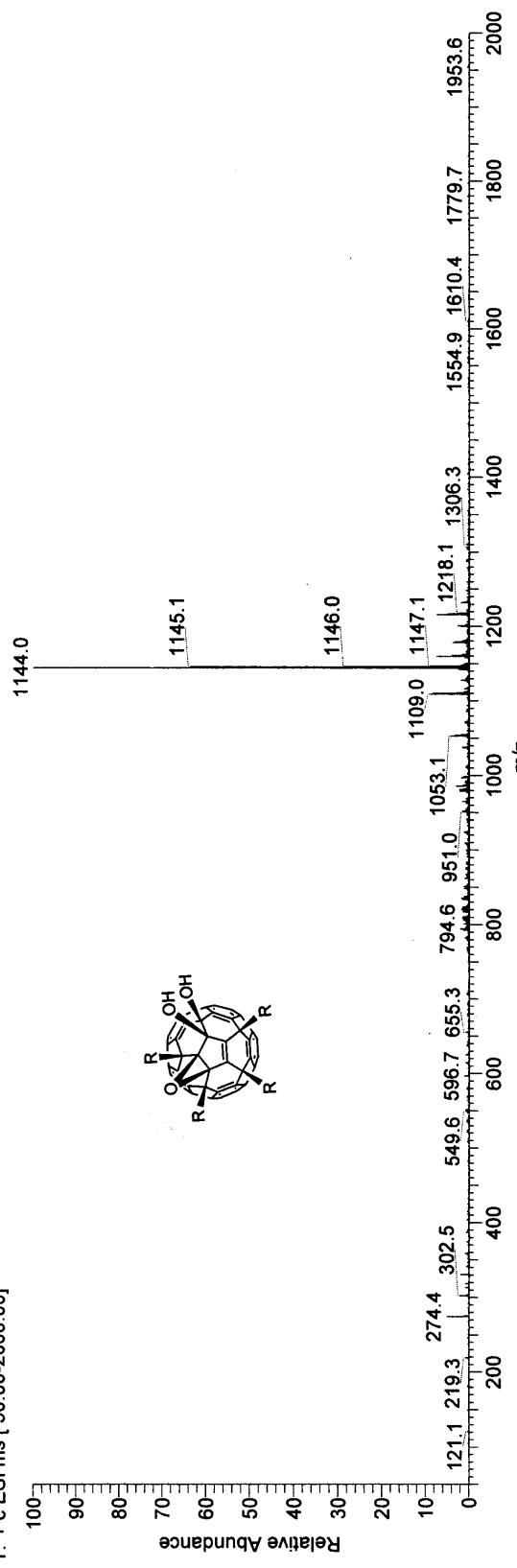
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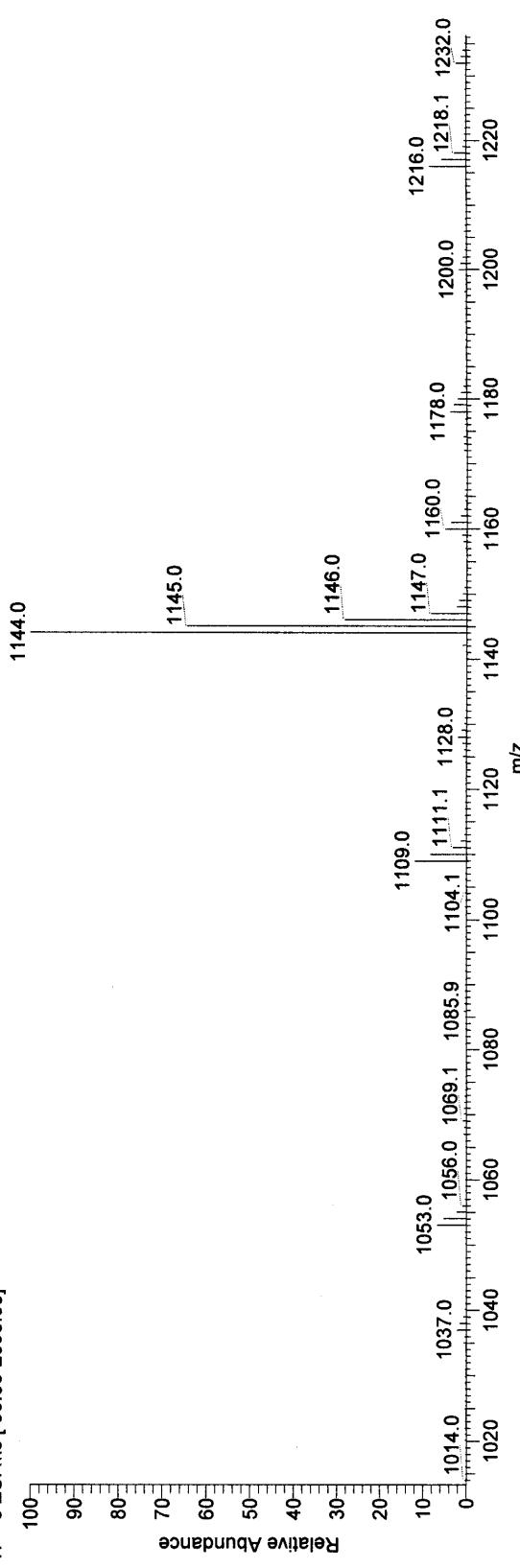
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03/19/2004 04:30:28 PM

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GAN031908 #18-26 RT: 0.50-0.73 AV: 9 NL: 8.77E8
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Current Data Parameters
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 PROCN0 1

F2 - Acquisition Parameters

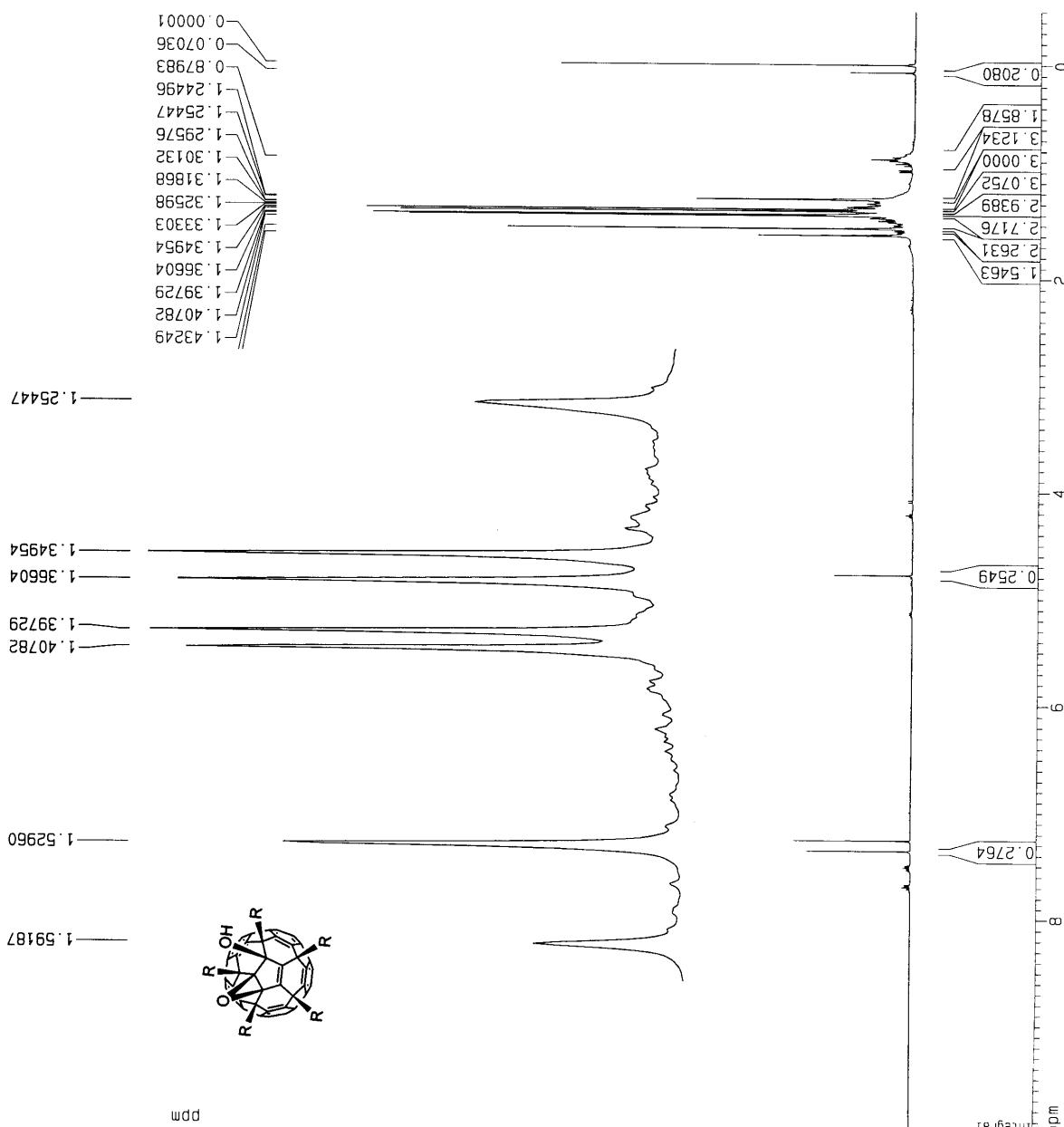
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 NS 32
 DS 0
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 FIDRES 0.195625 Hz
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 RG 715
 DW 78.000 usec
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 NUCLEUS 1H

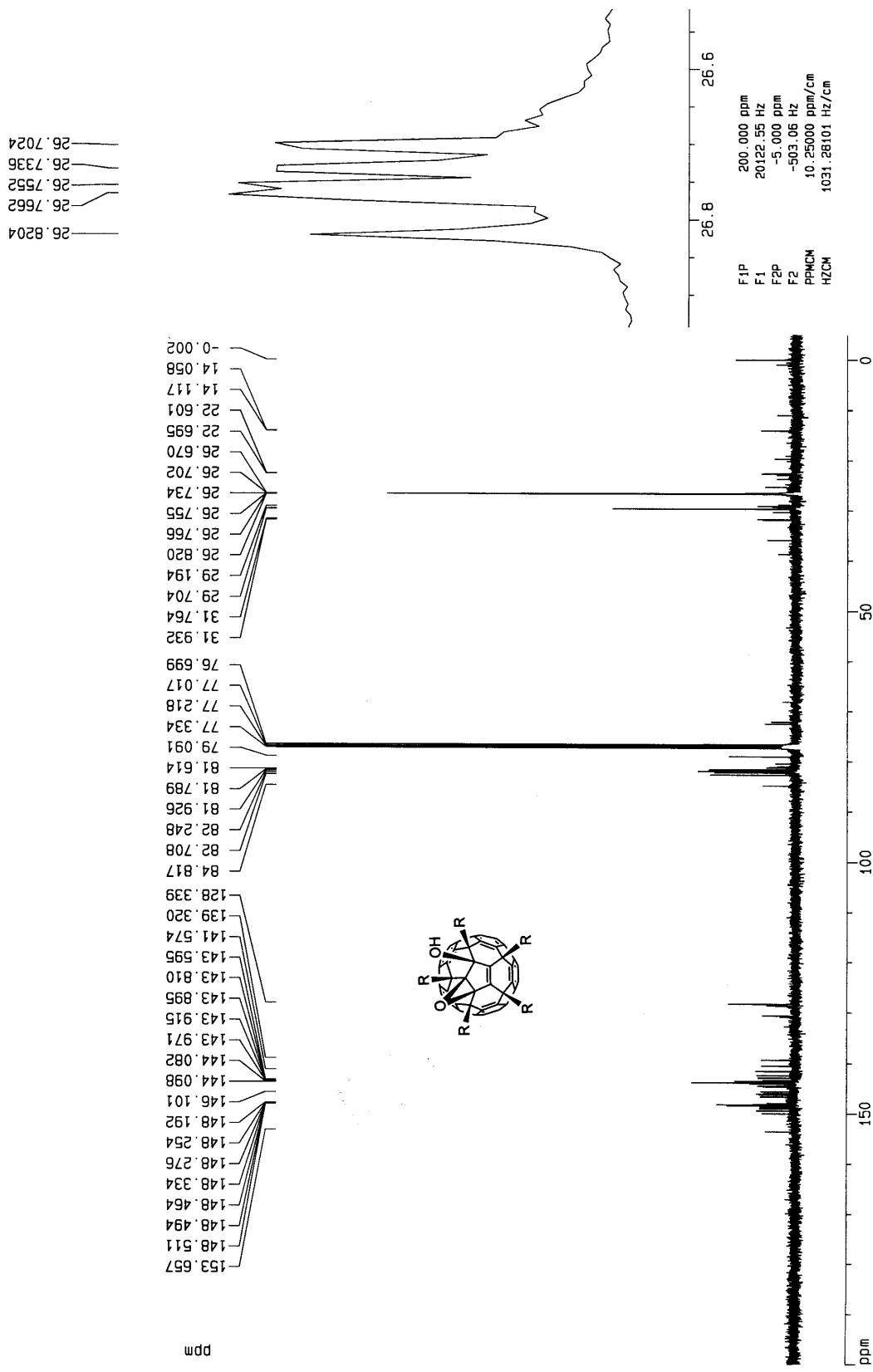
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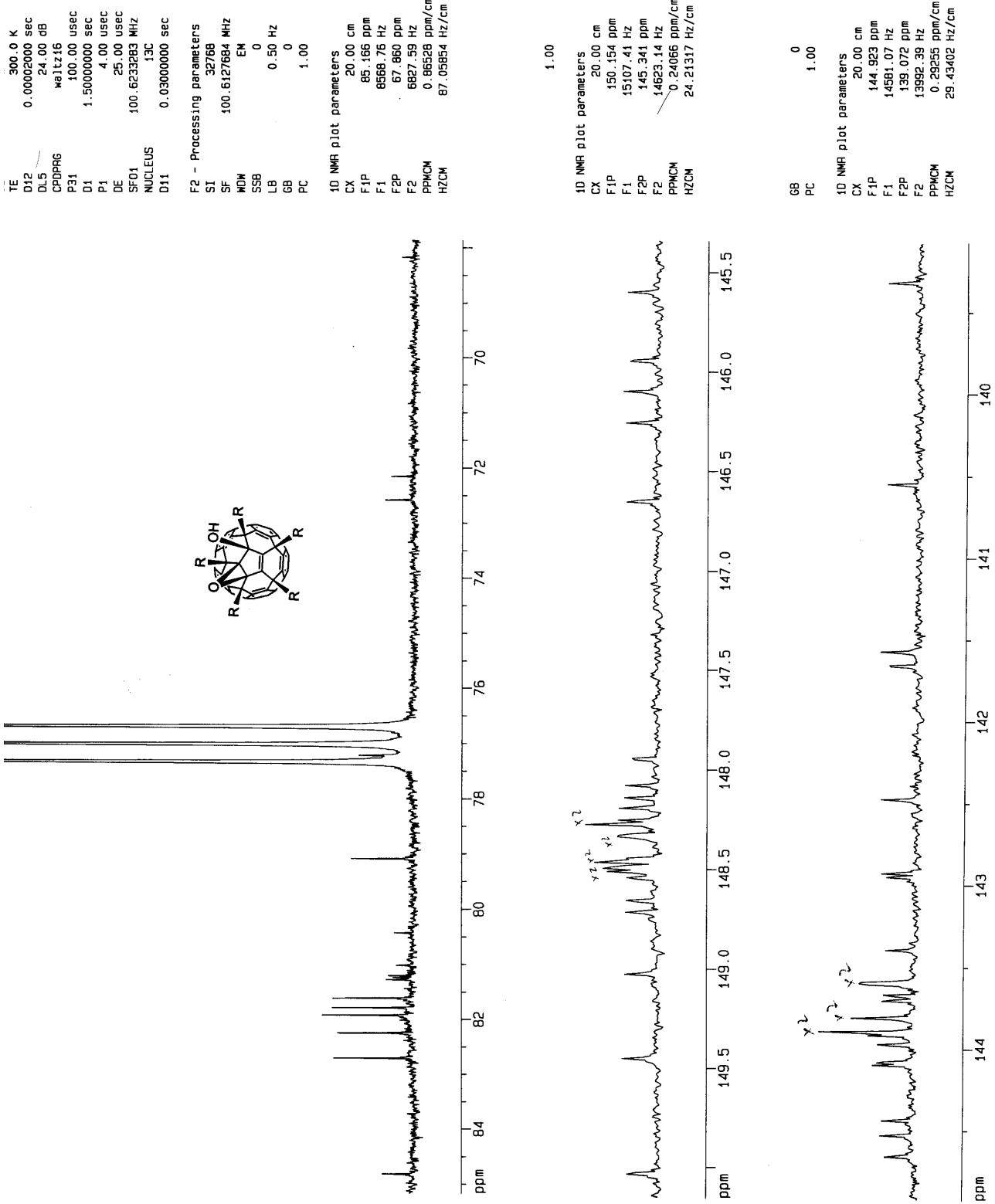
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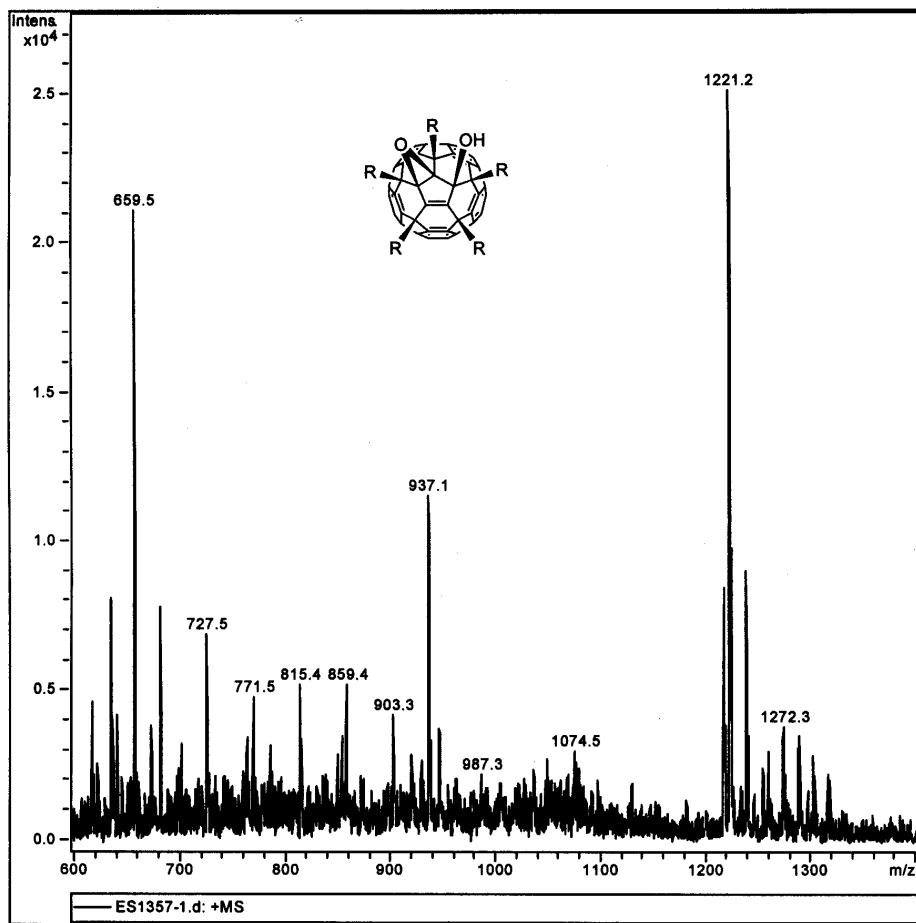
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 F1 4001.30 Hz
 F2P -0.500 ppm
 F2 -200.07 Hz
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 HZCM 210.06825 Hz/cm









Current Data Parameters
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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20040705
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 INSTRUM ARX400
 PROBHD 5 mm Multinu
 PULPROG 2g
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559340 sec
 RG 128
 DW 78.000 usec
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 NUCLEUS 1H

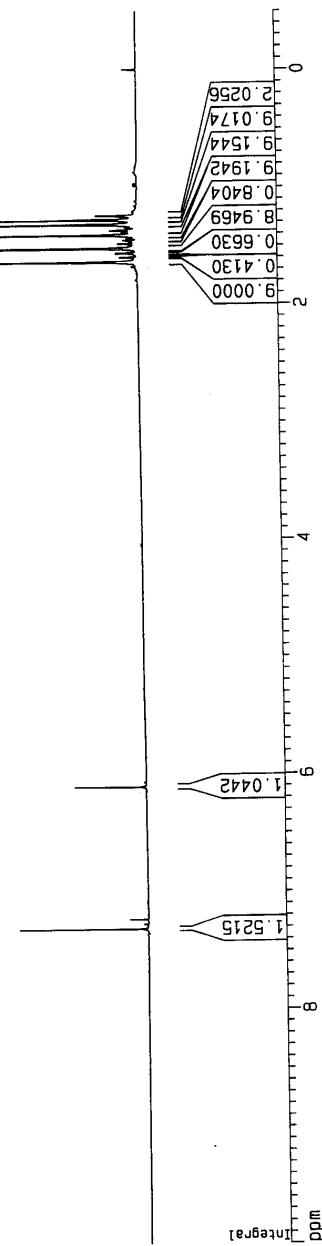
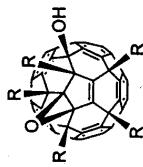
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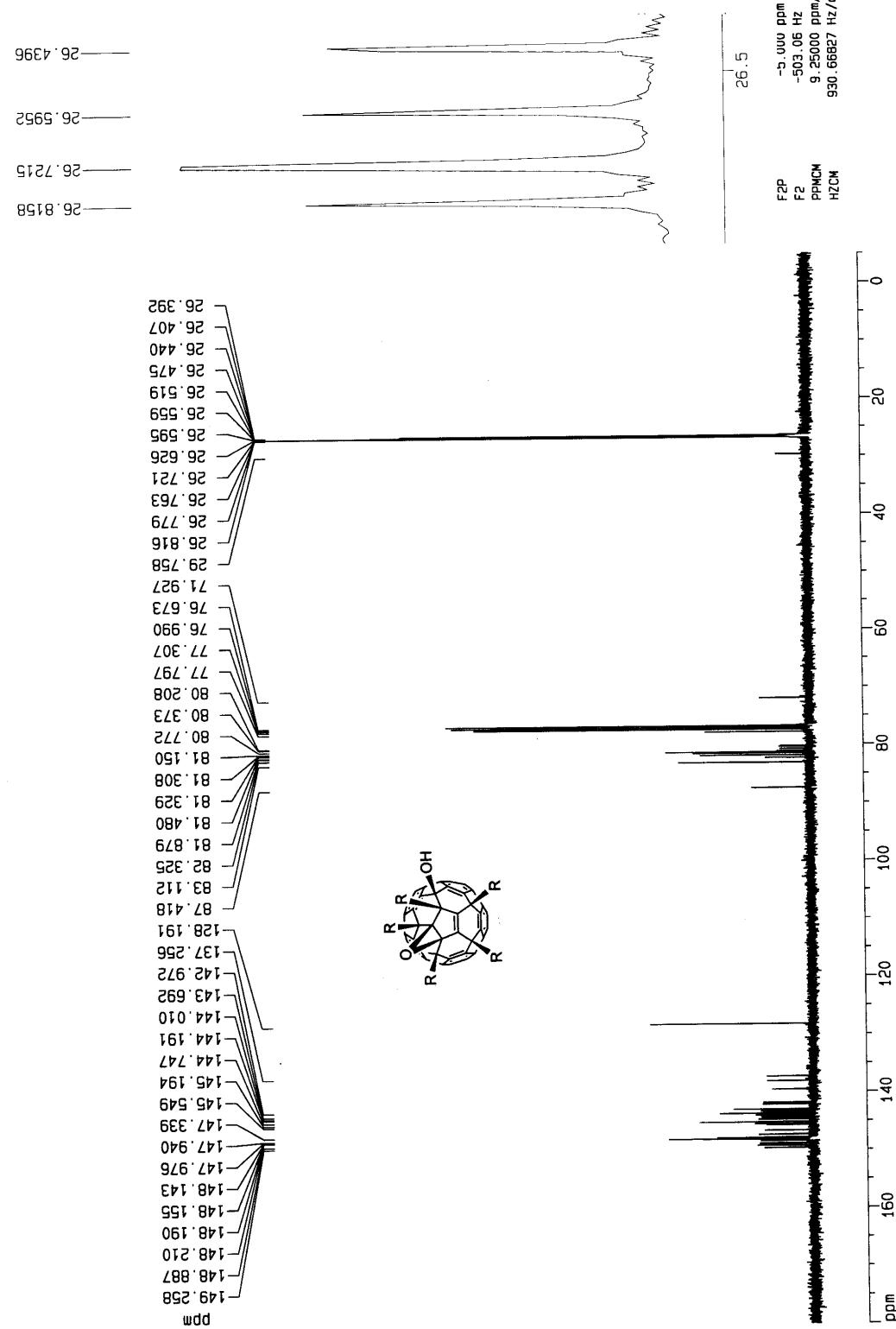
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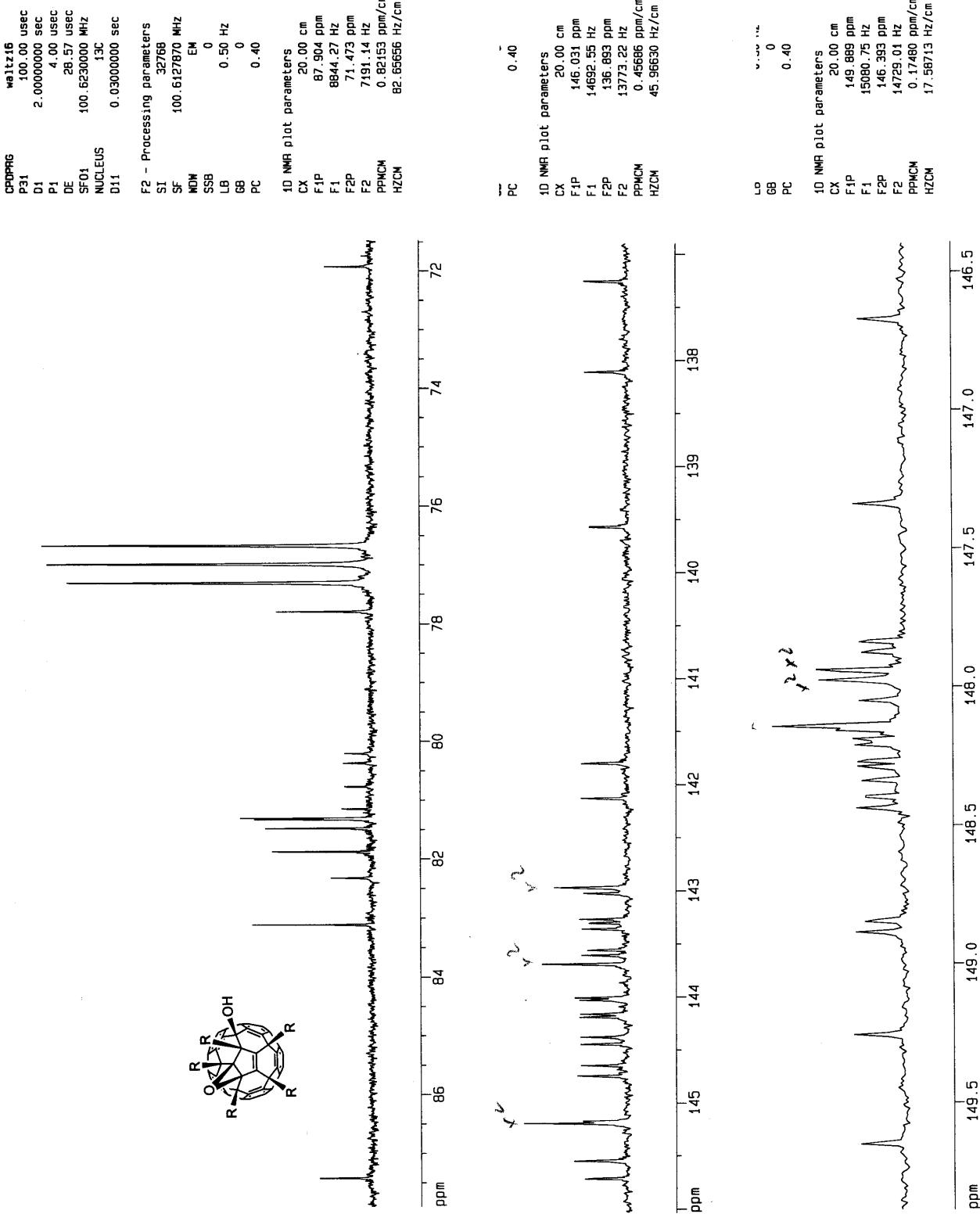
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7.3179

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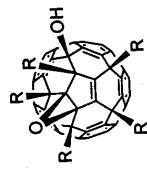
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25
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15
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5
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Relative Abundance

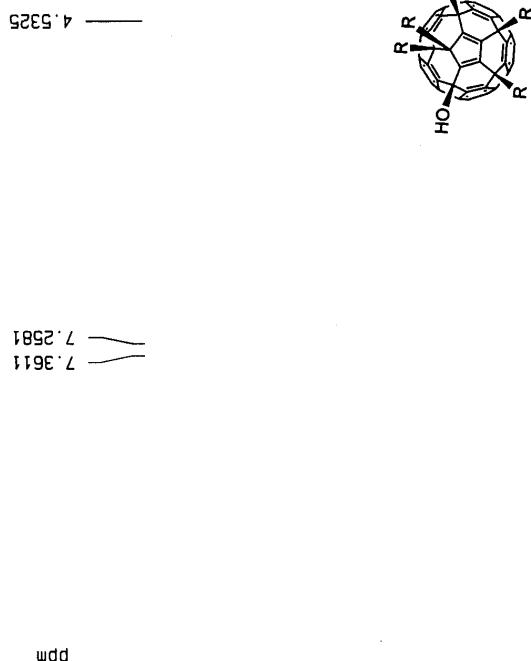
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1217.1
1218.1
1221.0
1222.0
1229.1
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1332.1
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1418.5
1453.4



Current Data Parameters
 NAME h29689
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

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 PULPROG 2g
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 360
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 SFO1 400.1317965 MHz
 NUCLEUS 1H



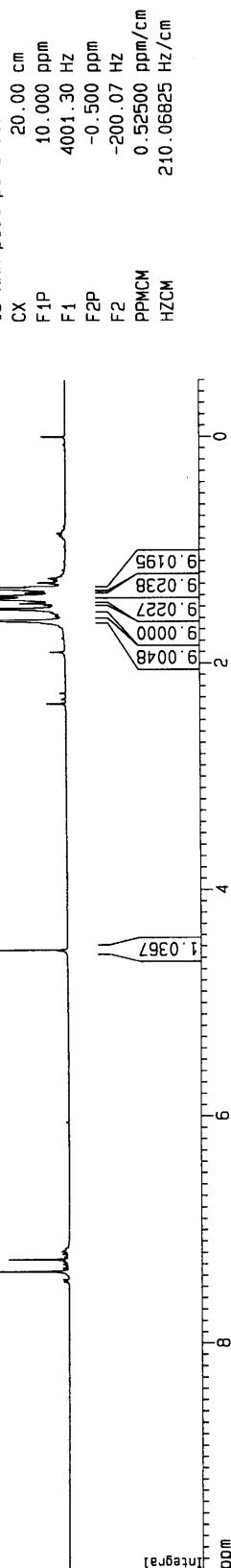
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4.5325

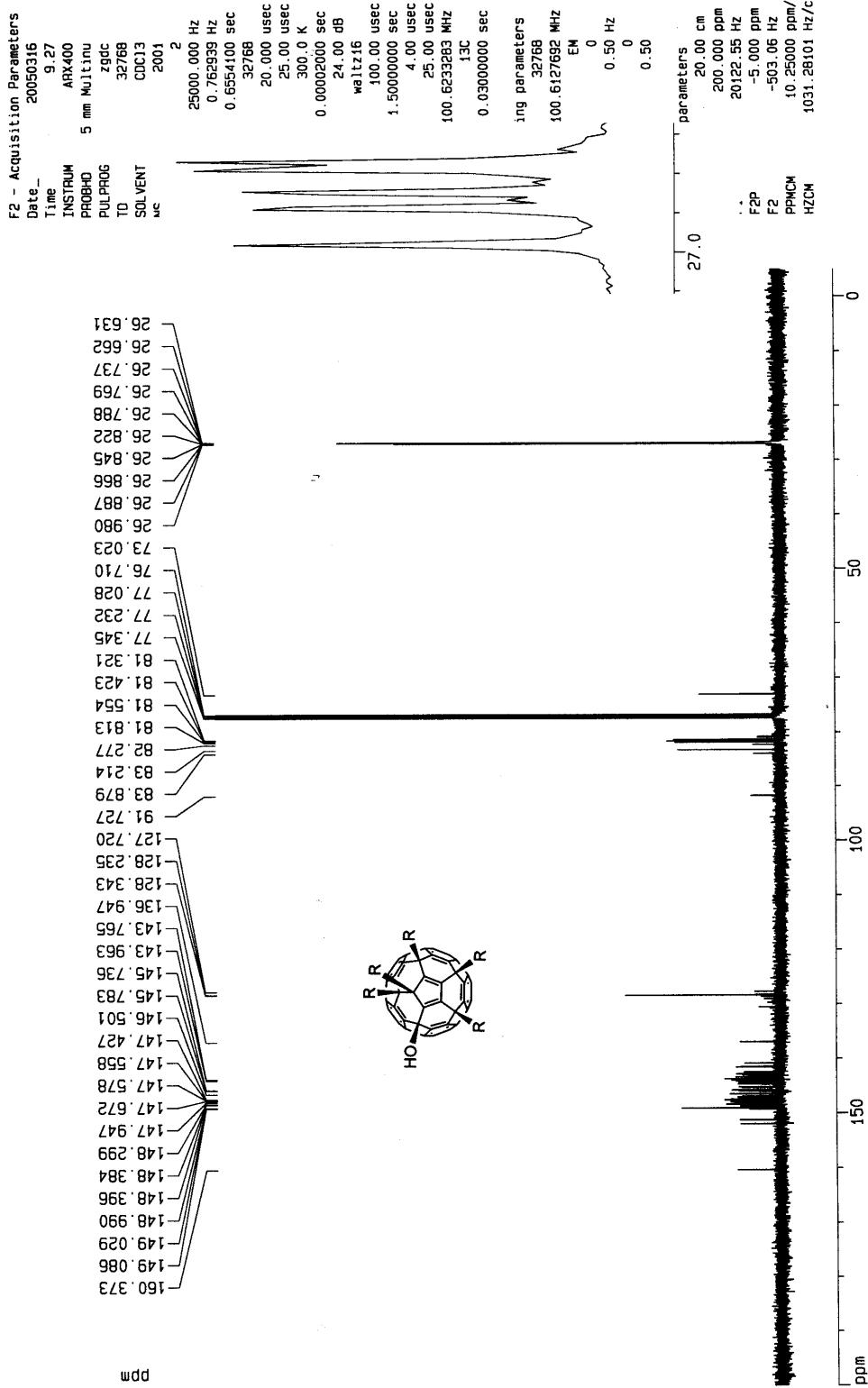
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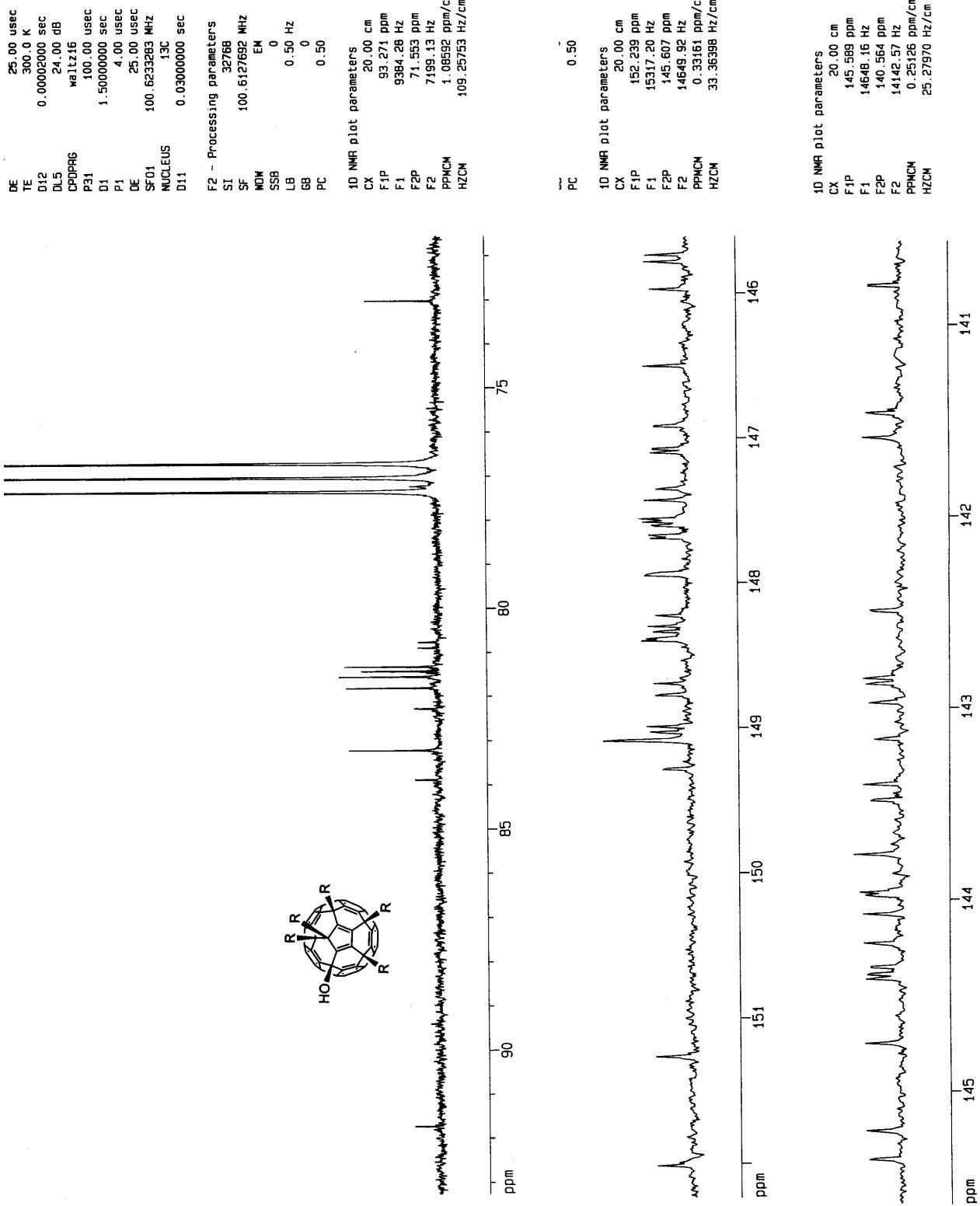
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1D NMR plot parameters



Current Data Parameters
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 PROCNO 1

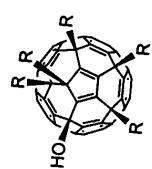




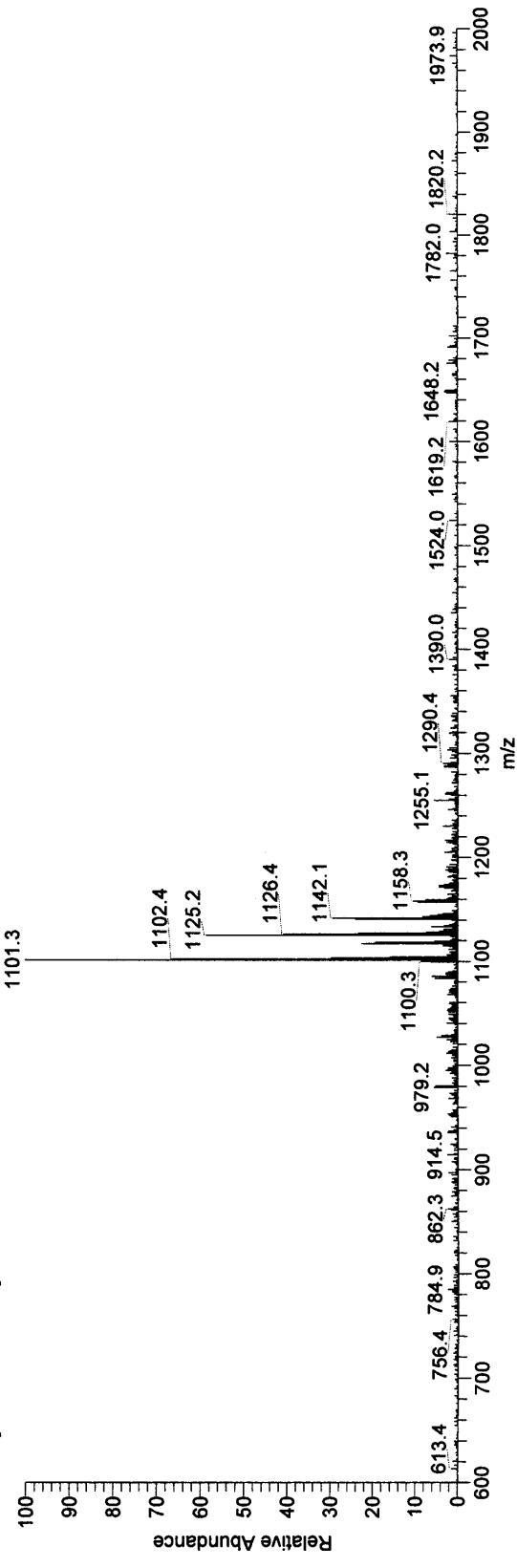
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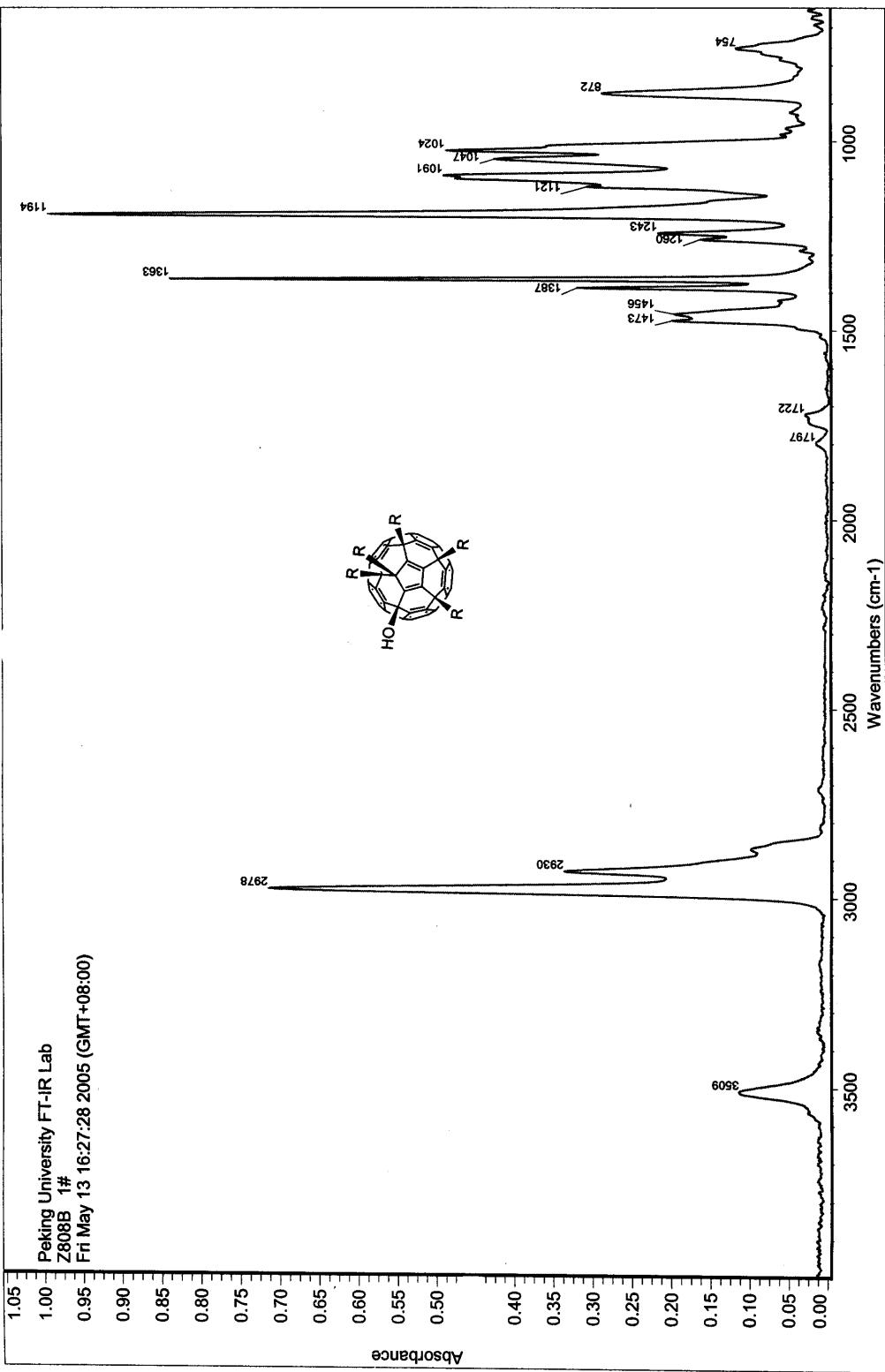
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T: - c ESI ms [600.00-2000.00]



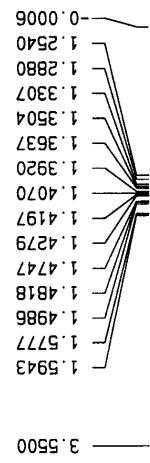


Current Data Parameters

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EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

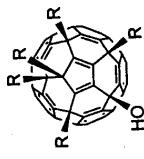
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RG	180
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TE	300.0 K
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NUCLEUS	¹ H



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7.3609

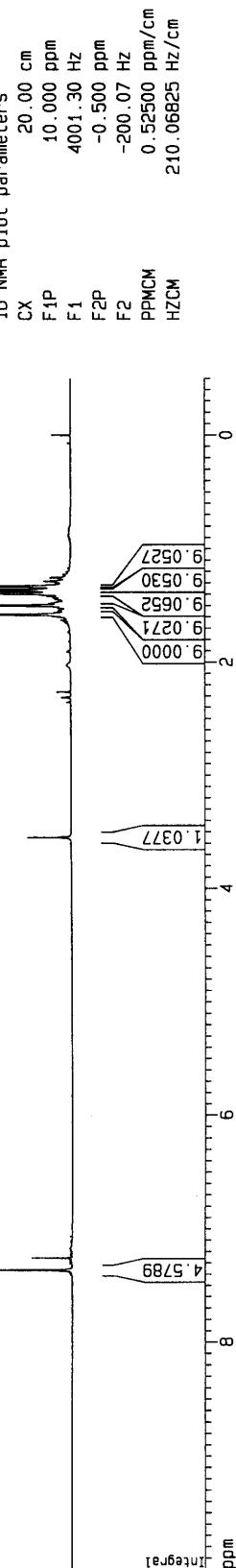
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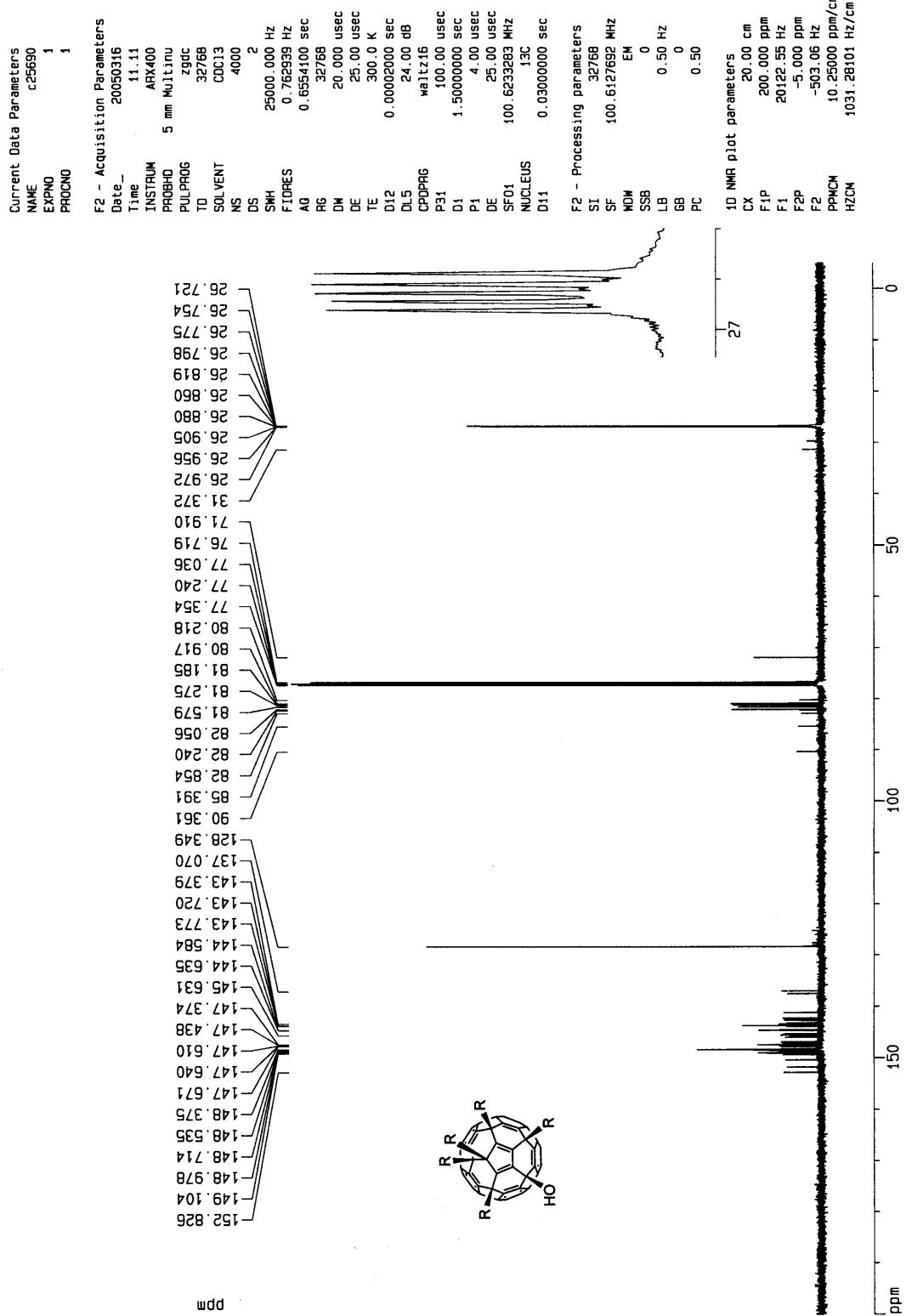


F2 - Processing parameters

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GB	0
PC	4.00

1D NMR plot parameters





wave -
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PUL PROG 79dc
TO 32768
SOLVENT C0C13
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DS 2
SWH 25000.000 Hz
FIDRES 0.765939 Hz
AQ 0.6554100 sec
RG 32768
DW 20.000 usec
DE 25.00 usec
TE 300.0 K
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D15 24.00 dB
CPDPRG Waltz16
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D1 1.500000 sec
P1 4.00 usec
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NUCLEUS ¹³C
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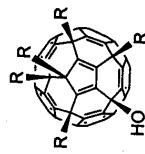
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HZCM 99.77399 Hz/cm

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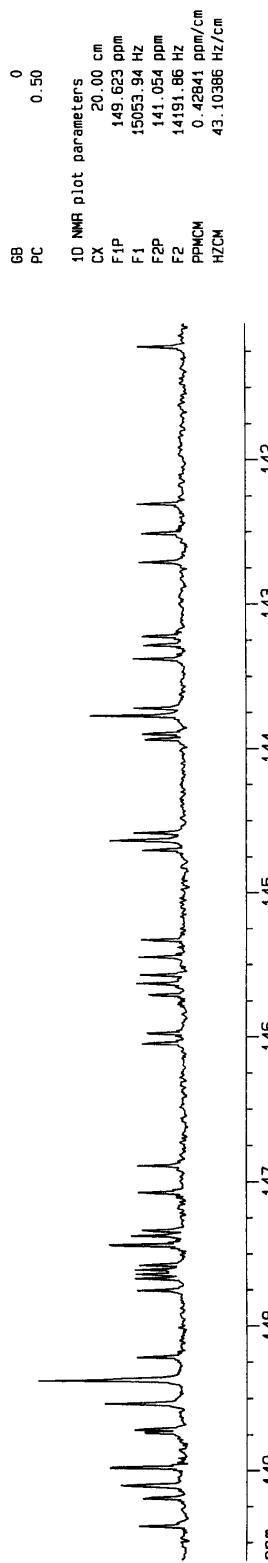
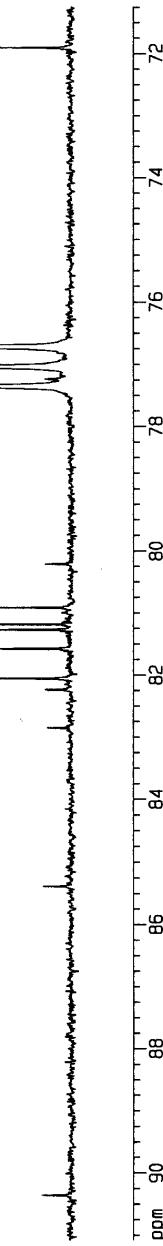
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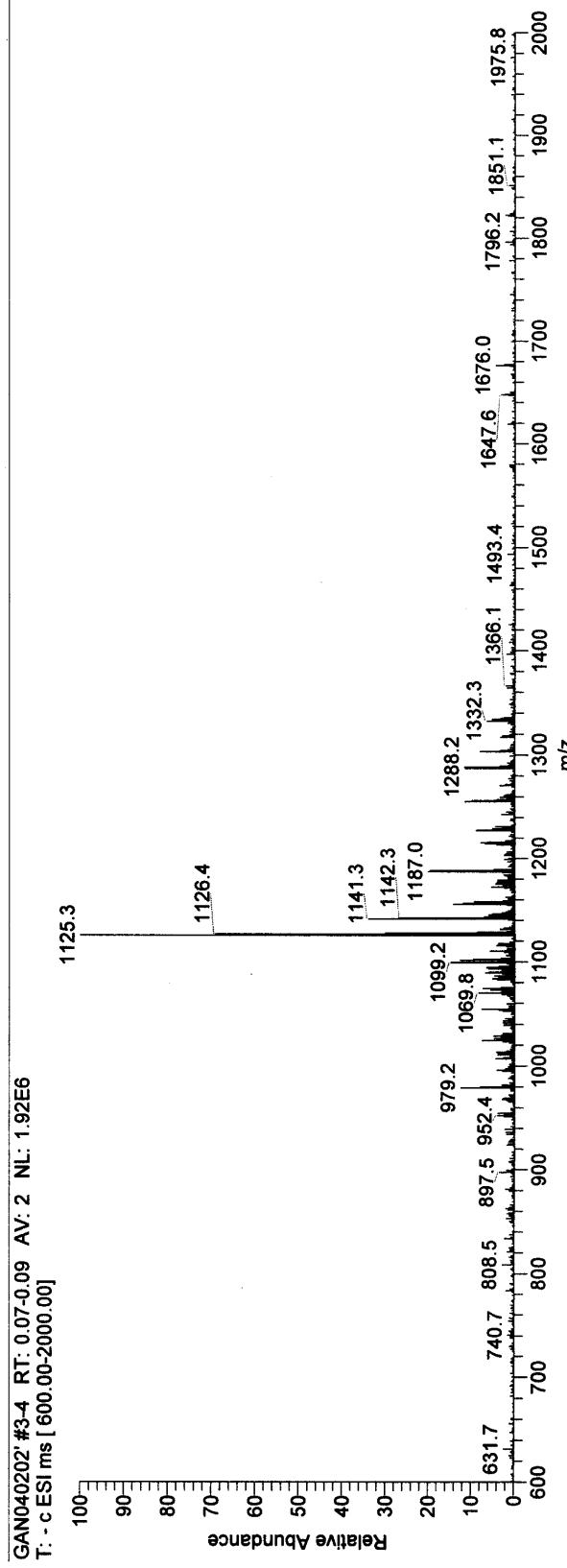
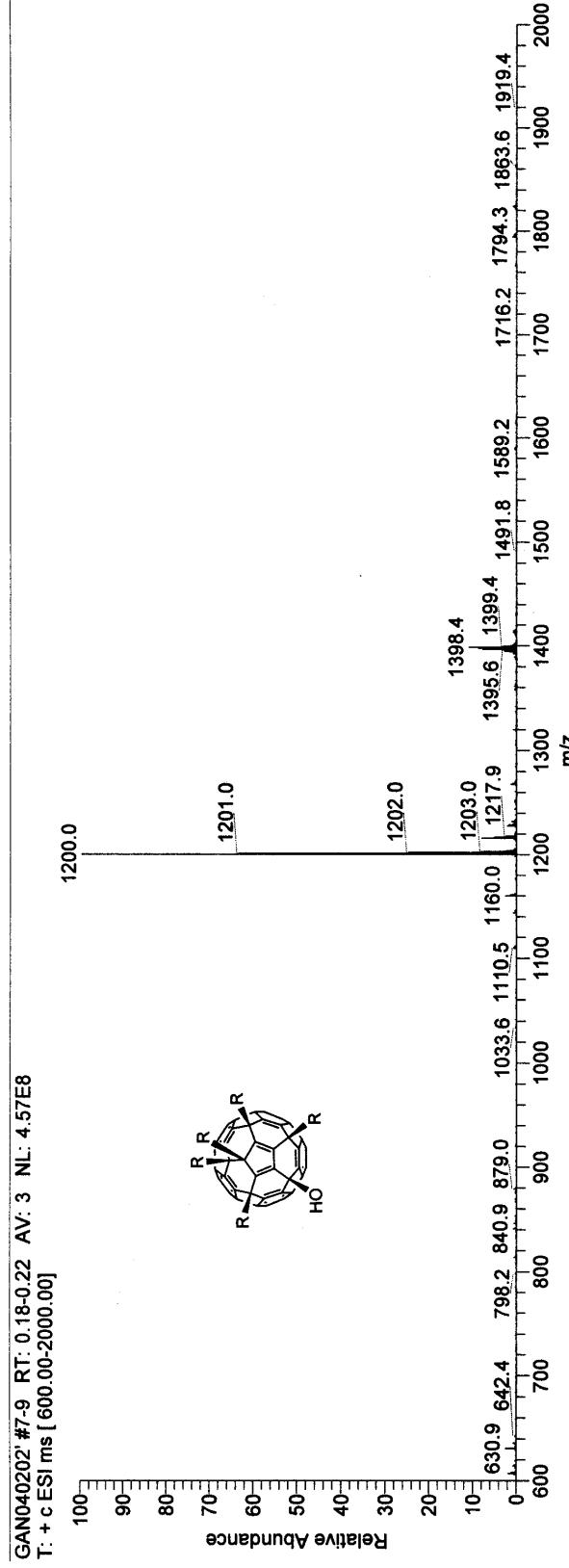
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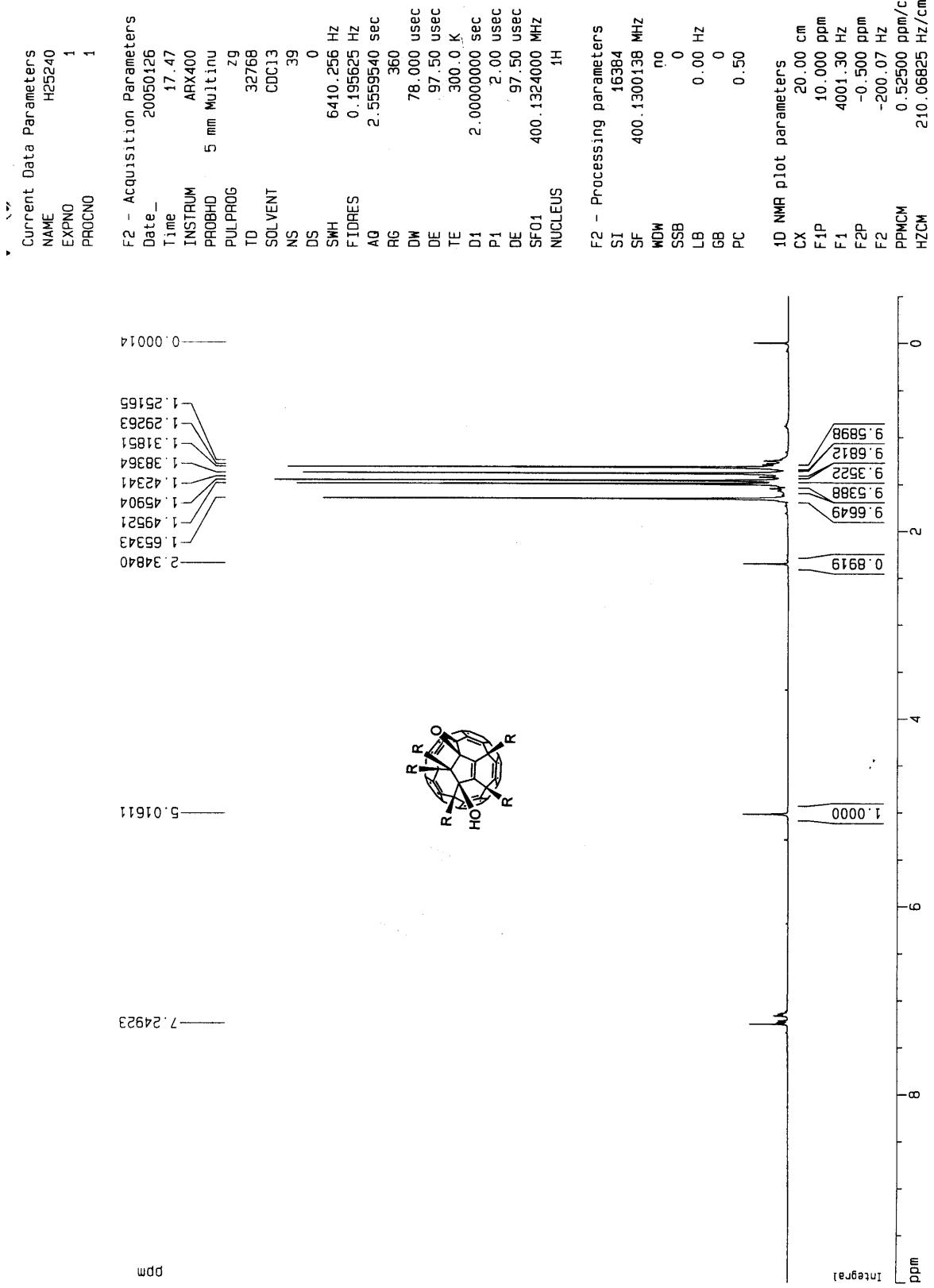
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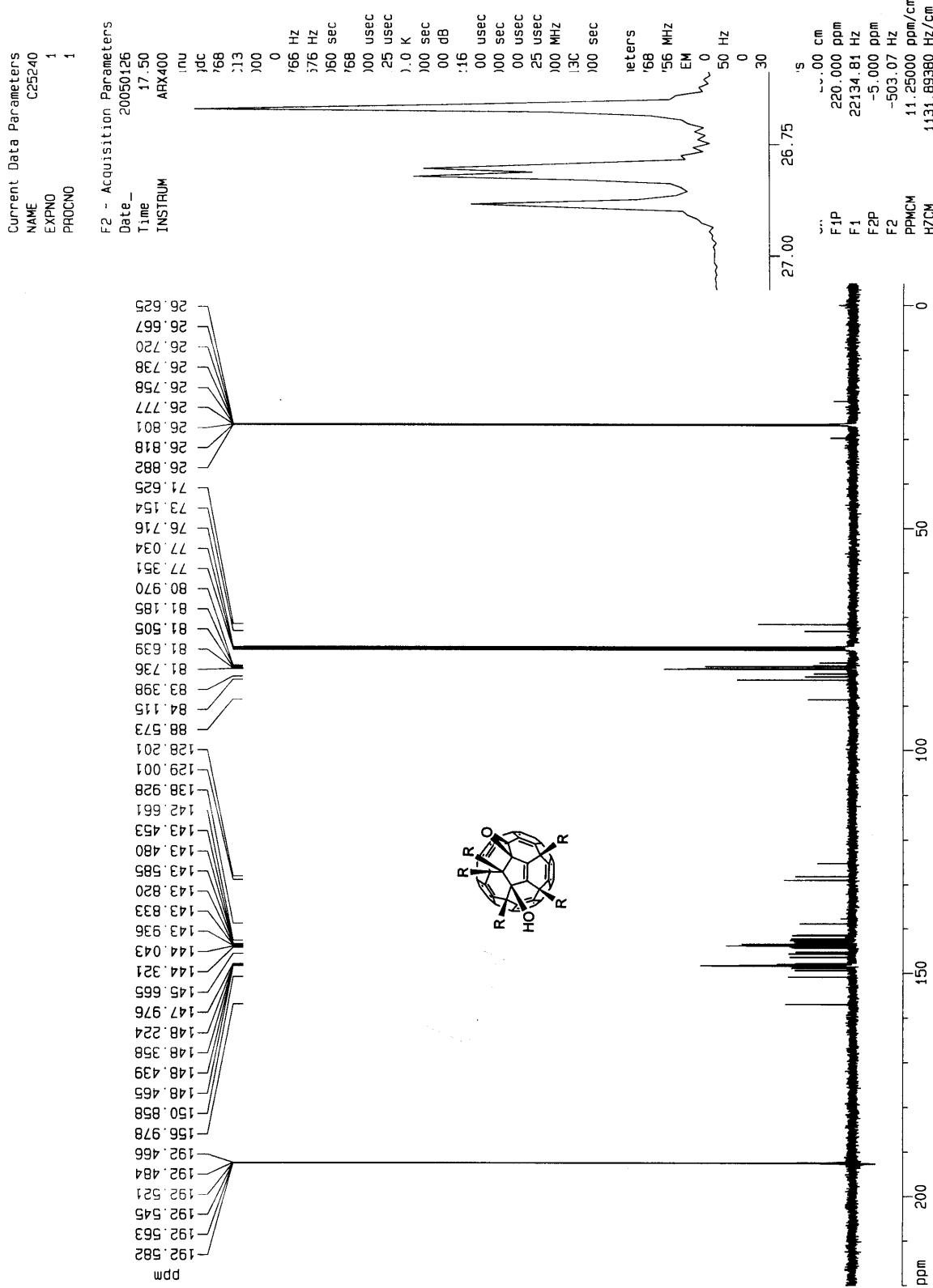


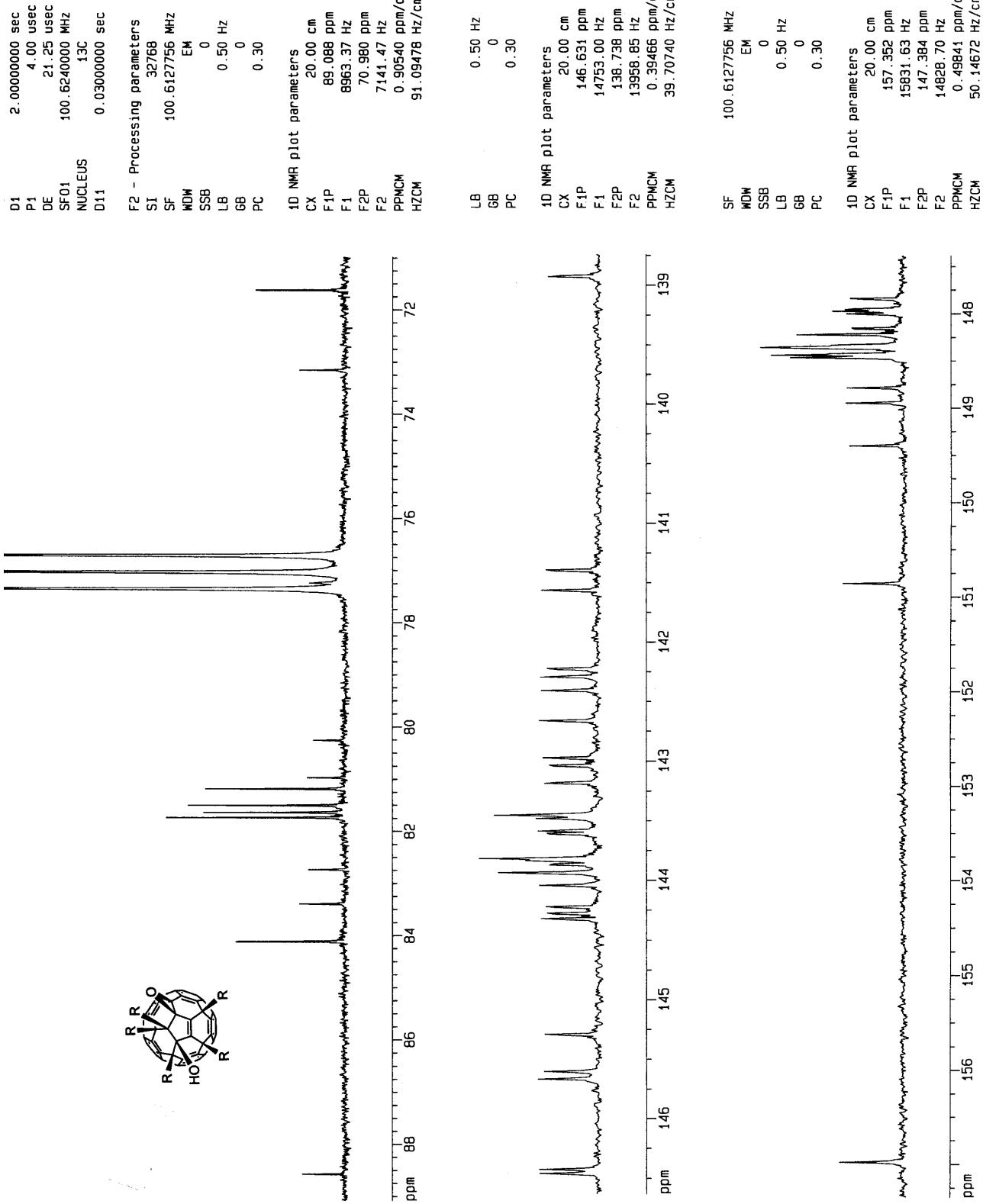
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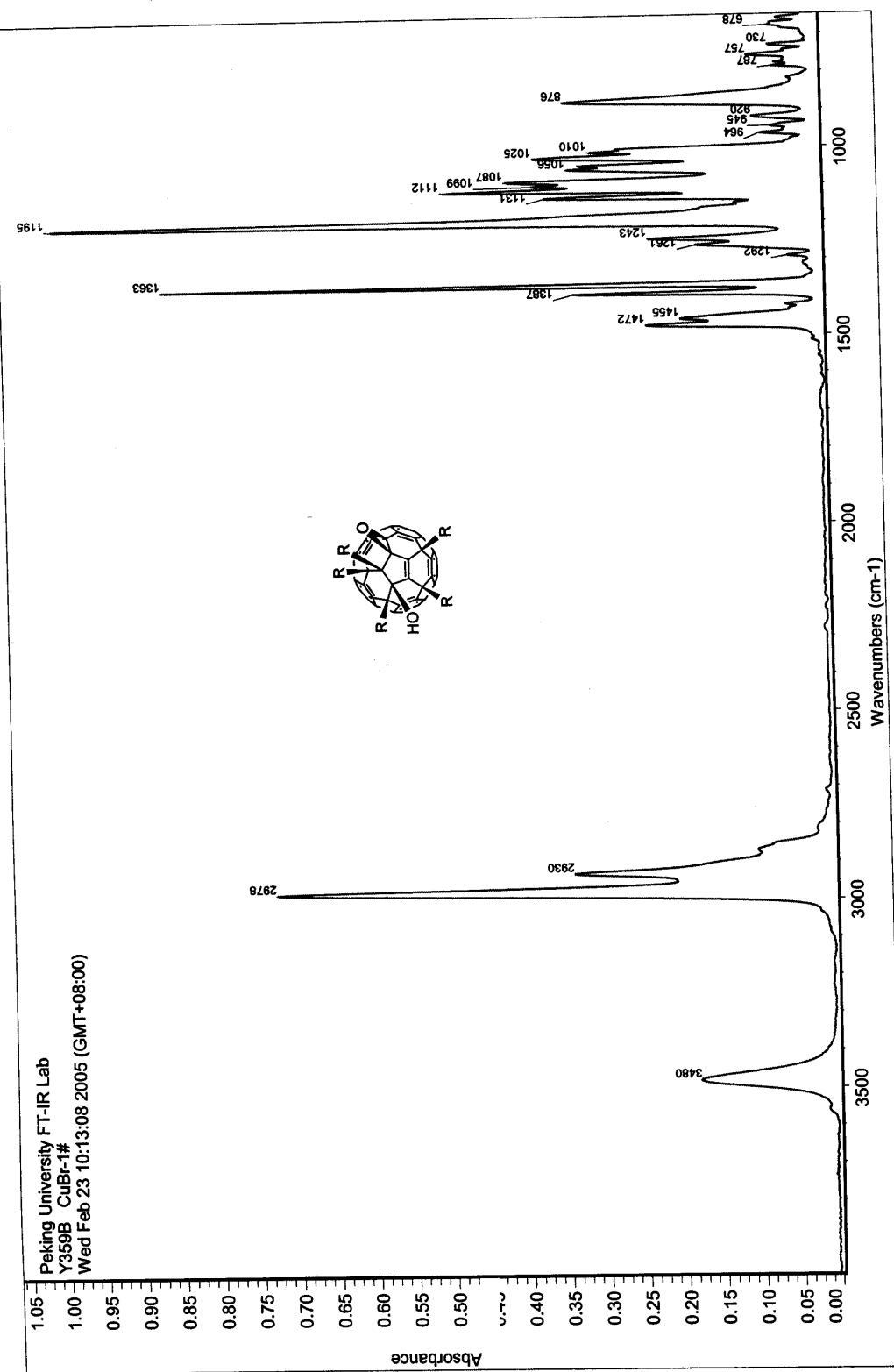












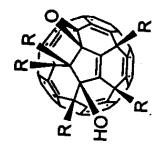
C:\Xcalibur\data\Zhou Jiang\GAN030412

03/05/2005 04:53:33 PM

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T: + c ESI ms [700.00-2000.00]

1215.9



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T: - c ESI ms [700.00-2000.00]

871.1

100

90

80

70

60

50

40

30

20

10

0

Relative Abundance

1161.2

1162.3

1164.1

870.1

872.2

832.9

832.9

917.8

1010.7

1054.8

1187.4

1354.2

1411.3

1488.3

1533.1

1583.6

1669.2

1758.9

1845.5

1921.0

1956.5

2000

m/z

Current Data Parameters
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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

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 RG 256
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 DE 97.50 usec
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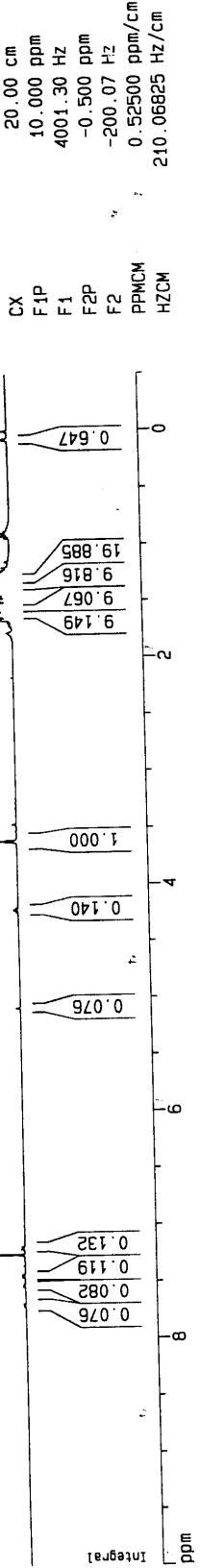
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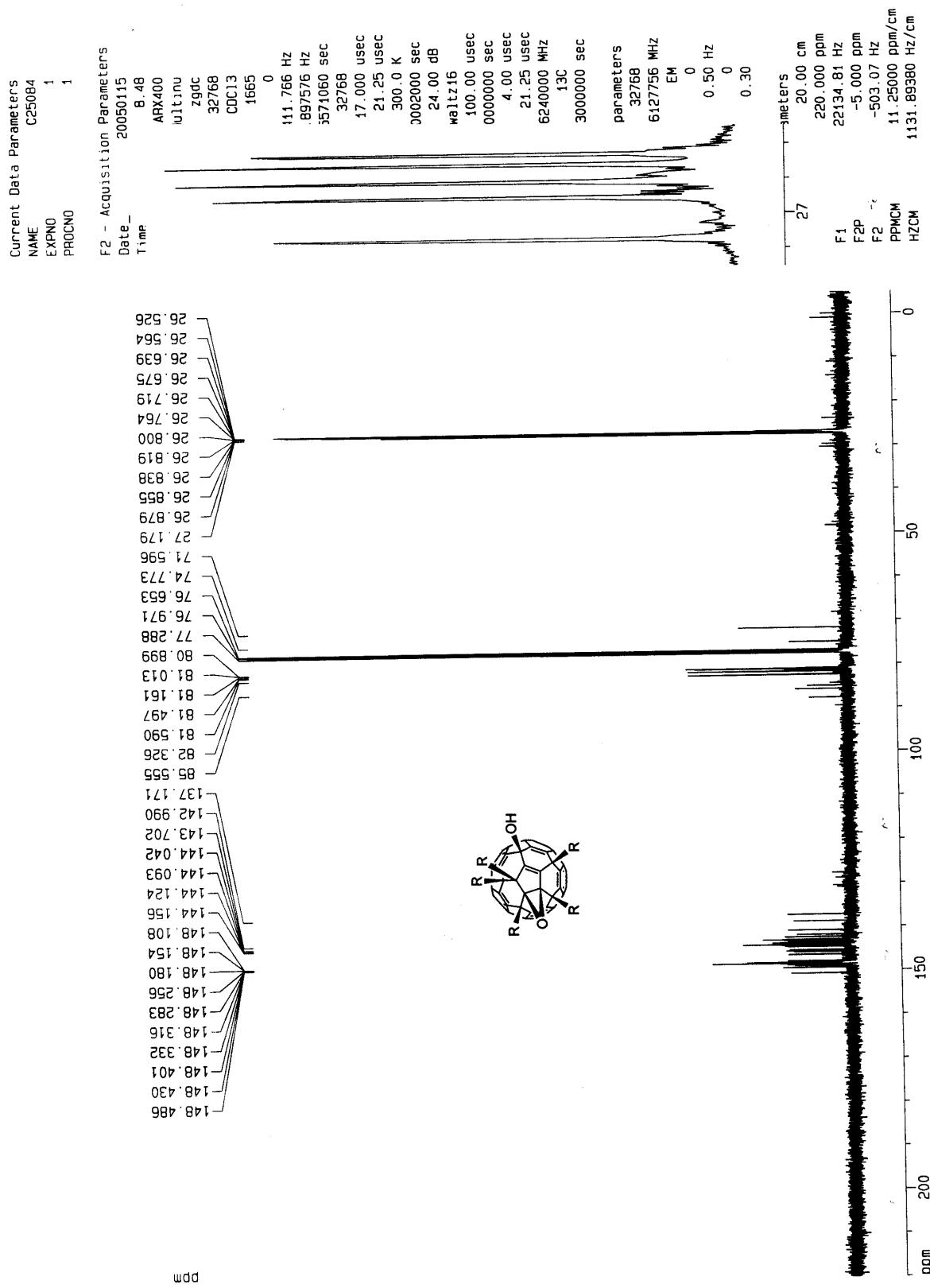


F2 - Processing parameters

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1D NMR plot parameters





CRDPG6
 P31
 D1
 P1
 DE
 SF01
 NUCLEUS
 D11

waitz16
 100.00 usec
 2.0000000 sec
 4.00 usec
 21.25 usec
 100.620000 MHz
 13C
 0.03000000 sec

F2 - Processing parameters

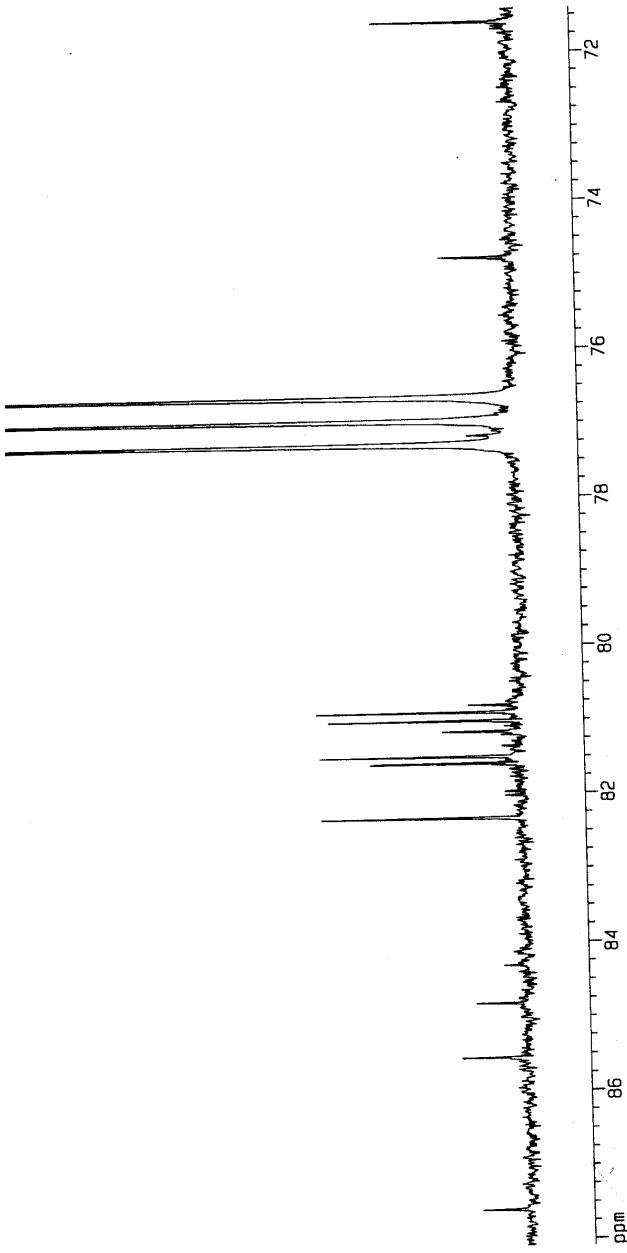
S1
 SF
 MDW
 SSB
 LB
 GB
 PC

32768
 100.6127756 MHz
 EM
 0
 0.50 Hz
 0
 0.30

1D NMR plot parameters

CX
 F1P
 F1
 F2P
 F2
 PPMCM
 HZCM

20.00 cm
 88.095 ppm
 8863.44 Hz
 71.403 ppm
 7184.06 Hz
 0.83457 ppm/cm
 83.96678 Hz/cm



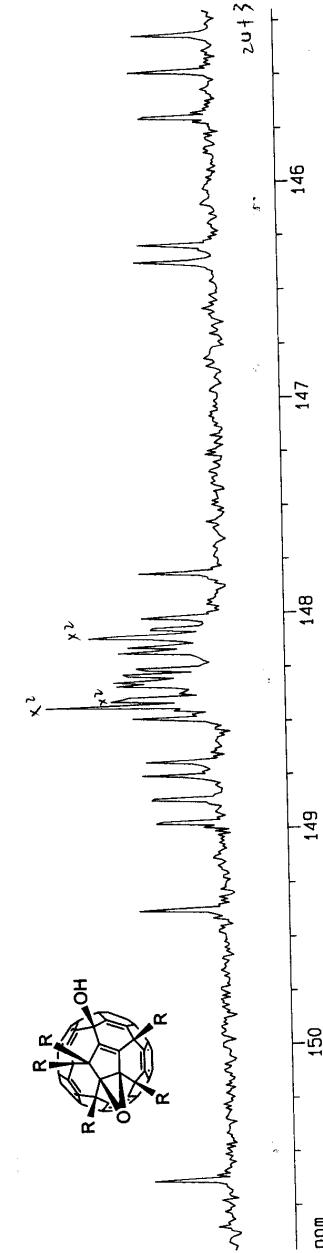
SSB
 LB
 GB
 PC

0
 0.50 Hz
 0
 0.30

1D NMR plot parameters

CX
 F1P
 F1
 F2P
 F2
 PPMCM
 HZCM

20.00 cm
 150.958 ppm
 15188.33 Hz
 145.199 ppm
 14608.87 Hz
 0.28797 ppm/cm
 28.97300 Hz/cm



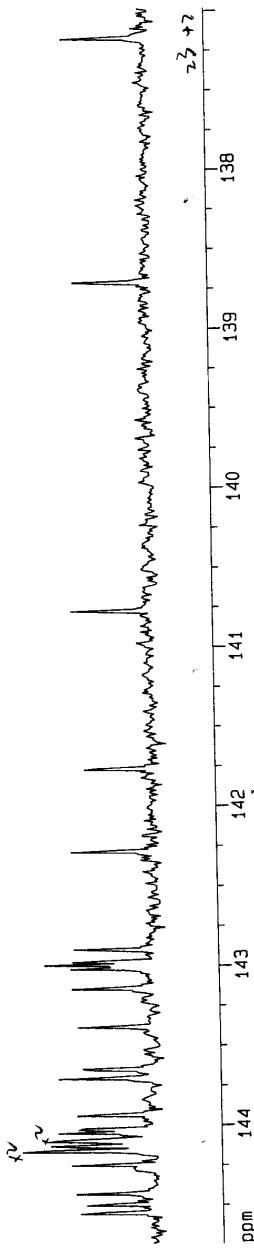
SSB
 LB
 GB
 PC

0
 0.50 Hz
 0
 0.30

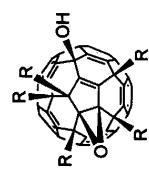
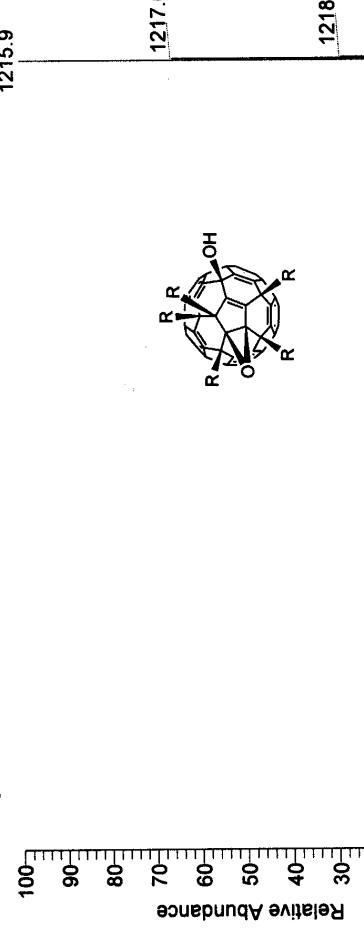
1D NMR plot parameters

CX
 F1P
 F1
 F2P
 F2
 PPMCM
 HZCM

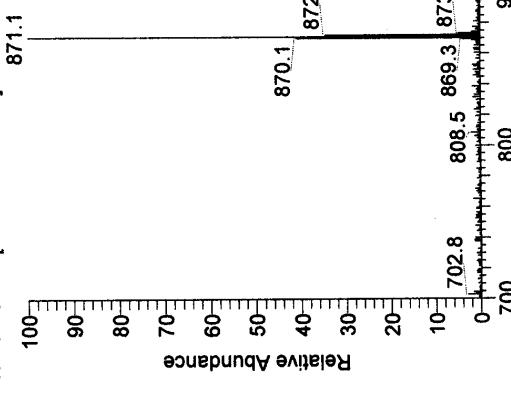
20.00 cm
 144.744 ppm
 14563.09 Hz
 136.983 ppm
 13782.20 Hz
 0.38807 ppm/cm
 39.04441 Hz/cm



GAN011811 #19-30 RT: 0.42-0.64 AV: 12 NL: 2.90E8
 T: + c ESI ms [700.00-2000.00]



GAN011811 #8-10 RT: 0.17-0.21 AV: 3 NL: 4.17E6
 T: - c ESI ms [700.00-2000.00]



Current Data Parameters
 NAME h24981
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

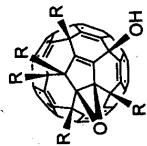
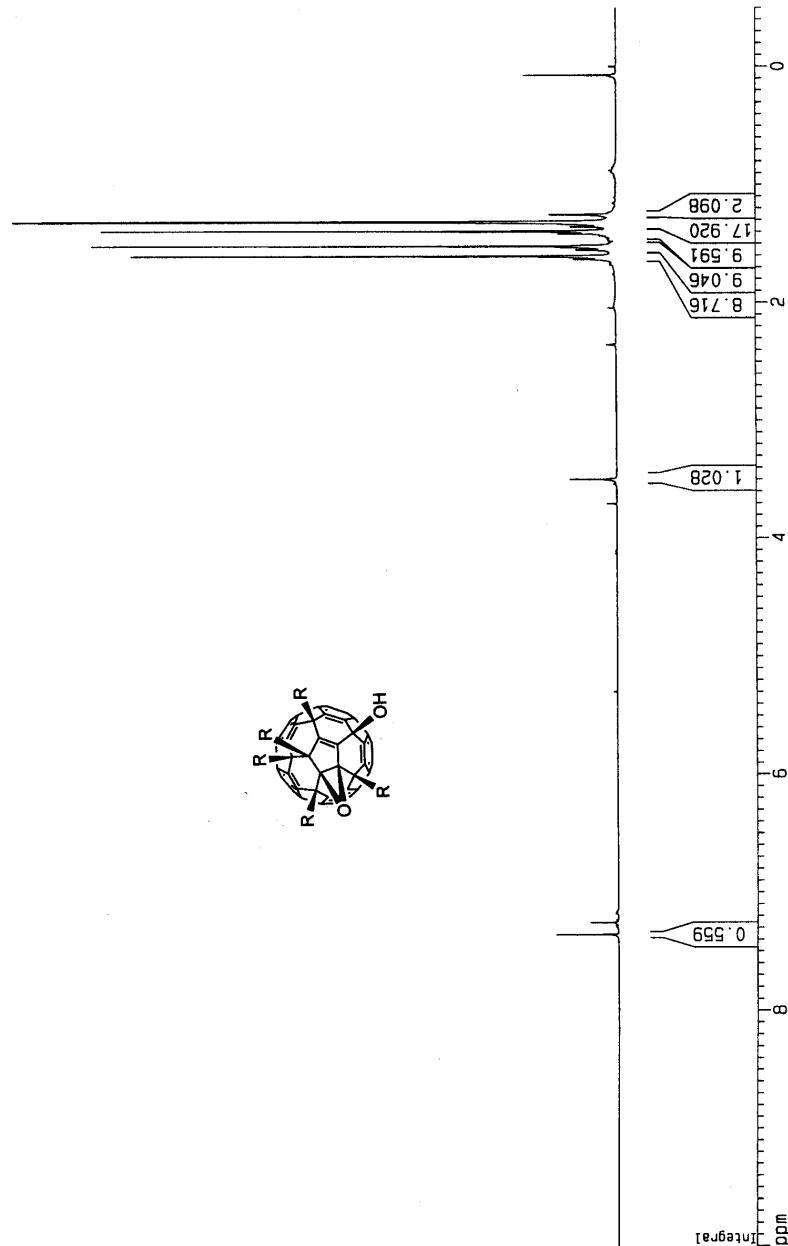
Date 20050106
 Time 14.16
 INSTRUM ARX400
 PROBHD 5 mm Multinu
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 128
 DW 78.000 usec
 DE 97.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 P1 4.00 usec
 DE 97.50 usec
 SF01 400.1317965 MHz
 NUCLEUS 1H

0.07248
 1.25486
 1.31444
 1.32029
 1.35178
 1.35778
 1.39576
 1.41774
 1.52222
 1.55489
 1.60658
 1.63555

-3.50064

7.35918
 7.25811

ppm

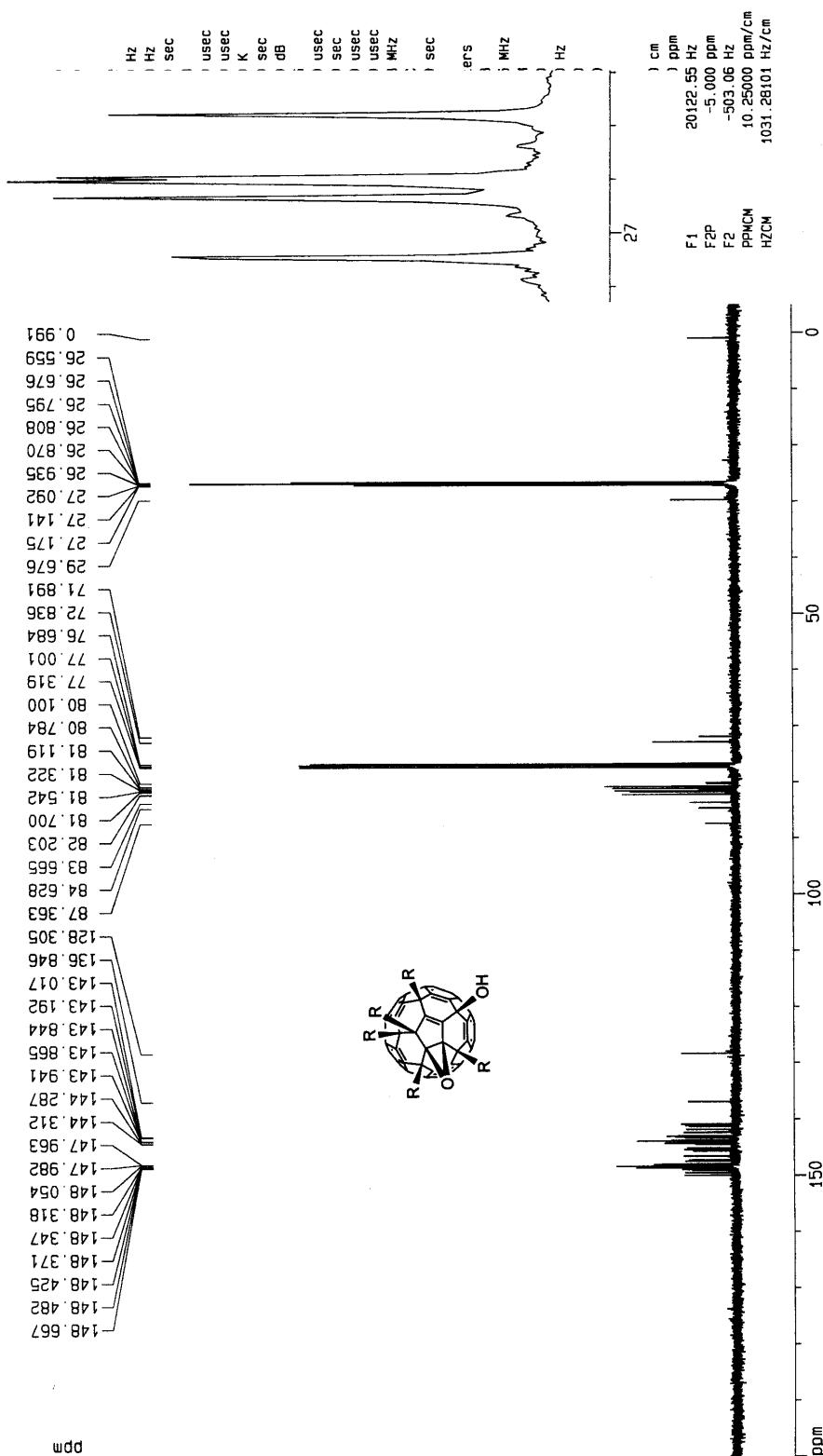


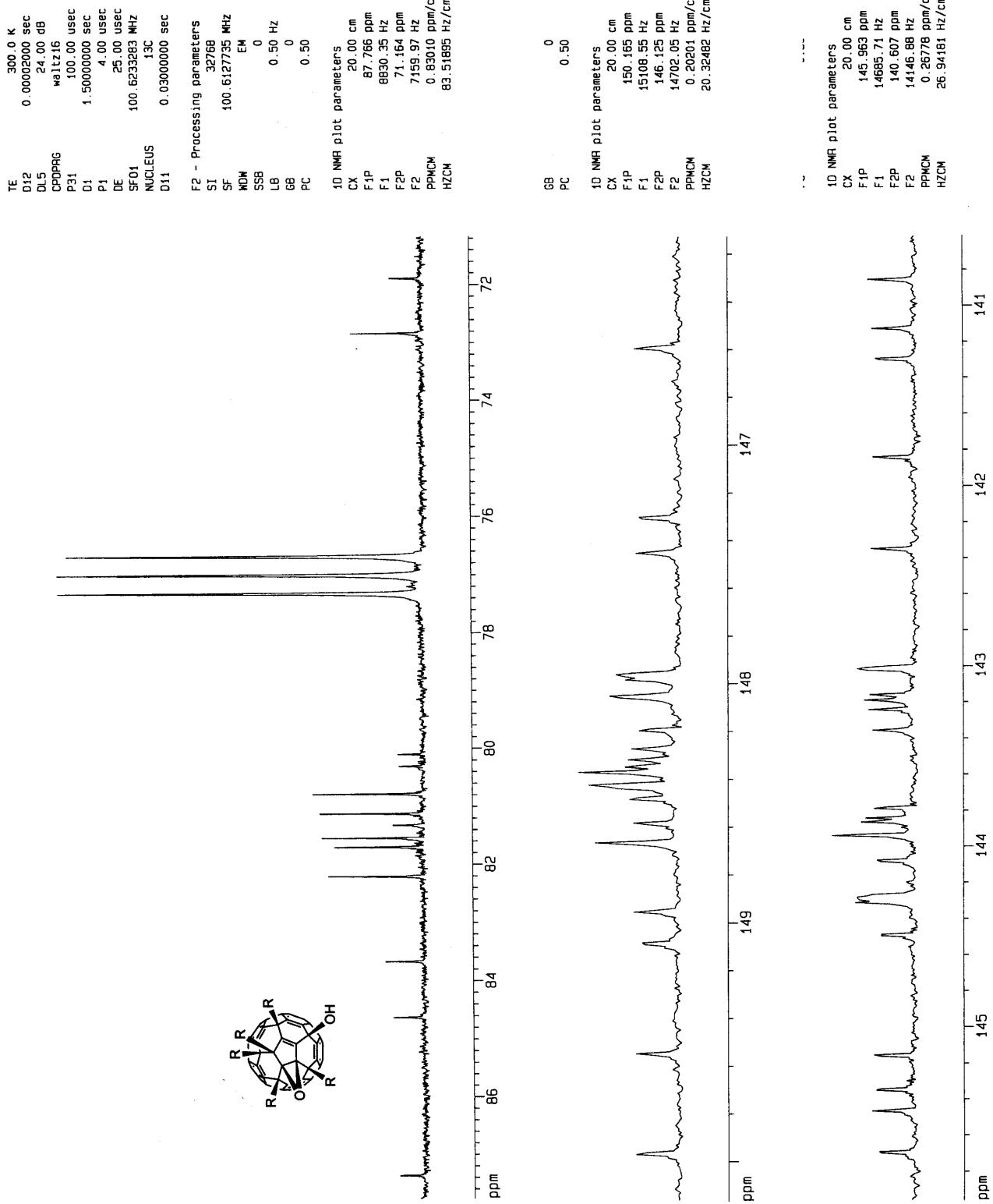
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Current Data Parameters
NAME      C249B1    1
EXPNO    PROCN0    1

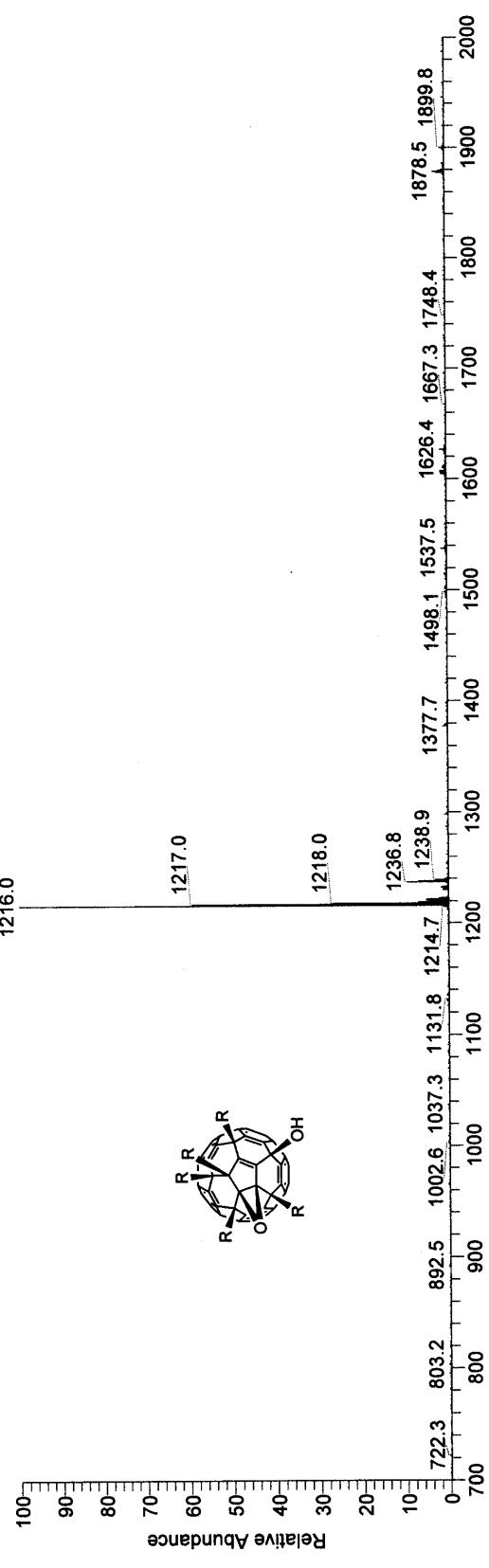
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F2 - Acquisition Parameters
Date _ 20050106

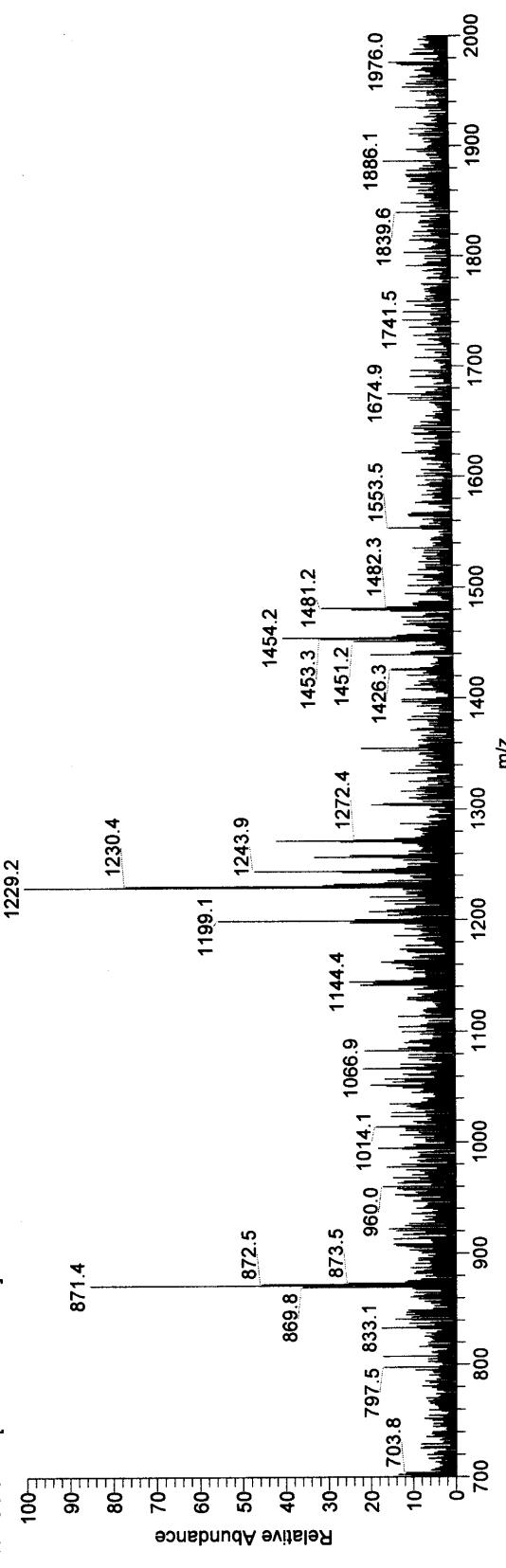




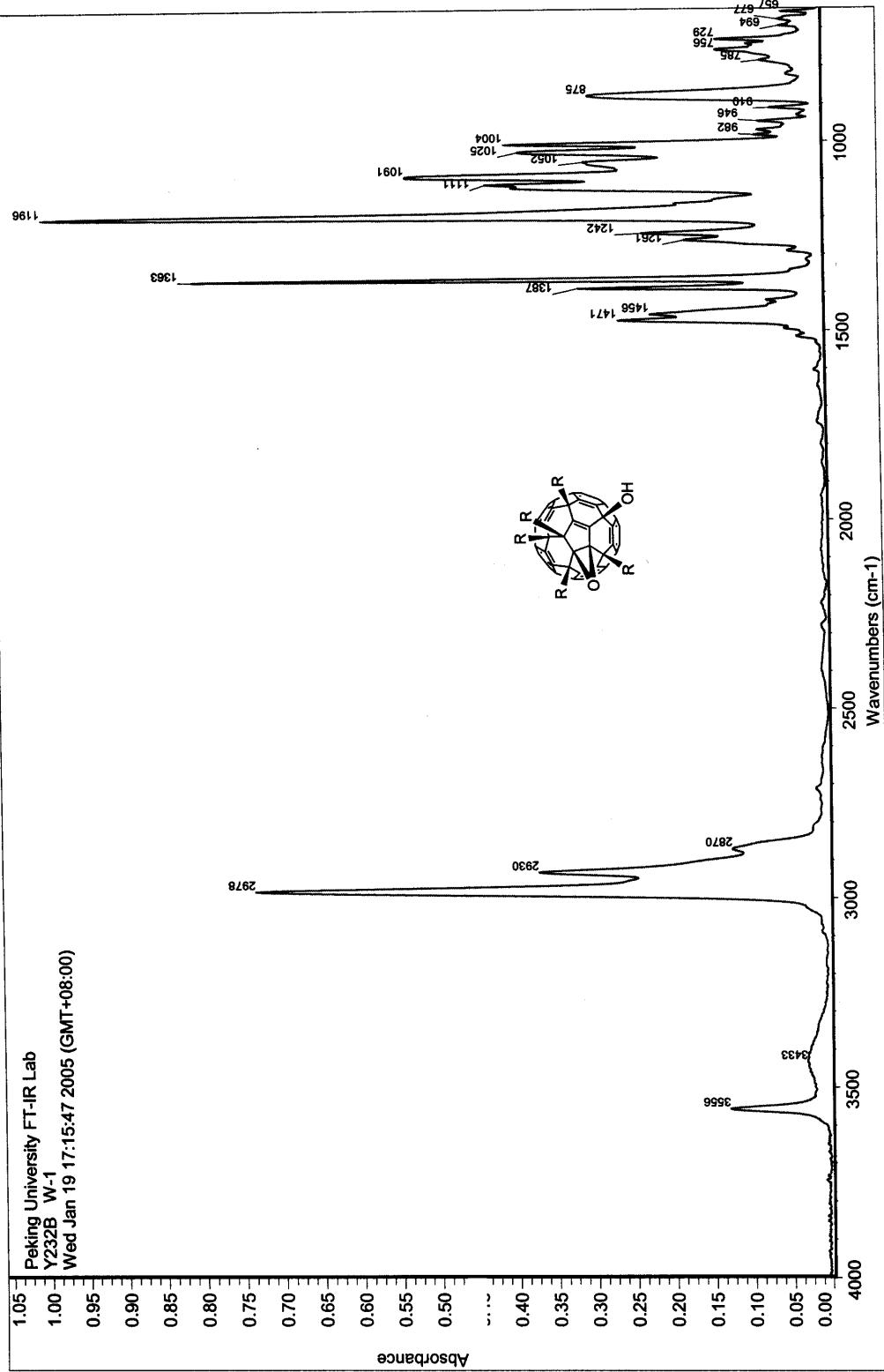
GAN011813 #16-18 RT: 0.34-0.39 AV: 3 NL: 6.28E8
T: + c ESI ms [700.00-2000.00]



GAN011813 #11-13 RT: 0.23-0.27 AV: 3 NL: 8.12E5
T: - c ESI ms [700.00-2000.00]



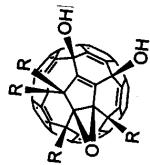
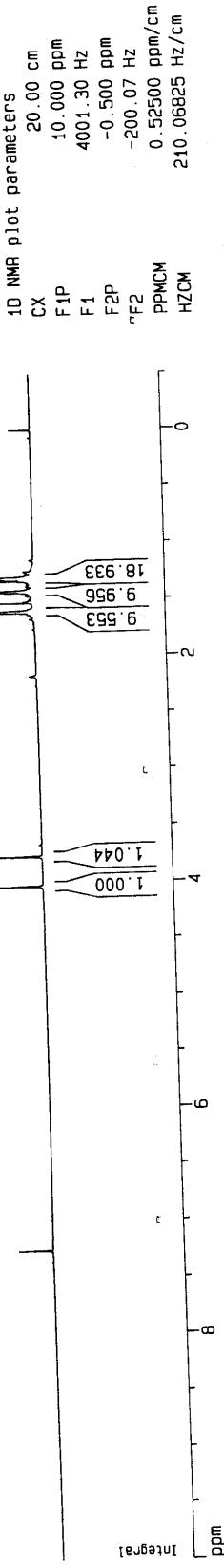
Peking University FT-IR Lab
Y232B W-1
Wed Jan 19 17:15:47 2005 (GMT+08:00)



Current Data Parameters
 NAME H25085
 EXPNO 1
 PROGNO

F2 - Acquisition Parameters
 Date 20050115
 Time 10.16
 INSTRUM ARX400
 PROBID 5 mm Multinu
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 33
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 715
 DW 78.000 usec
 DE 97.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 P1 2.00 usec
 DE 97.50 usec
 SF01 400.1324000 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 16384
 SF 400.1300087 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0.
 PC 0.50

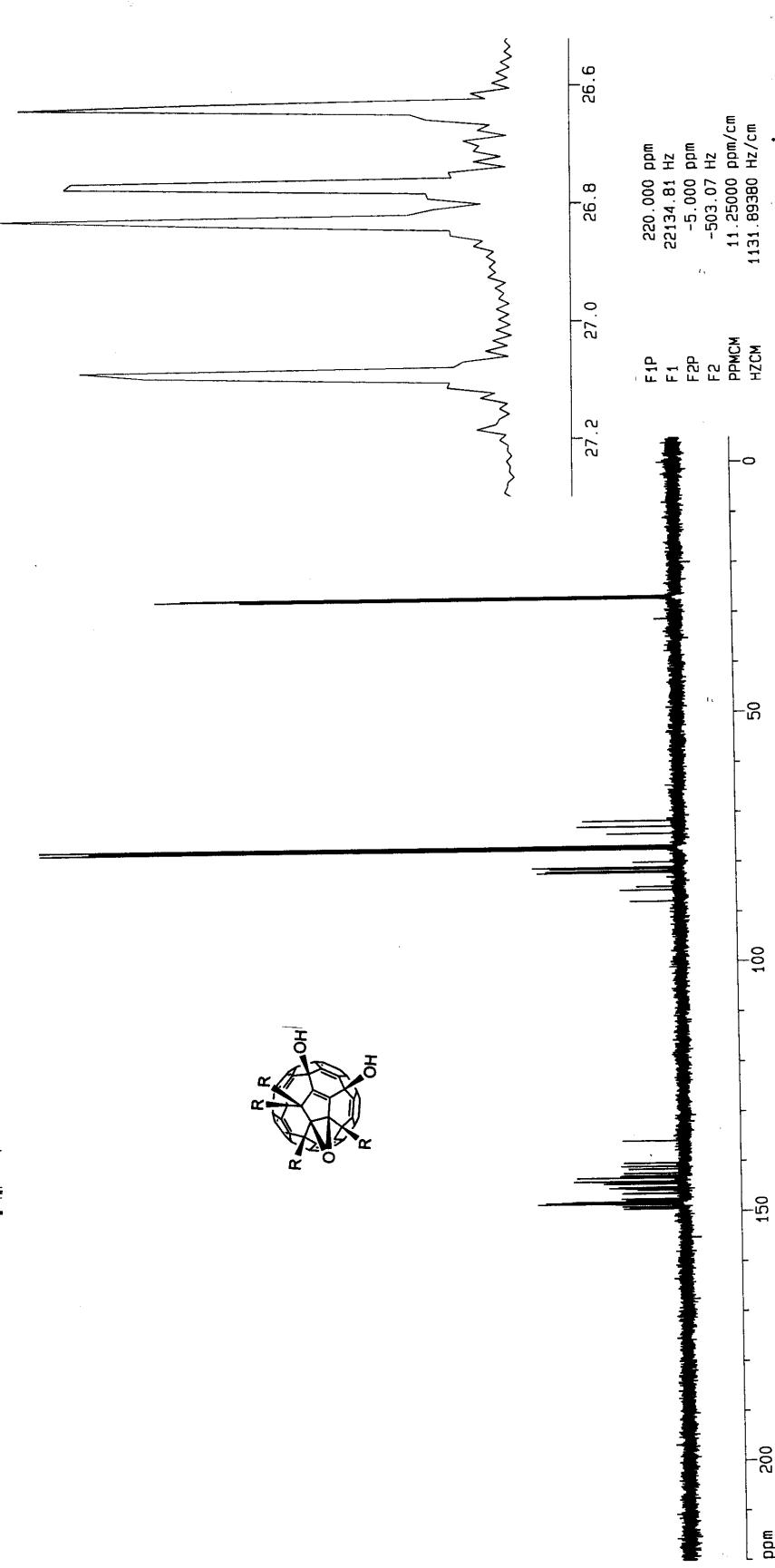


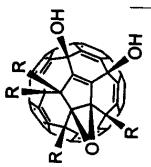
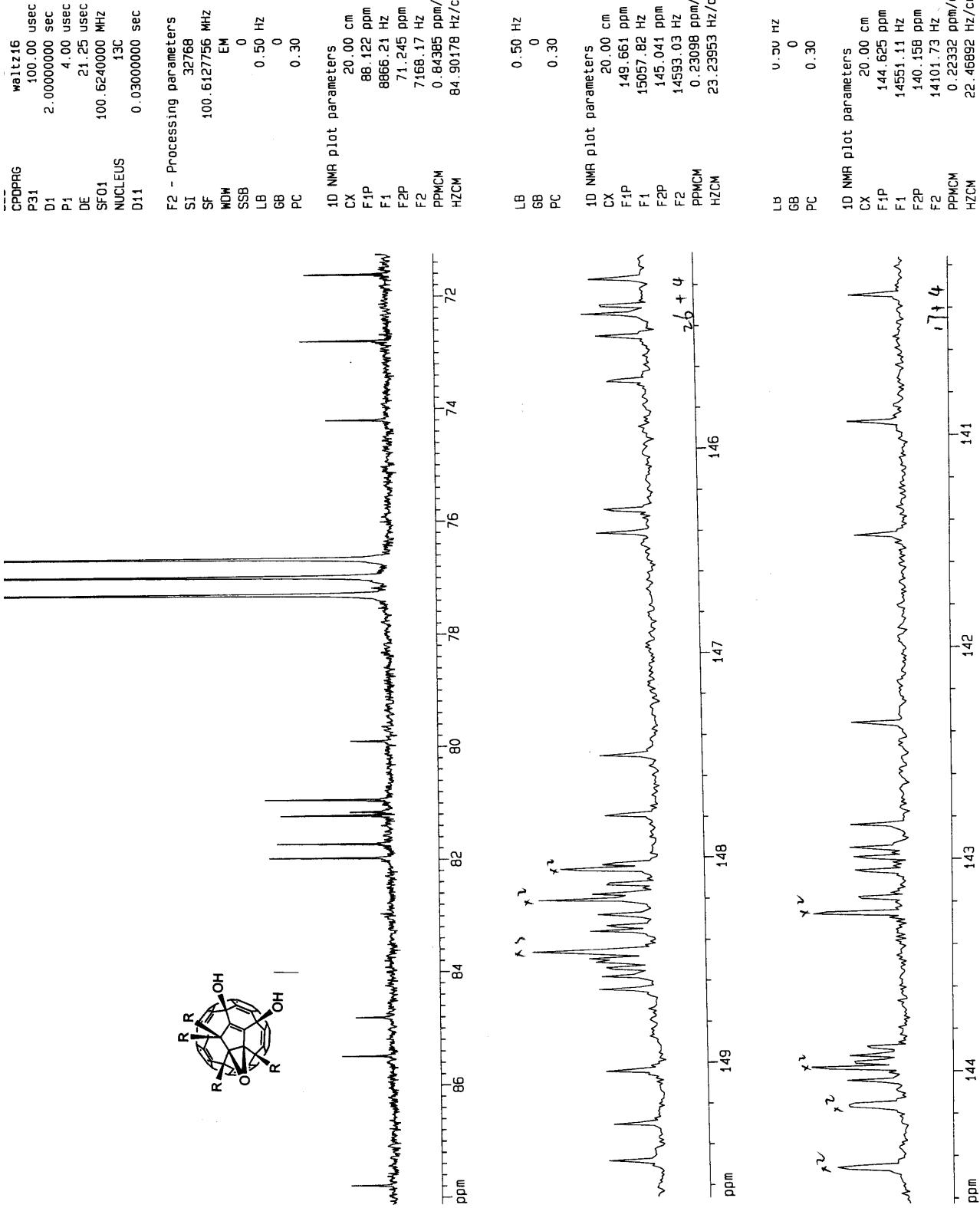
Current Data Parameters
NAME C25005
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

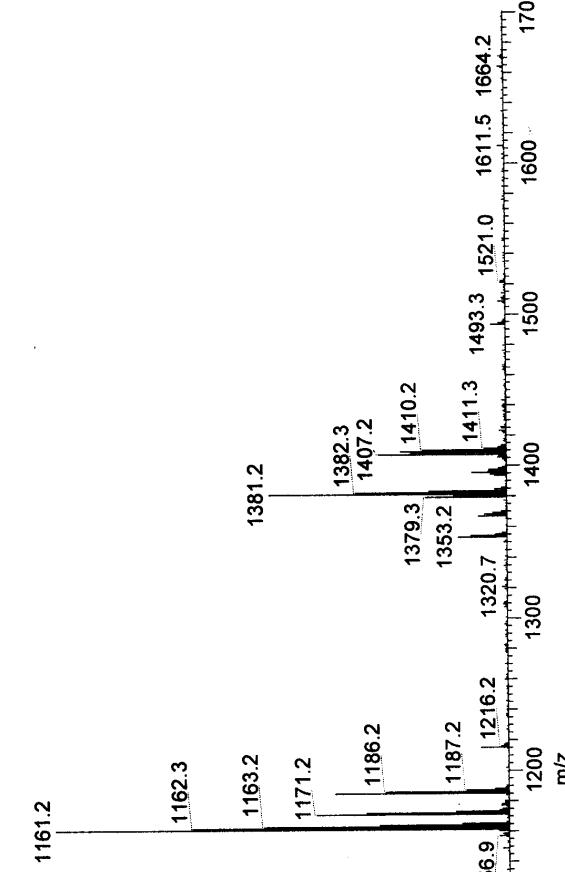
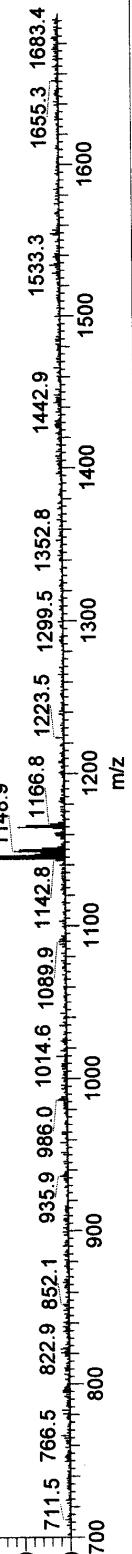
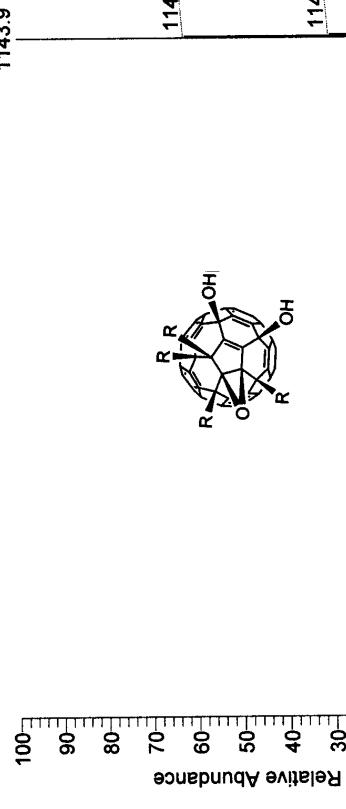
Date_ 20050115
Time 10.21
INSTRUM ARX400
PROBHD 5 mm Multinu
PULPROG PULPROG
TD 2048

26.616
26.639
26.696
26.709
26.729
26.770
26.829
26.871
27.090
27.184
71.617
72.787
74.200
76.661
76.978
77.295
79.901
80.936
81.156
81.217
81.721
81.730
85.484
87.787
135.854
143.254
143.925
143.982
144.043
144.161
144.454
145.336
148.050
148.173
148.199
148.272
148.351
148.450
148.487
148.501
148.637



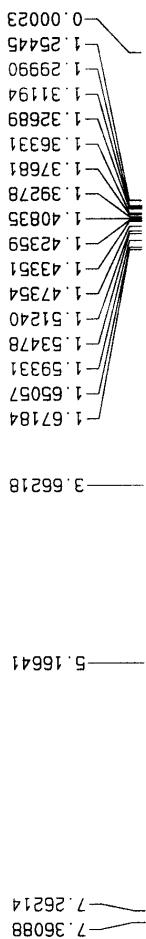


GAN011810 #11-12 RT: 0.26-0.28 AV: 2 NL: 1.06E8
 T: + c ESI ms [700.00-2000.00]

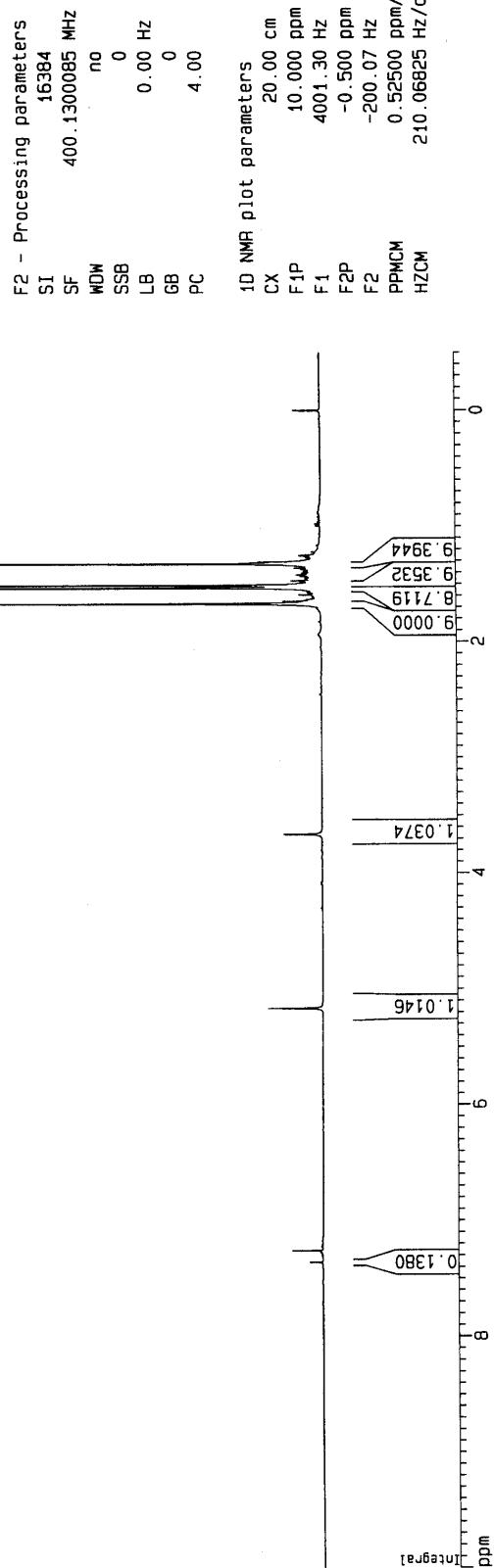


Current Data Parameters
 NAME h25125
 EXPNO 1
 PROCNO 1

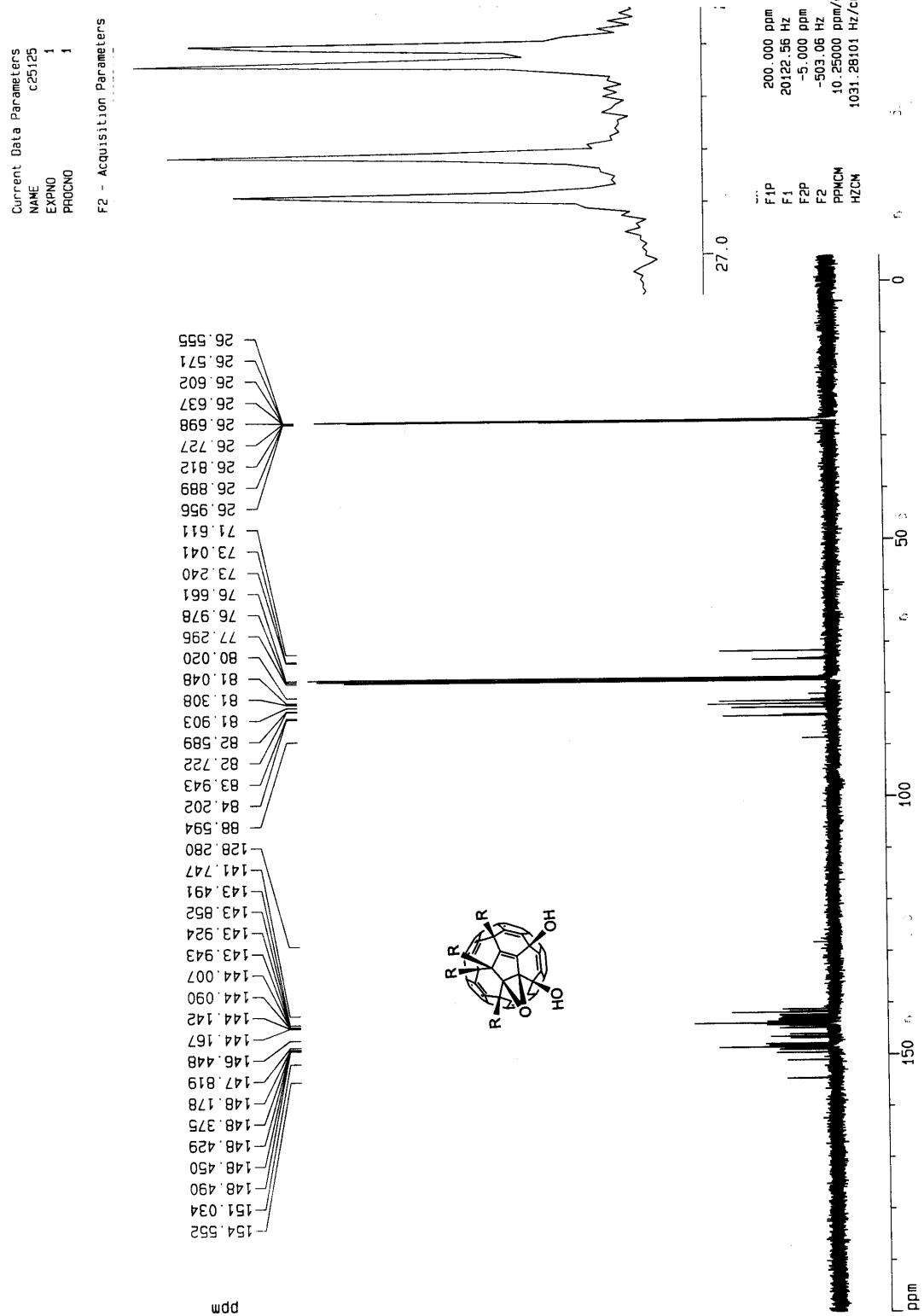
F2 - Acquisition Parameters
 Date_ 20050118
 Time 17.10
 INSTRUM ARX400
 PROBHD 5 mm Multinu
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 128
 DW 78.000 usec
 DE 97.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 P1 4.00 usec
 DE 97.50 usec
 SF01 400.1317985 MHz
 NUCLEUS 1H

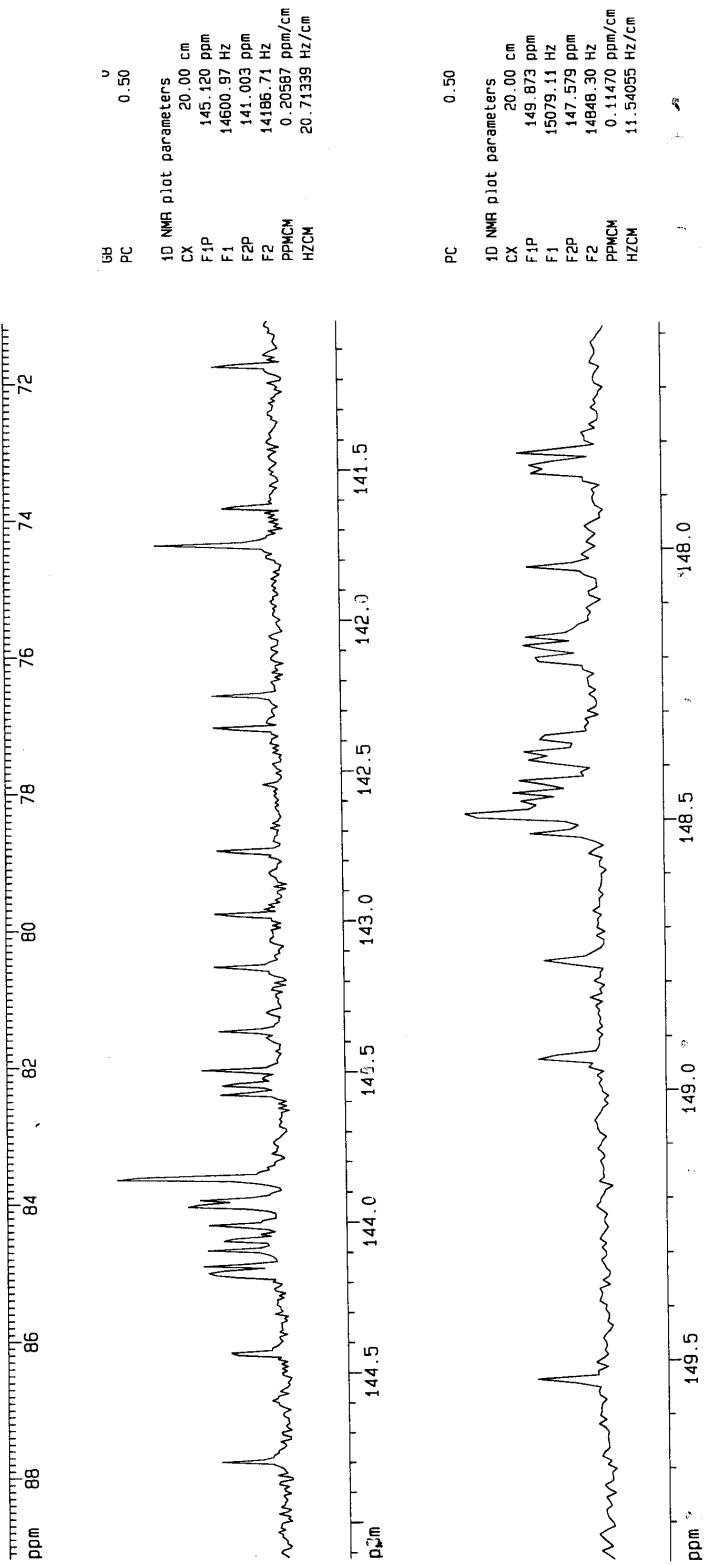
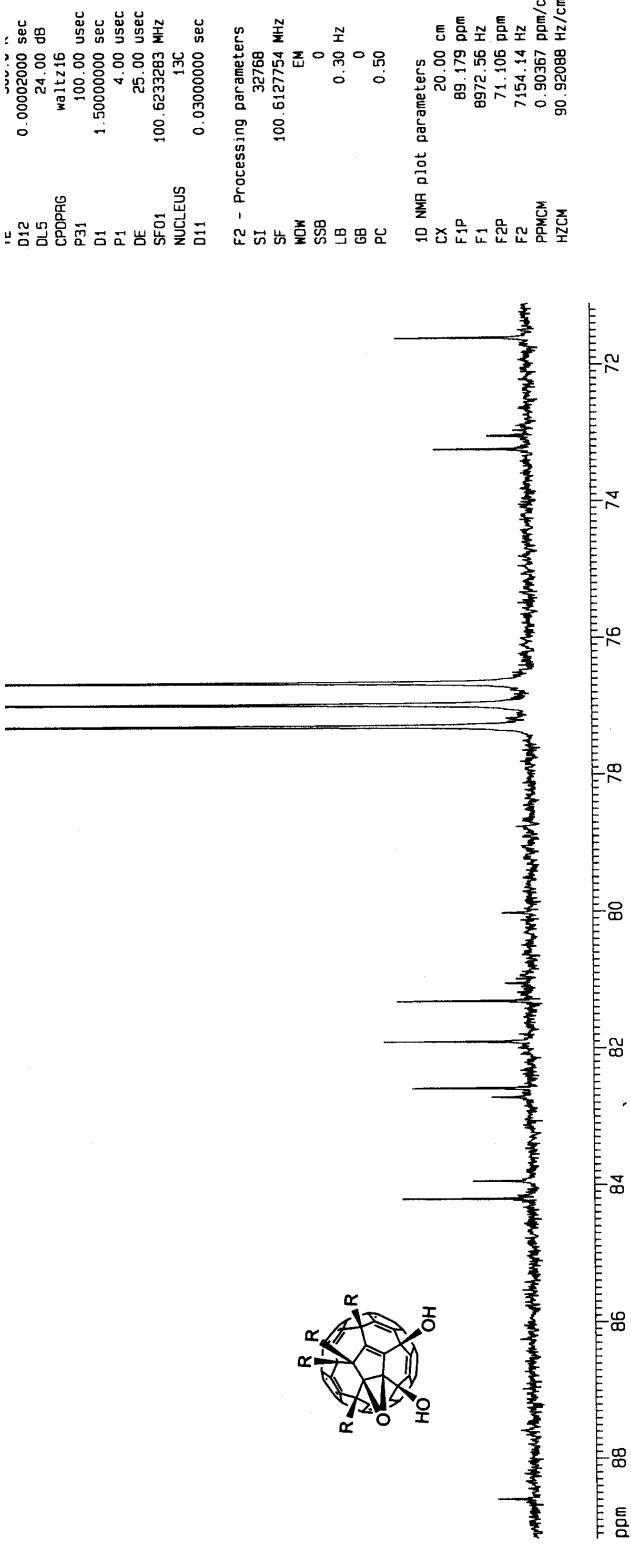


ppm



ppm
Integration





C:\Xcalibur\data\Zhou Jiang\GAN030411

4# 03/05/2005 04:49:09 PM

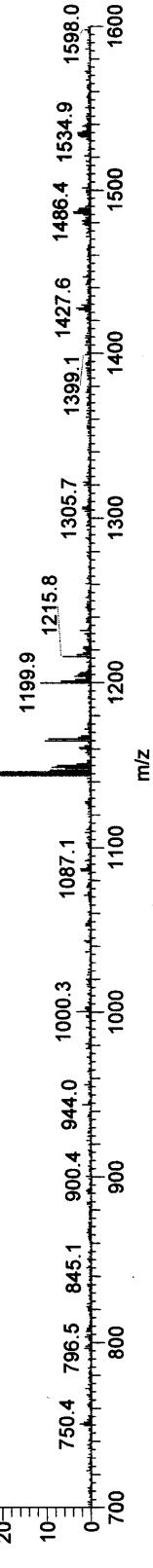
GAN030411 #54-56 RT: 1.16-1.20 AV: 3 NL: 1.10E8
T: + c ESI Full ms [700.00-2000.00]

T: - c ESI ms [700.00-2000.00]

Relative Abundance



1144.9
1146.0

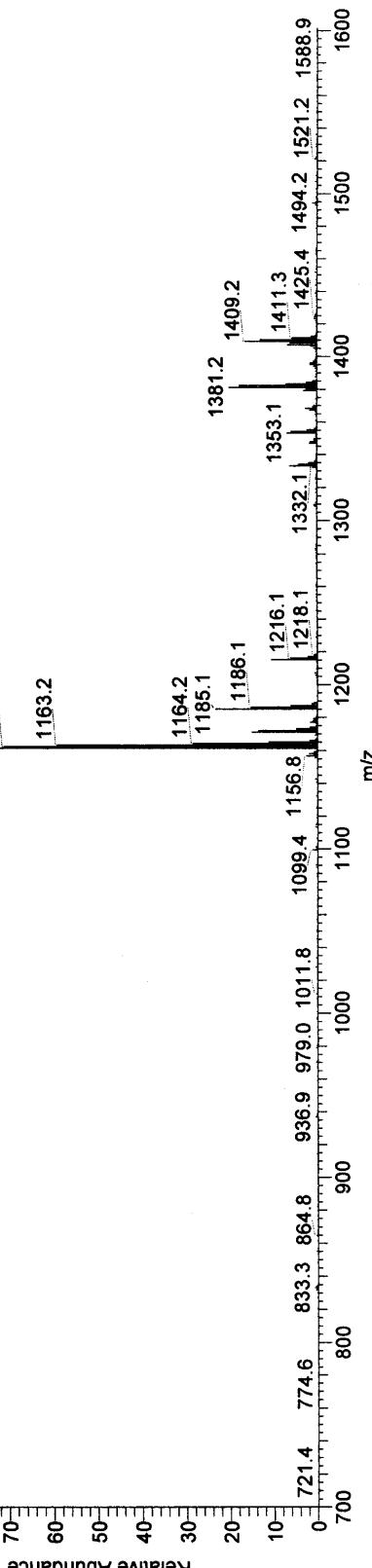


GAN030411 #13-16 RT: 0.35-0.40 AV: 4 NL: 6.57E7

T: - c ESI ms [700.00-2000.00]

Relative Abundance

1161.2
1162.3
1163.2



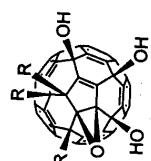
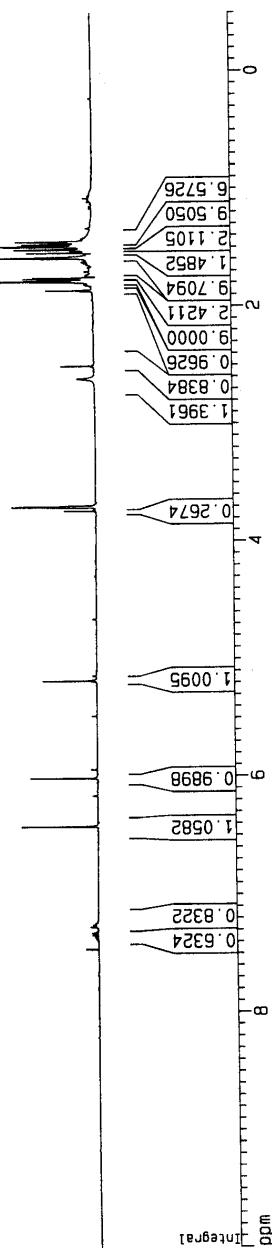
Current Data Parameters
NAME n5124
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

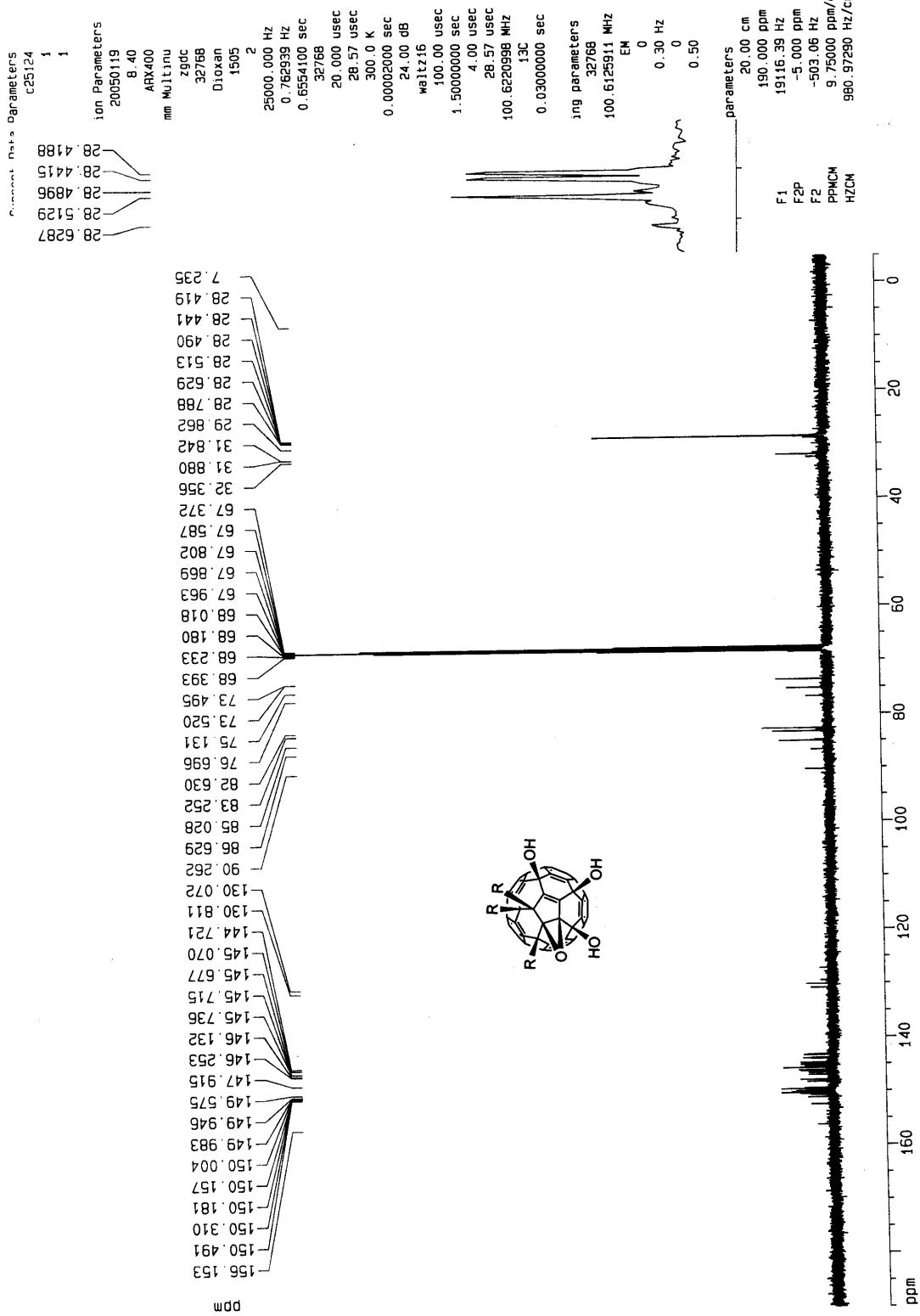
Date 20050119
Time 8.35
INSTRUM ARX400
PROBHD 5 mm Multinu
PULPROG 32768
TD 32768
SOLVENT Dioxan
NS 32
DS 0
SWH 5102.041 Hz
FIDRES 0.155702 Hz
AQ 3.2113140 sec
RG 256
DW 98.000 usec
DE 122.50 usec
TE 300.0 K
D1 2.0000000 sec
P1 4.00 usec
DE 122.50 usec
SF01 400.1318301 MHz
NUCLEUS ¹H

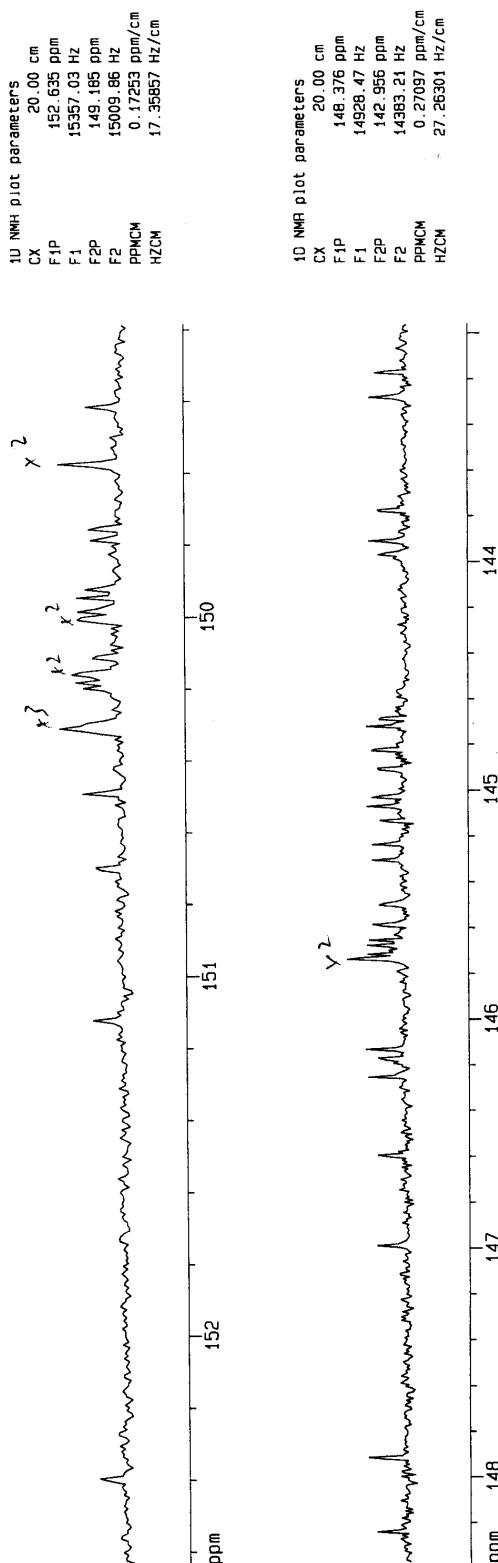
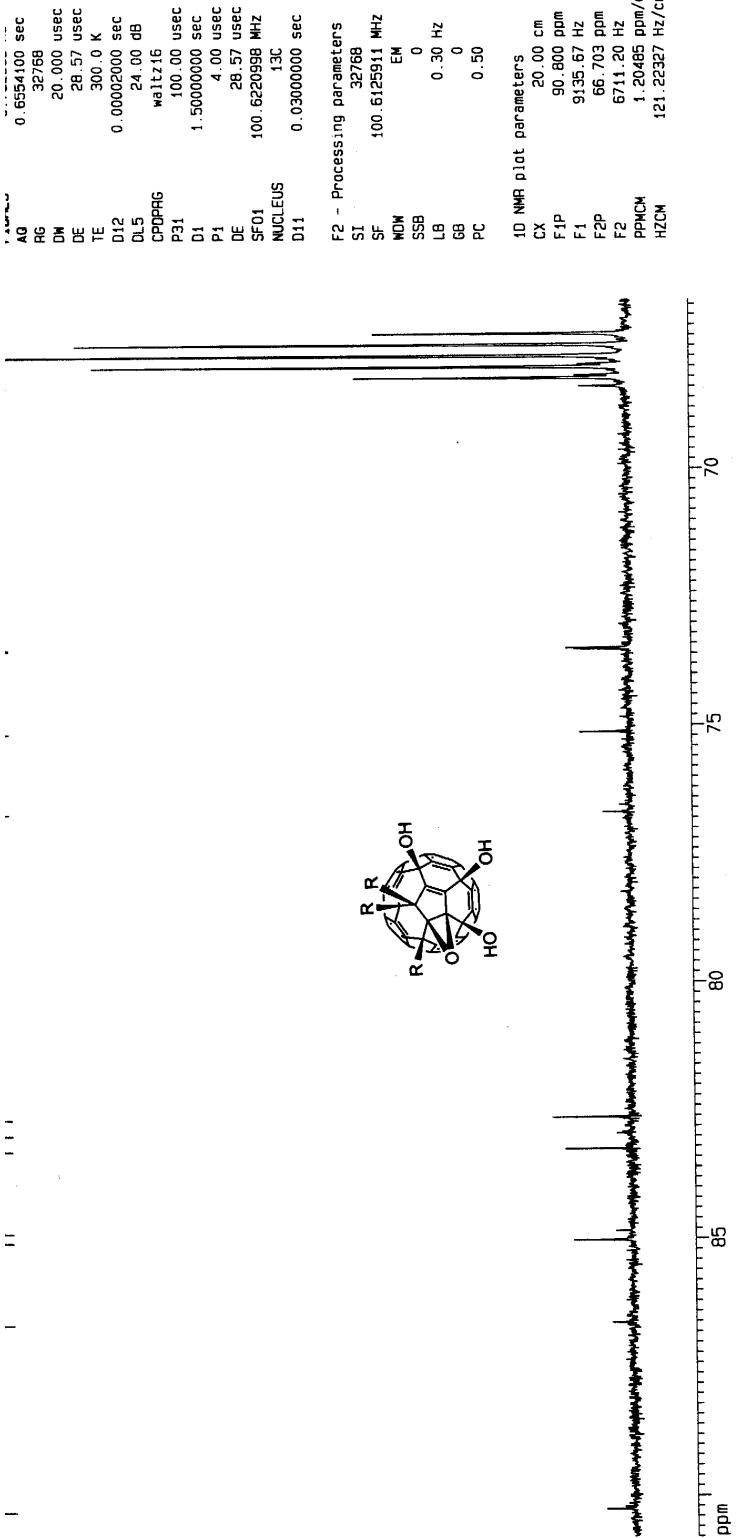
F2 - Processing parameters

SI 16384
SF 400.1299442 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00



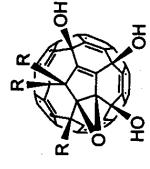
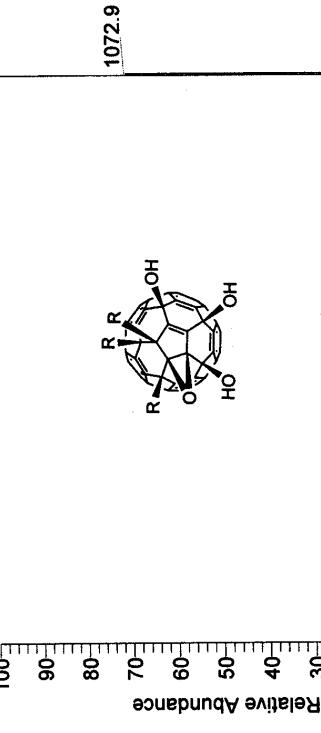
ppm





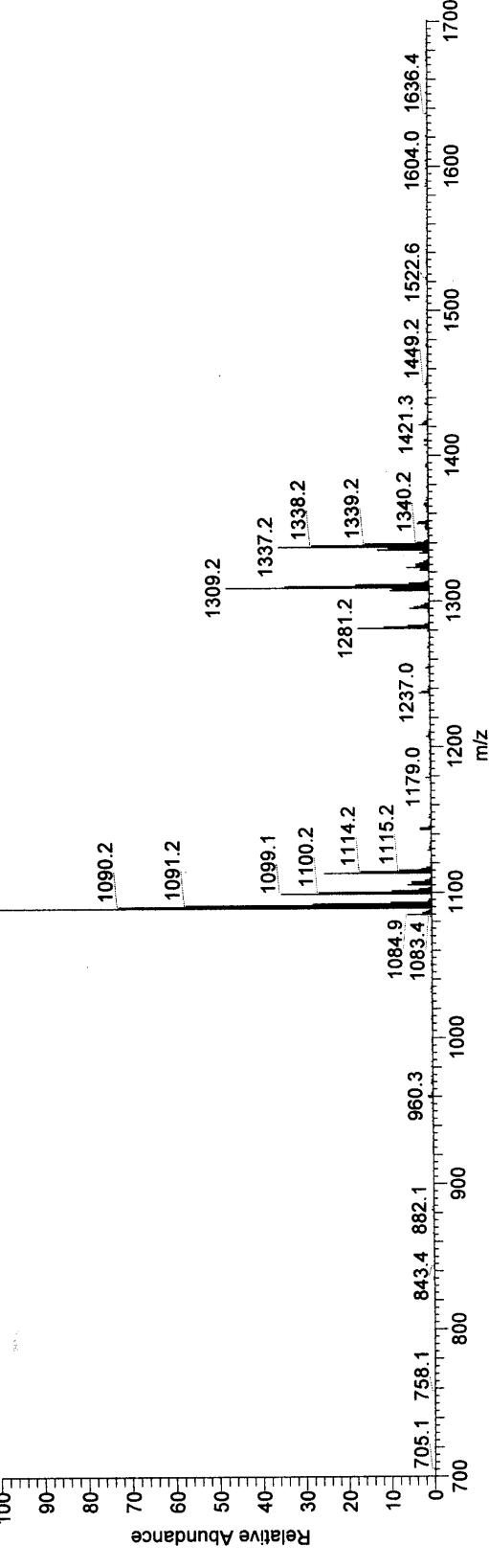
GAN011809 #15-19 RT: 0.32-0.41 AV: 5 NL: 3.55E7
 T: + c ESI ms [700.00-2000.00]

1071.8



GAN011809 #11-13 RT: 0.23-0.26 AV: 3 NL: 5.95E7
 T: - c ESI ms [700.00-2000.00]

1089.2



Current Data Parameters
 NAME h26276
 EXPNO 1
 PROCNO 1

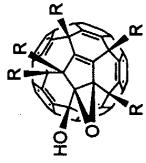
F2 - Acquisition Parameters

Date _ 20050425
 Time 11.29
 INSTRUM ARX400
 PROBHD 5 mm Multinu
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.198625 Hz
 AQ 2.555540 sec
 RG 360
 DW 78.000 usec
 DE 97.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 P1 4.00 usec
 DE 97.50 usec
 SF01 400.1317965 MHz
 NUCLEUS 1H

0.00095
 1.25536
 1.28580
 1.31289
 1.32151
 1.35054
 1.35745
 1.37404
 1.38899
 1.39401
 1.40642
 1.41736
 1.45258
 1.50908
 1.55400
 1.57343
 1.63562
 1.81455
 2.26511
 3.57112

— 7.26217 —

ppm



F2 - Processing parameters

SI 16384
 SF 400.1300085 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 4.00

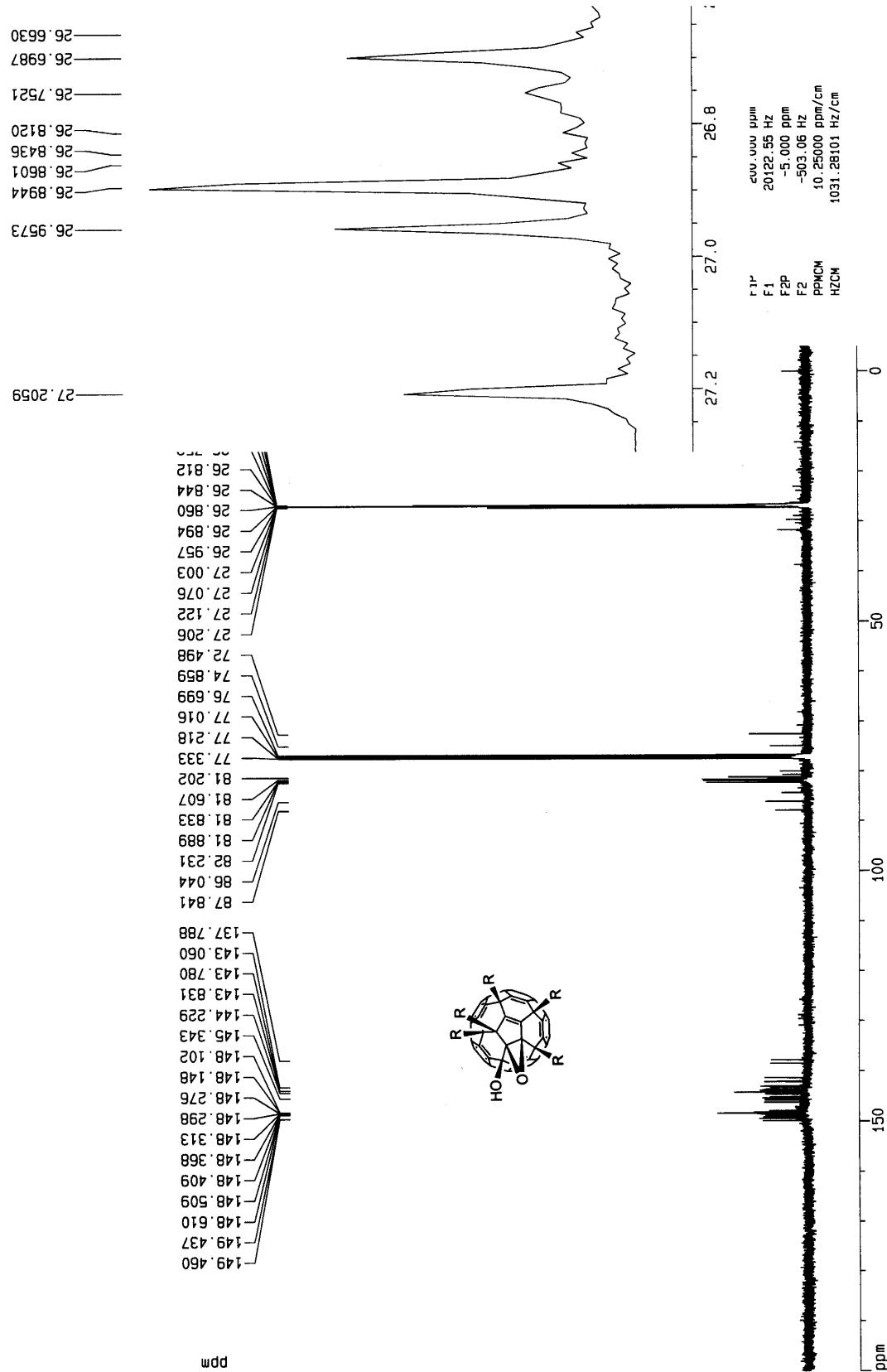
1D NMR plot parameters

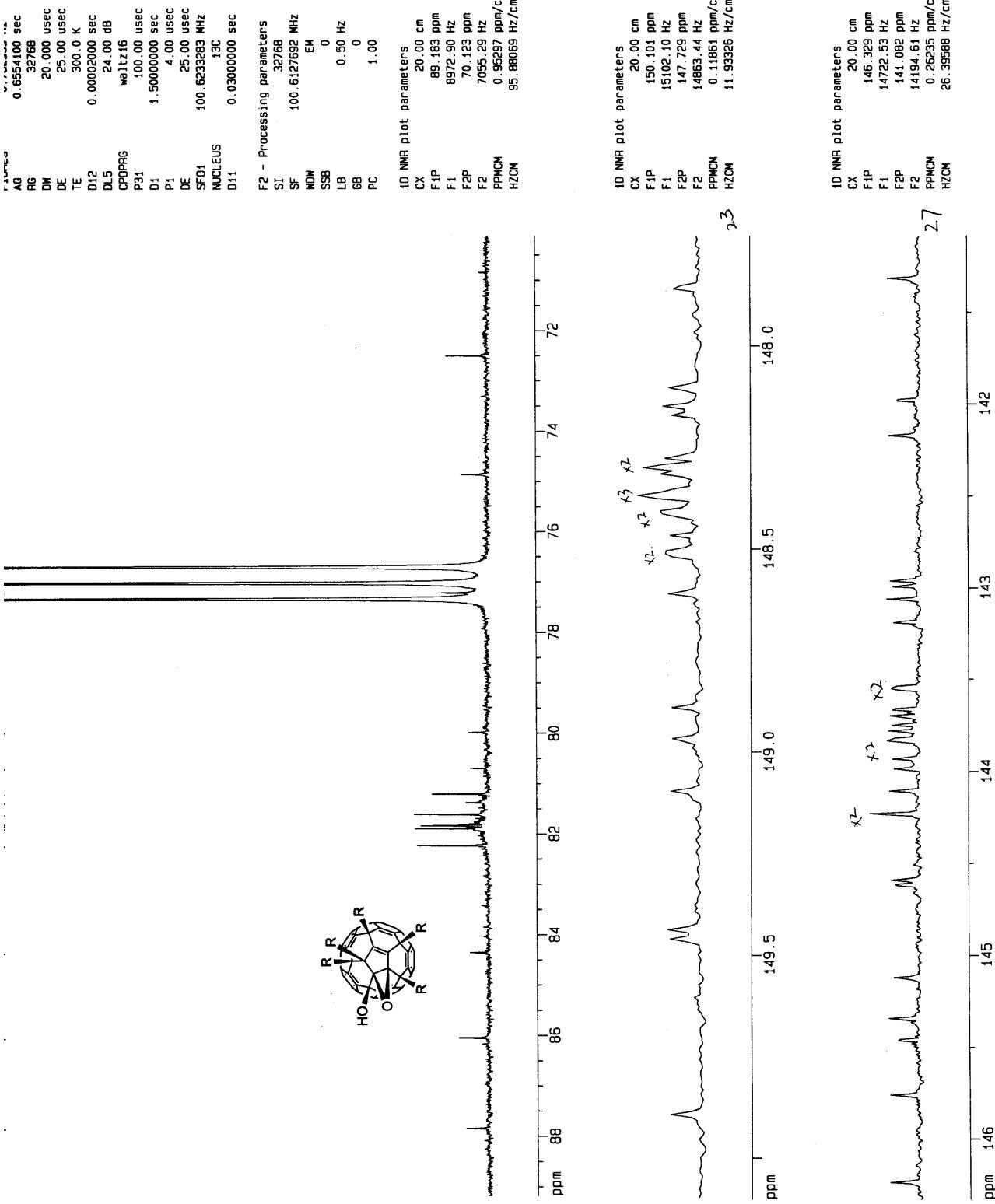
CX 20.00 cm
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 F2P -0.500 ppm
 F2 -200.07 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 210.06825 Hz/cm

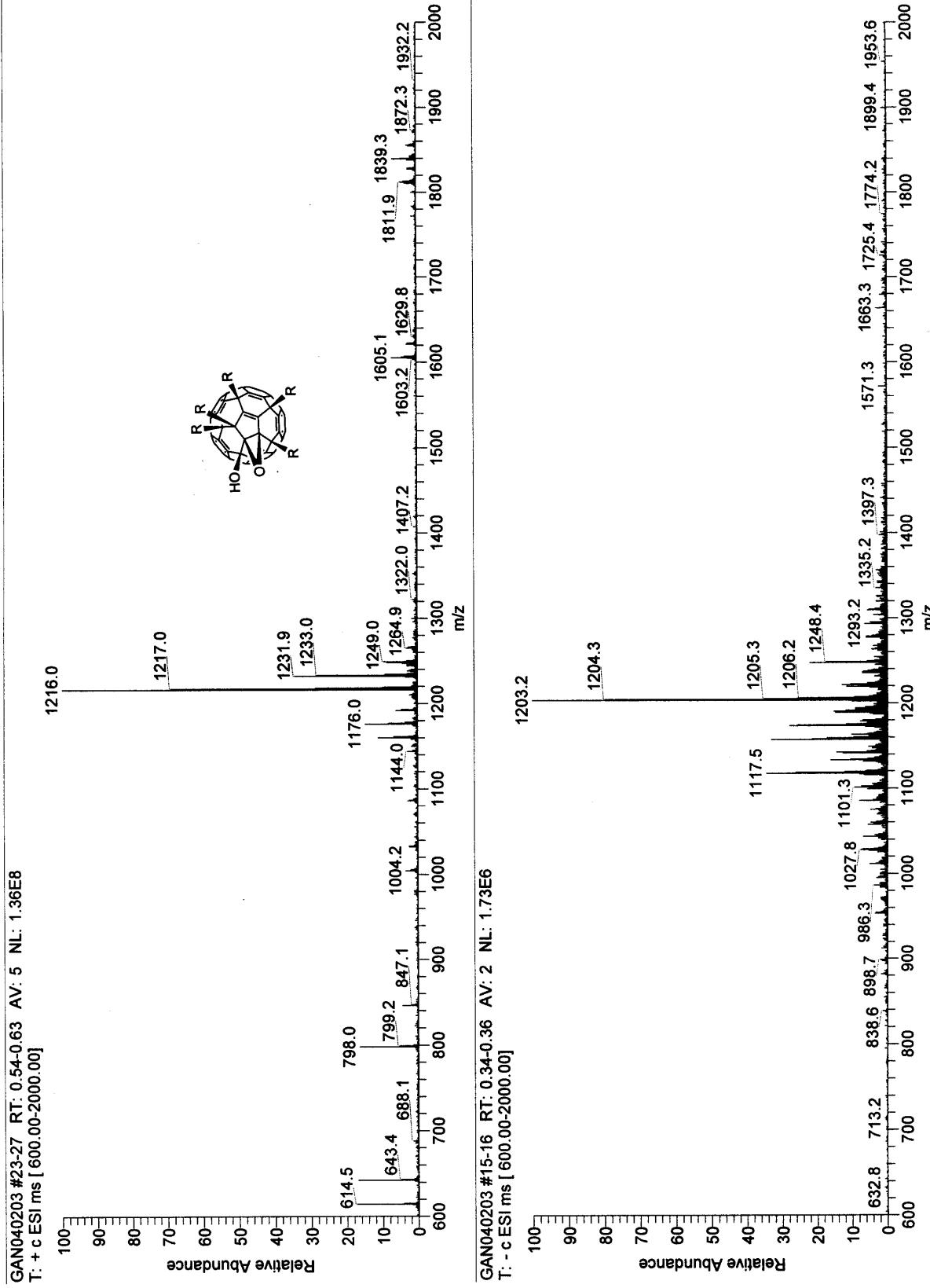
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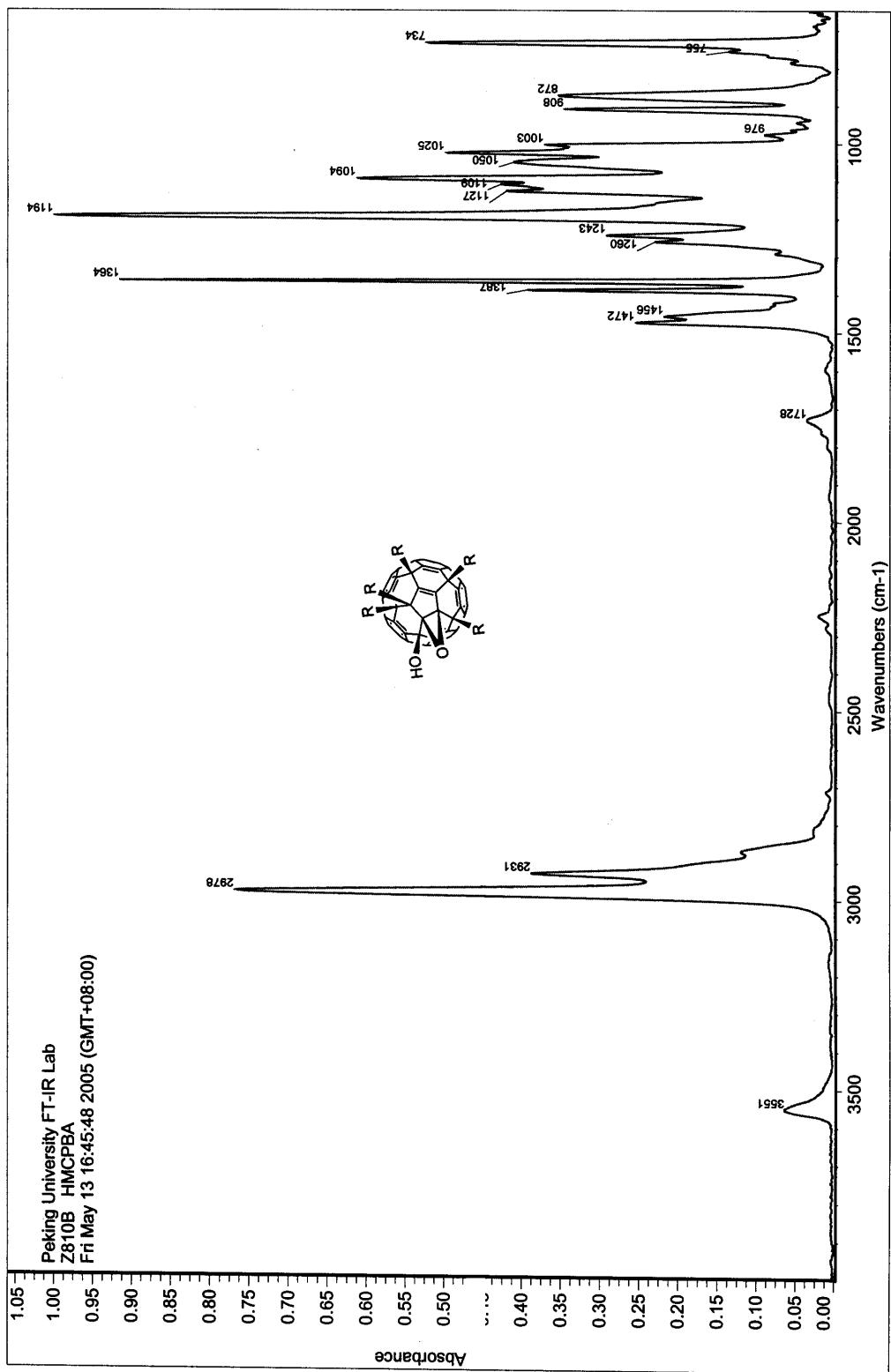
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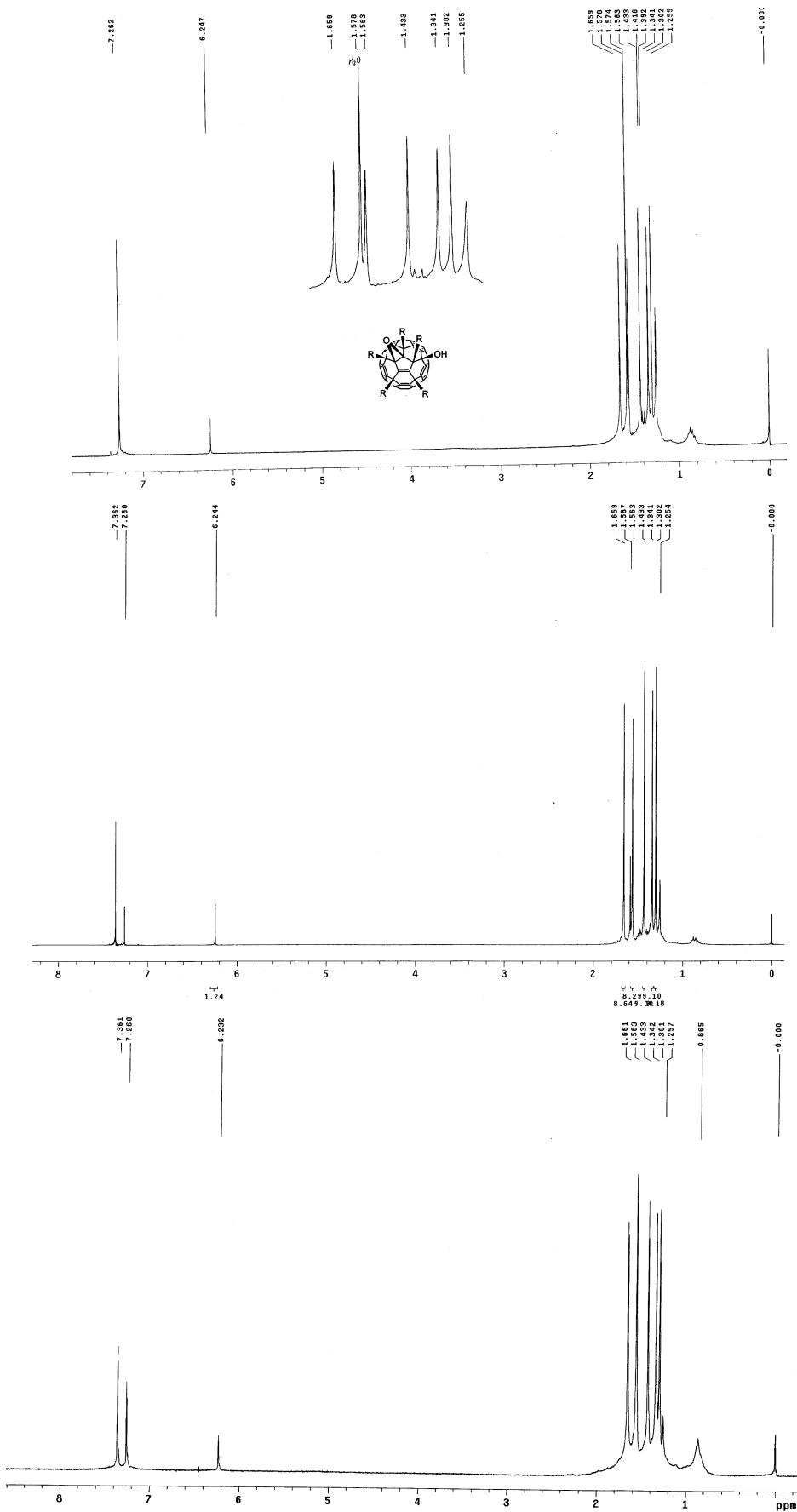
Integral



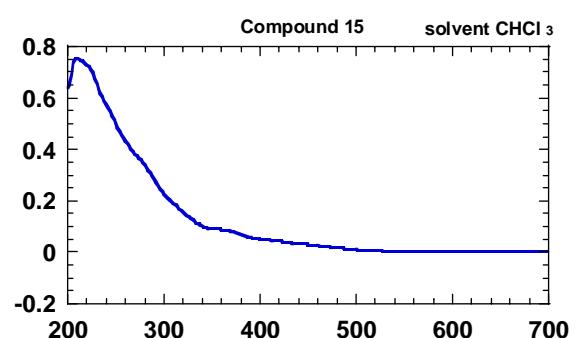
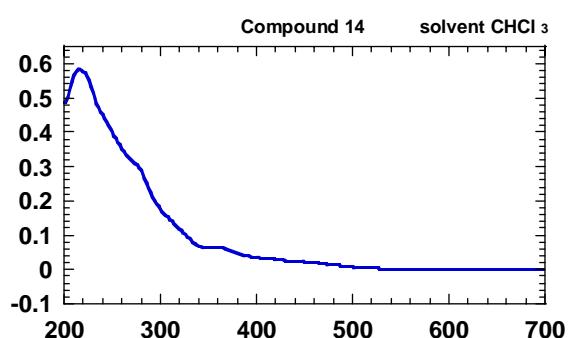
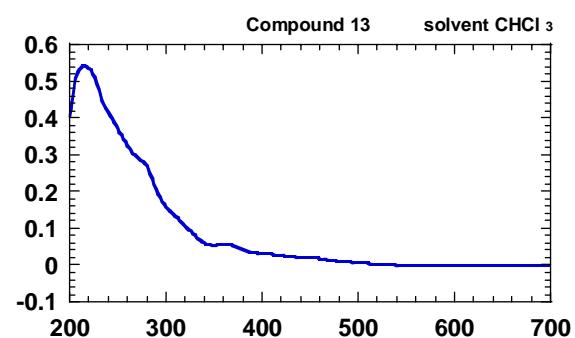
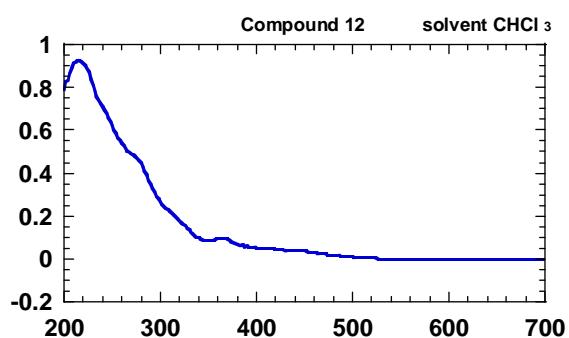
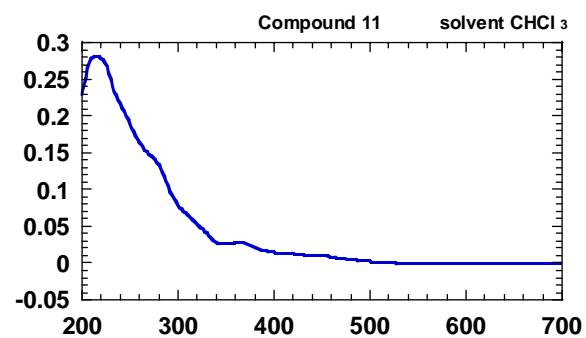
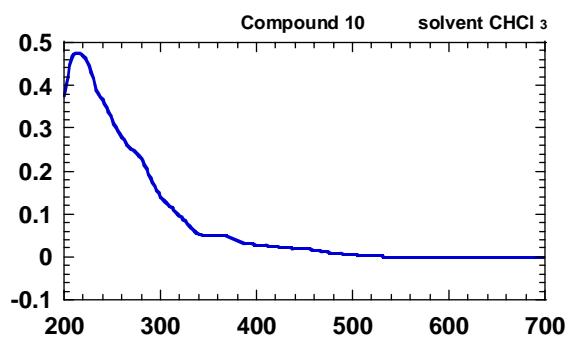
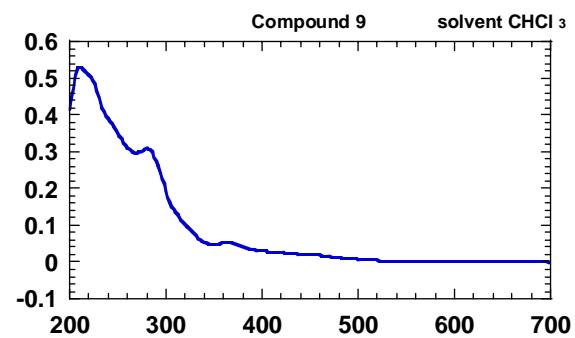
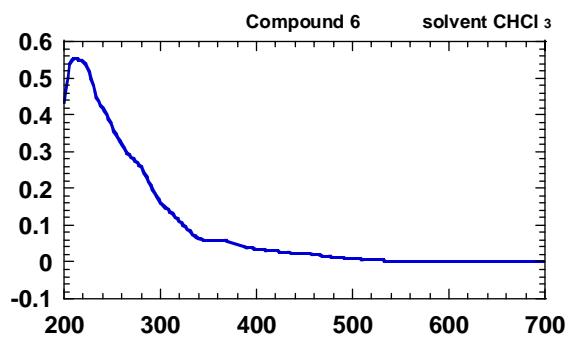








¹H NMR spectra of 6 in CDCl₃ at different concentrations



UV-Vis spectra in CHCl₃ at r.t.