

Supporting Information

Design and Synthesis of Potent Macrocyclic HIV-1 Protease Inhibitors
Involving P1-P2 Ligands

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2. Copies of ¹ H and ¹³ C spectra of compounds 7a-7d , 8a-8d , 23 , 24a-24d -----	S2~S27

General experimental details. All reactions were carried out under an inert atmosphere, either N₂ or Ar, using magnetic stirring and oven-dried glassware. All solvents were anhydrous and distilled prior to use. Dichloromethane and triethylamine were distilled from calcium hydride. Tetrahydrofuran, diethyl ether, and benzene were distilled from sodium/benzophenone. All other solvents were HPLC grade or better. Flash column chromatography was performed using EM Science 60-200 mesh silica gel. Thin-layer chromatography was performed using 60 F-254 E. Merck silica gel plates. ¹H- and ¹³C-NMR were recorded using Bruker AV-500, Avance DRX-500, Varian Mercury-Vx-300, and Gemini-2300 spectrometers and use Me₄Si as an internal standard. Infrared spectra were recorded on a ATI Mattson Genesis Series FT-IR. Optical rotations were recorded on a Perkin-Elmer 341 polarimeter. A Thermo Finnigan LCQ Classic mass was used for MS analyses.

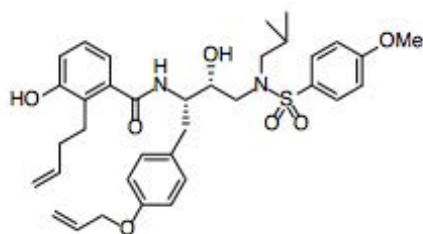
3-hydroxy-2-(3-butene)-benzamide-(4-allyloxybenze)-isostere-
N-isobutyl-N-4-methoxysulfonamide

Current Data Parameters
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PROCNO 1

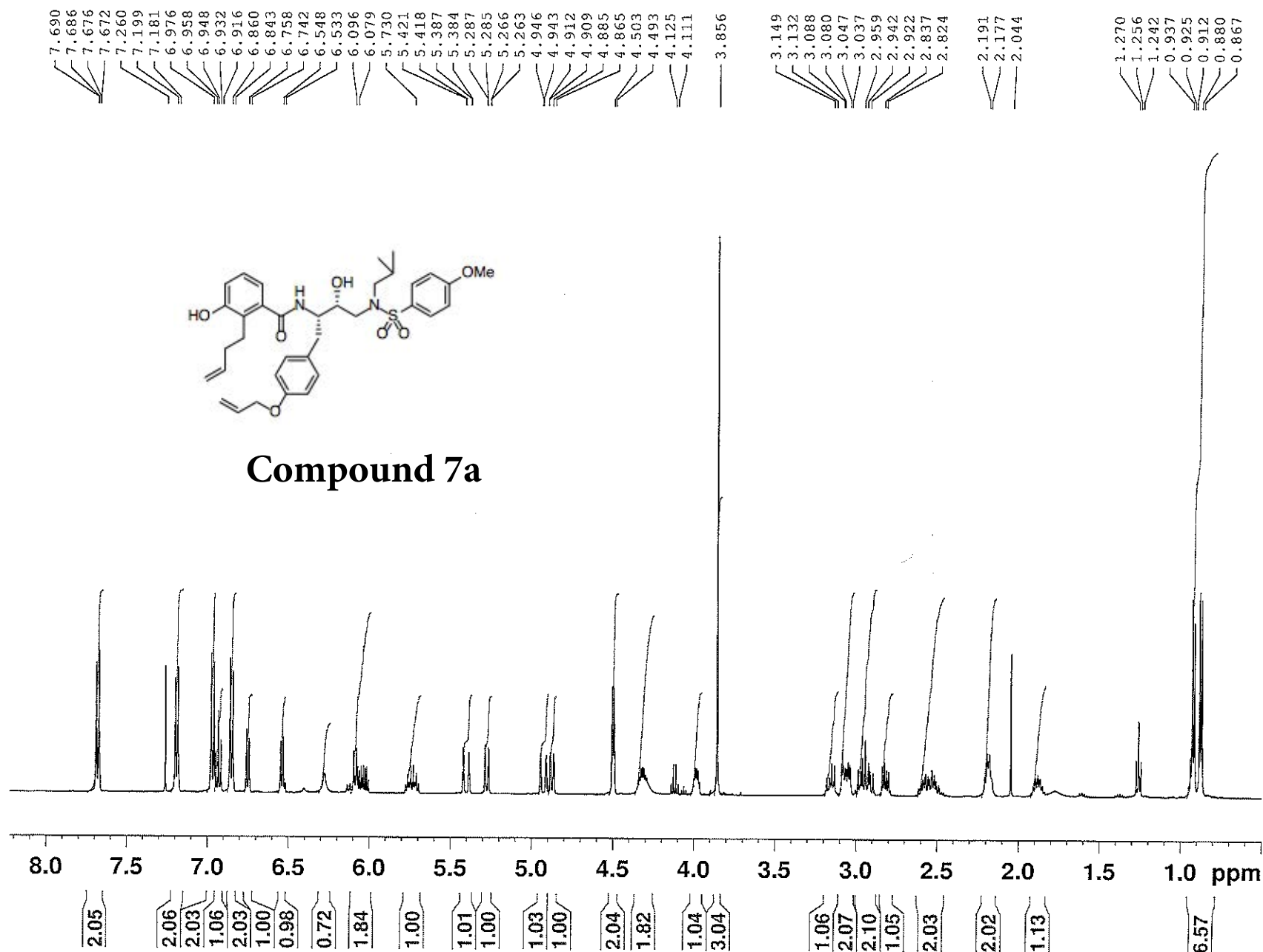
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Time 14.57
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7264305 sec
RG 101.6
DN 83.200 use
DE 6.00 use
TE 293.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 3.50 use
PL1 -2.00 dB
SFO1 500.6427535 MHz

F2 - Processing parameters
SI 32768
SF 500.6400128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

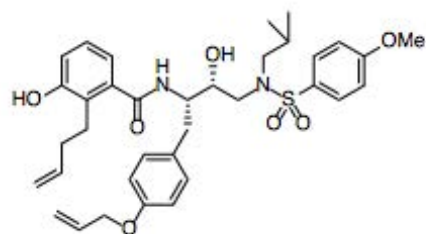


Compound 7a

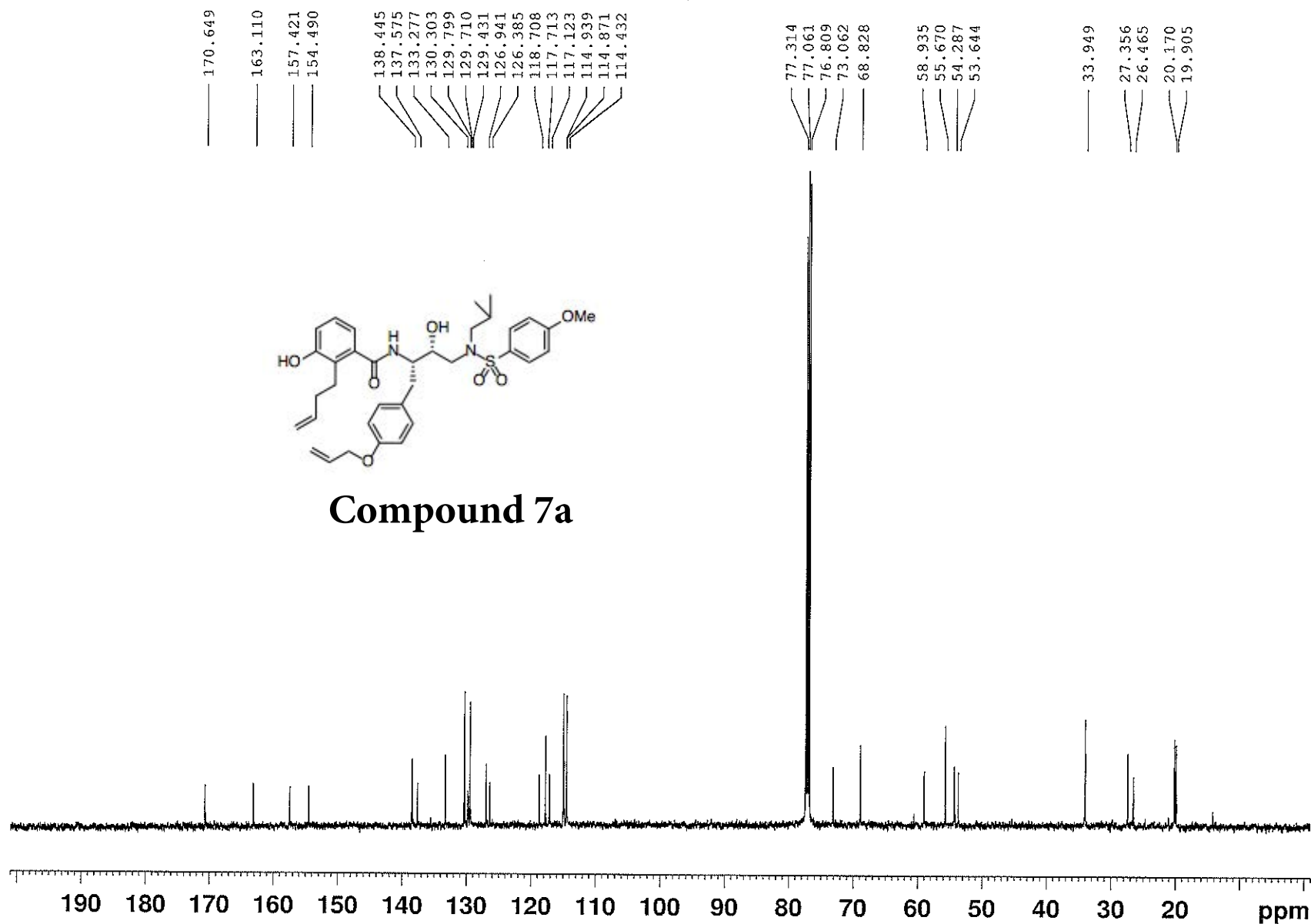


NO 1173
NB 738

3-hydroxy-2-(3-butene)-benzamide-(4-allyloxybenzene)-isostere-
N-isobutyl-N-4-methoxysulfonamide



Compound 7a



Current Data Parameters
NAME first
EXPNO 82
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040824
Time 15:07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 486
DS 2
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5407285 sec
RG 16384
DM 16.500 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

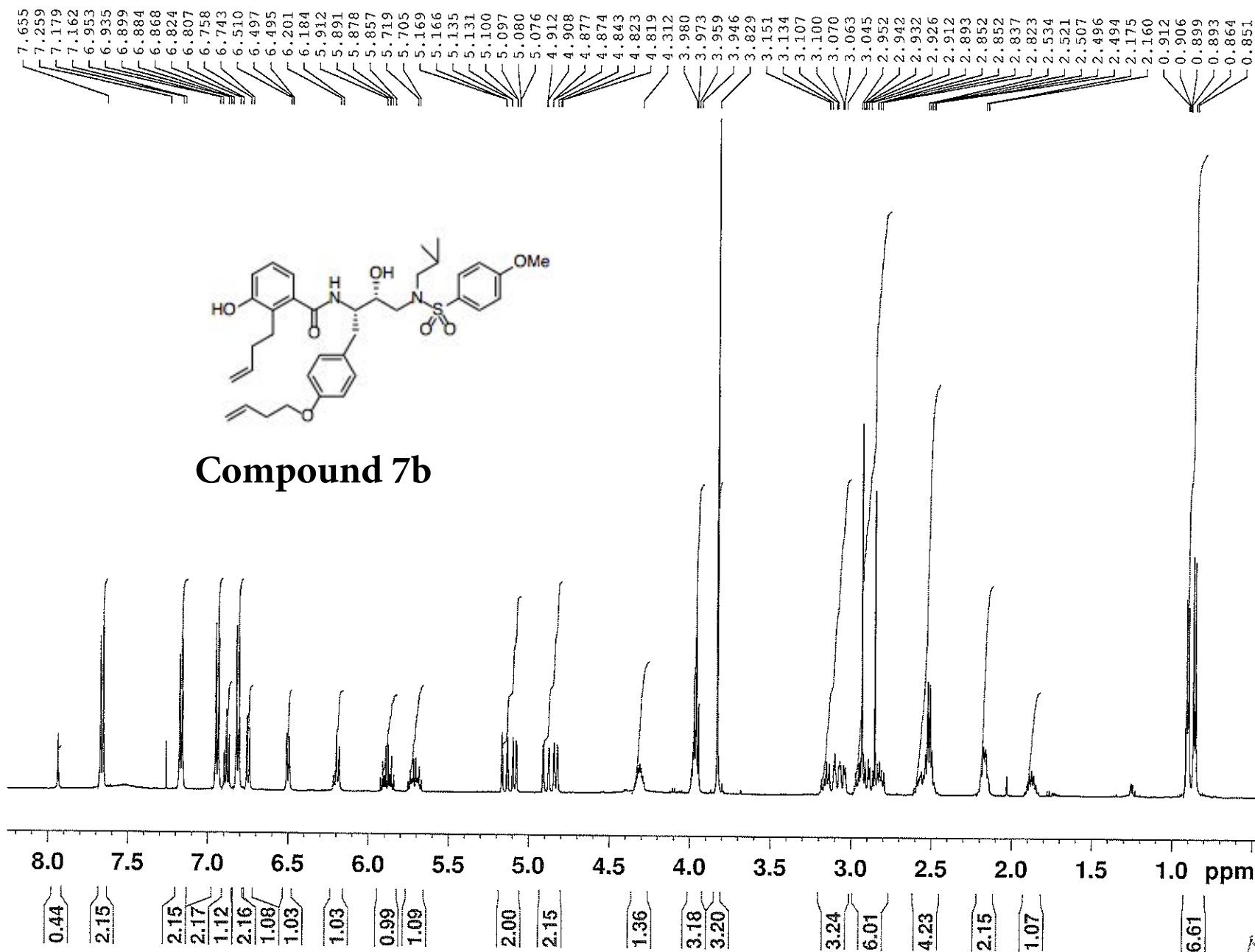
===== CHANNEL f1 =====
NUC1 13C
P1 2.75 usec
PL1 1.00 dB
SFO1 125.8998755 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 500.6422529 MHz

F2 - Processing parameters
ST 16384
SF 125.8860280 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

201173
1137-38

3-butenyl-aryl-3-butenyl-phenoxy



Current Data Parameters
NAME first
EXPNO 91
PROCNO 1

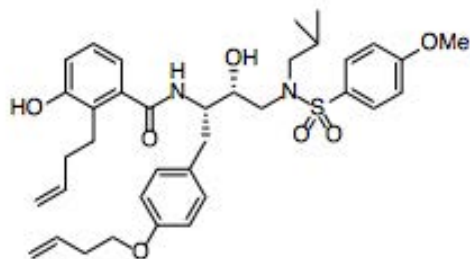
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INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7264309 sec
RG 32
DW 83.200 usec
DE 6.00 usec
TE 294.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 3.50 usec
PL1 -2.00 dB
SFO1 500.6427535 MHz

F2 - Processing parameters
SI 32768
SF 500.6400128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NO 1140
NB 7-63

3-butenyl-aryl-phenoxy-3-butenyl-aryl



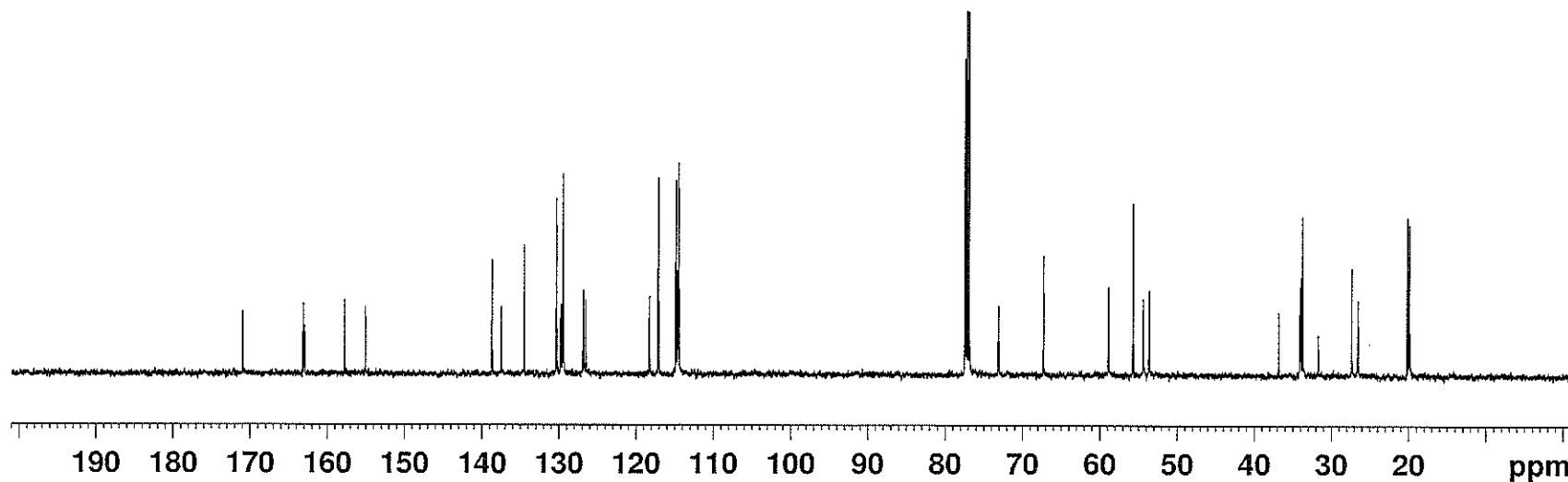
Compound 7b

Current Data Parameters
NAME Zifac
EXPNO 32
PROCNO 1
F2 - Acquisition Parameters
Date_ 20041001
Time 14.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 140
DS 2
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5407385 sec
RG 16384
OW 16.500 usec
DE 6.00 usec
TE 294.8 K
DL 2.00000000 sec
d11 0.03000000 sec
MCR2ST 0.00000000 sec
MCMRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 2.70 usec
PL1 1.00 dB
SFO1 125.8998755 MHz

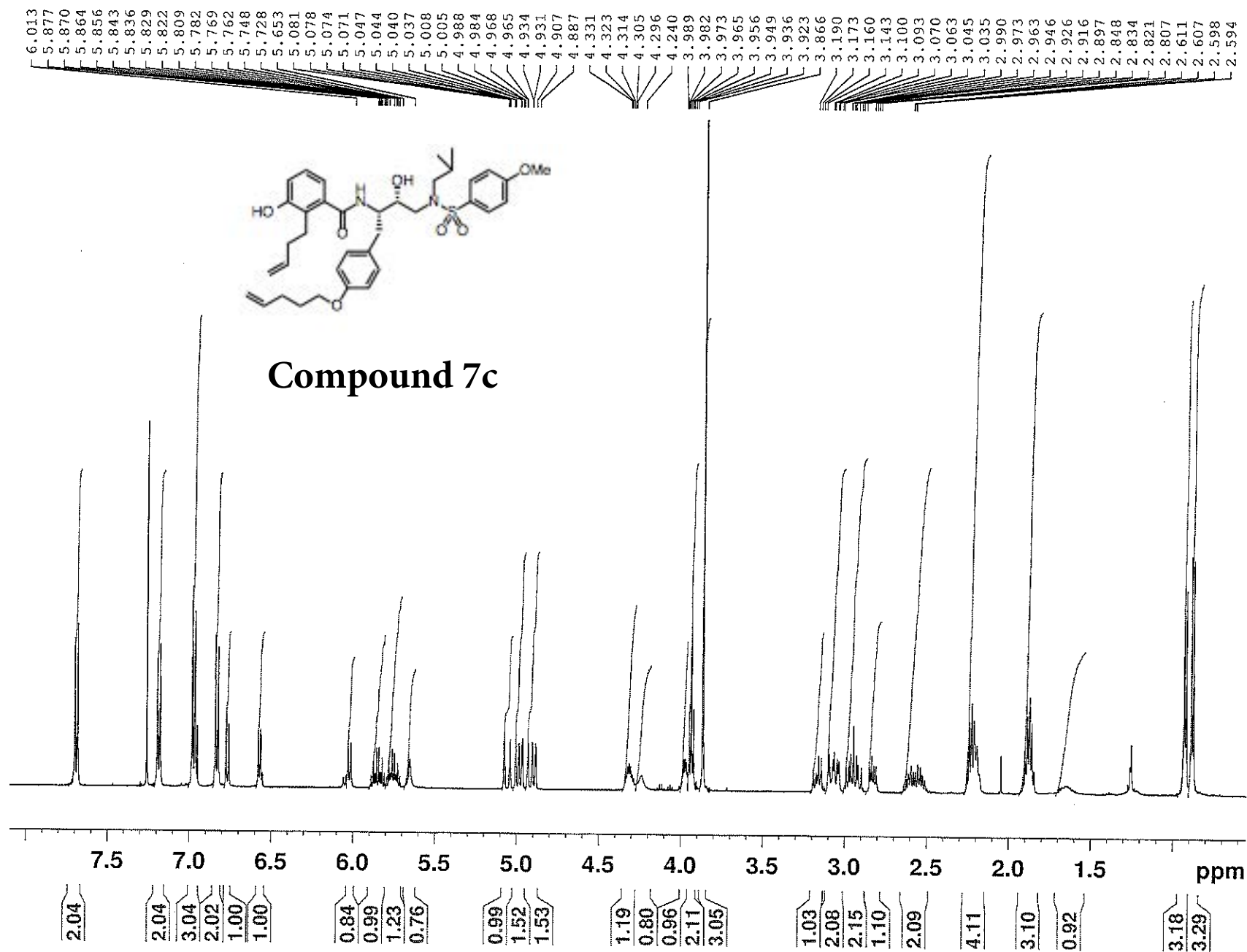
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 500.6425253 MHz

F2 - Processing parameters
SI 32768
SF 125.8950280 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00



pc 1151
MB 7-62

3-hydroxy-2-(3-butenyl)-4-(4-pentenyl)-phenylisostere



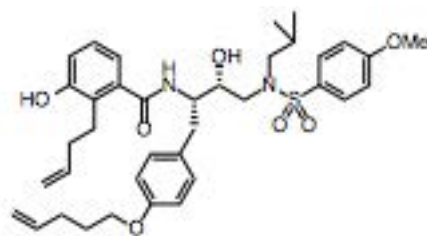
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NAME first
EXPNO 146
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041216
Time 11.32
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7264309 sec
RG 181
DW 83.200 use
DE 6.00 use
TE 294.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

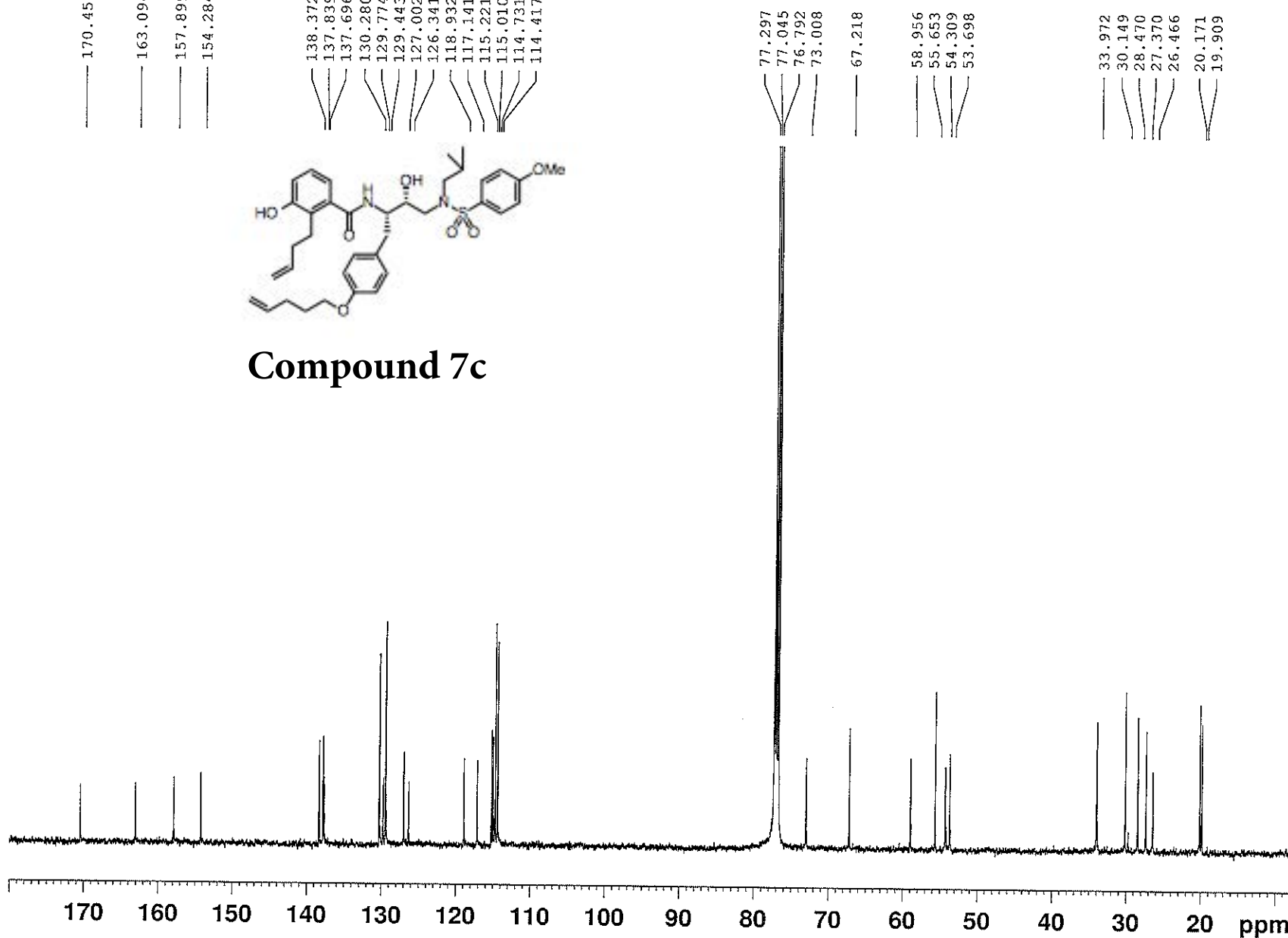
===== CHANNEL f1 =====
NUC1 1H
P1 3.50 use
PL1 -2.00 dB
SFO1 500.6427535 MHz

F2 - Processing parameters
SI 32768
SF 500.6400128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3-hydroxy-2-(3-butenyl)-4-(4-pentenyl)-phenyl



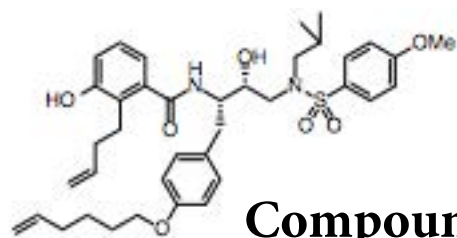
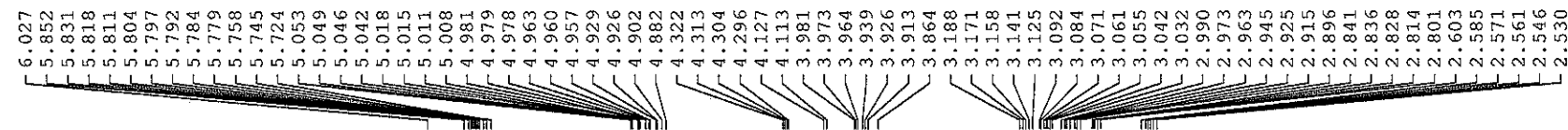
Compound 7c



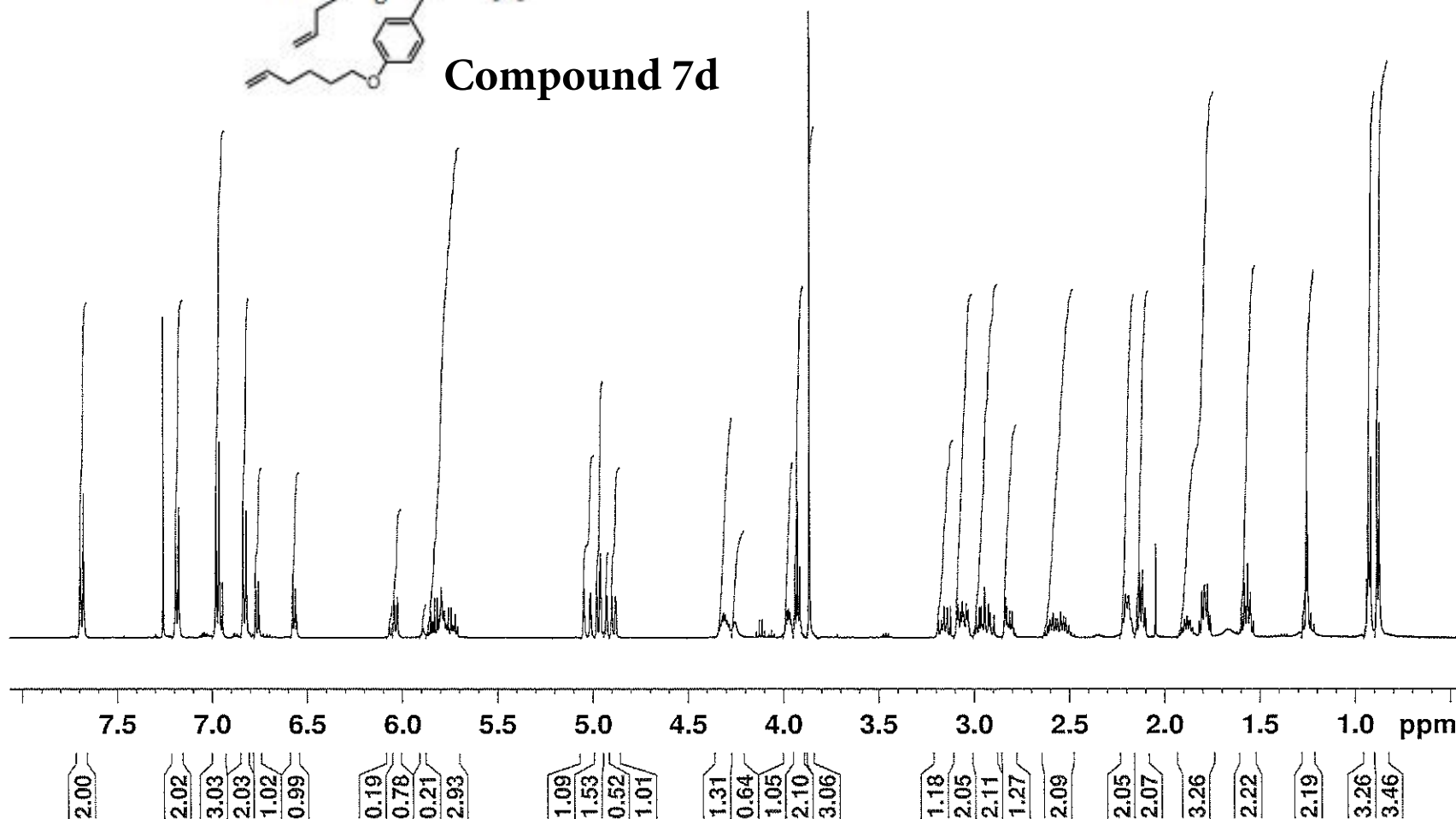
Current Data Parameters
NAME list
EXPNO 147
PROCNO 1
F2 - Acquisition Parameters
Date_ 20041216
Time 11:41
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 5569
DS 3
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5607385 sec
RG 16384
DW 16.500 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.03500000 sec
----- CHANNEL f1 -----
NUC1 13C
P1 2.70 usec
PL1 1.00 dB
SFO1 125.8996755 MHz
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 500.6422529 MHz
F2 - Processing parameters
SI 16384
SF 125.8860280 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

12-33
7-103
112

3-butenyl-(5-hexenyl)



Compound 7d



Current Data Parameters
NAME first
EXPNO 150
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041222
Time 18.55
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7264309 sec
RG 161.3
DW 83.200 use
DE 6.00 use
TE 292.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWVK 0.01500000 sec

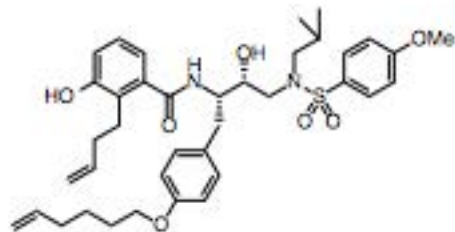
----- CHANNEL f1 -----
NUC1 1H
P1 3.50 use
PL1 -2.00 dB
SFO1 500.6427535 MHz

F2 - Processing parameters
SI 32768
SF 500.6400128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

MR 1036
MR 7-104
116

C13 standard parameters, BBO probe.

170.488
163.095
157.938
154.329
138.548
138.399
137.675
130.283
129.750
129.440
126.989
126.357
118.887
117.142
114.977
114.921
114.789
114.692
114.419

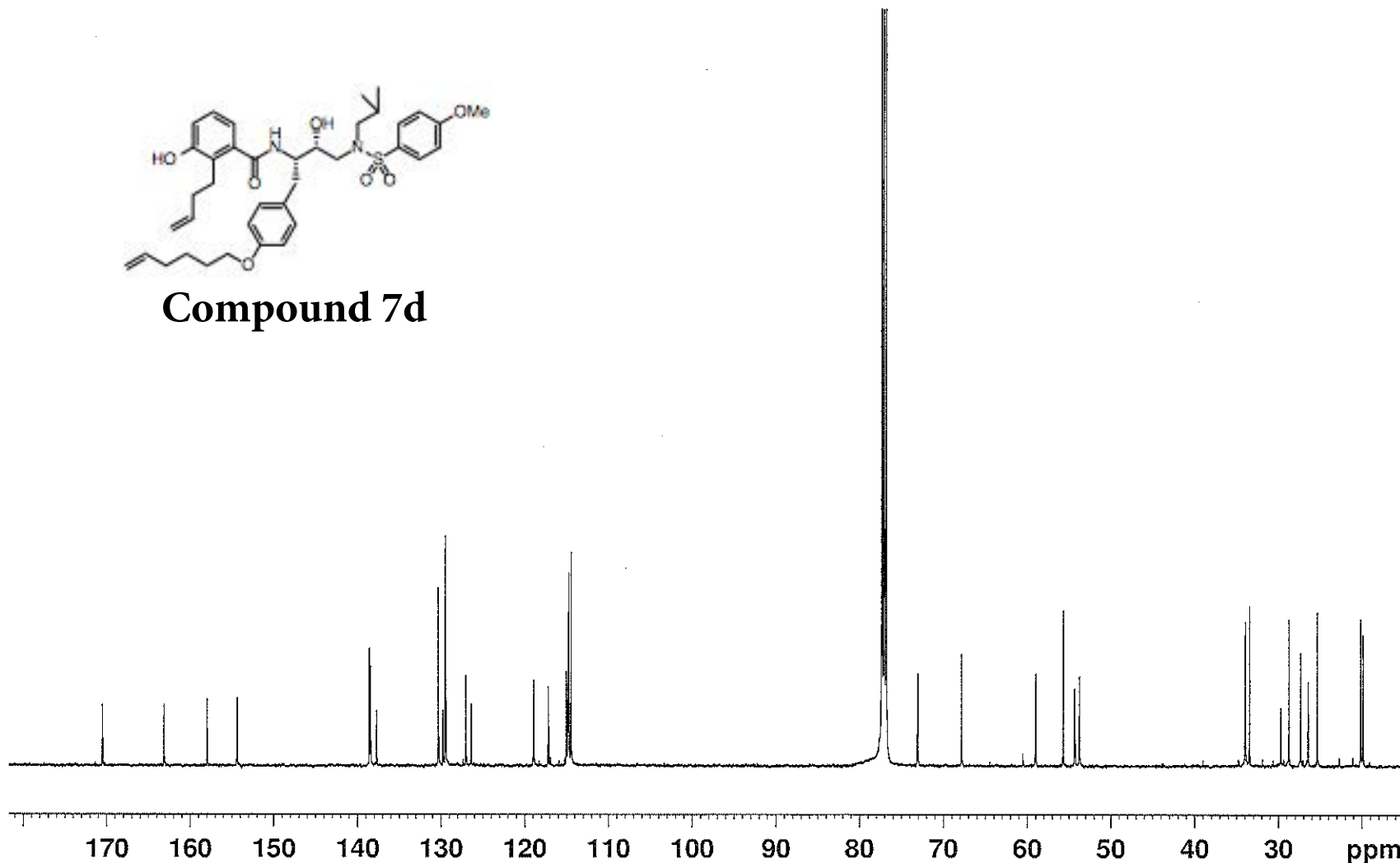


Compound 7d

77.619
77.303
77.048
76.795
73.076
73.019
67.792

58.957
55.654
54.293
53.695

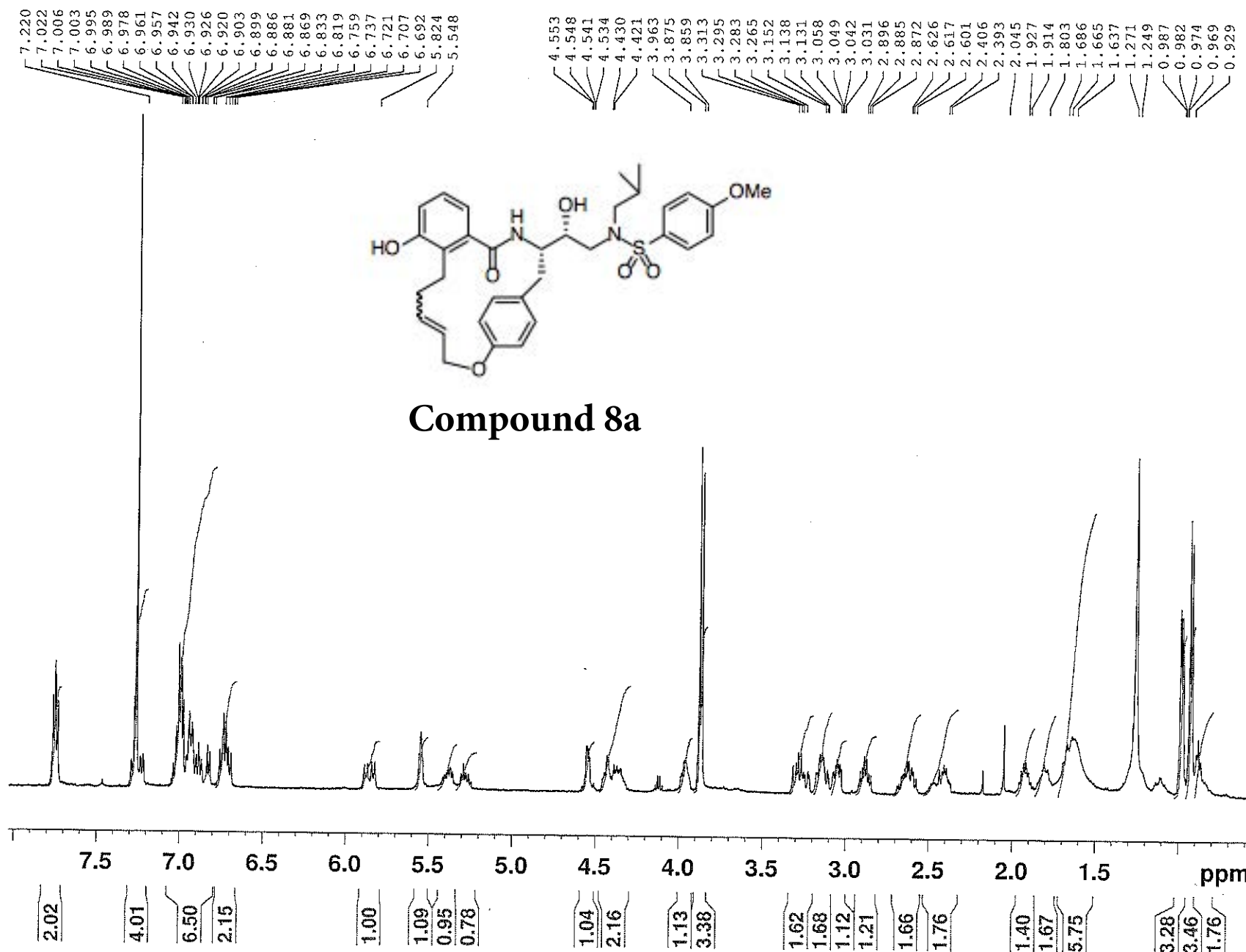
33.969
33.482
29.728
28.768
27.369
26.471
25.357
20.172
19.906



Current Data Parameters
NAME: 113
EXPNO: 131
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20041223
Time: 10.11
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 21335
DS: 2
SWH: 30502.031 Hz
FIDRES: 0.924776 Hz
AQ: 0.5407385 sec
RG: 16384
DW: 16.500 usec
DE: 5.00 usec
TE: 293.2 K
D1: 2.00000000 sec
d11: 0.01000000 sec
NOEST: 0.00000000 sec
NOH2: 0.01500000 sec
===== CHANNEL f1 =====
NUC1: 13C
P1: 2.70 usec
PL1: 1.00 dB
SFO1: 125.8998755 MHz
===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 80.00 usec
PL2: -2.00 dB
PL12: 17.00 dB
PL13: 20.00 dB
SFO2: 500.6422523 MHz
F2 - Processing parameters
S1: 16384
SF: 125.8860280 MHz
WDW: EM
SSB: 0
LB: 3.00 Hz
GB: 0
PC: 1.00

1037
7-104
113

H1 standard parameters, BBO probe.



Current Data Parameters
NAME first
EXPNO 87
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040916
Time 9.27
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7264309 sec
RG 32
DK 83.200 use
DE 6.00 use
TE 294.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRA 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 3.50 use
PL1 -2.90 dB
SFO1 500.6427535 MHz

F2 - Processing parameters
SI
SF 500.6400128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

001174
13 7-56

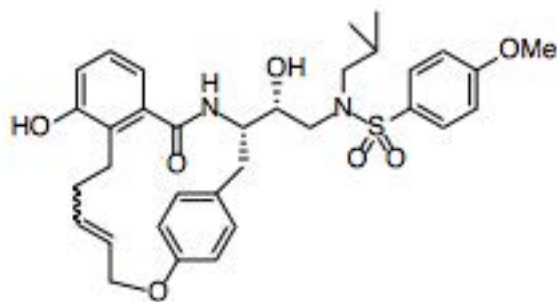
C13 standard parameters, BBO probe.

169.982
169.688
163.180
157.218
155.799
154.606
154.457
139.844
138.783
137.528
137.081
133.044
131.807
131.185
130.425
129.604
129.507
128.673
127.082
126.900
126.781
125.216
124.778
124.293
122.753
122.296
122.211
122.126
119.213
118.937
117.247
116.525
114.498

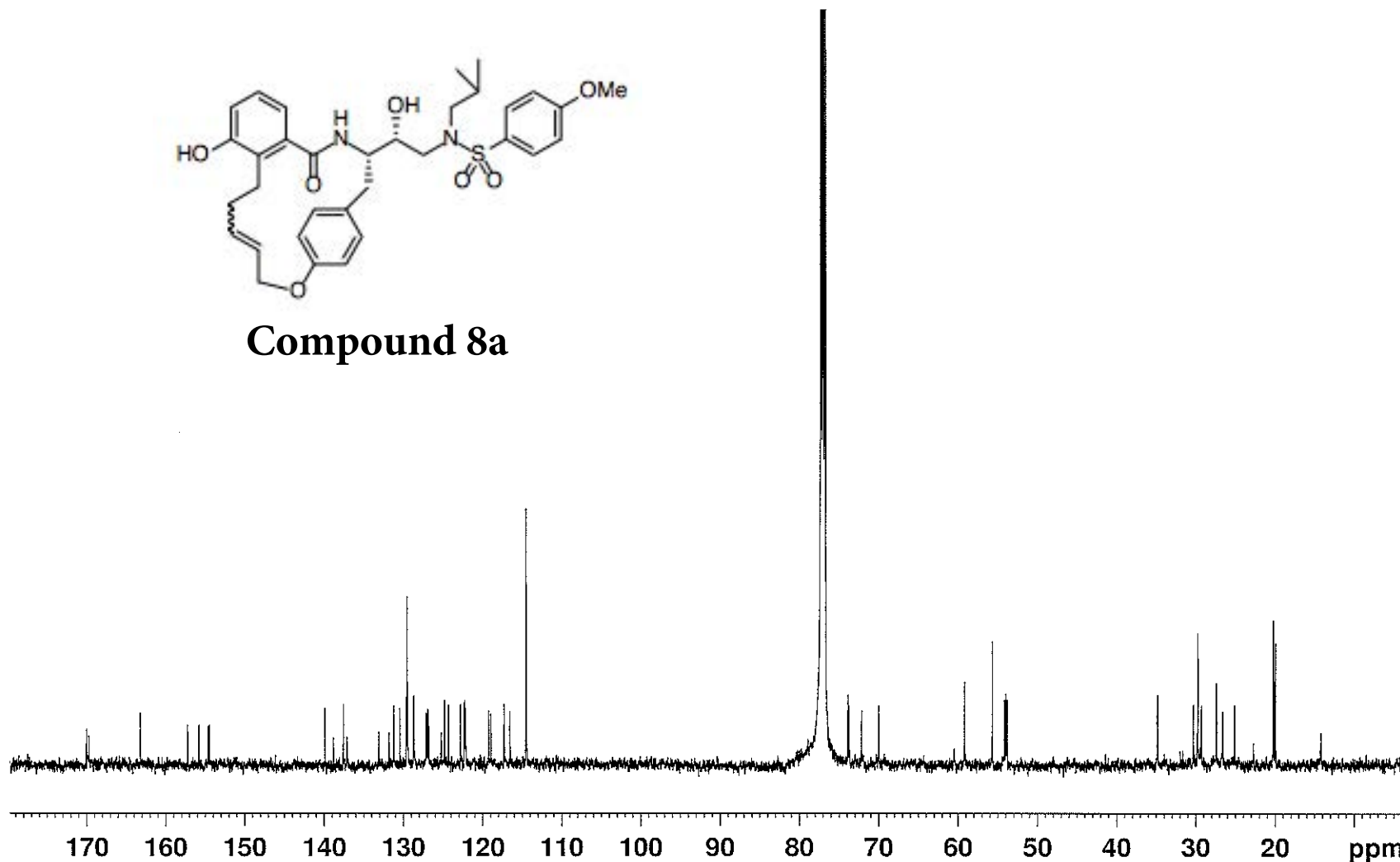
77.605
77.290
77.034
76.781
73.843
73.731
72.118
69.982

59.156
55.676
54.167
53.995
53.957
53.823

34.809
30.304
29.725
29.271
27.384
27.346
26.601
25.110
20.197
19.946
14.150



Compound 8a



Current Data Parameters
NAME first
EXPNO 86
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040916
Time 9.15
INSTRUM spect
PROBHD 5 mm BBO BB-H
PULPROG zgpg
TD 32768
FIDRES 0.3407385
RG 16384
DS 2
SWH 30303.031 Hz
FIDRES 0.9247775 Hz
AQ 0.5407385 sec
RG 16384
DW 16.500 usec
DE 6.00 usec
TE 294.7 K
D1 2.00000000 sec
d11 0.00000000 sec
MCOREST 0.00000000 sec
MCMRK 0.01500000 sec

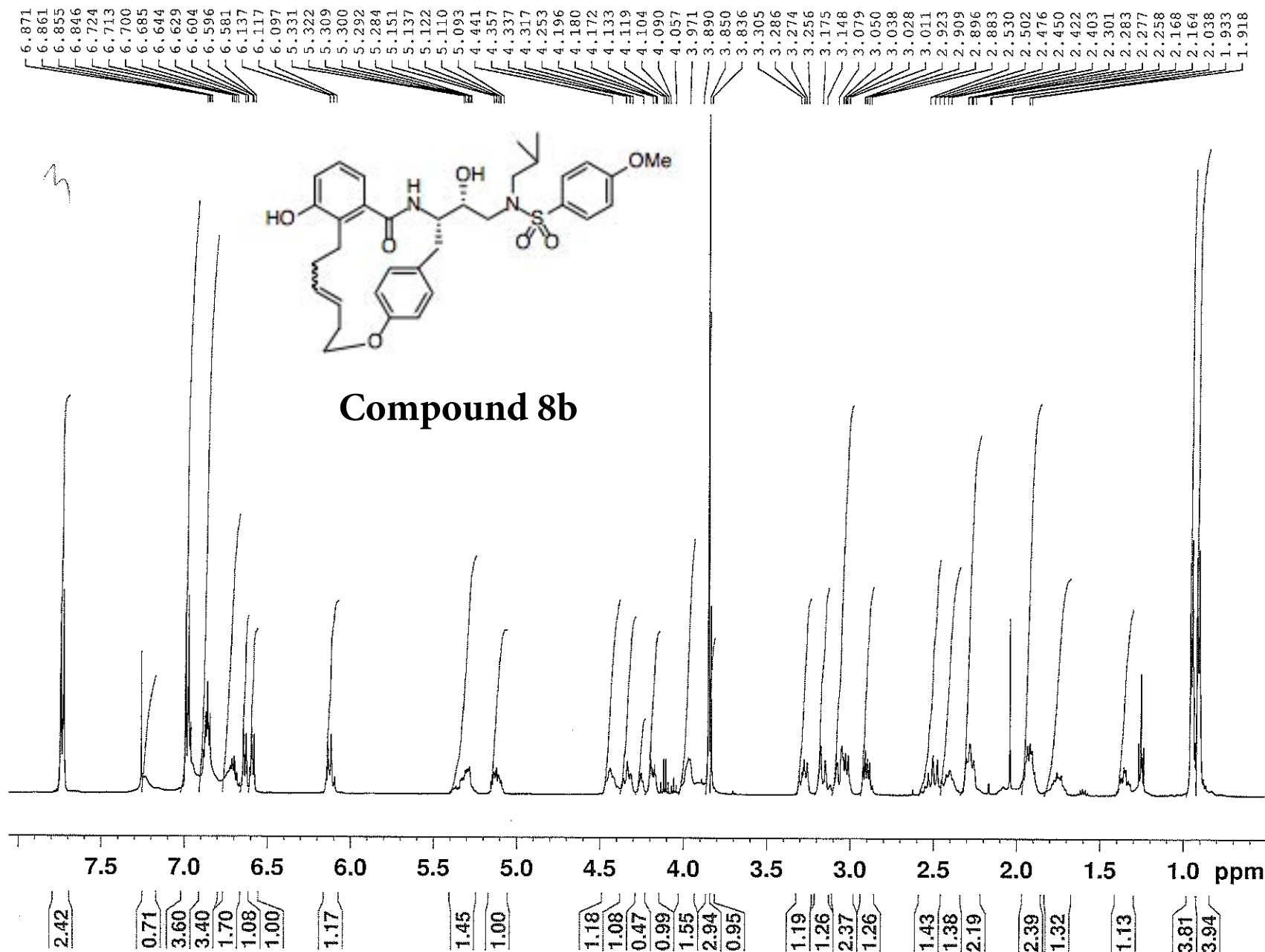
----- CHANNEL f1 -----
NUC1 13C
P1 2.70 usec
PL1 1.00 dB
SFO1 125.8998755 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 500.6422529 MHz

F2 - Processing parameters
S1 16384
SF 125.8960080 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

NC 1175
NB 7-58

3-butenyl-O-3-butenyl-RCM product



Current Data Parameters
NAME first 110
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041023
Time 13.16
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7264309 sec
RG 64
DW 83.200 usec
DE 6.00 usec
TE 294.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 3.50 usec
PL1 -2.00 dB
SFO1 500.6427535 MHz

F2 - Processing parameters
SI 32768
SF 500.6400128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00

NO 1194
NB 7-76

3-butenyl-3-O-butenyl-RCM product

170.477
163.196
158.629
154.527
138.667
133.097
129.593
129.513
126.701
126.298
125.516
118.089
116.335
114.534

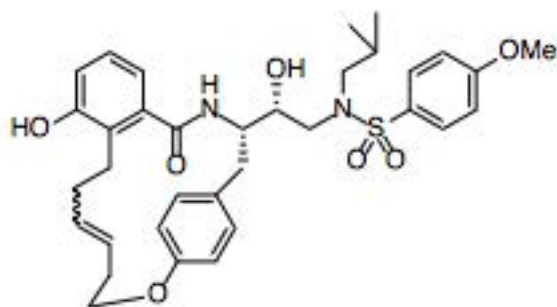
77.337
77.083
76.827
73.588

66.625

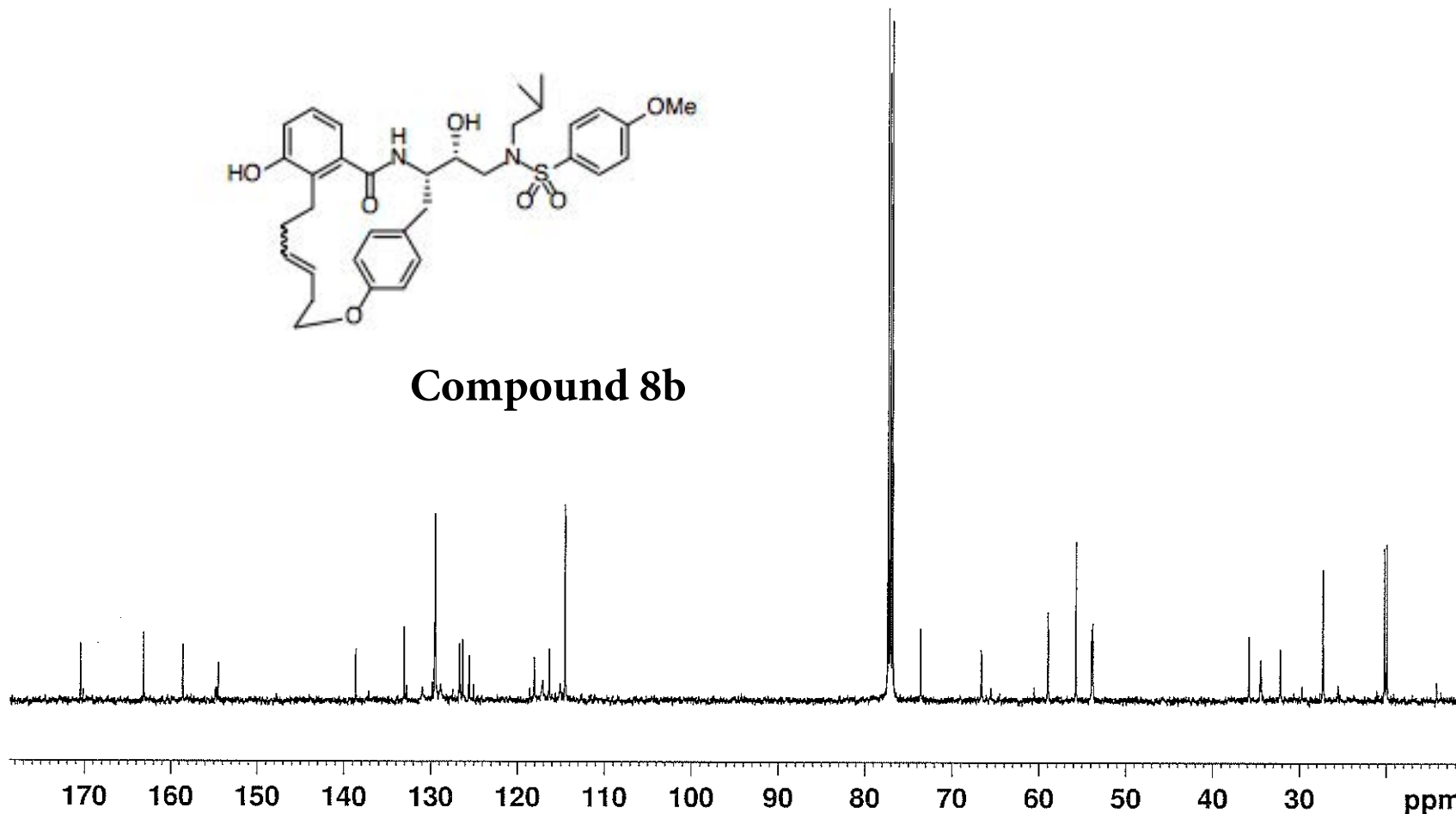
58.946
55.700
53.907
53.788

35.817
34.458
32.239
27.300

20.196
19.948



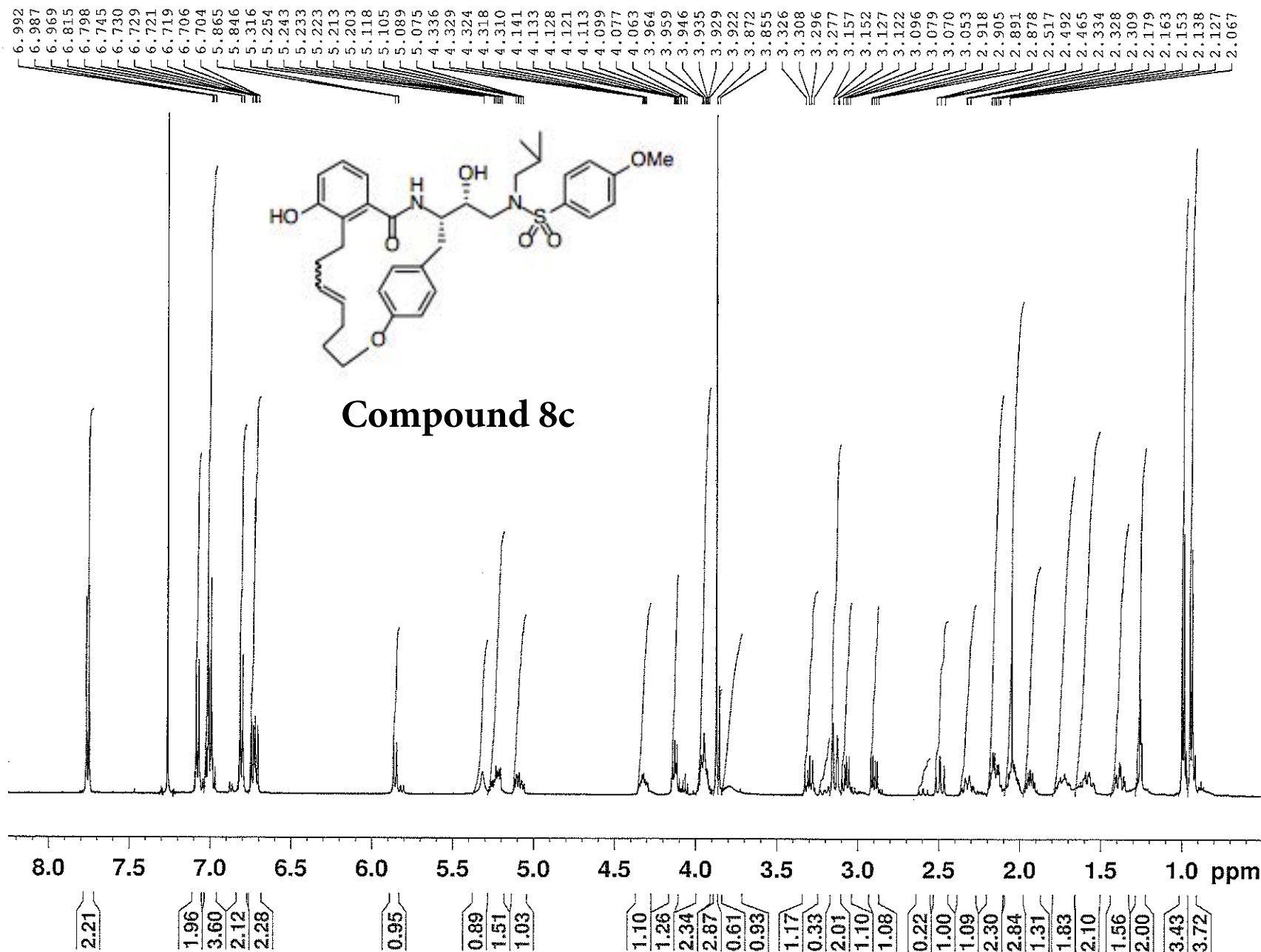
Compound 8b



Current Data Parameters
NAME 1195
EXPNO 111
PROCNO 1
F2 - Acquisition Parameters
Date_ 20041022
Time 15.22
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TE 32768
SOLVENT CDCl3
NS 512
DS 2
SWH 30303.031 KHz
FIDRES 0.924775 KHz
AQ 0.5467785 sec
RG 1.6384
DW 16.500 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWEX 0.01500000 sec
----- CHANNEL f1 -----
NUC1 13C
P1 2.70 usec
PL1 1.00 dB
SFO1 125.8998755 MHz
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 500.6422529 MHz
F2 - Processing parameters
SI 16384
SF 125.8860280 MHz
WDW EM
SSB 0
LB 3.00 KHz
GB 0
PC 1.00

NO 1195
MB 7-76

3-butenyl-(4-pentenyl)-RCM-product



Current Data Parameters

NAME	first
EXPNO	148
PROCNO	1

F2 - Acquisition Parameters

Date_	20041220
Time	19.07
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	8
DS	2
SWH	6009.615 Hz
FIDRES	0.163399 Hz
AQ	2.7264309 sec
RG	256
DW	83.200 use
DE	6.00 use
TE	294.7 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCHWK	0.01500000 sec

----- CHANNEL f1 -----

NUC1	1H
P1	3.50 use
PL1	-2.00 dB
SFO1	500.6427535 MHz

F2 - Processing parameters

SF	500.6400128 MHz
WDW	EM
SSE	0
GB	0.30 Hz
PC	1.00

1034
137-103
117

3-hydroxy-2-(3-butenyl)-4-(4-pentenyl)-phenyl

169.916

163.185

158.882

154.343

138.522

134.022

130.130

129.597

129.509

127.314

126.893

125.939

118.447

116.508

115.384

114.500

77.607

77.293

77.039

76.783

73.581

66.586

59.178

55.681

54.678

54.045

35.099

31.953

29.729

29.374

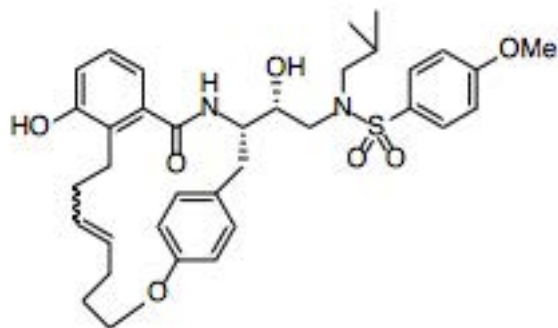
28.264

27.738

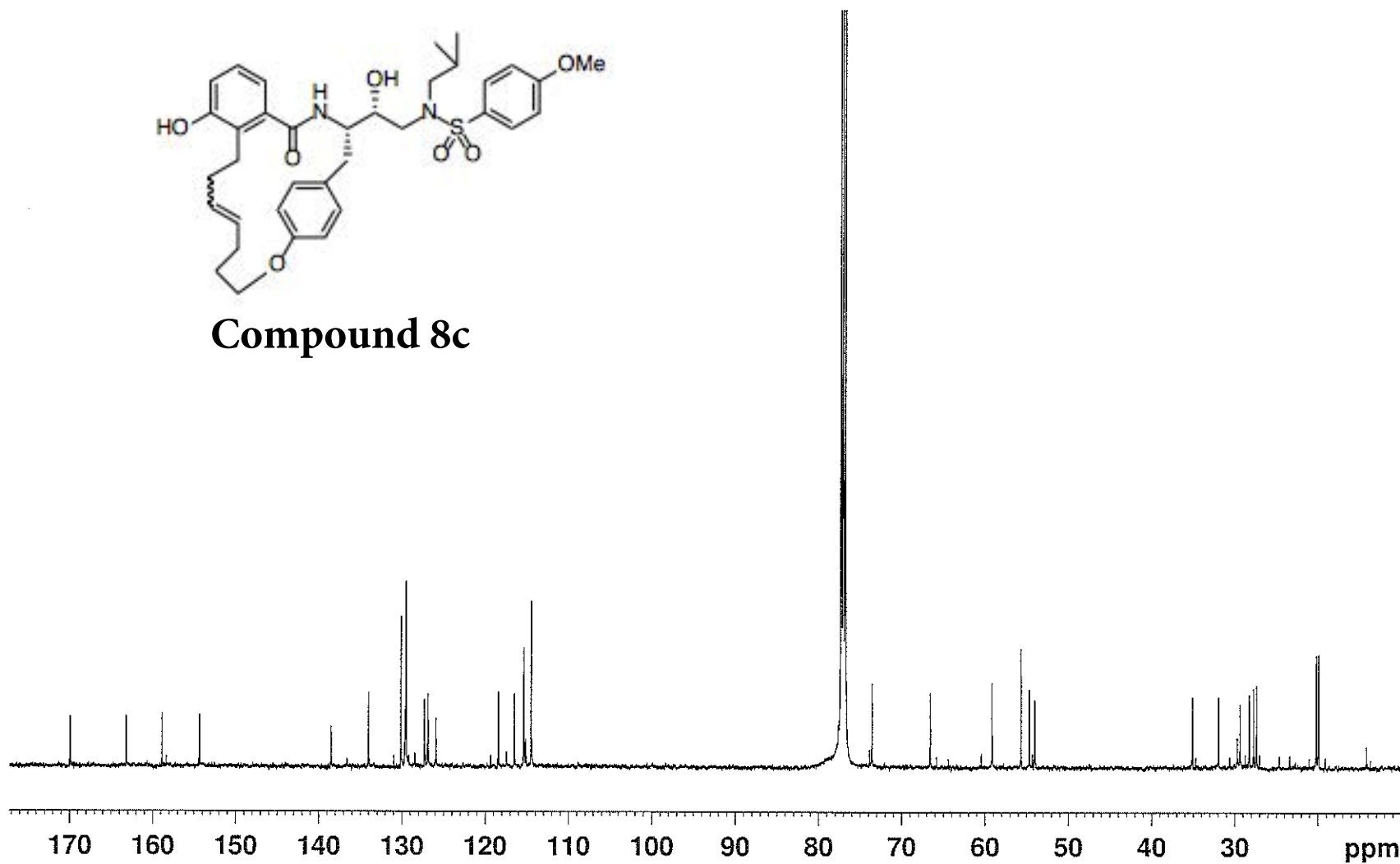
27.391

20.205

19.938



Compound 8c



Current Data Parameters
NAME: 11035
EXPNO: 149
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20041220
Time: 19.06
INSTRUM: spect
PROBHD: 5 mm 590 55-1H
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 22128
DS: 2
SWH: 30303.032 Hz
FIDRES: 0.924775 Hz
AQ: 0.5407385 sec
RG: 16284
DW: 16.500 usec
DE: 6.00 usec
TE: 294.7 K
D1: 2.00000000 sec
d11: 0.03000000 sec
WREST: 0.00000000 sec
MCWRR: 0.01500000 sec

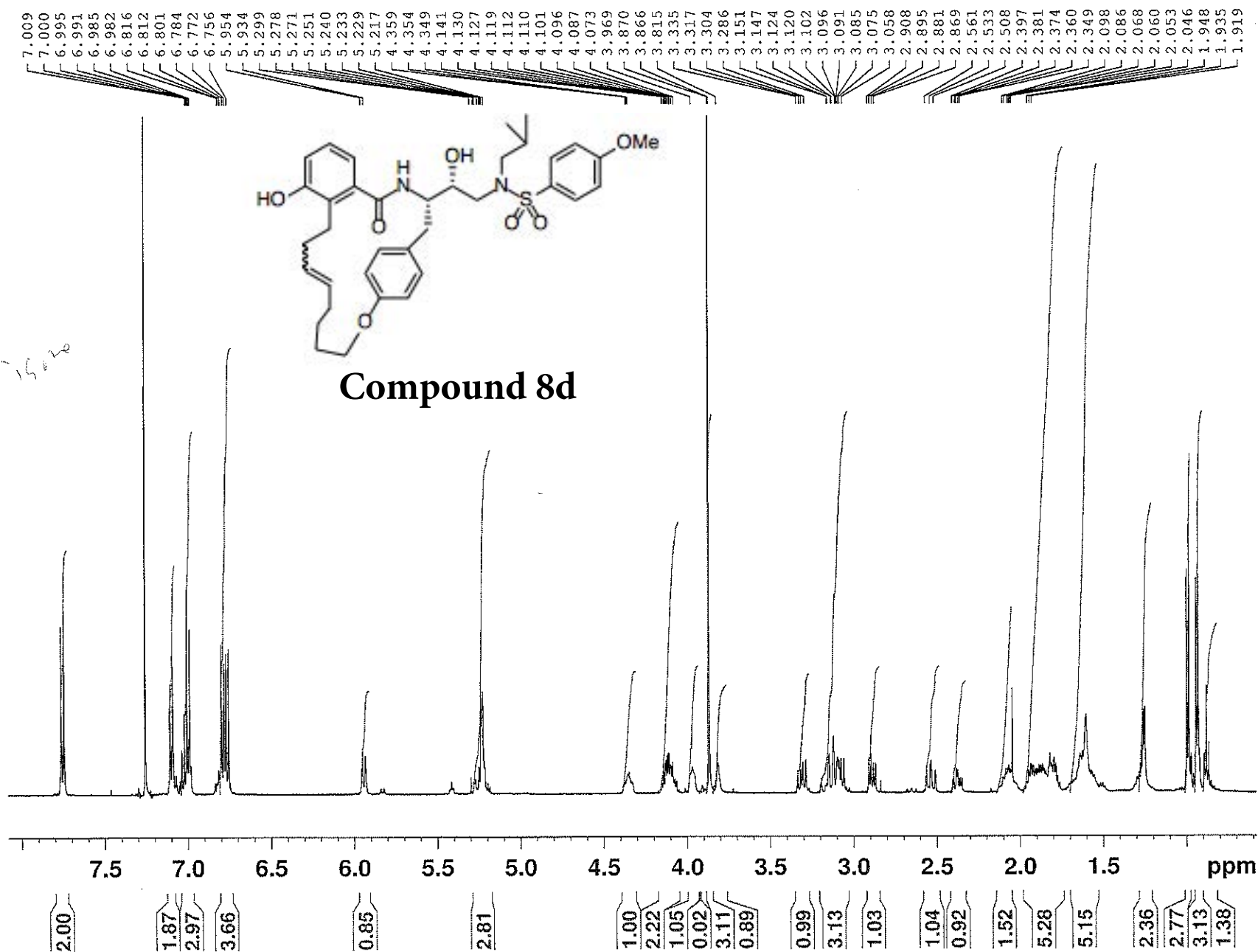
----- CHANNEL f1 -----
NUC1: 13C
P1: 2.70 usec
PL1: 1.00 dB
SFO1: 125.8998755 MHz

----- CHANNEL f2 -----
CHOPRG2: waltz16
NUC2: 1H
PCPD2: 80.00 usec
PL2: -2.00 dB
PL12: 17.00 dB
PL13: 20.00 dB
SFO2: 500.6422529 MHz

F2 - Processing parameters
SI: 6584
SF: 125.8998755 MHz
WDW: EM
SSB: 0
LB: 3.00 Hz
GB: 0
PC: 1.00

1035
7-1003
110

4 and 6 RCM product



Current Data Parameters
NAME first
EXPNO 152
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041223
Time 17.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 6009.615 Hz
FIDRES 0.181399 Hz
AQ 2.7264309 sec
RG 256
DN 83.200 use
DE 6.00 use
TE 292.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 3.50 use
PL1 -2.00 dB
SFO1 500.6427535 MHz

F2 - Processing parameters
SI 32768
SF 500.6400128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

AD 1238

137-106

1/5

4 and 6 RCM product

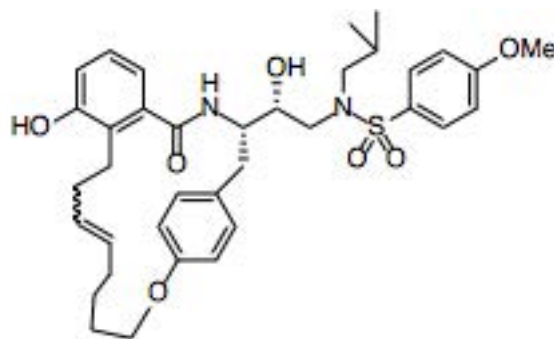
169.885
163.176
156.914
154.135

138.253
130.685
130.033
129.905
129.619
129.501
126.866
126.373
118.713
116.744
115.230
114.506

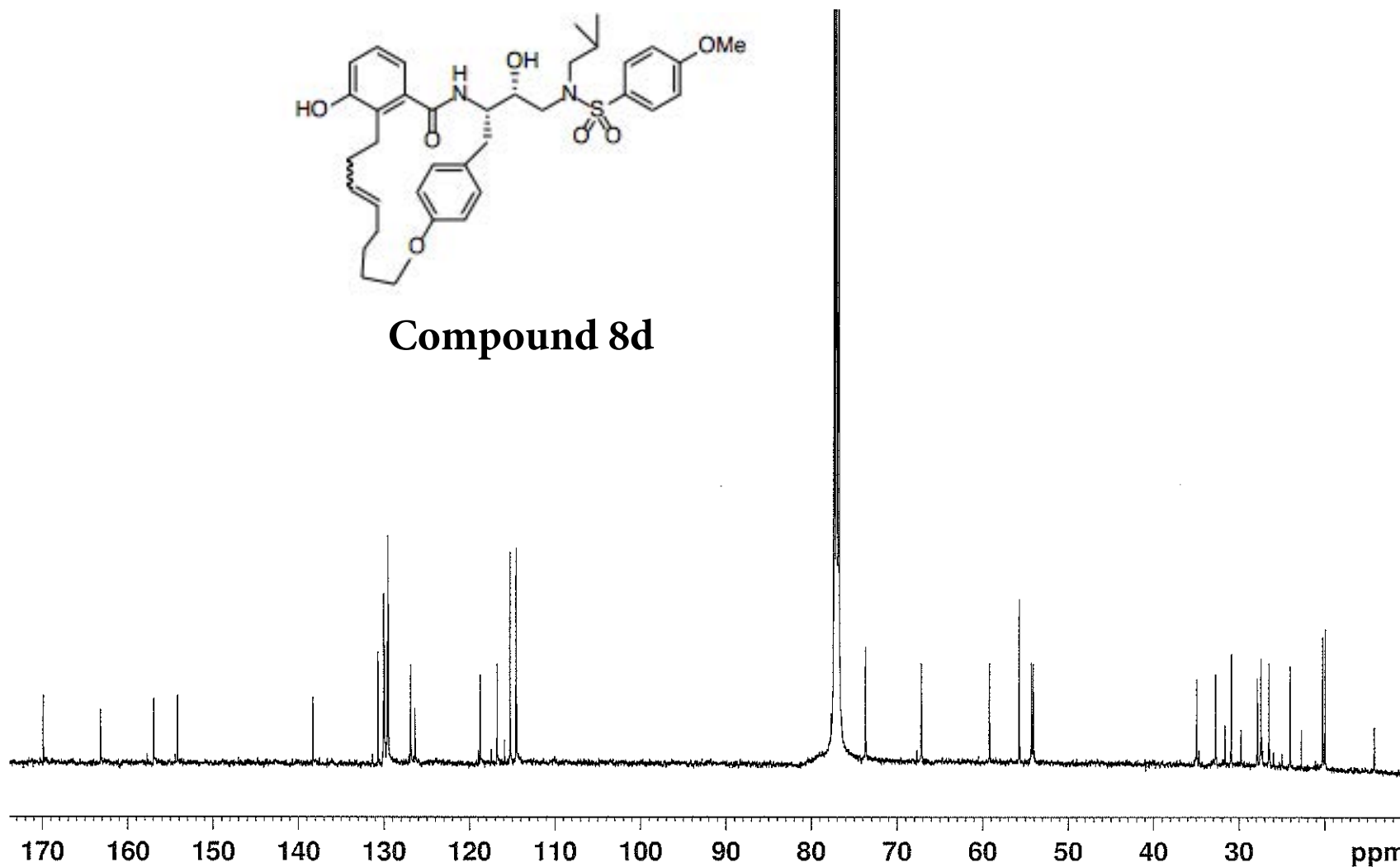
77.613
77.296
77.044
76.790
73.651
67.142

59.169
55.683
54.263
54.066

34.913
32.699
30.882
27.854
27.410
26.486
24.019
20.208
19.924

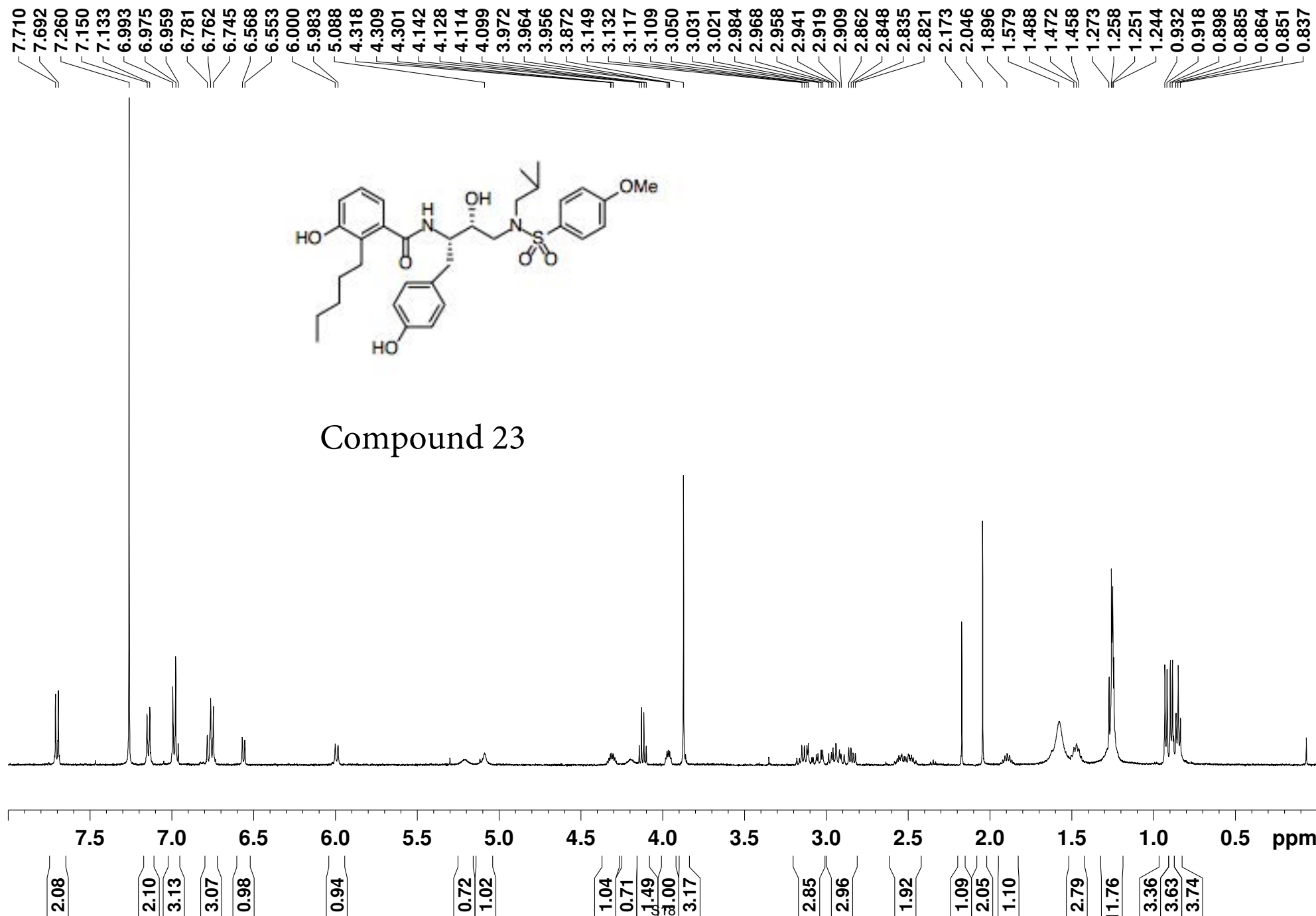


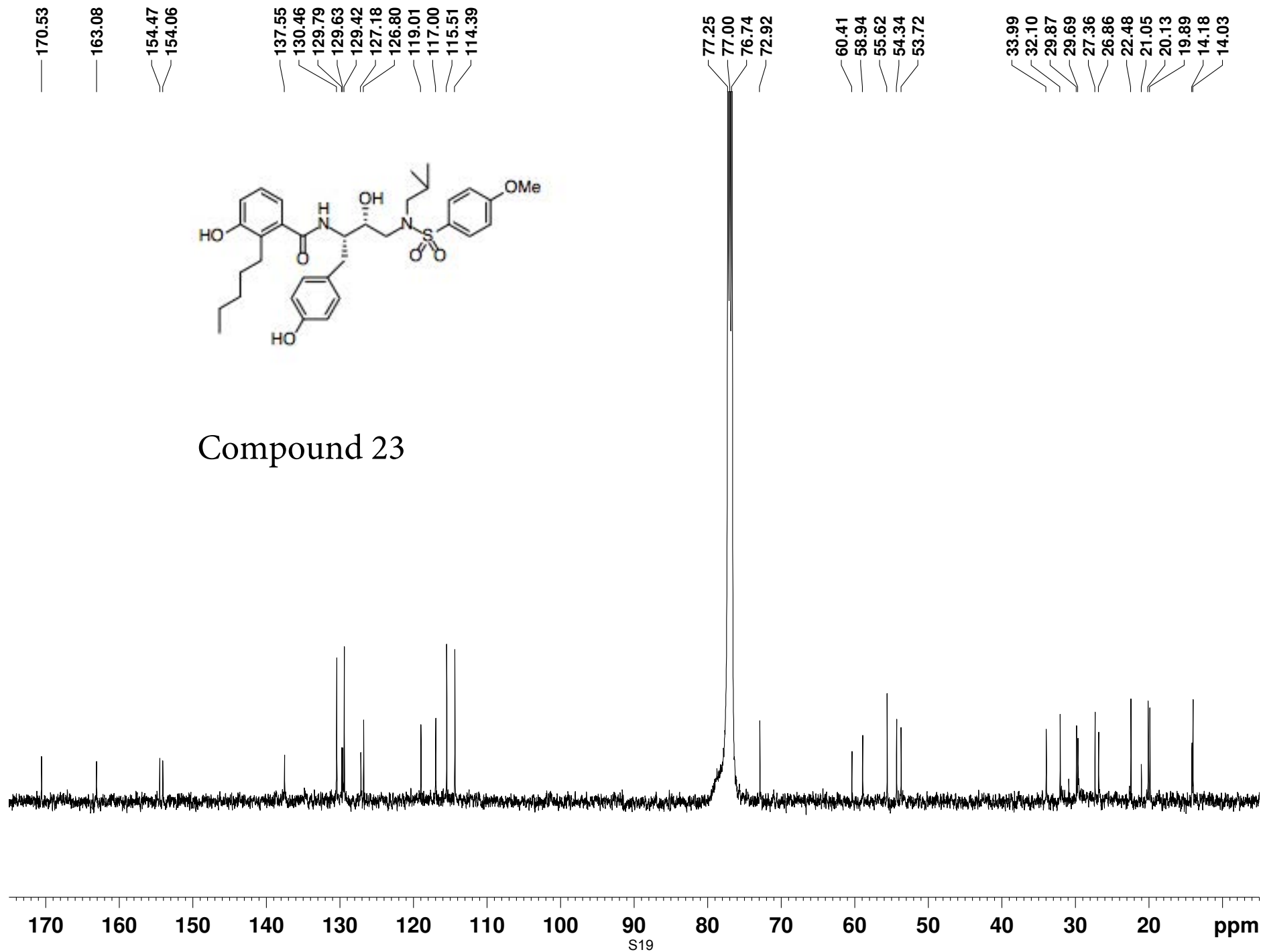
Compound 8d



Current Data Parameters
NAME first
EXPNO 153
PROCNO 1
F2 - Acquisition Parameters
Date_ 20041223
Time 18.01
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 23225
DS 2
SWH 30303.021 Hz
FIDRES 0.924775 Hz
AQ 0.5407385 sec
RG 16384
DW 16.500 usec
DE 6.00 usec
TE 292.3 K
D1 2.00000000 sec
d11 0.03000000 sec
WDEXT 0.00000000 sec
MCWEX 0.01500000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 2.70 usec
PL1 1.00 dB
SFO1 125.8996755 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 500.6422529 MHz
F2 - Processing parameters
SI 16384
SF 125.8860240 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1239
7-106
113

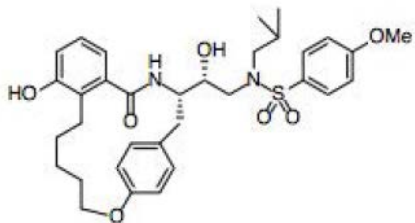




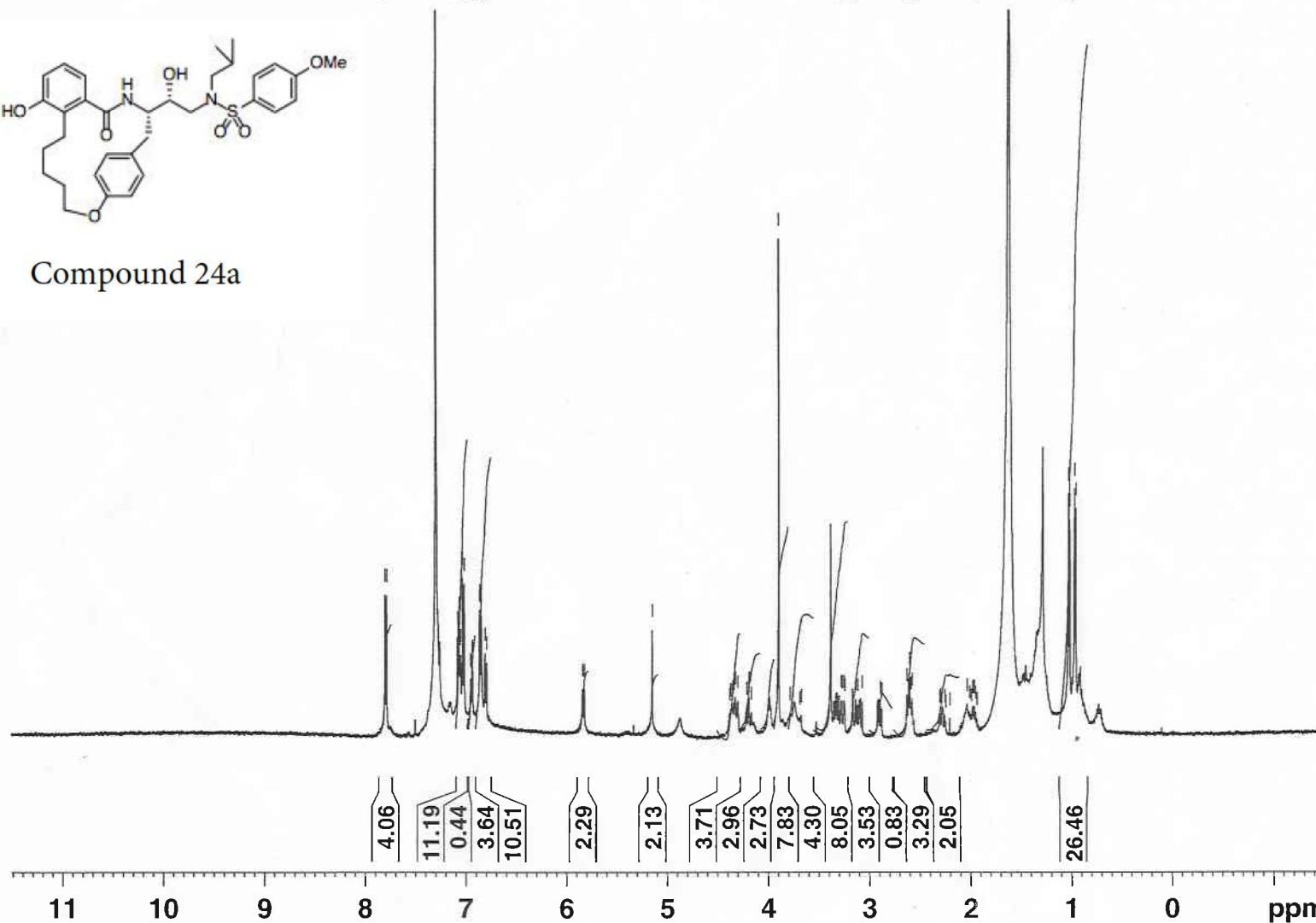
H1 standard parameters, cryoprobe (#02), CDCl3.



7.804
7.786
7.083
7.080
7.075
7.068
7.063
7.058
7.053
7.035
7.017
6.954
6.950
6.938
6.934
6.866
6.863
6.850
6.812
6.796
5.843
5.824
5.151
4.340
4.328
4.305
4.193
3.898
3.282
3.274
3.255
3.246
3.134
3.118
3.075
2.633
2.607
2.593
2.581
1.982
1.968
1.034
1.020
0.973
0.960



Compound 24a

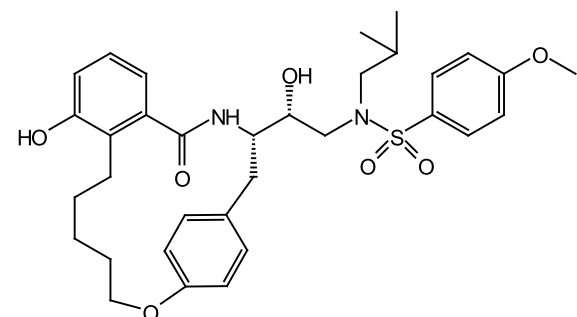


Current Data Parameters
NAME LR5-sample-3
EXPNO 1
PROCNO 1

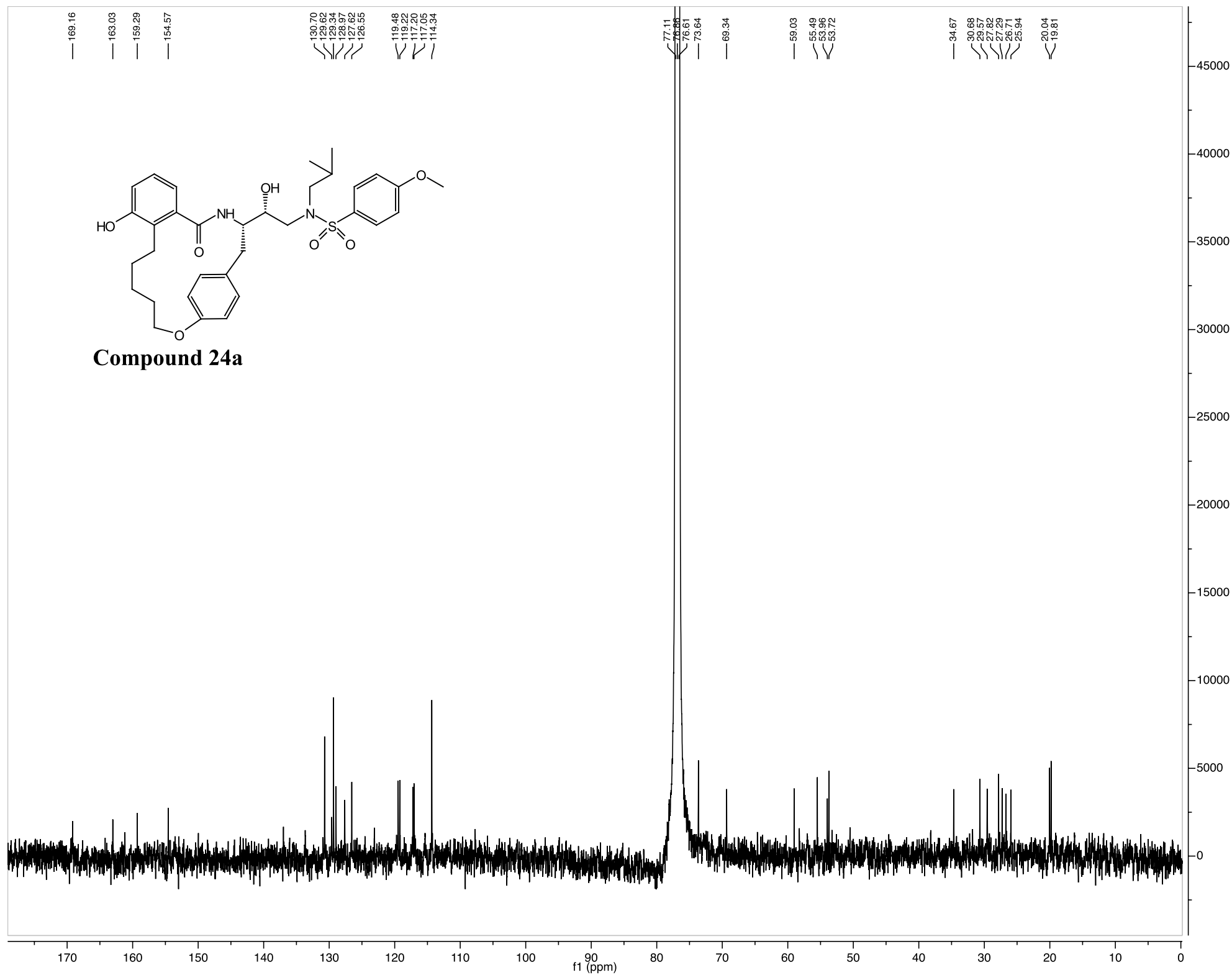
F2 - Acquisition Parameter
Date_ 20140622
Time 11.44
INSTRUM spect
PROBHD 5 mm CPTXI 1H-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 72
DS 2
SWH 6510.400 Hz
FIDRES 0.198682 Hz
AQ 2.5167158 se
RG 9
DW 76.800 us
DE 6.00 us
TE 298.0 K
D1 1.00000000 se
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.00 us
PL1 1.50 dB
SFO1 499.8925000 MHz

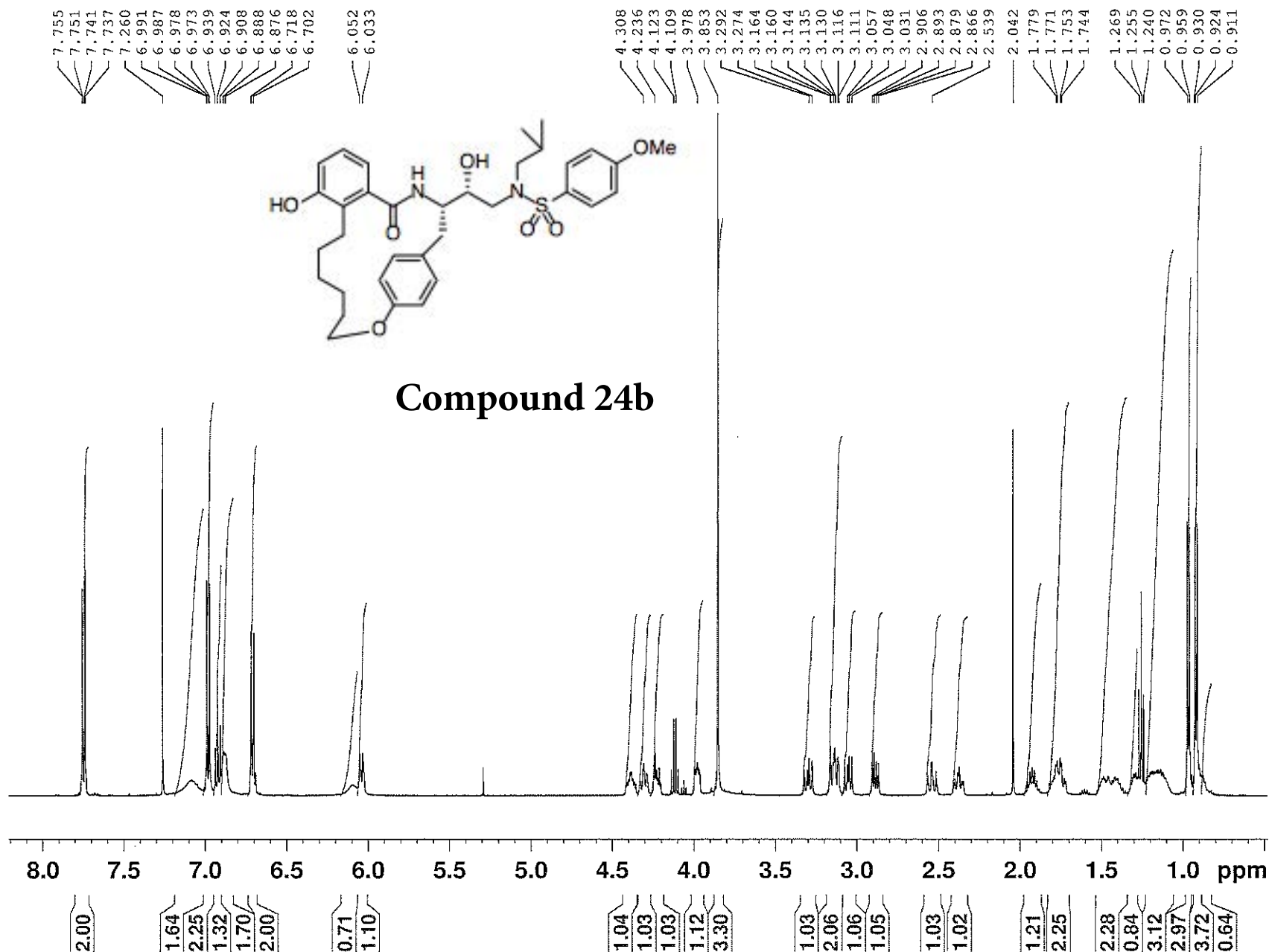
F2 - Processing parameters
SI 16384
SF 499.8899986 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Compound 24a



Aryl-3-butenyl-Aryl-O-3-butenyl-RCM AND Hydrogenation pdt



Current Data Parameters
NAME first
EXPNO 120
PROCNO 1

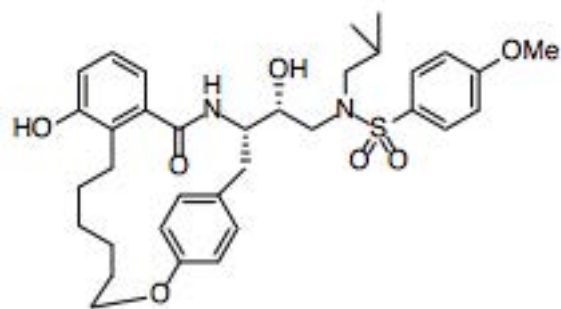
F2 - Acquisition Parameters
Date_ 20041026
Time 15.05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 6009.615 Hz
FIDRES 0.183359 Hz
AQ 2.7264309 sec
RG 90.5
DW 83.200 usec
DE 6.00 usec
TE 293.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCNRRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 3.50 usec
PL1 -2.00 dB
SFO1 500.6427535 MHz

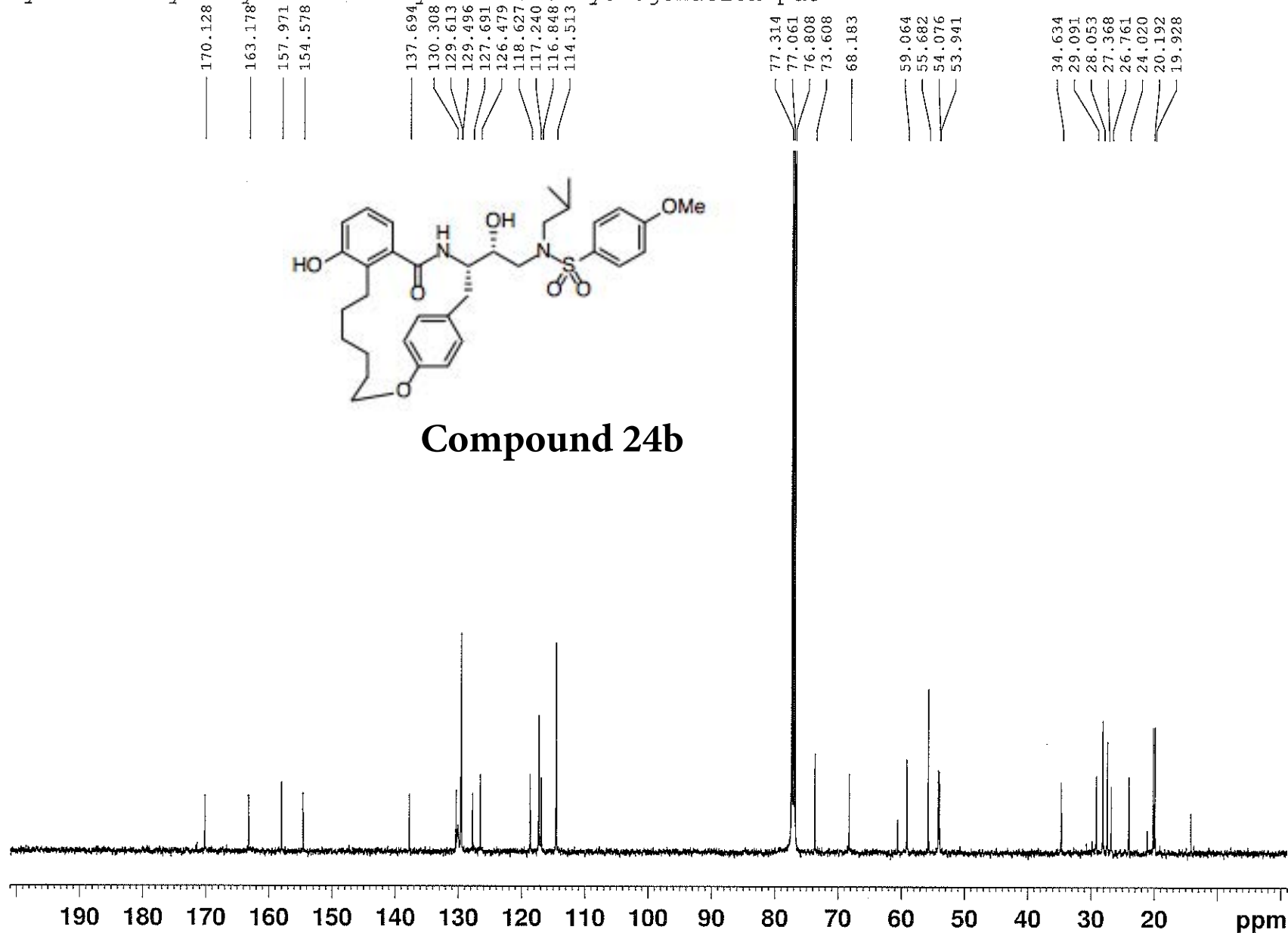
F2 - Processing parameters
SI 32768
SF 500.6400128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NO 1196
MS 7-77

Aryl-3-butenyl-Aryl-O-3-butenyl-RCM and hydrogenation pdt



Compound 24b



Current Data Parameters
NAME first
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20041026
Time 15:14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
ID 32768
SOLVENT CDCl3
NS 1300
DS 2
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5407385 sec
RG 16384
DE 16.500 usec
TE 294.2 K
D1 2.0000000 sec
d11 0.0300000 sec
d12 0.0000000 sec
d13 0.0000000 sec
MCWAX 0.0100000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 2.70 usec
PL1 1.00 dB
SFO1 125.8998755 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 500.6422529 MHz
F2 - Processing parameters
SI 16384
SF 125.8860280 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

NC1197
NB777

Compound 24c

Chemical Structure of Compound 24c:

COc1ccc(cc1)S(=O)(=O)CN(CC[C@H](O)C(=O)c2cc(O)ccc2)Cc3ccccc3

1H NMR Spectrum (CDCl₃):

Chemical Shifts (ppm): 7.260, 7.219, 7.088, 7.072, 7.056, 7.041, 7.003, 6.997, 6.993, 6.983, 6.979, 6.876, 6.874, 6.861, 6.859, 6.832, 6.815, 6.805, 6.803, 6.789, 6.787, 5.903, 5.885, 4.913, 4.378, 4.354, 4.260, 4.249, 4.152, 4.147, 4.141, 4.127, 4.113, 3.974, 3.969, 3.962, 3.956, 3.950, 3.864, 3.325, 3.307, 3.294, 3.276, 3.270, 3.170, 3.165, 3.139, 3.134, 3.079, 3.062, 3.053, 3.036, 2.889, 2.876, 2.862, 2.849, 2.678, 2.627, 2.603, 2.598, 2.574, 2.174, 2.174, 2.047, 2.006, 2.001, 1.942, 1.929, 1.925, 1.912, 1.898, 1.591, 1.467, 1.460, 1.454, 1.442.

Integration Values: 2.00, 3.06, 2.01, 1.03, 2.03, 1.03, 0.98, 0.91, 1.05, 1.11, 1.22, 1.15, 3.21, 1.04, 2.04, 1.06, 1.06, 1.06, 1.06, 1.16, 2.19, 3.29, 2.41, 1.44, 4.30, 5.86, 3.21, 3.33, 0.63.

N/ 1340
MB 7-105
115

4 and 5 RCM and H2 product

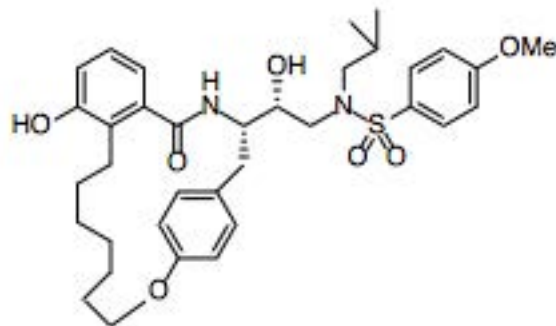
170.112
163.128
156.940
154.307

137.298
130.099
129.685
129.660
129.483
127.547
126.746
119.240
117.111
115.848
114.477

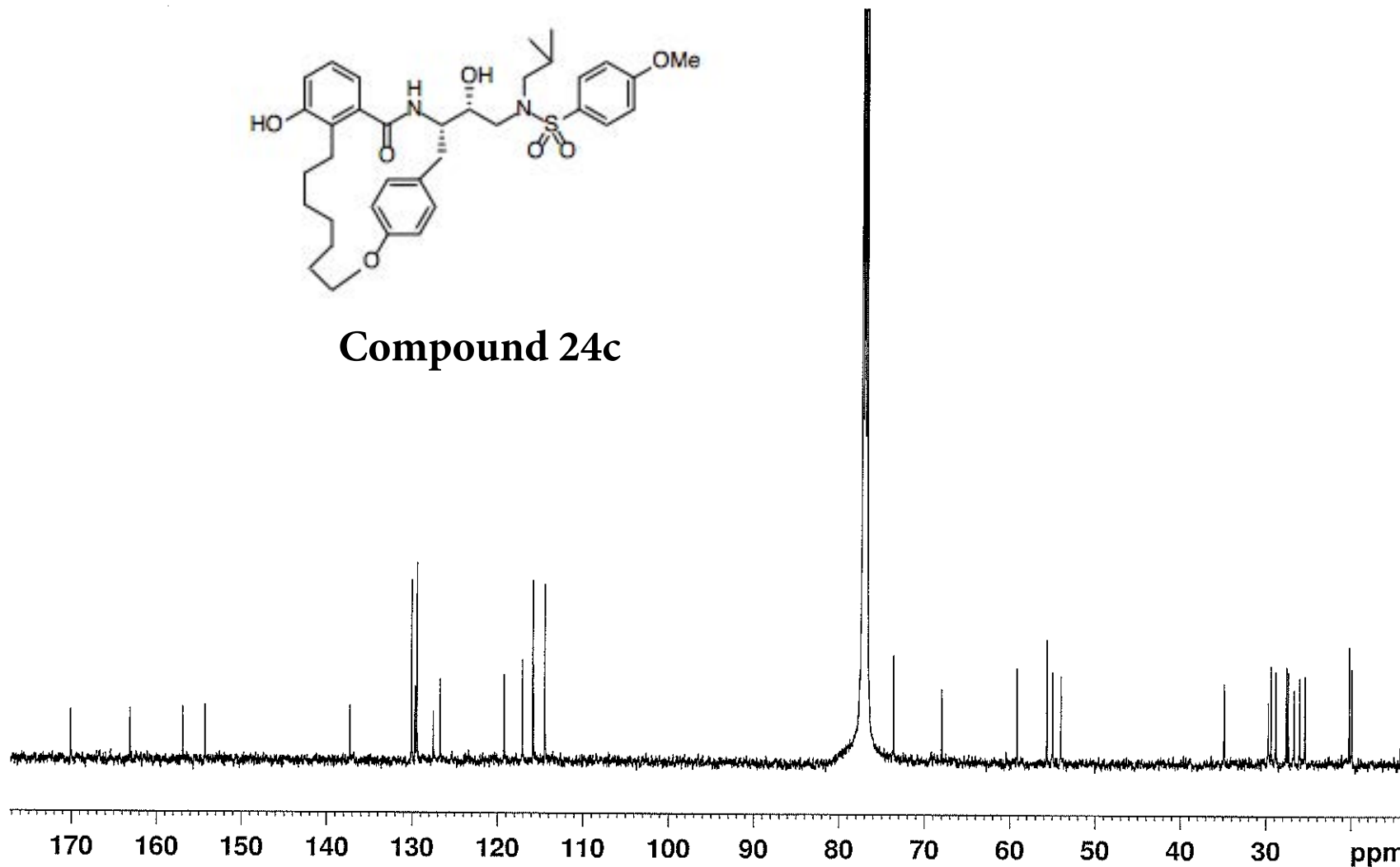
77.294
77.042
76.786
73.621
67.985

59.164
55.668
54.997
54.026

34.893
29.737
29.412
28.856
27.603
27.375
26.698
26.062
25.429
20.216
19.930



Compound 24c



Current Data Parameters
NAME first
EXPNO 155
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041228
Time 10.59
INSTRUM spect
PROBHD 5 mm BBO Hs-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 23560
DS 2
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5407383 sec
RG 16384
DW 16.500 usec
DE 6.00 usec
TE 290.1 K
D1 2.00000000 sec
d11 0.03000000 sec
MCRESST 0.00000000 sec
MCMRK 0.01500000 sec

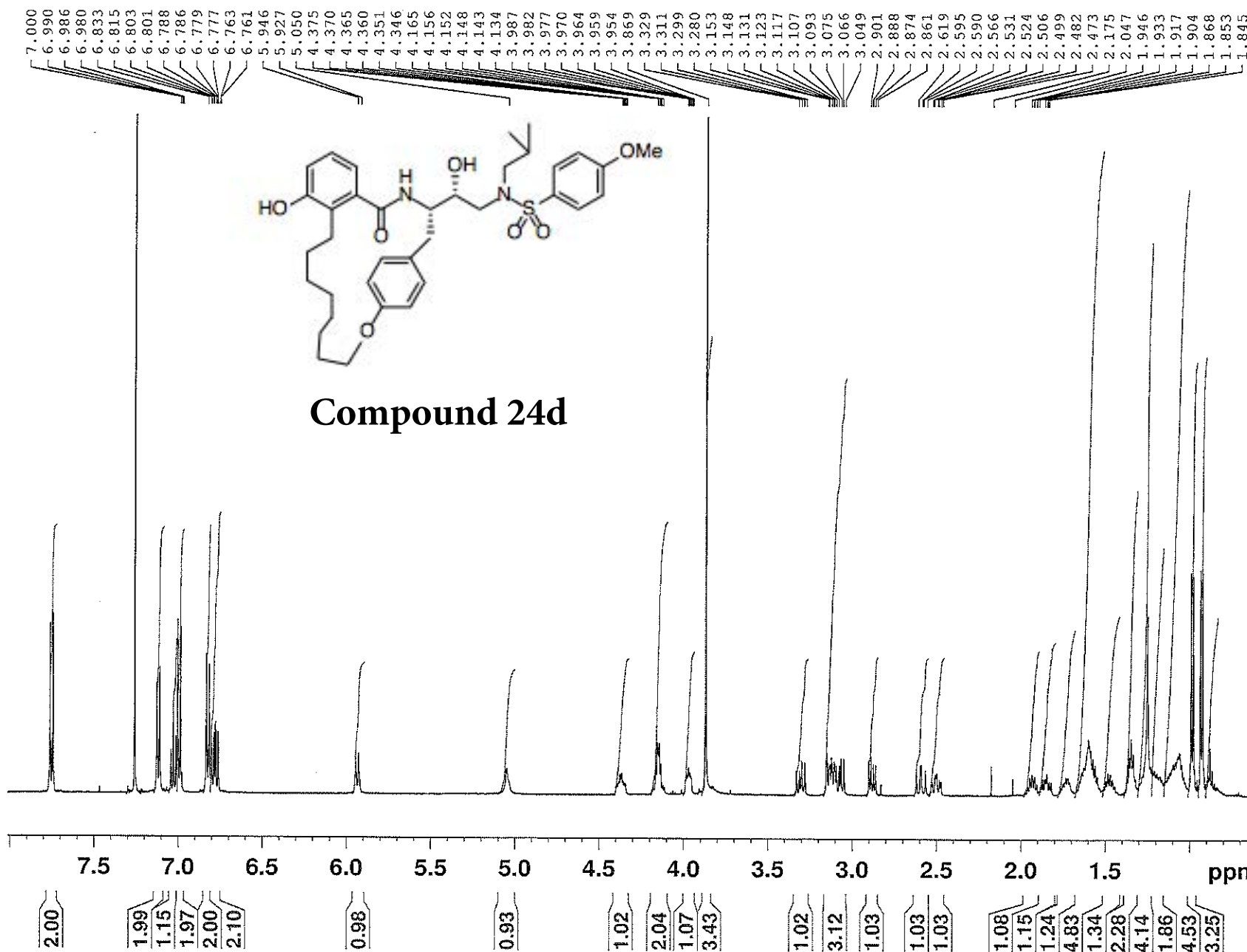
===== CHANNEL f1 =====
NUC1 13C
P1 2.70 usec
PL1 1.00 dB
SFO1 125.8998755 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 500.6422529 MHz

F2 - Processing parameters
SI 16384
SF 125.8960280 MHz
WDW EN
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1041
7-105
113

4 and 6 RCM and H2 product



Current Data Parameters
NAME first
EXPNO 156
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041228
Time 18.11
INSTRUM spect
PROBHD 5 mm BBO BB-IN
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 KHz
FIDRES 0.183389 KHz
AQ 2.7264309 Sec
RG 322.5
DW 83.200 usec
DE 6.00 usec
TE 291.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWREK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 3.50 usec
PL1 -2.00 dB
SFO1 500.6427555 MHz

F2 - Processing parameters
SI 32768
SF 500.6400128 MHz
WDW EM
SSB 0
LB 0.30 KHz
GB 0
PC 1.00

101242

137-107

115

4 and 6 RCM and H2 product

170.132

163.155

156.785

154.063

138.033

129.934

129.639

129.584

129.496

127.091

126.723

119.004

116.804

115.146

114.494

77.614

77.297

77.045

76.792

73.681

67.026

59.162

55.681

54.155

54.035

34.737

30.039

29.739

28.269

27.401

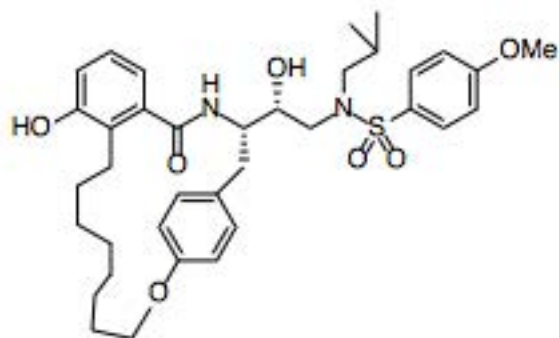
27.082

27.031

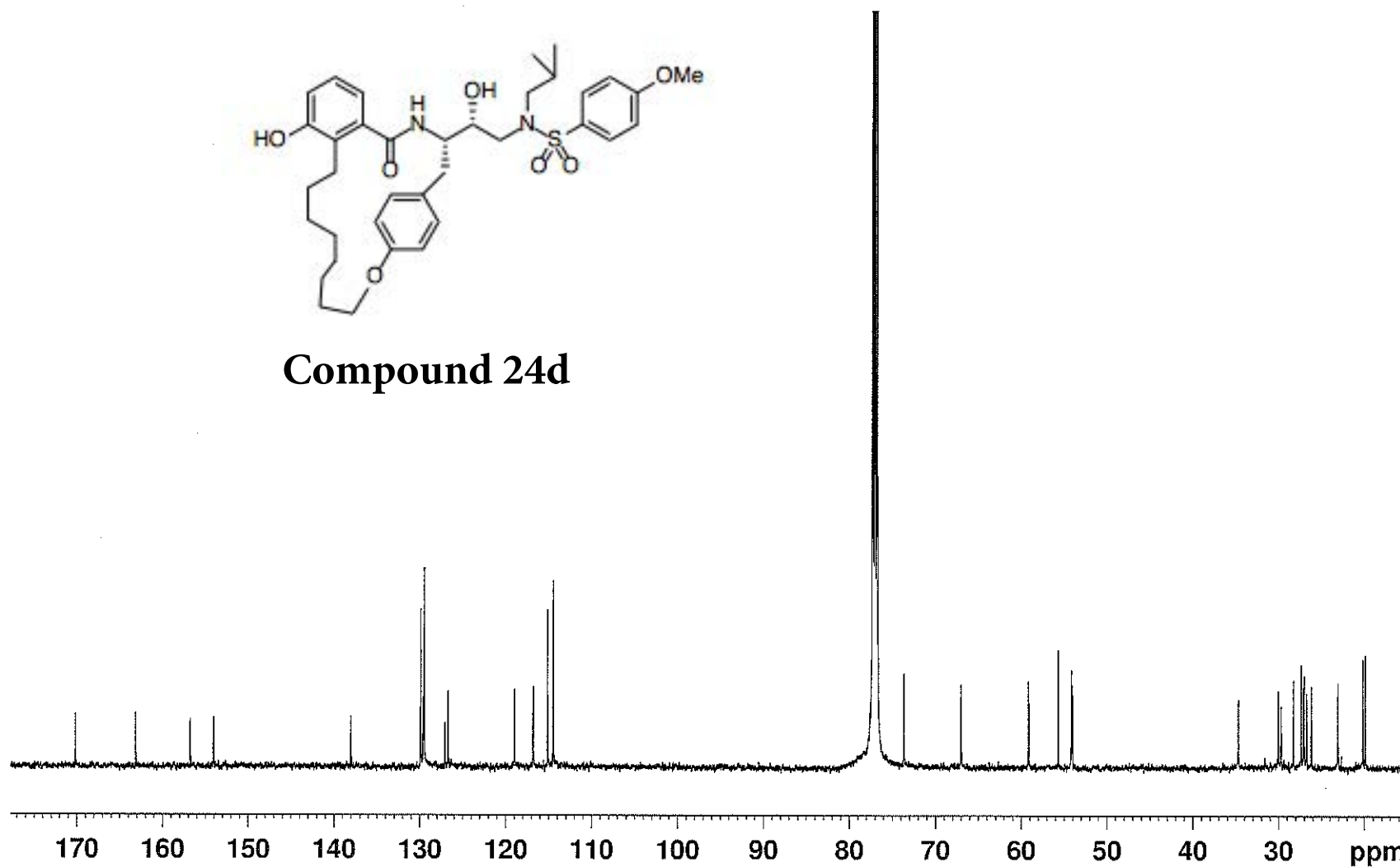
26.753

26.207

23.094



Compound 24d



Current Data Parameters
NAME first
EXPNO 157
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041229
Time 10.33
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 22650
DS 2
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5407385 sec
RG 16384
DW 16.500 usec
DE 5.00 usec
TE 293.6 K
D1 2.00000000 sec
d11 0.03000000 sec
WOREST 0.00000000 sec
MCWRE 0.01500000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 2.70 usec
PL1 1.00 dB
SFO1 125.8996755 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 500.6422529 MHz

F2 - Processing parameters
SI 16384
SF 125.8860286 MHz
WDW EN
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1243
7-107
114