Briaroxalides : Novel Bisepoxybriarane Diterpenes from an Okinawan gorgonian *Briareum* sp.

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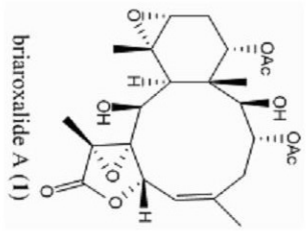
1432-1 Horinouchi, Hachioji, Tokyo 192-0392, Japan

List of Supplementaly Materials



δ / ppm

7.2598

6.0619
6.0493
6.0435
6.0309

5.5471
5.5318

5.2810
5.2661

5.1174
5.1076

4.5939
4.5878

4.0849
4.0789

3.8816
3.8646

3.0112
3.0013
2.9876
2.9755
2.9636
2.9578

2.6001
2.5831

2.3721

2.2334
2.2231

2.2167

2.1843

2.1555

2.0962

2.0282

1.8480

1.7437

1.6229

1.5261

1.0338

1.0

1.0012

0.994

0.9973

0.9876

0.9579

0.9814

2.0139

0.979

0.9776

0.902

0.8648

3.0651

4.1108

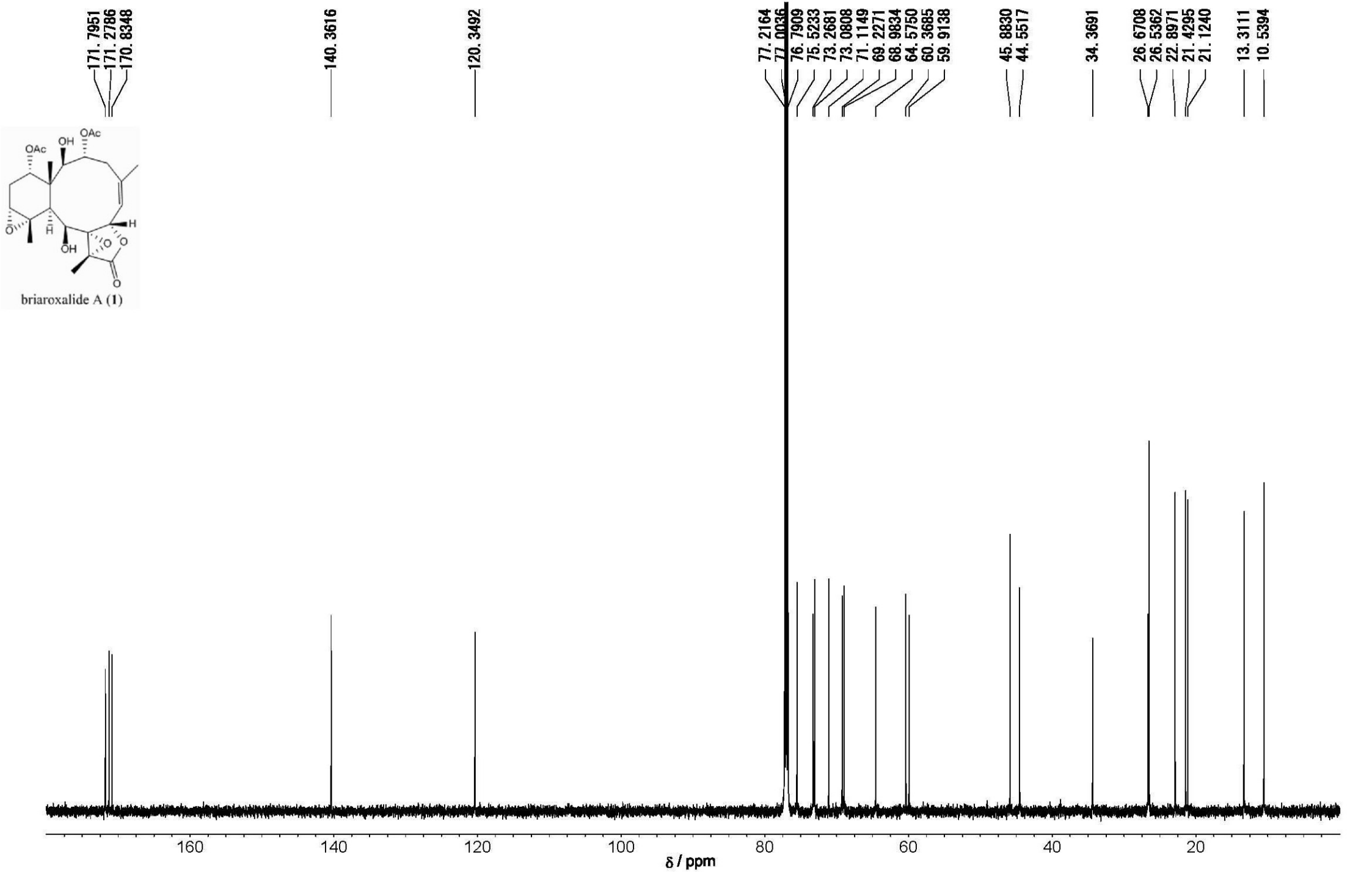
2.9093

1.1146

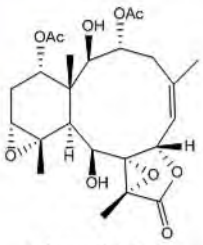
3.0747

2.9821

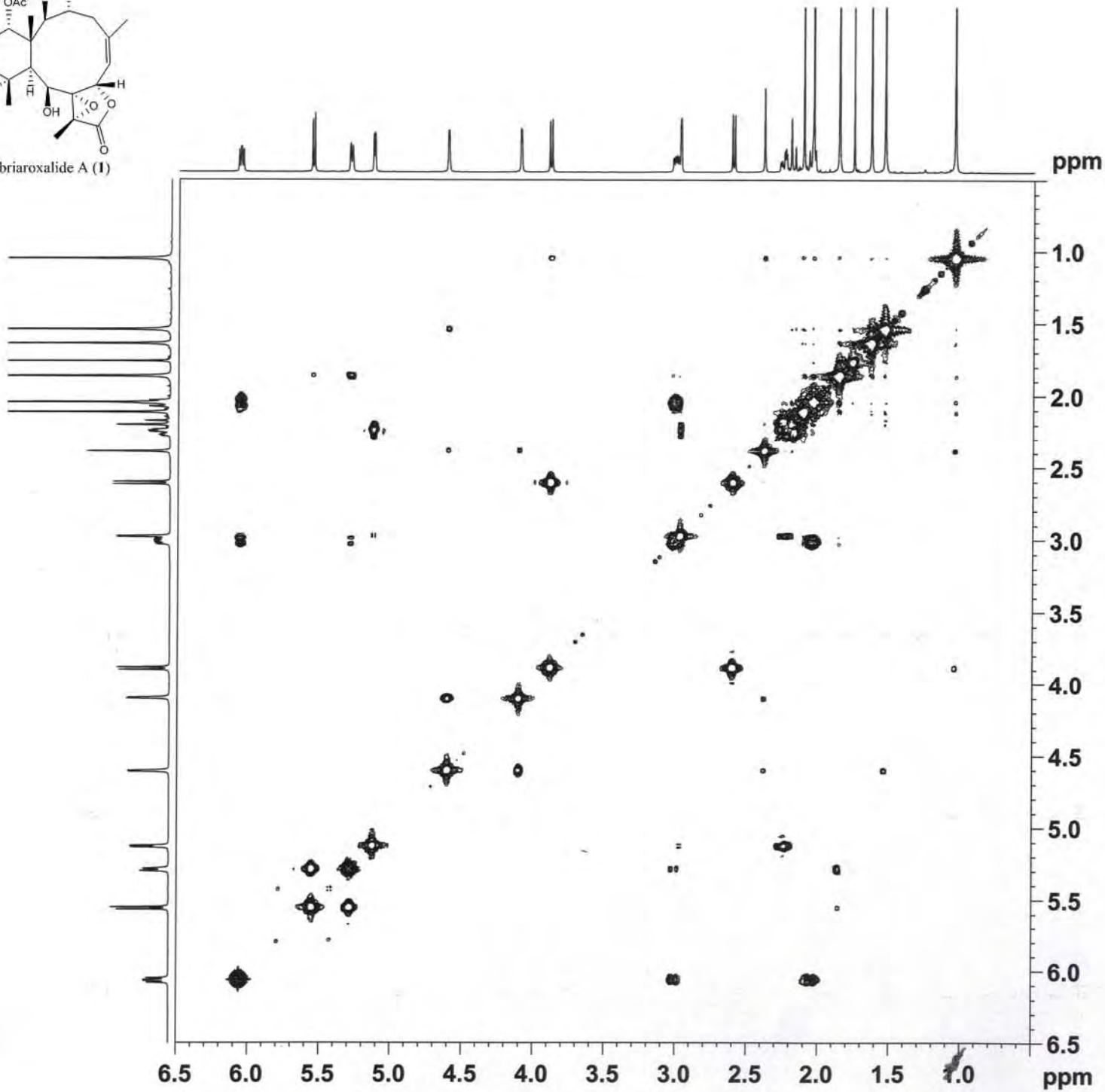
2.9407



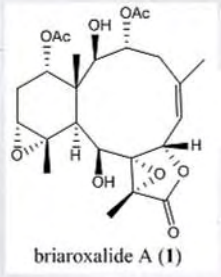
briaroxalide A (**1**)



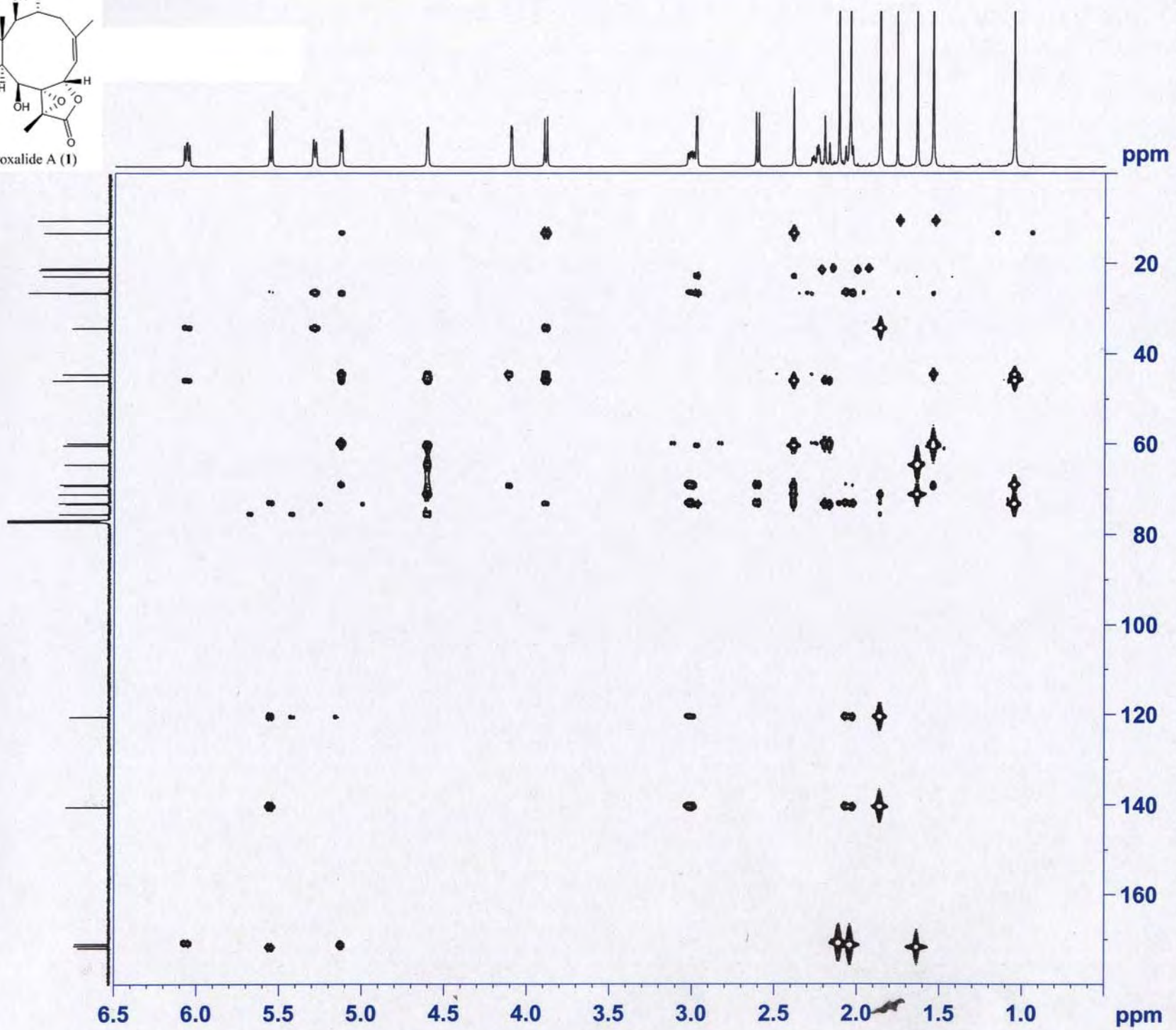
briaroxalide A (**1**)



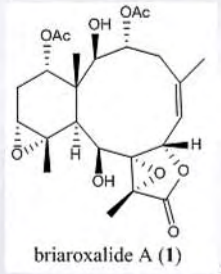
NAME	bsc119
EXPNO	11
PROCNO	1
Date_	20110725
Time	13.17
INSTRUM	AV600
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygpqf
TD	2048
SOLVENT	MeOD
NS	2
DS	8
SWH	6613.757 Hz
FIDRES	3.229373 Hz
AQ	0.1549544 sec
RG	40.3
DW	75.600 usec
DE	6.00 usec
TE	300.0 K
d0	0.00000300 sec
D1	2.00000000 sec
d13	0.00000400 sec
D16	0.00020000 sec
IN0	0.00015120 sec
======== CHANNEL f1 ========	
NUC1	1H
P0	10.20 usec
P1	10.20 usec
PL1	-4.10 dB
SFO1	600.1330006 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPZ1	10.00 %
GPZ2	10.00 %
P16	1000.00 usec
ND0	1
TD	256
SFO1	600.133 MHz
FIDRES	25.834988 Hz
SW	11.020 ppm
FnMODE	QF
SI	1024
SF	600.1300000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	600.1300000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0



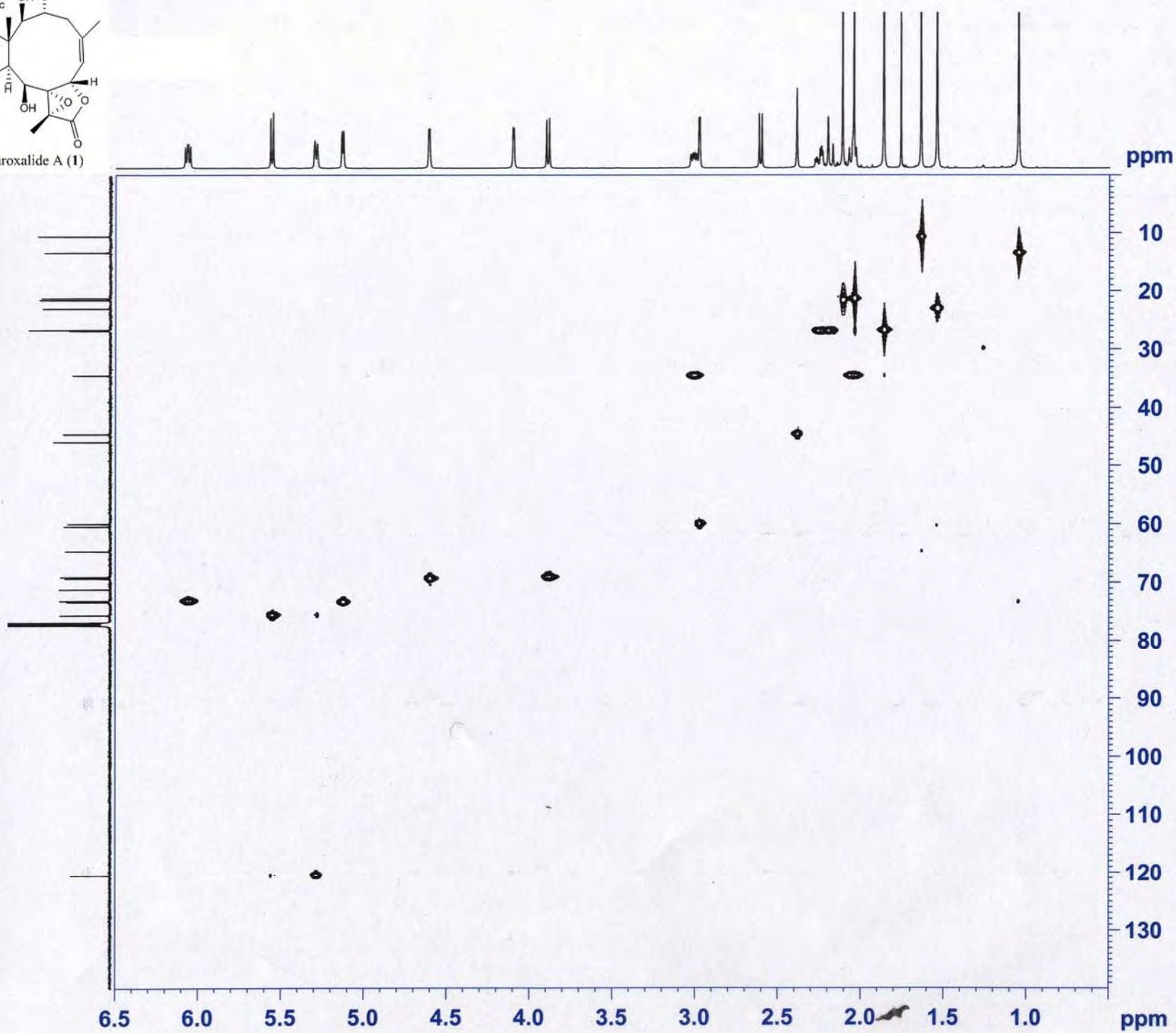
briaroxalide A (**1**)



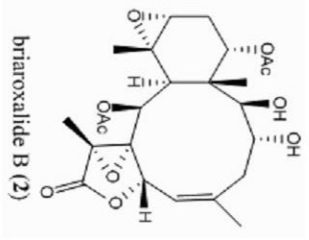
NAME	bsc119
EXPNO	14
PROCNO	1
Date_	20110725
Time	23.23
INSTRUM	AV600
PROBHD	5 mm CPTCI 1H-
PULPROG	hmbcgplpndqf
TD	2048
SOLVENT	CDCl3
NS	32
DS	16
SWH	6009.615 Hz
FIDRES	2.934382 Hz
AQ	0.1705268 sec
RG	16400
DW	83.200 usec
DE	6.00 usec
TE	300.0 K
CNST2	145.0000000
CNST13	8.0000000
d0	0.00000300 sec
D1	2.00000000 sec
d2	0.00344828 sec
d6	0.06250000 sec
D16	0.00020000 sec
IN0	0.00001505 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	10.20 usec
p2	20.40 usec
PL1	-4.10 dB
SFO1	600.1327006 MHz
======== CHANNEL f2 ========	
NUC2	13C
P3	15.50 usec
PL2	-4.80 dB
SFO2	150.9178993 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPNAM3	SINE.100
GPZ1	50.00 %
GPZ2	30.00 %
GPZ3	40.10 %
P16	1000.00 usec
ND0	2
TD	256
SFO1	150.9179 MHz
FIDRES	129.775742 Hz
SW	220.137 ppm
FnMODE	QF
SI	2048
SF	600.1300000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	150.9028090 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0



briaroxalide A (**1**)



NAME	bsc119
EXPNO	13
PROCNO	1
Date_	20110725
Time	20.55
INSTRUM	AV600
PROBHD	5 mm CPTCI 1H-
PULPROG	hsqcetgp
TD	2048
SOLVENT	CDCl3
NS	16
DS	16
SWH	7788.162 Hz
FIDRES	3.802814 Hz
AQ	0.1315958 sec
RG	10300
DW	64.200 usec
DE	6.00 usec
TE	300.0 K
CNST2	135.0000000
d0	0.00000300 sec
D1	2.00000000 sec
d4	0.00185185 sec
d11	0.03000000 sec
d13	0.00000400 sec
D16	0.00020000 sec
DELTA	0.00122640 sec
DELTA1	0.00084385 sec
IN0	0.00001950 sec
ST1CNT	0
ZGOPTNS	
======== CHANNEL f1 ========	
NUC1	1H
P1	10.20 usec
p2	20.40 usec
P28	0.00 usec
PL1	-4.10 dB
SFO1	600.1327006 MHz
======== CHANNEL f2 ========	
CPDPRG2	garp4
NUC2	13C
P3	15.50 usec
p4	31.00 usec
PCPD2	60.00 usec
PL2	-4.80 dB
PL12	6.96 dB
SFO2	150.9141267 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPZ1	80.00 %
GPZ2	20.10 %
P16	1000.00 usec
ND0	2
TD	256
SFO1	150.9141 MHz
FIDRES	100.160255 Hz
SW	169.905 ppm
FnMODE	Echo-Antiecho
SI	1024
SF	600.1300000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00
SI	1024
MC2	echo-antiecho
SF	150.9028090 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0



δ / ppm

7.2598

6.0619
6.0493
6.0435
6.0309

5.5471
5.5318

5.2810
5.2661

5.1174
5.1076

4.5939
4.5878

4.0849
4.0789

3.8816
3.8646

3.0112
3.0013
2.9876
2.9755
2.9636
2.9578

2.6001
2.5831

2.3721

2.2334
2.2231

2.2167
2.1843
2.1555
2.0962
2.0282
1.8480
1.7437
1.6229
1.5261

1.0338

1.0

1.0012

0.994

0.9973

0.9876

0.9579

0.9814

2.0139

0.979

0.9776

0.902

0.8648

3.0651

4.1108

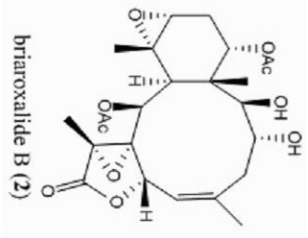
2.9093

1.1146

3.0747

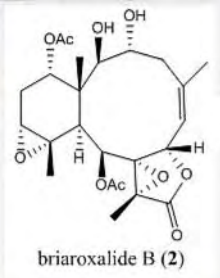
2.9821

2.9407

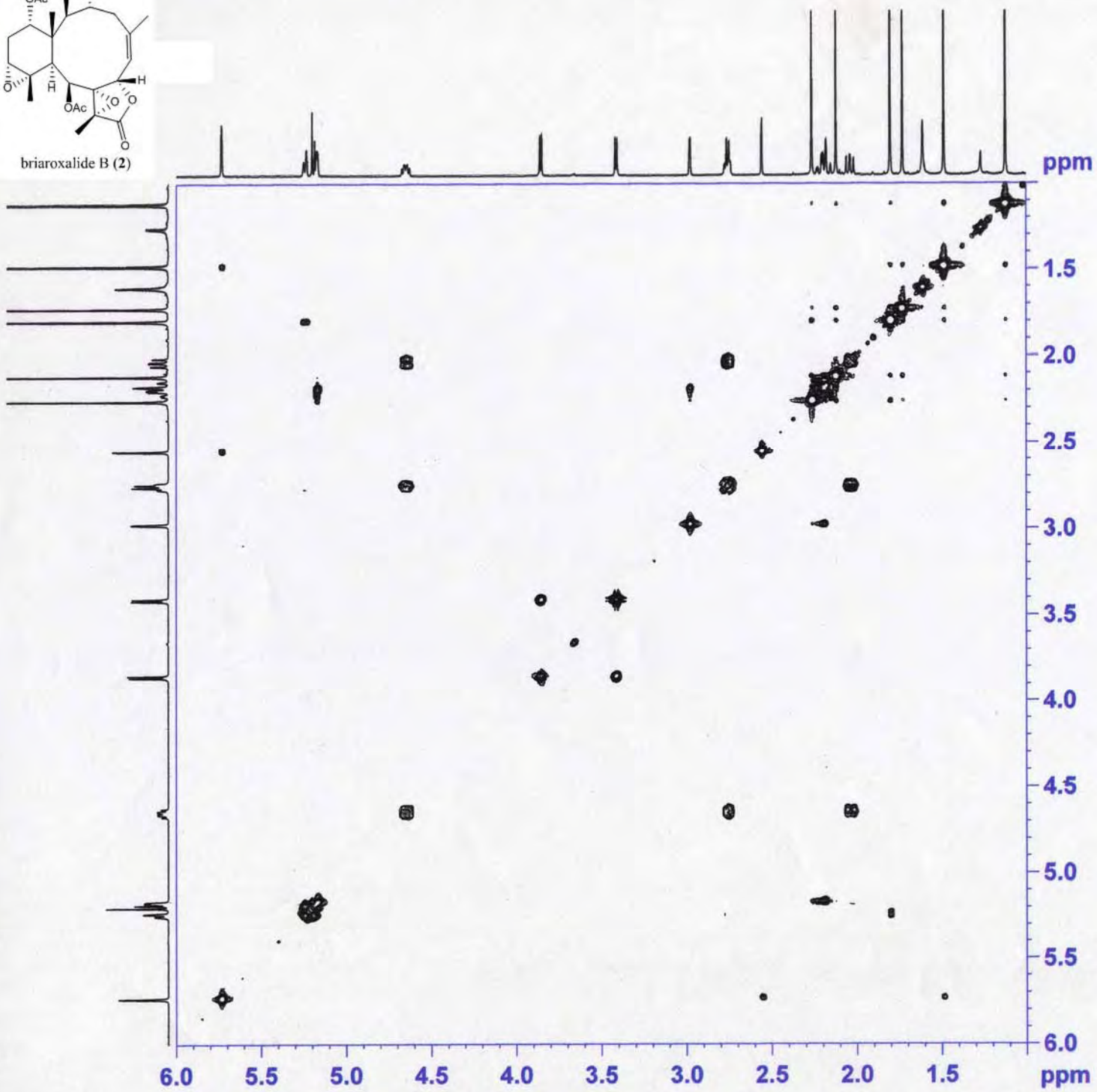


172.7189
170.3801
169.1198
141.2564
119.2635
77.2110
77.0000
76.7872
74.7303
73.7228
70.3219
68.8234
68.6397
68.4087
65.1424
59.7229
59.2664
46.1194
43.3842
39.3777
27.1728
26.3980
24.6812
21.2112
21.0839
13.7621
10.6031

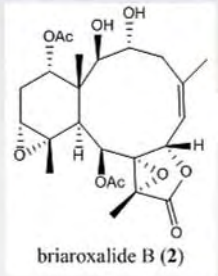
δ / ppm
160
140
120
100
80
60
40
20

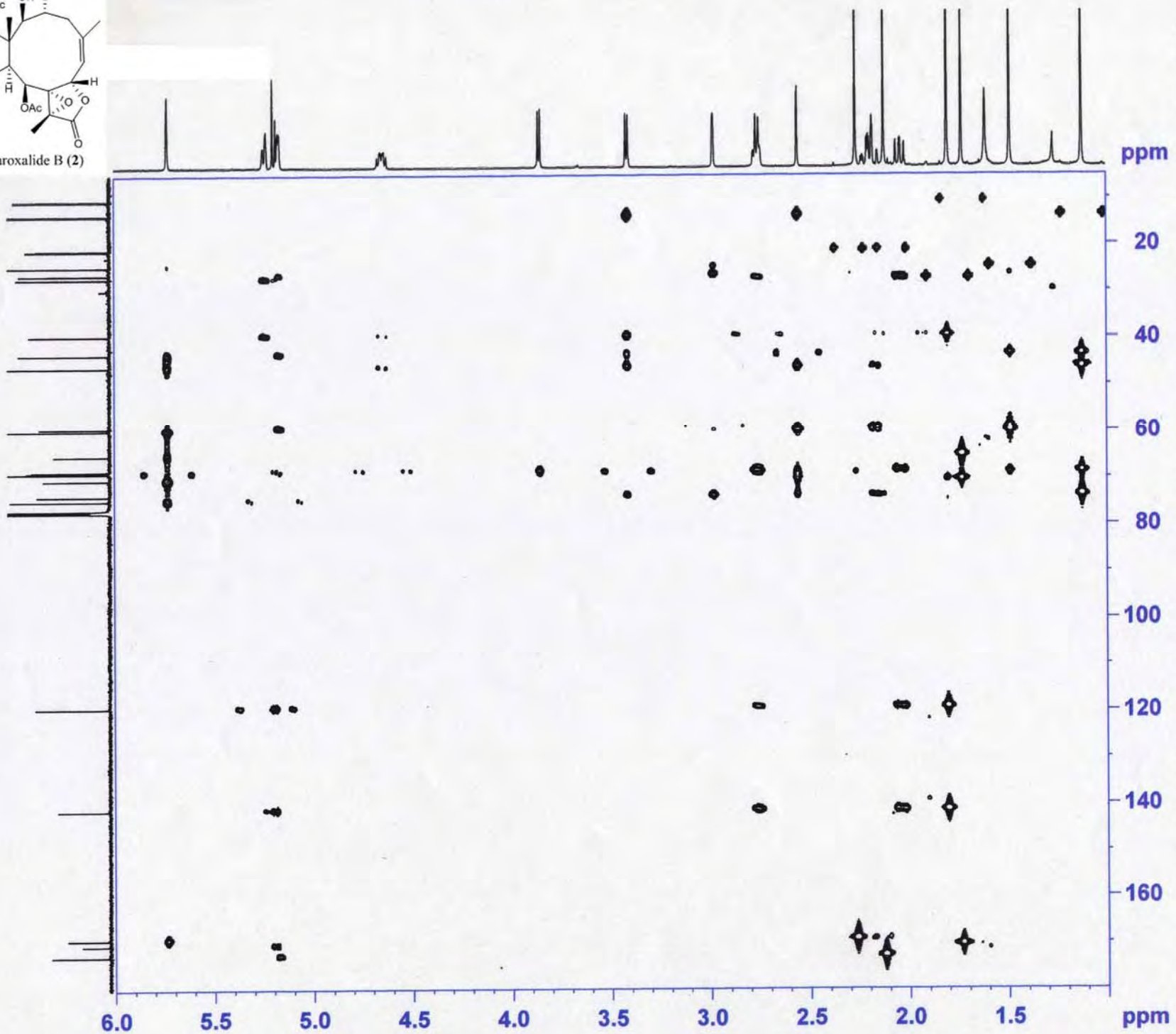


briaroxalide B (**2**)




```
Current Data Parameters
NAME                  sc117
EXPNO                    11
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110214
Time                 11.51
INSTRUM              AV600
PROBHD    5 mm CPTCI 1H-
PULPROG          cosygpqf
TD                   2048
SOLVENT              CDCl3
NS                      2
DS                      8
SWH               6009.615 Hz
FIDRES            2.934382 Hz
AQ                0.1705268 sec
RG                     90.5
DW                  83.200 usec
DE                   6.00 usec
TE                  300.0 K
d0              0.00000300 sec
D1              2.00000000 sec
d13             0.00000400 sec
D16             0.00020000 sec
IN0             0.00016640 sec

======== CHANNEL f1 ========
NUC1                    1H
P0                   10.00 usec
P1                   10.00 usec
PL1                  -4.10 dB
SFO1          600.1327006 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPZ1                10.00 %
GPZ2                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
ND0                     1
TD                    256
SFO1           600.1327 MHz
FIDRES        23.475060 Hz
SW              10.014 ppm
FnMODE                 QF

F2 - Processing parameters
SI                   1024
SF            600.1299811 MHz
WDW                  SINE
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.40

F1 - Processing parameters
SI                   1024
MC2                    QF
SF            600.1299811 MHz
WDW                  SINE
SSB                     0
LB                   0.00 Hz
GB                      0
```





Current Data Parameters
NAME sc117
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110214
Time 14.24
INSTRUM AV600
PROBHD 5 mm CPTCI 1H-
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 12
DS 16
SWH 6009.615 Hz
FIDRES 2.934382 Hz
AQ 0.1705268 sec
RG 20600
DW 83.200 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
CNST13 8.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d2 0.00344828 sec
d6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001440 sec

======== CHANNEL f1 ========
NUC1 1H
P1 9.80 usec
p2 19.60 usec
PL1 -3.60 dB
SFO1 600.1327006 MHz

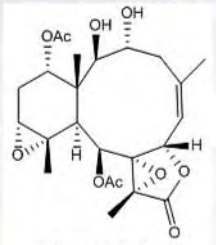
======== CHANNEL f2 ========
NUC2 13C
P3 15.40 usec
PL2 -6.00 dB
SFO2 150.9194083 MHz

====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

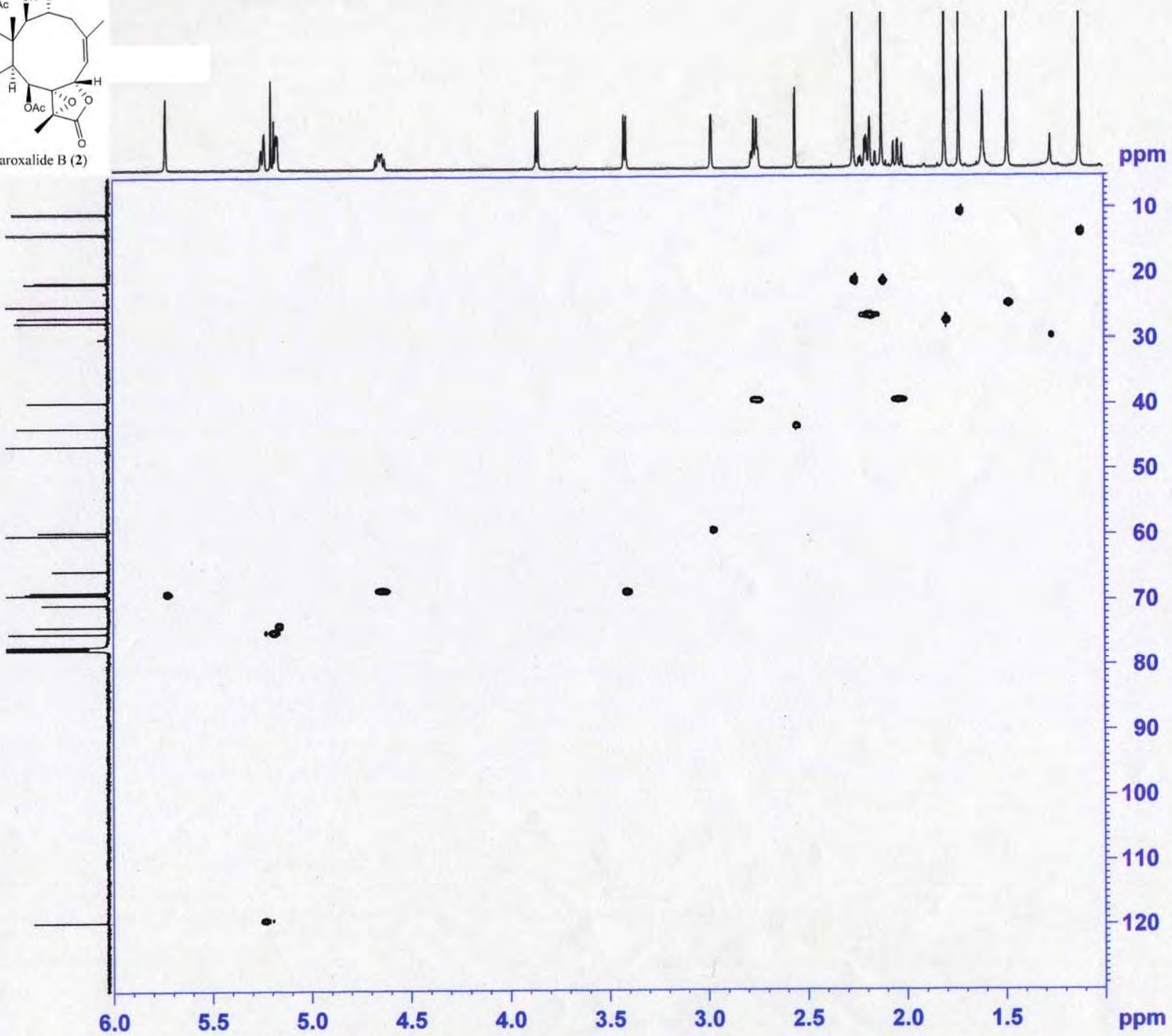
F1 - Acquisition parameters
ND0 2
TD 256
SFO1 150.9194 MHz
FIDRES 135.633682 Hz
SW 230.071 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

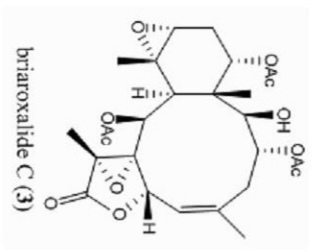
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028090 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0



briaroxalide B (**2**)




```
Current Data Parameters
NAME                  scl17
EXPNO                    13
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110214
Time                 13.28
INSTRUM              AV600
PROBHD   5 mm CPTCI 1H-
PULPROG           hsqcetgp
TD                    2048
SOLVENT               CDCl3
NS                        6
DS                       16
SWH                7788.162 Hz
FIDRES             3.802814 Hz
AQ                 0.1315958 sec
RG                    20600
DW                   64.200 usec
DE                    6.00 usec
TE                   300.0 K
CNST2             135.0000000
d0                 0.00000300 sec
D1                 2.00000000 sec
d4                 0.00185185 sec
d11                0.03000000 sec
d13                0.00000400 sec
D16                0.00020000 sec
DELTA              0.00122600 sec
DELTA1             0.00084385 sec
IN0                0.00002070 sec
ST1CNT                   128
ZGOPTNS

======== CHANNEL f1 ========
NUC1                     1H
P1                    10.00 usec
p2                    20.00 usec
P28                    0.00 usec
PL1                   -4.10 dB
SFO1           600.1327006 MHz

======== CHANNEL f2 ========
CPDPRG2                garp4
NUC2                     13C
P3                    15.50 usec
p4                    31.00 usec
PCPD2                 60.00 usec
PL2                   -4.80 dB
PL12                   6.96 dB
SFO2           150.9141267 MHz

====== GRADIENT CHANNEL =====
GPNAM1              SINE.100
GPNAM2              SINE.100
GPZ1                  80.00 %
GPZ2                  20.10 %
P16                 1000.00 usec

F1 - Acquisition parameters
ND0                       2
TD                      256
SFO1           150.9141 MHz
FIDRES          94.353867 Hz
SW                160.055 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                     1024
SF           600.1300000 MHz
WDW                   QSINE
SSB                       2
LB                    0.00 Hz
GB                        0
PC                    1.00

F1 - Processing parameters
SI                     1024
MC2         echo-antiecho
SF           150.9028090 MHz
WDW                   QSINE
SSB                       2
LB                    0.00 Hz
GB                        0
```



7.2597

5.7113
5.6991
5.6931
5.6806
5.6418

5.3000
5.2851
5.2758

5.1372
5.1284

3.9254

3.0544
3.0421
3.0309
3.0186
2.9395
2.9340

2.6129
2.6110

2.2527
2.2217
2.1821
2.1184
2.0395

1.8603

1.7260

1.3976

0.9512

1.0102

2.0977

1.0065

0.9762

1.0251

1.0376

0.9638

1.0594

3.5074

3.143

3.2815

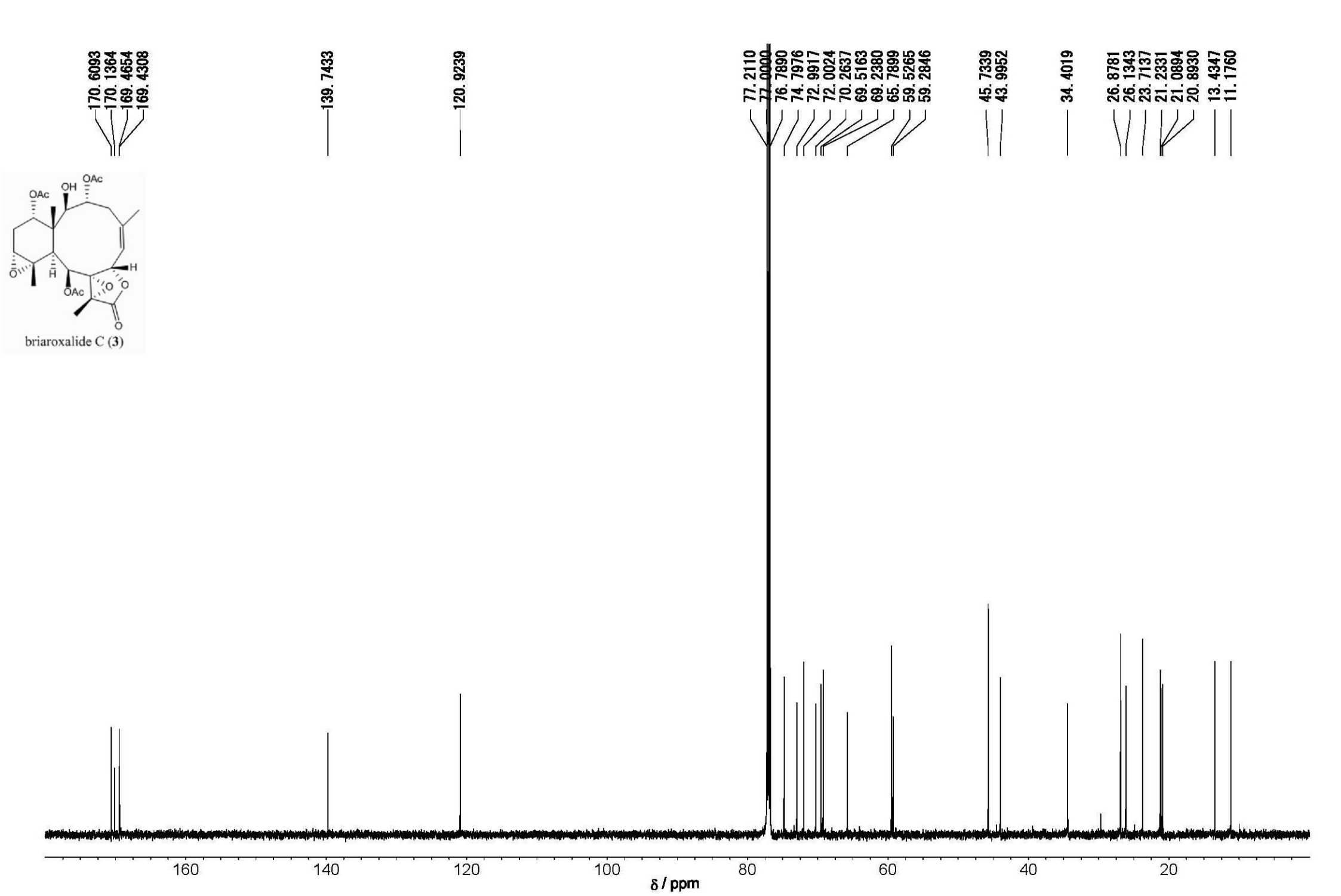
2.9797

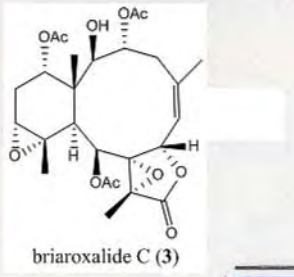
2.9409

2.8703

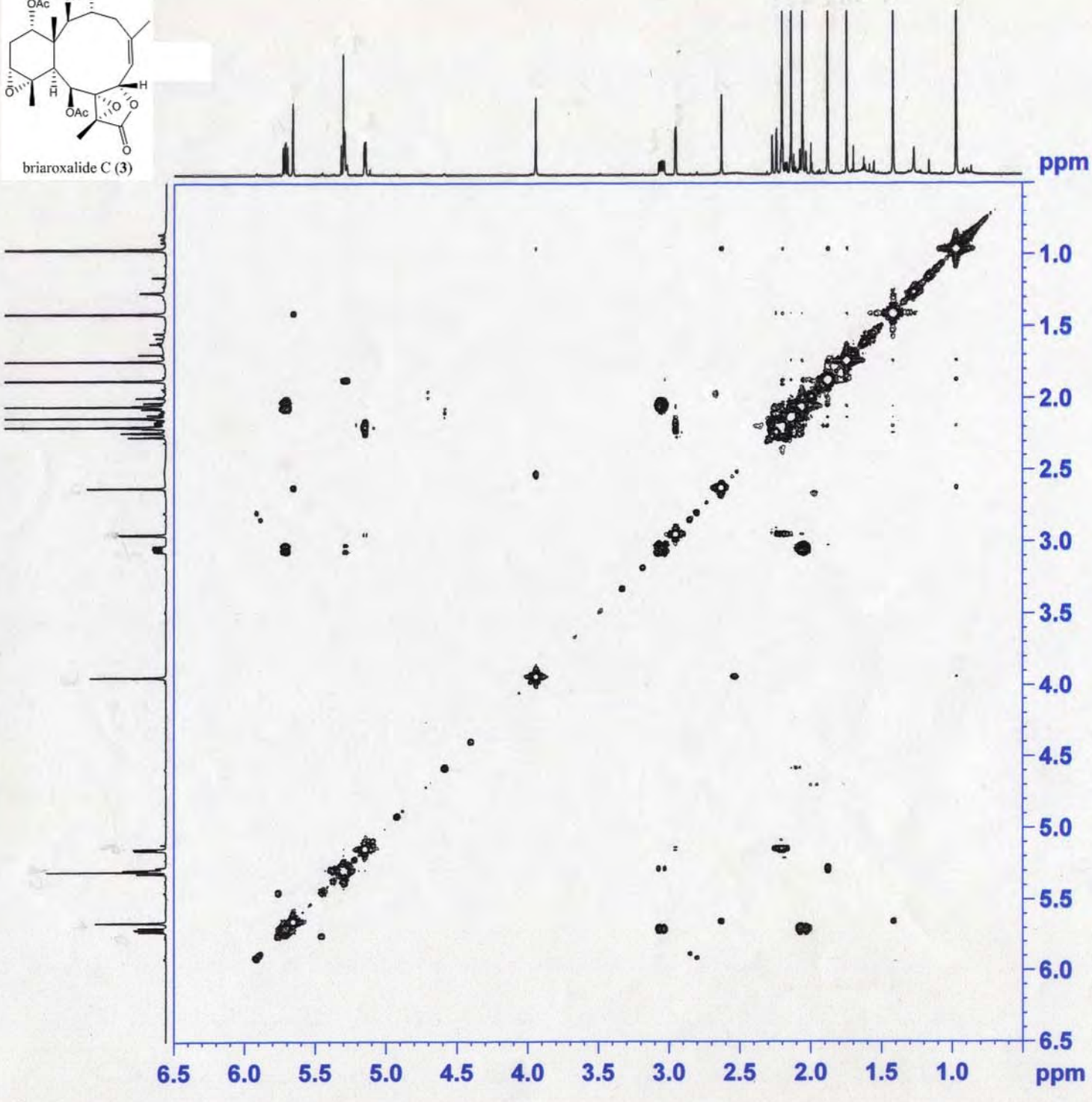
2.9175

δ / ppm

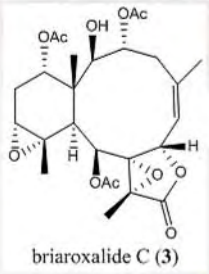

170.6093
170.1364
169.4654
169.4308
139.7433
120.9239
77.2110
77.0000
76.7890
74.7976
72.9917
72.0024
70.2637
69.5163
69.2380
65.7899
59.5265
59.2846
45.7339
43.9952
34.4019
26.8781
26.1343
23.7137
21.2331
21.0894
20.8930
13.4347
11.1760
OAc
OH
OAc
OAc
H
H
O
O
O
O
briaroxalide C (3)
160
140
120
100
80
60
40
20
δ / ppm



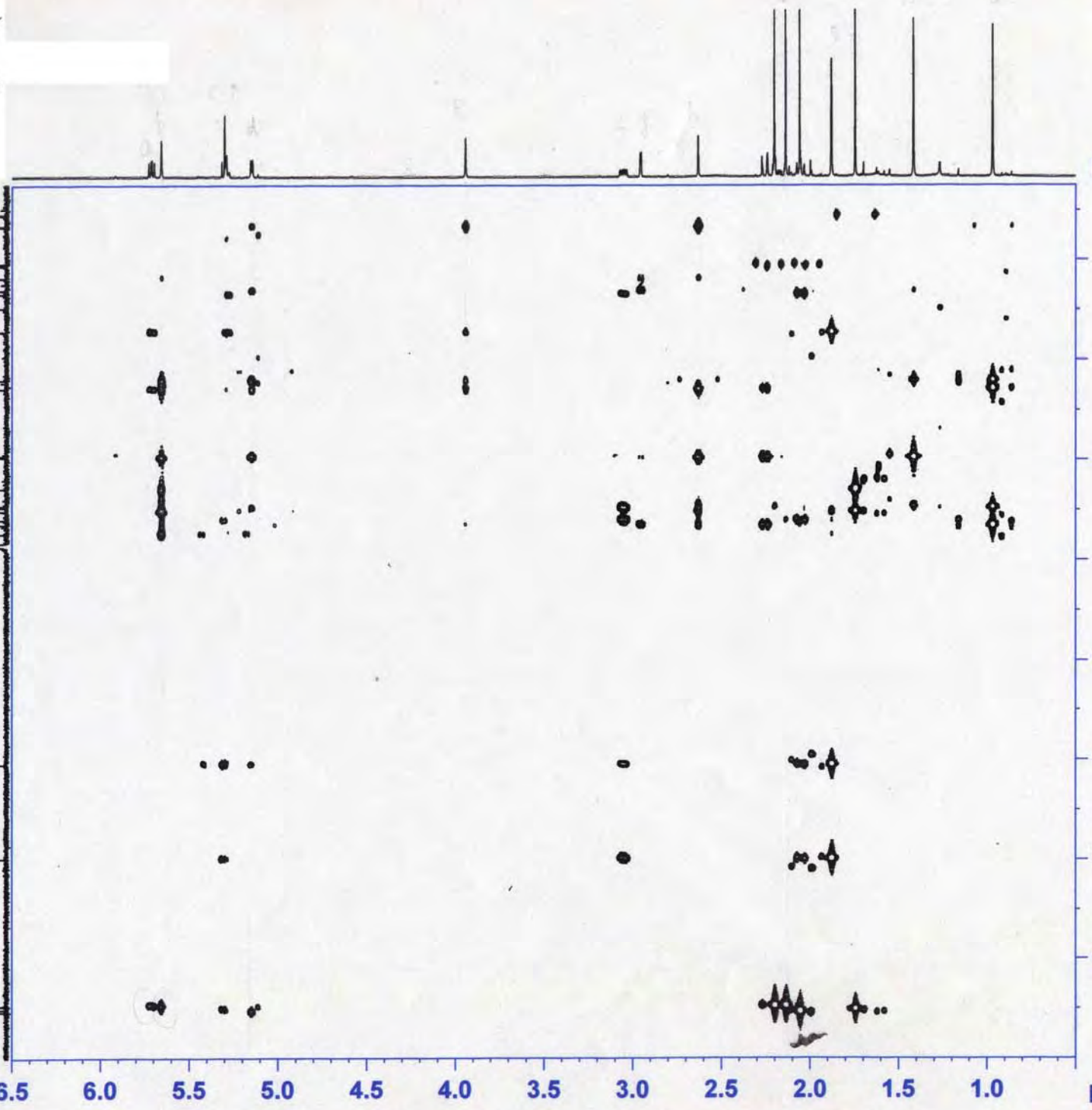
briaroxalide C (**3**)




```
Current Data Parameters
NAME                  sc82
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20110117
Time                  13.41
INSTRUM               AV600
PROBHD   5 mm CPTCI 1H-
PULPROG           cosygpqf
TD                    2048
SOLVENT               MeOD
NS                       2
DS                       8
SWH                6613.757 Hz
FIDRES             3.229373 Hz
AQ                0.1549544 sec
RG                     80.6
DW                  75.600 usec
DE                   6.00 usec
TE                   300.0 K
d0              0.00000300 sec
D1              2.00000000 sec
d13             0.00000400 sec
D16             0.00020000 sec
IN0             0.00015120 sec

======== CHANNEL f1 ========
NUC1                    1H
P0                   10.20 usec
P1                   10.20 usec
PL1                  -4.10 dB
SFO1          600.1330006 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPZ1                10.00 %
GPZ2                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
ND0                      1
TD                     256
SFO1             600.133 MHz
FIDRES         25.834988 Hz
SW                 11.020 ppm
FnMODE                  QF

F2 - Processing parameters
SI                    1024
SF            600.1300000 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF            600.1300000 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
```

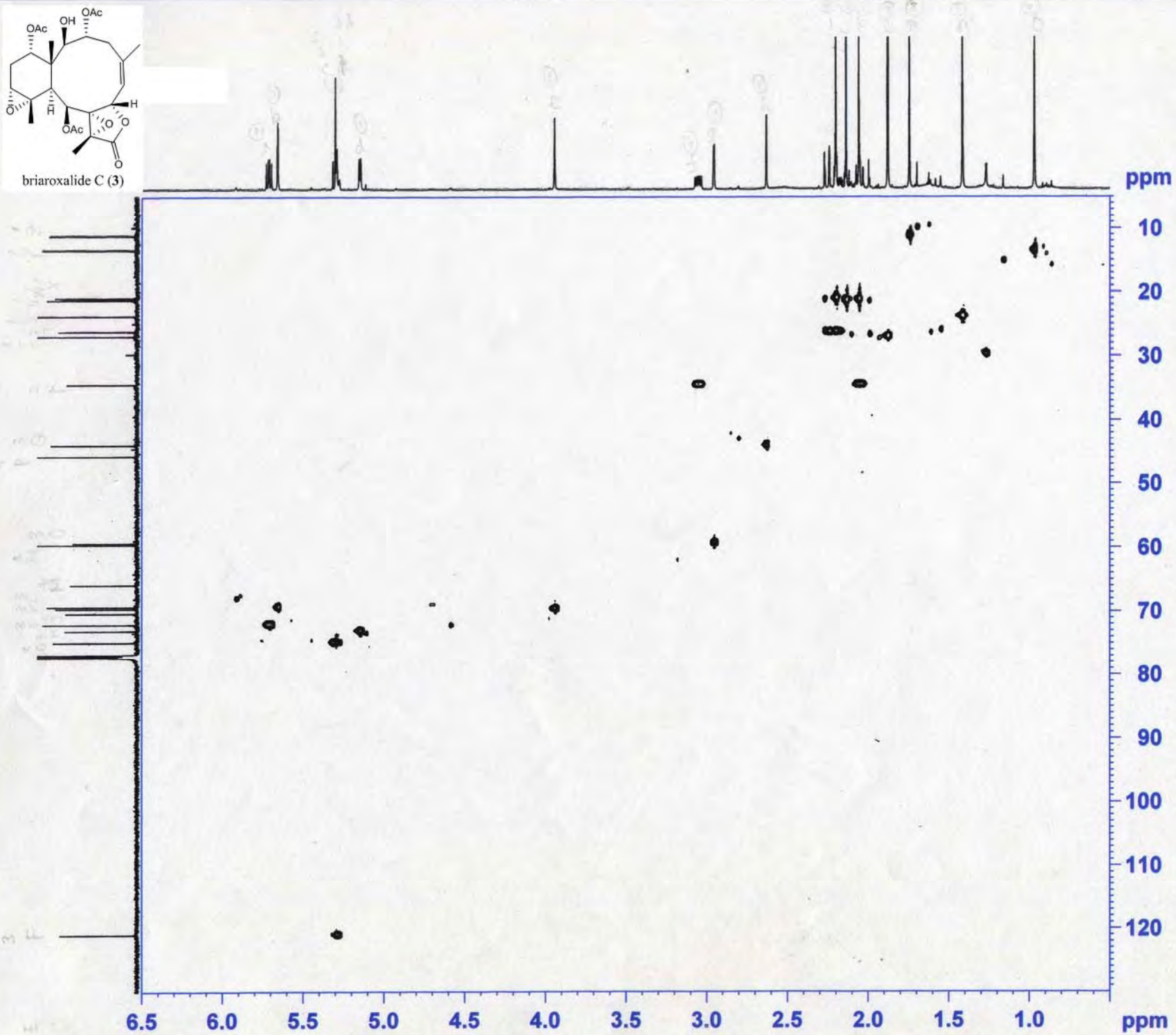


briaroxalide C (**3**)

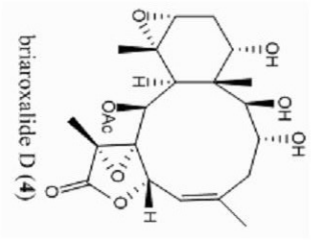



```
Current Data Parameters
NAME                  sc82
EXPNO                   14
PROCNO                   1

F2 - Acquisition Parameters
Date_              20110117
Time                 11.07
INSTRUM              AV600
PROBHD    5 mm CPTCI 1H-
PULPROG     hmbcgplpndqf
TD                    2048
SOLVENT               CDCl3
NS                      16
DS                      16
SWH               6009.615 Hz
FIDRES            2.934382 Hz
AQ                0.1705268 sec
RG                    16400
DW                 83.200 usec
DE                  6.00 usec
TE                  300.0 K
CNST2           145.0000000
CNST13            8.0000000
d0                0.00000300 sec
D1                2.00000000 sec
d2                0.00344828 sec
d6                0.06250000 sec
D16               0.00020000 sec
IN0               0.00001505 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                  10.20 usec
p2                  20.40 usec
PL1                 -4.10 dB
SFO1           600.1327006 MHz

======== CHANNEL f2 ========
NUC2                   13C
P3                  15.50 usec
PL2                 -4.80 dB
SFO2           150.9178993 MHz

====== GRADIENT CHANNEL =====
GPNAM1            SINE.100
GPNAM2            SINE.100
GPNAM3            SINE.100
GPZ1                50.00 %
GPZ2                30.00 %
GPZ3                40.10 %
P16               1000.00 usec

F1 - Acquisition parameters
ND0                     2
TD                    256
SFO1           150.9179 MHz
FIDRES         129.775742 Hz
SW               220.137 ppm
FnMODE                 QF

F2 - Processing parameters
SI                    2048
SF           600.1300000 MHz
WDW                   SINE
SSB                      0
LB                  0.00 Hz
GB                       0
PC                   1.40

F1 - Processing parameters
SI                    1024
MC2                    QF
SF           150.9028090 MHz
WDW                   SINE
SSB                      0
LB                  0.00 Hz
GB                       0
```

briaroxalide C (**3**)




```
Current Data Parameters
NAME                  sc82
EXPNO                   13
PROCNO                   1

F2 - Acquisition Parameters
Date_              20110117
Time                  9.52
INSTRUM              AV600
PROBHD    5 mm CPTCI 1H-
PULPROG           hsqcetgp
TD                    2048
SOLVENT               CDCl3
NS                       8
DS                      16
SWH                7788.162 Hz
FIDRES             3.802814 Hz
AQ                 0.1315958 sec
RG                     11500
DW                    64.200 usec
DE                     6.00 usec
TE                    300.0 K
CNST2          135.0000000
d0               0.00000300 sec
D1               2.00000000 sec
d4               0.00185185 sec
d11              0.03000000 sec
d13              0.00000400 sec
D16              0.00020000 sec
DELTA            0.00122640 sec
DELTA1           0.00084385 sec
IN0              0.00001950 sec
ST1CNT                  128
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                    10.20 usec
p2                    20.40 usec
P28                    0.00 usec
PL1                   -4.10 dB
SFO1           600.1327006 MHz

======== CHANNEL f2 ========
CPDPRG2               garp4
NUC2                    13C
P3                    15.50 usec
p4                    31.00 usec
PCPD2                 60.00 usec
PL2                   -4.80 dB
PL12                   6.96 dB
SFO2           150.9141267 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPZ1                  80.00 %
GPZ2                  20.10 %
P16                 1000.00 usec

F1 - Acquisition parameters
ND0                      2
TD                     256
SFO1           150.9141 MHz
FIDRES         100.160255 Hz
SW                 169.905 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                    1024
SF             600.1300000 MHz
WDW                  QSINE
SSB                      2
LB                    0.00 Hz
GB                       0
PC                    1.00

F1 - Processing parameters
SI                    1024
MC2          echo-antiecho
SF             150.9028090 MHz
WDW                  QSINE
SSB                      2
LB                    0.00 Hz
GB                       0
```

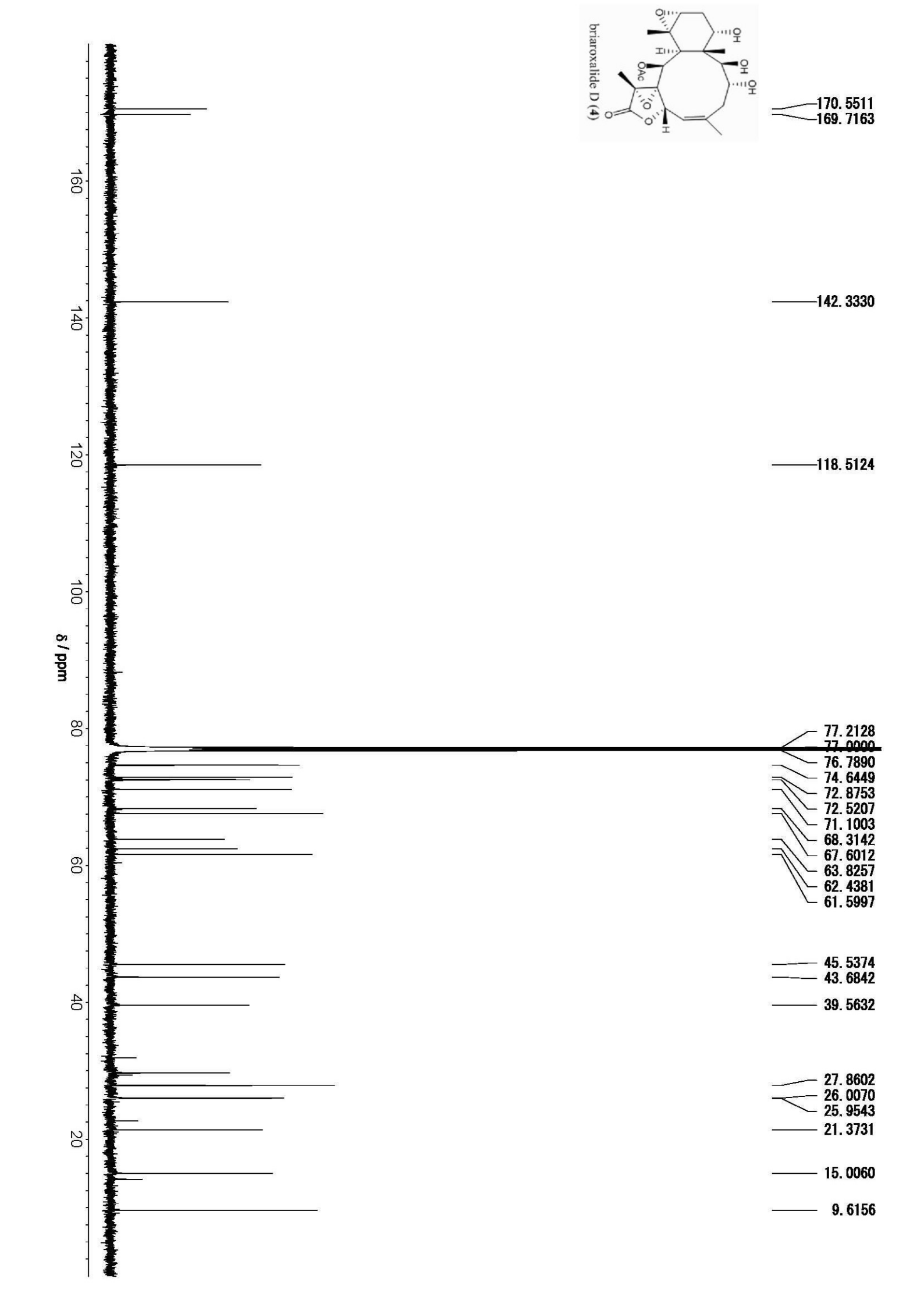


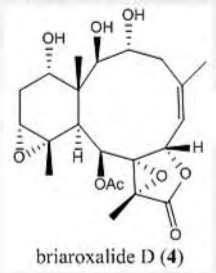
δ / ppm

1 2 3 4 5 6 7

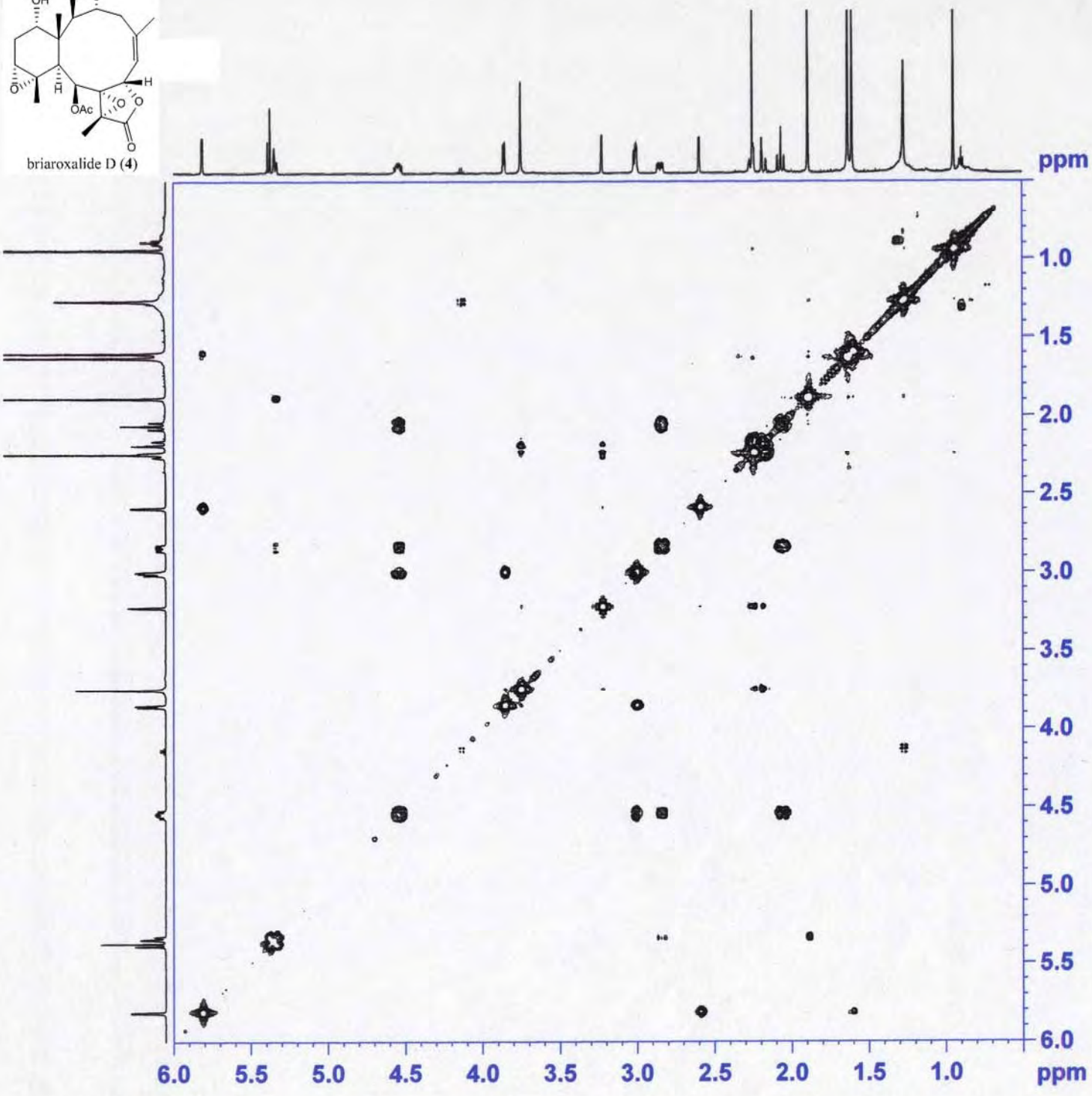
1.0
2.0781
1.0152
0.9953
1.8916
0.9913
1.7608
0.996
0.9785
3.9234
0.962
1.0763
2.8876
7.968
2.8208

7.2600
5.7996
5.7944
5.3727
5.3567
5.3299
5.3140
4.5506
4.5346
4.5236
4.5038
3.8447
3.8349
3.7333
3.2067
2.9993
2.9892
2.9834
2.8429
2.8350
2.8193
2.8116
2.5773
2.5721
2.2502
2.2315
2.2252
2.1711
2.1438
2.0669
2.0444
2.0236
1.8724
1.8709
1.6135
1.5858
0.9295
0.0673

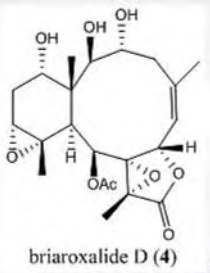

briaroxalide D (4)
170.5511
169.7163
142.3330
118.5124
77.2128
77.0000
76.7890
74.6449
72.8753
72.5207
71.1003
68.3142
67.6012
63.8257
62.4381
61.5997
45.5374
43.6842
39.5632
27.8602
26.0070
25.9543
21.3731
15.0060
9.6156
δ / ppm
160
140
120
100
80
60
40
20



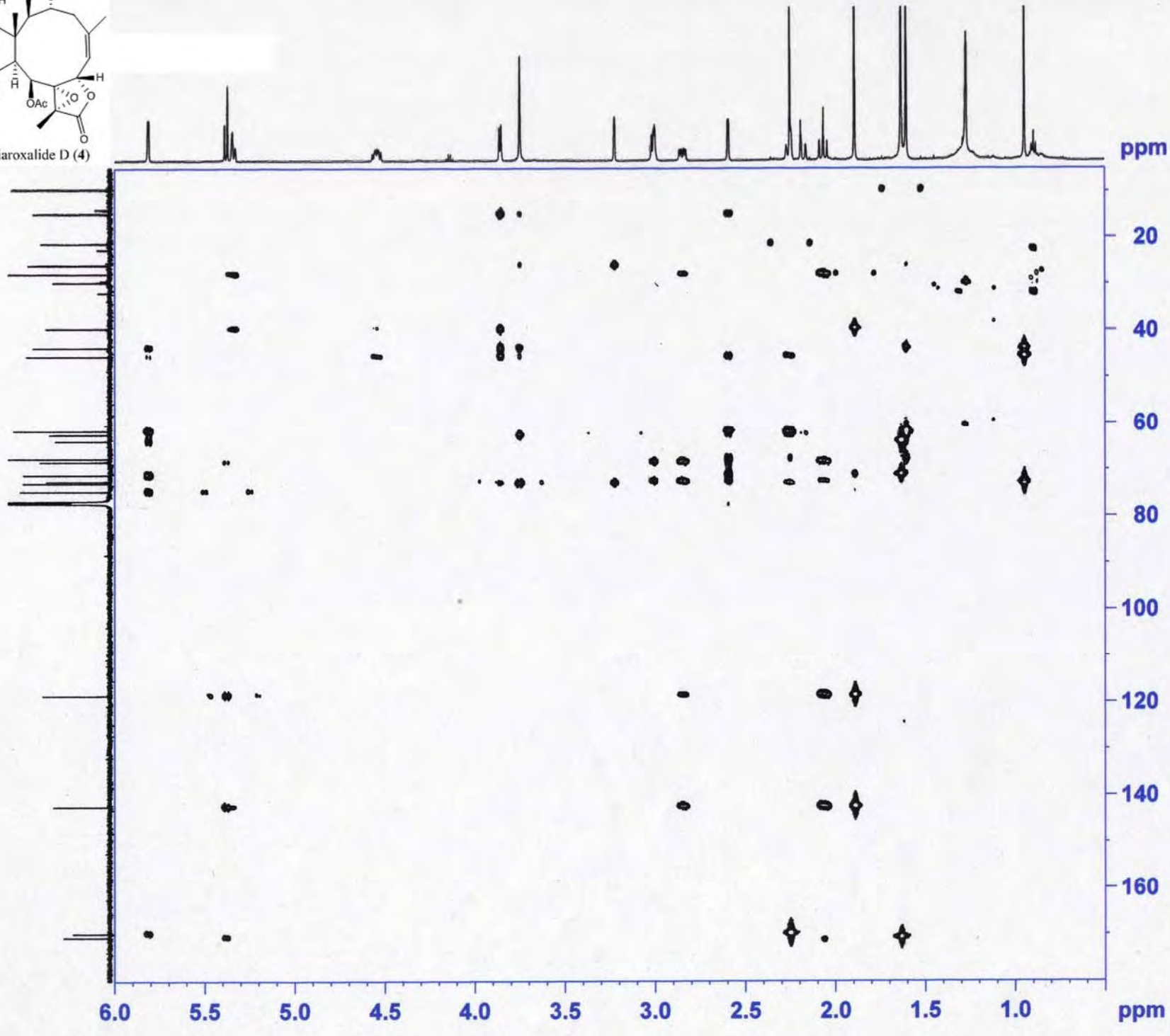
briaroxalide D (**4**)



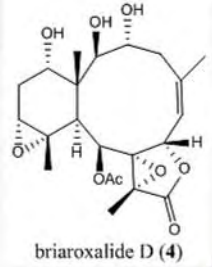

```
Current Data Parameters
NAME                  sc132
EXPNO                    11
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110222
Time                  13.38
INSTRUM                AV600
PROBHD    5 mm CPTCI 1H-
PULPROG           cosygpqf
TD                     2048
SOLVENT                MeOD
NS                        2
DS                        8
SWH                6613.757 Hz
FIDRES             3.229373 Hz
AQ                 0.1549544 sec
RG                      144
DW                   75.600 usec
DE                    6.00 usec
TE                   300.0 K
d0                0.00000300 sec
D1                2.00000000 sec
d13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00015120 sec

======== CHANNEL f1 ========
NUC1                      1H
P0                    10.20 usec
P1                    10.20 usec
PL1                   -4.10 dB
SFO1           600.1330006 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPZ1                 10.00 %
GPZ2                 10.00 %
P16                1000.00 usec

F1 - Acquisition parameters
ND0                       1
TD                      256
SFO1             600.133 MHz
FIDRES          25.834988 Hz
SW                 11.020 ppm
FnMODE                 QF

F2 - Processing parameters
SI                     1024
SF             600.1300000 MHz
WDW                    SINE
SSB                       0
LB                    0.00 Hz
GB                        0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2                    QF
SF             600.1300000 MHz
WDW                    SINE
SSB                       0
LB                    0.00 Hz
GB                        0
```



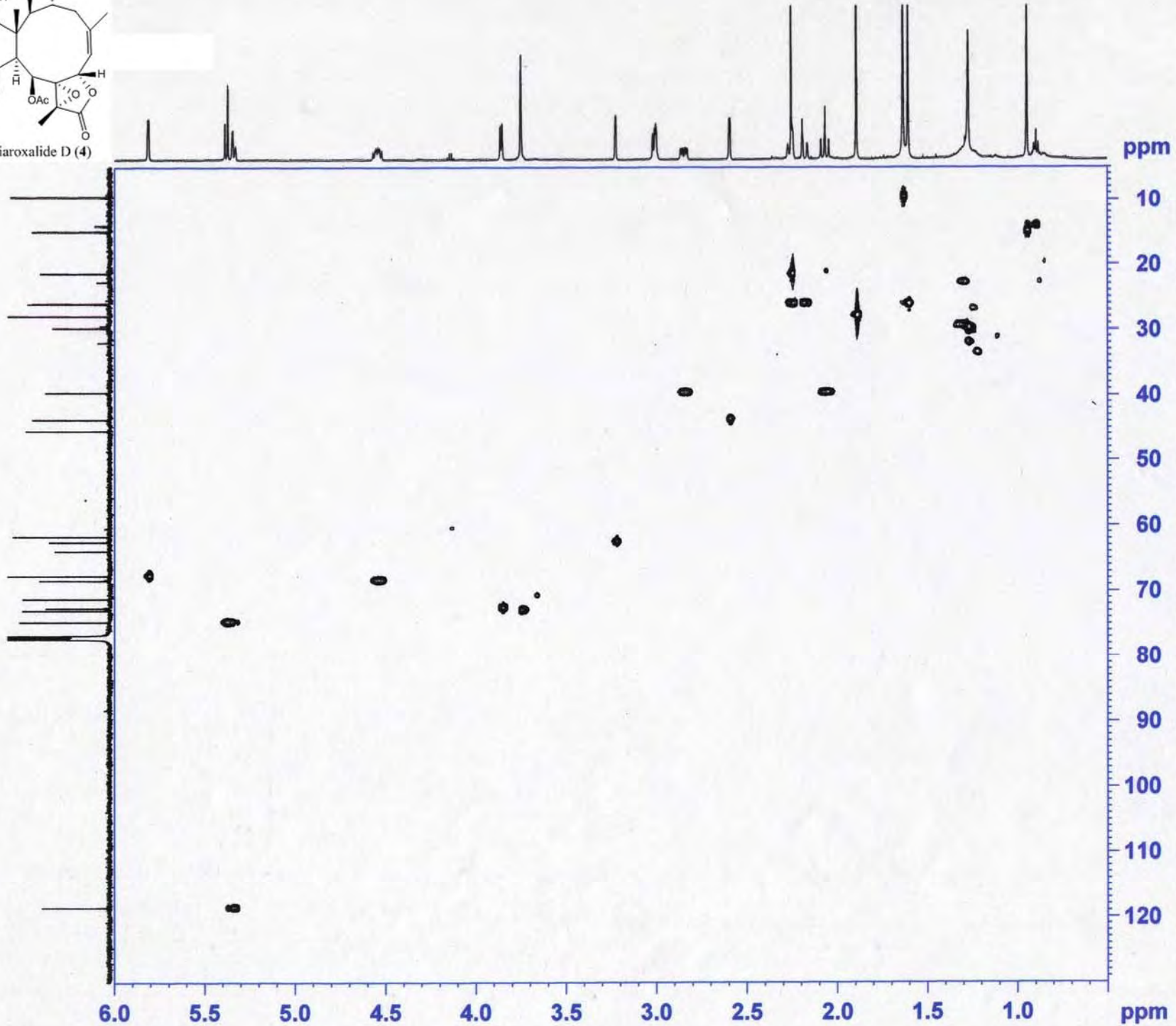
briaroxalide D (**4**)



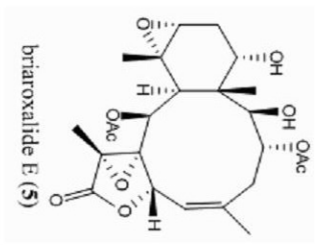

```
Current Data Parameters
NAME                  sc132
EXPNO                    14
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110222
Time               17.18
INSTRUM            AV600
PROBHD    5 mm CPTCI 1H-
PULPROG    hmbcgplpndqf
TD                   2048
SOLVENT              CDCl3
NS                     32
DS                     16
SWH              6009.615 Hz
FIDRES           2.934382 Hz
AQ               0.1705268 sec
RG                   26000
DW                83.200 usec
DE                 6.00 usec
TE                 300.0 K
CNST2          145.0000000
CNST13           8.0000000
d0               0.00000300 sec
D1               2.00000000 sec
d2               0.00344828 sec
d6               0.06250000 sec
D16              0.00020000 sec
IN0              0.00001505 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                10.20 usec
p2                20.40 usec
PL1               -4.10 dB
SFO1         600.1327006 MHz

======== CHANNEL f2 ========
NUC2                  13C
P3                15.50 usec
PL2               -4.80 dB
SFO2         150.9178993 MHz

======= GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPNAM3          SINE.100
GPZ1              50.00 %
GPZ2              30.00 %
GPZ3              40.10 %
P16             1000.00 usec

F1 - Acquisition parameters
ND0                    2
TD                   256
SFO1         150.9179 MHz
FIDRES       129.775742 Hz
SW           220.137 ppm
FnMODE                 QF

F2 - Processing parameters
SI                  2048
SF           600.1300000 MHz
WDW                 SINE
SSB                    0
LB                0.00 Hz
GB                     0
PC                 1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           150.9028090 MHz
WDW                 SINE
SSB                    0
LB                0.00 Hz
GB                     0
```



briaroxalide D (**4**)




```
Current Data Parameters
NAME                  sc132
EXPNO                    13
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110222
Time                  14.50
INSTRUM               AV600
PROBHD   5 mm CPTCI 1H-
PULPROG            hsqcetgp
TD                     2048
SOLVENT               CDCl3
NS                       16
DS                       16
SWH                7788.162 Hz
FIDRES             3.802814 Hz
AQ                 0.1315958 sec
RG                     26000
DW                  64.200 usec
DE                   6.00 usec
TE                   300.0 K
CNST2            135.0000000
d0                0.00000300 sec
D1                2.00000000 sec
d4                0.00185185 sec
d11               0.03000000 sec
d13               0.00000400 sec
D16               0.00020000 sec
DELTA             0.00122640 sec
DELTA1            0.00084385 sec
IN0               0.00001950 sec
ST1CNT                  128
ZGOPTNS

======== CHANNEL f1 =========
NUC1                     1H
P1                   10.20 usec
p2                   20.40 usec
P28                   0.00 usec
PL1                  -4.10 dB
SFO1           600.1327006 MHz

======== CHANNEL f2 =========
CPDPRG2                garp4
NUC2                     13C
P3                   15.50 usec
p4                   31.00 usec
PCPD2                60.00 usec
PL2                  -4.80 dB
PL12                  6.96 dB
SFO2           150.9141267 MHz

====== GRADIENT CHANNEL =====
GPNAM1              SINE.100
GPNAM2              SINE.100
GPZ1                 80.00 %
GPZ2                 20.10 %
P16                1000.00 usec

F1 - Acquisition parameters
ND0                       2
TD                      256
SFO1           150.9141 MHz
FIDRES         100.160255 Hz
SW                169.905 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                     1024
SF           600.1300000 MHz
WDW                   QSINE
SSB                       2
LB                   0.00 Hz
GB                        0
PC                    1.00

F1 - Processing parameters
SI                     1024
MC2         echo-antiecho
SF           150.9028090 MHz
WDW                   QSINE
SSB                       2
LB                   0.00 Hz
GB                        0
```



δ / ppm

7.2603

1.0
0.9978
1.0108
0.938

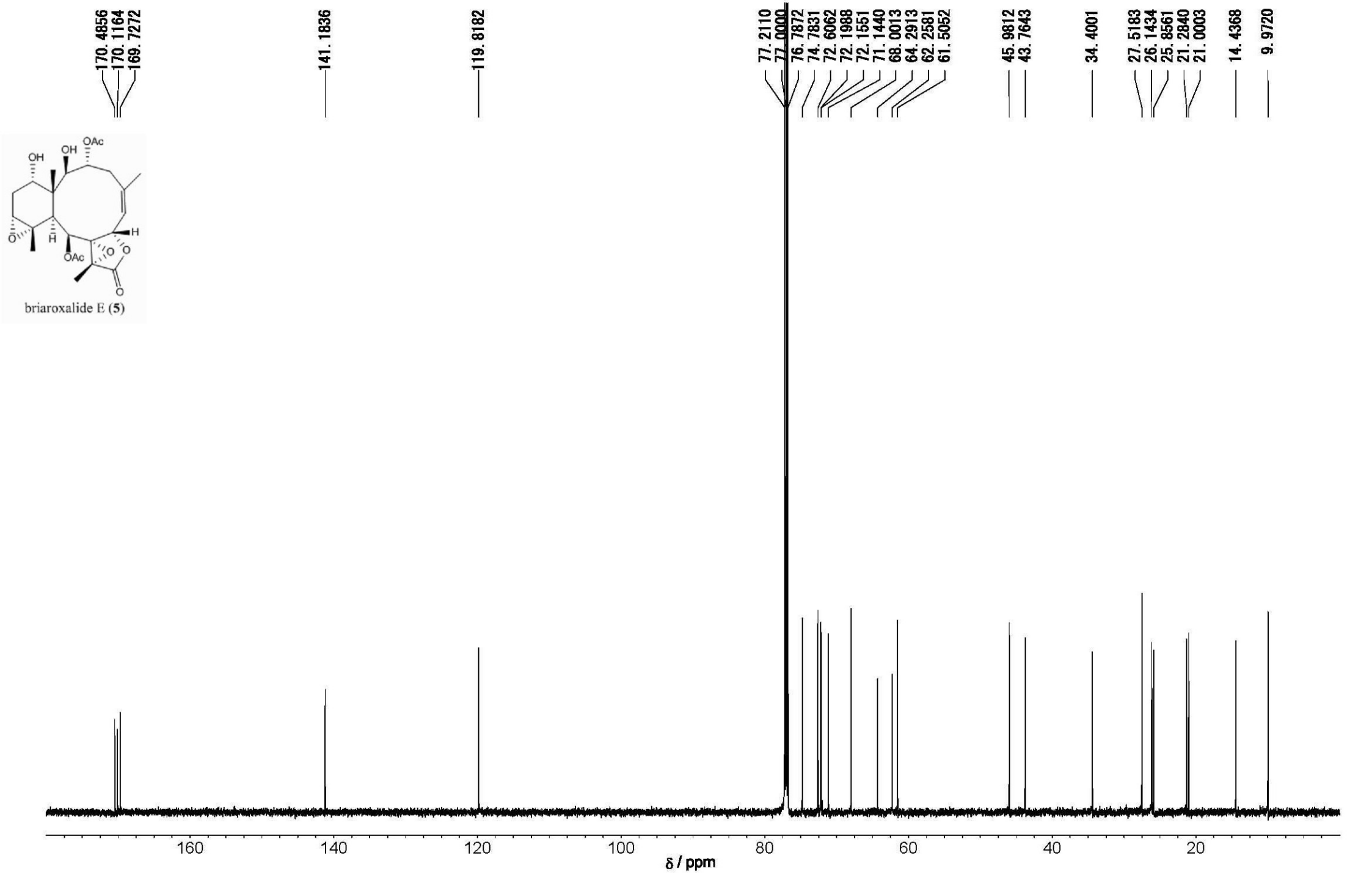
5.8251
5.6168
5.6009
5.5491
5.5387
5.5293
5.5187
5.3594
5.3436

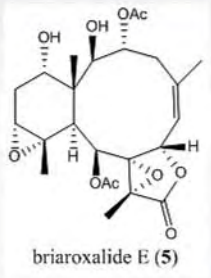
1.0211
1.0226
0.9441
1.0186
1.0024
0.8193
0.9792
0.9868
3.1834
2.9731
2.8124
2.9196
2.9285

4.328

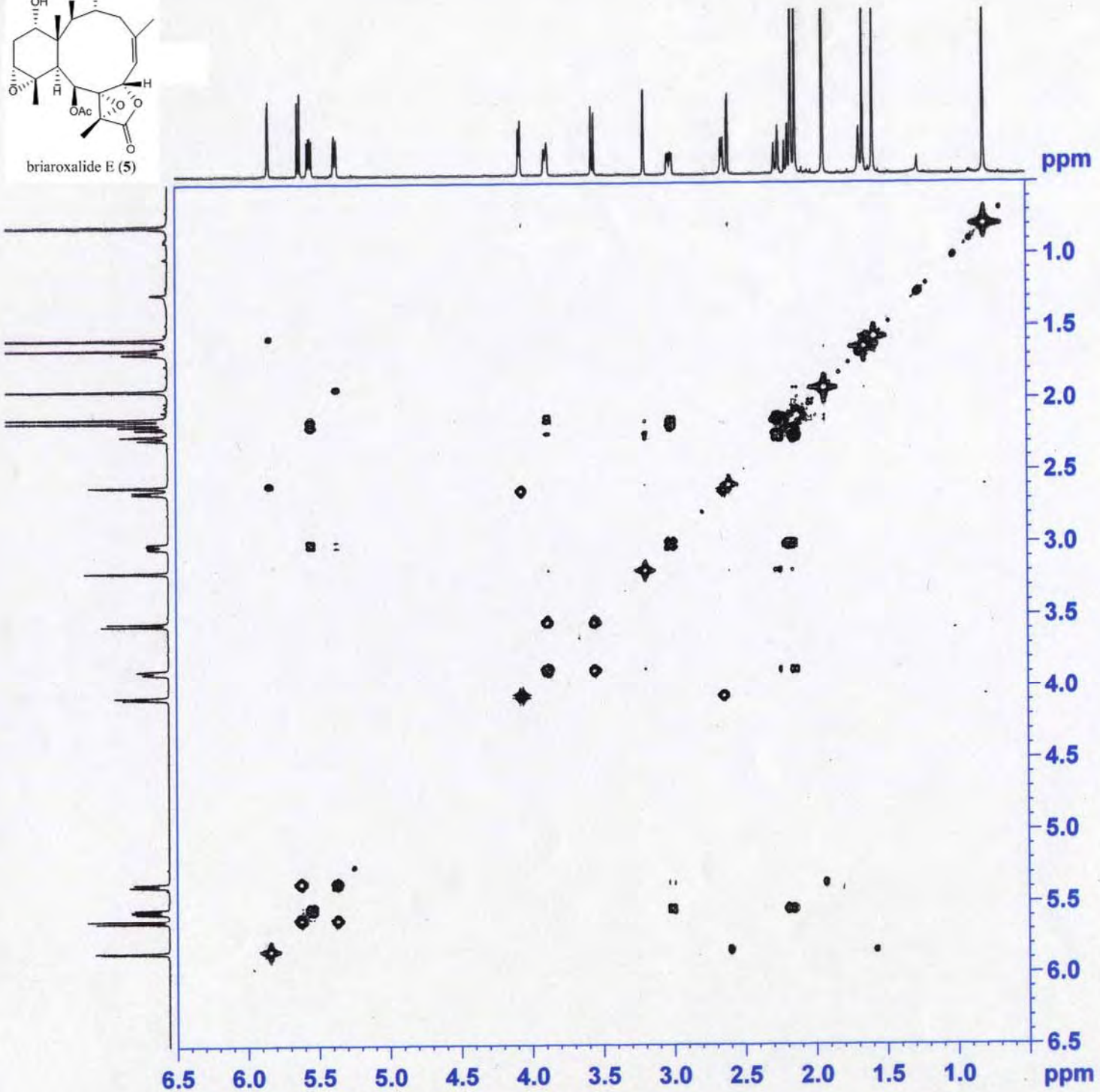
4.0577
4.0453
3.8774
3.8595
3.5464
3.5284
3.1776
3.0111
3.0009
2.9881
2.9780
2.6314
2.6184
2.5882
2.5841
2.2559
2.2288
2.1800
2.1588
2.1349
2.1077
1.9138
1.6317
1.5614

0.7821

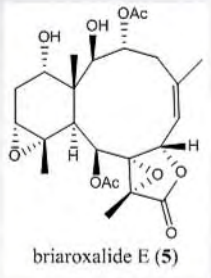

170.4856
170.1164
169.7272
141.1836
119.8182
77.2110
77.0000
76.7872
74.7831
72.6062
72.1988
72.1551
71.1440
68.0013
64.2913
62.2581
61.5052
45.9812
43.7643
34.4001
27.5183
26.1434
25.8561
21.2840
21.0003
14.4368
9.9720
OAc
OH
OH
H
H
OAc
O
O
O
O
briaroxalide E (5)
160
140
120
100
80
60
40
20
δ / ppm



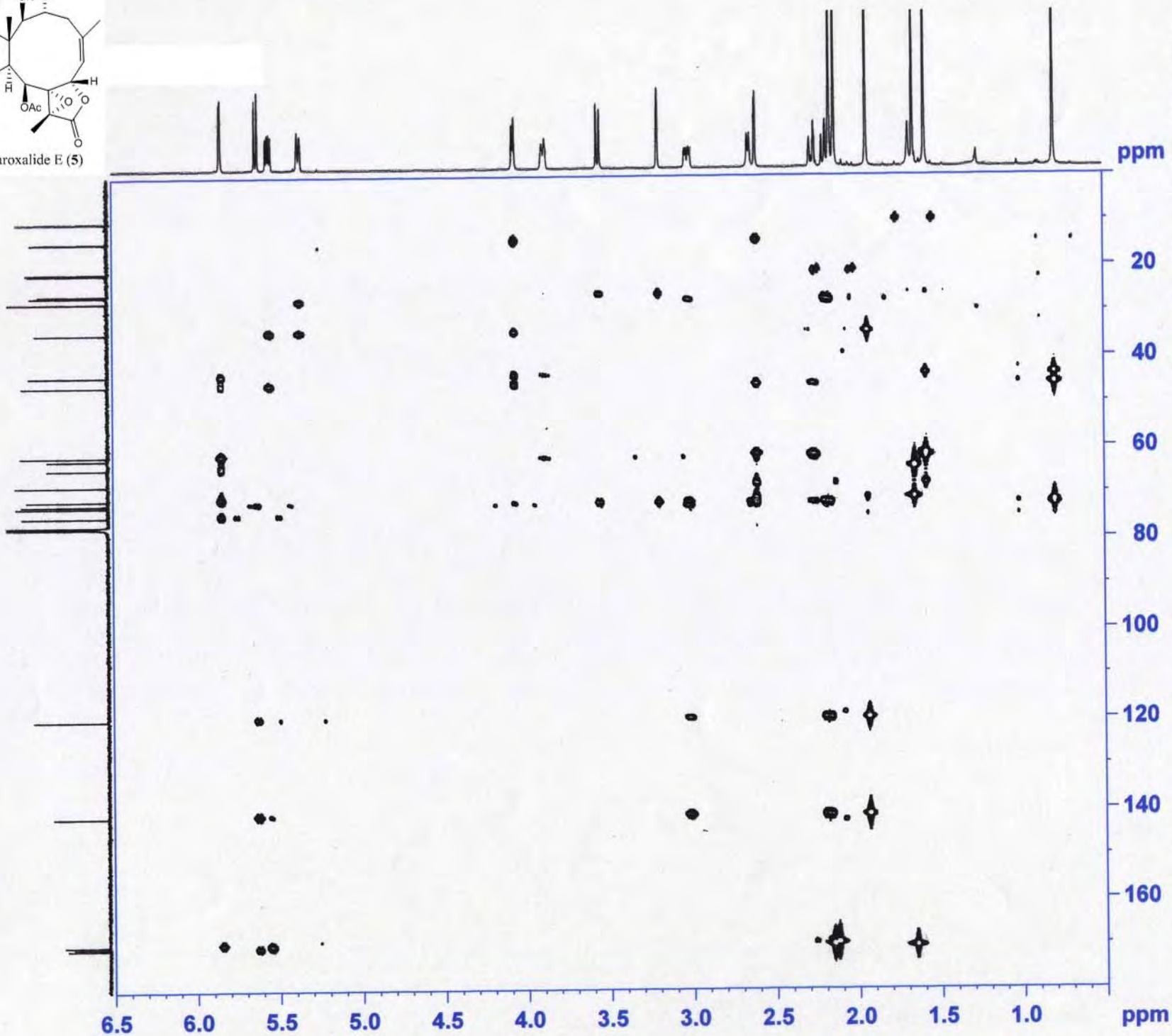
briaroxalide E (**5**)



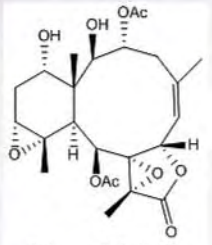

```
Current Data Parameters
NAME                  sc147
EXPNO                    11
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110303
Time                 20.52
INSTRUM              AV600
PROBHD    5 mm CPTCI 1H-
PULPROG           cosygpqf
TD                    2048
SOLVENT              CDCl3
NS                       2
DS                       8
SWH               6009.615 Hz
FIDRES            2.934382 Hz
AQ                0.1705268 sec
RG                      57
DW                 83.200 usec
DE                  6.00 usec
TE                 300.0 K
d0                0.00000300 sec
D1                2.00000000 sec
d13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00016640 sec

======== CHANNEL f1 ========
NUC1                     1H
P0                  10.00 usec
P1                  10.00 usec
PL1                 -4.10 dB
SFO1          600.1327006 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPZ1                10.00 %
GPZ2                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
ND0                      1
TD                     256
SFO1            600.1327 MHz
FIDRES         23.475060 Hz
SW                 10.014 ppm
FnMODE                  QF

F2 - Processing parameters
SI                    1024
SF            600.1300000 MHz
WDW                   SINE
SSB                      0
LB                  0.00 Hz
GB                       0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF            600.1300000 MHz
WDW                   SINE
SSB                      0
LB                  0.00 Hz
GB                       0
```



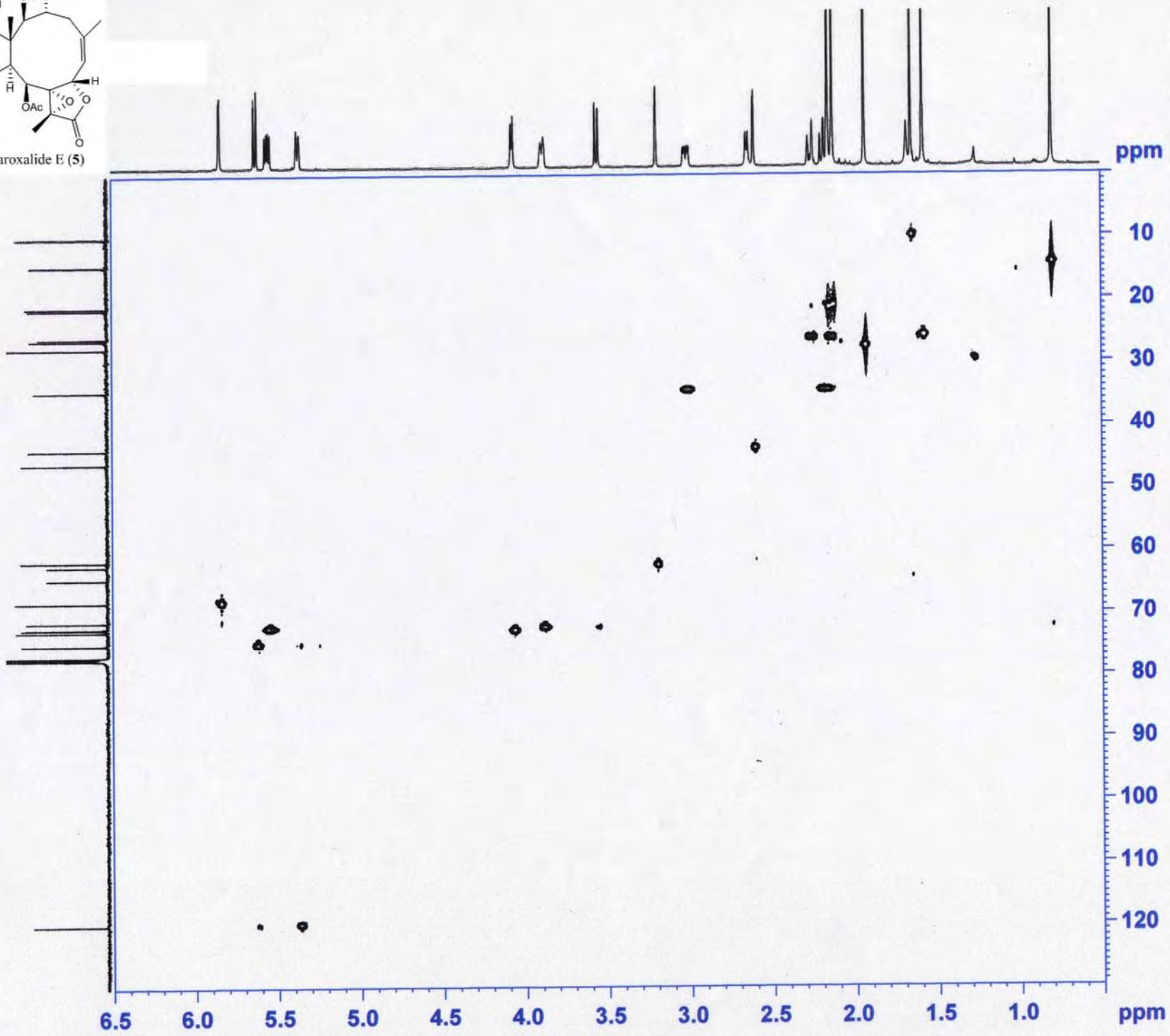
briaroxalide E (**5**)



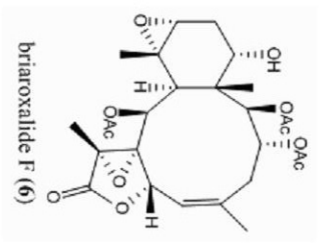

```
Current Data Parameters
NAME                  sc147
EXPNO                    14
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110303
Time                 18.19
INSTRUM              AV600
PROBHD   5 mm CPTCI 1H-
PULPROG     hmbcgplpndqf
TD                    2048
SOLVENT                D2O
NS                       16
DS                       16
SWH              6009.615 Hz
FIDRES           2.934382 Hz
AQ               0.1705268 sec
RG                   10300
DW                83.200 usec
DE                 6.00 usec
TE                 300.0 K
CNST2          145.0000000
CNST13           8.0000000
d0               0.00000300 sec
D1               2.00000000 sec
d2               0.00344828 sec
d6               0.06250000 sec
D16              0.00020000 sec
IN0              0.00001440 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
p2                 20.00 usec
PL1                -4.10 dB
SFO1         600.1327006 MHz

======== CHANNEL f2 ========
NUC2                   13C
P3                 15.50 usec
PL2                -4.80 dB
SFO2         150.9194083 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPNAM3           SINE.100
GPZ1               50.00 %
GPZ2               30.00 %
GPZ3               40.10 %
P16              1000.00 usec

F1 - Acquisition parameters
ND0                    2
TD                   256
SFO1         150.9194 MHz
FIDRES       135.633682 Hz
SW             230.071 ppm
FnMODE                 QF

F2 - Processing parameters
SI                  2048
SF           600.1300000 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           150.9028090 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0
```



briaroxalide E (**5**)




```
Current Data Parameters
NAME                  sc147
EXPNO                    13
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110303
Time                 17.04
INSTRUM              AV600
PROBHD    5 mm CPTCI 1H-
PULPROG            hsqcetgp
TD                     2048
SOLVENT               CDCl3
NS                        8
DS                       16
SWH                7788.162 Hz
FIDRES             3.802814 Hz
AQ                 0.1315958 sec
RG                     10300
DW                    64.200 usec
DE                     6.00 usec
TE                    300.0 K
CNST2             135.0000000
d0                 0.00000300 sec
D1                 2.00000000 sec
d4                 0.00185185 sec
d11                0.03000000 sec
d13                0.00000400 sec
D16                0.00020000 sec
DELTA              0.00122600 sec
DELTA1             0.00084385 sec
IN0                0.00002070 sec
ST1CNT                   128
ZGOPTNS

======== CHANNEL f1 ========
NUC1                      1H
P1                    10.00 usec
p2                    20.00 usec
P28                    0.00 usec
PL1                   -4.10 dB
SFO1           600.1327006 MHz

======== CHANNEL f2 ========
CPDPRG2                garp4
NUC2                      13C
P3                    15.50 usec
p4                    31.00 usec
PCPD2                 60.00 usec
PL2                   -4.80 dB
PL12                   6.96 dB
SFO2           150.9141267 MHz

====== GRADIENT CHANNEL =====
GPNAM1              SINE.100
GPNAM2              SINE.100
GPZ1                  80.00 %
GPZ2                  20.10 %
P16                 1000.00 usec

F1 - Acquisition parameters
ND0                       2
TD                      256
SFO1           150.9141 MHz
FIDRES          94.353867 Hz
SW                160.055 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                     1024
SF           600.1300000 MHz
WDW                   QSINE
SSB                       2
LB                     0.00 Hz
GB                        0
PC                     1.00

F1 - Processing parameters
SI                     1024
MC2         echo-antiecho
SF           150.9028090 MHz
WDW                   QSINE
SSB                       2
LB                     0.00 Hz
GB                        0
```



δ / ppm

7.2600

1.0
0.994
0.9985
0.9844
1.017

5.8768
5.8707
5.7538
5.7378
5.5642
5.5548
5.5438
5.5342
5.4464
5.4305
5.2761

0.9742
1.0339
0.9903
0.97
0.9999

3.6271
3.6085
3.4740
3.4554
3.1683
2.9082
2.8920
2.8377
2.8316

1.8935
2.0295

8.0268

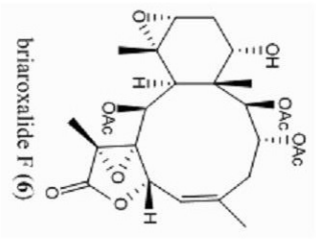
2.2633
2.2485
2.2416
2.2209
2.1261
2.1171
2.1103
2.0984
2.0858

7.586

1.6045
1.5952

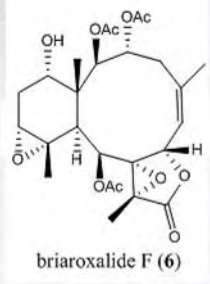
2.7849

0.8450

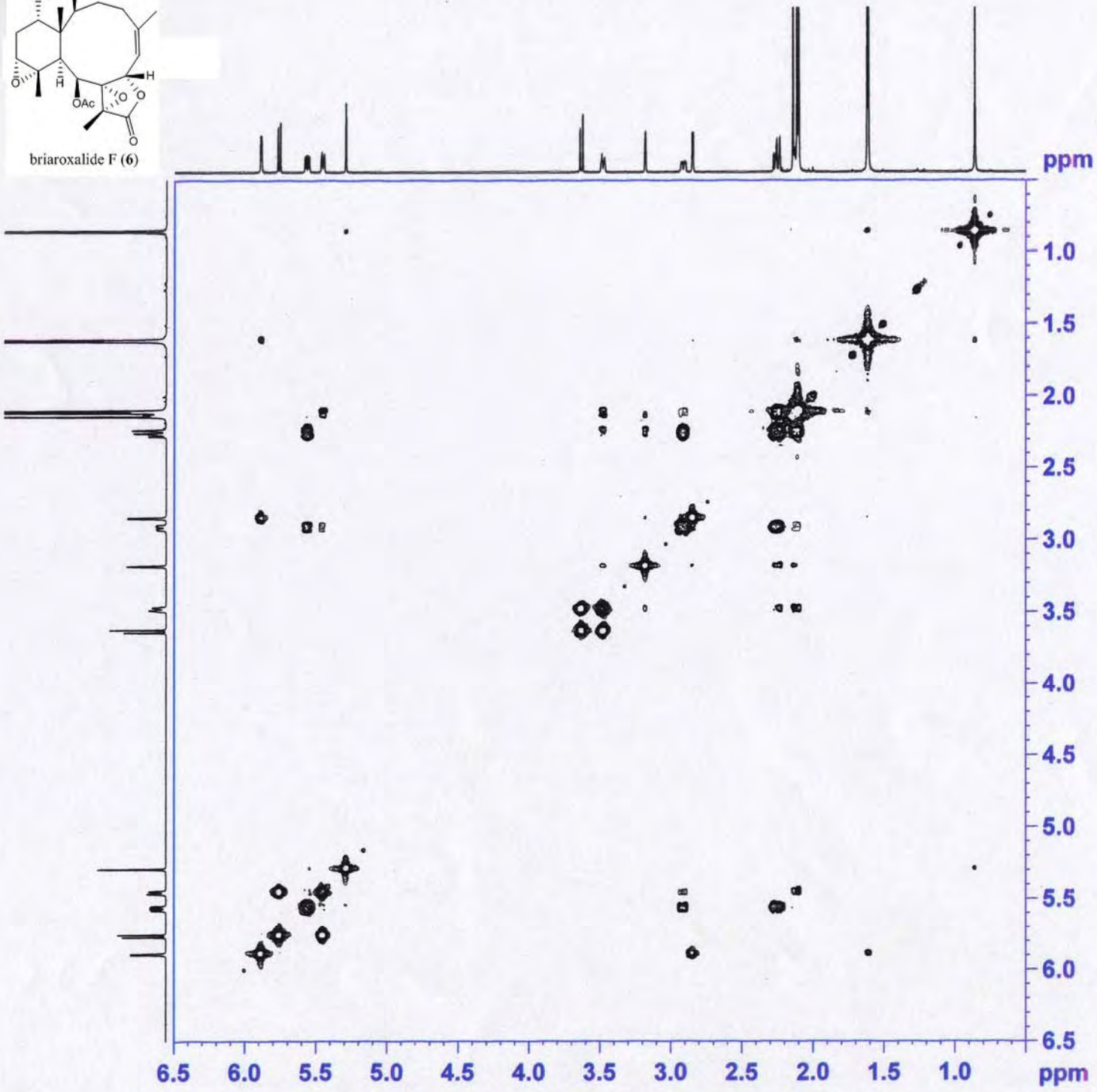


170.7402
170.3674
169.9255
169.8455
141.4964
120.2328
77.2110
77.0000
76.7890
74.5194
73.7574
72.2788
71.2822
70.8384
67.5067
63.7148
61.9780
61.2360
45.6829
42.1020
34.8675
26.7545
26.3307
25.8324
21.2276
21.0712
20.7384
15.7644
9.6228

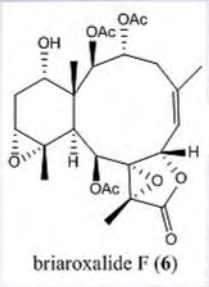
δ / ppm

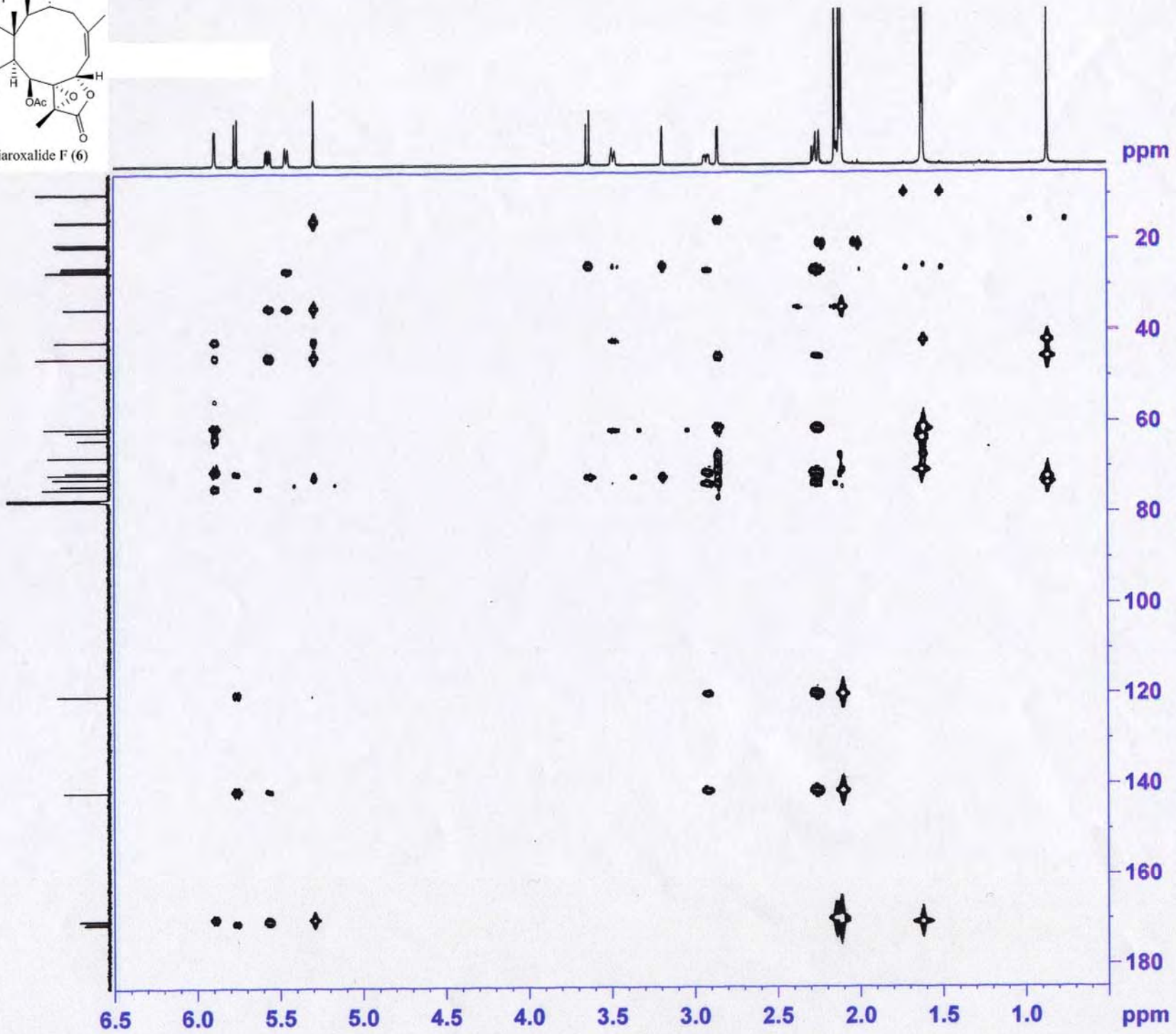


briaroxalide F (**6**)




```
Current Data Parameters
NAME                  bsc79
EXPNO                    12
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110704
Time                  14.19
INSTRUM               AV600
PROBHD   5 mm CPTCI 1H-
PULPROG           cosygpqf
TD                    2048
SOLVENT                MeOD
NS                        2
DS                        8
SWH                6613.757 Hz
FIDRES             3.229373 Hz
AQ                 0.1549544 sec
RG                      71.8
DW                   75.600 usec
DE                    6.00 usec
TE                   300.0 K
d0                0.00000300 sec
D1                2.00000000 sec
d13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00015120 sec

======== CHANNEL f1 ========
NUC1                      1H
P0                    10.20 usec
P1                    10.20 usec
PL1                   -4.10 dB
SFO1           600.1330006 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPZ1                  10.00 %
GPZ2                  10.00 %
P16                 1000.00 usec

F1 - Acquisition parameters
ND0                       1
TD                      256
SFO1             600.133 MHz
FIDRES          25.834988 Hz
SW                 11.020 ppm
FnMODE                 QF

F2 - Processing parameters
SI                     1024
SF             600.1300000 MHz
WDW                    SINE
SSB                       0
LB                    0.00 Hz
GB                        0
PC                    1.40

F1 - Processing parameters
SI                     1024
MC2                      QF
SF             600.1300000 MHz
WDW                    SINE
SSB                       0
LB                    0.00 Hz
GB                        0
```





Current Data Parameters
NAME bsc79
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110704
Time 15.53
INSTRUM AV600
PROBHD 5 mm CPTCI 1H-
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 16
DS 16
SWH 6009.615 Hz
FIDRES 2.934382 Hz
AQ 0.1705268 sec
RG 16400
DW 83.200 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
CNST13 8.0000000
d0 0.00000300 sec
D1 2.00000000 sec
d2 0.00344828 sec
d6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001505 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.20 usec
p2 20.40 usec
PL1 -4.10 dB
SFO1 600.1327006 MHz

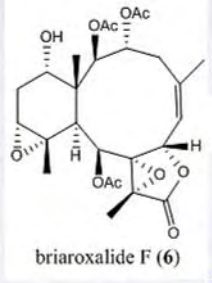
======== CHANNEL f2 ========
NUC2 13C
P3 15.50 usec
PL2 -4.80 dB
SFO2 150.9178993 MHz

====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

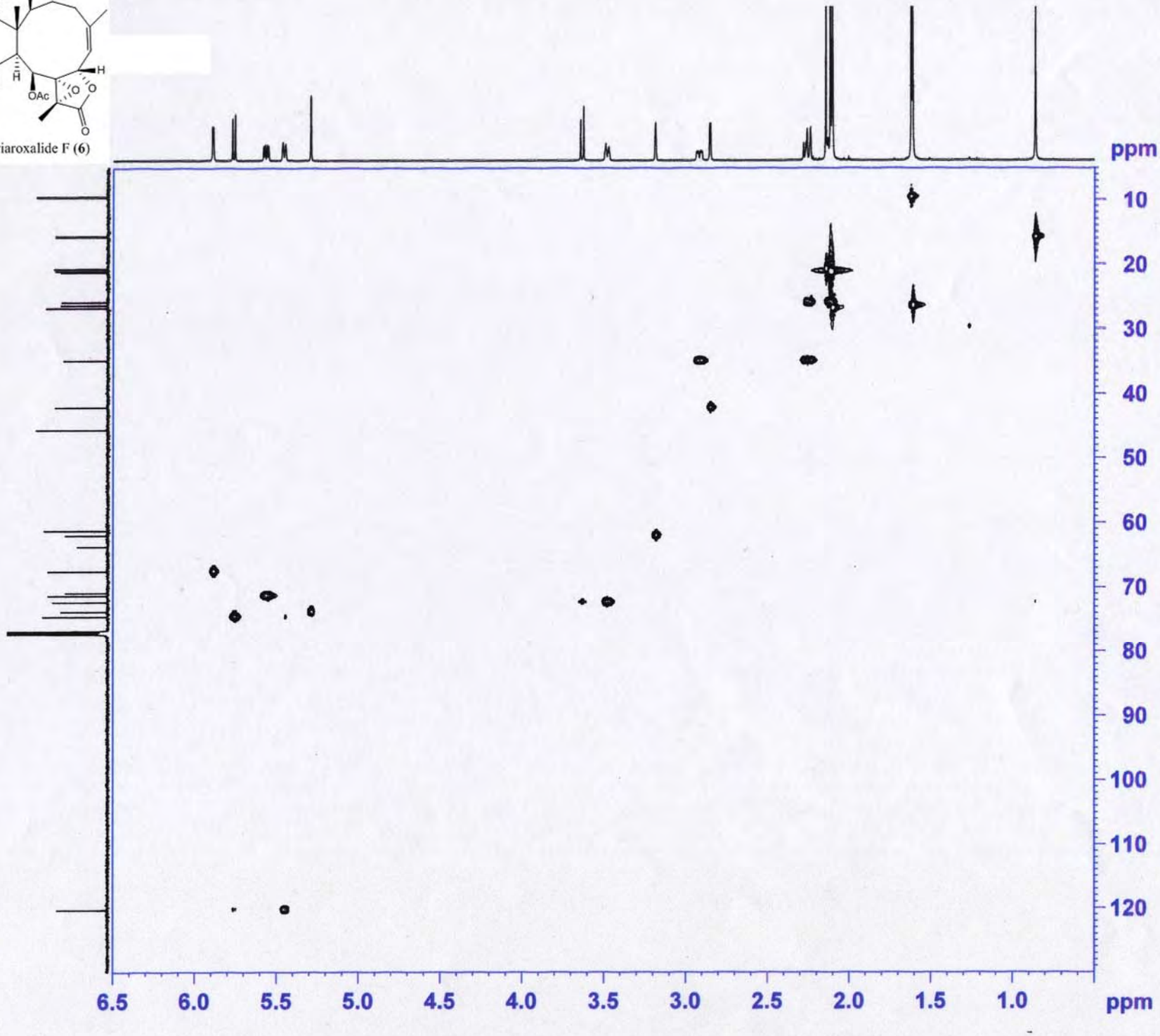
F1 - Acquisition parameters
ND0 2
TD 256
SFO1 150.9179 MHz
FIDRES 129.775742 Hz
SW 220.137 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

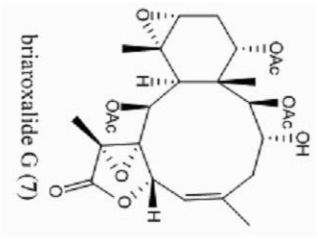
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028090 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0



briaroxalide F (**6**)




```
Current Data Parameters
NAME                  bsc79
EXPNO                    13
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110704
Time_                 14.39
INSTRUM              AV600
PROBHD   5 mm CPTCI 1H-
PULPROG          hsqcetgp
TD                    2048
SOLVENT              CDCl3
NS                       8
DS                      16
SWH                7788.162 Hz
FIDRES             3.802814 Hz
AQ                 0.1315958 sec
RG                     10300
DW                    64.200 usec
DE                     6.00 usec
TE                    300.0 K
CNST2            135.0000000
d0                 0.00000300 sec
D1                 2.00000000 sec
d4                 0.00185185 sec
d11                0.03000000 sec
d13                0.00000400 sec
D16                0.00020000 sec
DELTA              0.00122640 sec
DELTA1             0.00084385 sec
IN0                0.00001950 sec
ST1CNT                   128
ZGOPTNS

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.20 usec
p2                     20.40 usec
P28                     0.00 usec
PL1                    -4.10 dB
SFO1           600.1327006 MHz

======== CHANNEL f2 ========
CPDPRG2                garp4
NUC2                     13C
P3                     15.50 usec
p4                     31.00 usec
PCPD2                  60.00 usec
PL2                    -4.80 dB
PL12                    6.96 dB
SFO2           150.9141267 MHz

====== GRADIENT CHANNEL =====
GPNAM1              SINE.100
GPNAM2              SINE.100
GPZ1                   80.00 %
GPZ2                   20.10 %
P16                  1000.00 usec

F1 - Acquisition parameters
NDO                       2
TD                      256
SFO1             150.9141 MHz
FIDRES           100.160255 Hz
SW                  169.905 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                     1024
SF             600.1300000 MHz
WDW                   QSINE
SSB                       2
LB                     0.00 Hz
GB                        0
PC                     1.00

F1 - Processing parameters
SI                     1024
MC2         echo-antiecho
SF              150.9028090 MHz
WDW                   QSINE
SSB                       2
LB                     0.00 Hz
GB                        0
```



δ / ppm

7.2602

5.8965
5.8926

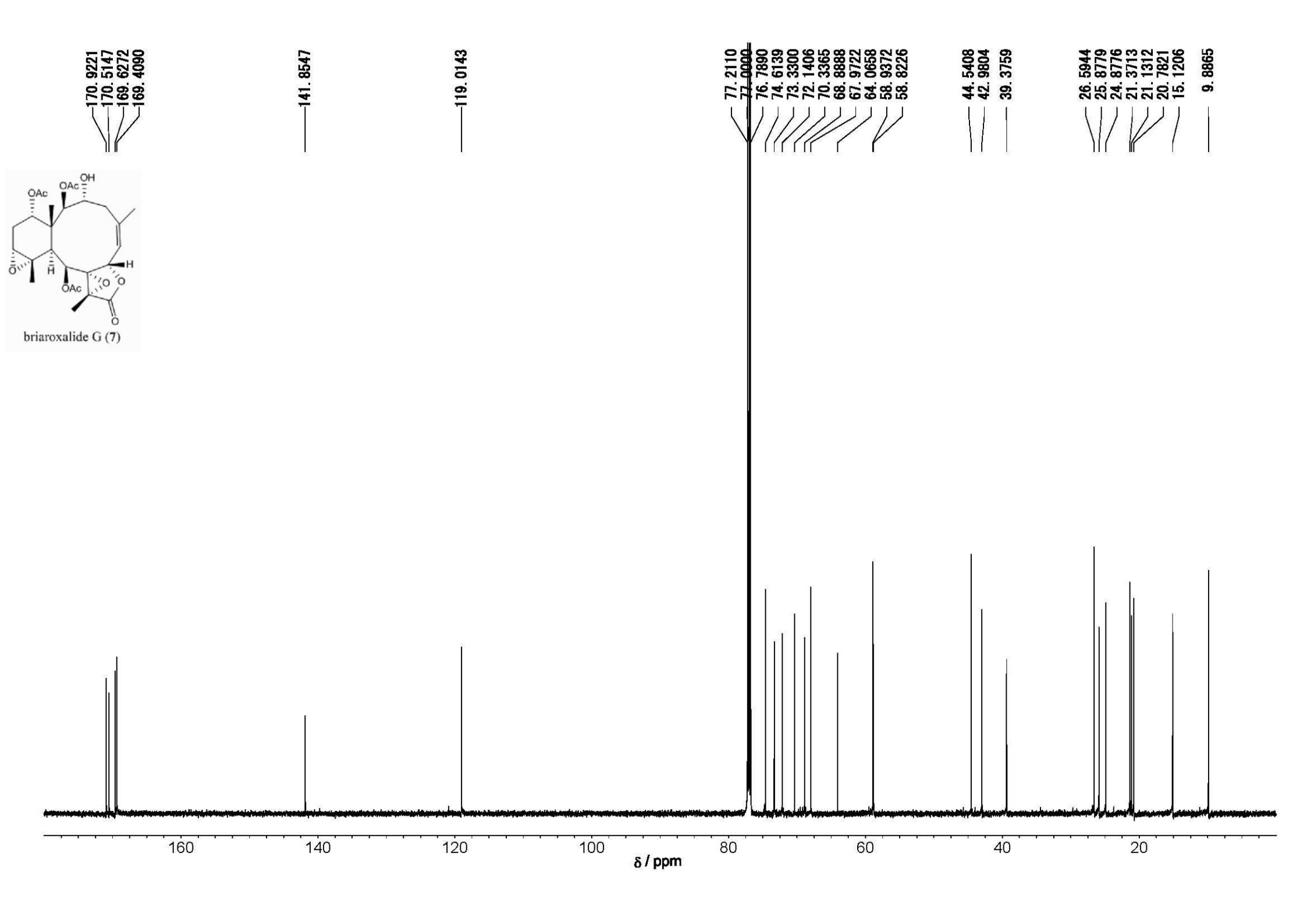
5.3606
5.3455
5.2794
5.2643
5.0906

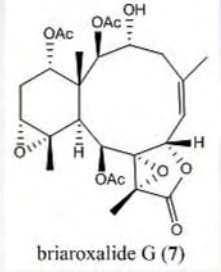
4.6967
4.6864
4.6808
4.6704
4.6605
4.5679
4.5635

2.9323
2.7809
2.7765
2.6594
2.6517
2.6355
2.6261

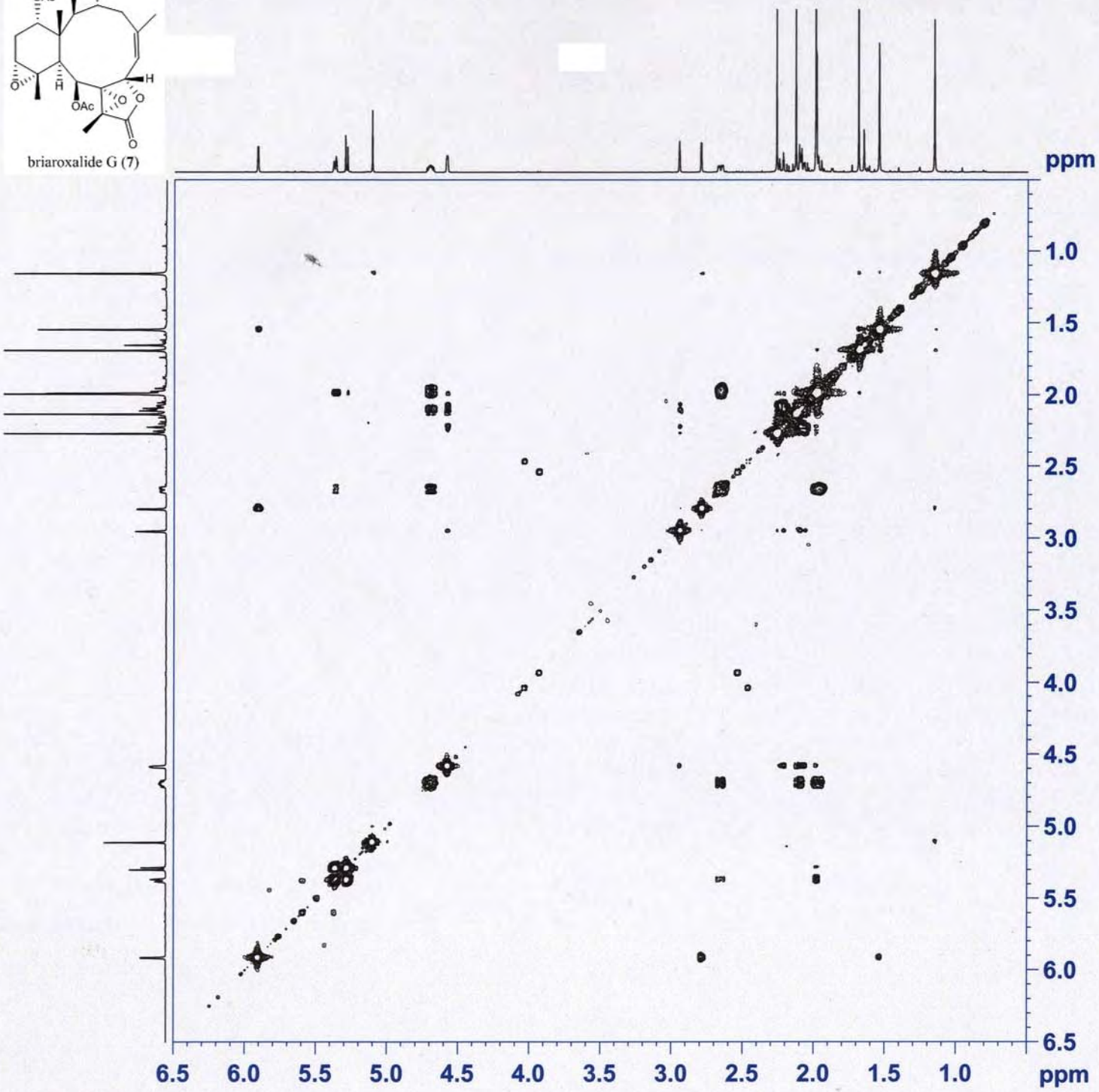
2.2485
2.2304
2.2024
2.1132
2.0899
2.0830
2.0792
2.0726
2.0623
2.0586
2.0546
2.0509
1.9741
1.9695
1.6726
1.5280
1.1396

1.0
1.0205
1.0277
1.0097
1.0288
1.0149
1.0201
0.9555
0.9241
3.9907
3.0102
1.8677
7.0953
2.9636
2.8881
2.9391

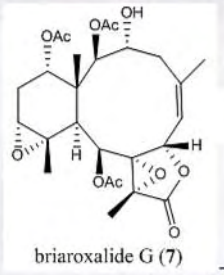

170.9221
170.5147
169.6272
169.4090
141.8547
119.0143
77.2110
77.0000
76.7890
74.6139
73.3300
72.1406
70.3365
68.8888
67.9722
64.0658
58.9372
58.8226
44.5408
42.9804
39.3759
26.5944
25.8779
24.8776
21.3713
21.1312
20.7821
15.1206
9.8865
OAc
OAc
OH
OAc
H
H
O
O
O
O
briaroxalide G (7)
160
140
120
100
80
60
40
20
δ / ppm

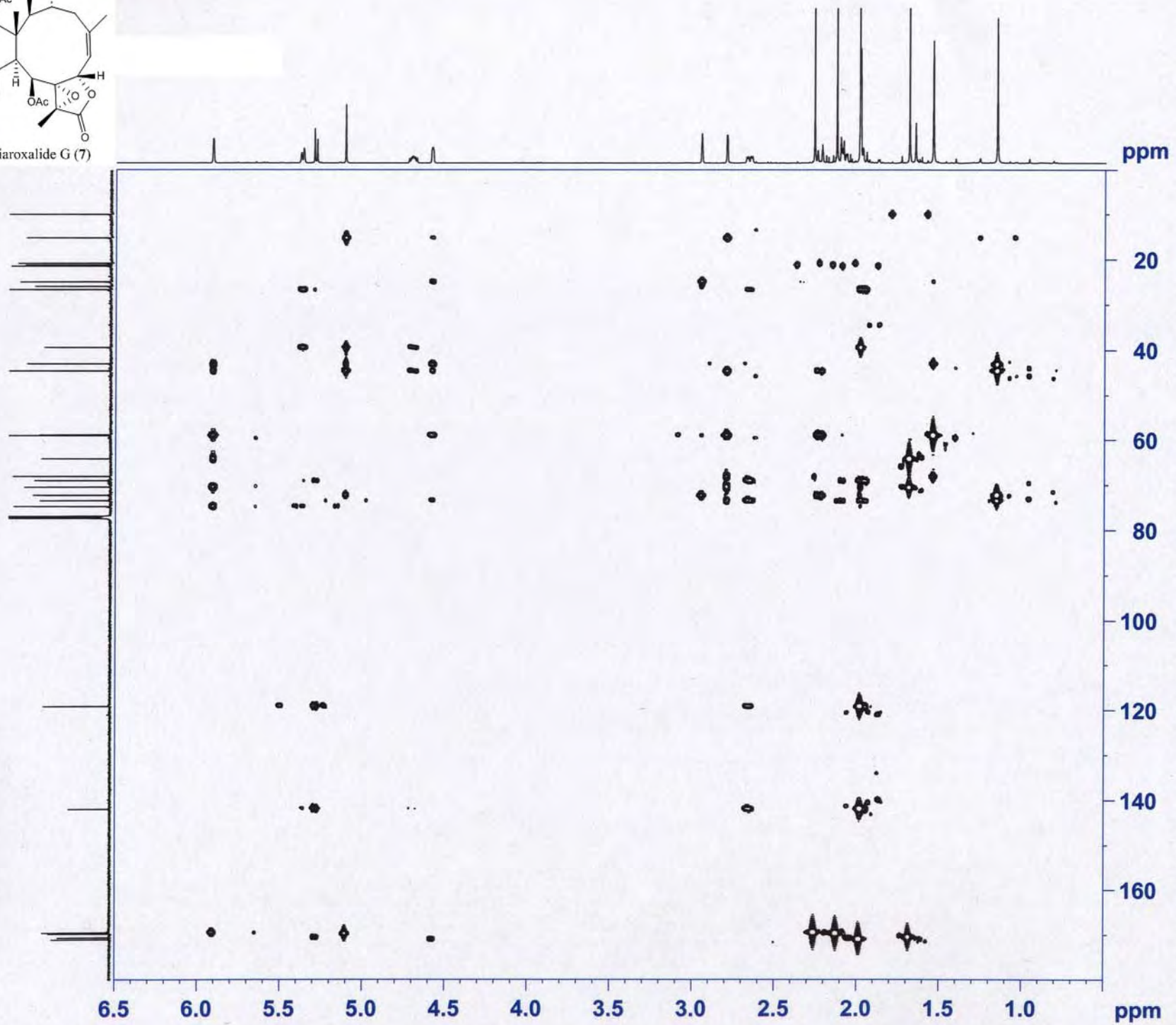


briaroxalide G (7)

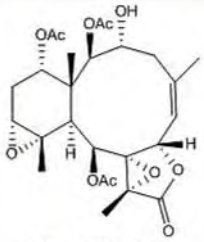


NAME	bsc127
EXPNO	11
PROCNO	1
Date_	20110728
Time	13.32
INSTRUM	AV600
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygpqf
TD	2048
SOLVENT	MeOD
NS	2
DS	8
SWH	6613.757 Hz
FIDRES	3.229373 Hz
AQ	0.1549544 sec
RG	40.3
DW	75.600 usec
DE	6.00 usec
TE	300.0 K
d0	0.00000300 sec
D1	2.00000000 sec
d13	0.00000400 sec
D16	0.00020000 sec
IN0	0.00015120 sec
======== CHANNEL f1 ========	
NUC1	1H
P0	10.20 usec
P1	10.20 usec
PL1	-4.10 dB
SFO1	600.1330006 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPZ1	10.00 %
GPZ2	10.00 %
P16	1000.00 usec
ND0	1
TD	256
SFO1	600.133 MHz
FIDRES	25.834988 Hz
SW	11.020 ppm
FnMODE	QF
SI	1024
SF	600.1300000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	600.1300000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

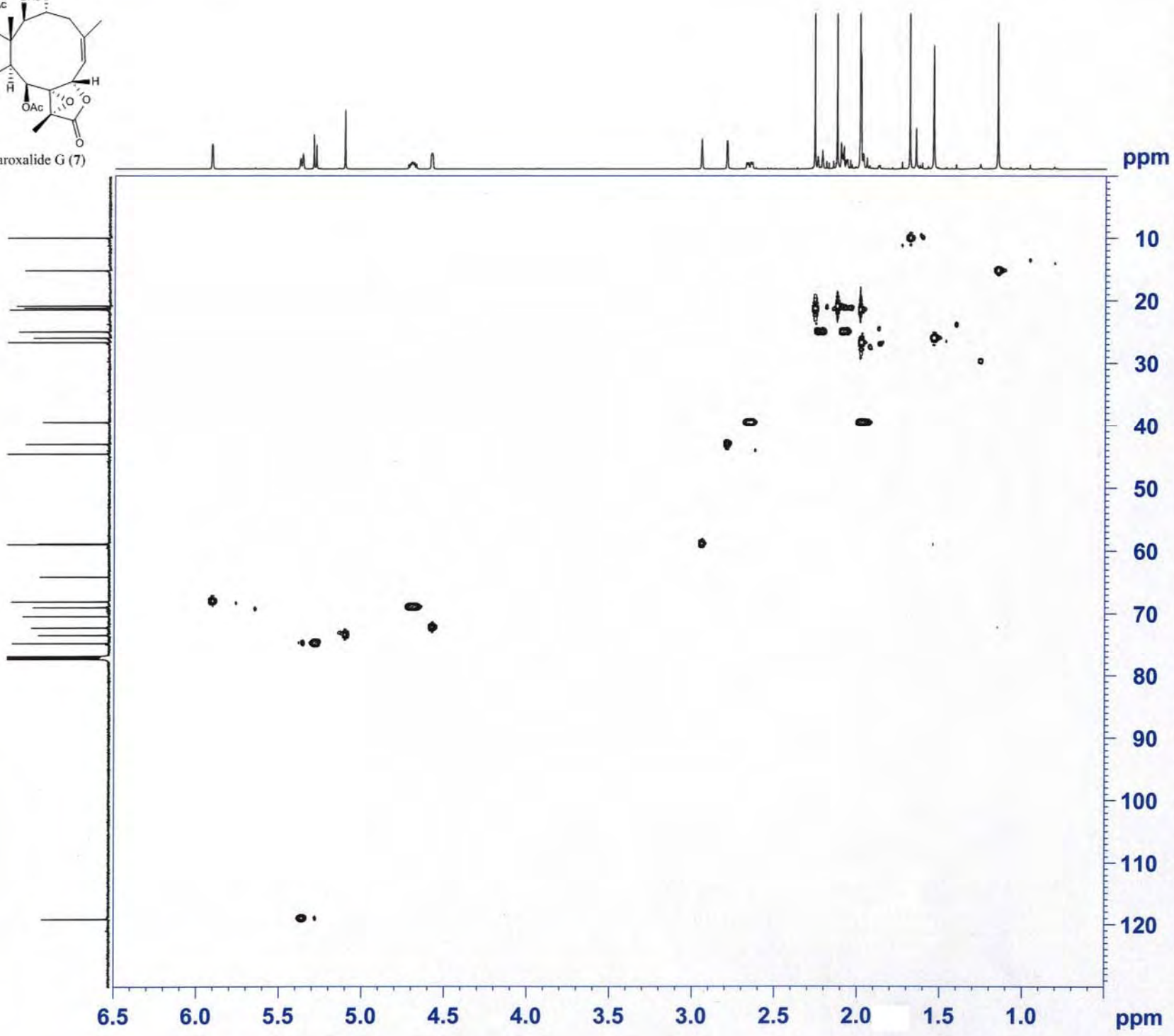




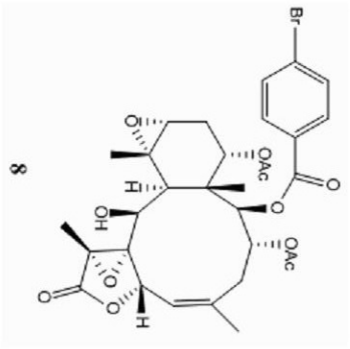
NAME	bsc127
EXPNO	14
PROCNO	1
Date_	20110728
Time	10.57
INSTRUM	AV600
PROBHD	5 mm CPTCI 1H-
PULPROG	hmbcgplpndqf
TD	2048
SOLVENT	CDCl3
NS	16
DS	16
SWH	6009.615 Hz
FIDRES	2.934382 Hz
AQ	0.1705268 sec
RG	16400
DW	83.200 usec
DE	6.00 usec
TE	300.0 K
CNST2	145.0000000
CNST13	8.0000000
d0	0.00000300 sec
D1	2.00000000 sec
d2	0.00344828 sec
d6	0.06250000 sec
D16	0.00020000 sec
IN0	0.00001505 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	10.20 usec
p2	20.40 usec
PL1	-4.10 dB
SFO1	600.1327006 MHz
======== CHANNEL f2 ========	
NUC2	13C
P3	15.50 usec
PL2	-4.80 dB
SFO2	150.9178993 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPNAM3	SINE.100
GPZ1	50.00 %
GPZ2	30.00 %
GPZ3	40.10 %
P16	1000.00 usec
ND0	2
TD	256
SFO1	150.9179 MHz
FIDRES	129.775742 Hz
SW	220.137 ppm
FnMODE	QF
SI	2048
SF	600.1300000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	150.9028090 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0



briaroxalide G (7)



NAME	bsc127
EXPNO	13
PROCNO	1
Date_	20110728
Time	9.43
INSTRUM	AV600
PROBHD	5 mm CPTCI 1H-
PULPROG	hsqcetgp
TD	2048
SOLVENT	CDCl3
NS	8
DS	16
SWH	7788.162 Hz
FIDRES	3.802814 Hz
AQ	0.1315958 sec
RG	10300
DW	64.200 usec
DE	6.00 usec
TE	300.0 K
CNST2	135.0000000
d0	0.00000300 sec
D1	2.00000000 sec
d4	0.00185185 sec
d11	0.03000000 sec
d13	0.00000400 sec
D16	0.00020000 sec
DELTA	0.00122640 sec
DELTA1	0.00084385 sec
IN0	0.00001950 sec
ST1CNT	0
ZGOPTNS	
======== CHANNEL f1 ========	
NUC1	1H
P1	10.20 usec
p2	20.40 usec
P28	0.00 usec
PL1	-4.10 dB
SFO1	600.1327006 MHz
======== CHANNEL f2 ========	
CPDPRG2	garp4
NUC2	13C
P3	15.50 usec
p4	31.00 usec
PCPD2	60.00 usec
PL2	-4.80 dB
PL12	6.96 dB
SFO2	150.9141267 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPZ1	80.00 %
GPZ2	20.10 %
P16	1000.00 usec
ND0	2
TD	256
SFO1	150.9141 MHz
FIDRES	100.160255 Hz
SW	169.905 ppm
FnMODE	Echo-Antiecho
SI	1024
SF	600.1300000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00
SI	1024
MC2	echo-antiecho
SF	150.9028090 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0



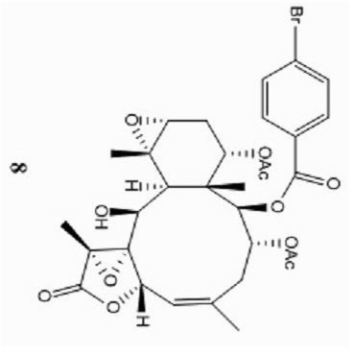
8

δ / ppm

1 2 3 4 5 6 7

1.9931
2.0282
1.0
1.0371
1.0063
1.018
0.986
1.0141
0.9497
0.9927
0.9624
0.9922
2.18
4.2644
2.939
2.8621
1.0072
3.4509
2.8477
2.8344
2.7255

7.8818
7.8780
7.8749
7.8669
7.8637
7.8599
7.6080
7.6050
7.5969
7.5939
7.2600
6.1281
6.1184
6.1077
6.0977
5.7497
5.7351
5.5172
5.3718
5.3572
4.6809
4.5882
4.5818
3.9270
2.9365
2.9318
2.8482
2.8308
2.6766
2.1742
2.1151
2.0145
1.9262
1.8923
1.8720
1.8471
1.6948
1.5282
1.2635
1.0365
0.8796
0.0659



8

δ / ppm

160
140
120
100
80
60
40
20

171.5532
171.4604
170.8548
164.5569
139.8815
131.9194
131.1811
128.7659
128.4604
120.4292
77.2110
77.0000
76.7890
75.5760
72.8026
72.0169
71.8696
71.0949
69.0871
64.2713
59.7229
59.5828
45.7048
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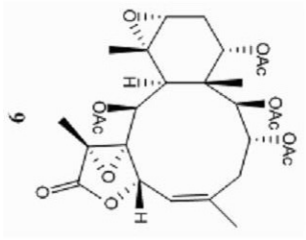
34.5947
30.9301
26.4198
25.9906
24.1575
21.4931
15.0733
10.3139



7.2600

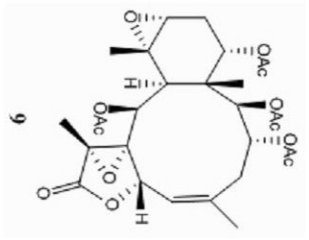
1.0
0.9788
0.957
0.9698
0.9834
0.9833

5.8665
5.8628
5.6388
5.6289
5.6194
5.6095
5.5601
5.5452
5.3726
5.3576
5.1946
4.7133
4.7075

0.9879
0.9181
0.9811
1.0725
0.9667
2.8107
3.1327
2.3042
2.8357
2.8287
2.8515
2.6903
2.8444

2.9280
2.8538
2.8374
2.8012
2.7973
2.2309
2.2258
2.1975
2.1711
2.1440
2.1056
2.0844
2.0578
2.0375
2.0332
2.0136
1.9816
1.9491
1.6833
1.6528
1.4928
1.0250

δ / ppm



9

170.8203
170.4856
170.3256
170.0928
169.7291
140.3616
120.5038
77.2110
77.0000
76.7890
74.8485
72.0788
71.7969
71.4277
70.2401
68.4233
64.6041
58.9881
58.7899
44.7136
42.7931
35.0002
26.5872
25.3287
25.2177
21.3495
21.2713
20.9930
20.6948
15.0497
10.3212

160
140
120
100
80
60
40
20

δ / ppm

Table 1. Crystal data and structure refinement for *p*-bromobenzoate **8**.

Identification code	p21	
Empirical formula	C62 H80 Br2 O27	
Formula weight	1417.08	
Temperature	90 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 10.1791(6) Å	α= 90°.
	b = 17.2512(9) Å	β= 104.3150(10)°.
	c = 19.3528(10) Å	γ = 90°.
Volume	3292.9(3) $Å^3$	
Z	2	
Density (calculated)	1.429 Mg/m^3	
Absorption coefficient	1.314 mm^{-1}	
F(000)	1476	
Crystal size	0.27 x 0.23 x 0.16 mm^3	
Theta range for data collection	2.06 to 25.02°.	
Index ranges	-11<=h<=12, -9<=k<=20, -22<=l<=23	
Reflections collected	15768	
Independent reflections	7667 [R(int) = 0.0217]	
Completeness to theta = 25.02°	99.7 %	
Absorption correction	Analytical	
Max. and min. transmission	0.8172 and 0.7179	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7667 / 56 / 864	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0224, wR2 = 0.0512	
R indices (all data)	R1 = 0.0242, wR2 = 0.0517	
Absolute structure parameter	0.003(3)	
Largest diff. peak and hole	0.234 and -0.314 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *p*-bromobenzoate **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	-77(1)	3304(1)	8579(1)	23(1)
Br(1B)	7144(1)	4307(1)	-4342(1)	23(1)
C(1)	-78(2)	5592(1)	4448(1)	12(1)
C(2)	1233(2)	5594(1)	5083(1)	13(1)
C(3)	2589(2)	5259(1)	4992(1)	15(1)
C(4)	3805(2)	5765(2)	5342(1)	19(1)
C(5)	3625(2)	6611(2)	5106(1)	18(1)
C(6)	3427(2)	6835(2)	4434(1)	17(1)
C(7)	3434(2)	6341(1)	3798(1)	16(1)
C(8)	2097(2)	6304(1)	3230(1)	13(1)
C(9)	955(2)	5758(1)	3281(1)	12(1)
C(10)	88(2)	6088(1)	3786(1)	12(1)
C(11)	-1318(2)	6351(1)	3310(1)	15(1)
C(12)	-2556(2)	6342(1)	3574(1)	19(1)
C(13)	-2571(2)	6033(1)	4289(1)	17(1)
C(14)	-1156(2)	5970(1)	4783(1)	14(1)
C(15)	-570(2)	4761(1)	4239(1)	16(1)
C(16)	3636(3)	7190(2)	5687(2)	27(1)
C(17)	2376(2)	6568(1)	2551(1)	15(1)
C(18)	1674(2)	6385(1)	1796(1)	17(1)
C(19)	3851(3)	6784(2)	2727(1)	19(1)
C(20)	-1590(2)	6369(2)	2505(1)	20(1)
C(21)	-1041(2)	7042(1)	5583(1)	18(1)
C(22)	-311(3)	7788(2)	5825(2)	25(1)
C(23)	1101(2)	5496(2)	6308(1)	16(1)
C(24)	807(2)	4944(1)	6842(1)	16(1)
C(25)	773(2)	4152(1)	6733(1)	19(1)
C(26)	514(3)	3654(2)	7250(1)	22(1)
C(27)	284(2)	3971(2)	7865(1)	18(1)
C(28)	304(3)	4761(2)	7987(1)	21(1)
C(29)	567(3)	5242(2)	7469(1)	22(1)
C(30)	3402(2)	3947(1)	5039(1)	18(1)
C(31)	3603(3)	3231(2)	5484(2)	28(1)
C(1B)	7709(2)	4176(1)	290(1)	12(1)
C(2B)	6438(2)	4570(1)	-208(1)	14(1)

C(3B)	5020(2)	4275(1)	-214(1)	15(1)
C(4B)	3932(2)	4908(1)	-387(1)	17(1)
C(5B)	4195(2)	5541(1)	173(1)	17(1)
C(6B)	4452(2)	5402(1)	874(1)	16(1)
C(7B)	4368(2)	4635(1)	1226(1)	15(1)
C(8B)	5686(2)	4293(1)	1692(1)	14(1)
C(9B)	6683(2)	3786(1)	1420(1)	13(1)
C(10B)	7723(2)	4273(1)	1107(1)	13(1)
C(11B)	9173(2)	4181(1)	1600(1)	16(1)
C(12B)	10392(2)	4232(1)	1319(1)	17(1)
C(13B)	10316(2)	4337(2)	546(1)	16(1)
C(14B)	8933(2)	4612(1)	122(1)	14(1)
C(15B)	7862(2)	3319(2)	81(1)	15(1)
C(16B)	4182(3)	6360(2)	-101(2)	27(1)
C(17B)	5471(2)	4194(1)	2415(1)	16(1)
C(18B)	6081(3)	3632(2)	2995(1)	20(1)
C(19B)	4089(2)	4511(1)	2389(1)	17(1)
C(20B)	9390(2)	3796(2)	2320(1)	21(1)
C(21B)	9234(2)	5944(1)	-148(1)	17(1)
C(22B)	8935(3)	6761(1)	12(2)	22(1)
C(23B)	6482(2)	5122(1)	-1354(1)	17(1)
C(24B)	6627(2)	4914(1)	-2078(1)	14(1)
C(25B)	6603(2)	4141(1)	-2295(1)	19(1)
C(26B)	6766(3)	3965(2)	-2969(1)	20(1)
C(27B)	6944(2)	4558(2)	-3413(1)	18(1)
C(28B)	6970(2)	5331(2)	-3211(1)	20(1)
C(29B)	6808(2)	5505(2)	-2540(1)	20(1)
C(30B)	3745(2)	3146(1)	-630(1)	20(1)
C(31B)	3446(3)	2566(2)	-1230(2)	27(1)
O(1)	4507(2)	6988(1)	2322(1)	27(1)
O(2)	4393(2)	6703(1)	3435(1)	20(1)
O(3)	1699(2)	7079(1)	2965(1)	16(1)
O(4)	1479(2)	5007(1)	3476(1)	15(1)
O(5)	-1817(2)	7060(1)	3572(1)	20(1)
O(6)	-645(2)	6744(1)	5032(1)	16(1)
O(7)	-1874(2)	6744(1)	5851(1)	24(1)
O(8)	885(2)	5173(1)	5663(1)	14(1)
O(9)	1475(2)	6161(1)	6437(1)	24(1)
O(10)	2784(2)	4498(1)	5336(1)	21(1)
O(11)	3754(2)	4040(1)	4493(1)	31(1)

O(1B)	3535(2)	4549(1)	2870(1)	26(1)
O(2B)	3516(2)	4778(1)	1730(1)	17(1)
O(3B)	6300(2)	4830(1)	2257(1)	16(1)
O(4B)	5982(2)	3212(1)	949(1)	17(1)
O(5B)	9956(2)	4898(1)	1671(1)	19(1)
O(6B)	8766(2)	5442(1)	256(1)	14(1)
O(7B)	9816(2)	5751(1)	-605(1)	25(1)
O(8B)	6605(2)	4497(1)	-934(1)	15(1)
O(9B)	6292(2)	5772(1)	-1161(1)	22(1)
O(10B)	4689(2)	3660(1)	-740(1)	18(1)
O(11B)	3213(2)	3183(1)	-144(1)	24(1)
O(1S)	4821(2)	2197(1)	1716(1)	25(1)
O(2S)	7708(2)	2012(1)	2262(1)	28(1)
O(3S)	6836(2)	7822(1)	6575(1)	34(1)
O(4S)	2525(2)	2747(1)	1990(1)	36(1)
O(5S)	94(2)	7013(1)	8468(1)	35(1)

Table 3. Bond lengths [Å] and angles [°] for *p*-bromobenzoate **8**.

Br(1)-C(27)	1.903(2)
Br(1B)-C(27B)	1.907(2)
C(1)-C(15)	1.538(3)
C(1)-C(14)	1.551(3)
C(1)-C(2)	1.575(3)
C(1)-C(10)	1.583(3)
C(2)-O(8)	1.451(3)
C(2)-C(3)	1.546(3)
C(2)-H(2)	1.0000
C(3)-O(10)	1.463(3)
C(3)-C(4)	1.530(3)
C(3)-H(3)	1.0000
C(4)-C(5)	1.526(4)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.322(4)
C(5)-C(16)	1.502(4)
C(6)-C(7)	1.498(4)
C(6)-H(6)	0.9500
C(7)-O(2)	1.475(3)
C(7)-C(8)	1.524(3)
C(7)-H(7)	1.0000
C(8)-O(3)	1.453(3)
C(8)-C(17)	1.484(3)
C(8)-C(9)	1.519(3)
C(9)-O(4)	1.416(3)
C(9)-C(10)	1.578(3)
C(9)-H(9)	1.0000
C(10)-C(11)	1.565(3)
C(10)-H(10)	1.0000
C(11)-O(5)	1.461(3)
C(11)-C(12)	1.472(3)
C(11)-C(20)	1.515(3)
C(12)-O(5)	1.449(3)
C(12)-C(13)	1.487(4)
C(12)-H(12)	1.0000
C(13)-C(14)	1.523(3)
C(13)-H(13A)	0.9900

C(13)-H(13B)	0.9900
C(14)-O(6)	1.469(3)
C(14)-H(14)	1.0000
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-O(3)	1.472(3)
C(17)-C(18)	1.492(3)
C(17)-C(19)	1.502(3)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-O(1)	1.201(3)
C(19)-O(2)	1.352(3)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-O(7)	1.213(3)
C(21)-O(6)	1.332(3)
C(21)-C(22)	1.503(4)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-O(9)	1.214(3)
C(23)-O(8)	1.336(3)
C(23)-C(24)	1.489(4)
C(24)-C(25)	1.382(4)
C(24)-C(29)	1.394(4)
C(25)-C(26)	1.393(4)
C(25)-H(25)	0.9500
C(26)-C(27)	1.381(4)
C(26)-H(26)	0.9500
C(27)-C(28)	1.382(4)
C(28)-C(29)	1.377(4)
C(28)-H(28)	0.9500
C(29)-H(29)	0.9500
C(30)-O(11)	1.207(3)

C(30)-O(10)	1.345(3)
C(30)-C(31)	1.490(4)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(1B)-C(15B)	1.549(3)
C(1B)-C(14B)	1.557(3)
C(1B)-C(2B)	1.565(3)
C(1B)-C(10B)	1.587(3)
C(2B)-O(8B)	1.460(3)
C(2B)-C(3B)	1.528(3)
C(2B)-H(2B)	1.0000
C(3B)-O(10B)	1.451(3)
C(3B)-C(4B)	1.532(3)
C(3B)-H(3B)	1.0000
C(4B)-C(5B)	1.514(3)
C(4B)-H(4B1)	0.9900
C(4B)-H(4B2)	0.9900
C(5B)-C(6B)	1.339(3)
C(5B)-C(16B)	1.508(4)
C(6B)-C(7B)	1.501(3)
C(6B)-H(6B)	0.9500
C(7B)-O(2B)	1.478(3)
C(7B)-C(8B)	1.538(3)
C(7B)-H(7B)	1.0000
C(8B)-O(3B)	1.451(3)
C(8B)-C(17B)	1.478(3)
C(8B)-C(9B)	1.528(3)
C(9B)-O(4B)	1.414(3)
C(9B)-C(10B)	1.585(3)
C(9B)-H(9B)	1.0000
C(10B)-C(11B)	1.555(3)
C(10B)-H(10B)	1.0000
C(11B)-O(5B)	1.459(3)
C(11B)-C(12B)	1.475(3)
C(11B)-C(20B)	1.510(3)
C(12B)-O(5B)	1.458(3)
C(12B)-C(13B)	1.489(3)
C(12B)-H(12B)	1.0000
C(13B)-C(14B)	1.519(3)

C(13B)-H(13C)	0.9900
C(13B)-H(13D)	0.9900
C(14B)-O(6B)	1.473(3)
C(14B)-H(14B)	1.0000
C(15B)-H(15D)	0.9800
C(15B)-H(15E)	0.9800
C(15B)-H(15F)	0.9800
C(16B)-H(16D)	0.9800
C(16B)-H(16E)	0.9800
C(16B)-H(16F)	0.9800
C(17B)-O(3B)	1.462(3)
C(17B)-C(18B)	1.496(3)
C(17B)-C(19B)	1.499(3)
C(18B)-H(18D)	0.9800
C(18B)-H(18E)	0.9800
C(18B)-H(18F)	0.9800
C(19B)-O(1B)	1.202(3)
C(19B)-O(2B)	1.345(3)
C(20B)-H(20D)	0.9800
C(20B)-H(20E)	0.9800
C(20B)-H(20F)	0.9800
C(21B)-O(7B)	1.225(3)
C(21B)-O(6B)	1.332(3)
C(21B)-C(22B)	1.489(4)
C(22B)-H(22D)	0.9800
C(22B)-H(22E)	0.9800
C(22B)-H(22F)	0.9800
C(23B)-O(9B)	1.213(3)
C(23B)-O(8B)	1.337(3)
C(23B)-C(24B)	1.488(4)
C(24B)-C(25B)	1.398(3)
C(24B)-C(29B)	1.398(4)
C(25B)-C(26B)	1.389(4)
C(25B)-H(25B)	0.9500
C(26B)-C(27B)	1.375(4)
C(26B)-H(26B)	0.9500
C(27B)-C(28B)	1.388(4)
C(28B)-C(29B)	1.381(4)
C(28B)-H(28B)	0.9500
C(29B)-H(29B)	0.9500

C(30B)-O(11B)	1.198(3)
C(30B)-O(10B)	1.363(3)
C(30B)-C(31B)	1.506(4)
C(31B)-H(31D)	0.9800
C(31B)-H(31E)	0.9800
C(31B)-H(31F)	0.9800
O(4)-H(4)	0.8400
O(4B)-H(4B3)	0.8400
O(1S)-H(1A)	0.947(11)
O(1S)-H(1B)	0.947(11)
O(2S)-H(2C)	0.947(11)
O(2S)-H(2D)	0.947(11)
O(3S)-H(3D)	0.947(11)
O(3S)-H(3C)	0.947(11)
O(4S)-H(4C)	0.947(11)
O(4S)-H(4D)	0.947(11)
O(5S)-H(5B)	0.947(11)
O(5S)-H(5A)	0.947(11)

C(15)-C(1)-C(14)	106.48(18)
C(15)-C(1)-C(2)	111.39(19)
C(14)-C(1)-C(2)	102.87(18)
C(15)-C(1)-C(10)	112.63(18)
C(14)-C(1)-C(10)	109.76(18)
C(2)-C(1)-C(10)	113.04(18)
O(8)-C(2)-C(3)	107.27(18)
O(8)-C(2)-C(1)	106.33(17)
C(3)-C(2)-C(1)	121.2(2)
O(8)-C(2)-H(2)	107.1
C(3)-C(2)-H(2)	107.1
C(1)-C(2)-H(2)	107.1
O(10)-C(3)-C(4)	107.84(18)
O(10)-C(3)-C(2)	107.92(19)
C(4)-C(3)-C(2)	112.6(2)
O(10)-C(3)-H(3)	109.5
C(4)-C(3)-H(3)	109.5
C(2)-C(3)-H(3)	109.5
C(5)-C(4)-C(3)	112.9(2)
C(5)-C(4)-H(4A)	109.0
C(3)-C(4)-H(4A)	109.0

C(5)-C(4)-H(4B)	109.0
C(3)-C(4)-H(4B)	109.0
H(4A)-C(4)-H(4B)	107.8
C(6)-C(5)-C(16)	120.9(2)
C(6)-C(5)-C(4)	123.4(2)
C(16)-C(5)-C(4)	115.7(2)
C(5)-C(6)-C(7)	127.7(2)
C(5)-C(6)-H(6)	116.2
C(7)-C(6)-H(6)	116.2
O(2)-C(7)-C(6)	106.78(19)
O(2)-C(7)-C(8)	104.64(19)
C(6)-C(7)-C(8)	115.6(2)
O(2)-C(7)-H(7)	109.9
C(6)-C(7)-H(7)	109.9
C(8)-C(7)-H(7)	109.9
O(3)-C(8)-C(17)	60.15(14)
O(3)-C(8)-C(9)	116.25(18)
C(17)-C(8)-C(9)	124.3(2)
O(3)-C(8)-C(7)	109.76(18)
C(17)-C(8)-C(7)	107.10(19)
C(9)-C(8)-C(7)	122.7(2)
O(4)-C(9)-C(8)	109.96(18)
O(4)-C(9)-C(10)	113.40(18)
C(8)-C(9)-C(10)	111.70(18)
O(4)-C(9)-H(9)	107.1
C(8)-C(9)-H(9)	107.1
C(10)-C(9)-H(9)	107.1
C(11)-C(10)-C(9)	108.10(19)
C(11)-C(10)-C(1)	111.58(18)
C(9)-C(10)-C(1)	119.55(18)
C(11)-C(10)-H(10)	105.5
C(9)-C(10)-H(10)	105.5
C(1)-C(10)-H(10)	105.5
O(5)-C(11)-C(12)	59.21(15)
O(5)-C(11)-C(20)	110.38(19)
C(12)-C(11)-C(20)	113.7(2)
O(5)-C(11)-C(10)	112.63(19)
C(12)-C(11)-C(10)	122.0(2)
C(20)-C(11)-C(10)	121.3(2)
O(5)-C(12)-C(11)	60.02(15)

O(5)-C(12)-C(13)	115.7(2)
C(11)-C(12)-C(13)	122.2(2)
O(5)-C(12)-H(12)	115.7
C(11)-C(12)-H(12)	115.7
C(13)-C(12)-H(12)	115.7
C(12)-C(13)-C(14)	112.6(2)
C(12)-C(13)-H(13A)	109.1
C(14)-C(13)-H(13A)	109.1
C(12)-C(13)-H(13B)	109.1
C(14)-C(13)-H(13B)	109.1
H(13A)-C(13)-H(13B)	107.8
O(6)-C(14)-C(13)	110.20(18)
O(6)-C(14)-C(1)	106.87(18)
C(13)-C(14)-C(1)	115.1(2)
O(6)-C(14)-H(14)	108.1
C(13)-C(14)-H(14)	108.1
C(1)-C(14)-H(14)	108.2
C(1)-C(15)-H(15A)	109.5
C(1)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(1)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(5)-C(16)-H(16A)	109.5
C(5)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(5)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
O(3)-C(17)-C(8)	58.87(14)
O(3)-C(17)-C(18)	118.95(19)
C(8)-C(17)-C(18)	130.7(2)
O(3)-C(17)-C(19)	107.72(19)
C(8)-C(17)-C(19)	105.9(2)
C(18)-C(17)-C(19)	119.0(2)
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5

H(18B)-C(18)-H(18C)	109.5
O(1)-C(19)-O(2)	122.5(2)
O(1)-C(19)-C(17)	127.6(2)
O(2)-C(19)-C(17)	109.9(2)
C(11)-C(20)-H(20A)	109.5
C(11)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(11)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(7)-C(21)-O(6)	124.1(2)
O(7)-C(21)-C(22)	125.0(2)
O(6)-C(21)-C(22)	110.9(2)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
O(9)-C(23)-O(8)	123.9(2)
O(9)-C(23)-C(24)	124.6(2)
O(8)-C(23)-C(24)	111.5(2)
C(25)-C(24)-C(29)	119.7(2)
C(25)-C(24)-C(23)	121.9(2)
C(29)-C(24)-C(23)	118.5(2)
C(24)-C(25)-C(26)	120.1(2)
C(24)-C(25)-H(25)	120.0
C(26)-C(25)-H(25)	120.0
C(27)-C(26)-C(25)	118.5(2)
C(27)-C(26)-H(26)	120.7
C(25)-C(26)-H(26)	120.7
C(26)-C(27)-C(28)	122.6(2)
C(26)-C(27)-Br(1)	119.36(19)
C(28)-C(27)-Br(1)	118.0(2)
C(29)-C(28)-C(27)	117.9(2)
C(29)-C(28)-H(28)	121.1
C(27)-C(28)-H(28)	121.1
C(28)-C(29)-C(24)	121.2(2)
C(28)-C(29)-H(29)	119.4
C(24)-C(29)-H(29)	119.4

O(11)-C(30)-O(10)	123.4(2)
O(11)-C(30)-C(31)	126.0(2)
O(10)-C(30)-C(31)	110.6(2)
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(15B)-C(1B)-C(14B)	105.60(18)
C(15B)-C(1B)-C(2B)	112.02(18)
C(14B)-C(1B)-C(2B)	104.10(18)
C(15B)-C(1B)-C(10B)	112.62(18)
C(14B)-C(1B)-C(10B)	110.23(18)
C(2B)-C(1B)-C(10B)	111.74(18)
O(8B)-C(2B)-C(3B)	107.34(17)
O(8B)-C(2B)-C(1B)	106.27(17)
C(3B)-C(2B)-C(1B)	119.65(19)
O(8B)-C(2B)-H(2B)	107.7
C(3B)-C(2B)-H(2B)	107.7
C(1B)-C(2B)-H(2B)	107.7
O(10B)-C(3B)-C(2B)	107.67(18)
O(10B)-C(3B)-C(4B)	109.76(17)
C(2B)-C(3B)-C(4B)	113.2(2)
O(10B)-C(3B)-H(3B)	108.7
C(2B)-C(3B)-H(3B)	108.7
C(4B)-C(3B)-H(3B)	108.7
C(5B)-C(4B)-C(3B)	111.52(19)
C(5B)-C(4B)-H(4B1)	109.3
C(3B)-C(4B)-H(4B1)	109.3
C(5B)-C(4B)-H(4B2)	109.3
C(3B)-C(4B)-H(4B2)	109.3
H(4B1)-C(4B)-H(4B2)	108.0
C(6B)-C(5B)-C(16B)	120.4(2)
C(6B)-C(5B)-C(4B)	123.6(2)
C(16B)-C(5B)-C(4B)	116.1(2)
C(5B)-C(6B)-C(7B)	126.8(2)
C(5B)-C(6B)-H(6B)	116.6
C(7B)-C(6B)-H(6B)	116.6
O(2B)-C(7B)-C(6B)	105.11(18)

O(2B)-C(7B)-C(8B)	104.20(19)
C(6B)-C(7B)-C(8B)	117.8(2)
O(2B)-C(7B)-H(7B)	109.8
C(6B)-C(7B)-H(7B)	109.8
C(8B)-C(7B)-H(7B)	109.8
O(3B)-C(8B)-C(17B)	59.86(14)
O(3B)-C(8B)-C(9B)	115.24(17)
C(17B)-C(8B)-C(9B)	121.8(2)
O(3B)-C(8B)-C(7B)	110.32(19)
C(17B)-C(8B)-C(7B)	106.74(19)
C(9B)-C(8B)-C(7B)	125.1(2)
O(4B)-C(9B)-C(8B)	110.53(18)
O(4B)-C(9B)-C(10B)	113.75(18)
C(8B)-C(9B)-C(10B)	113.05(19)
O(4B)-C(9B)-H(9B)	106.3
C(8B)-C(9B)-H(9B)	106.3
C(10B)-C(9B)-H(9B)	106.3
C(11B)-C(10B)-C(9B)	109.50(18)
C(11B)-C(10B)-C(1B)	111.94(17)
C(9B)-C(10B)-C(1B)	118.85(18)
C(11B)-C(10B)-H(10B)	105.1
C(9B)-C(10B)-H(10B)	105.1
C(1B)-C(10B)-H(10B)	105.1
O(5B)-C(11B)-C(12B)	59.59(15)
O(5B)-C(11B)-C(20B)	109.50(18)
C(12B)-C(11B)-C(20B)	114.9(2)
O(5B)-C(11B)-C(10B)	112.66(19)
C(12B)-C(11B)-C(10B)	121.7(2)
C(20B)-C(11B)-C(10B)	120.7(2)
O(5B)-C(12B)-C(11B)	59.64(15)
O(5B)-C(12B)-C(13B)	115.3(2)
C(11B)-C(12B)-C(13B)	122.5(2)
O(5B)-C(12B)-H(12B)	115.8
C(11B)-C(12B)-H(12B)	115.8
C(13B)-C(12B)-H(12B)	115.8
C(12B)-C(13B)-C(14B)	113.08(19)
C(12B)-C(13B)-H(13C)	109.0
C(14B)-C(13B)-H(13C)	109.0
C(12B)-C(13B)-H(13D)	109.0
C(14B)-C(13B)-H(13D)	109.0

H(13C)-C(13B)-H(13D)	107.8
O(6B)-C(14B)-C(13B)	109.87(19)
O(6B)-C(14B)-C(1B)	107.45(18)
C(13B)-C(14B)-C(1B)	114.79(19)
O(6B)-C(14B)-H(14B)	108.2
C(13B)-C(14B)-H(14B)	108.2
C(1B)-C(14B)-H(14B)	108.2
C(1B)-C(15B)-H(15D)	109.5
C(1B)-C(15B)-H(15E)	109.5
H(15D)-C(15B)-H(15E)	109.5
C(1B)-C(15B)-H(15F)	109.5
H(15D)-C(15B)-H(15F)	109.5
H(15E)-C(15B)-H(15F)	109.5
C(5B)-C(16B)-H(16D)	109.5
C(5B)-C(16B)-H(16E)	109.5
H(16D)-C(16B)-H(16E)	109.5
C(5B)-C(16B)-H(16F)	109.5
H(16D)-C(16B)-H(16F)	109.5
H(16E)-C(16B)-H(16F)	109.5
O(3B)-C(17B)-C(8B)	59.15(14)
O(3B)-C(17B)-C(18B)	119.33(19)
C(8B)-C(17B)-C(18B)	130.8(2)
O(3B)-C(17B)-C(19B)	107.71(18)
C(8B)-C(17B)-C(19B)	106.48(19)
C(18B)-C(17B)-C(19B)	118.3(2)
C(17B)-C(18B)-H(18D)	109.5
C(17B)-C(18B)-H(18E)	109.5
H(18D)-C(18B)-H(18E)	109.5
C(17B)-C(18B)-H(18F)	109.5
H(18D)-C(18B)-H(18F)	109.5
H(18E)-C(18B)-H(18F)	109.5
O(1B)-C(19B)-O(2B)	122.6(2)
O(1B)-C(19B)-C(17B)	127.5(2)
O(2B)-C(19B)-C(17B)	109.9(2)
C(11B)-C(20B)-H(20D)	109.5
C(11B)-C(20B)-H(20E)	109.5
H(20D)-C(20B)-H(20E)	109.5
C(11B)-C(20B)-H(20F)	109.5
H(20D)-C(20B)-H(20F)	109.5
H(20E)-C(20B)-H(20F)	109.5

O(7B)-C(21B)-O(6B)	123.6(2)
O(7B)-C(21B)-C(22B)	124.6(2)
O(6B)-C(21B)-C(22B)	111.8(2)
C(21B)-C(22B)-H(22D)	109.5
C(21B)-C(22B)-H(22E)	109.5
H(22D)-C(22B)-H(22E)	109.5
C(21B)-C(22B)-H(22F)	109.5
H(22D)-C(22B)-H(22F)	109.5
H(22E)-C(22B)-H(22F)	109.5
O(9B)-C(23B)-O(8B)	123.7(2)
O(9B)-C(23B)-C(24B)	125.0(2)
O(8B)-C(23B)-C(24B)	111.3(2)
C(25B)-C(24B)-C(29B)	119.8(2)
C(25B)-C(24B)-C(23B)	121.0(2)
C(29B)-C(24B)-C(23B)	119.2(2)
C(26B)-C(25B)-C(24B)	119.6(2)
C(26B)-C(25B)-H(25B)	120.2
C(24B)-C(25B)-H(25B)	120.2
C(27B)-C(26B)-C(25B)	119.3(2)
C(27B)-C(26B)-H(26B)	120.4
C(25B)-C(26B)-H(26B)	120.4
C(26B)-C(27B)-C(28B)	122.3(2)
C(26B)-C(27B)-Br(1B)	118.72(19)
C(28B)-C(27B)-Br(1B)	118.95(19)
C(29B)-C(28B)-C(27B)	118.3(2)
C(29B)-C(28B)-H(28B)	120.8
C(27B)-C(28B)-H(28B)	120.8
C(28B)-C(29B)-C(24B)	120.6(2)
C(28B)-C(29B)-H(29B)	119.7
C(24B)-C(29B)-H(29B)	119.7
O(11B)-C(30B)-O(10B)	124.1(2)
O(11B)-C(30B)-C(31B)	126.7(2)
O(10B)-C(30B)-C(31B)	109.2(2)
C(30B)-C(31B)-H(31D)	109.5
C(30B)-C(31B)-H(31E)	109.5
H(31D)-C(31B)-H(31E)	109.5
C(30B)-C(31B)-H(31F)	109.5
H(31D)-C(31B)-H(31F)	109.5
H(31E)-C(31B)-H(31F)	109.5
C(19)-O(2)-C(7)	111.93(18)

C(8)-O(3)-C(17)	60.98(15)
C(9)-O(4)-H(4)	109.5
C(12)-O(5)-C(11)	60.76(15)
C(21)-O(6)-C(14)	117.45(18)
C(23)-O(8)-C(2)	119.93(18)
C(30)-O(10)-C(3)	117.75(19)
C(19B)-O(2B)-C(7B)	112.44(17)
C(8B)-O(3B)-C(17B)	60.98(14)
C(9B)-O(4B)-H(4B3)	109.5
C(12B)-O(5B)-C(11B)	60.77(14)
C(21B)-O(6B)-C(14B)	117.08(19)
C(23B)-O(8B)-C(2B)	119.99(18)
C(30B)-O(10B)-C(3B)	114.66(19)
H(1A)-O(1S)-H(1B)	100.9(13)
H(2C)-O(2S)-H(2D)	100.9(13)
H(3D)-O(3S)-H(3C)	100.9(13)
H(4C)-O(4S)-H(4D)	100.9(13)
H(5B)-O(5S)-H(5A)	100.9(13)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *p*-bromobenzoate **8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	32(1)	22(1)	18(1)	7(1)	12(1)	2(1)
Br(1B)	28(1)	30(1)	14(1)	0(1)	8(1)	-4(1)
C(1)	13(1)	14(1)	8(1)	0(1)	3(1)	2(1)
C(2)	15(1)	13(1)	10(1)	0(1)	4(1)	-2(1)
C(3)	18(1)	15(1)	12(1)	4(1)	3(1)	4(1)
C(4)	15(1)	26(1)	16(1)	1(1)	2(1)	1(1)
C(5)	10(1)	22(1)	21(2)	-5(1)	3(1)	-6(1)
C(6)	12(1)	15(1)	25(2)	-1(1)	4(1)	-4(1)
C(7)	14(1)	17(1)	19(1)	5(1)	8(1)	1(1)
C(8)	12(1)	12(1)	17(1)	0(1)	5(1)	2(1)
C(9)	12(1)	12(1)	12(1)	2(1)	2(1)	1(1)
C(10)	13(1)	10(1)	12(1)	0(1)	4(1)	0(1)
C(11)	17(1)	13(1)	15(1)	2(1)	4(1)	2(1)
C(12)	14(1)	20(1)	21(1)	3(1)	4(1)	3(1)
C(13)	13(1)	19(1)	21(1)	-2(1)	7(1)	-1(1)
C(14)	17(1)	9(1)	16(1)	-1(1)	6(1)	0(1)
C(15)	20(1)	13(1)	15(1)	-1(1)	7(1)	-1(1)
C(16)	32(2)	29(2)	22(2)	-4(1)	9(1)	-10(1)
C(17)	16(1)	14(1)	18(1)	2(1)	9(1)	3(1)
C(18)	21(1)	16(1)	16(1)	4(1)	8(1)	2(1)
C(19)	19(1)	18(1)	21(2)	4(1)	9(1)	2(1)
C(20)	15(1)	28(1)	17(1)	5(1)	5(1)	5(1)
C(21)	19(1)	15(1)	22(1)	-2(1)	6(1)	3(1)
C(22)	33(2)	17(1)	28(2)	-7(1)	14(1)	-2(1)
C(23)	16(1)	20(1)	14(1)	0(1)	4(1)	2(1)
C(24)	16(1)	20(1)	12(1)	3(1)	3(1)	1(1)
C(25)	22(1)	24(2)	13(1)	-1(1)	5(1)	3(1)
C(26)	30(2)	19(1)	17(1)	1(1)	8(1)	-2(1)
C(27)	16(1)	24(1)	14(1)	10(1)	6(1)	3(1)
C(28)	25(1)	25(1)	14(1)	-2(1)	8(1)	-2(1)
C(29)	30(2)	16(1)	20(1)	-3(1)	9(1)	-2(1)
C(30)	13(1)	17(1)	23(2)	-1(1)	0(1)	-1(1)
C(31)	23(1)	20(1)	39(2)	4(1)	4(1)	4(1)
C(1B)	14(1)	12(1)	12(1)	-1(1)	6(1)	-2(1)
C(2B)	19(1)	13(1)	10(1)	-1(1)	4(1)	0(1)

C(3B)	19(1)	14(1)	10(1)	-3(1)	4(1)	0(1)
C(4B)	14(1)	22(1)	15(1)	1(1)	3(1)	1(1)
C(5B)	13(1)	18(1)	21(1)	2(1)	6(1)	5(1)
C(6B)	15(1)	15(1)	20(1)	-1(1)	7(1)	3(1)
C(7B)	14(1)	17(1)	16(1)	-1(1)	8(1)	2(1)
C(8B)	16(1)	12(1)	15(1)	-1(1)	3(1)	-3(1)
C(9B)	15(1)	12(1)	14(1)	0(1)	5(1)	-2(1)
C(10B)	15(1)	10(1)	15(1)	-1(1)	6(1)	1(1)
C(11B)	18(1)	15(1)	14(1)	-3(1)	5(1)	-4(1)
C(12B)	14(1)	17(1)	20(1)	0(1)	4(1)	-3(1)
C(13B)	11(1)	18(1)	20(1)	0(1)	6(1)	-1(1)
C(14B)	18(1)	11(1)	16(1)	-1(1)	8(1)	-1(1)
C(15B)	18(1)	14(1)	13(1)	1(1)	6(1)	2(1)
C(16B)	38(2)	18(1)	26(2)	4(1)	12(1)	10(1)
C(17B)	17(1)	17(1)	15(1)	-1(1)	6(1)	-2(1)
C(18B)	20(1)	27(1)	15(1)	4(1)	8(1)	2(1)
C(19B)	20(1)	15(1)	18(1)	-1(1)	7(1)	-1(1)
C(20B)	15(1)	30(2)	16(1)	2(1)	1(1)	-6(1)
C(21B)	17(1)	16(1)	18(1)	1(1)	3(1)	-1(1)
C(22B)	28(1)	17(1)	25(2)	1(1)	12(1)	-2(1)
C(23B)	12(1)	17(1)	21(1)	4(1)	4(1)	0(1)
C(24B)	12(1)	18(1)	12(1)	2(1)	0(1)	1(1)
C(25B)	22(1)	19(1)	15(1)	5(1)	3(1)	-1(1)
C(26B)	24(1)	16(1)	18(1)	0(1)	5(1)	-1(1)
C(27B)	15(1)	29(1)	10(1)	0(1)	3(1)	0(1)
C(28B)	22(1)	22(1)	16(1)	5(1)	2(1)	-2(1)
C(29B)	20(1)	18(1)	19(1)	3(1)	2(1)	0(1)
C(30B)	16(1)	20(2)	22(2)	-6(1)	3(1)	-4(1)
C(31B)	24(2)	30(2)	29(2)	-12(1)	7(1)	-7(1)
O(1)	21(1)	38(1)	24(1)	7(1)	11(1)	-1(1)
O(2)	12(1)	30(1)	20(1)	3(1)	7(1)	-3(1)
O(3)	18(1)	14(1)	17(1)	2(1)	7(1)	3(1)
O(4)	21(1)	13(1)	14(1)	1(1)	10(1)	4(1)
O(5)	23(1)	17(1)	24(1)	4(1)	11(1)	6(1)
O(6)	20(1)	10(1)	19(1)	-2(1)	8(1)	-1(1)
O(7)	32(1)	21(1)	27(1)	-3(1)	20(1)	0(1)
O(8)	19(1)	15(1)	10(1)	3(1)	4(1)	1(1)
O(9)	39(1)	19(1)	16(1)	-2(1)	10(1)	-8(1)
O(10)	26(1)	16(1)	22(1)	6(1)	11(1)	8(1)
O(11)	38(1)	33(1)	25(1)	2(1)	9(1)	14(1)

O(1B)	28(1)	33(1)	20(1)	3(1)	15(1)	8(1)
O(2B)	17(1)	21(1)	17(1)	0(1)	10(1)	3(1)
O(3B)	19(1)	18(1)	13(1)	-4(1)	7(1)	-4(1)
O(4B)	20(1)	11(1)	21(1)	-1(1)	9(1)	-6(1)
O(5B)	20(1)	19(1)	21(1)	-6(1)	9(1)	-8(1)
O(6B)	18(1)	11(1)	14(1)	-1(1)	8(1)	-2(1)
O(7B)	37(1)	18(1)	25(1)	0(1)	20(1)	-2(1)
O(8B)	19(1)	15(1)	12(1)	2(1)	5(1)	1(1)
O(9B)	33(1)	15(1)	20(1)	2(1)	9(1)	4(1)
O(10B)	18(1)	20(1)	17(1)	-7(1)	5(1)	-5(1)
O(11B)	23(1)	28(1)	23(1)	-8(1)	9(1)	-10(1)
O(1S)	29(1)	20(1)	28(1)	-3(1)	8(1)	-7(1)
O(2S)	27(1)	28(1)	29(1)	8(1)	9(1)	5(1)
O(3S)	41(1)	36(1)	30(1)	0(1)	16(1)	11(1)
O(4S)	38(1)	43(1)	29(1)	0(1)	10(1)	8(1)
O(5S)	42(1)	30(1)	37(1)	8(1)	18(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for *p*-bromobenzoate **8**.

	x	y	z	U(eq)
H(2)	1407	6144	5242	15
H(3)	2544	5200	4472	18
H(4A)	3948	5739	5866	23
H(4B)	4627	5555	5222	23
H(6)	3261	7372	4345	21
H(7)	3744	5806	3956	19
H(9)	338	5717	2792	15
H(10)	556	6576	3993	14
H(12)	-3428	6297	3200	22
H(13A)	-2998	5514	4232	20
H(13B)	-3131	6377	4510	20
H(14)	-1219	5656	5208	17
H(15A)	175	4456	4140	24
H(15B)	-1325	4776	3812	24
H(15C)	-873	4522	4632	24
H(16A)	3496	7711	5482	41
H(16B)	4511	7168	6040	41
H(16C)	2907	7067	5919	41
H(18A)	705	6305	1758	26
H(18B)	2063	5913	1648	26
H(18C)	1792	6817	1488	26
H(20A)	-1585	5839	2324	30
H(20B)	-883	6673	2366	30
H(20C)	-2476	6607	2304	30
H(22A)	-845	8099	6081	37
H(22B)	-191	8078	5409	37
H(22C)	578	7675	6143	37
H(25)	927	3947	6304	23
H(26)	496	3109	7182	26
H(28)	141	4966	8414	25
H(29)	586	5788	7541	26
H(31A)	3939	2814	5229	42
H(31B)	2738	3075	5578	42
H(31C)	4265	3332	5936	42

H(2B)	6472	5135	-87	17
H(3B)	5037	4054	266	17
H(4B1)	3919	5137	-858	21
H(4B2)	3032	4675	-416	21
H(6B)	4715	5835	1181	19
H(7B)	3918	4246	860	18
H(9B)	7234	3504	1845	16
H(10B)	7476	4828	1159	15
H(12B)	11211	3953	1600	21
H(13C)	10531	3839	347	19
H(13D)	11009	4720	493	19
H(14B)	8889	4544	-396	17
H(15D)	8137	3300	-369	22
H(15E)	6993	3051	24	22
H(15F)	8552	3065	456	22
H(16D)	4250	6724	295	40
H(16E)	3335	6452	-462	40
H(16F)	4953	6435	-313	40
H(18D)	5497	3174	2955	30
H(18E)	6163	3879	3460	30
H(18F)	6981	3476	2949	30
H(20D)	9132	3249	2256	32
H(20E)	8831	4054	2597	32
H(20F)	10348	3836	2574	32
H(22D)	9545	7111	-159	34
H(22E)	9072	6824	528	34
H(22F)	7993	6884	-228	34
H(25B)	6476	3738	-1983	23
H(26B)	6756	3442	-3122	24
H(28B)	7095	5731	-3527	24
H(29B)	6821	6030	-2392	24
H(31D)	3100	2087	-1068	41
H(31E)	4280	2454	-1379	41
H(31F)	2765	2780	-1634	41
H(4)	1948	4864	3198	22
H(4B3)	5654	2883	1180	25
H(1A)	4002(17)	2369(15)	1814(17)	52
H(1B)	4560(30)	1699(10)	1526(17)	52
H(4C)	1720(20)	2474(17)	1780(13)	52
H(4D)	2560(30)	2682(19)	2481(6)	52

H(5B)	120(30)	6552(12)	8736(15)	52
H(5A)	860(20)	6940(17)	8277(15)	52
H(3D)	6670(30)	8251(12)	6261(13)	52
H(3C)	7200(30)	7462(13)	6304(13)	52
H(2C)	6751(11)	2047(19)	2126(15)	52
H(2D)	7840(30)	1713(18)	2684(11)	52