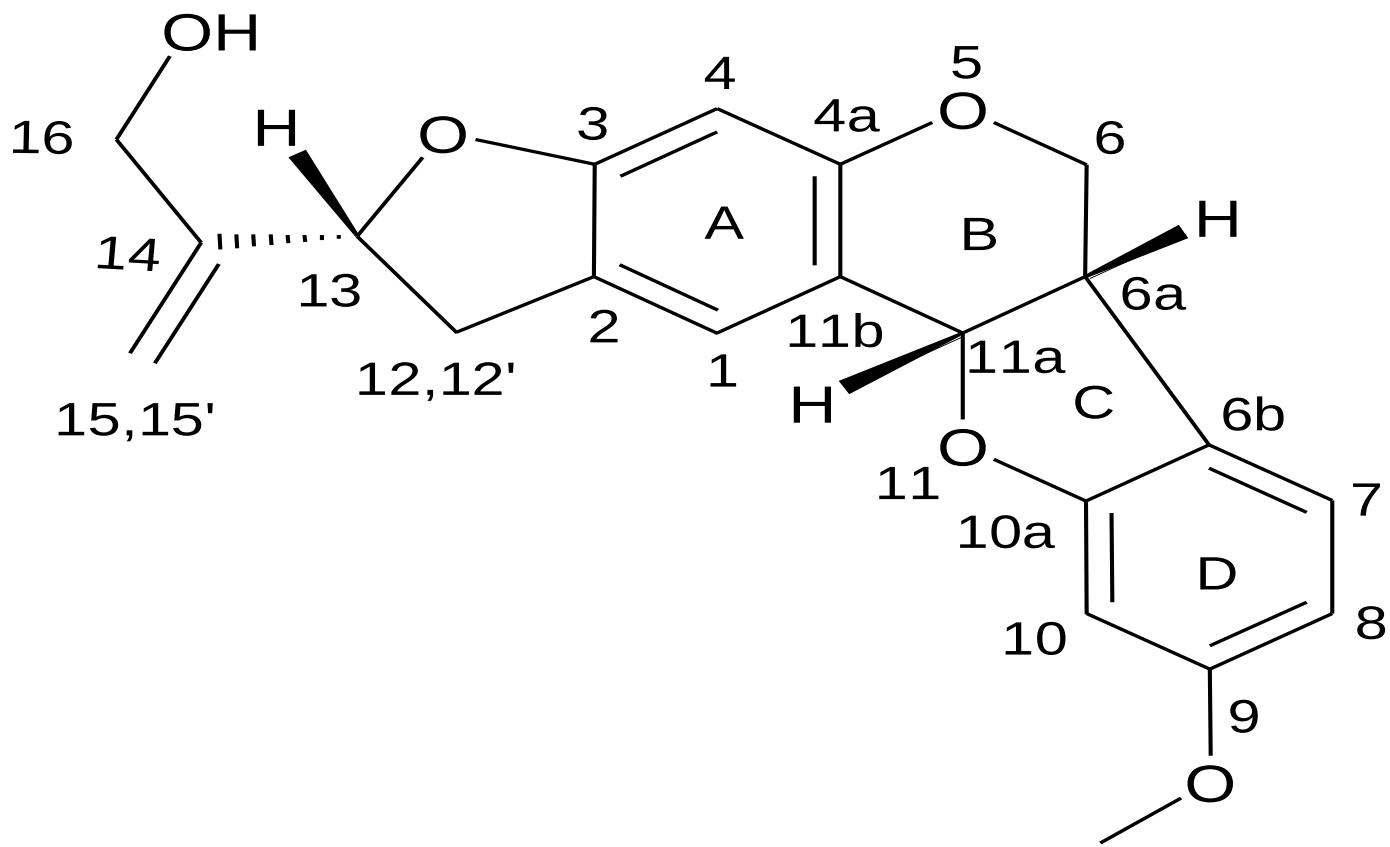
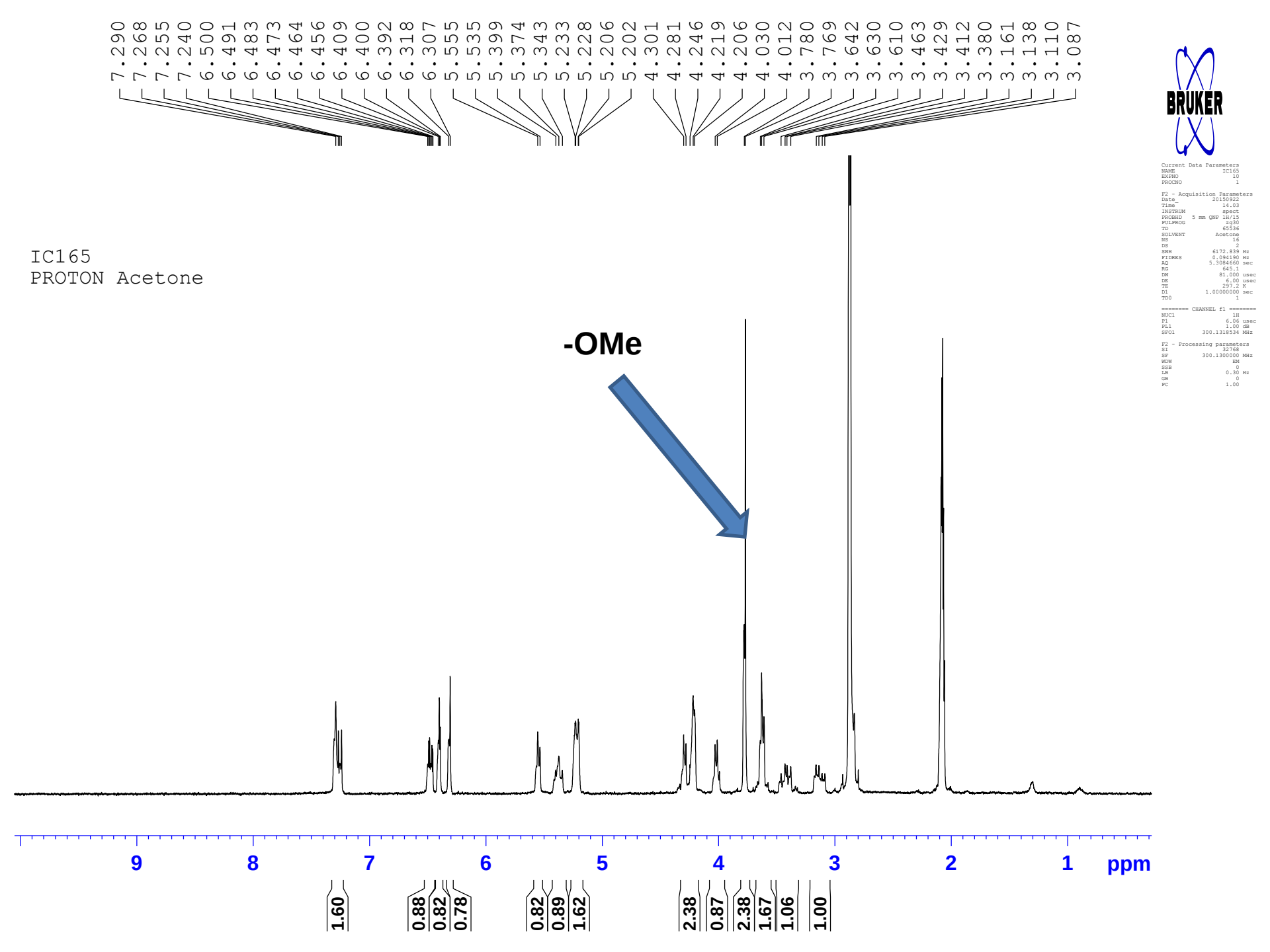
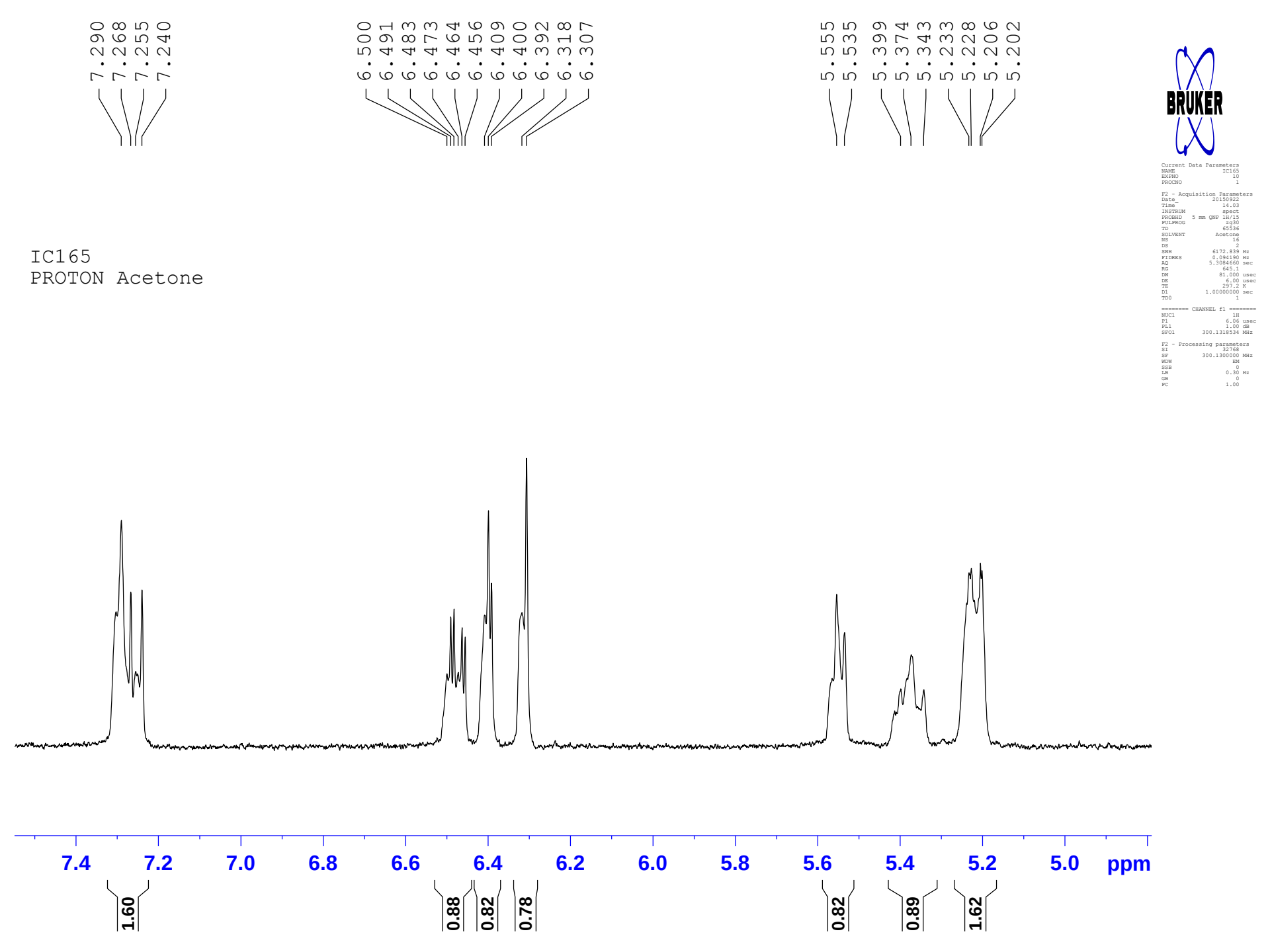
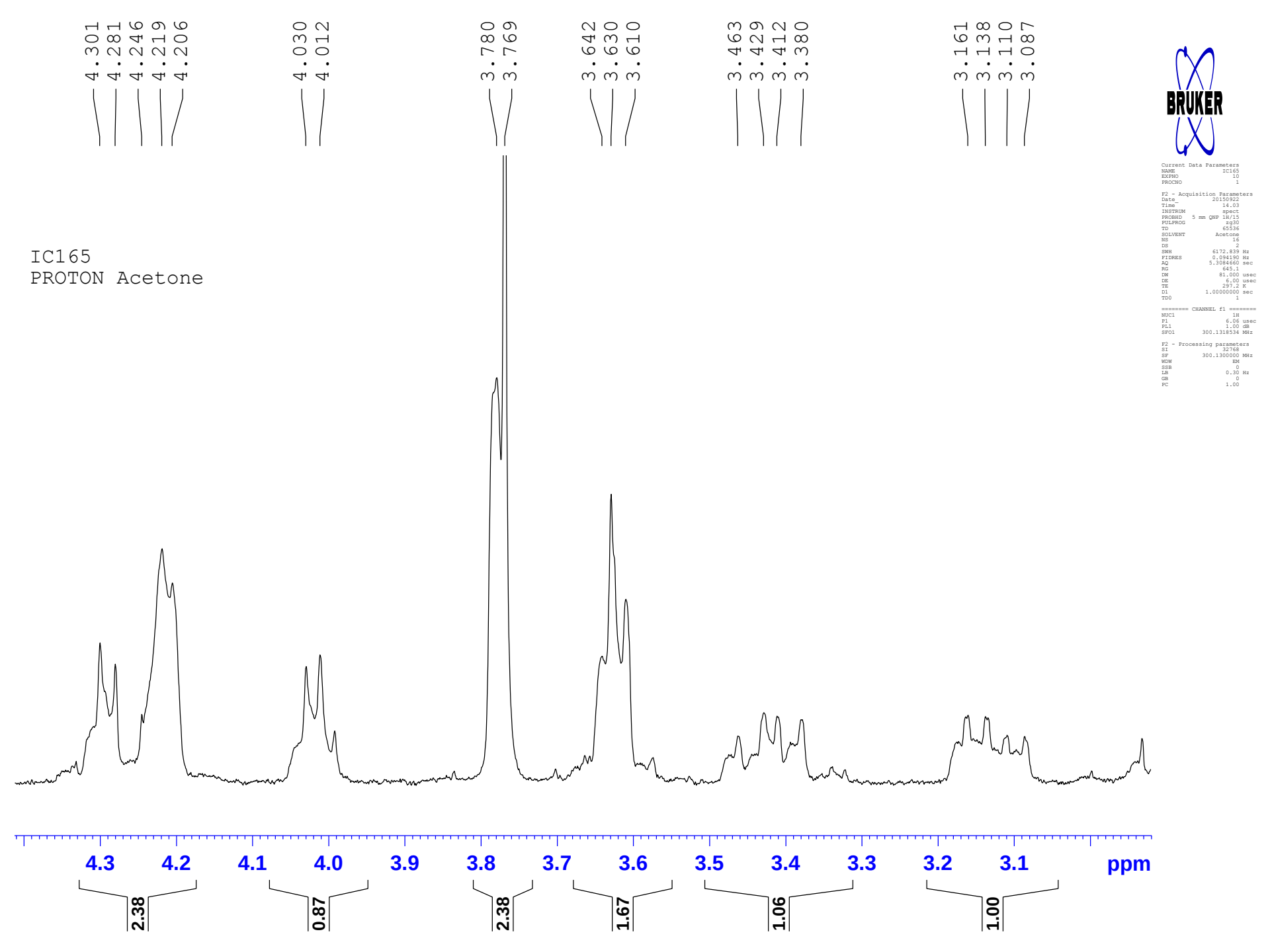


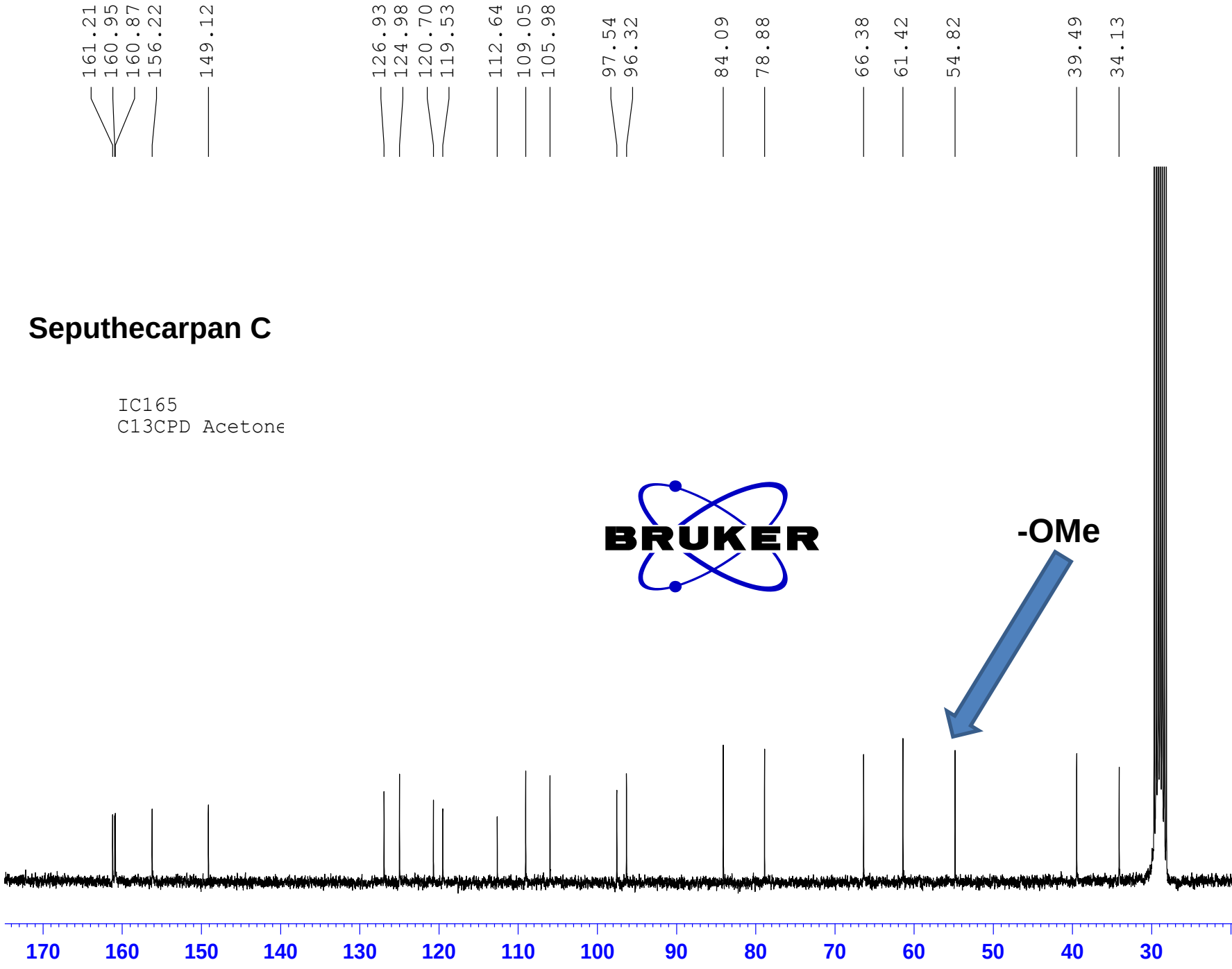
1

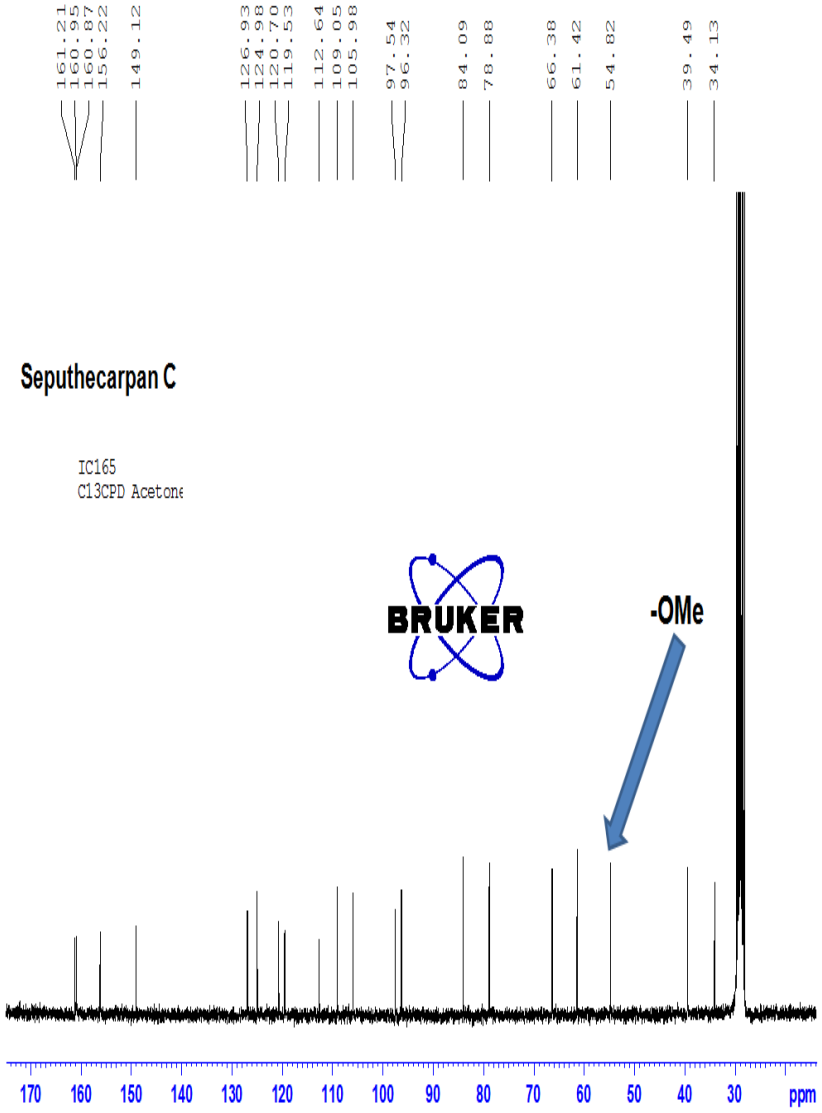
Seputhecarpan C

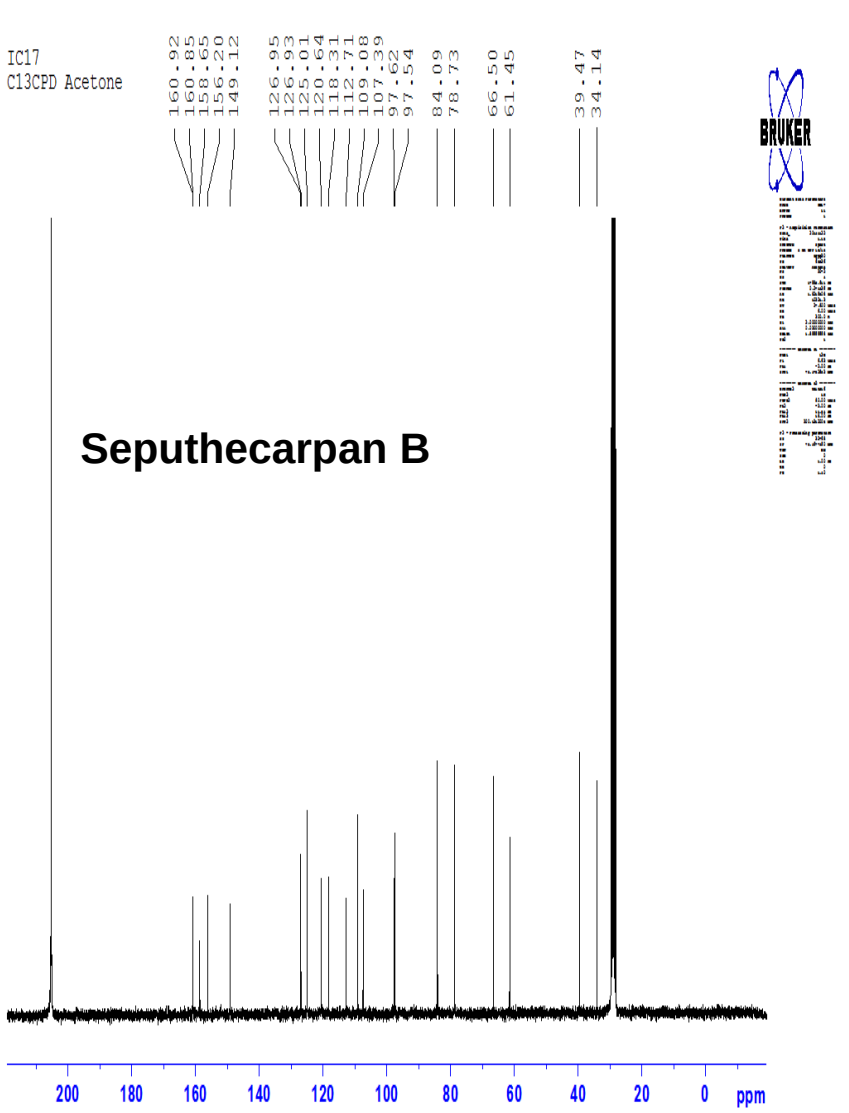

7.290
7.268
7.255
7.240
6.500
6.491
6.483
6.473
6.464
6.456
6.409
6.400
6.392
6.318
6.307
5.555
5.535
5.399
5.374
5.343
5.233
5.228
5.206
5.202
4.301
4.281
4.246
4.219
4.206
4.030
4.012
3.780
3.769
3.642
3.630
3.610
3.463
3.429
3.412
3.380
3.161
3.138
3.110
3.087
BRUKER
Current Data Parameters
NAME IC165
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150922
Time 14.03
INSTRUM spect
PROBHD 5 mm QNP 1H/15
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 645.1
DW 81.000 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.06 usec
PL1 1.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
IC165
PROTON Acetone
-OMe
9
8
7
6
5
4
3
2
1
ppm
1.60
0.88
0.82
0.78
0.82
0.89
1.62
2.38
0.87
2.38
1.67
1.06
1.00

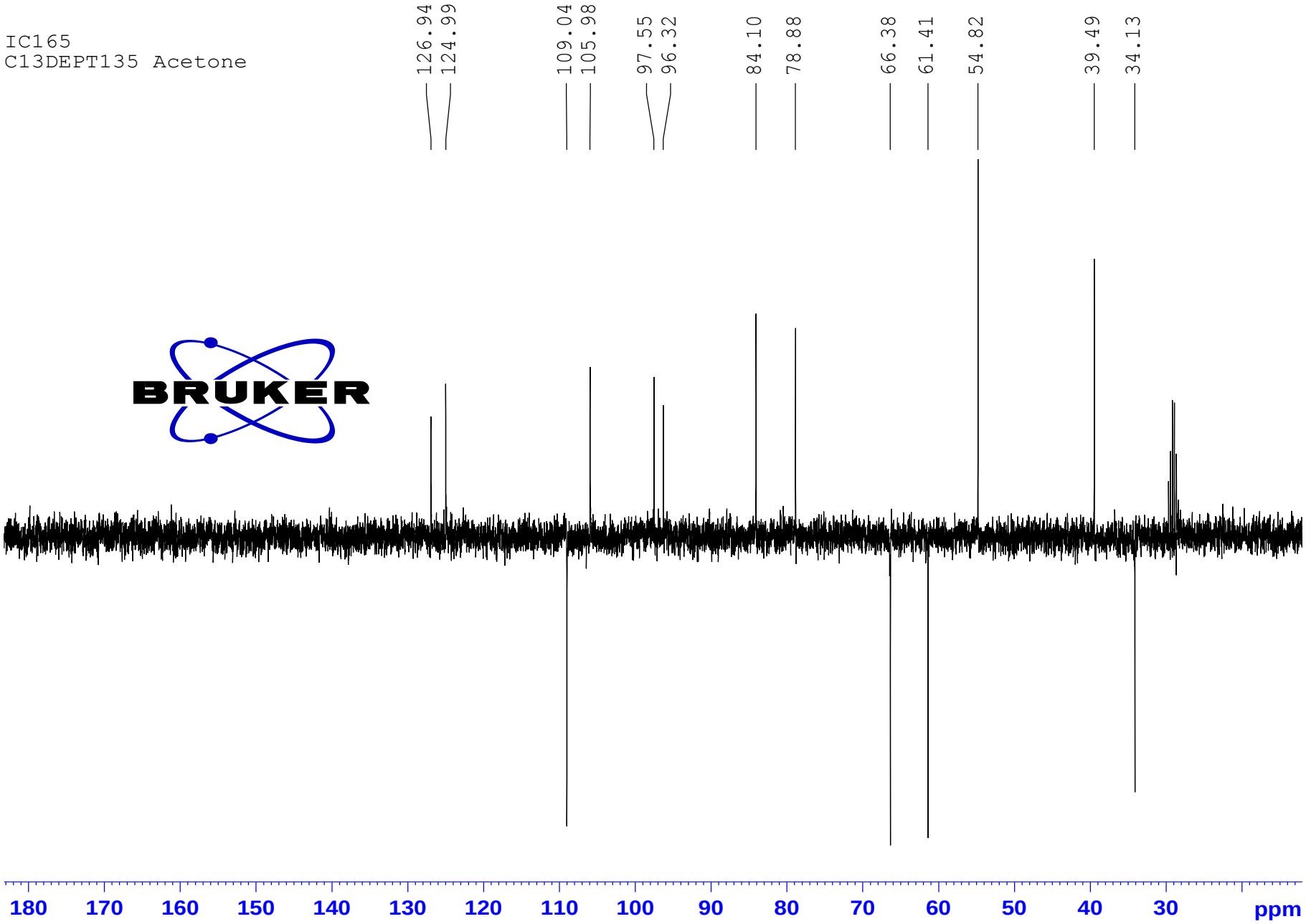

7.290
7.268
7.255
7.240
6.500
6.491
6.483
6.473
6.464
6.456
6.409
6.400
6.392
6.318
6.307
5.555
5.535
5.399
5.374
5.343
5.233
5.228
5.206
5.202
BRUKER
Current Data Parameters
NAME IC165
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150922
Time 14.03
INSTRUM spect
PROBHD 5 mm QNP 1H/15
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 645.1
DW 81.000 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.06 usec
PL1 1.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
IC165
PROTON Acetone
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
ppm
1.60
0.88
0.82
0.78
0.82
0.89
1.62

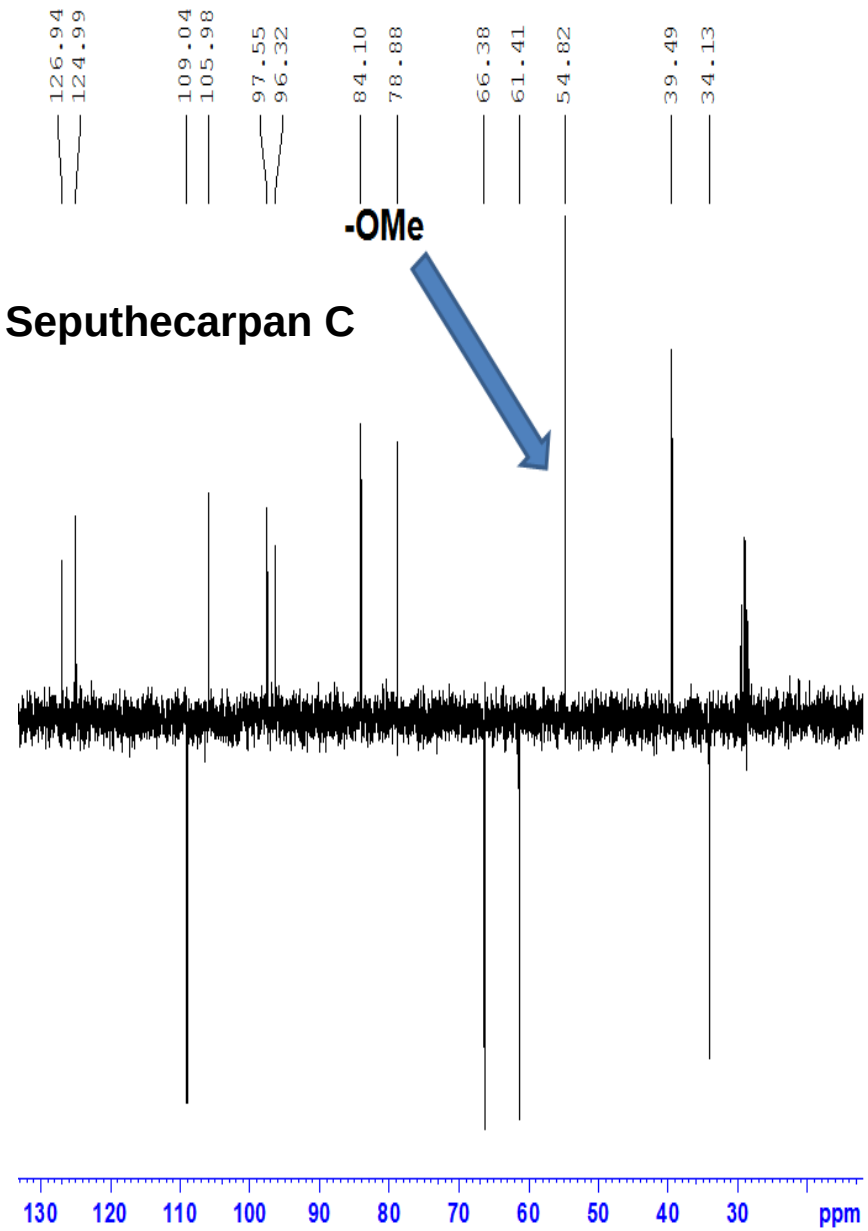

4.301
4.281
4.246
4.219
4.206
4.030
4.012
3.780
3.769
3.642
3.630
3.610
3.463
3.429
3.412
3.380
3.161
3.138
3.110
3.087
IC165
PROTON Acetone
Current Data Parameters
NAME IC165
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150922
Time 14.03
INSTRUM spect
PROBHD 5 mm QNP 1H/15
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 645.1
DW 81.000 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 6.06 usec
PL1 1.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
4.3
4.2
4.1
4.0
3.9
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
ppm
2.38
0.87
2.38
1.67
1.06
1.00

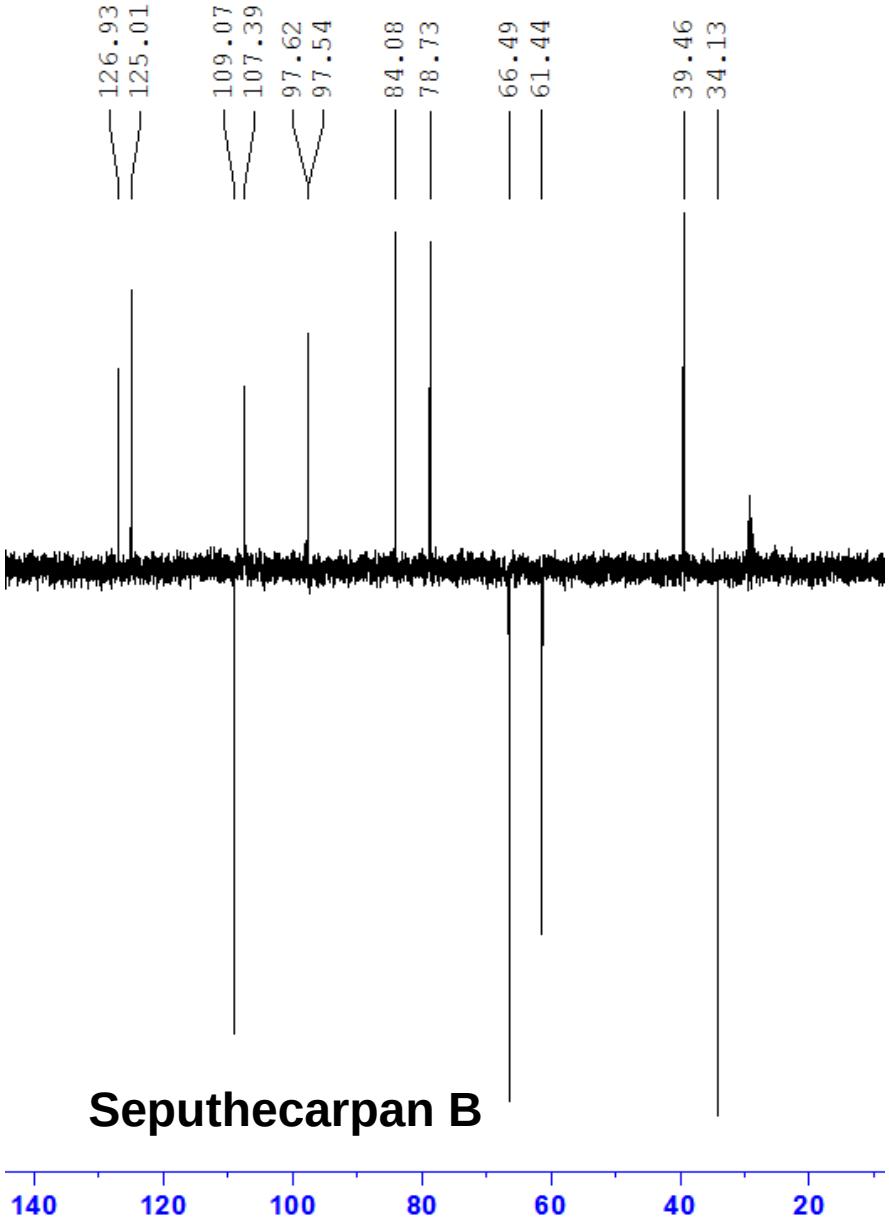

161.21
160.95
160.87
156.22
149.12
126.93
124.98
120.70
119.53
112.64
109.05
105.98
97.54
96.32
84.09
78.88
66.38
61.42
54.82
39.49
34.13
Seputhecarpan C
IC165
C13CPD Acetone
BRUKER
-OMe
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

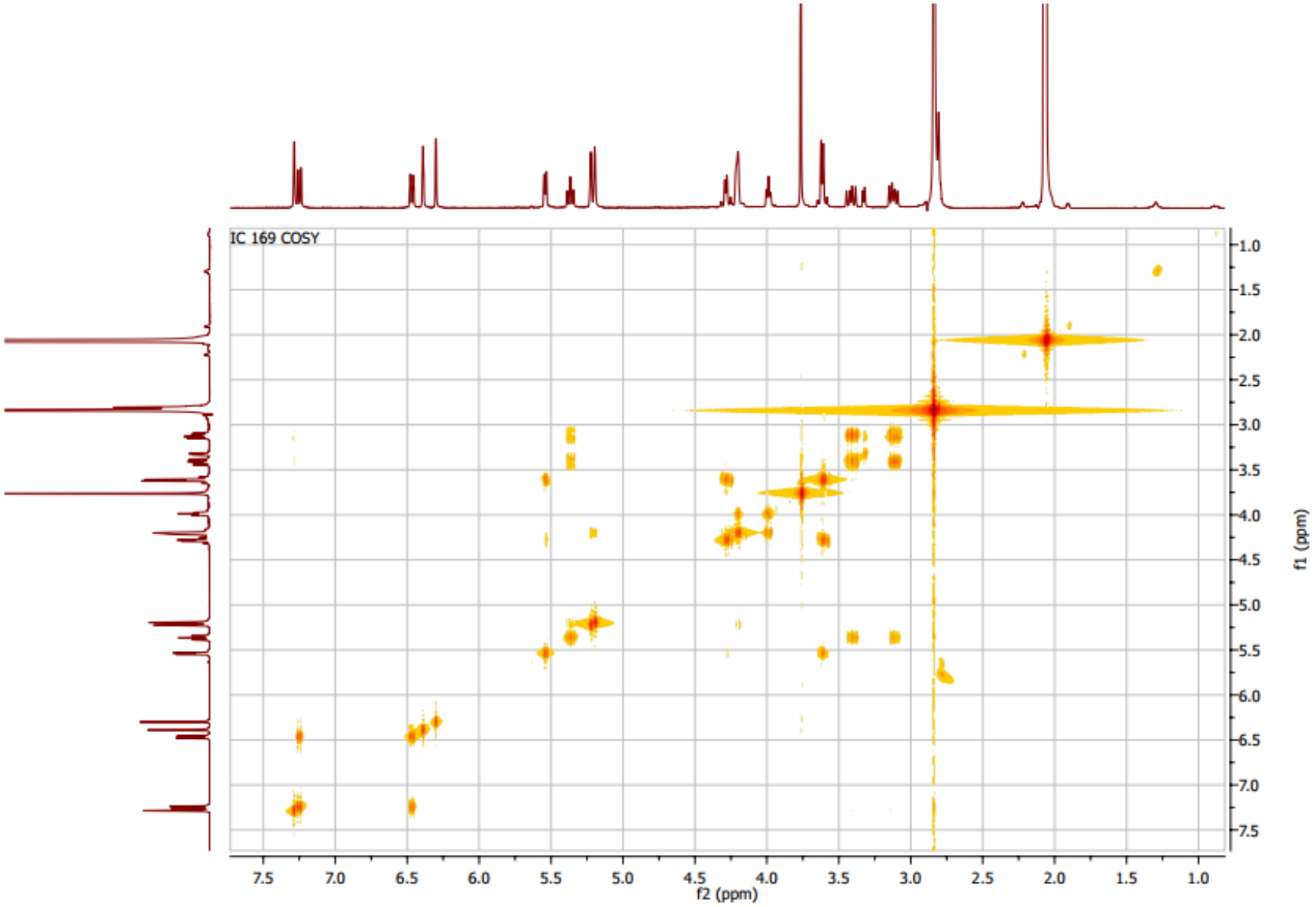

161.21
160.95
160.87
156.22
149.12
126.93
124.98
120.70
119.53
112.64
109.05
105.98
97.54
96.32
84.09
78.88
66.38
61.42
54.82
39.49
34.13
Seputhecarpan C
IC165
C13CPD Acetone
BRUKER
-OMe
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm


IC17
C13CPD Acetone
160.92
160.85
158.65
156.20
149.12
126.95
126.93
125.01
120.64
118.31
112.71
109.08
107.39
97.62
97.54
84.09
78.73
66.50
61.45
39.47
34.14
BRUKER
Seputhecarpan B
200
180
160
140
120
100
80
60
40
20
0
ppm

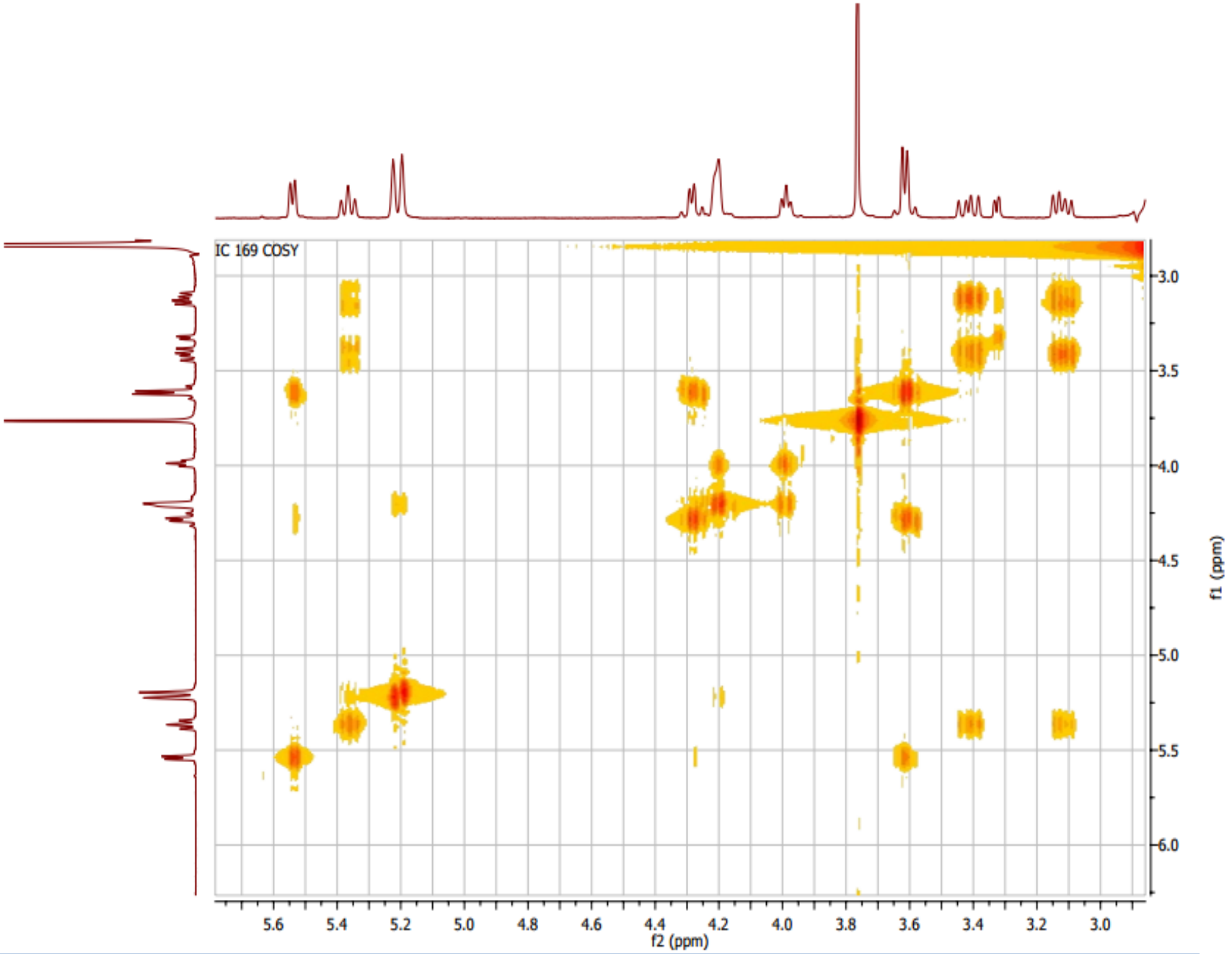

IC165
C13DEPT135 Acetone
126.94
124.99
109.04
105.98
97.55
96.32
84.10
78.88
66.38
61.41
54.82
39.49
34.13
BRUKER
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm


126.94
124.99
109.04
105.98
97.55
96.32
84.10
78.88
66.38
61.41
54.82
39.49
34.13
-OMe
Seputhecarpan C
130
120
110
100
90
80
70
60
50
40
30
ppm

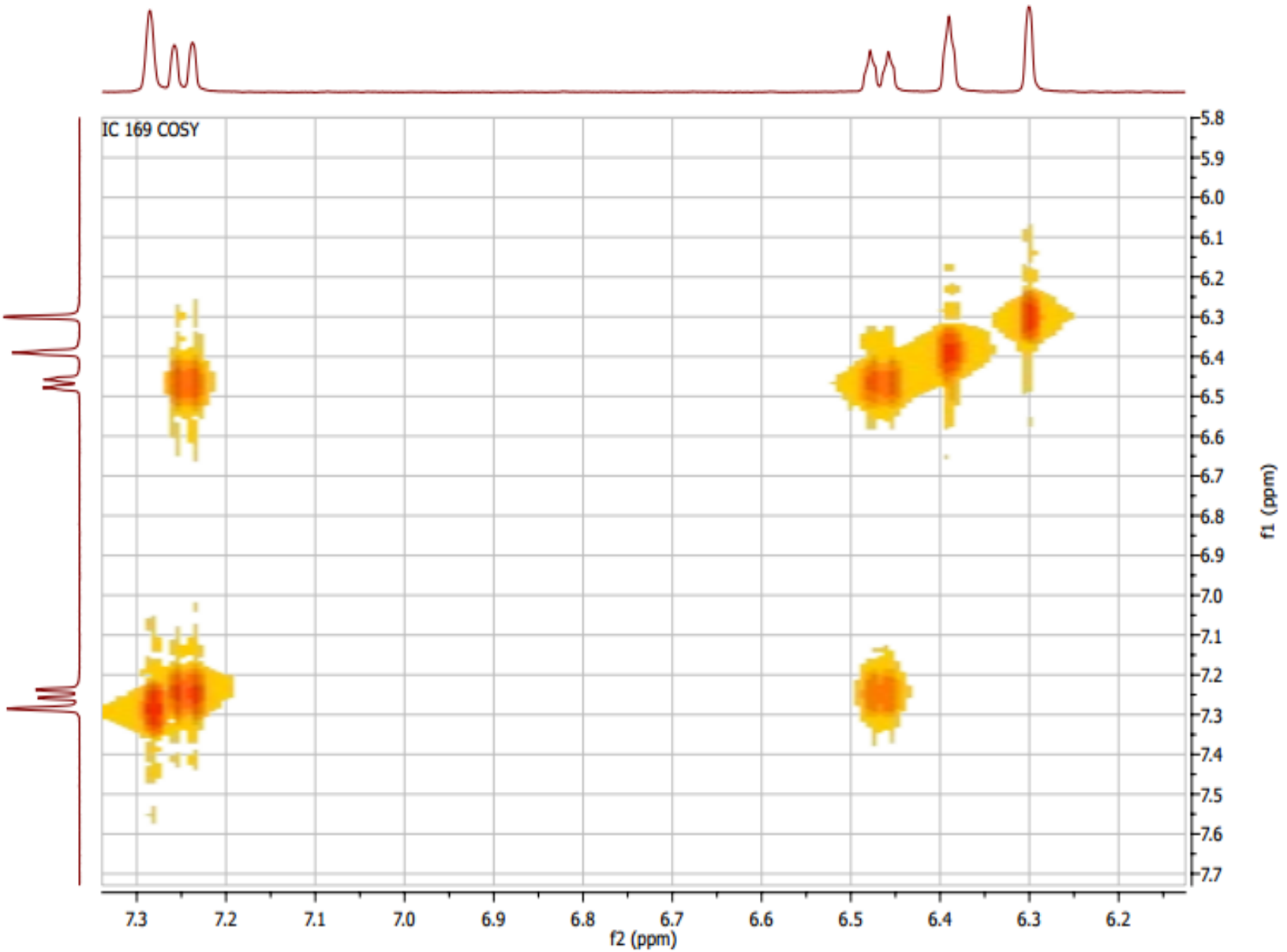

126.93
125.01
109.07
107.39
97.62
97.54
84.08
78.73
66.49
61.44
39.46
34.13
Seputhecarpan B
140
120
100
80
60
40
20



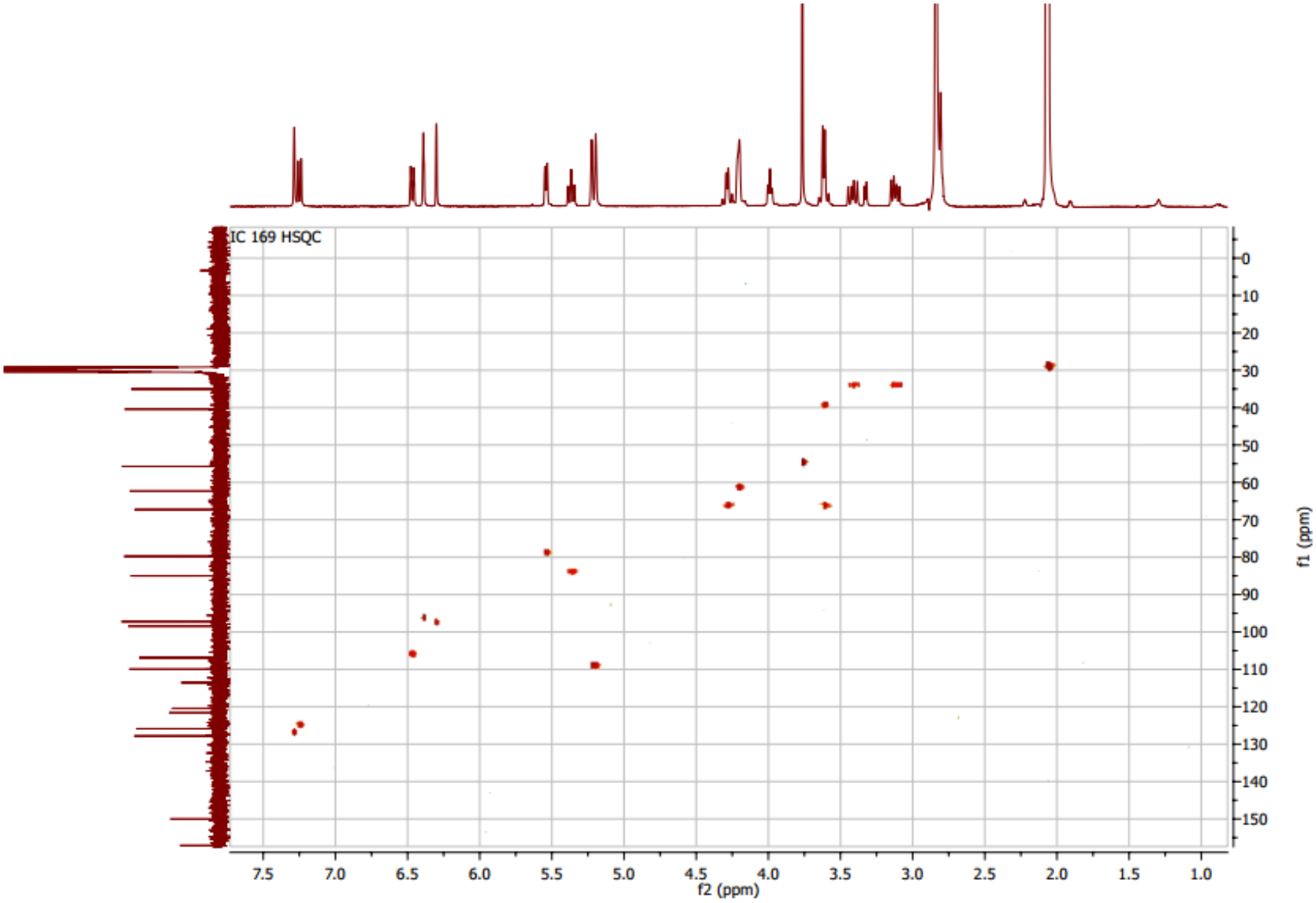
Full COSY spectrum of compound 1



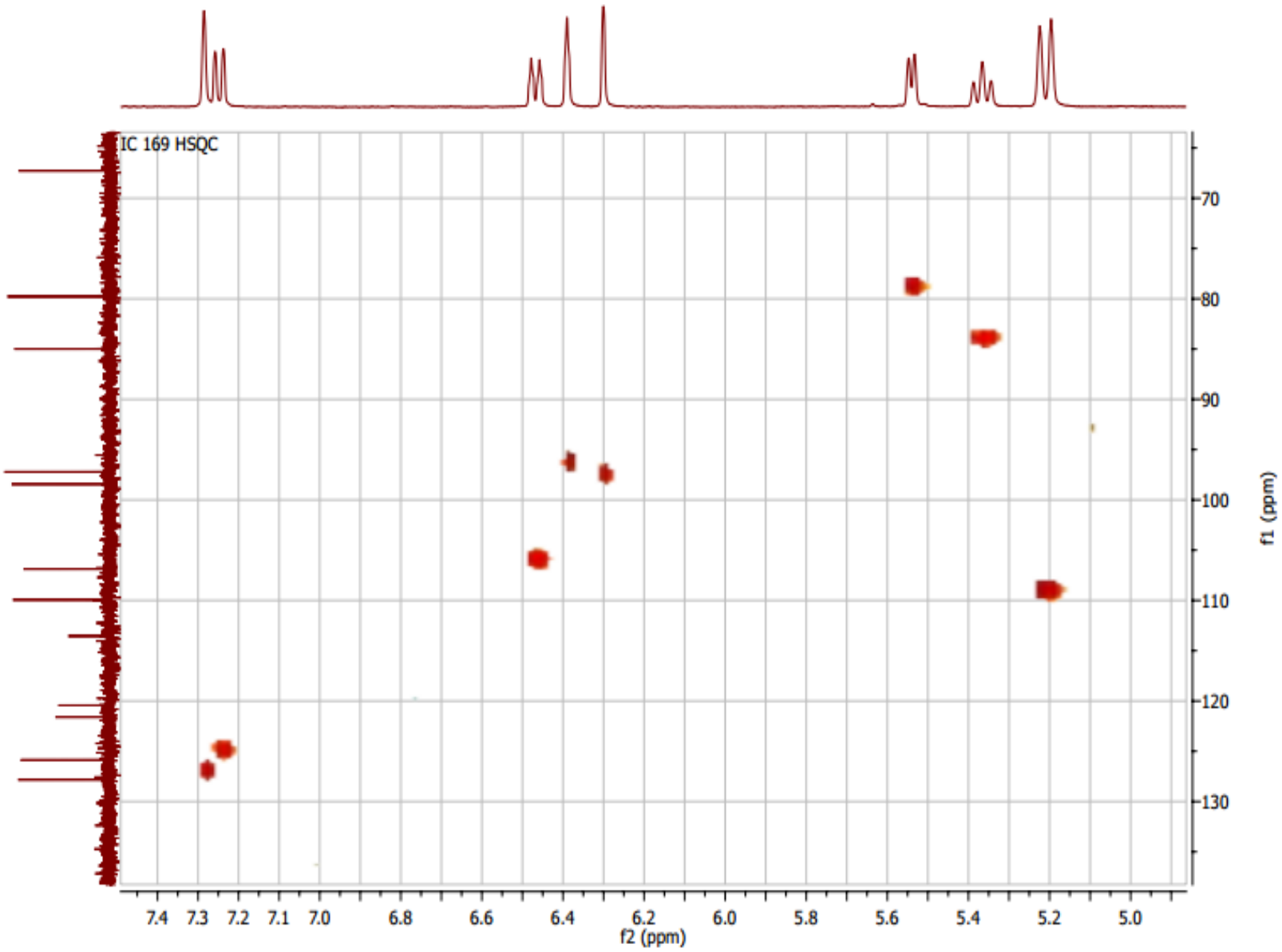
COSY spectrum of compound 1 (aliphatic region)



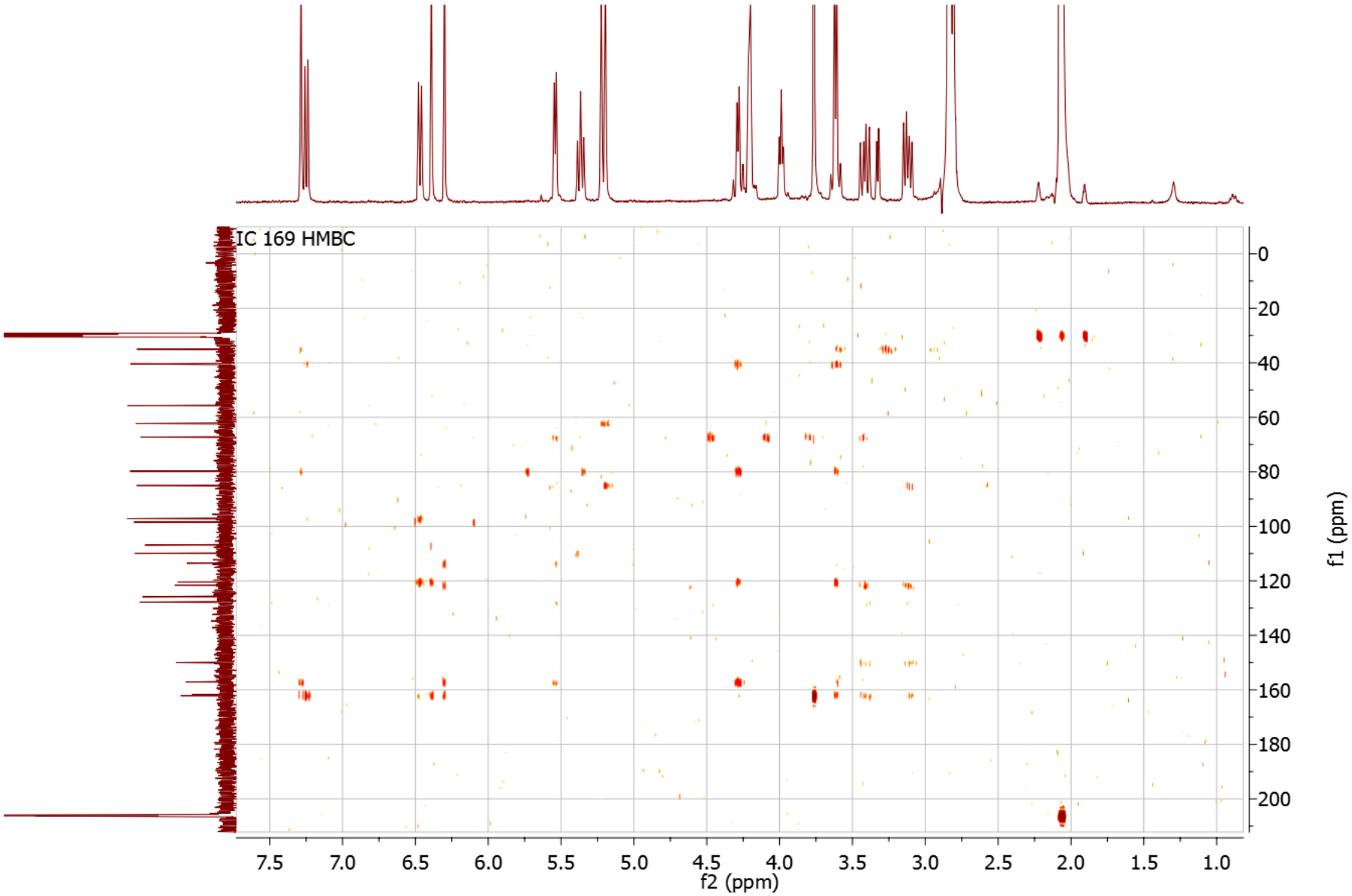
COSY spectrum of compound 1 (aromatic region)



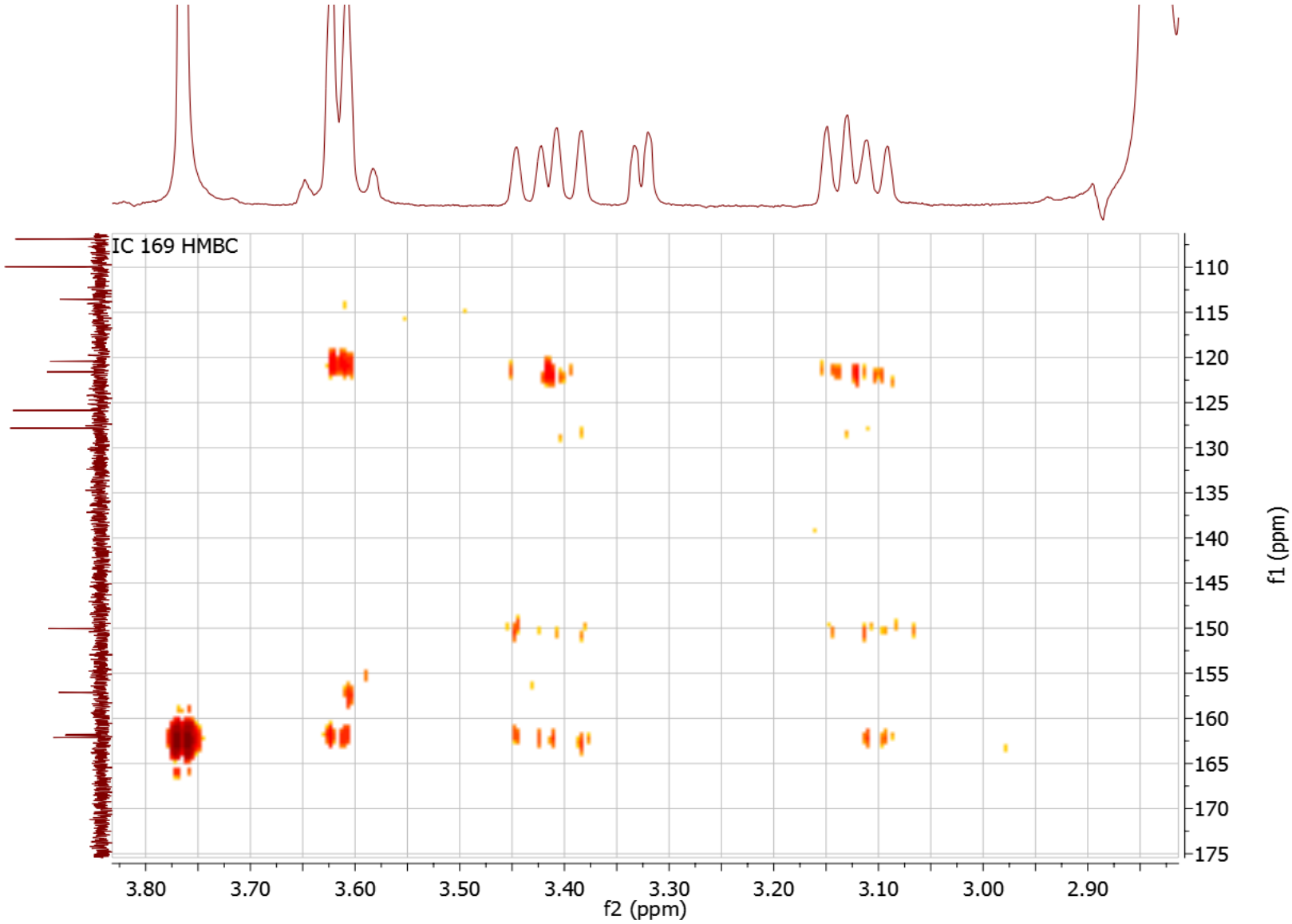
Full HSQC spectrum of compound 1



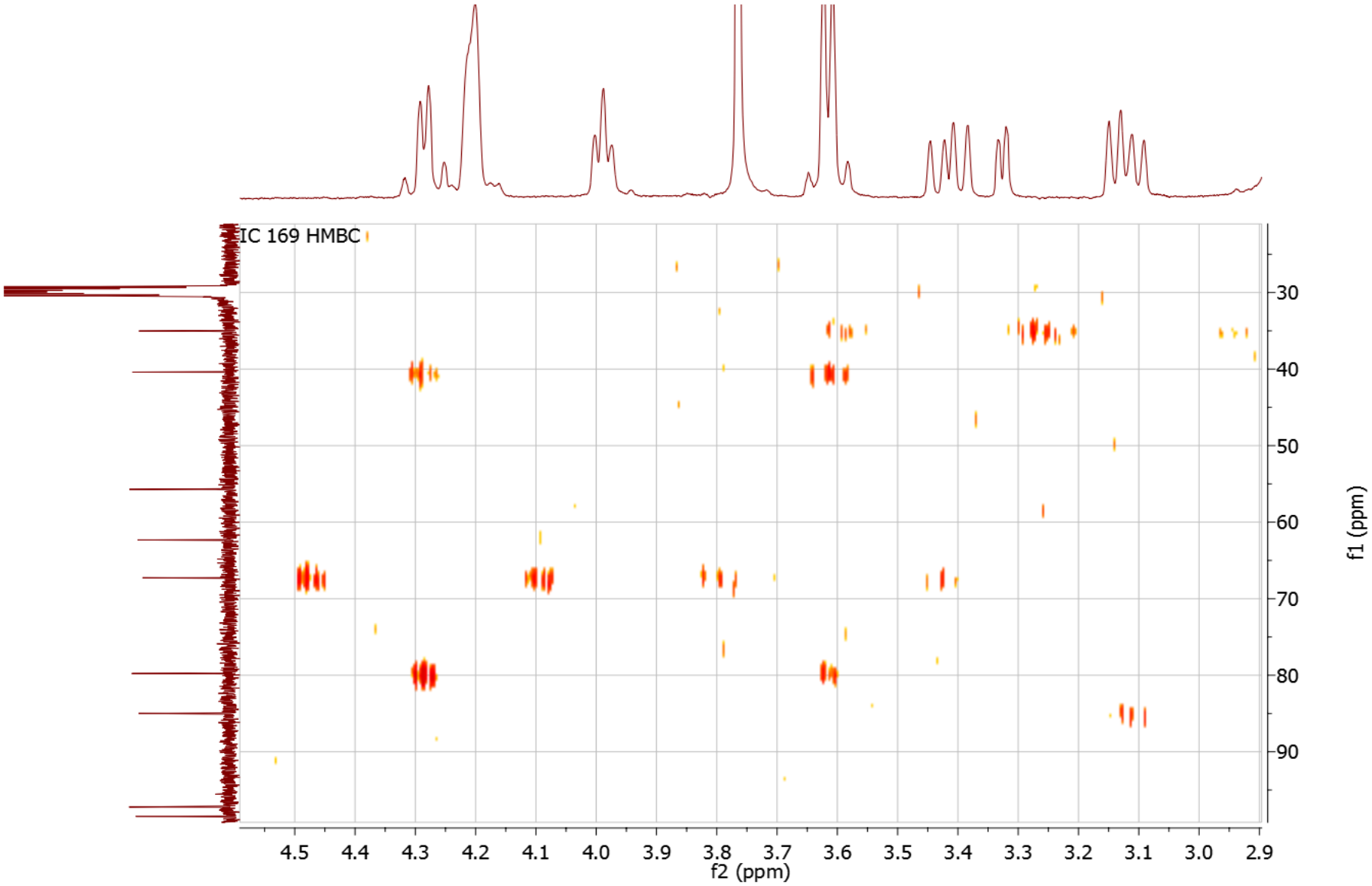
HSQC spectrum of compound 1 continued



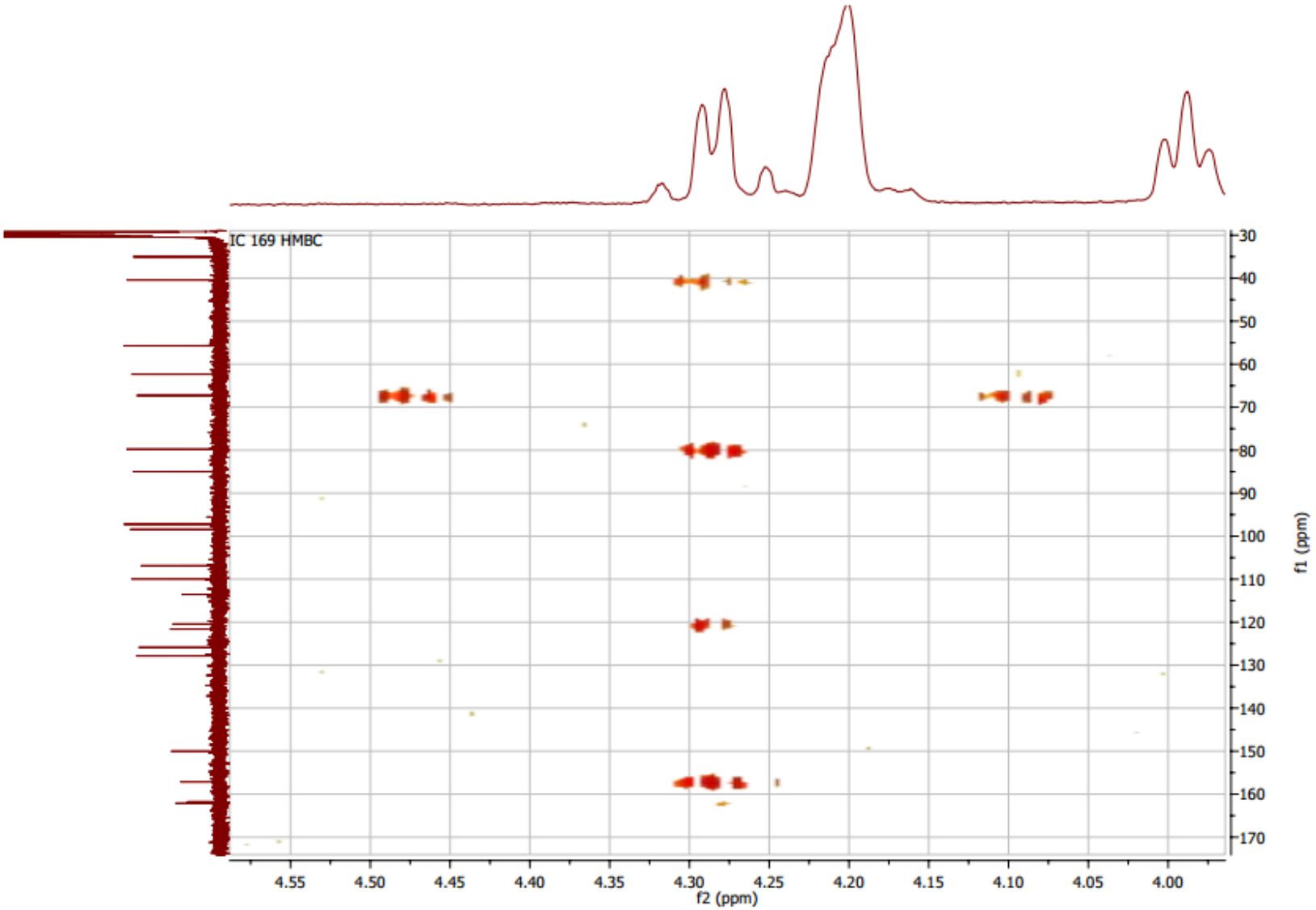
Full HMBC spectrum of compound 1



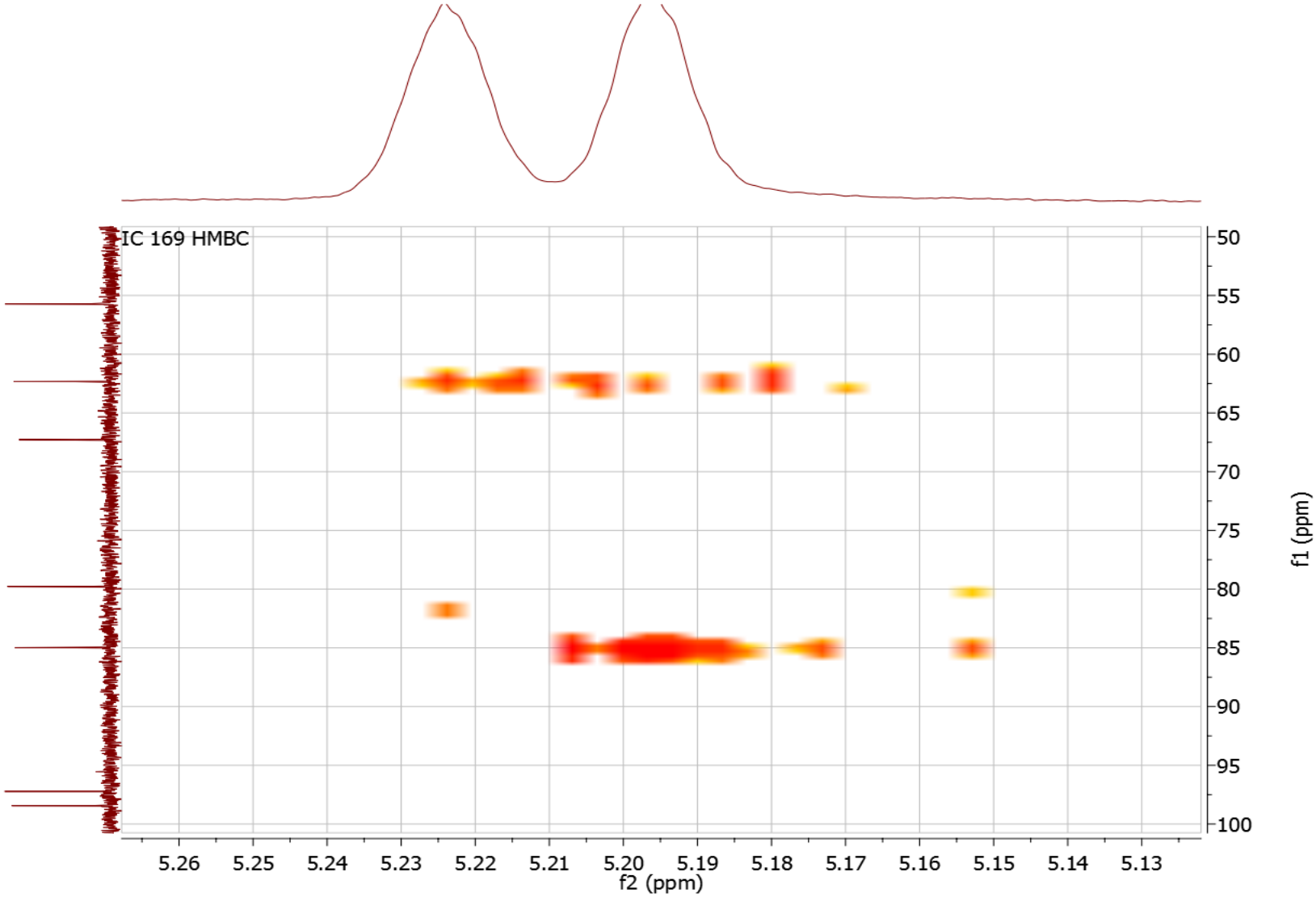
HMBC spectrum of compound 1 (aliphatic region)



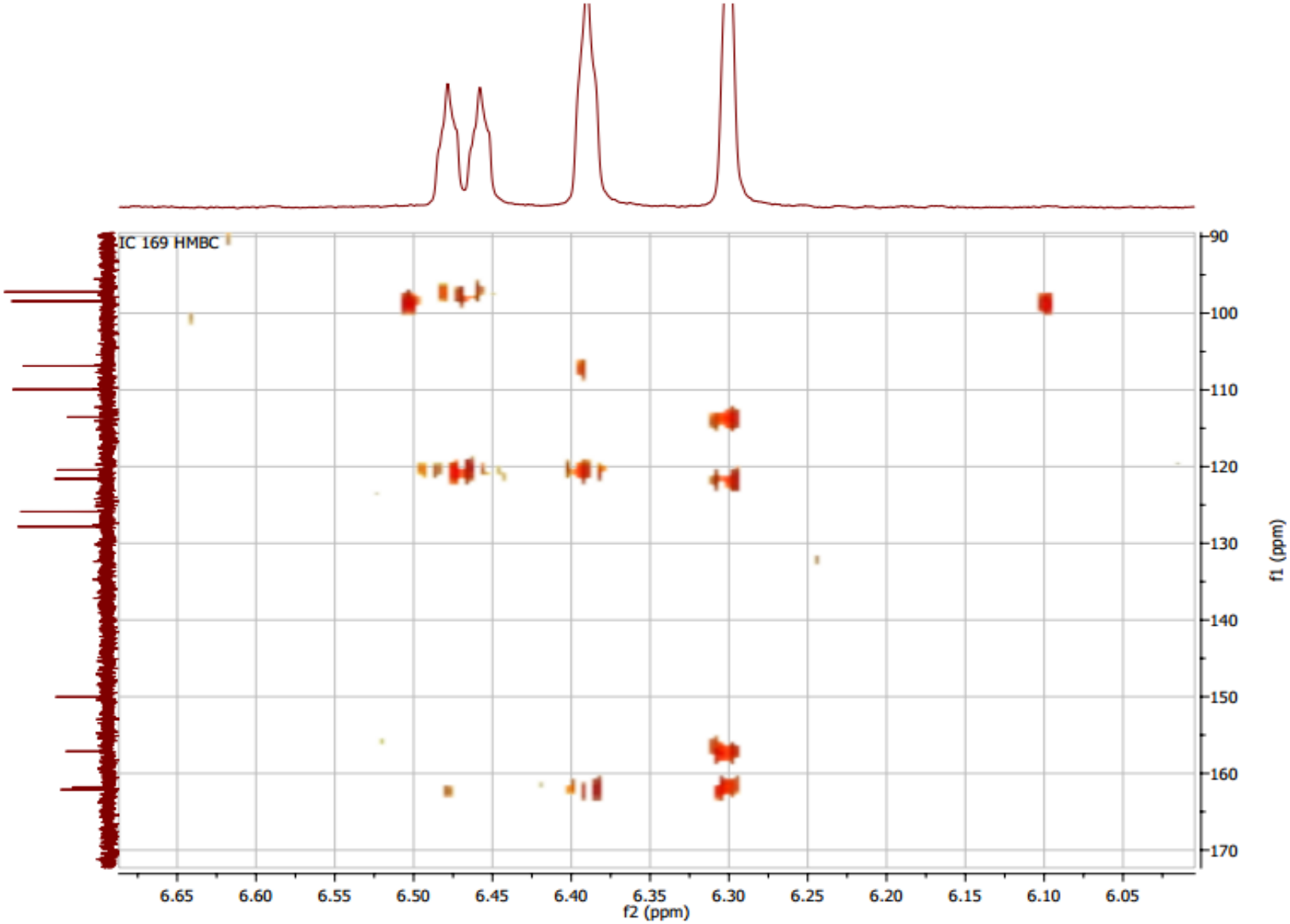
HMBC spectrum of compound 1 (aliphatic region) continued



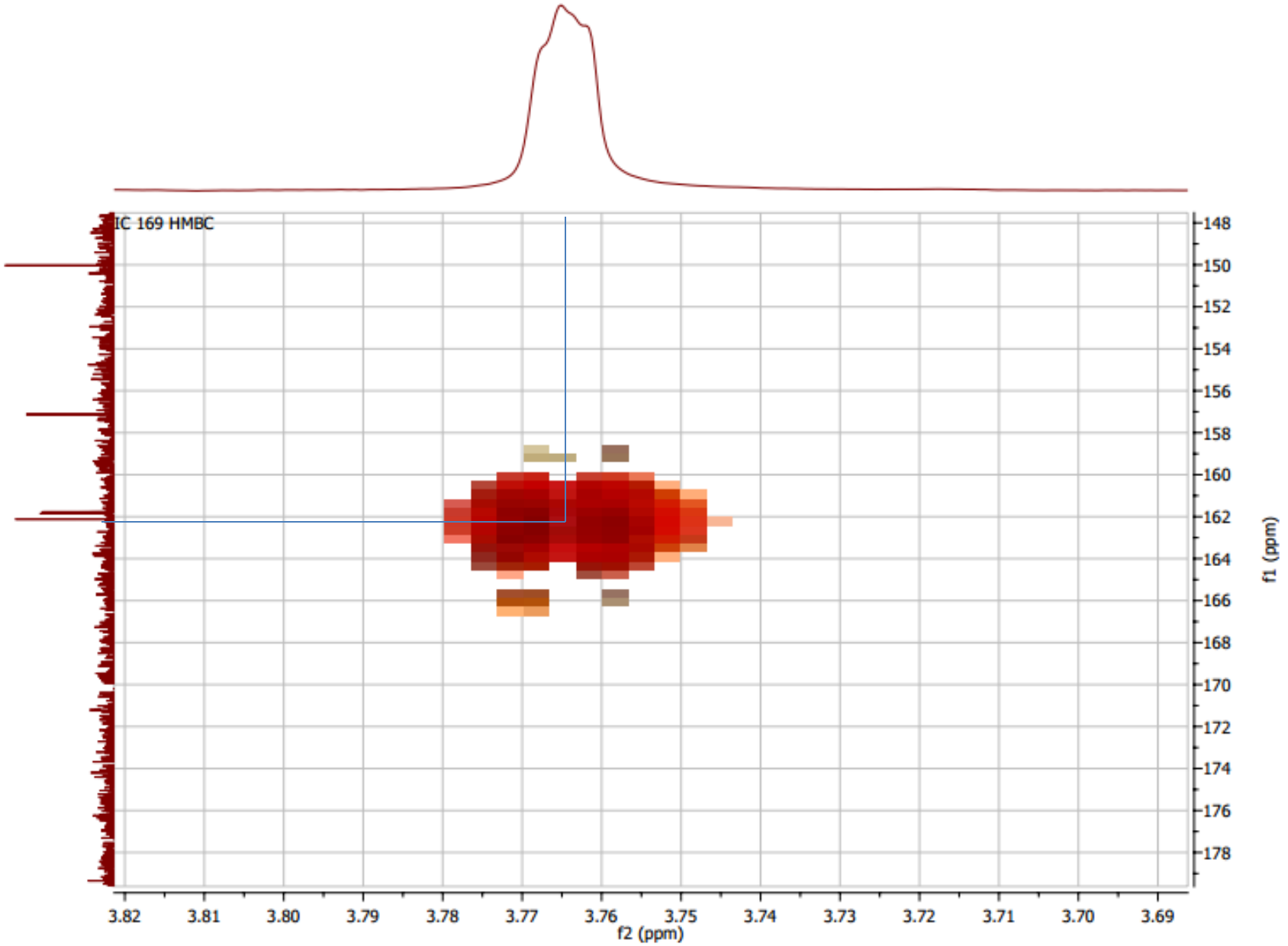
HMBC spectrum of compound 1 (aliphatic region) continued



HMBC spectrum of compound 1 (correlations of H-15,15' with C-13 and C-16)



HMBC spectrum of compound 1 (aromatic region)



HMBC correlation of the methoxyl (δ 3.77) group with C-9 (δ 162.1)