Supplementary material

Oxygenated cembrene diterpenes from *Sarcophyton convolutum:* cytotoxic sarcoconvolutum A-E

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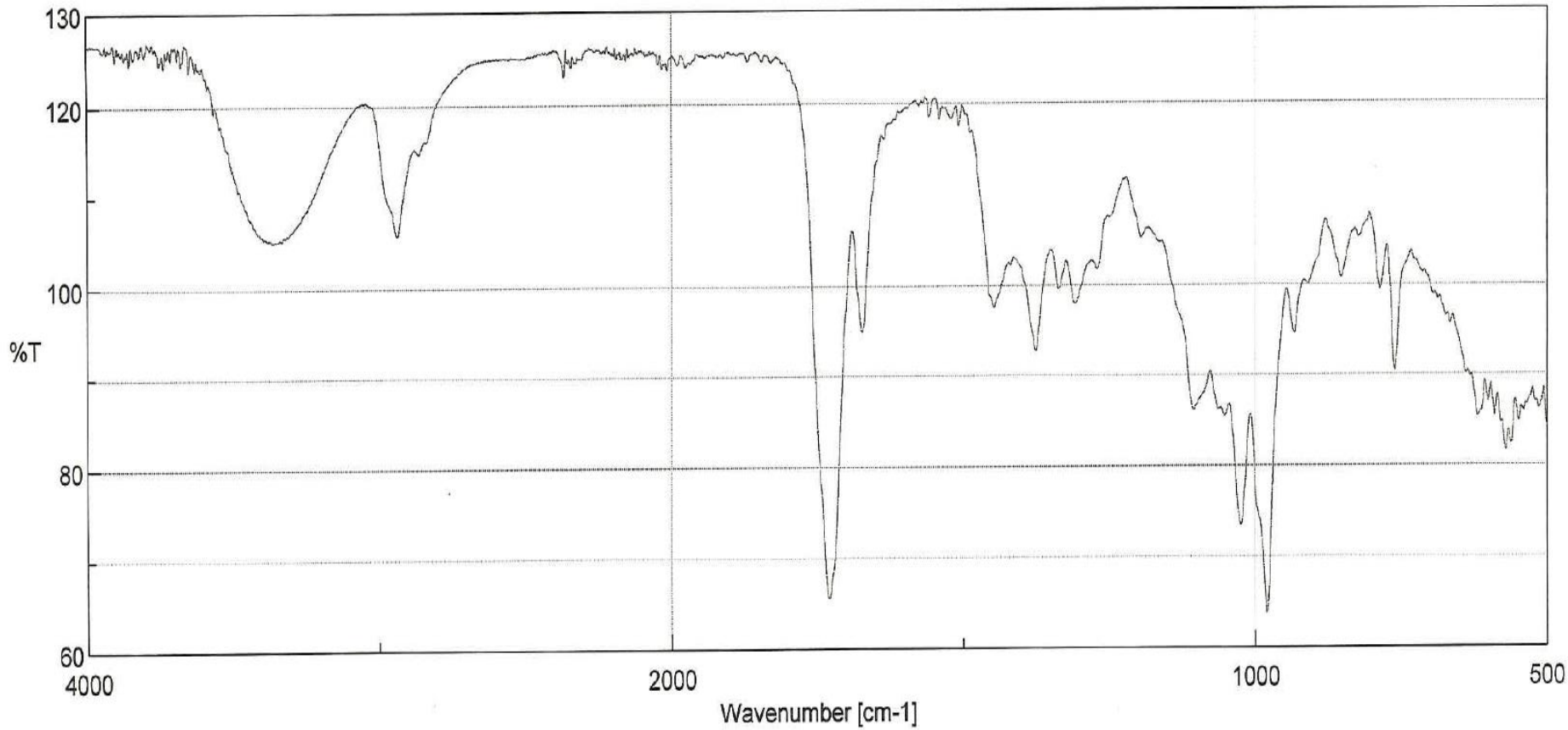
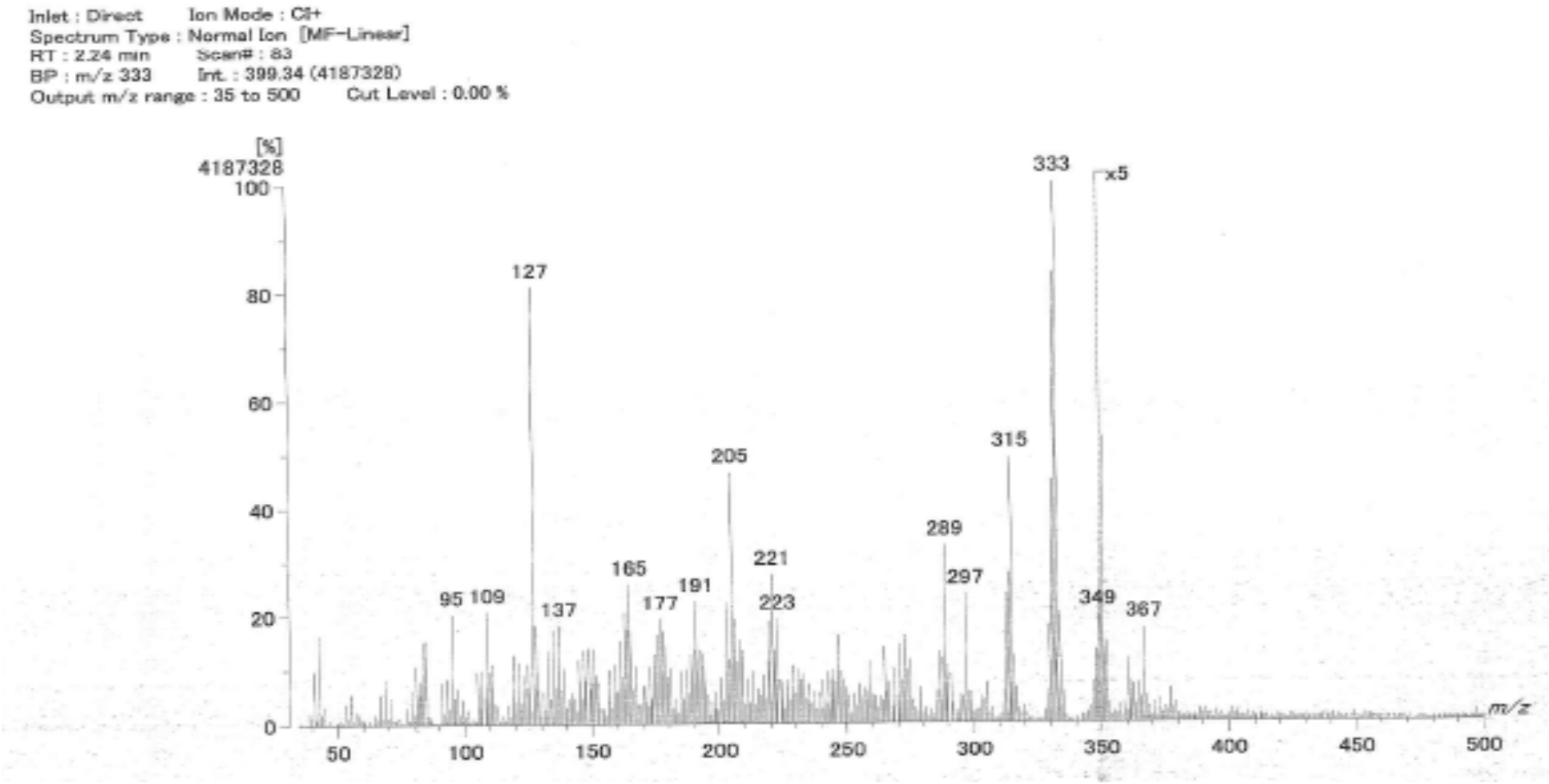


S1: FTIR of **1**

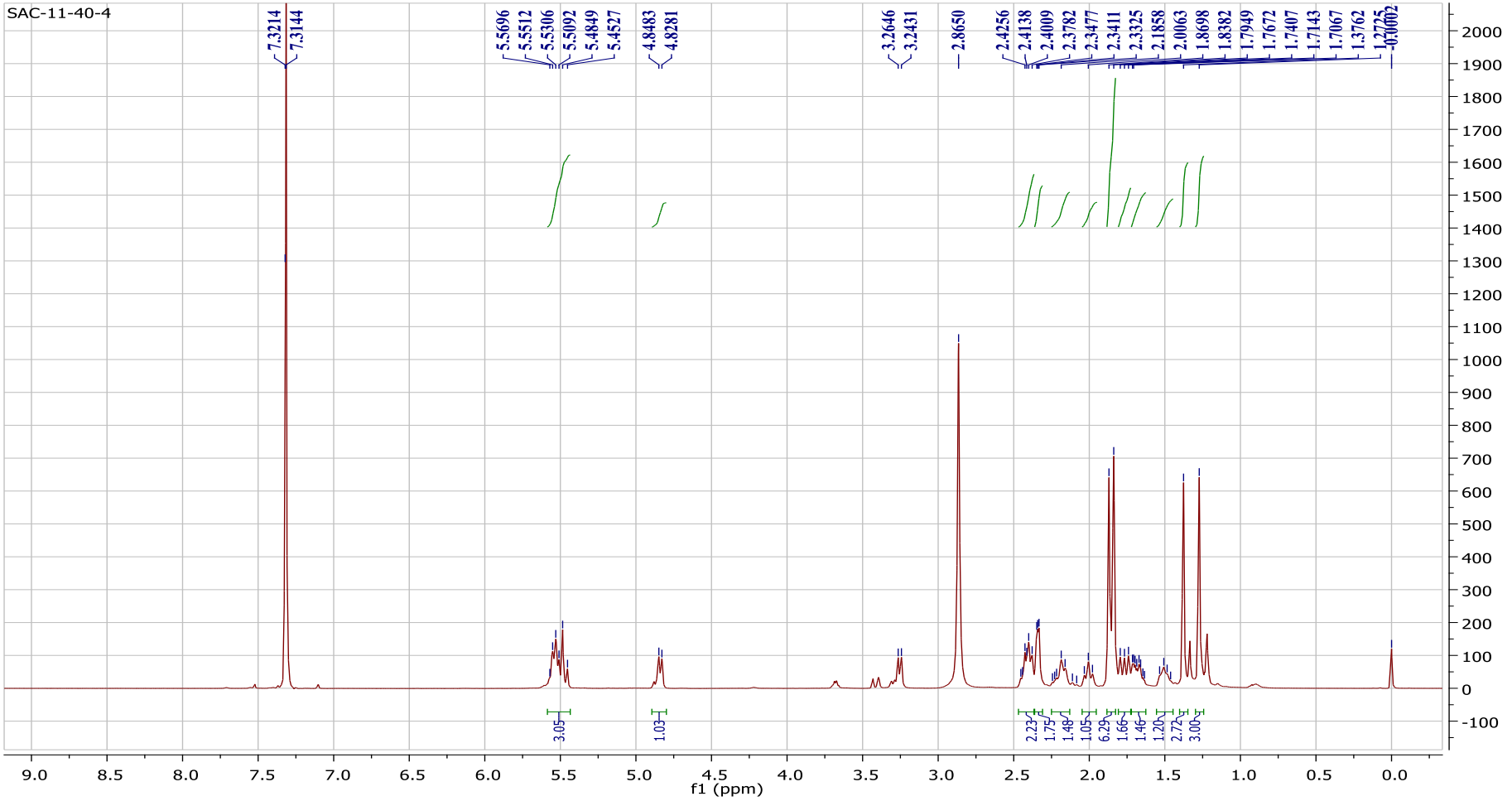


S2: LRCIMS of **1**

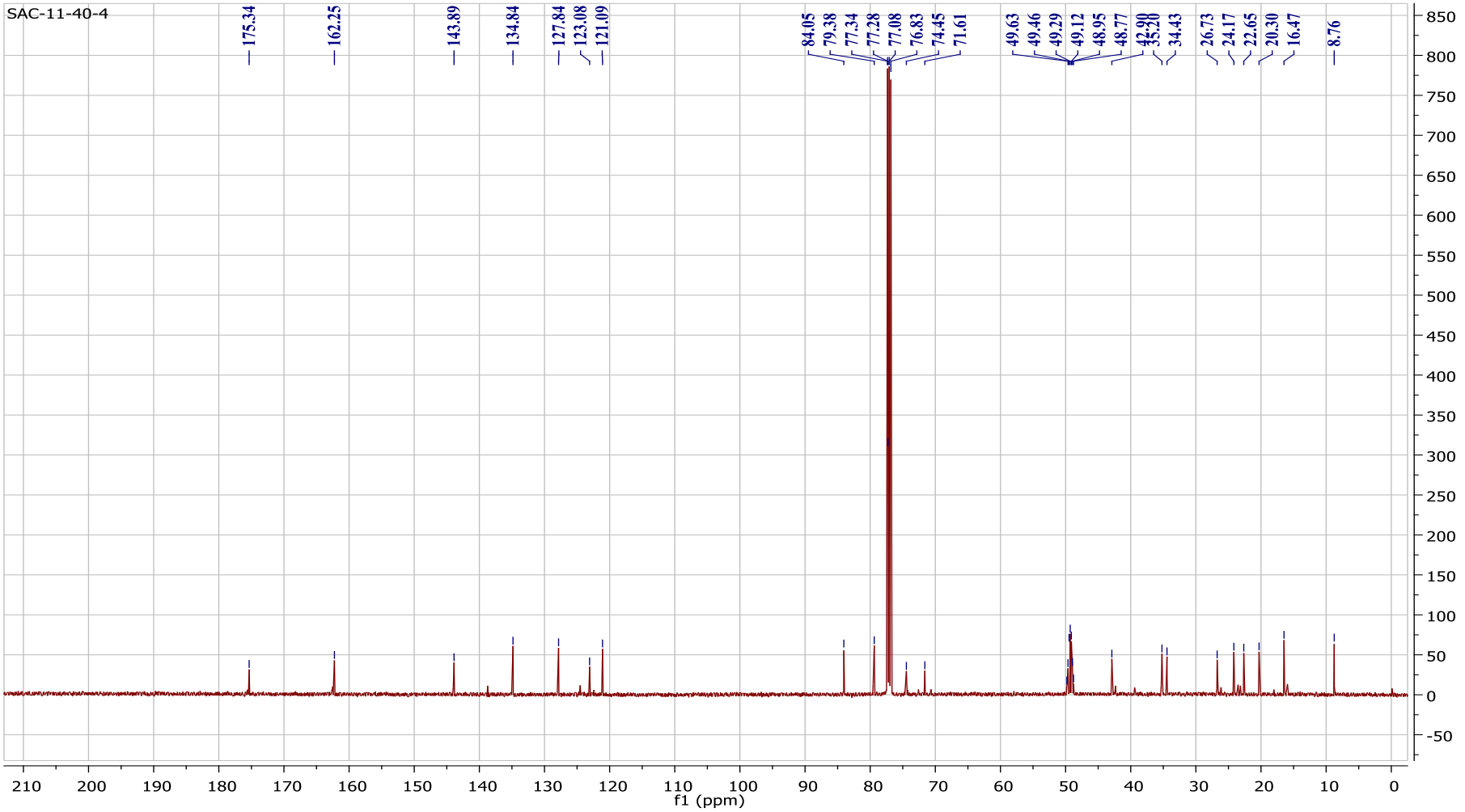
Note : MStation
Inlet : Direct Ion Mode : CI+
RT : 1.92 min Scan# : 49
Elements : C 150/0, H 250/0, O 50/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : 0.0 – 15.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	367.2122	4.78	+0.4 / +0.1	5.5	C20 H31 O6

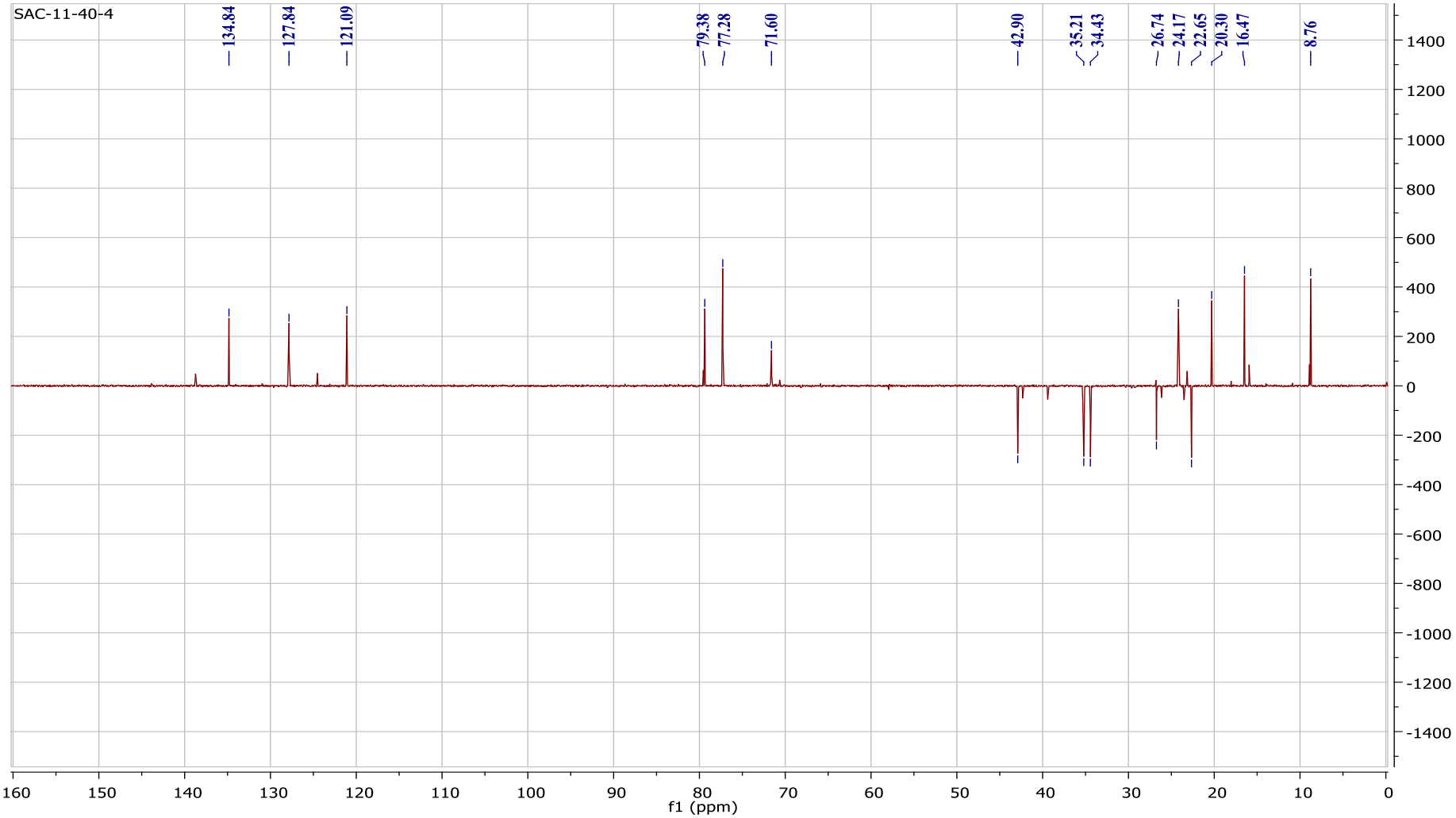
S3: HRCIMS of **1**



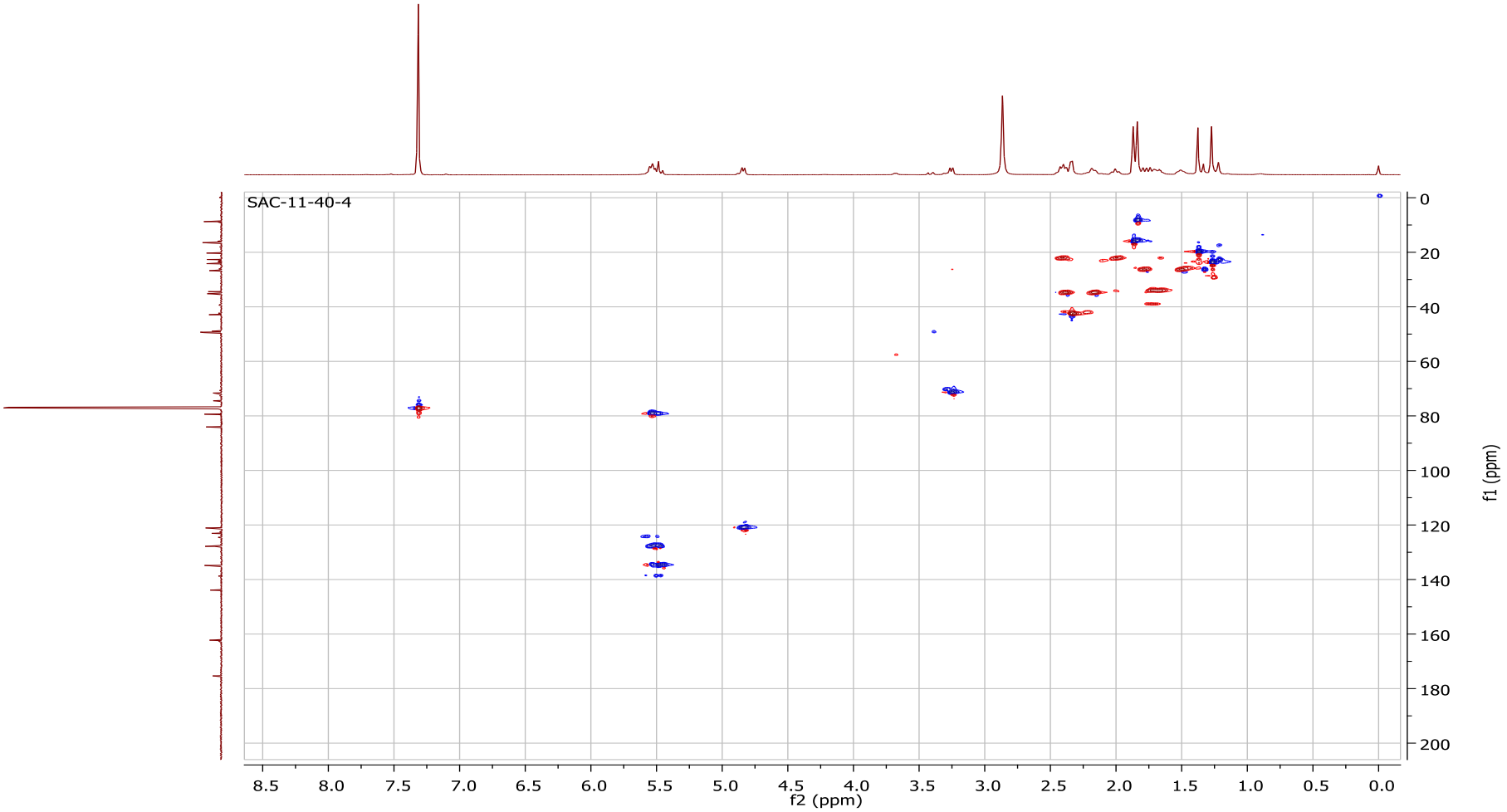
S4: ^{1}H NMR of **1** (500 Hz, $CDCl_3$)



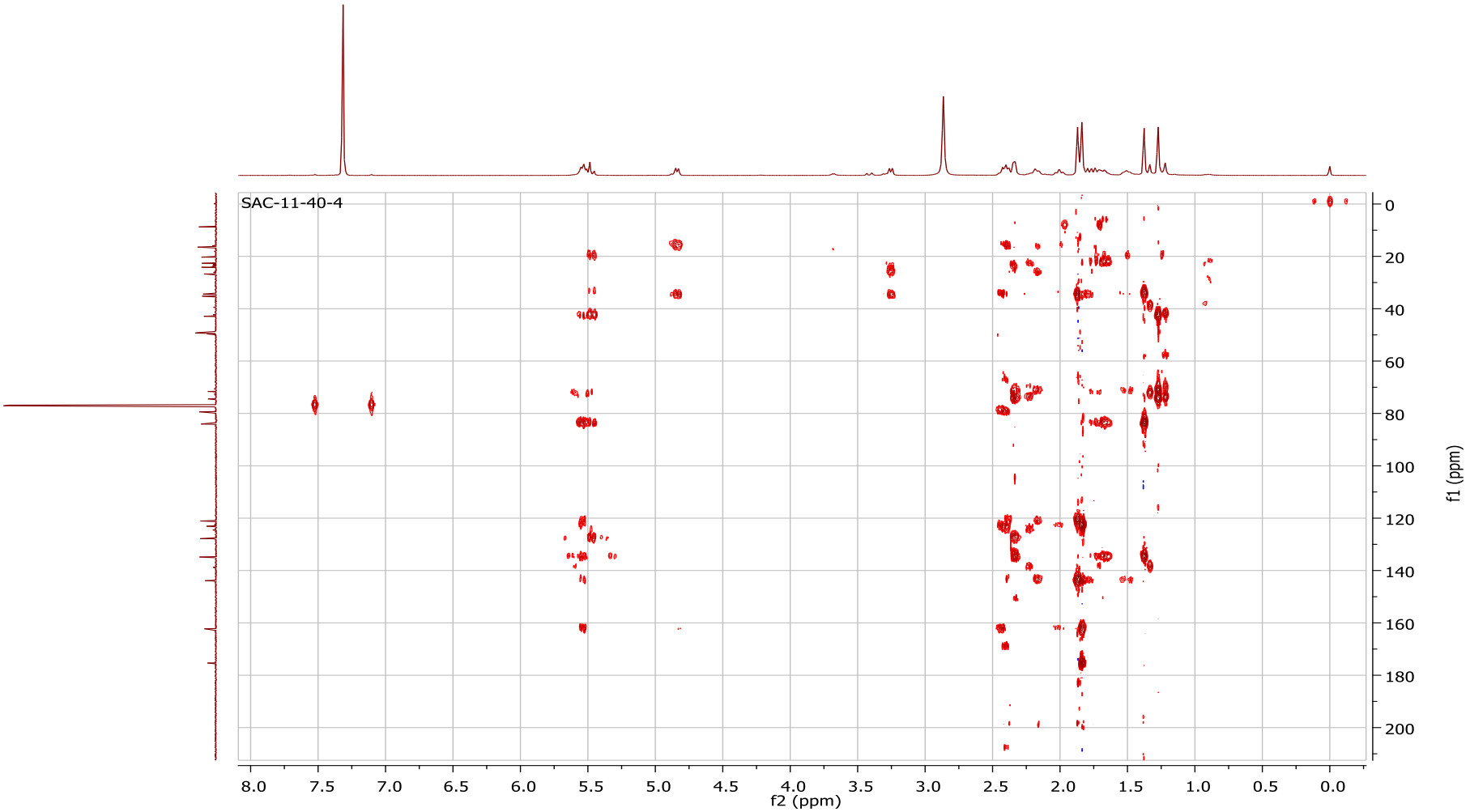
S5: ^{13}C NMR of **1** (125 Hz, $CDCl_3$)


SAC-11-40-4
134.84
127.84
121.09
79.38
77.28
71.60
42.90
35.21
34.43
26.74
24.17
22.65
20.30
16.47
8.76
1400
1200
1000
800
600
400
200
0
-200
-400
-600
-800
-1000
-1200
-1400
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

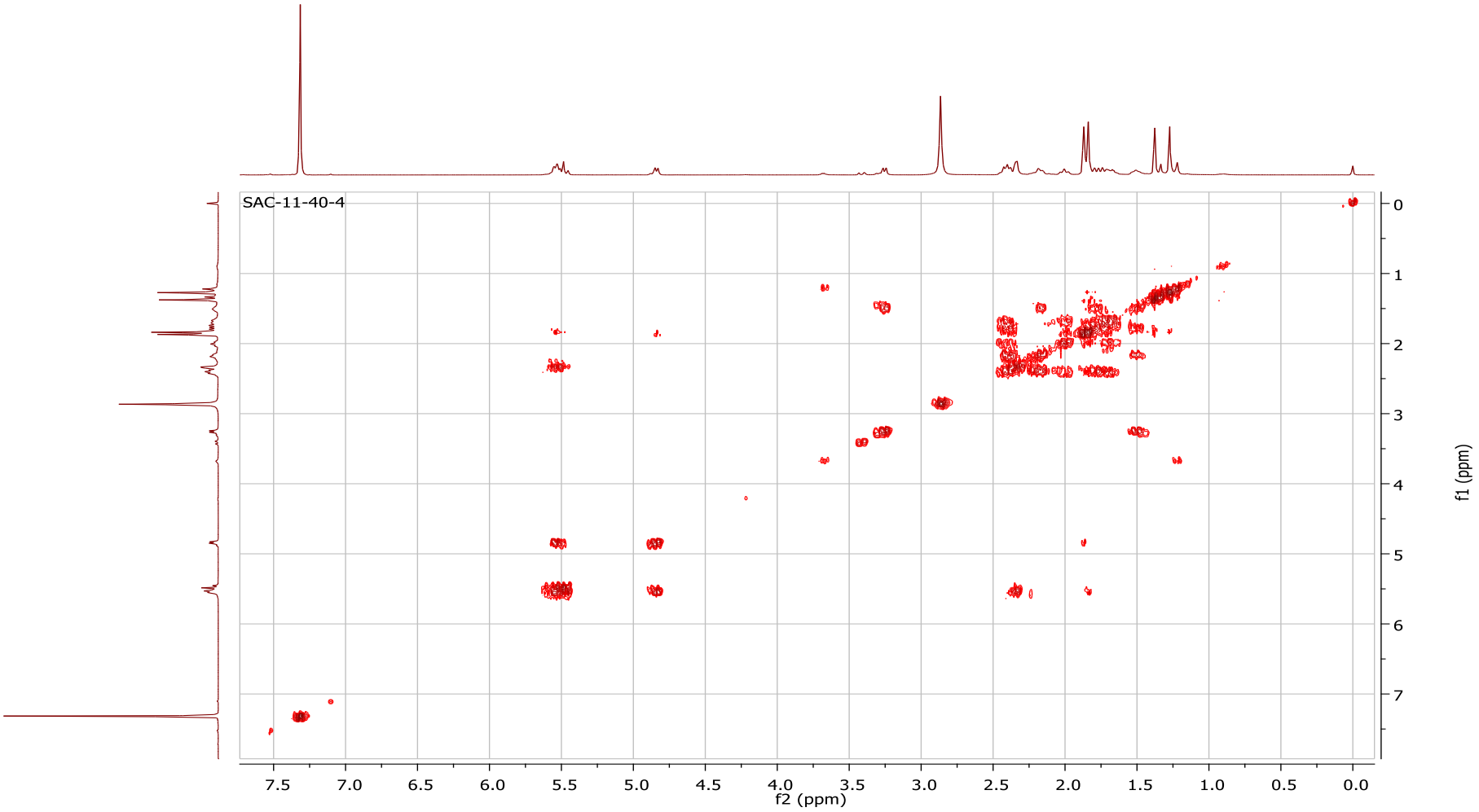
S6: DEPT of **1**


SAC-11-40-4
f2 (ppm)
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
180
200

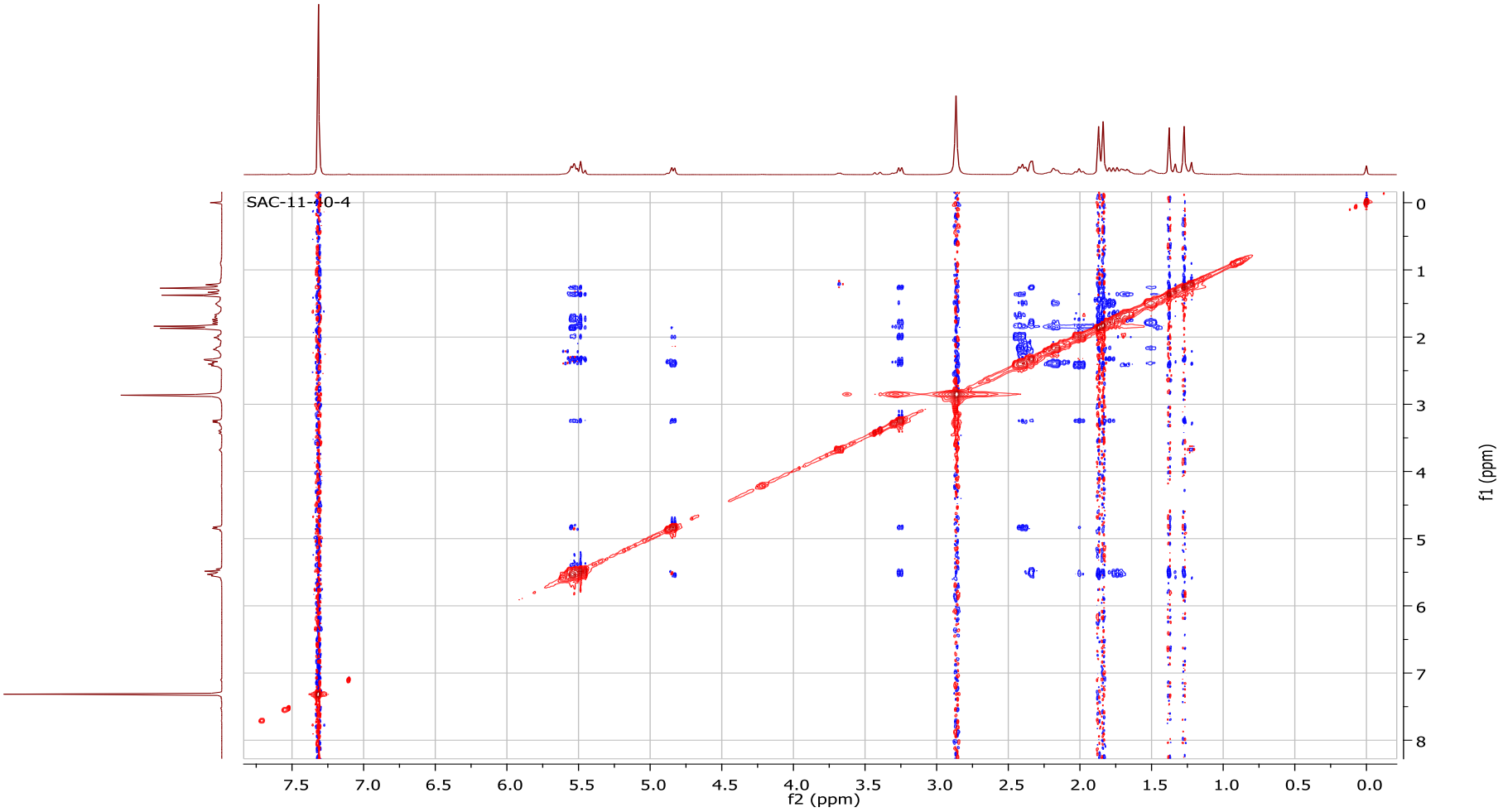
S7: HSQC of **1**


SAC-11-40-4
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f2 (ppm)
0
20
40
60
80
100
120
140
160
180
200
f1 (ppm)

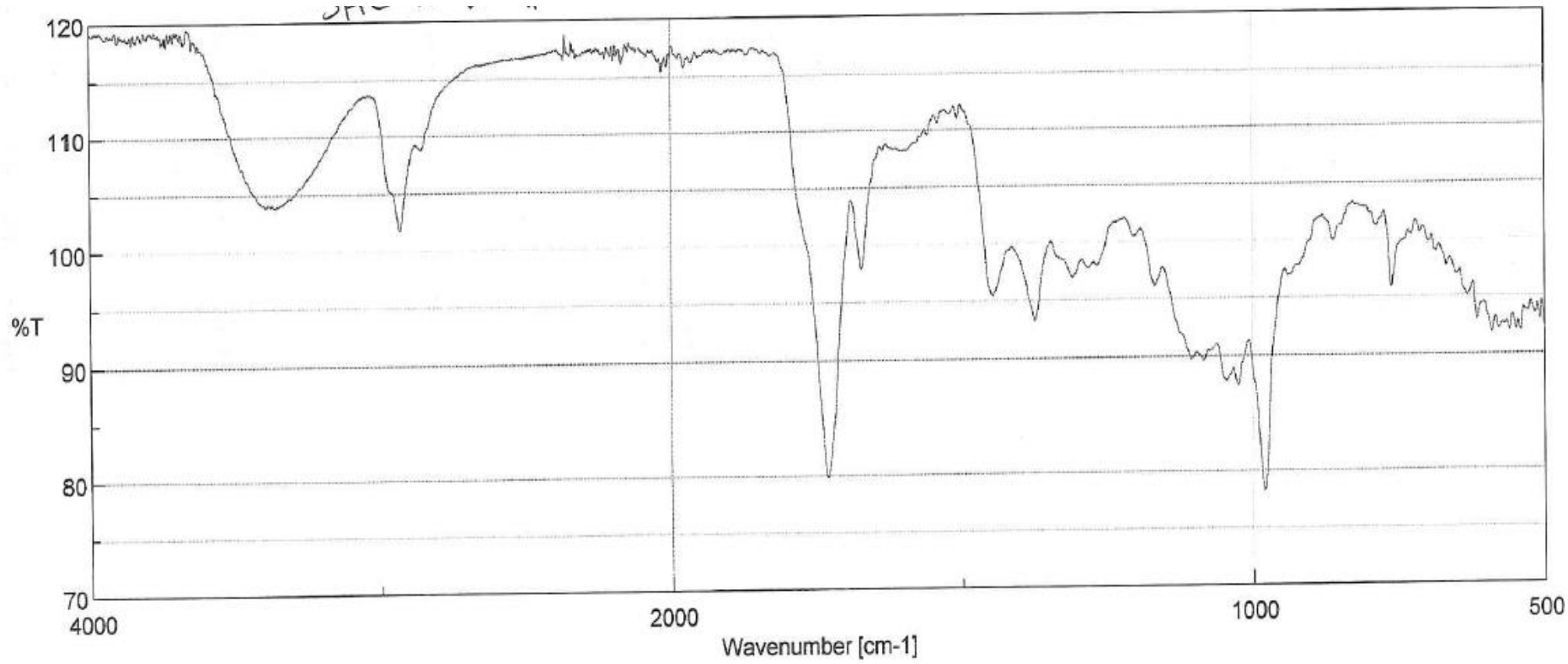
S8: HMBC of **1**



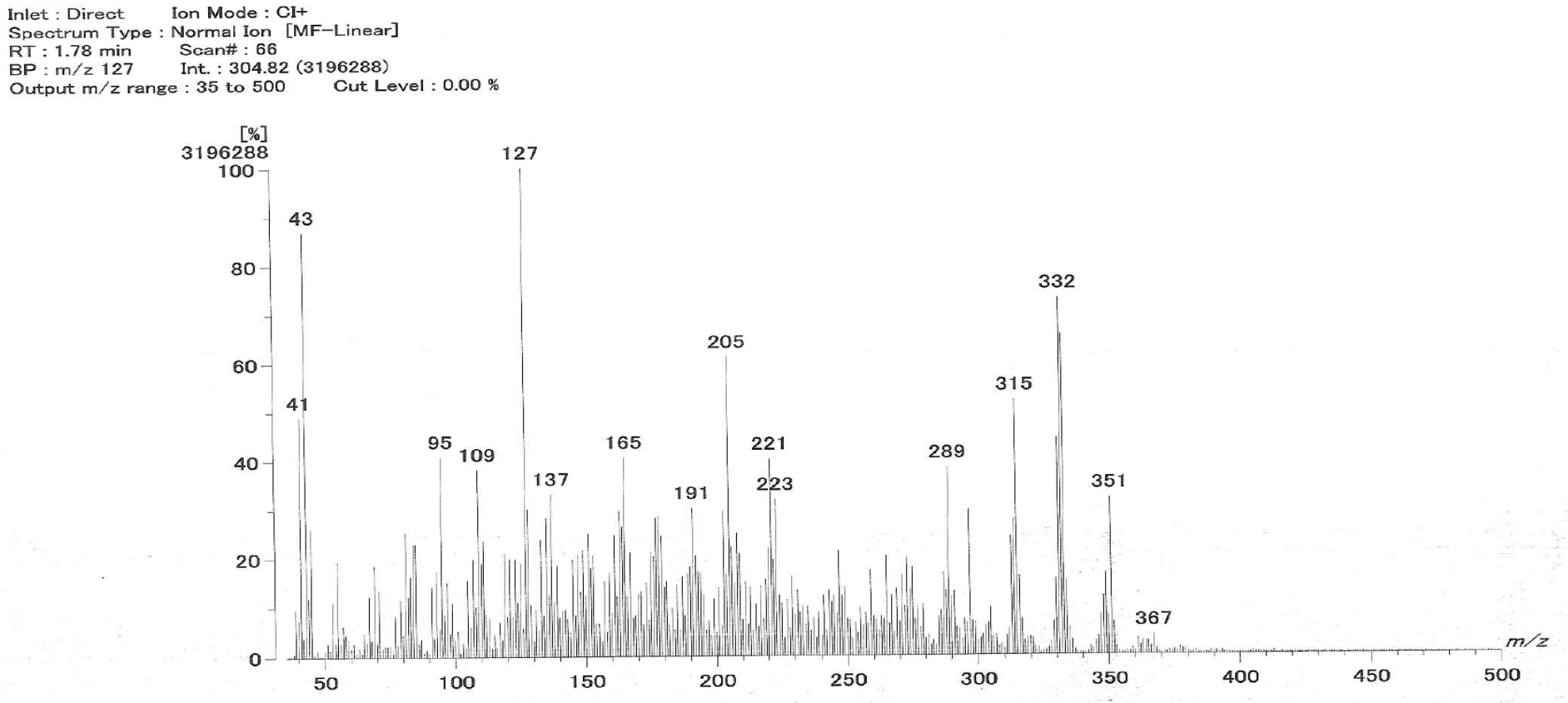
S9: ^{1}H ^{1}H COSY of 1



S10: NOESY of **1**



S11: FTIR of **2**

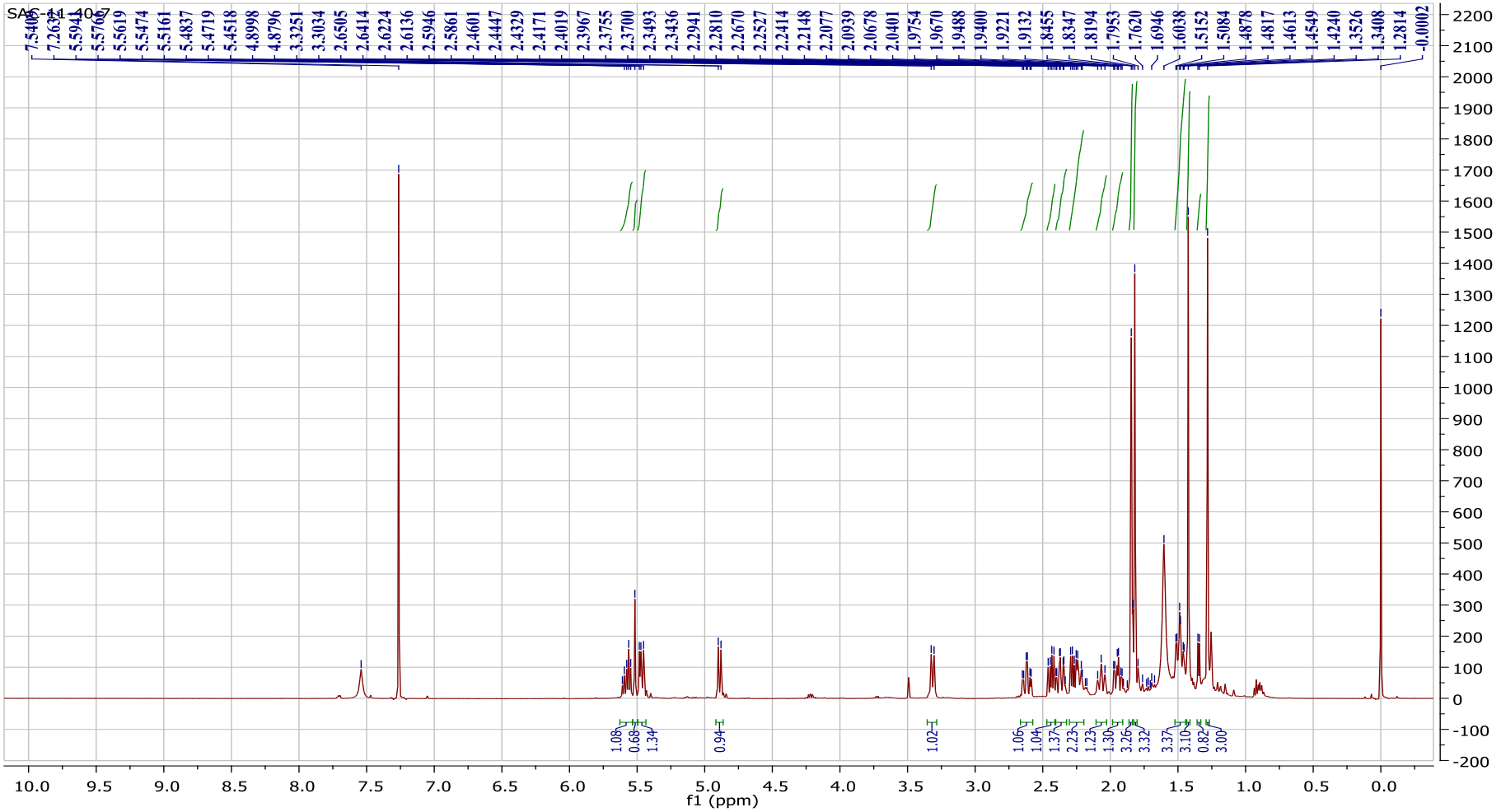


S12: LRCIMS of **2**

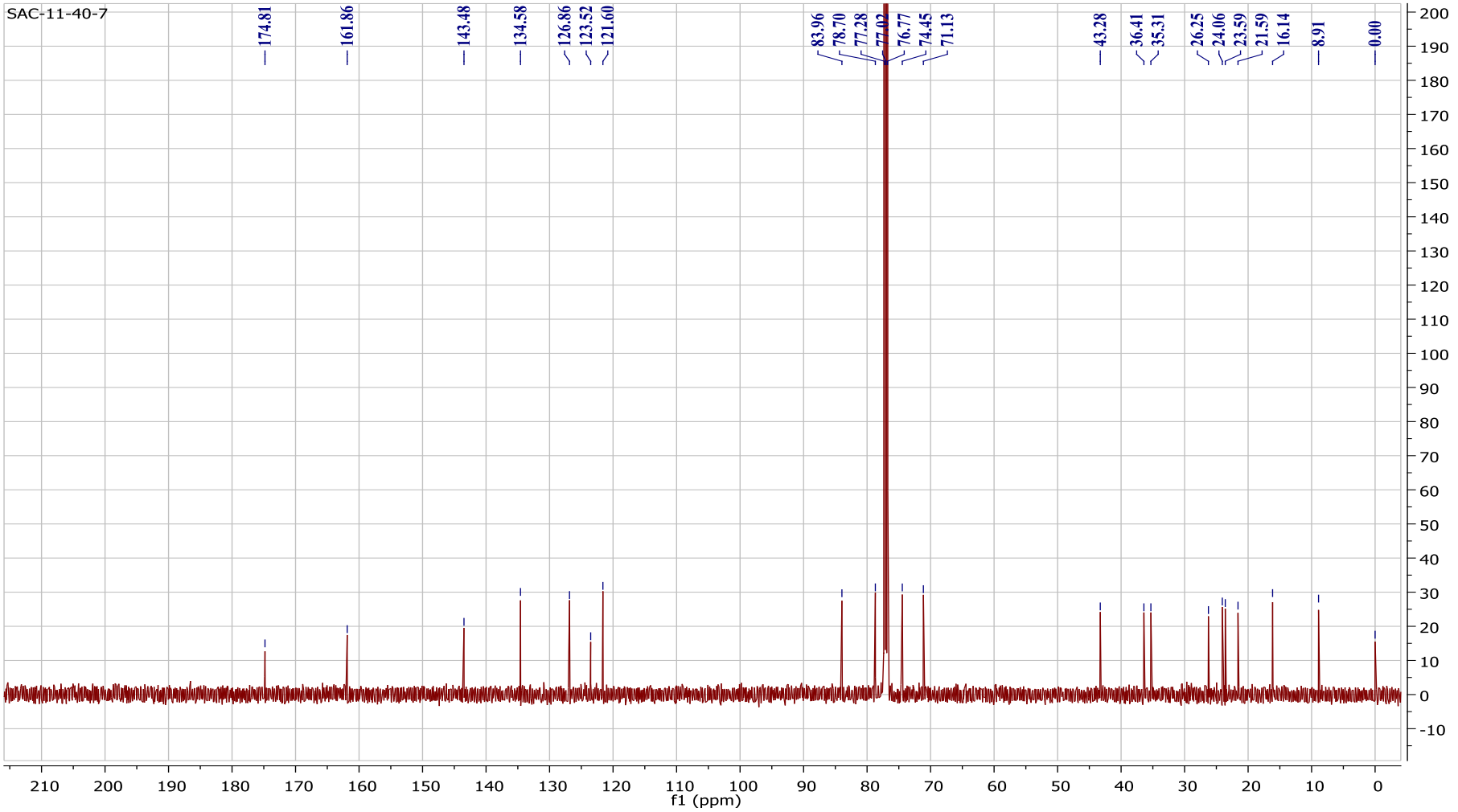
Note : MStation
Inlet : Direct Ion Mode : CI+
RT : 1.92 min Scan# : 49
Elements : C 150/0, H 250/0, O 50/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : 0.0 – 15.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	367.2122	4.78	+0.4 / +0.1	5.5	C20 H31 O6

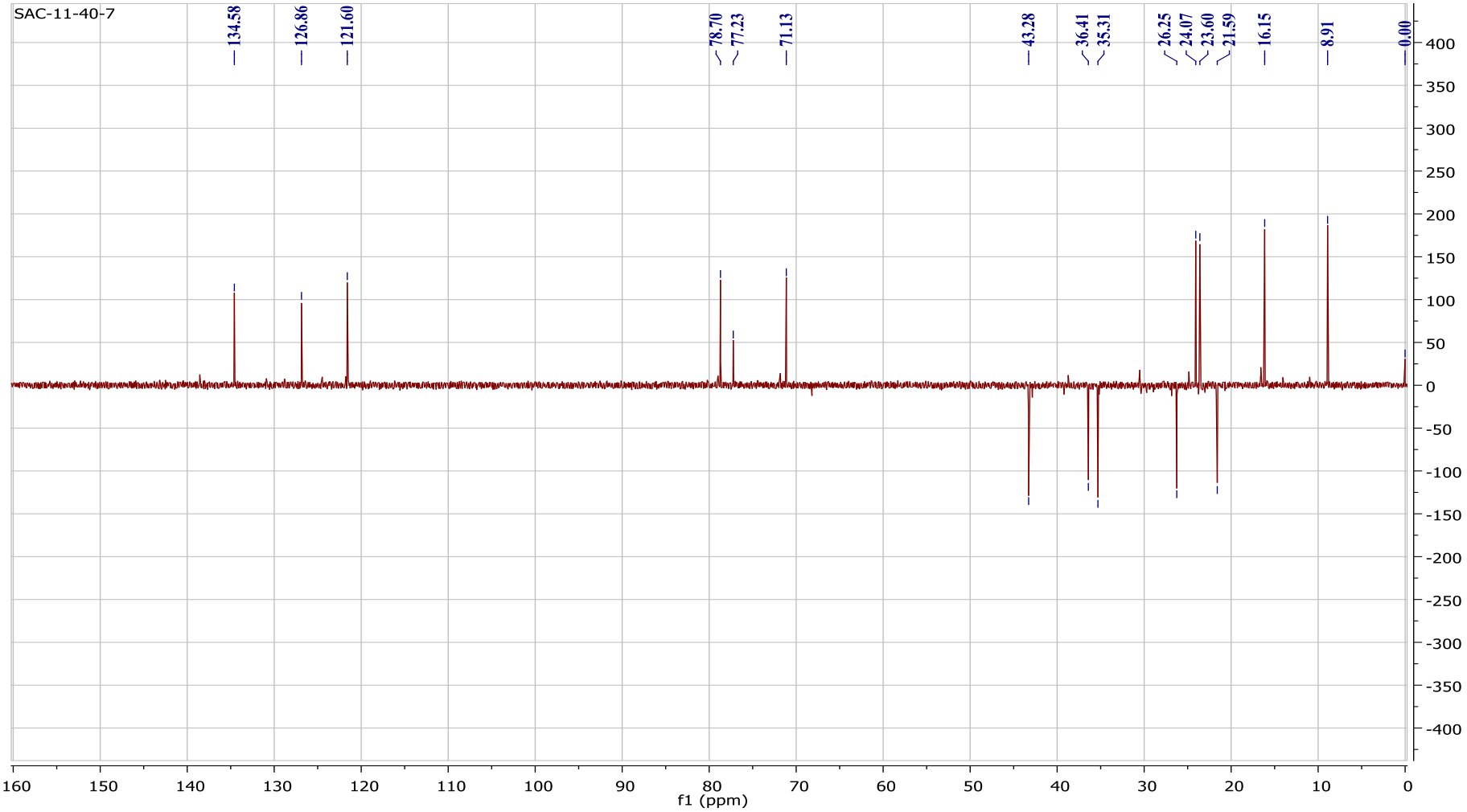
S13: HRCIMS of **2**



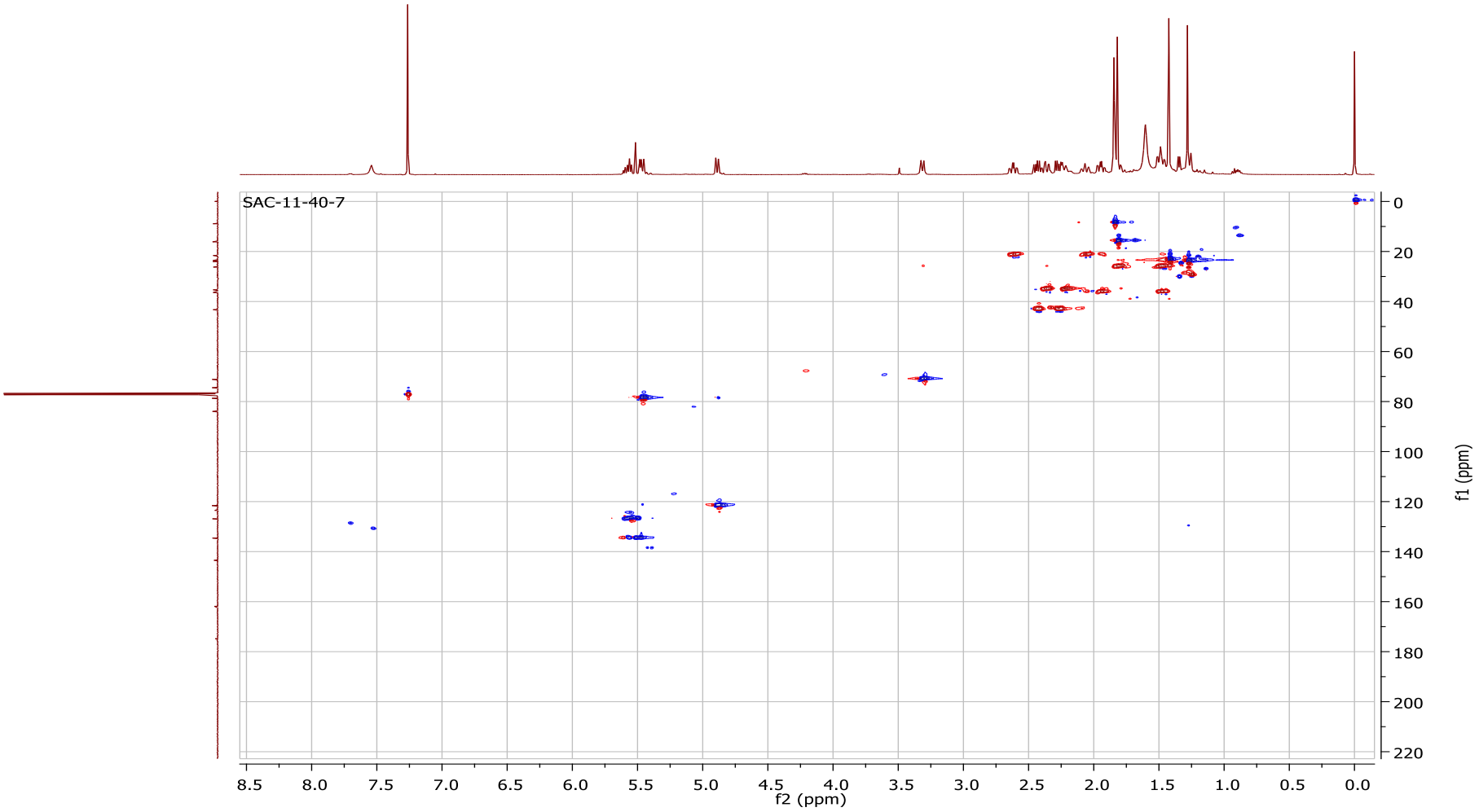
S14: ^{1}H NMR of **2**



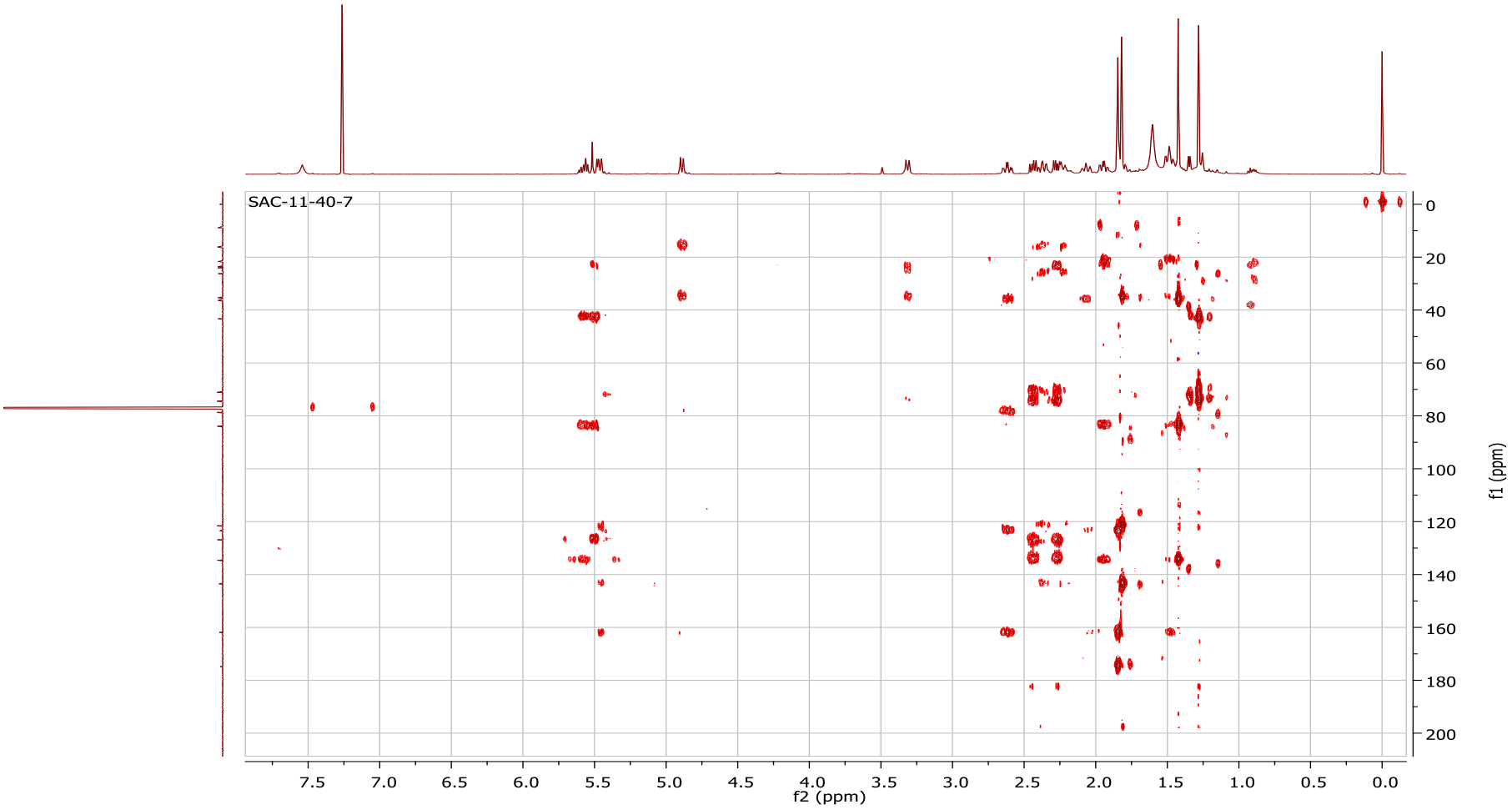
S15: ^{13}C NMR of **2**


SAC-11-40-7
134.58
126.86
121.60
78.70
77.23
71.13
43.28
36.41
35.31
26.25
24.07
23.60
21.59
16.15
8.91
0.00
f1 (ppm)

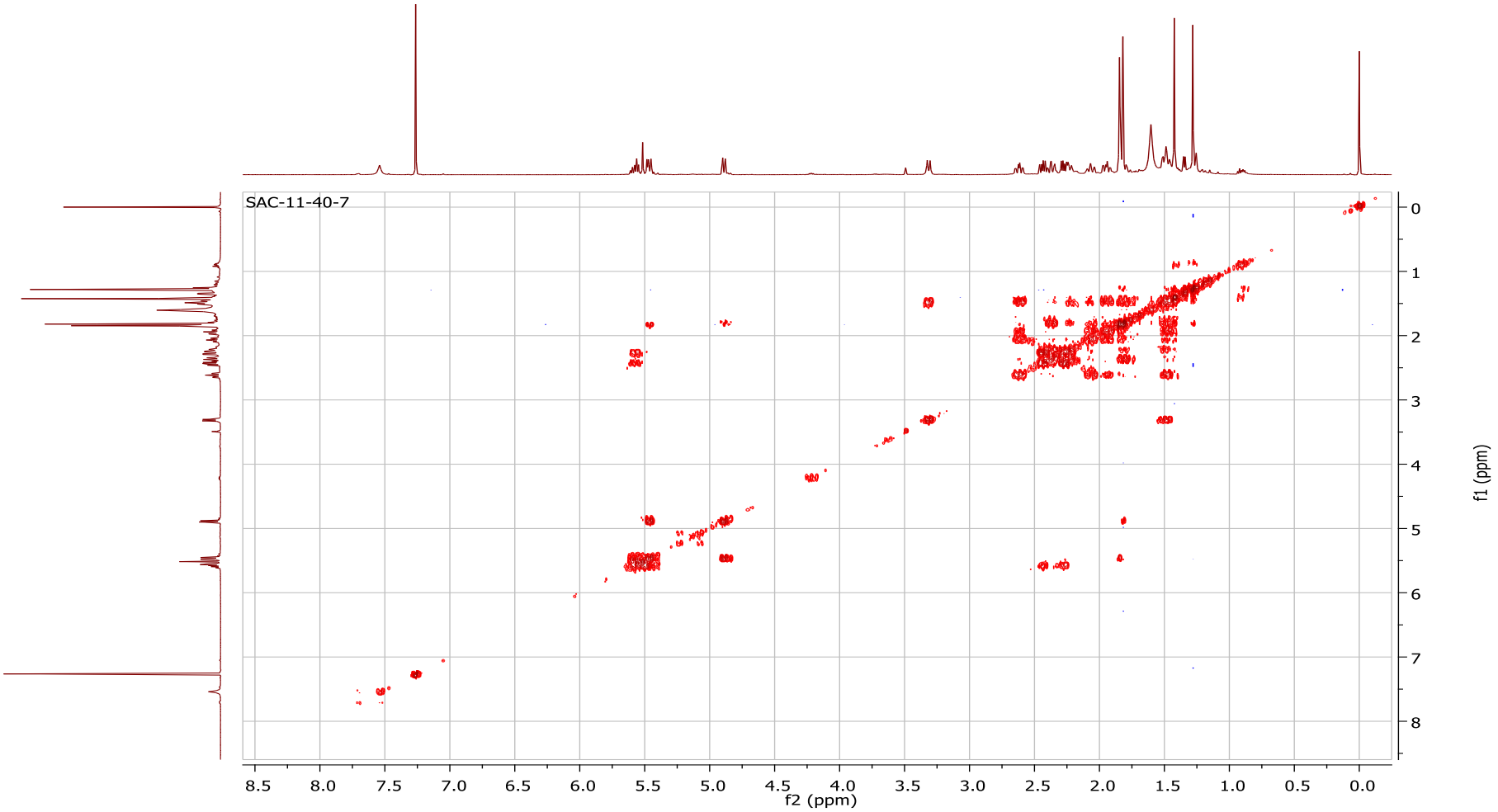
S16: DEPT of **2**



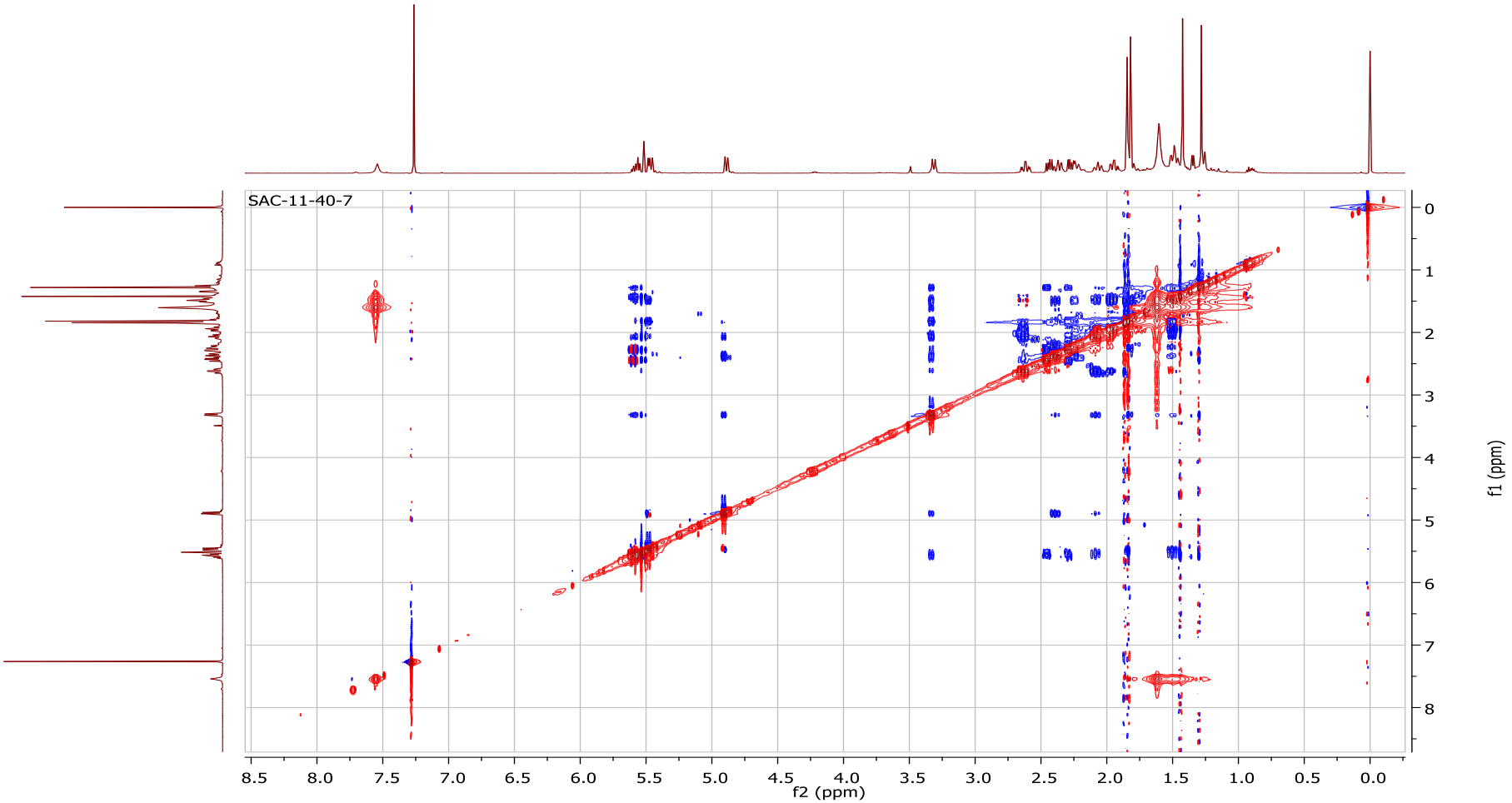
S17: HSQC of **2**


SAC-11-40-7
f2 (ppm)
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
180
200

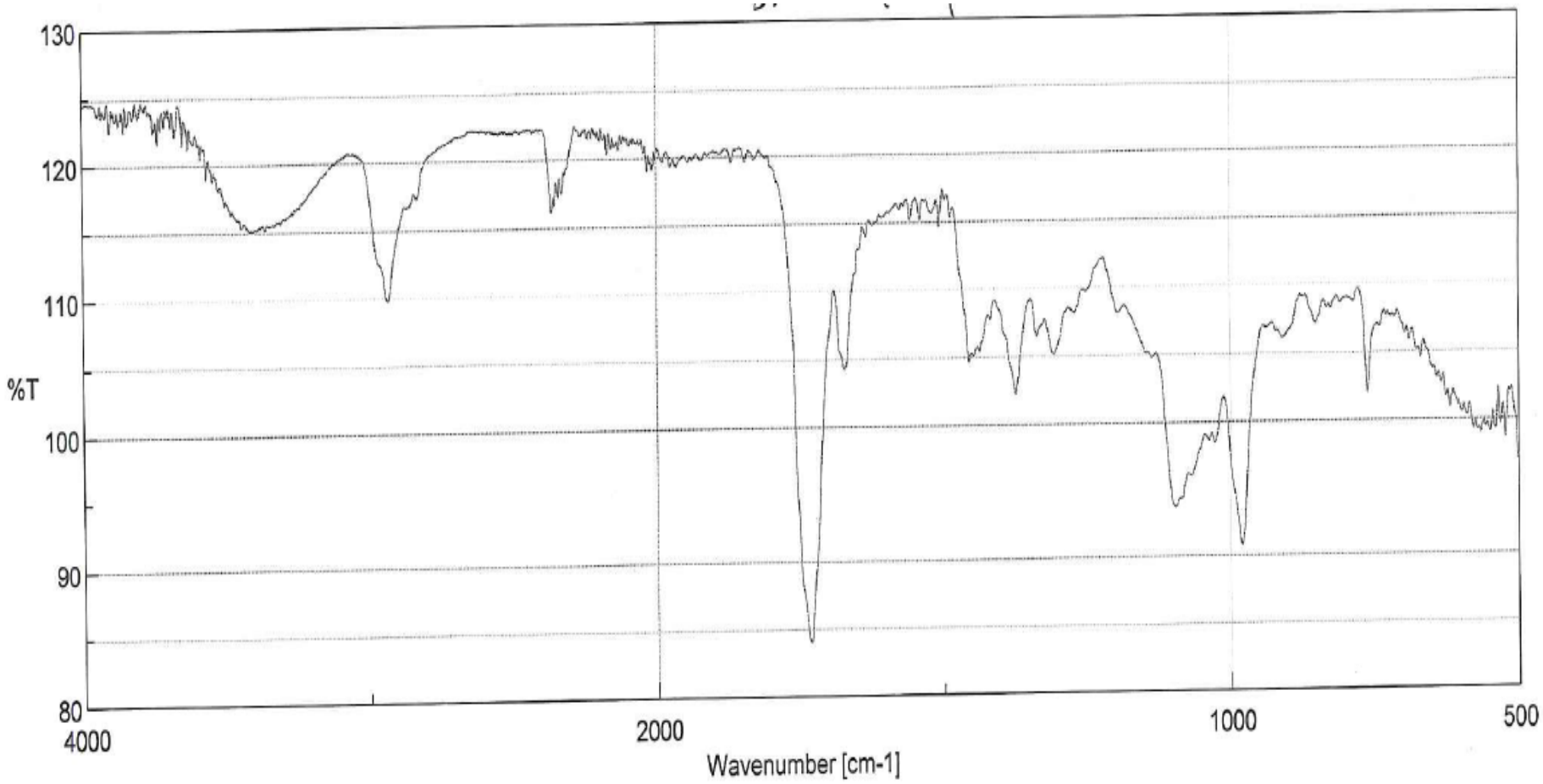
S18: HMBC of **2**



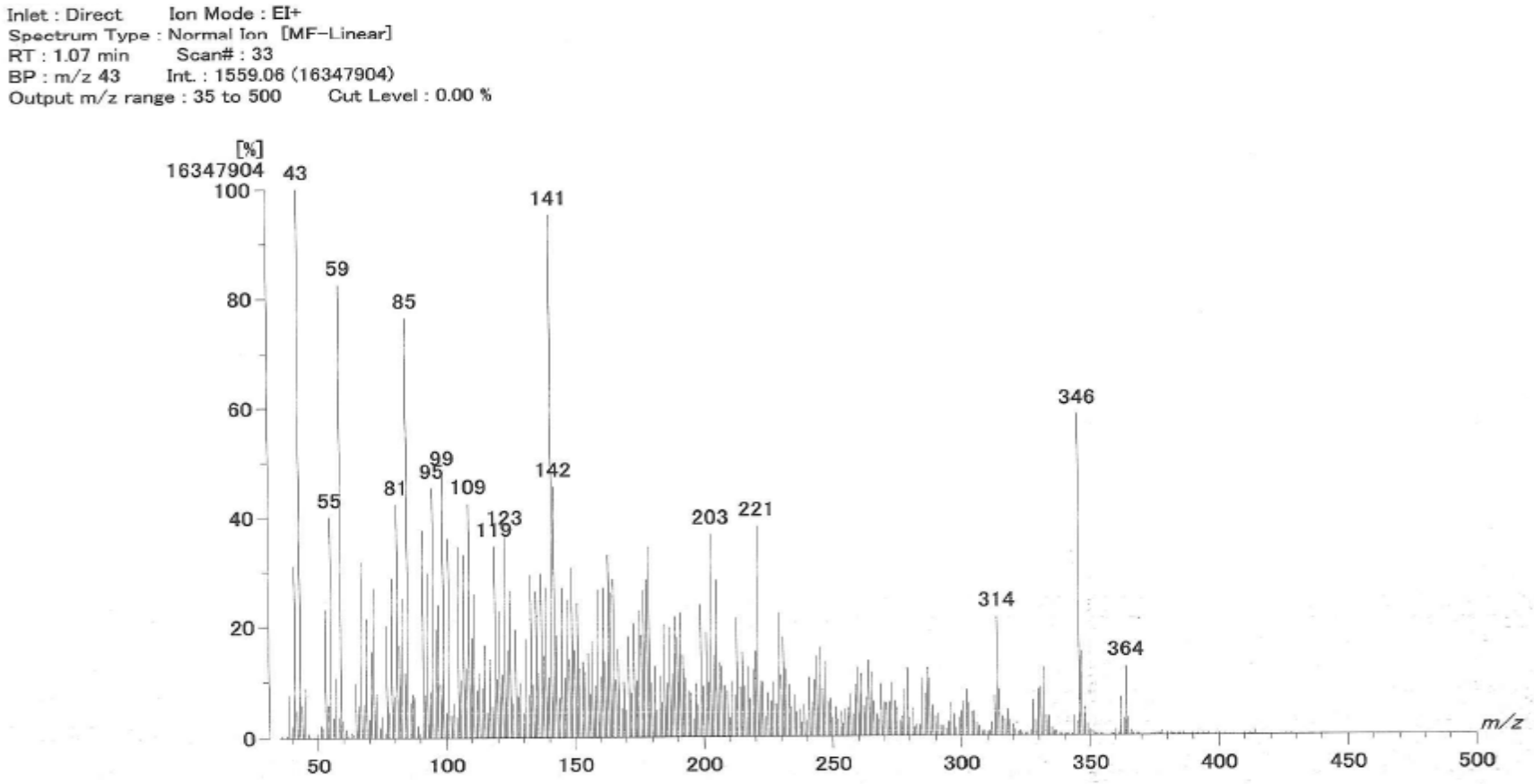
S19: ^{1}H ^{1}H COSY of **2**



S20: NOESY of **2**



S21: LRCIMS of **3**

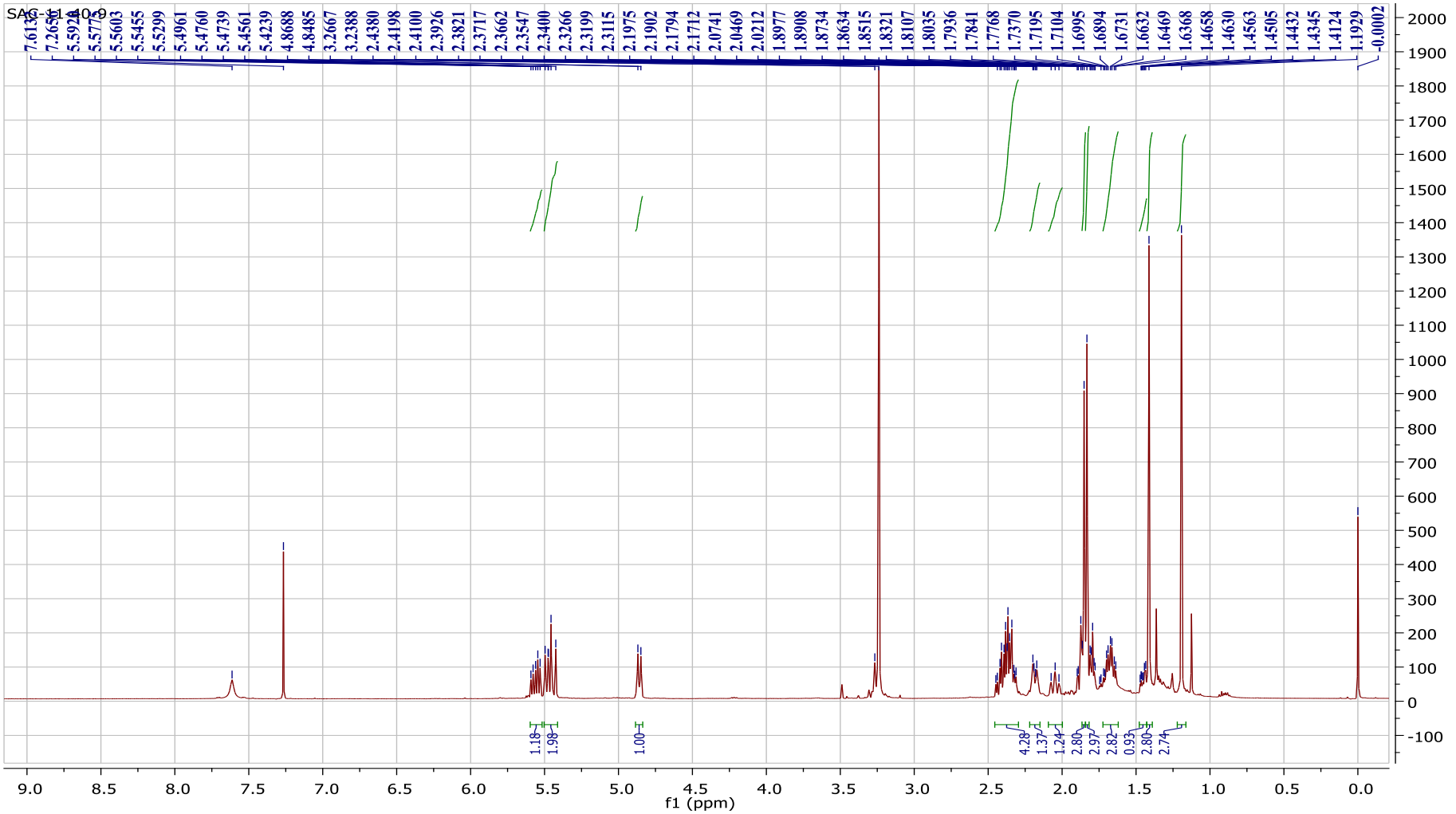


S22: LREIMS of **3**

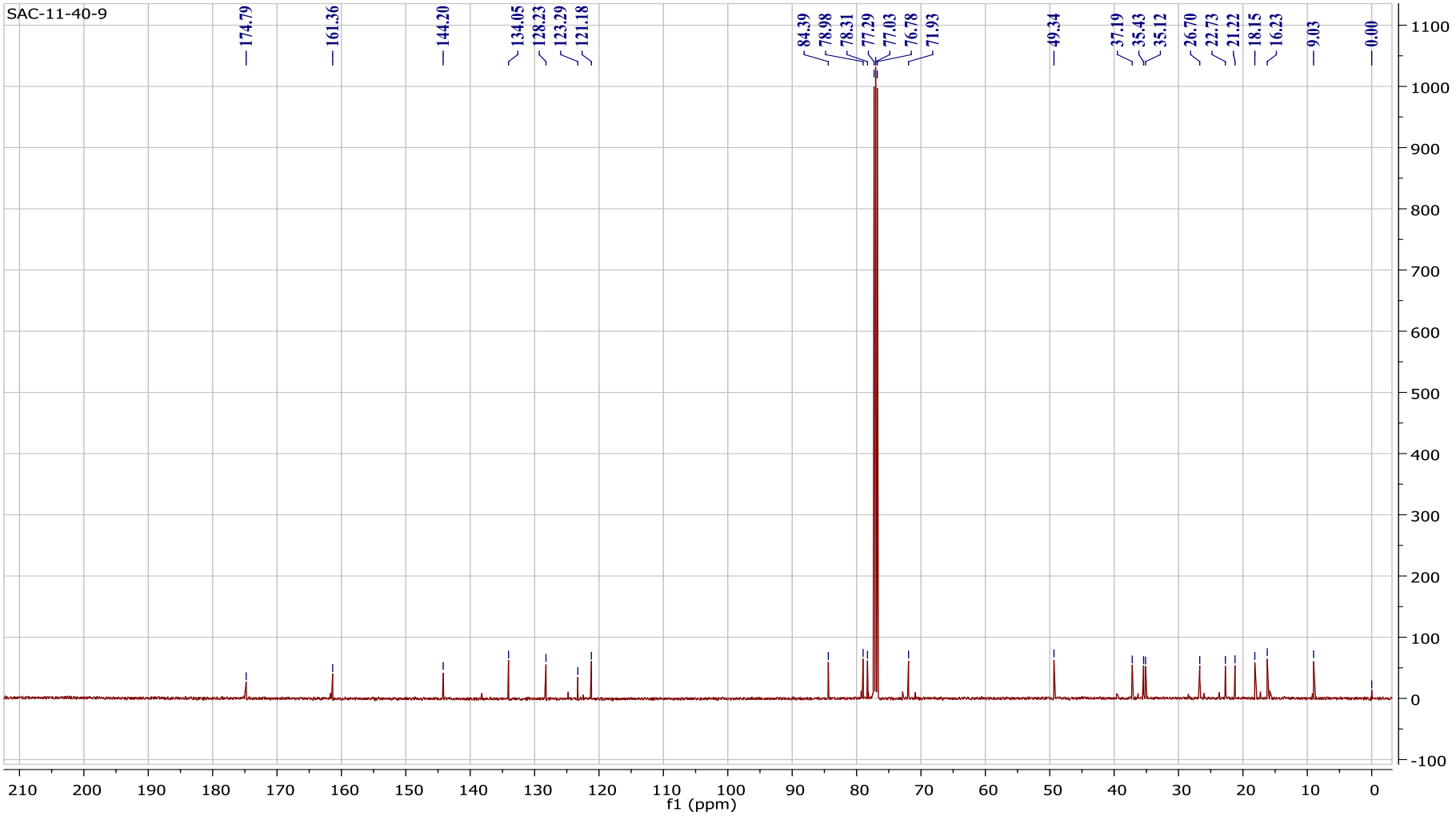
Inlet : Direct Ion Mode : EI+
RT : 1.48 min Scan# : 38
Elements : C 150/0, H 250/0, O 50/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : 0.0 – 20.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	364.2258	21.08	+2.3 / +0.8	6.0	C21 H32 O5

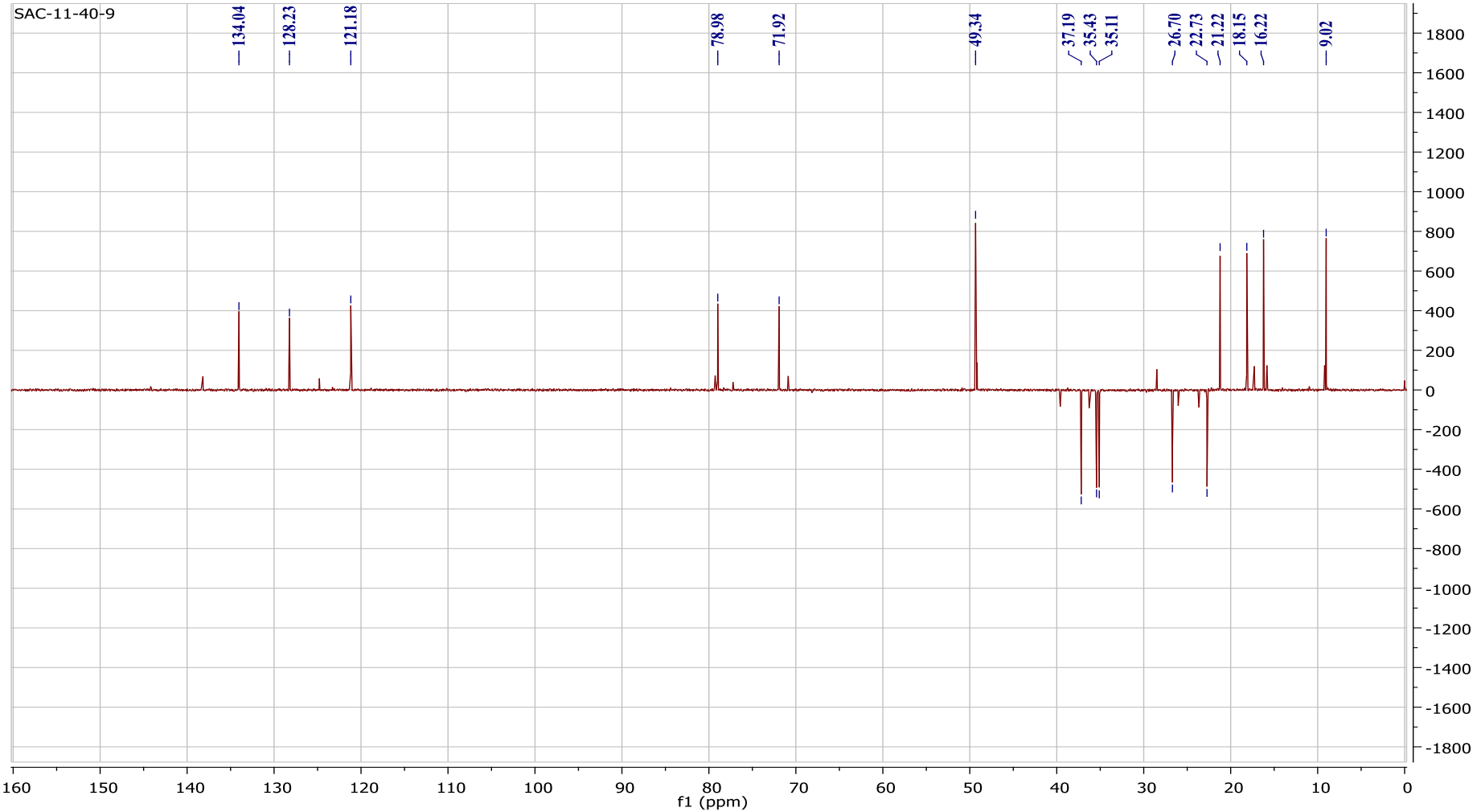
S23: HREIMS of **3**



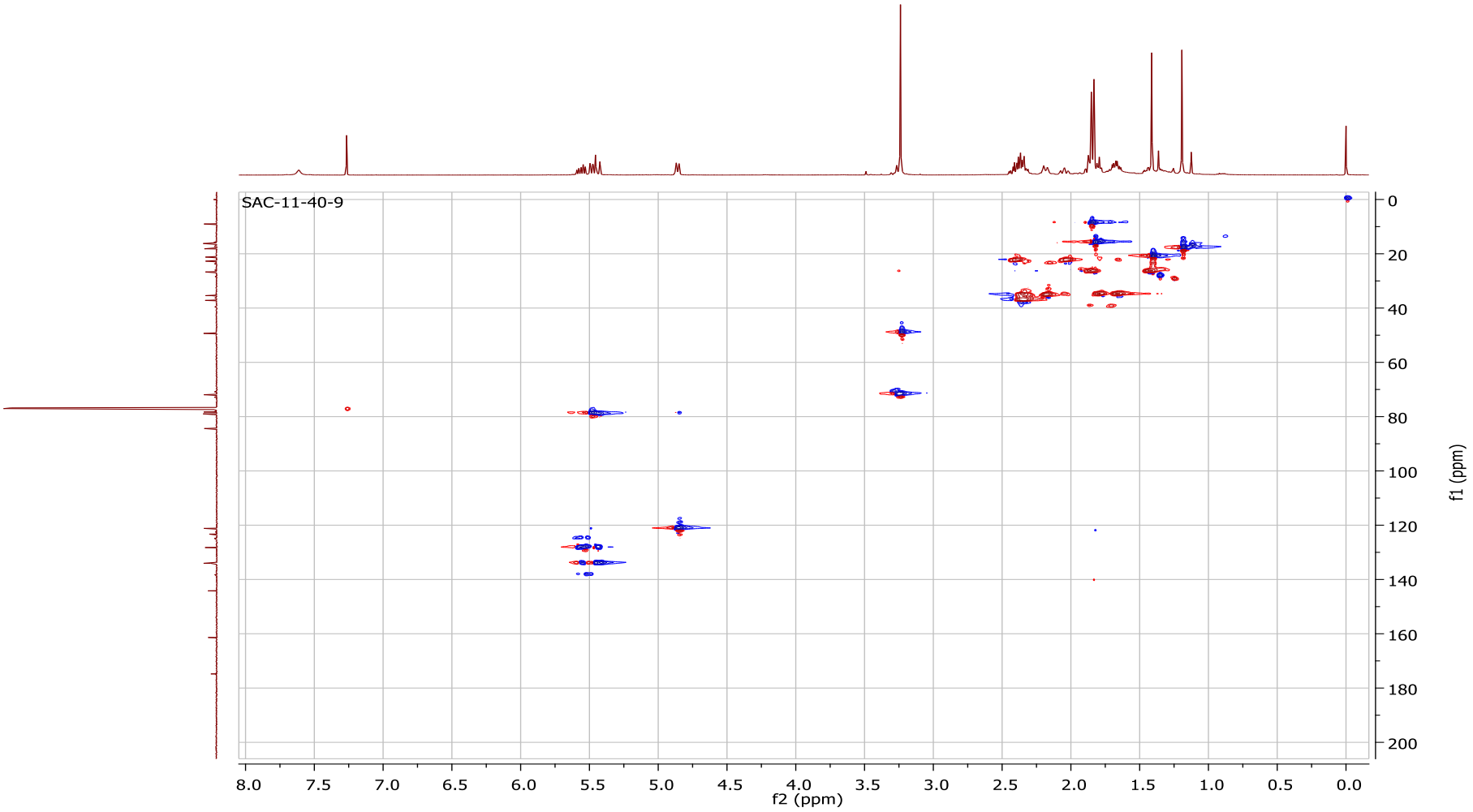
S24: ^{1}H NMR of **3**



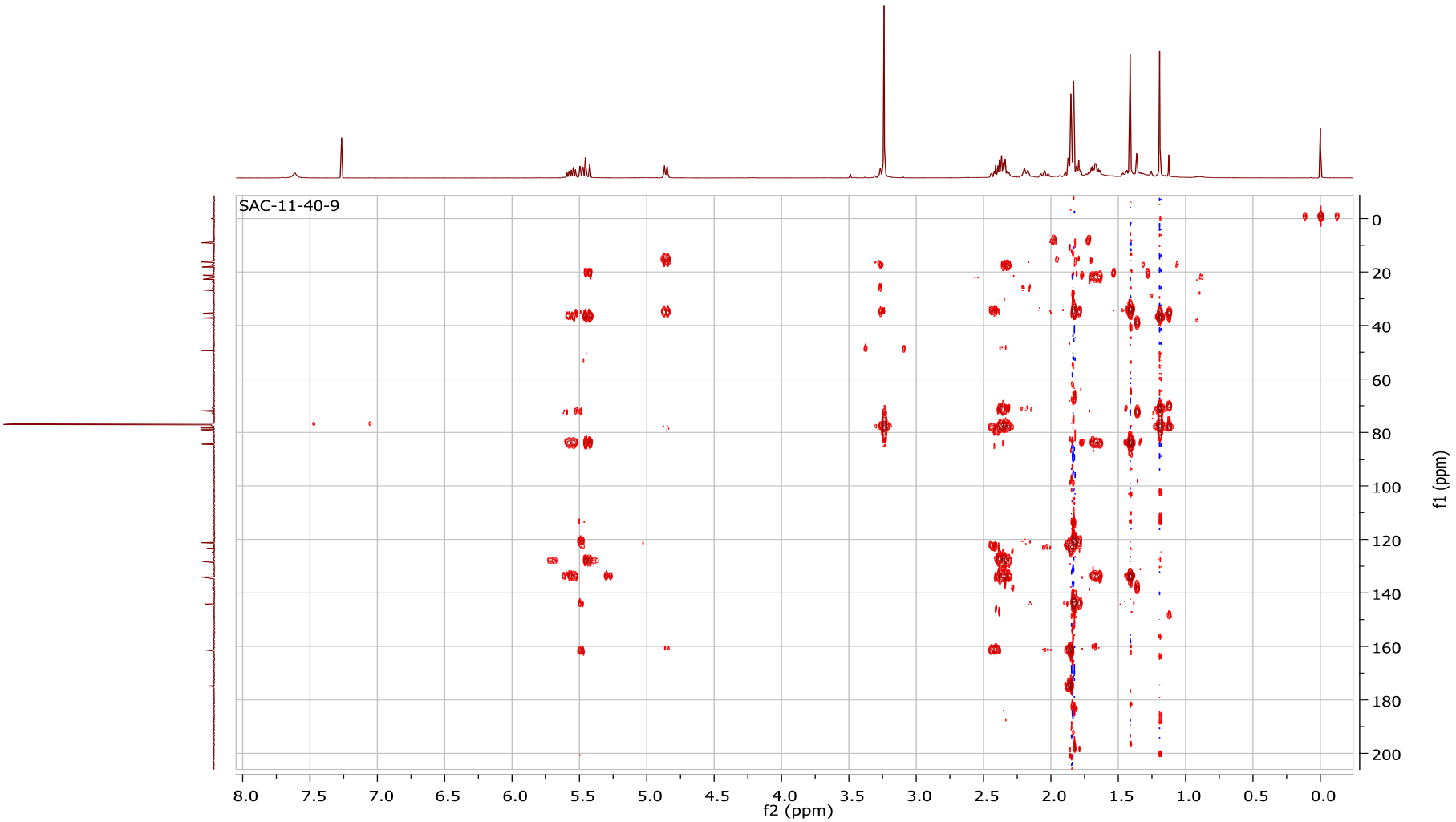
S25: ^{13}C NMR of **3**


SAC-11-40-9
134.04
128.23
121.18
78.98
71.92
49.34
37.19
35.43
35.11
26.70
22.73
21.22
18.15
16.22
9.02
f1 (ppm)

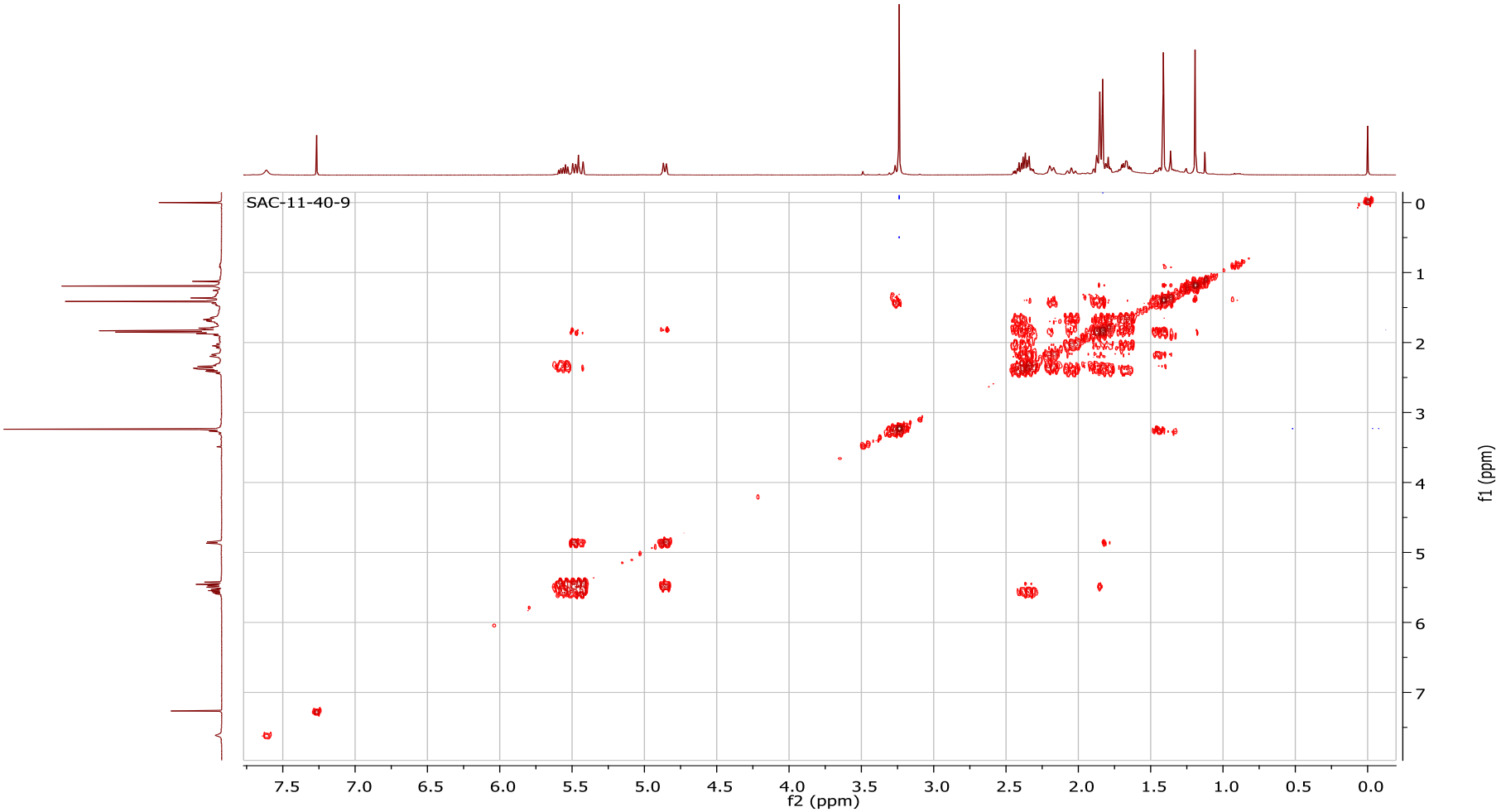
S26: DEPT of **3**


SAC-11-40-9
f2 (ppm)
f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
180
200

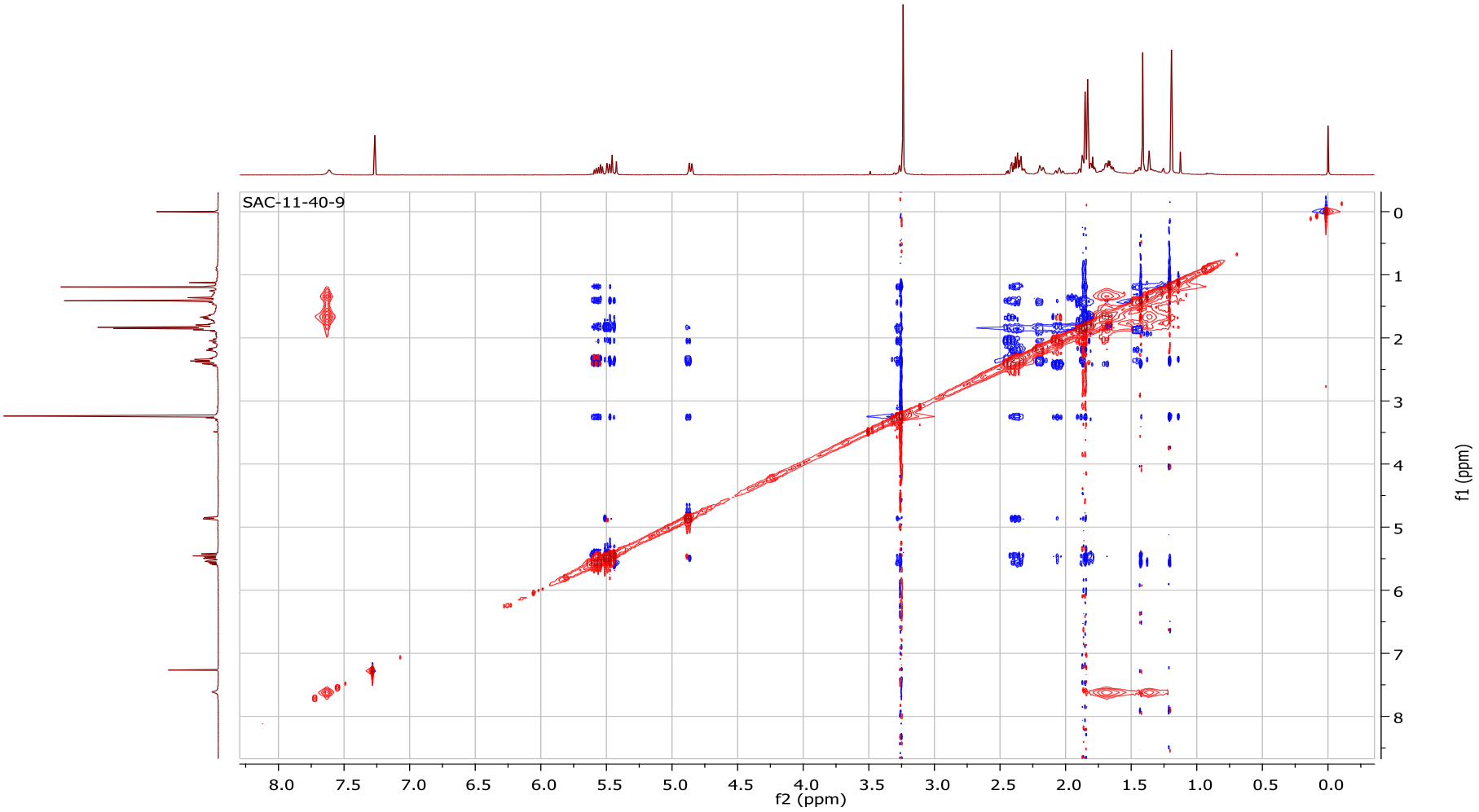
S27: HSQC of **3**



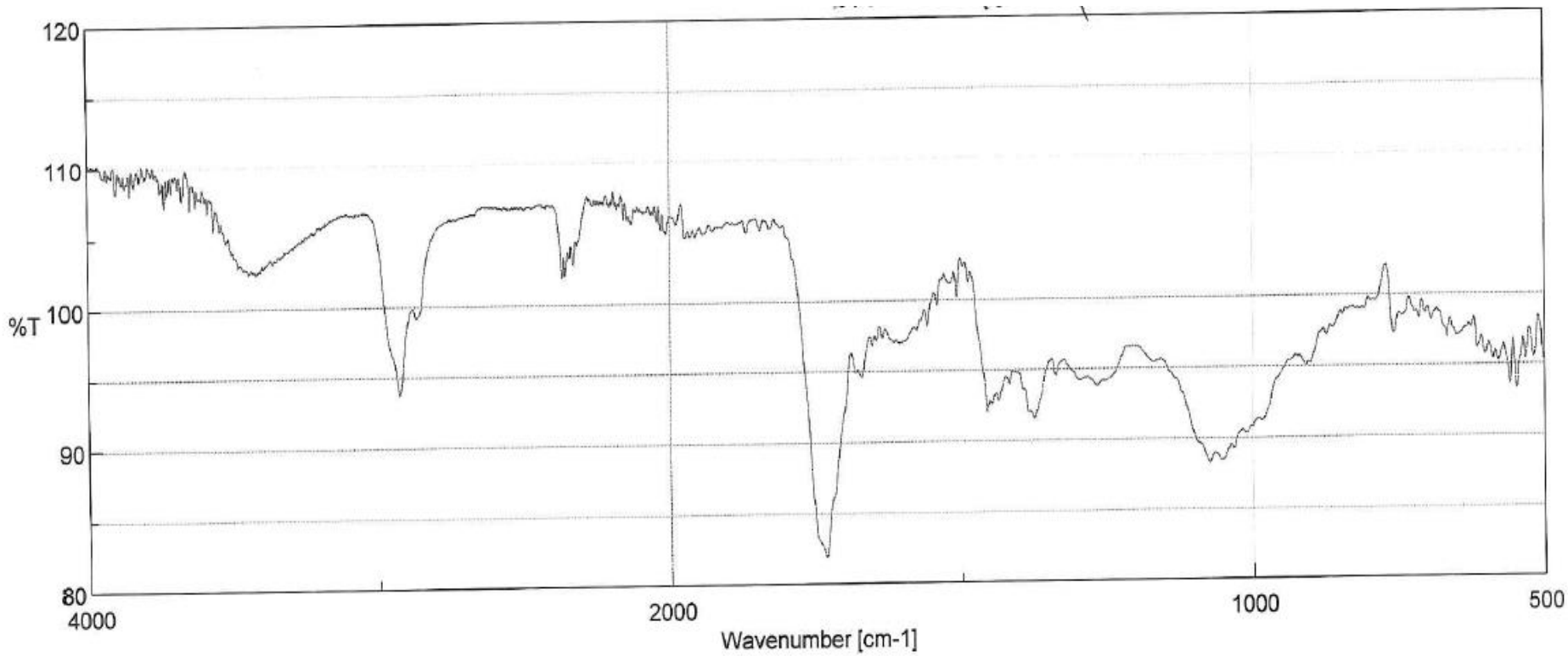
S28: HMBC of **3**



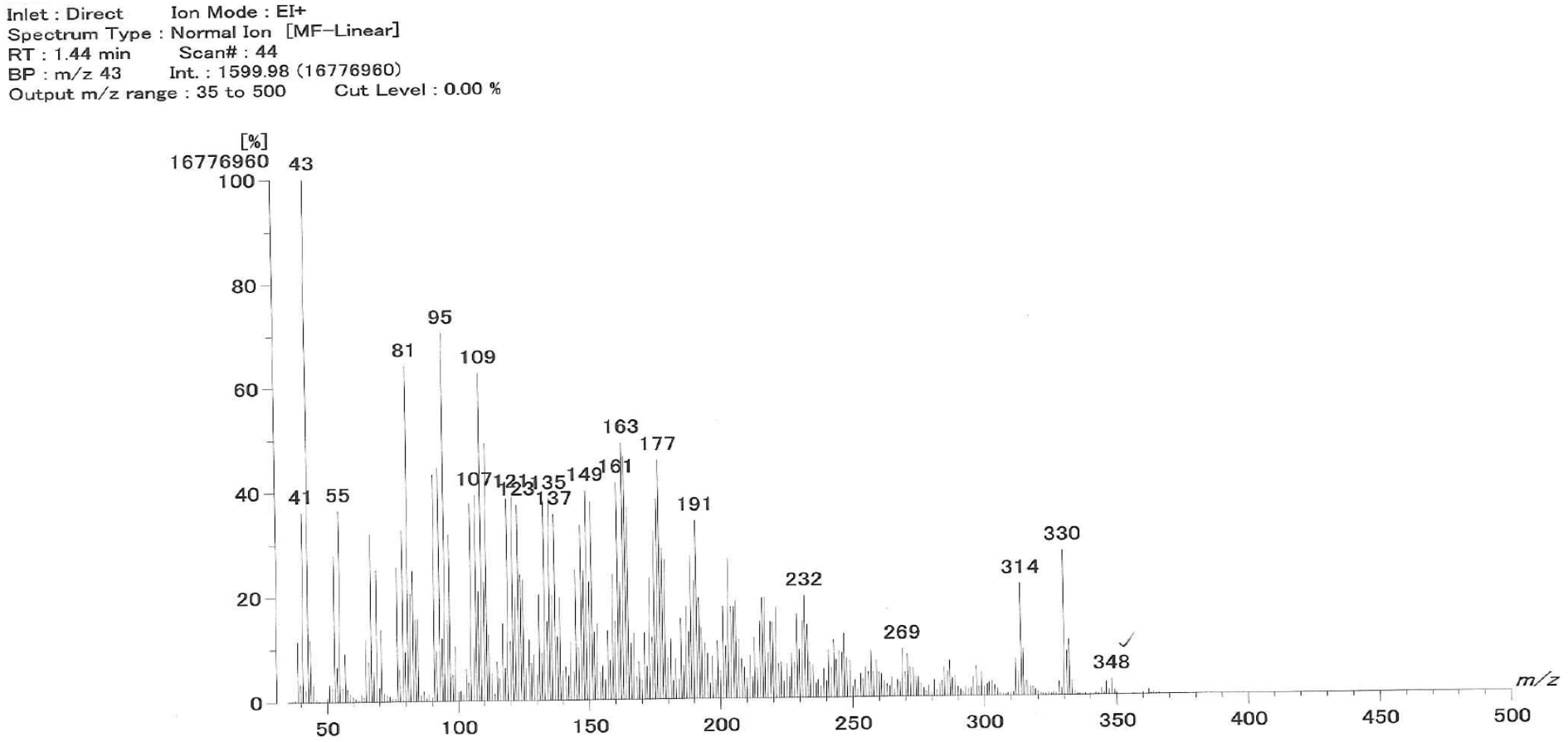
S29: ^{1}H ^{1}H COSY of **3**



S30: NOESY of **3**



S31: FTIR of **4**

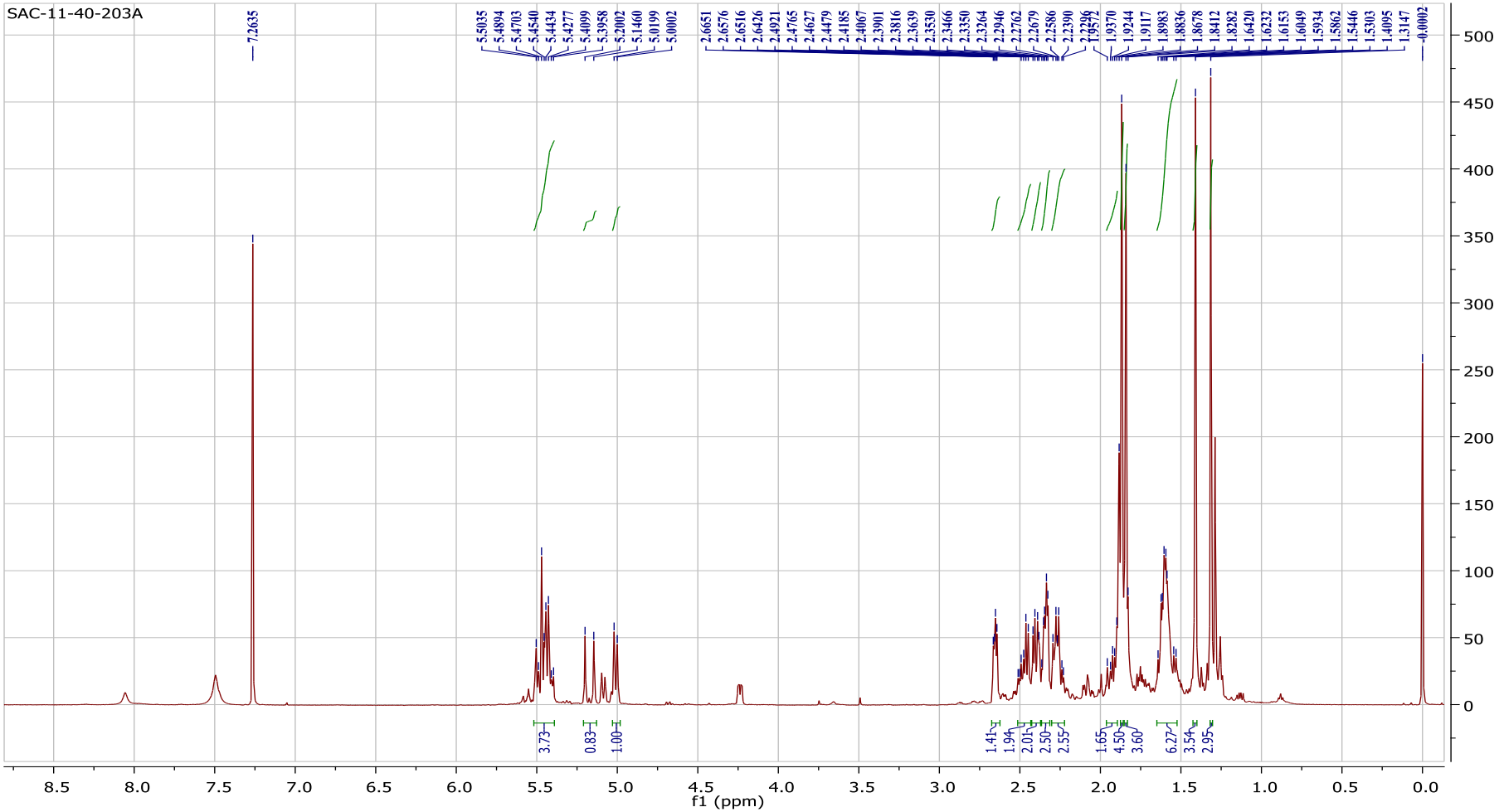


S32: LREIMS of **4**

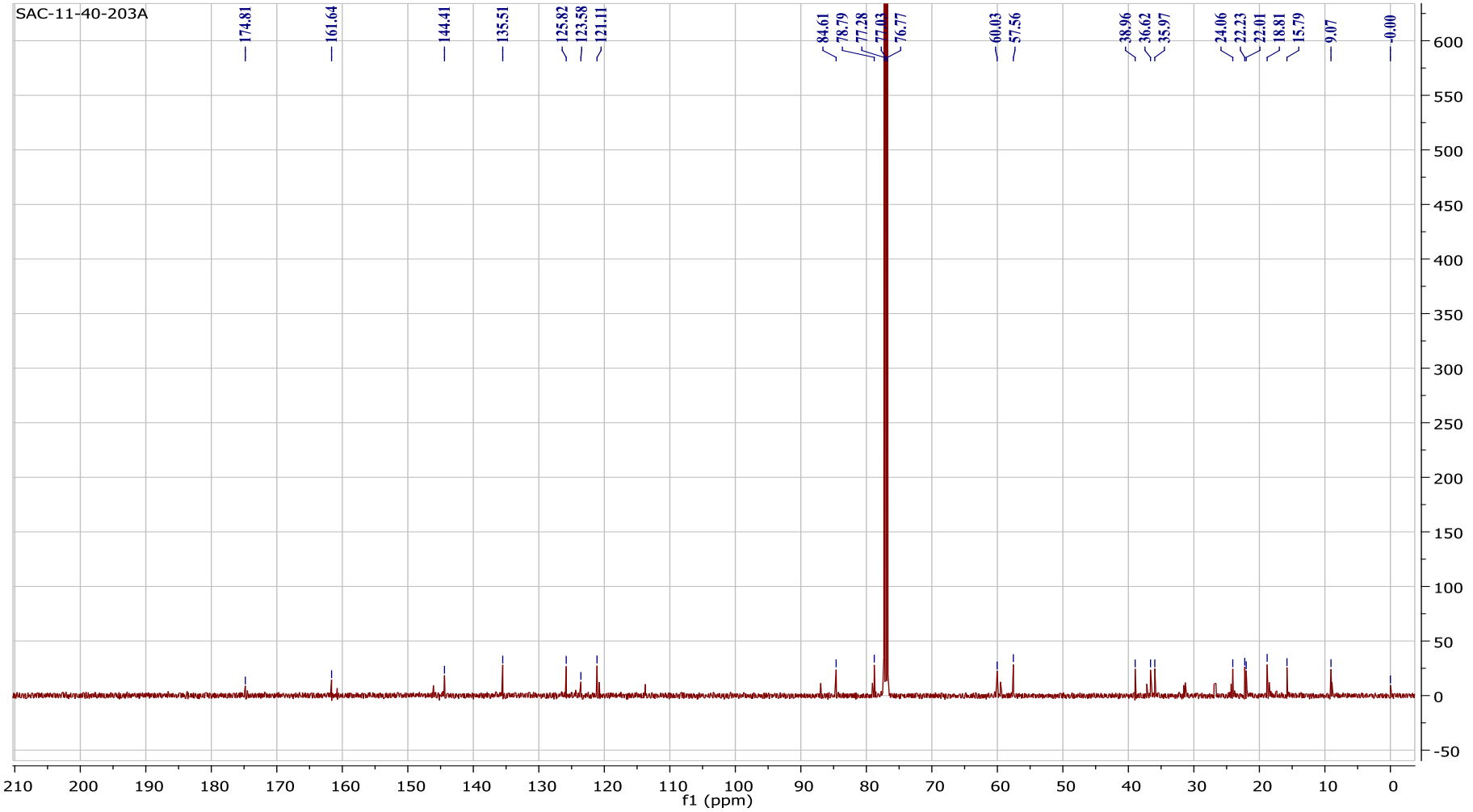
Inlet : Direct Ion Mode : EI+
RT : 2.08 min Scan# : 53
Elements : C 150/0, H 250/0, O 50/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : 0.0 – 15.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	348.1939	5.37	+0.6 / +0.2	7.0	C20 H28 O5

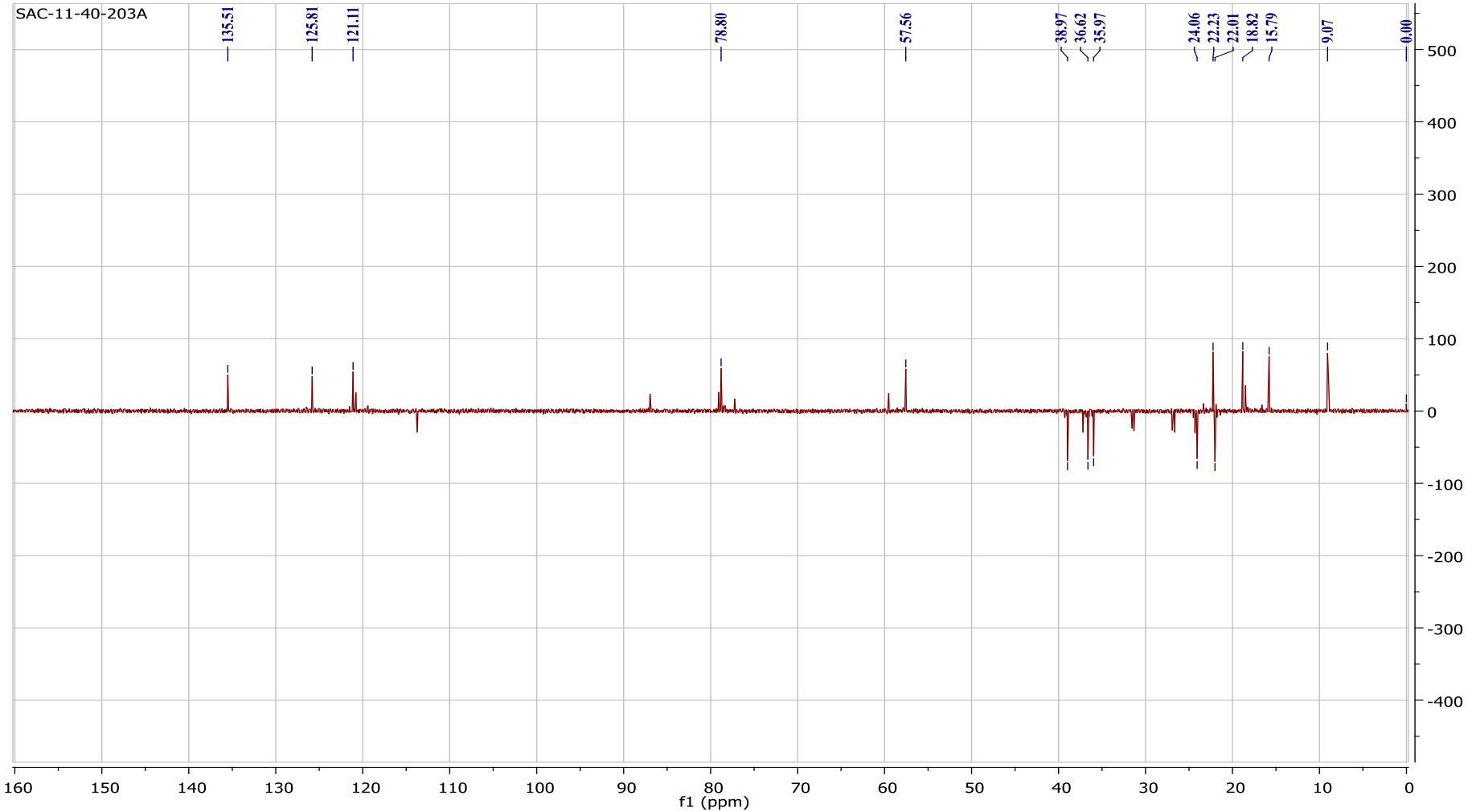
S33: HRCIMS of **4**



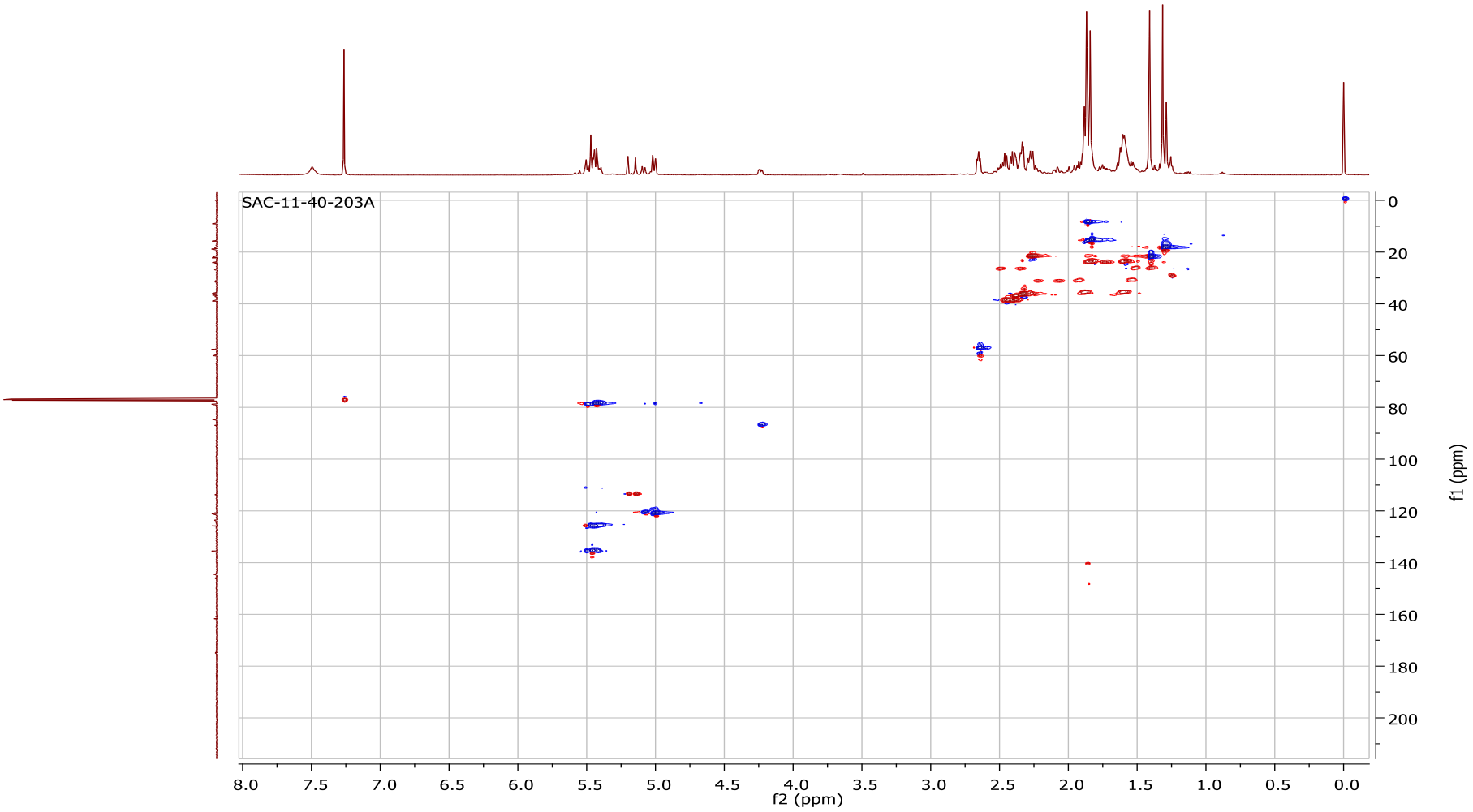
S34: ^{1}H NMR of **4**



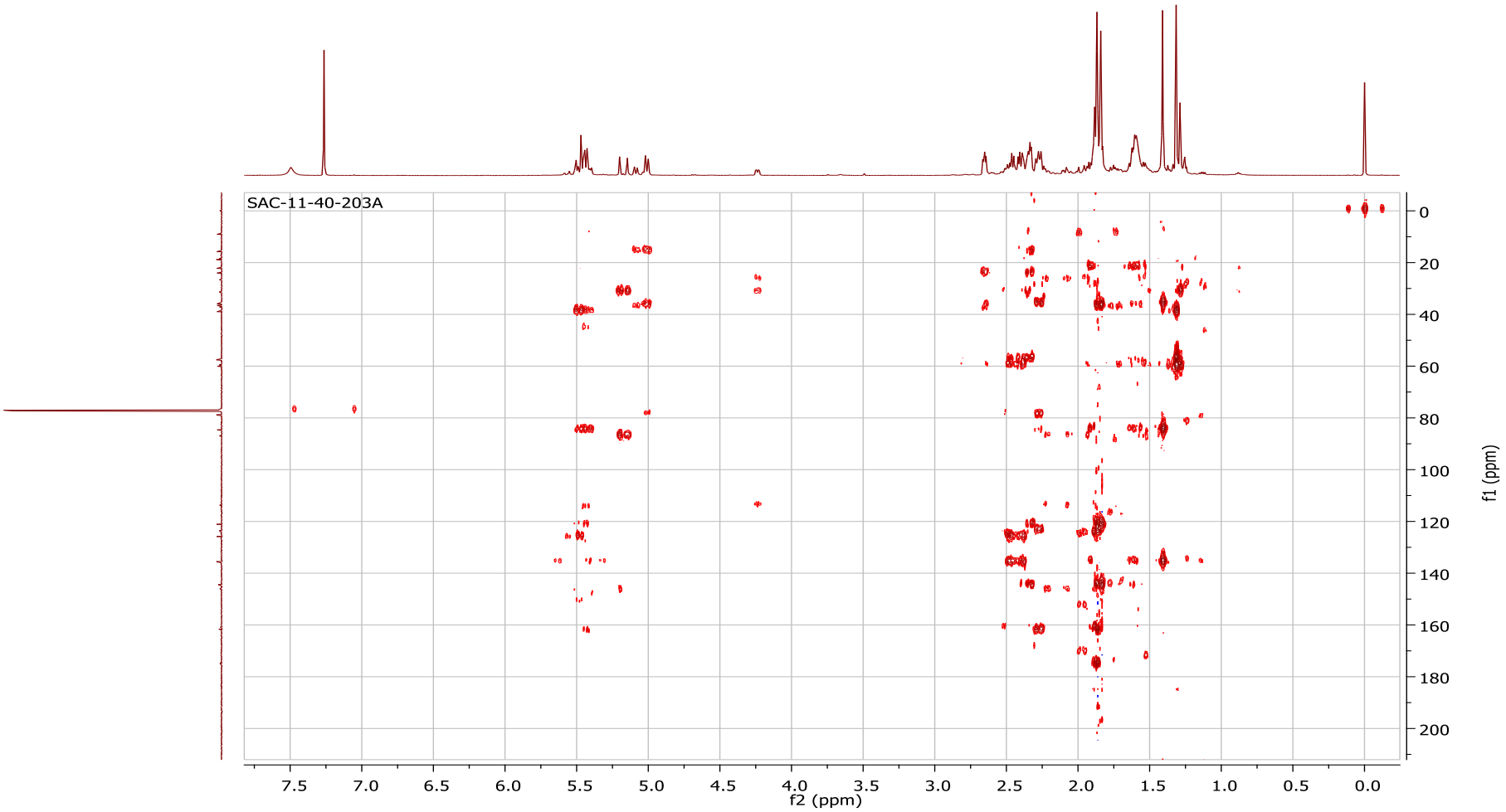
S35: ^{13}C NMR of **4**


SAC-11-40-203A
135.51
125.81
121.11
78.80
57.56
38.97
36.62
35.97
24.06
22.23
22.01
18.82
15.79
9.07
0.00
500
400
300
200
100
0
-100
-200
-300
-400
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

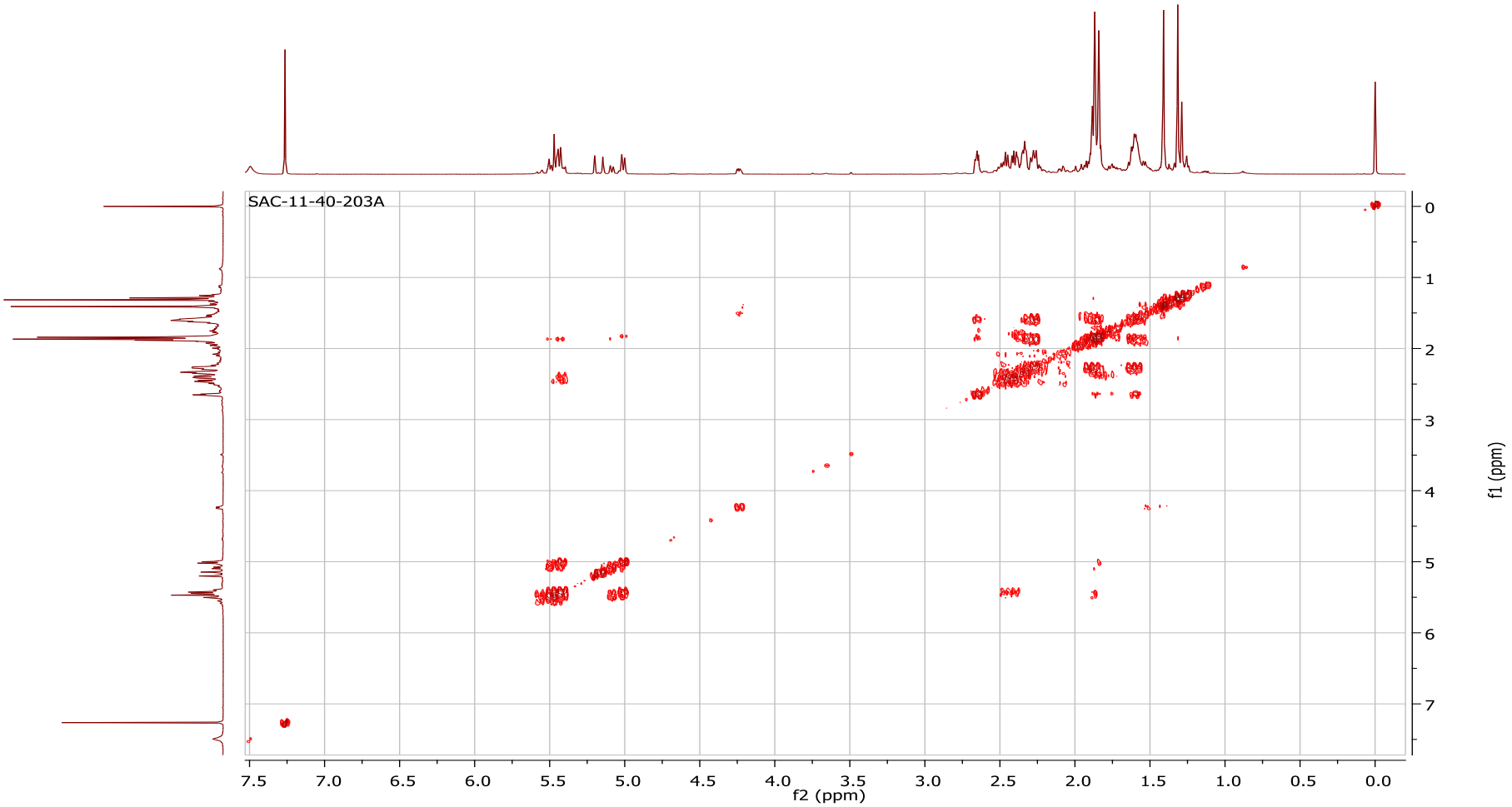
S36: DEPT of **4**


SAC-11-40-203A
f2 (ppm)
f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
180
200

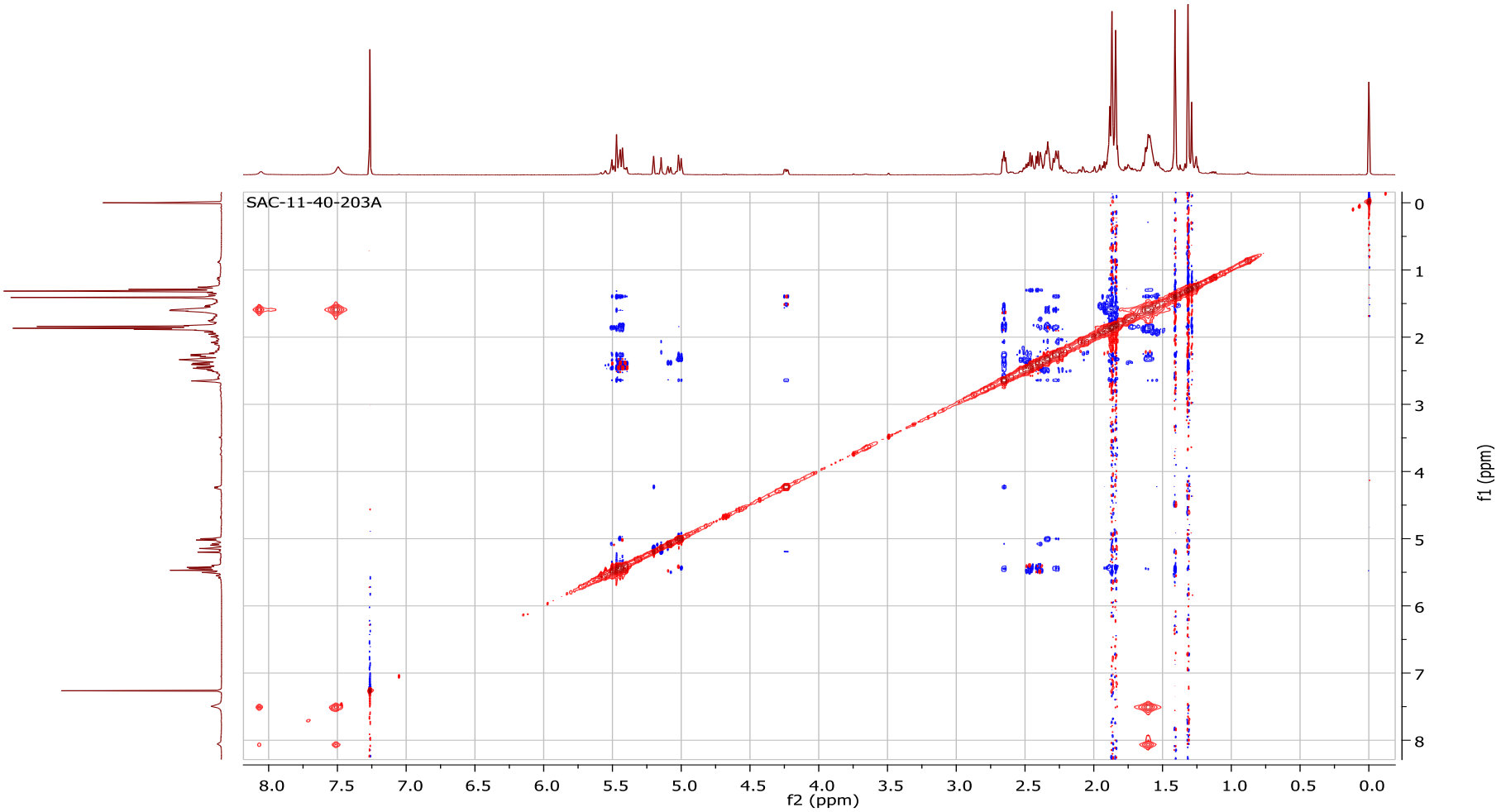
S37: HSQC of **4**



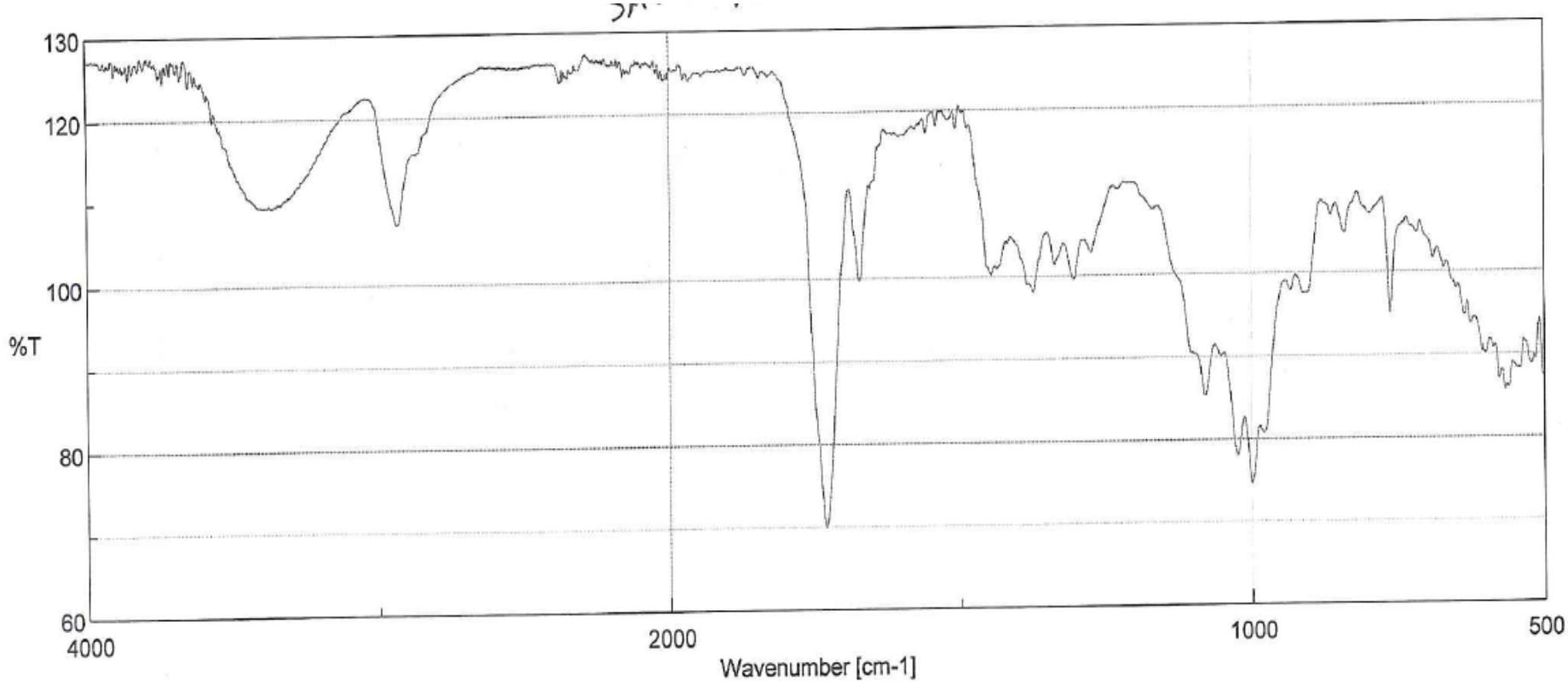
S38: HMBC of **4**



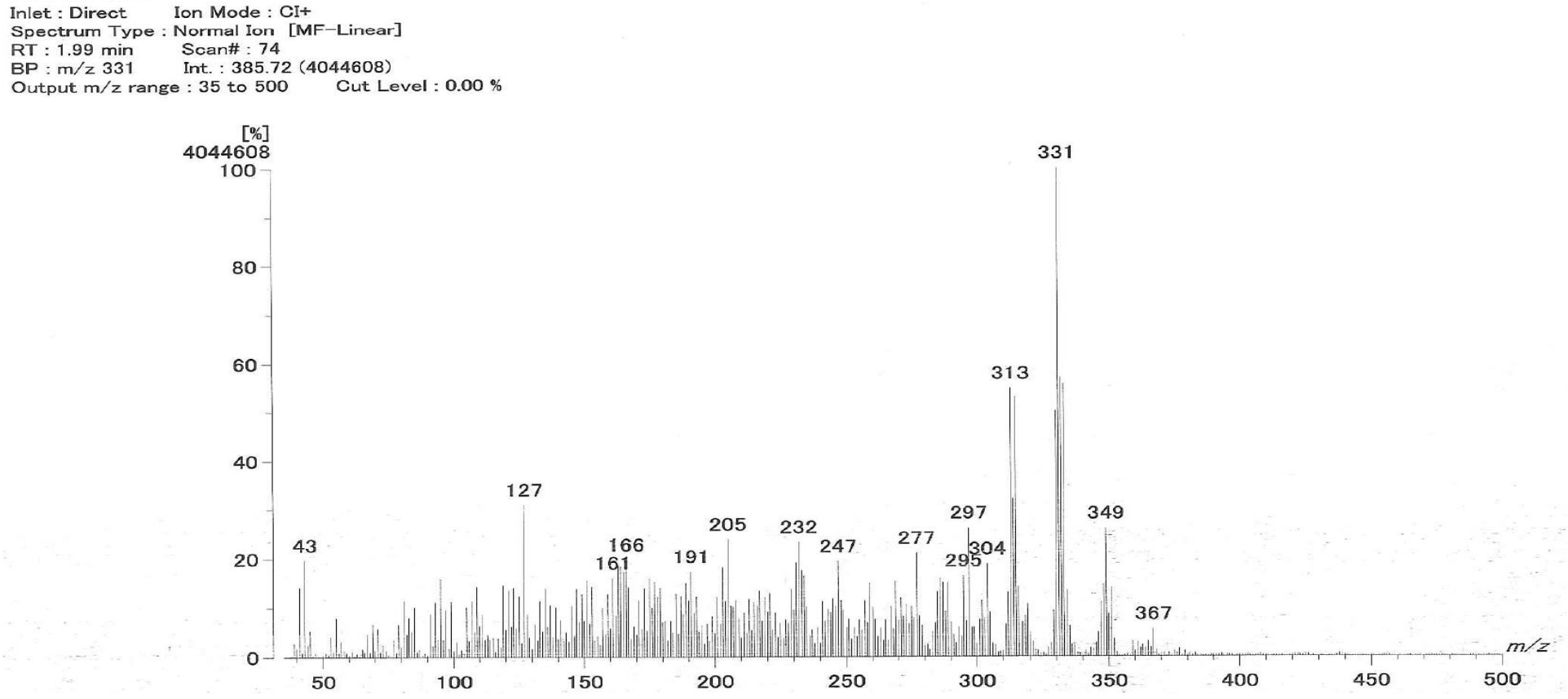
S39: ^{1}H ^{1}H COSY of **4**



S40: NOESY of **4**



S41: FTIR of **5**

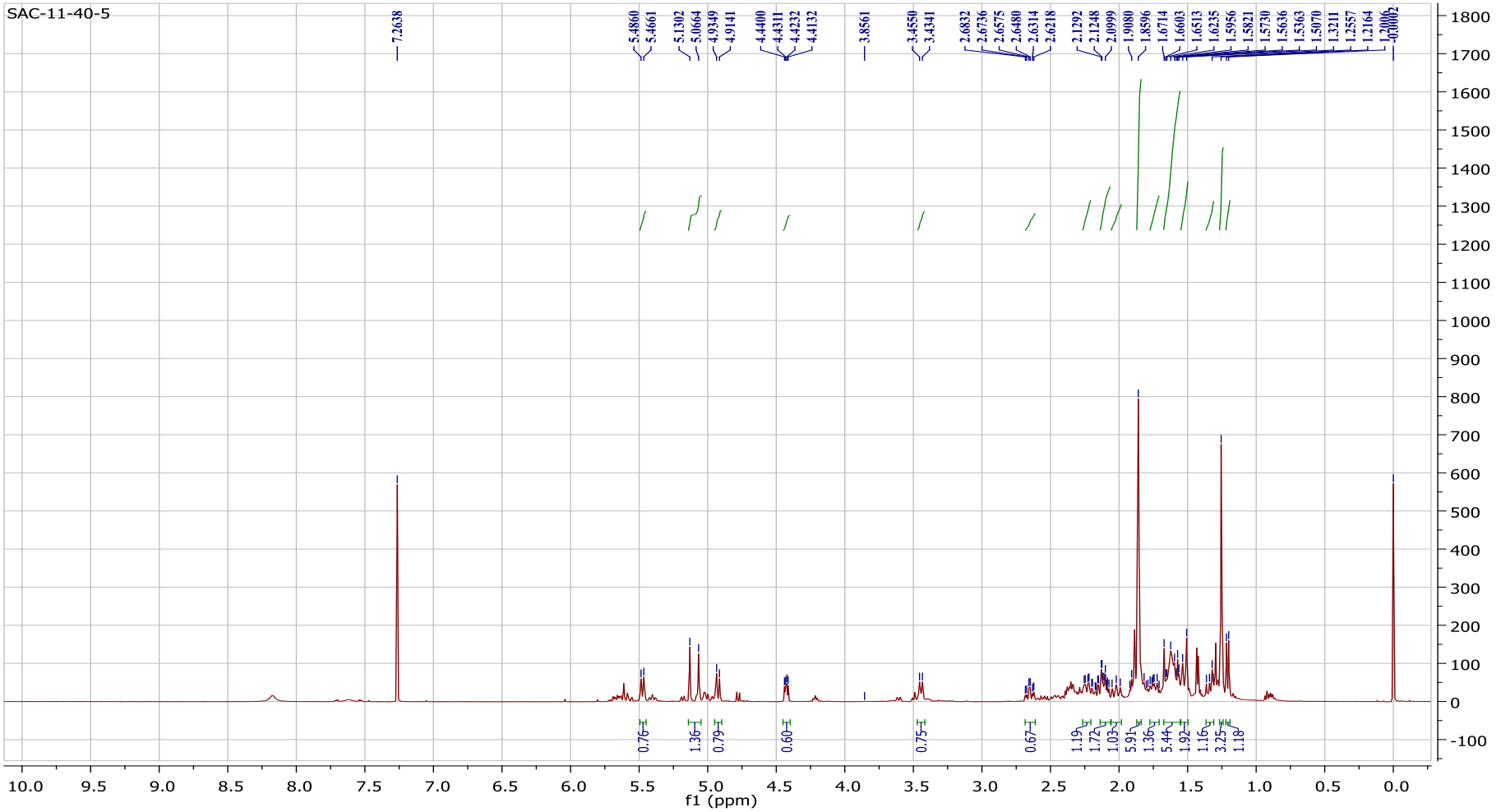


S42: LRCIMS of **5**

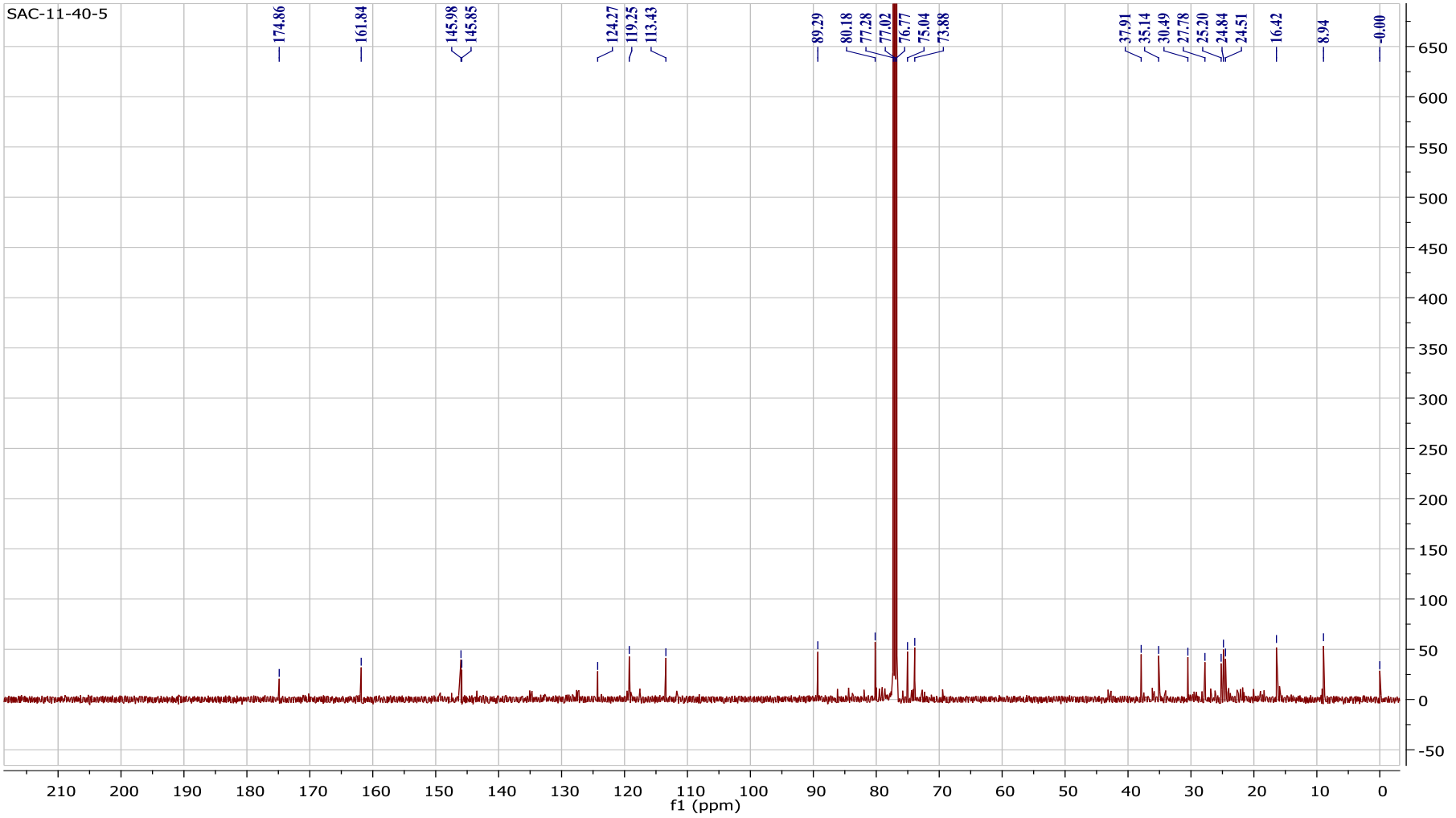
Inlet : Direct Ion Mode : CI+
RT : 1.64 min Scan# : 42
Elements : C 150/0, H 250/0, O 50/0
Mass Tolerance : 5mmu
Unsaturation (U.S.) : 0.0 – 15.0

	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	367.2130	3.63	+2.5 / +0.9	5.5	C20 H31 O6

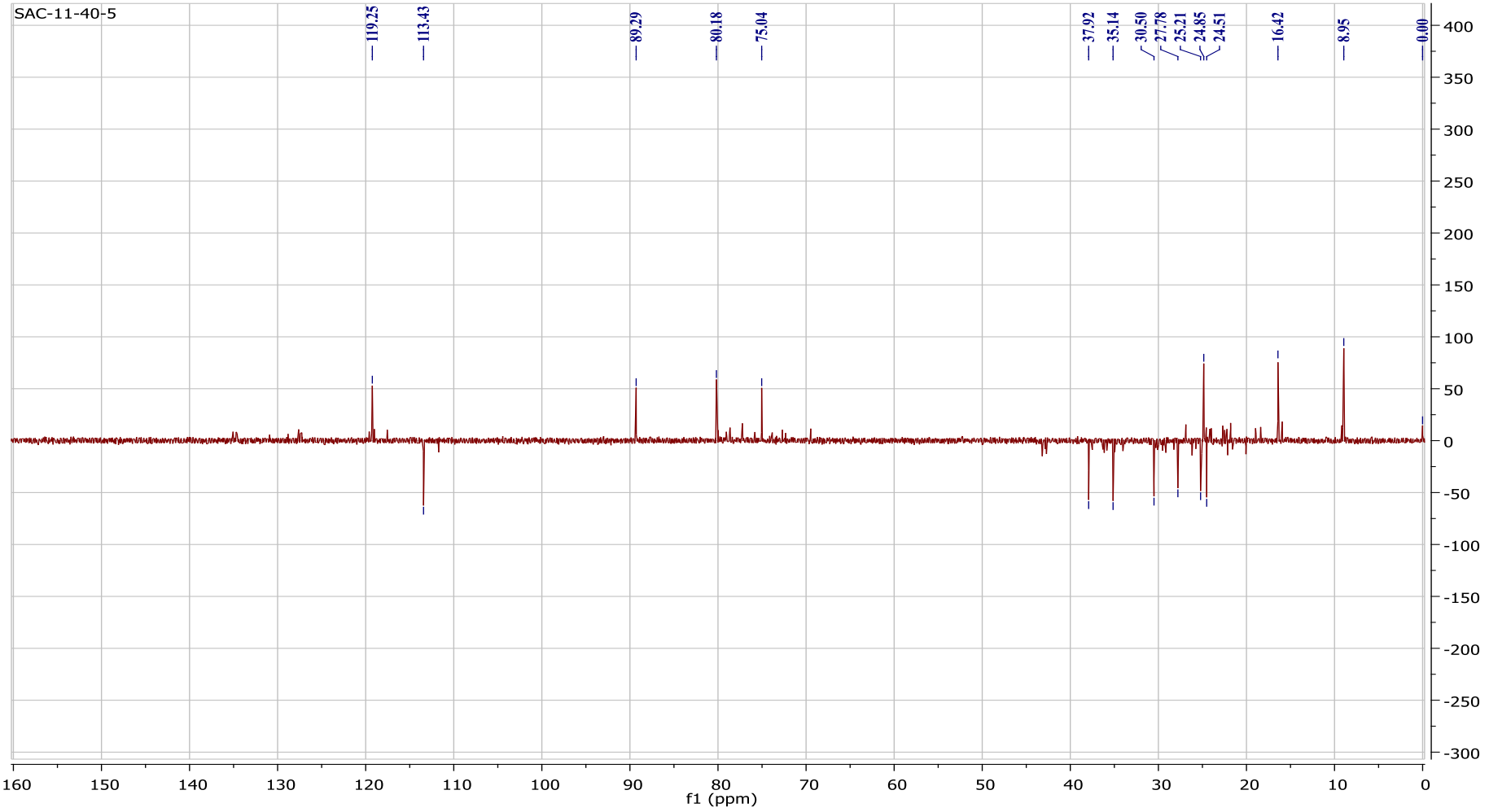
S43: HRCIMS of **5**



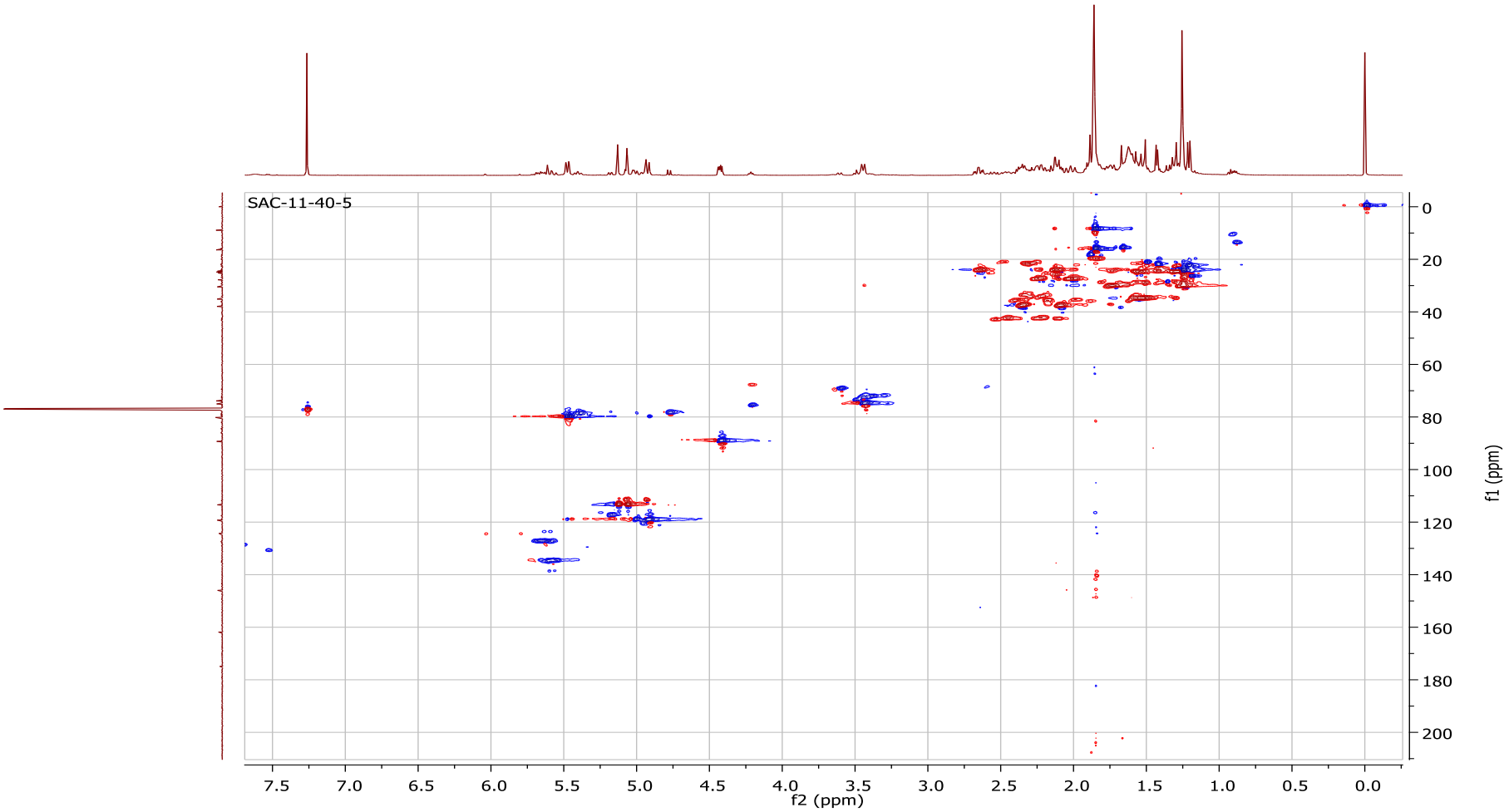
S44: ^{1}H NMR of **5**



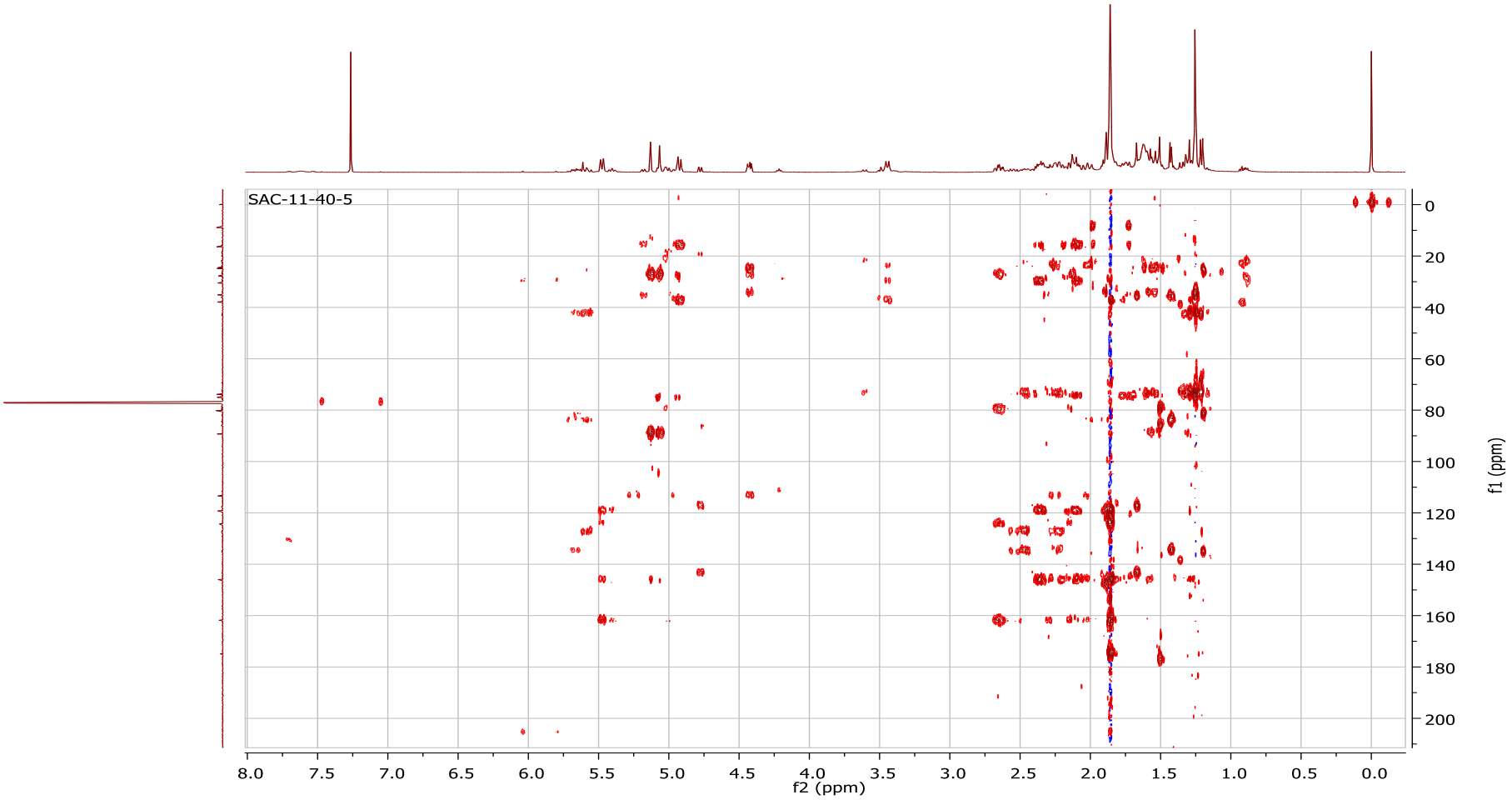
S45: ^{13}C NMR of **5**


SAC-11-40-5
119.25
113.43
89.29
80.18
75.04
37.92
35.14
30.50
27.78
25.21
24.85
24.51
16.42
8.95
0.00
f1 (ppm)

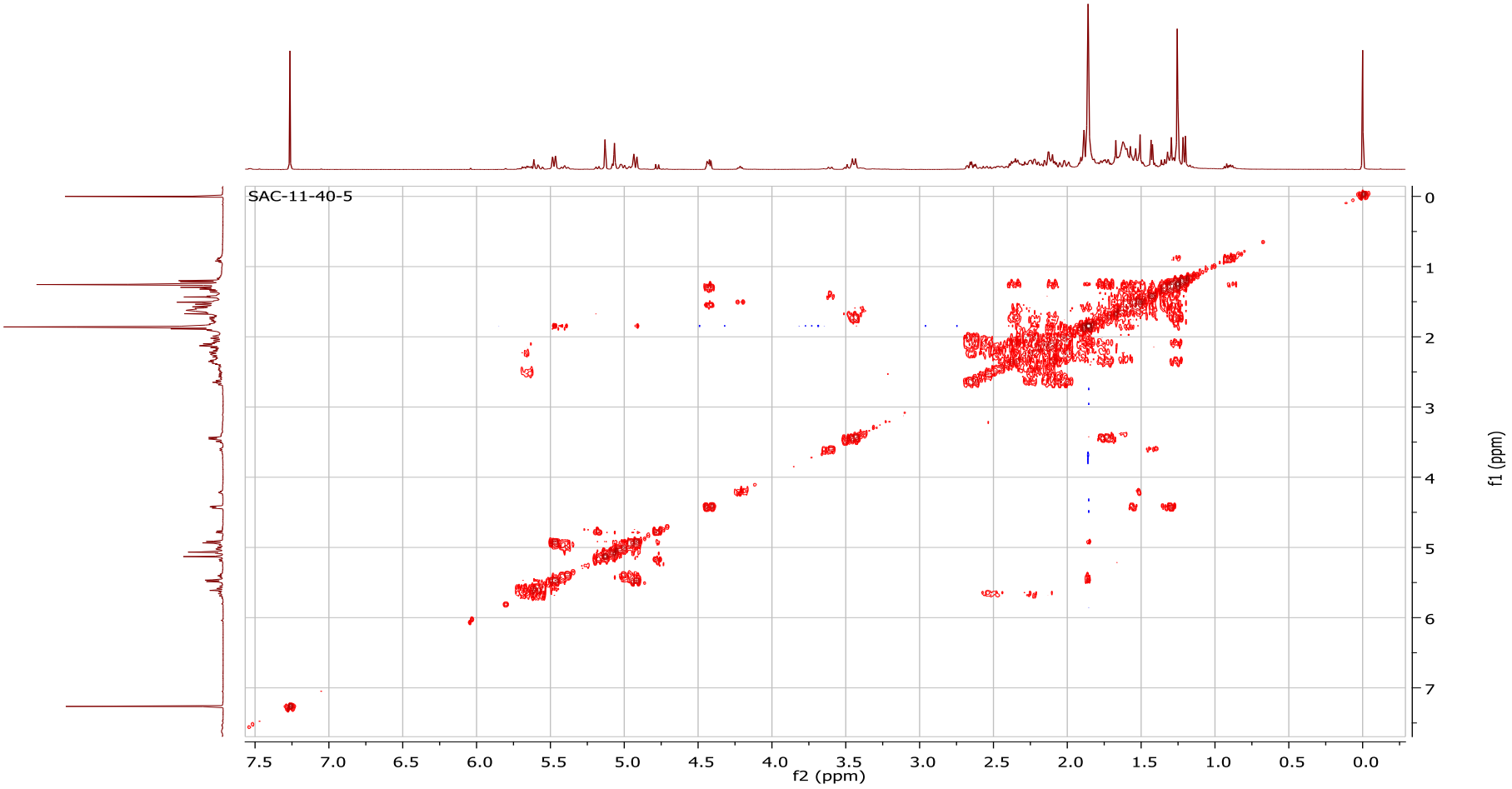
S46: DEPT of **5**


SAC-11-40-5
f2 (ppm)
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
180
200

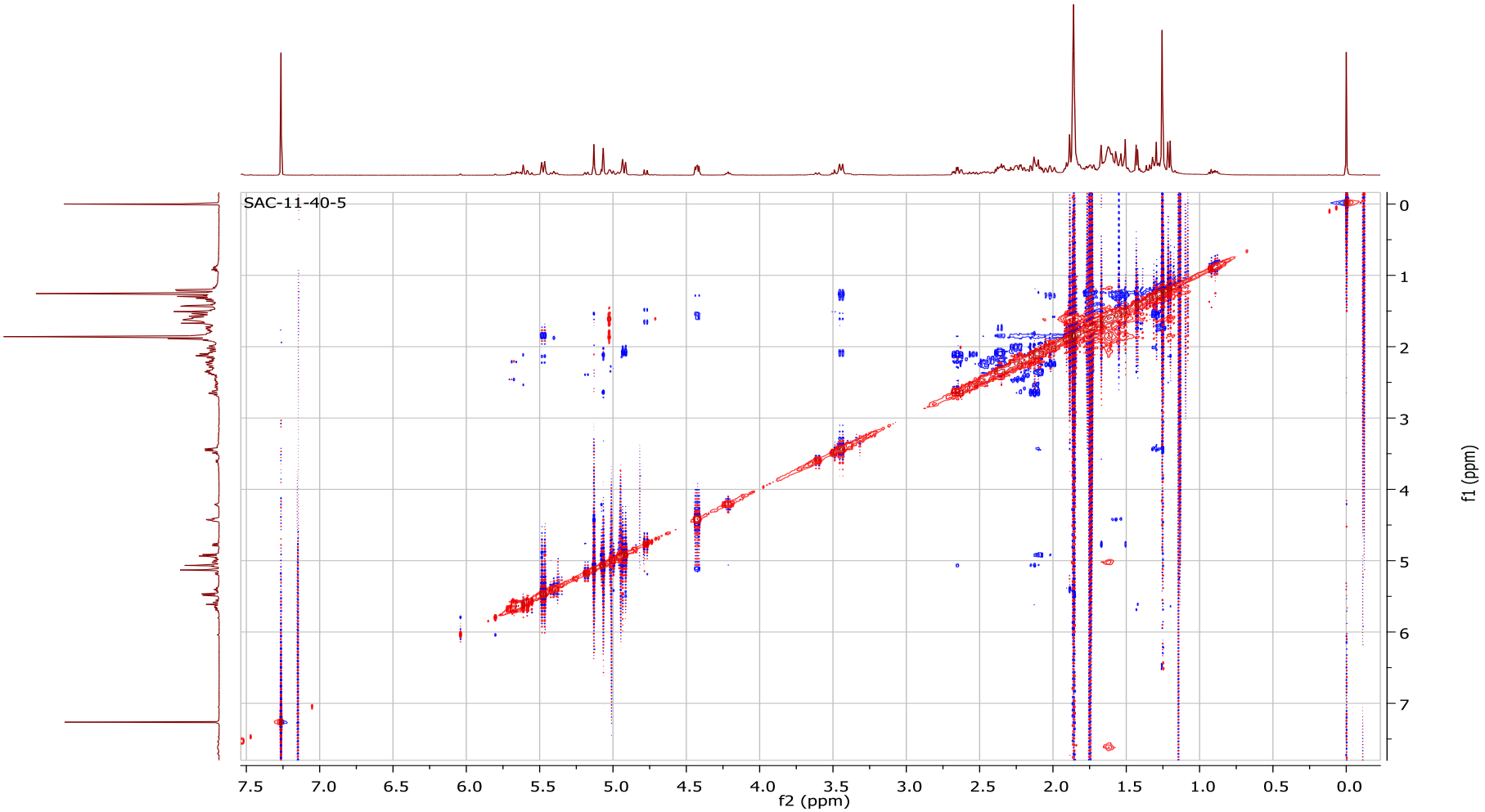
S47: HSQC of **5**


SAC-11-40-5
f2 (ppm)
f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
120
140
160
180
200

S48: HMBC of **5**



S49: ^{1}H ^{1}H COSY of **5**



S50: NOESY of **5**