Supporting Information

Part 2

Synthesis of unstrained Criegee intermediates: inverse α-effect and other protective stereoelectronic forces can stop Baeyer-Villiger rearrangement of γ-hydroperoxy-γ-peroxylactones

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[b] Department of Chemistry and Biochemistry Florida State University, Tallahassee, 32309, USA.

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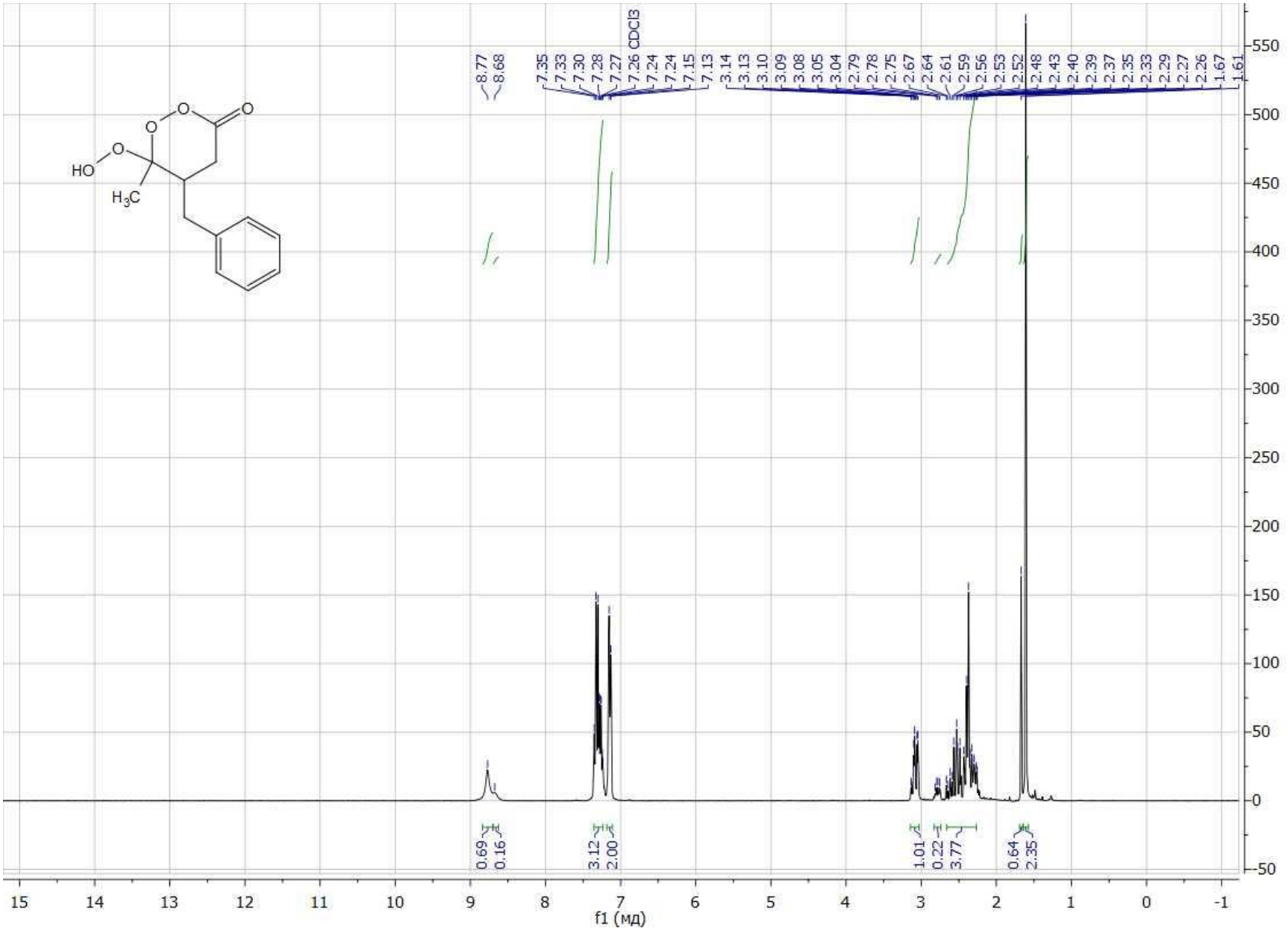
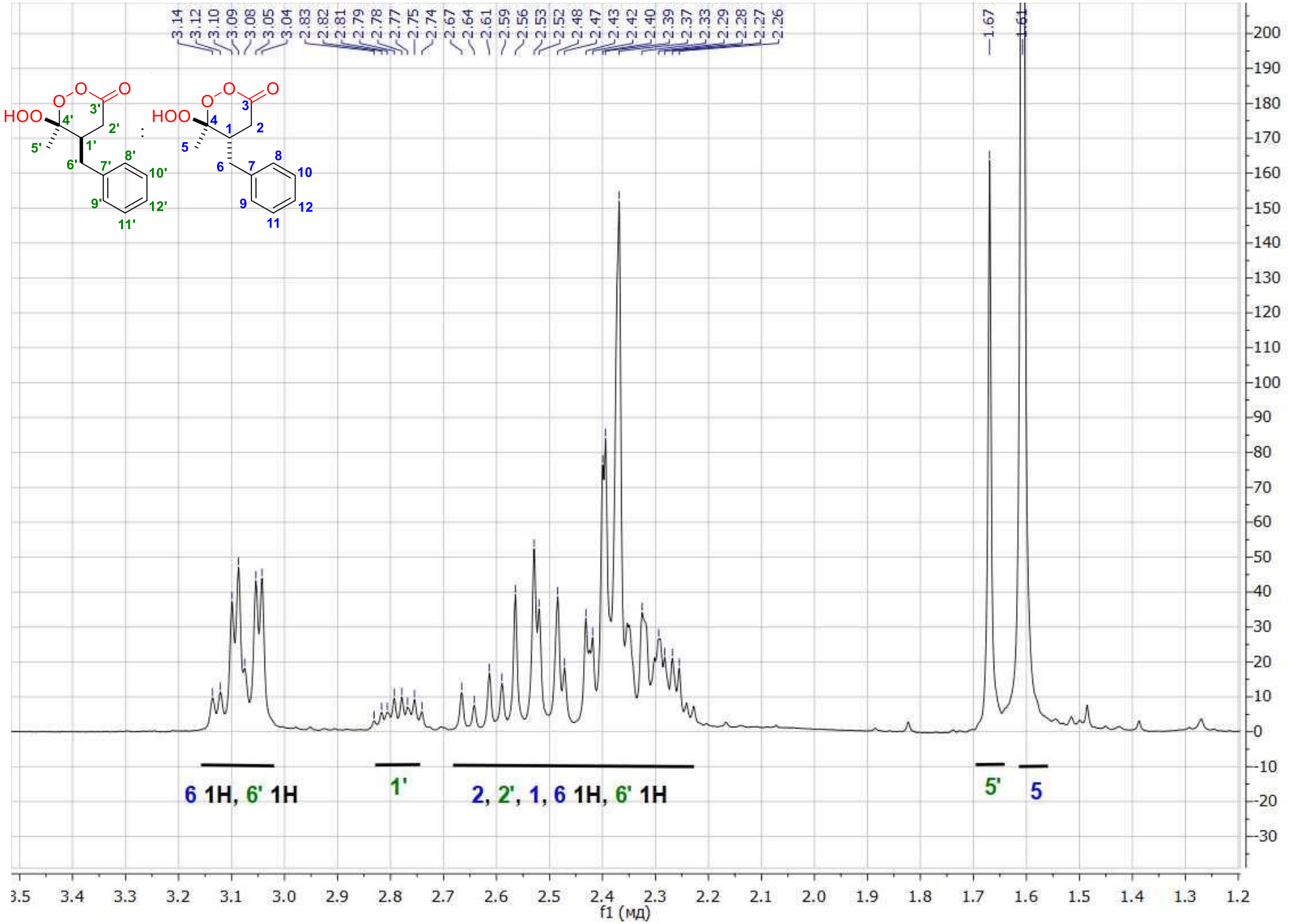
NMR of γ-hydroperoxy-γ-peroxylactones 2 and other products

5-Benzyl-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2a

^{1}H NMR

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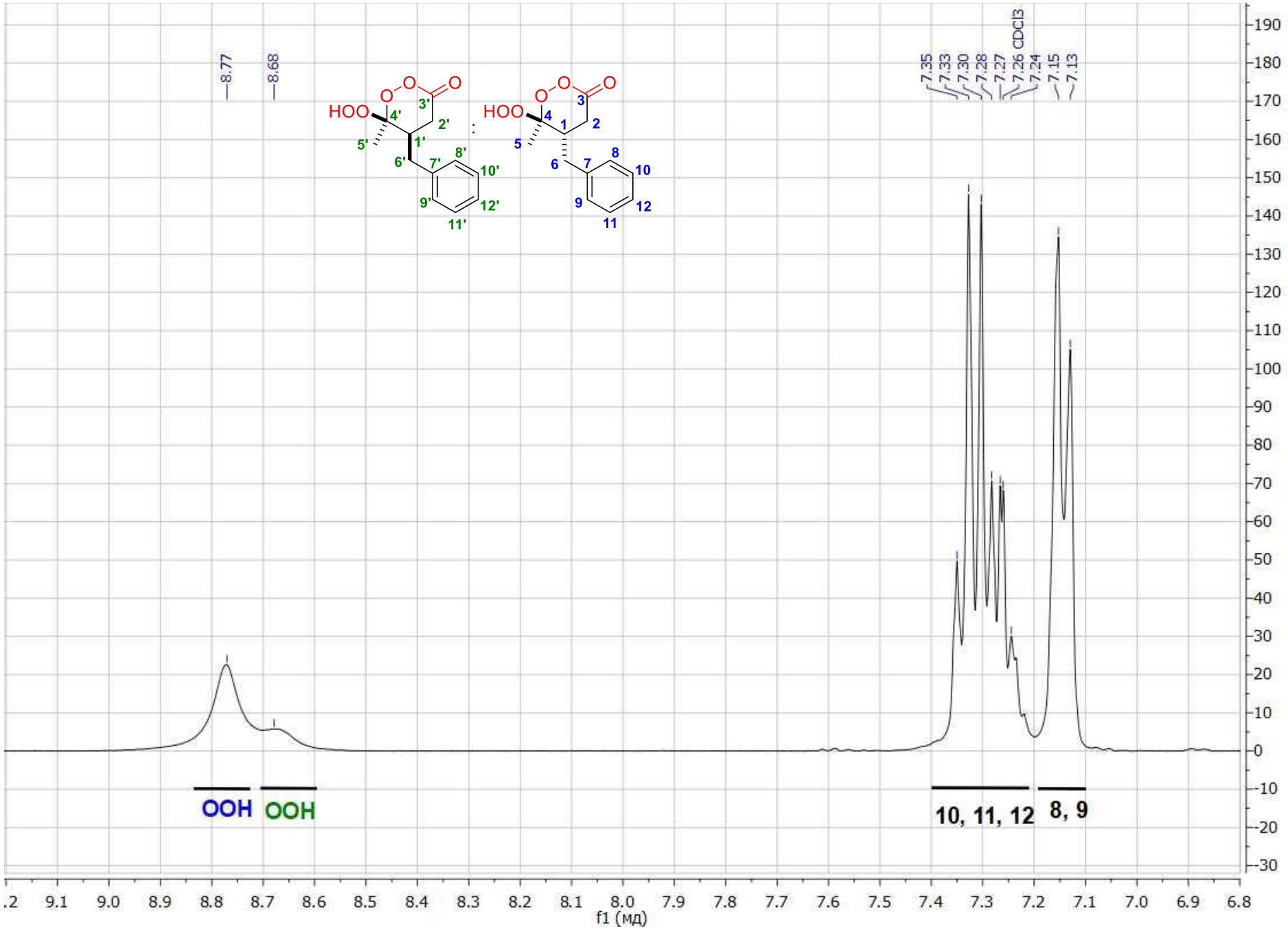
1.67
1.61
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
6 1H, 6' 1H
1'
2, 2', 1, 6 1H, 6' 1H
5'
5
f1 (мд)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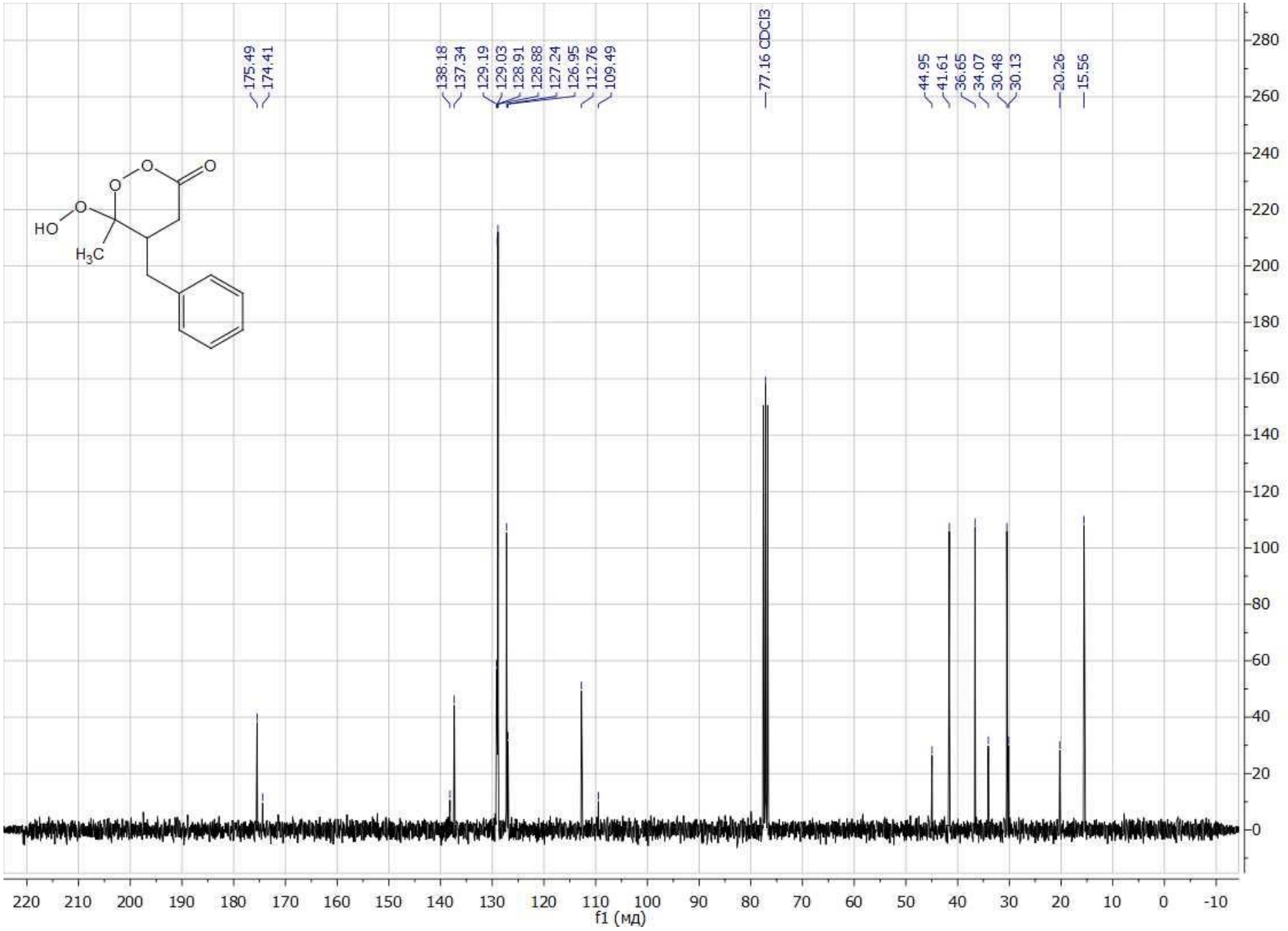
8.68
7.35
7.33
7.30
7.28
7.27
7.26 CDCl3
7.24
7.15
7.13
HOO
O
O
O
O
HOO
O
O
O
O
OOH
OOH
10, 11, 12
8, 9
f1 (мд)

^{13}C NMR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174.41
138.18
137.34
129.19
129.03
128.91
128.88
127.24
126.95
112.76
109.49
77.16 CDCl3
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36.65
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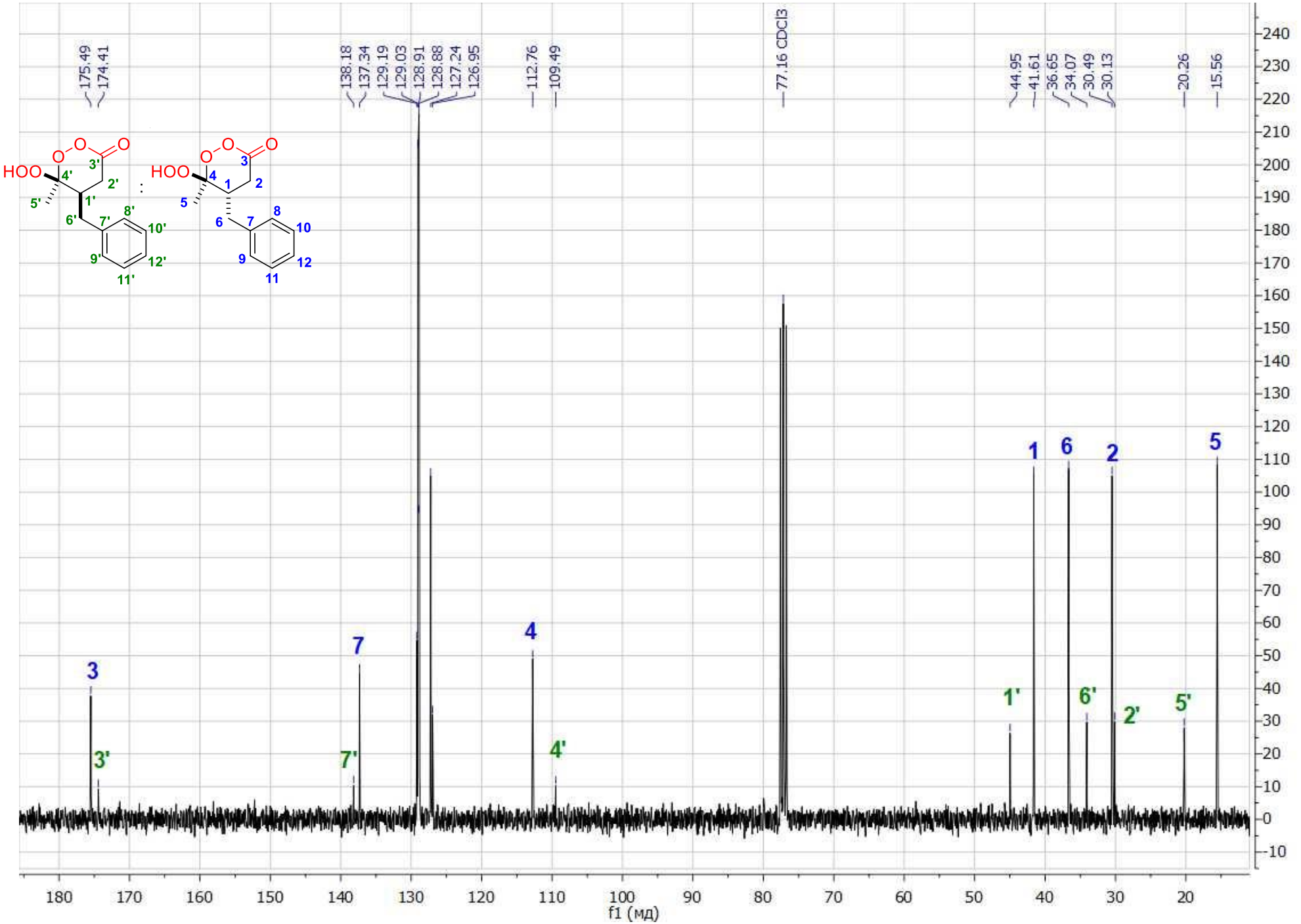
30.48
30.13
20.26
15.56
HO
H3C
f1 (мд)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174.41
138.18
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129.19
129.03
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128.88
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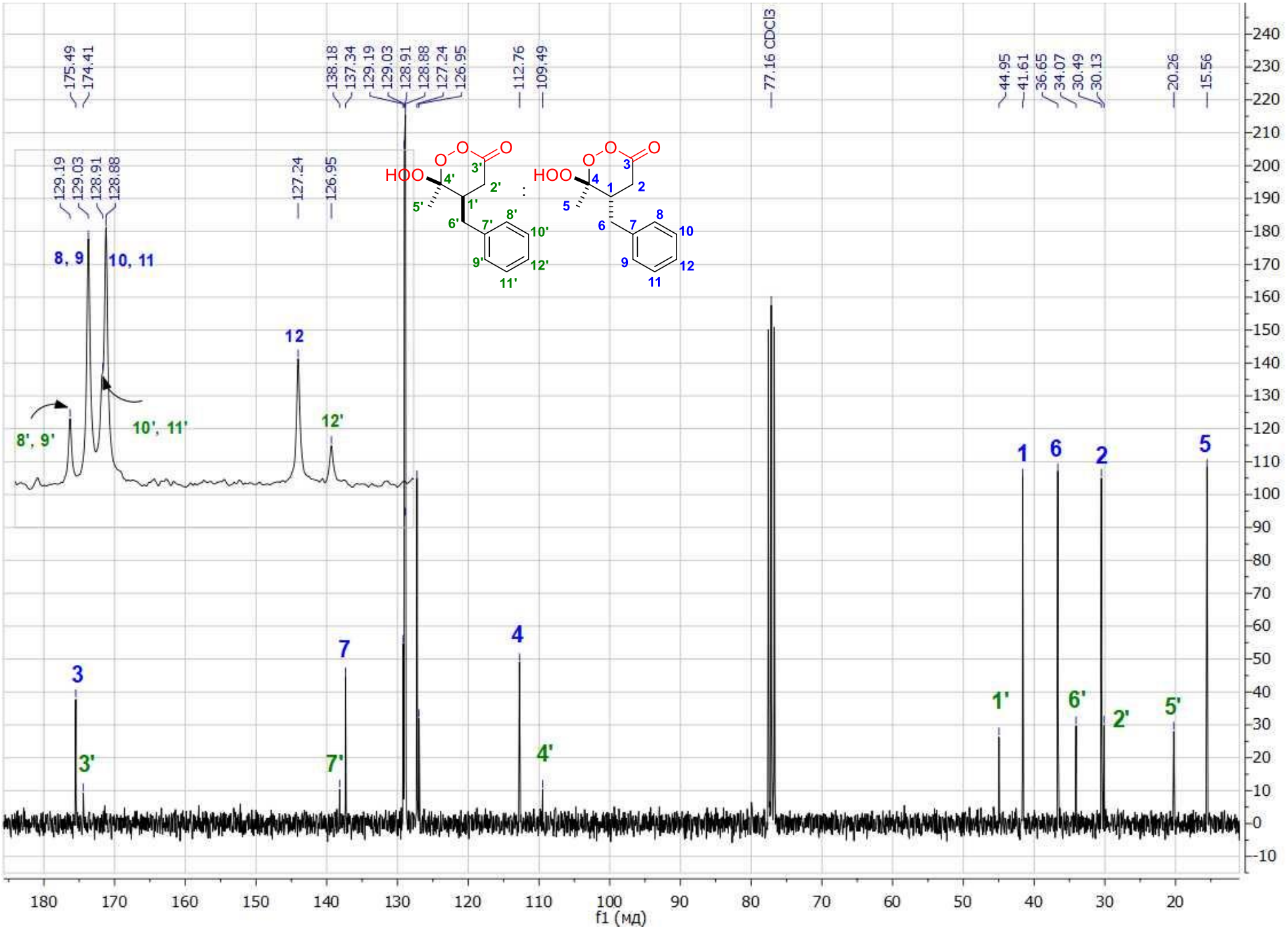
126.95
112.76
109.49
77.16 CDCl3
44.95
41.61
36.65
34.07
30.49
30.13
20.26
15.56
HOO
HOO
3
3'
7
7'
4
4'
1
1'
6
6'
2
2'
5
5'
f1 (мд)


175.49
174.41
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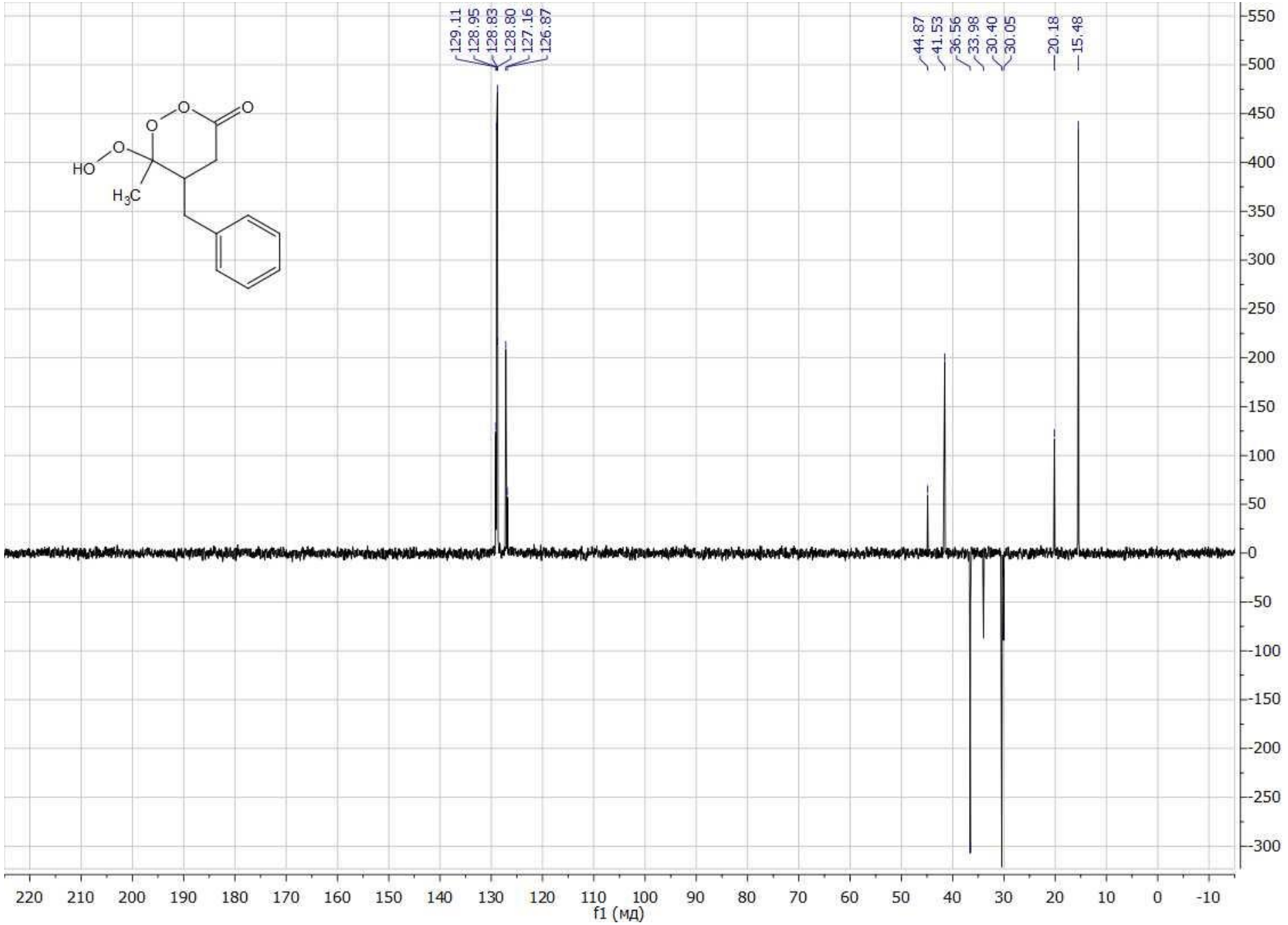
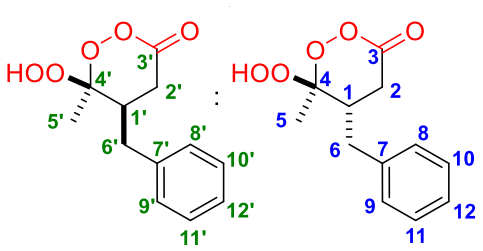
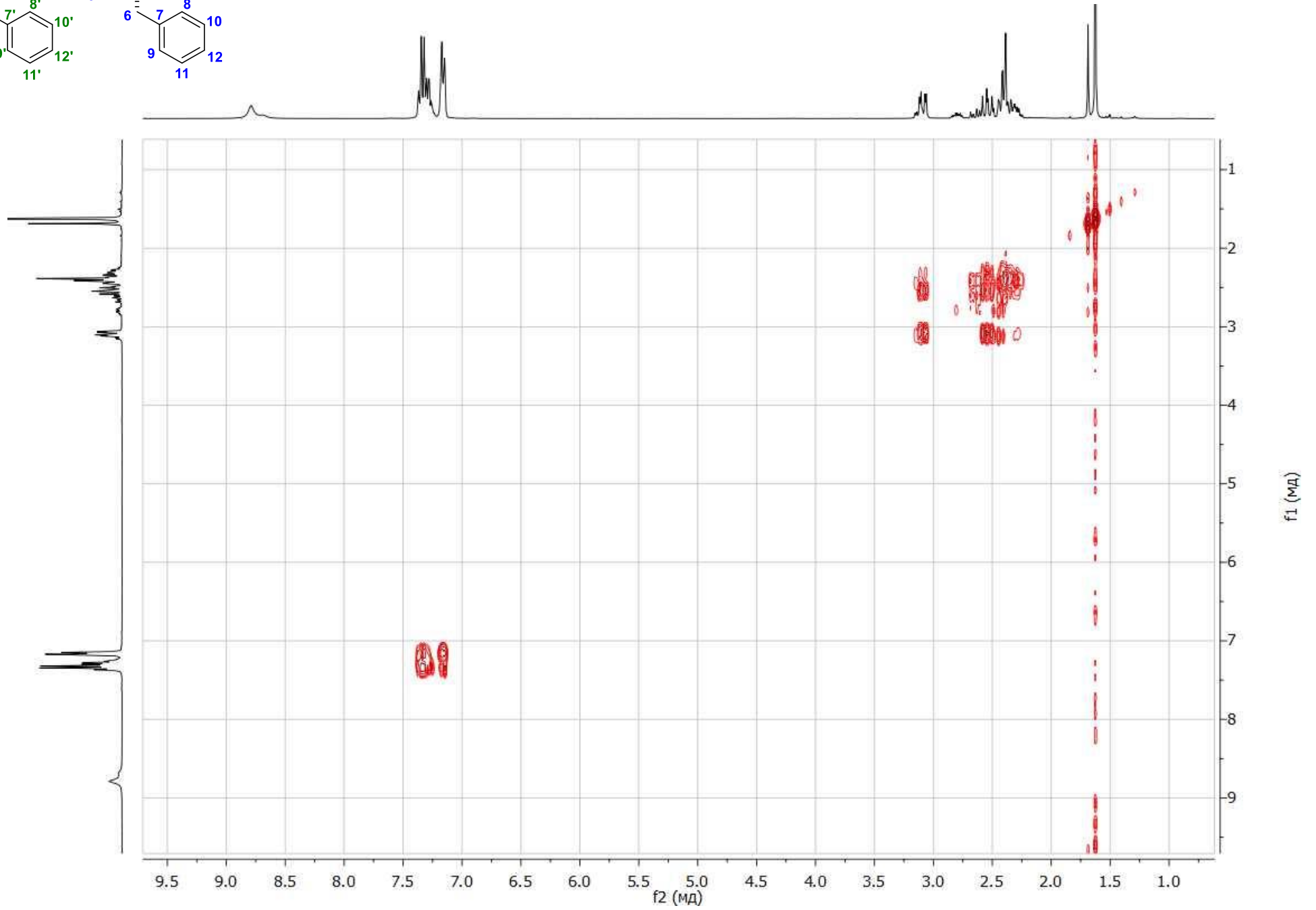
137.34
129.19
129.03
128.91
128.88
127.24
126.95
112.76
109.49
77.16 CDCl3
44.95
41.61
36.65
34.07
30.49
30.13
20.26
15.56
HOO
8, 9
10, 11
12
8', 9'
10', 11'
12'
3
3'
7
7'
4
4'
1
6
2
5
1'
6'
2'
5'
f1 (мд)

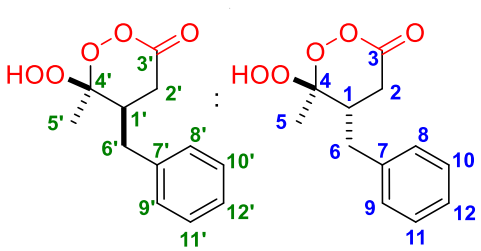
^{13}C_deptsp135



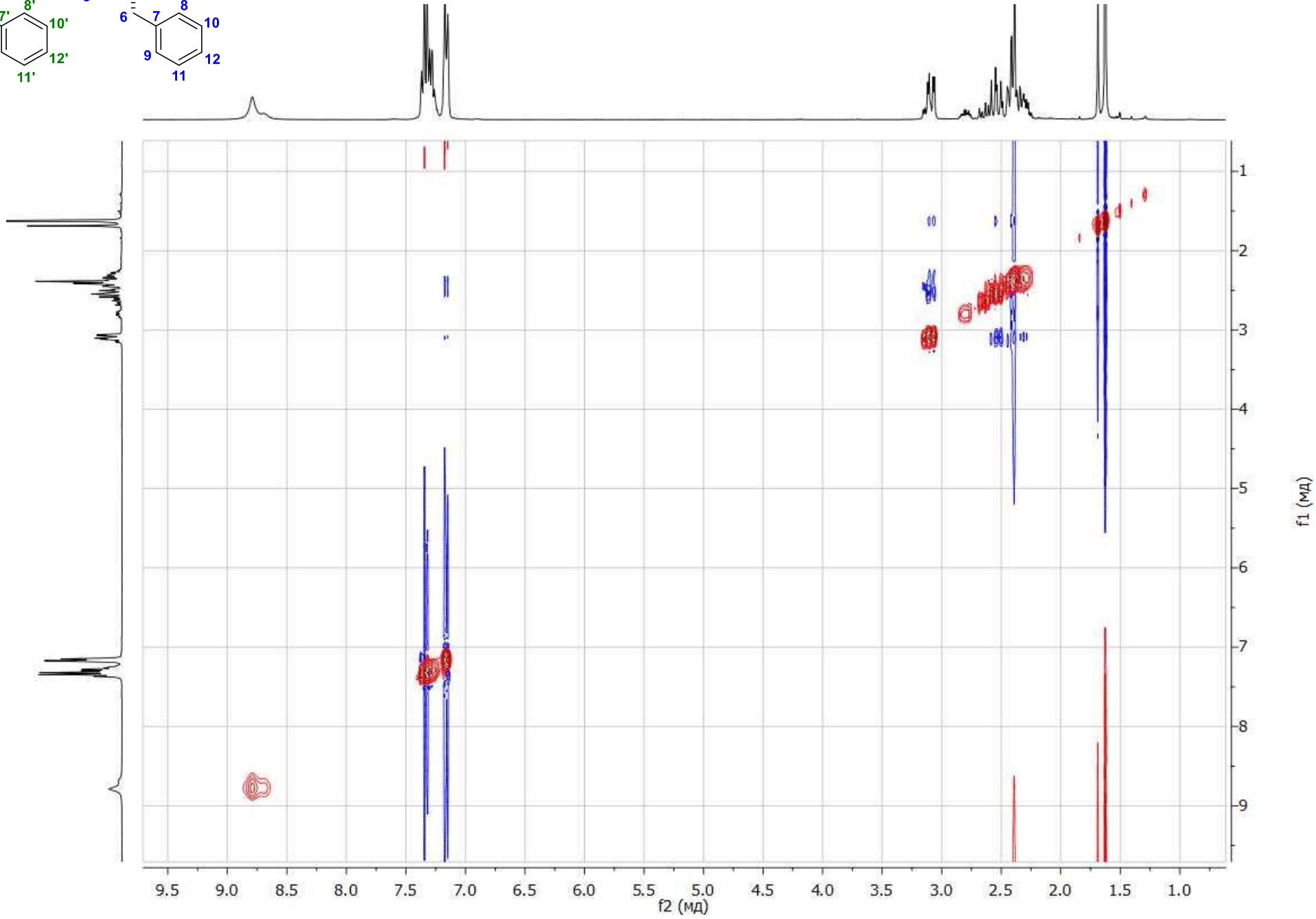

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
:
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11

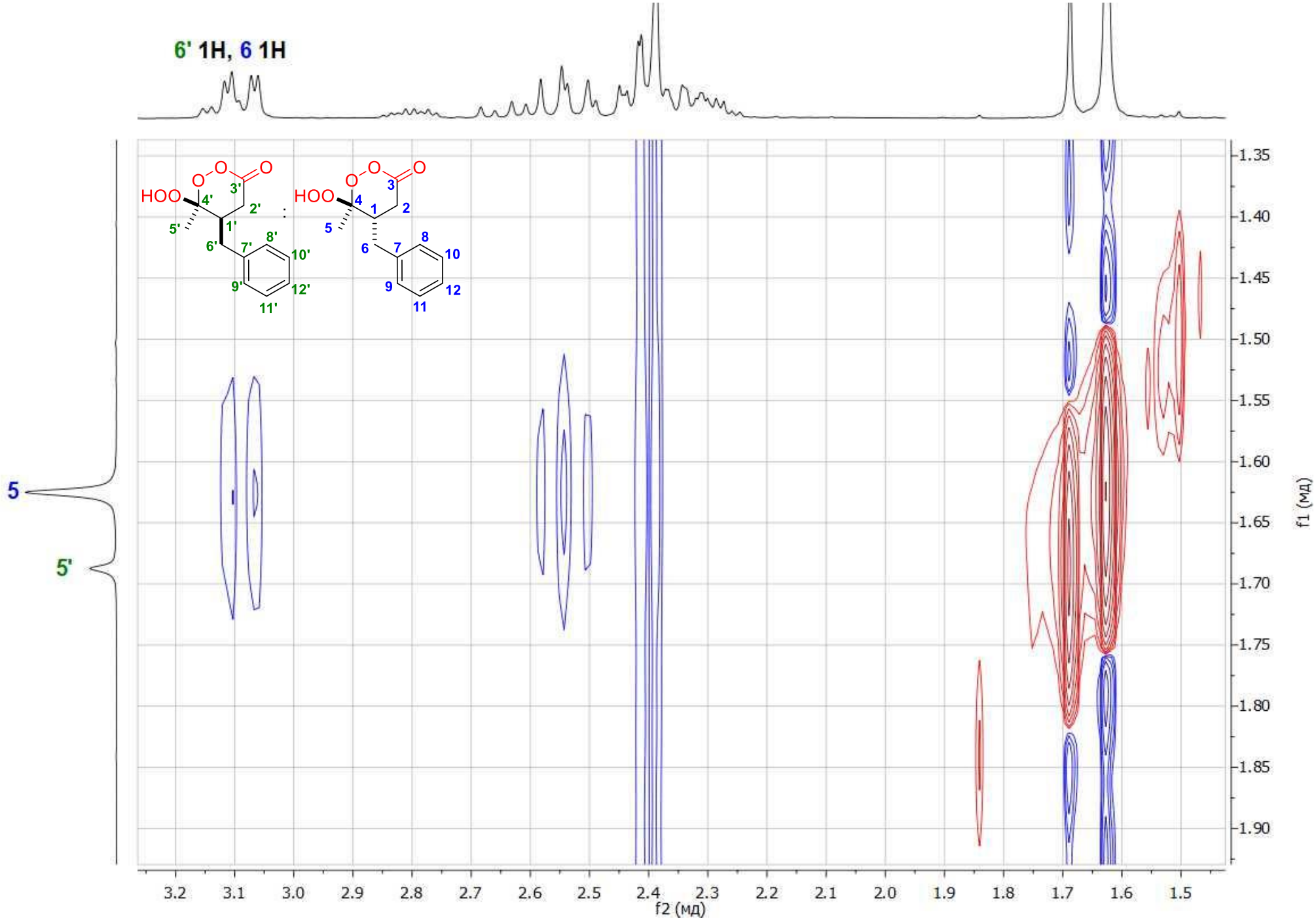
{^{1}H-^{1}H} COSY

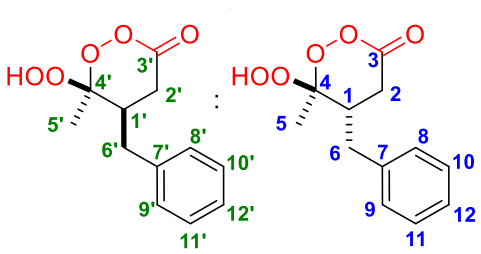

f2 (мд)
f1 (мд)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
1
2
3
4
5
6
7
8
9


HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11

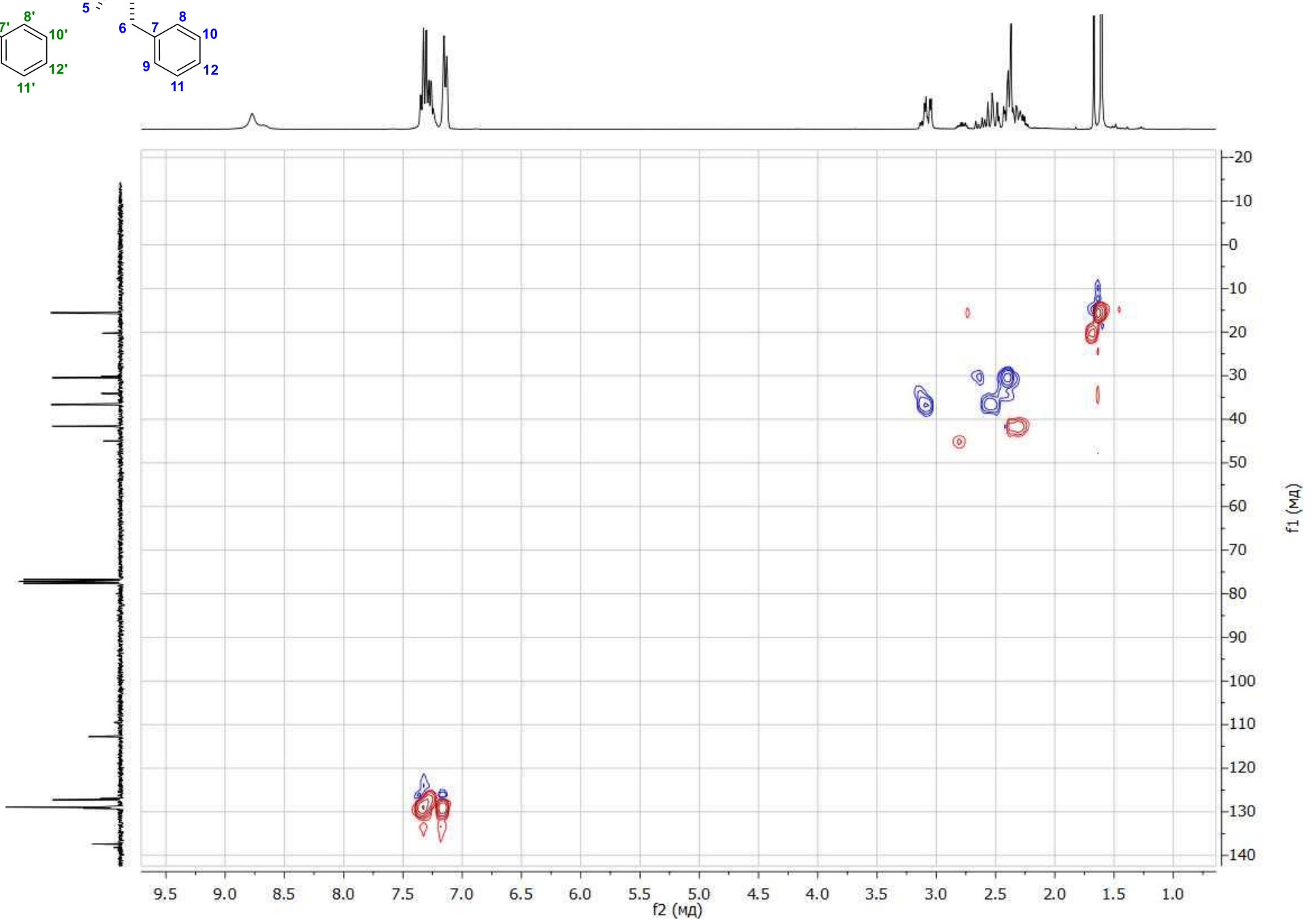
{^{1}H-^{1}H} NOESY


9.5
9.0
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
f2 (мд)
1
2
3
4
5
6
7
8
9
f1 (мд)


6' 1H, 6 1H
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
5
5'
f2 (мд)
f1 (мд)
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.35
1.40
1.45
1.50
1.55
1.60
1.65
1.70
1.75
1.80
1.85
1.90


HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11

{^{1}H-^{13}C} HSQC


f2 (мд)
f1 (мд)
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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
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-10
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20
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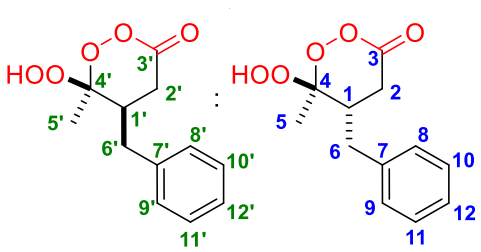
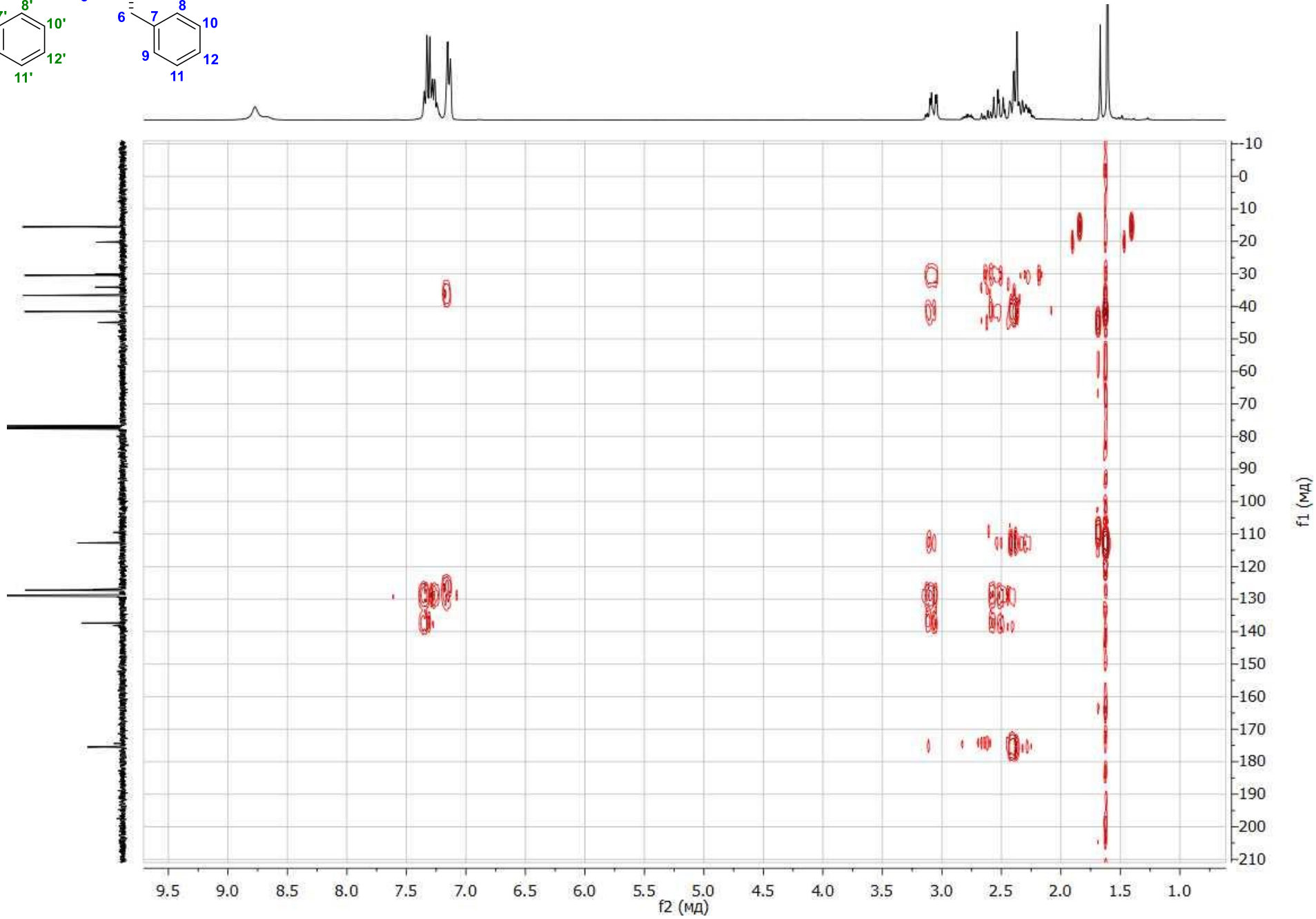
70
80
90
100
110
120
130
140

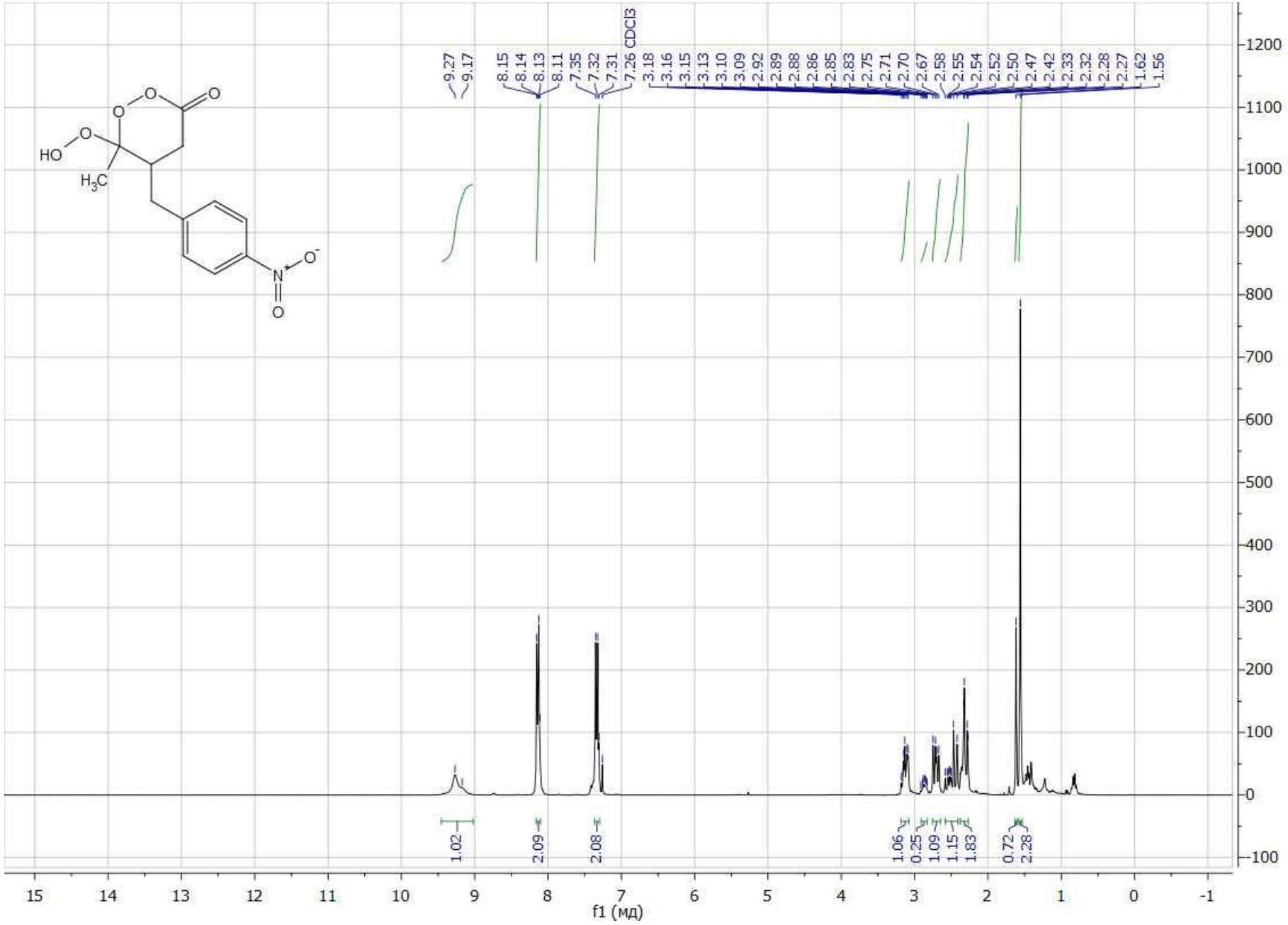

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11

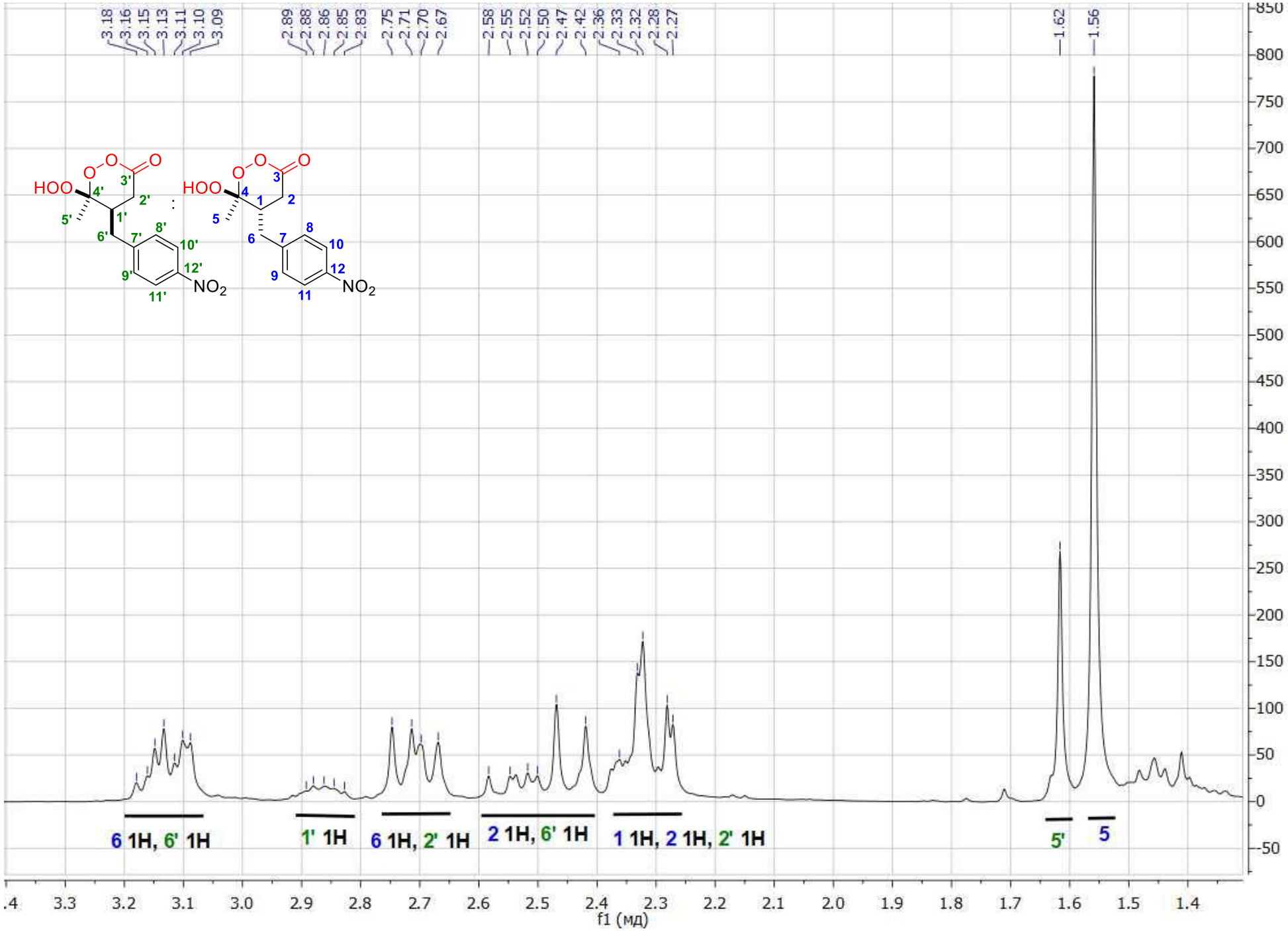
{^{1}H-^{13}C} HMBC

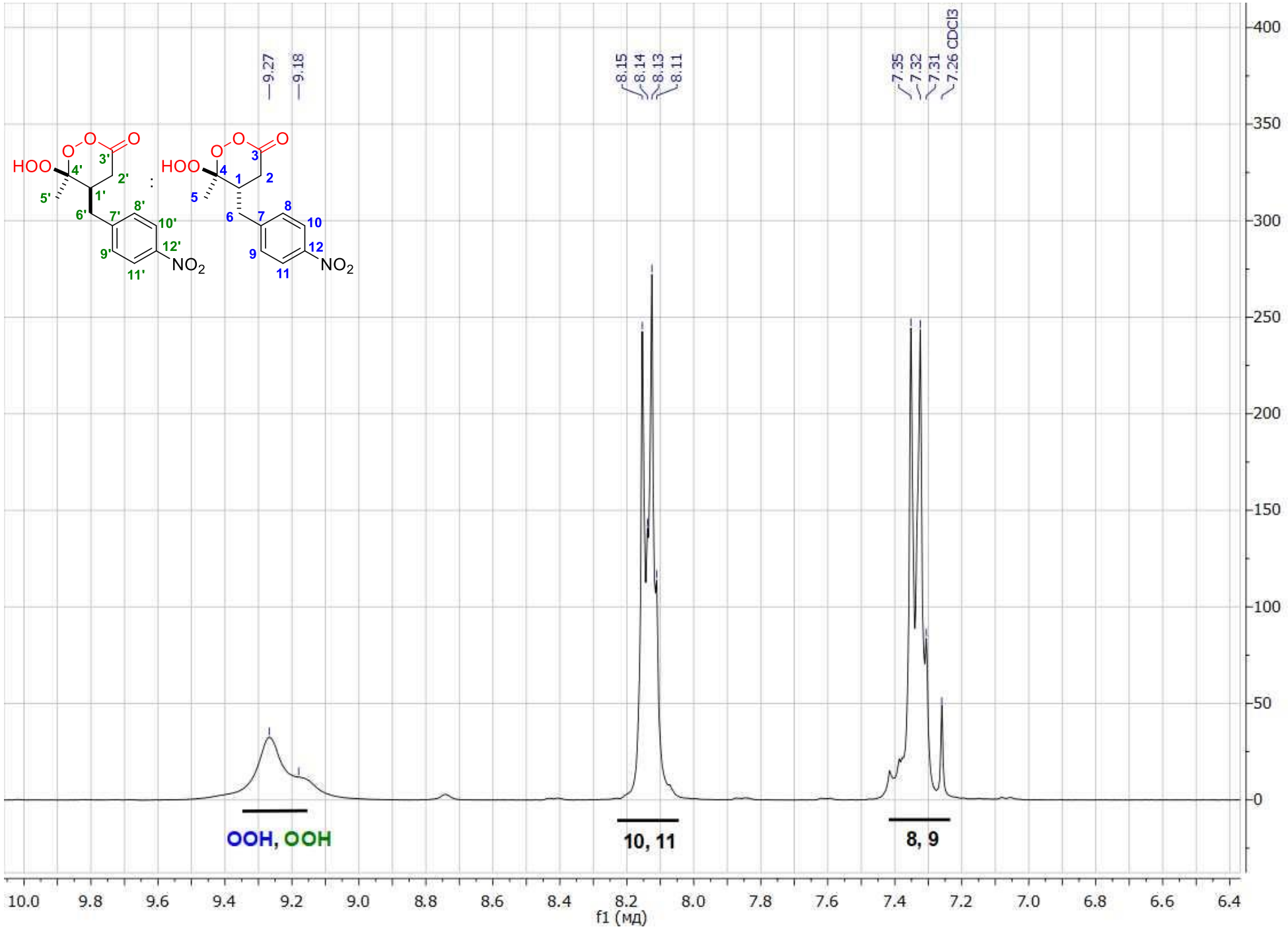

f2 (мд)
f1 (мд)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210

6-Hydroperoxy-6-methyl-5-(4-nitrobenzyl)-1,2-dioxan-3-one, 2b

^{1}H NMR




3.18
3.16
3.15
3.13
3.11
3.10
3.09
2.89
2.88
2.86
2.85
2.83
2.75
2.71
2.70
2.67
2.58
2.55
2.52
2.50
2.47
2.42
2.36
2.33
2.32
2.28
2.27
1.62
1.56
HOO
O-O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
12'
9'
11'
NO2
HOO
O-O
O
3
4
1
2
5
6
7
8
10
12
9
11
NO2
6 1H, 6' 1H
1' 1H
6 1H, 2' 1H
2 1H, 6' 1H
1 1H, 2 1H, 2' 1H
5'
5
f1 (мд)


9.27
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8.14
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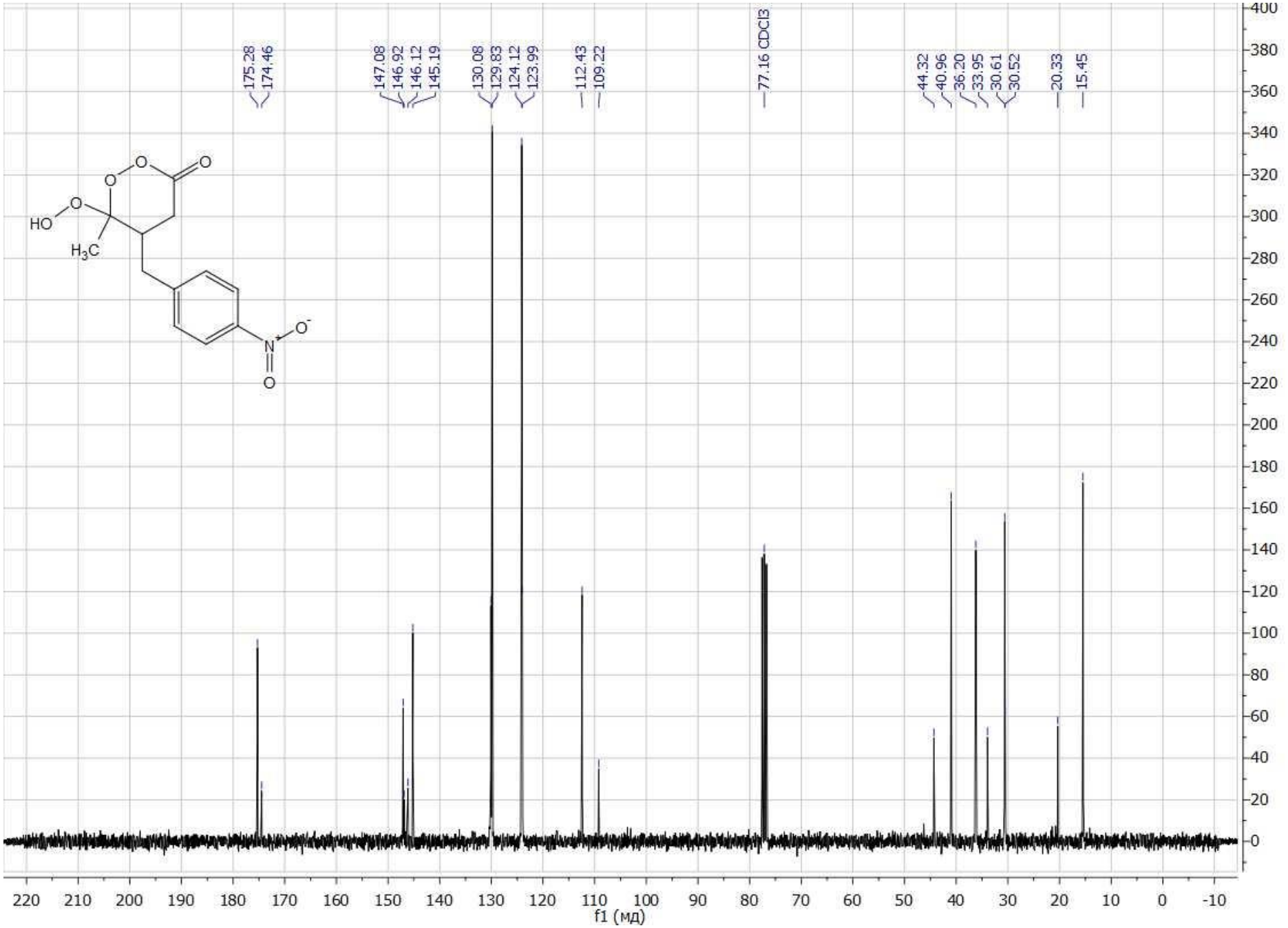
8.11
7.35
7.32
7.31
7.26 CDCl3
HOO
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
10'
12'
9'
11'
NO2
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
NO2
OOH, OOH
10, 11
8, 9
400
350
300
250
200
150
100
50
0
10.0
9.8
9.6
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
f1 (мд)

^{13}C NMR


175.28
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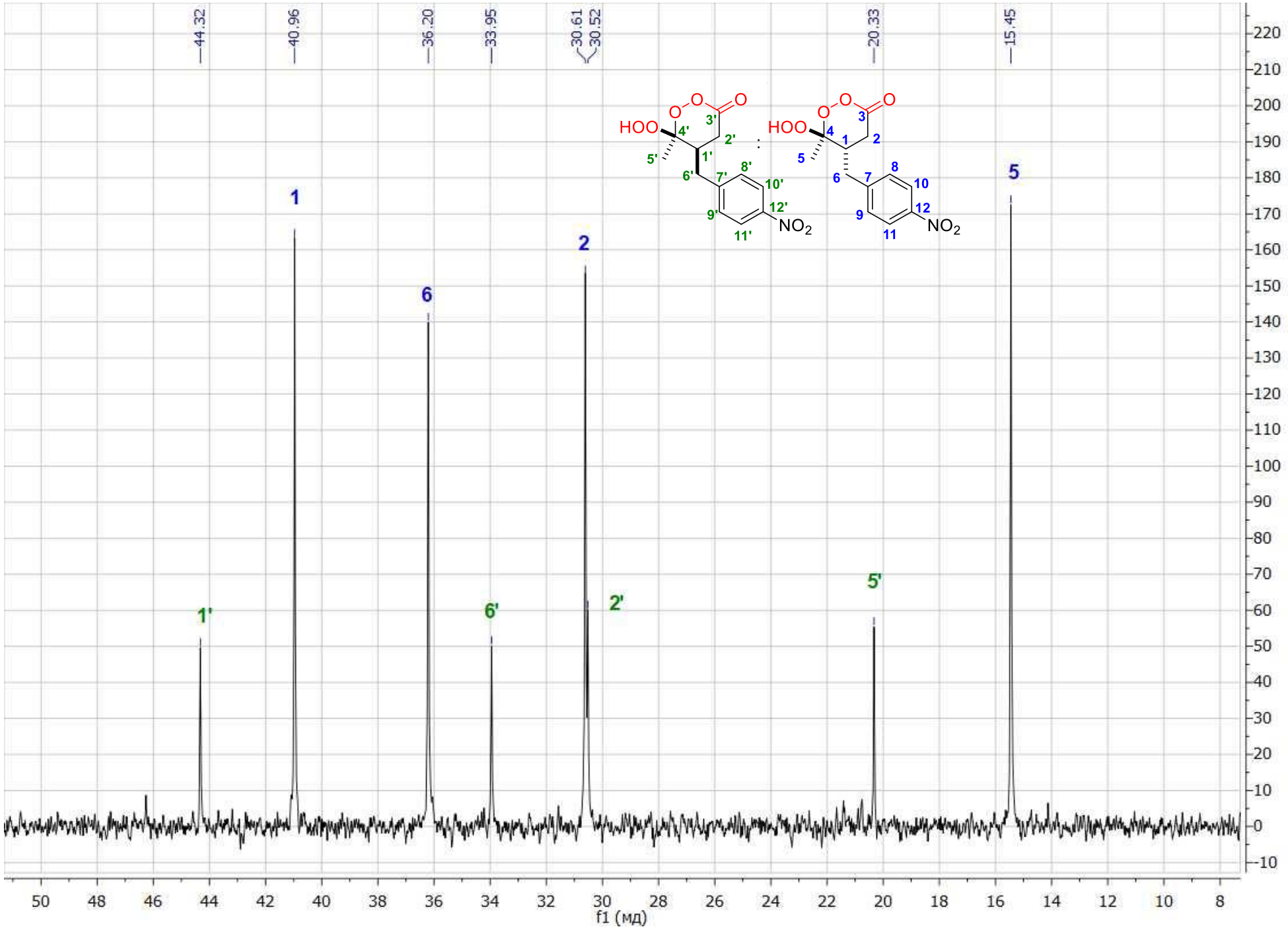
146.92
146.12
145.19
130.08
129.83
124.12
123.99
112.43
109.22
77.16 CDCl3
44.32
40.96
36.20
33.95
30.61
30.52
20.33
15.45
HO
O
O
O
O
H_3C
N
O
O
f1 (мд)


44.32
40.96
36.20
33.95
30.61
30.52
20.33
15.45
1
6
2
5
1'
6'
2'
5'
HOO
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
10'
12'
9'
11'
NO2
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
NO2
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
50
48
46
44
42
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38
36
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32
30
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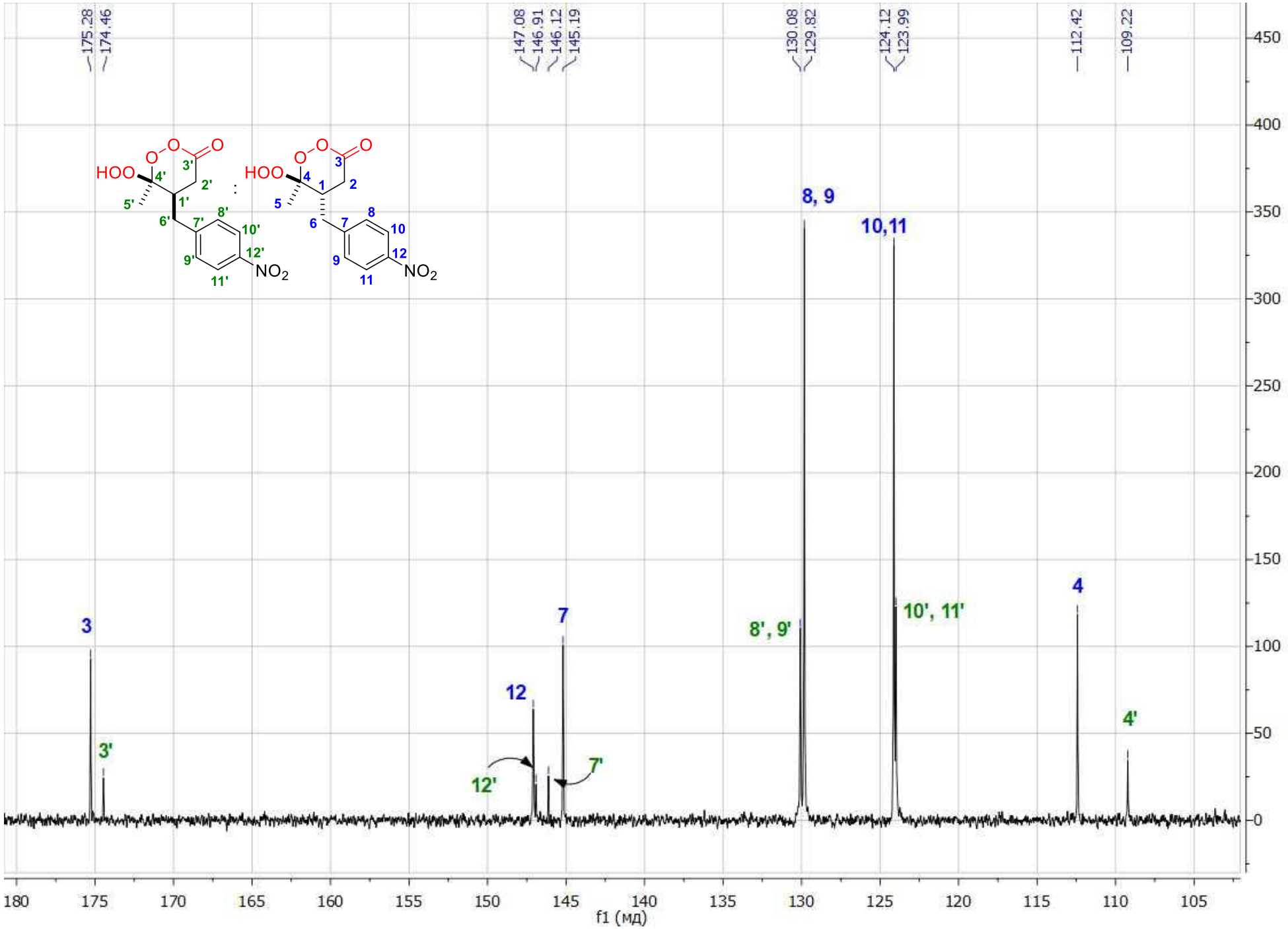
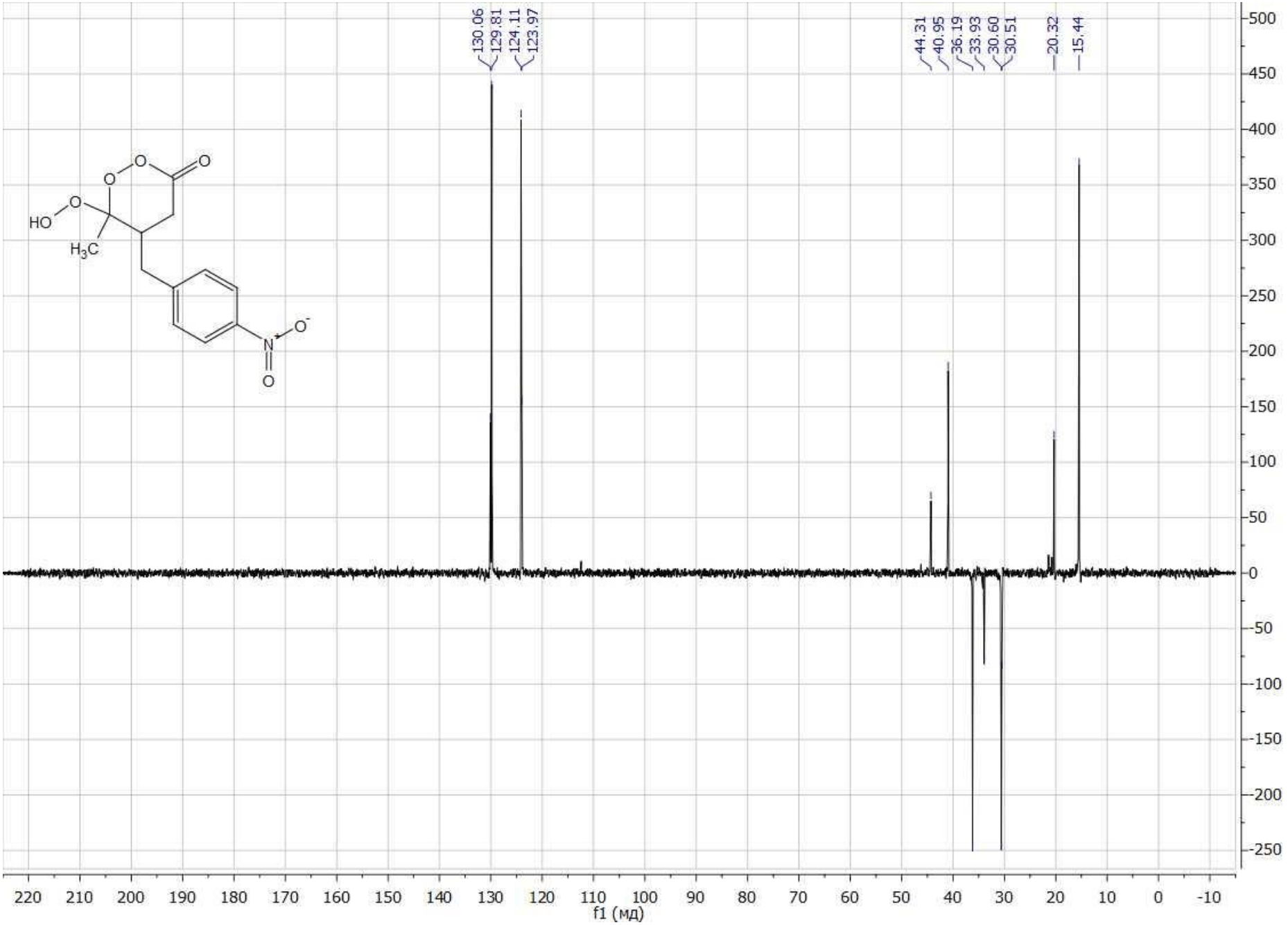
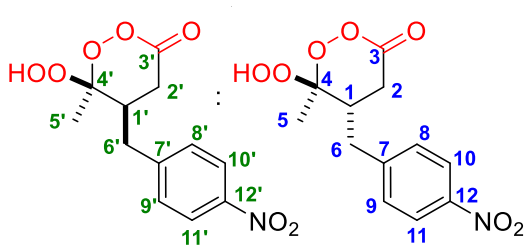
26
24
22
20
18
16
14
12
10
8
f1 (мд)

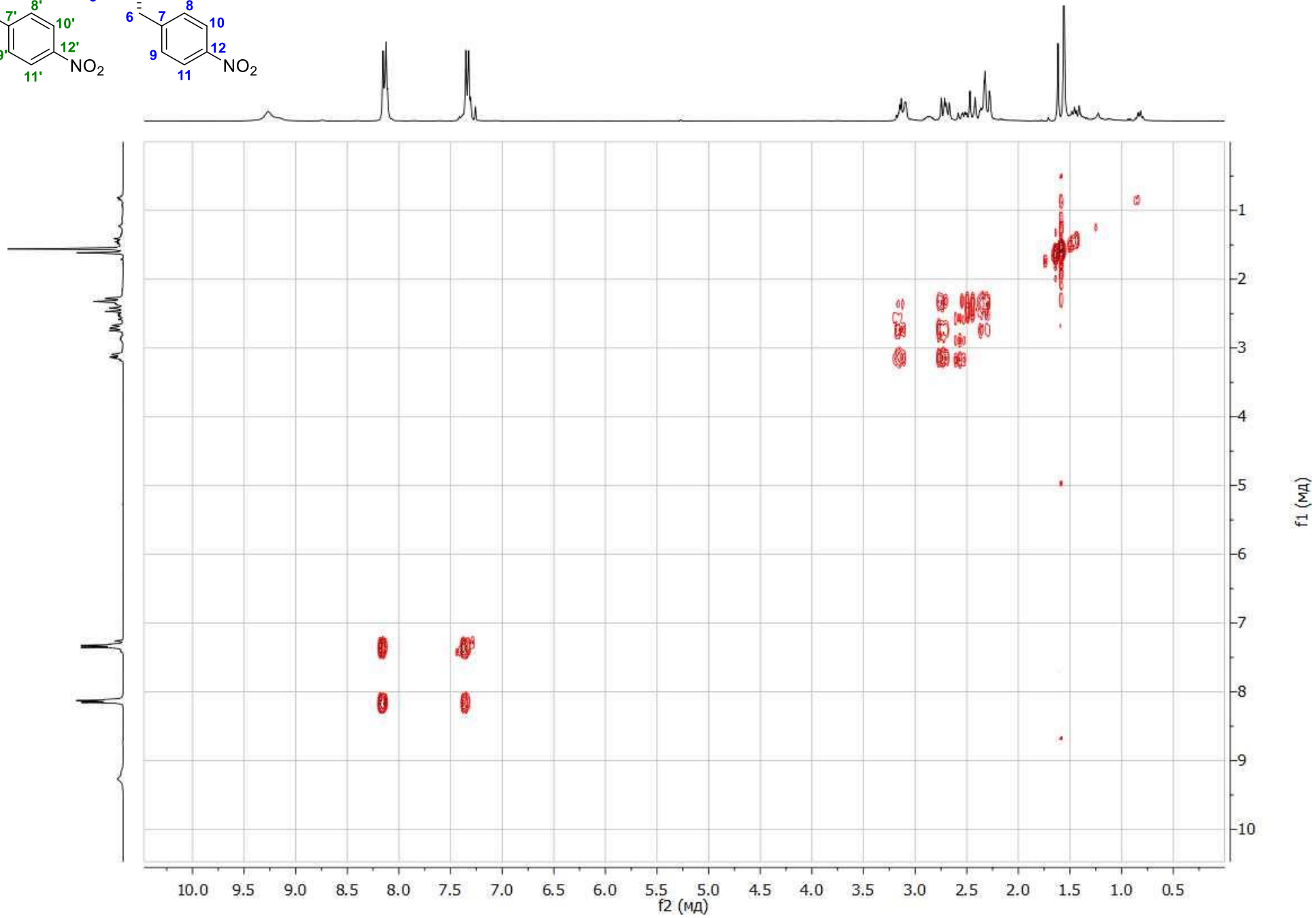

175.28
174.46
147.08
146.91
146.12
145.19
130.08
129.82
124.12
123.99
112.42
109.22
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
12'
9'
11'
NO2
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
NO2
8, 9
10,11
3
3'
12
7
12'
7'
8', 9'
10', 11'
4
4'
450
400
350
300
250
200
150
100
50
0
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
f1 (мд)

^{13}C_deptsp135




HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
12'
9'
11'
NO2
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
NO2

{^{1}H-^{1}H} COSY


f1 (мд)
f2 (мд)
10.0
9.5
9.0
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
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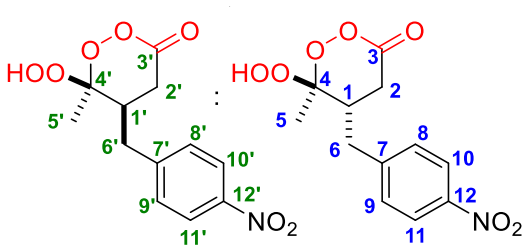
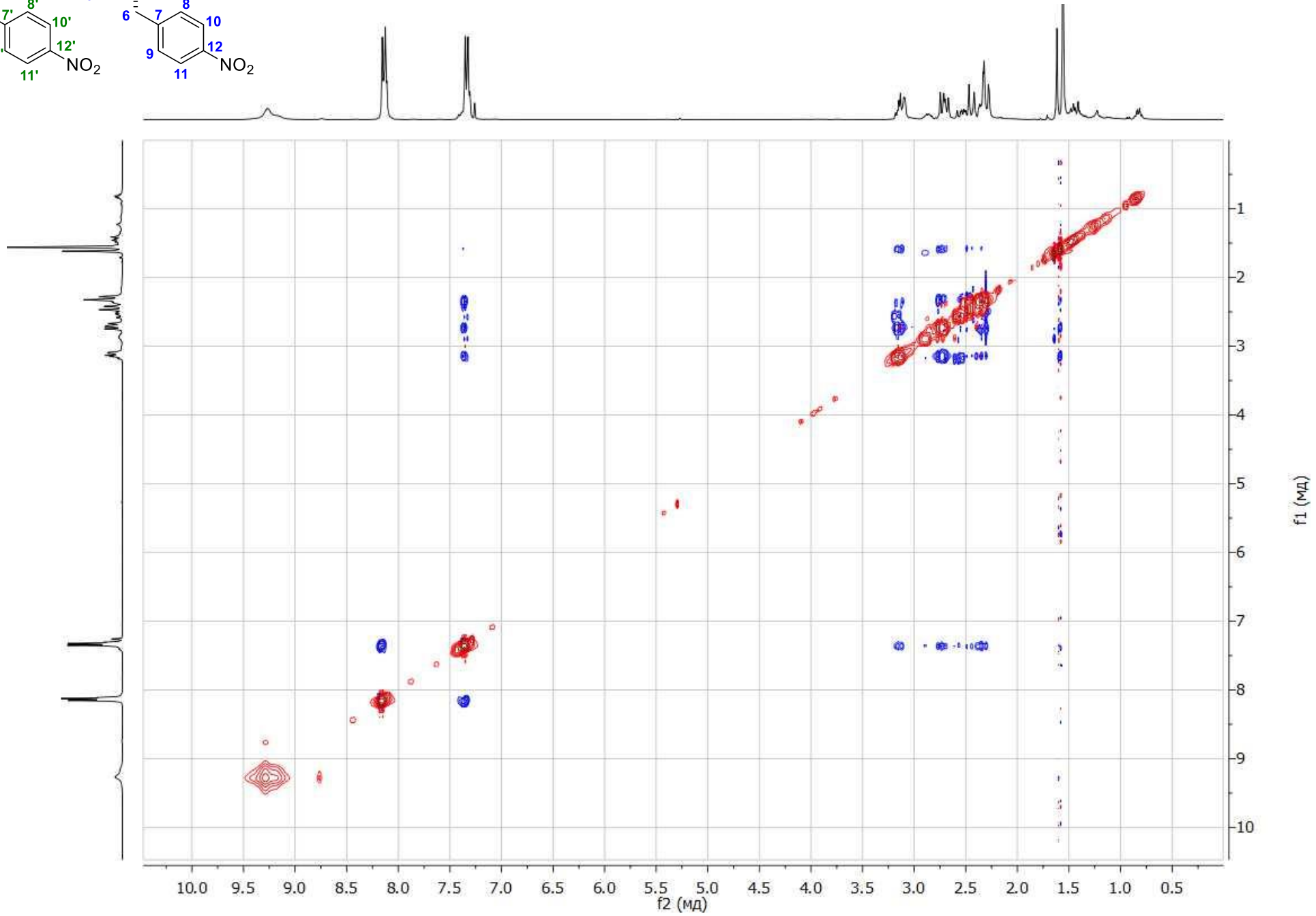
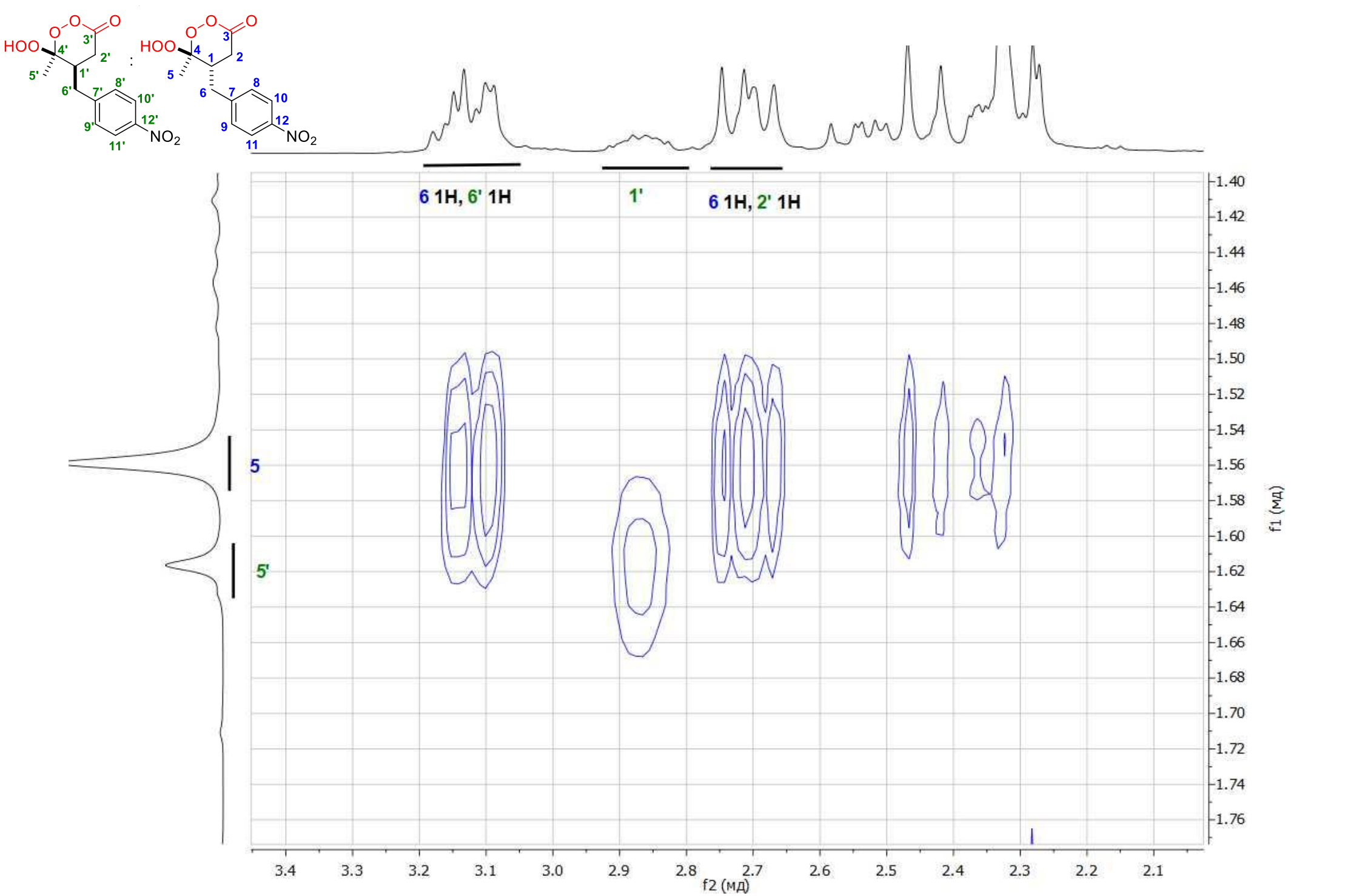
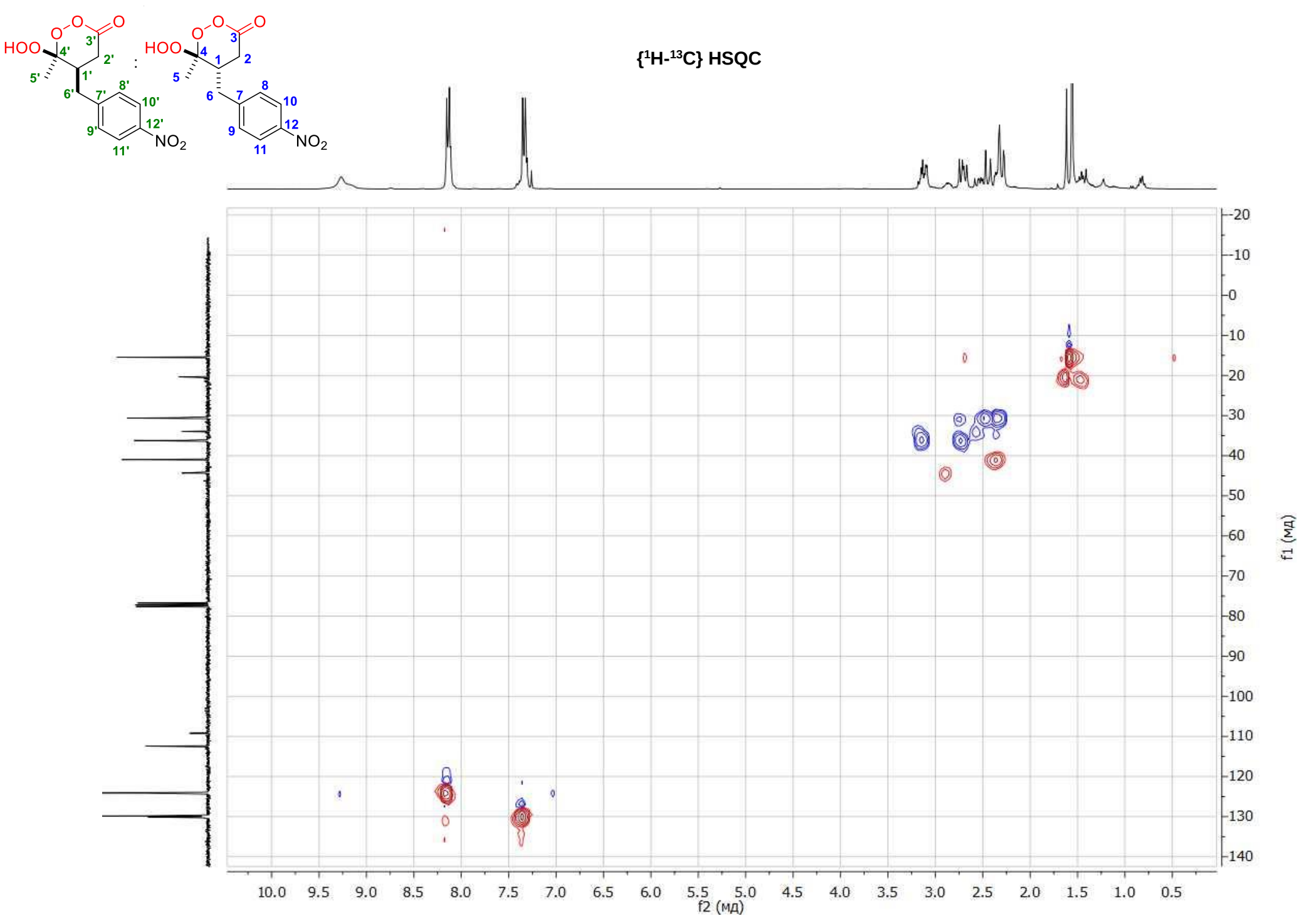
3
4
5
6
7
8
9
10

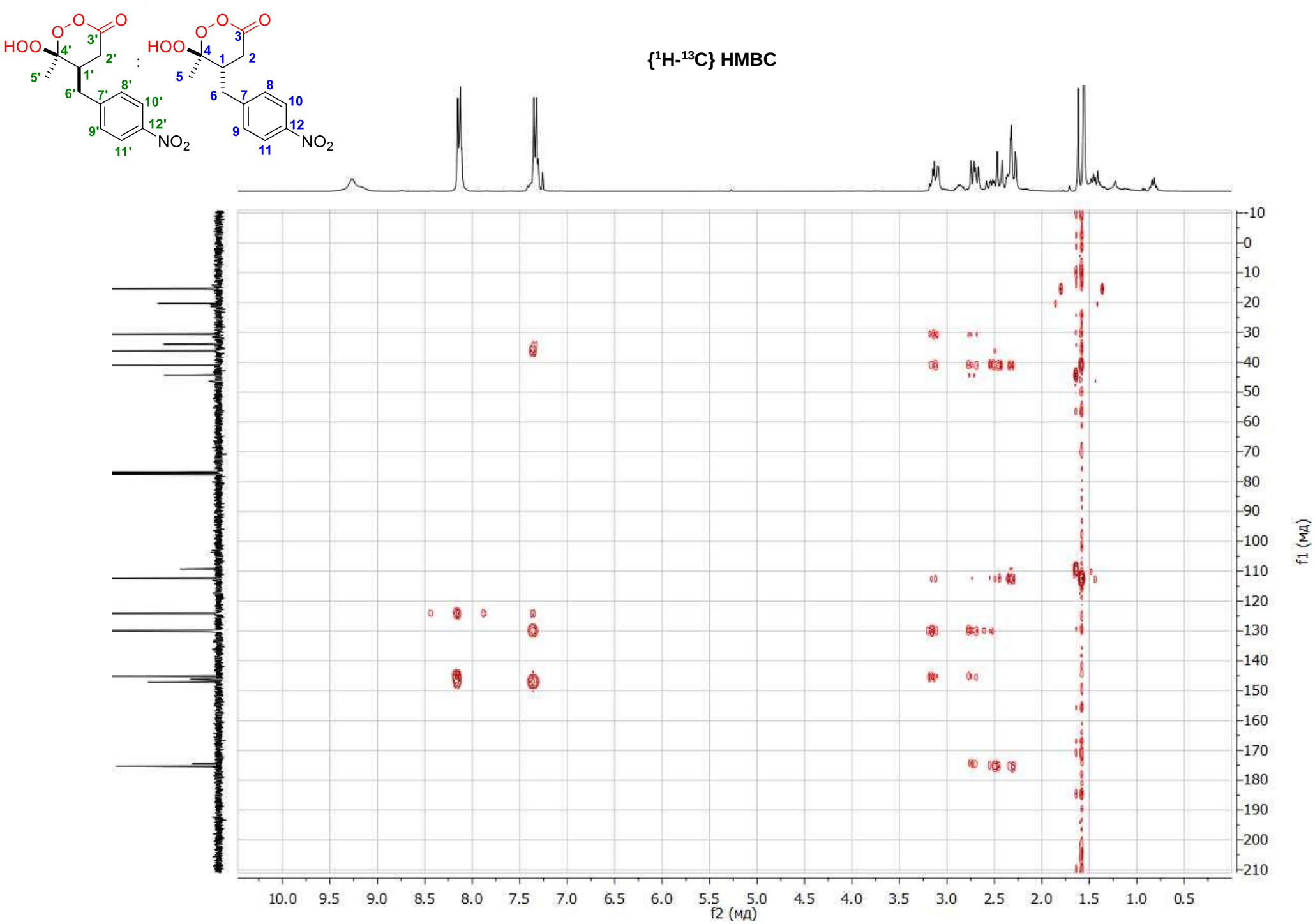

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
12'
9'
11'
NO2
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
NO2

{^{1}H-^{1}H} NOESY


10.0
9.5
9.0
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
f2 (мд)
1
2
3
4
5
6
7
8
9
10
f1 (мд)

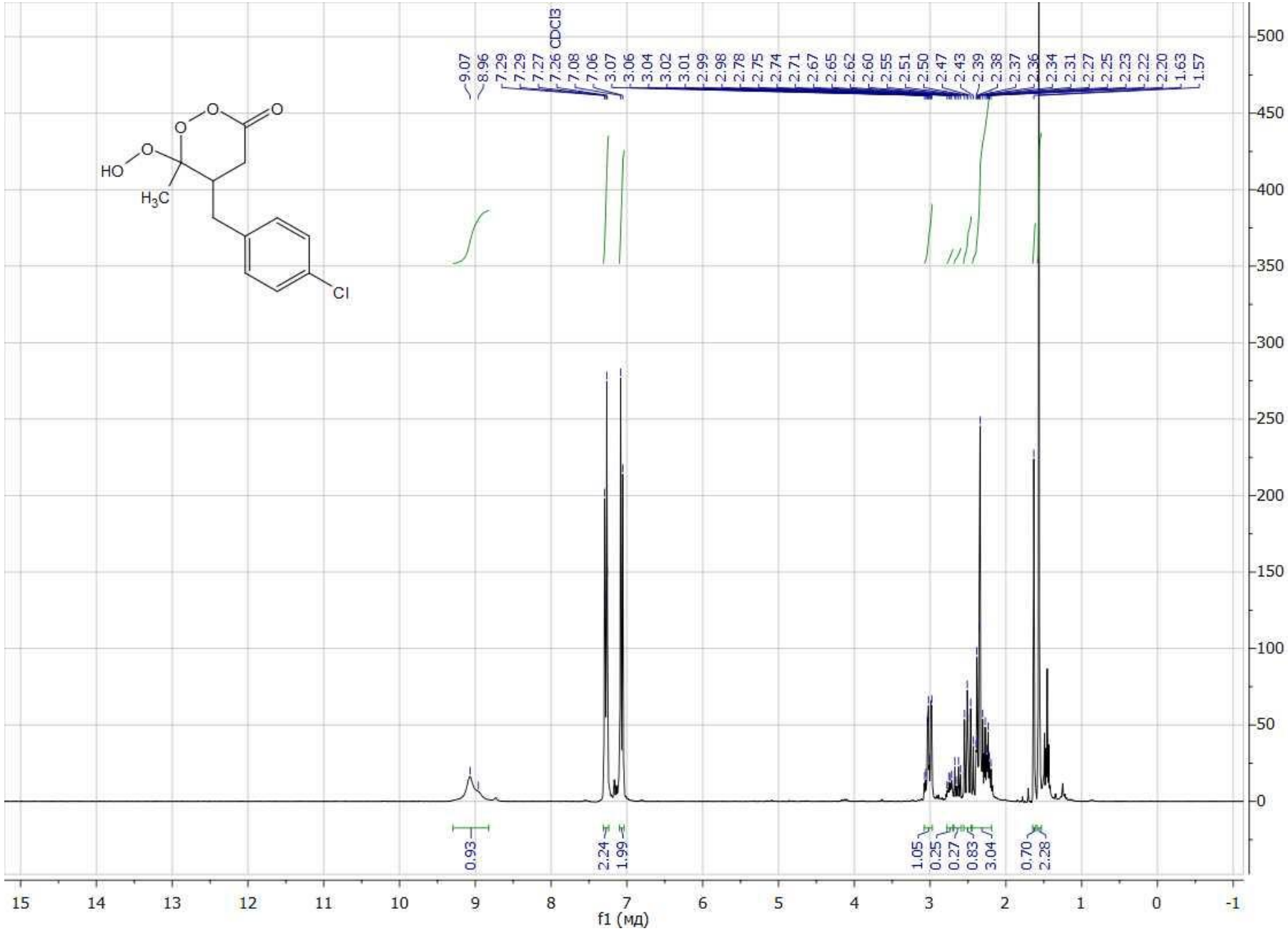

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
12'
9'
11'
NO2
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
NO2
6 1H, 6' 1H
1'
6 1H, 2' 1H
5
5'
1.40
1.42
1.44
1.46
1.48
1.50
1.52
1.54
1.56
1.58
1.60
1.62
1.64
1.66
1.68
1.70
1.72
1.74
1.76
f1 (мд)
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
f2 (мд)

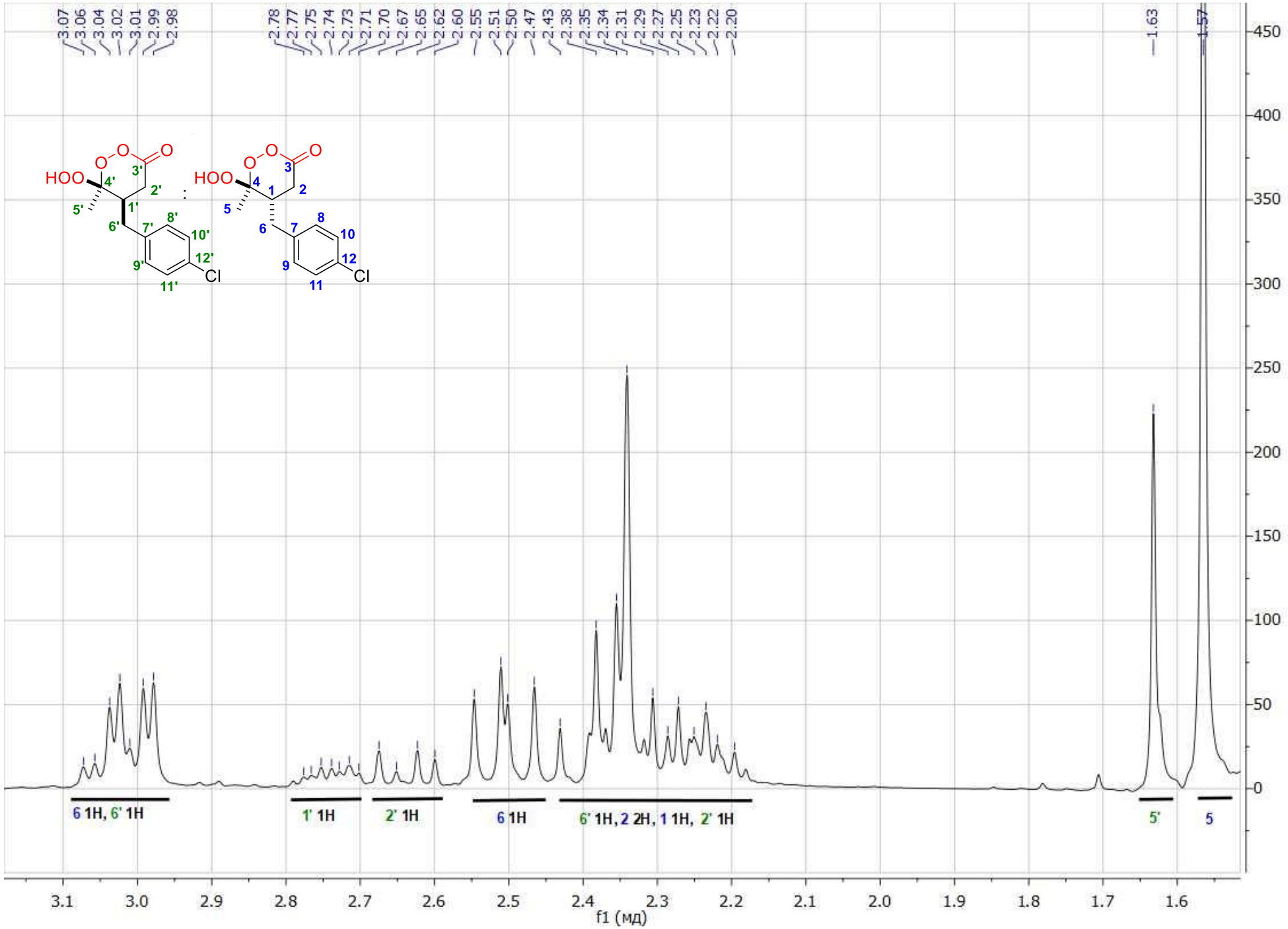

{1H-13C} HSQC
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
NO2
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
NO2
f2 (мд)
f1 (мд)

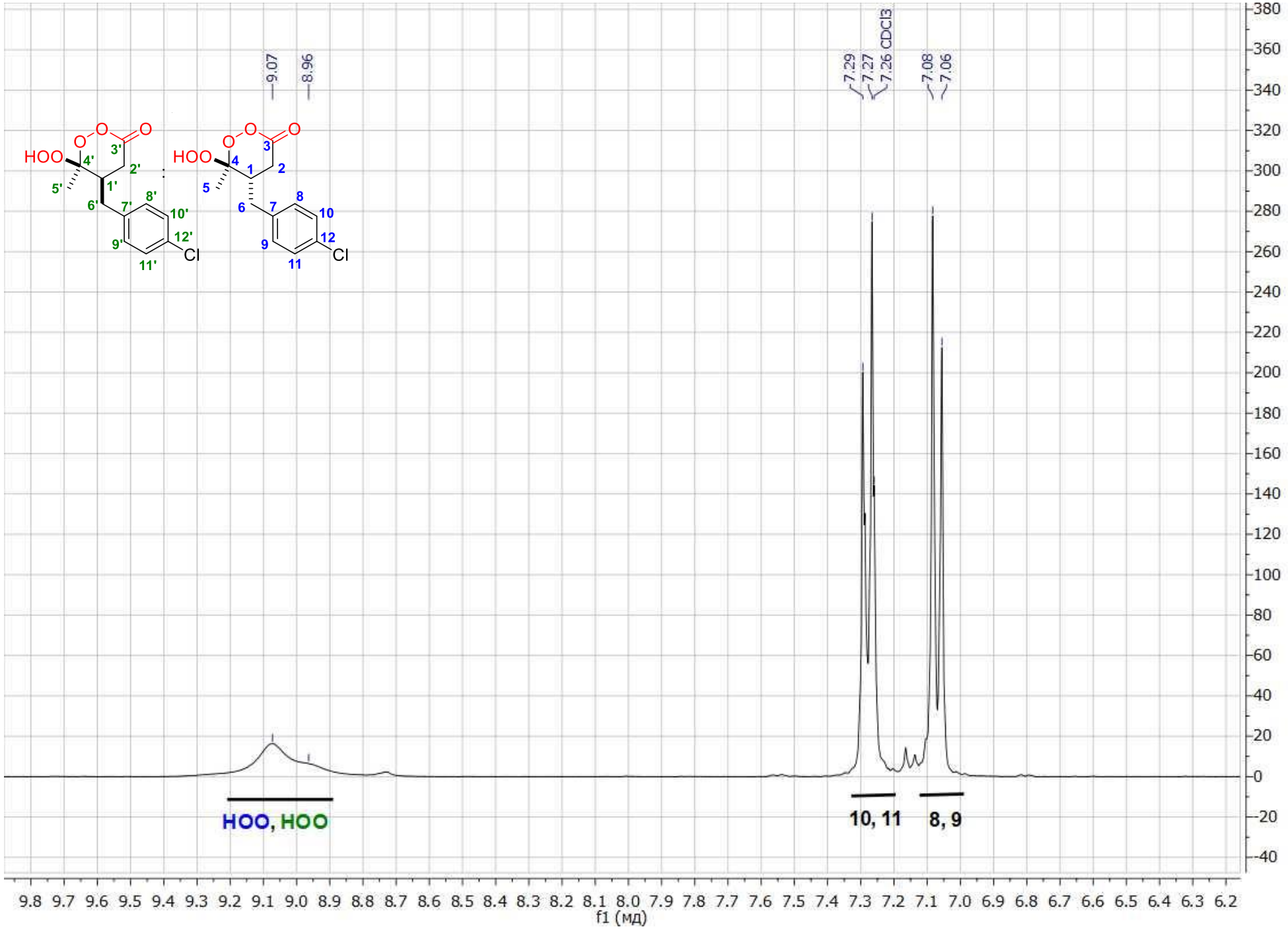

{1H-13C} HMBC
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
12'
9'
11'
NO2
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
NO2
f2 (мд)
f1 (мд)

5-(4-Chlorobenzyl)-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2c

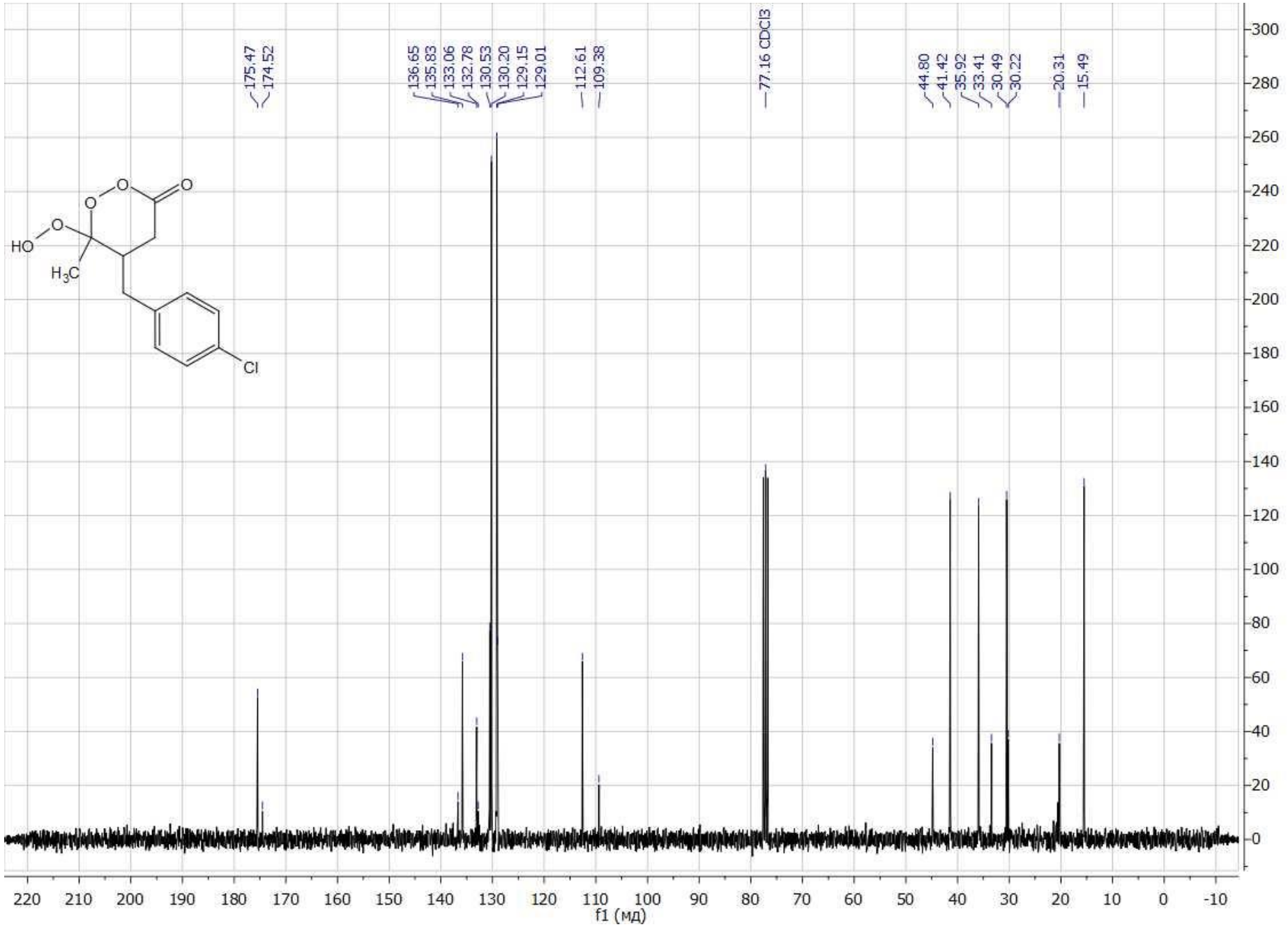
^{1}H NMR

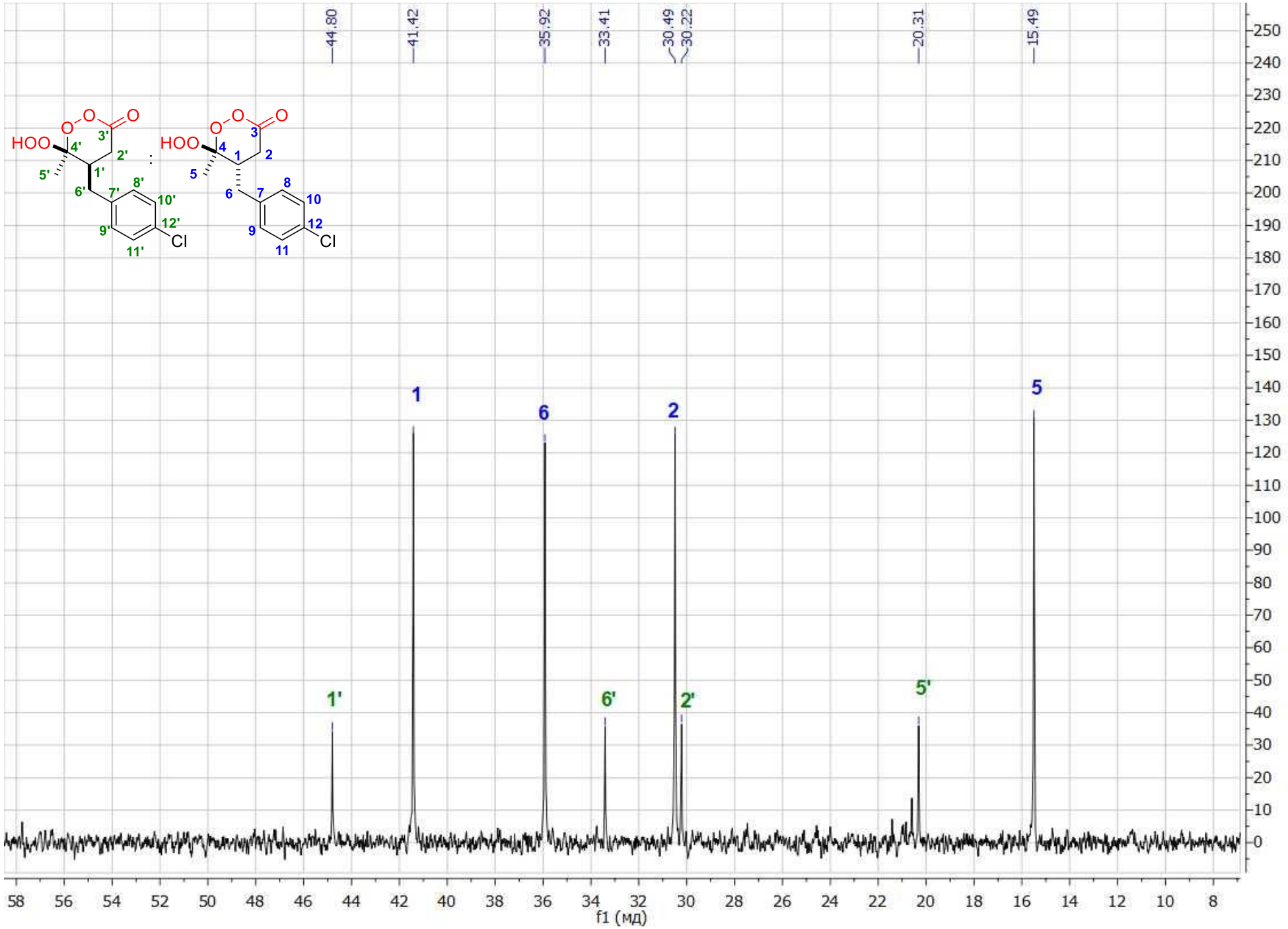


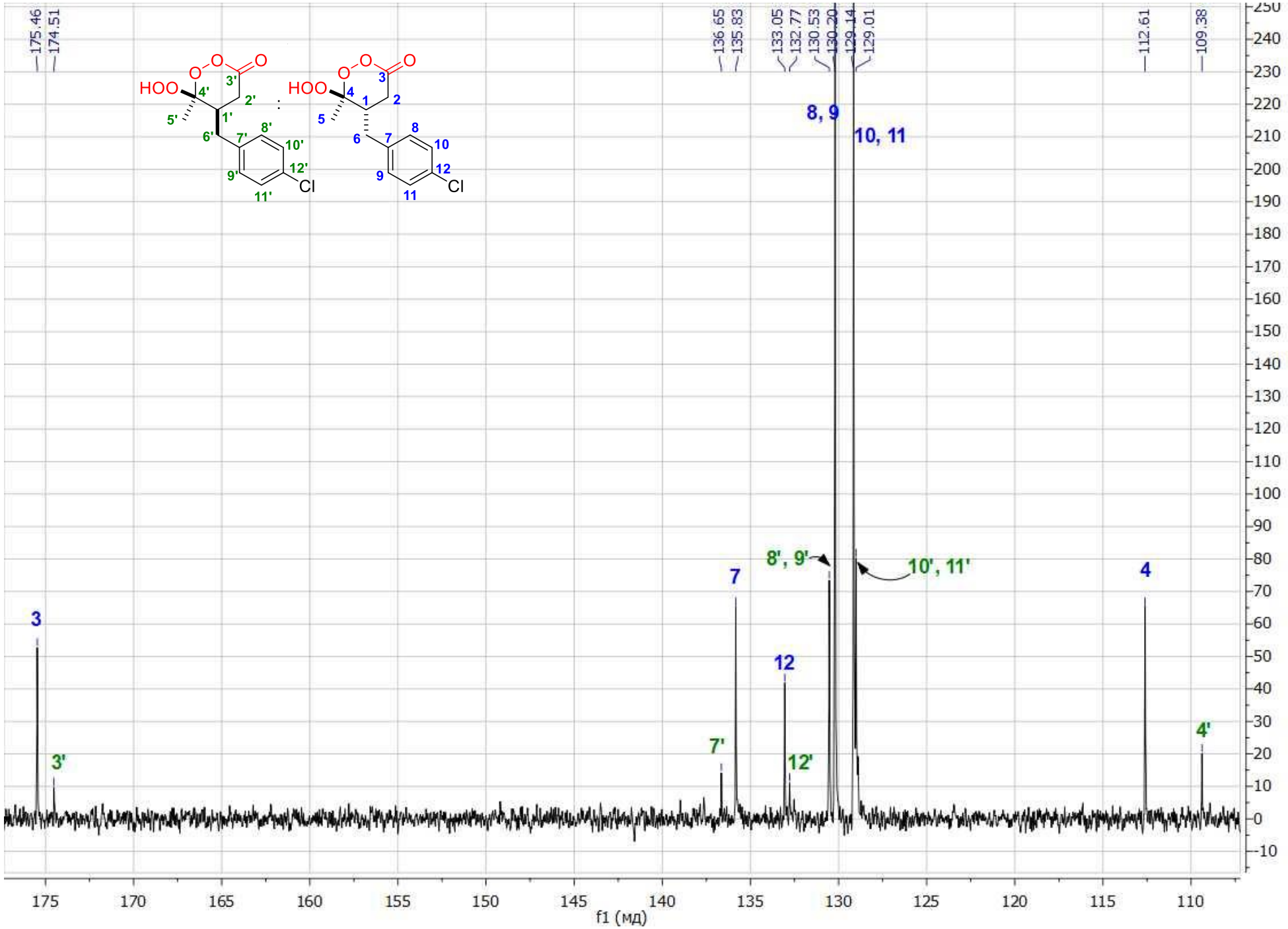

3.07 3.06 3.04 3.02 3.01 2.99 2.98
2.78 2.77 2.75 2.74 2.73 2.71 2.70 2.67 2.65 2.62 2.60 2.55 2.51 2.50 2.47 2.43 2.38 2.35 2.34 2.31 2.29 2.27 2.25 2.23 2.22 2.20
1.63 1.57
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
Cl
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
Cl
6 1H, 6' 1H
1' 1H
2' 1H
6 1H
6' 1H, 2 2H, 1 1H, 2' 1H
5'
5
450
400
350
300
250
200
150
100
50
0
3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6
f1 (мд)


9.07
8.96
7.29
7.27
7.26 CDCl3
7.08
7.06
HOO
HOO
Cl
Cl
HOO, HOO
10, 11
8, 9
f1 (мд)

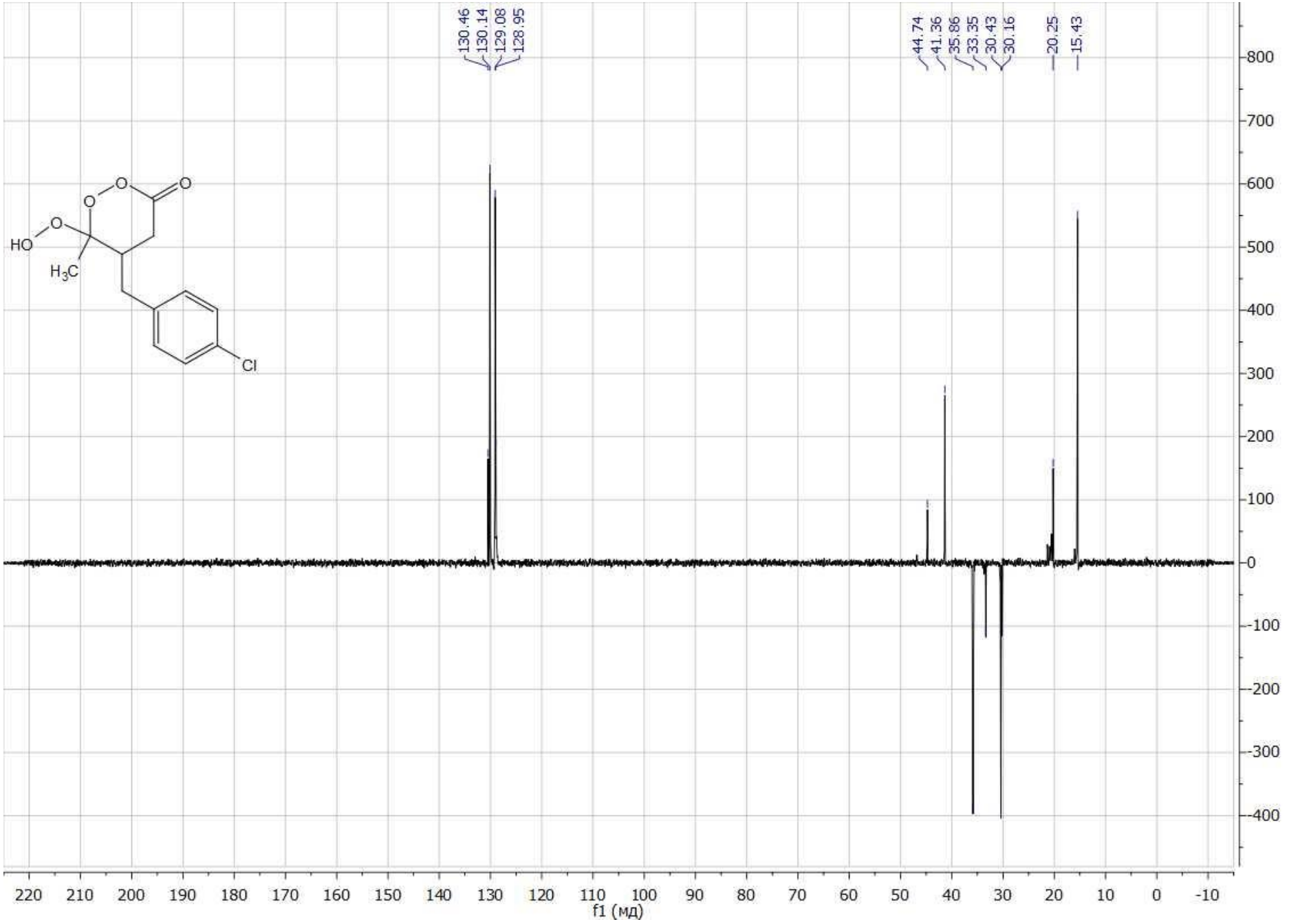
^{13}C NMR

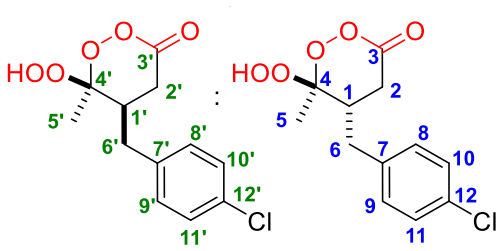

175.47
174.52
136.65
135.83
133.06
132.78
130.53
130.20
129.15
129.01
112.61
109.38
77.16 CDCl3
44.80
41.42
35.92
33.41
30.49
30.22
20.31
15.49
HO
O
O
O
O
H3C
Cl
f1 (мд)


44.80
41.42
35.92
33.41
30.49
30.22
20.31
15.49
HOO
Cl
1
6
2
5
1'
6'
2'
5'
f1 (мд)

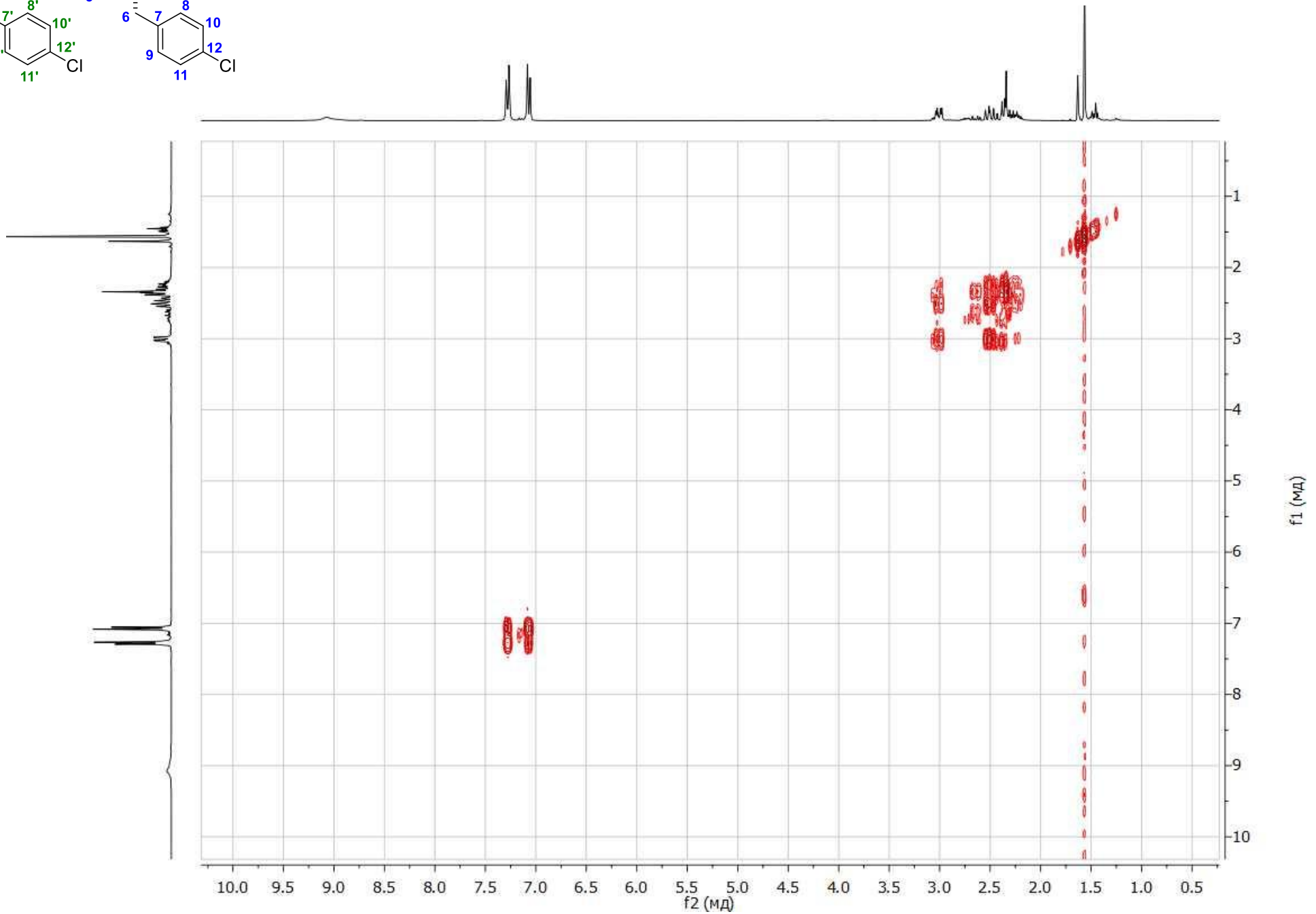

175.46
174.51
136.65
135.83
133.05
132.77
130.53
130.20
129.14
129.01
112.61
109.38
HOO
Cl
8, 9
10, 11
8', 9'
10', 11'
3
7
12
4
3'
7'
12'
4'
f1 (мд)

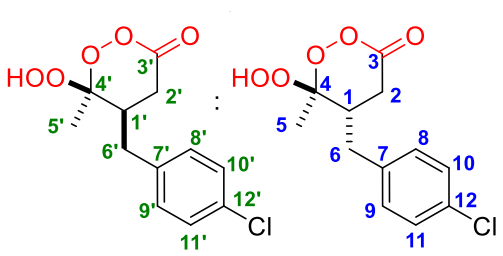
^{13}C_deptsp135



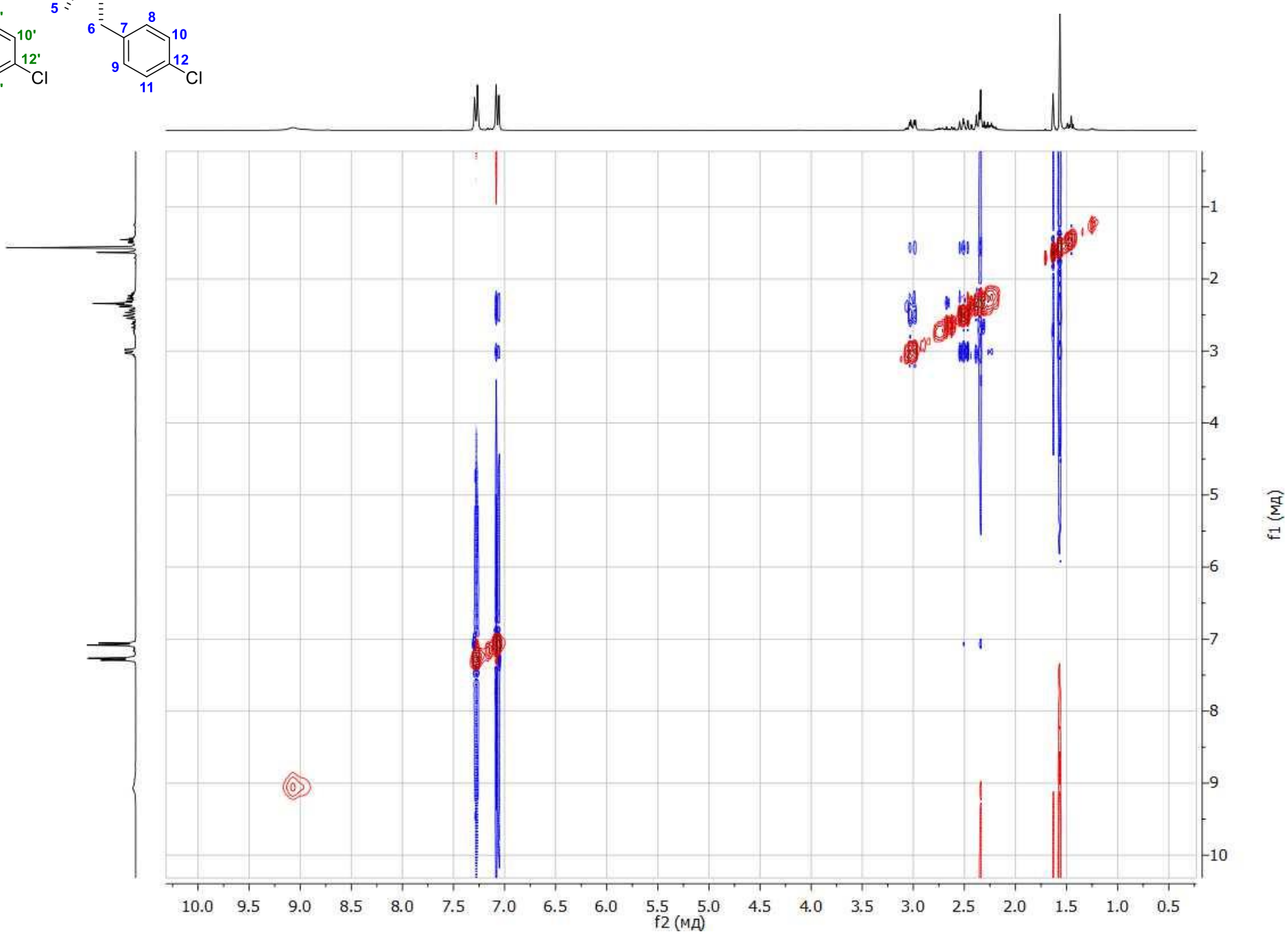

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
Cl
:
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
Cl

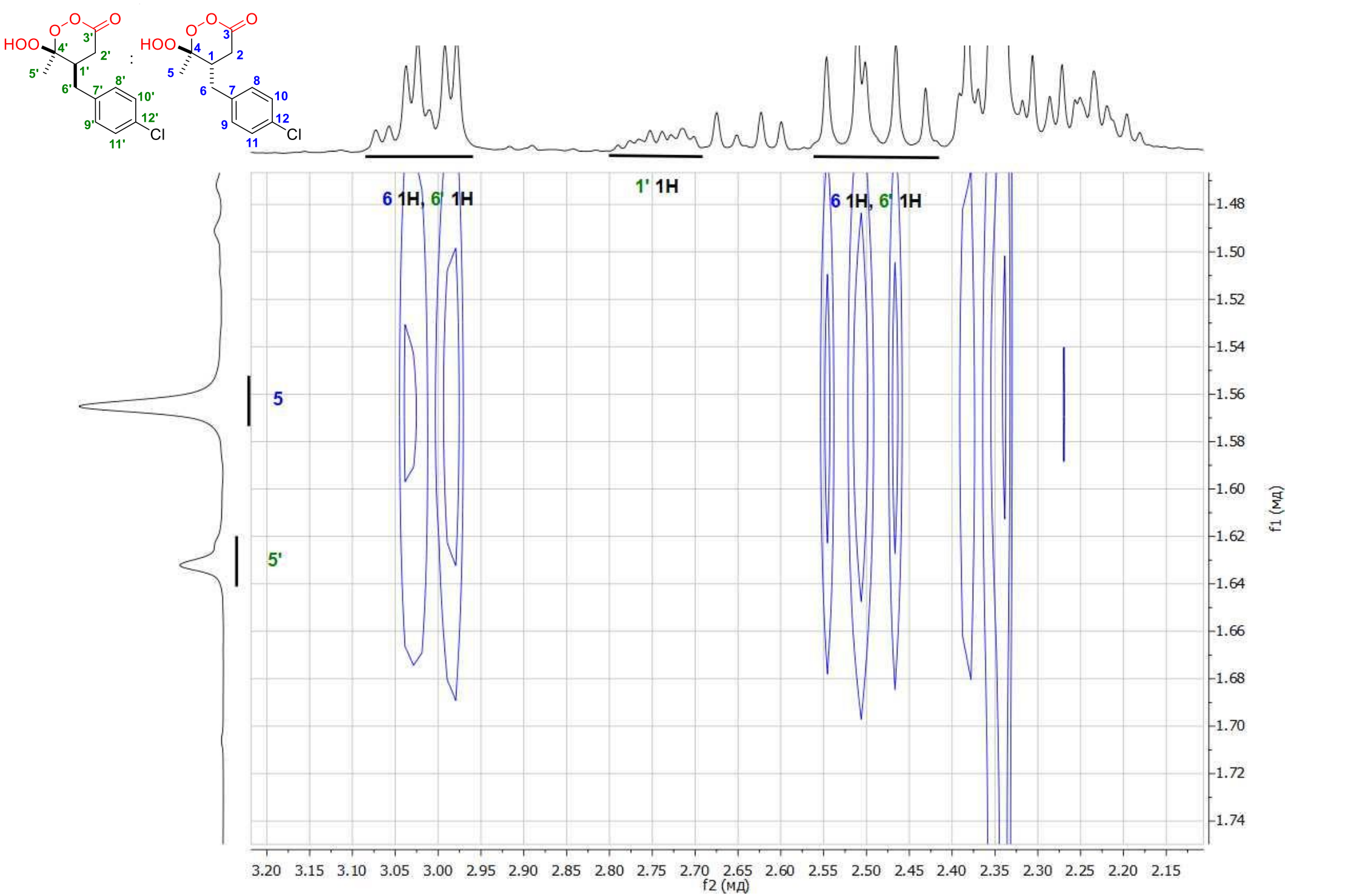
{^{1}H-^{1}H} COSY

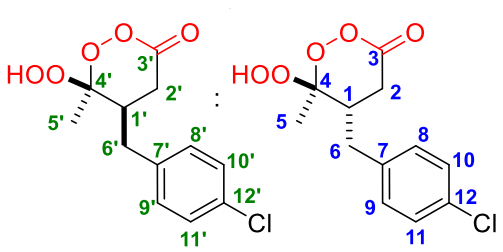

f2 (мд)
f1 (мд)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
1
2
3
4
5
6
7
8
9
10


HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
12'
9'
11'
Cl
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
Cl

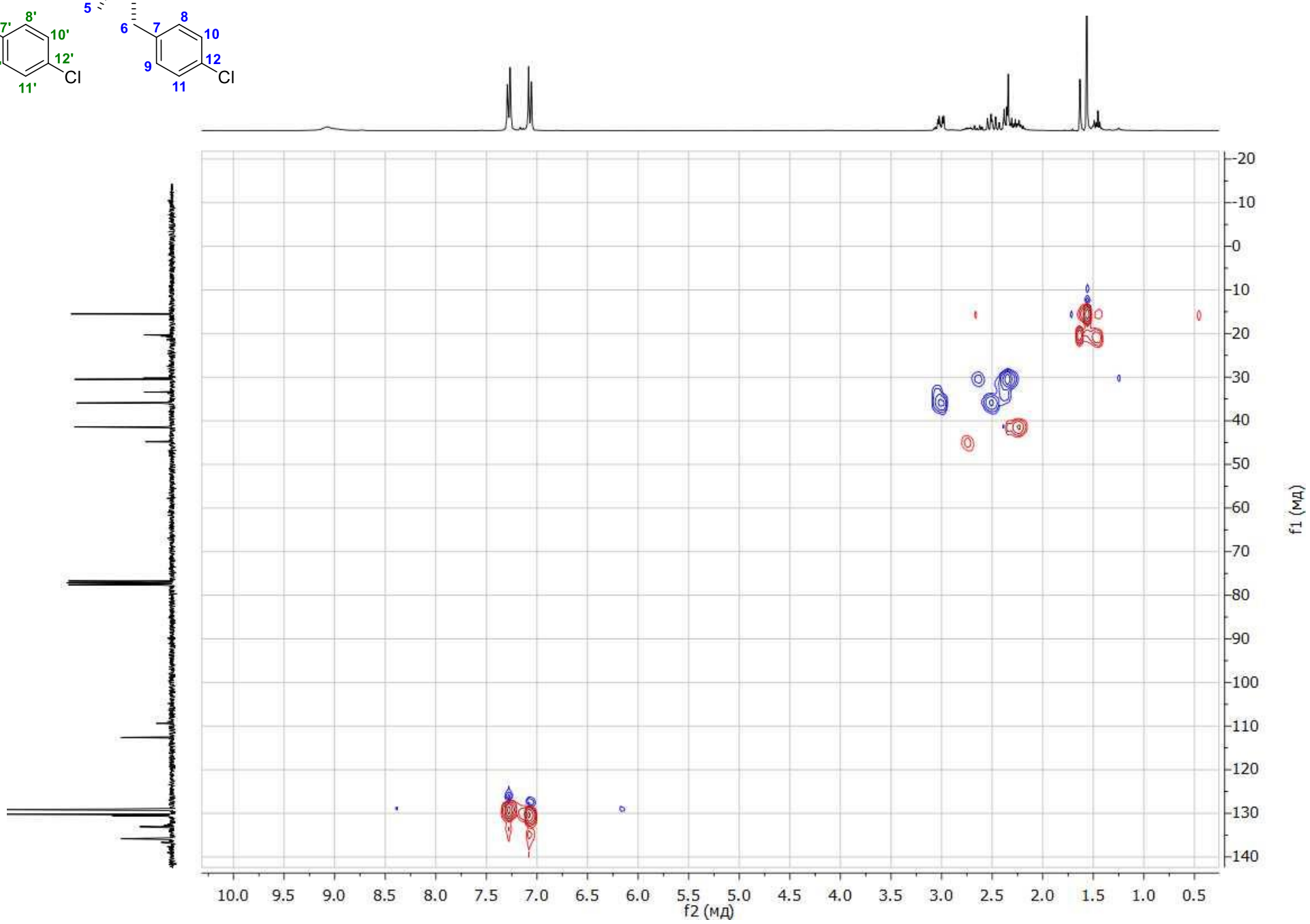
{^{1}H-^{1}H} NOESY

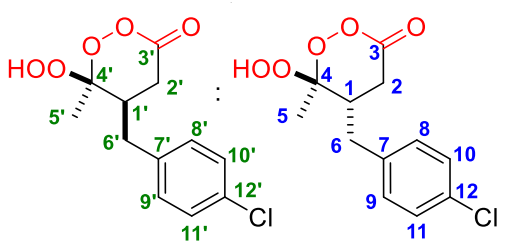

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (мд)
1
2
3
4
5
6
7
8
9
10
f1 (мд)


HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
Cl
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
Cl
6 1H, 6' 1H
1' 1H
6 1H, 6' 1H
5
5'
1.48
1.50
1.52
1.54
1.56
1.58
1.60
1.62
1.64
1.66
1.68
1.70
1.72
1.74
f1 (мд)
3.20
3.15
3.10
3.05
3.00
2.95
2.90
2.85
2.80
2.75
2.70
2.65
2.60
2.55
2.50
2.45
2.40
2.35
2.30
2.25
2.20
2.15
f2 (мд)

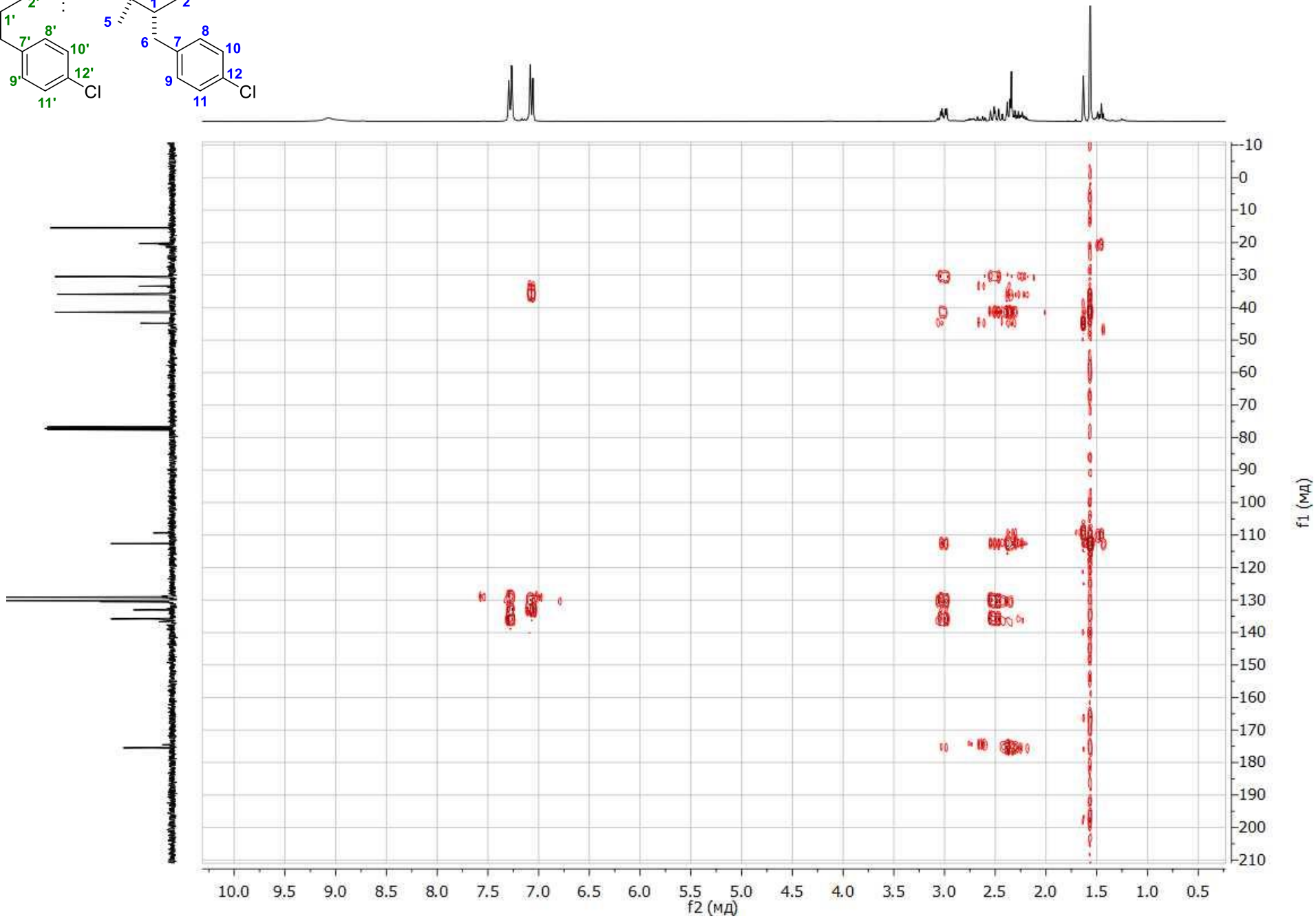

HOO
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
10'
12'
9'
11'
Cl
:
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
Cl

{^{1}H-^{13}C} HSQC


-20
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
f1 (мд)
10.0
9.5
9.0
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
f2 (мд)

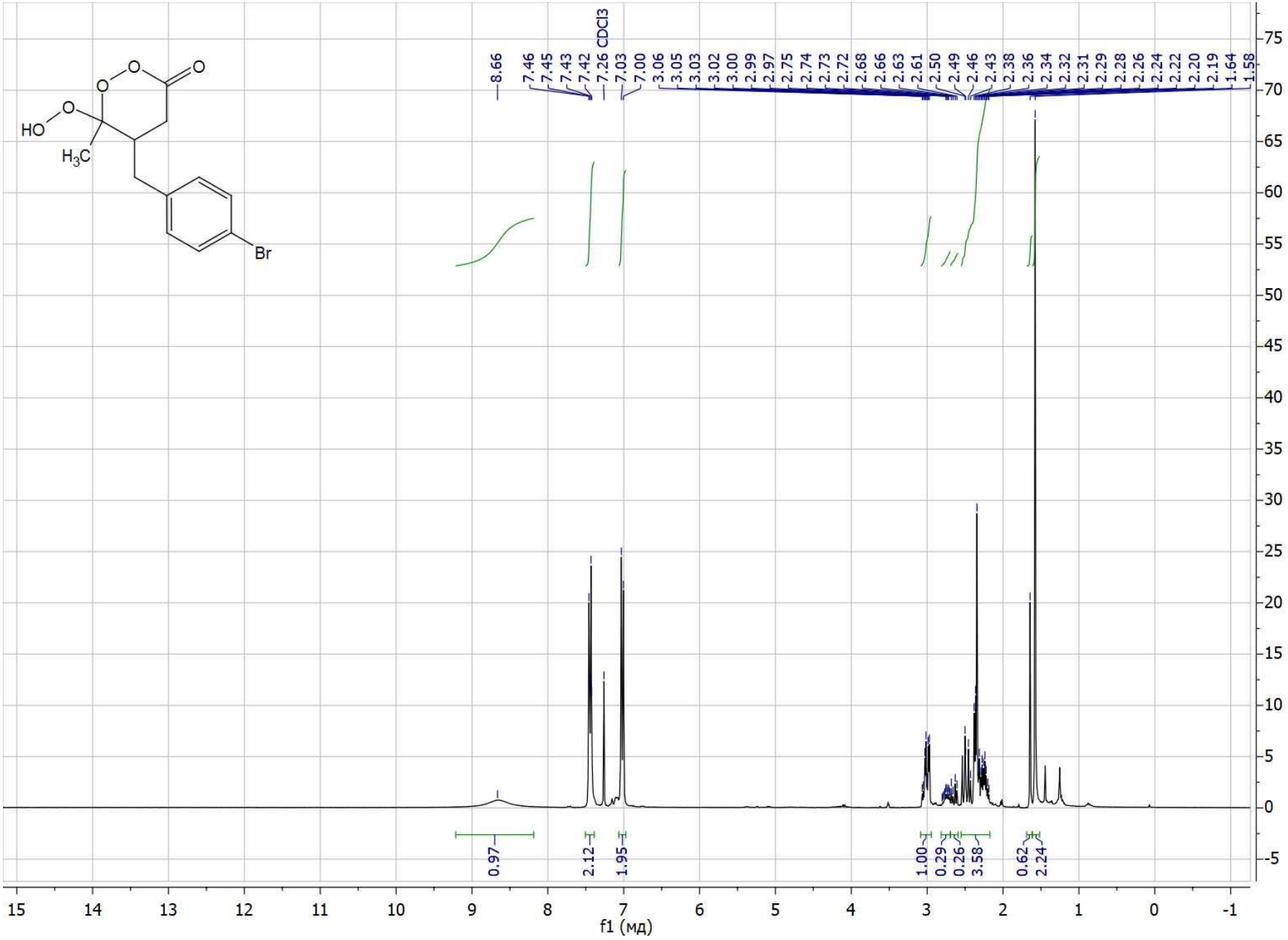

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
12'
9'
11'
Cl
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
Cl

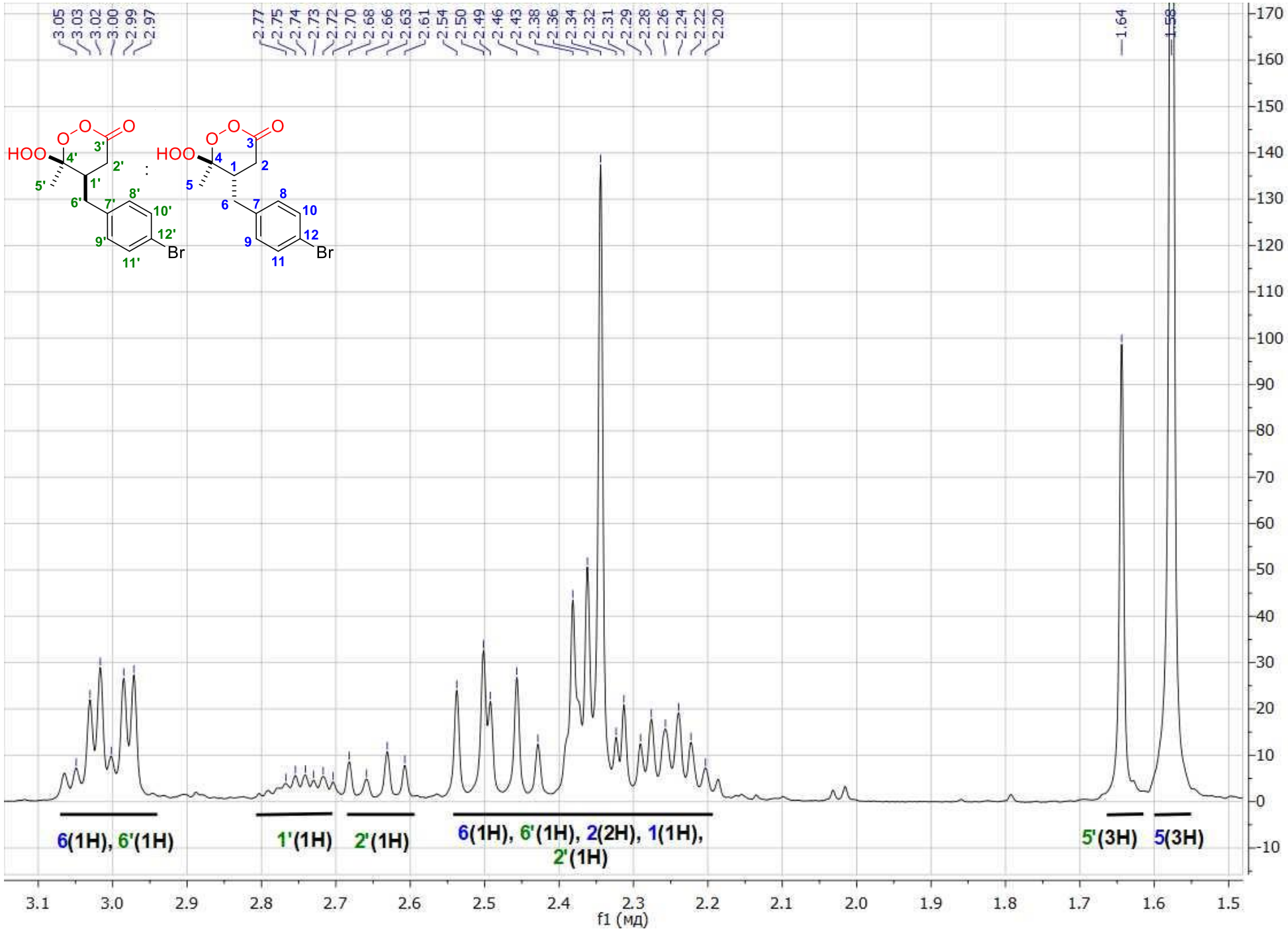
{^{1}H-^{13}C} HMBC

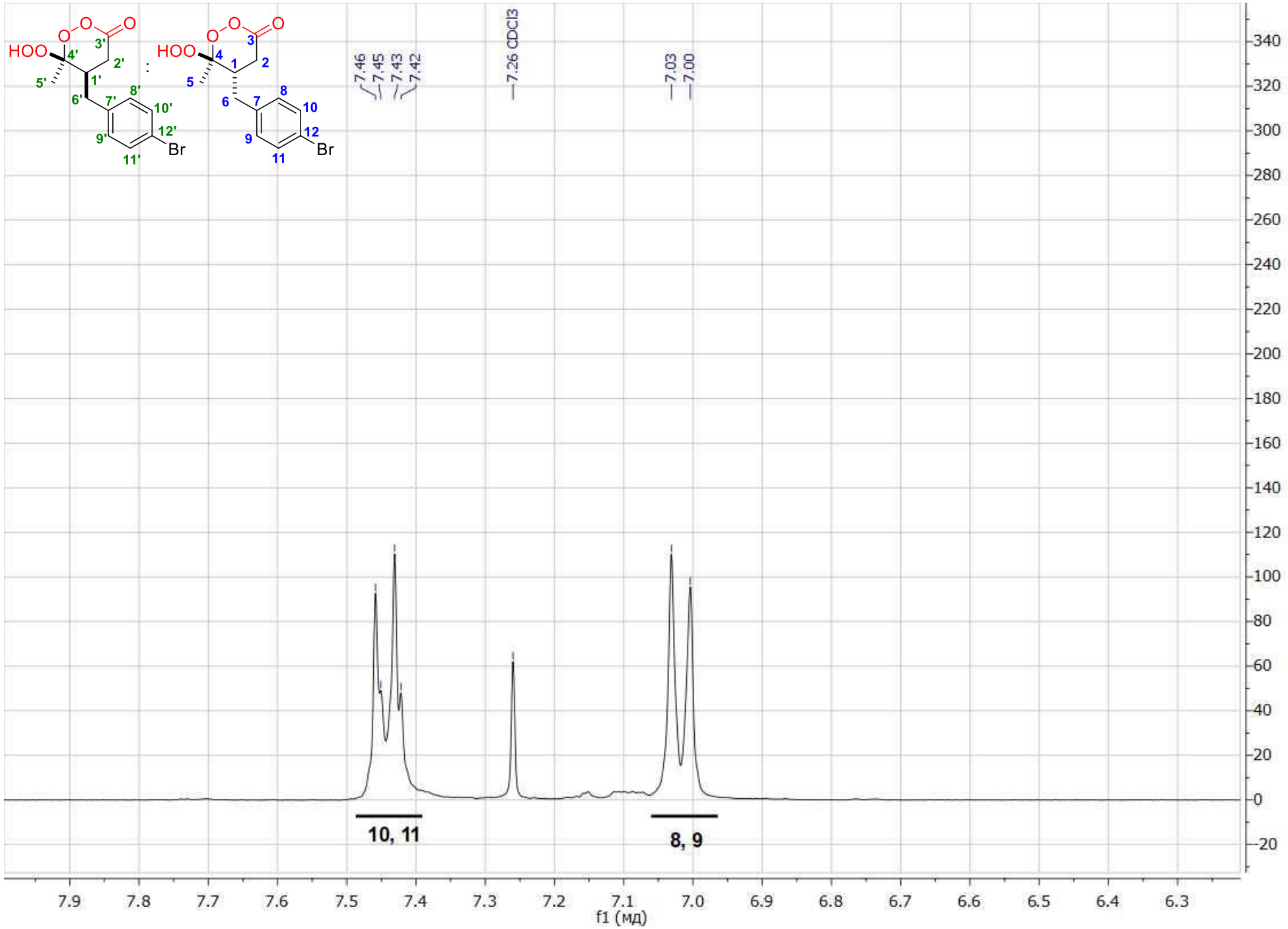

f2 (мд)
f1 (мд)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210

5-(4-Bromobenzyl)-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2d

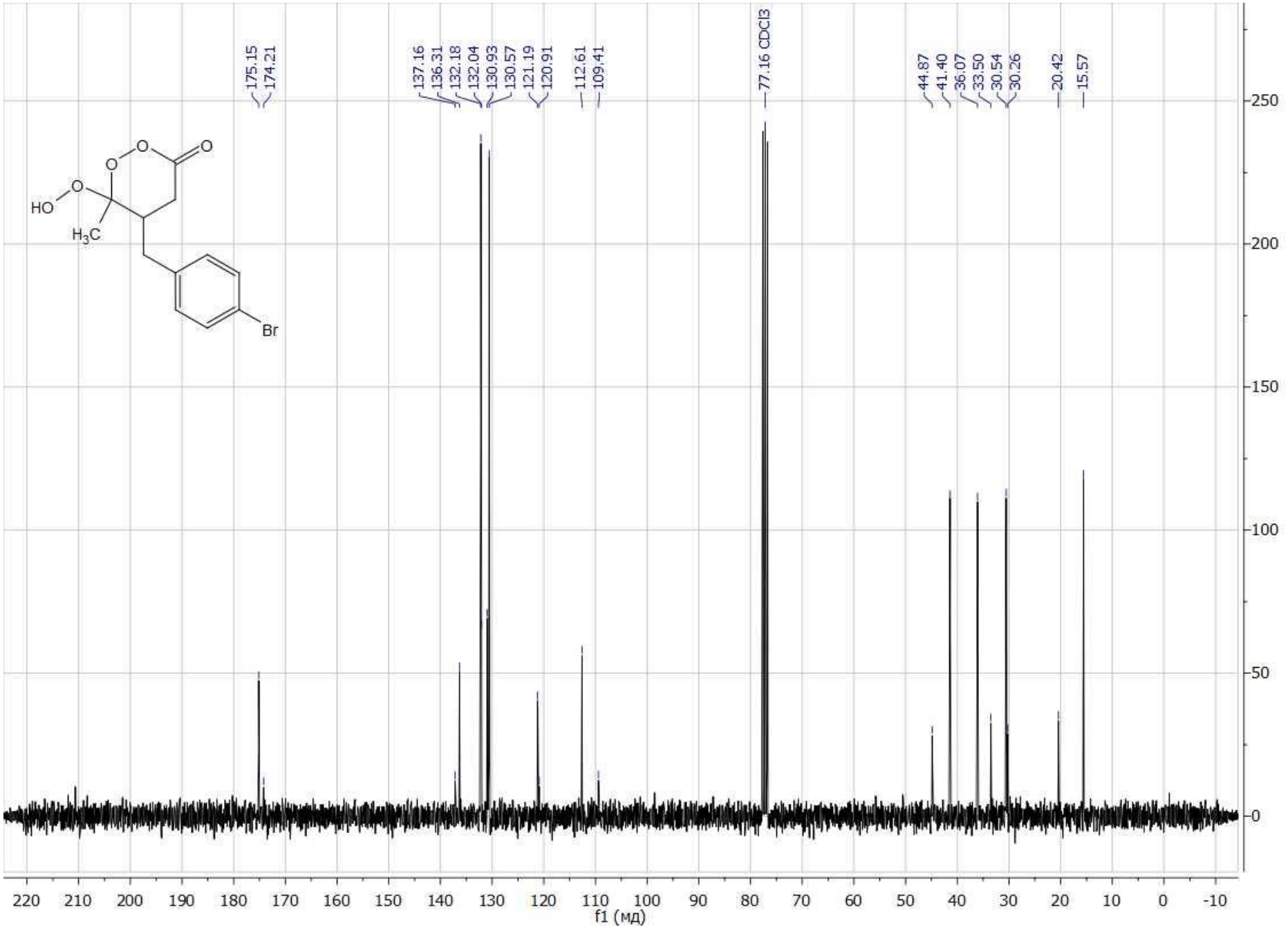
^{1}H NMR

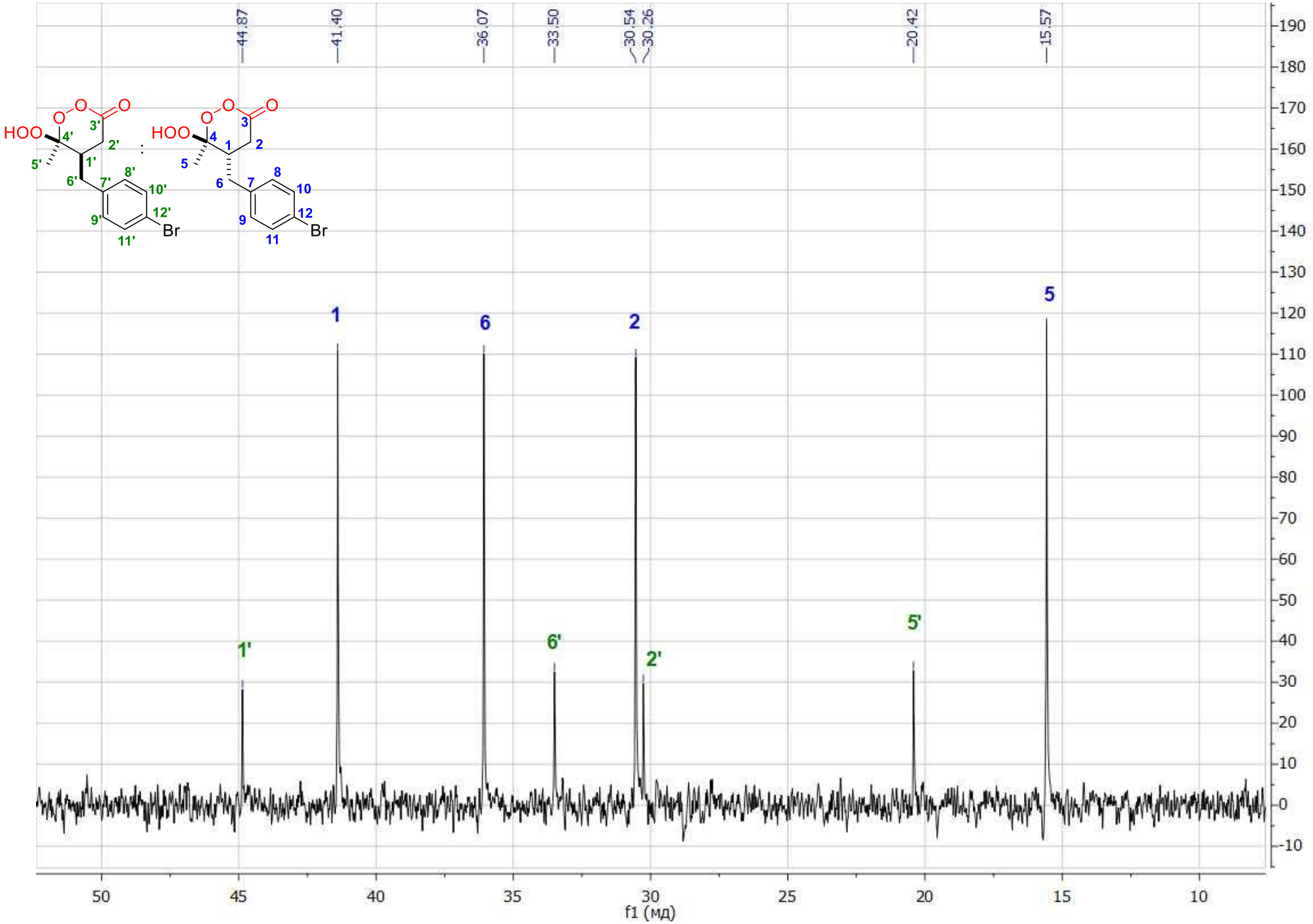


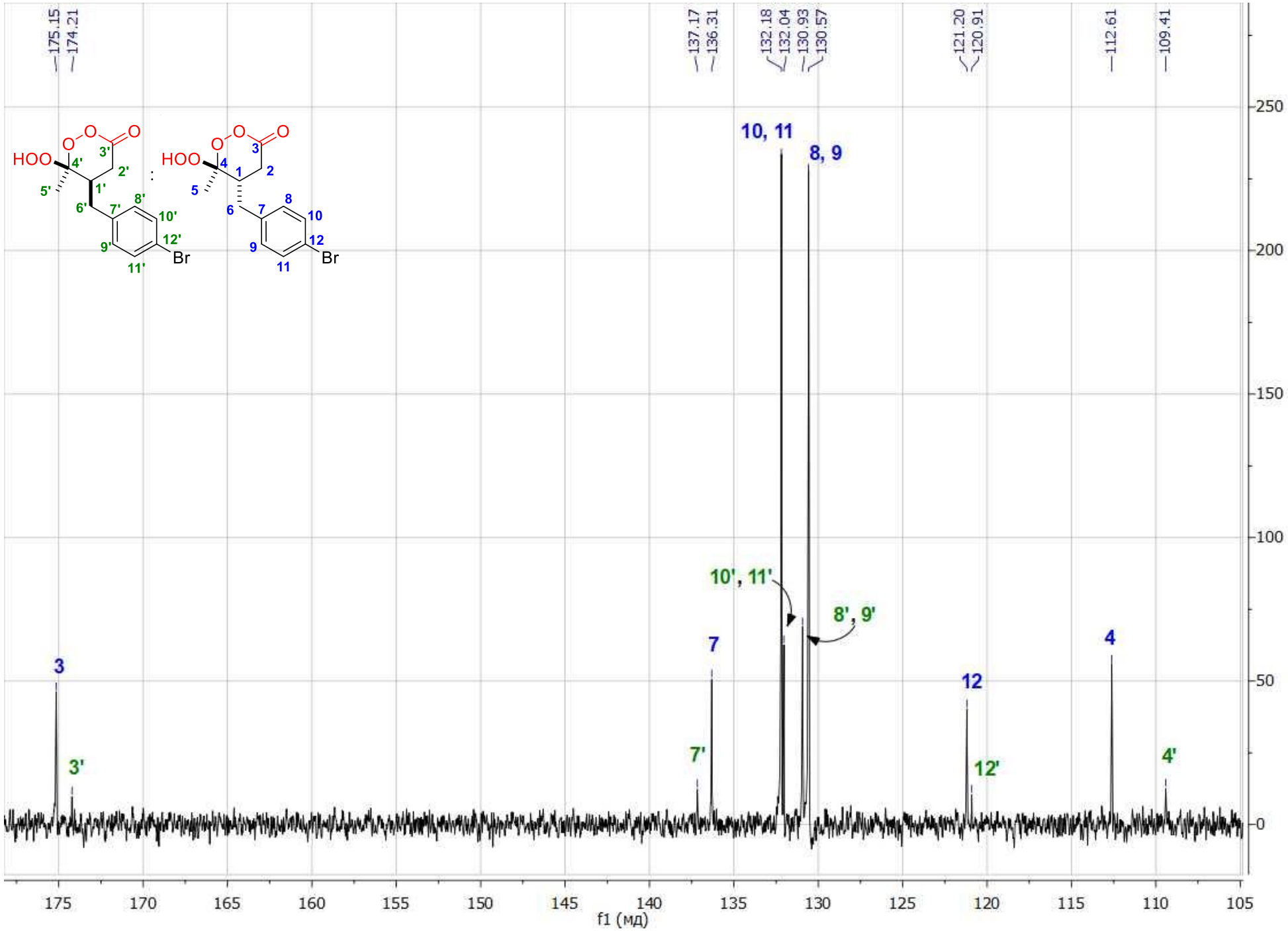

3.05
3.03
3.02
3.00
2.99
2.97
2.77
2.75
2.74
2.73
2.72
2.70
2.68
2.66
2.63
2.61
2.54
2.50
2.49
2.46
2.43
2.38
2.36
2.34
2.32
2.31
2.29
2.28
2.26
2.24
2.22
2.20
1.64
1.58
HOO
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
10'
12'
9'
11'
Br
:
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
Br
6(1H), 6'(1H)
1'(1H)
2'(1H)
6(1H), 6'(1H), 2(2H), 1(1H),
2'(1H)
5'(3H)
5(3H)
f1 (мд)


7.46
7.45
7.43
7.42
7.26 CDCl3
7.03
7.00
10, 11
8, 9
f1 (мд)

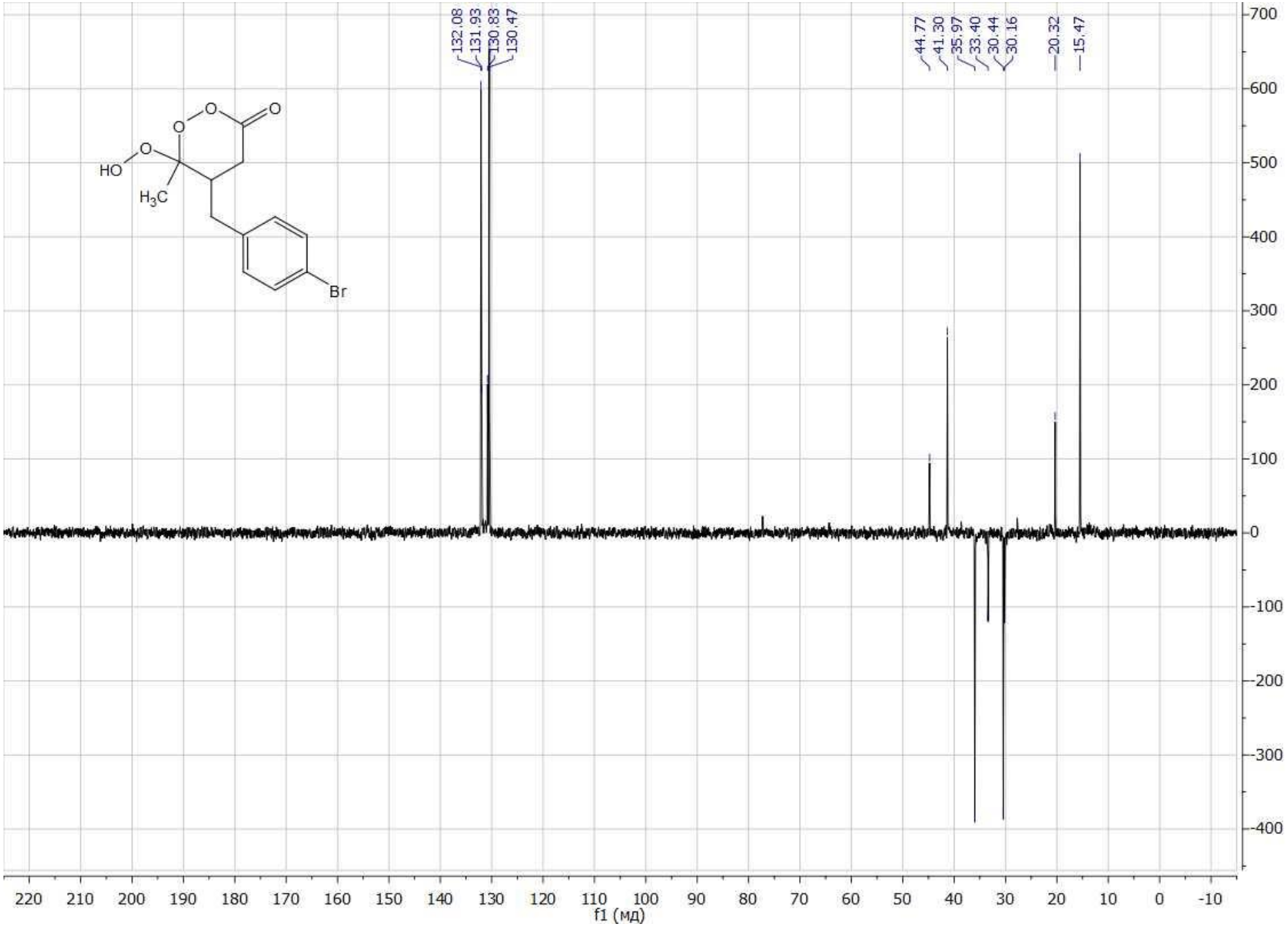
^{13}C NMR

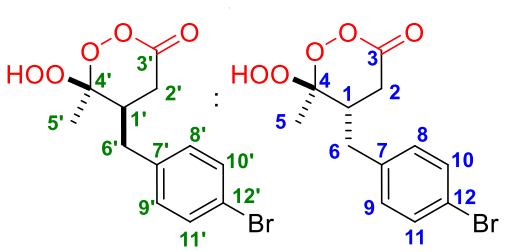

175.15
174.21
137.16
136.31
132.18
132.04
130.93
130.57
121.19
120.91
112.61
109.41
77.16 CDCl3
44.87
41.40
36.07
33.50
30.54
30.26
20.42
15.57
HO
O
O
O
O
H3C
Br
250
200
150
100
50
0
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (мд)


44.87
41.40
36.07
33.50
30.54
30.26
20.42
15.57
HOO
Br
1
6
2
5
1'
6'
2'
5'
f1 (мд)

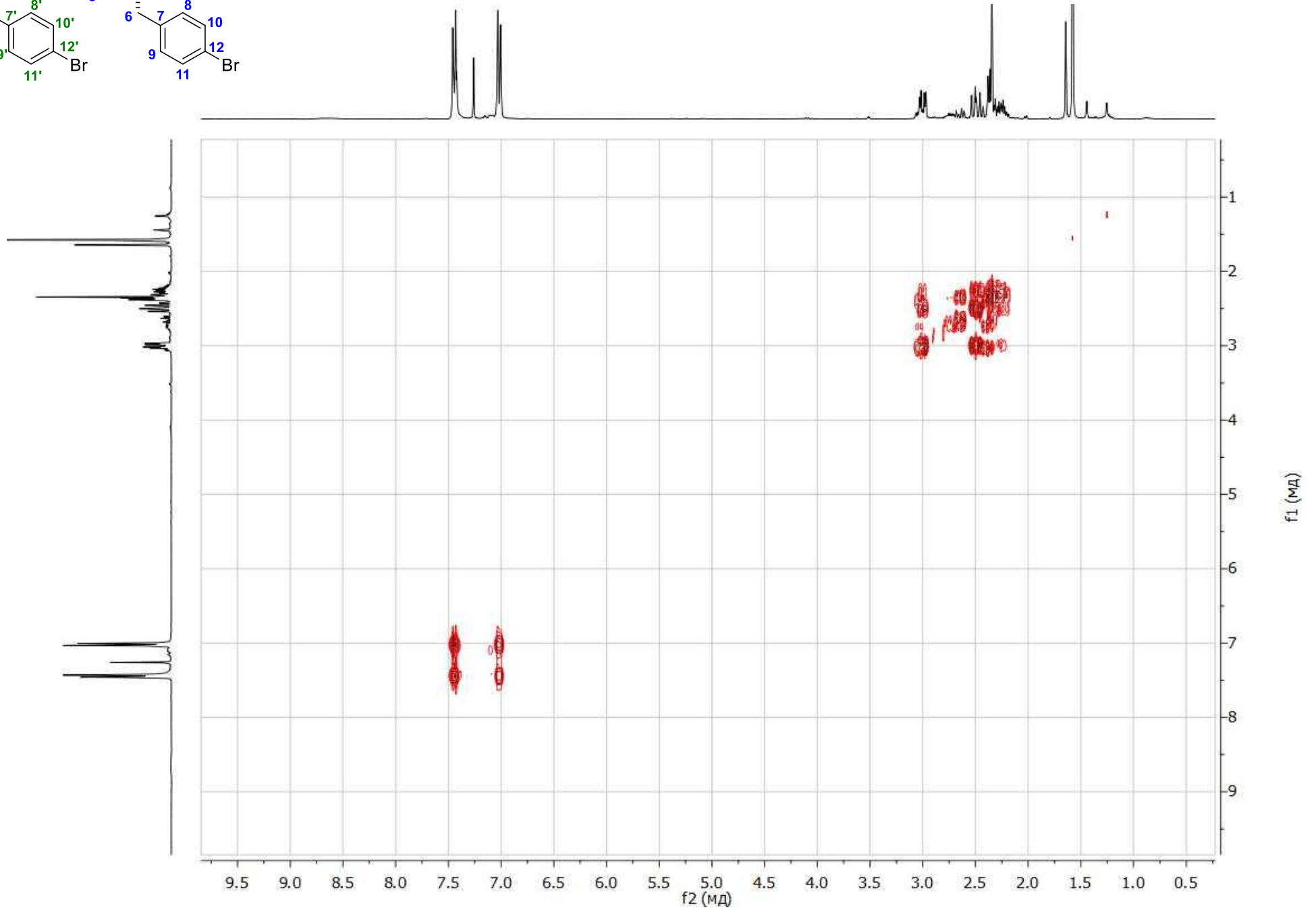

175.15
174.21
137.17
136.31
132.18
132.04
130.93
130.57
121.20
120.91
112.61
109.41
HOO
Br
10, 11
8, 9
10', 11'
8', 9'
7
7'
3
3'
12
12'
4
4'
250
200
150
100
50
0
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
f1 (мд)

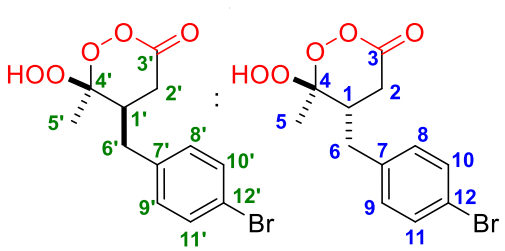
^{13}C_deptsp135



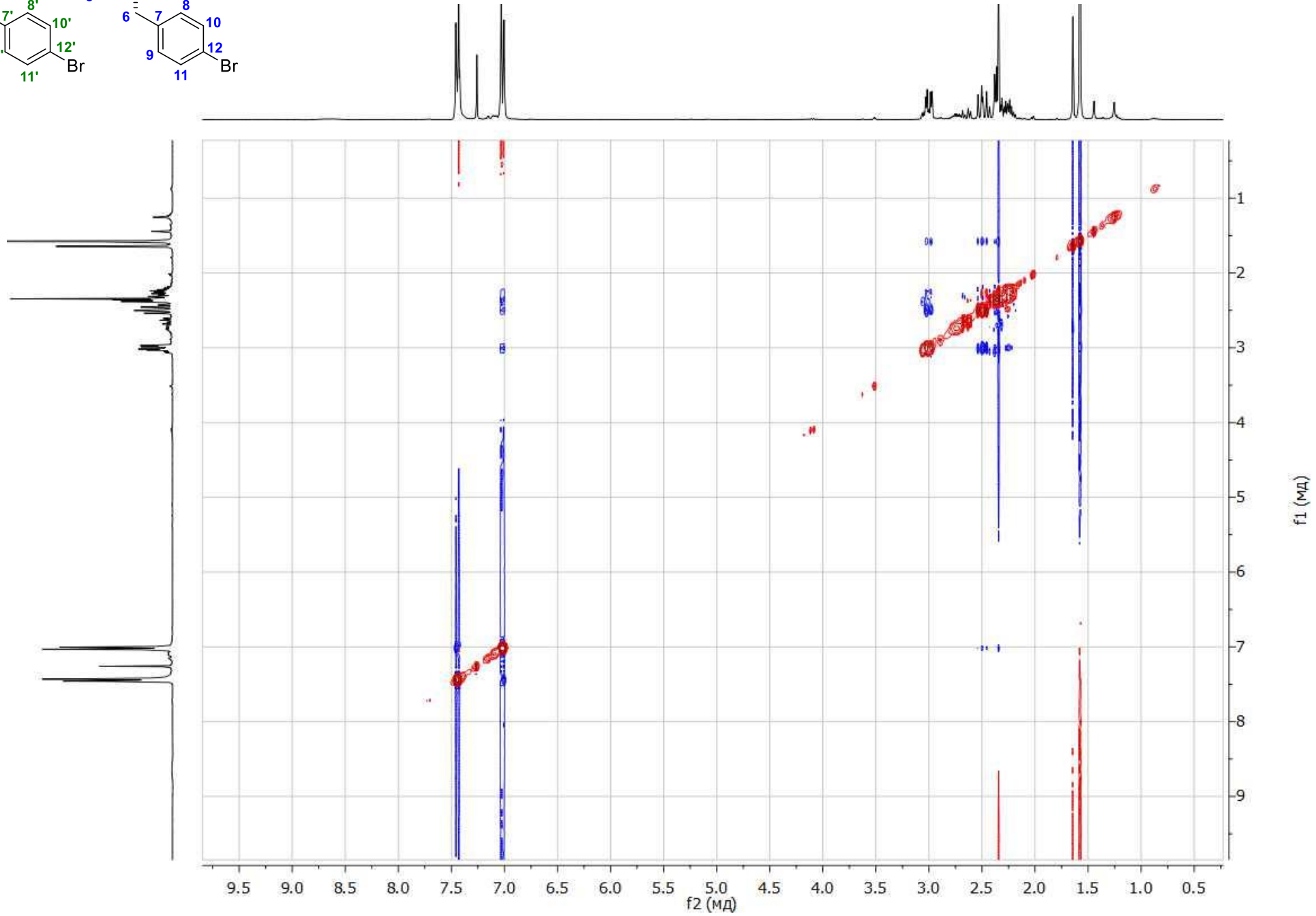

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
Br
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
Br

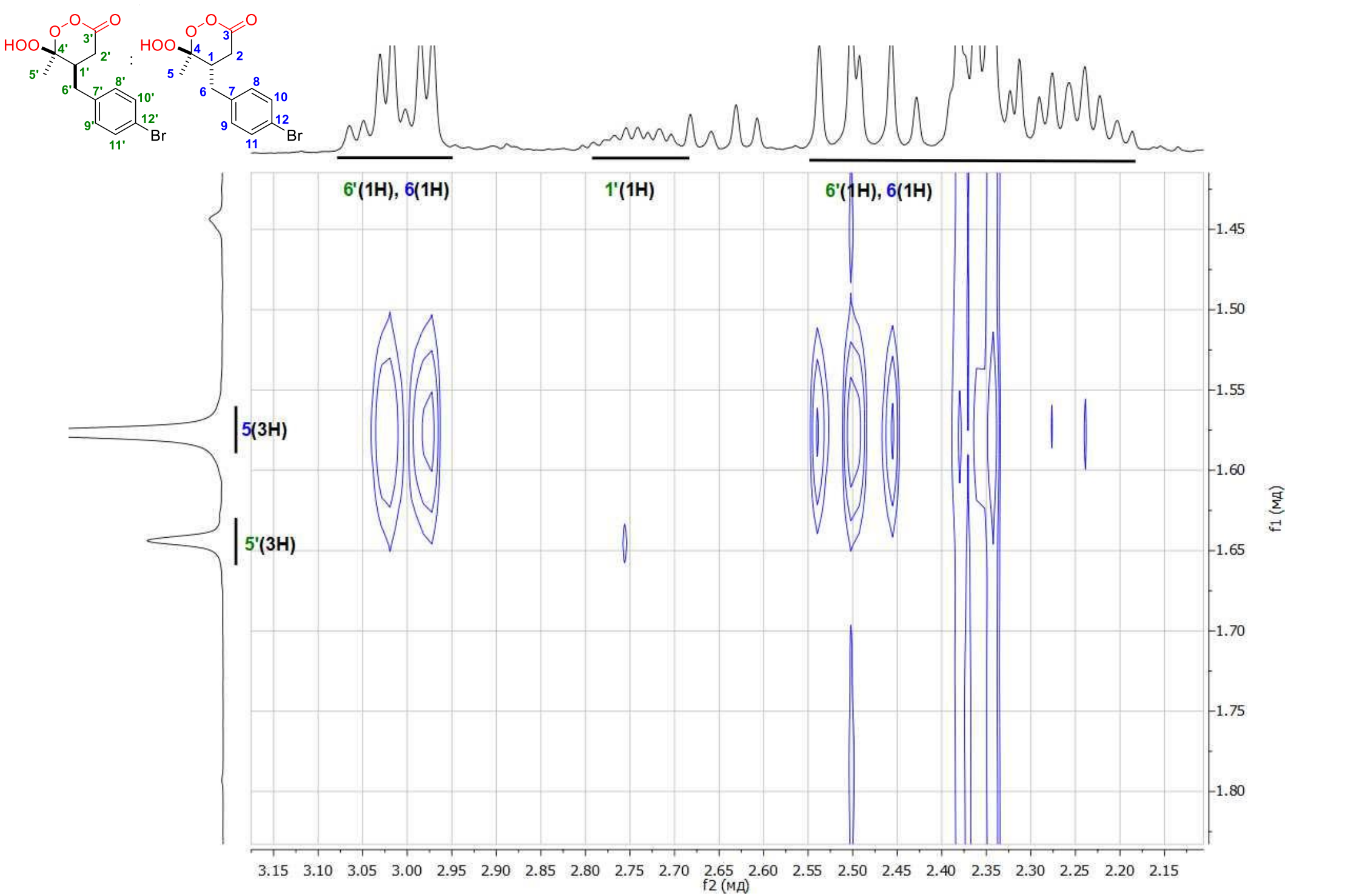
{^{1}H-^{1}H} COSY

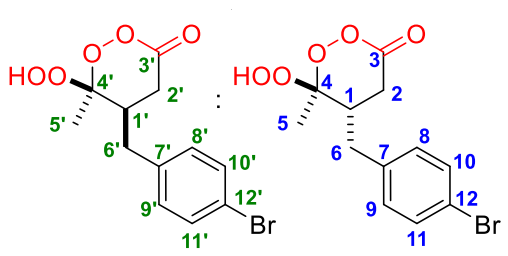

f1 (мд)
f2 (мд)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
1
2
3
4
5
6
7
8
9


HOO
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
9'
10'
11'
12'
Br
HOO
O
O
O
3
4
1
2
5
6
7
8
9
10
11
12
Br

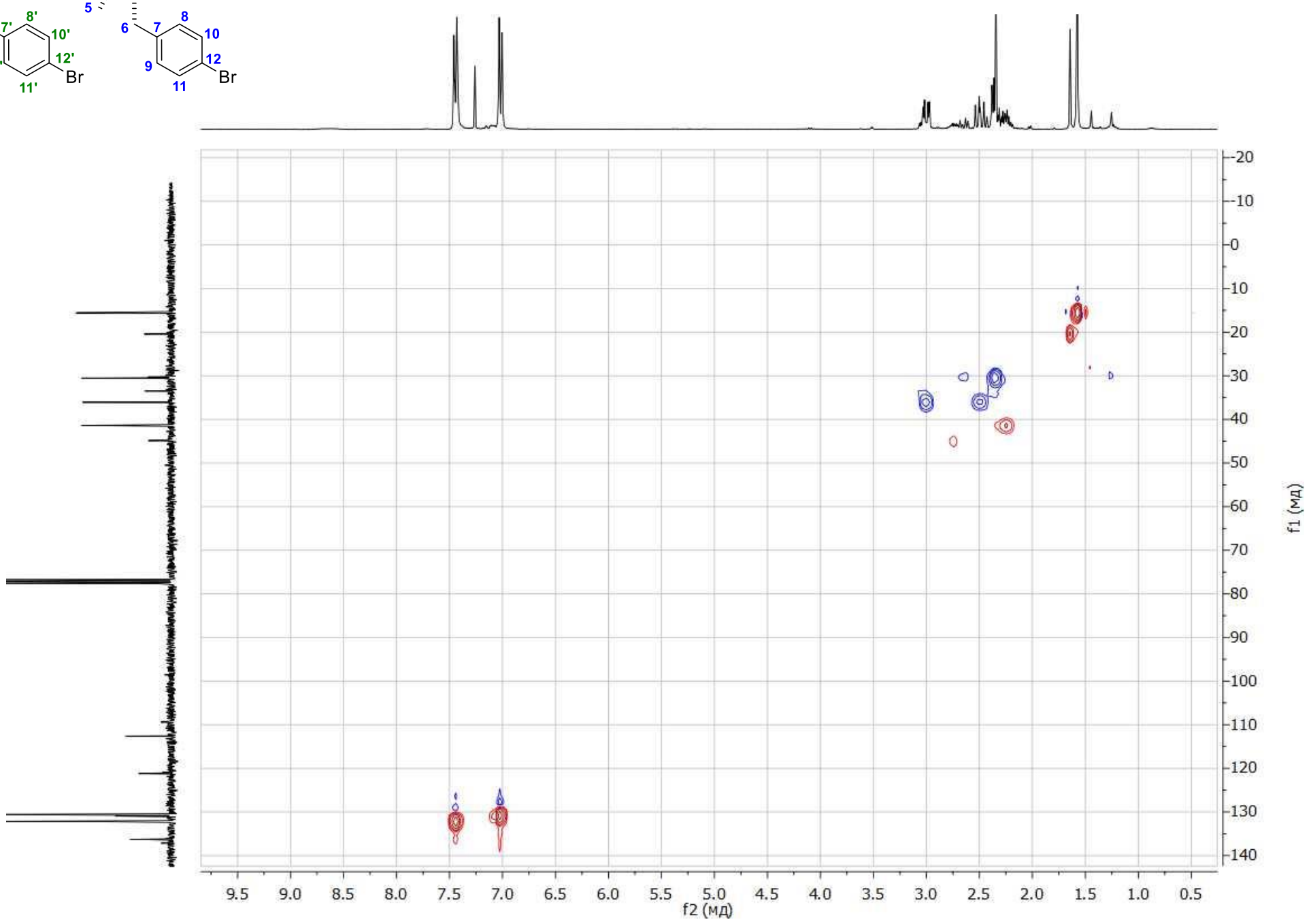
{^{1}H-^{1}H} NOESY

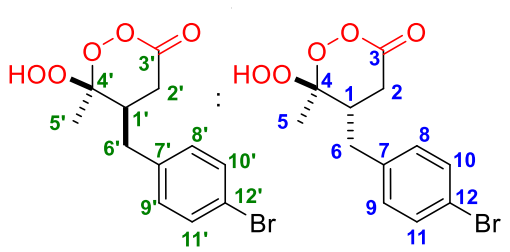

9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (мд)
1
2
3
4
5
6
7
8
9
f1 (мд)


HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
Br
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
Br
6'(1H), 6(1H)
1'(1H)
6'(1H), 6(1H)
5(3H)
5'(3H)
1.45
1.50
1.55
1.60
1.65
1.70
1.75
1.80
f1 (мд)
3.15
3.10
3.05
3.00
2.95
2.90
2.85
2.80
2.75
2.70
2.65
2.60
2.55
2.50
2.45
2.40
2.35
2.30
2.25
2.20
2.15
f2 (мд)

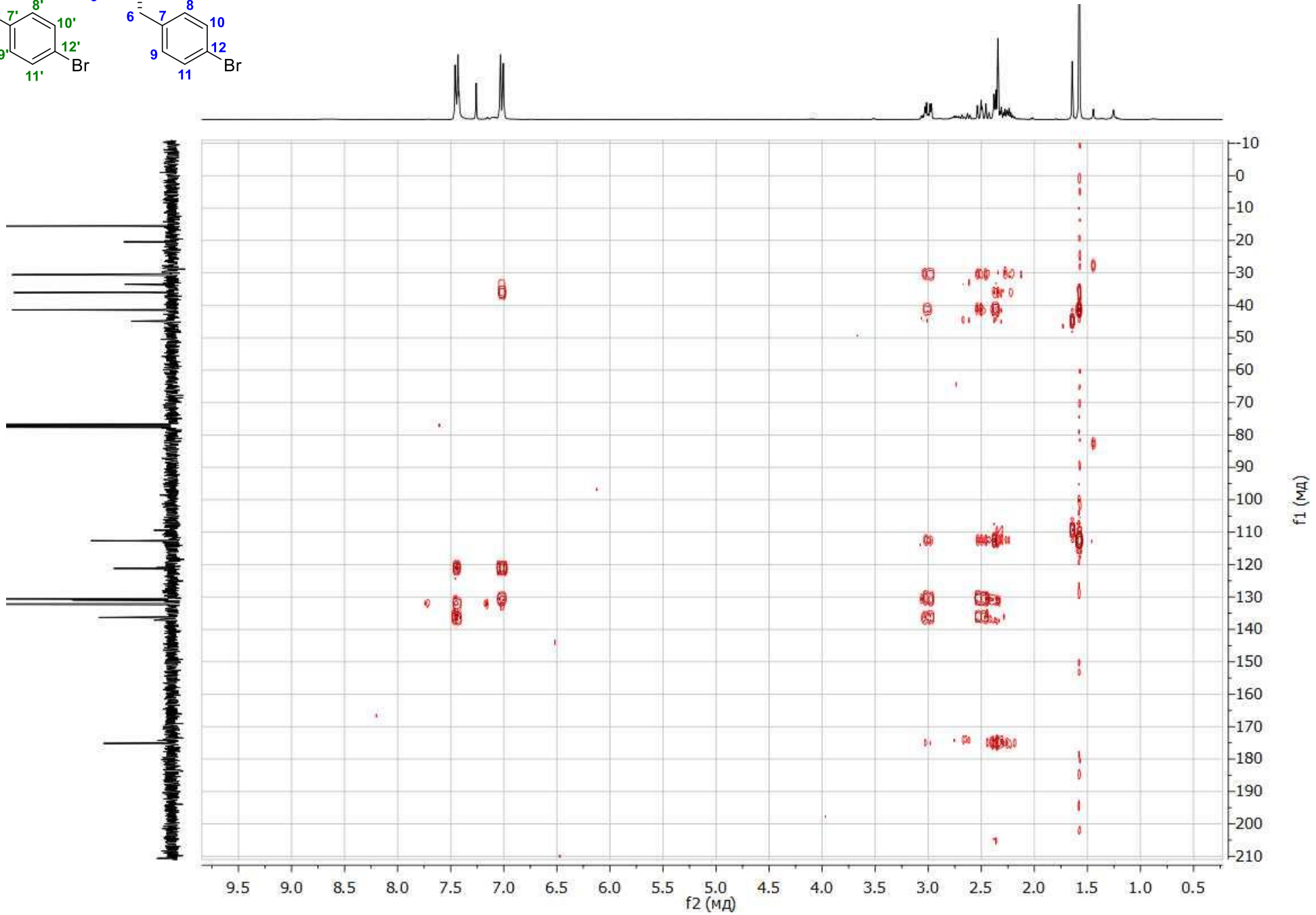

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
12'
9'
11'
Br
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
Br

{^{1}H-^{13}C} HSQC


f2 (мд)
f1 (мд)
9.5
9.0
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
-20
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140

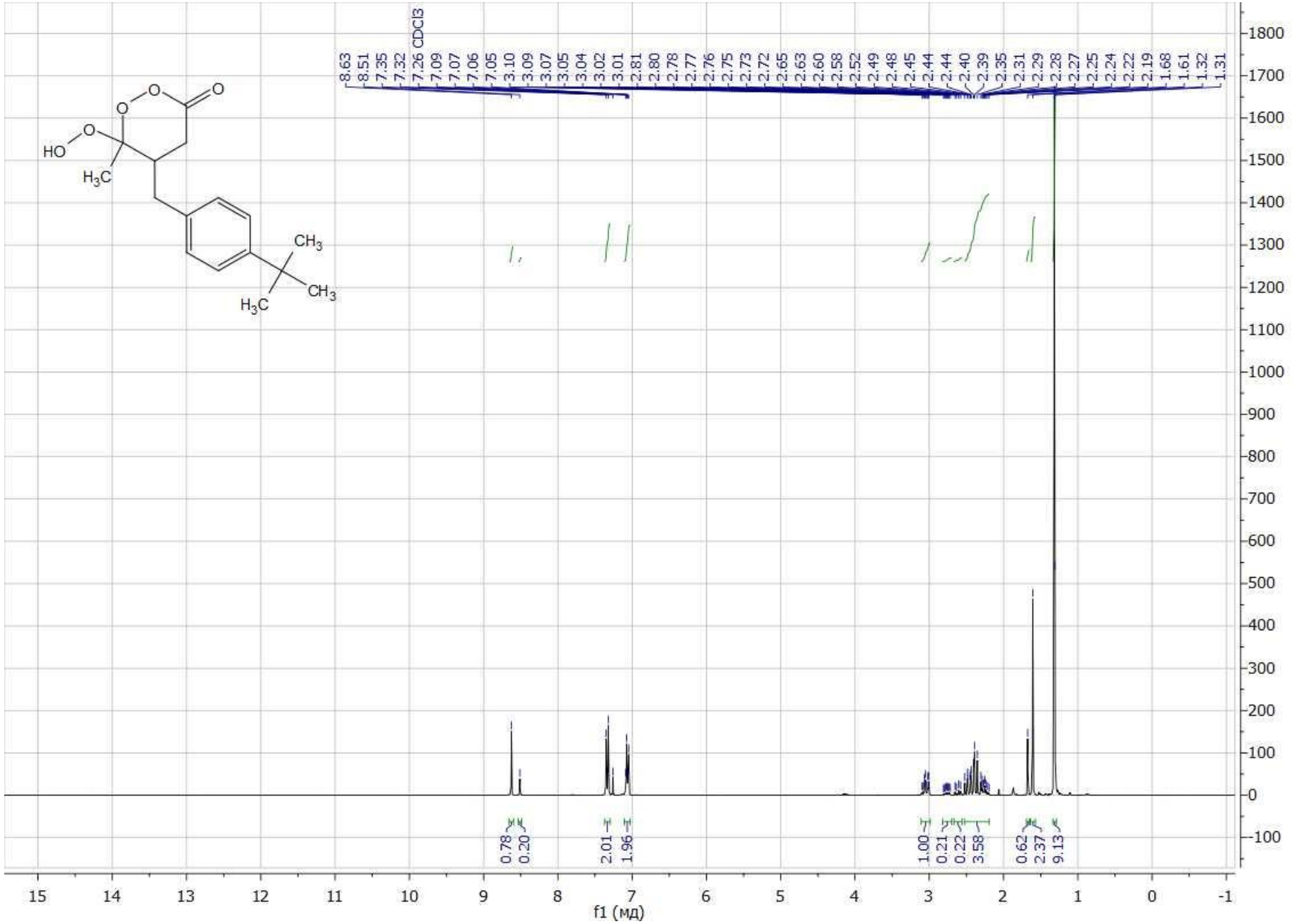

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
Br
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
Br

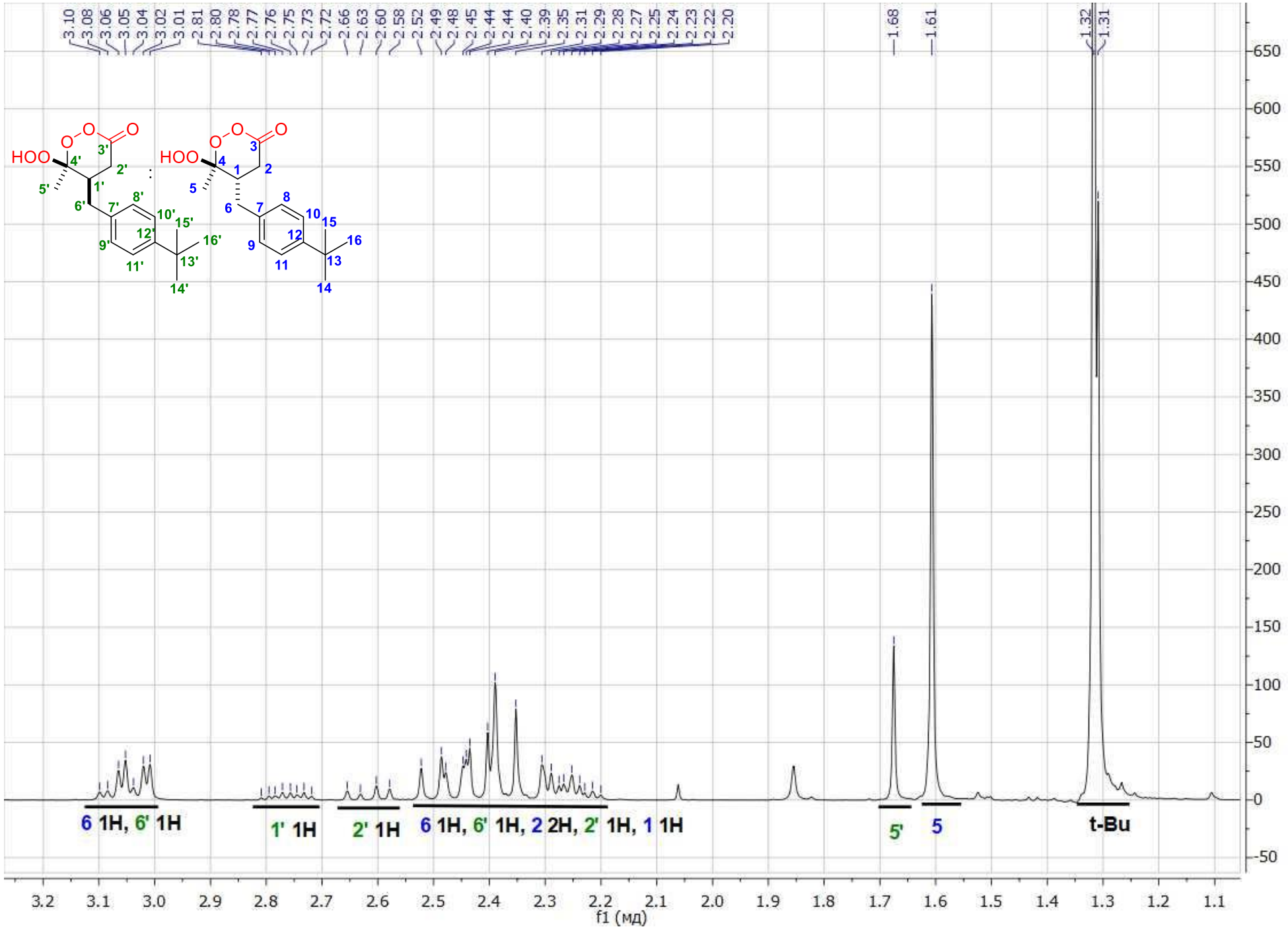
{^{1}H-^{13}C} HMBC

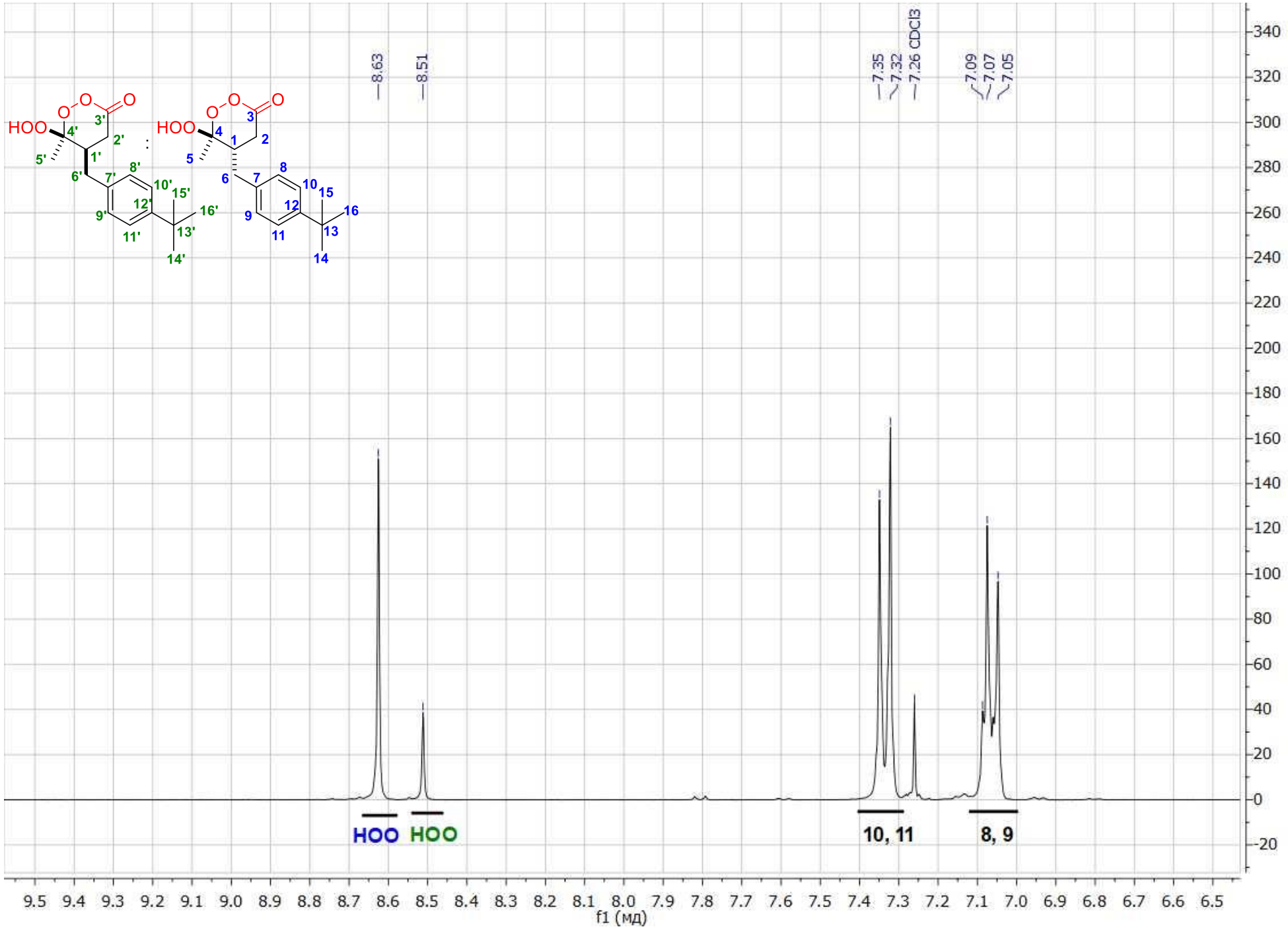

f2 (мд)
f1 (мд)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210

5-(4-(*Tert*-butyl)benzyl)-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2e

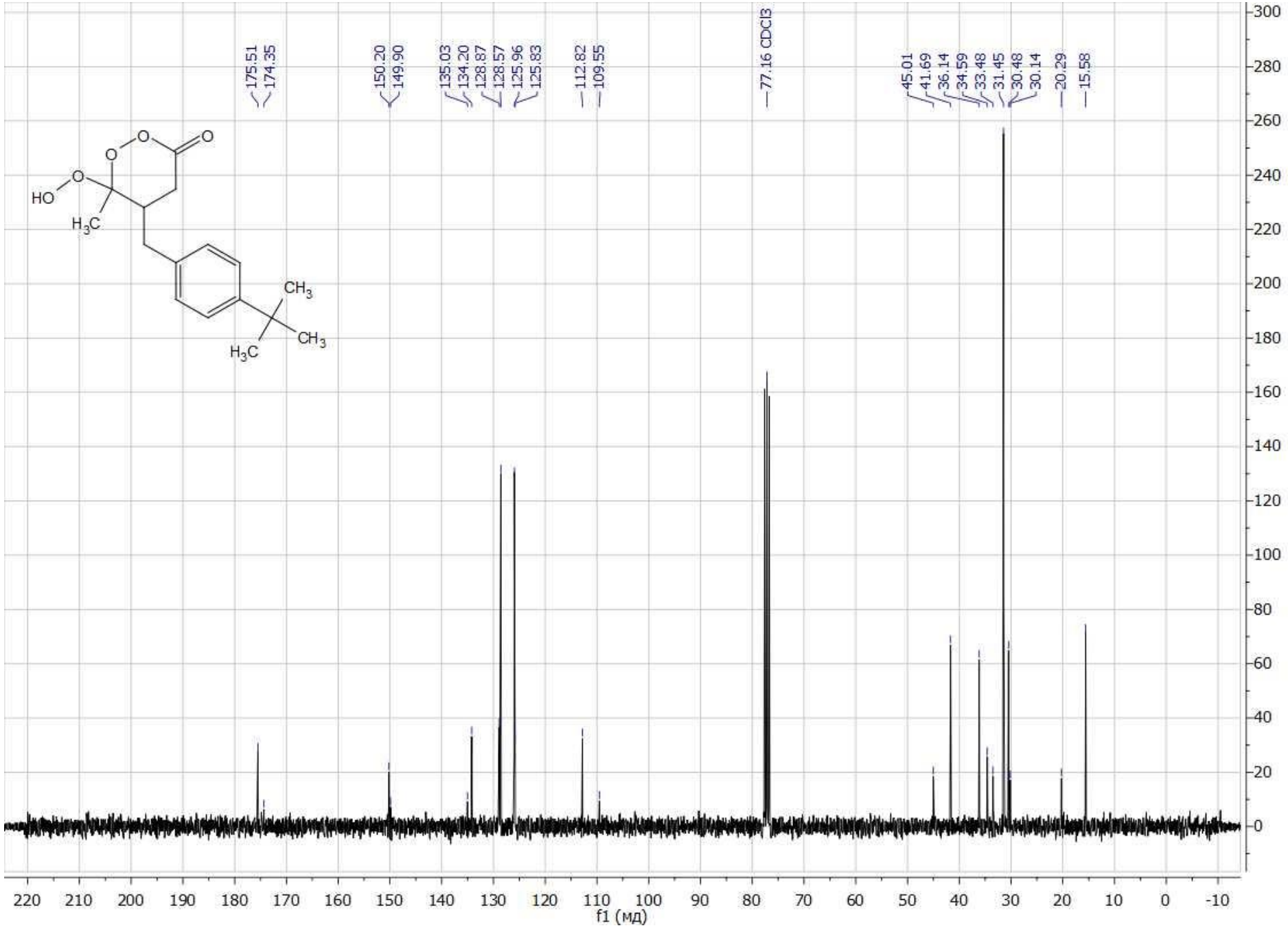
^{1}H NMR

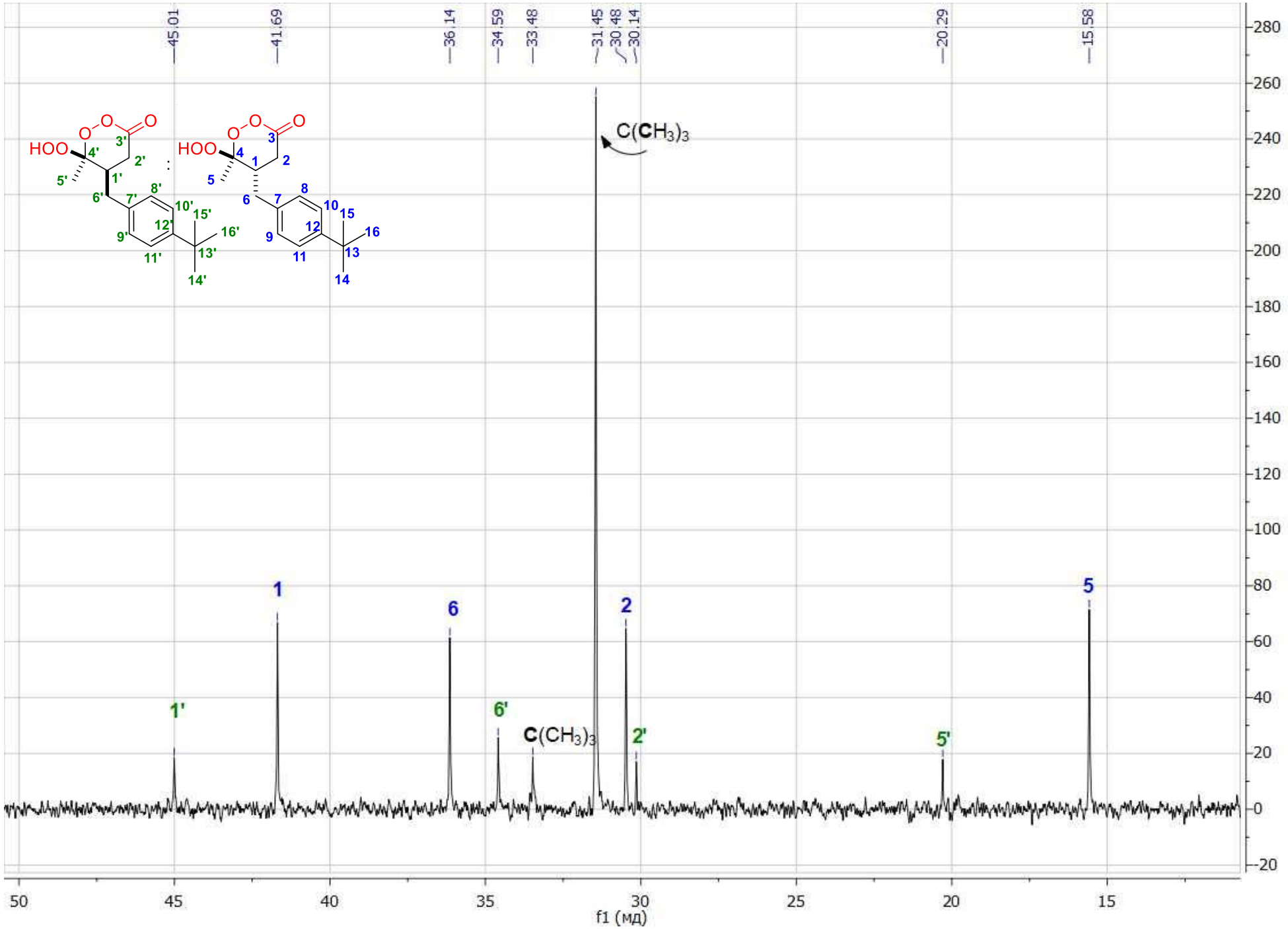


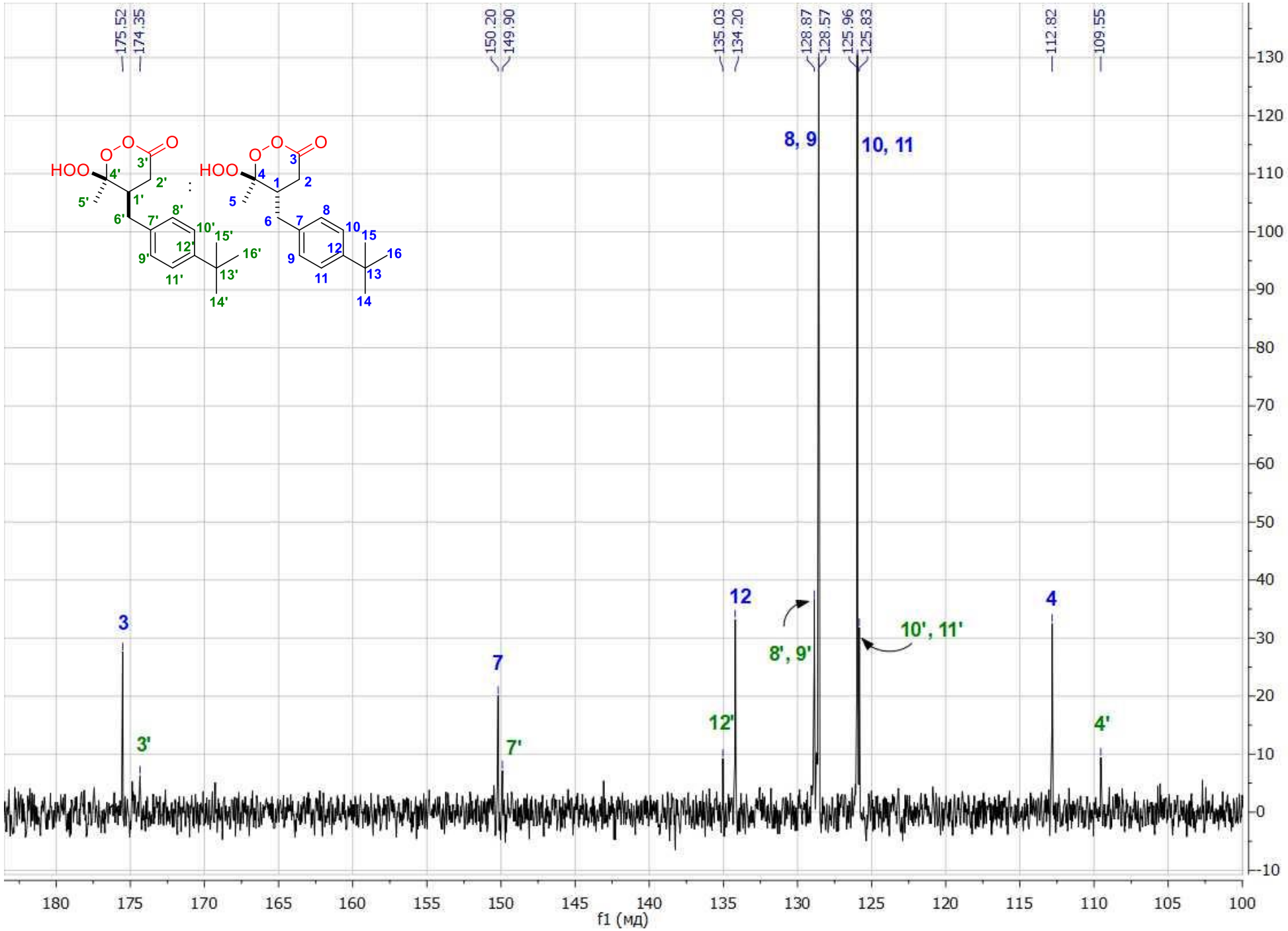

3.10 3.08 3.06 3.05 3.04 3.02 3.01 2.81 2.80 2.78 2.77 2.76 2.75 2.73 2.72 2.66 2.63 2.60 2.58 2.52 2.49 2.48 2.45 2.44 2.44 2.40 2.39 2.35 2.31 2.29 2.28 2.27 2.25 2.24 2.23 2.22 2.20
1.68 1.61
1.32 1.31
HOO
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
9'
10'
11'
12'
13'
14'
15'
16'
HOO
O
O
O
3
4
1
2
5
6
7
8
9
10
11
12
13
14
15
16
6 1H, 6' 1H
1' 1H
2' 1H
6 1H, 6' 1H, 2 2H, 2' 1H, 1 1H
5'
5
t-Bu
650 600 550 500 450 400 350 300 250 200 150 100 50 0 -50
3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1
f1 (мд)


8.63
8.51
7.35
7.32
7.26 CDCl3
7.09
7.07
7.05
HOO
HOO
10, 11
8, 9
f1 (мд)

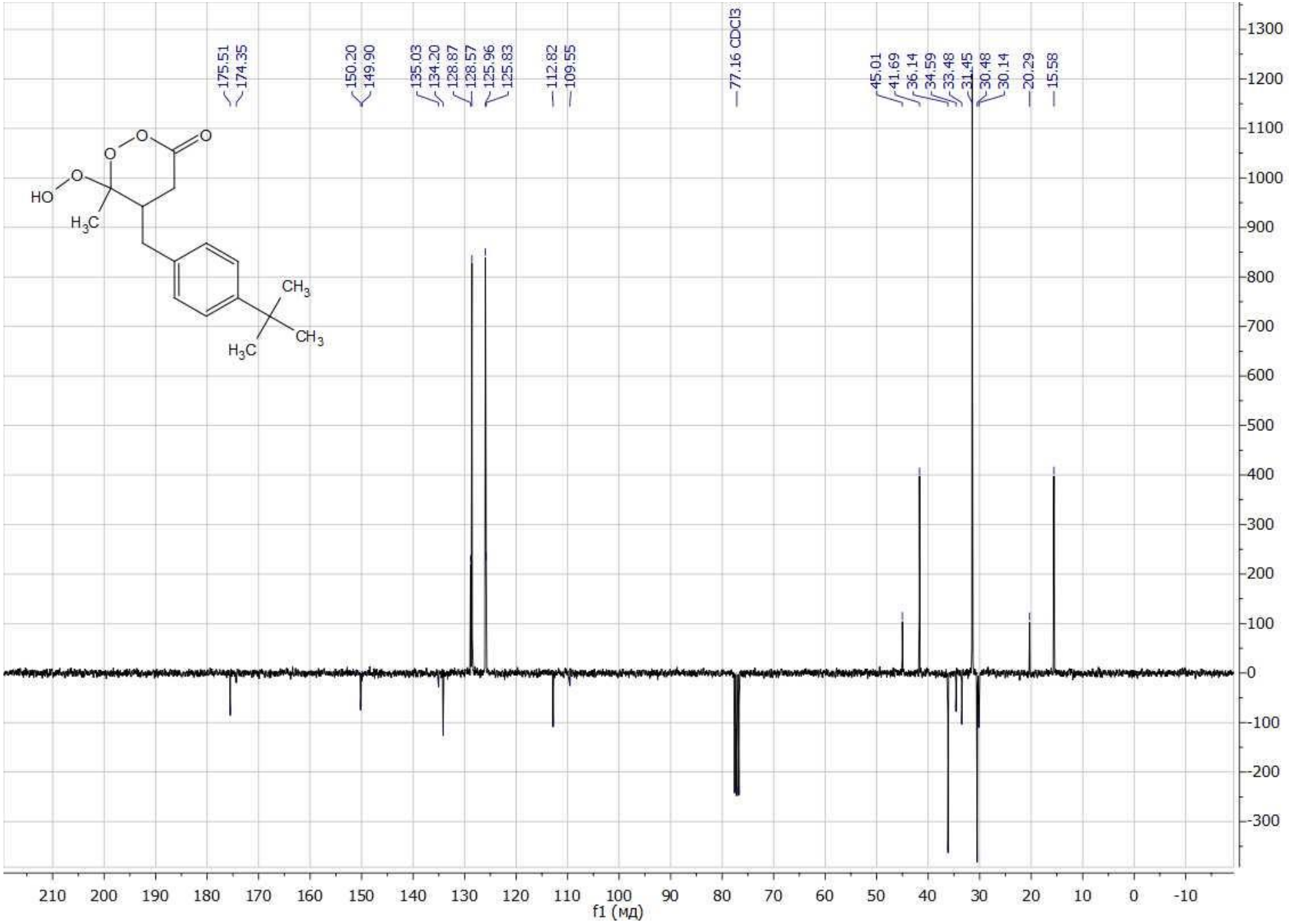
^{13}C NMR

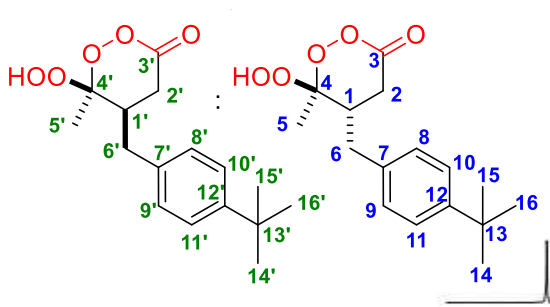

175.51
174.35
150.20
149.90
135.03
134.20
128.87
128.57
125.96
125.83
112.82
109.55
77.16 CDCl3
45.01
41.69
36.14
34.59
33.48
31.45
30.48
30.14
20.29
15.58
HO
O
O
O
O
H3C
CH3
CH3
H3C
f1 (мд)


45.01
41.69
36.14
34.59
33.48
31.45
30.48
30.14
20.29
15.58
C(CH3)3
1
6
2
5
1'
6'
C(CH3)3
2'
5'
50
45
40
35
30
25
20
15
f1 (мд)

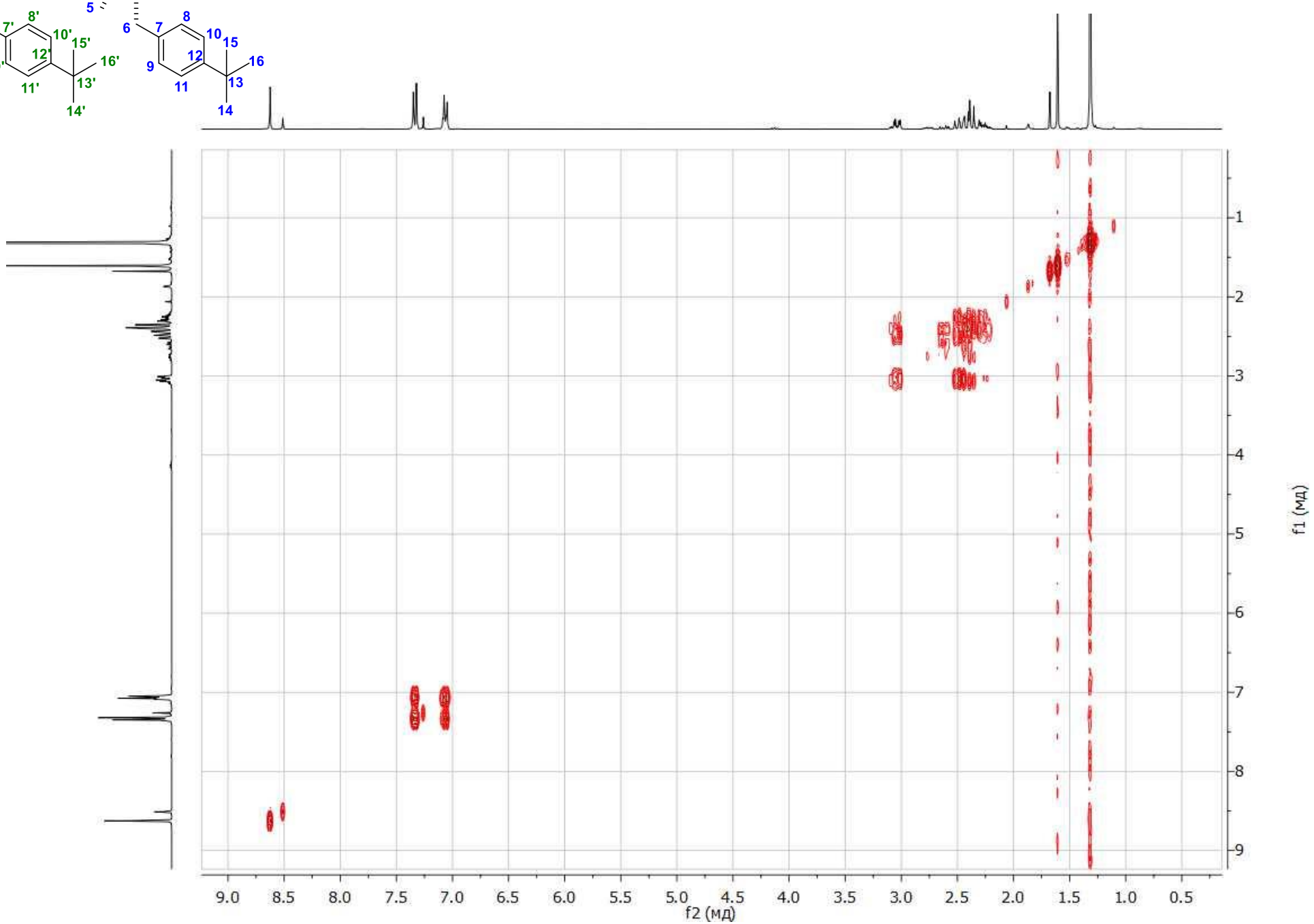

175.52
174.35
150.20
149.90
135.03
134.20
128.87
128.57
125.96
125.83
112.82
109.55
8, 9
10, 11
3
3'
7
7'
12
12'
8', 9'
10', 11'
4
4'
HOO
O
O
O
O
HOO
O
O
O
O
f1 (мд)

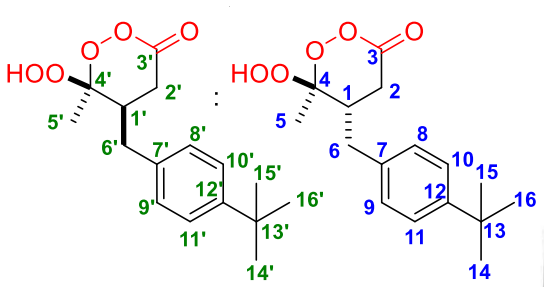
^{13}C_apt_jmod


175.51
174.35
150.20
149.90
135.03
134.20
128.87
128.57
125.96
125.83
112.82
109.55
77.16 CDCl3
45.01
41.69
36.14
34.59
33.48
31.45
30.48
30.14
20.29
15.58
HO
O
O
O
O
H3C
CH3
CH3
H3C
f1 (мд)

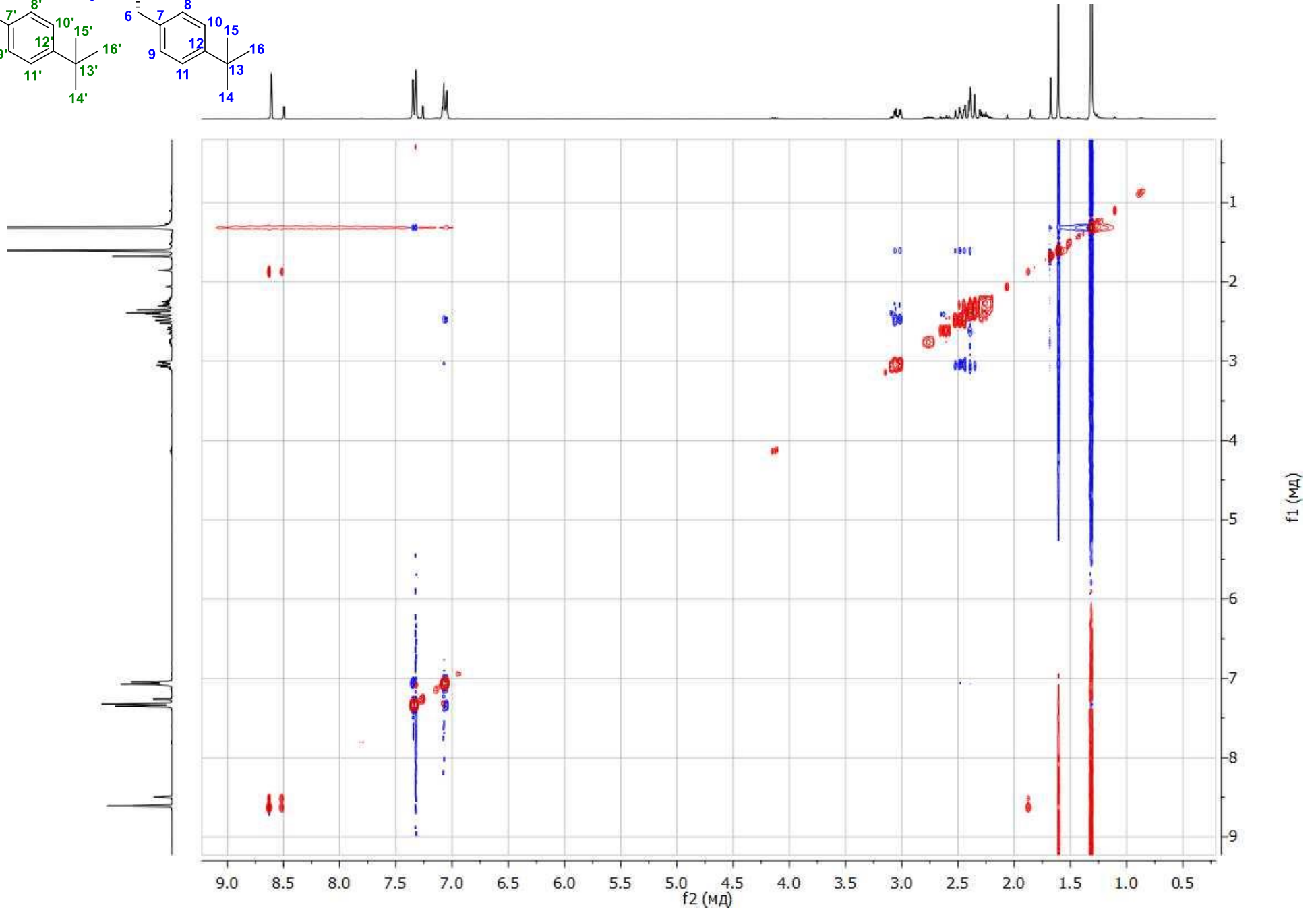

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
12'
15'
16'
9'
11'
13'
14'
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
15
16
9
11
13
14

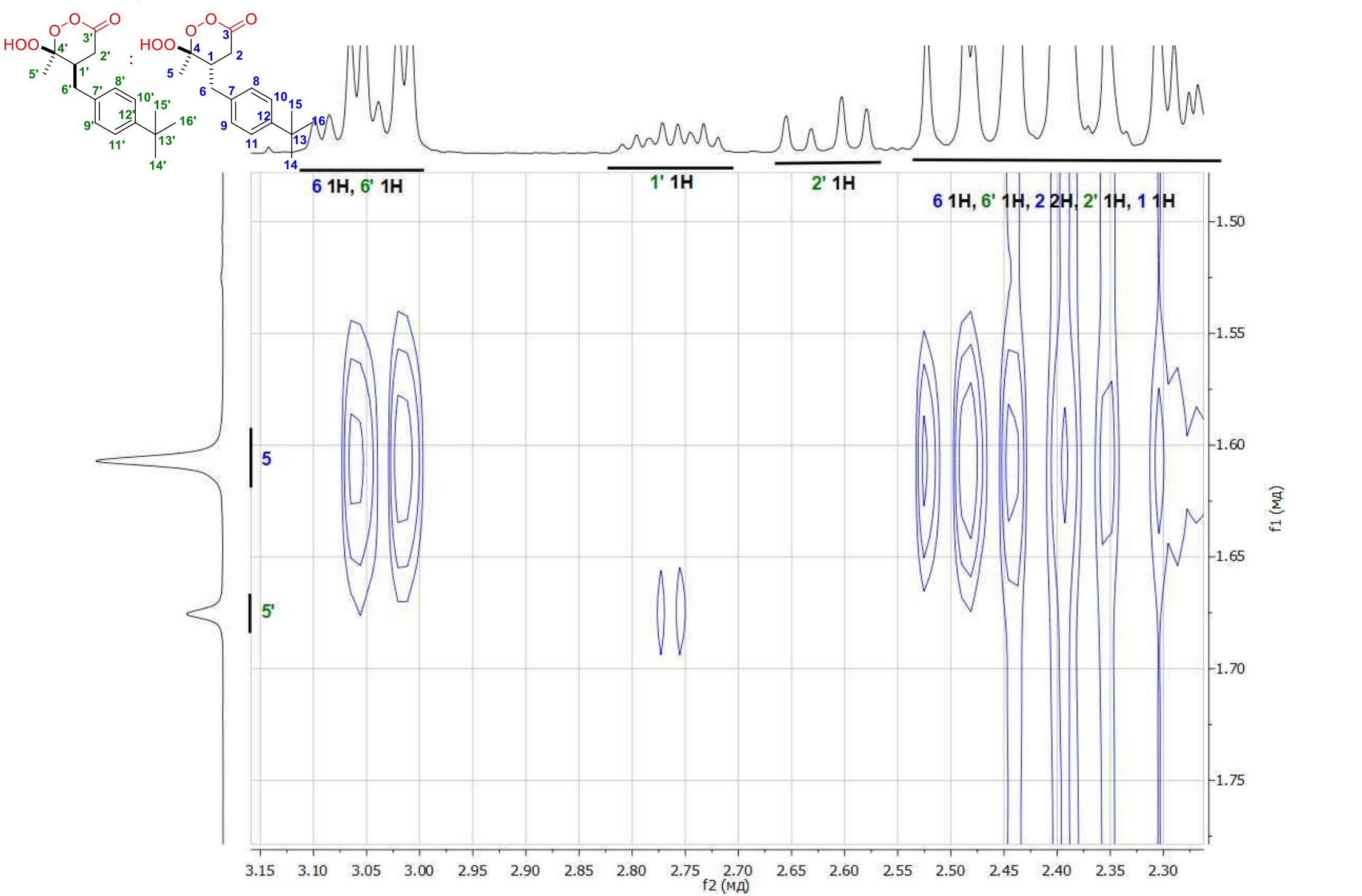
{^{1}H-^{1}H} COSY

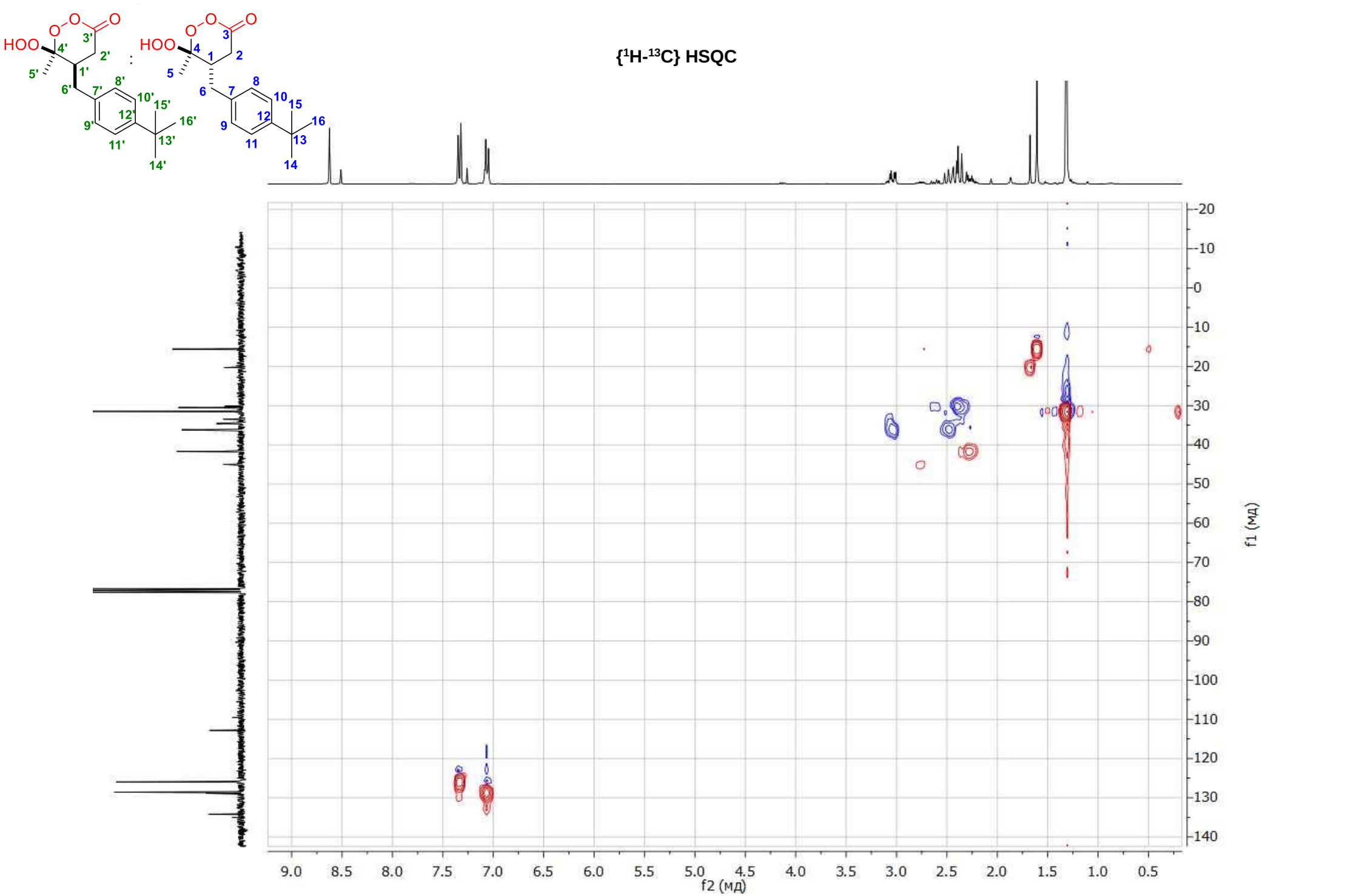

9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (мд)
1
2
3
4
5
6
7
8
9
f1 (мд)

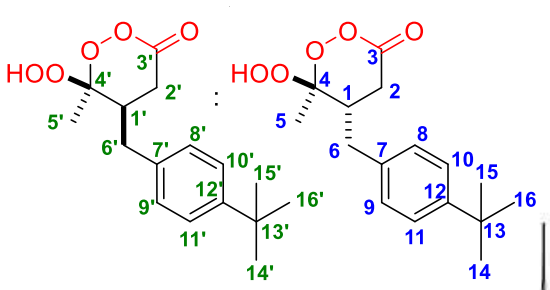

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
15'
16'
12'
9'
11'
13'
14'
:
HOO
O
O
O
3
4
2
1
5
6
7
8
10
15
16
12
9
11
13
14

{^{1}H-^{1}H} NOESY

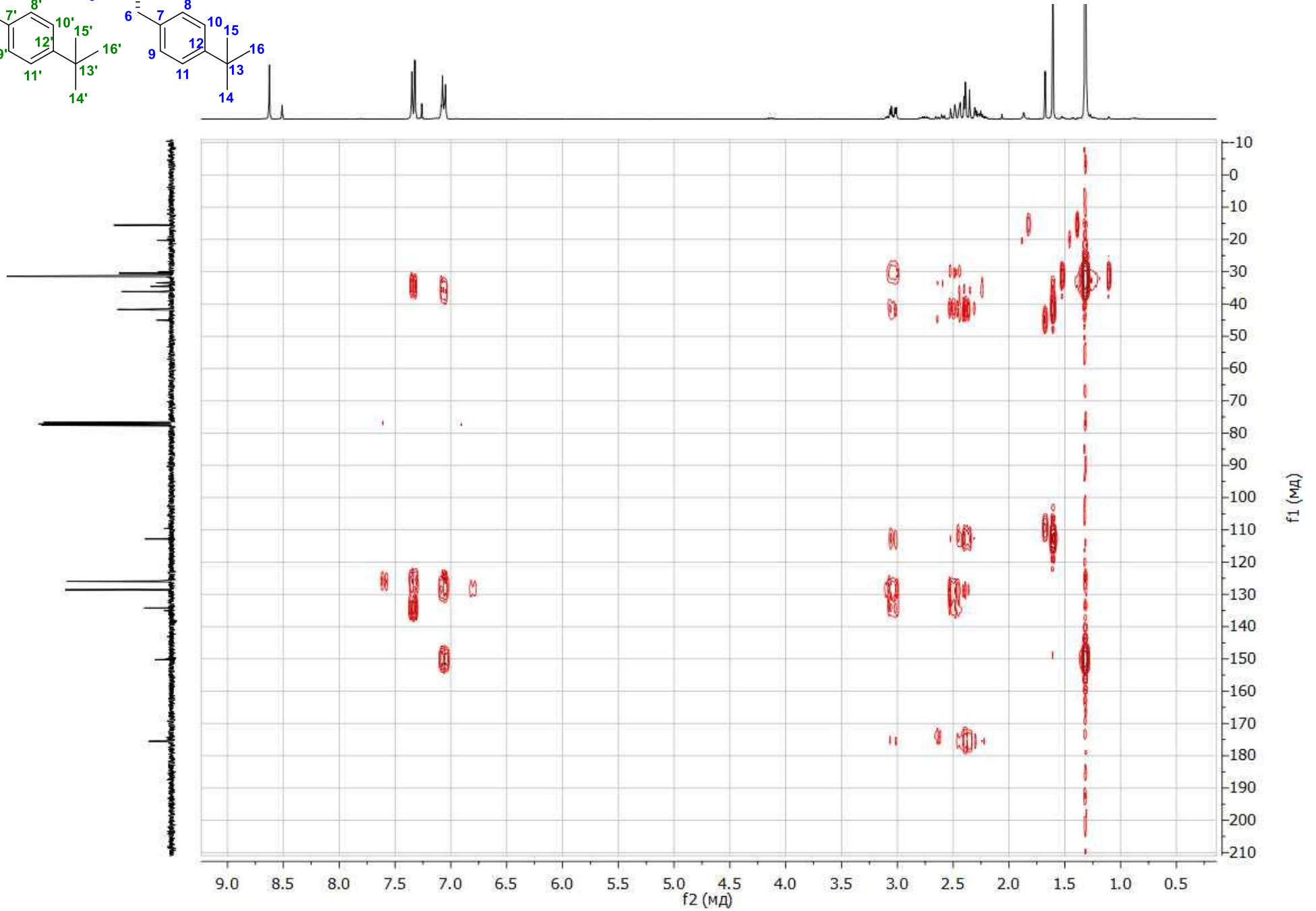

9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (мд)
1
2
3
4
5
6
7
8
9
f1 (мд)


6 1H, 6' 1H
1' 1H
2' 1H
6 1H, 6' 1H, 2 2H, 2' 1H, 1 1H
5
5'
1.50
1.55
1.60
1.65
1.70
1.75
f1 (мд)
3.15
3.10
3.05
3.00
2.95
2.90
2.85
2.80
2.75
2.70
2.65
2.60
2.55
2.50
2.45
2.40
2.35
2.30
f2 (мд)


{1H-13C} HSQC
HOO
O
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
9'
10'
11'
12'
13'
14'
15'
16'
HOO
O
O
O
3
4
2
1
5
6
7
8
9
10
11
12
13
14
15
16
f2 (мд)
f1 (мд)

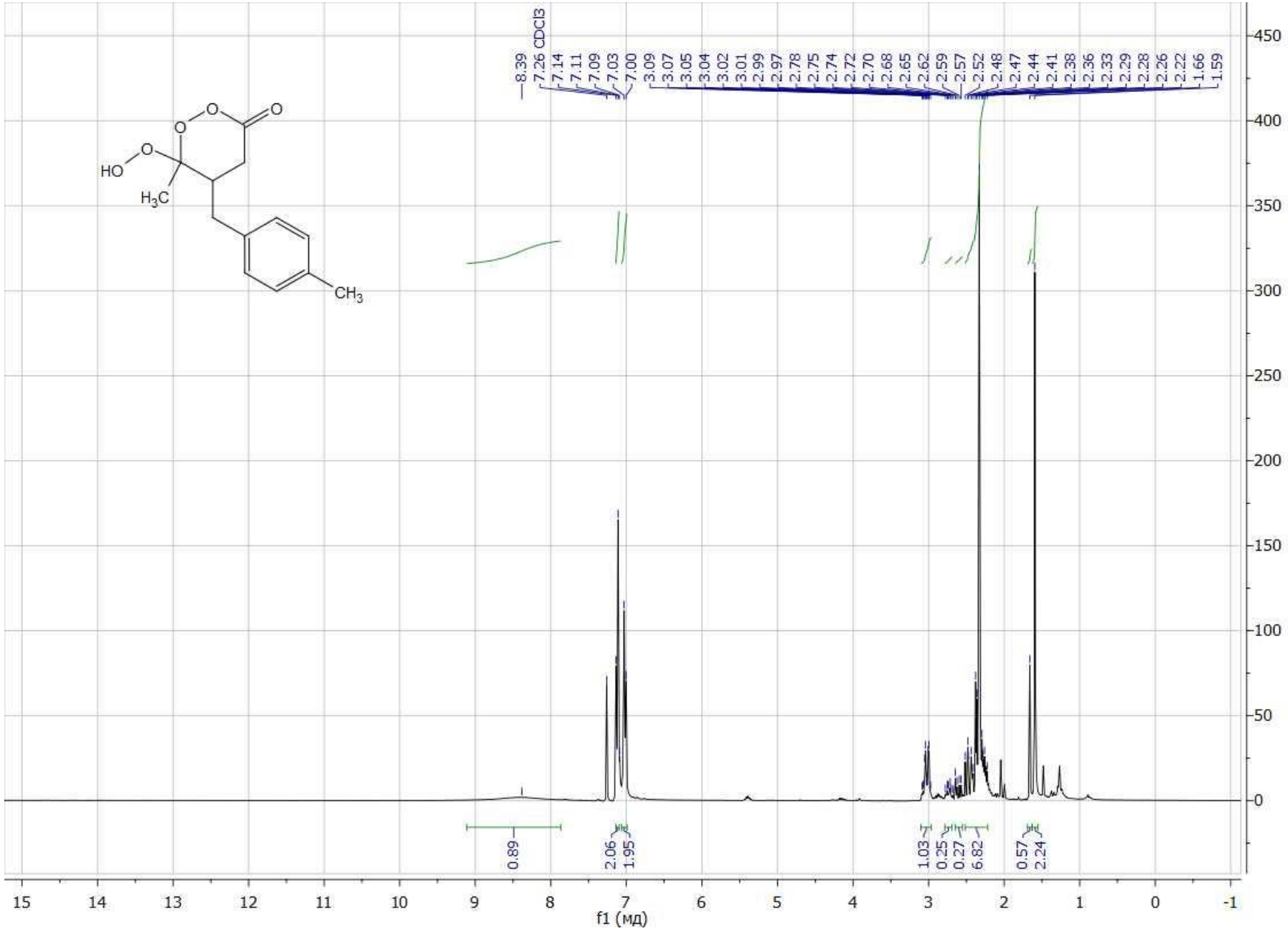

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
10'
11'
12'
13'
14'
15'
16'
:
HOO
O
O
O
3
4
2
1
5
6
7
8
9
10
11
12
13
14
15
16

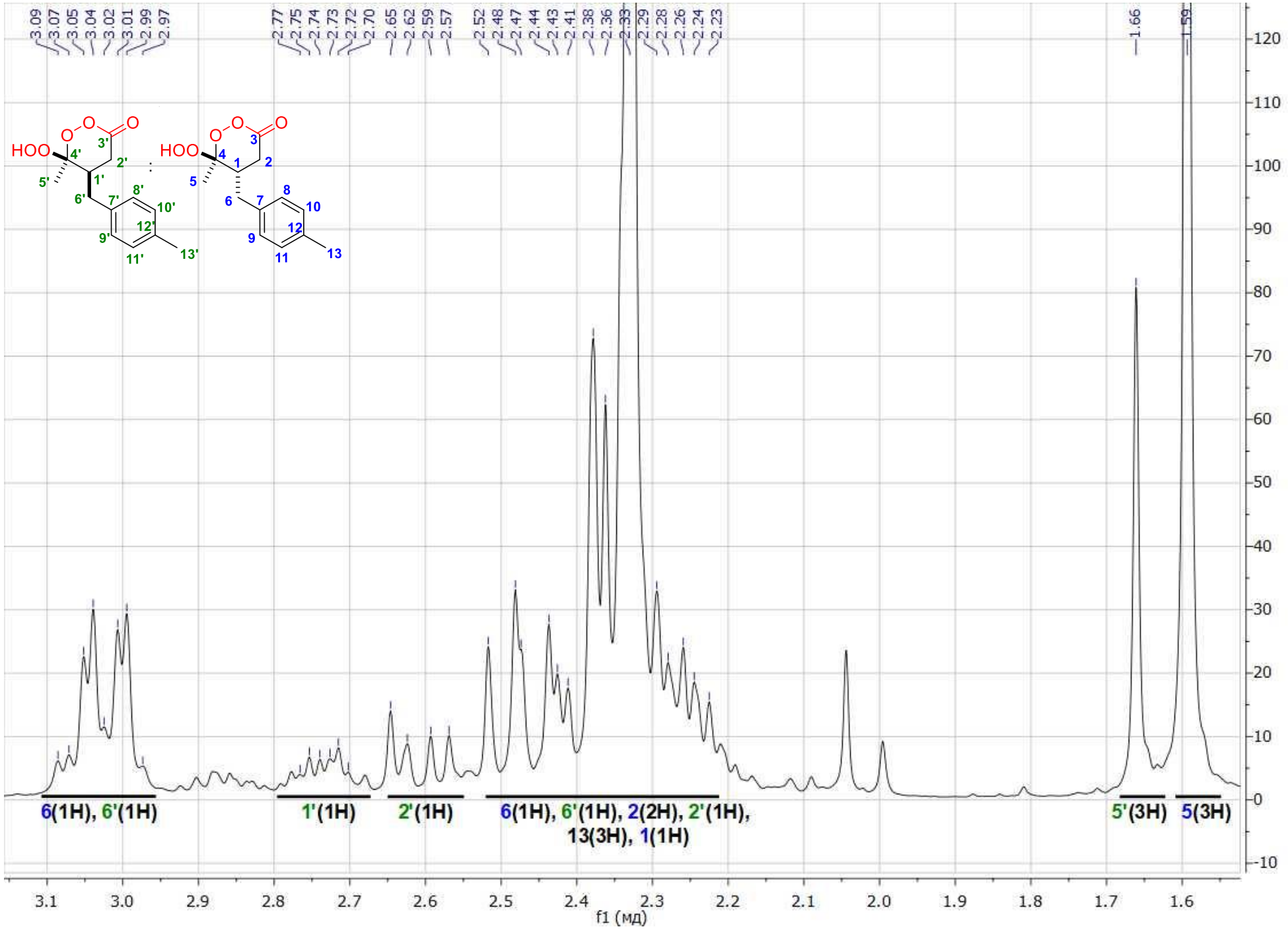
{^{1}H-^{13}C} HMBC

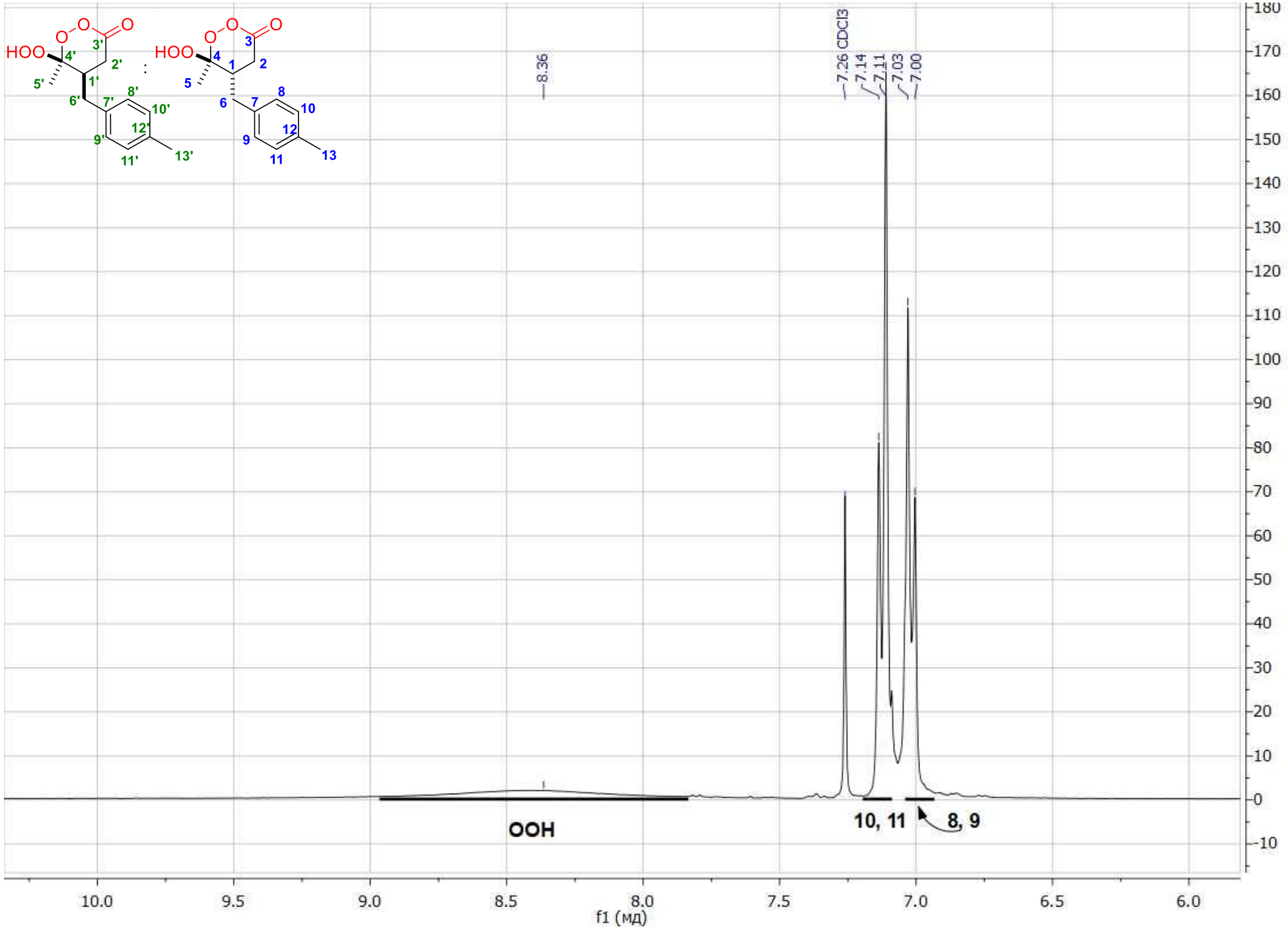

f2 (мд)
f1 (мд)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210

6-Hydroperoxy-6-methyl-5-(4-methylbenzyl)-1,2-dioxan-3-one, 2f

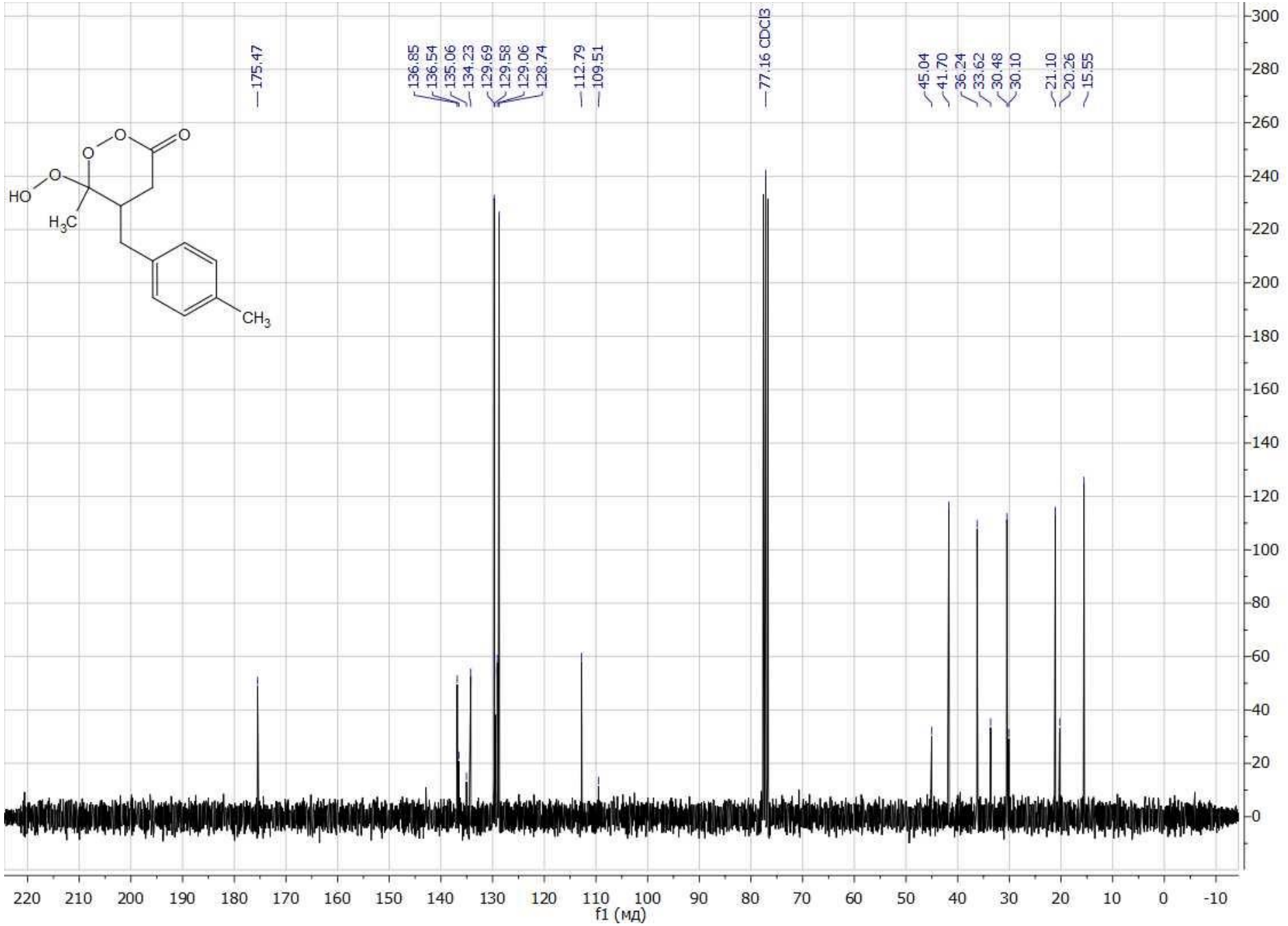
^{1}H NMR

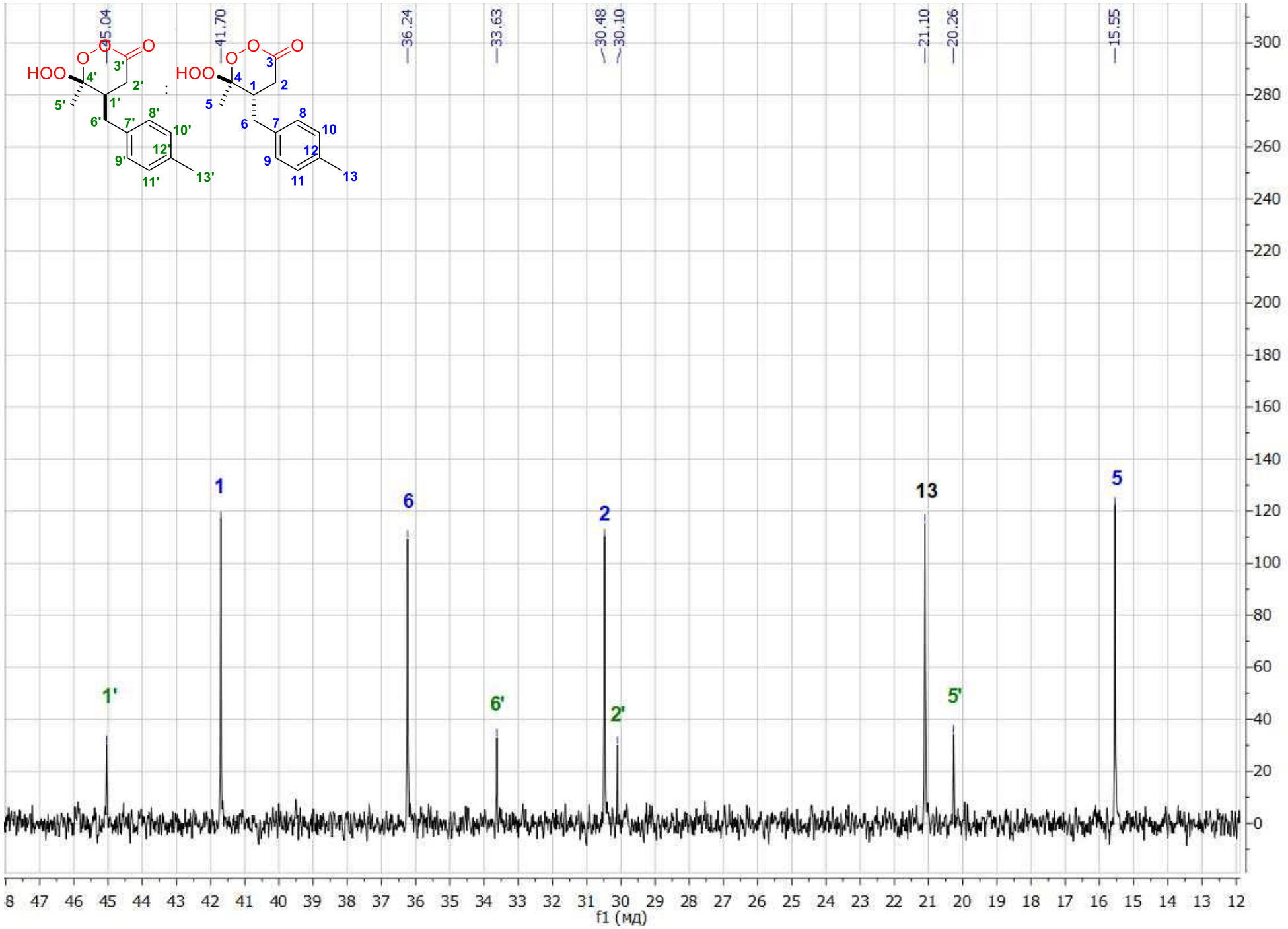


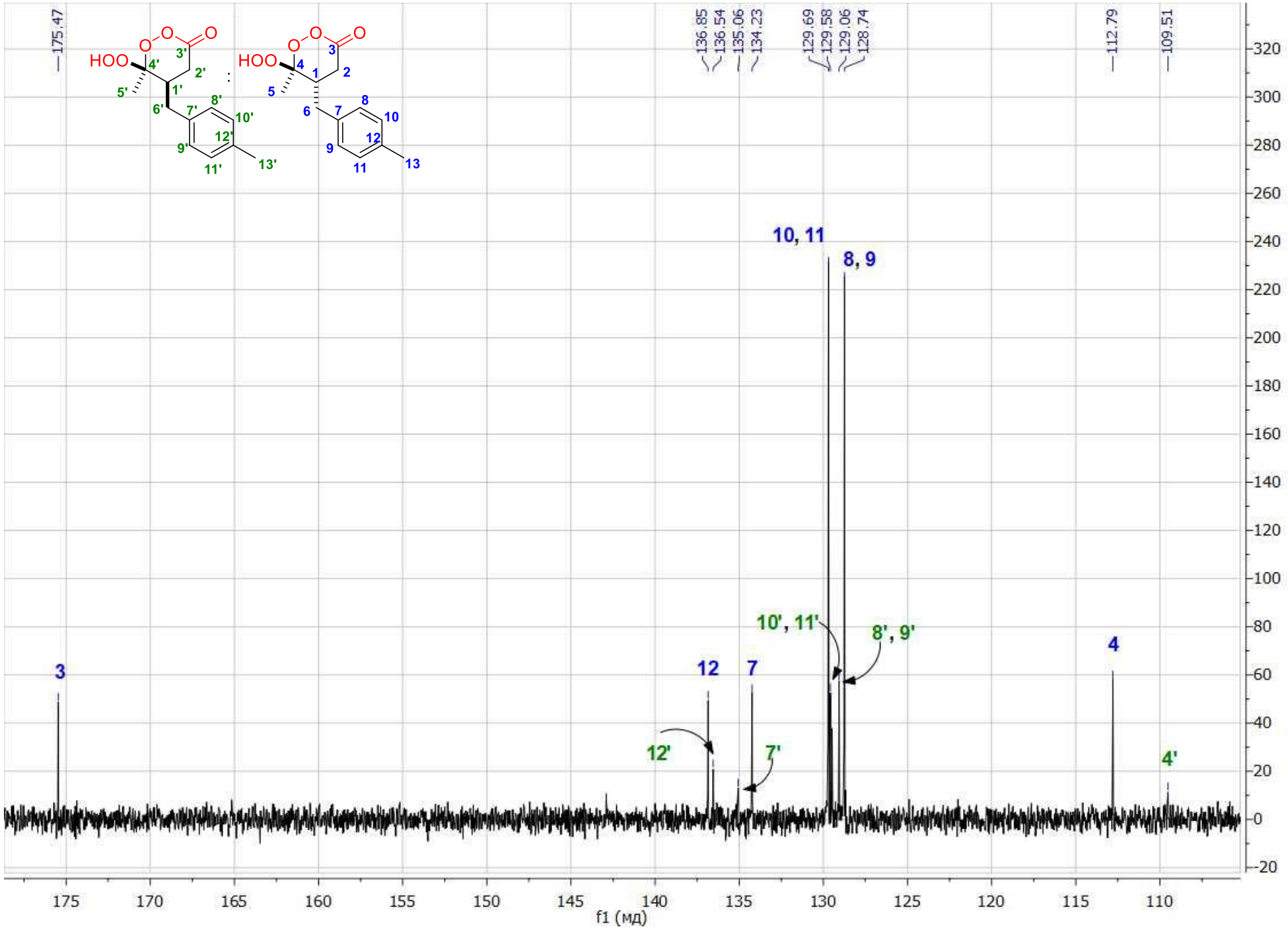

3.09 3.07 3.05 3.04 3.02 3.01 2.99 2.97
2.77 2.75 2.74 2.73 2.72 2.70 2.65 2.62 2.59 2.57 2.52 2.48 2.47 2.44 2.43 2.41 2.38 2.36 2.33 2.29 2.28 2.26 2.24 2.23
1.66 1.59
HOO
HOO
6(1H), 6'(1H)
1'(1H)
2'(1H)
6(1H), 6'(1H), 2(2H), 2'(1H), 13(3H), 1(1H)
5'(3H)
5(3H)
f1 (мд)


8.36
7.26 CDCl3
7.14
7.11
7.03
7.00
OOH
10, 11
8, 9
f1 (мд)

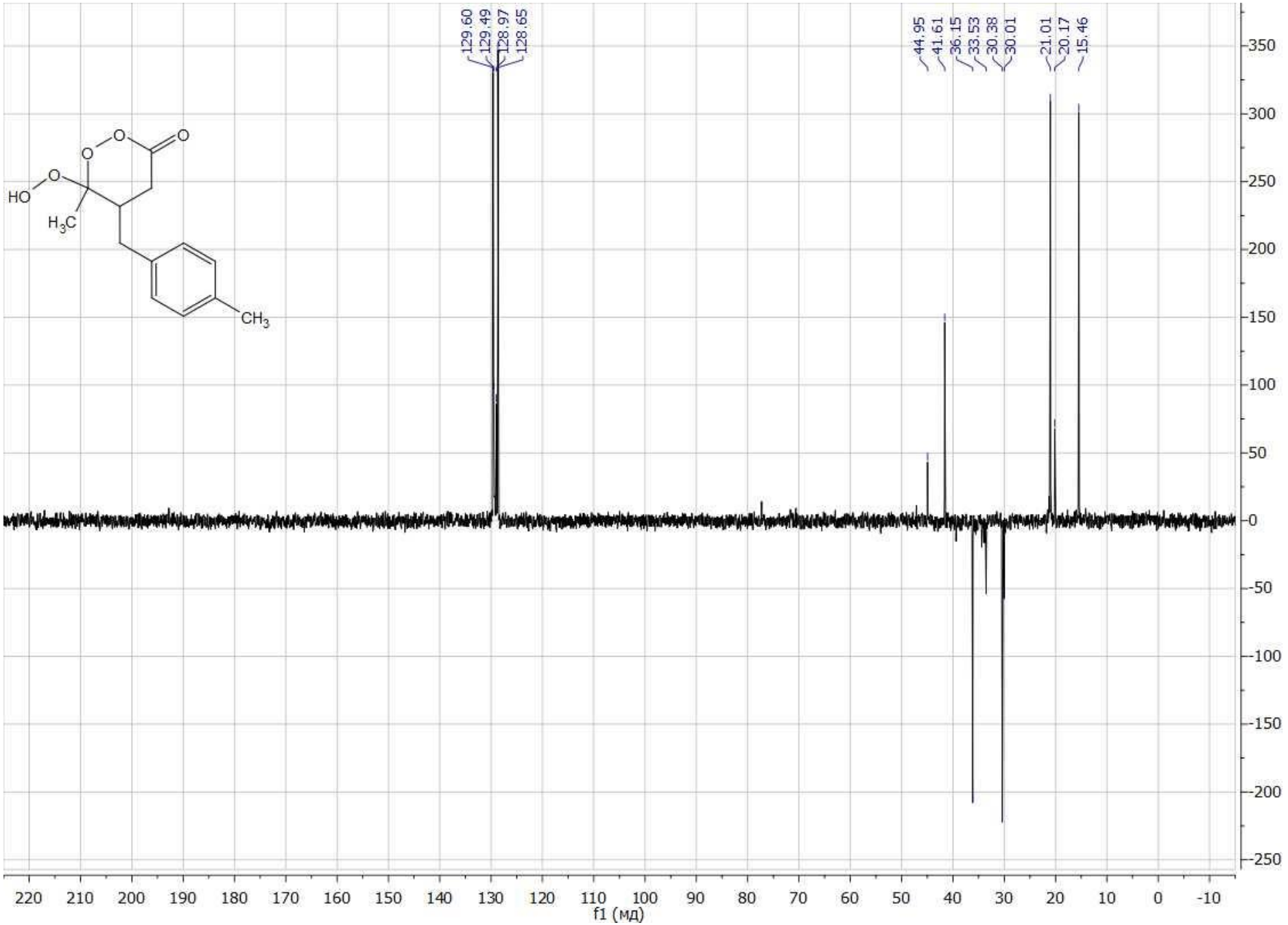
^{13}C NMR

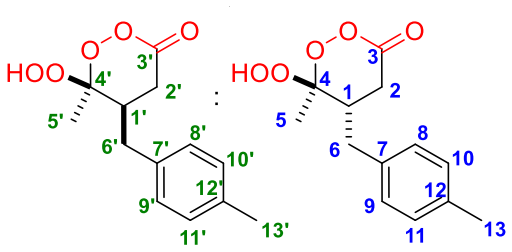

175.47
136.85
136.54
135.06
134.23
129.69
129.58
129.06
128.74
112.79
109.51
77.16 CDCl3
45.04
41.70
36.24
33.62
30.48
30.10
21.10
20.26
15.55
HO
O
O
O
O
H3C
CH3
f1 (мд)


HOO
O
O
O
HOO
O
O
O
45.04
41.70
36.24
33.63
30.48
30.10
21.10
20.26
15.55
1
6
2
13
5
1'
6'
2'
5'
f1 (мд)

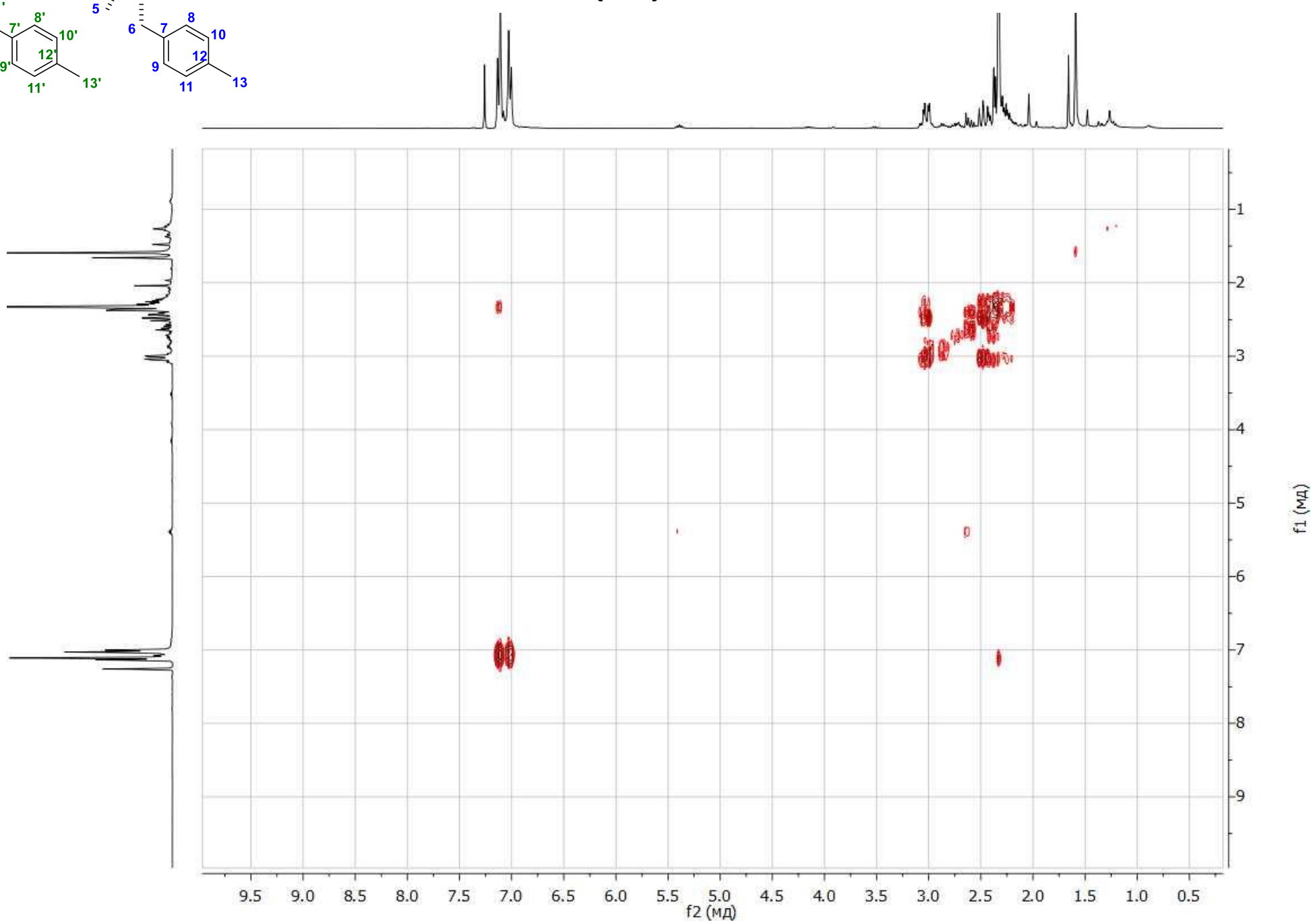

175.47
136.85
136.54
135.06
134.23
129.69
129.58
129.06
128.74
112.79
109.51
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
12'
9'
11'
13'
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
13
10, 11
8, 9
10', 11'
8', 9'
3
12
7
4
12'
7'
4'
320
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
175
170
165
160
155
150
145
140
135
130
125
120
115
110
f1 (мд)

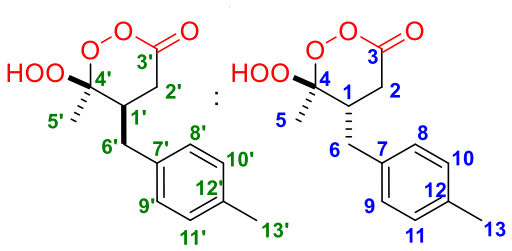
^{13}C_deptsp135



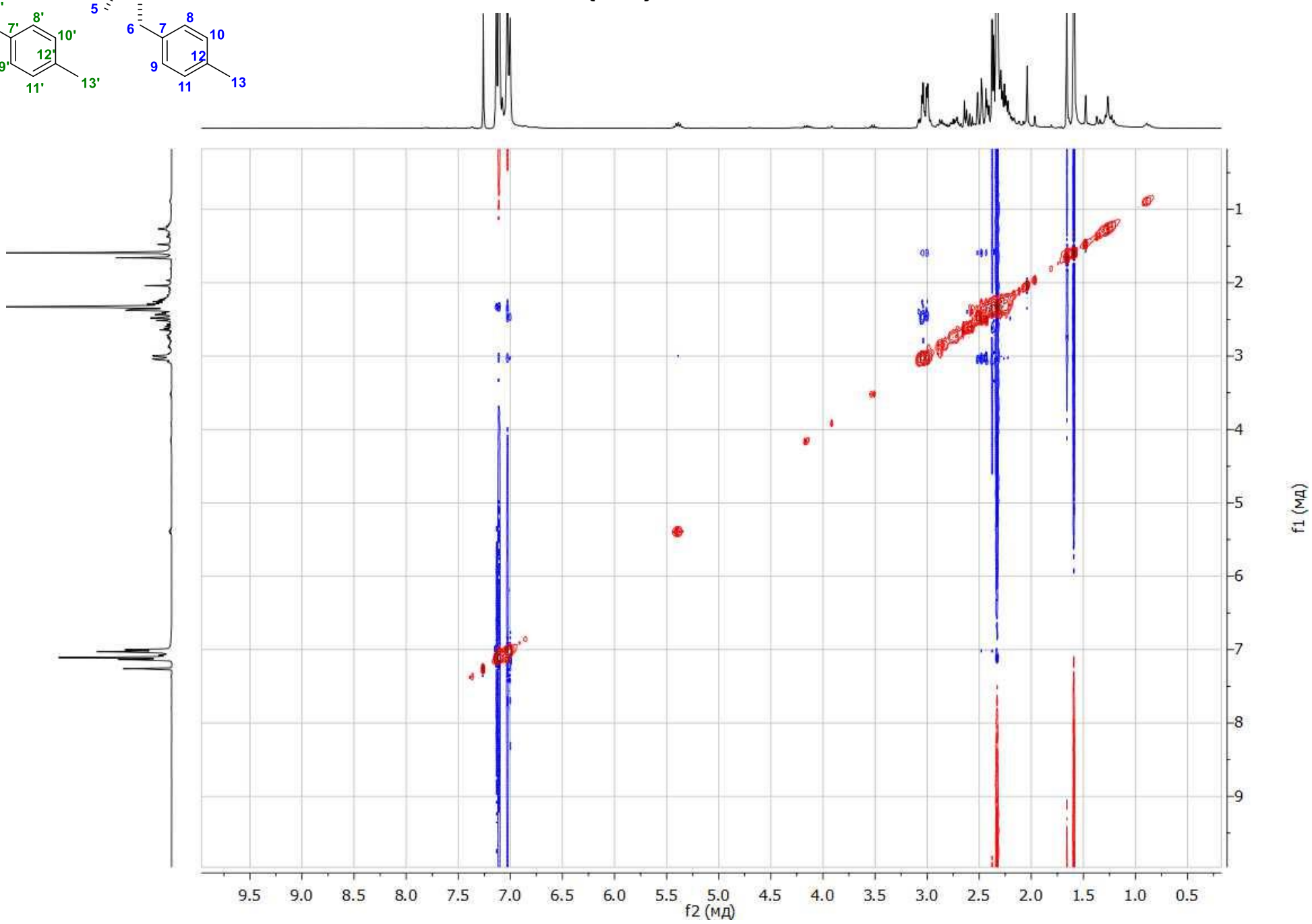

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
12'
9'
11'
13'
:
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
13

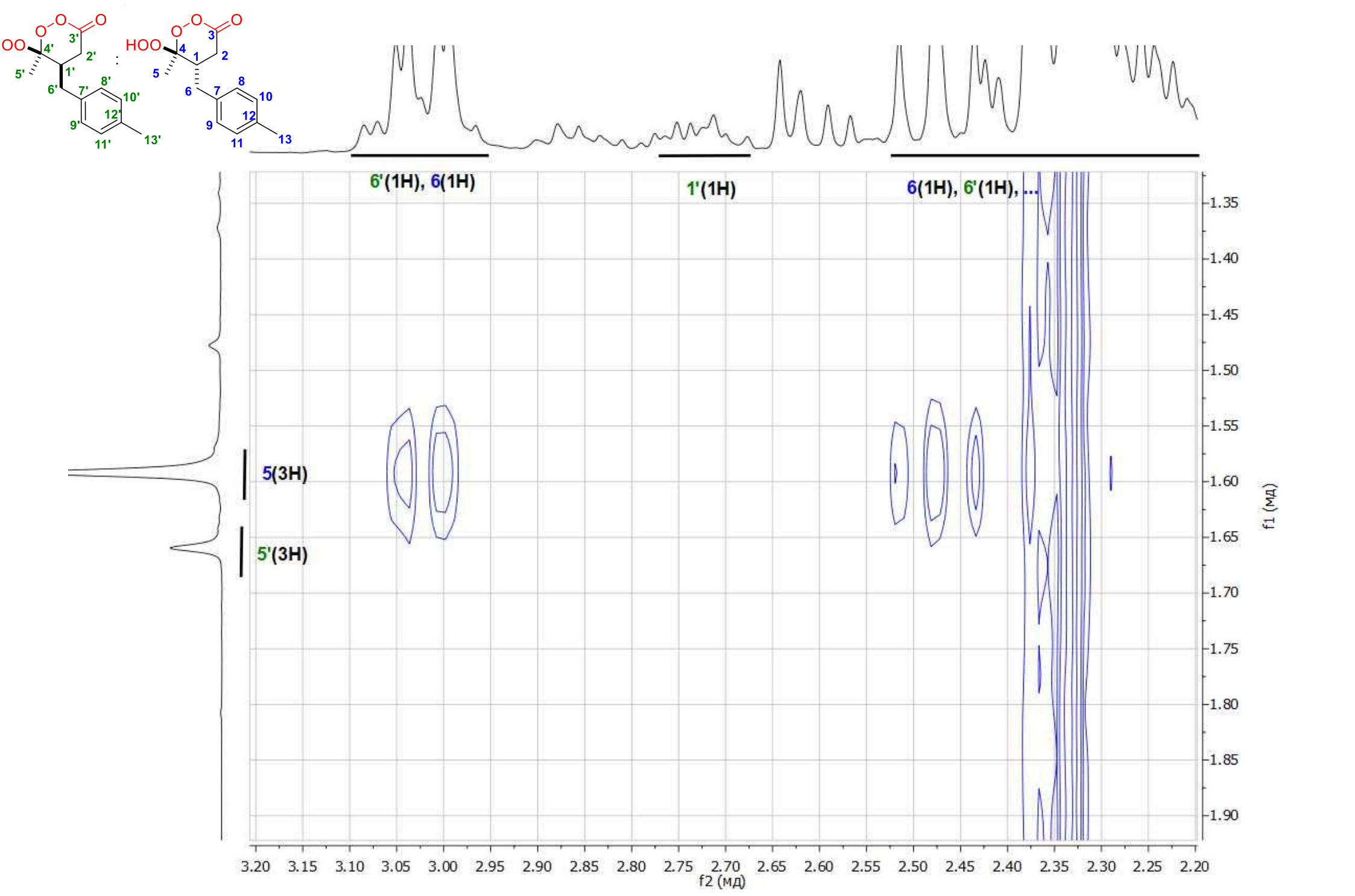
{^{1}H-^{1}H} COSY

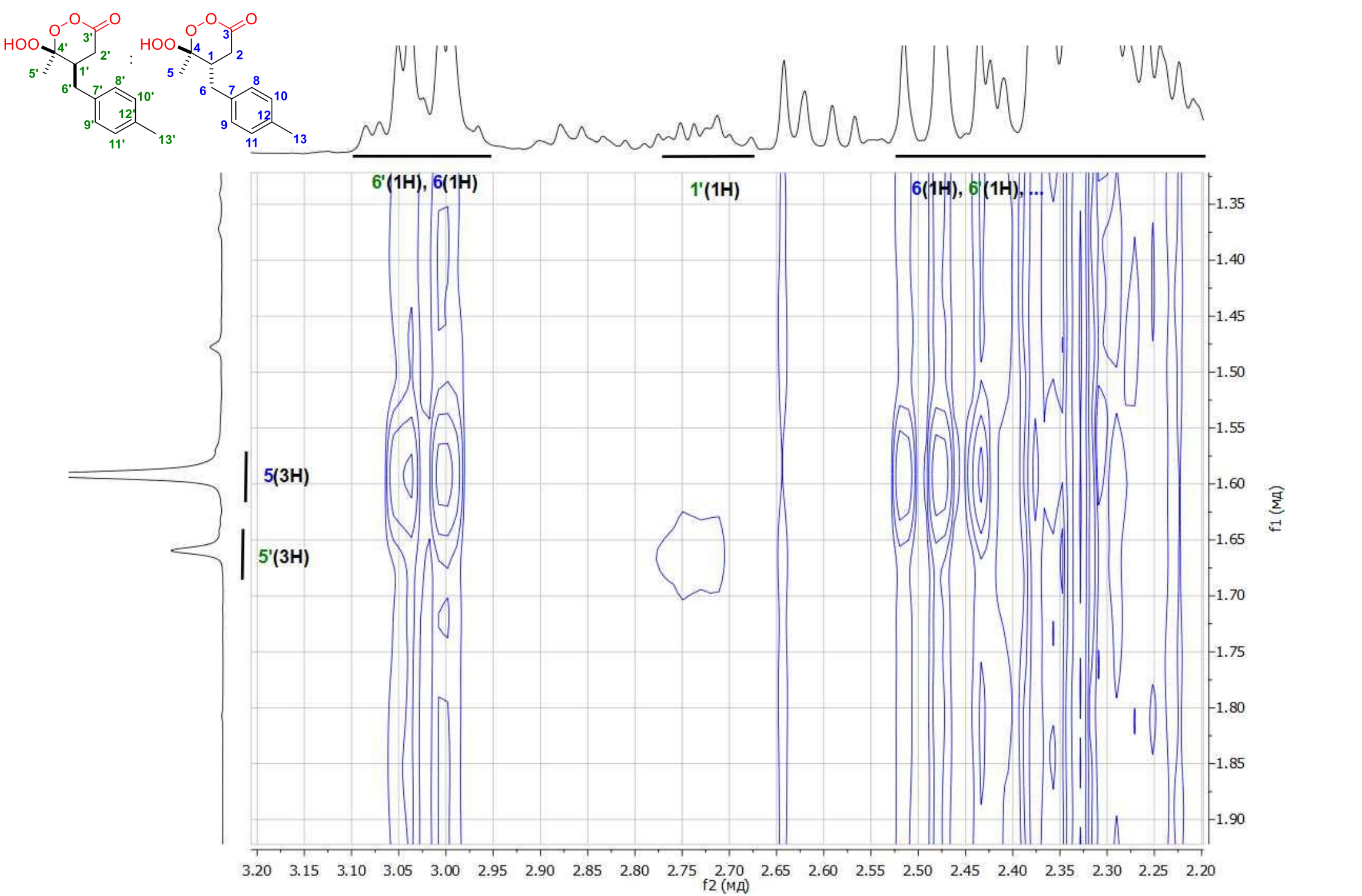

f1 (мд)
f2 (мд)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
1
2
3
4
5
6
7
8
9

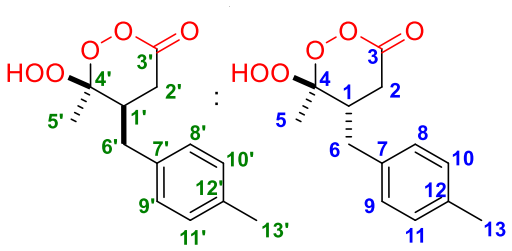

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
13'
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
13

{^{1}H-^{1}H} NOESY

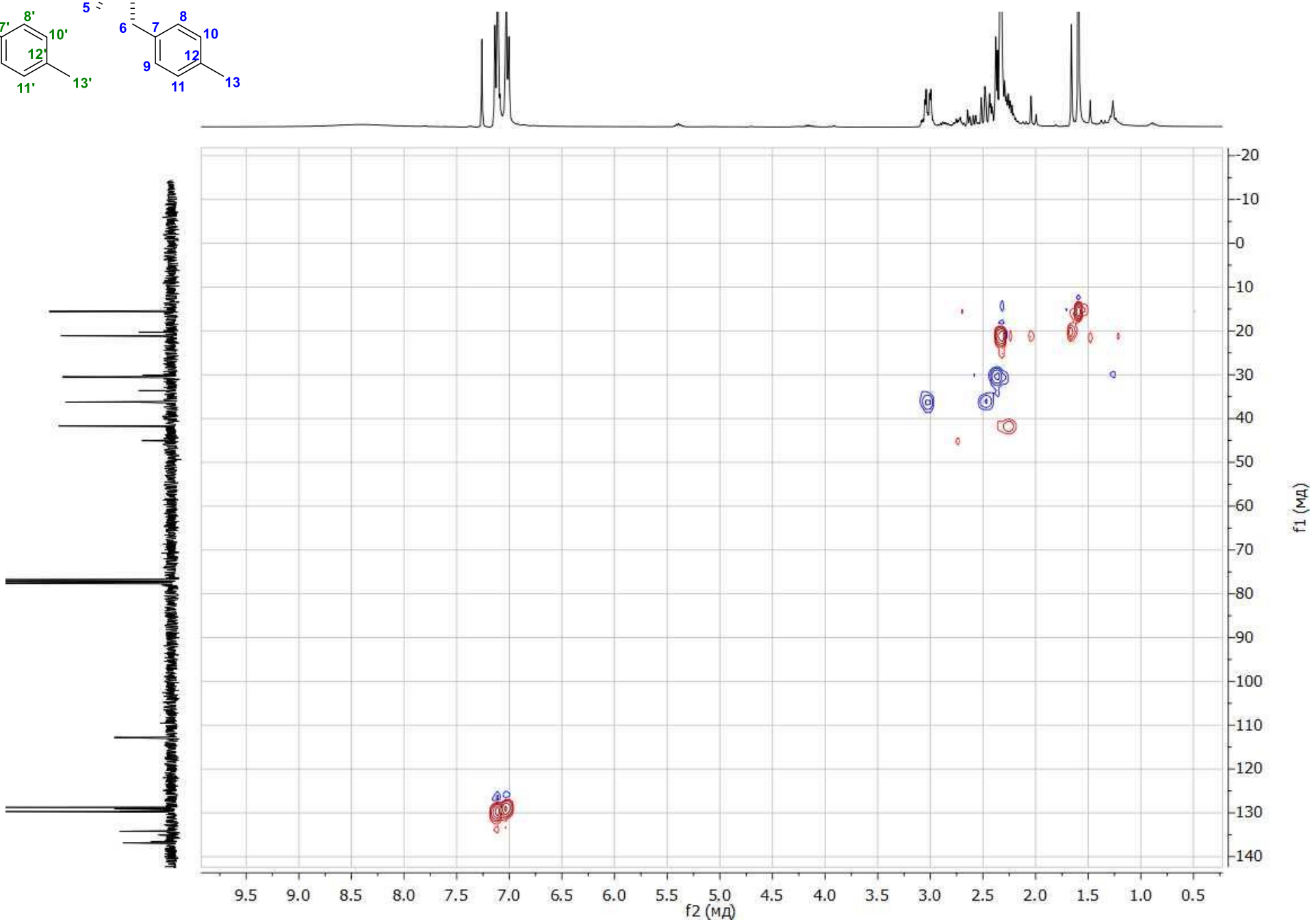

9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (мд)
1
2
3
4
5
6
7
8
9
f1 (мд)

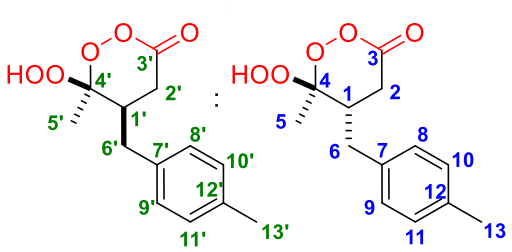

6'(1H), 6(1H)
1'(1H)
6(1H), 6'(1H), ...
5(3H)
5'(3H)
f2 (мд)
f1 (мд)


6'(1H), 6(1H)
1'(1H)
6(1H), 6'(1H), ...
5(3H)
5'(3H)
f2 (мд)
f1 (мд)

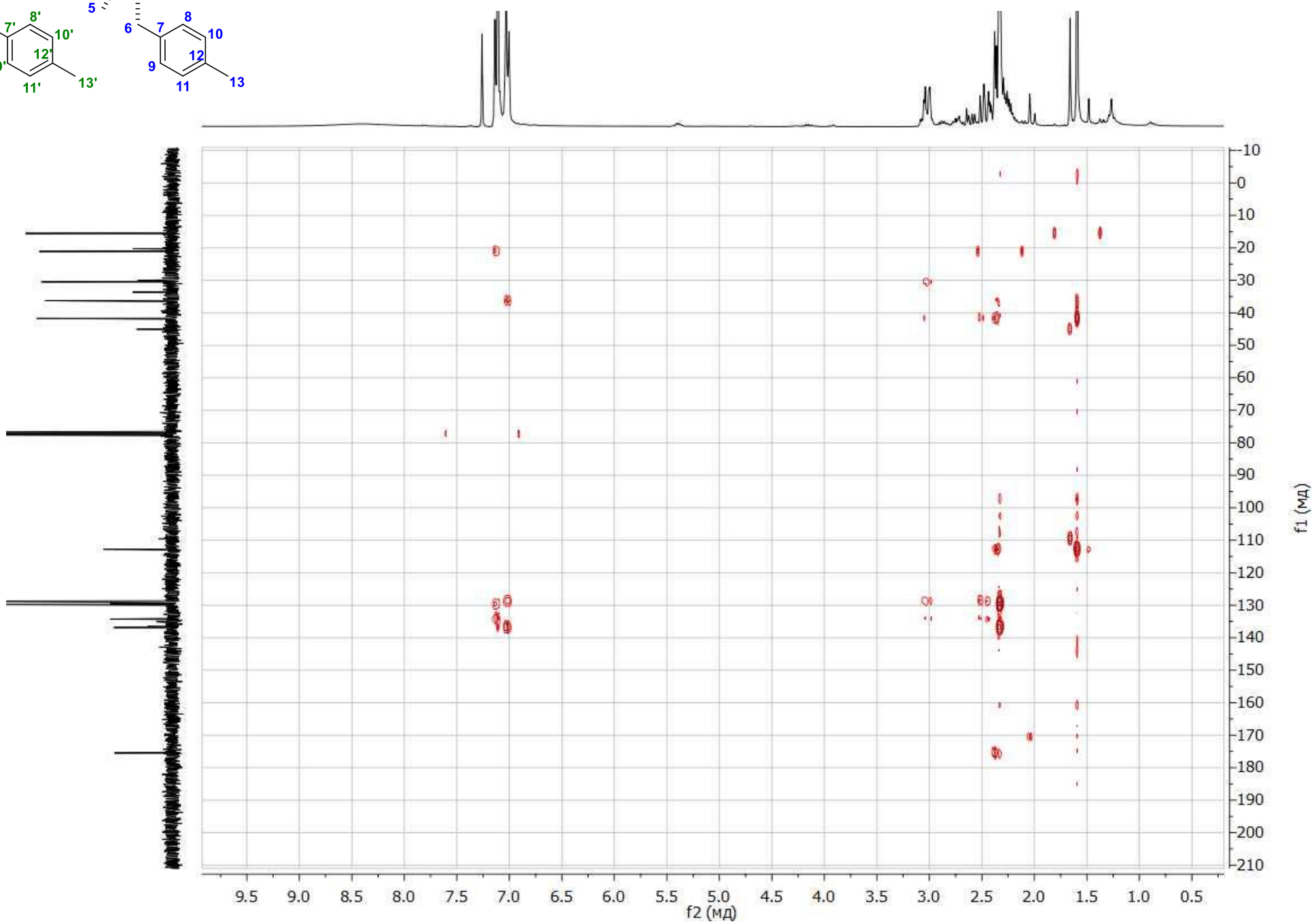

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
12'
9'
11'
13'
:
HOO
O
O
O
3
4
1
2
5
6
7
8
10
12
9
11
13

{^{1}H-^{13}C} HSQC


-20
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
f1 (мд)
9.5
9.0
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
f2 (мд)

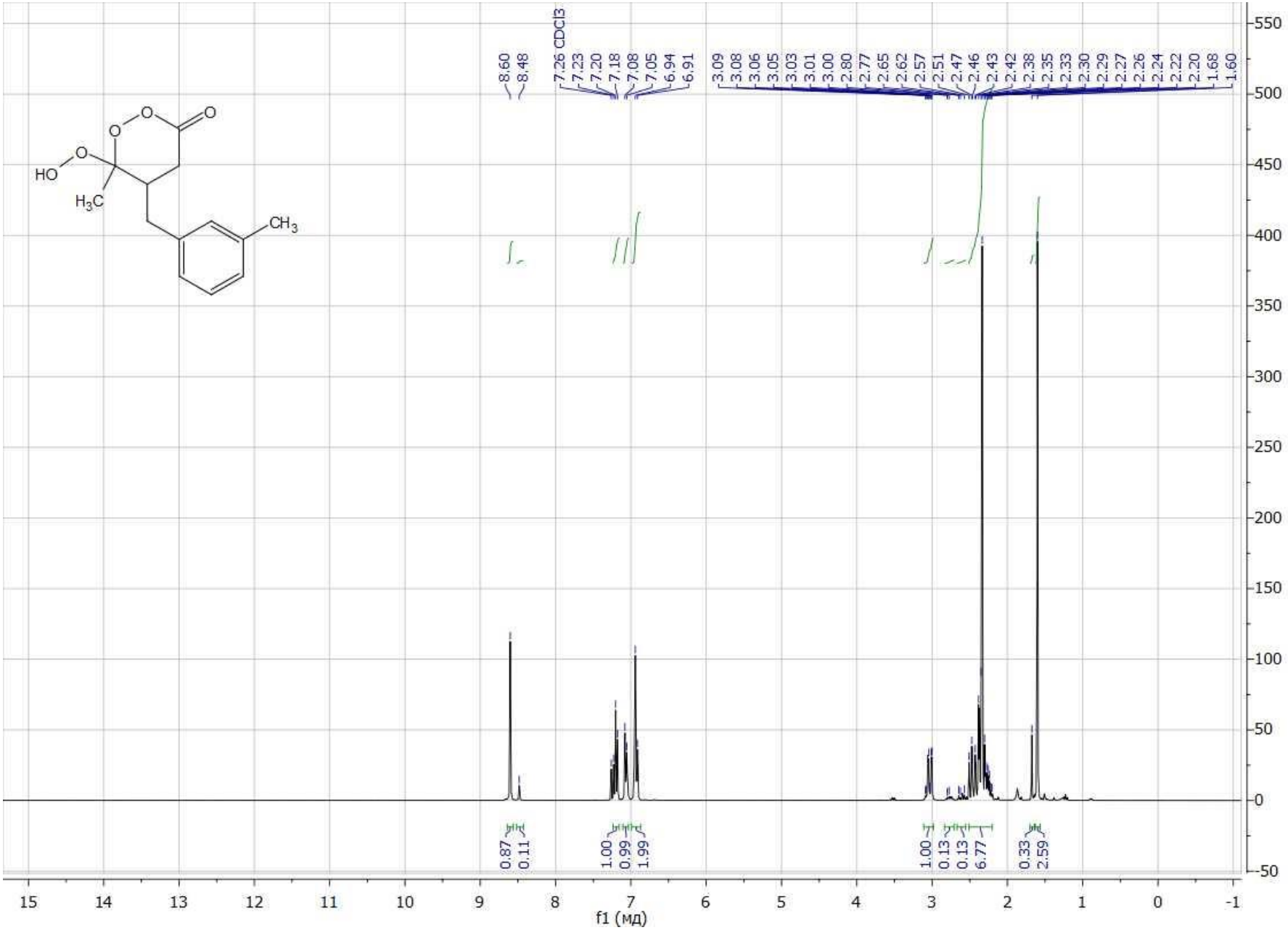

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
13'
:
HOO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
13

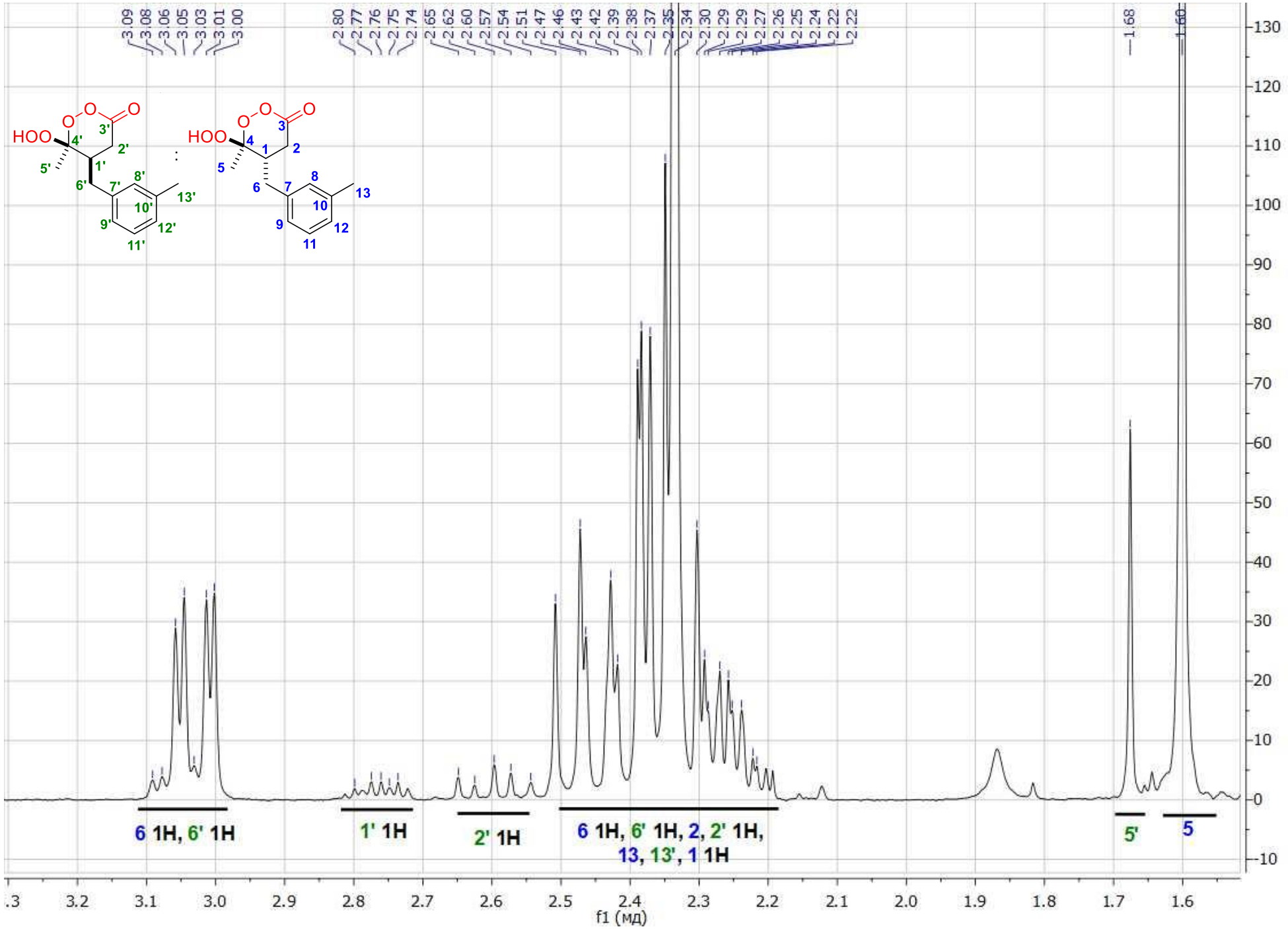
{^{1}H-^{13}C} HMBC

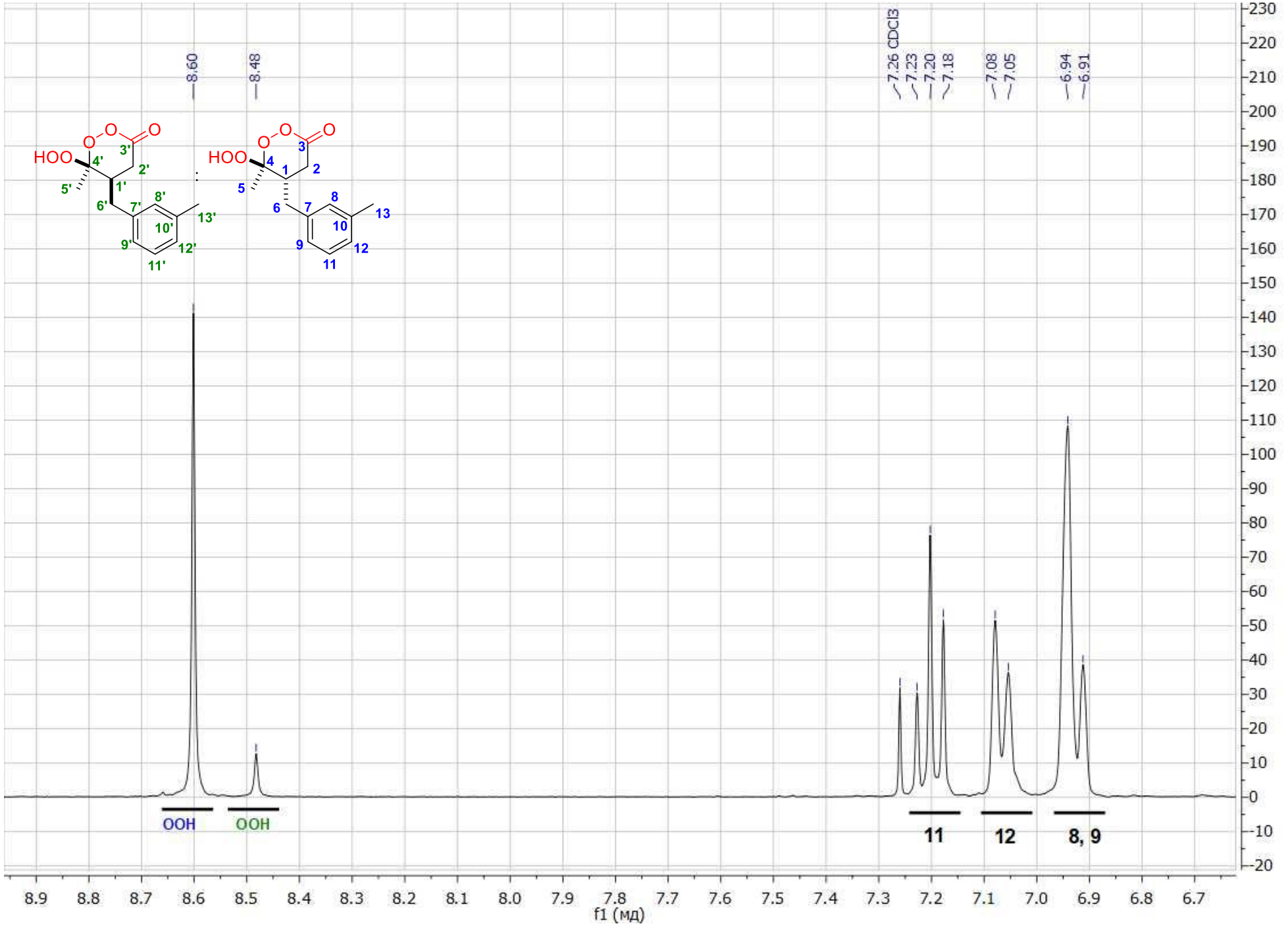

f2 (мд)
f1 (мд)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210

6-Hydroperoxy-6-methyl-5-(3-methylbenzyl)-1,2-dioxan-3-one, 2g

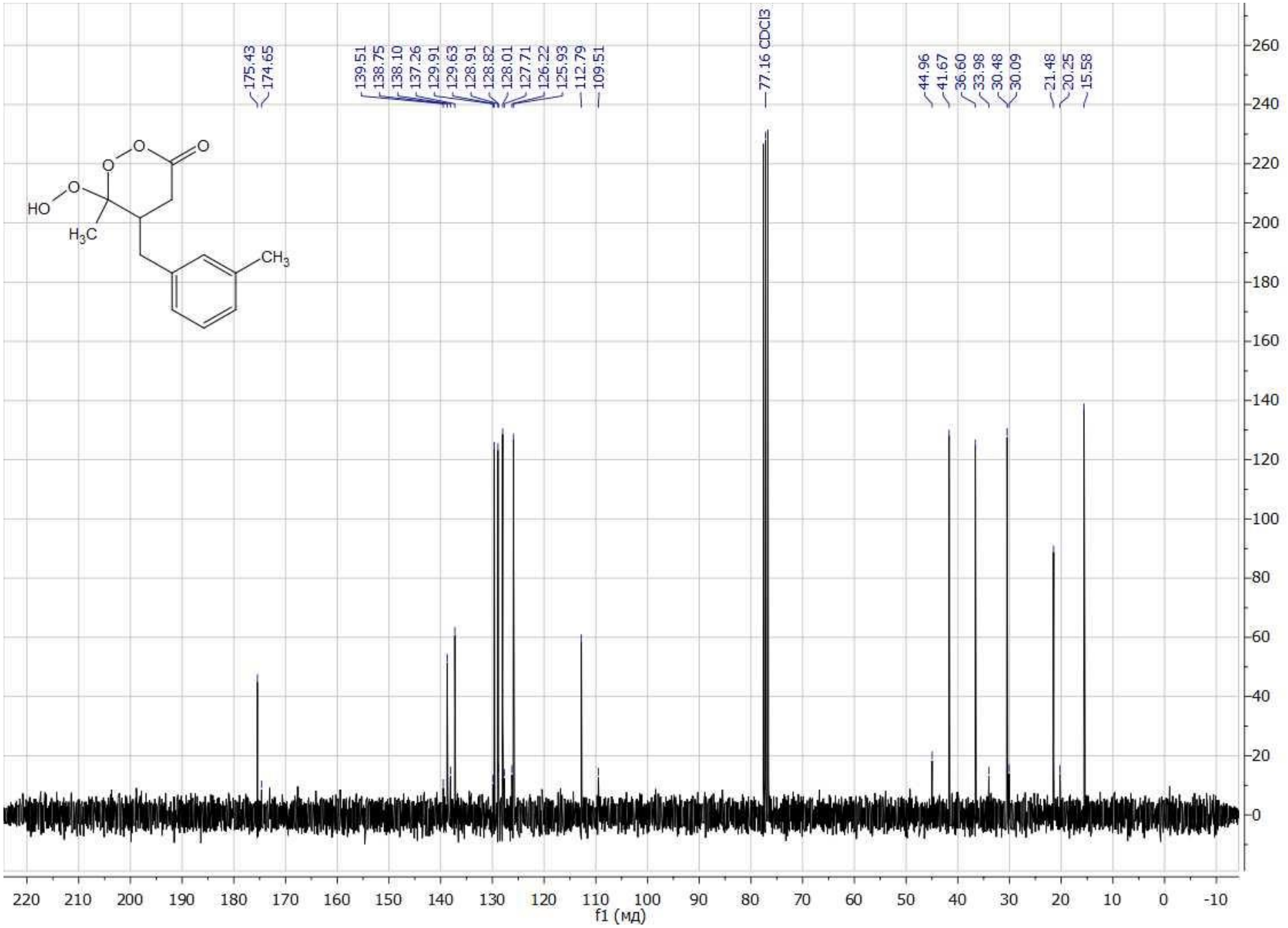
^{1}H NMR

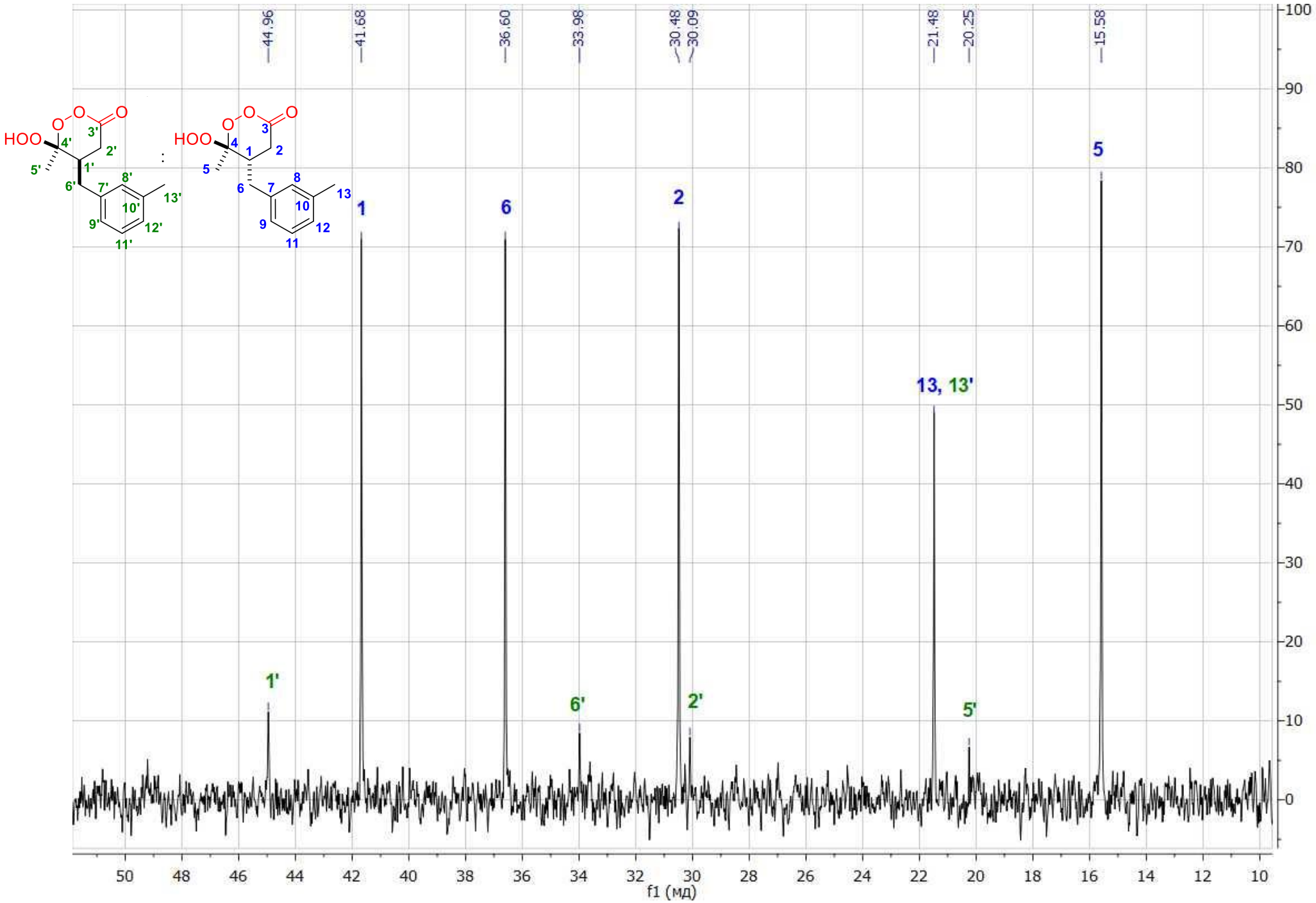


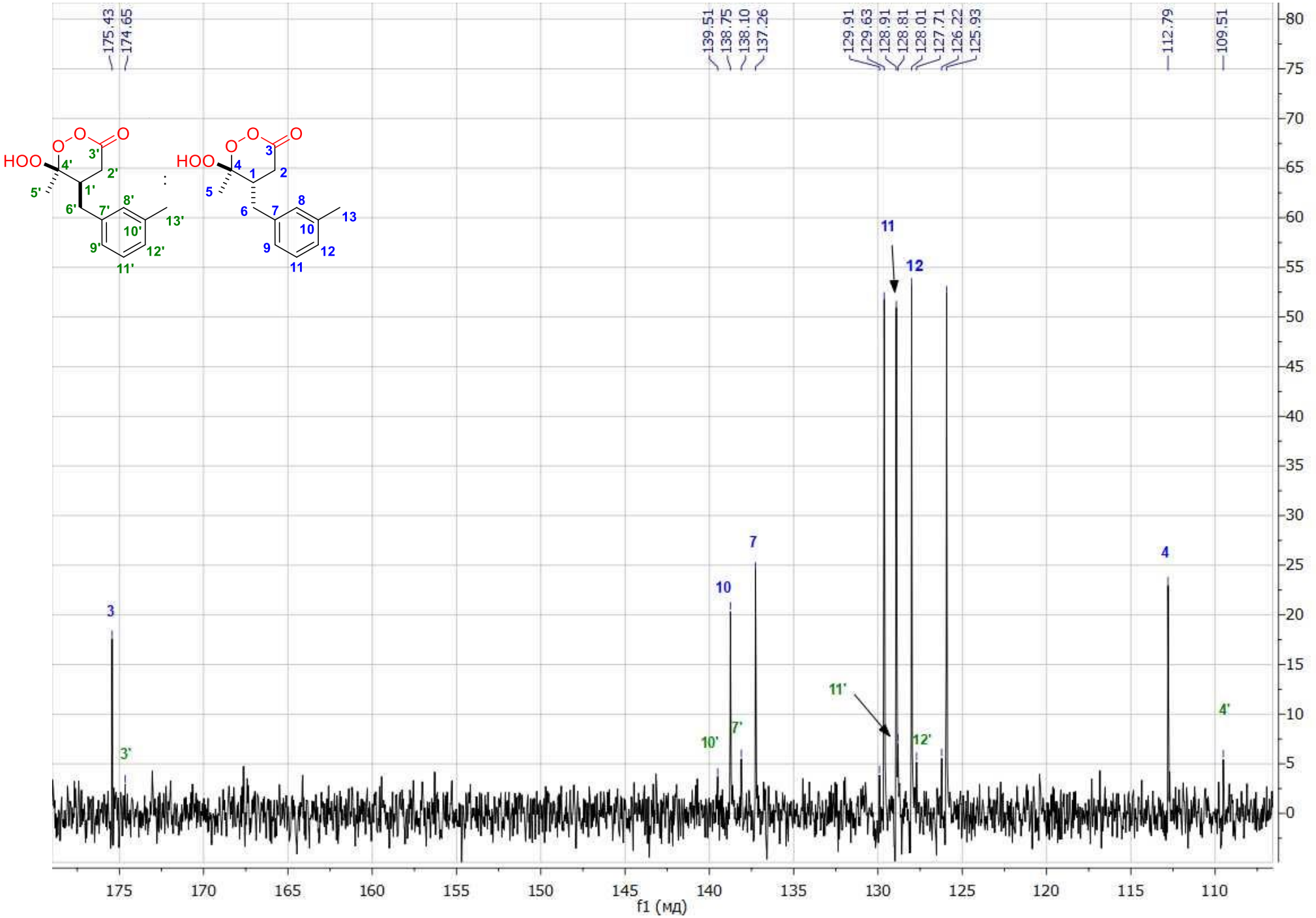

3.09 3.08 3.06 3.05 3.03 3.01 3.00
2.80 2.77 2.76 2.75 2.74 2.65 2.62 2.60 2.57 2.54 2.51 2.47 2.46 2.43 2.42 2.39 2.38 2.37 2.35 2.34 2.30 2.29 2.29 2.27 2.26 2.25 2.24 2.22 2.22
1.68
1.60
HOO
HOO
6 1H, 6' 1H
1' 1H
2' 1H
6 1H, 6' 1H, 2, 2' 1H,
13, 13', 1 1H
5'
5
f1 (мд)


8.60
8.48
7.26 CDCl3
7.23
7.20
7.18
7.08
7.05
6.94
6.91
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
13'
10'
9'
12'
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
13
10
9
12
11
OOH
OOH
11
12
8, 9
f1 (мд)

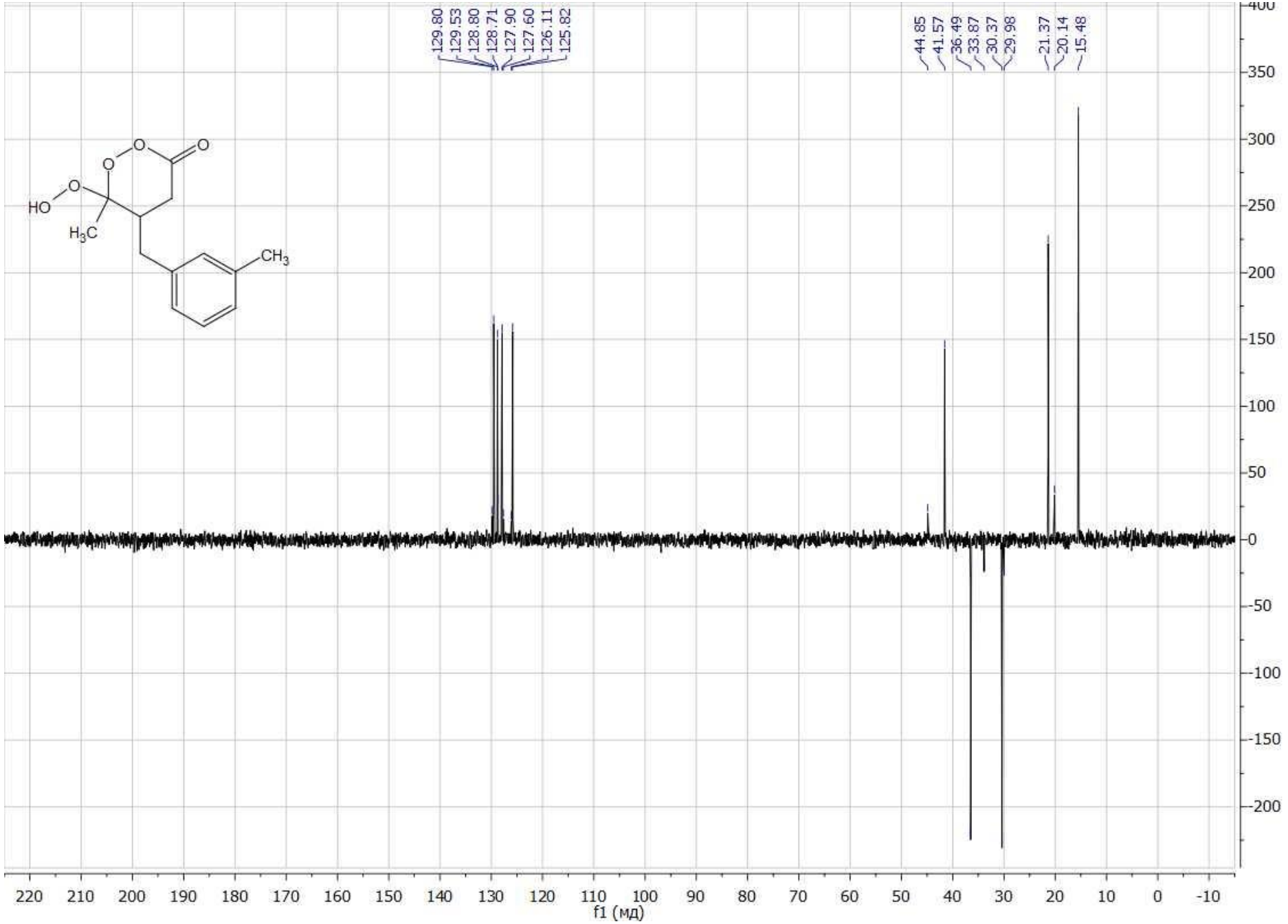
^{13}C NMR

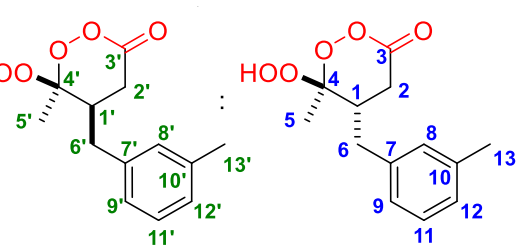

175.43
174.65
139.51
138.75
138.10
137.26
129.91
129.63
128.91
128.82
128.01
127.71
126.22
125.93
112.79
109.51
77.16 CDCl3
44.96
41.67
36.60
33.98
30.48
30.09
21.48
20.25
15.58
HO
O
O
O
O
H3C
CH3
f1 (мд)


44.96
41.68
36.60
33.98
30.48
30.09
21.48
20.25
15.58
HOO
1
6
2
5
13, 13'
1'
6'
2'
5'
f1 (мд)

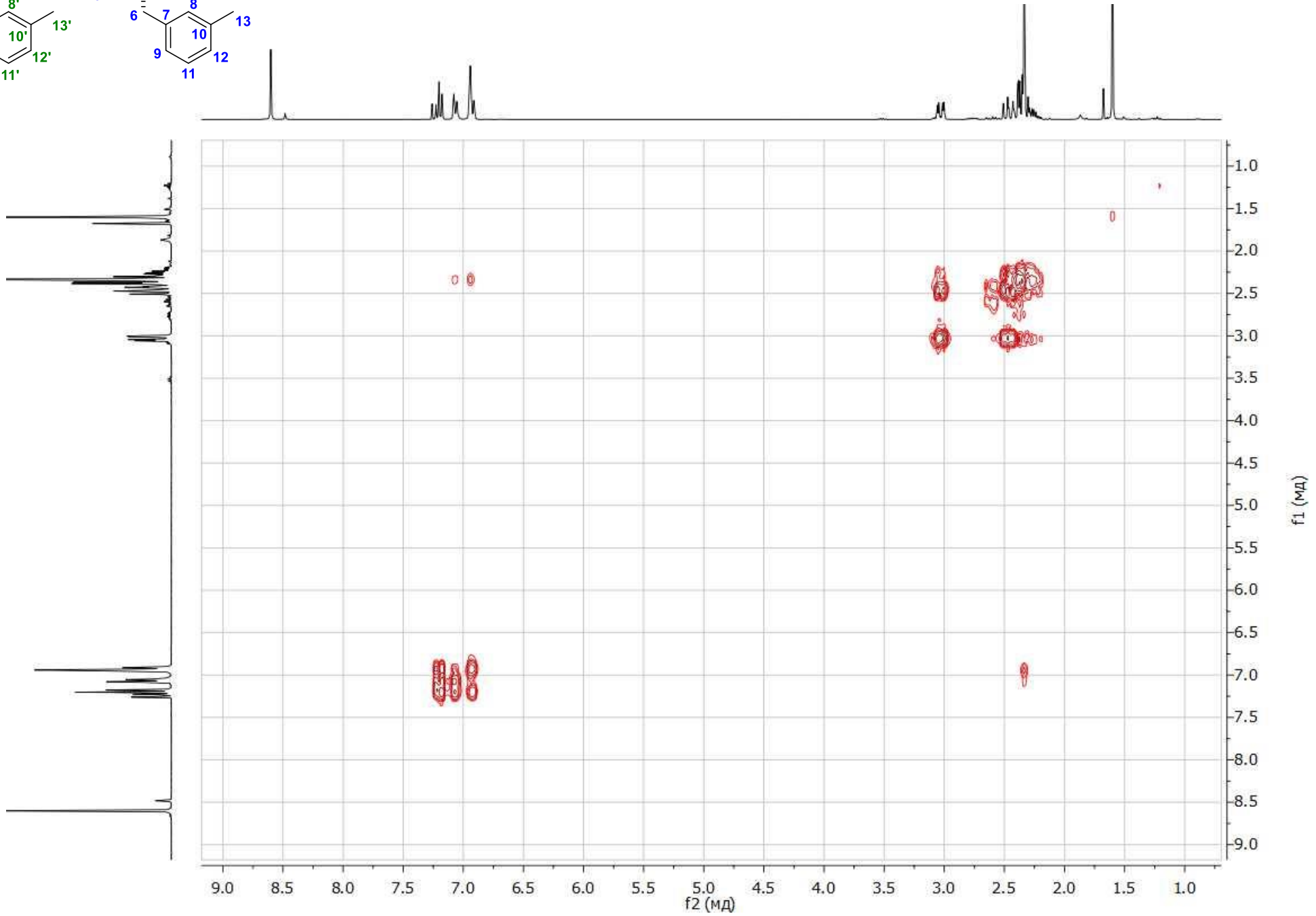

175.43
174.65
139.51
138.75
138.10
137.26
129.91
129.63
128.91
128.81
128.01
127.71
126.22
125.93
112.79
109.51
HOO
HOO
3
10
7
11
12
4
11'
10'
7'
12'
3'
4'
f1 (мд)

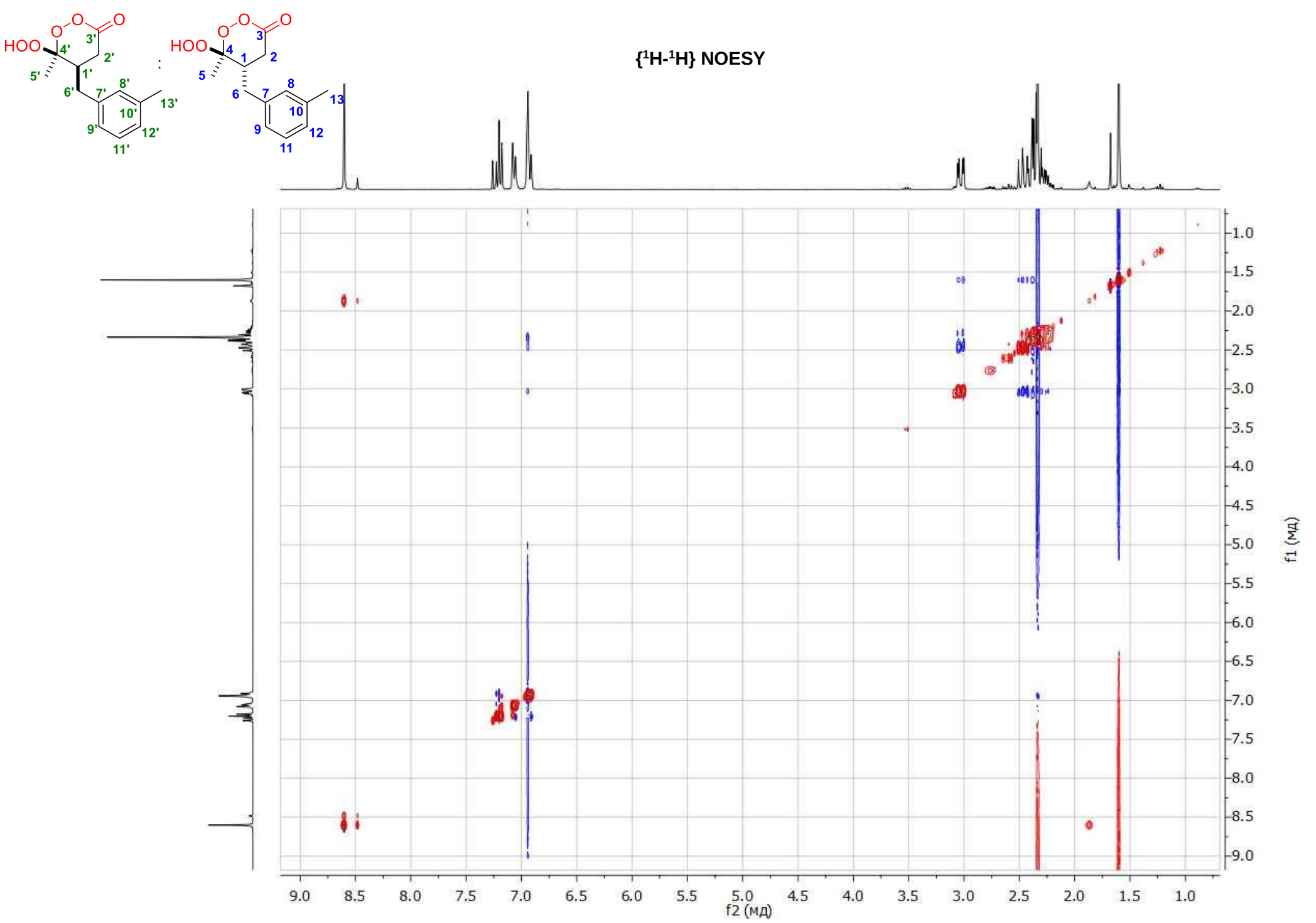
^{13}C_deptsp135

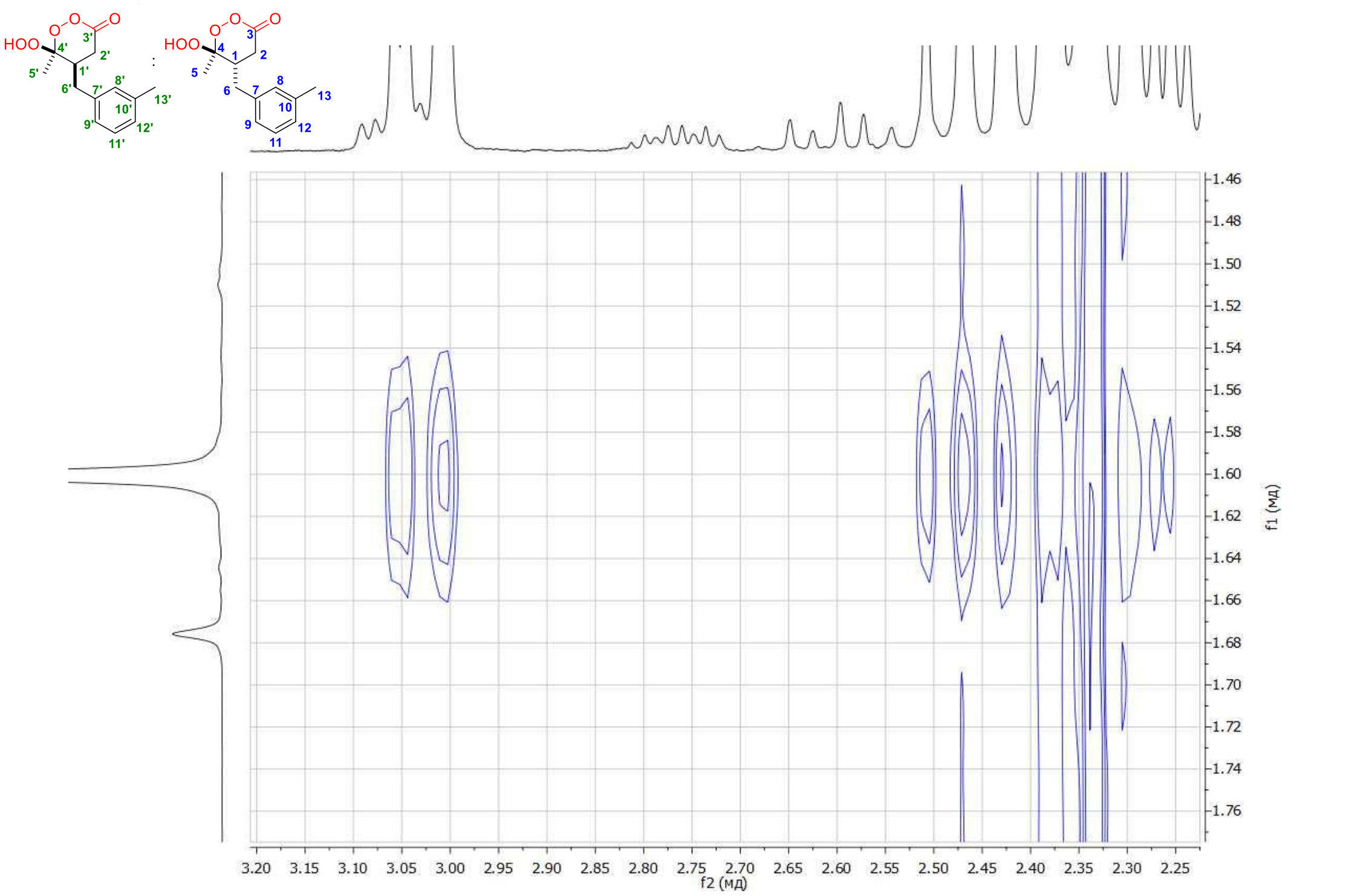


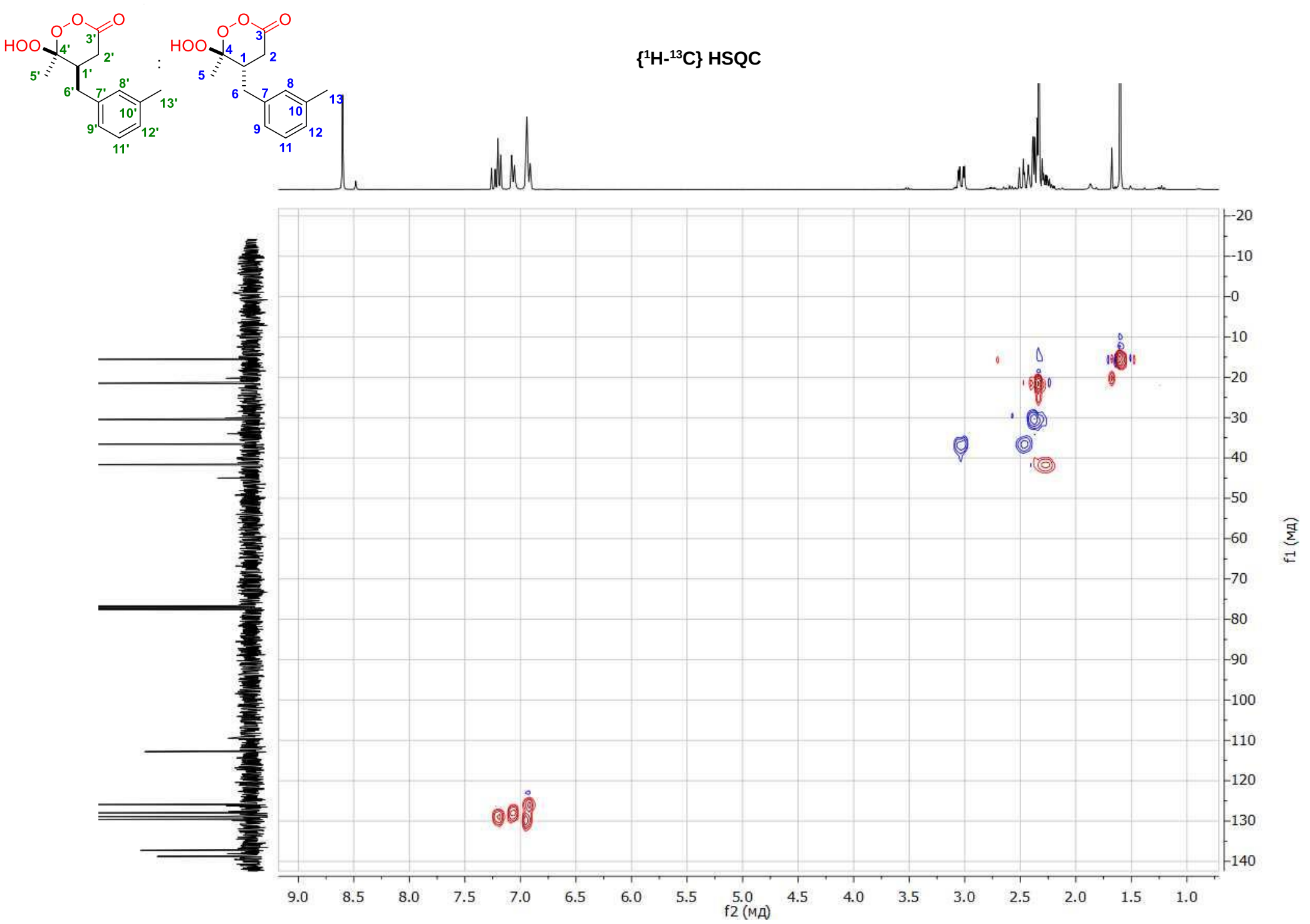

HOO
O
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
13'
10'
9'
12'
11'
HOO
O
O
O
3
4
2
1
5
6
7
8
13
10
9
12
11

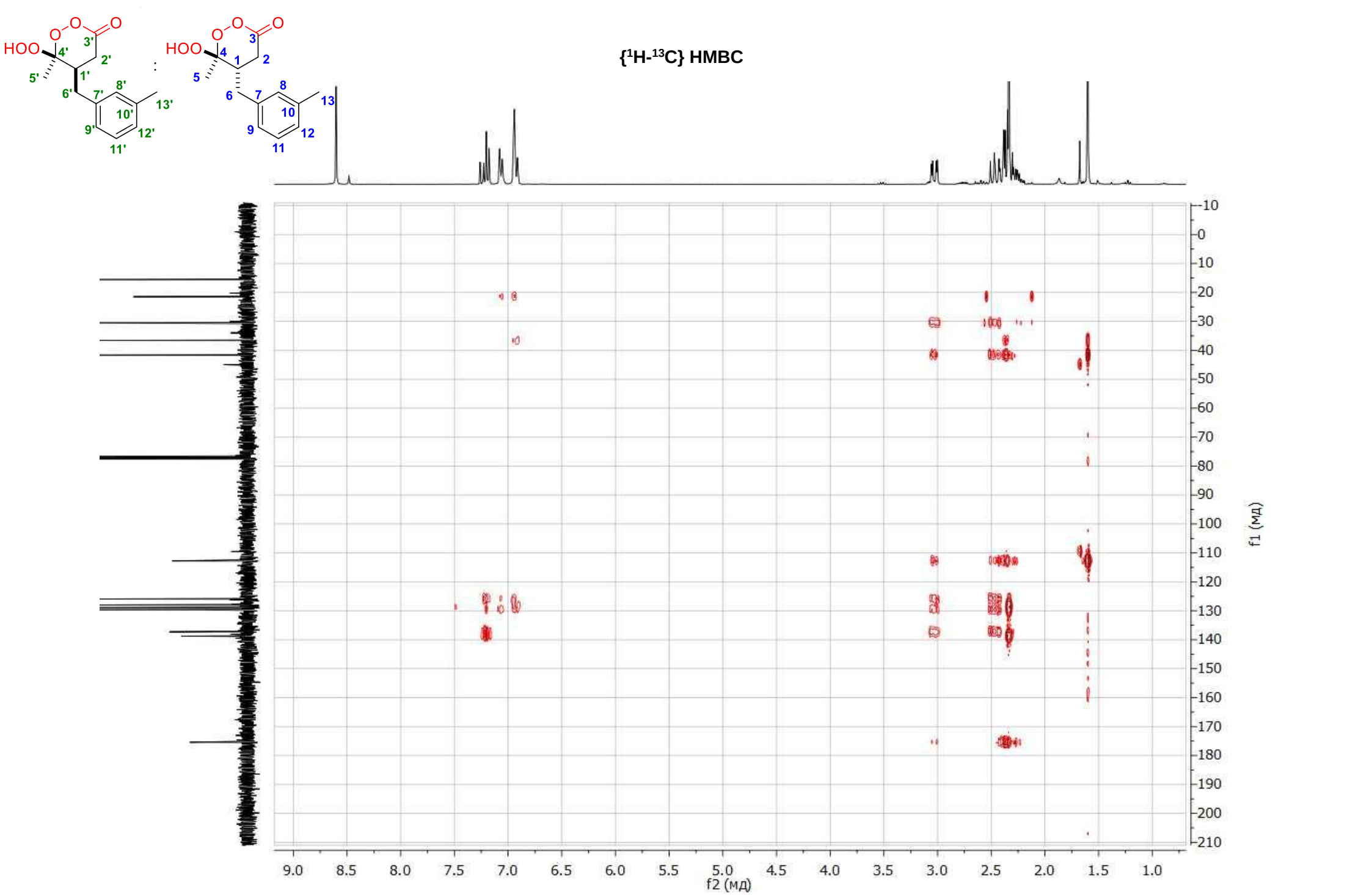
{^{1}H-^{1}H} COSY


f2 (мд)
f1 (мд)
9.0
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
9.0
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


{1H-1H} NOESY
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
13'
10'
9'
12'
11'
HOO
O
O
O
3
4
2
1
5
6
7
8
13
10
9
12
11
f2 (мд)
f1 (мд)

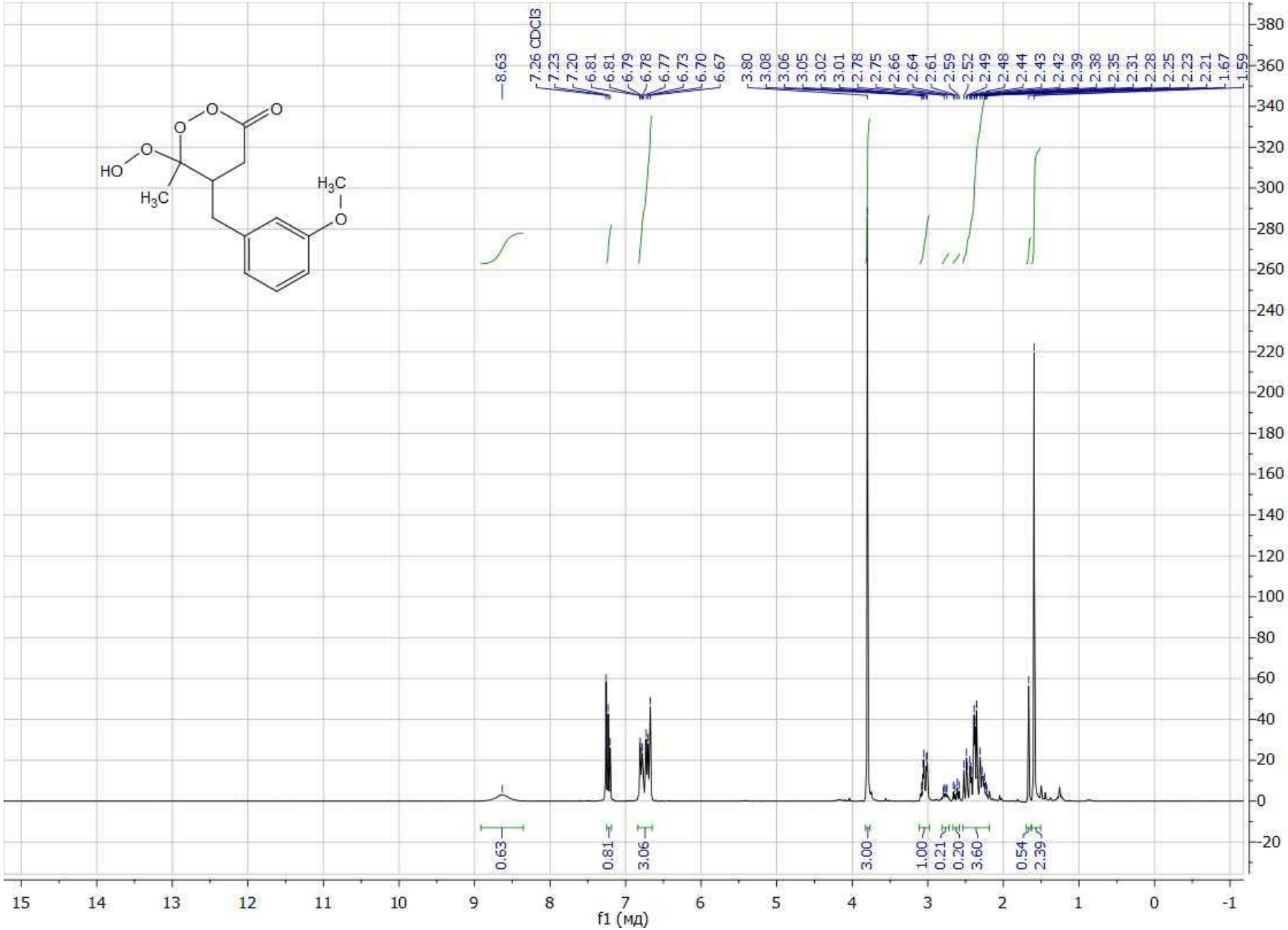

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
13'
10'
9'
12'
11'
HOO
O
O
O
3
4
2
1
5
6
7
8
13
10
9
12
11
1.46
1.48
1.50
1.52
1.54
1.56
1.58
1.60
1.62
1.64
1.66
1.68
1.70
1.72
1.74
1.76
f1 (мд)
3.20
3.15
3.10
3.05
3.00
2.95
2.90
2.85
2.80
2.75
2.70
2.65
2.60
2.55
2.50
2.45
2.40
2.35
2.30
2.25
f2 (мд)

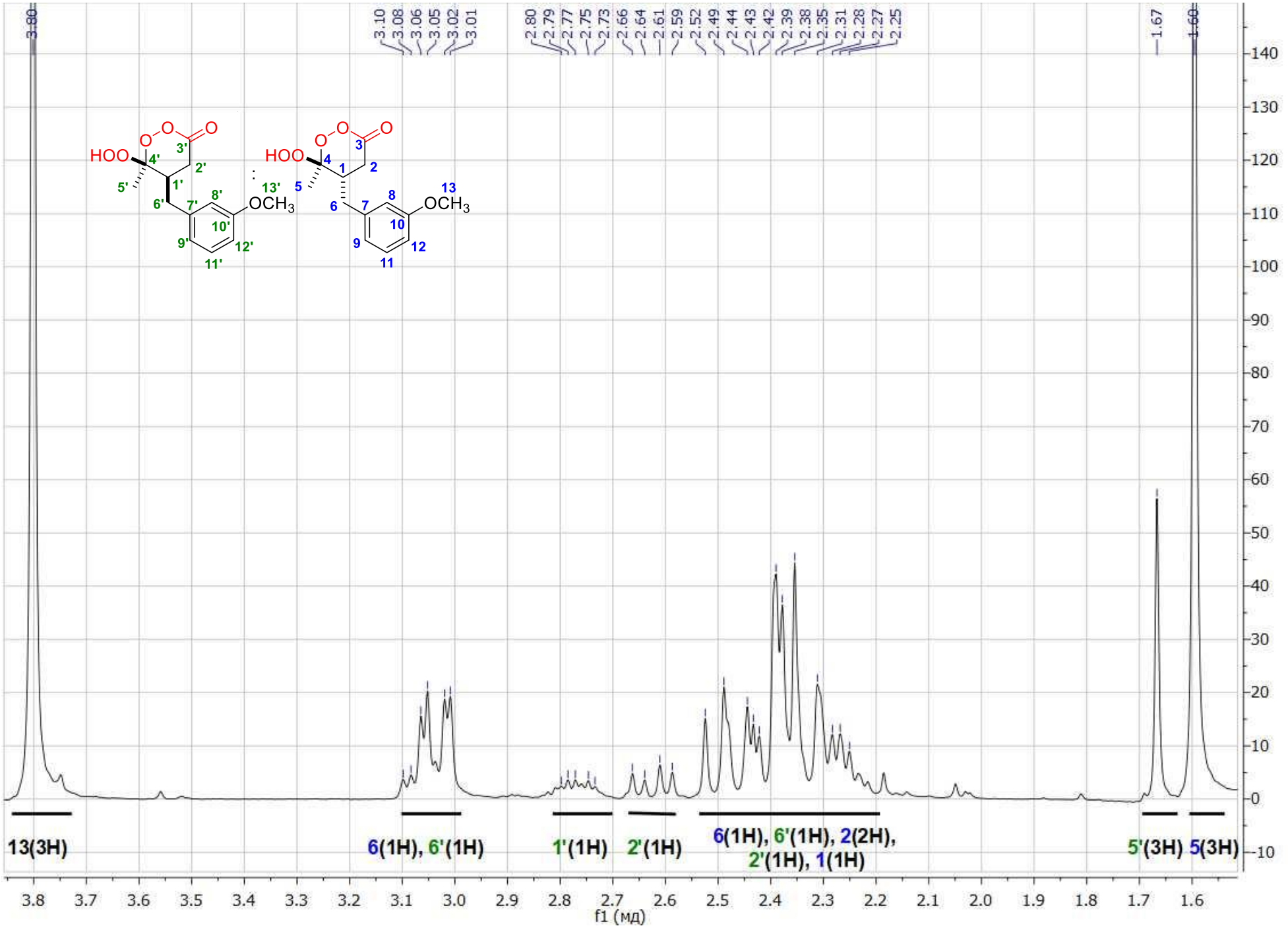

{1H-13C} HSQC
HOO
O
O
O
3'
2'
4'
1'
5'
6'
7'
8'
10'
9'
12'
11'
13'
HOO
O
O
O
3
2
4
1
5
6
7
8
10
9
12
11
13
f2 (мд)
f1 (мд)

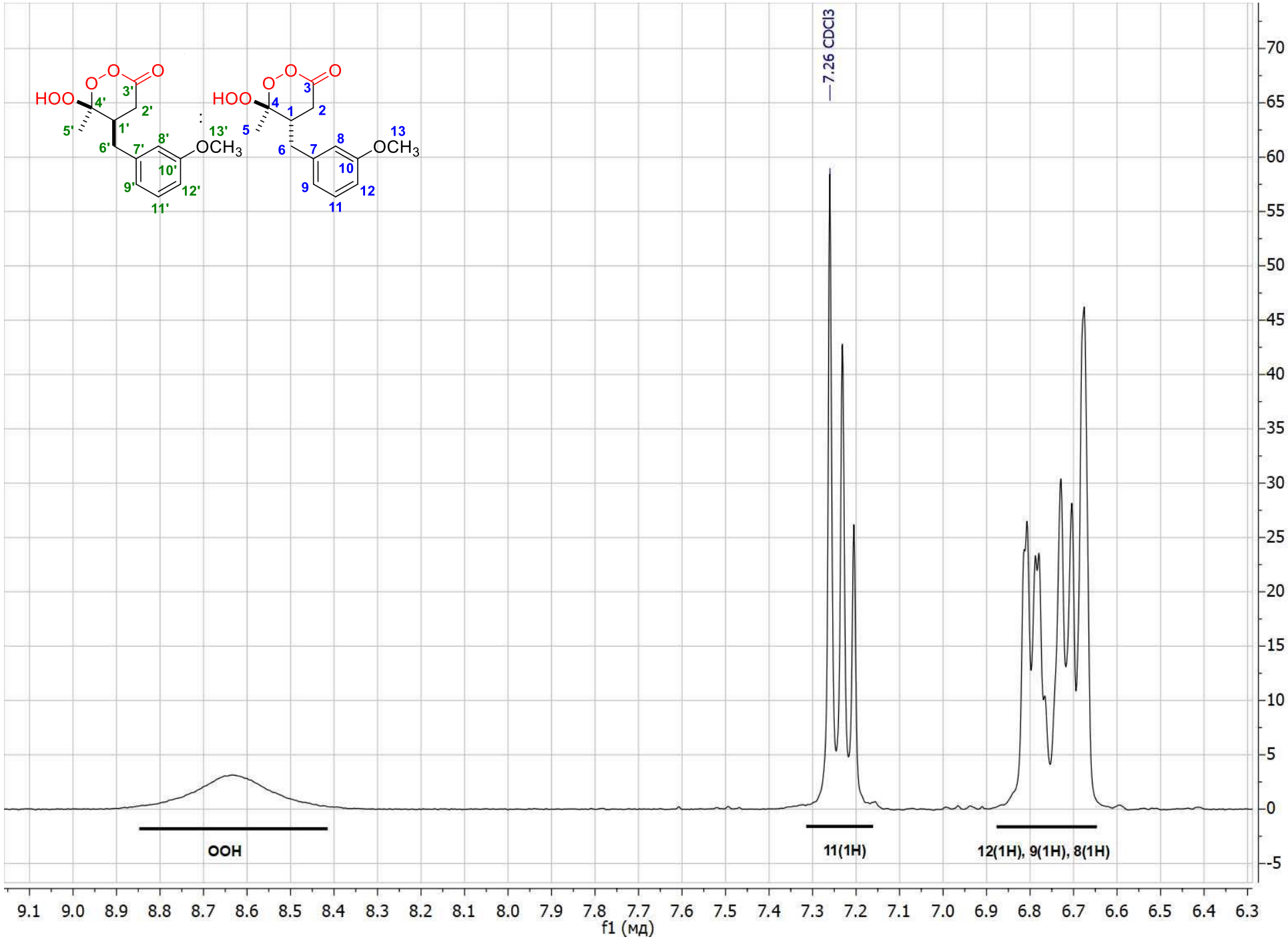

{1H-13C} HMBC
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
13'
10'
9'
12'
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
13
10
9
12
11
f2 (мд)
f1 (мд)

6-Hydroperoxy-6-methyl-5-(3-methoxybenzyl)-1,2-dioxan-3-one, 2h

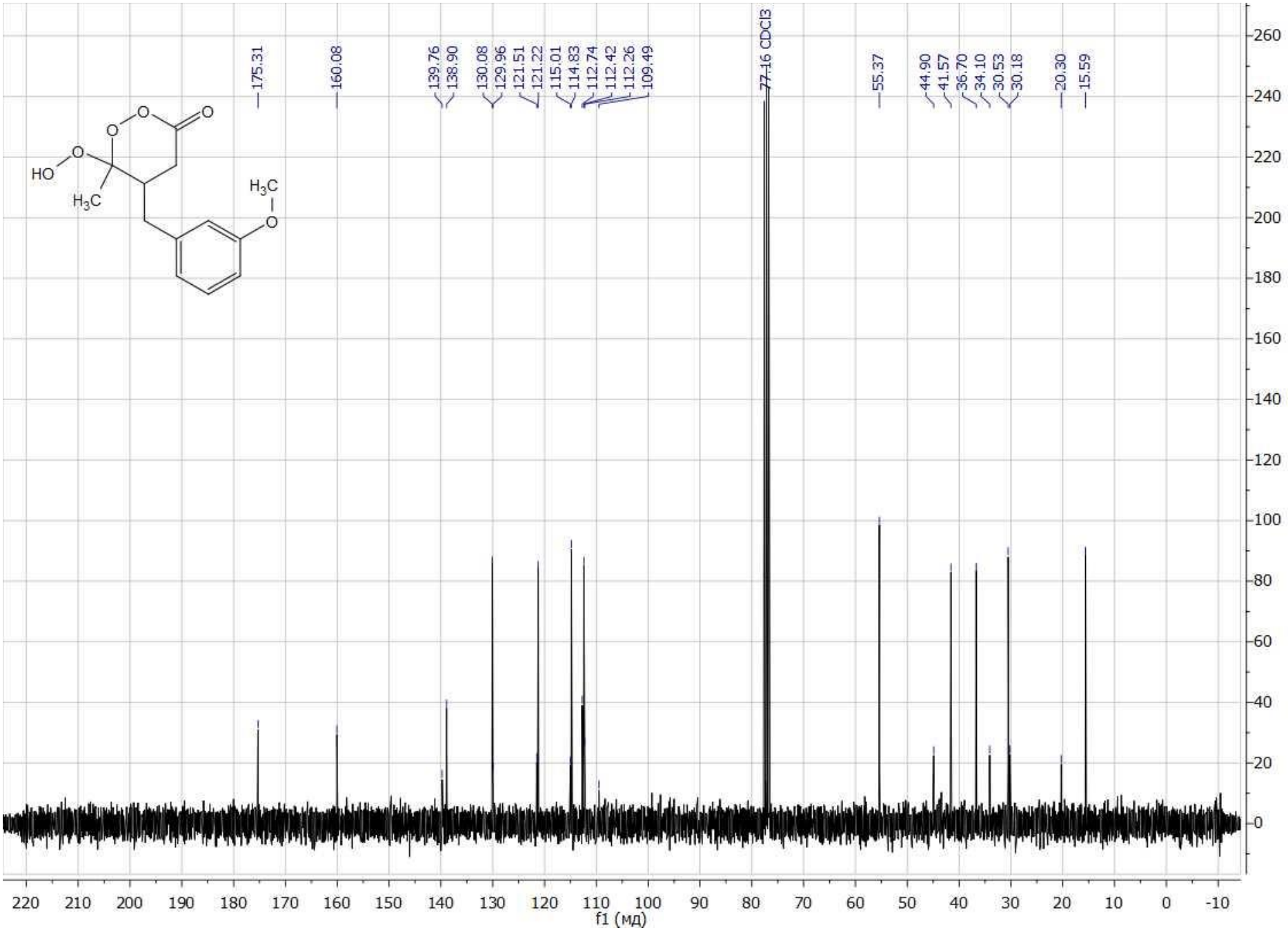
^{1}H NMR

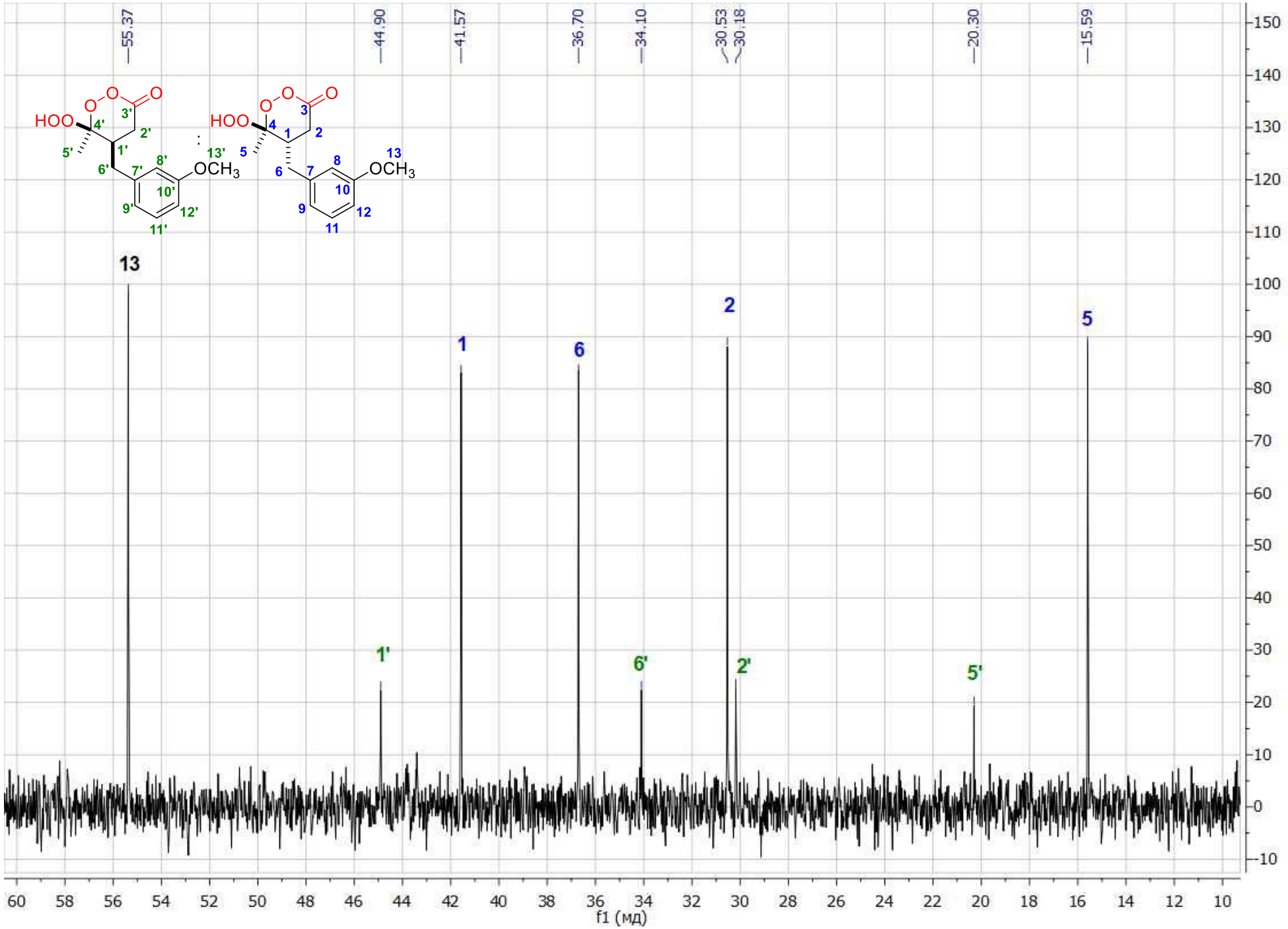


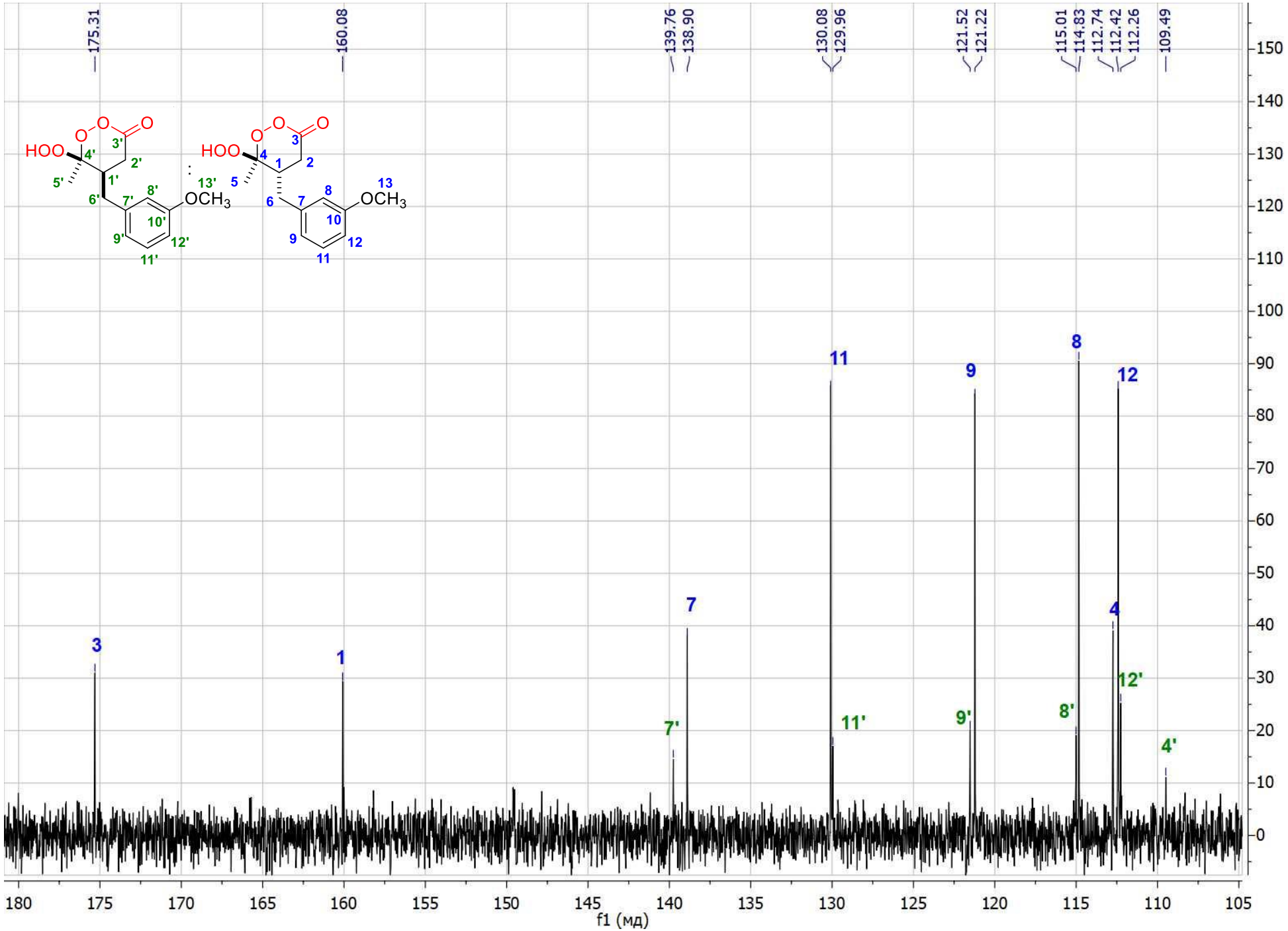

3.80
3.10
3.08
3.06
3.05
3.02
3.01
2.80
2.79
2.77
2.75
2.73
2.66
2.64
2.61
2.59
2.52
2.49
2.44
2.43
2.42
2.39
2.38
2.35
2.31
2.28
2.27
2.25
1.67
1.60
HOO
OCH3
13(3H)
6(1H), 6'(1H)
1'(1H)
2'(1H)
6(1H), 6'(1H), 2(2H), 2'(1H), 1(1H)
5'(3H) 5(3H)
f1 (мд)


7.26 CDCl3
OOH
11(1H)
12(1H), 9(1H), 8(1H)
f1 (мд)

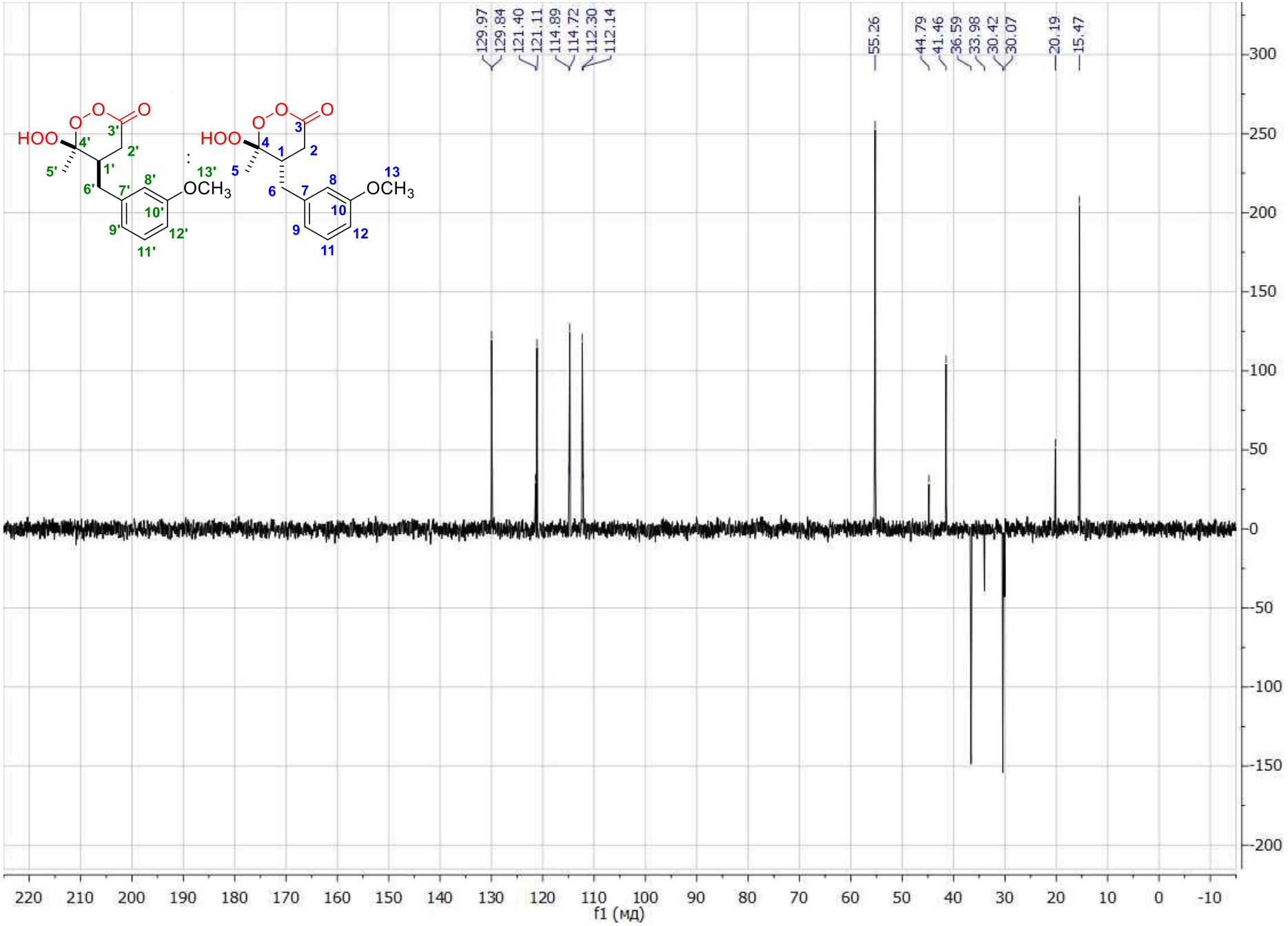
^{13}C NMR

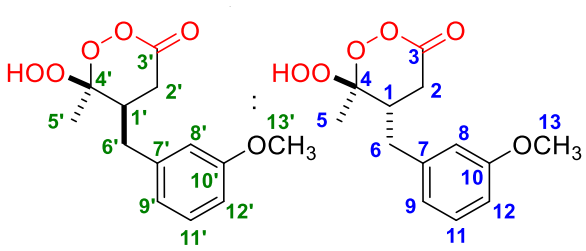

175.31
160.08
139.76
138.90
130.08
129.96
121.51
121.22
115.01
114.83
112.74
112.42
112.26
109.49
77.16 CDCl3
55.37
44.90
41.57
36.70
34.10
30.53
30.18
20.30
15.59
HO
O
O
O
O
H3C
H3C
O
f1 (мд)


55.37
44.90
41.57
36.70
34.10
30.53
30.18
20.30
15.59
HOO
OCH3
13
1
6
2
5
1'
6'
2'
5'
f1 (мд)

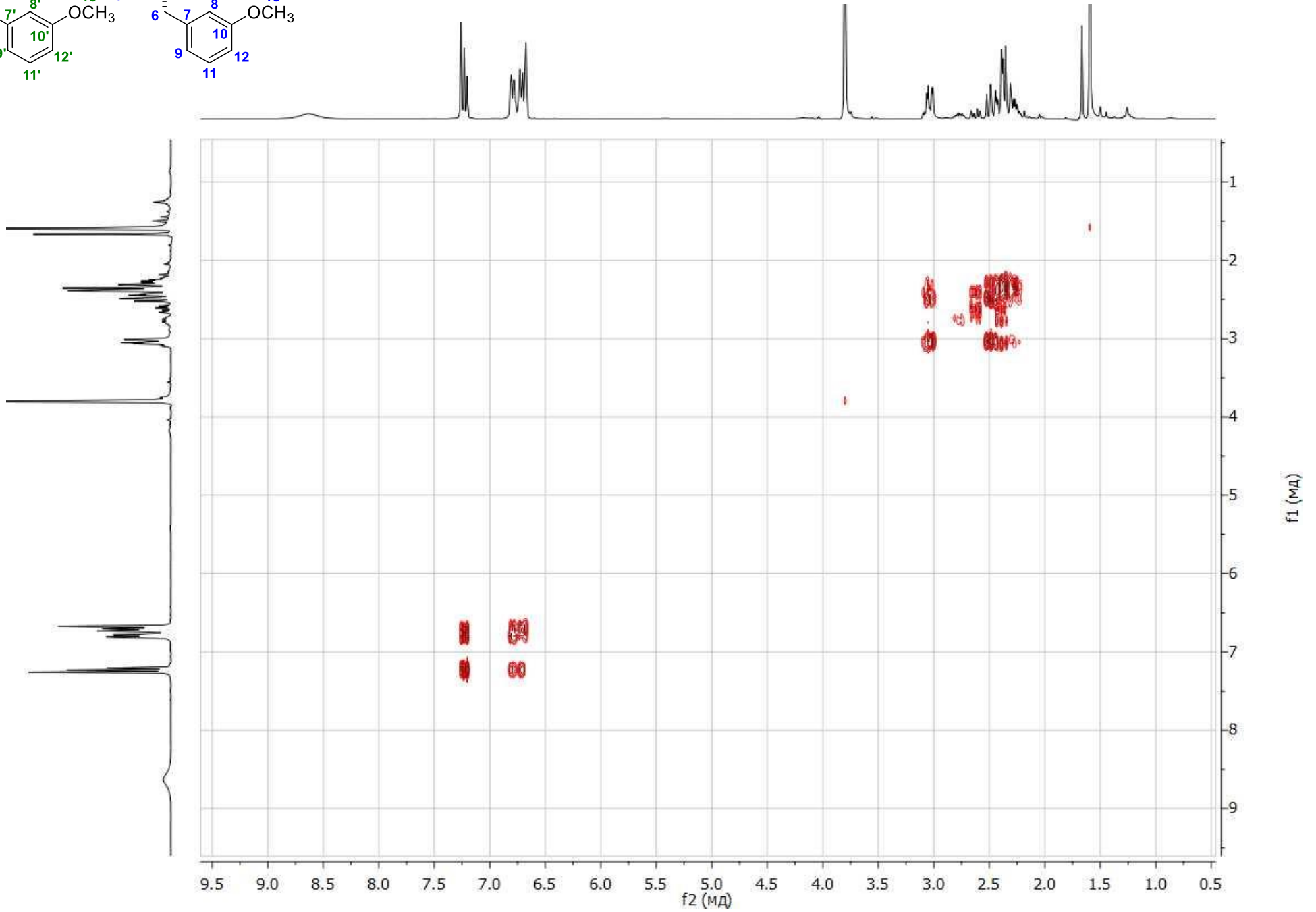

175.31
160.08
139.76
138.90
130.08
129.96
121.52
121.22
115.01
114.83
112.74
112.42
112.26
109.49
HOO
OCH3
3
1
7
11
9
8
12
4
7'
11'
9'
8'
12'
4'
f1 (мд)

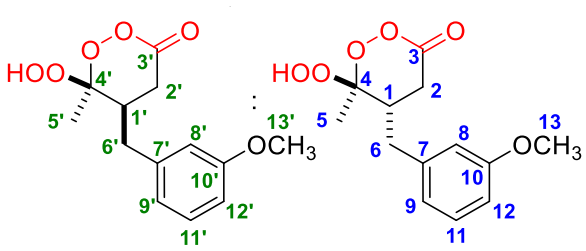
^{13}C_deptsp135



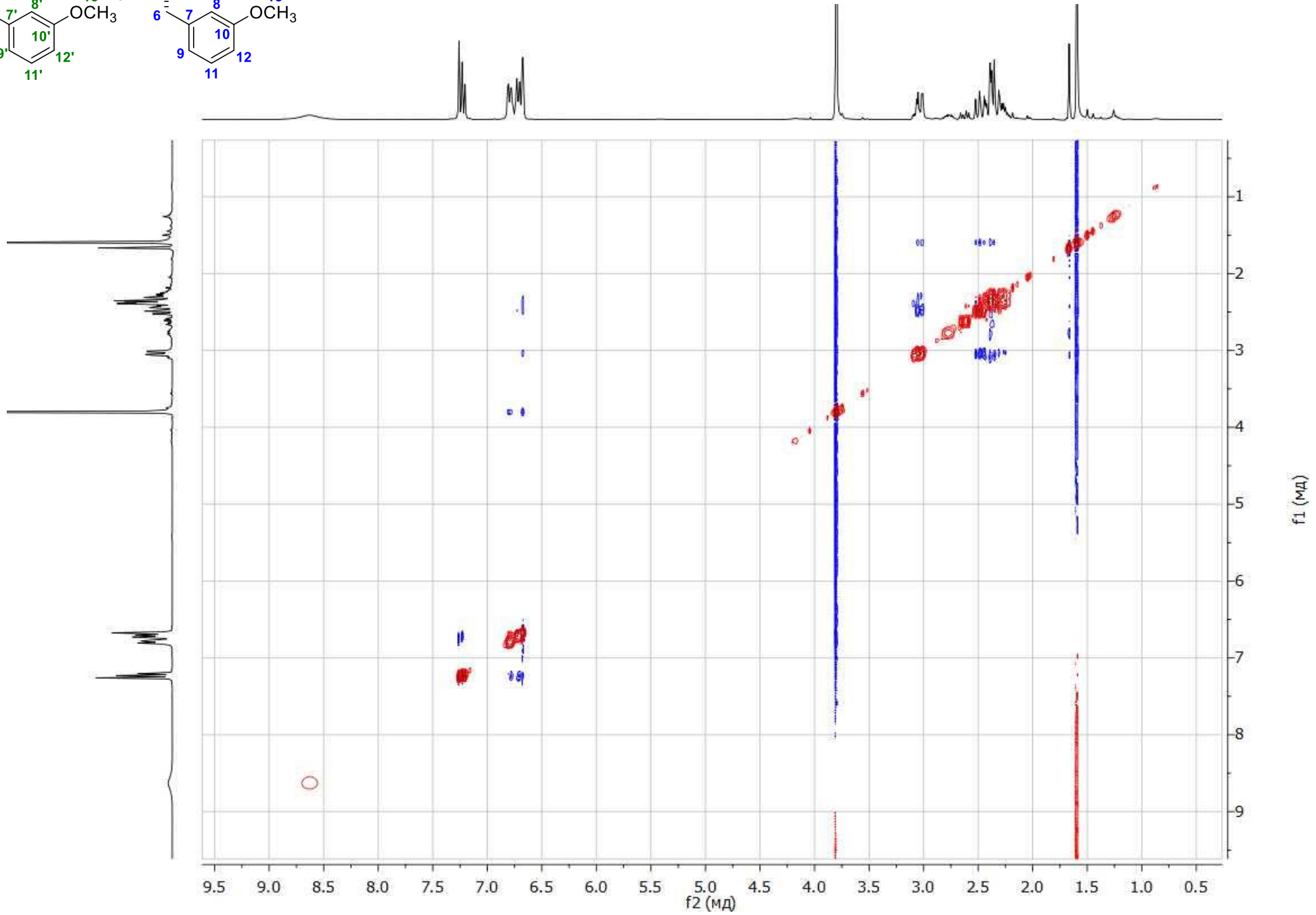

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
13'
OCH3
10'
9'
12'
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
13
OCH3
10
9
12
11

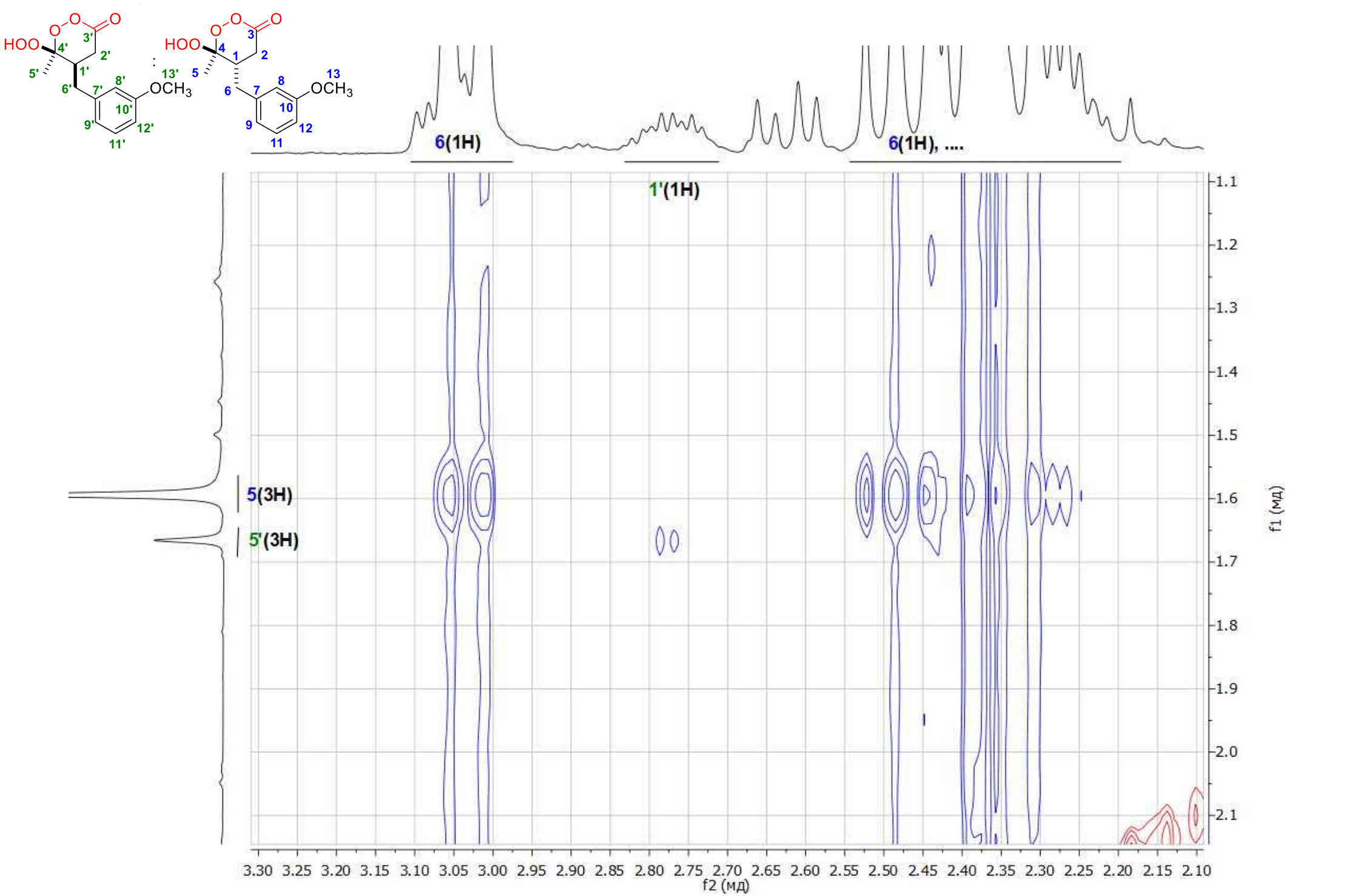
{^{1}H-^{1}H} COSY

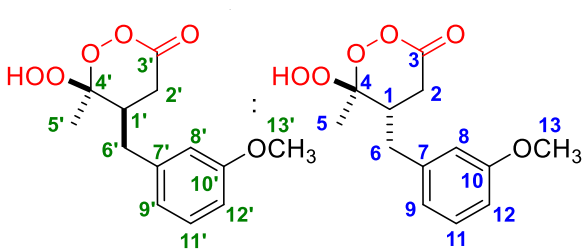

f1 (мд)
f2 (мд)
1
2
3
4
5
6
7
8
9
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5


HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
13'
OCH3
10'
9'
12'
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
13
OCH3
10
9
12
11

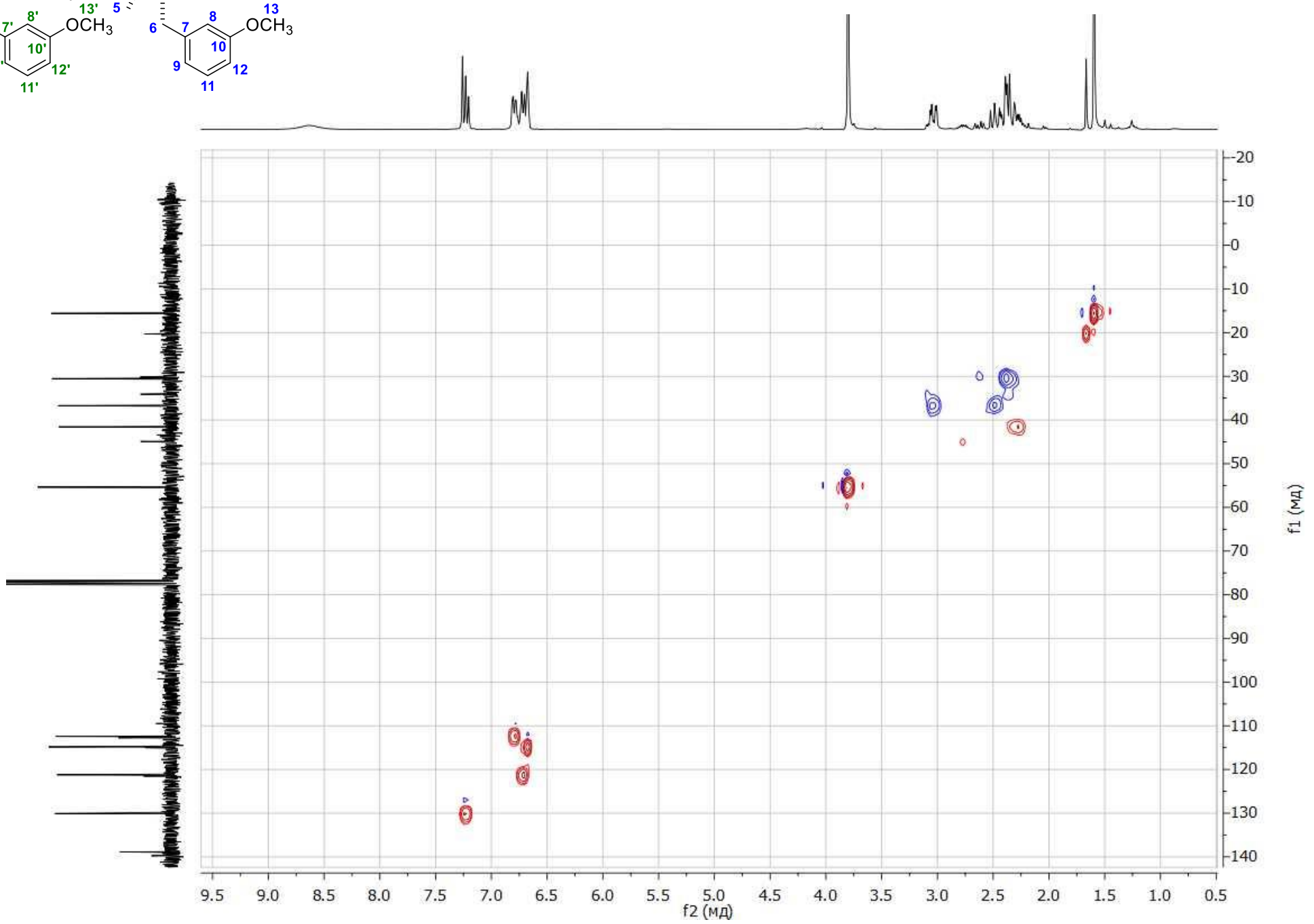
{^{1}H-^{1}H} NOESY

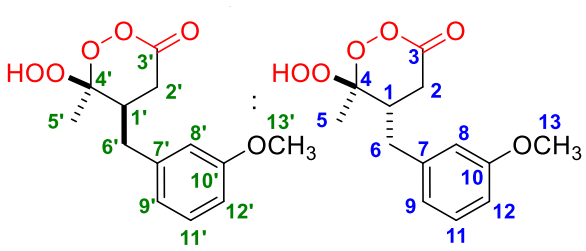

f2 (мд)
f1 (мд)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
1
2
3
4
5
6
7
8
9


HOO
OCH3
6(1H)
6(1H), ...
1'(1H)
5(3H)
5'(3H)
f1 (мд)
f2 (мд)

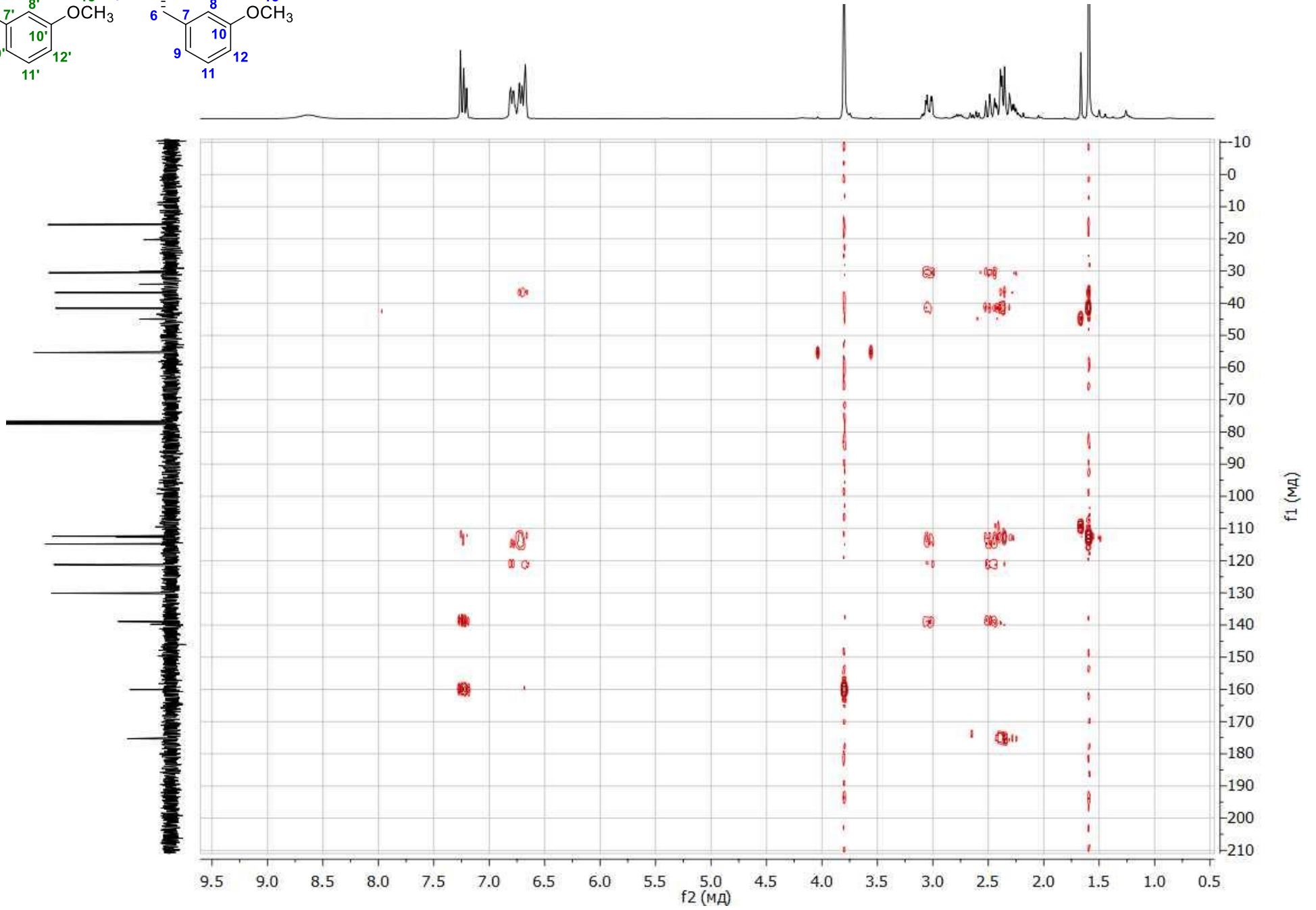

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
13'
OCH3
10'
9'
12'
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
13
OCH3
10
9
12
11

{^{1}H-^{13}C} HSQC


-20
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
f1 (мд)
9.5
9.0
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
f2 (мд)

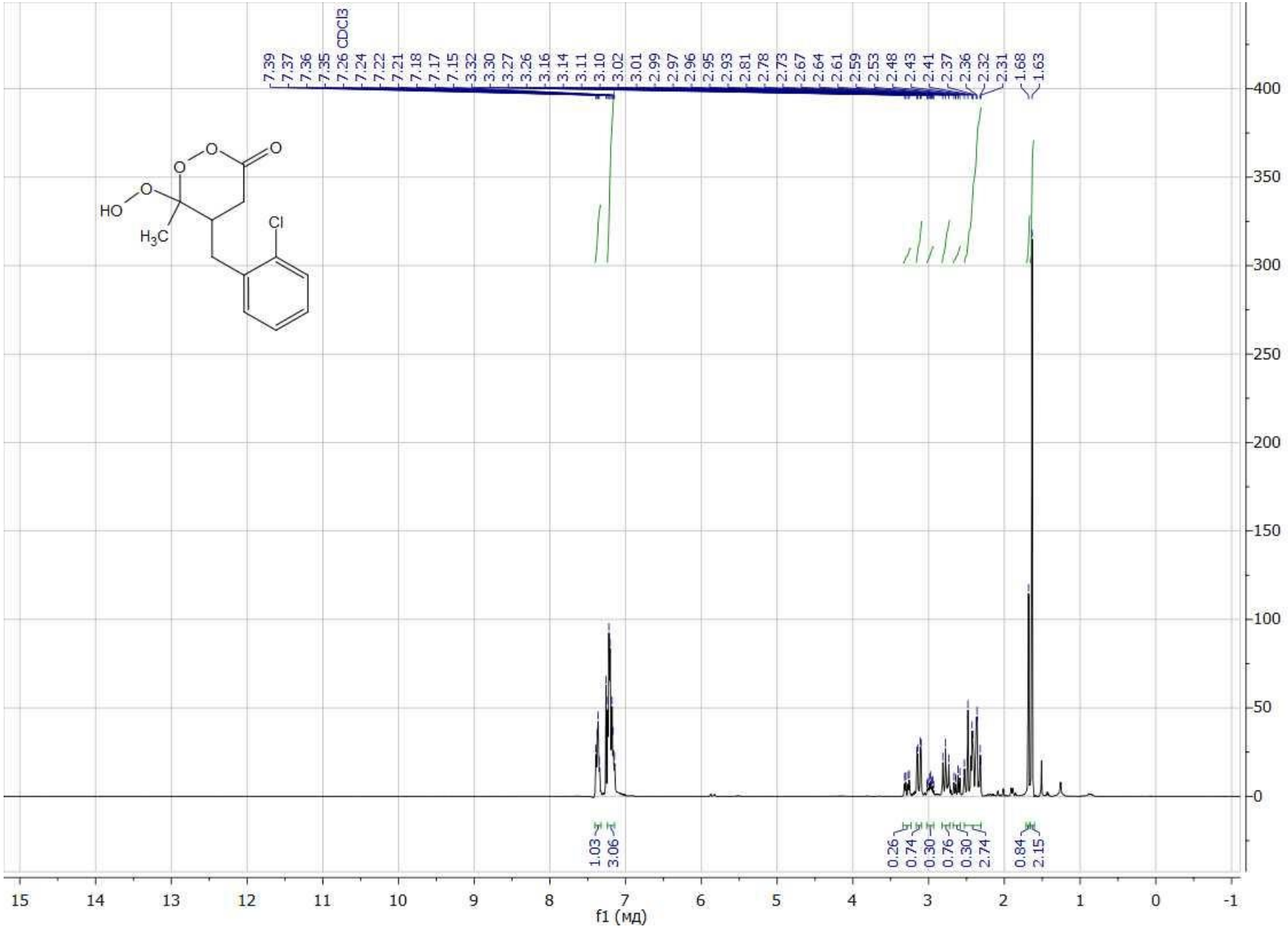

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
13'
OCH3
10'
9'
12'
11'
HOO
O
O
O
3
4
2
1
5
6
7
8
13
OCH3
10
9
12
11

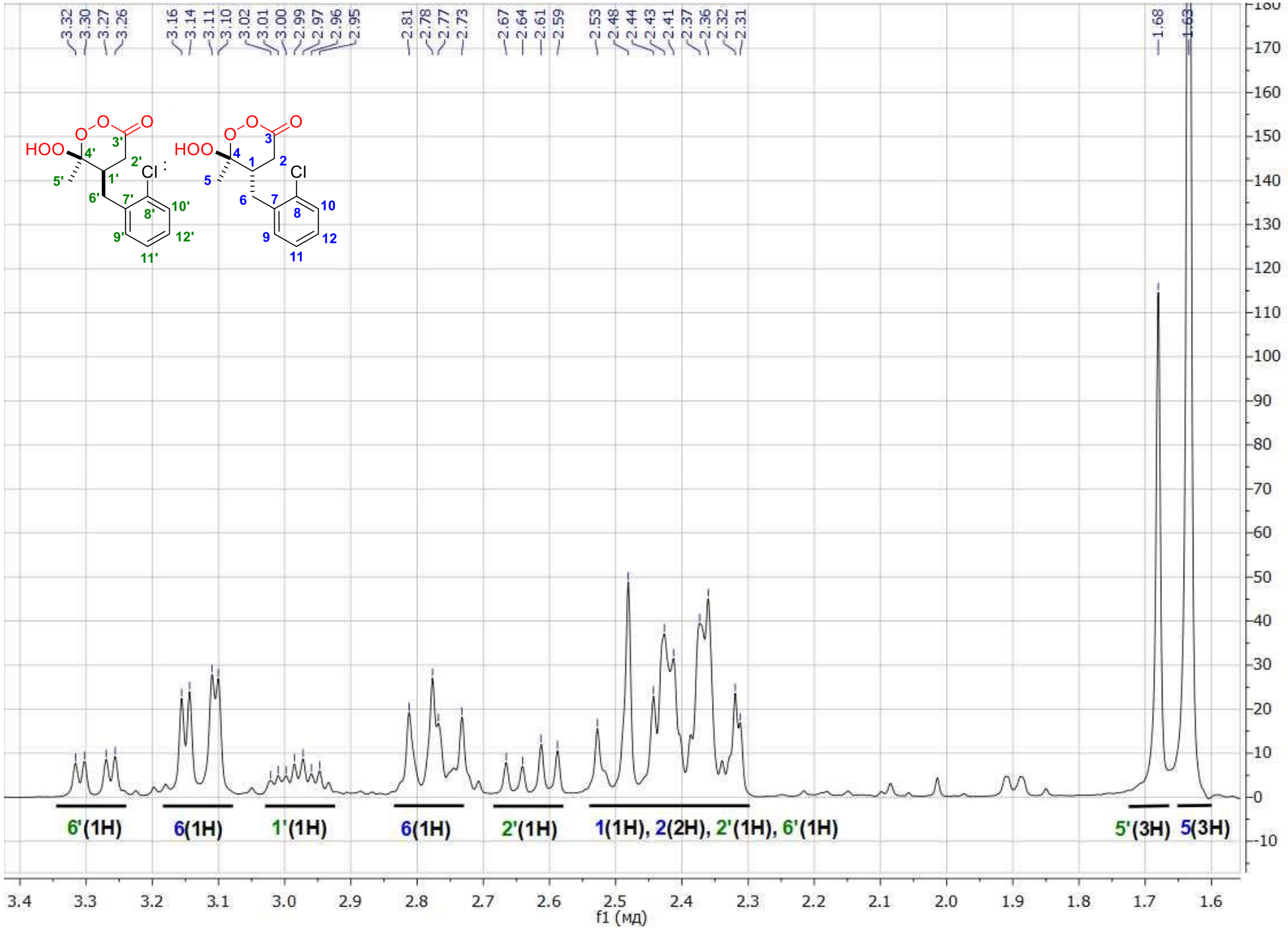
{^{1}H-^{13}C} HMBC

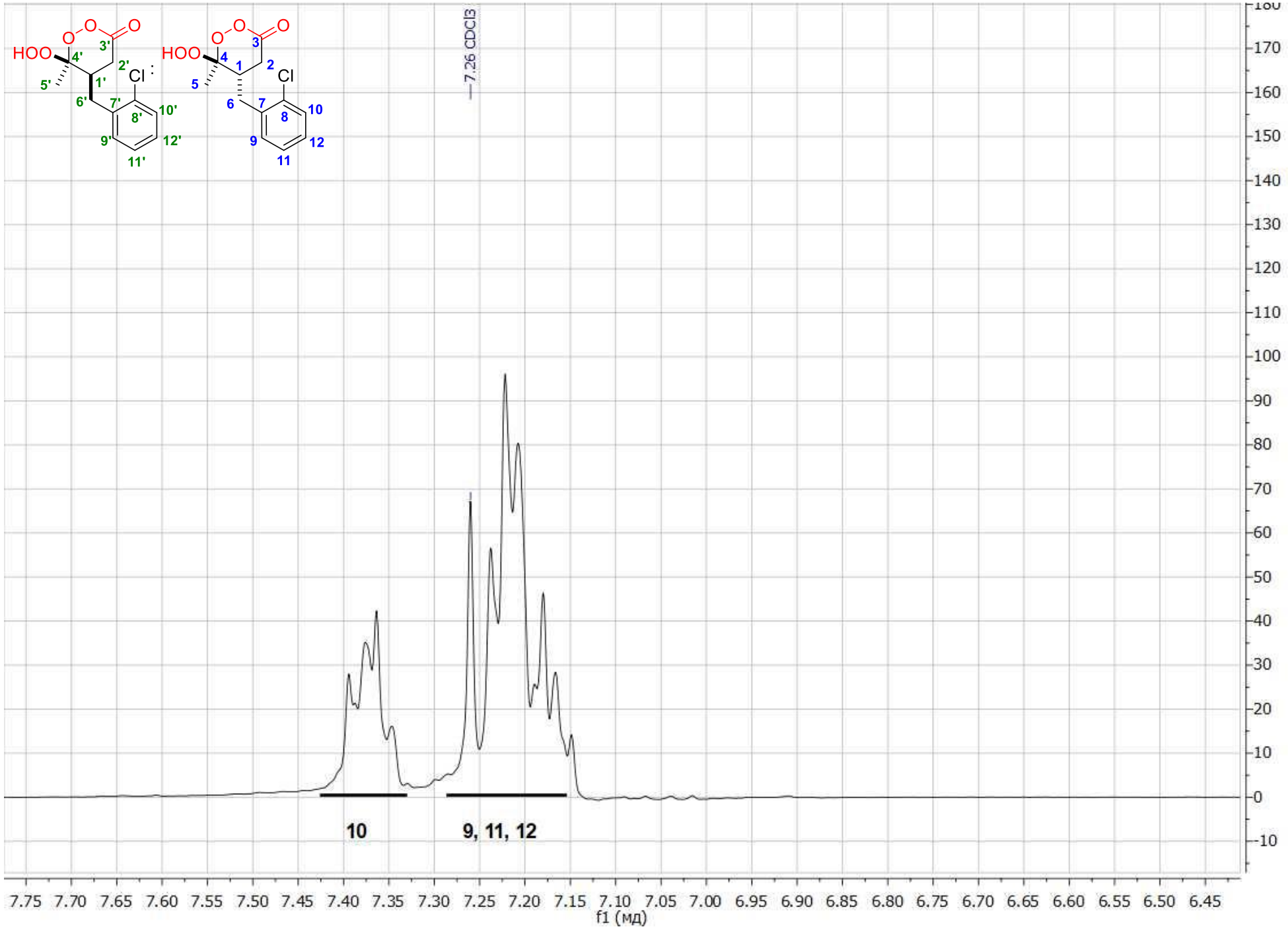

f2 (мд)
f1 (мд)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210

5-(2-Chlorobenzyl)-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2i

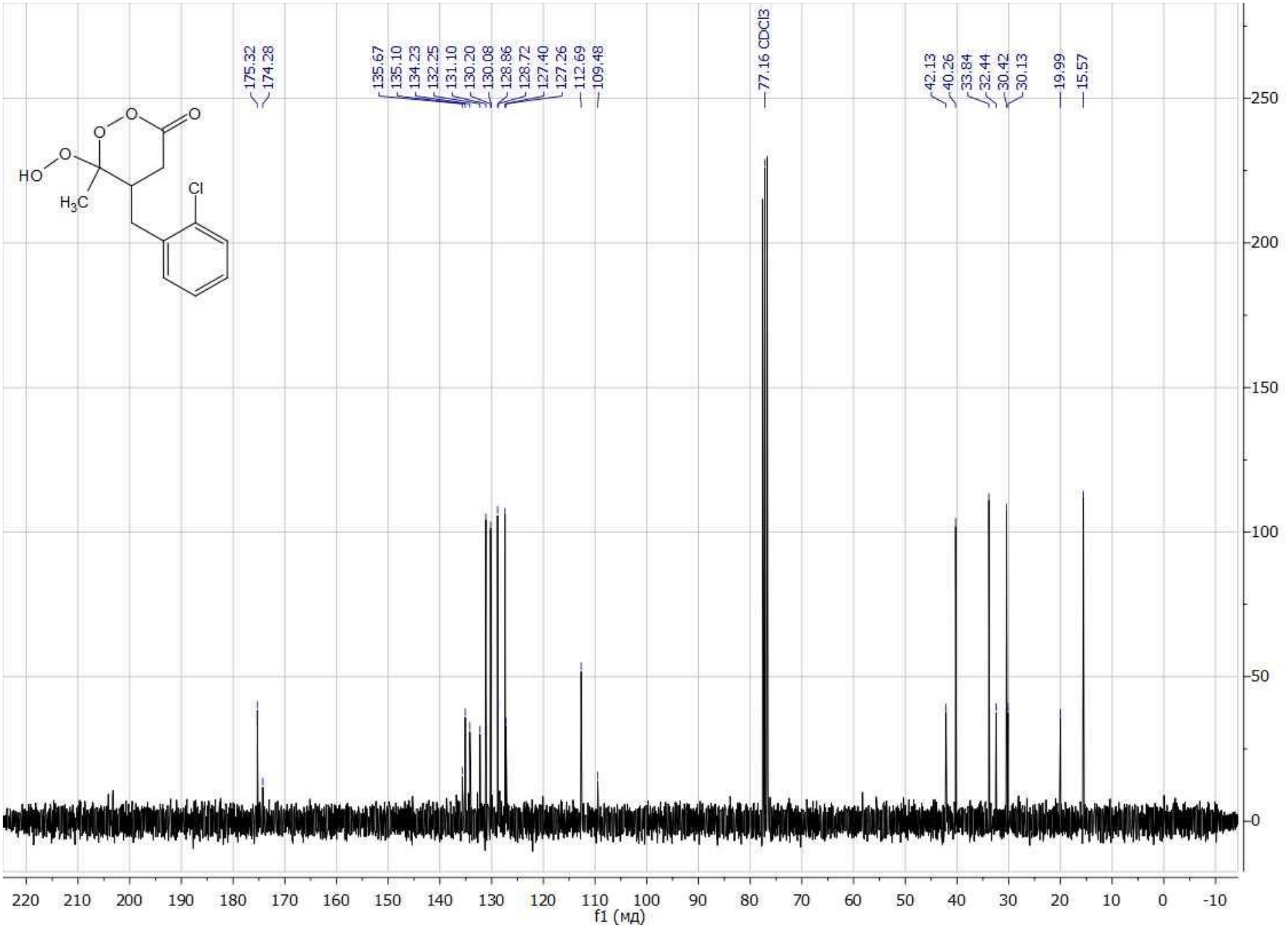
^{1}H NMR

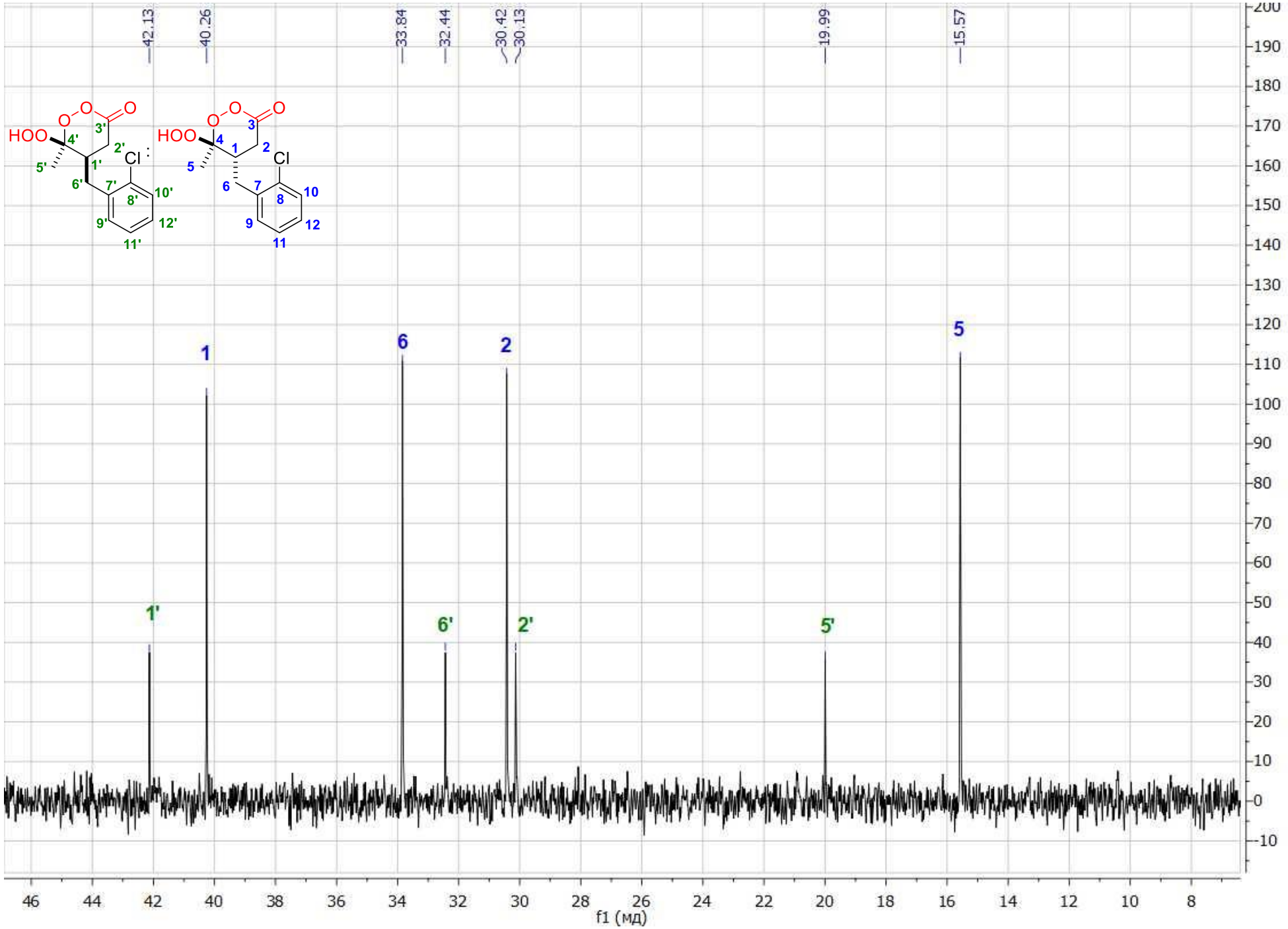


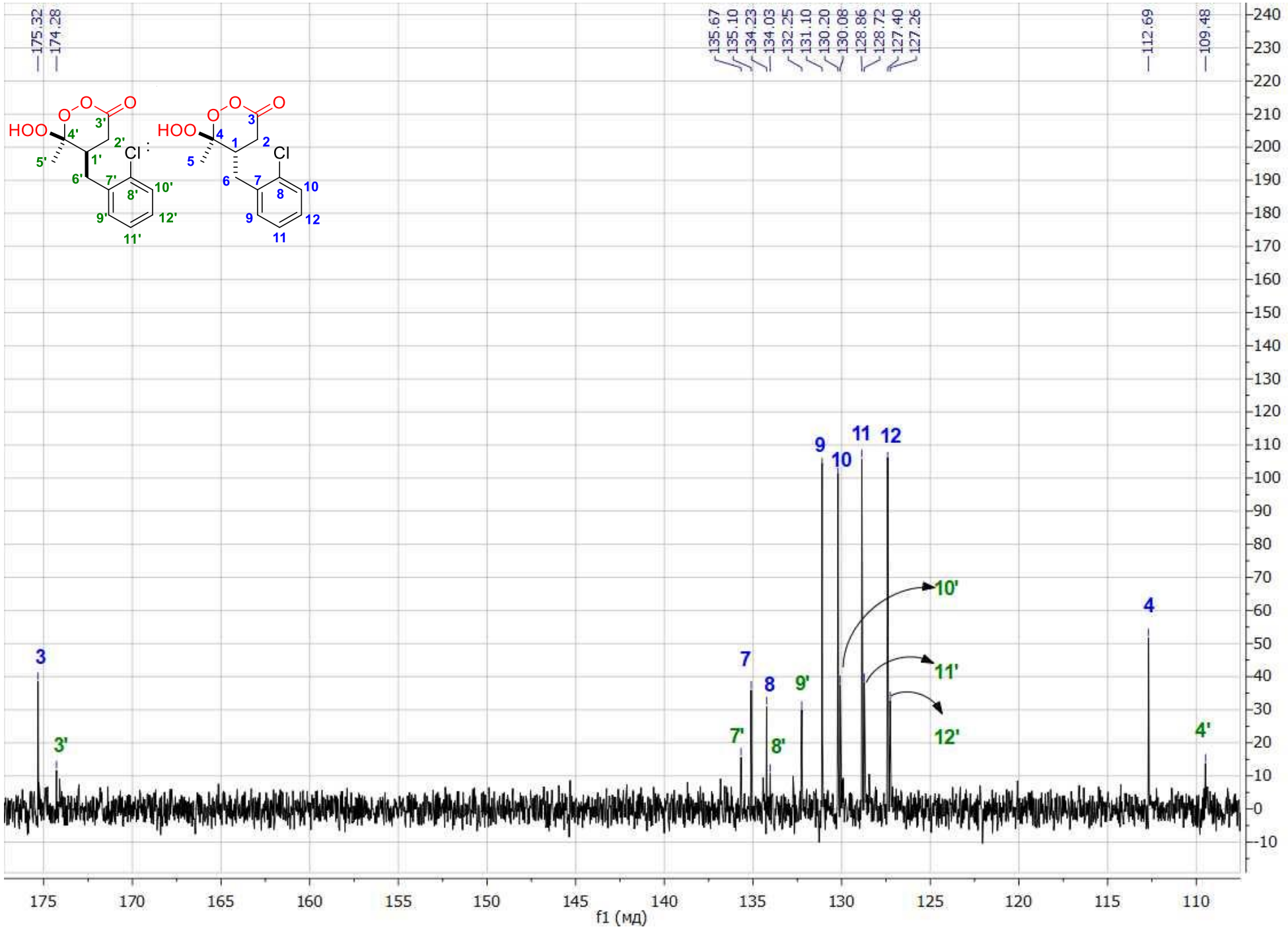

3.32
3.30
3.27
3.26
3.16
3.14
3.11
3.10
3.02
3.01
3.00
2.99
2.97
2.96
2.95
2.81
2.78
2.77
2.73
2.67
2.64
2.61
2.59
2.53
2.48
2.44
2.43
2.41
2.37
2.36
2.32
2.31
1.68
1.63
HOO
Cl
6'(1H)
6(1H)
1'(1H)
6(1H)
2'(1H)
1(1H), 2(2H), 2'(1H), 6'(1H)
5'(3H)
5(3H)
f1 (мд)


HOO
Cl
HOO
Cl
7.26 CDCl3
10
9, 11, 12
7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85 6.80 6.75 6.70 6.65 6.60 6.55 6.50 6.45
f1 (мд)

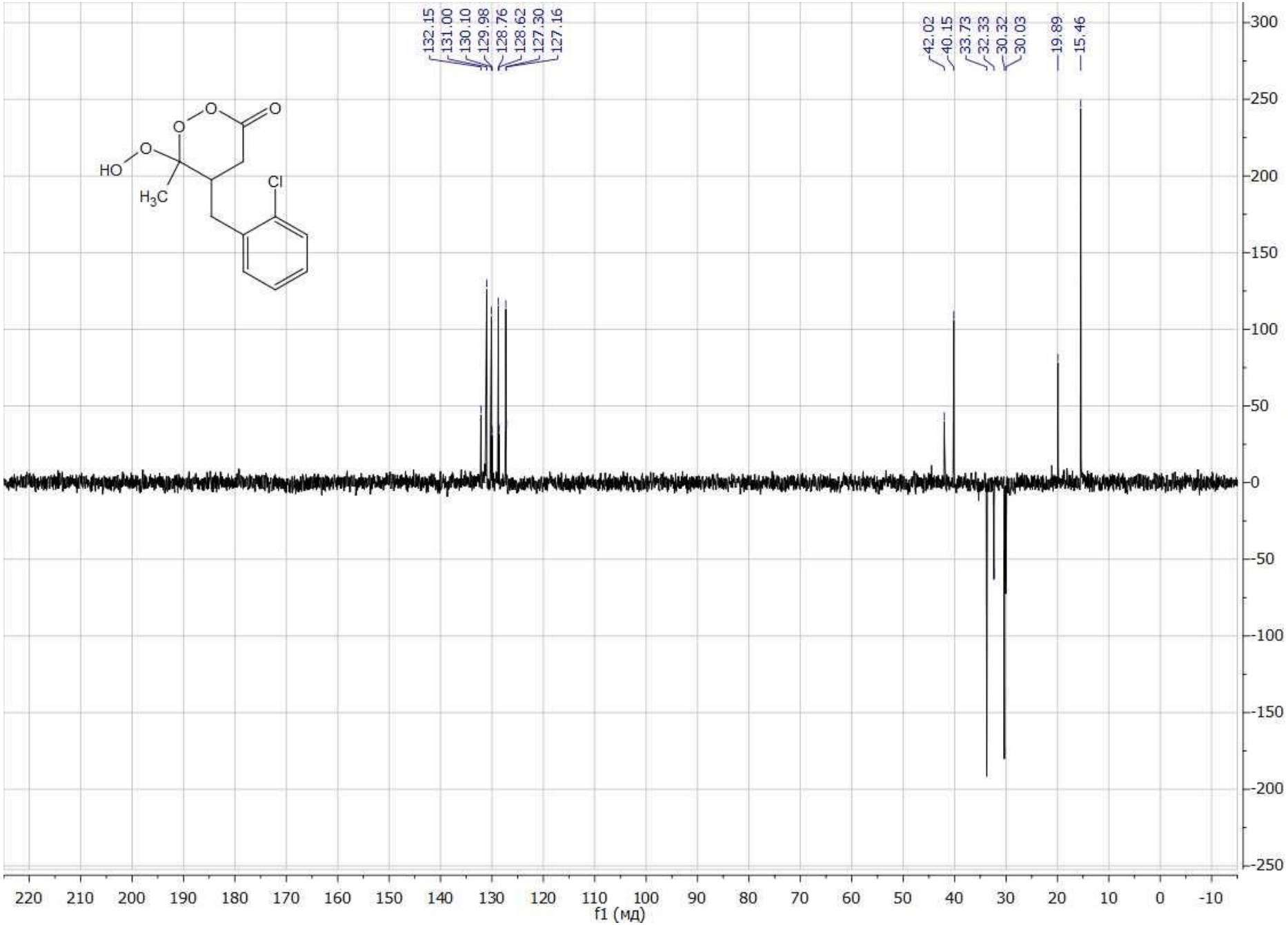
^{13}C NMR

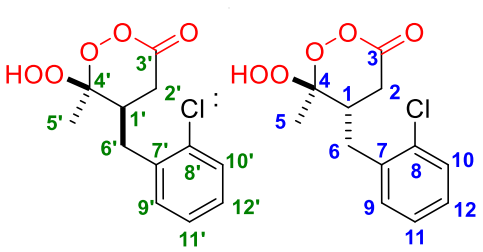

175.32
174.28
135.67
135.10
134.23
132.25
131.10
130.20
130.08
128.86
128.72
127.40
127.26
112.69
109.48
77.16 CDCl3
42.13
40.26
33.84
32.44
30.42
30.13
19.99
15.57
HO
O
O
O
O
H3C
Cl
250
200
150
100
50
0
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (мд)


42.13
40.26
33.84
32.44
30.42
30.13
19.99
15.57
HOO
Cl
1
6
2
5
1'
6'
2'
5'
f1 (мд)

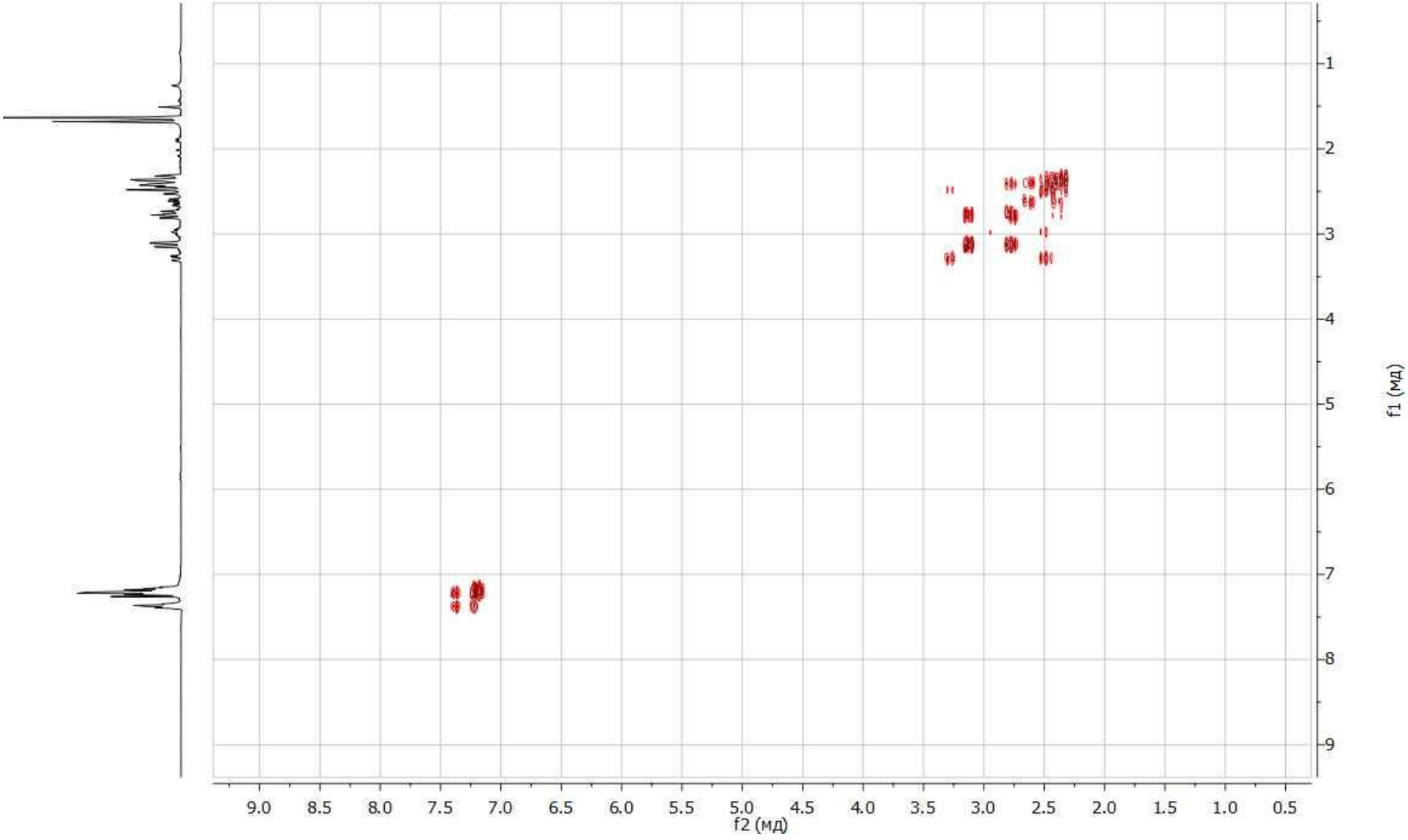

175.32
174.28
135.67
135.10
134.23
134.03
132.25
131.10
130.20
130.08
128.86
128.72
127.40
127.26
112.69
109.48
HOO
Cl
3
3'
7
8
9'
7'
8'
9
10
11
12
10'
11'
12'
4
4'
f1 (мд)

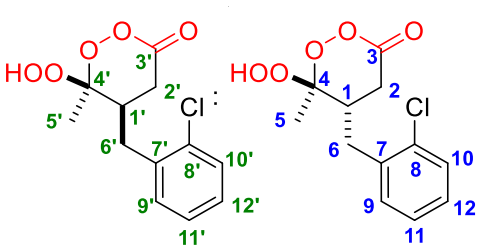
^{13}C_deptsp135



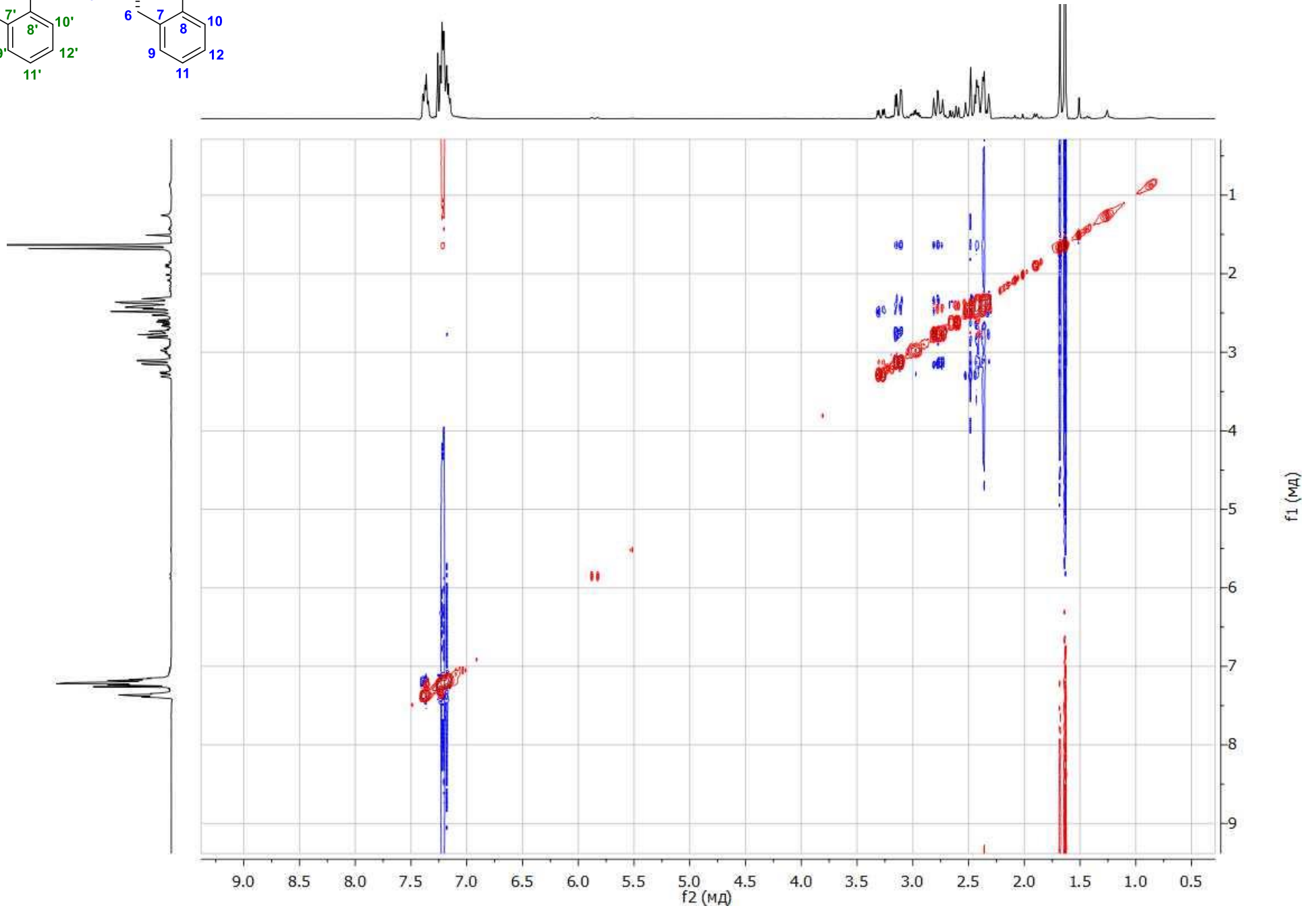

HOO
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
9'
10'
11'
12'
Cl
:
HOO
O
O
O
3
4
1
2
5
6
7
8
9
10
11
12
Cl

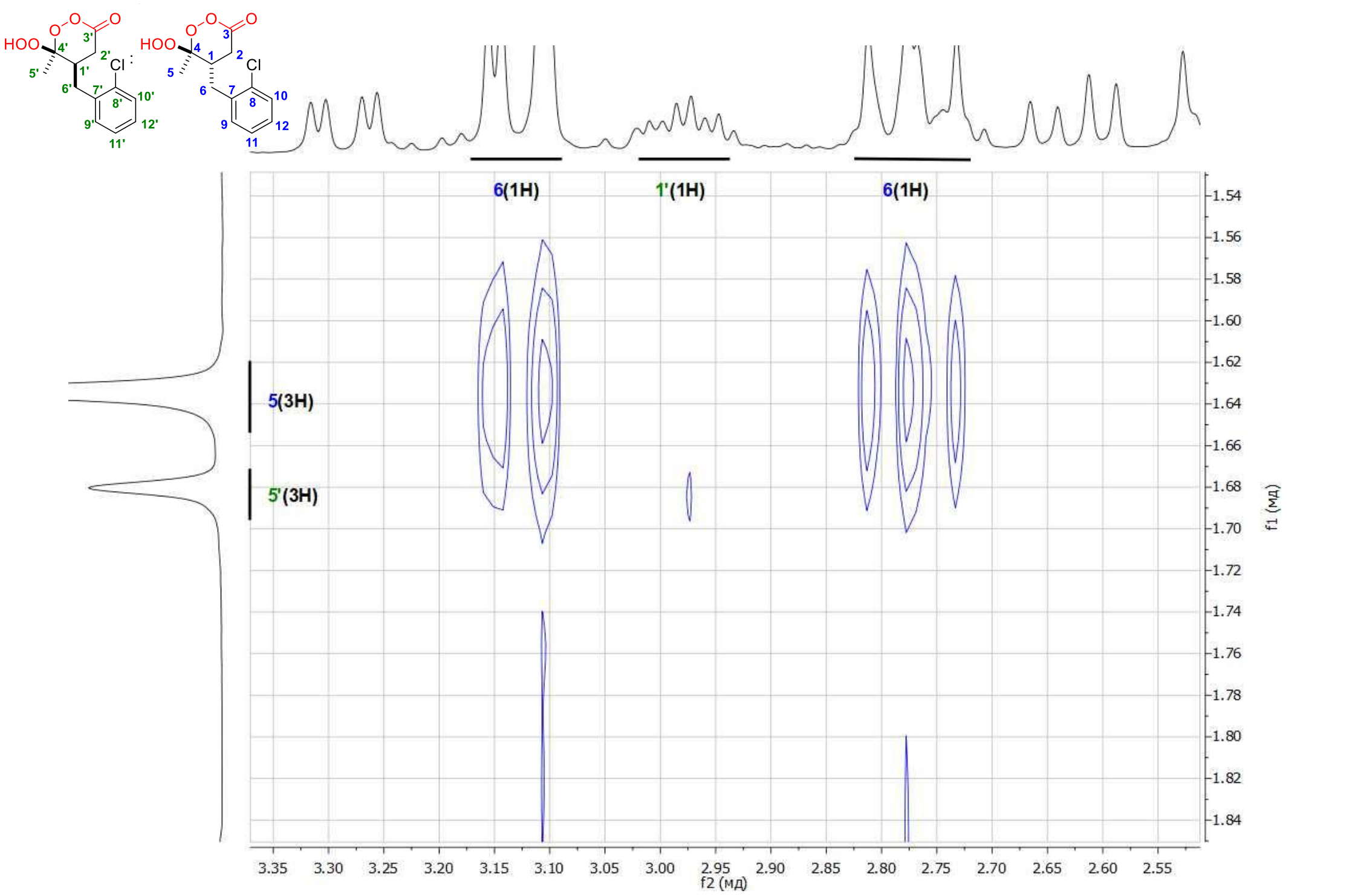
{^{1}H-^{1}H} COSY

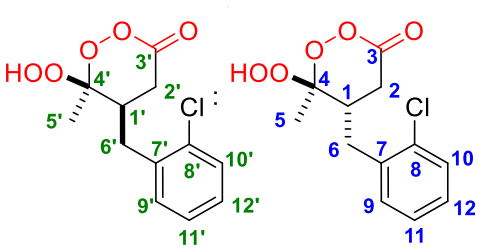

9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (мд)
1
2
3
4
5
6
7
8
9
f1 (мд)


HOO
O
O
O
3'
4'
2'
5'
1'
Cl
6'
7'
8'
10'
9'
12'
11'
HOO
O
O
O
3
4
1
2
5
Cl
6
7
8
10
9
12
11

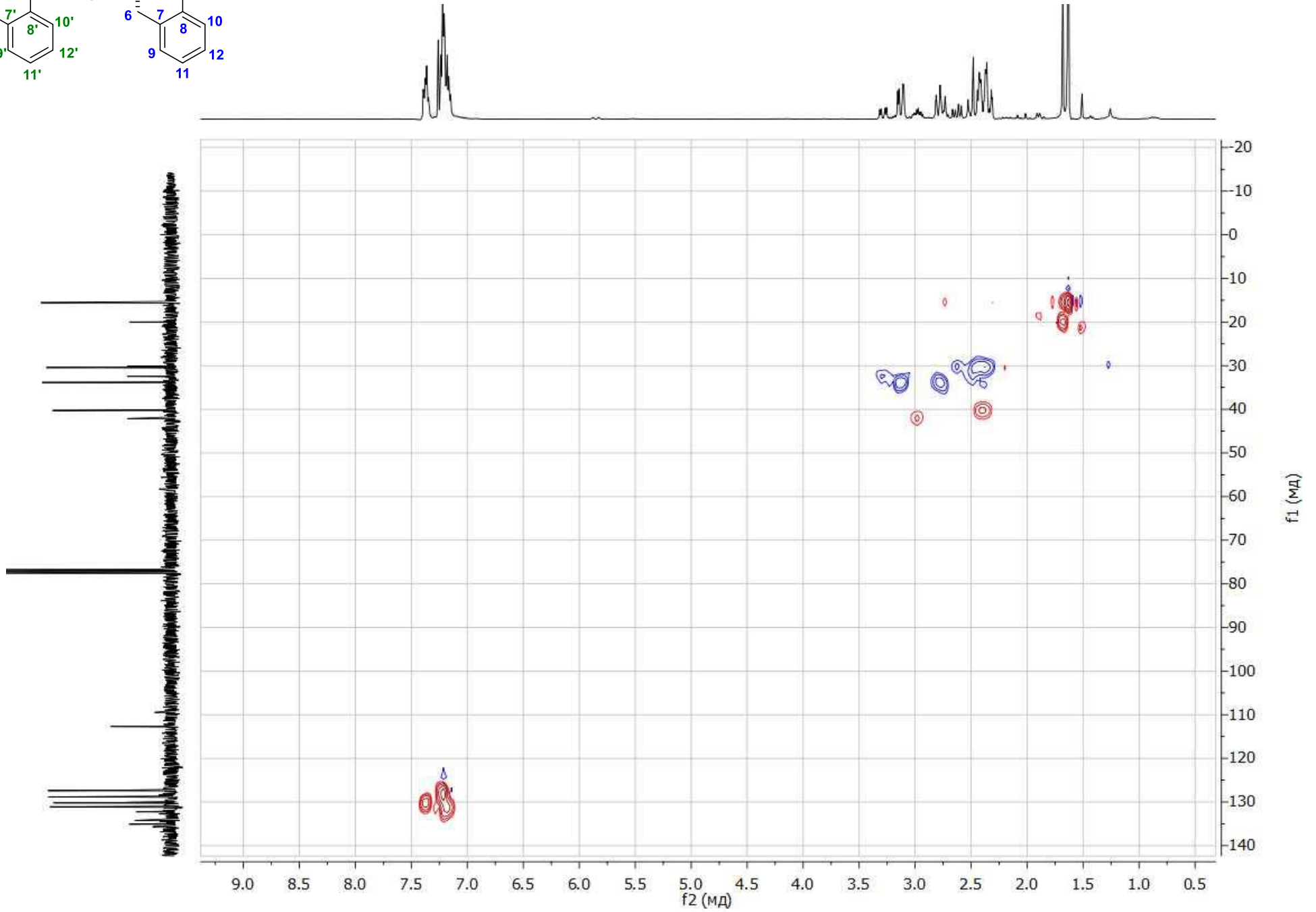
{^{1}H-^{1}H} NOESY

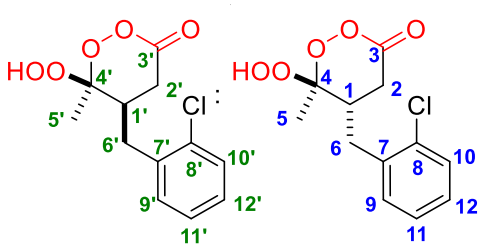

9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (мд)
1
2
3
4
5
6
7
8
9
f1 (мд)


6(1H)
1'(1H)
6(1H)
5(3H)
5'(3H)
f2 (мд)
f1 (мд)

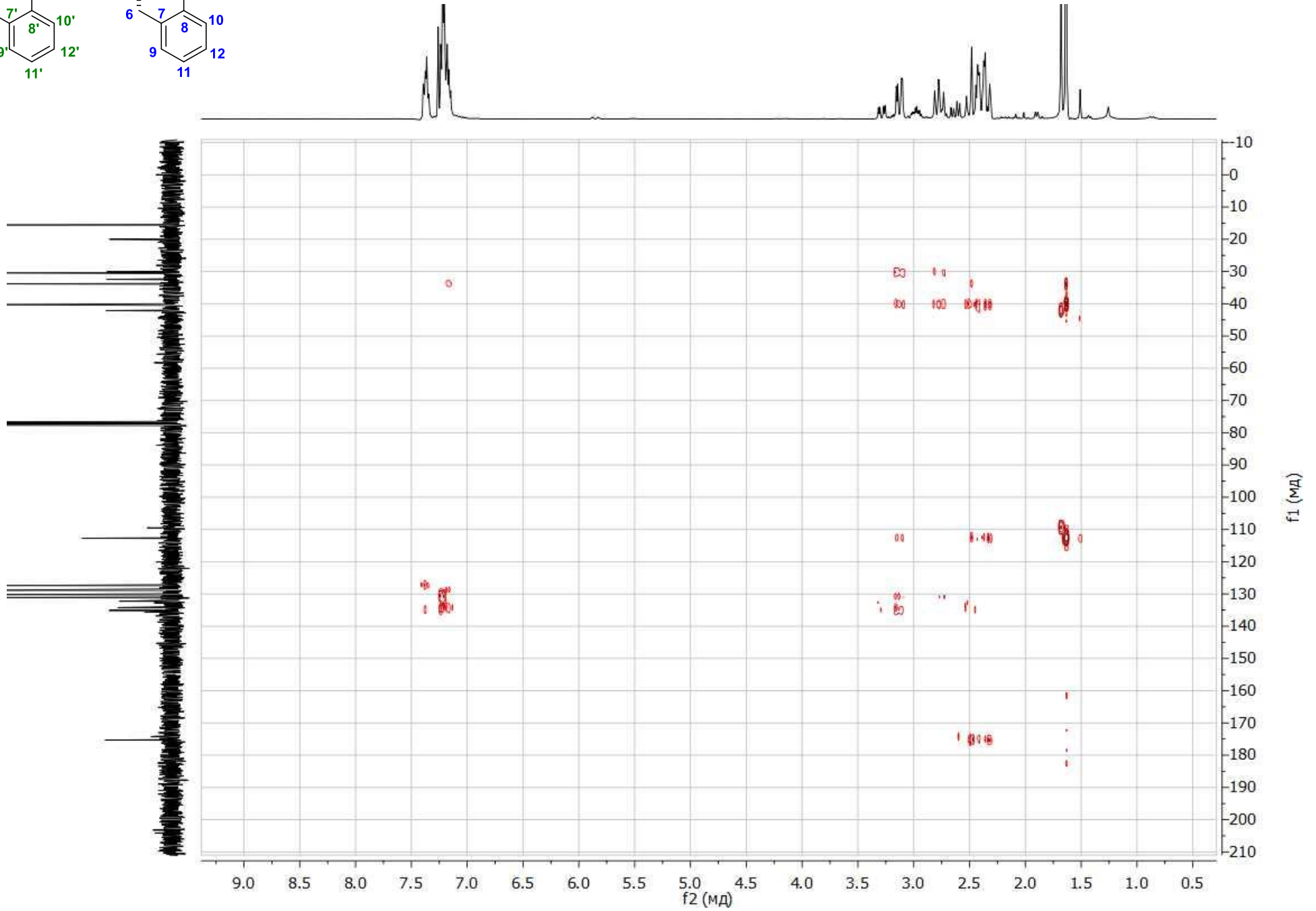

HOO
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
9'
10'
11'
12'
Cl
HOO
O
O
O
3
4
1
2
5
6
7
8
9
10
11
12
Cl

{^{1}H-^{13}C} HSQC


f2 (мд)
f1 (мд)
9.0
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
-20
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140

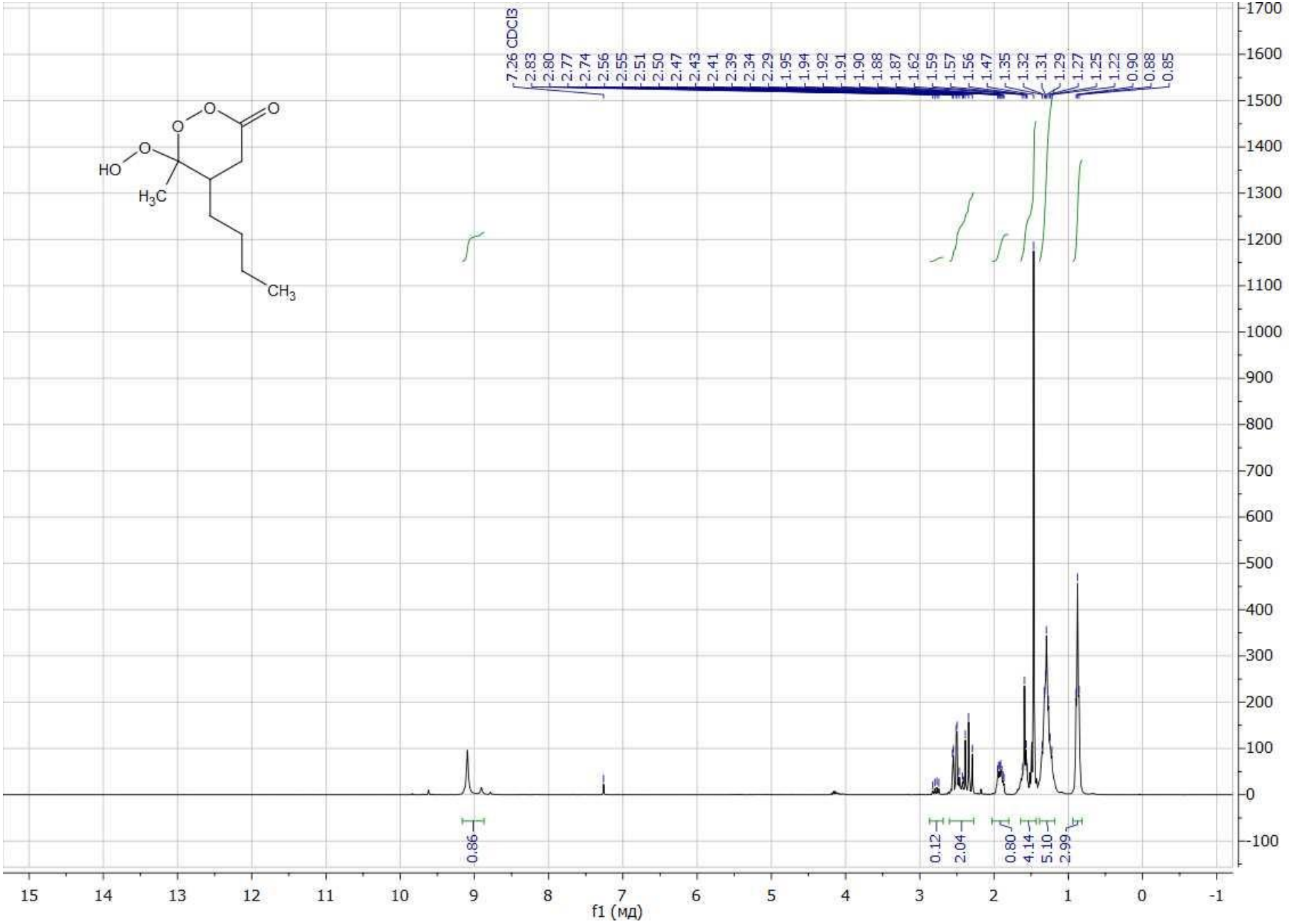

HOO
O
O
O
3'
4'
2'
5'
1'
Cl
6'
7'
8'
10'
9'
12'
11'
HOO
O
O
O
3
4
1
2
5
Cl
6
7
8
10
9
12
11

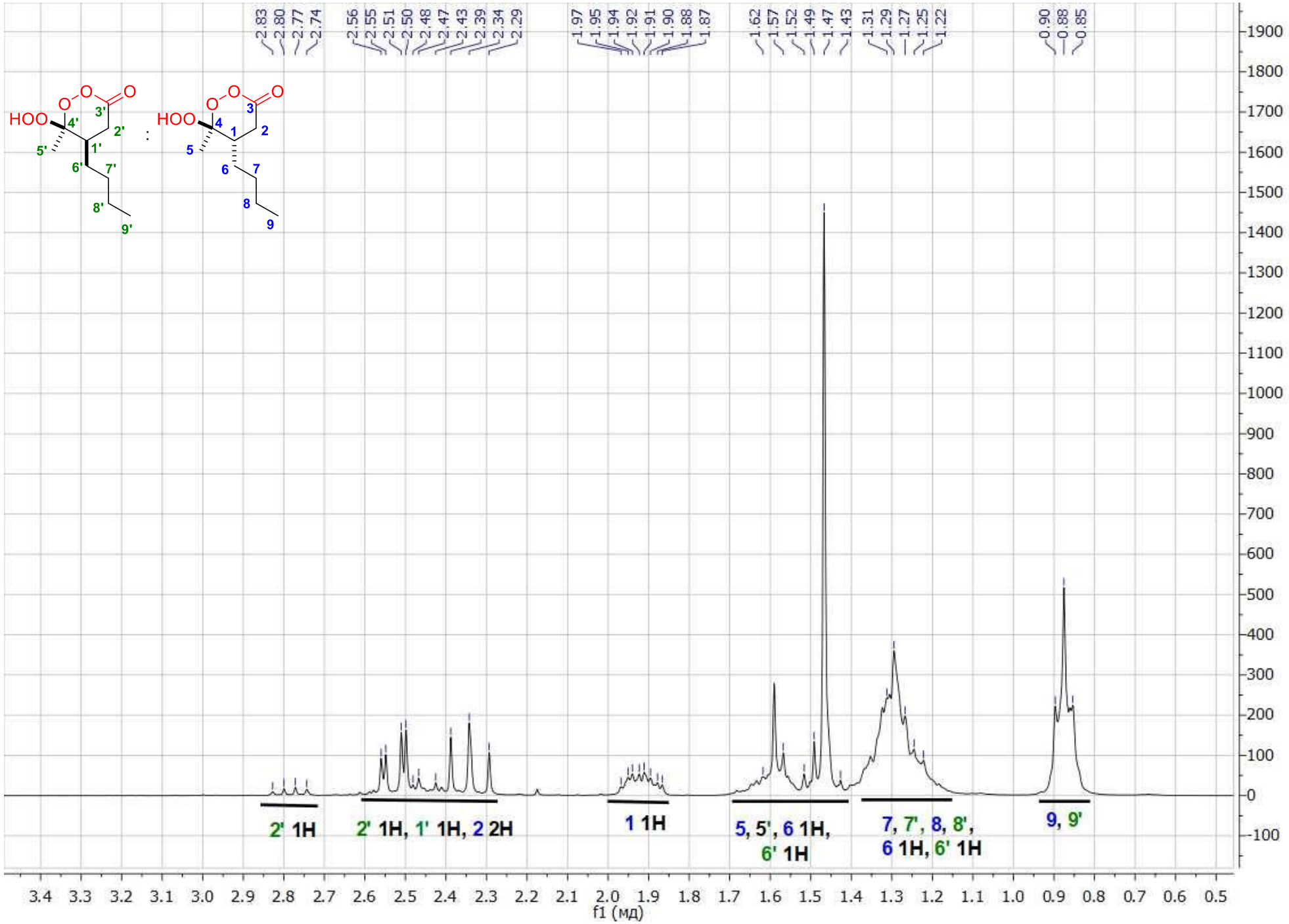
{^{1}H-^{13}C} HMBC


f2 (мд)
f1 (мд)
9.0
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
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210

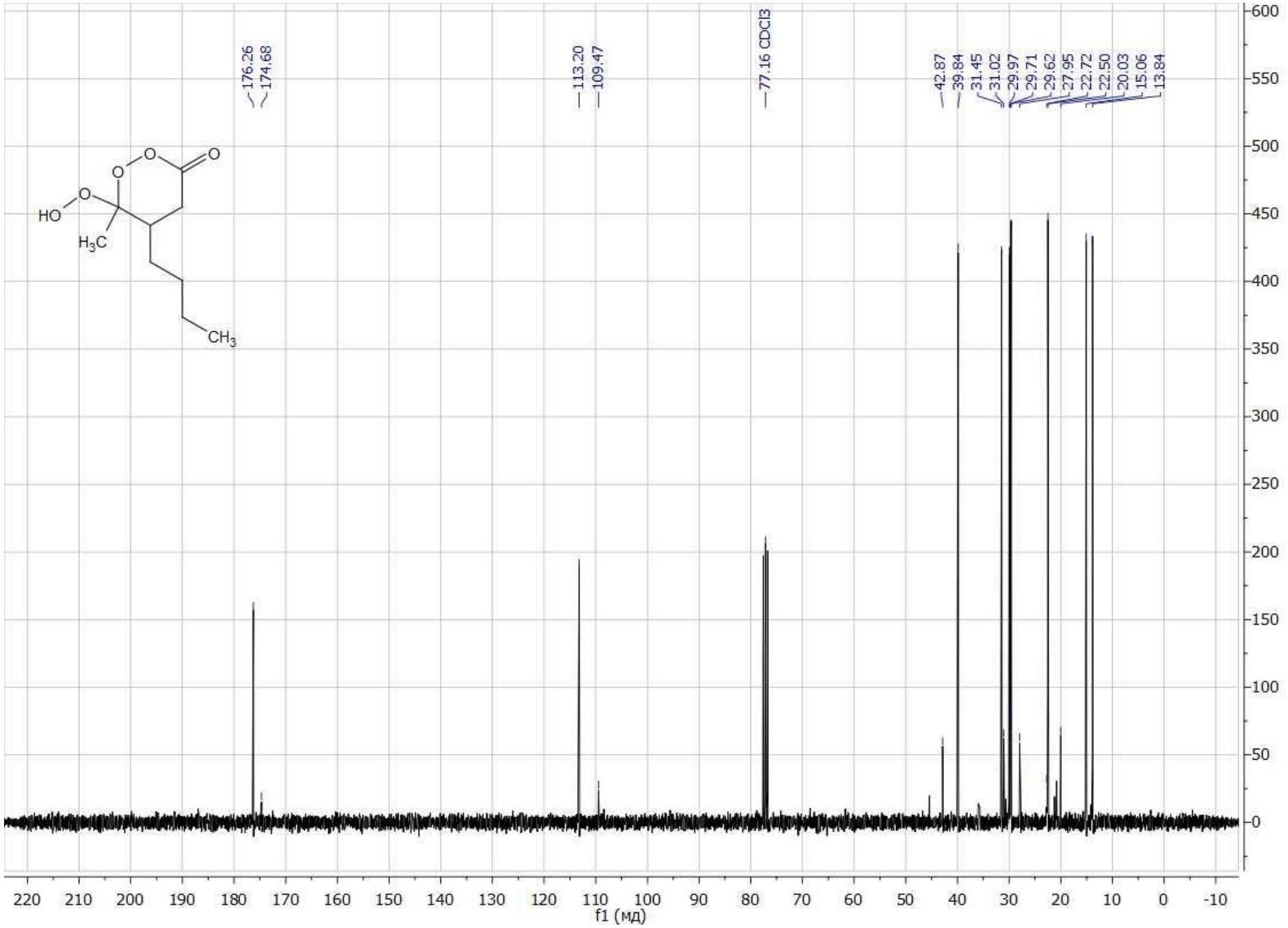
5-Butyl-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2j

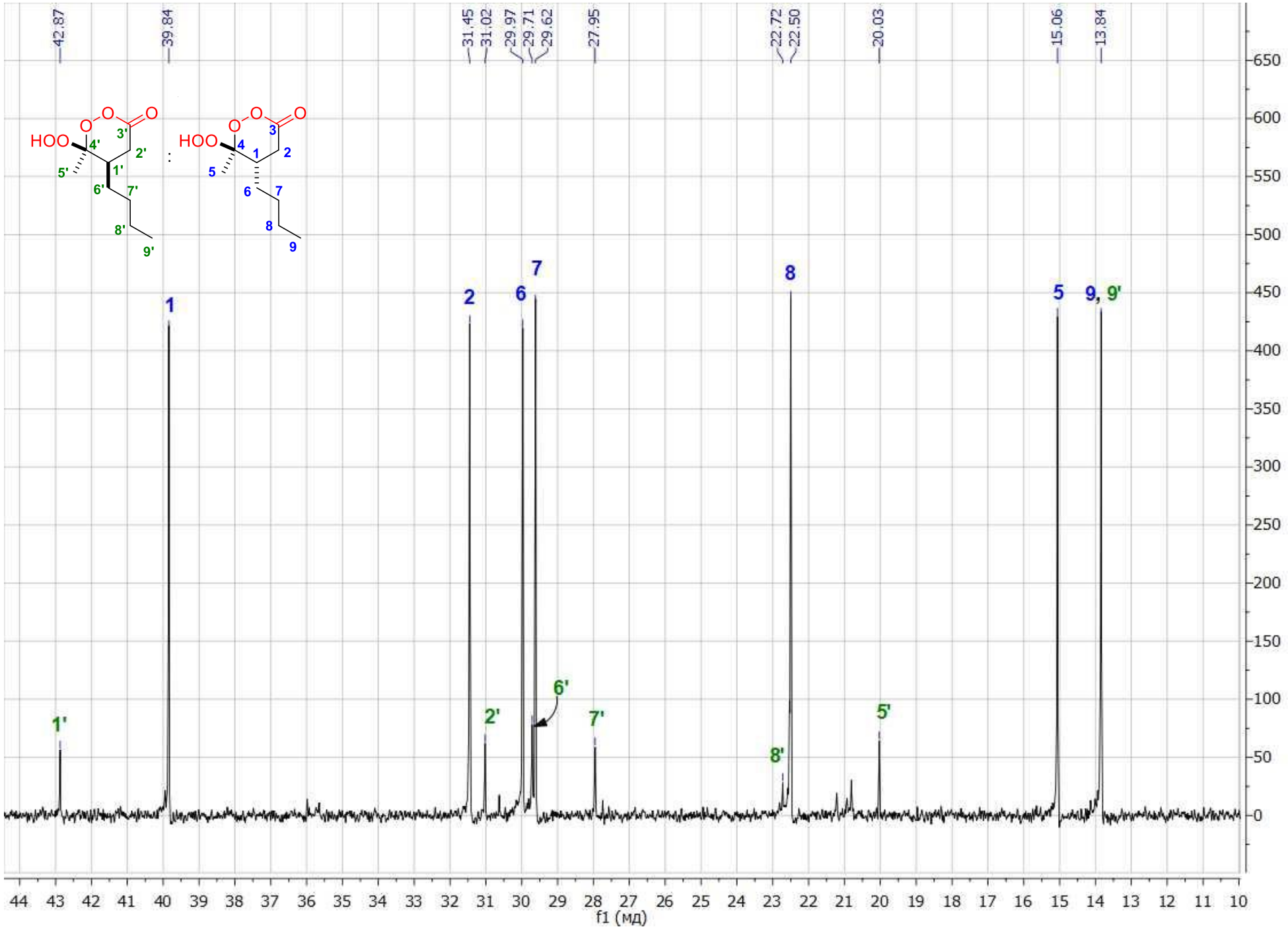
^{1}H NMR

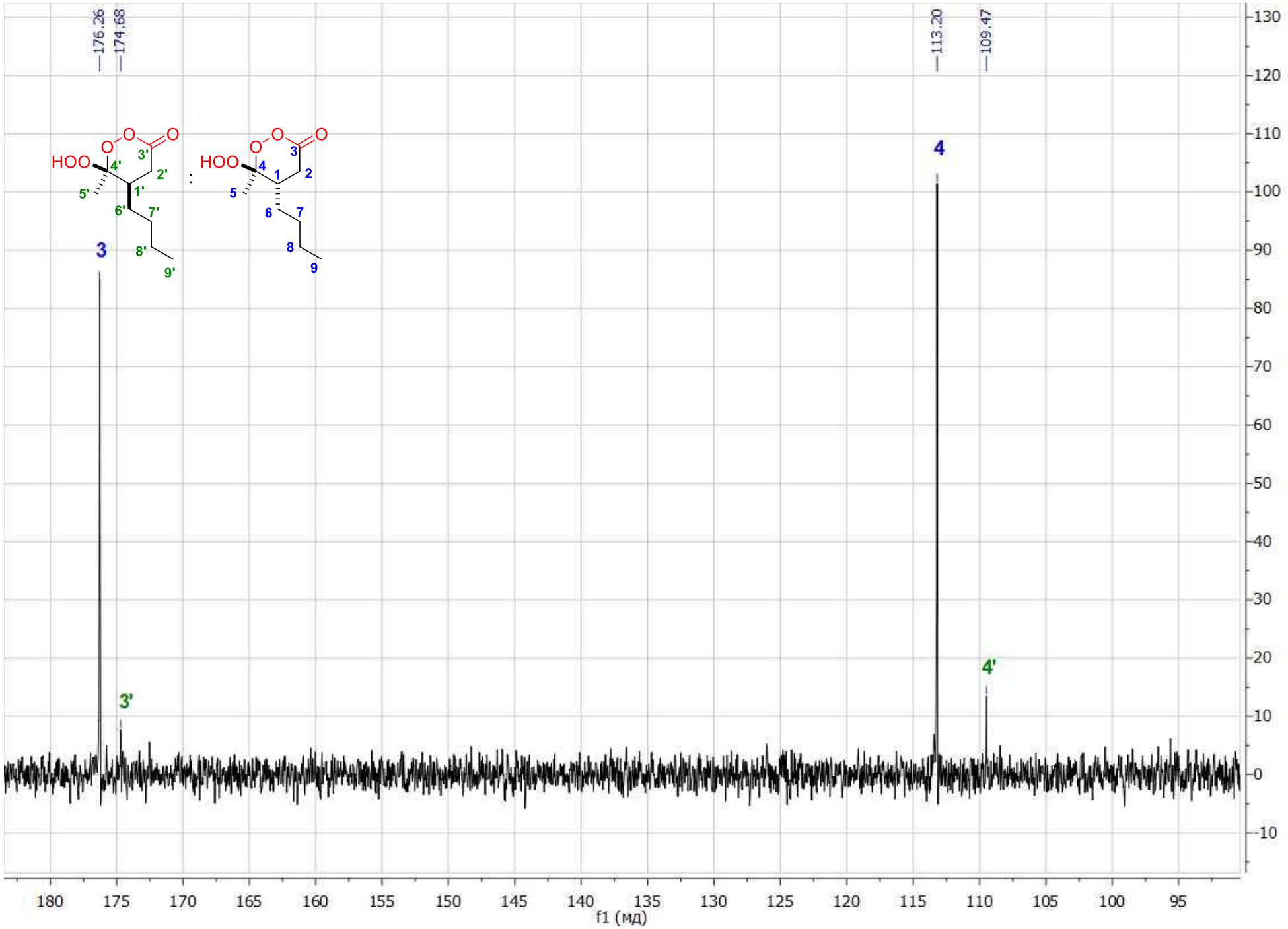



2.83 2.80 2.77 2.74 2.56 2.55 2.51 2.50 2.48 2.47 2.43 2.39 2.34 2.29 1.97 1.95 1.94 1.92 1.91 1.90 1.88 1.87 1.62 1.57 1.52 1.49 1.47 1.43 1.31 1.29 1.27 1.25 1.22 0.90 0.88 0.85
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
HOO
O
O
O
3
4
1
2
5
6
7
8
9
2' 1H
2' 1H, 1' 1H, 2 2H
1 1H
5, 5', 6 1H, 6' 1H
7, 7', 8, 8', 6 1H, 6' 1H
9, 9'
f1 (мд)

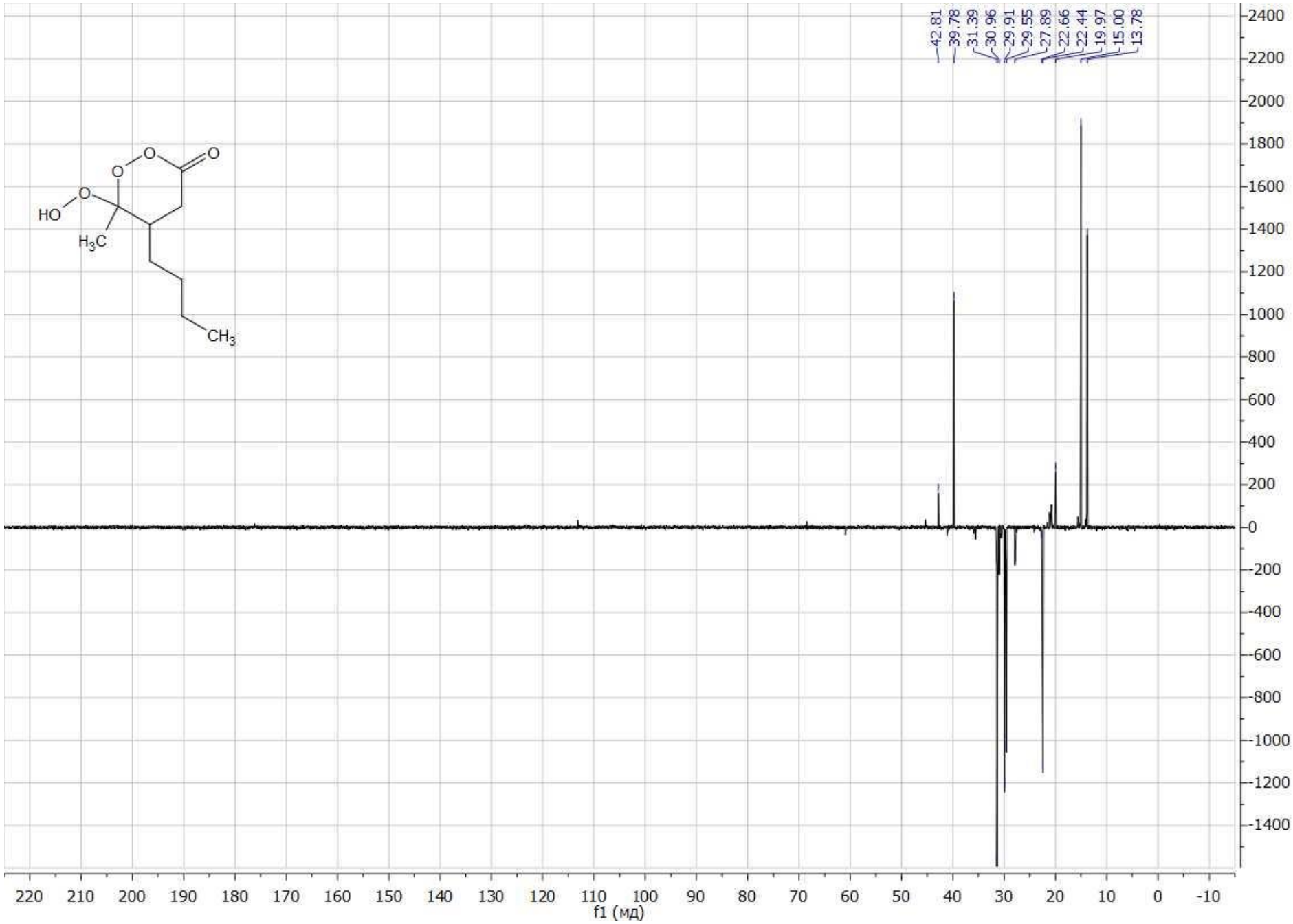
^{13}C NMR

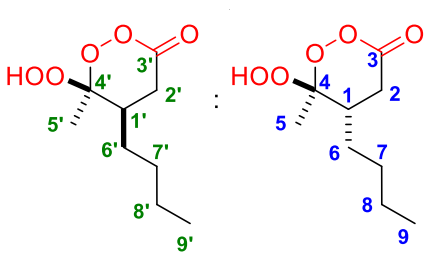

176.26
174.68
113.20
109.47
77.16 CDCl3
42.87
39.84
31.45
31.02
29.97
29.71
29.62
27.95
22.72
22.50
20.03
15.06
13.84
HO
O
O
O
O
H3C
CH3
600
550
500
450
400
350
300
250
200
150
100
50
0
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (мд)


42.87
39.84
31.45
31.02
29.97
29.71
29.62
27.95
22.72
22.50
20.03
15.06
13.84
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
HOO
O
O
O
3
4
1
2
5
6
7
8
9
1
2
6
7
8
5
9, 9'
1'
2'
6'
7'
8'
5'
650
600
550
500
450
400
350
300
250
200
150
100
50
0
44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26 25 24 23 22 21 20 19 18 17 16 15 14 13 12 11 10
f1 (мд)

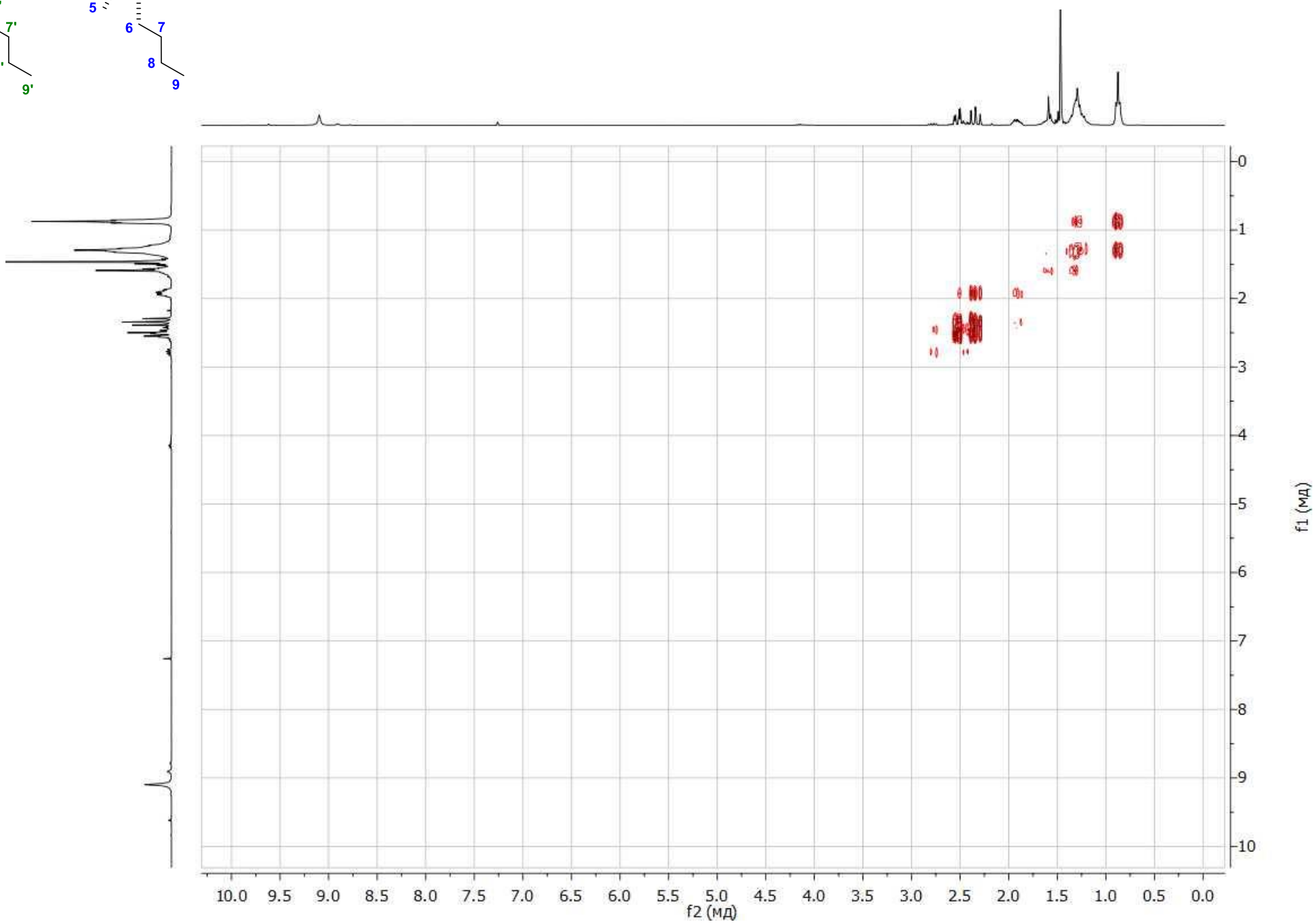

176.26
174.68
113.20
109.47
HOO
3'
4'
2'
5'
1'
6'
7'
8'
9'
3
HOO
3
4
1
2
5
6
7
8
9
4
3'
4'
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
95
f1 (мд)

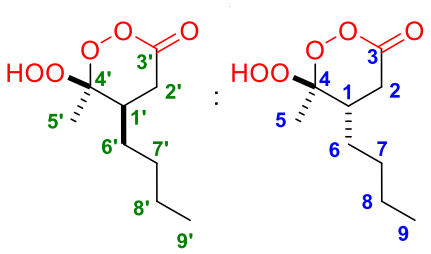
^{13}C_deptsp135



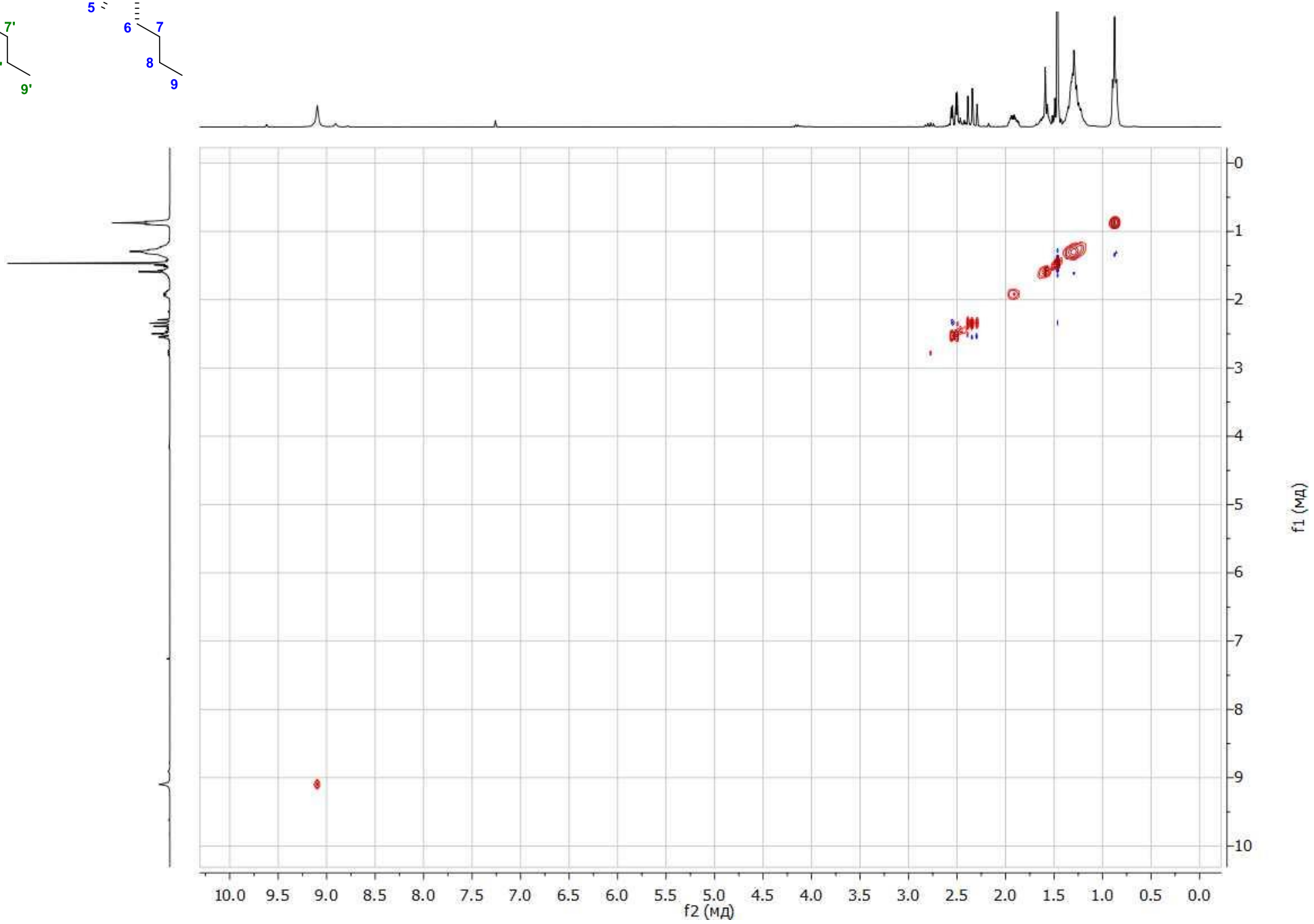

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
:
HOO
O
O
O
3
4
1
2
5
6
7
8
9

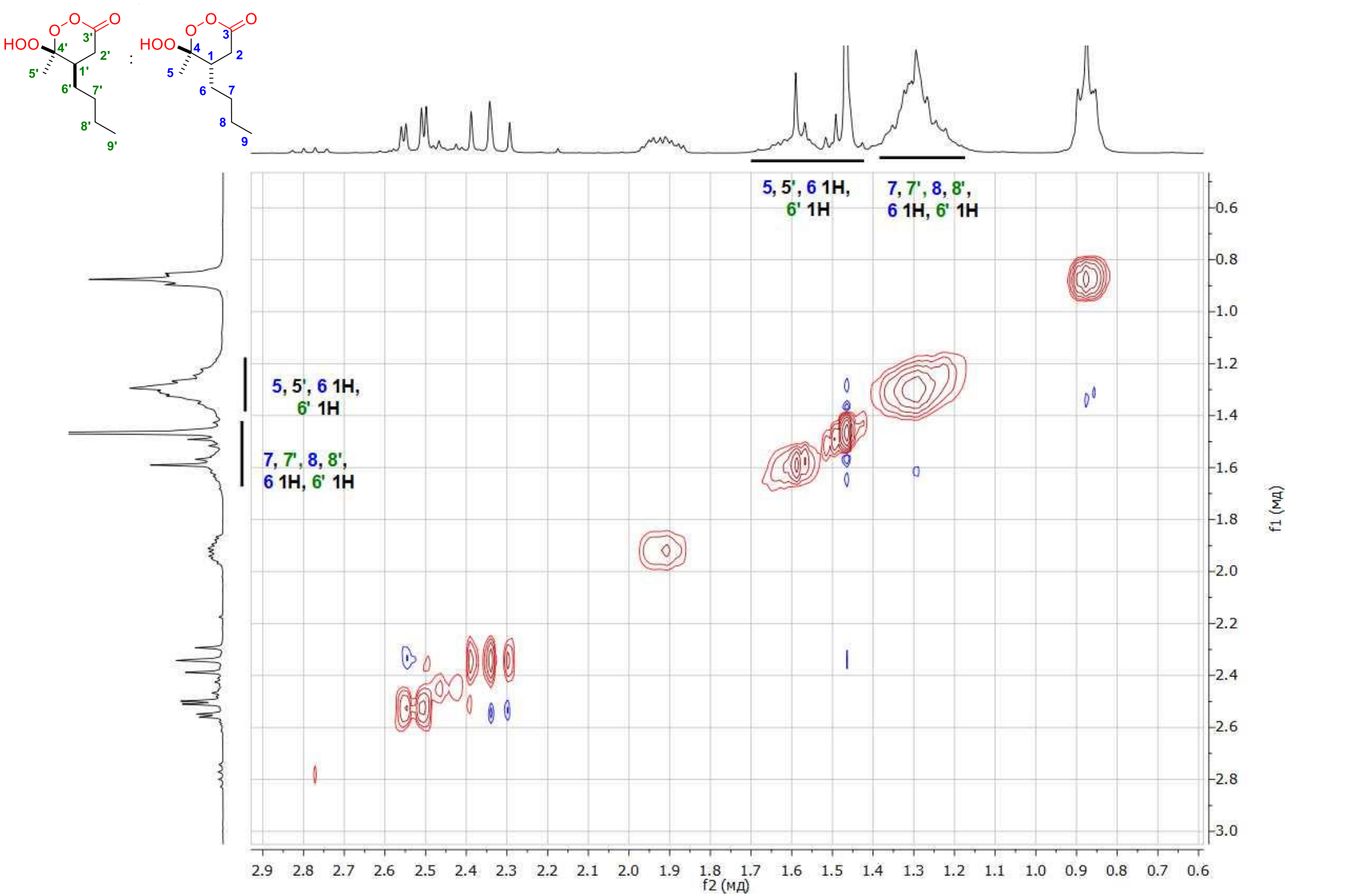
{^{1}H-^{1}H} COSY

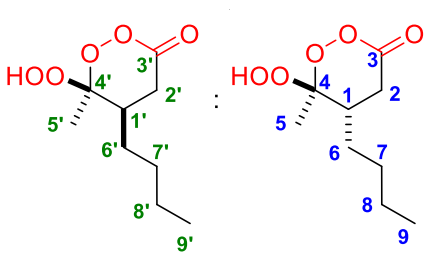

0
1
2
3
4
5
6
7
8
9
10
f1 (мд)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f2 (мд)


HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
:
HOO
O
O
O
3
4
2
1
5
6
7
8
9

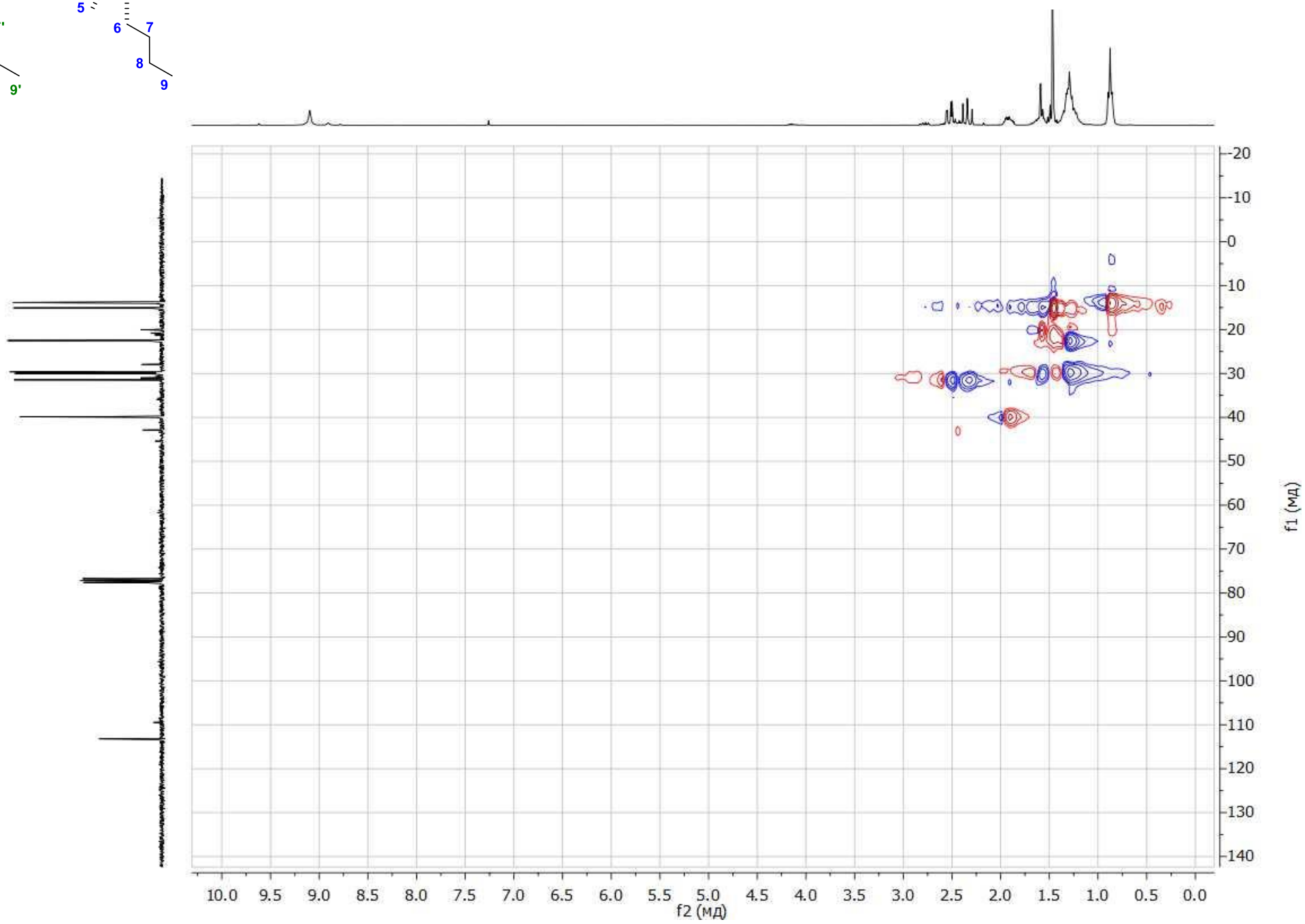
{^{1}H-^{1}H} NOESY

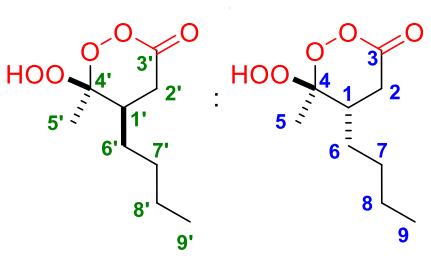

0
1
2
3
4
5
6
7
8
9
10
f1 (мд)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f2 (мд)


HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
:
HOO
O
O
O
3
4
2
1
5
6
7
8
9
5, 5', 6 1H,
6' 1H
7, 7', 8, 8',
6 1H, 6' 1H
5, 5', 6 1H,
6' 1H
7, 7', 8, 8',
6 1H, 6' 1H
f2 (мд)
f1 (мд)

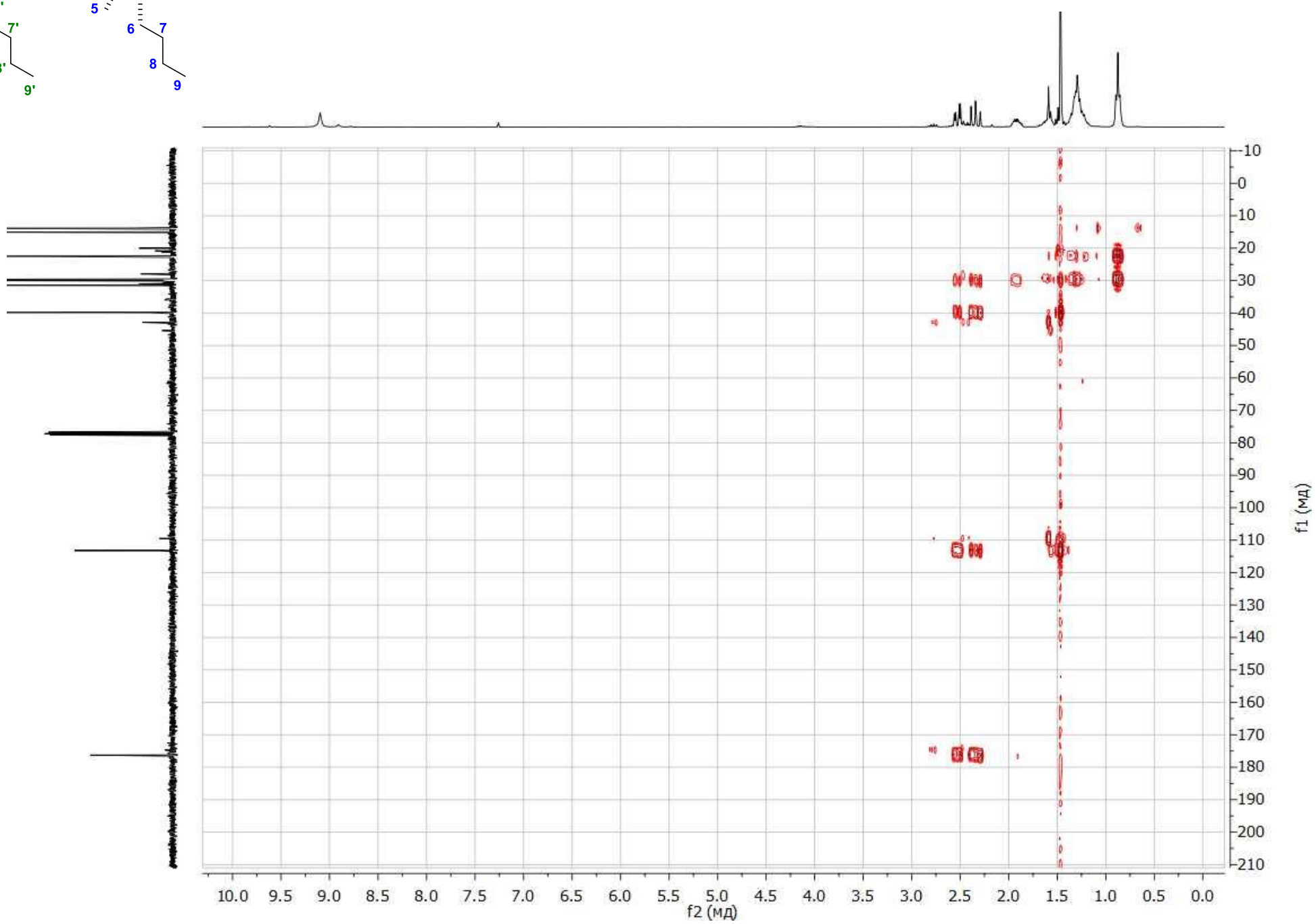

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
:
HOO
O
O
O
3
4
1
2
5
6
7
8
9

{^{1}H-^{13}C} HSQC


-20
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
f1 (мд)
10.0
9.5
9.0
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
f2 (мд)

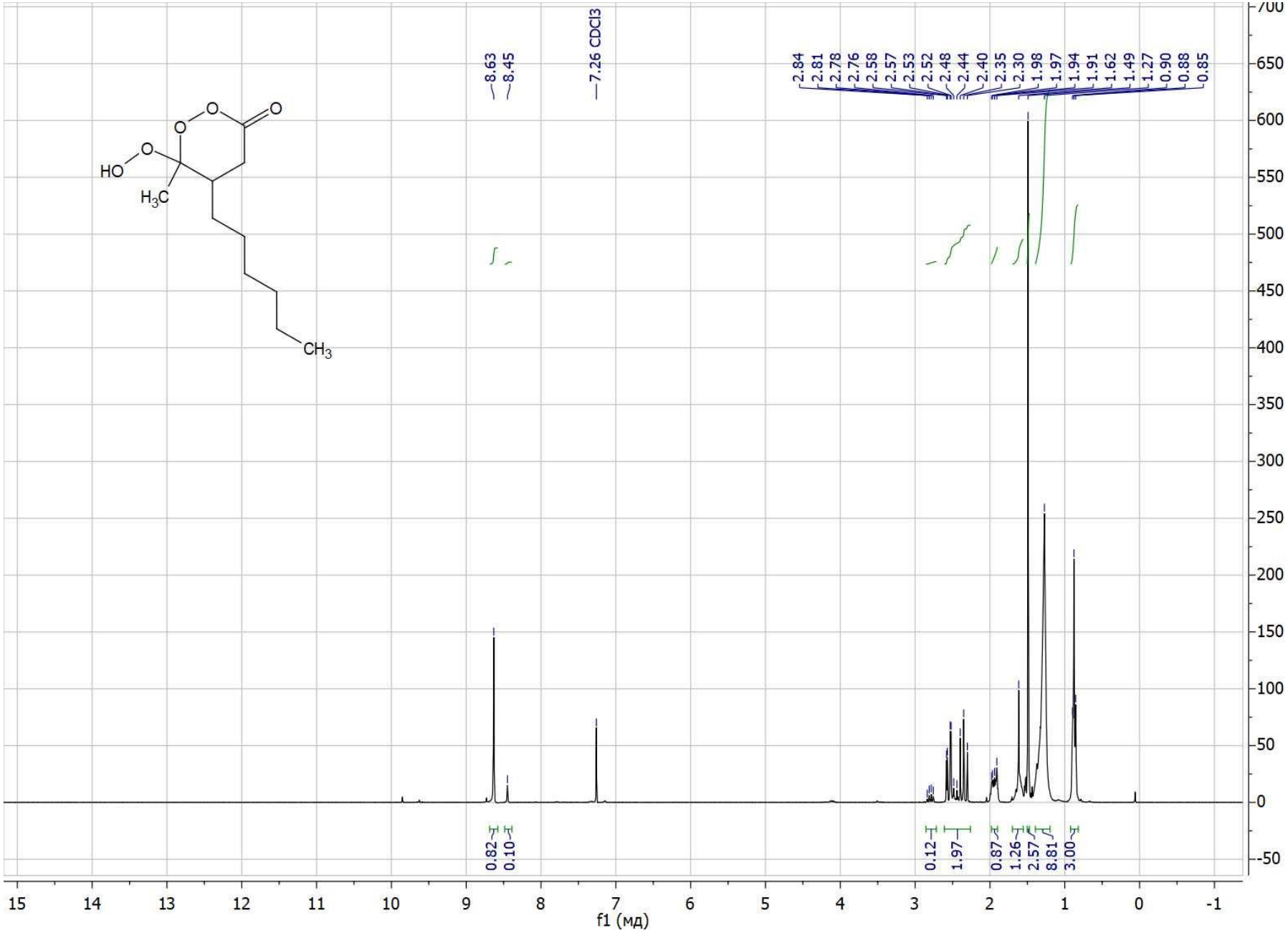

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
HOO
O
O
3
4
1
2
5
6
7
8
9

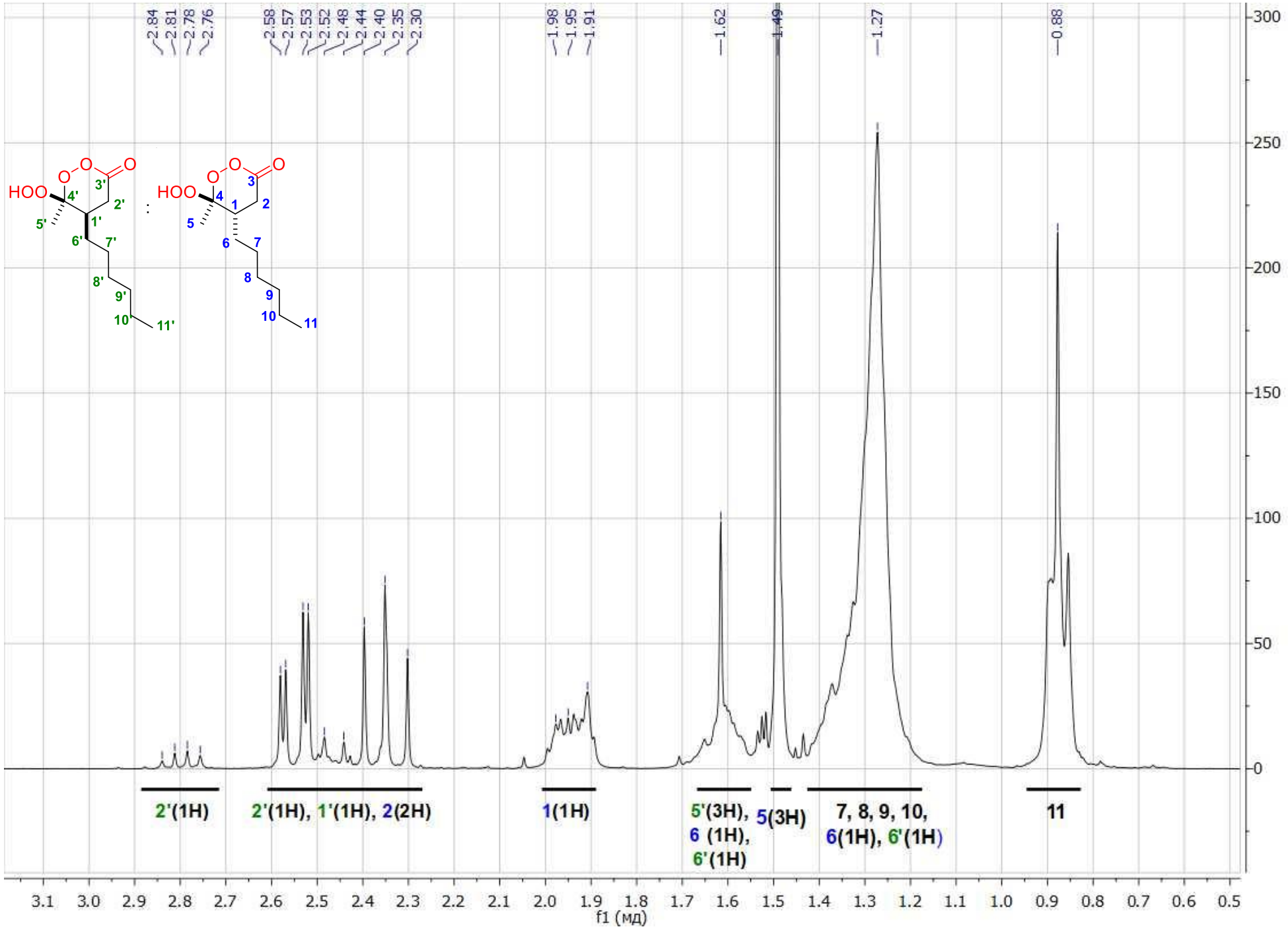
{^{1}H-^{13}C} HMBC


10.0
9.5
9.0
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
f2 (мд)
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
f1 (мд)

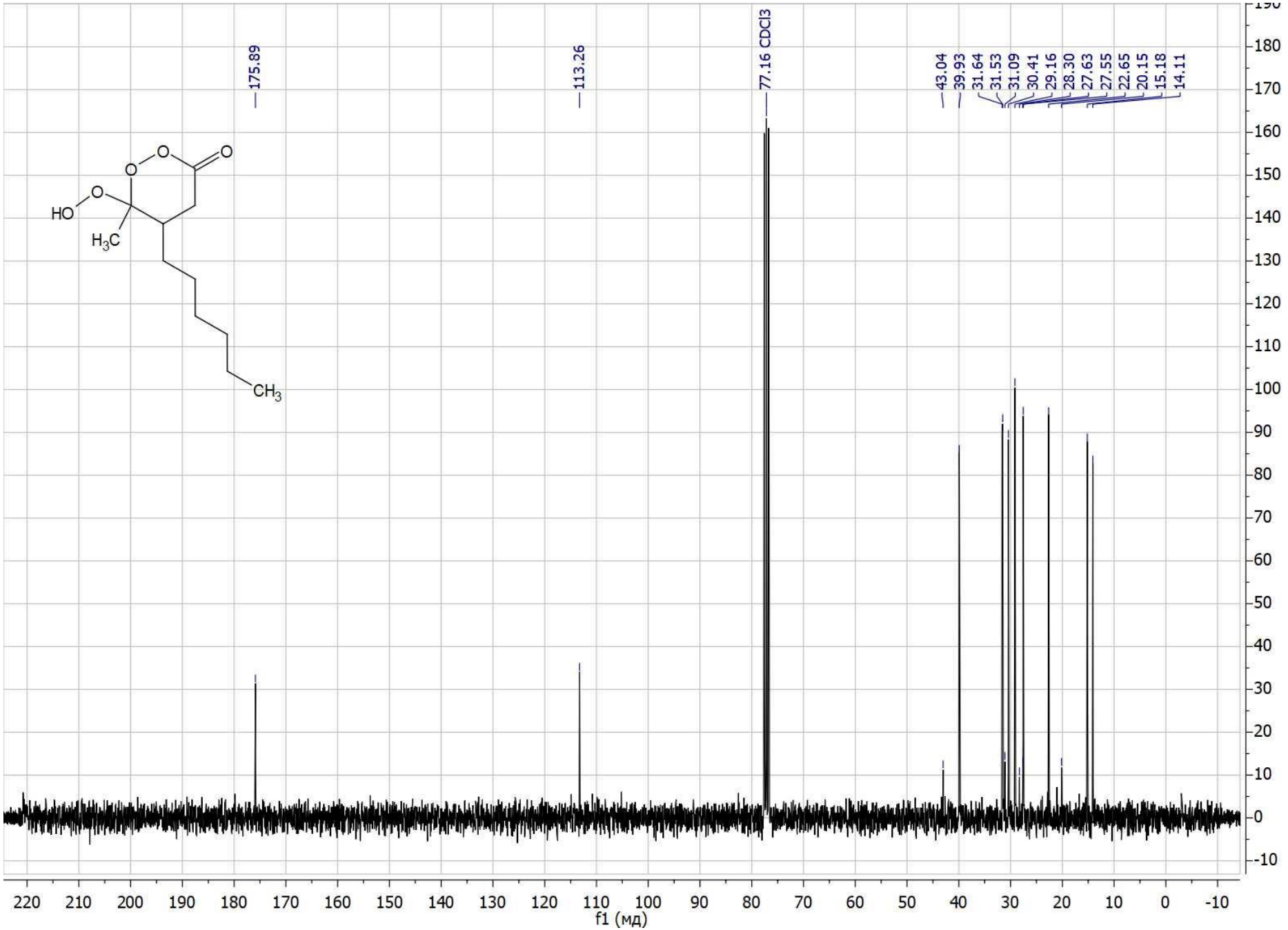
5-Hexyl-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2k

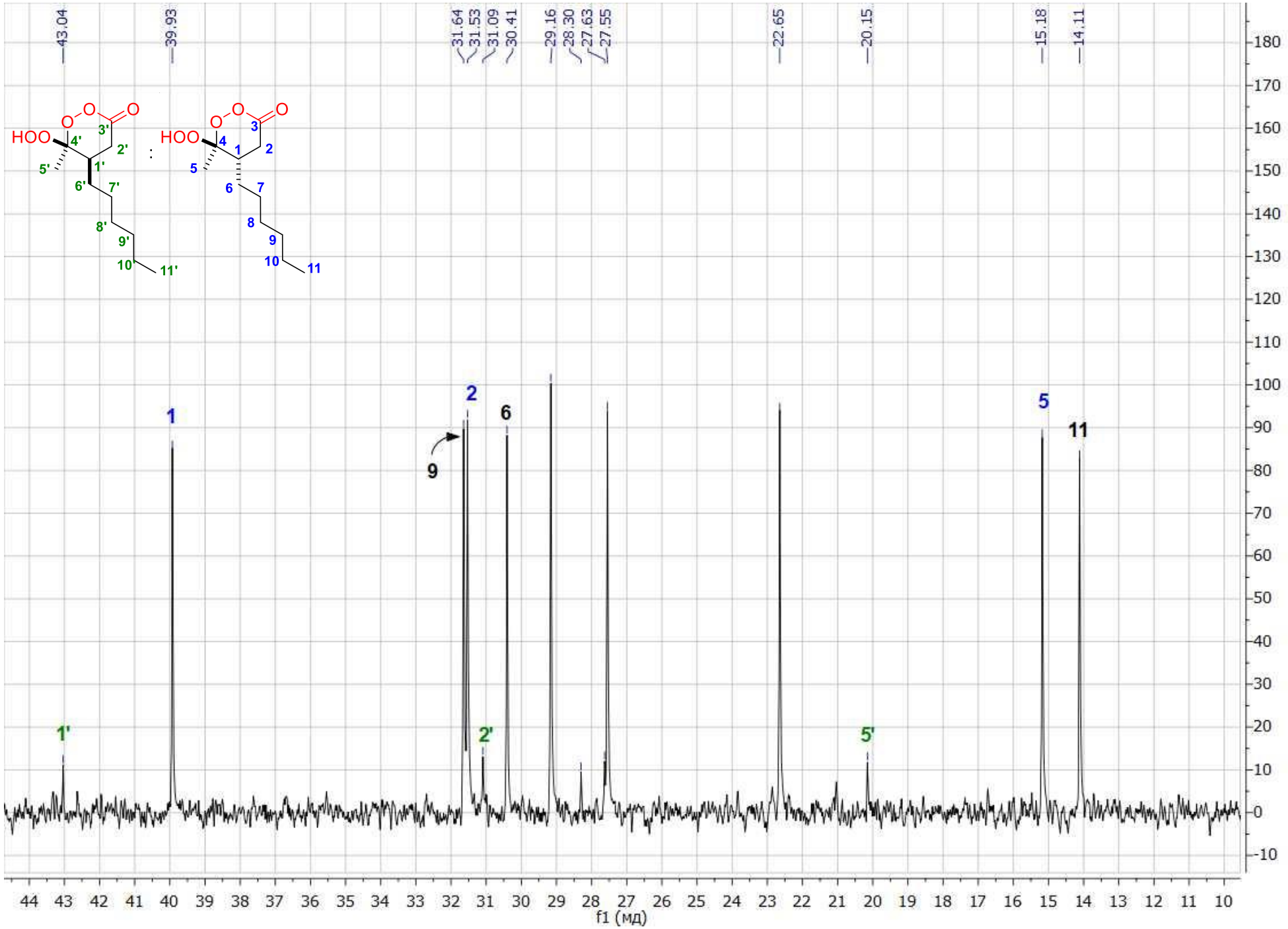
^{1}H NMR

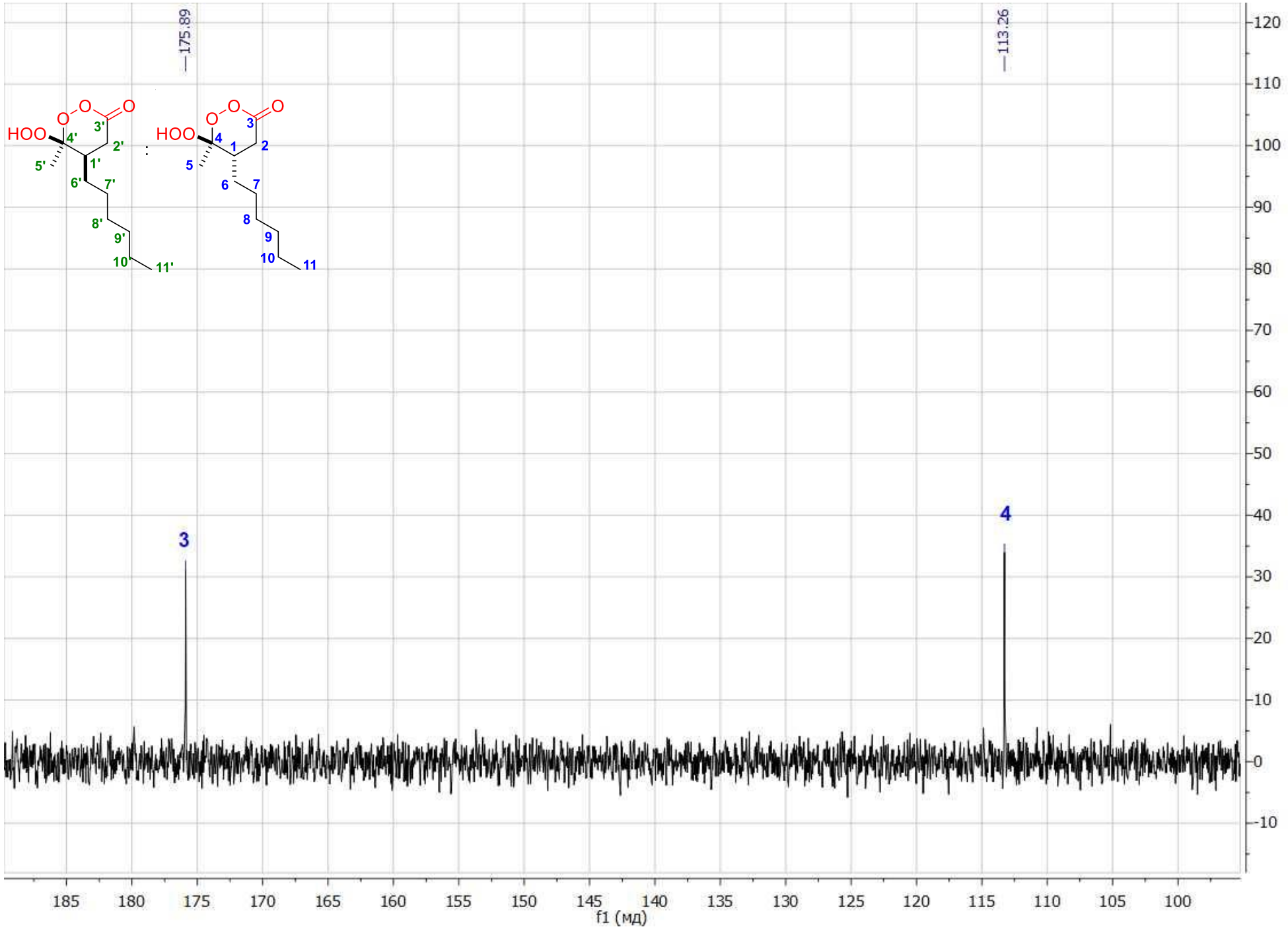



2.84
2.81
2.78
2.76
2.58
2.57
2.53
2.52
2.48
2.44
2.40
2.35
2.30
1.98
1.95
1.91
1.62
1.49
1.27
0.88
HOO
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
9'
10
11'
:
HOO
O
O
O
3
4
1
2
5
6
7
8
9
10
11
2'(1H)
2'(1H), 1'(1H), 2(2H)
1(1H)
5'(3H),
6 (1H),
6'(1H)
5(3H)
7, 8, 9, 10,
6(1H), 6'(1H)
11
f1 (мд)

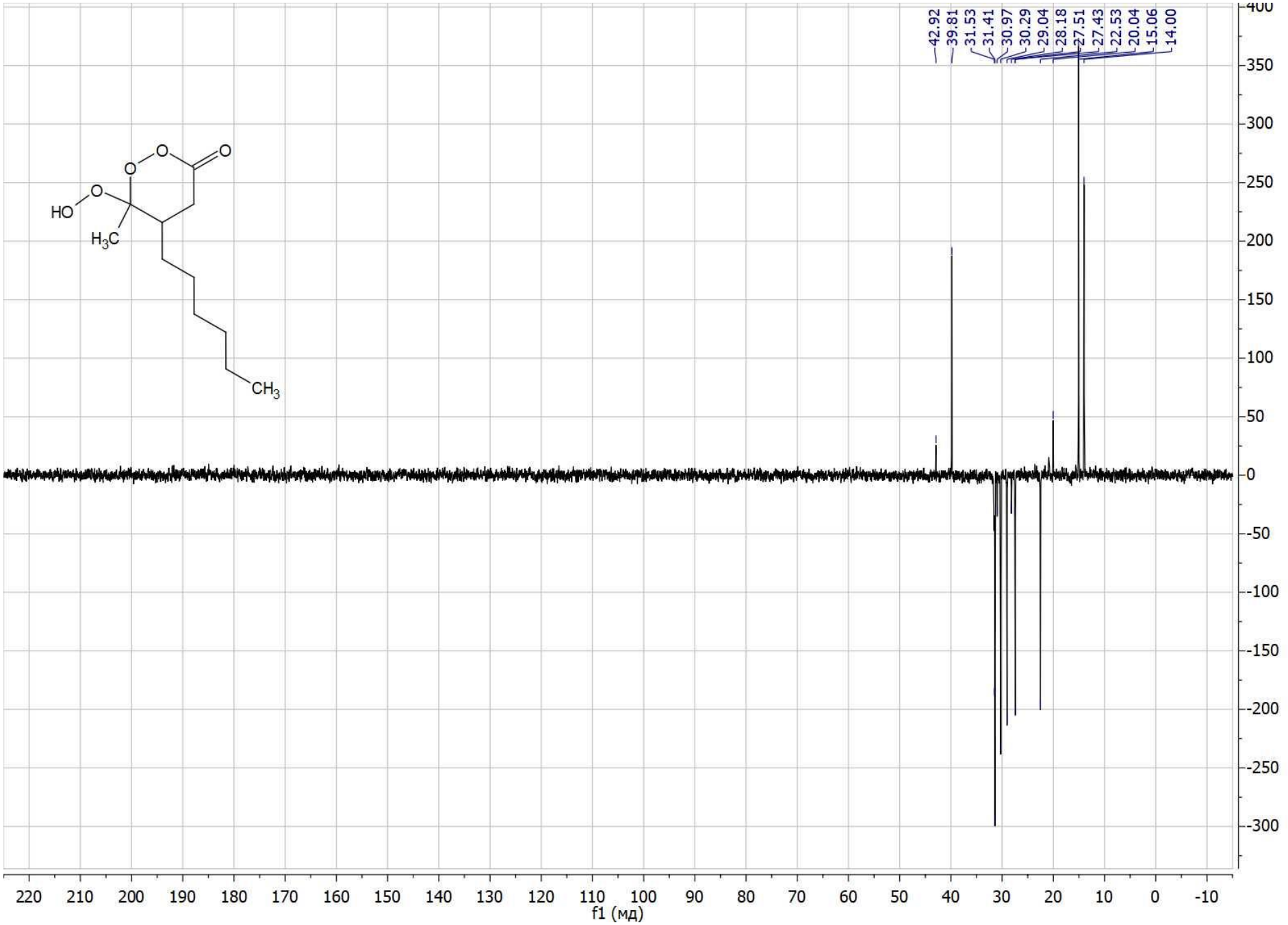
^{13}C NMR

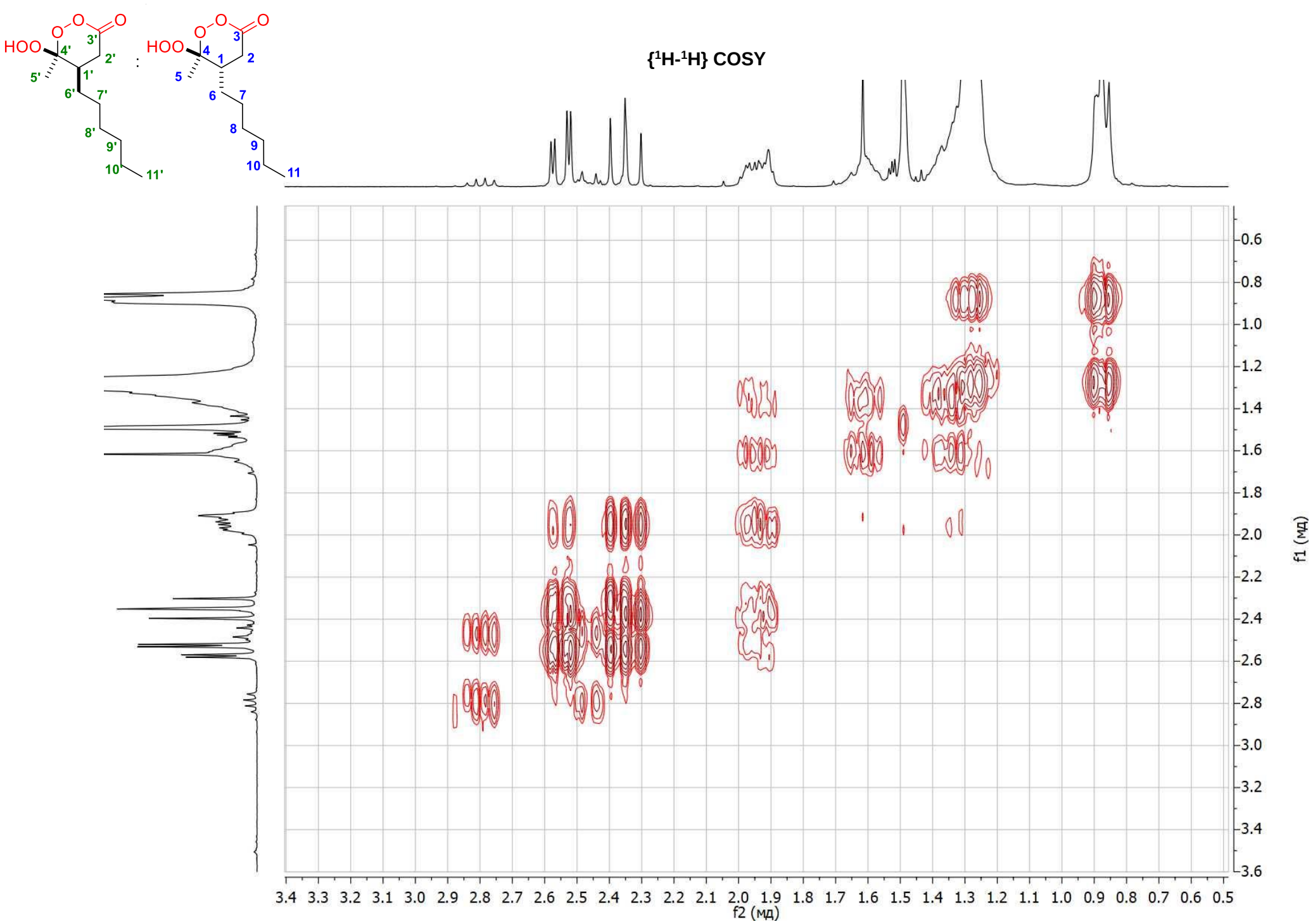

175.89
113.26
77.16 CDCl3
43.04
39.93
31.64
31.53
31.09
30.41
29.16
28.30
27.63
27.55
22.65
20.15
15.18
14.11
HO
H3C
CH3
f1 (мд)

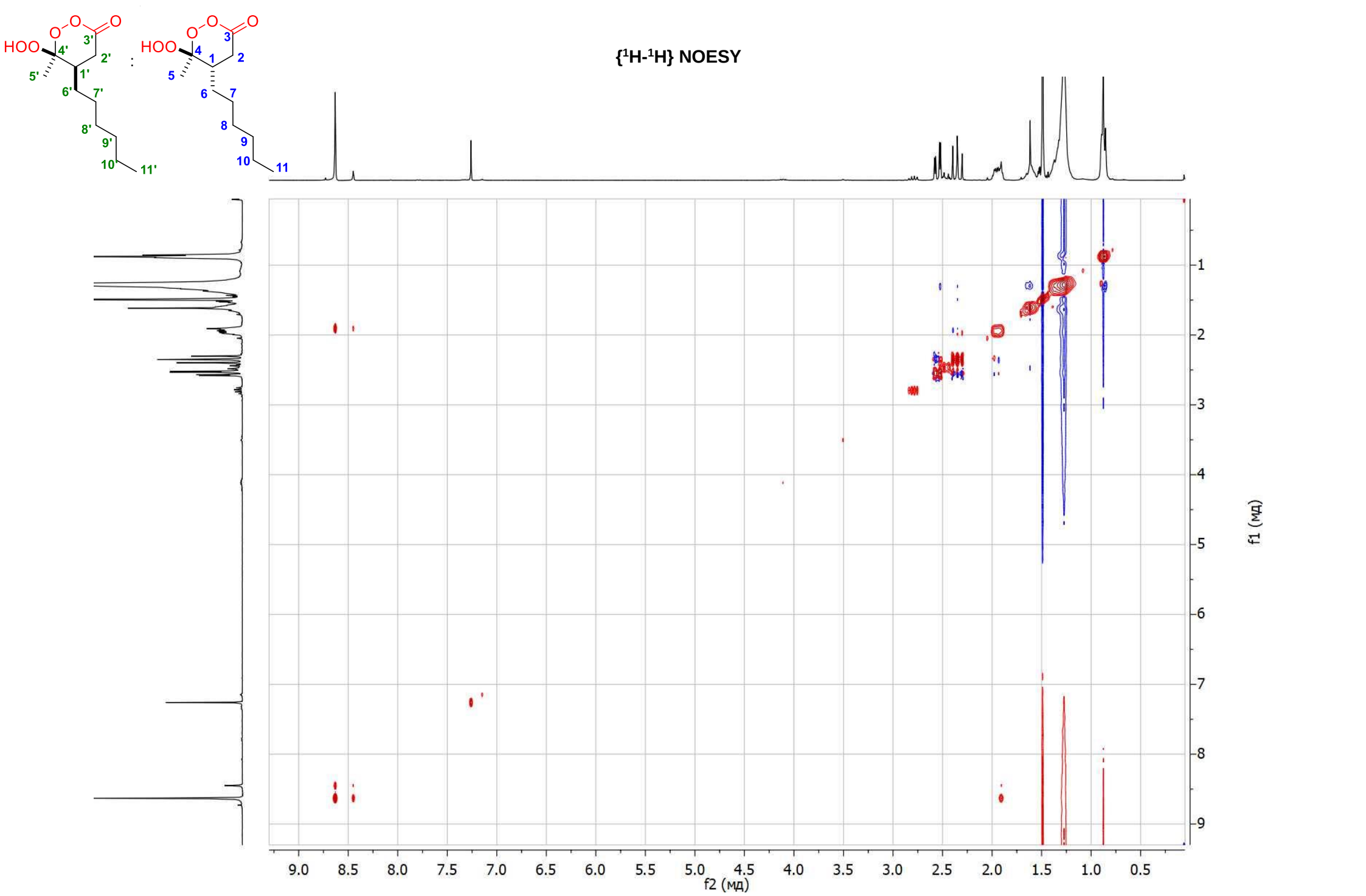

43.04
39.93
31.64
31.53
31.09
30.41
29.16
28.30
27.63
27.55
22.65
20.15
15.18
14.11
HOO
HOO
1
2
6
9
5
11
1'
2'
5'
f1 (мд)

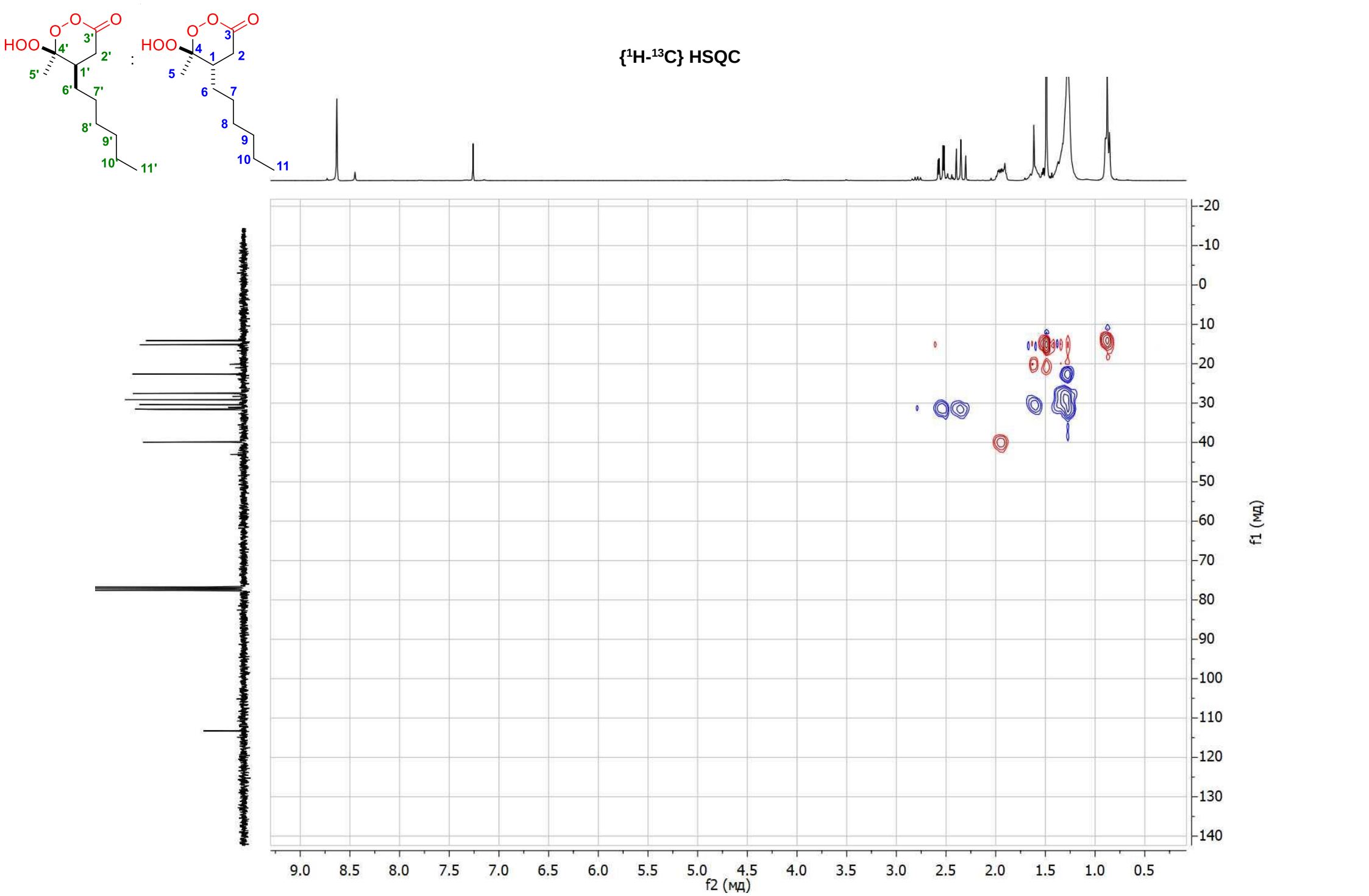

175.89
113.26
HOO
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
9'
10'
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
9
10
11
3
4
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
185
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
f1 (мд)

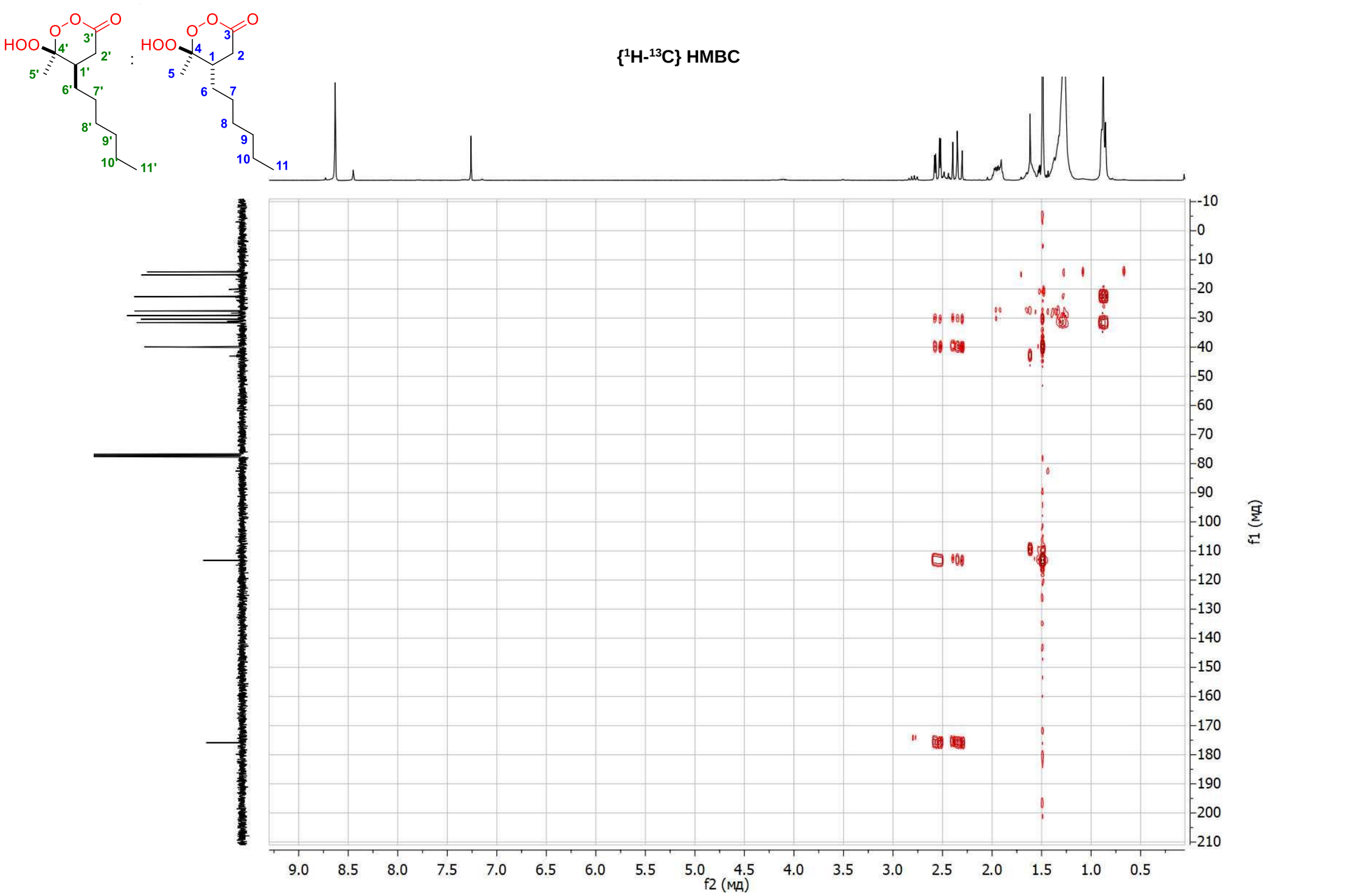
^{13}C_deptsp135




{1H-1H} COSY
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
10
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
9
10
11
f1 (мд)
f2 (мд)
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2
2.4
2.6
2.8
3.0
3.2
3.4
3.6
3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7 0.6 0.5

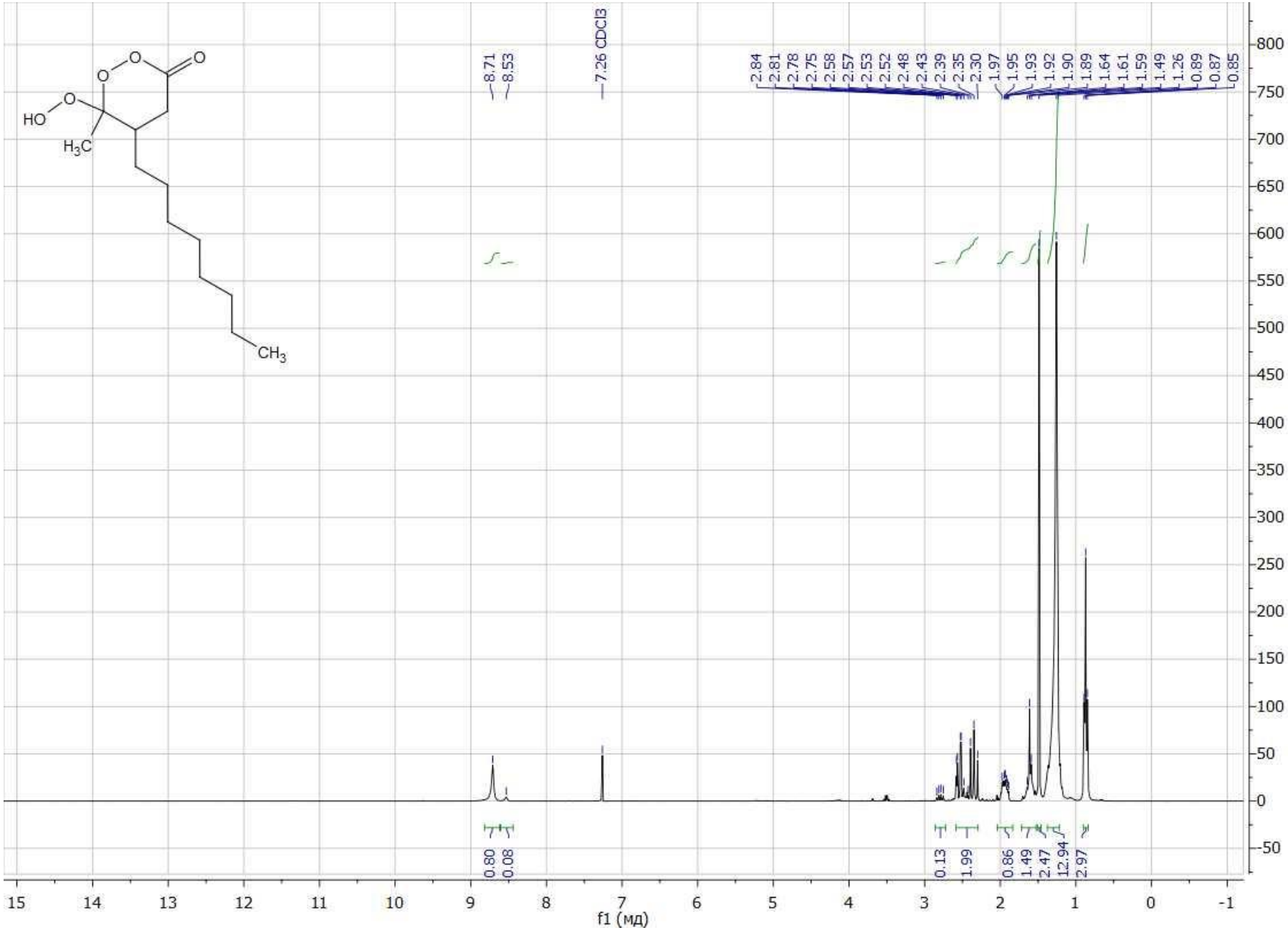

{1H-1H} NOESY
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
10
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
9
10
11
f1 (мд)
f2 (мд)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
1
2
3
4
5
6
7
8
9

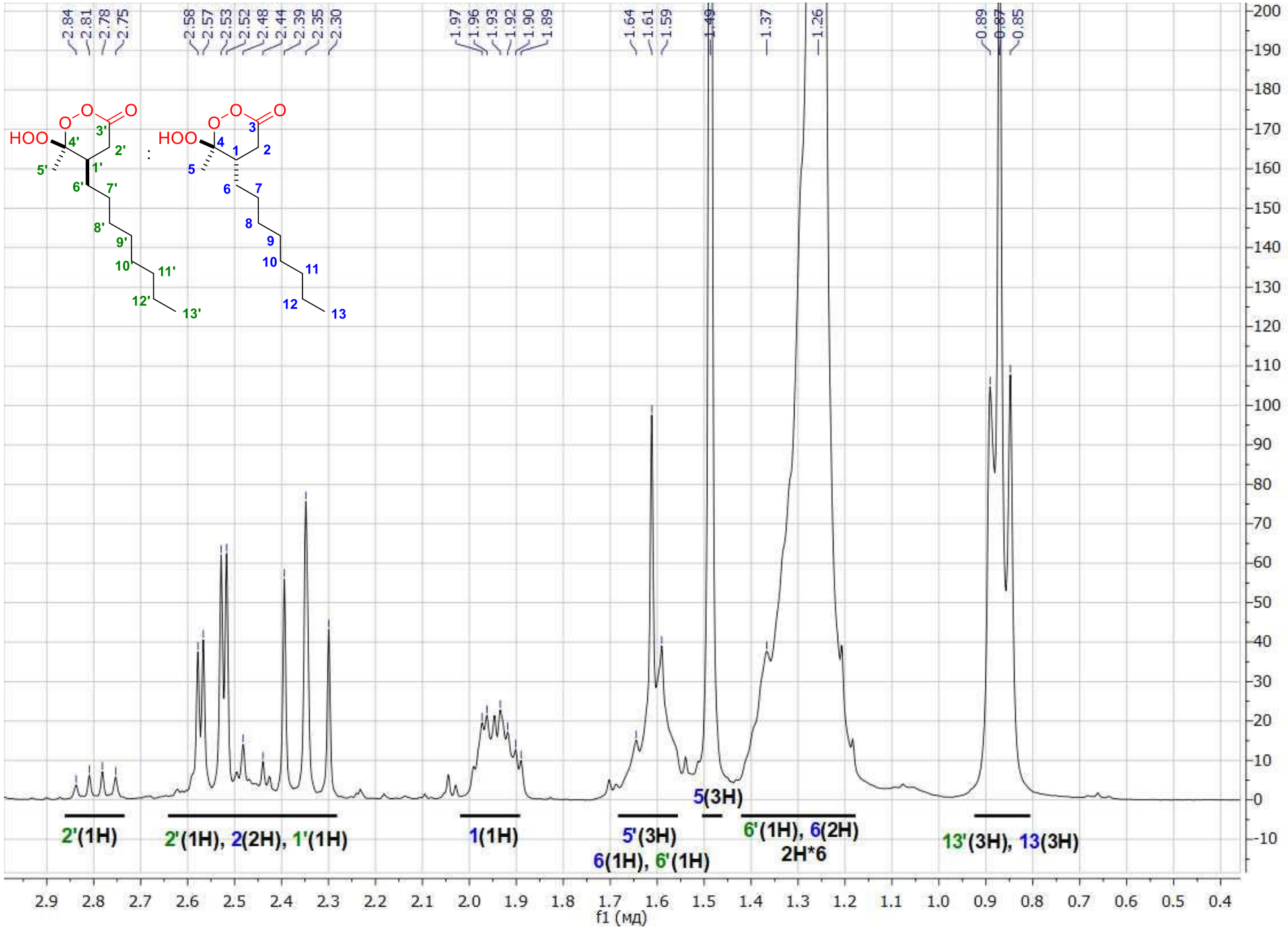

{1H-13C} HSQC
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
10
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
9
10
11
f2 (мд)
f1 (мд)


{1H-13C} HMBC
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
10'
11'
HOO
O
O
O
3
4
1
2
5
6
7
8
9
10
11
f2 (мд)
f1 (мд)

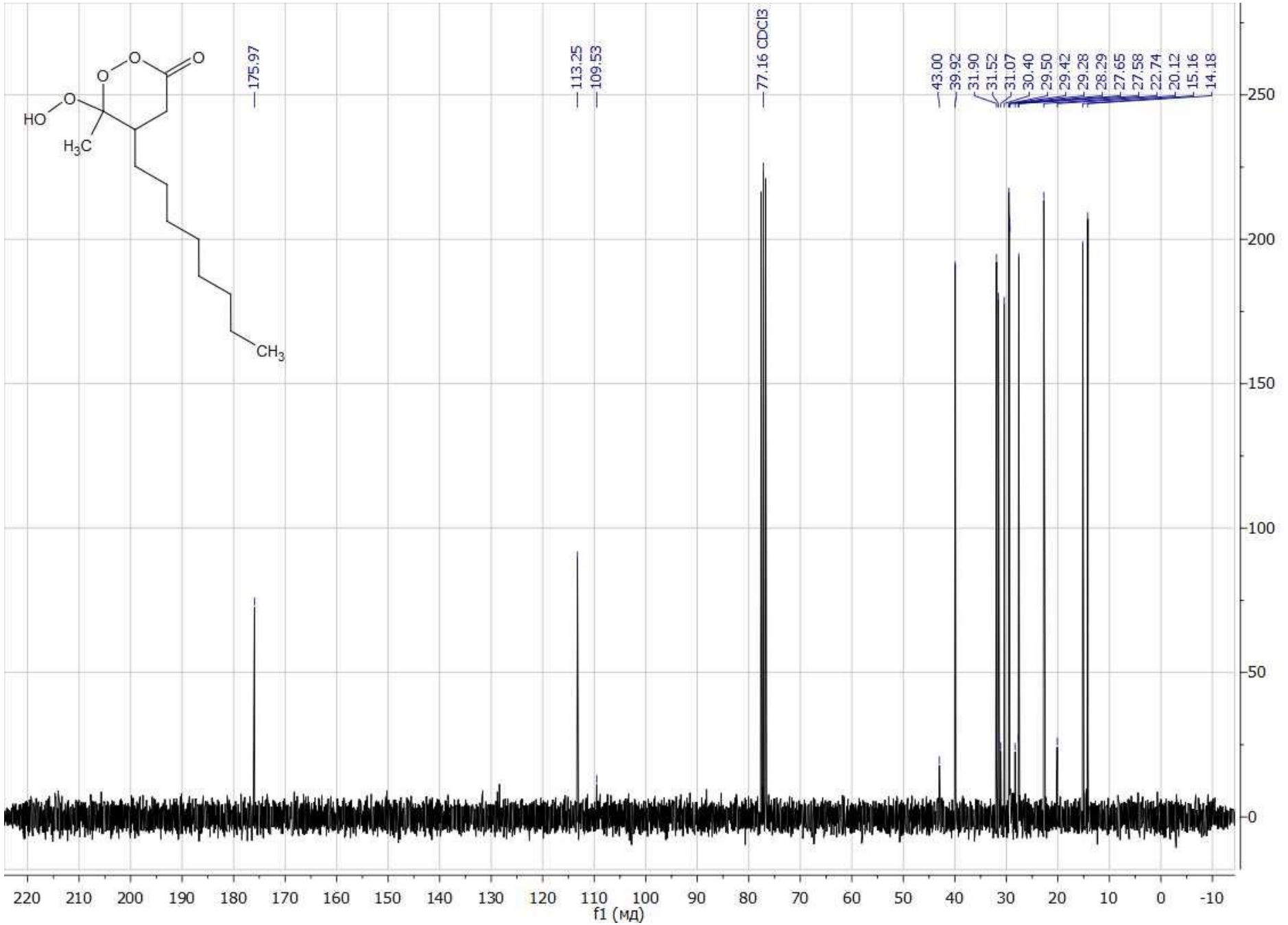
6-Hydroperoxy-6-methyl-5-octyl-1,2-dioxan-3-one, 2l

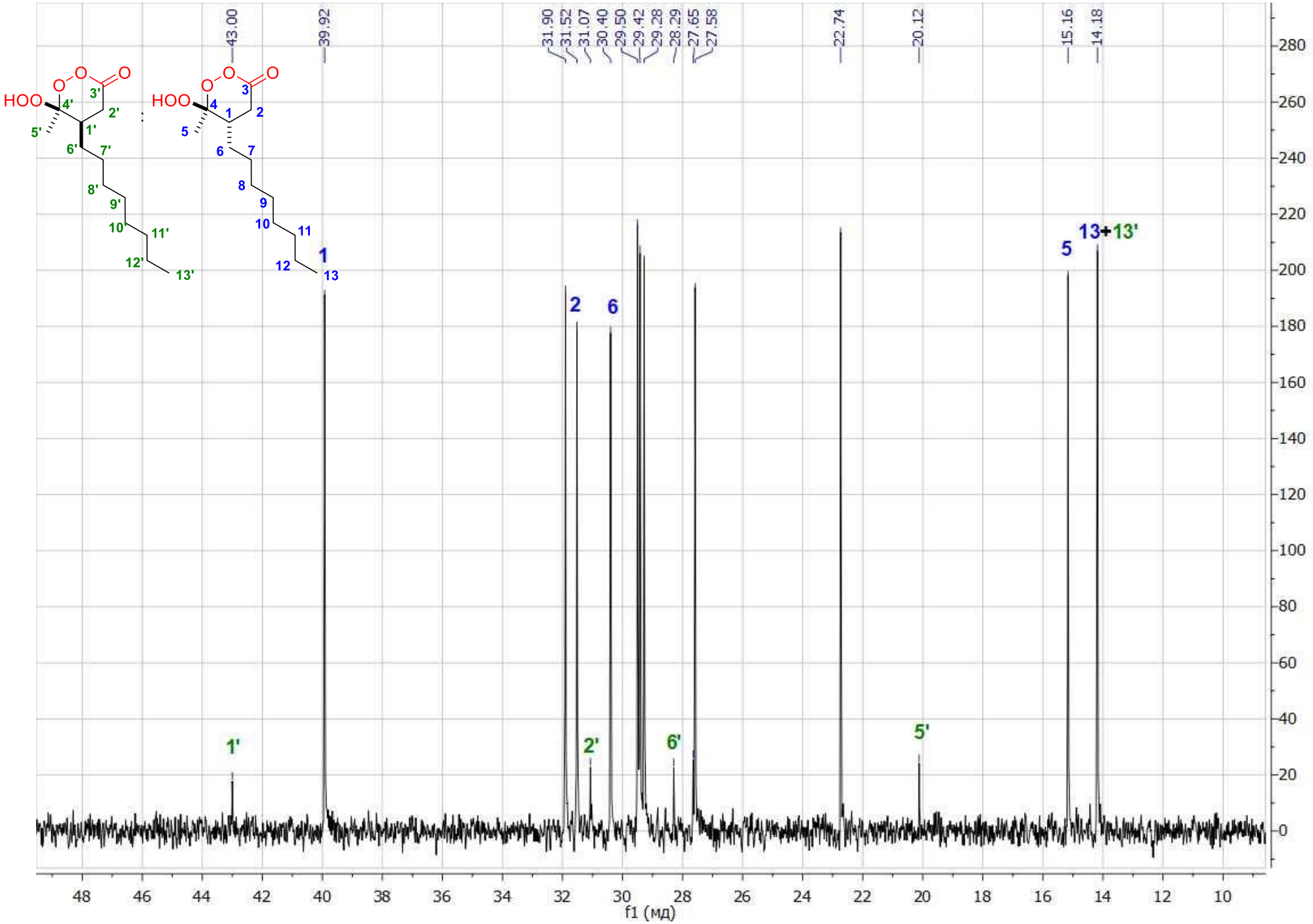
^{1}H NMR

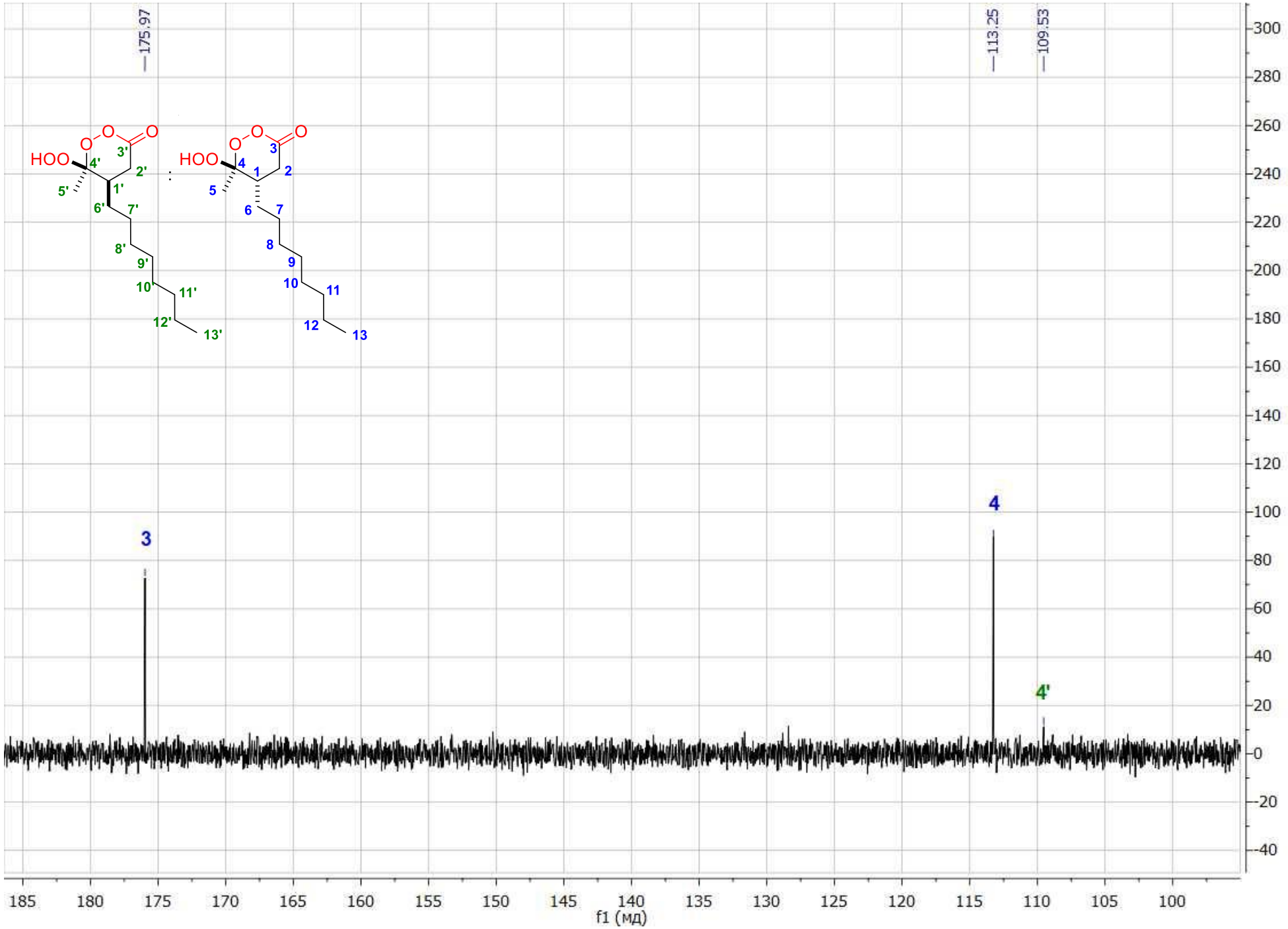



2.84
2.81
2.78
2.75
2.58
2.57
2.53
2.52
2.48
2.44
2.39
2.35
2.30
1.97
1.96
1.93
1.92
1.90
1.89
1.64
1.61
1.59
1.49
1.37
1.26
0.89
0.87
0.85
HOO
O
O
O
4'
3'
2'
1'
5'
6'
7'
8'
9'
10
11'
12'
13'
HOO
O
O
O
4
3
2
1
5
6
7
8
9
10
11
12
13
2'(1H)
2'(1H), 2(2H), 1'(1H)
1(1H)
5'(3H)
6(1H), 6'(1H)
5(3H)
6'(1H), 6(2H)
2H*6
13'(3H), 13(3H)
f1 (мд)

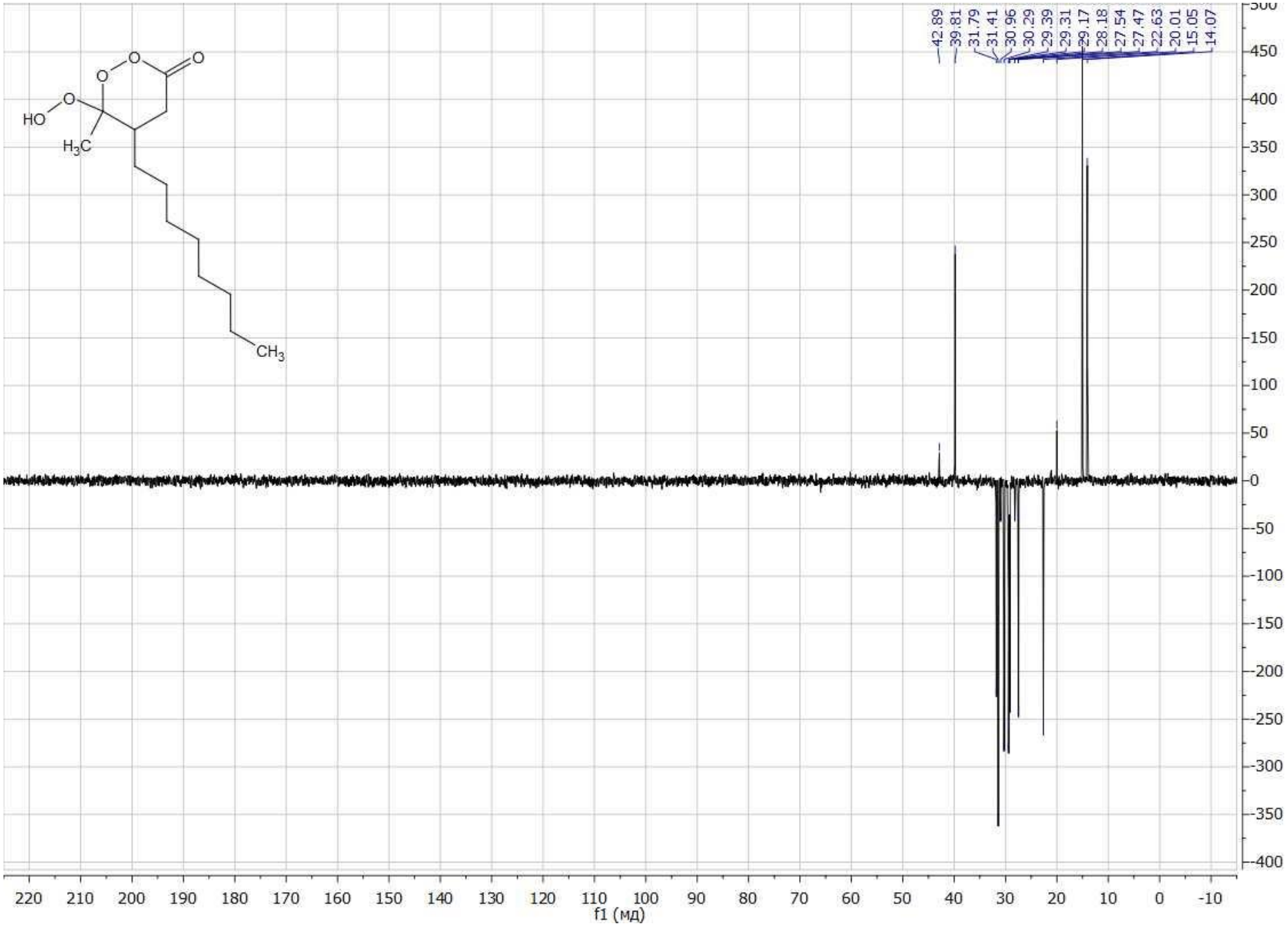
^{13}C NMR

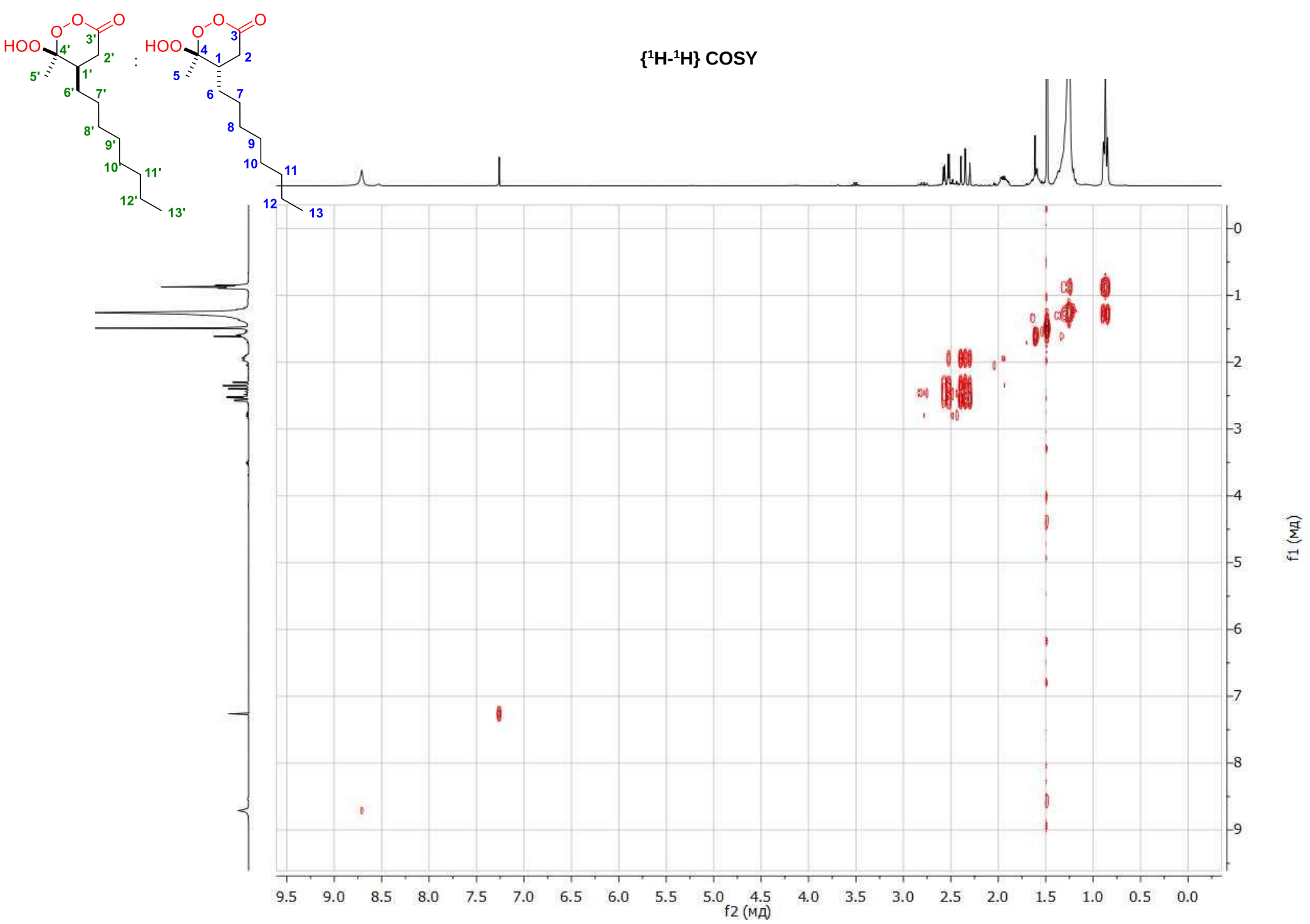

175.97
113.25
109.53
77.16 CDCl3
43.00
39.92
31.90
31.52
31.07
30.40
29.50
29.42
29.28
28.29
27.65
27.58
22.74
20.12
15.16
14.18
HO
O
O
O
O
H3C
CH3
250
200
150
100
50
0
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (мд)

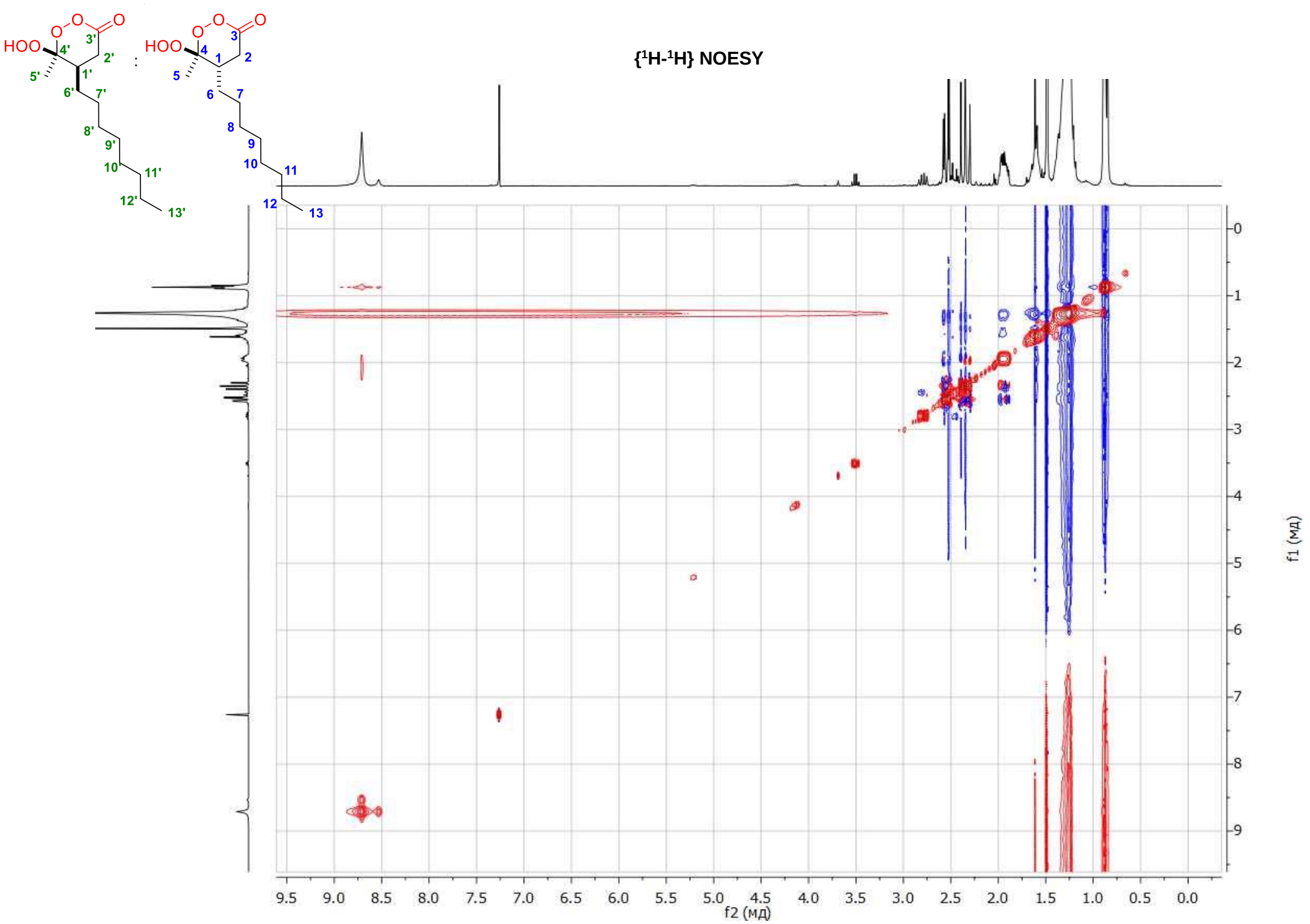

HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
10'
11'
12'
13'
HOO
O
O
O
3
4
1
2
5
6
7
8
9
10
11
12
13
43.00
39.92
31.90
31.52
31.07
30.40
29.50
29.42
29.28
28.29
27.65
27.58
22.74
20.12
15.16
14.18
1'
2'
6'
5'
2
6
5
13+13'
1
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
48
46
44
42
40
38
36
34
32
30
28
26
24
22
20
18
16
14
12
10
f1 (мд)

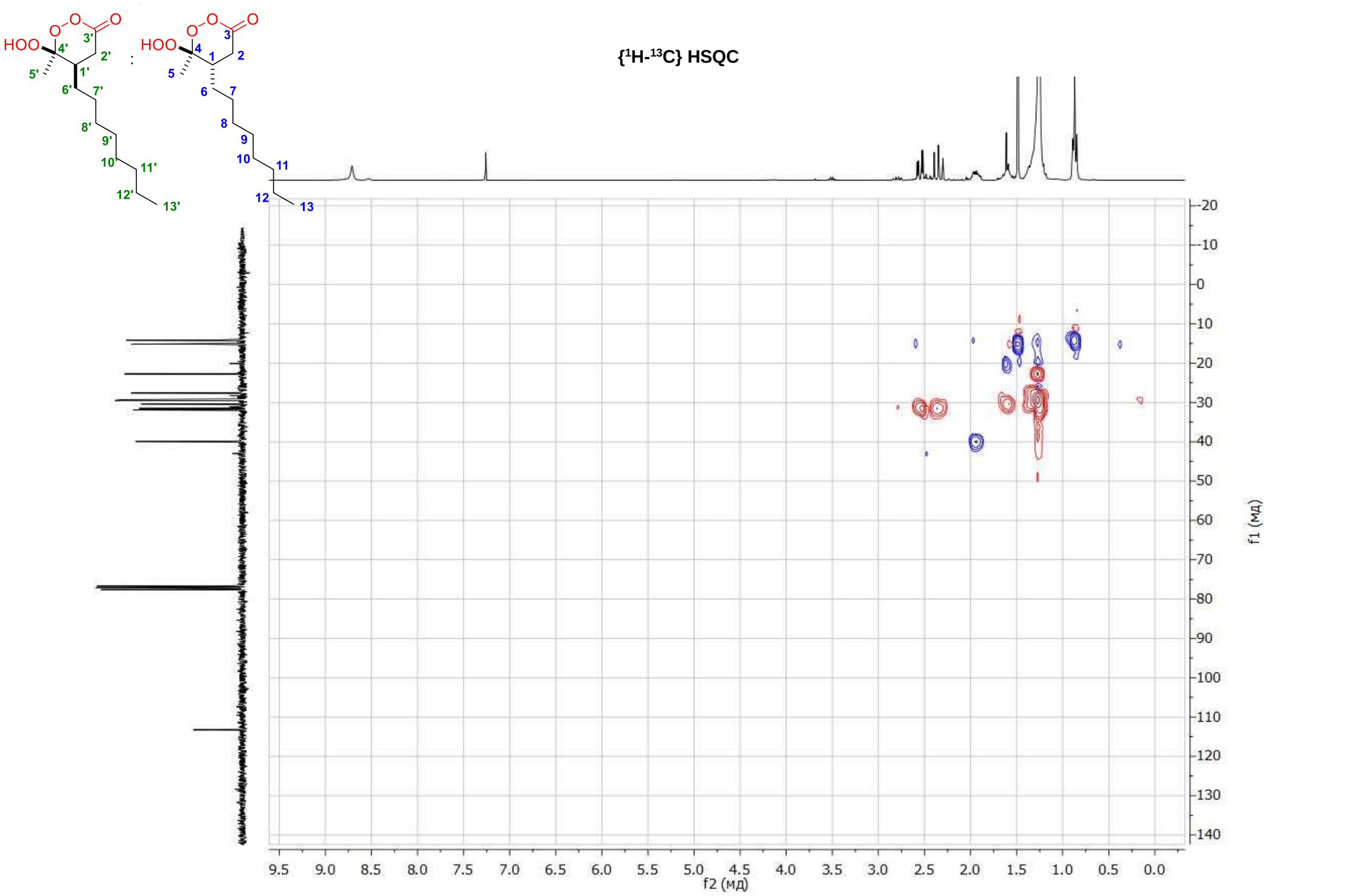

175.97
113.25
109.53
HOO
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
9'
10
11'
12'
13'
HOO
O
O
O
3
4
1
2
5
6
7
8
9
10
11
12
13
3
4
4'
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
-40
185
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
f1 (мд)

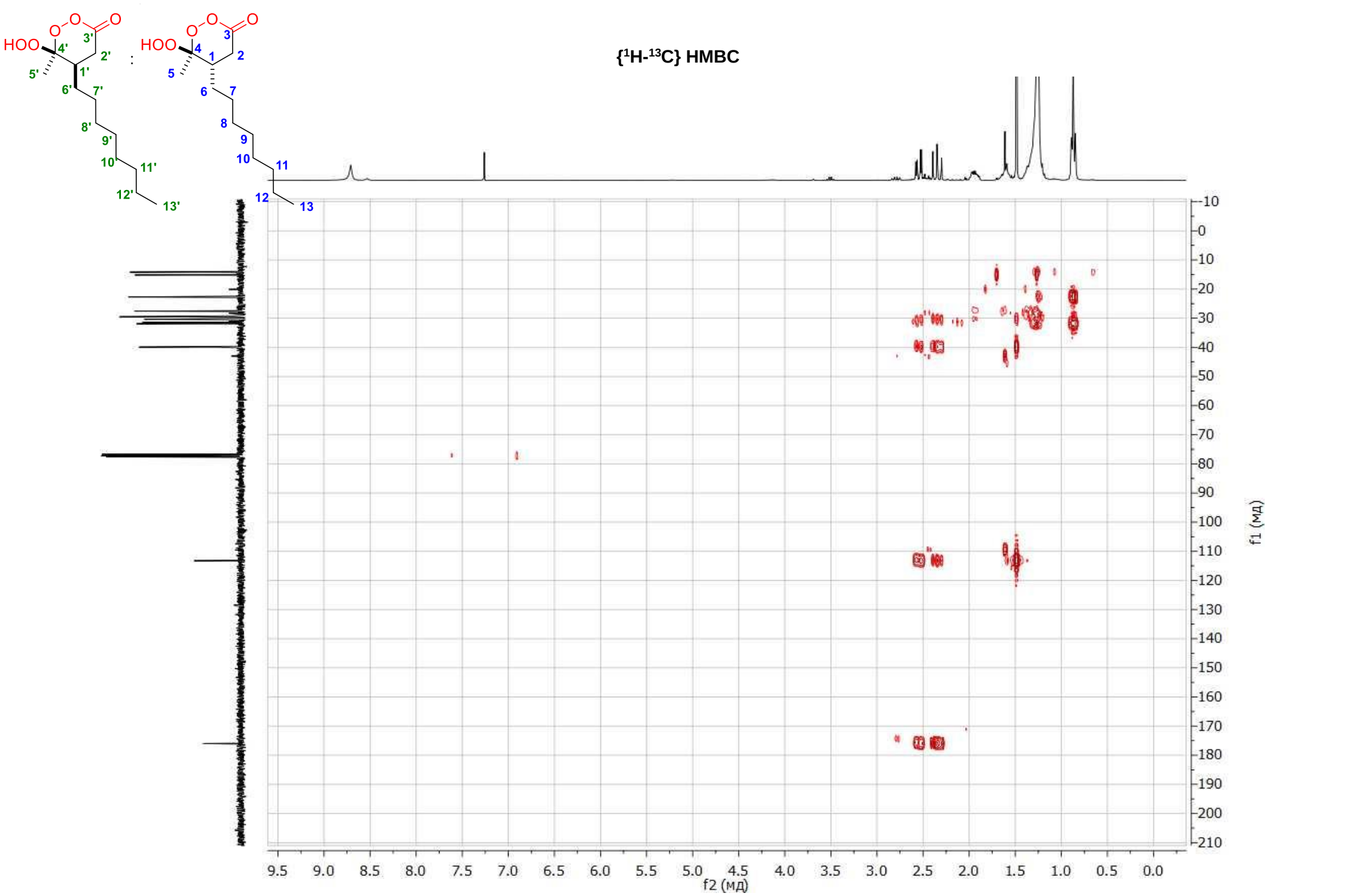
^{13}C_deptsp135




{1H-1H} COSY
HOO
O
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
10'
11'
12'
13'
HOO
O
O
O
3
4
2
1
5
6
7
8
9
10
11
12
13
f2 (мд)
f1 (мд)

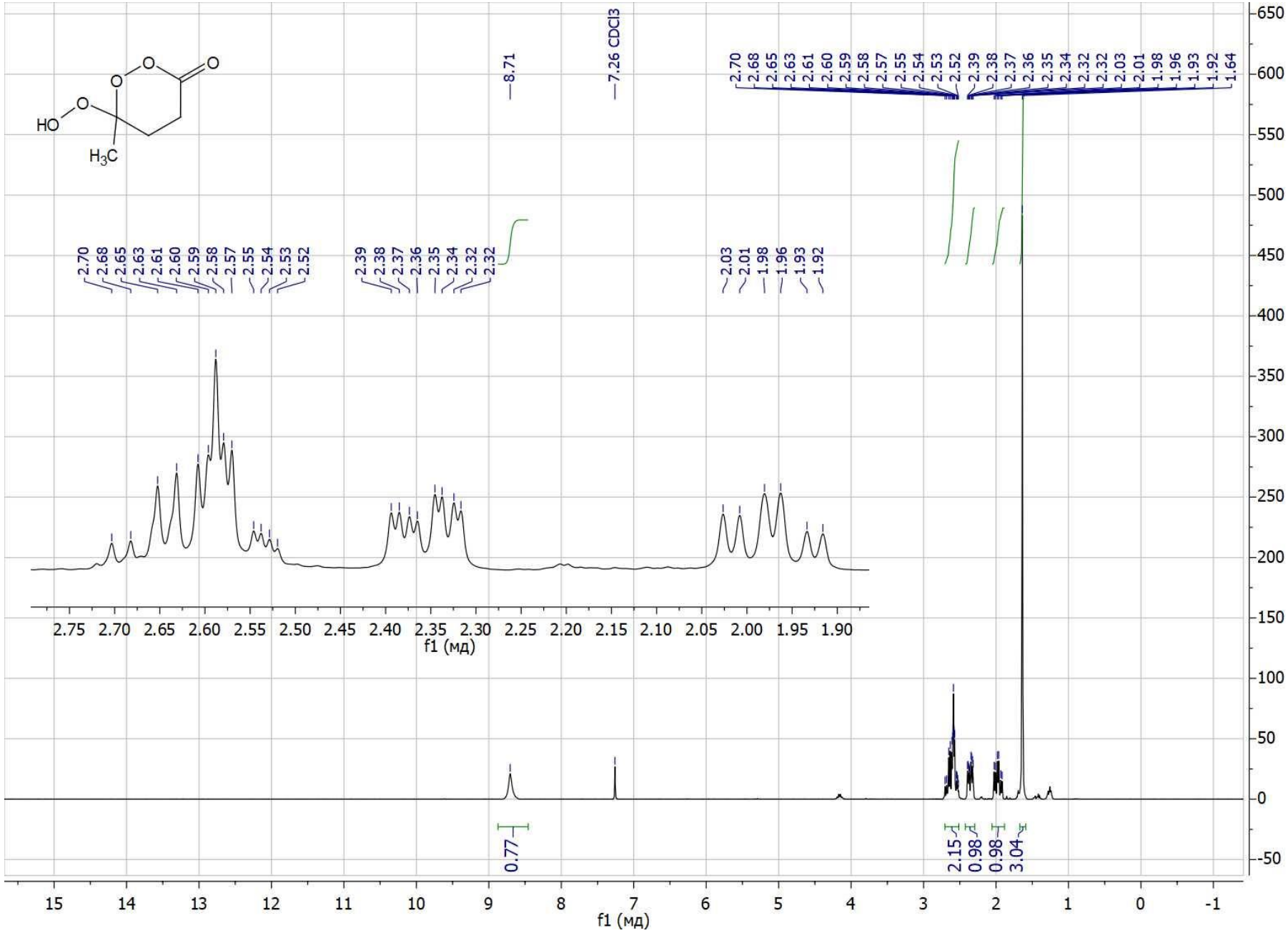

{1H-1H} NOESY
HOO
O
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
9'
10
11'
12'
13'
HOO
O
O
O
3
4
2
1
5
6
7
8
9
10
11
12
13
f2 (мд)
f1 (мд)


{1H-13C} HSQC
HOO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
10
11'
12'
13'
HOO
O
O
O
3
4
1
2
5
6
7
8
9
10
11
12
13
f2 (мд)
f1 (мд)

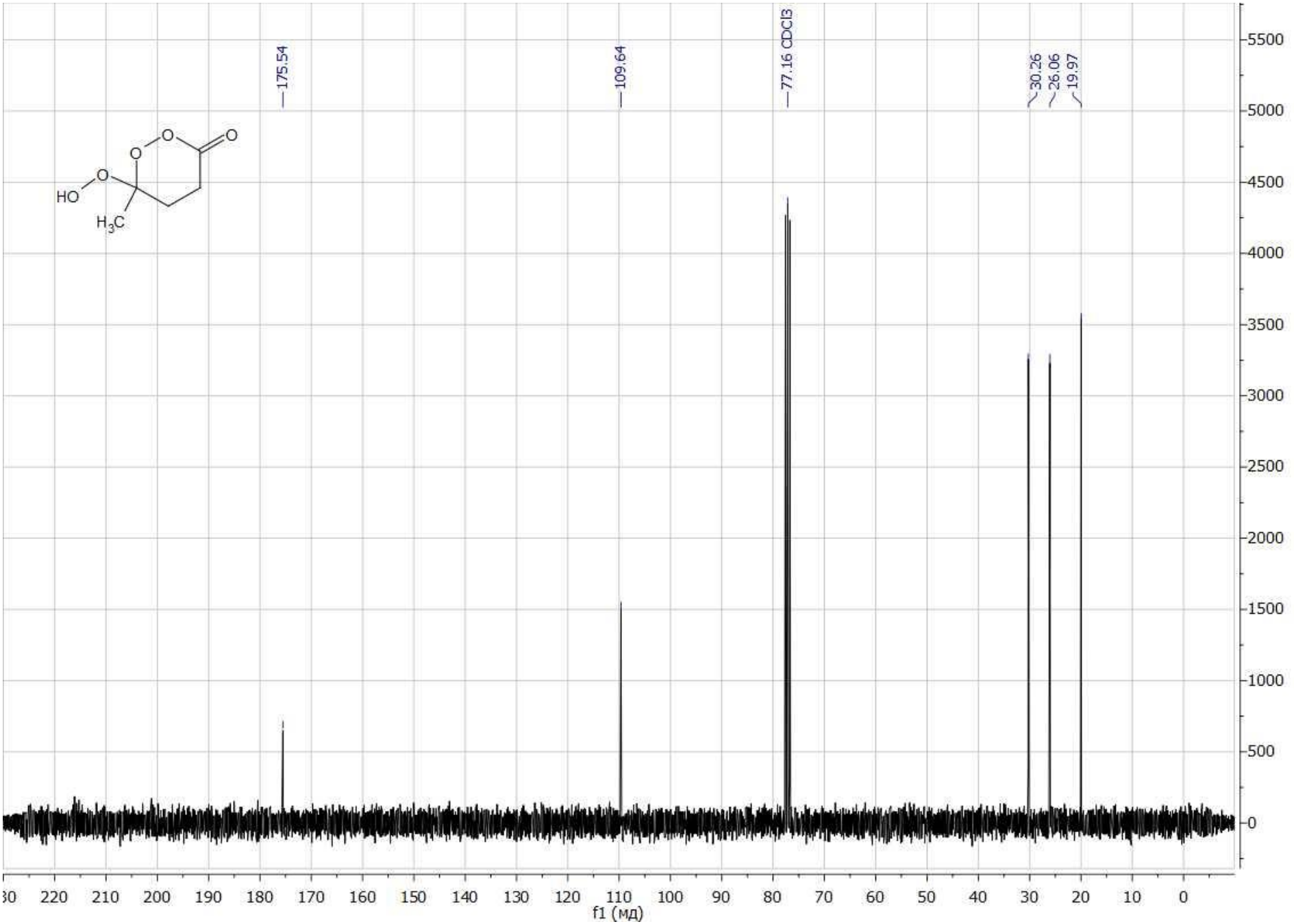

{1H-13C} HMBC
HOO
O
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
9'
10
11'
12'
13'
HOO
O
O
O
3
4
2
1
5
6
7
8
9
10
11
12
13
f2 (мд)
f1 (мд)

6-Hydroperoxy-6-methyl-1,2-dioxan-3-one, 2m

^{1}H NMR

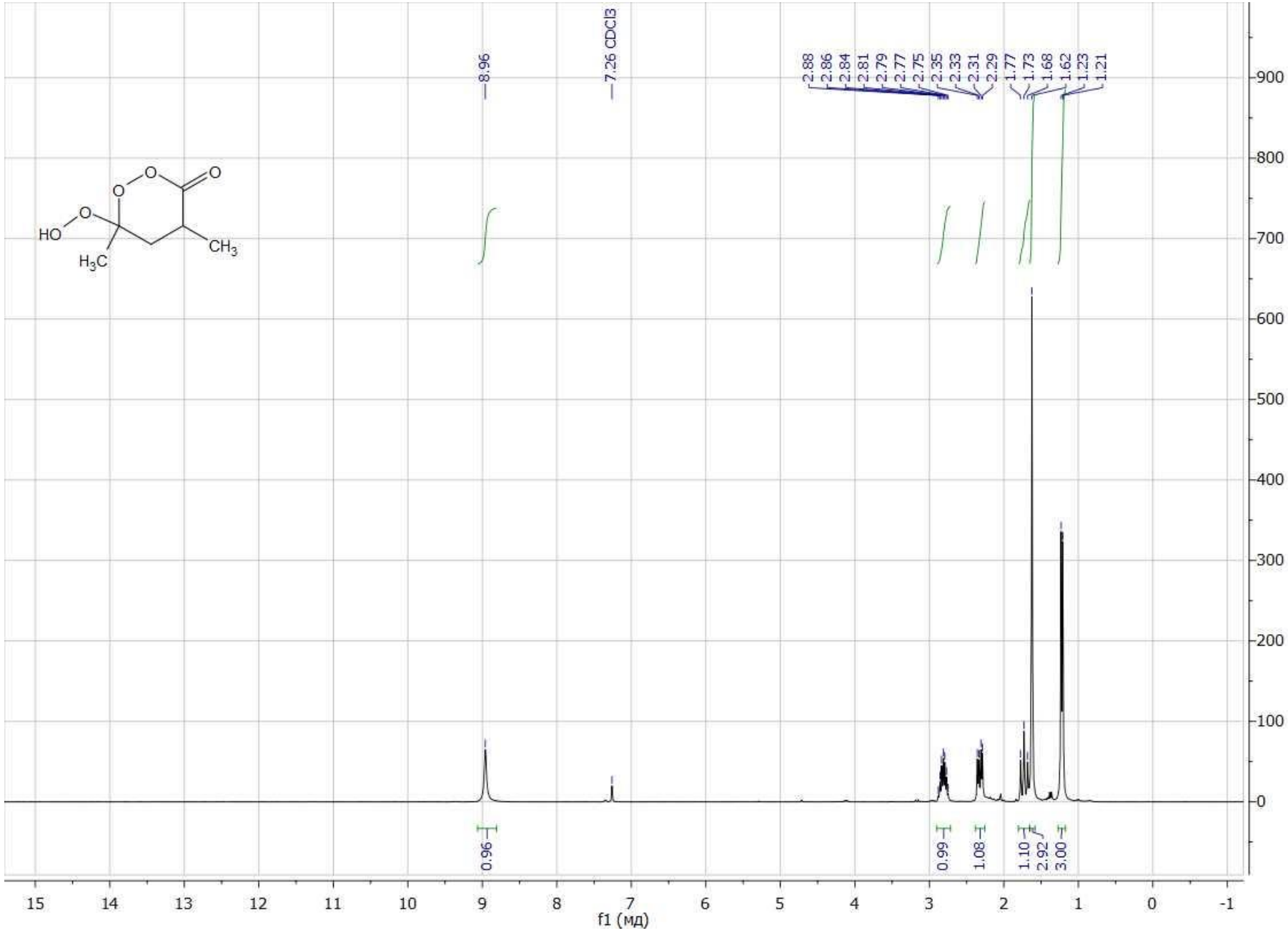


^{13}C NMR

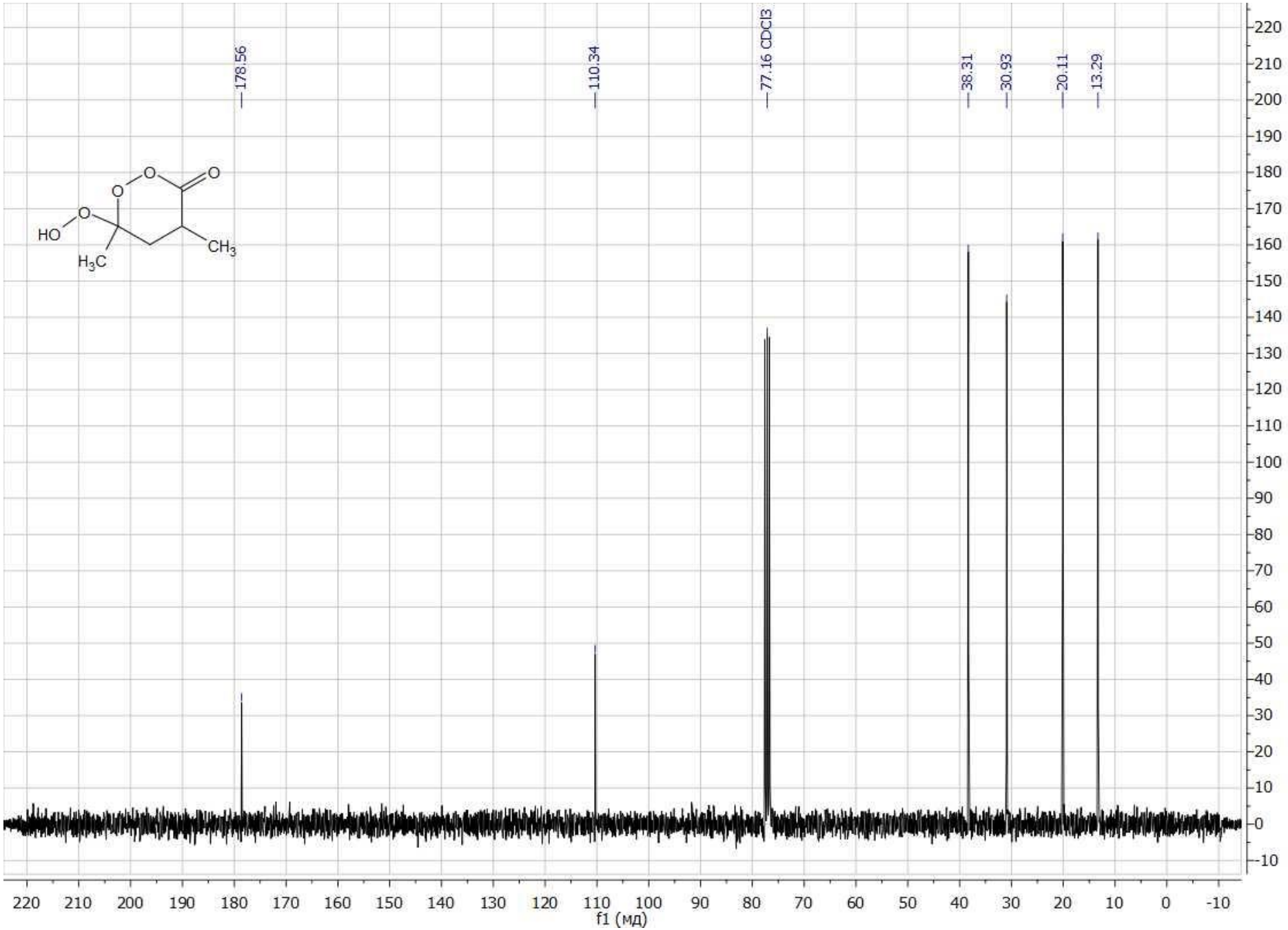

175.54
109.64
77.16 CDCl3
30.26
26.06
19.97
HO
O
O
O
O
H3C
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (мд)

6-Hydroperoxy-4,6-dimethyl-1,2-dioxan-3-one, 2n

^{1}H NMR

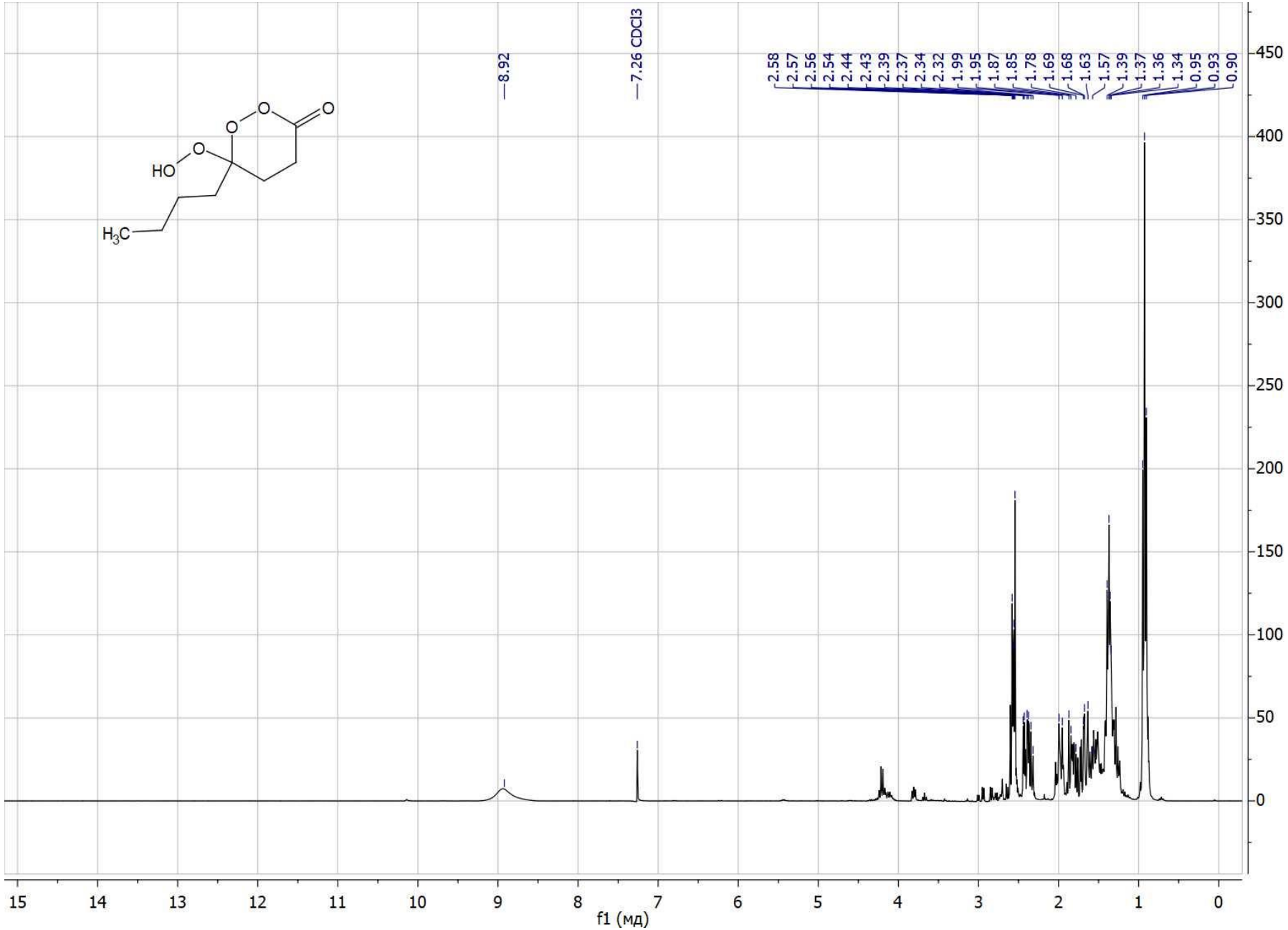


^{13}C NMR

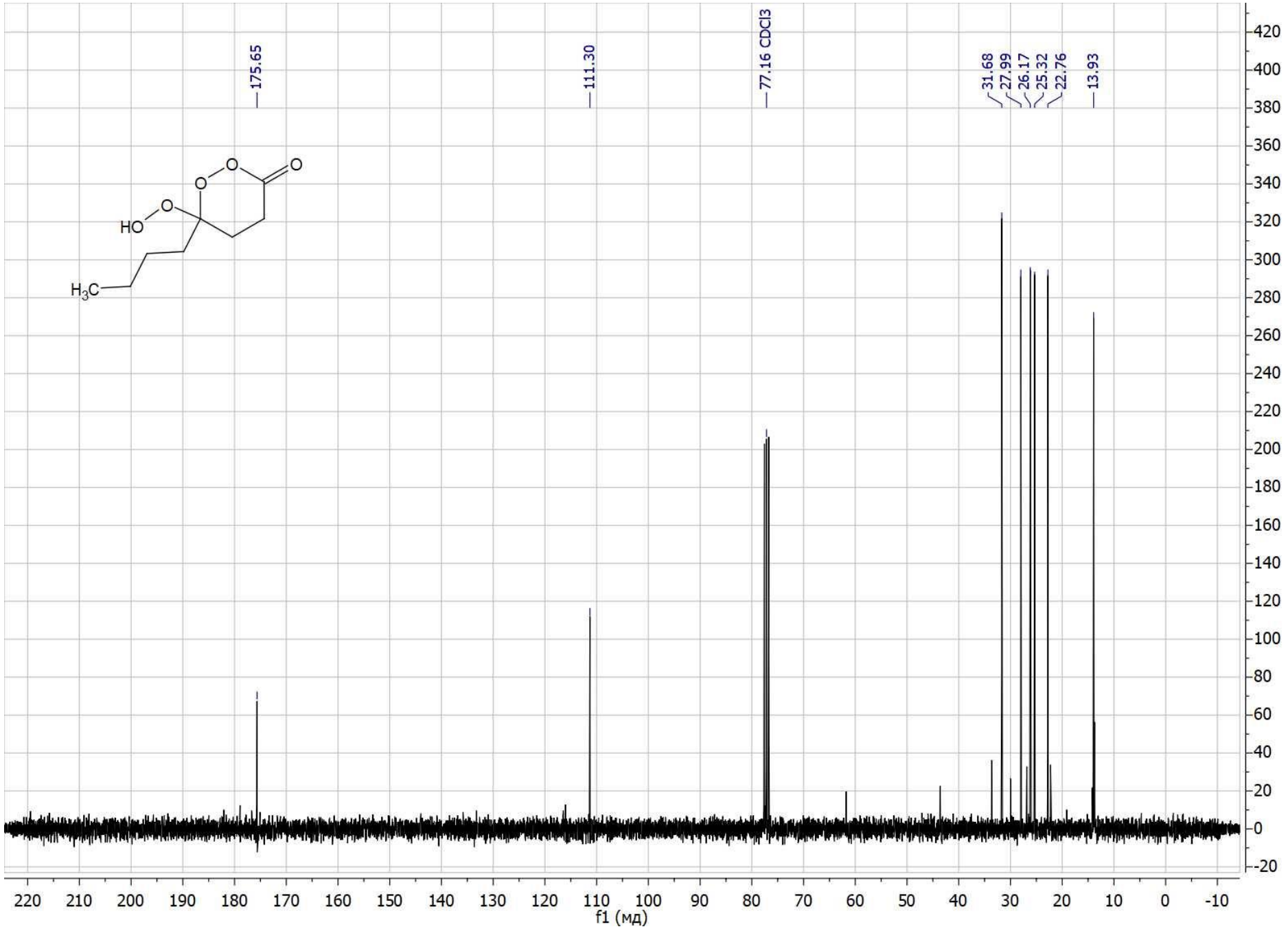

178.56
110.34
77.16 CDCl3
38.31
30.93
20.11
13.29
HO
O
O
O
O
H3C
CH3
f1 (мд)

6-Butyl-6-hydroperoxy-1,2-dioxan-3-one, 2o

^{1}H NMR

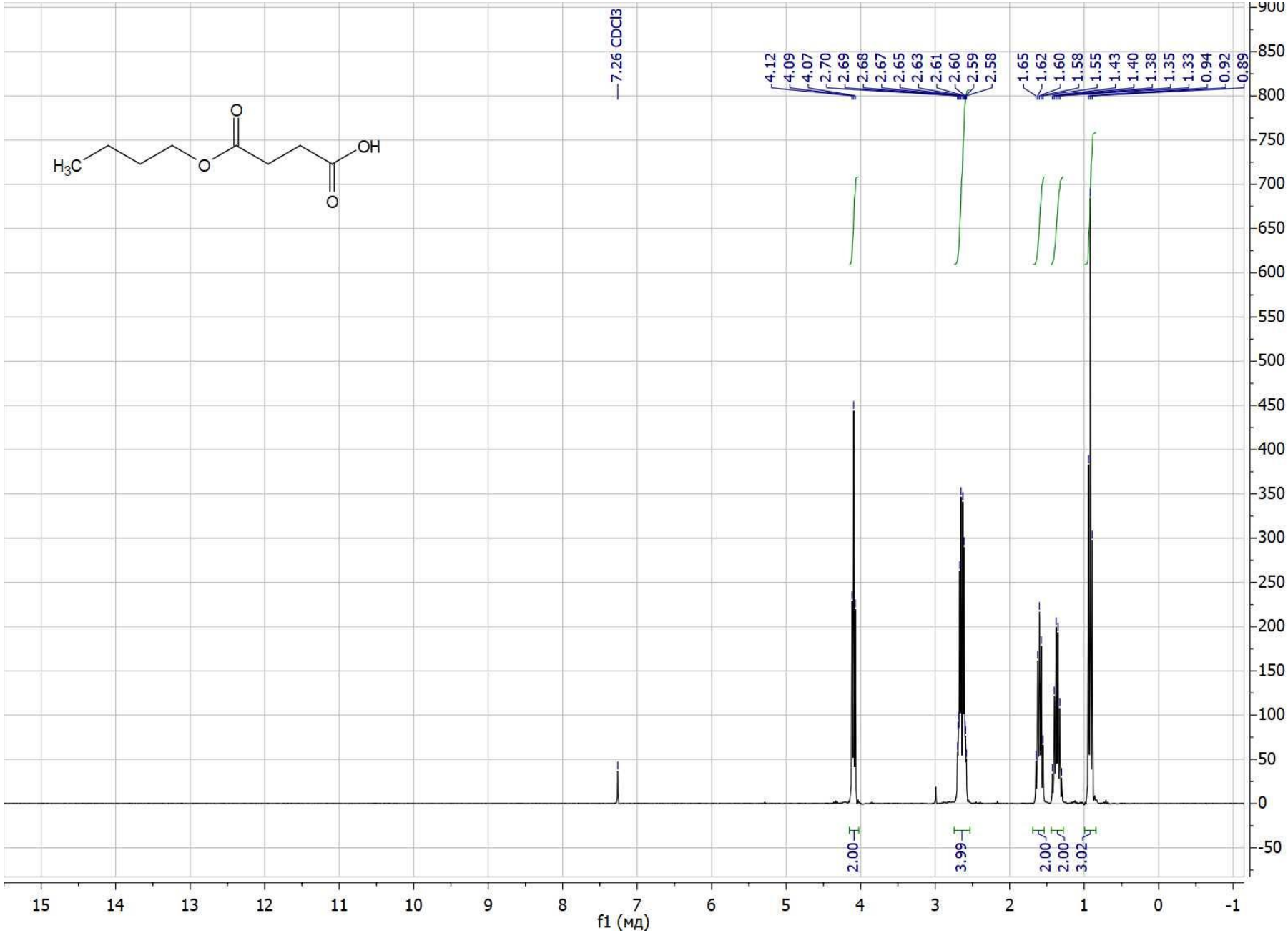


^{13}C NMR

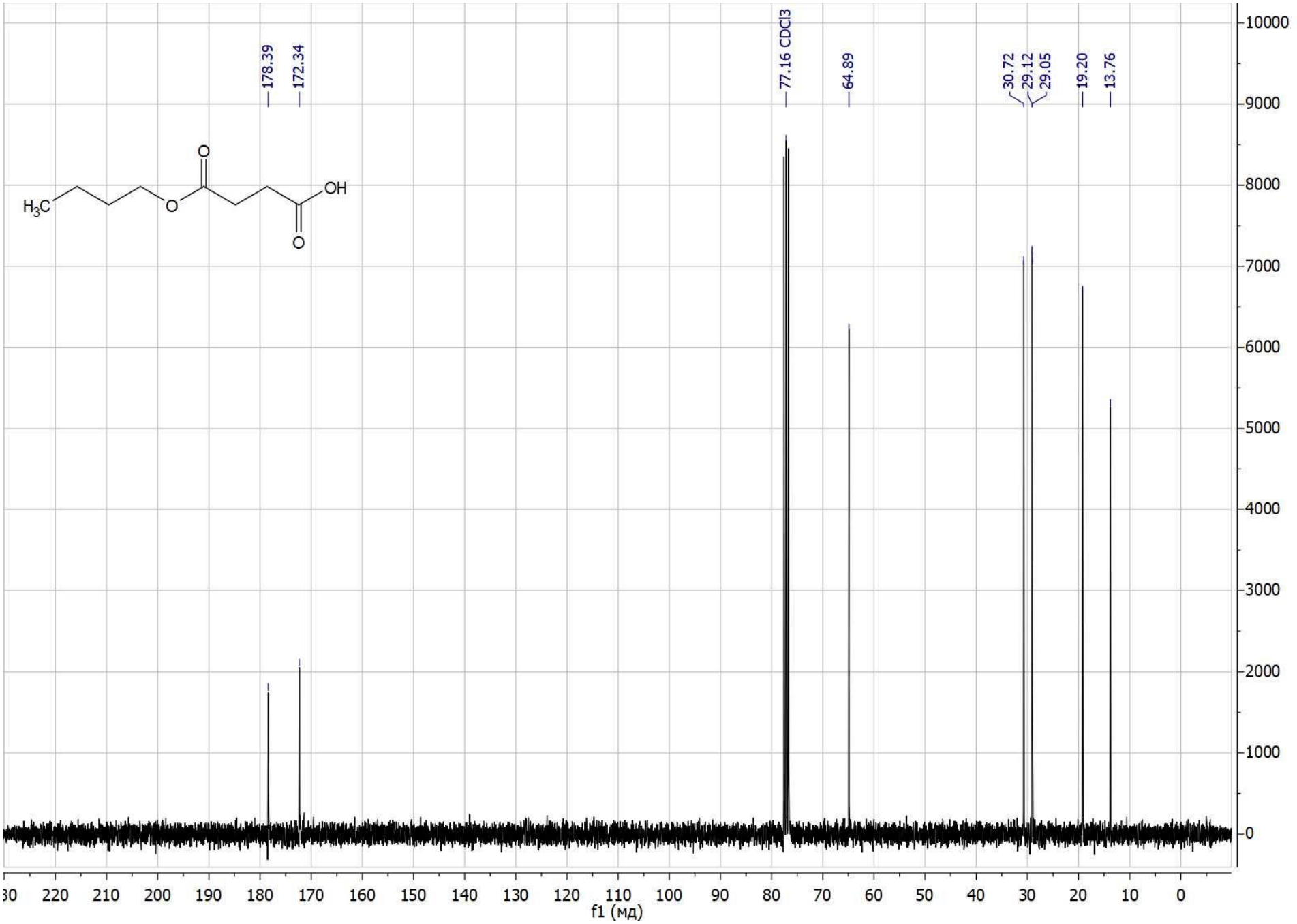

175.65
111.30
77.16 CDCl3
31.68
27.99
26.17
25.32
22.76
13.93
HO
O
O
O
O
H3C
f1 (мд)

4-Butoxy-4-oxobutanoic acid, 6o

^{1}H NMR

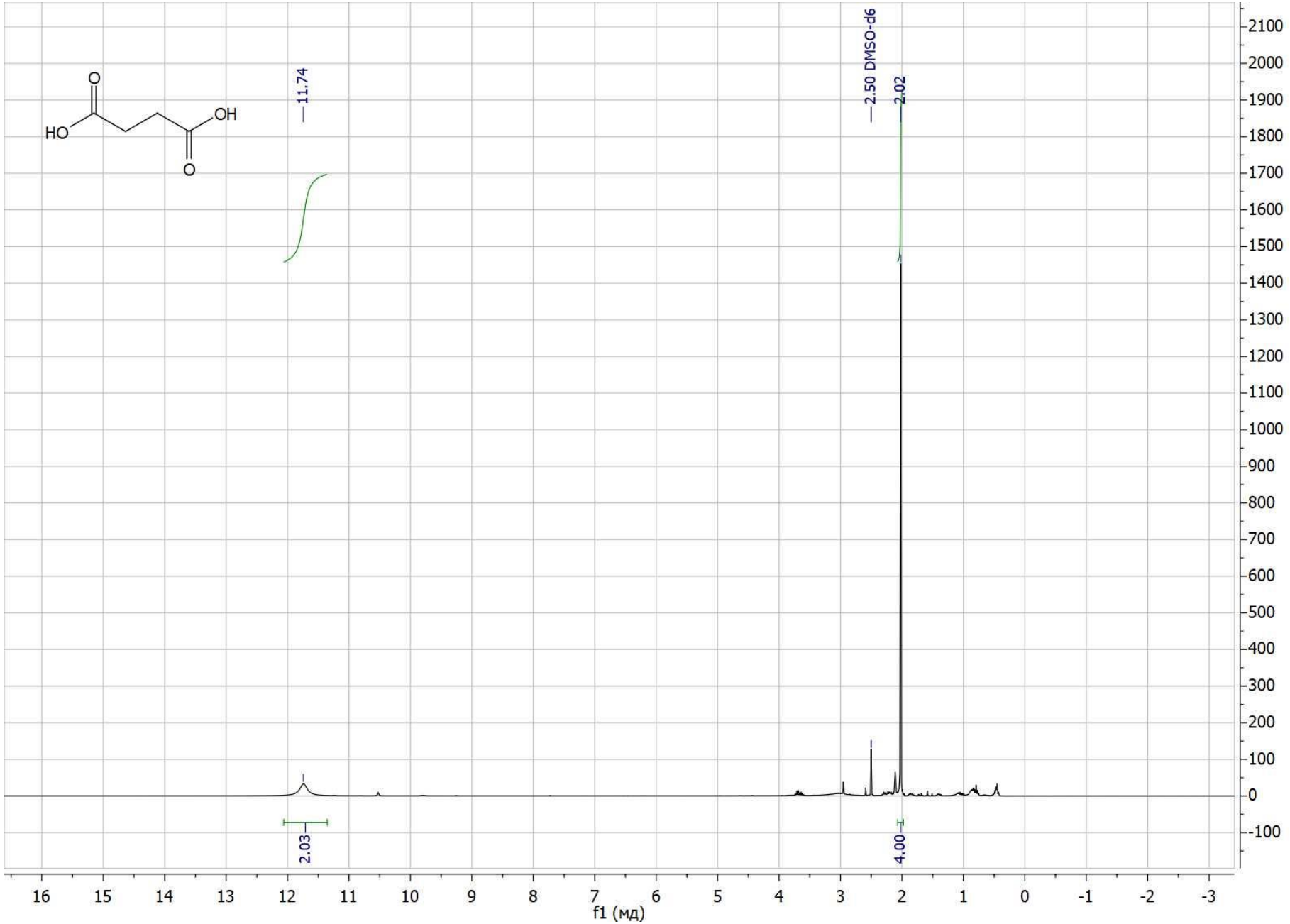


^{13}C NMR

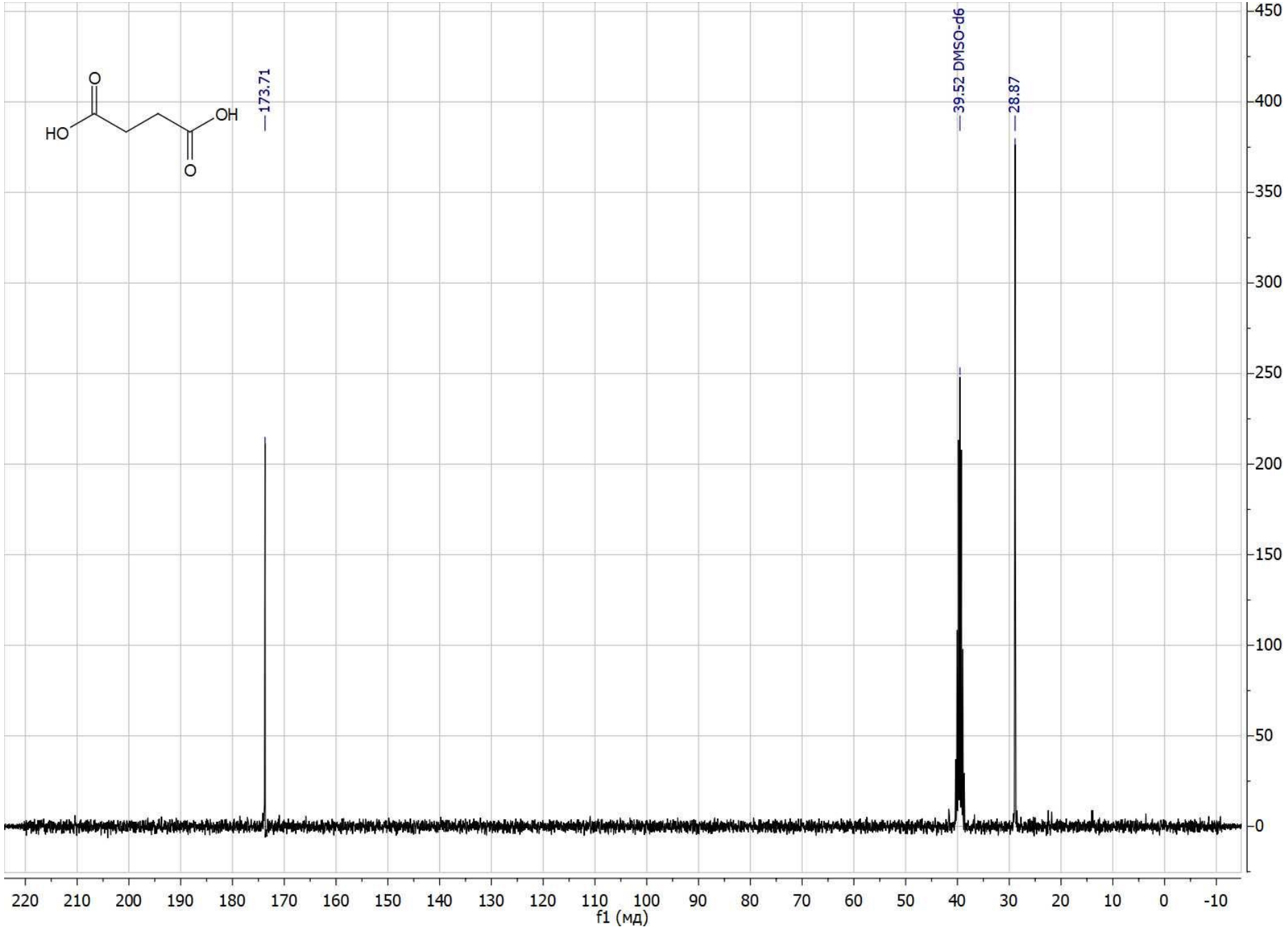

178.39
172.34
77.16 CDCl3
64.89
30.72
29.12
29.05
19.20
13.76
H3C
O
O
OH
O
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (мд)

Succinic acid, 7

^{1}H NMR

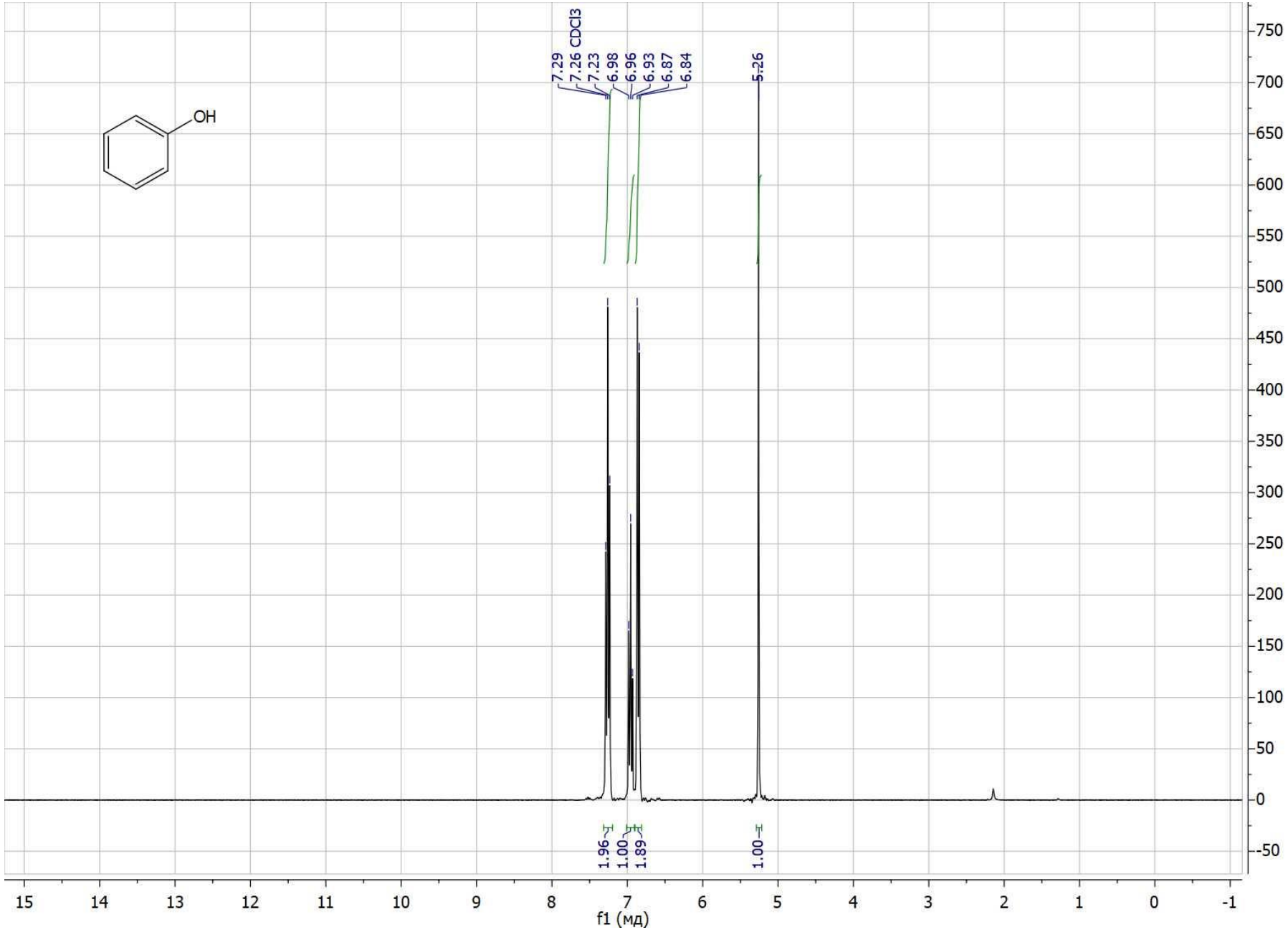


^{13}C NMR

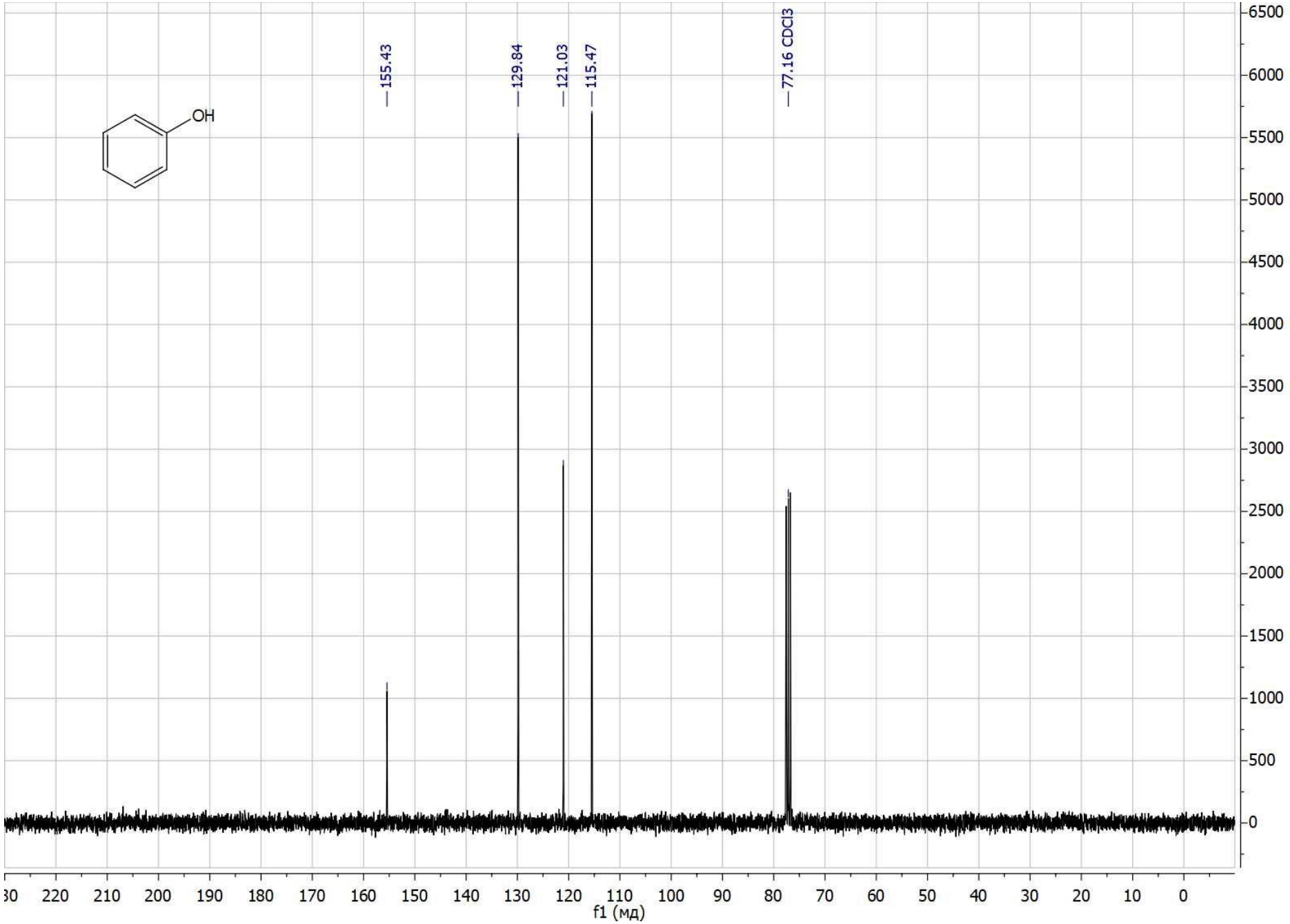

HO
O
OH
O
173.71
39.52 DMSO-d6
28.87
450
400
350
300
250
200
150
100
50
0
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (мд)

Phenol

^{1}H NMR

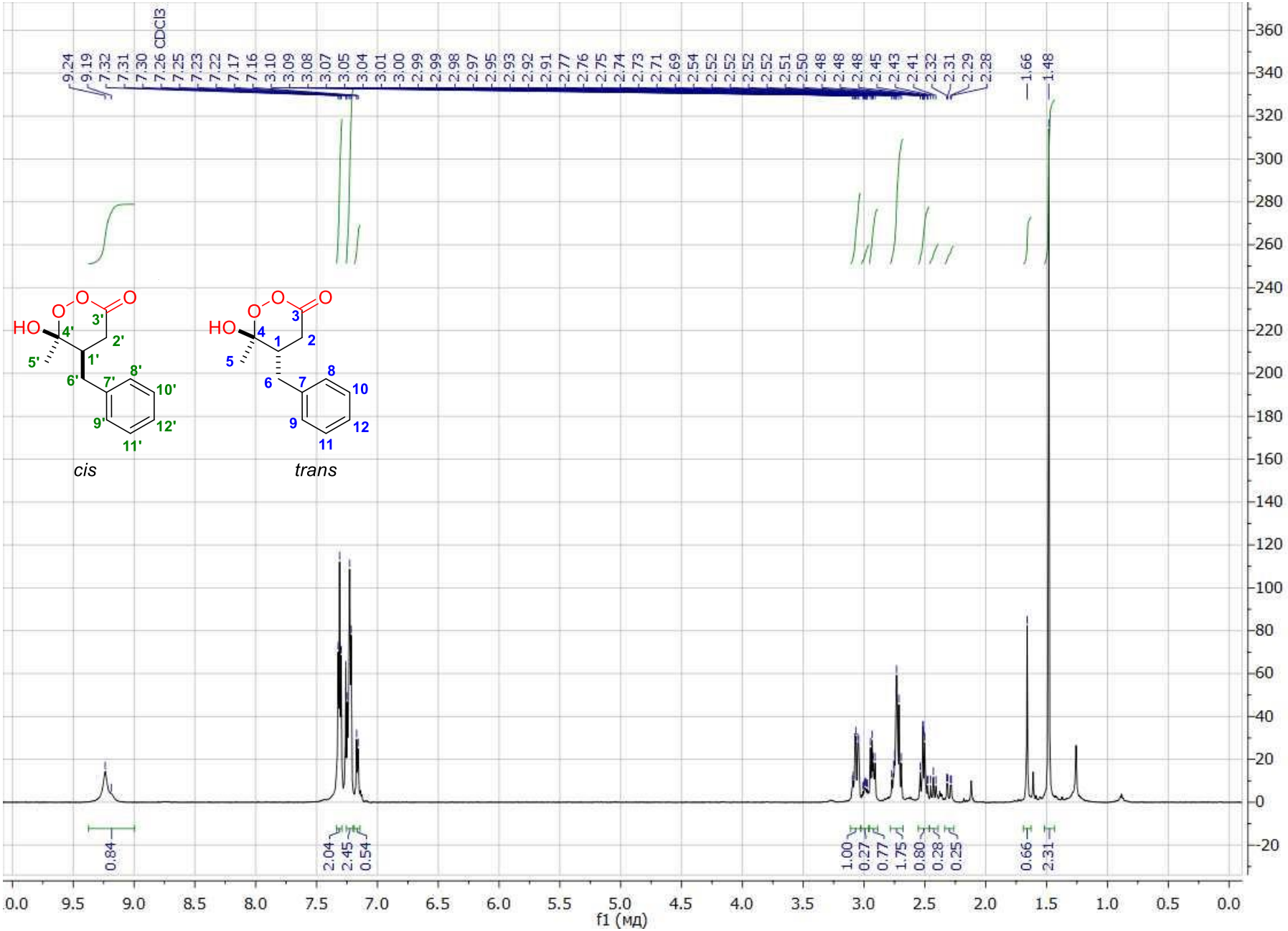


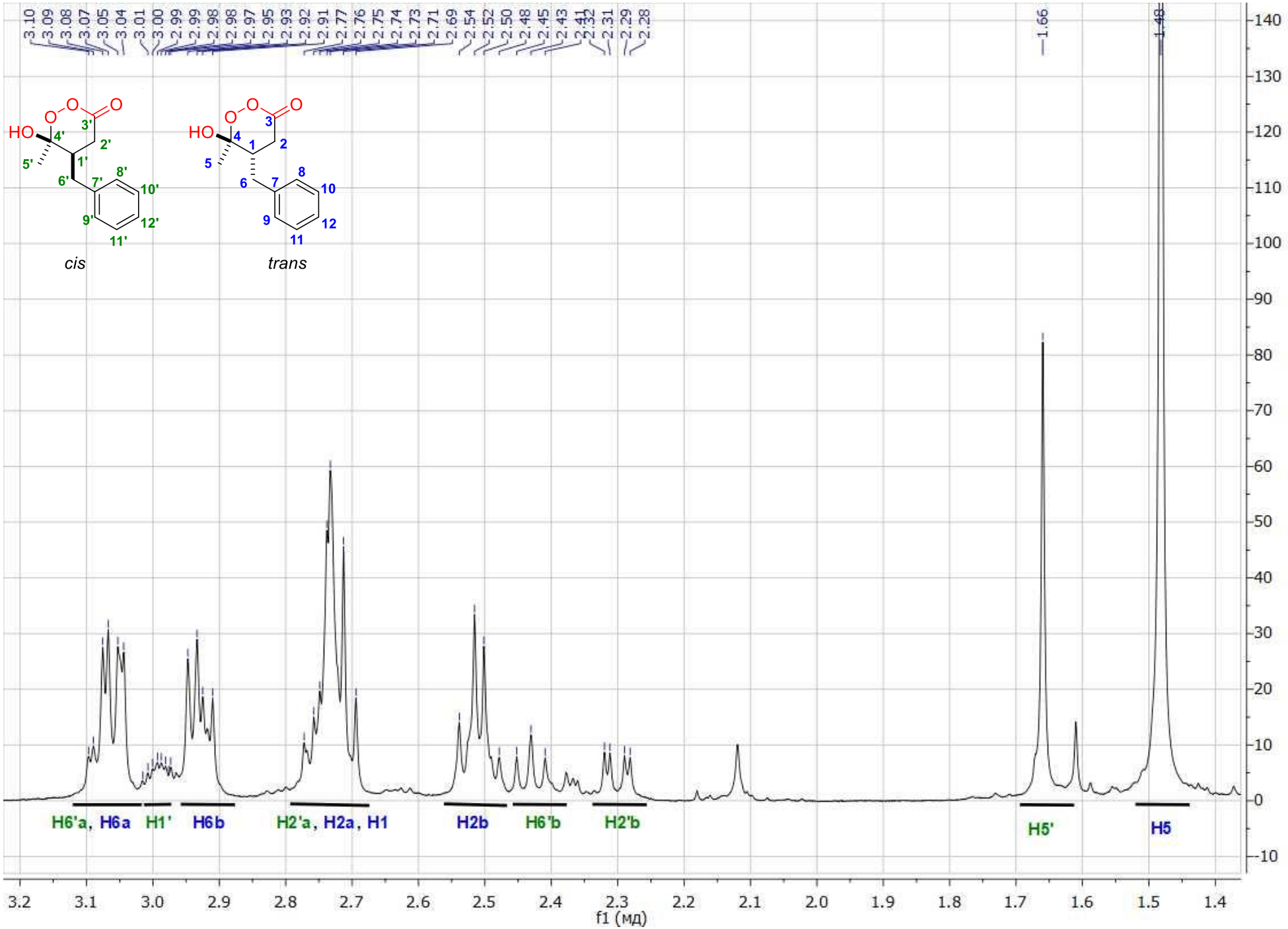
^{13}C NMR

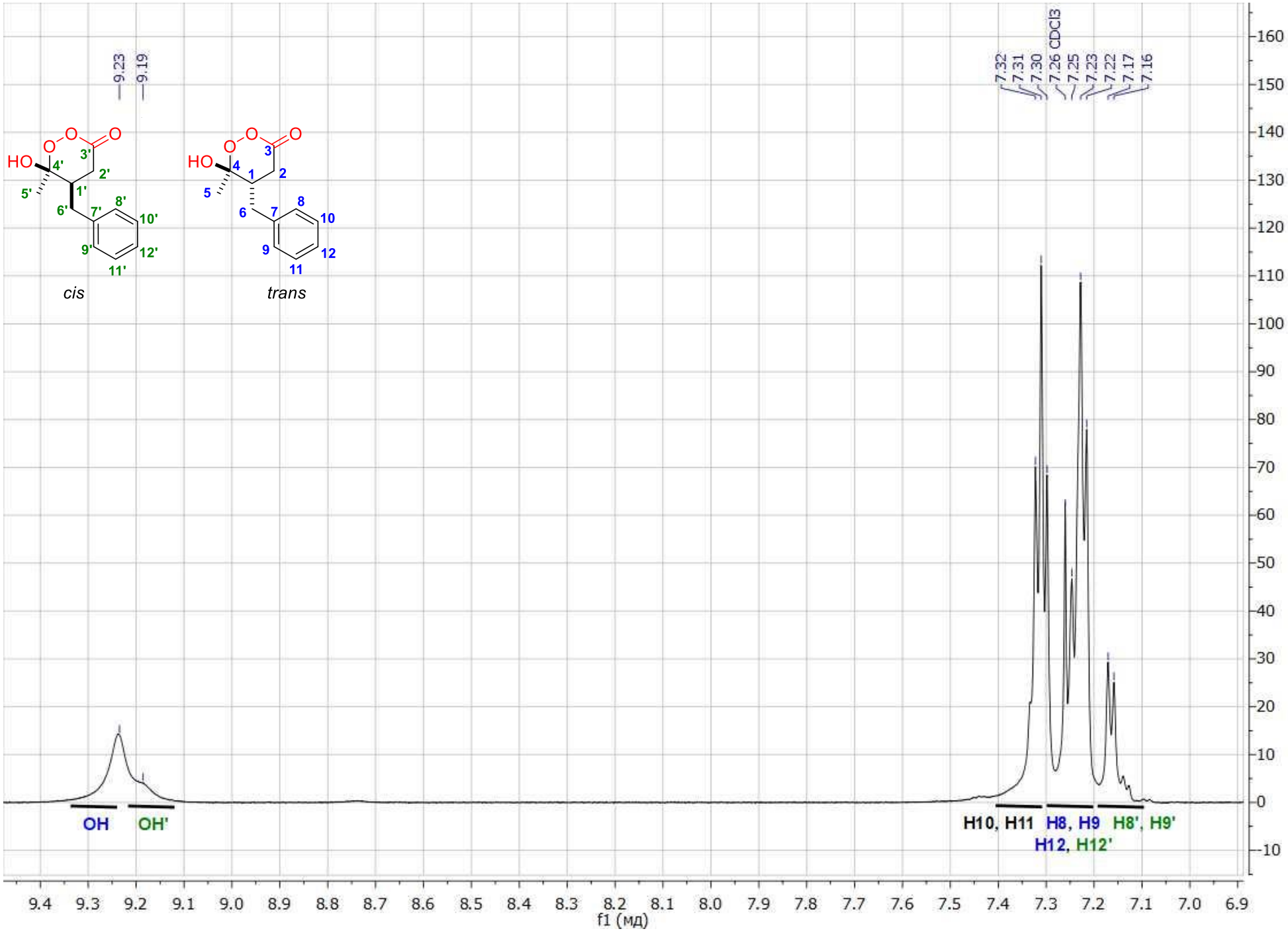

OH
155.43
129.84
121.03
115.47
77.16 CDCl3
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (мд)

5-Benzyl-6-hydroxy-6-methyl-1,2-dioxan-3-one, 3a

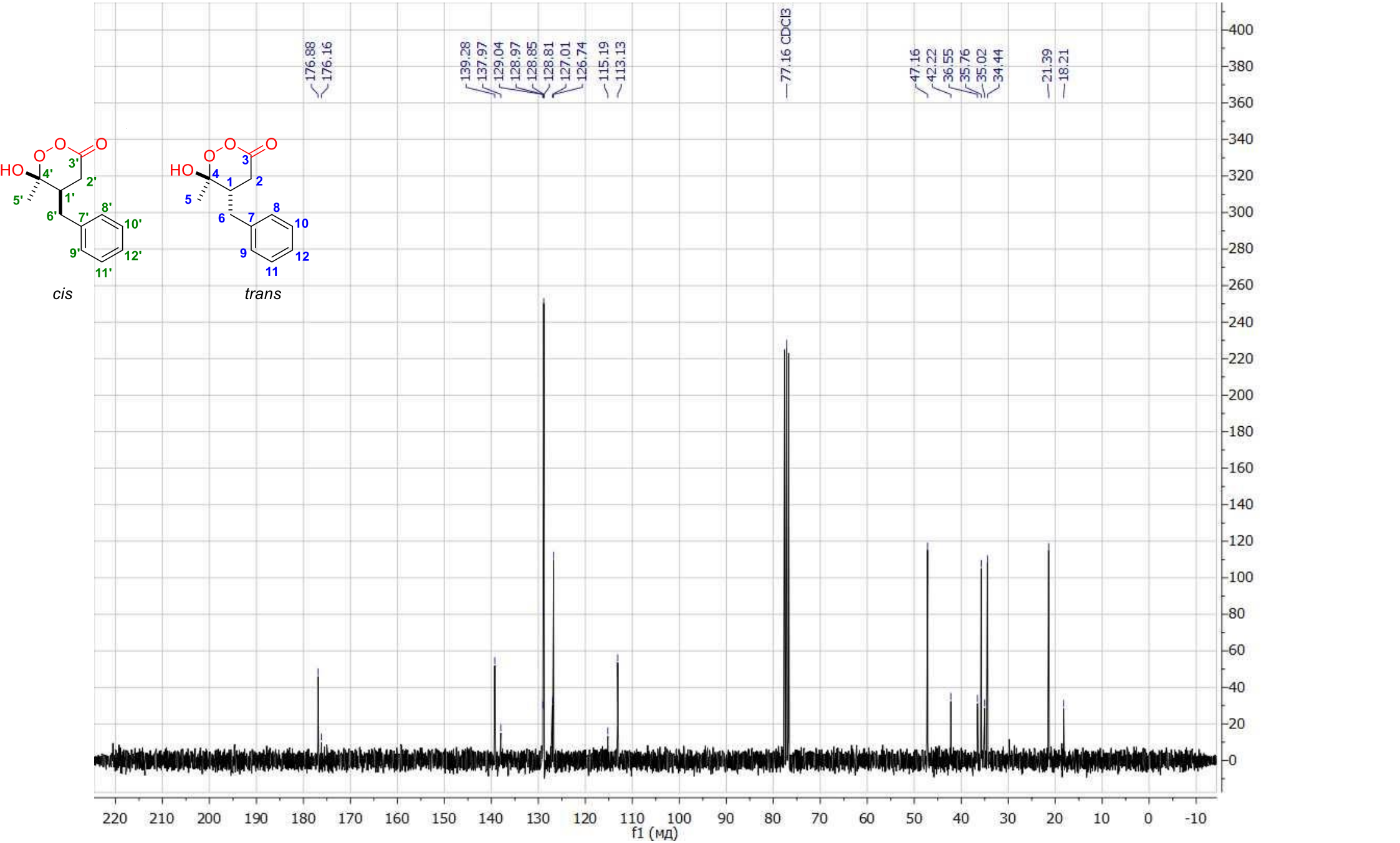
^{1}H NMR

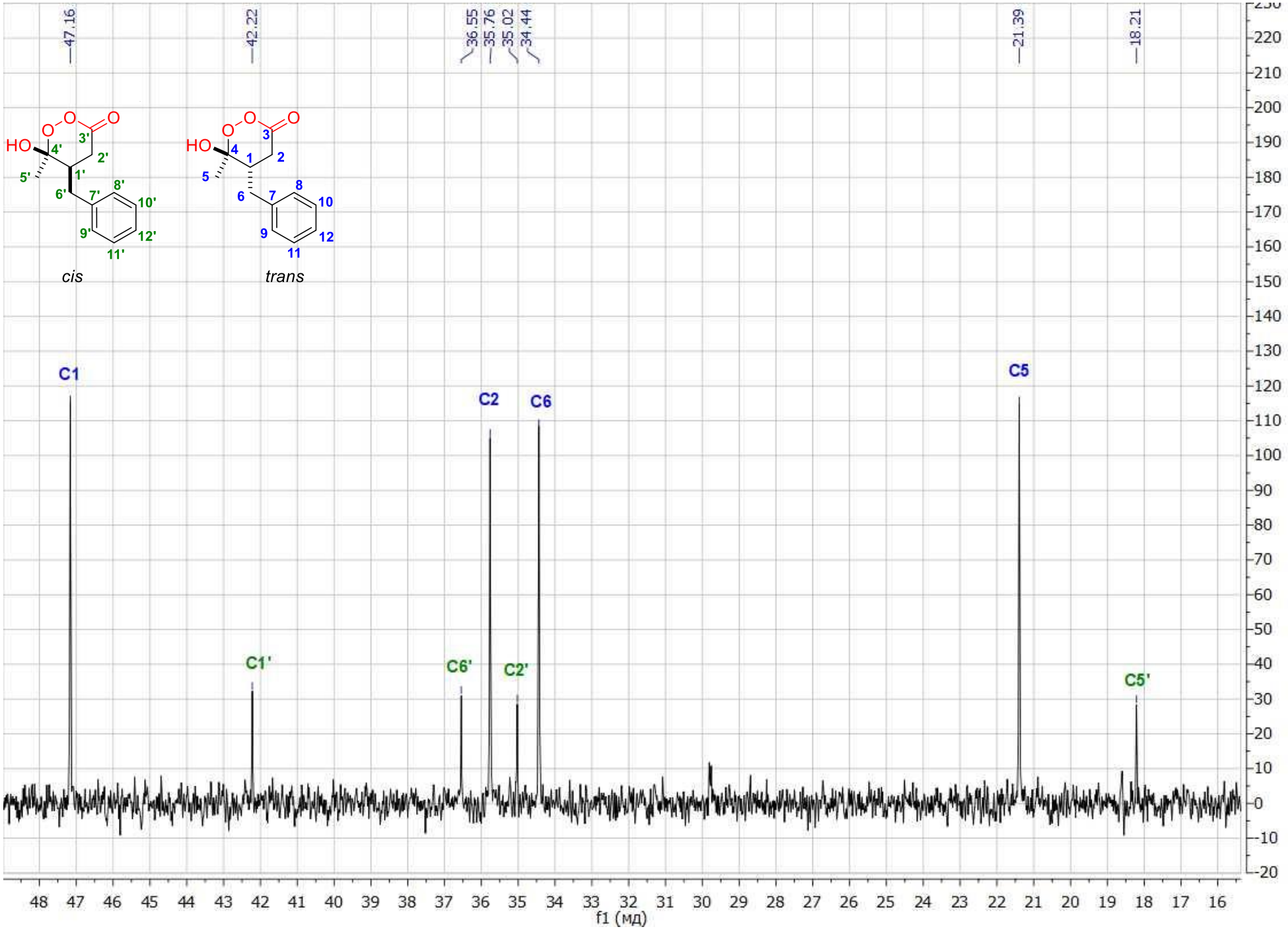


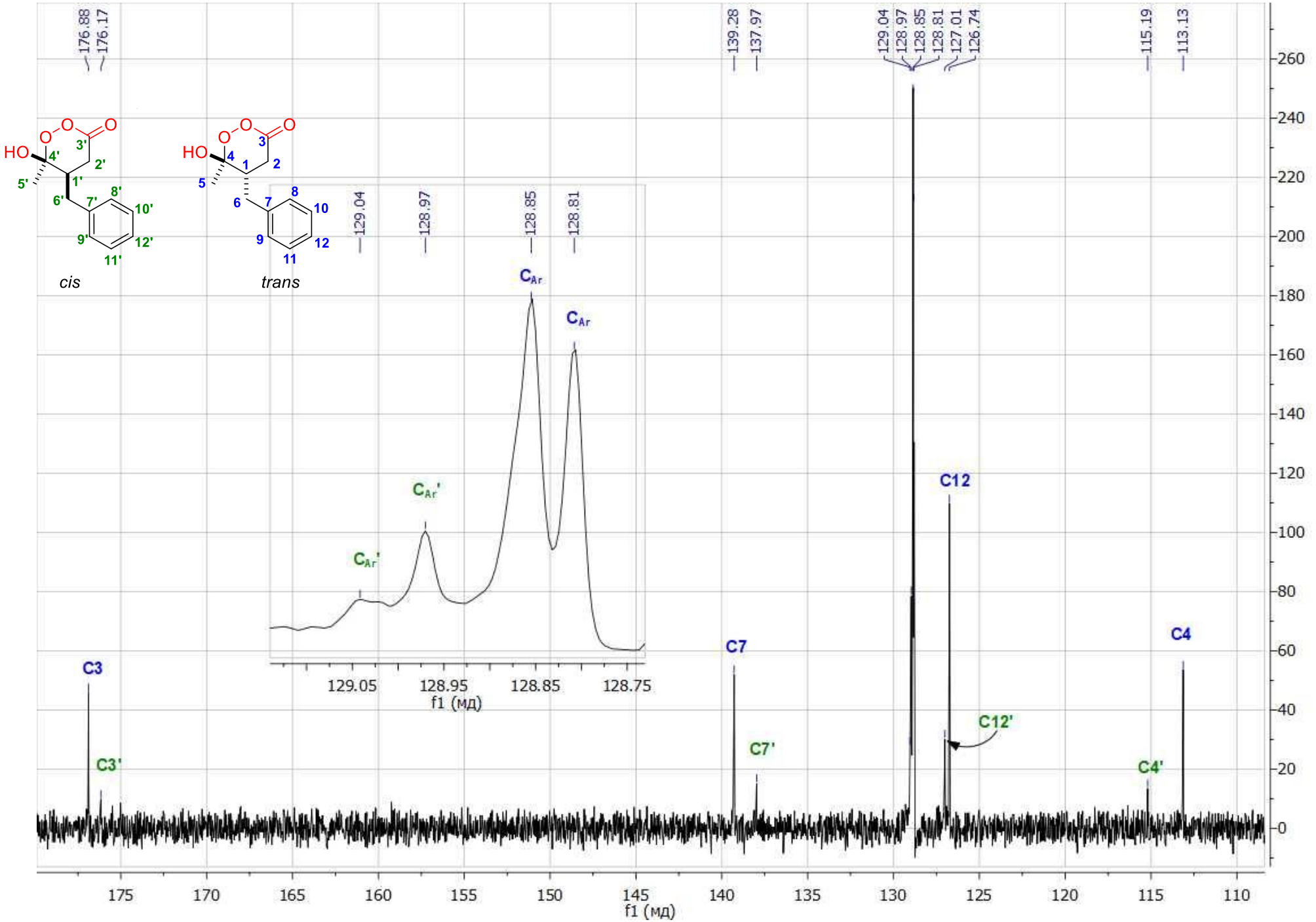

cis
trans
H6'a, H6a
H1'
H6b
H2'a, H2a, H1
H2b
H6'b
H2'b
H5'
H5
f1 (мд)

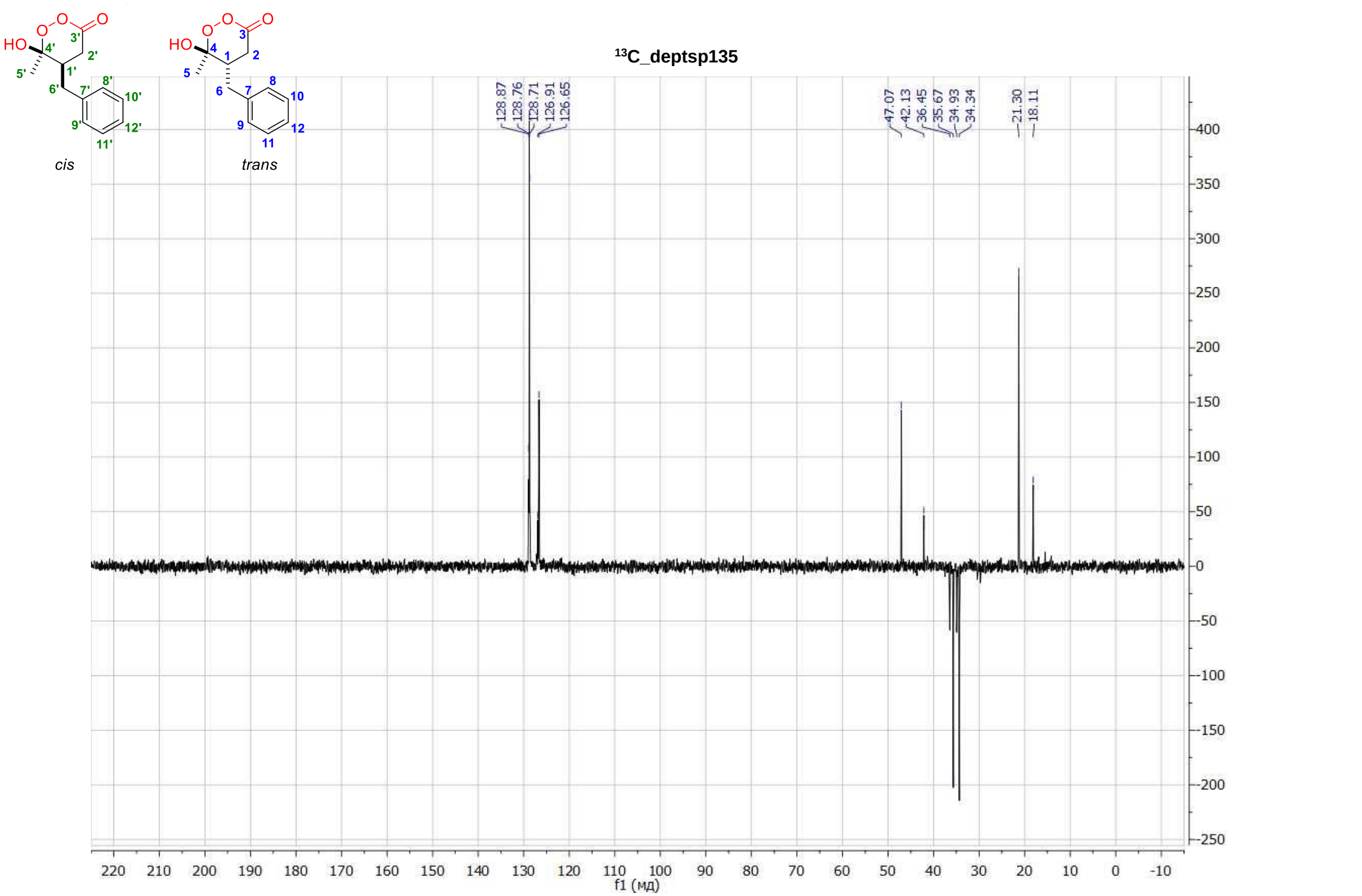

9.23
9.19
7.32
7.31
7.30
7.26 CDCl3
7.25
7.23
7.22
7.17
7.16
HO
O
O
O
3'
4'
2'
1'
5'
6'
7'
8'
10'
9'
12'
11'
cis
HO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
trans
OH
OH'
H10, H11
H8, H9
H8', H9'
H12, H12'
f1 (мд)

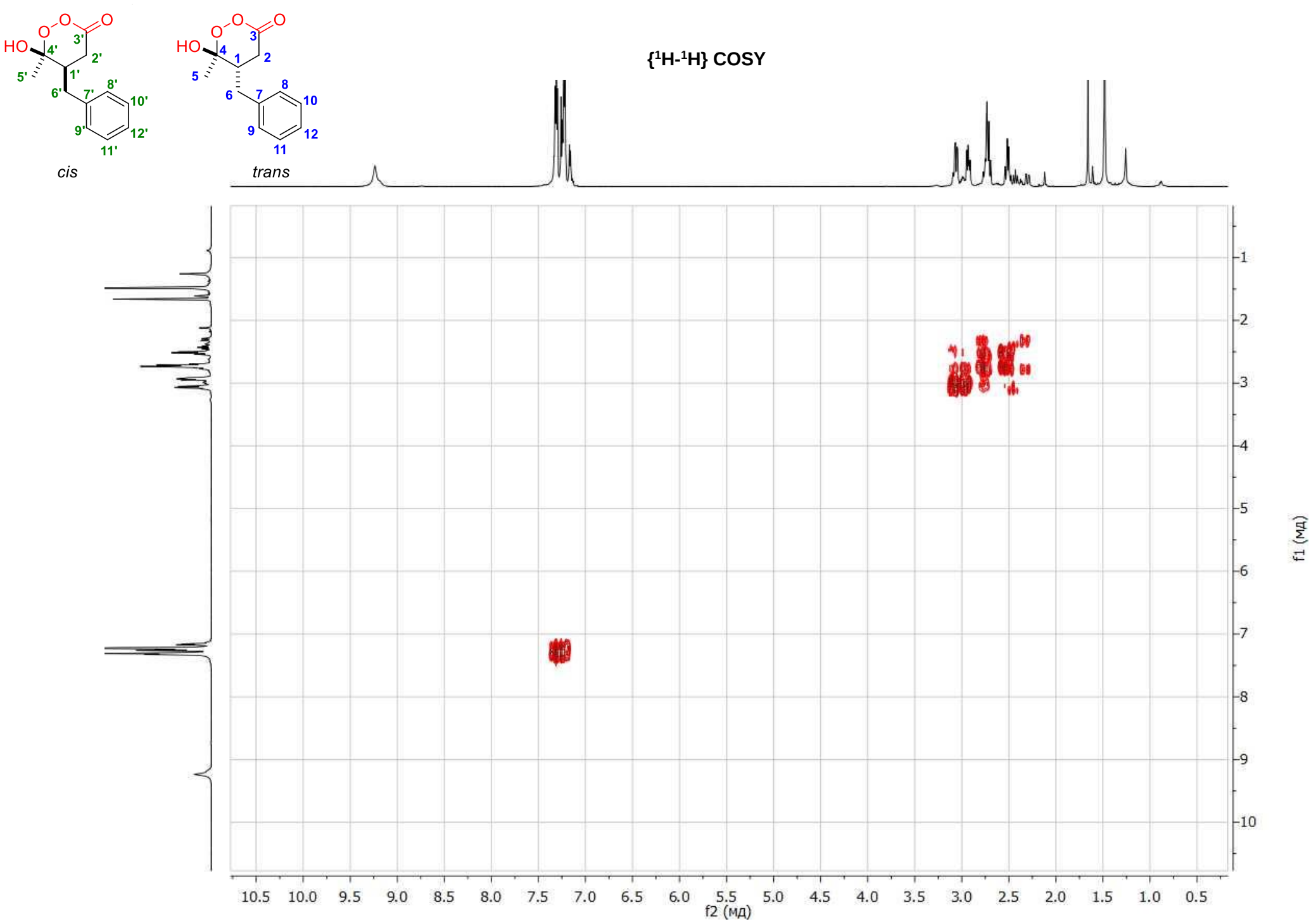
^{13}C NMR

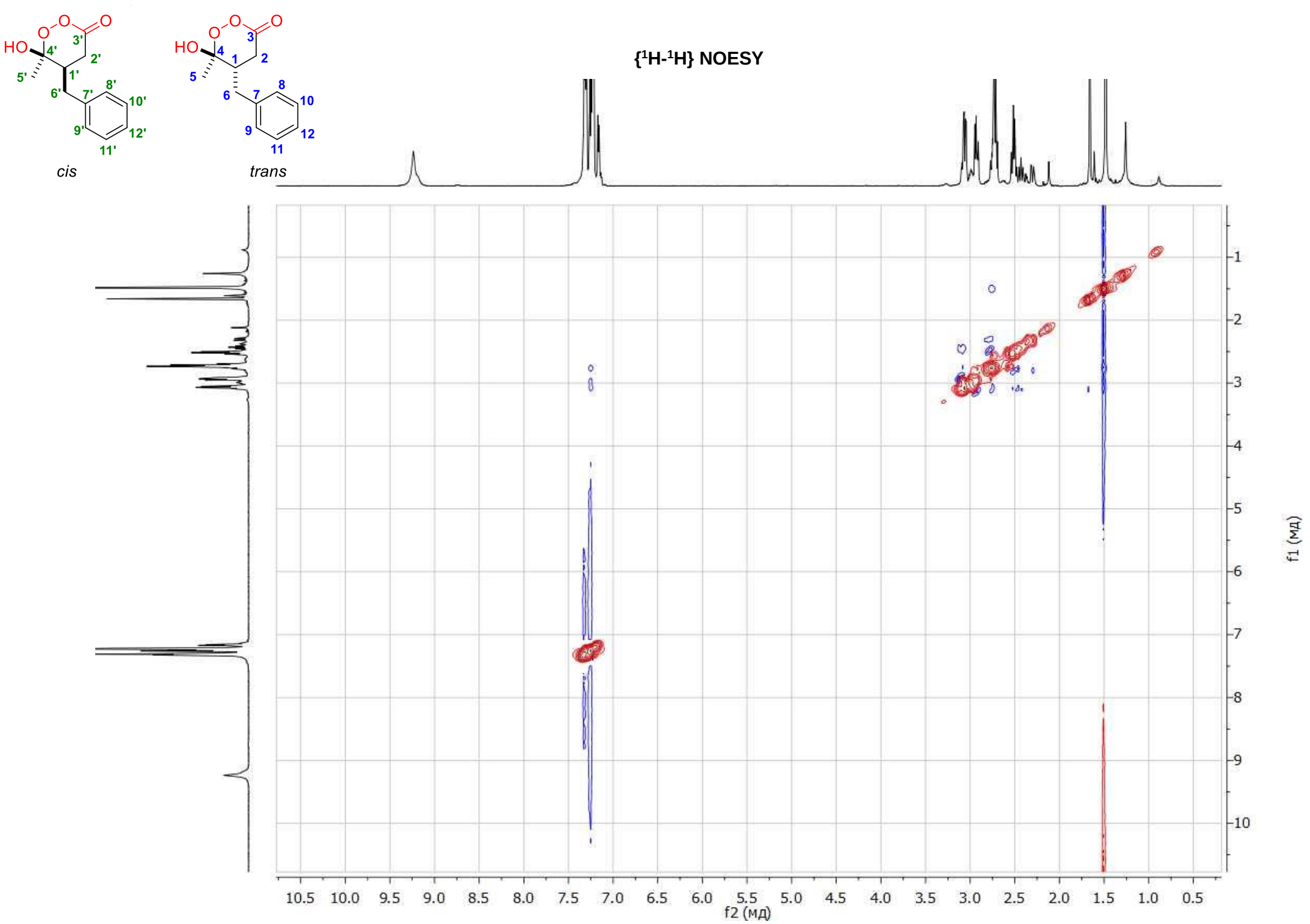

176.88
176.16
139.28
137.97
129.04
128.97
128.85
128.81
127.01
126.74
115.19
113.13
77.16 CDCl3
47.16
42.22
36.55
35.76
35.02
34.44
21.39
18.21
HO
cis
trans
f1 (мд)

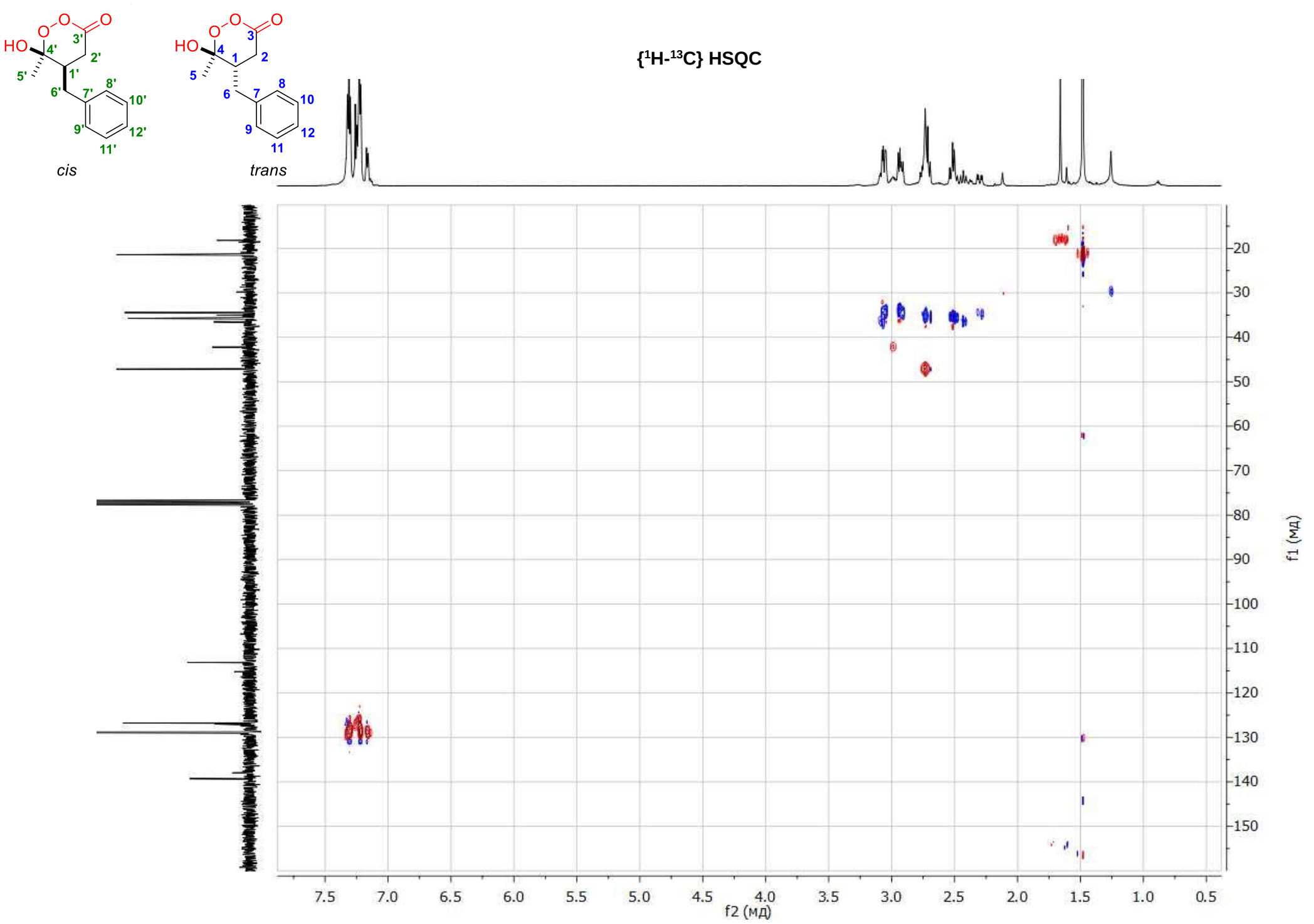

47.16
42.22
36.55
35.76
35.02
34.44
21.39
18.21
HO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
cis
HO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
trans
C1
C2
C6
C5
C1'
C6'
C2'
C5'
f1 (мд)

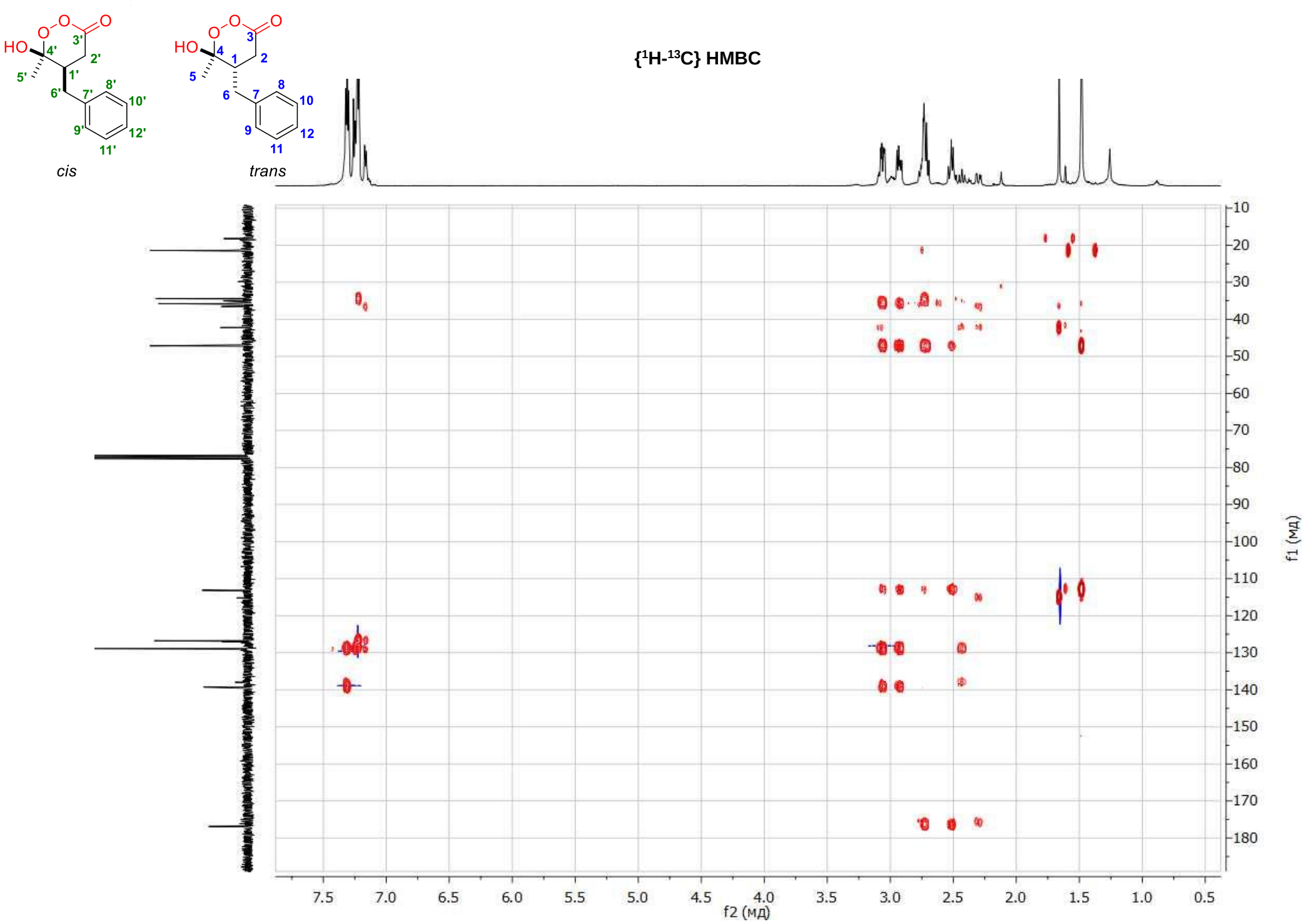

176.88
176.17
139.28
137.97
129.04
128.97
128.85
128.81
127.01
126.74
115.19
113.13
HO
O
O
O
3'
4'
2'
5'
1'
6'
7'
8'
10'
9'
12'
11'
cis
HO
O
O
O
3
4
1
2
5
6
7
8
10
9
12
11
trans
129.04
128.97
128.85
128.81
C_Ar
C_Ar
C_Ar'
C_Ar'
129.05
128.95
128.85
128.75
f1 (мд)
C3
C3'
C7
C7'
C12
C12'
C4
C4'
260
240
220
200
180
160
140
120
100
80
60
40
20
0
175
170
165
160
155
150
145
140
135
130
125
120
115
110
f1 (мд)

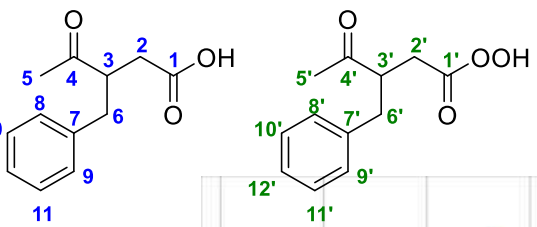

cis
trans
13C_deptsp135
128.87
128.76
128.71
126.91
126.65
47.07
42.13
36.45
35.67
34.93
34.34
21.30
18.11
f1 (мд)


cis
trans
{1H-1H} COSY
f2 (мд)
f1 (мд)


{1H-1H} NOESY
cis
trans
f2 (мд)
f1 (мд)

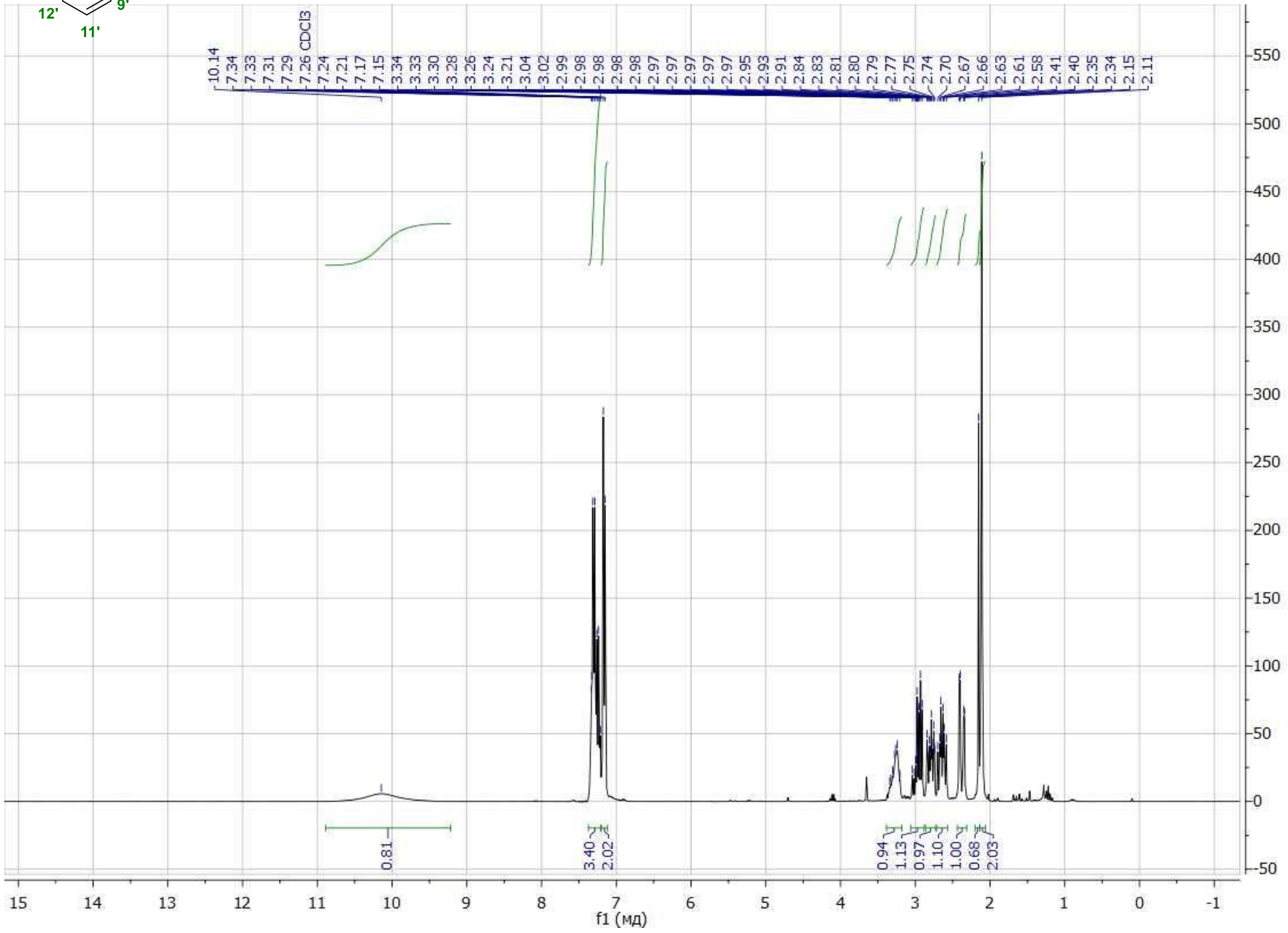

{1H-13C} HSQC
cis
trans
f2 (мд)
f1 (мд)

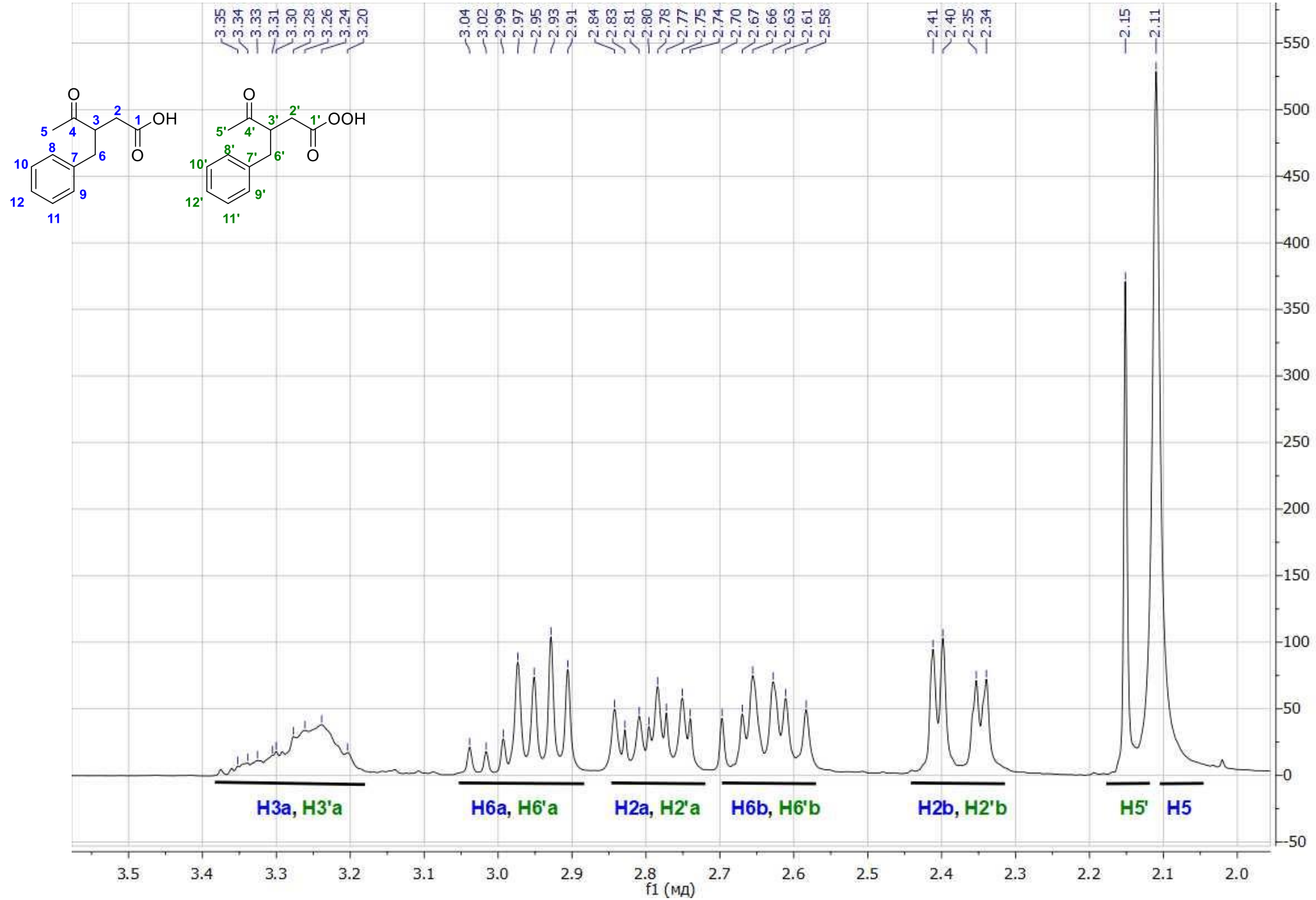

cis
trans
{1H-13C} HMBC
f2 (мд)
f1 (мд)

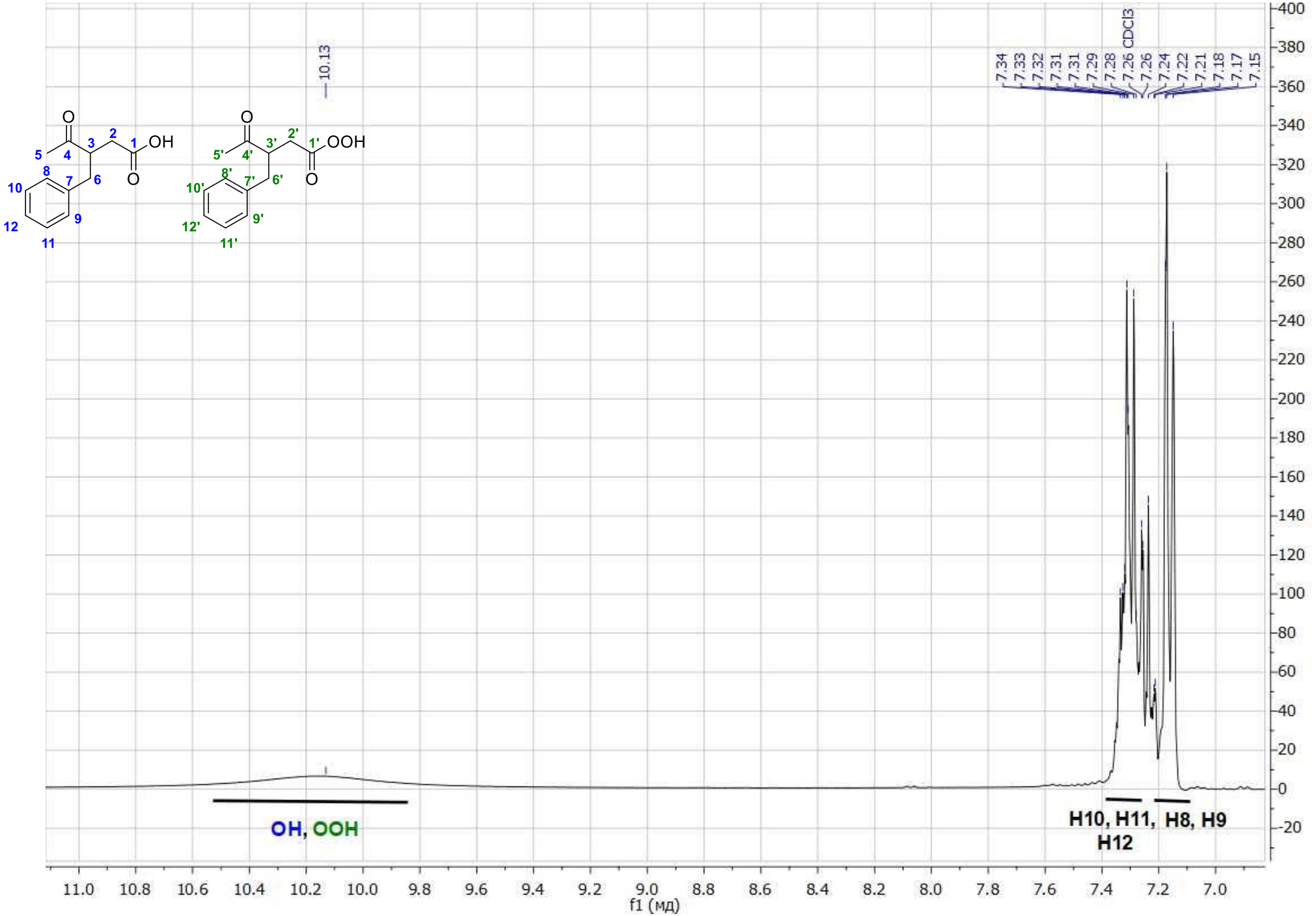


3-Benzyl-4-oxopentaneperoxoic acid (4a) and 3-benzyl-4-oxopentanoic acid (5a)

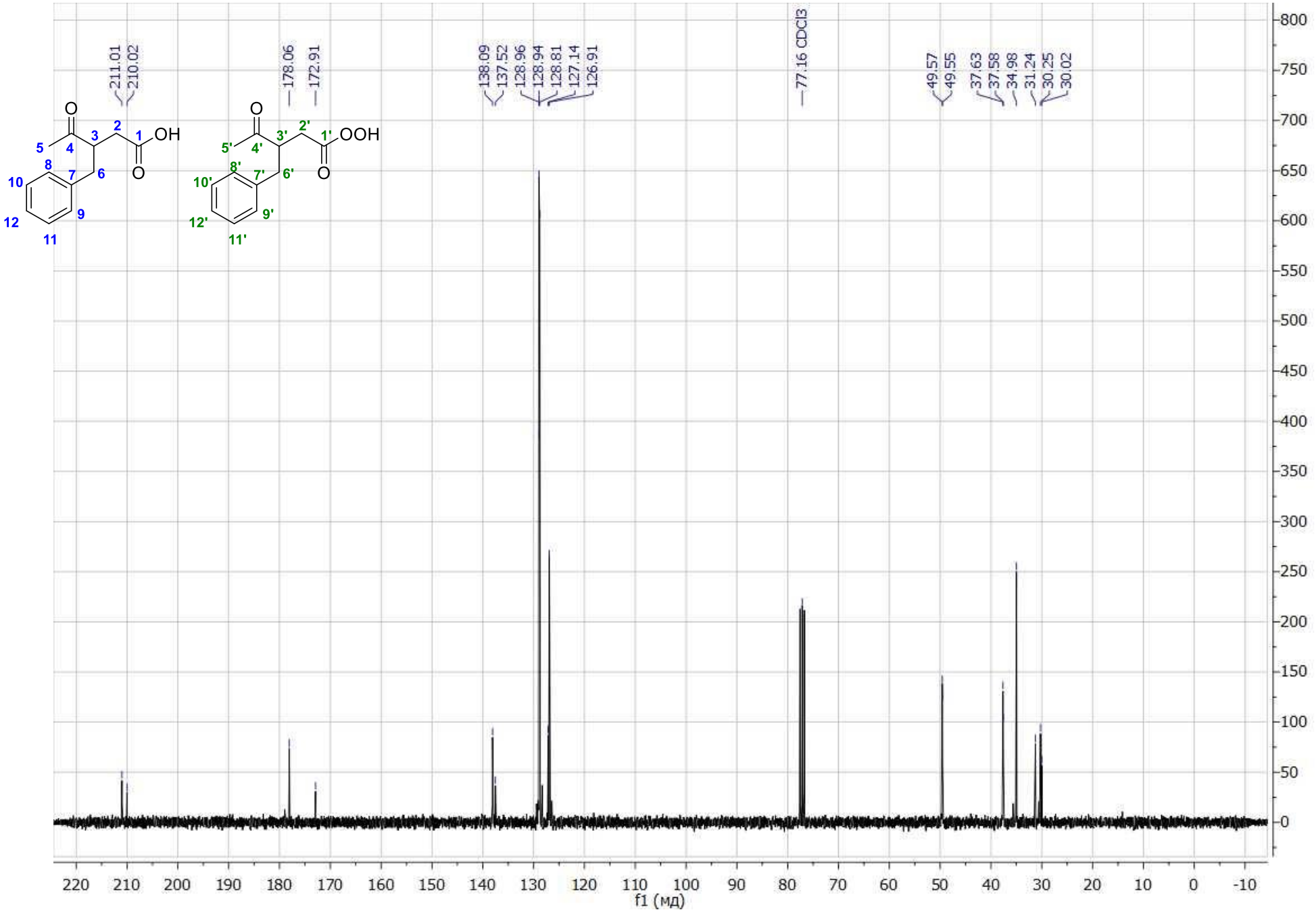
^{1}H NMR

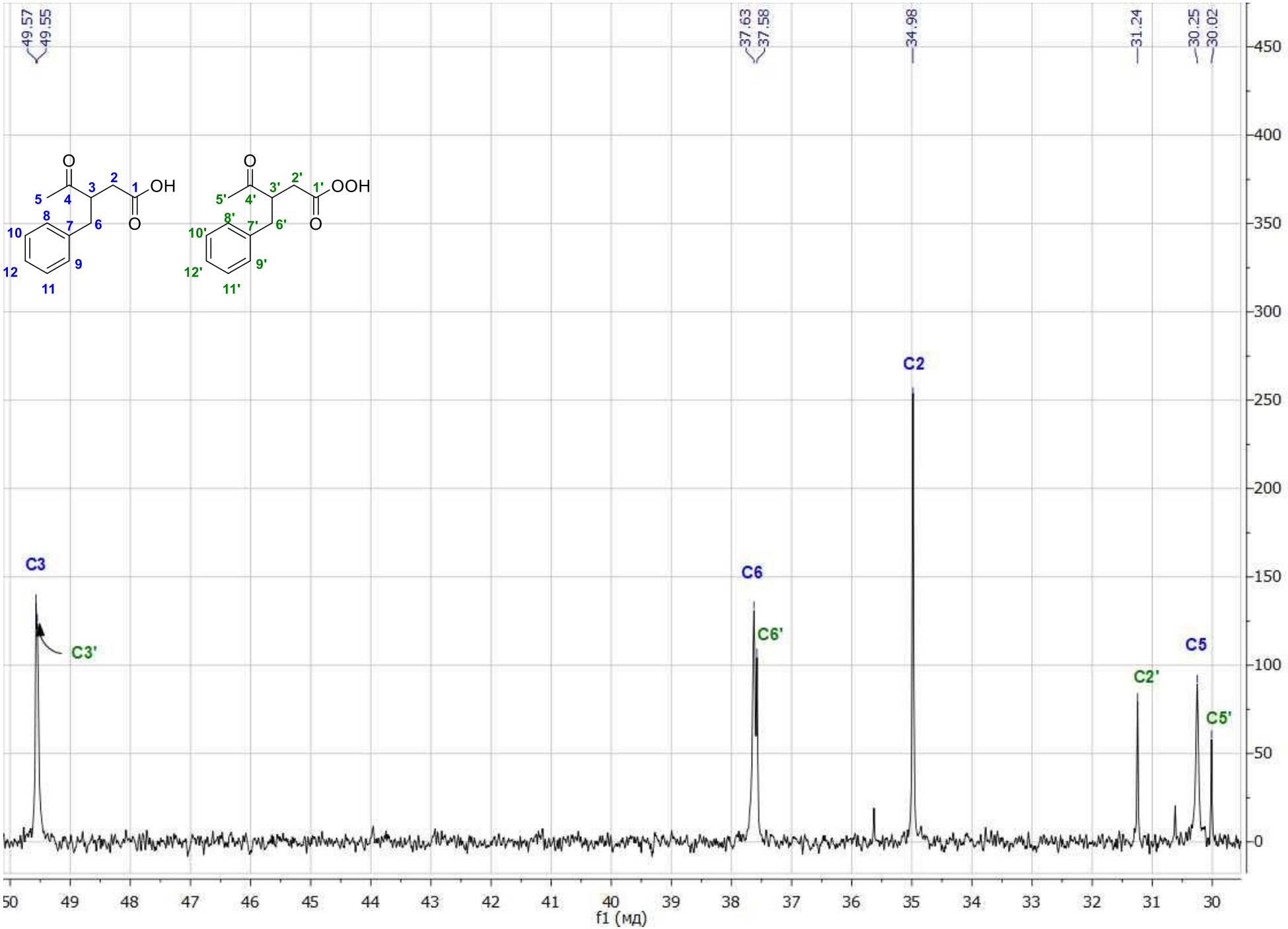


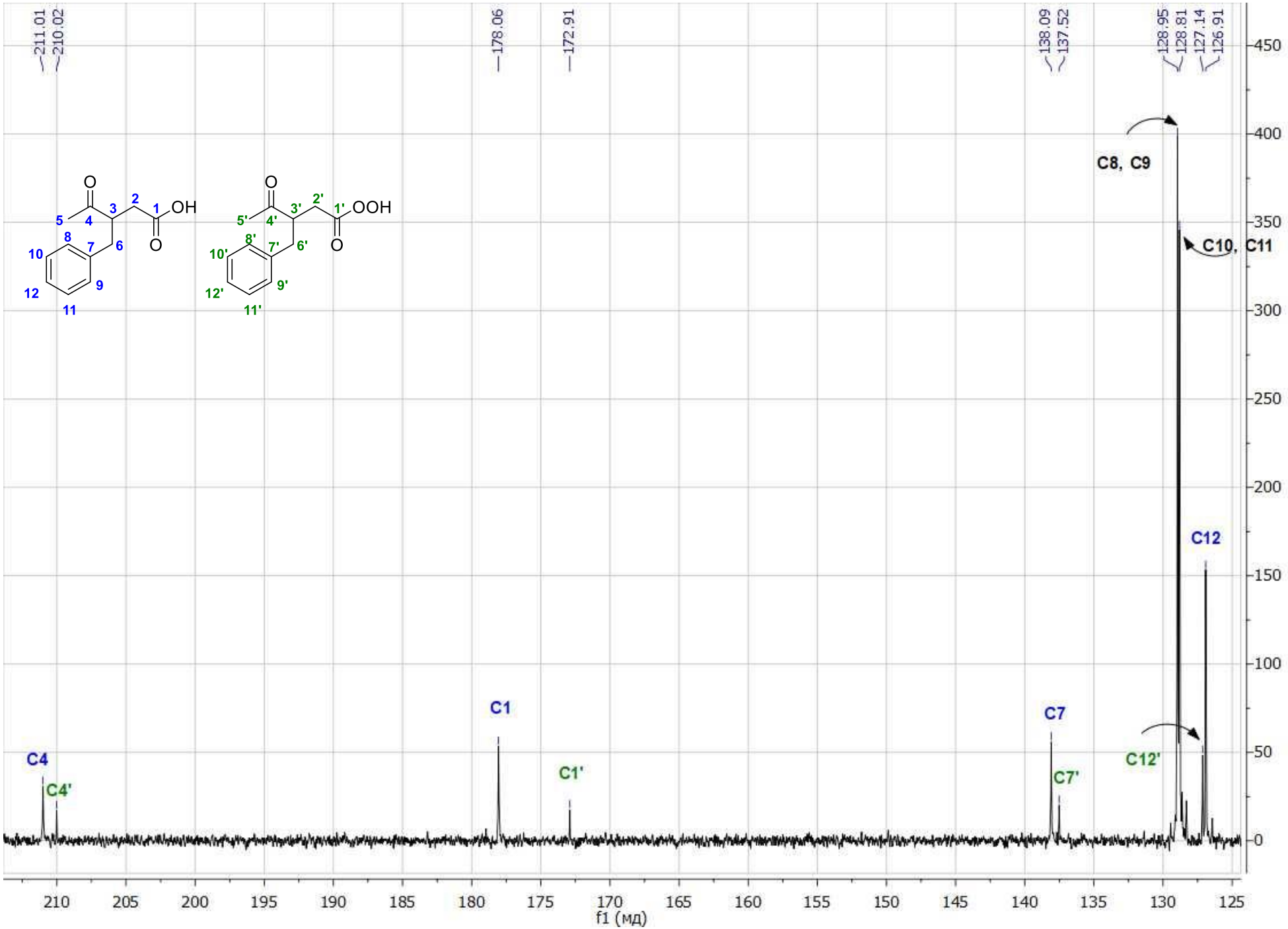

3.35
3.34
3.33
3.31
3.30
3.28
3.26
3.24
3.20
3.04
3.02
2.99
2.97
2.95
2.93
2.91
2.84
2.83
2.81
2.80
2.78
2.77
2.75
2.74
2.70
2.67
2.66
2.63
2.61
2.58
2.41
2.40
2.35
2.34
2.15
2.11
OH
OOH
H3a, H3'a
H6a, H6'a
H2a, H2'a
H6b, H6'b
H2b, H2'b
H5'
H5
f1 (мд)

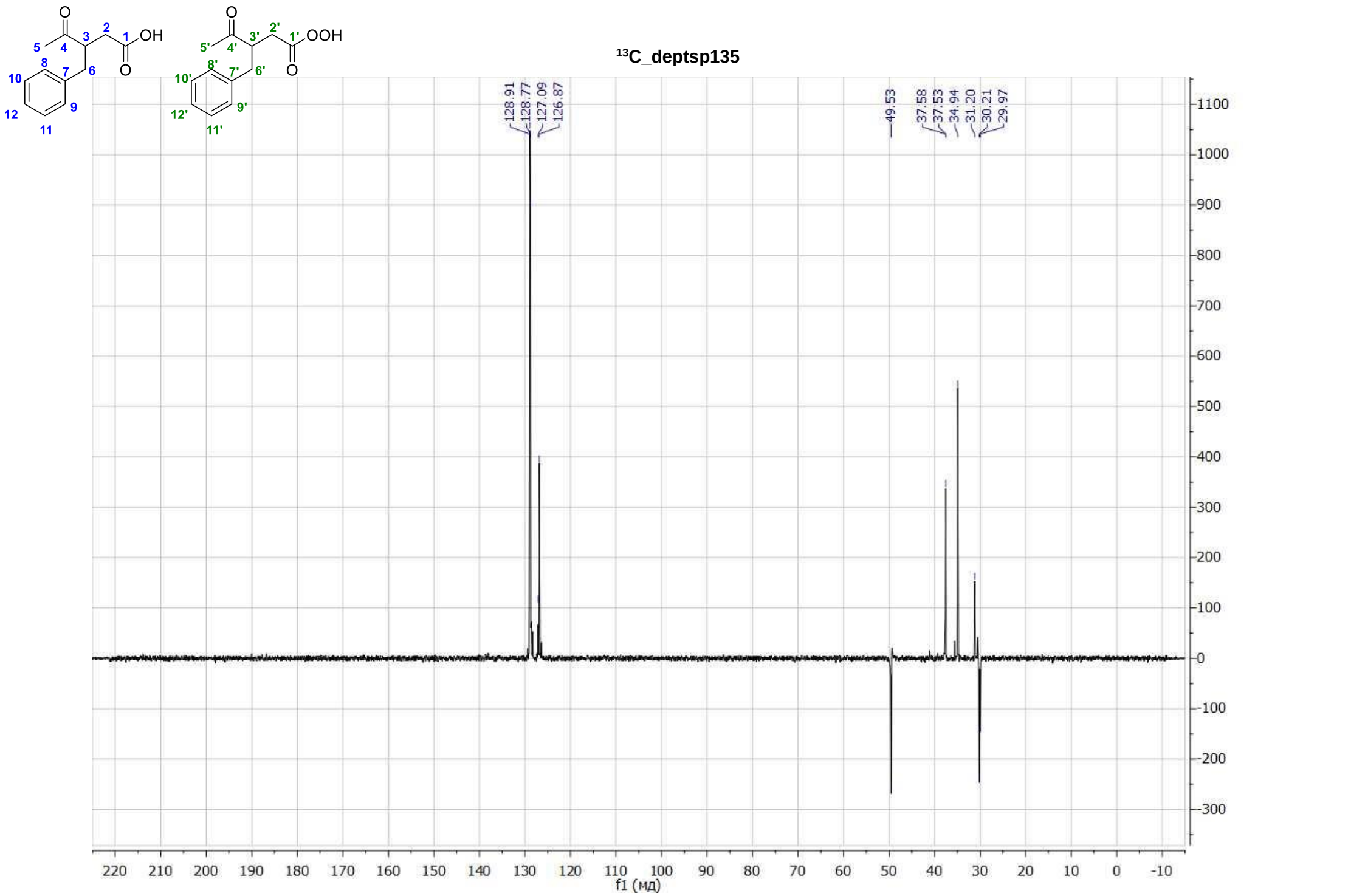

10.13
7.34
7.33
7.32
7.31
7.31
7.29
7.28
7.26 CDCl3
7.26
7.24
7.22
7.21
7.18
7.17
7.15
OH
OOH
OH, OOH
H10, H11, H8, H9
H12
f1 (мд)

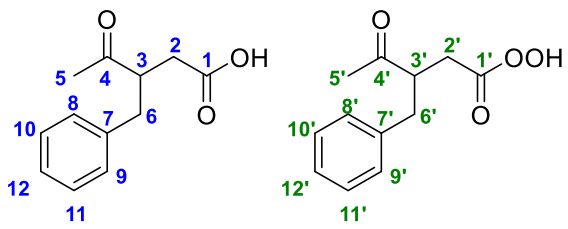
^{13}C NMR


211.01
210.02
178.06
172.91
138.09
137.52
128.96
128.94
128.81
127.14
126.91
77.16 CDCl3
49.57
49.55
37.63
37.58
34.98
31.24
30.25
30.02
OH
OOH
f1 (мд)

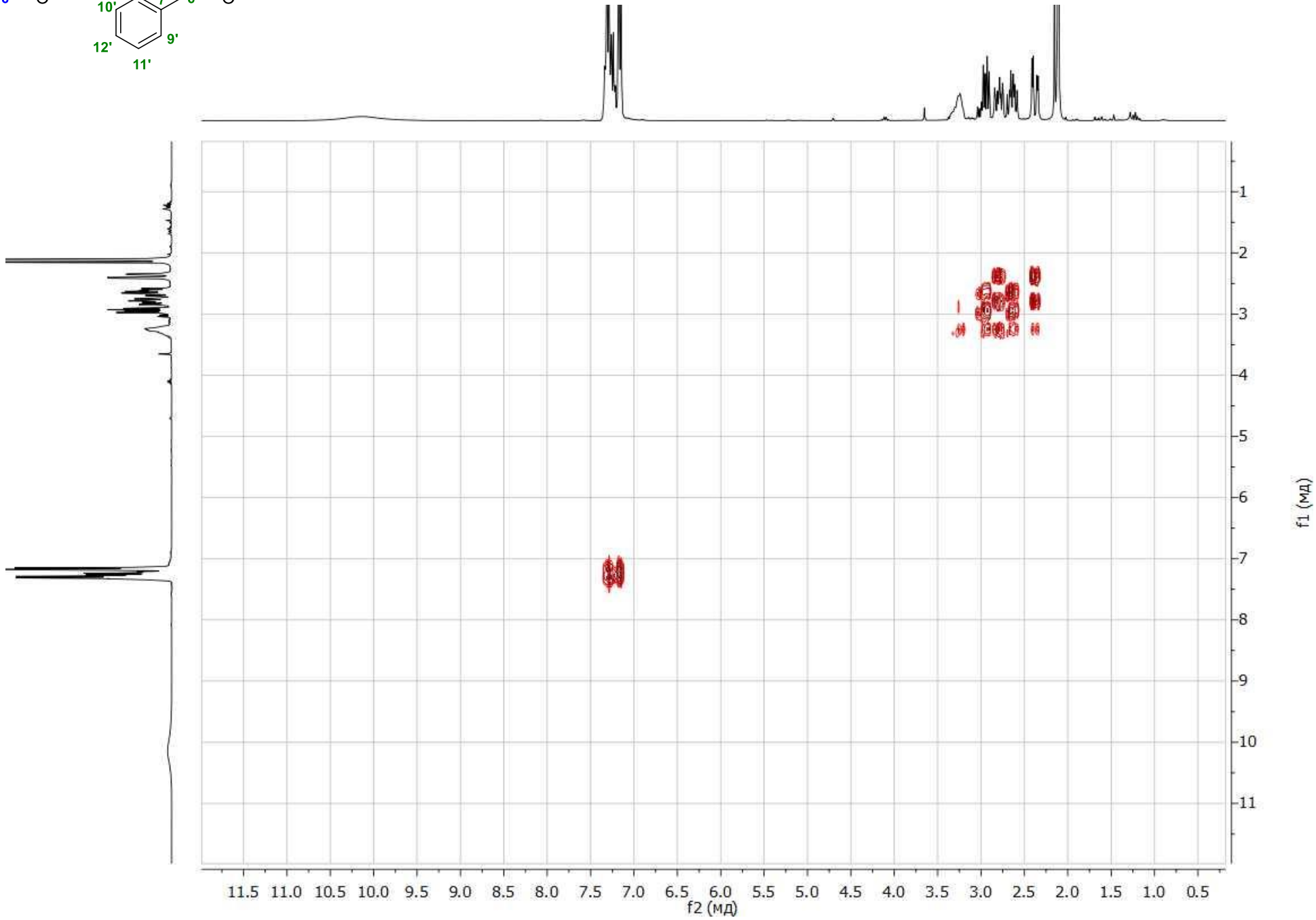

49.57
49.55
37.63
37.58
34.98
31.24
30.25
30.02
OH
OOH
C3
C3'
C6
C6'
C2
C2'
C5
C5'
f1 (мд)

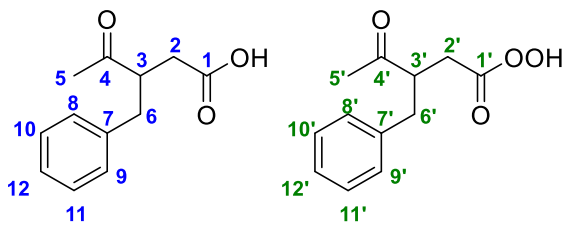

211.01
210.02
178.06
172.91
138.09
137.52
128.95
128.81
127.14
126.91
C8, C9
C10, C11
C12
C1
C7
C4
C4'
C1'
C7'
C12'
f1 (мд)


13C_deptsp135
128.91
128.77
127.09
126.87
49.53
37.58
37.53
34.94
31.20
30.21
29.97
f1 (мд)

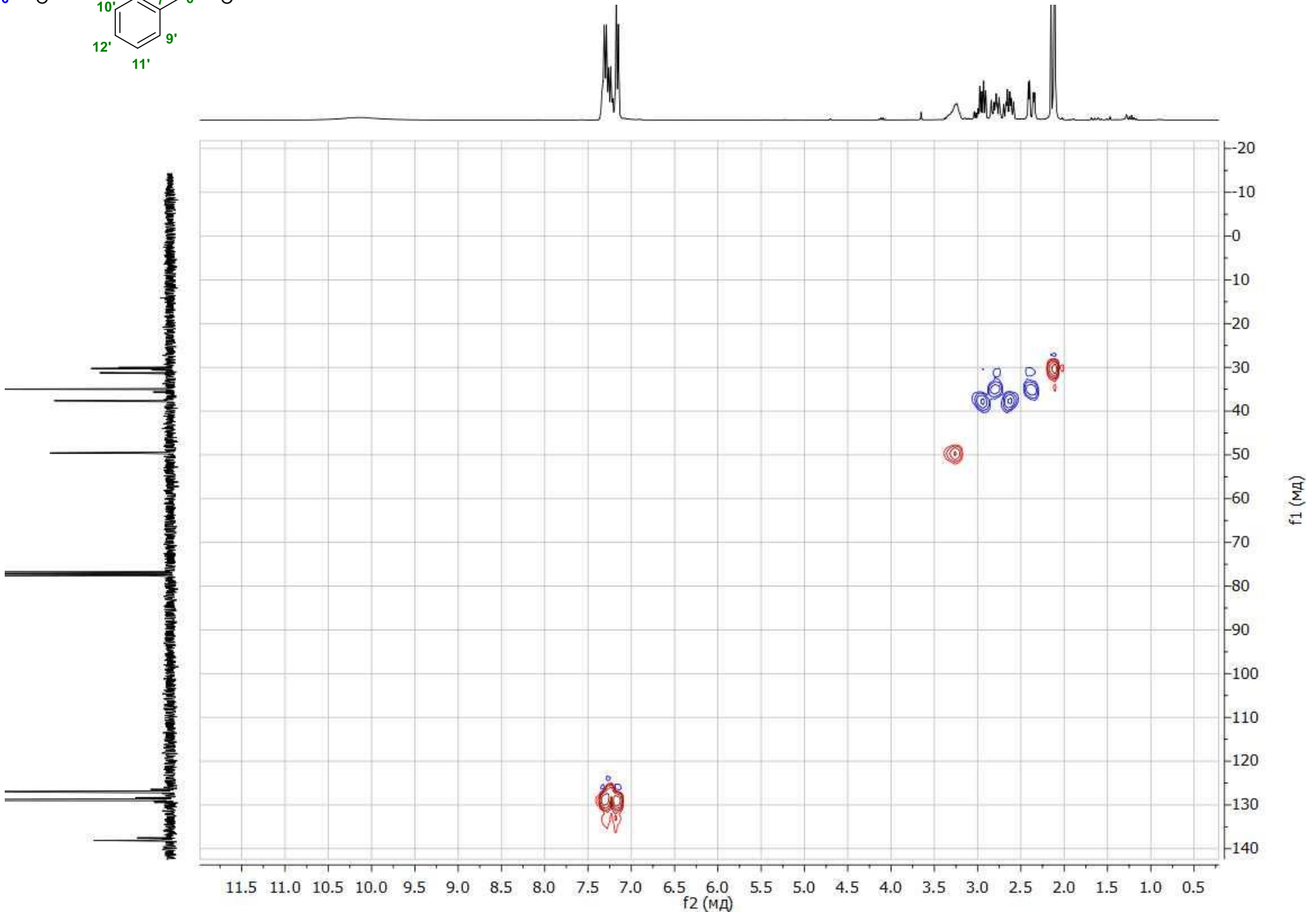

O
OH
O
1
2
3
4
5
6
7
8
9
10
11
12
O
OOH
O
1'
2'
3'
4'
5'
6'
7'
8'
9'
10'
11'
12'

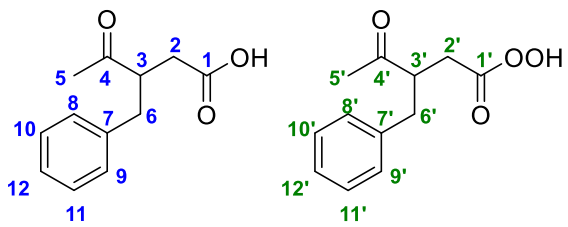
{^{1}H-^{1}H} COSY


f1 (мд)
f2 (мд)
1
2
3
4
5
6
7
8
9
10
11
11.5 11.0 10.5 10.0 9.5 9.0 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

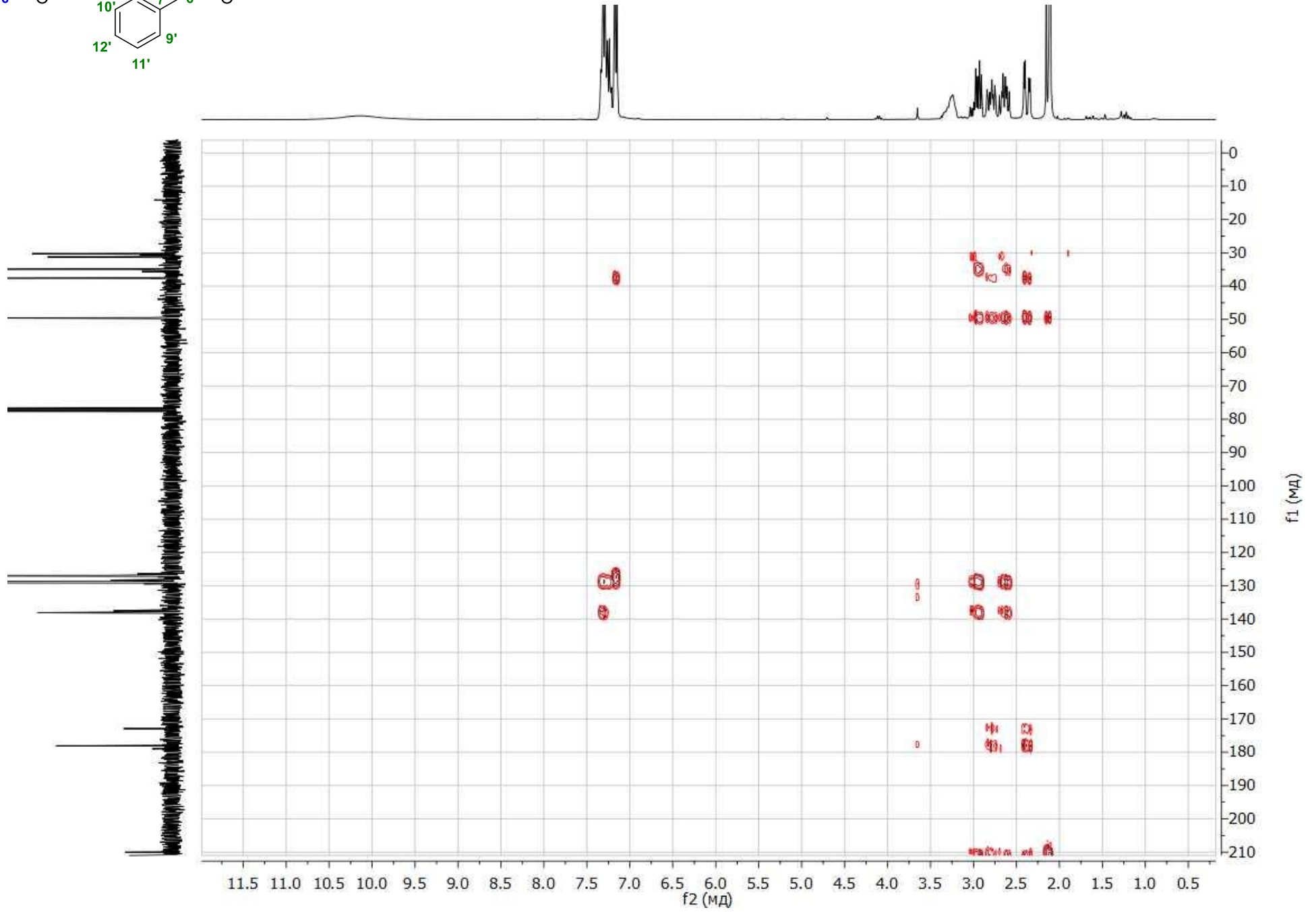


{^{1}H-^{13}C} HSQC



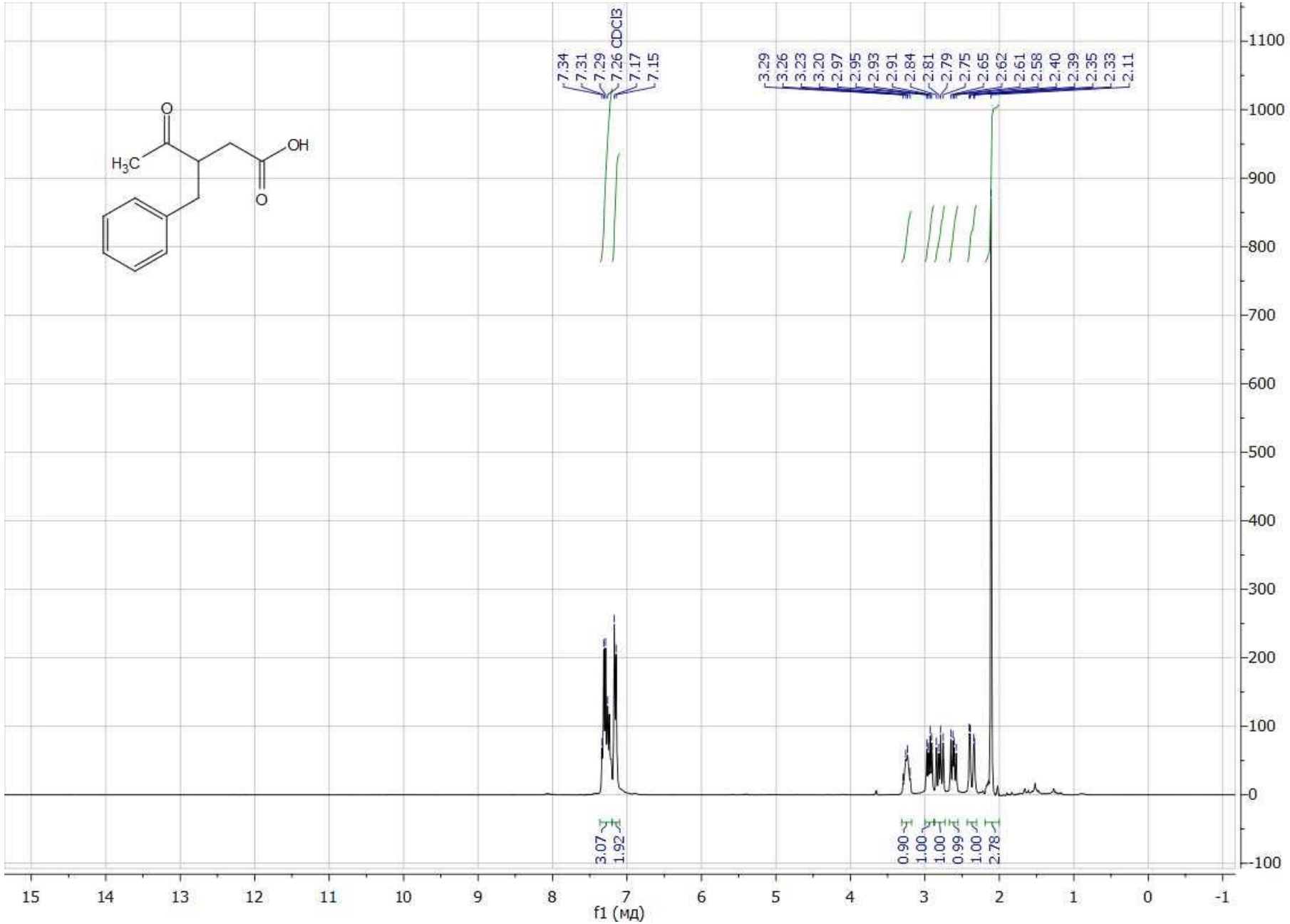

O
OH
1
2
3
4
5
6
7
8
9
10
11
12
O
OOH
1'
2'
3'
4'
5'
6'
7'
8'
9'
10'
11'
12'

{^{1}H-^{13}C} HMBC

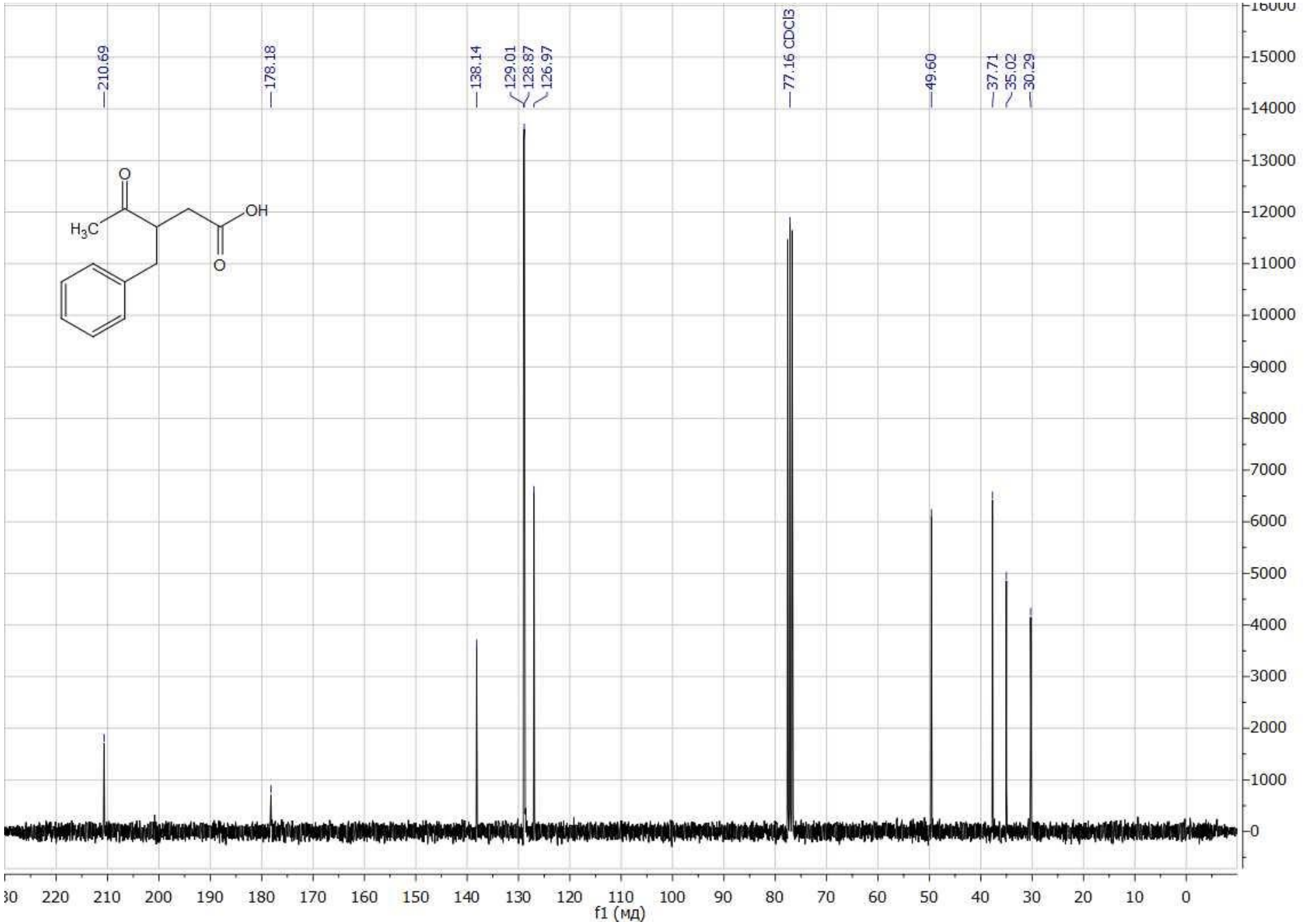

f2 (мд)
f1 (мд)
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210

3-Benzyl-4-oxopentanoic acid, 5a

^{1}H NMR



^{13}C NMR


210.69
178.18
138.14
129.01
128.87
126.97
77.16 CDCl3
49.60
37.71
35.02
30.29
O
H3C
OH
O
f1 (мд)

HRMS data of γ-hydroperoxy-γ-peroxylactones 2 and other products
5-Benzyl-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2a

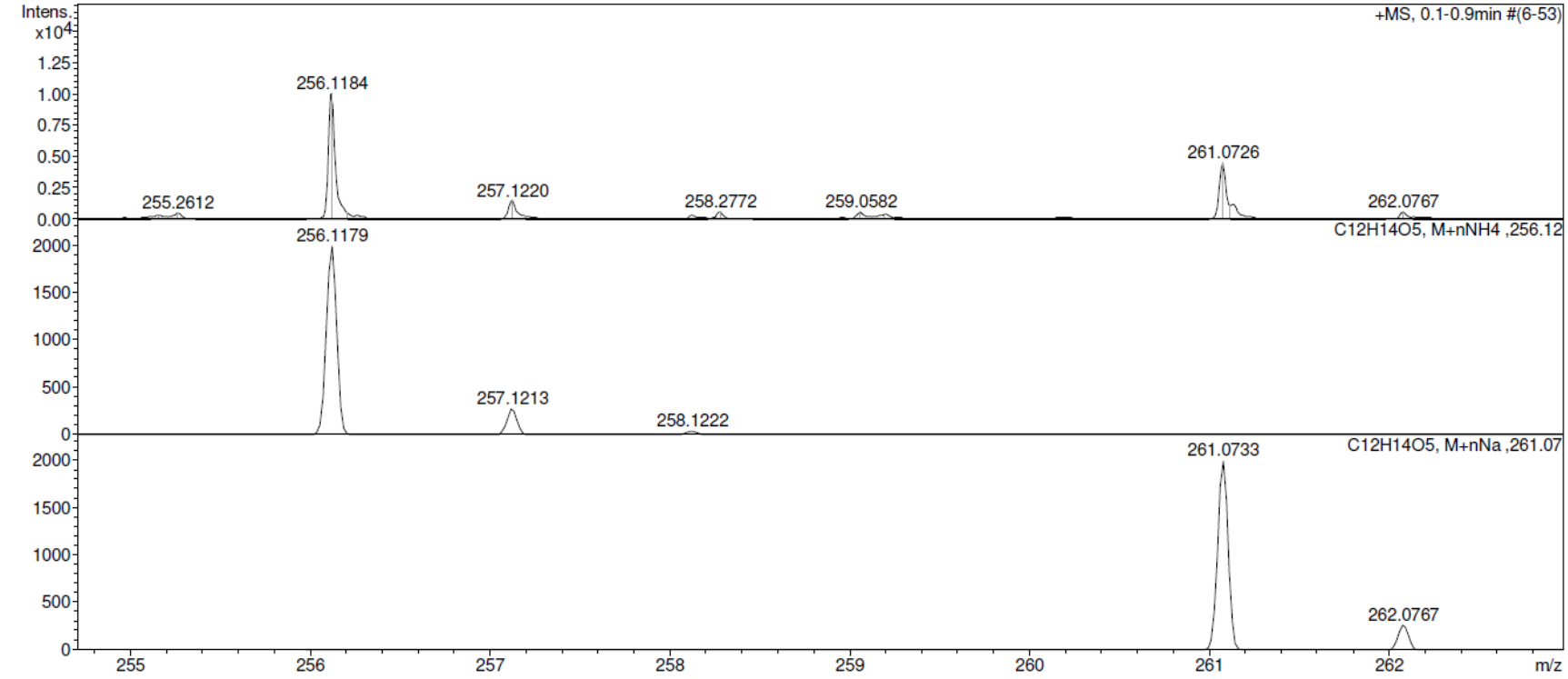
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Vil\0903033.d	Acquisition Date	03.09.2019 17:06:22
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN BB2137	Instrument / Ser#	micrOTOF 10248
Comment	C12H14O5 mH 239.0914 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Bruker Compass DataAnalysis 4.0 printed: 03.09.2019 17:09:46 Page 1 of 1

6-Hydroperoxy-6-methyl-5-(4-nitrobenzyl)-1,2-dioxan-3-one, 2b

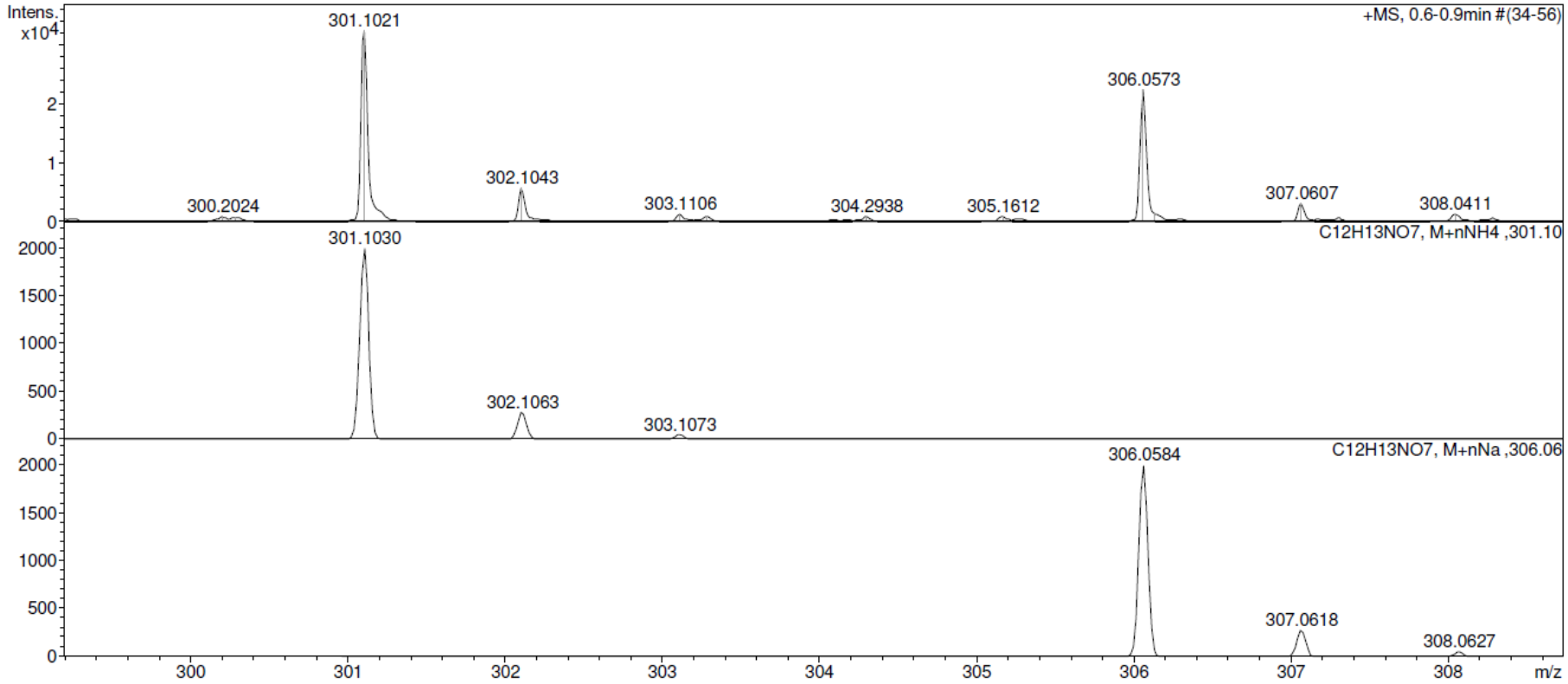
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Vil\0903031.d	Acquisition Date	03.09.2019 16:53:48
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN BB2150	Instrument / Ser#	micrOTOF 10248
Comment	C12H13NO7 mH 284.0764 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



5-(4-Chlorobenzyl)-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2c

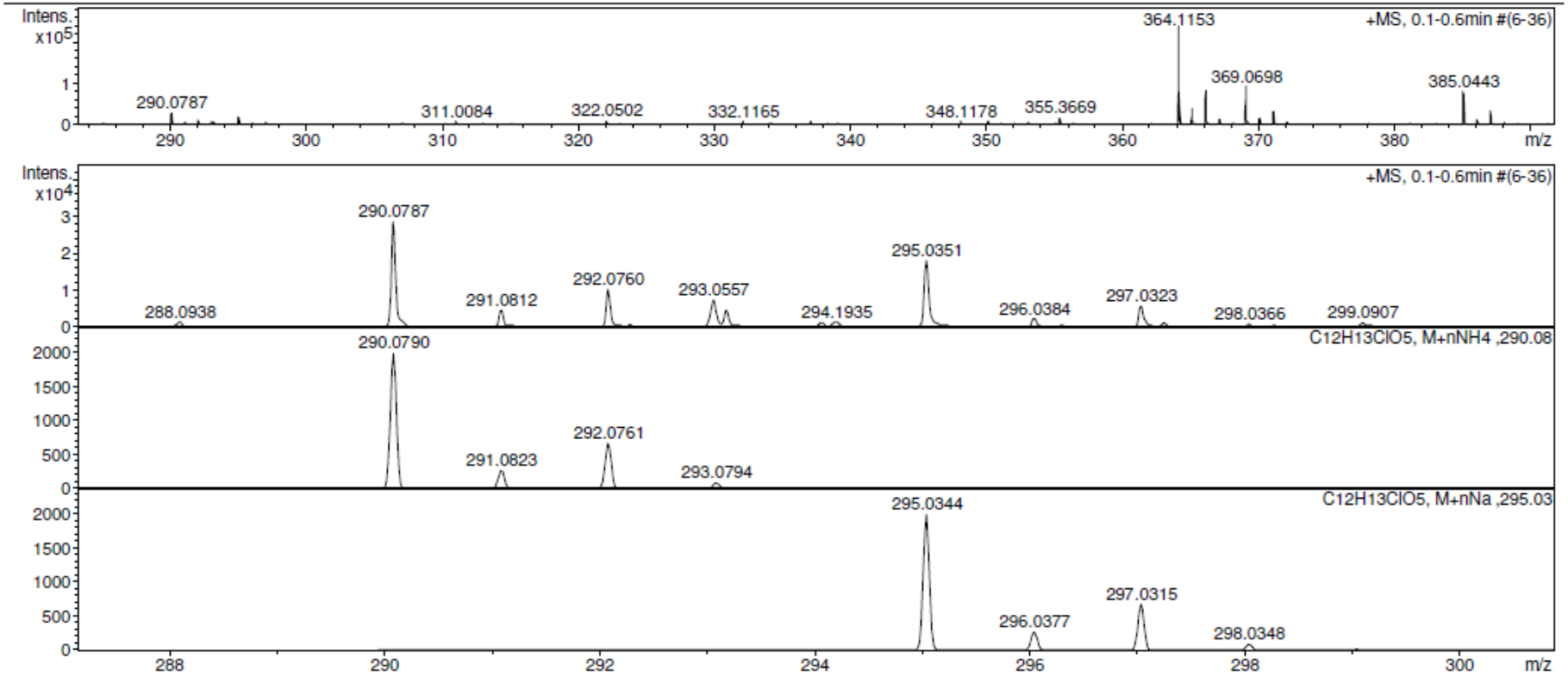
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Vil\0905009.d	Acquisition Date	05.09.2019 15:18:14
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN BB2153	Instrument / Ser#	micrOTOF 10248
Comment	C12H13ClO5 mH 273.0524 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



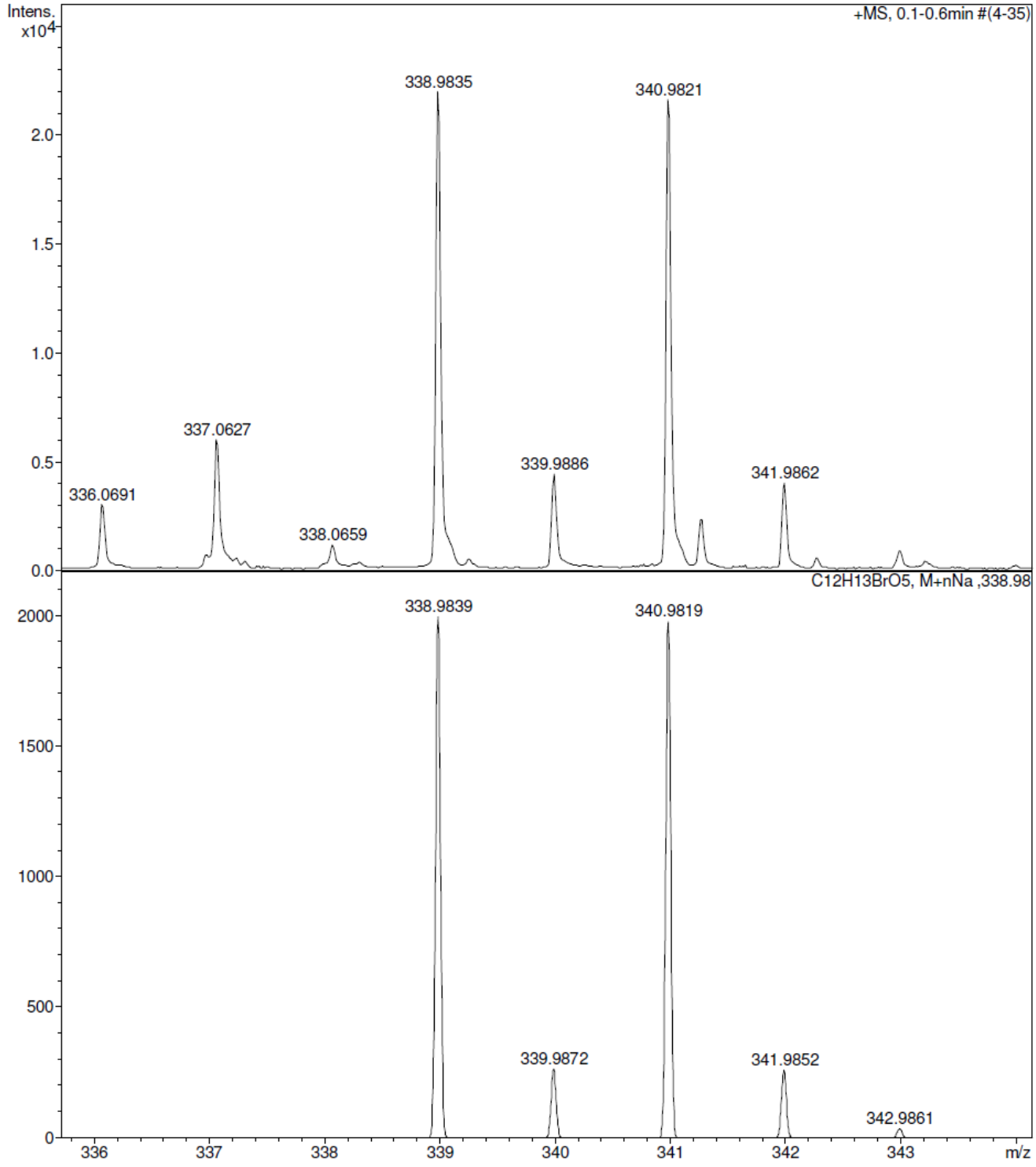
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Barsegyan\1120063.d	Acquisition Date	20.11.2019 18:29:26
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN Brs362	Instrument / Ser#	micrOTOF 10248
Comment	C12H13BrO5 mH 317.0030 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



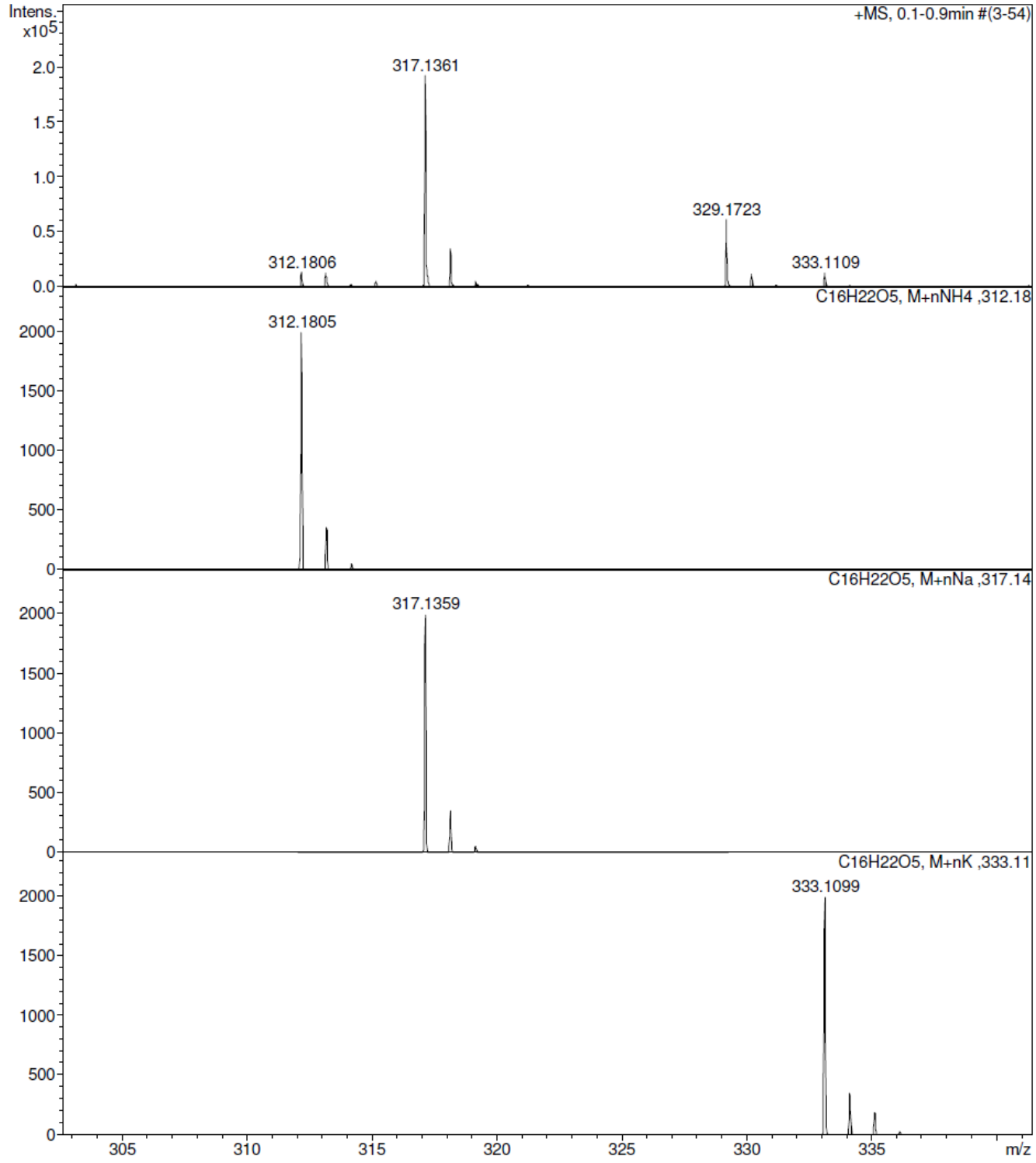
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Vil\0905010.d	Acquisition Date	05.09.2019 15:27:15
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN BB2155	Instrument / Ser#	micrOTOF 10248
Comment	C16H22O5 mH 295.1540 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



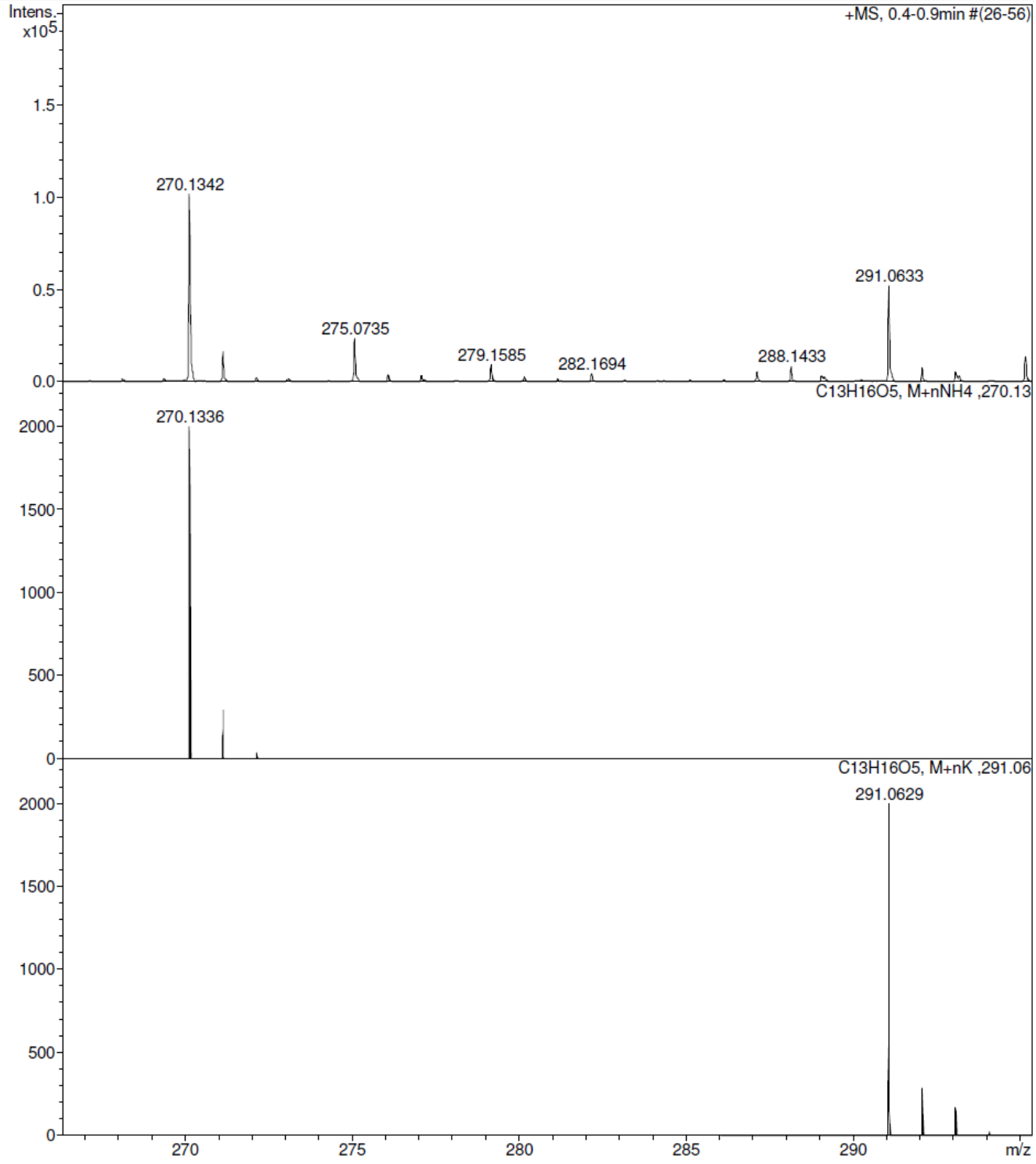
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Barseg'yan\1205035.d	Acquisition Date	05.12.2019 16:20:39
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN Brs391	Instrument / Ser#	micrOTOF 10248
Comment	C13H16O5 mH 253.1070 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



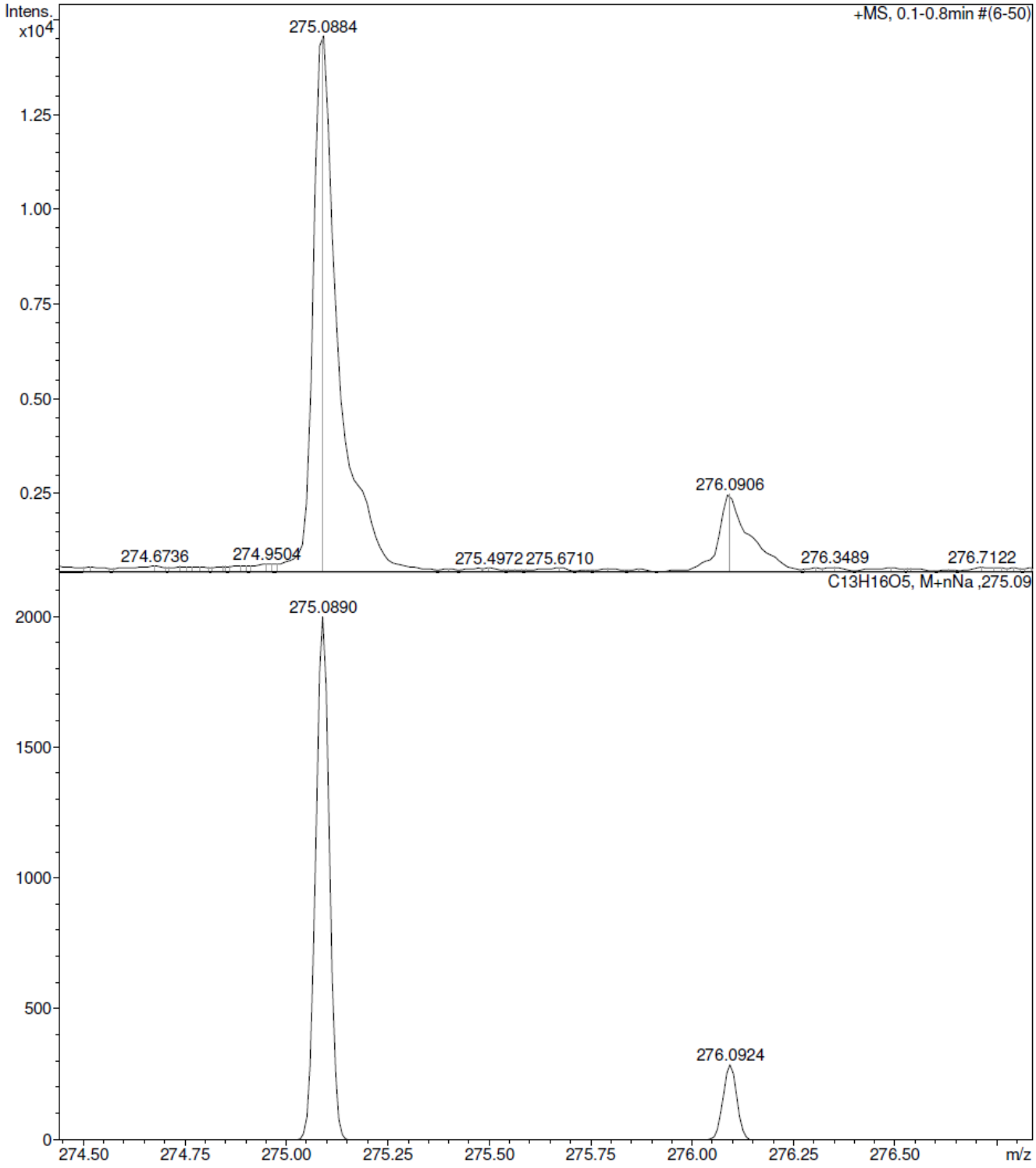
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Vil\1017025.d	Acquisition Date	17.10.2019 17:06:52
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN SE-30	Instrument / Ser#	micrOTOF 10248
Comment	C13H16O5 mH 253.1070 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



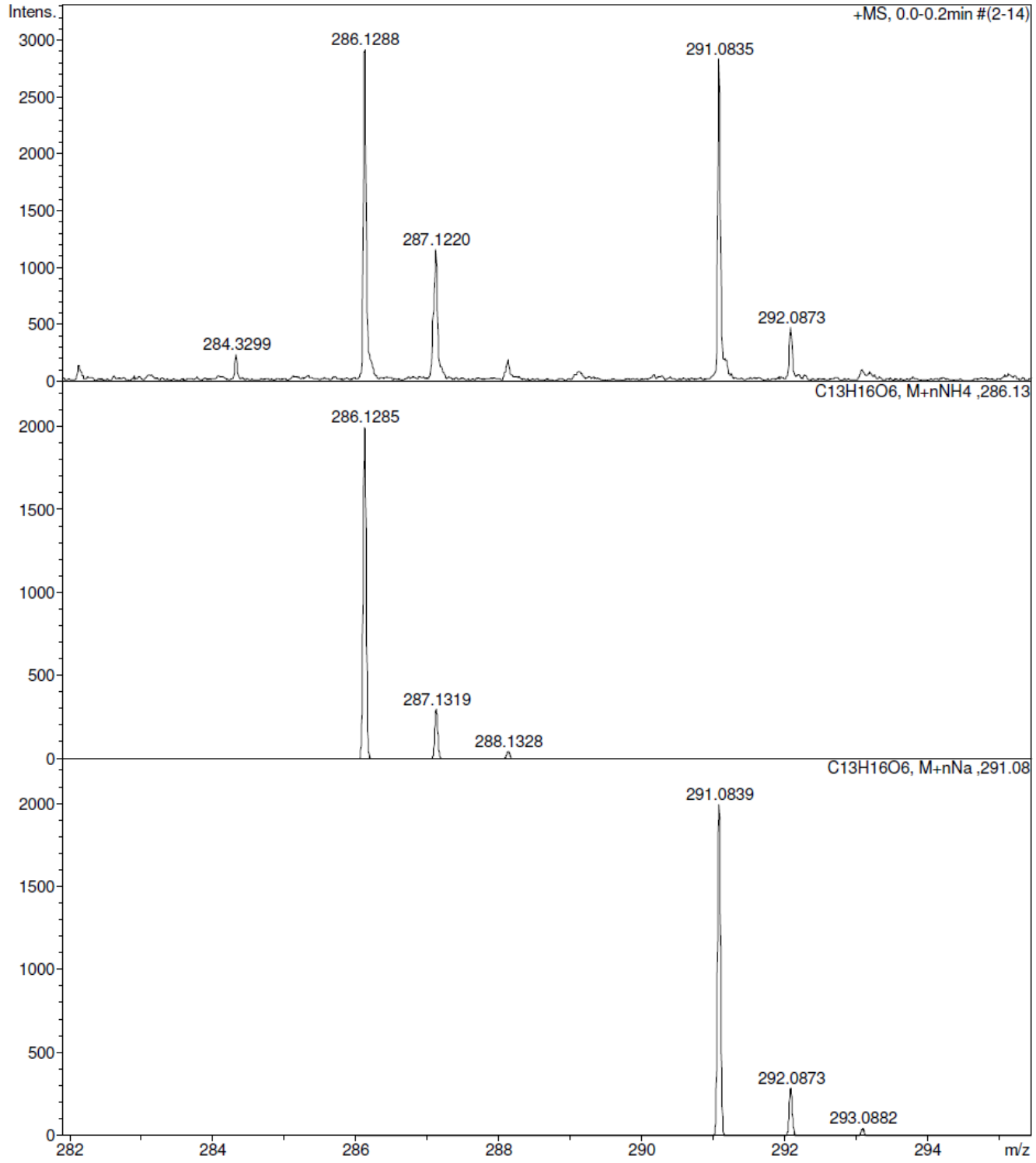
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Barsegyan\1113017.d	Acquisition Date	13.11.2019 17:00:22
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN Brs371	Instrument / Ser#	micrOTOF 10248
Comment	C13H16O6 mH 269.1019 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



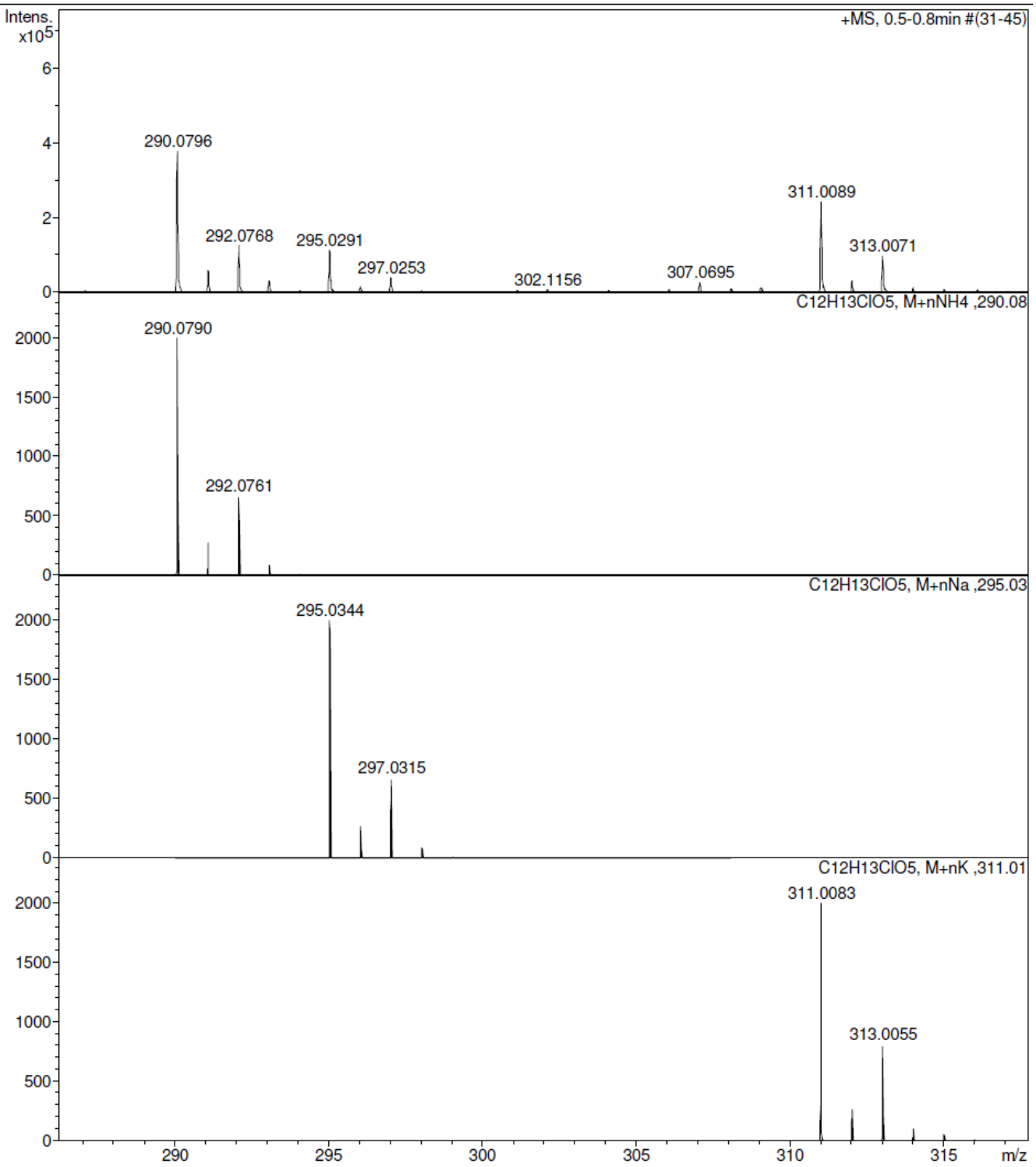
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Barsegyan\1128034.d	Acquisition Date	28.11.2019 16:31:52
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN Brs383	Instrument / Ser#	micrOTOF 10248
Comment	C12H13ClO5 mH 273.0524 calibrant added CH3CN		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



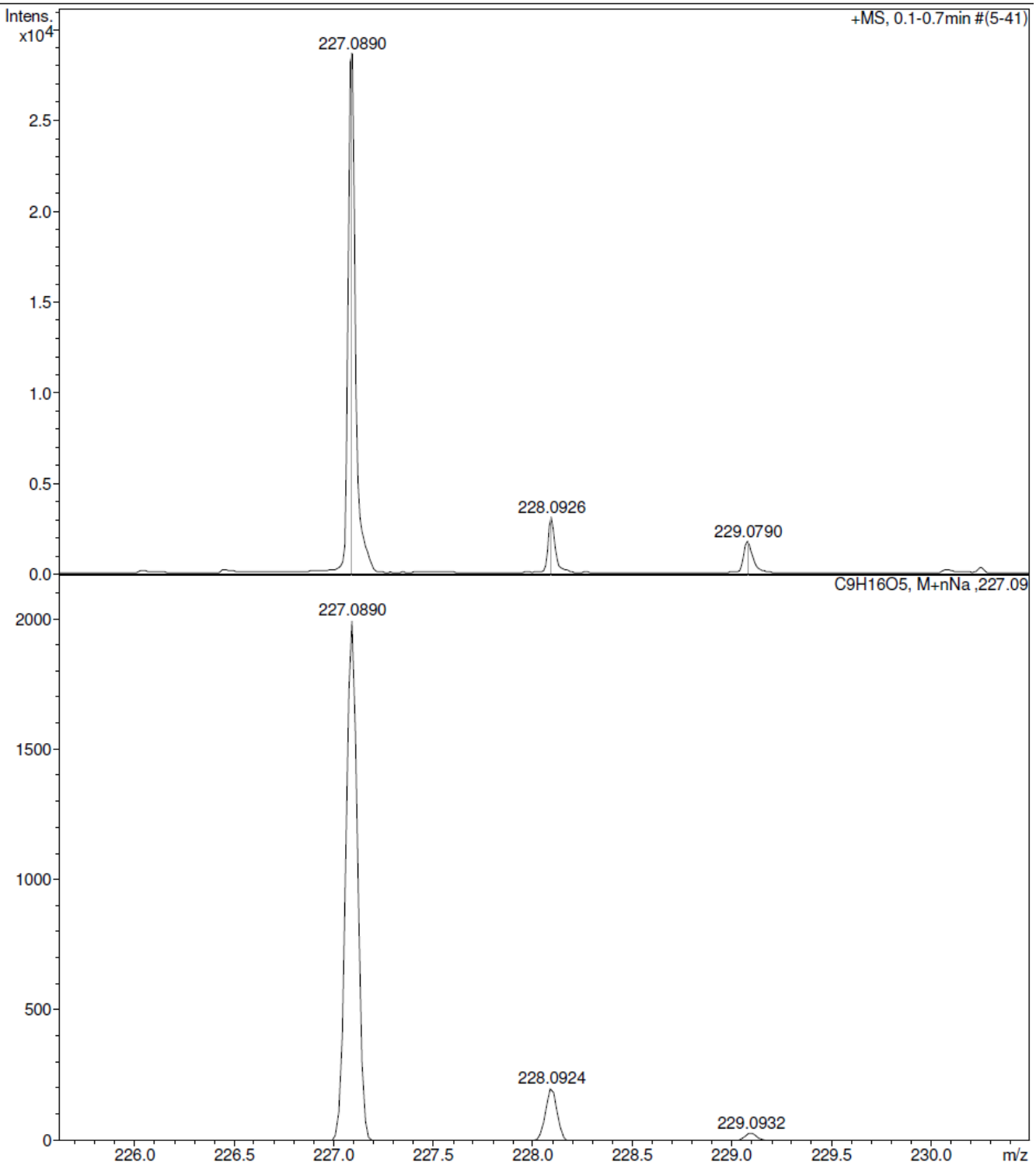
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Barsegyan\0925015.d	Acquisition Date	25.09.2019 15:06:00
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN Brs328	Instrument / Ser#	micrOTOF 10248
Comment	C9H16O5 mH 205.1070 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



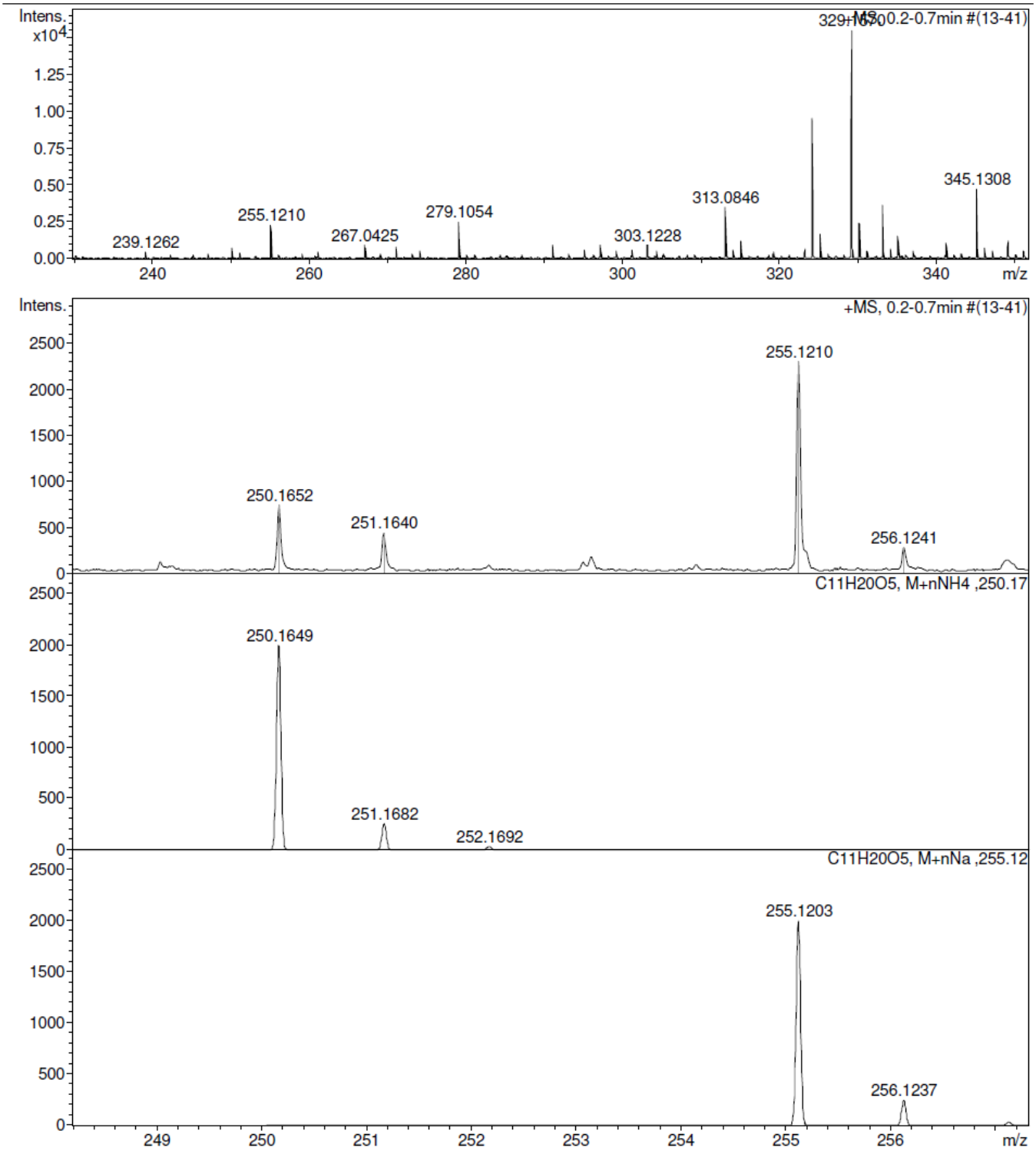
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Barsegyan\1113020.d	Acquisition Date	13.11.2019 17:32:15
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN Brs361	Instrument / Ser#	micrOTOF 10248
Comment	C11H20O5 mH 233.1383 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



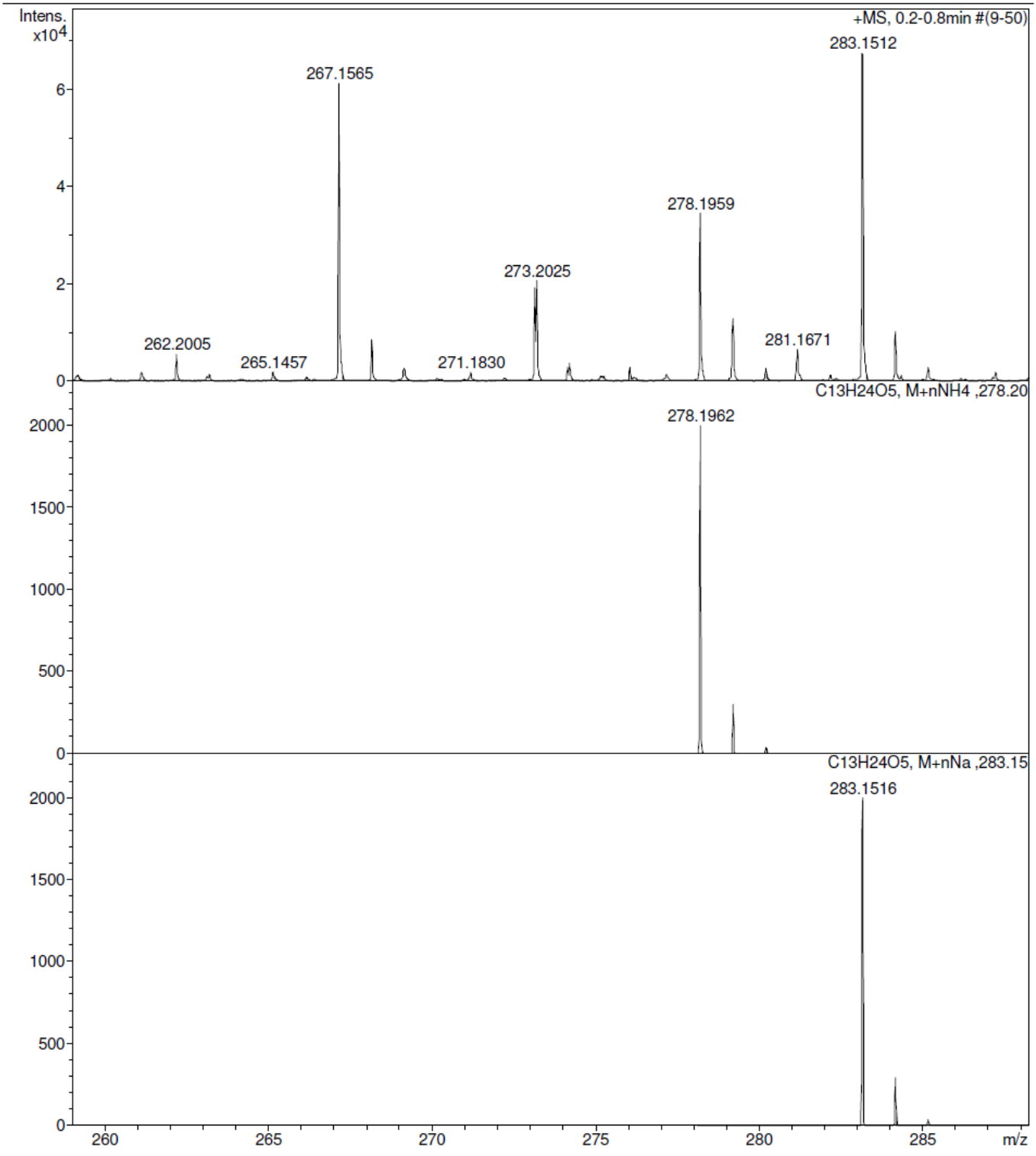
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Barsegyan\1010028.d	Acquisition Date	10.10.2019 18:24:46
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN Brs331	Instrument / Ser#	micrOTOF 10248
Comment	C13H24O5 mH 261.1696 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



6-Hydroperoxy-6-methyl-1,2-dioxan-3-one, 2m

Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2017\Vil\0912020.d	Acquisition Date	12.09.2017 14:56:25
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/TERN ME-14	Instrument / Ser#	micrOTOF 10248
Comment	C5H8O5 mH 149.0444 clb added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
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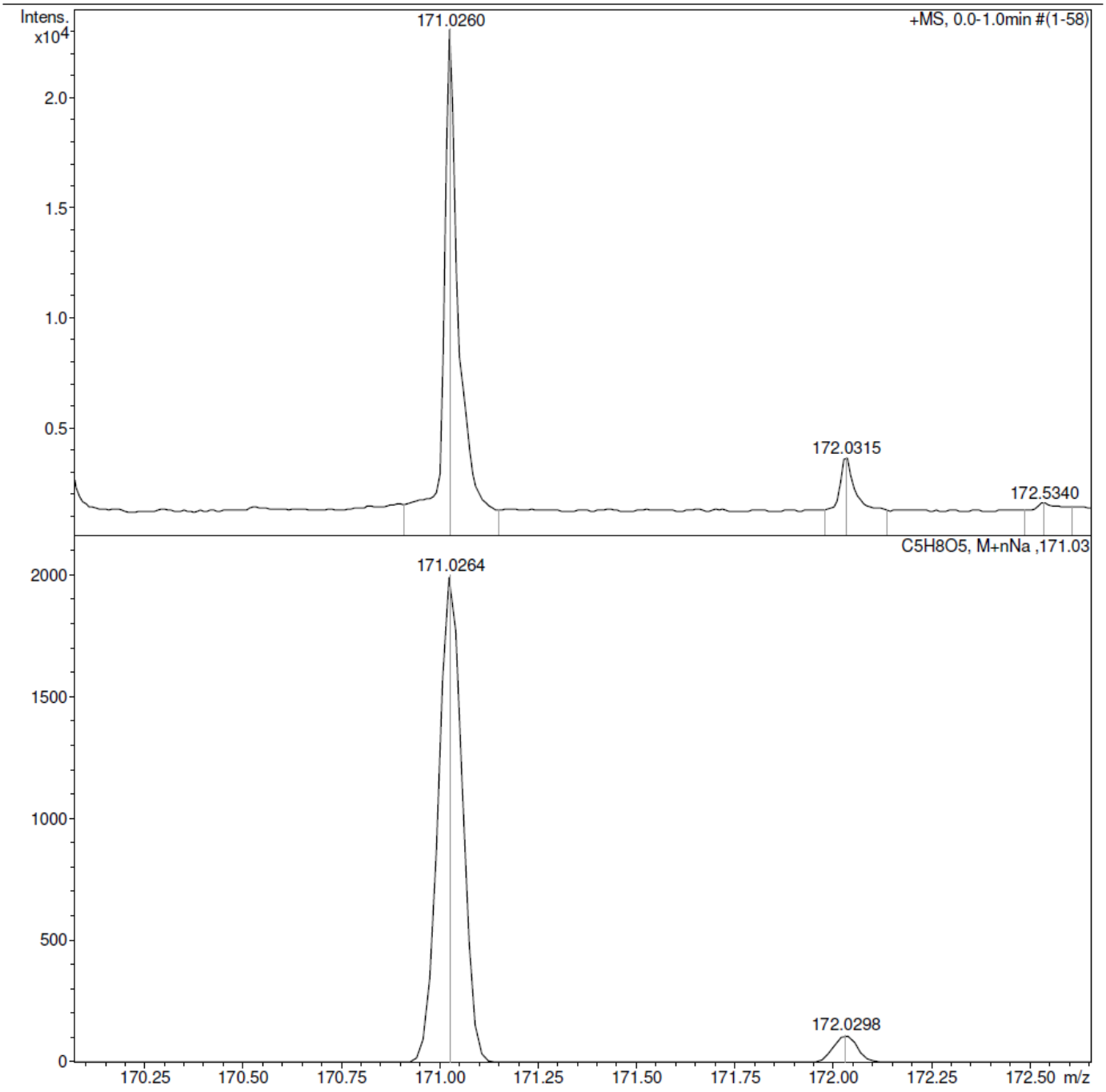
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



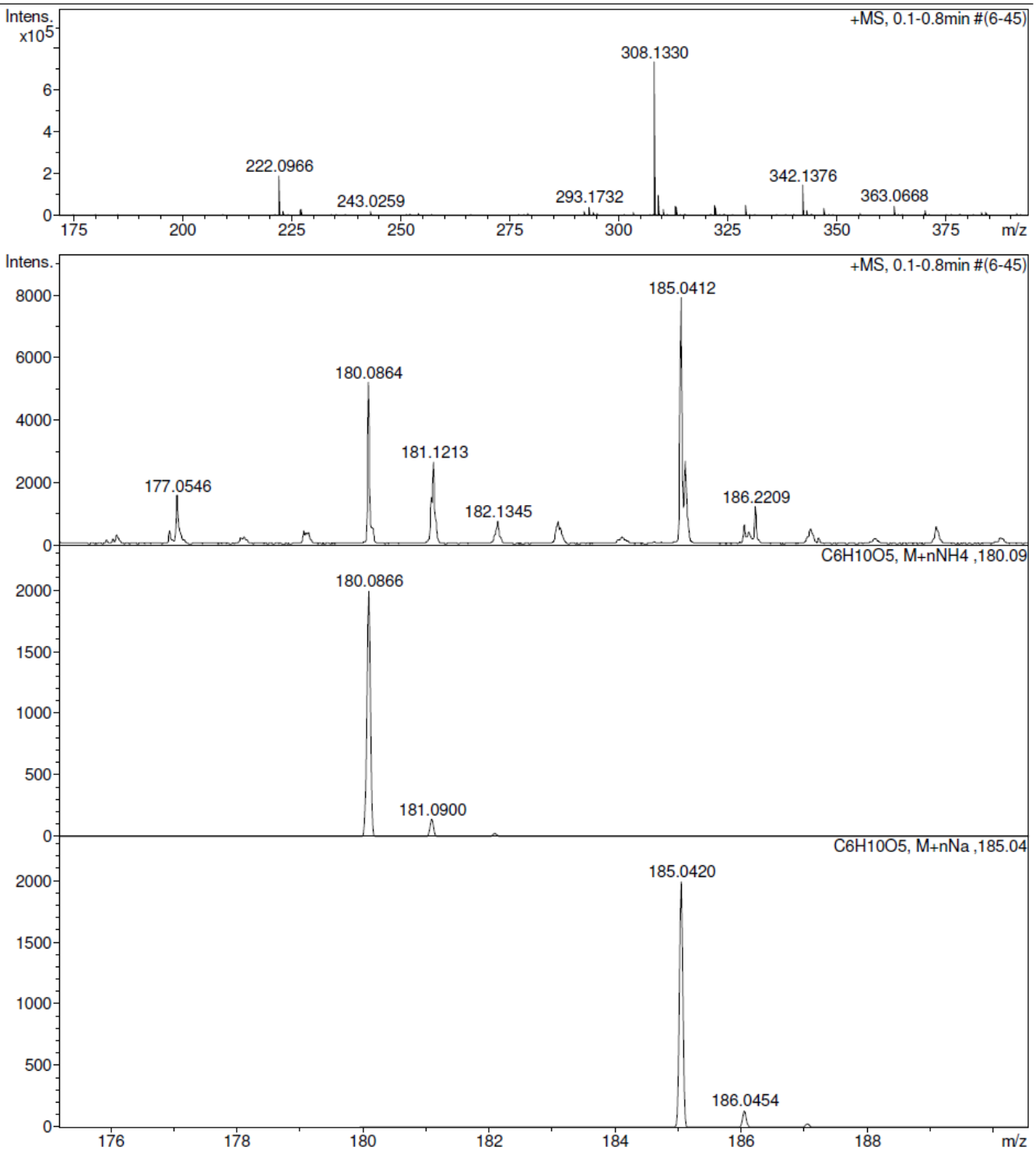
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Barsegyan\0912023.d	Acquisition Date	12.09.2019 15:15:40
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN Brs284	Instrument / Ser#	micrOTOF 10248
Comment	C6H10O5 mH 163.0601 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2019\Vil\1119020.d		
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN BB2139	Instrument / Ser#	micrOTOF 10248
Comment	C8H14O5 mH 191.0924 calibrant added	Acquisition Date	19.11.2019 15:52:42

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
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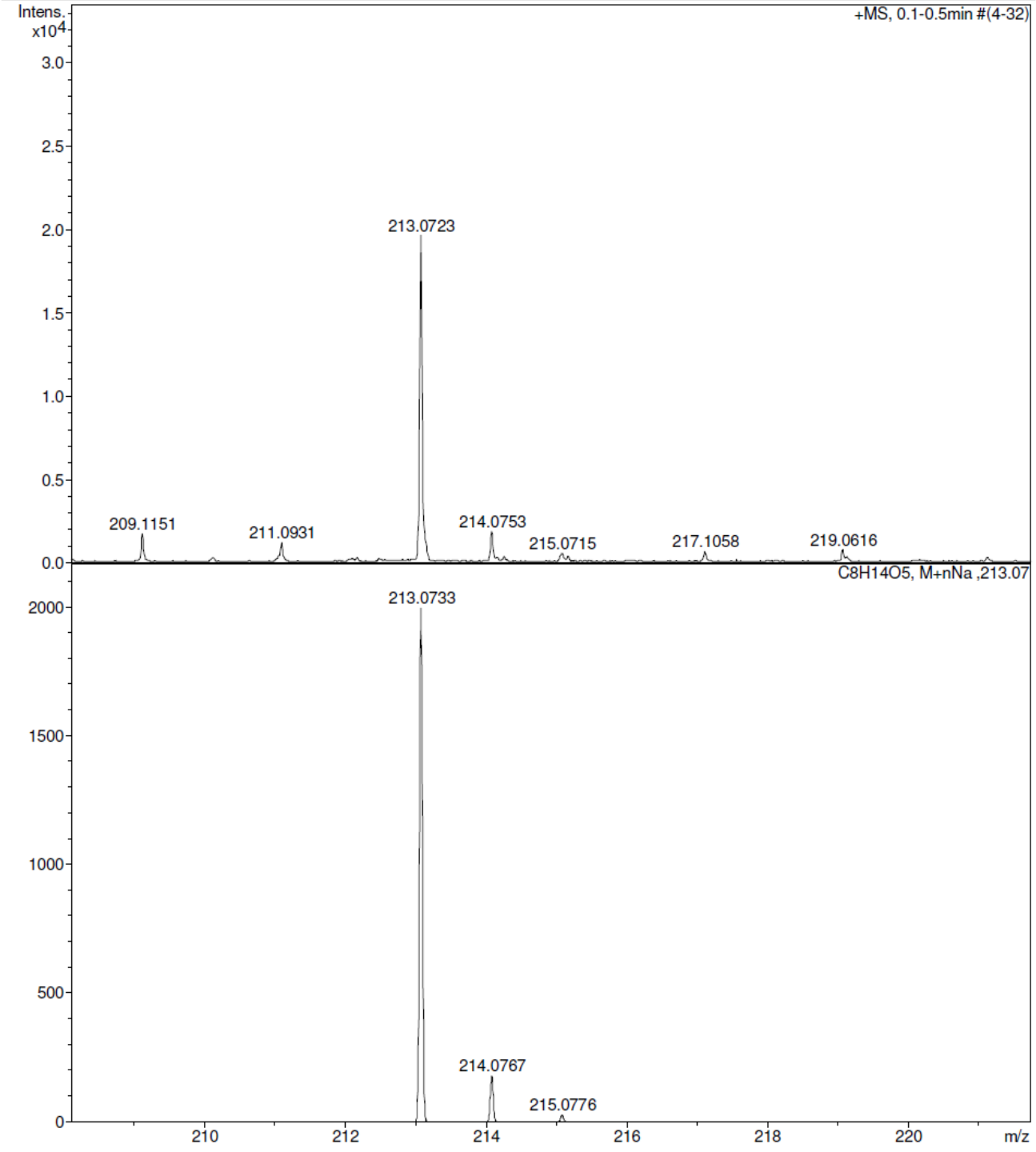
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



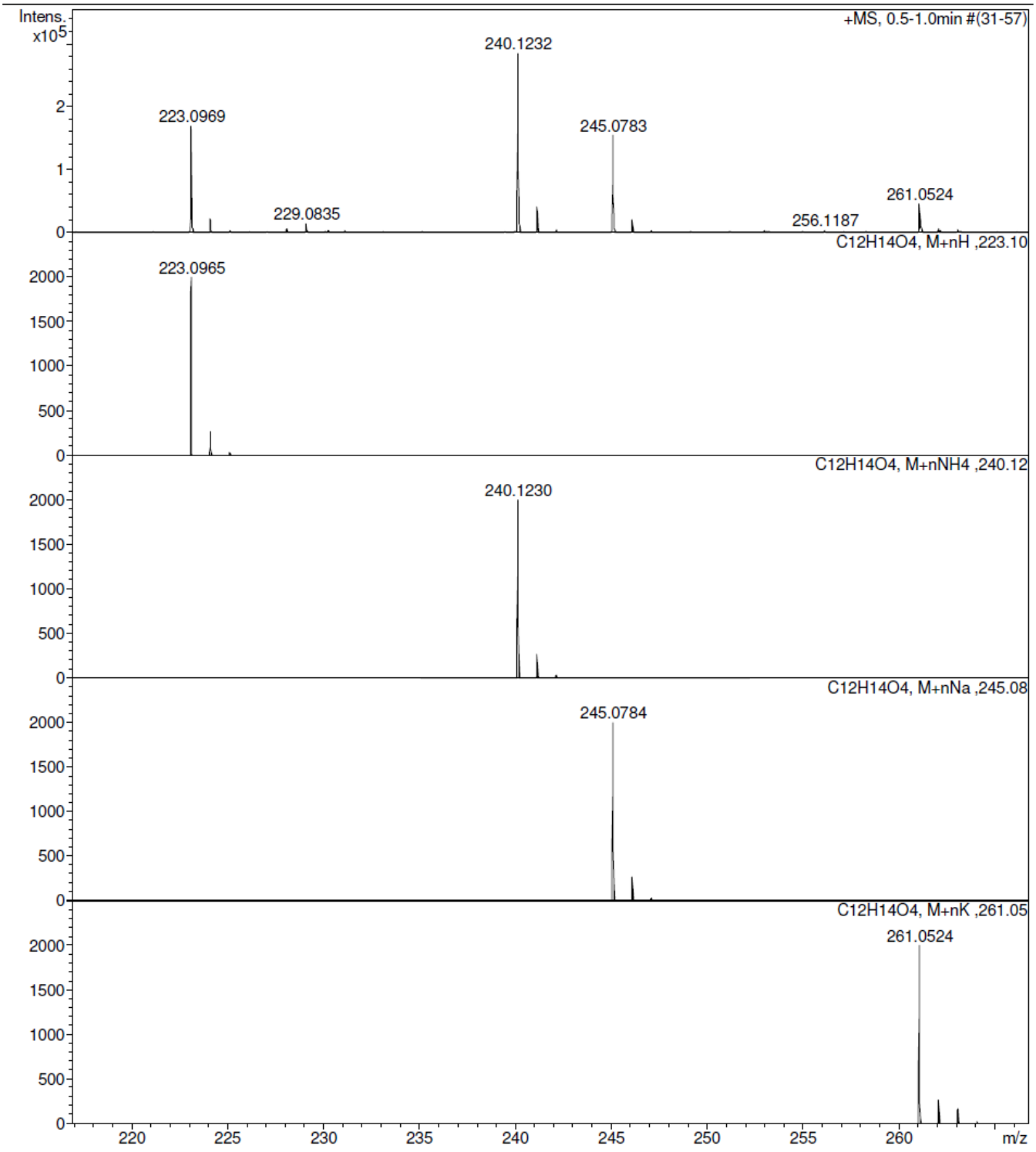
Display Report

Analysis Info

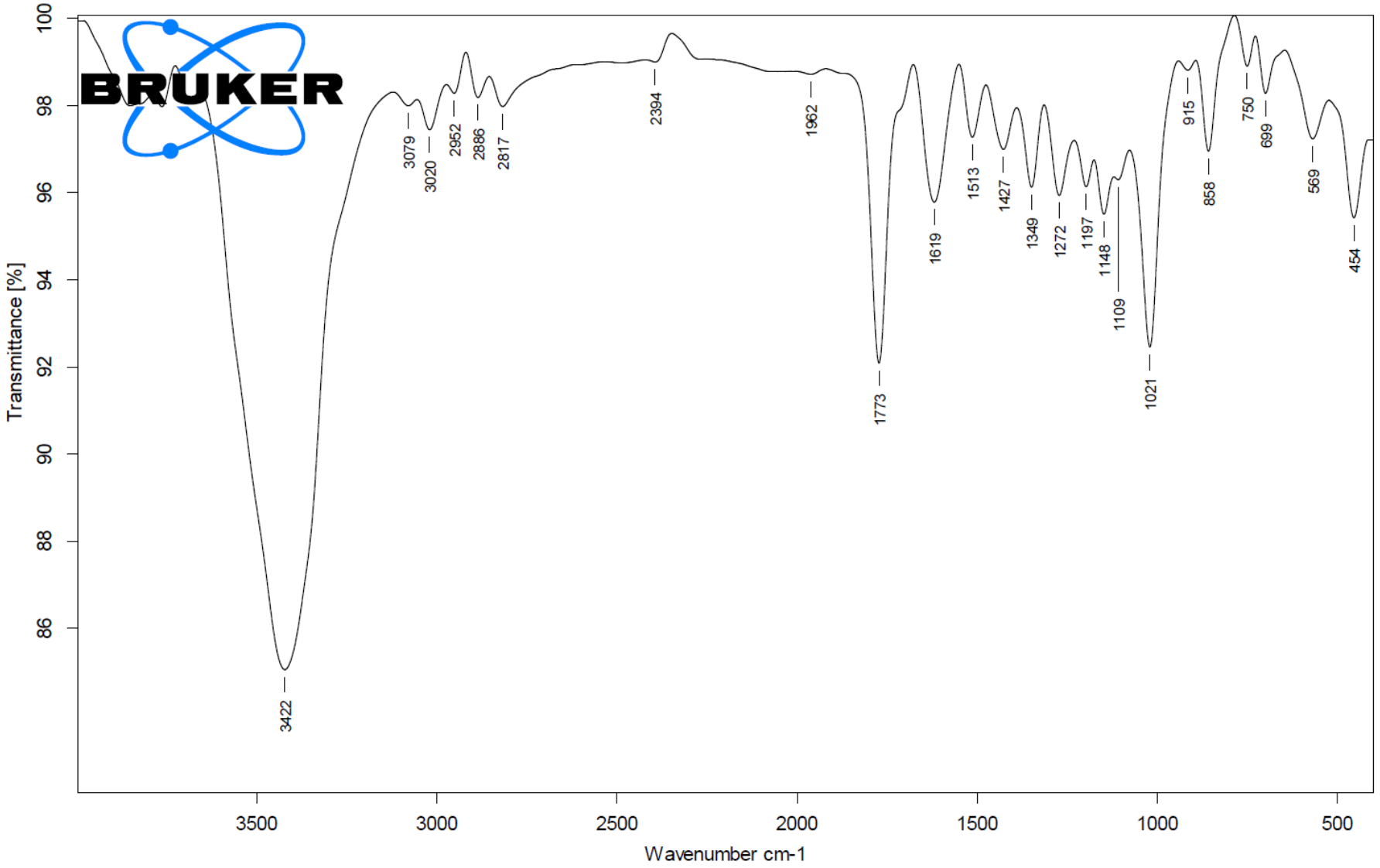
Analysis Name	D:\Data\Kolotyrkina\2019\Vil\1009027.d	Acquisition Date	09.10.2019 18:15:54
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/TERN BB-2184	Instrument / Ser#	micrOTOF 10248
Comment	C12H14O4 mH 223.0964 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

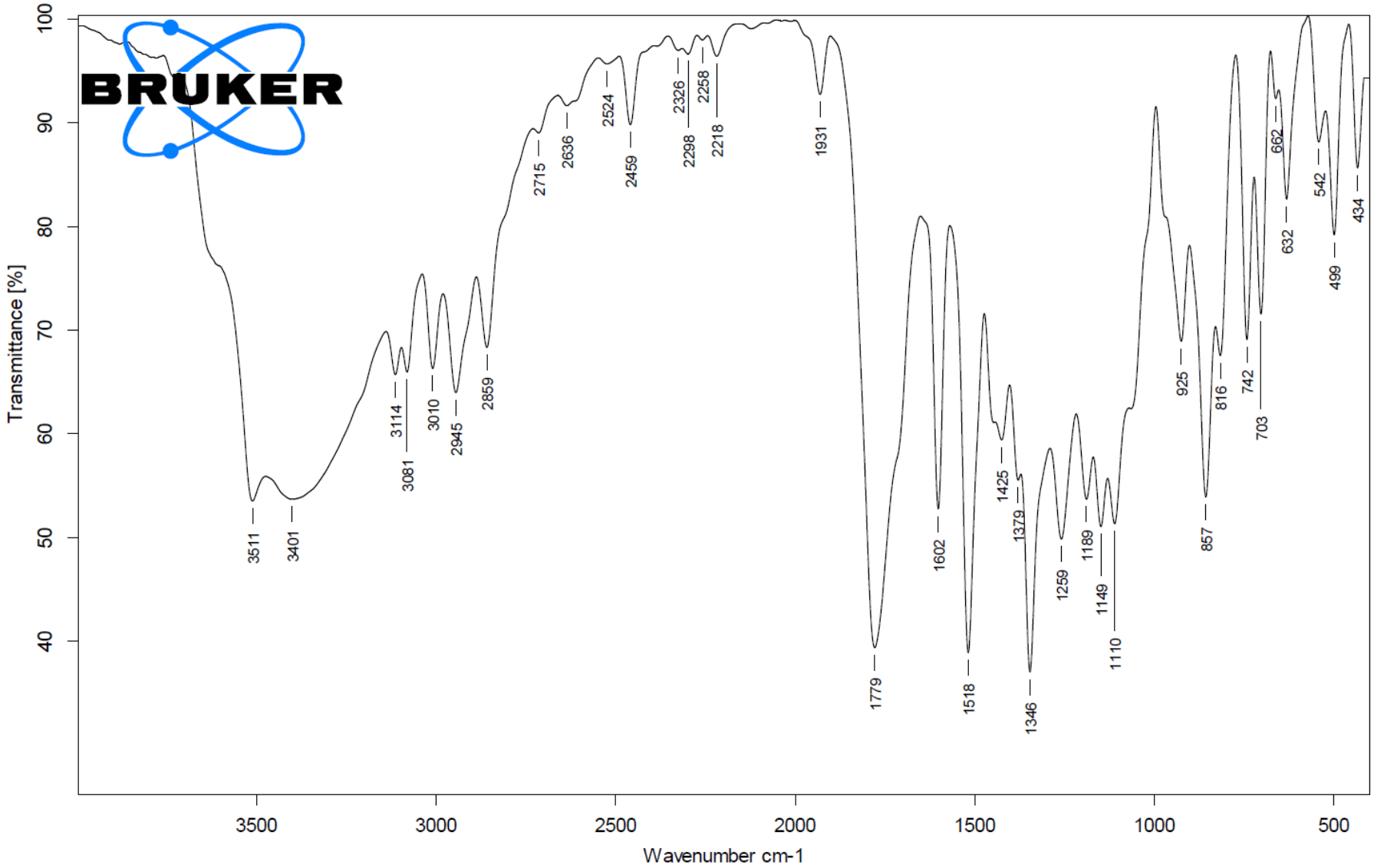


IR spectra of γ-hydroperoxy-γ-peroxylactones 2 and other products
5-Benzyl-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2a



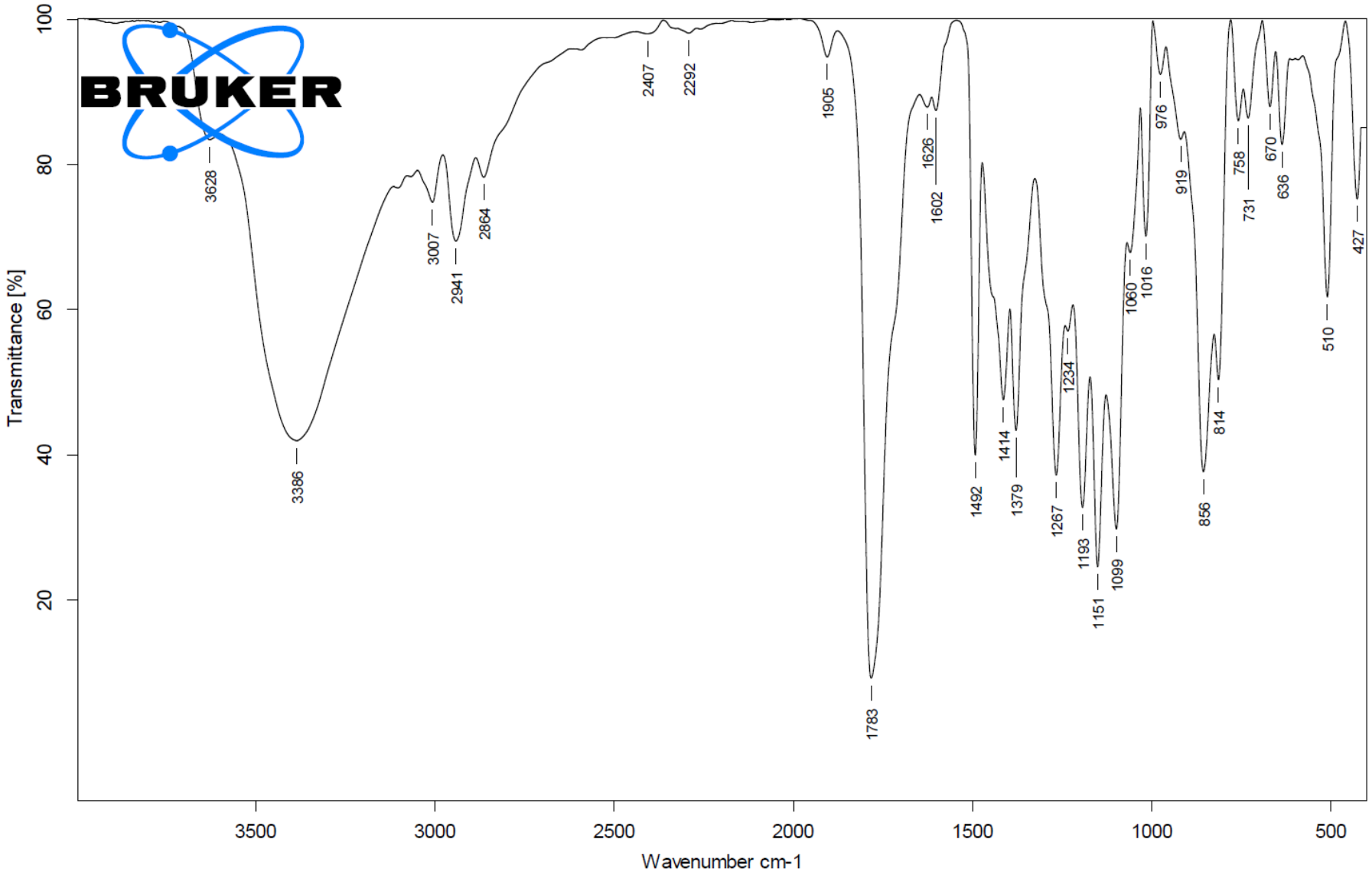
D:\IrB\Виль ВВ-2137.0	Виль ВВ-2137	KBr прессовка	18.10.2019

6-Hydroperoxy-6-methyl-5-(4-nitrobenzyl)-1,2-dioxan-3-one, 2b



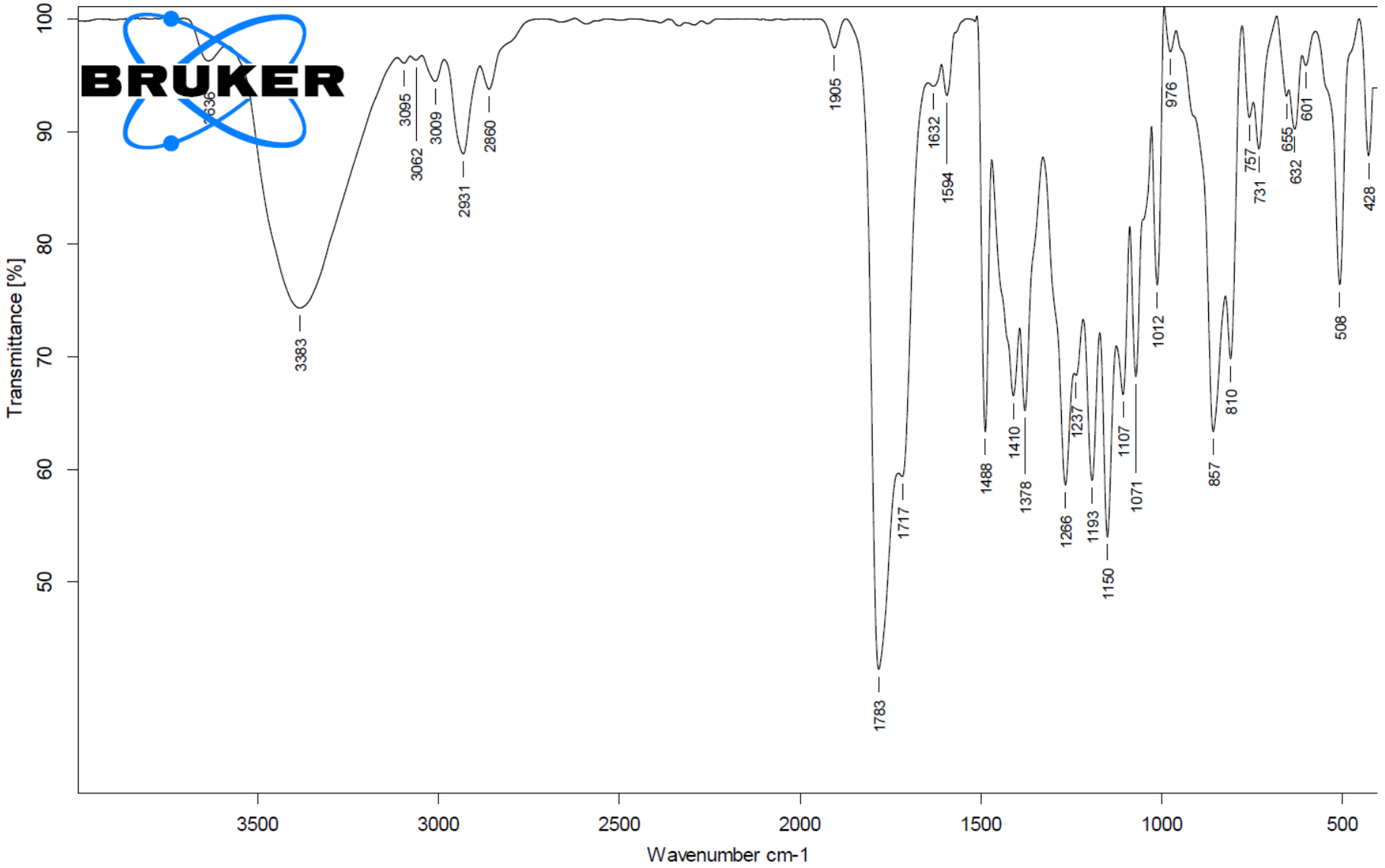
D:\IrB\Виль ВВ2150.0	Виль ВВ2150	KBr тонкий слой	18.10.2019

5-(4-Chlorobenzyl)-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2c



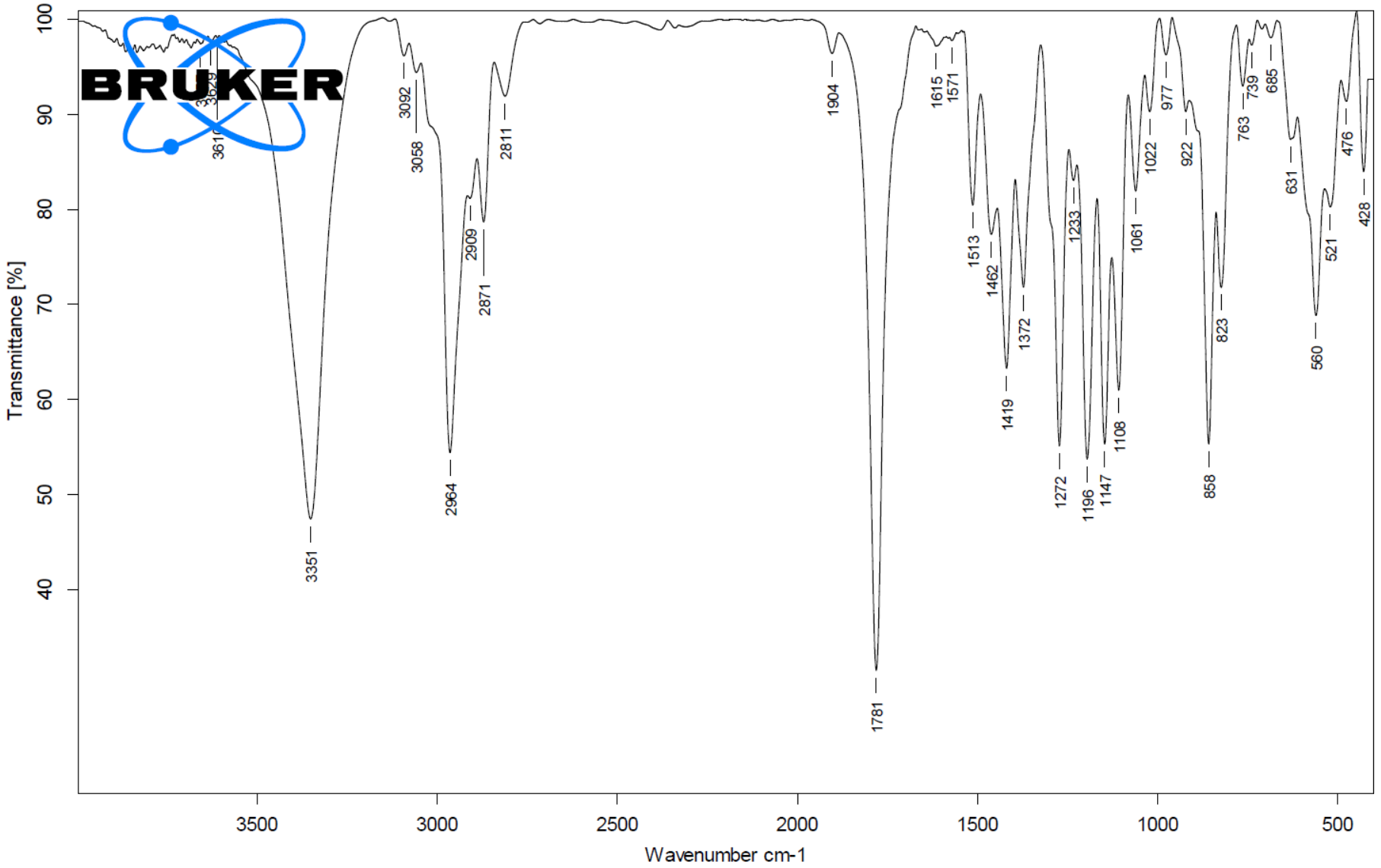
D:\IrB\Виль BB2153.0	Виль BB2153	KBr тонкий слой	18.10.2019

5-(4-Bromobenzyl)-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2d



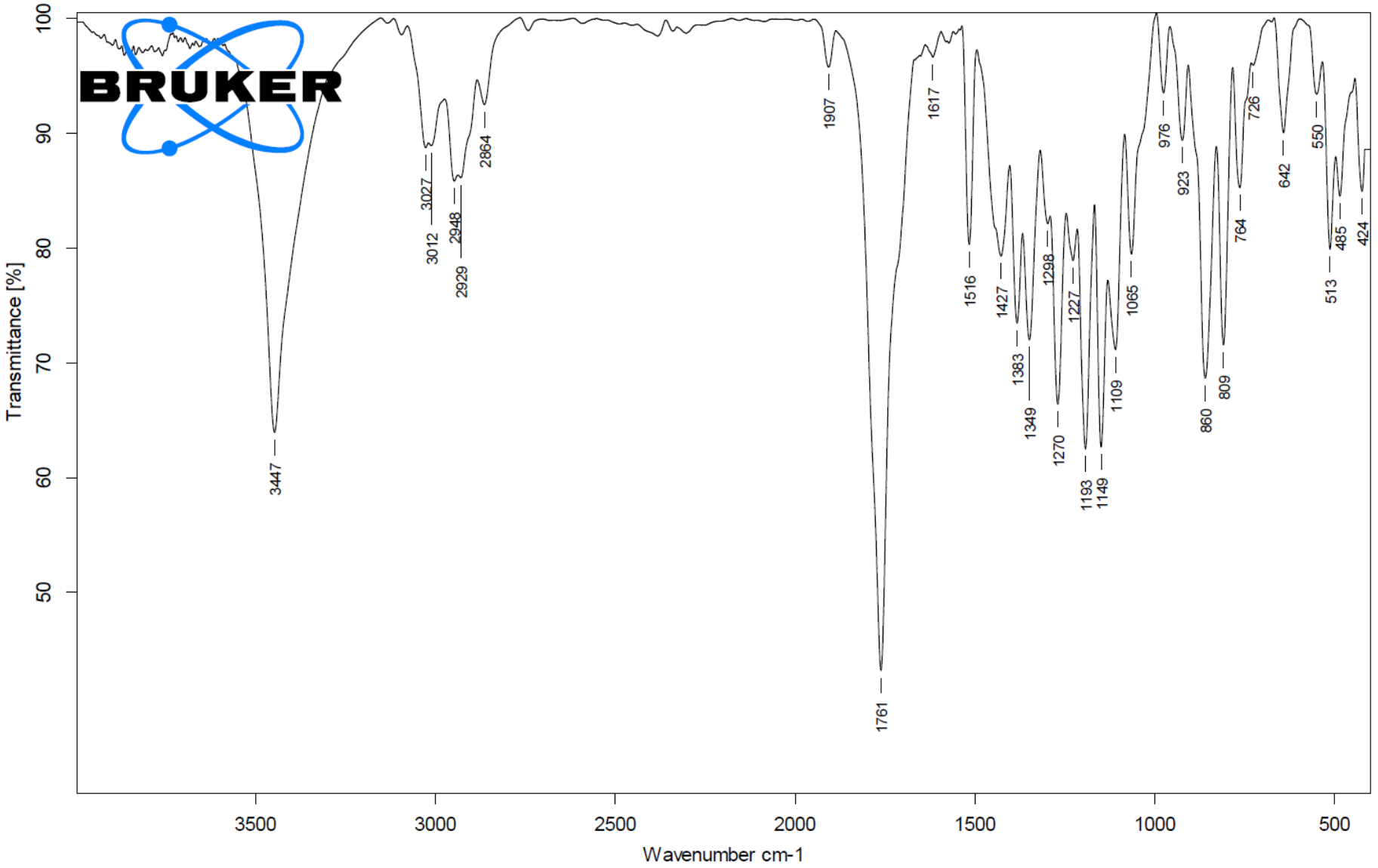
D:\IrB\Барсегян Brs362.0	Барсегян Brs362	KBr тонкий слой	11.12.2019

5-(4-(*Tert*-butyl)benzyl)-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2e



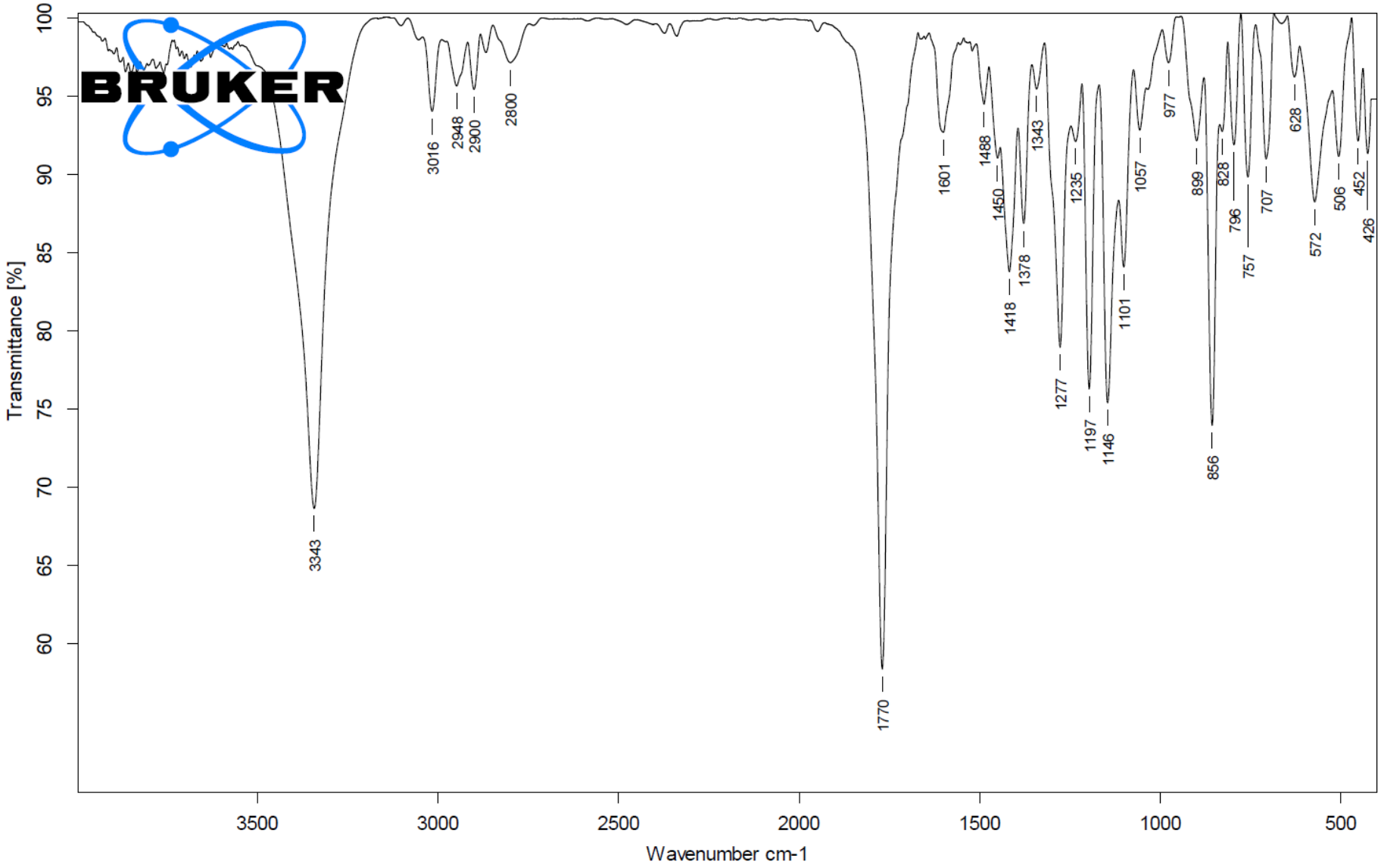
D:\IrB\Барсегян BB2155.0	Барсегян BB2155	KBr прессовка	11.12.2019

6-Hydroperoxy-6-methyl-5-(4-methylbenzyl)-1,2-dioxan-3-one, 2f



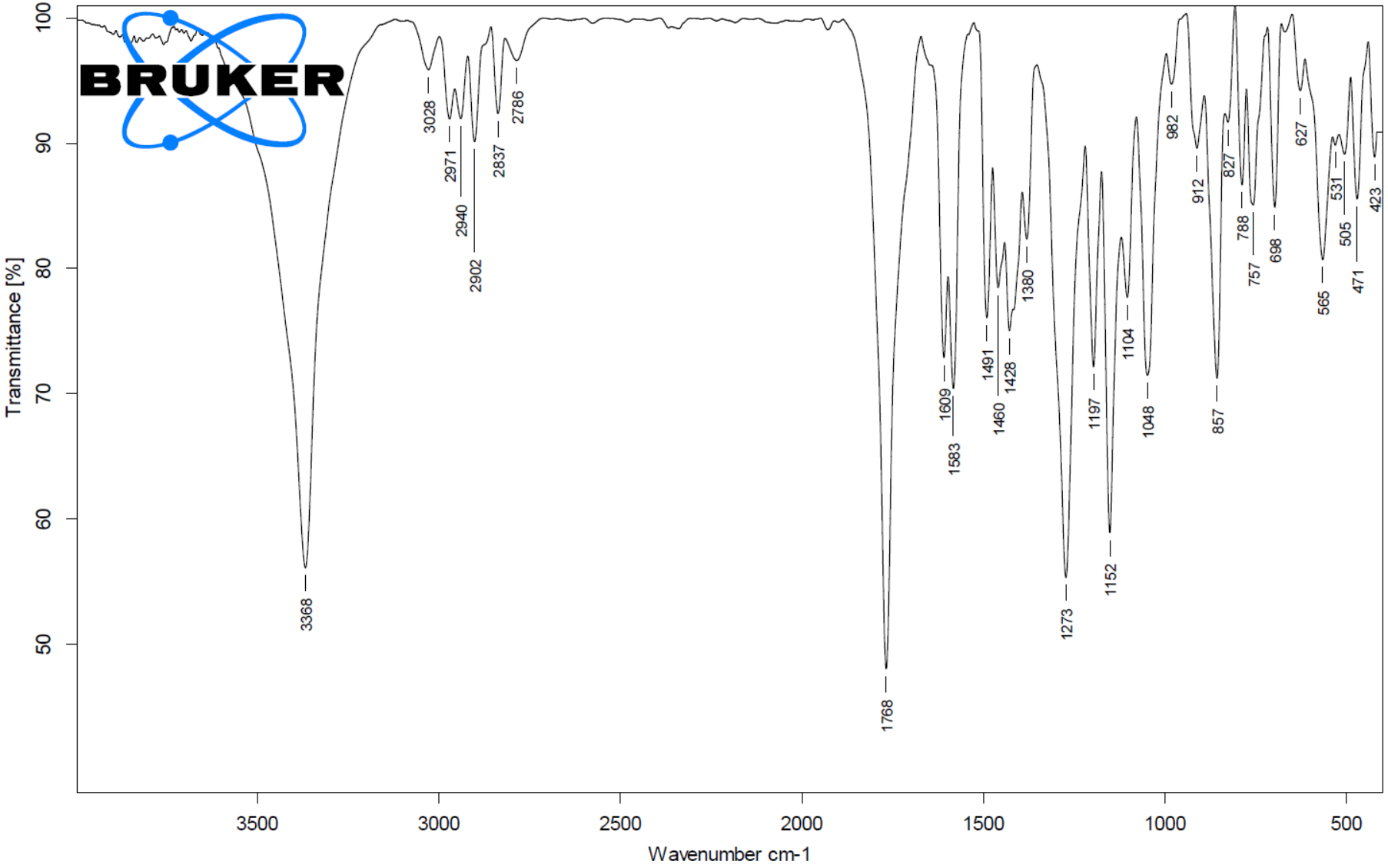
D:\IrB\Барсегян Brs391.1	Барсегян Brs391	KBr прессовка	11.12.2019

6-Hydroperoxy-6-methyl-5-(3-methylbenzyl)-1,2-dioxan-3-one, 2g



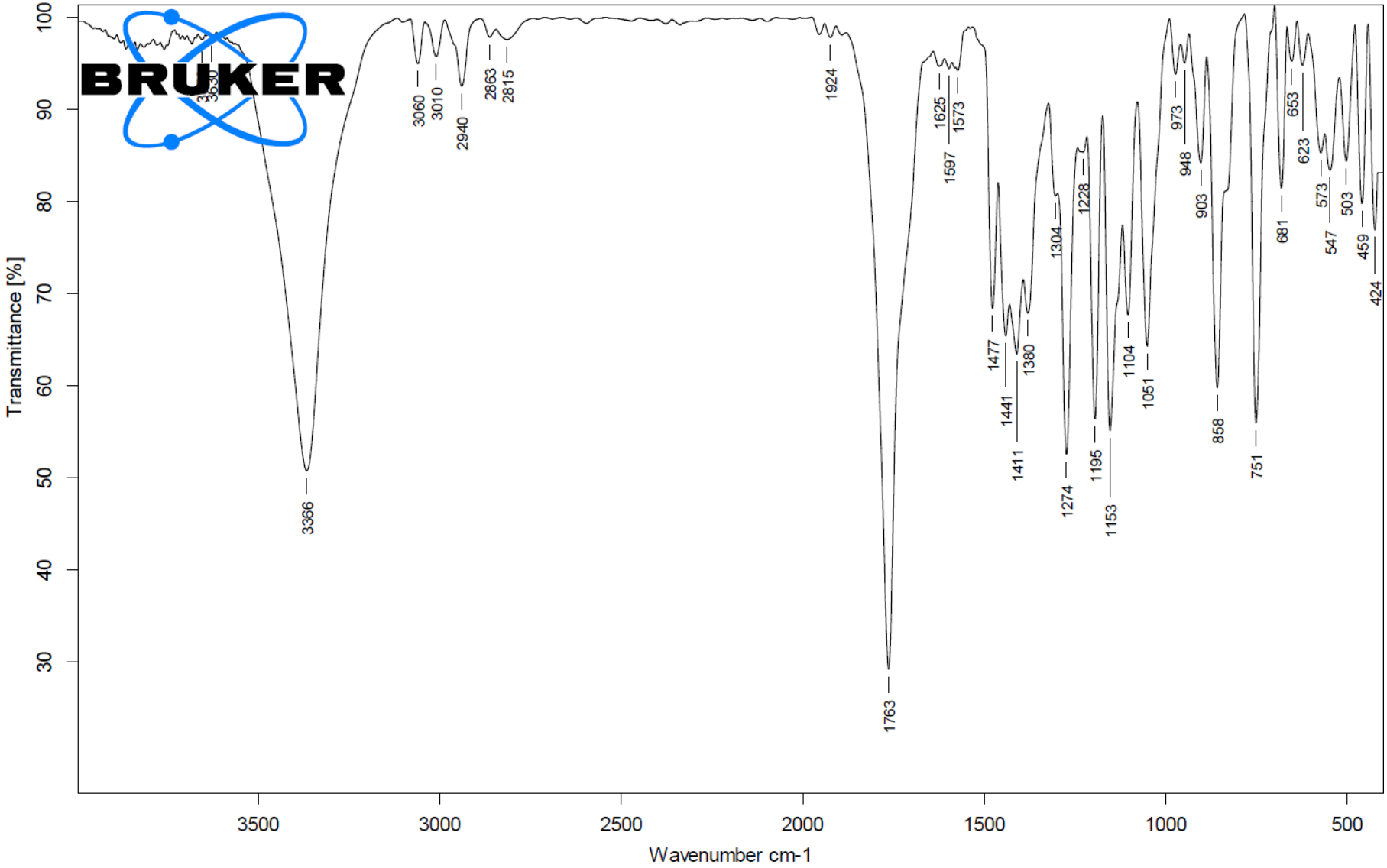
D:\IrB\Барсегян SE-30.0	Барсегян SE-30	KBr прессовка	11.12.2019

6-Hydroperoxy-5-(3-methoxybenzyl)-6-methyl-1,2-dioxan-3-one, 2h



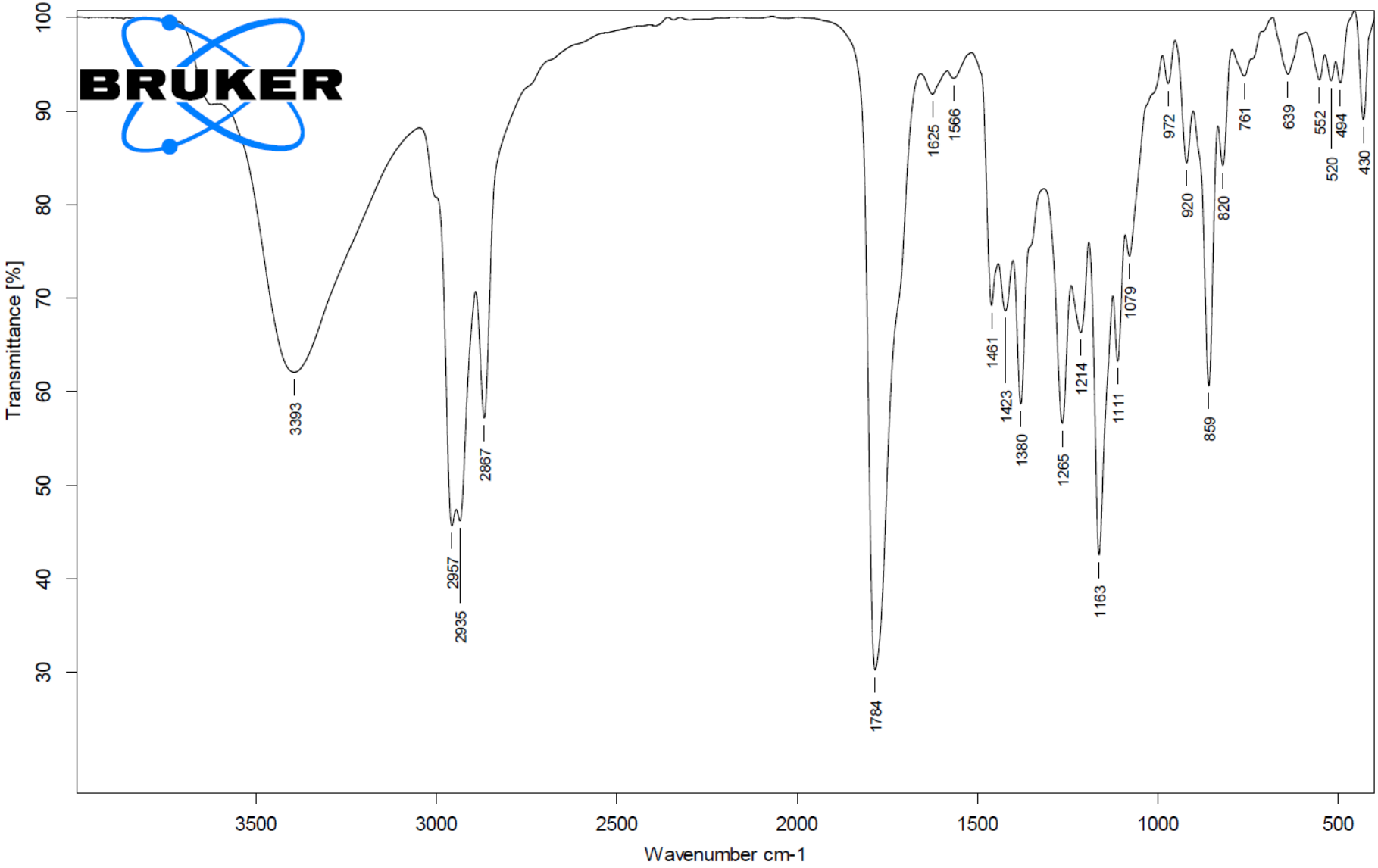
D:\IrB\Барсегян Brs371.0	Барсегян Brs371	KBr прессовка	20.11.2019

5-(2-Chlorobenzyl)-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2i



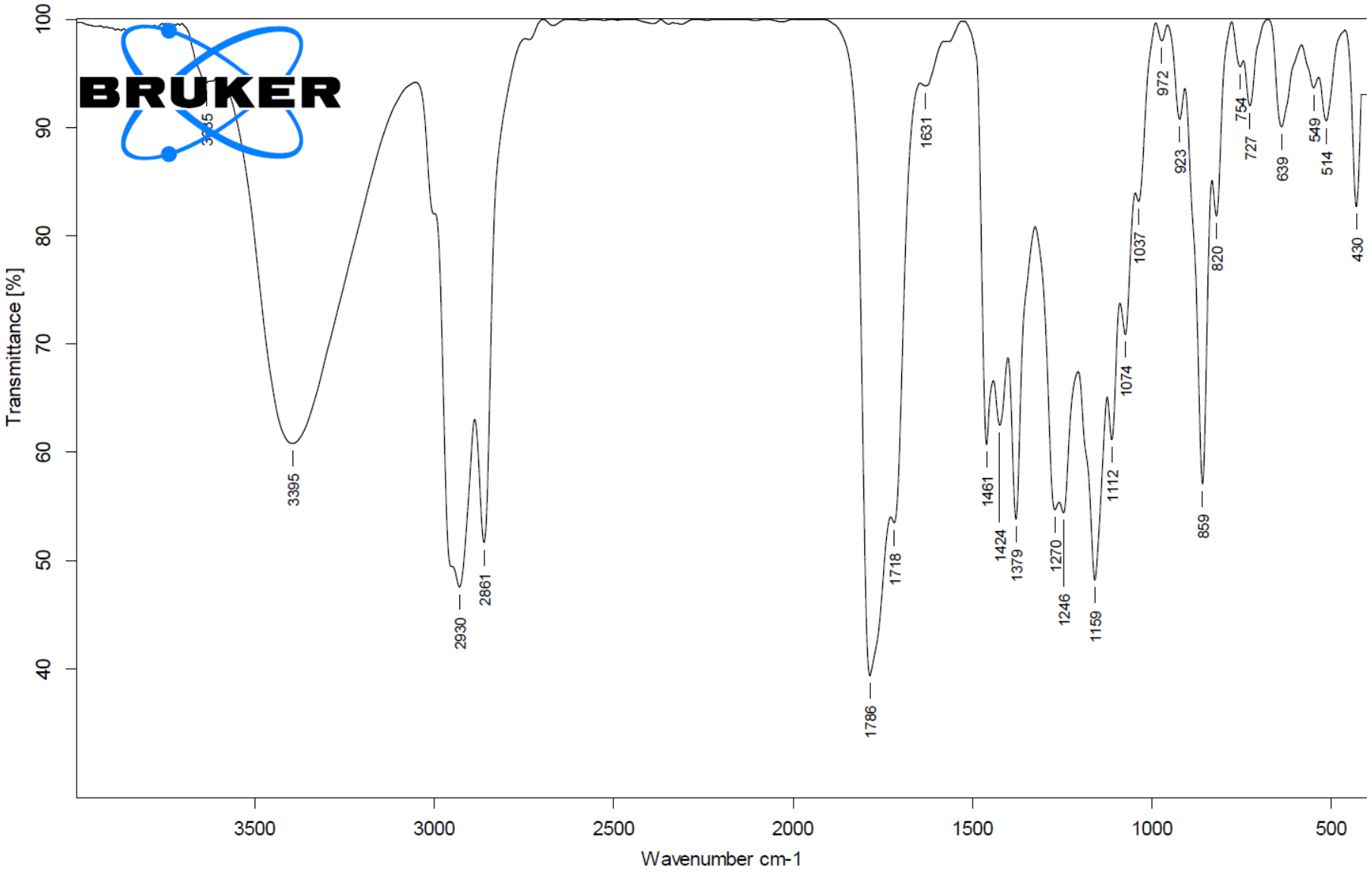
D:\IrB\Барсегян Brs383.0	Барсегян Brs383	KBr прессовка	11.12.2019

5-Butyl-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2j



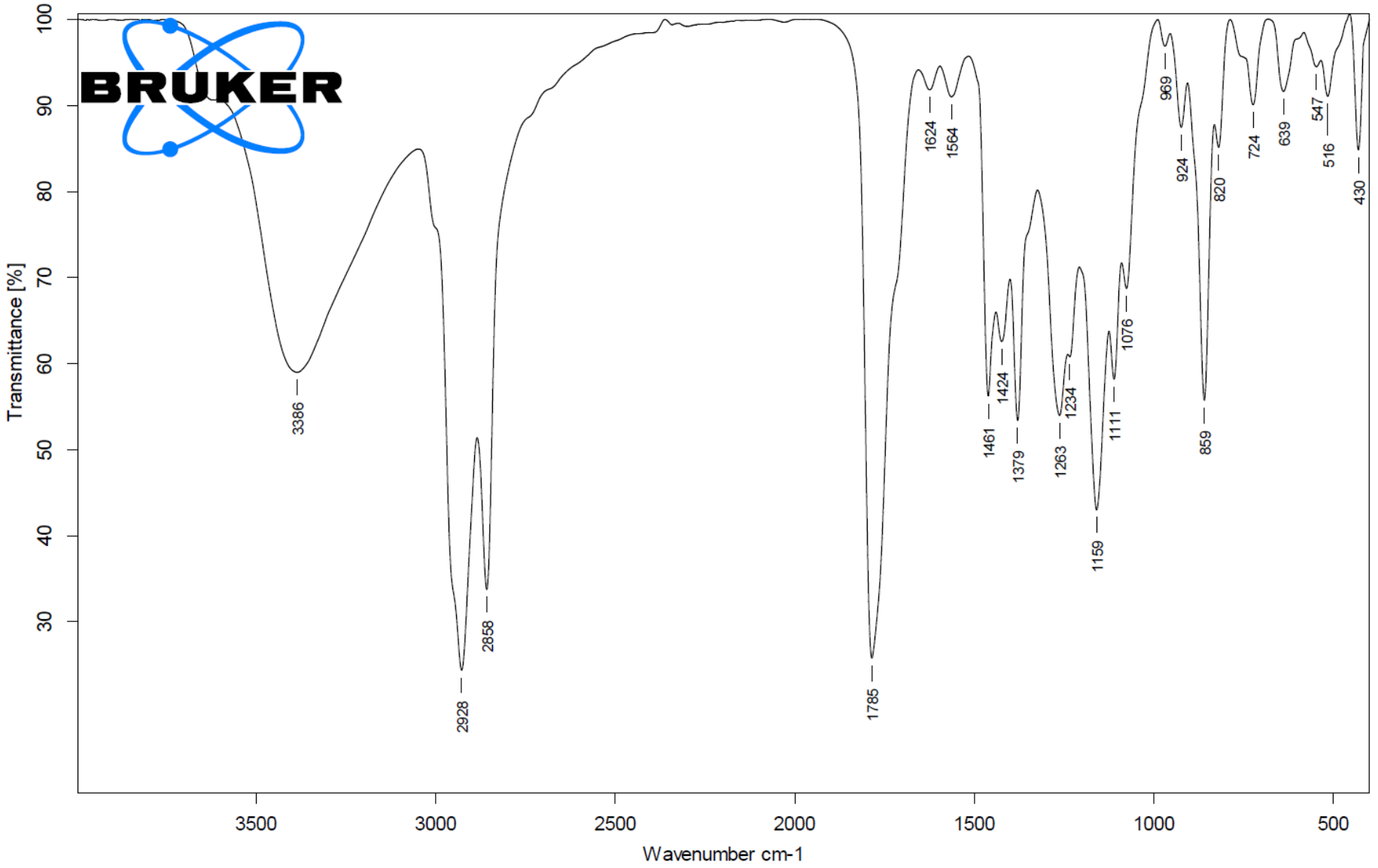
D:\IrB\Барсегян Brs328.0	Барсегян Brs328	KBr тонкий слой	16.10.2019

5-Hexyl-6-hydroperoxy-6-methyl-1,2-dioxan-3-one, 2k



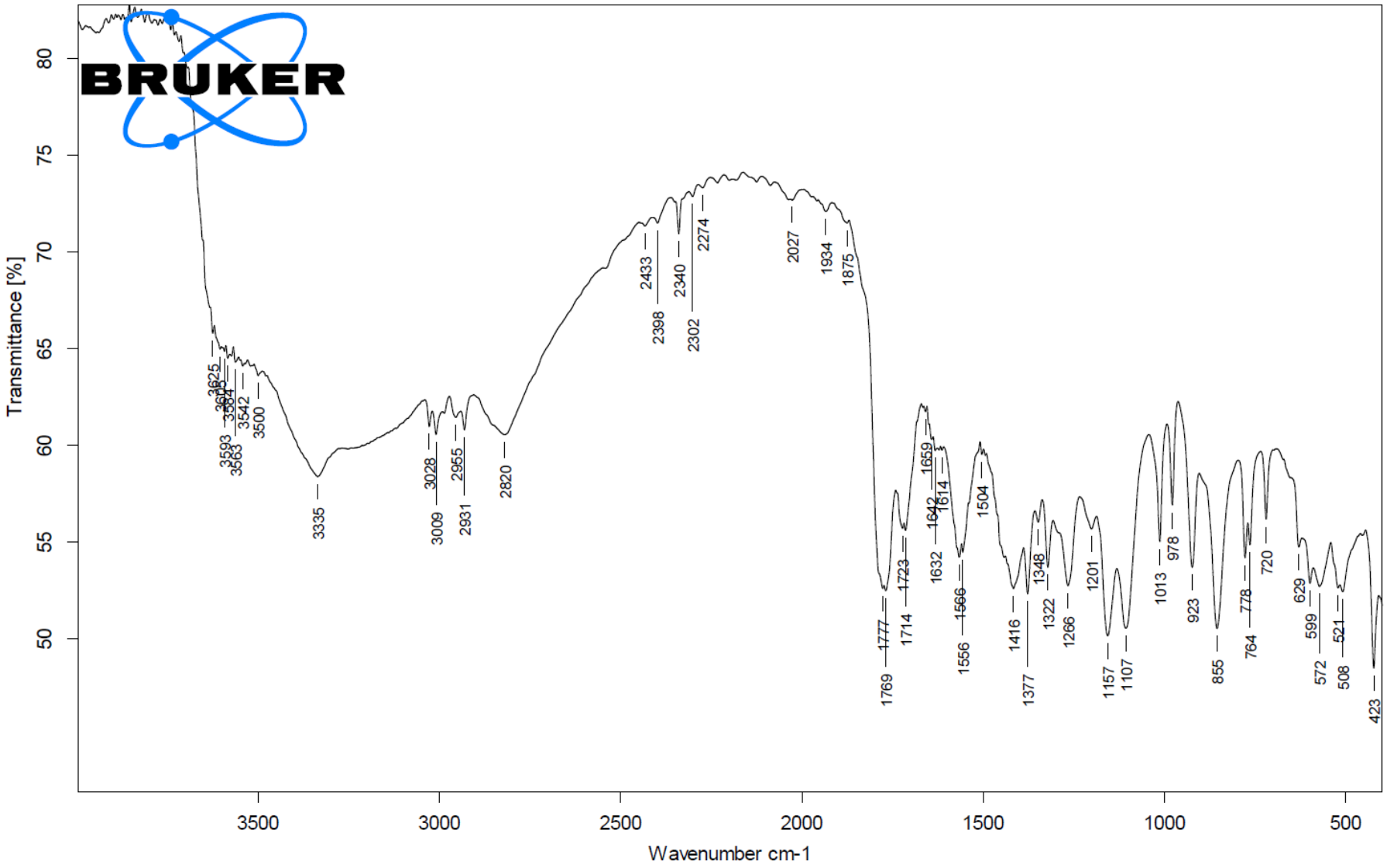
D:\IrB\Барсегян Brs361.0	Барсегян Brs361	KBr тонкий слой	20.11.2019

6-Hydroperoxy-6-methyl-5-octyl-1,2-dioxan-3-one, 2l



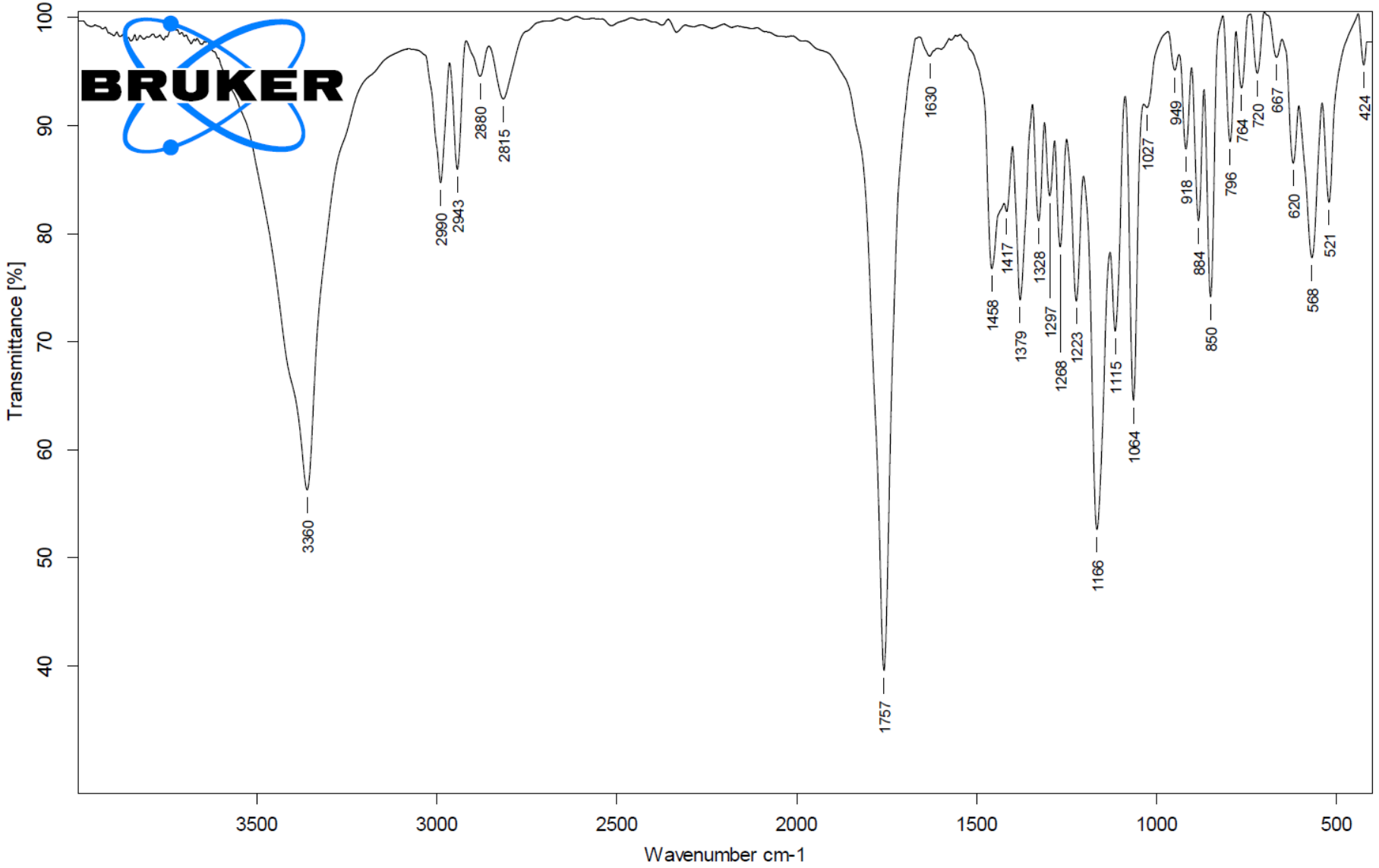
D:\IrB\Барсегян Brs331.0	Барсегян Brs331	KBr тонкий слой	16.10.2019

6-Hydroperoxy-6-methyl-1,2-dioxan-3-one, 2m



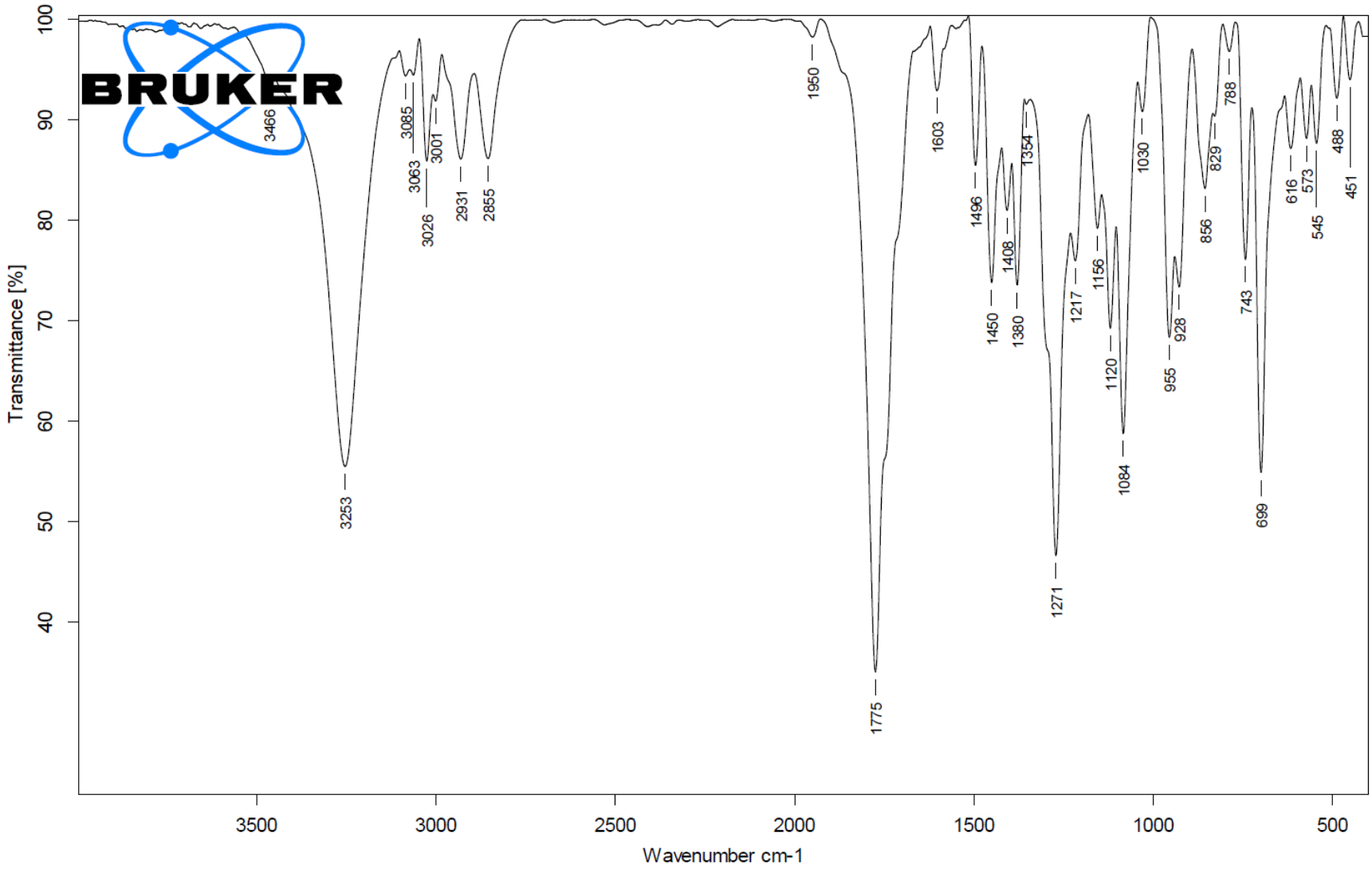
D:\IrB\Виль ВВ 2133-1.0	Виль ВВ 2133-1	KBr тонкий слой	25.07.2019

6-Hydroperoxy-4,6-dimethyl-1,2-dioxan-3-one, 2n



D:\IrB\Барсегян Brs284.0	Барсегян Brs284	KBr прессовка	25.10.2019

5-Benzyl-6-hydroxy-6-methyl-1,2-dioxan-3-one, 3a



D:\IrB\Виль ВВ2184.0	Виль ВВ2184	KBr прессовка	28.01.2020