N-alkylation of anthracycline antibiotics by natural sesquiterpene lactones as a way to obtain antitumor agents with reduced side effects

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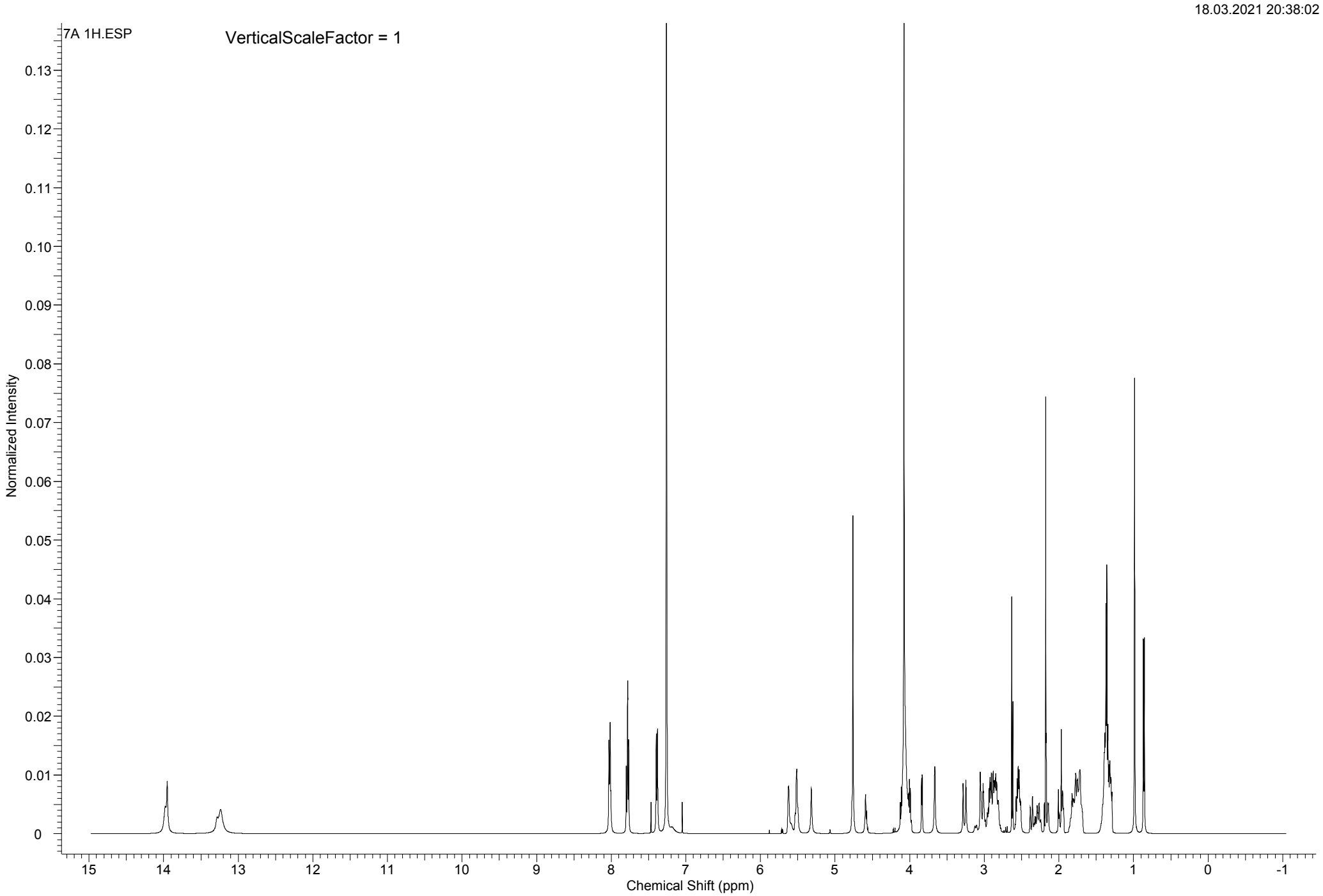
^{1}H and ^{13}C NMR spectra were recorded on Bruker AVANCE III instruments (operating frequency 500.13 and 125.78 MHz) in CDCl3, internal standard is the residual solvent signal, subscripts “alpha” and “beta” denote nonequivalent protons at one carbon atom. To refine the multiplicity in the proton spectra analysis, we used the multiplication by the TRAF function. For some weakly intense ^{13}C spectra, the Convolution difference was used to increase the signal-to-noise ratio.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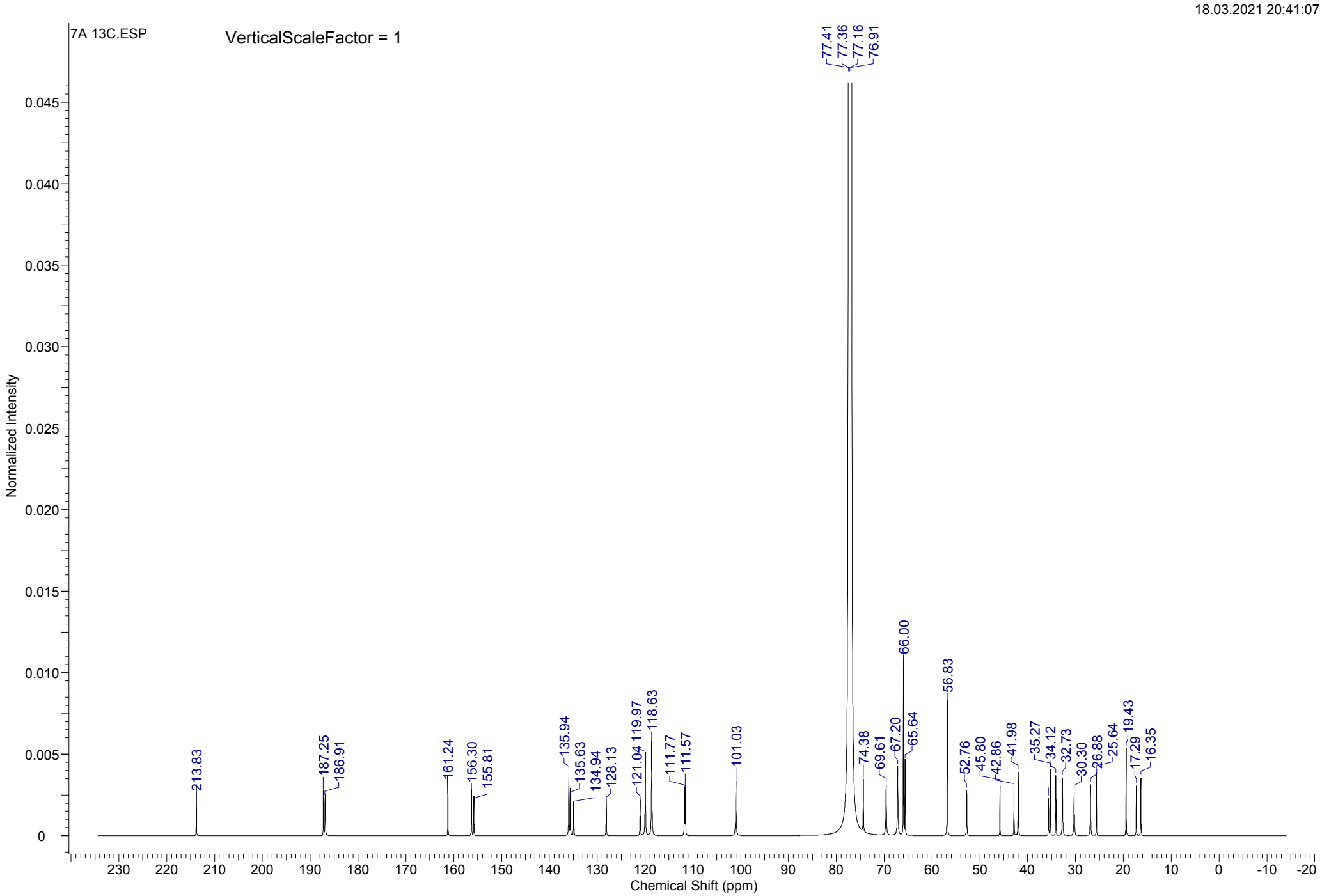
0.11
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
Chemical Shift (ppm)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Chemical Shift (ppm)
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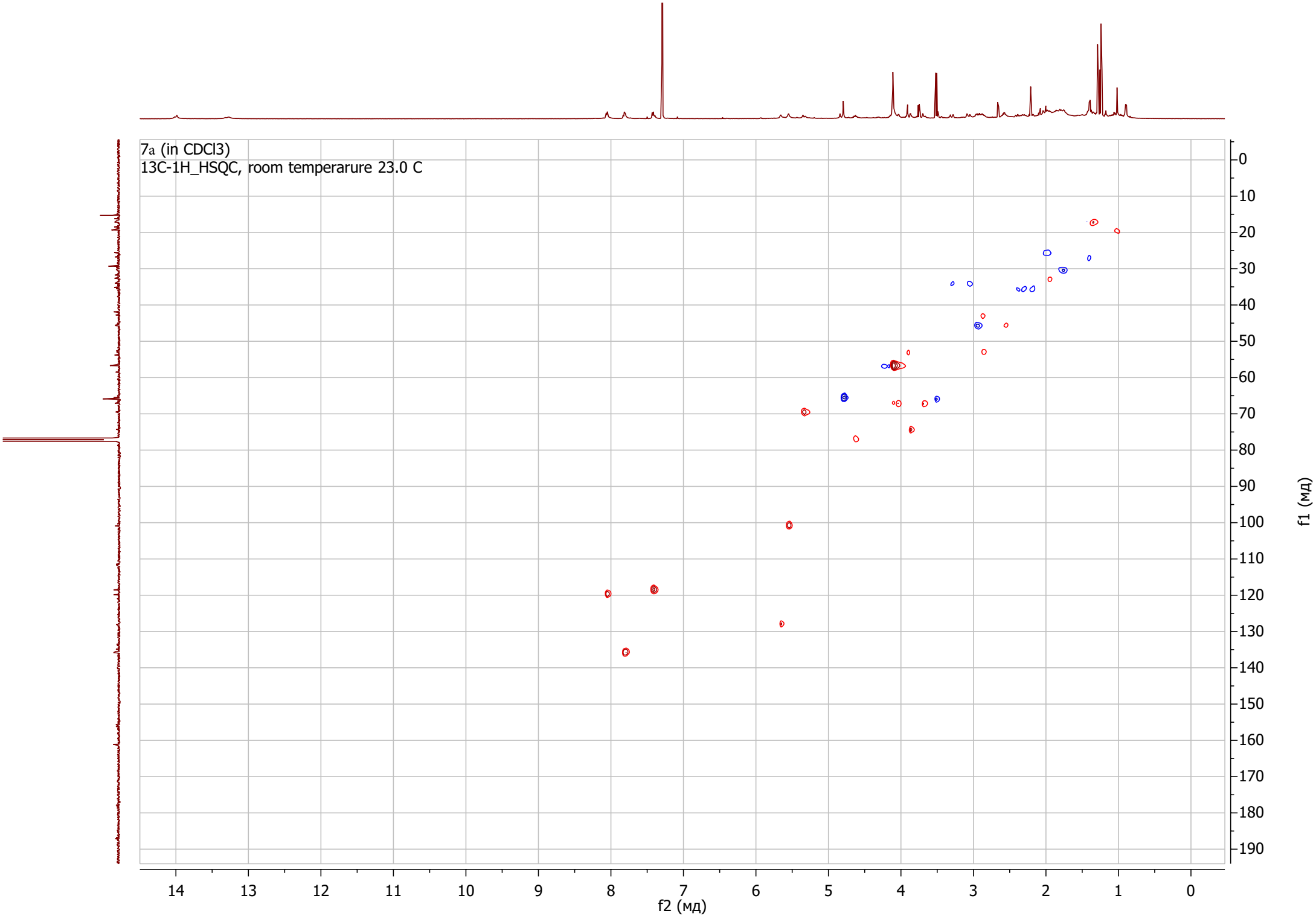
77.36
77.16
76.91
213.83
187.25
186.91
161.24
156.30
155.81
135.94
135.63
134.94
128.13
121.04
119.97
118.63
111.77
111.57
101.03
74.38
69.61
67.20
66.00
65.64
56.83
52.76
45.80
42.86
41.98
35.27
34.12
32.73
30.30
26.88
25.64
19.43
17.29
16.35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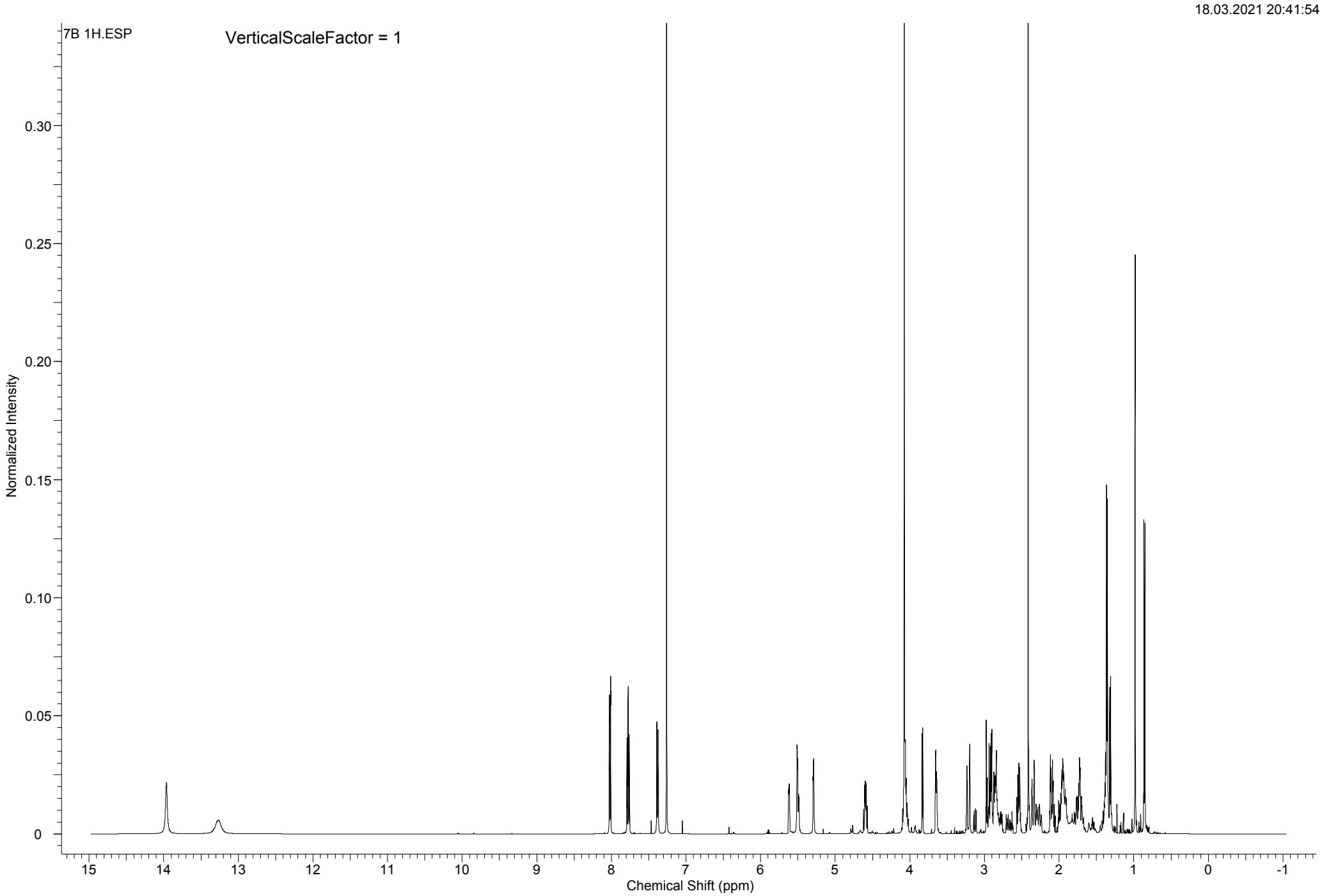
13C-1H_HSQC, room temperarure 23.0 C
f2 (мд)
f1 (мд)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7B 1H.ESP
VerticalScaleFactor = 1
Normalized Intensity
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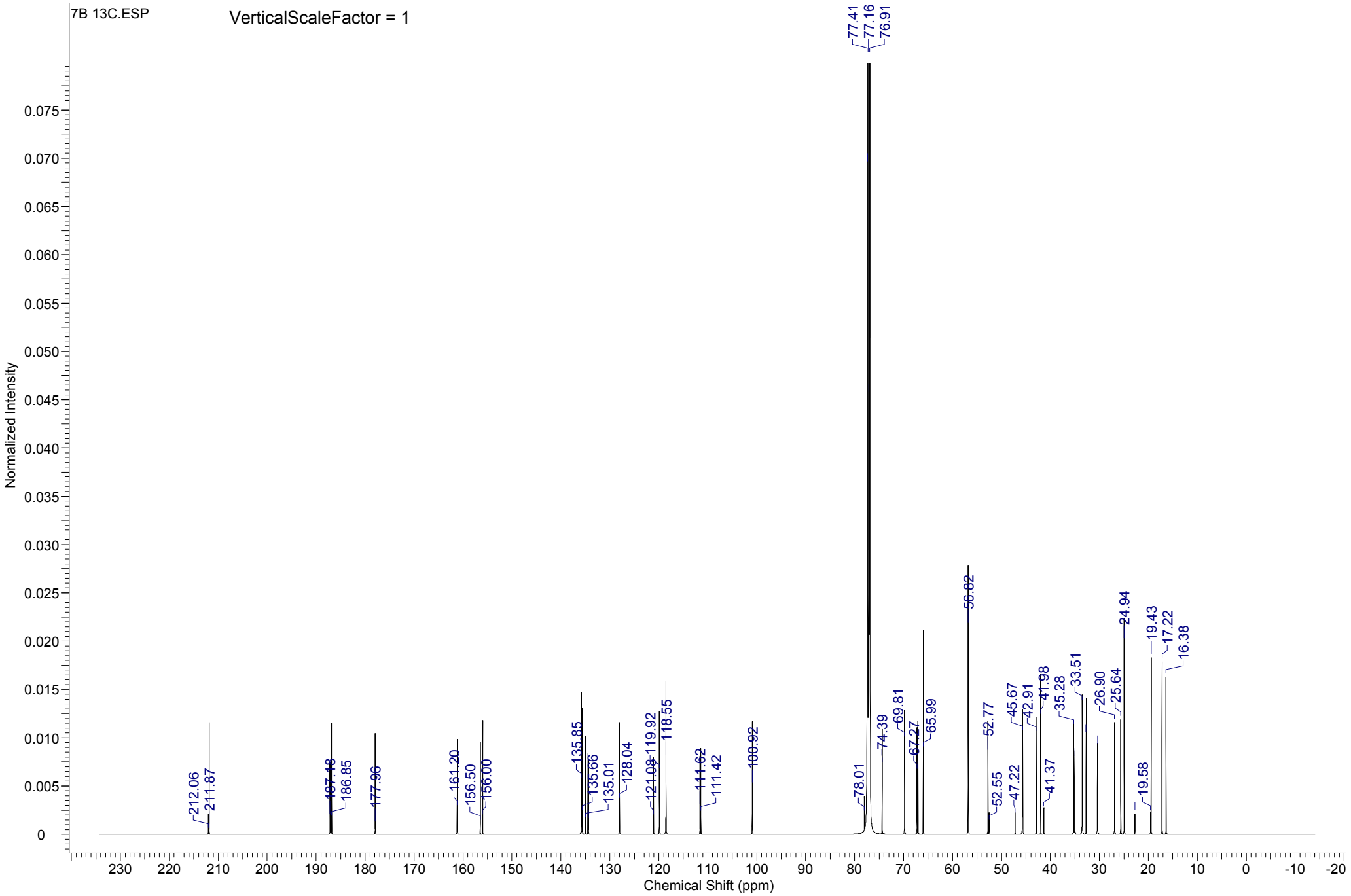
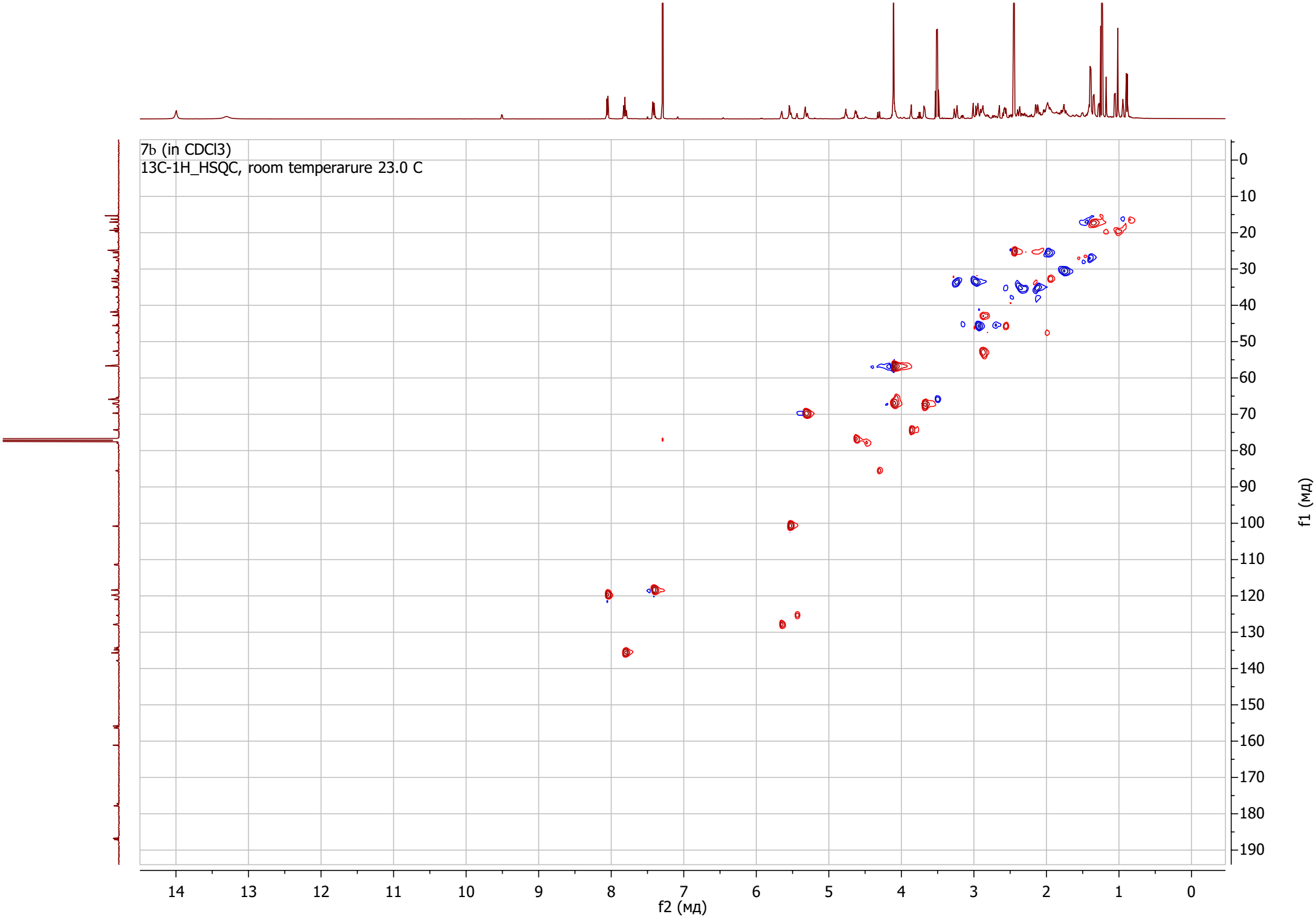
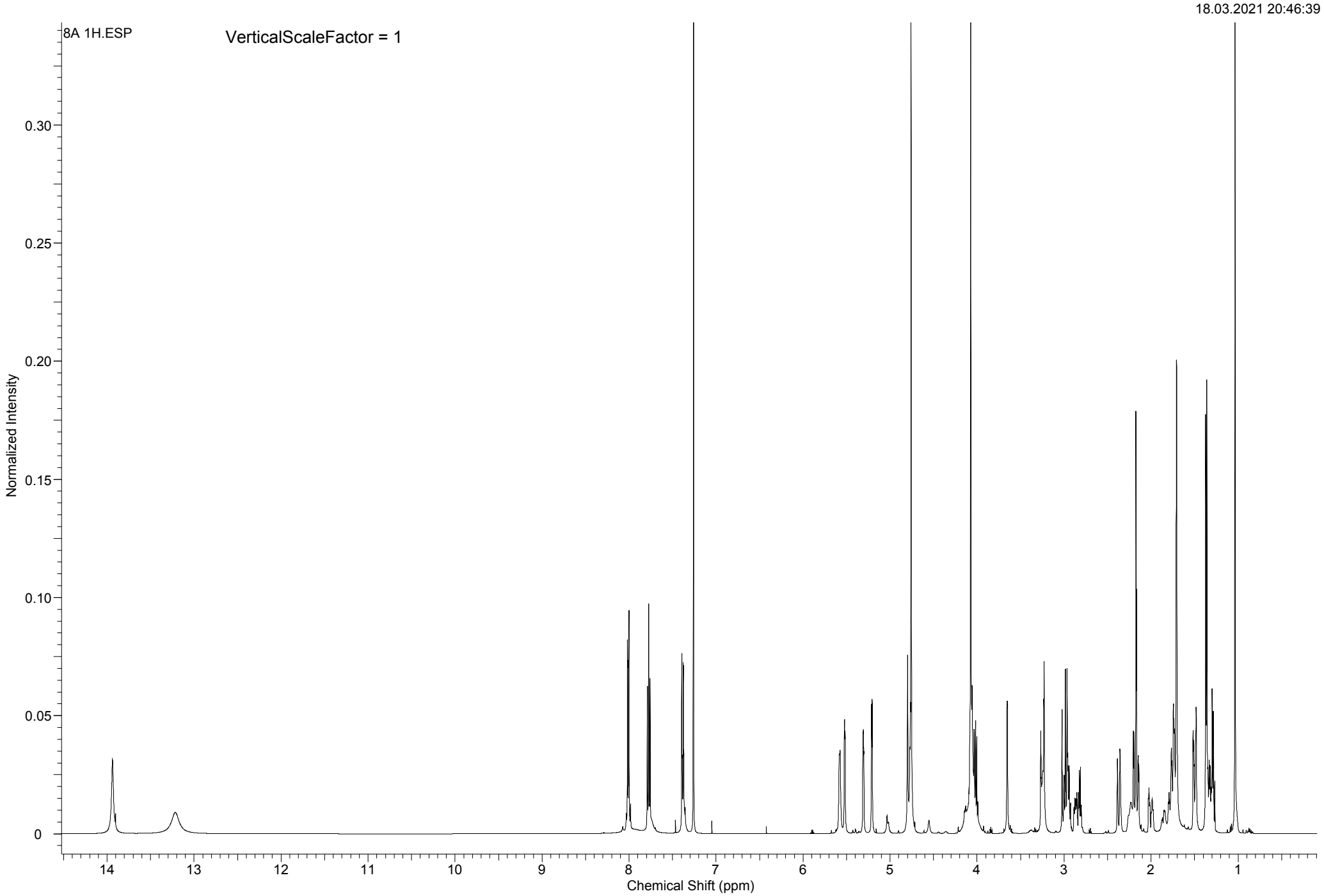
0.25
0.20
0.15
0.10
0.05
0
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
Chemical Shift (ppm)

18.03.2021 20:45:42




7b (in CDCl3)
13C-1H_HSQC, room temperarure 23.0 C
f2 (мд)
f1 (мд)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Normalized Intensity
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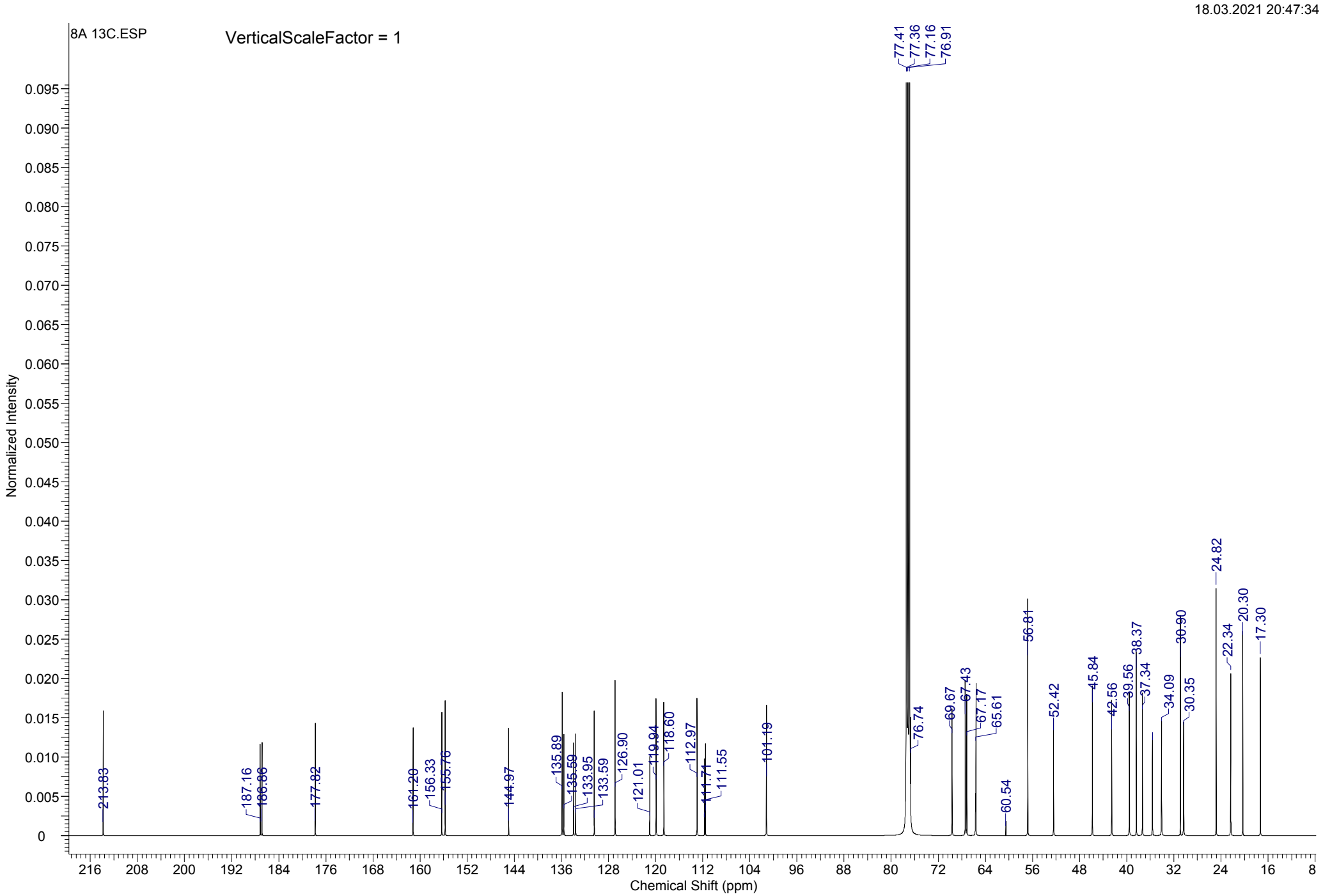
0.25
0.20
0.15
0.10
0.05
0
14
13
12
11
10
9
8
7
6
5
4
3
2
1
Chemical Shift (ppm)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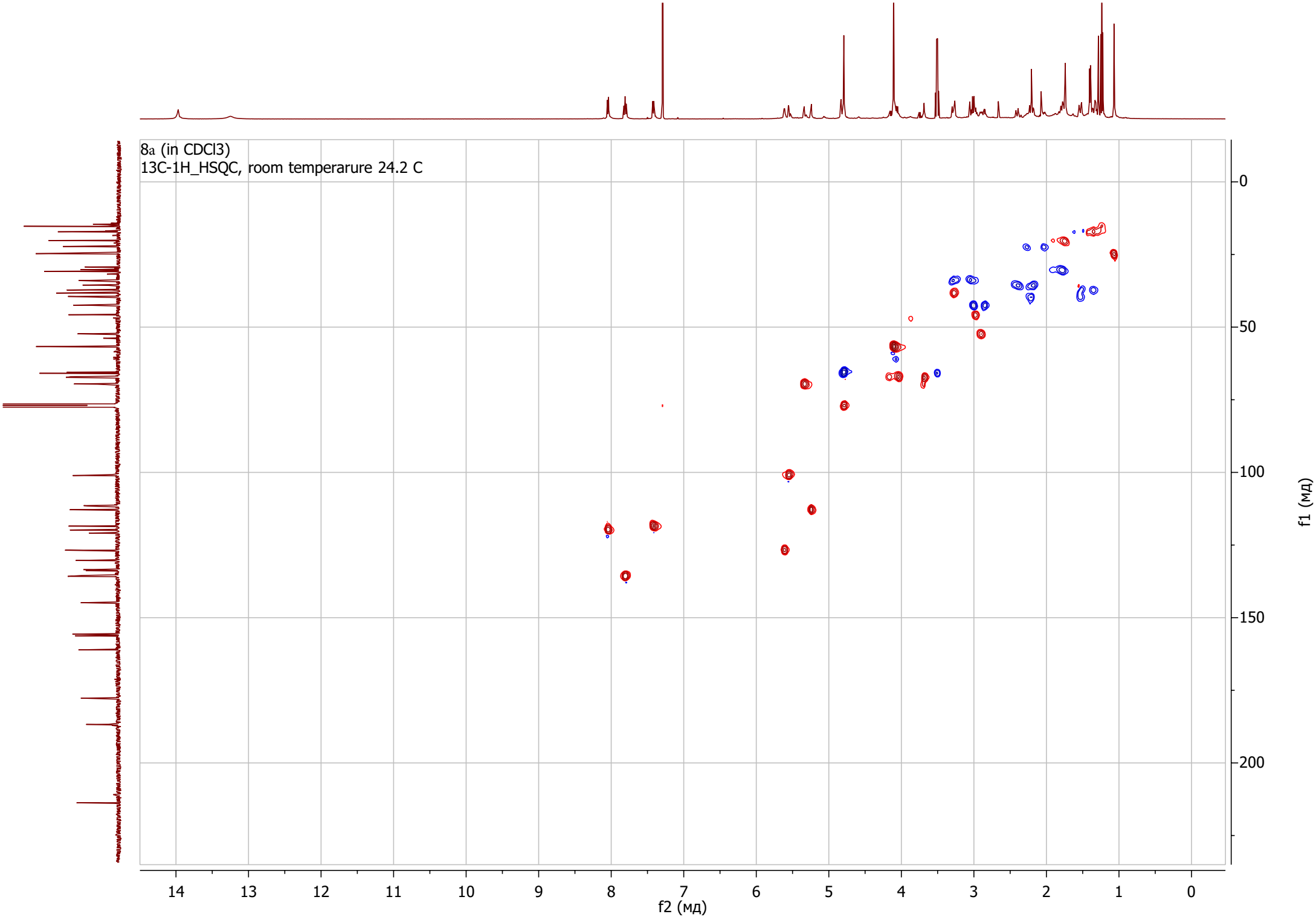
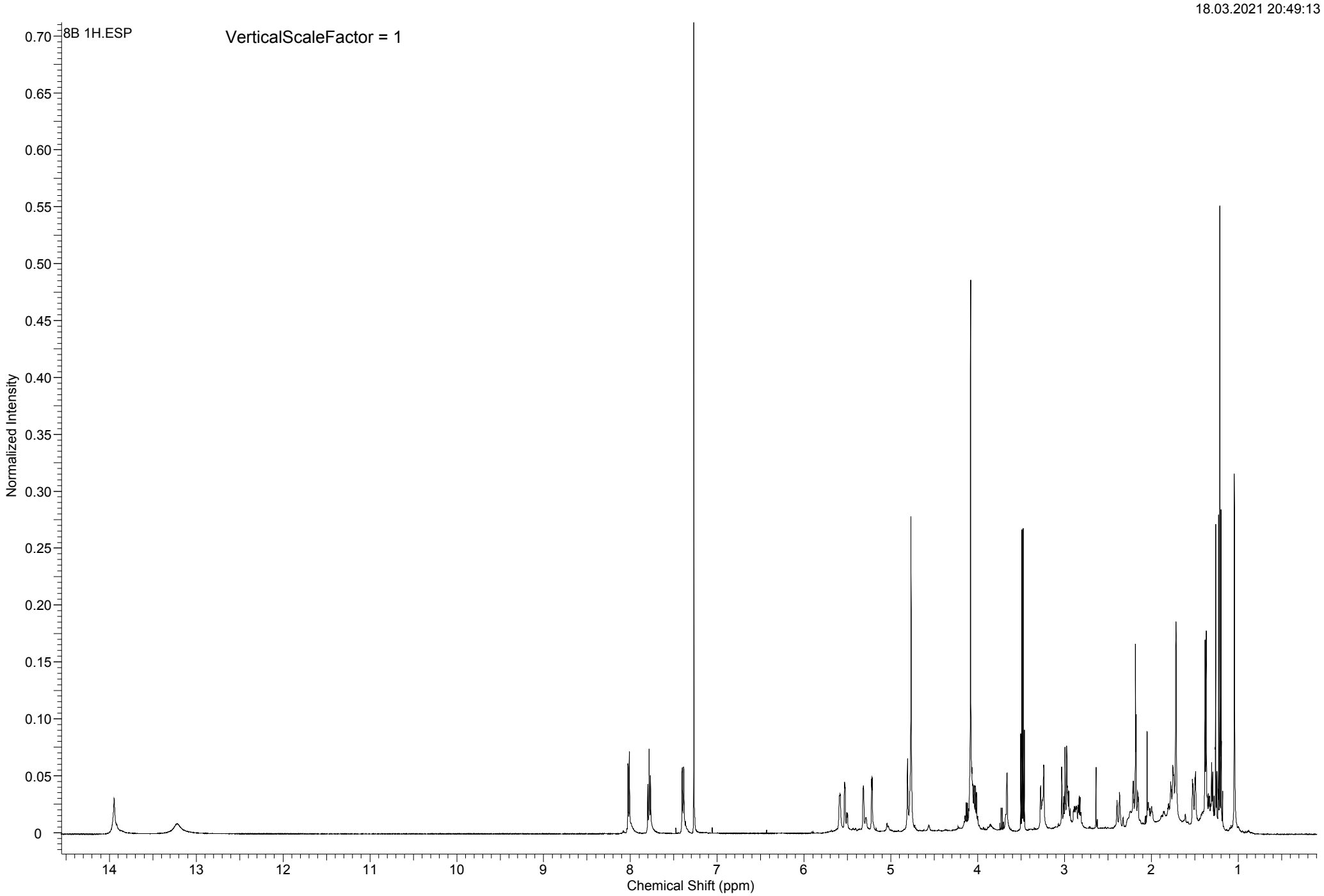
Normalized Intensity
Chemical Shift (ppm)
213.83
187.16
186.88
177.82
161.20
156.33
155.76
144.97
135.89
135.59
133.95
133.59
126.90
121.01
119.94
118.60
112.97
111.71
111.55
101.19
77.41
77.36
77.16
76.91
76.74
69.67
67.43
67.17
65.61
60.54
56.81
52.42
45.84
42.56
39.56
38.37
37.34
34.09
30.90
30.35
24.82
22.34
20.30
17.30


8a (in CDCl3)
13C-1H_HSQC, room temperarure 24.2 C
f2 (мд)
f1 (мд)
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
0
50
100
150
200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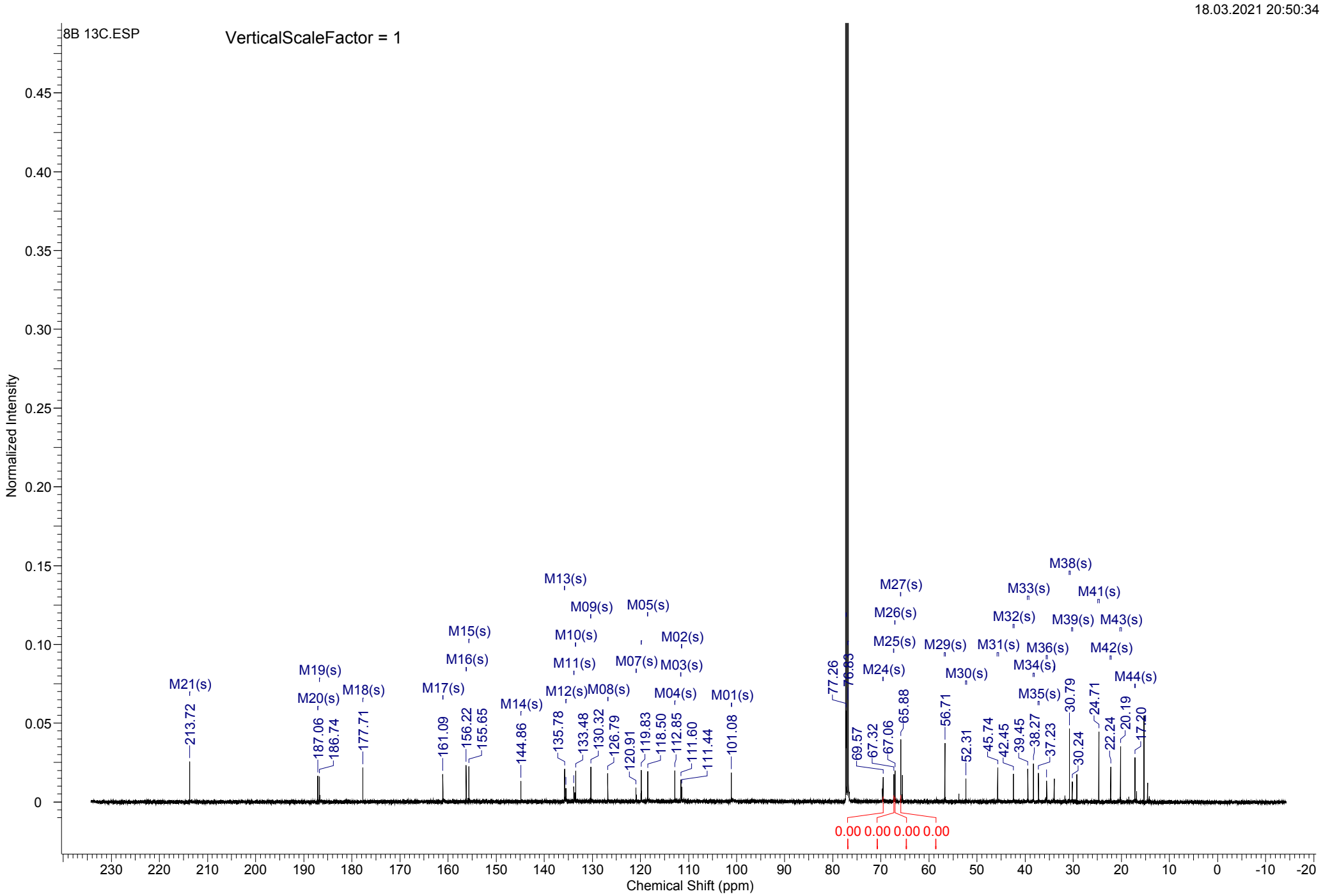
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0
14
13
12
11
10
9
8
7
6
5
4
3
2
1
Chemical Shift (ppm)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8B 13C.ESP
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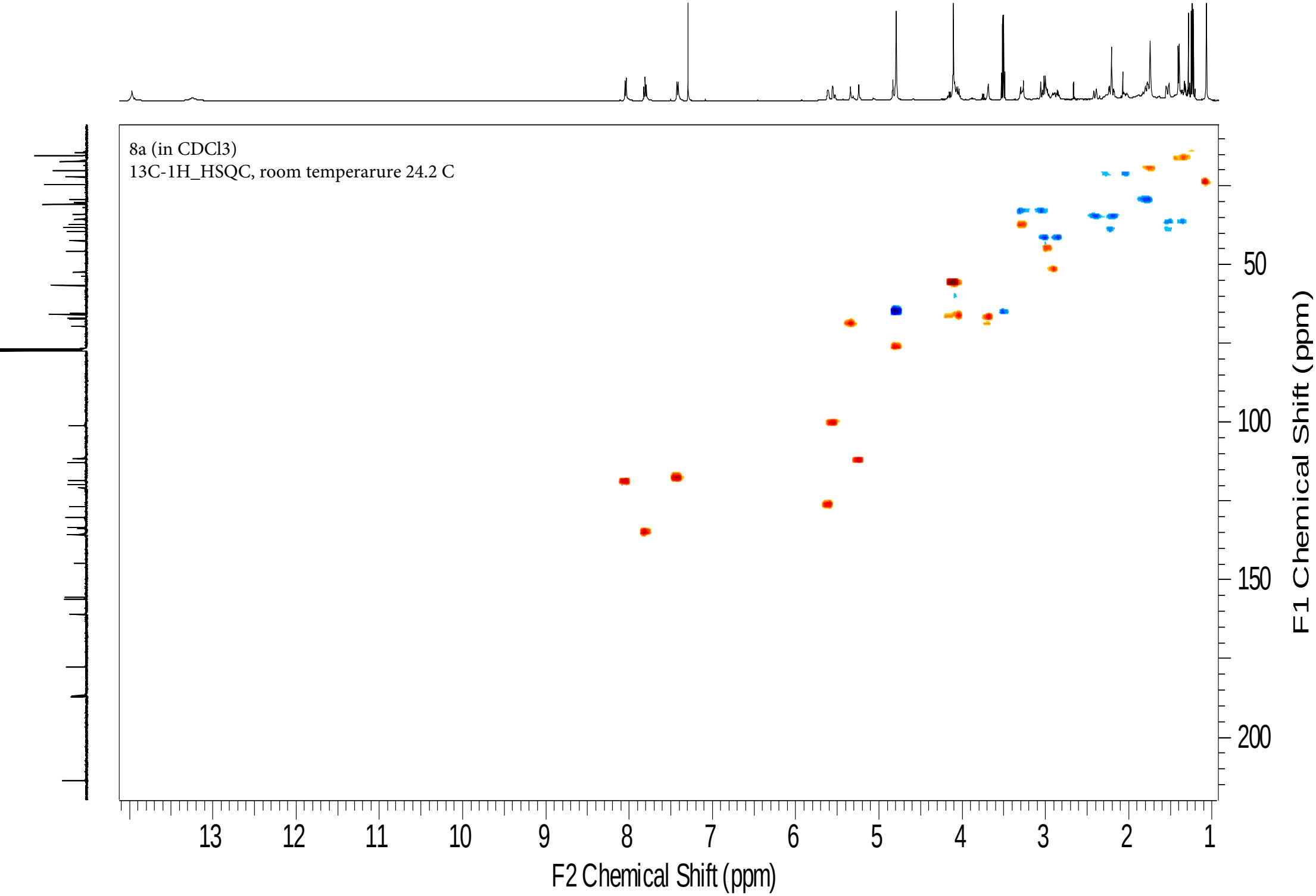
Normalized Intensity
Chemical Shift (ppm)
M01(s)
M02(s)
M03(s)
M04(s)
M05(s)
M07(s)
M08(s)
M09(s)
M10(s)
M11(s)
M12(s)
M13(s)
M14(s)
M15(s)
M16(s)
M17(s)
M18(s)
M19(s)
M20(s)
M21(s)
M24(s)
M25(s)
M26(s)
M27(s)
M29(s)
M30(s)
M31(s)
M32(s)
M33(s)
M34(s)
M35(s)
M36(s)
M38(s)
M39(s)
M41(s)
M42(s)
M43(s)
M44(s)
213.72
187.06
186.74
177.71
161.09
156.22
155.65
144.86
135.78
133.48
130.32
126.79
120.91
119.83
118.50
112.85
111.60
111.44
101.08
77.26
76.93
69.57
67.32
67.06
65.88
56.71
52.31
45.74
42.45
39.45
38.27
37.23
30.79
30.24
24.71
22.24
20.19
17.20
0.00 0.00 0.00 0.00


8a (in CDCl3)
13C-1H_HSQC, room temperarure 24.2 C
F2 Chemical Shift (ppm)
F1 Chemical Shift (ppm)
13
12
11
10
9
8
7
6
5
4
3
2
1
50
100
150
200