Supporting information (NMR spectra)

Generation of singlet oxygen from fragmentation of monoactivated 1,1-dihydroperoxides

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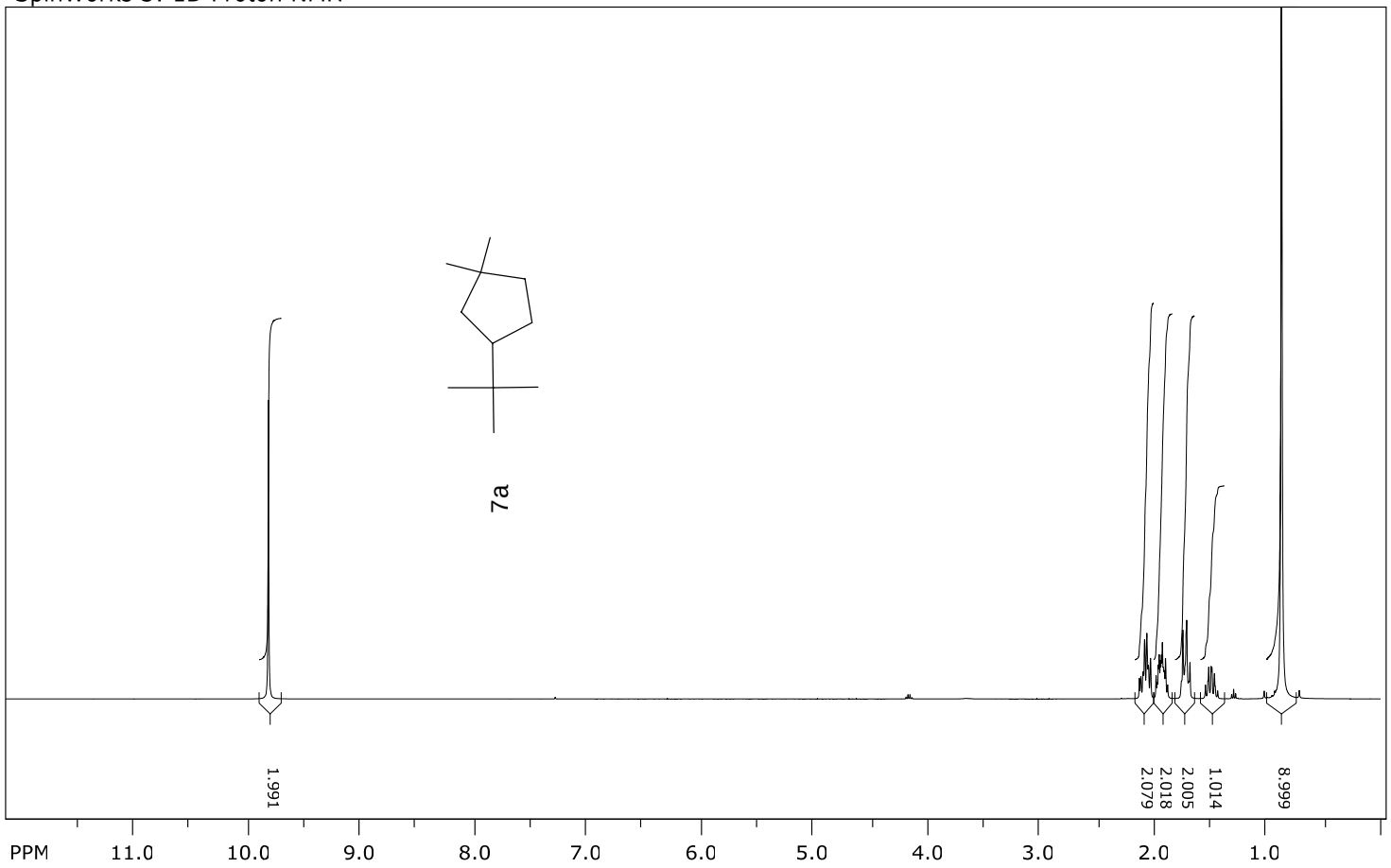
SpinWorks 3: 1D Proton NMR



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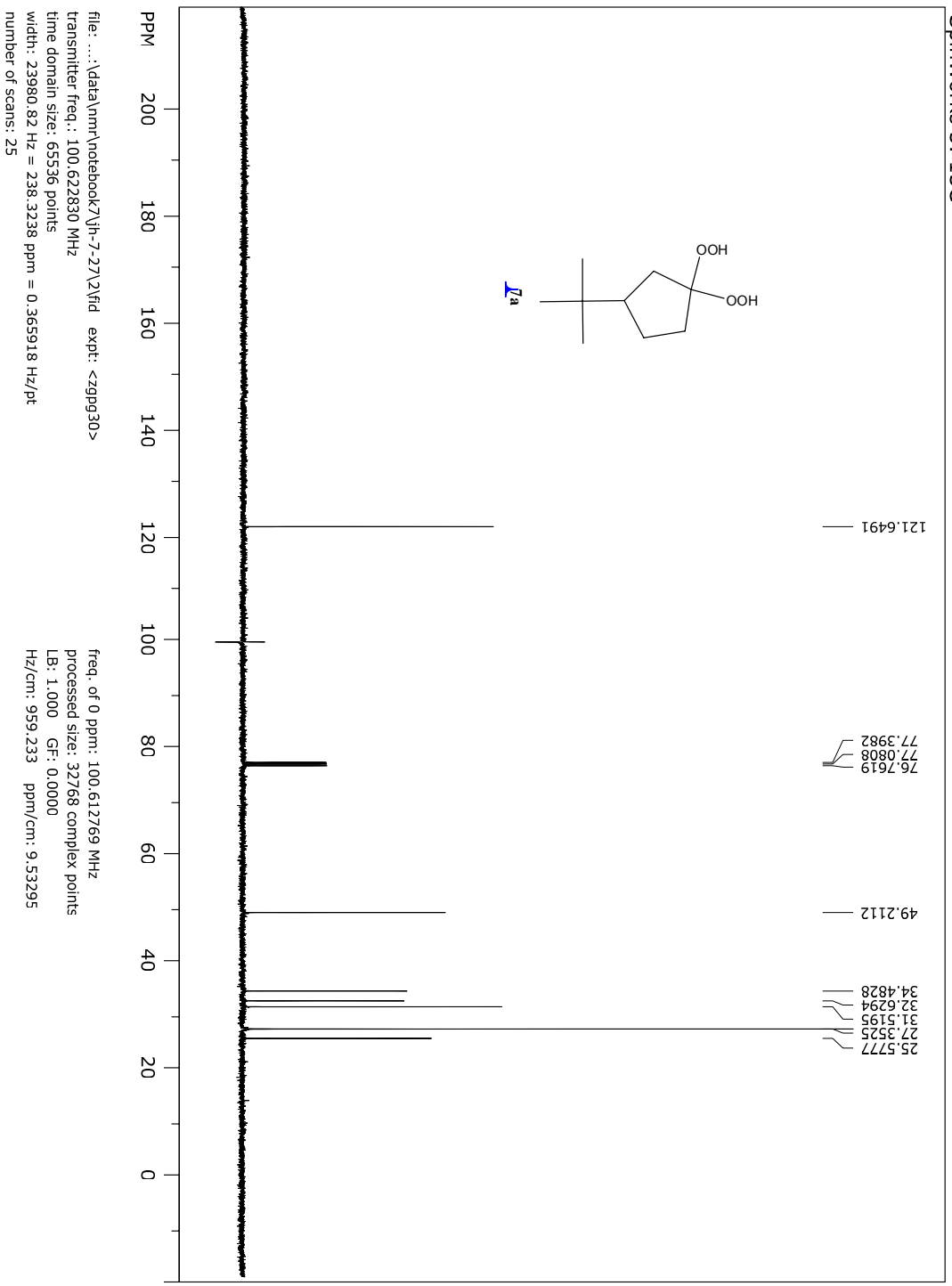
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140
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7a
OOH
OOH
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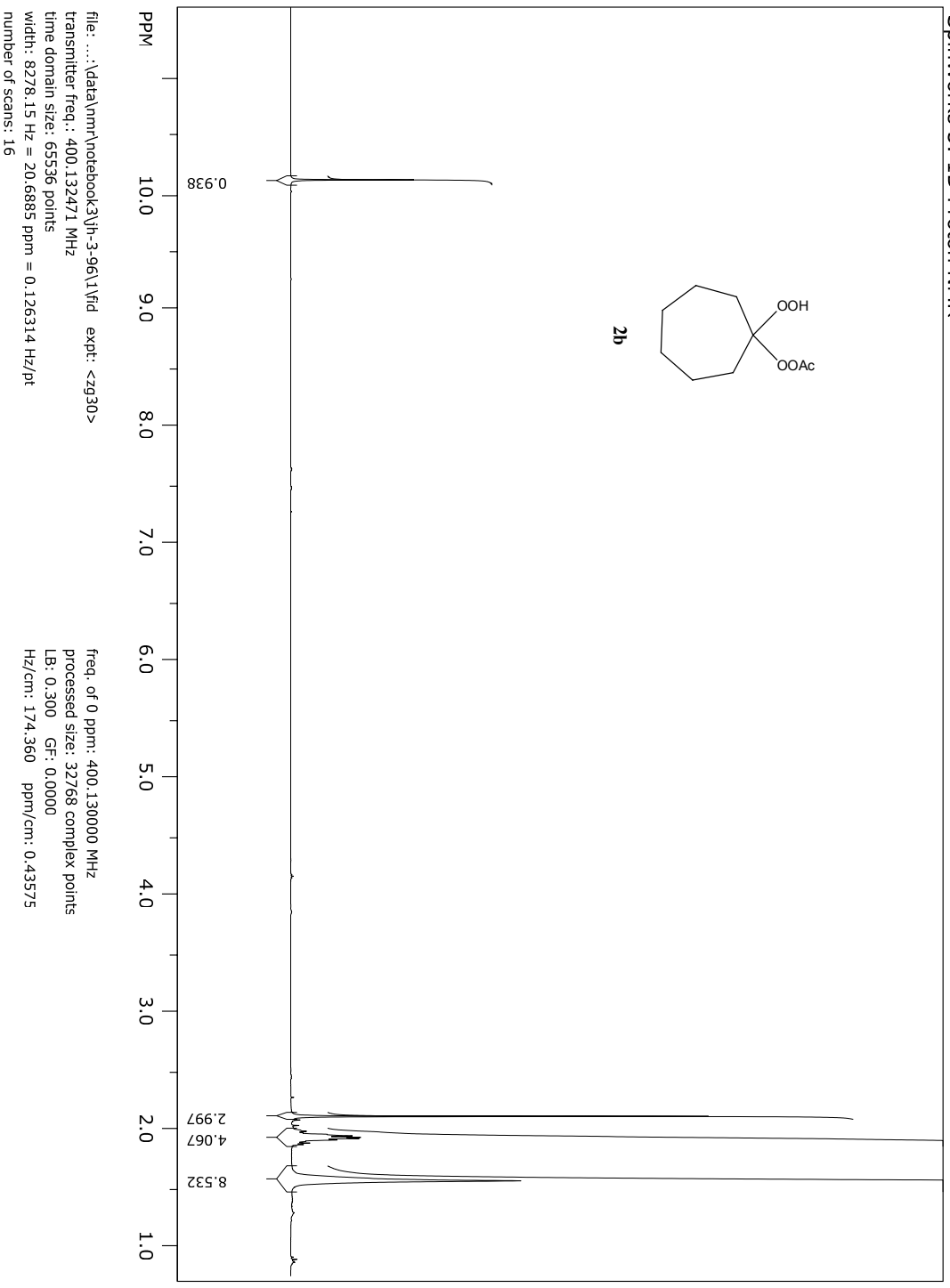
Hz/cm: 959.233 ppm/cm: 9.53295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PPM
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8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
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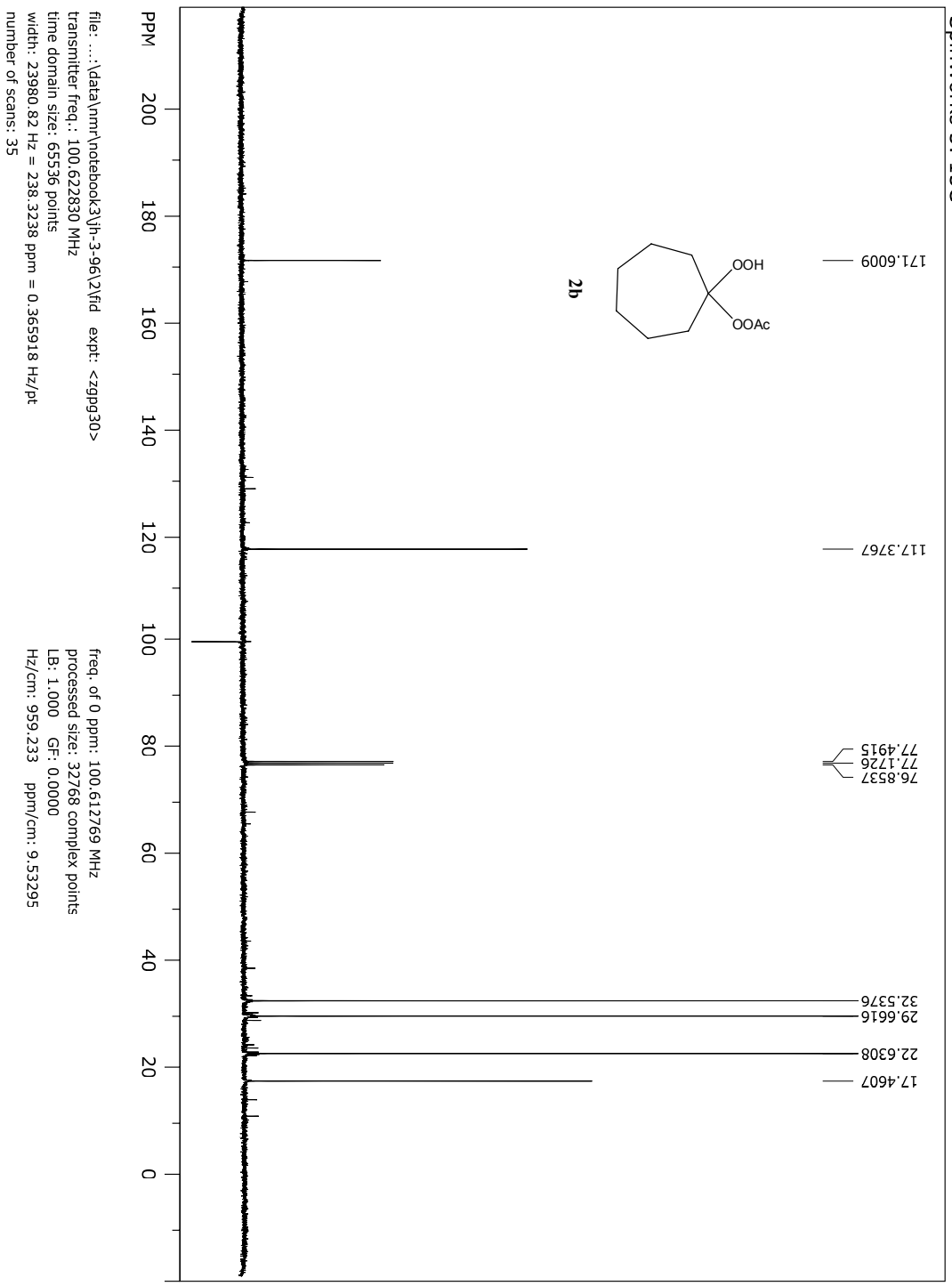
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120
100
80
60
40
20
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77.1726
77.4915
32.5376
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OOH
OOAc
2b
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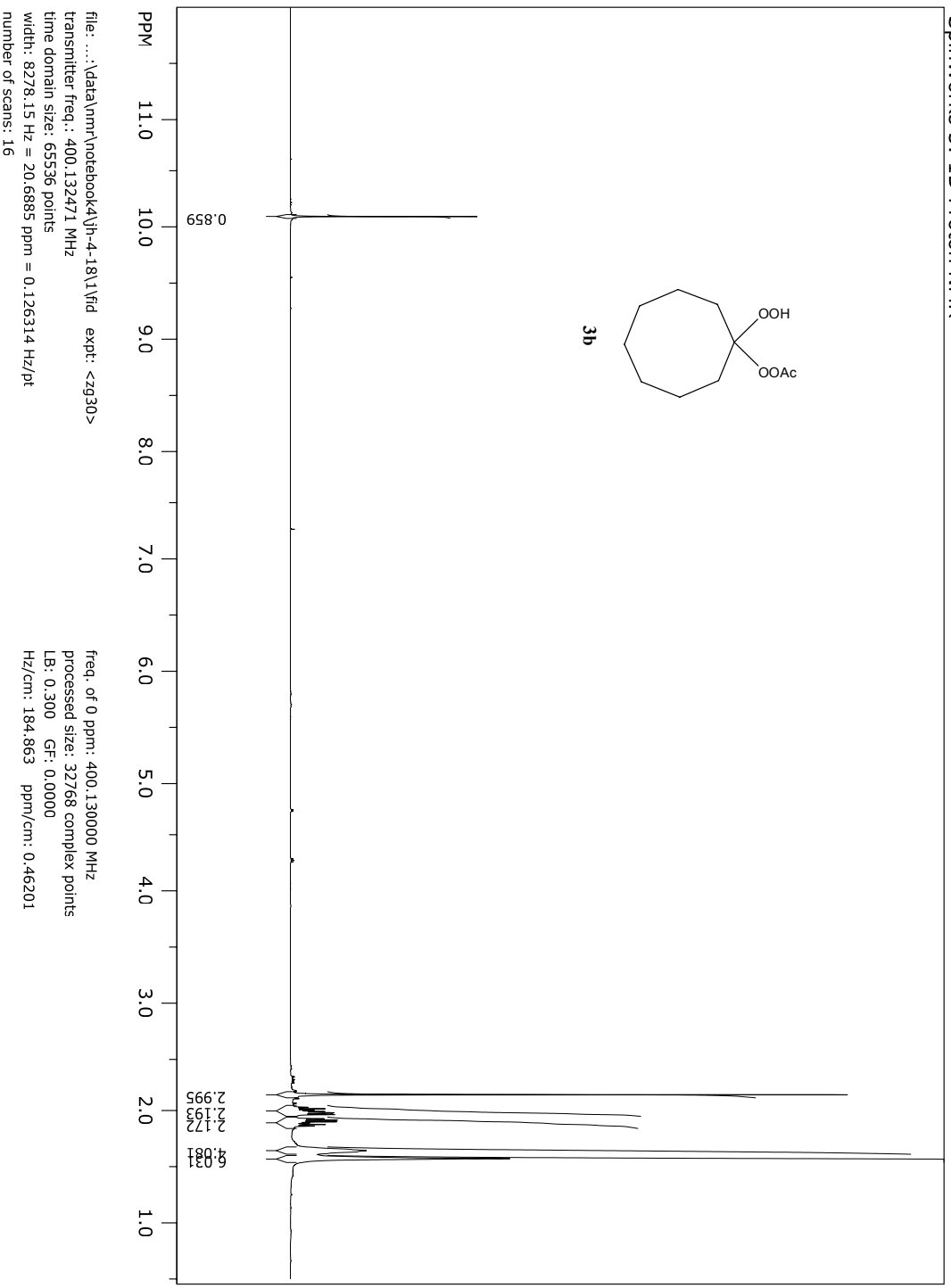
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 959.233 ppm/cm: 9.53295

.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3b
OOH
OOAc
0.859
6.031
4.081
2.172
2.193
2.995
PPM
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10.0
9.0
8.0
7.0
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5.0
4.0
3.0
2.0
1.0
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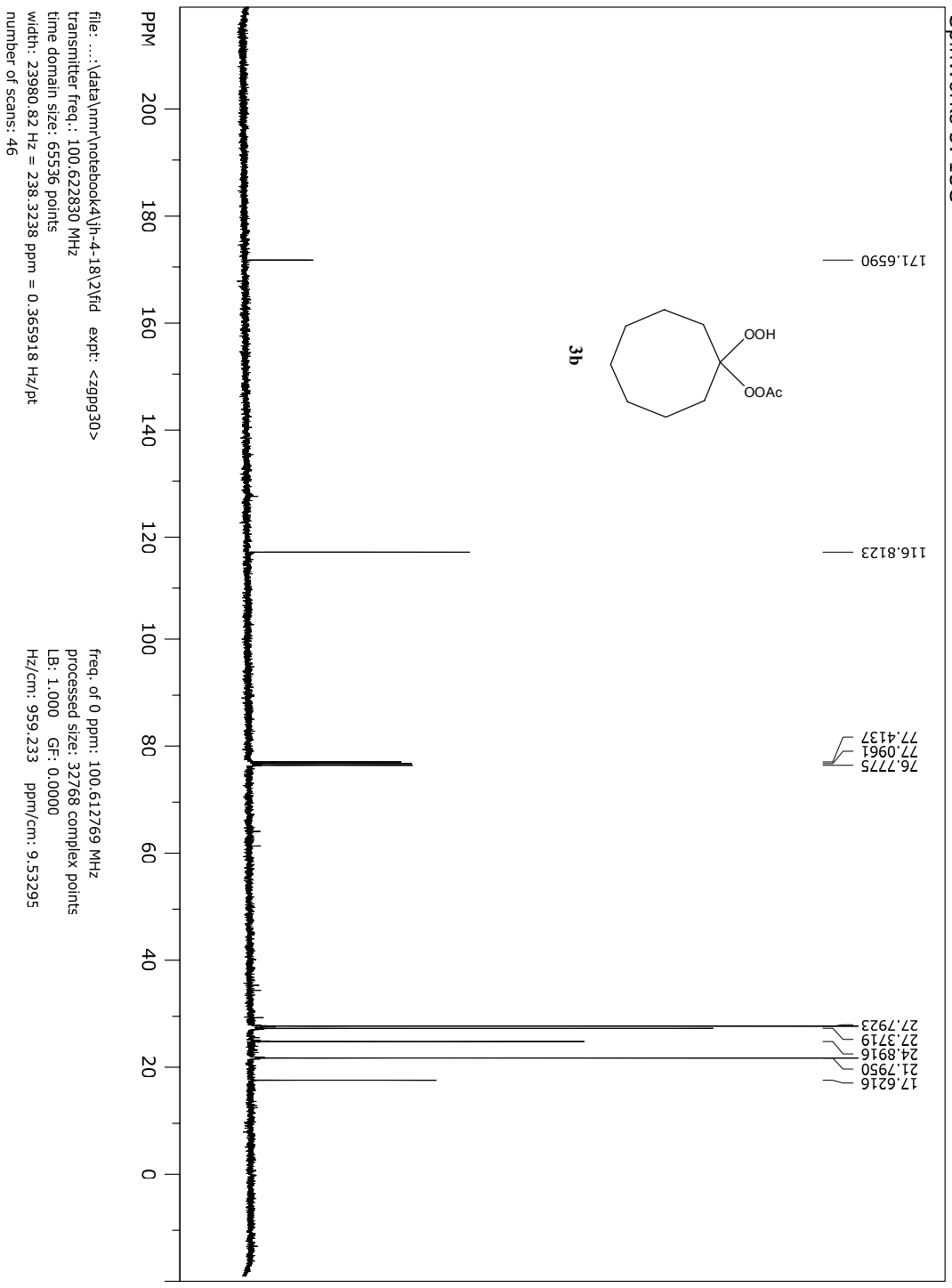
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27.3719
24.8916
21.7950
17.6216
PPM
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180
160
140
120
100
80
60
40
20
0
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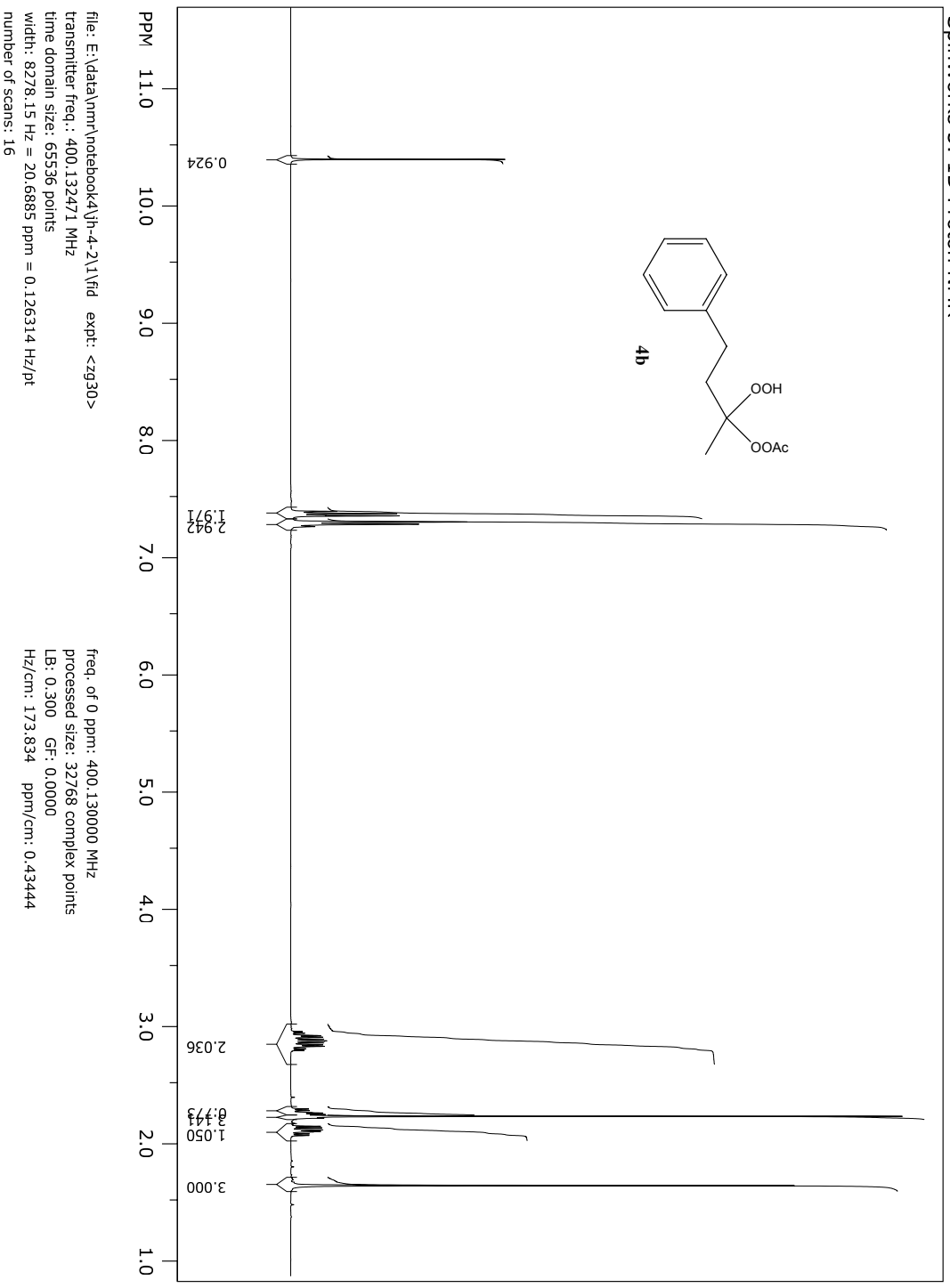
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 959.233 ppm/cm: 9.53295

.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4b
OOH
OOAc
0.924
2.942
1.971
2.036
1.050
3.441
0.793
3.000
PPM 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0
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LB: 0.300 GF: 0.0000
Hz/cm: 173.834 ppm/cm: 0.43444

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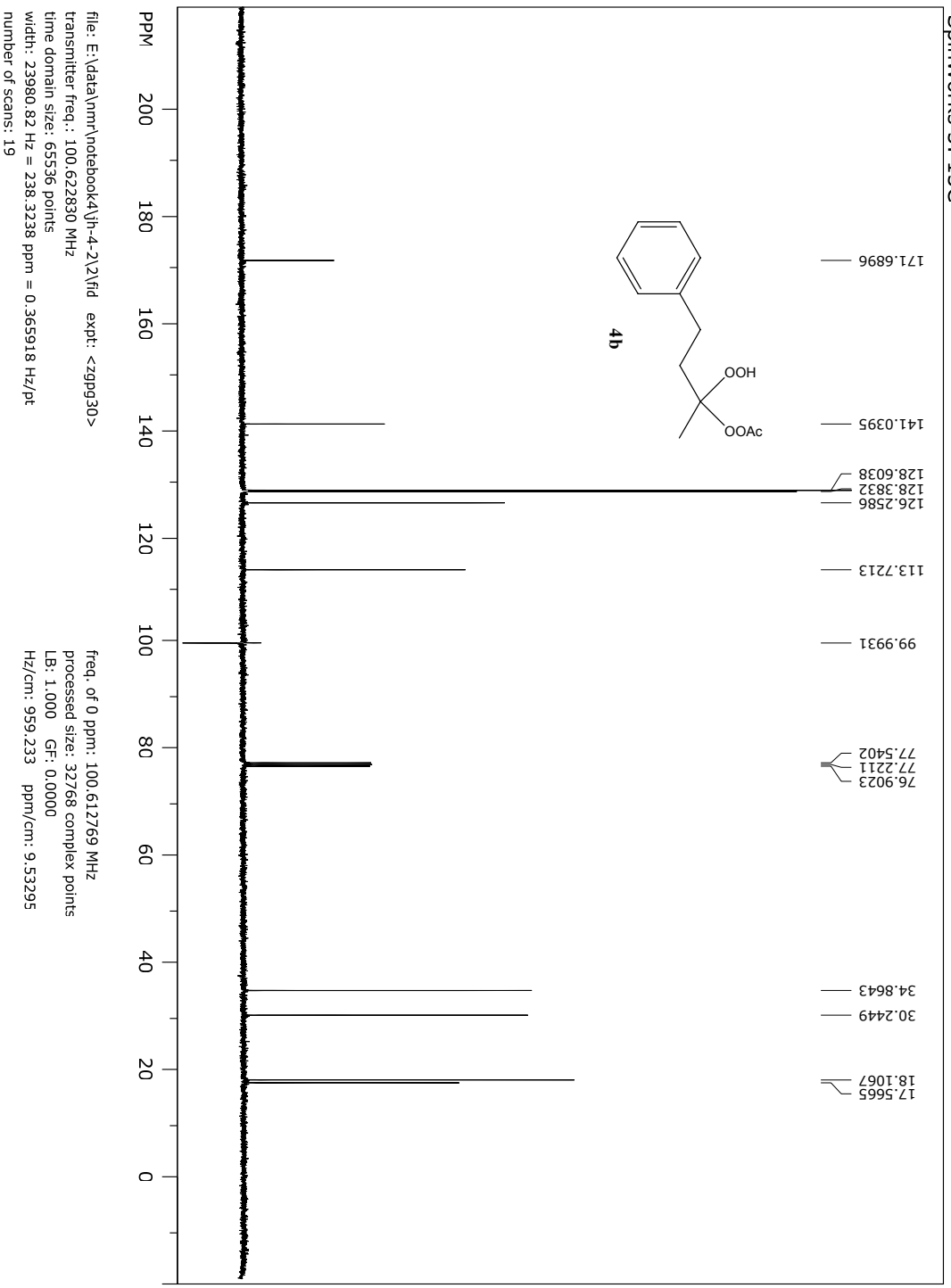
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180
160
140
120
100
80
60
40
20
0
4b
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OOAc
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141.0395
128.6038
128.3832
126.2586
113.7213
99.9931
76.9023
77.2211
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18.1067
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LB: 1.000 GF: 0.0000
Hz/cm: 959.233 ppm/cm: 9.53295

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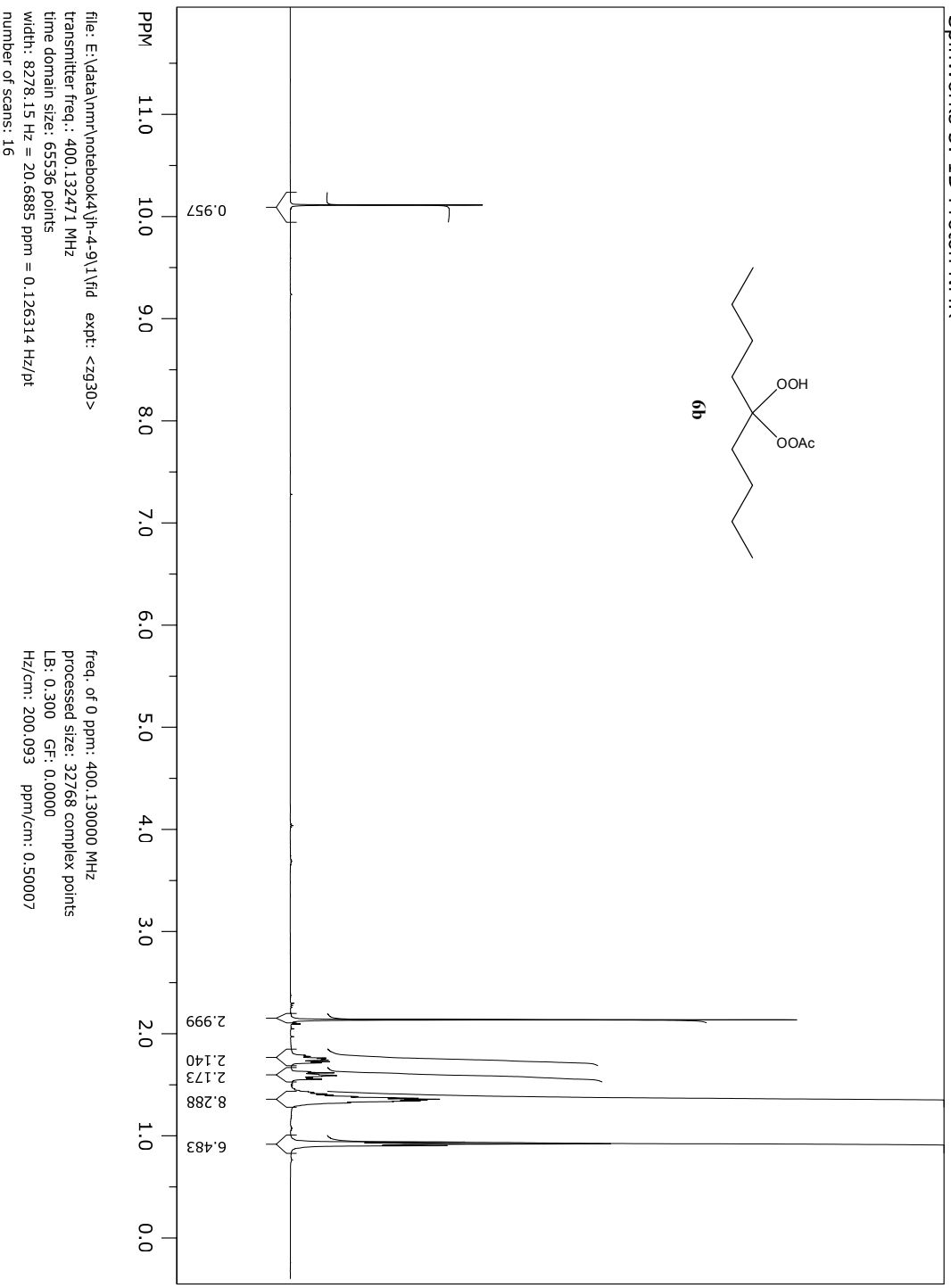
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5.0
4.0
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2.0
1.0
0.0
0.957
2.999
2.140
2.173
8.288
6.483
OOH
OOAc
6b
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time domain size: 65536 points
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freq. of 0 ppm: 400.130000 MHz
processed size: 32768 complex points
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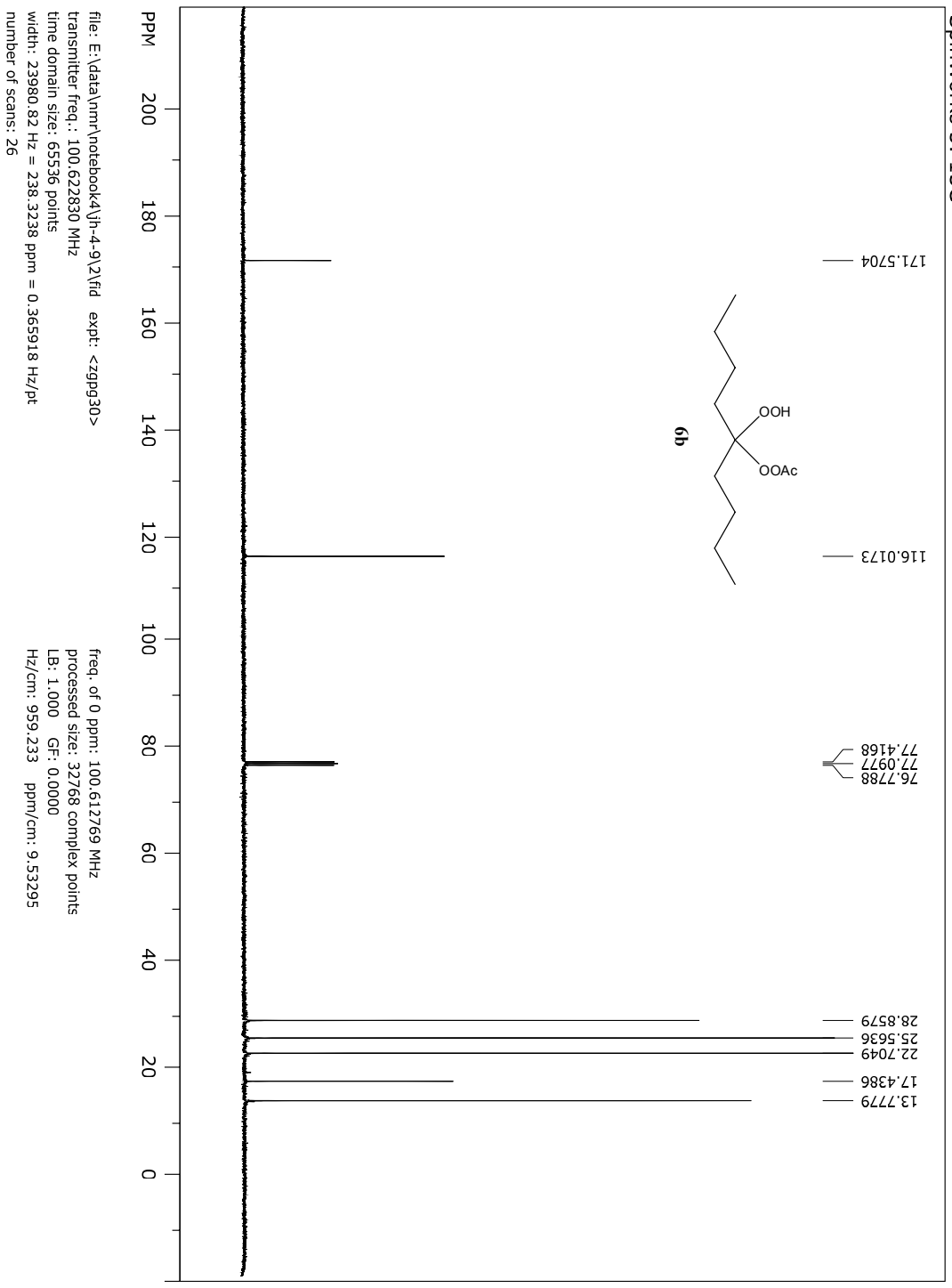
Hz/cm: 200.093 ppm/cm: 0.50007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22.7049
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13.7779
6b
OOH
OOAc
PPM
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180
160
140
120
100
80
60
40
20
0
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processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 959.233 ppm/cm: 9.53295

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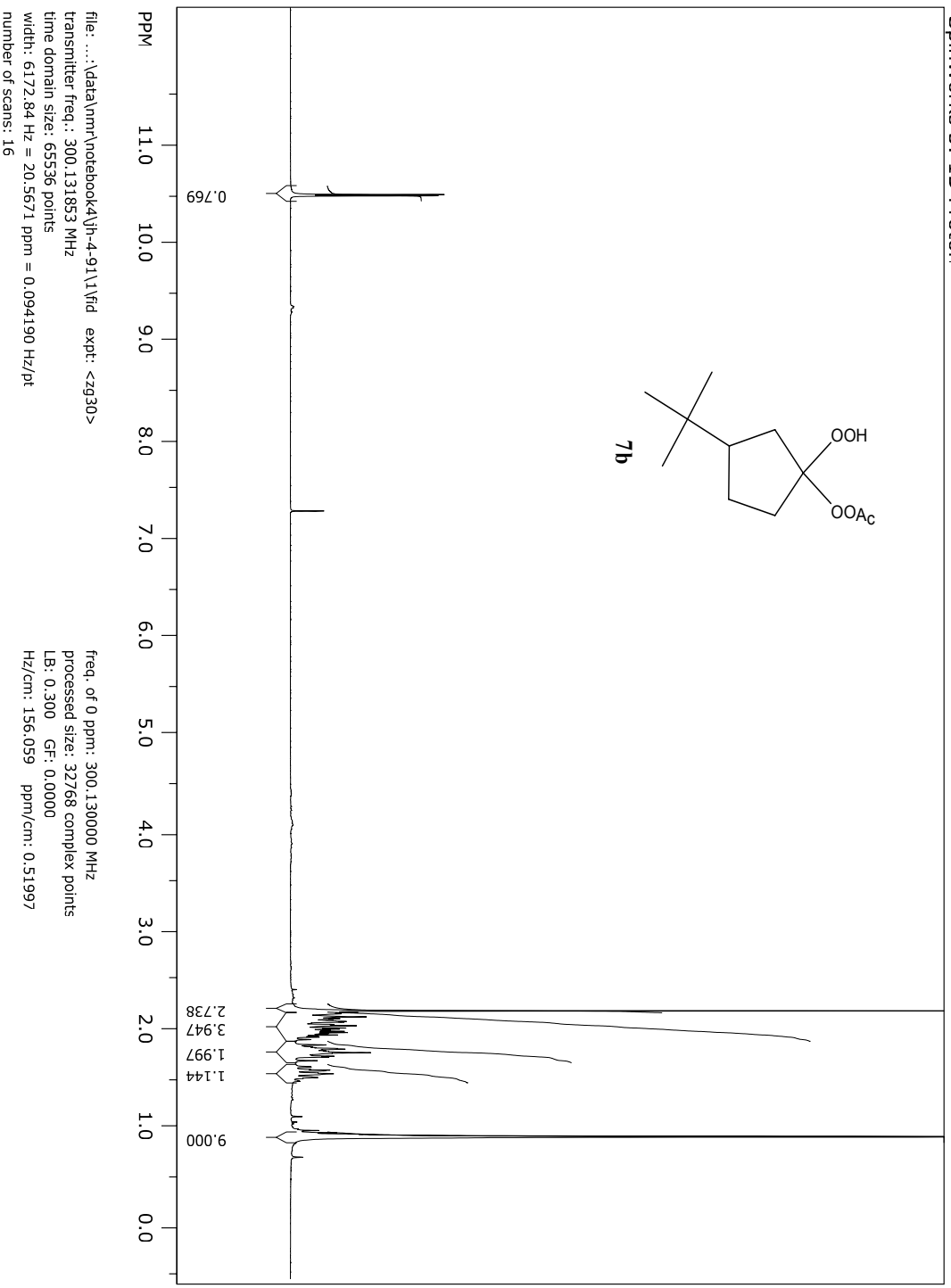
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7b
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OOAc
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1.997
3.947
2.738
PPM
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9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
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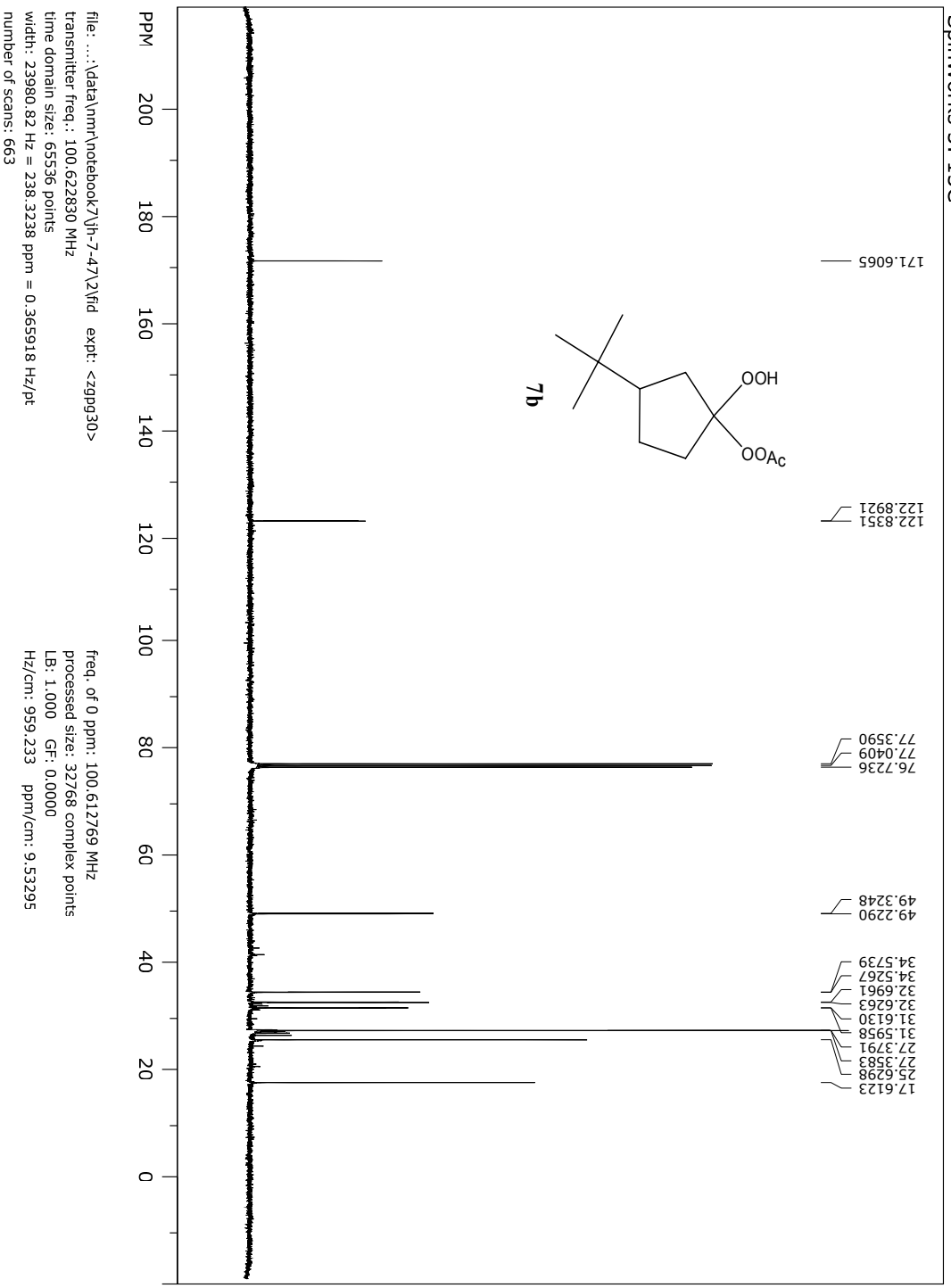
Hz/cm: 156.059 ppm/cm: 0.51997

.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160
140
120
100
80
60
40
20
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122.8921
76.7236
77.0409
77.3590
49.2290
49.3248
34.5739
34.5267
32.6961
32.6263
31.6130
31.5958
27.3791
27.3583
25.6298
17.6123
7b
OOH
OOAc
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time domain size: 65536 points
width: 23980.82 Hz = 238.3238 ppm = 0.365918 Hz/pt
number of scans: 663
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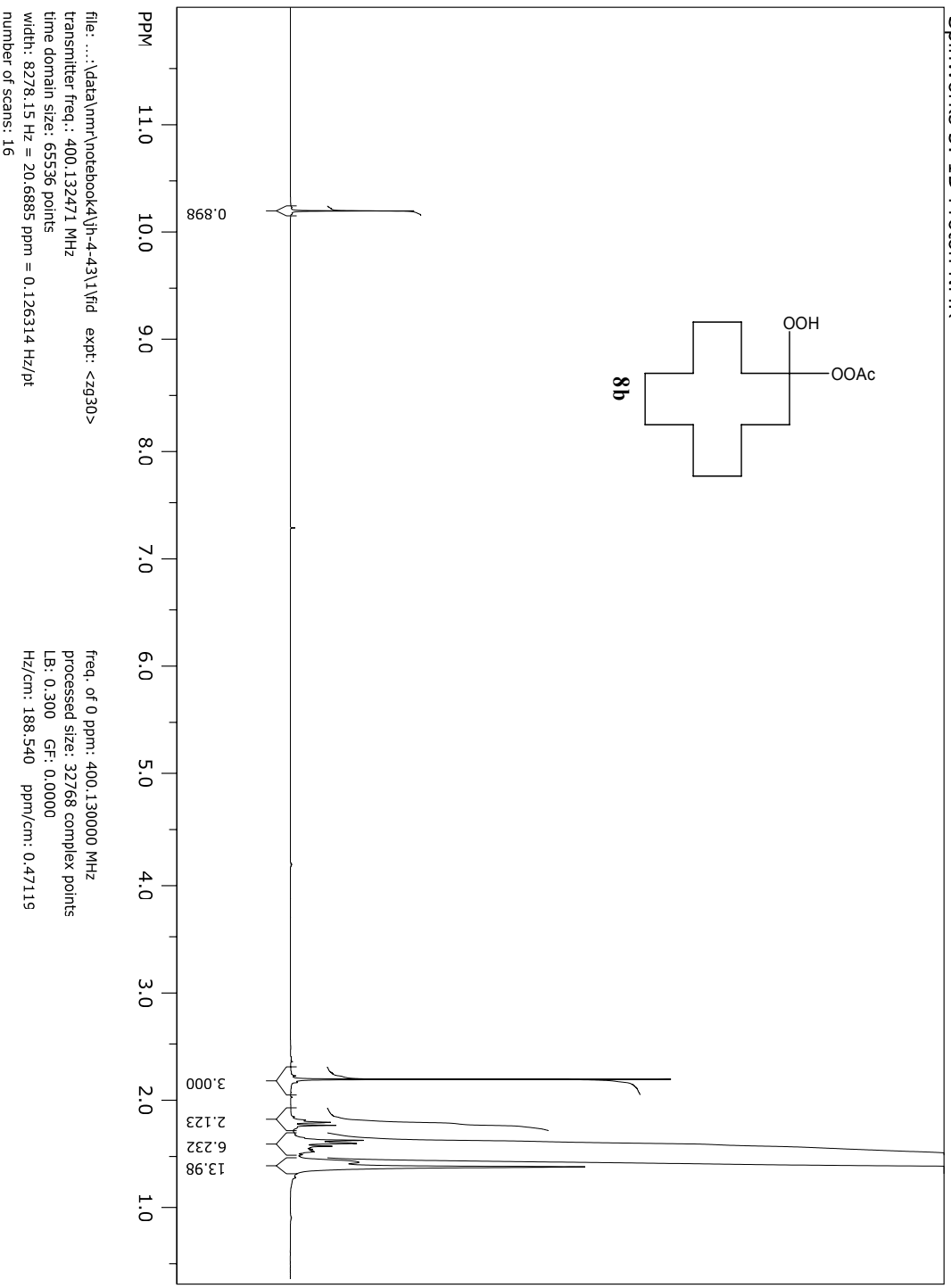
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 959.233 ppm/cm: 9.53295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OOH
OOAc
8b
0.898
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6.232
13.98
PPM
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9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
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processed size: 32768 complex points
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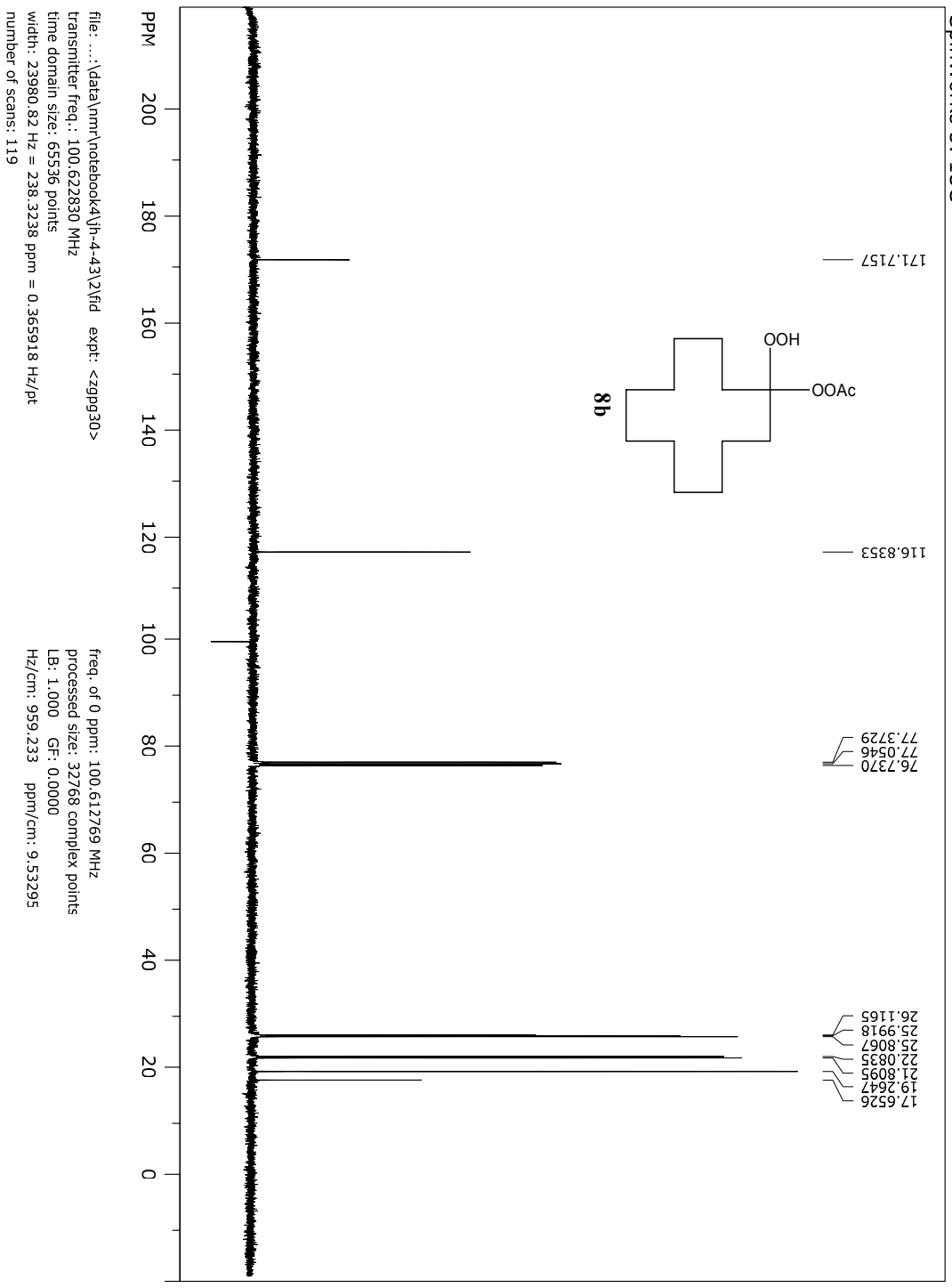
Hz/cm: 188.540 ppm/cm: 0.47119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120
100
80
60
40
20
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77.0546
77.3729
26.1165
25.9918
25.8067
22.0835
21.8095
19.2647
17.6526
8b
OOH
OOAc
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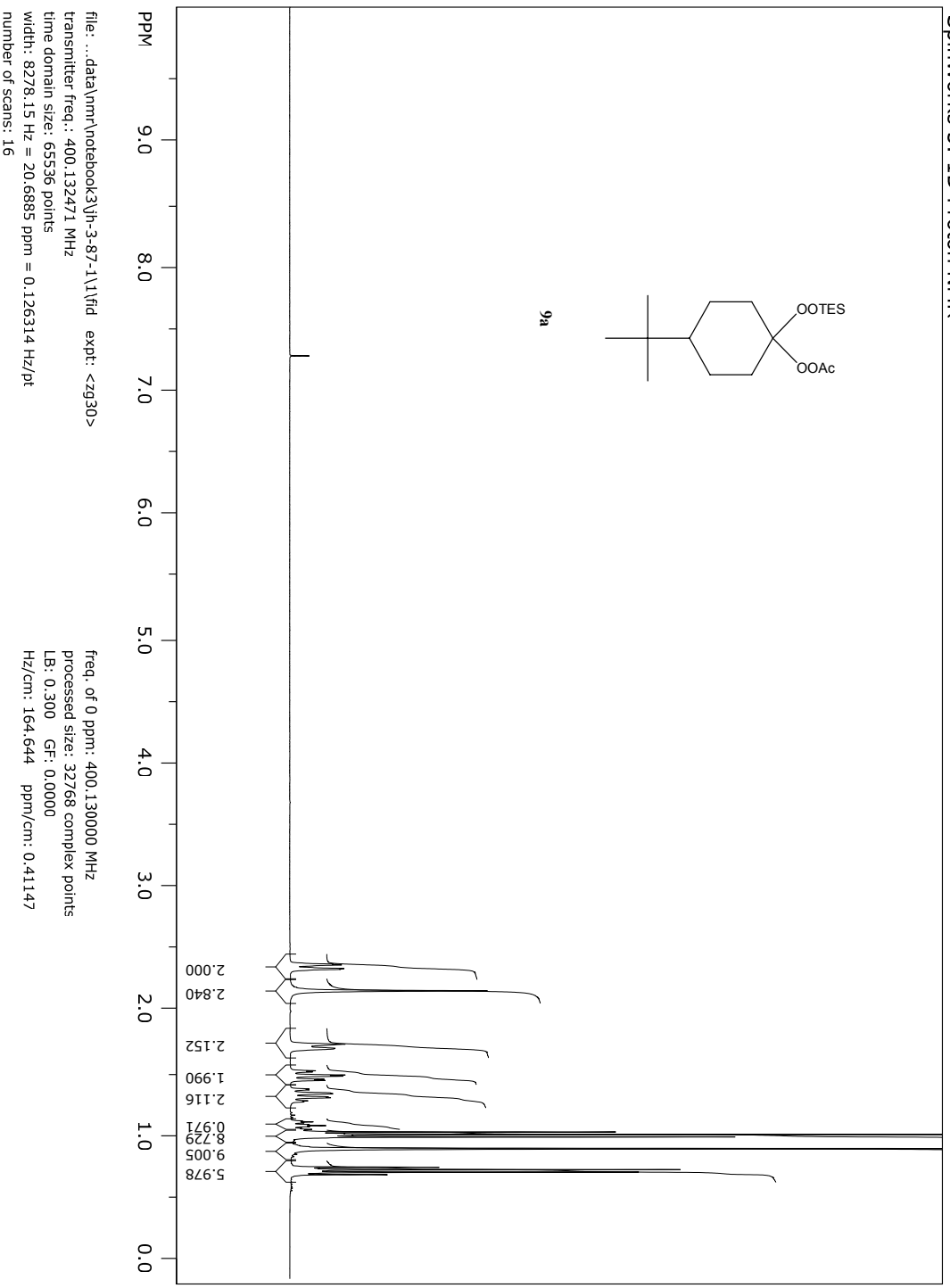
LB: 1.000 GF: 0.0000
Hz/cm: 959.233 ppm/cm: 9.53295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2.0
1.0
0.0
2.000
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2.116
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9.005
5.978
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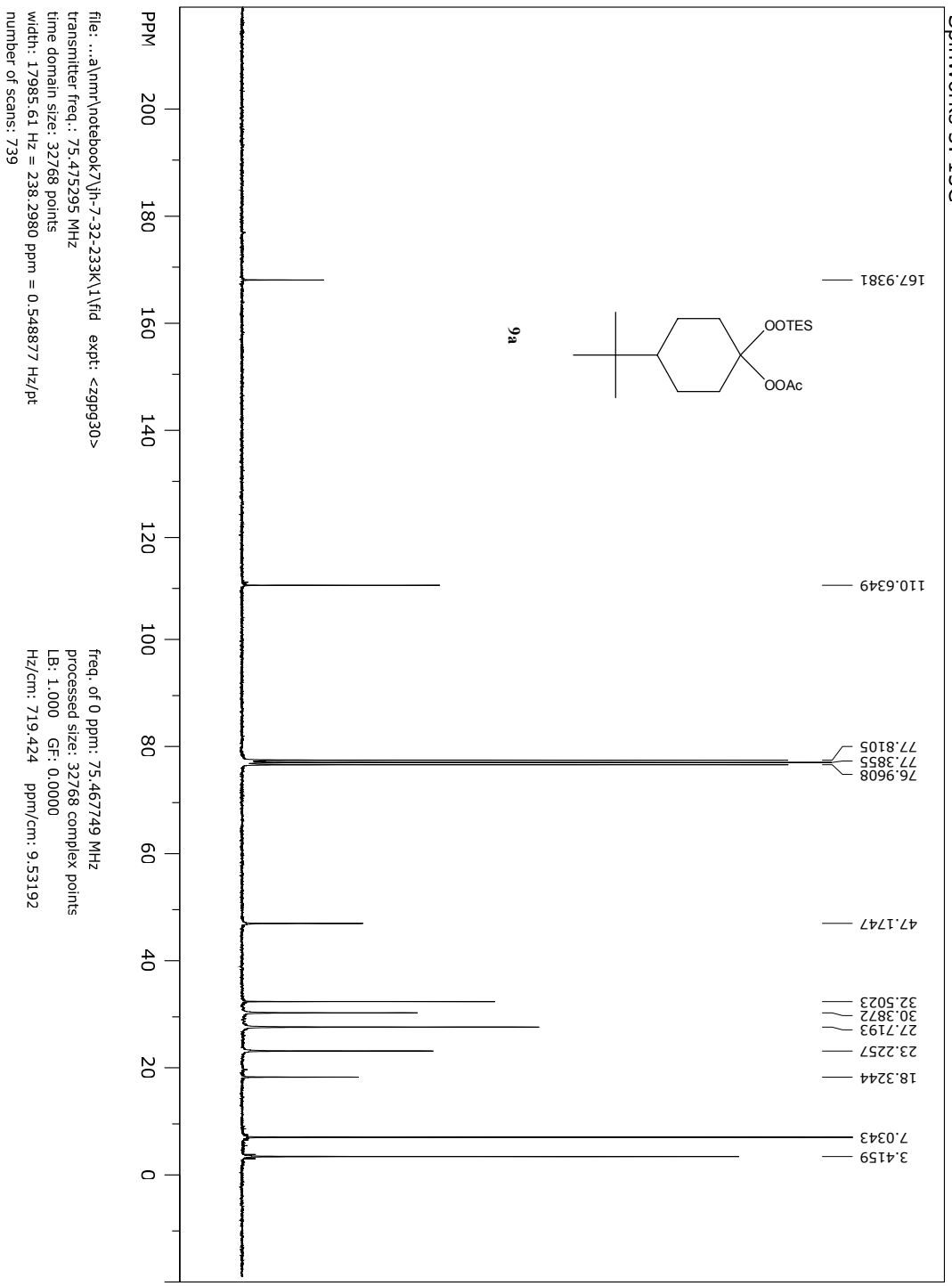
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77.3855
76.9608
47.1747
32.5023
30.3872
27.7193
23.2257
18.3244
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3.4159
9a
OOTES
OOAc
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time domain size: 32768 points
width: 17985.61 Hz = 238.2980 ppm = 0.548877 Hz/pt
number of scans: 739
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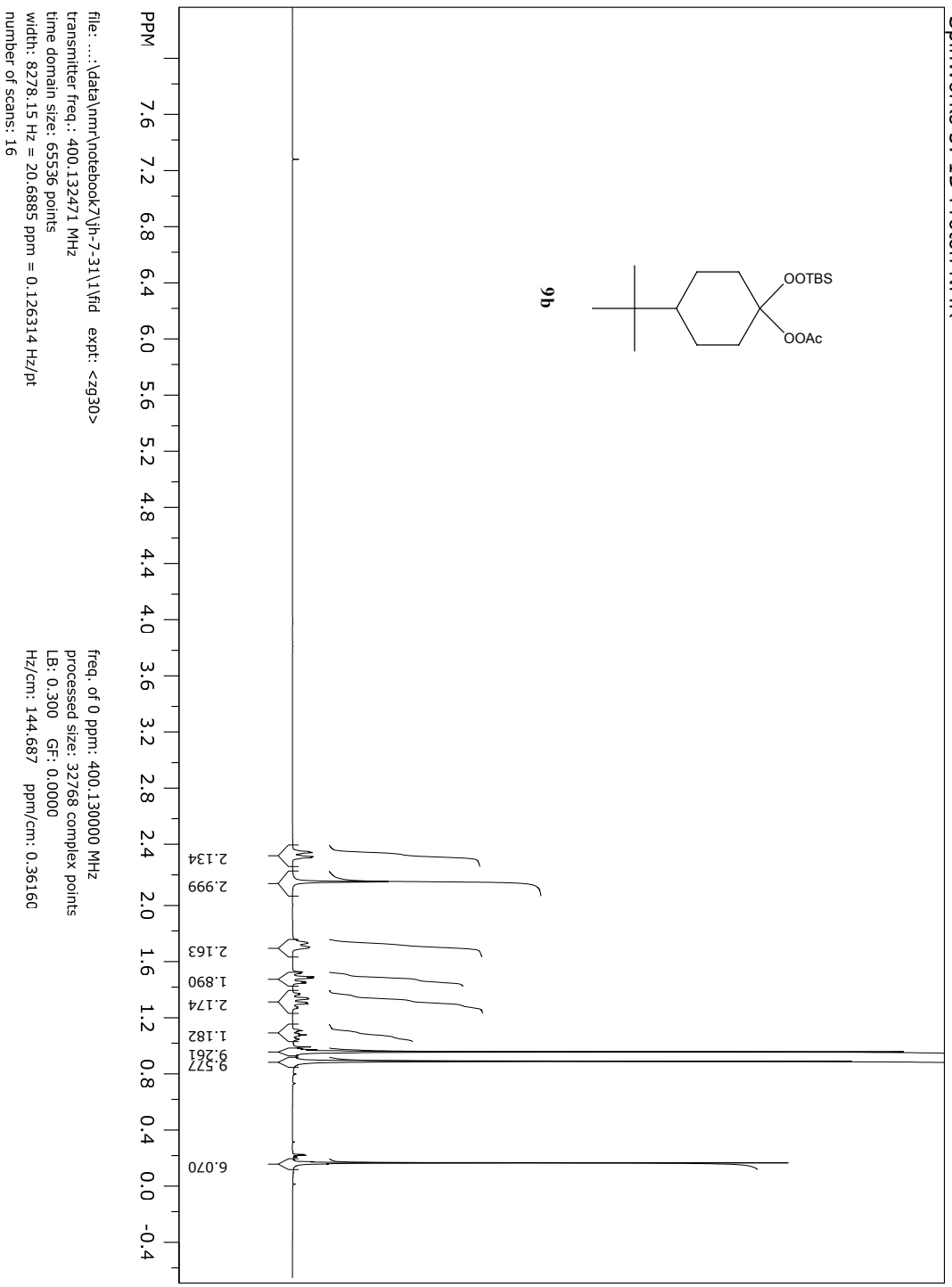
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 719.424 ppm/cm: 9.53192


SpinWorks 3: 1D Proton NMR
OOTBS
OOAc
9b
PPM
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
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6.070
9.577
9.261
1.182
2.174
1.890
2.163
2.999
2.134
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time domain size: 65536 points
width: 8278.15 Hz = 20.6885 ppm = 0.126314 Hz/pt
number of scans: 16
freq. of 0 ppm: 400.130000 MHz
processed size: 32768 complex points
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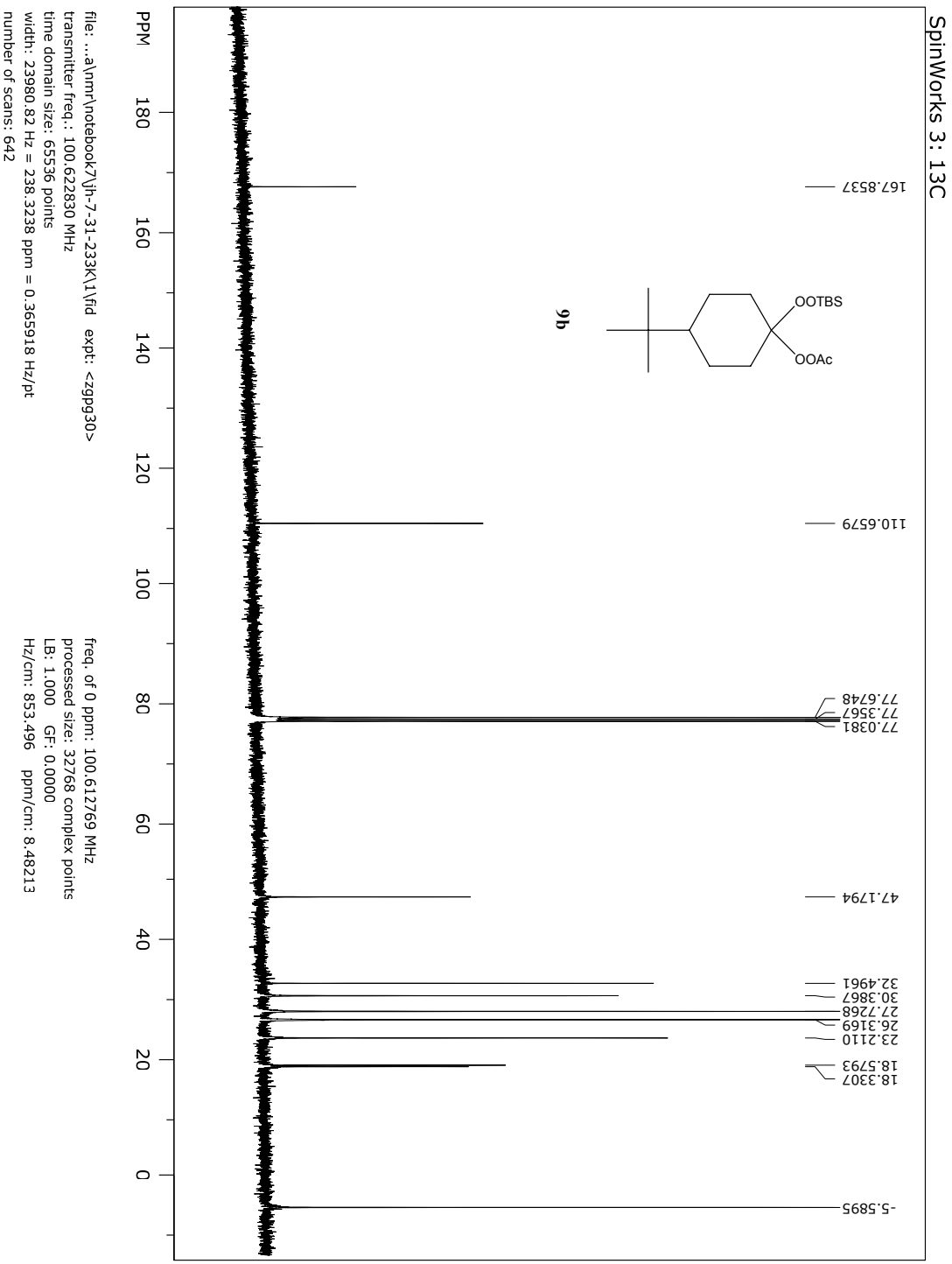
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PPM
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160
140
120
100
80
60
40
20
0
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110.6579
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77.3567
77.6748
47.1794
32.4961
30.3867
27.7268
26.3169
23.2110
18.5793
18.3307
-5.5895
9b
OOTBS
OOAc
file: ...a\nmr\notebook7\jh-7-31-233K\1\fid expt: <zgpg30>
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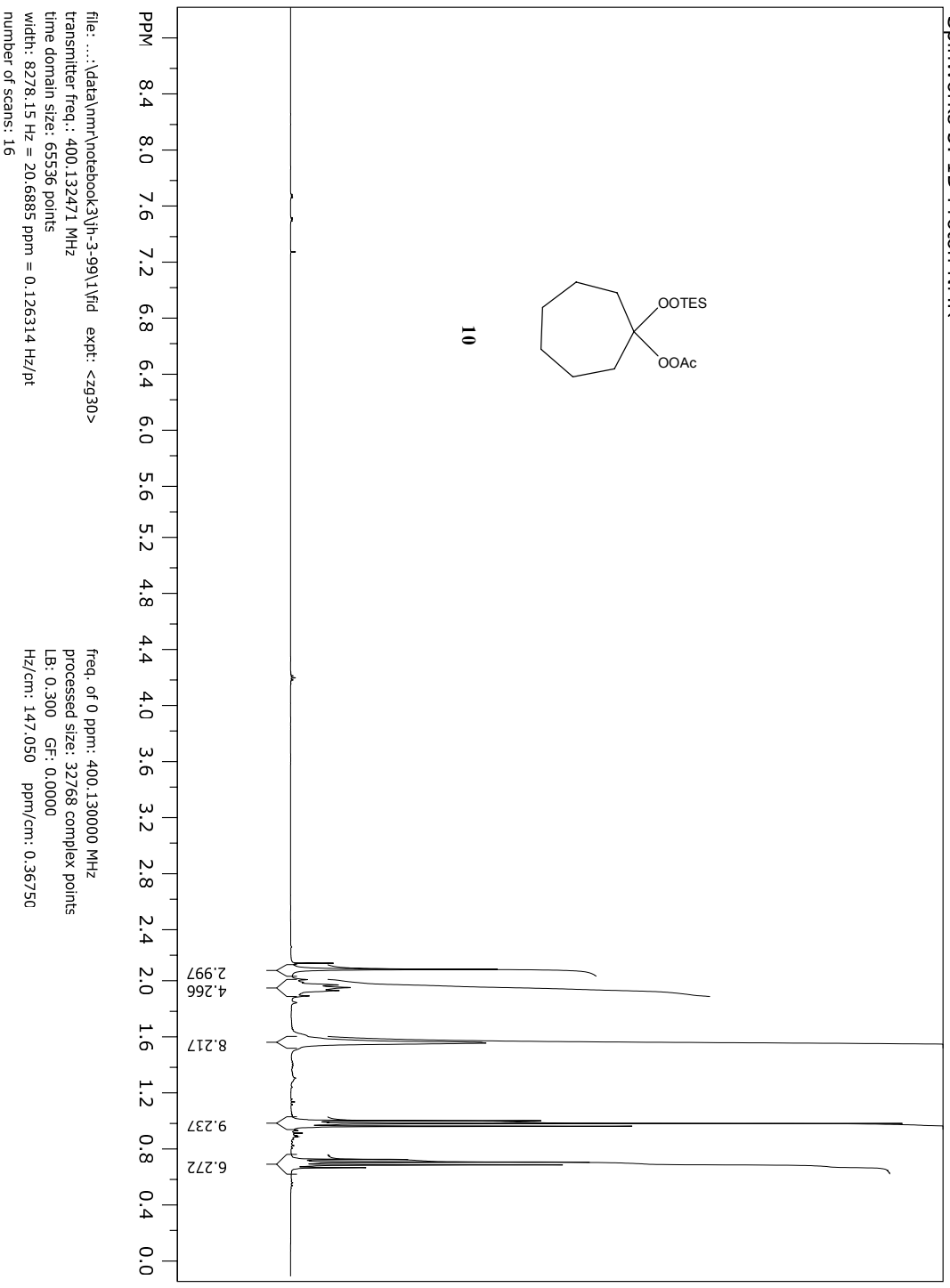
time domain size: 65536 points
width: 23980.82 Hz = 238.3238 ppm = 0.365918 Hz/pt
number of scans: 642
freq. of 0 ppm: 100.612769 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 853.496 ppm/cm: 8.48213


SpinWorks 3: 1D Proton NMR
10
OOTES
OOAc
6.272
9.237
8.217
4.266
2.997
PPM 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0
file: ...\data\nmr\notebook3\jh-3-99\1\fid expt: <zg30>
transmitter freq.: 400.132471 MHz
time domain size: 65536 points
width: 8278.15 Hz = 20.6885 ppm = 0.126314 Hz/pt
number of scans: 16
freq. of 0 ppm: 400.130000 MHz
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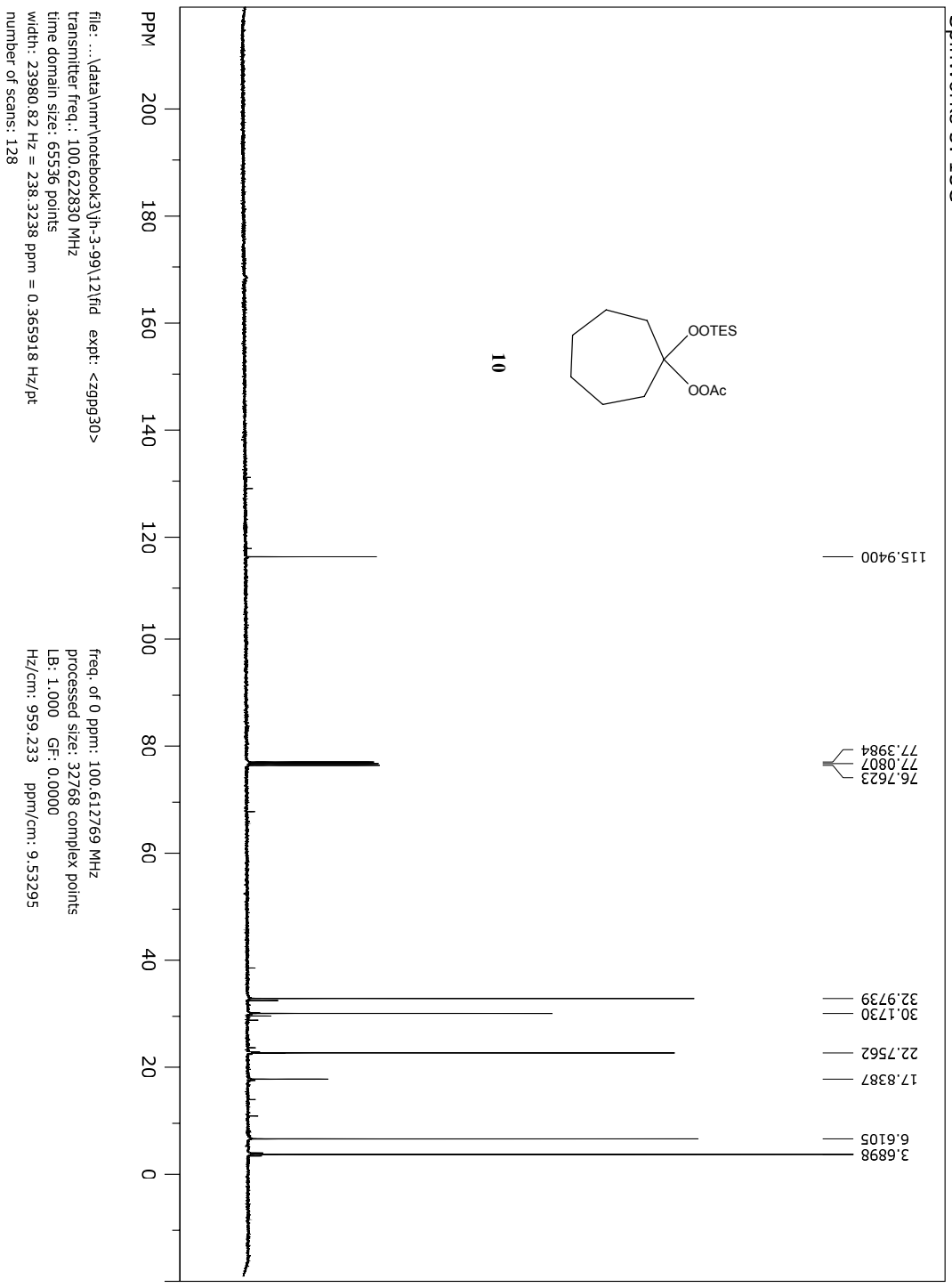
Hz/cm: 147.050 ppm/cm: 0.36750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OOAc
115.9400
76.7623
77.0807
77.3984
32.9739
30.1730
22.7562
17.8387
6.6105
3.6898
PPM
200
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140
120
100
80
60
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20
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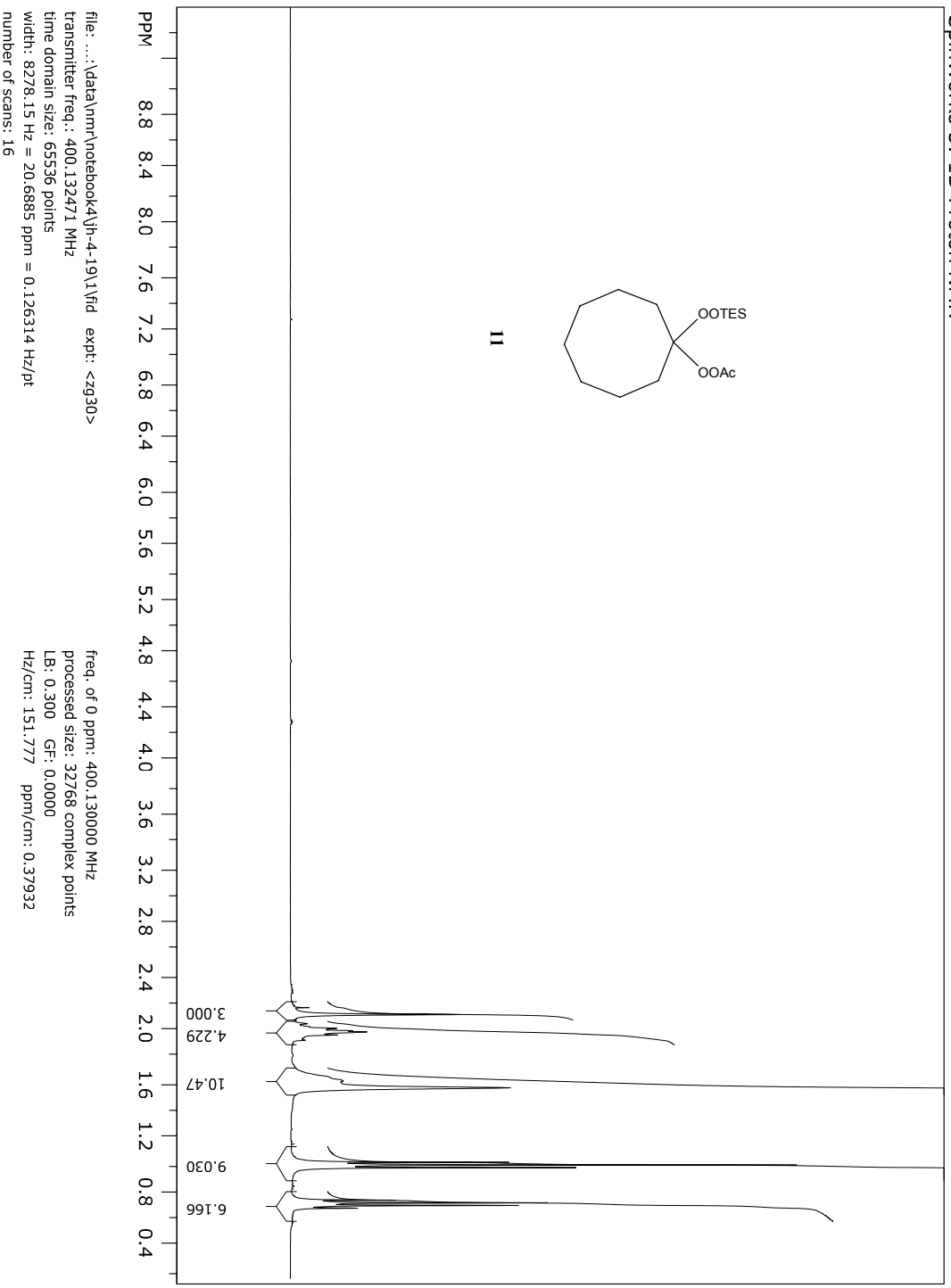
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 959.233 ppm/cm: 9.53295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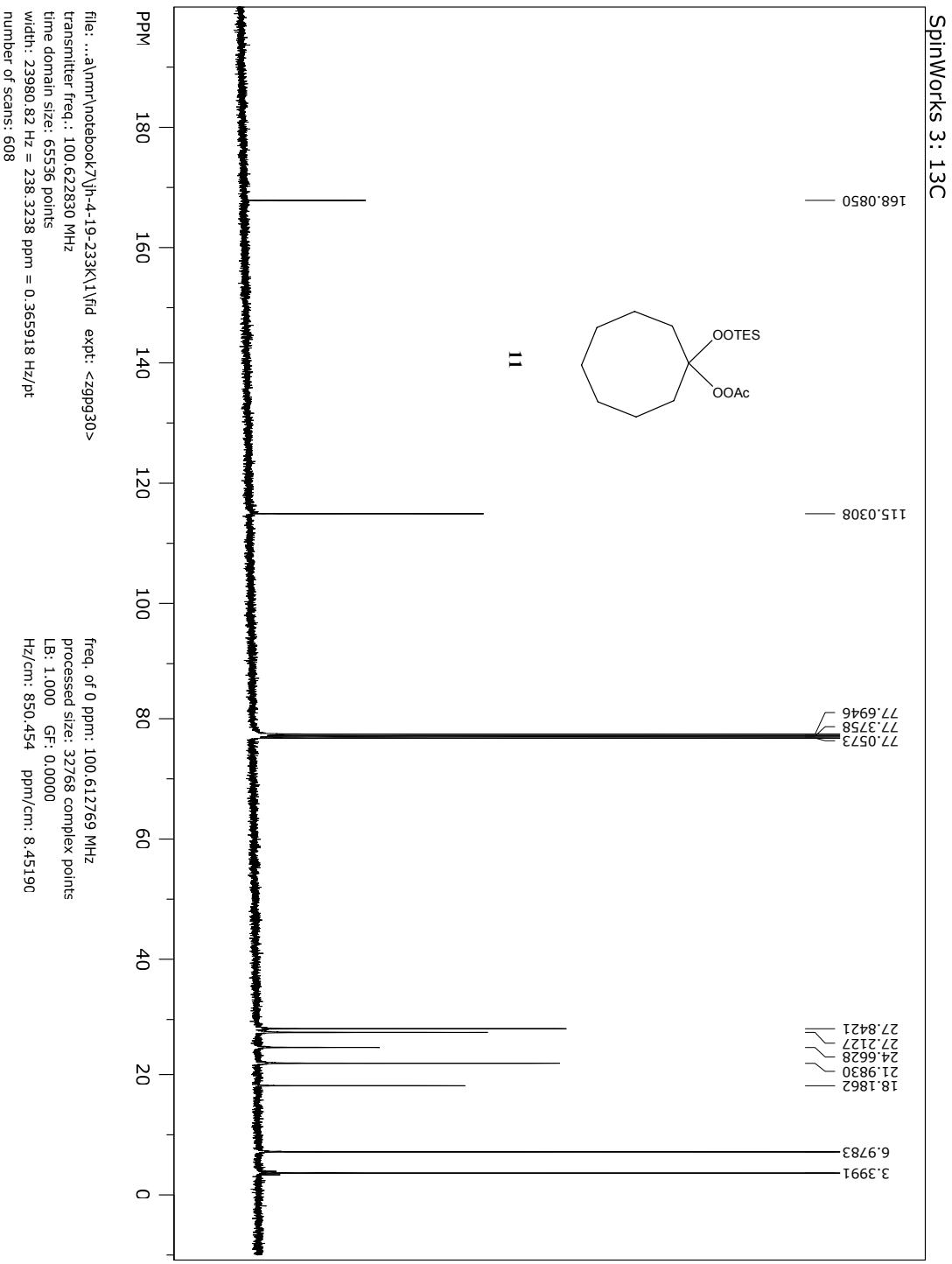
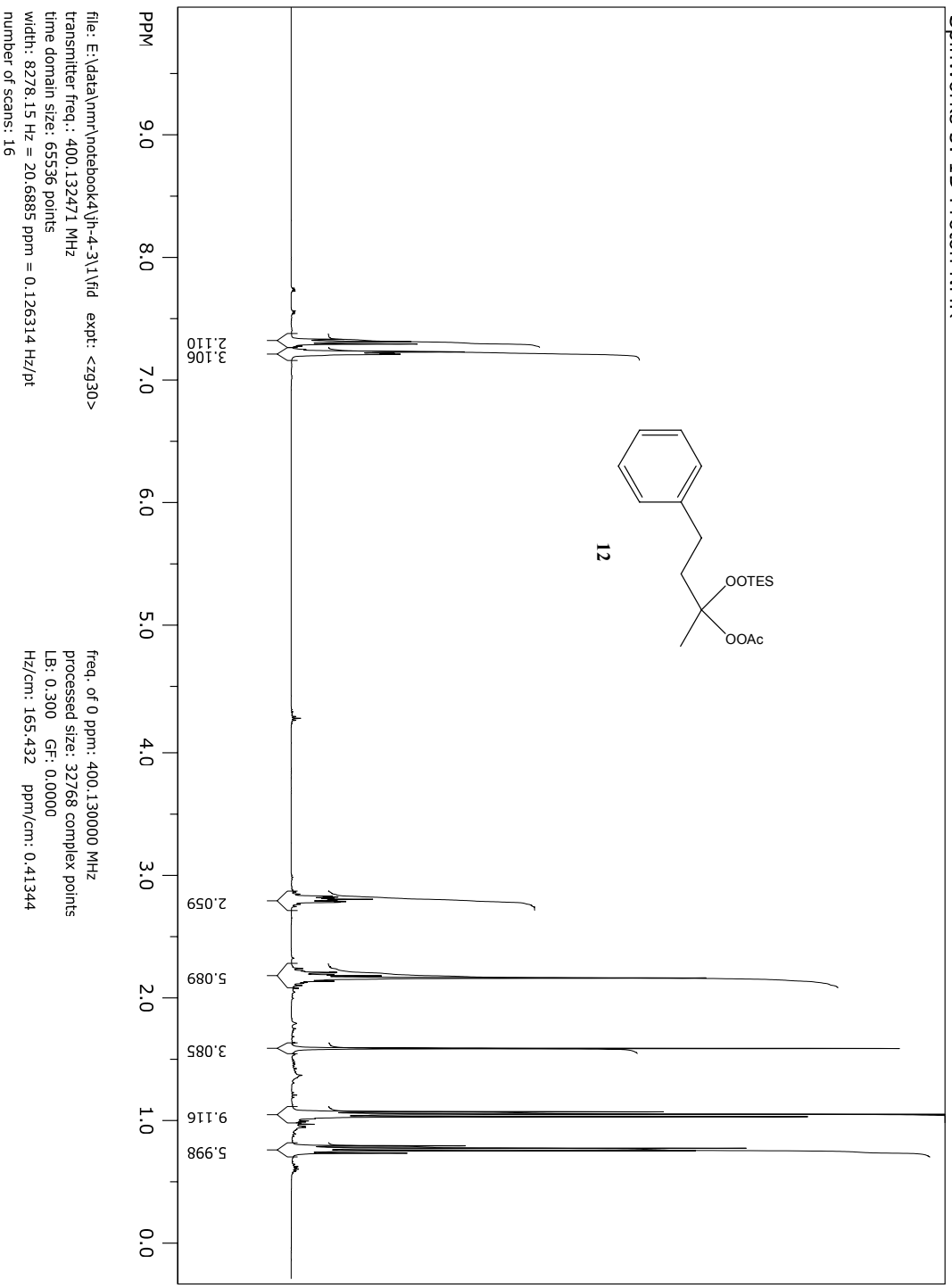
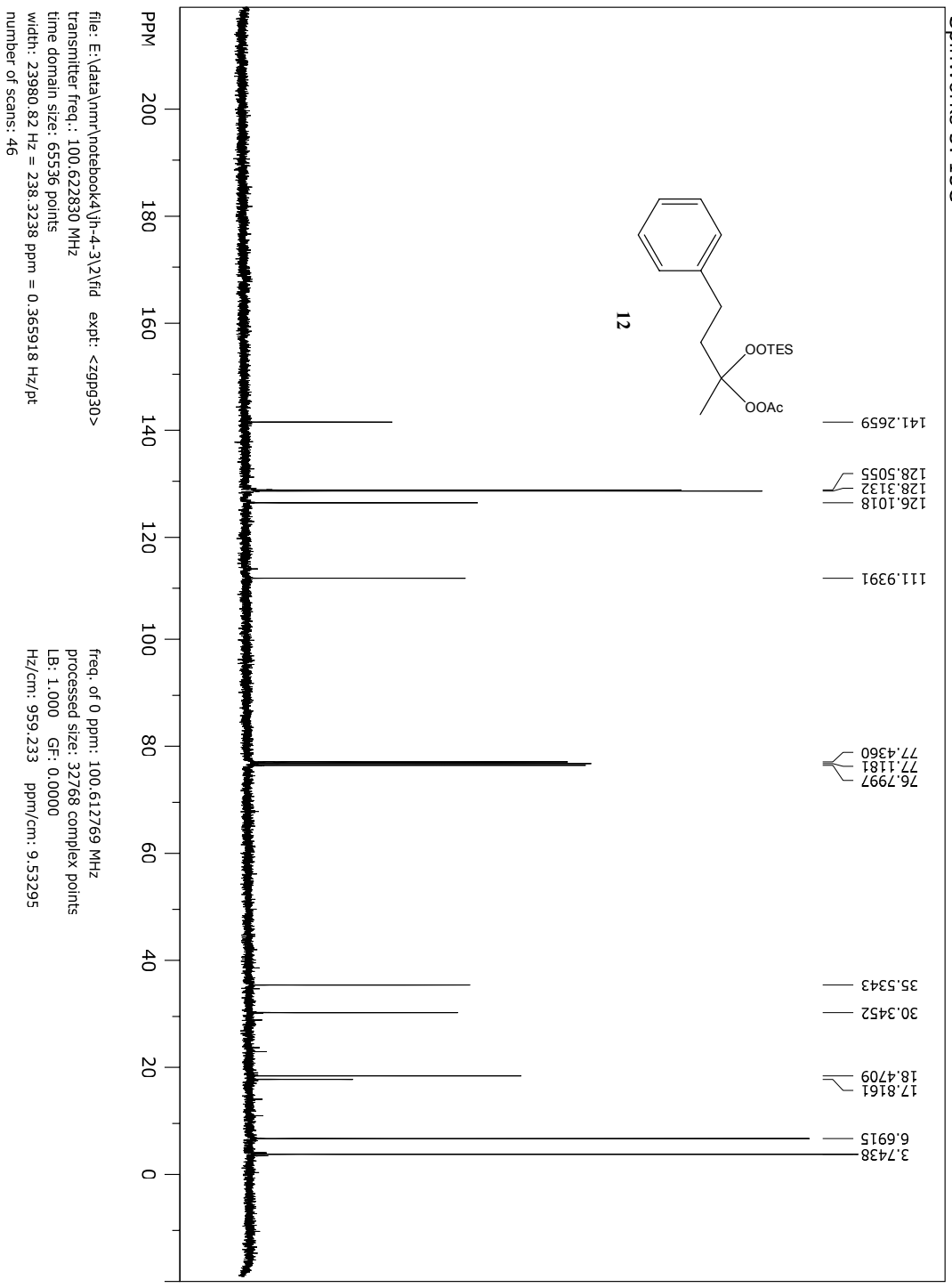
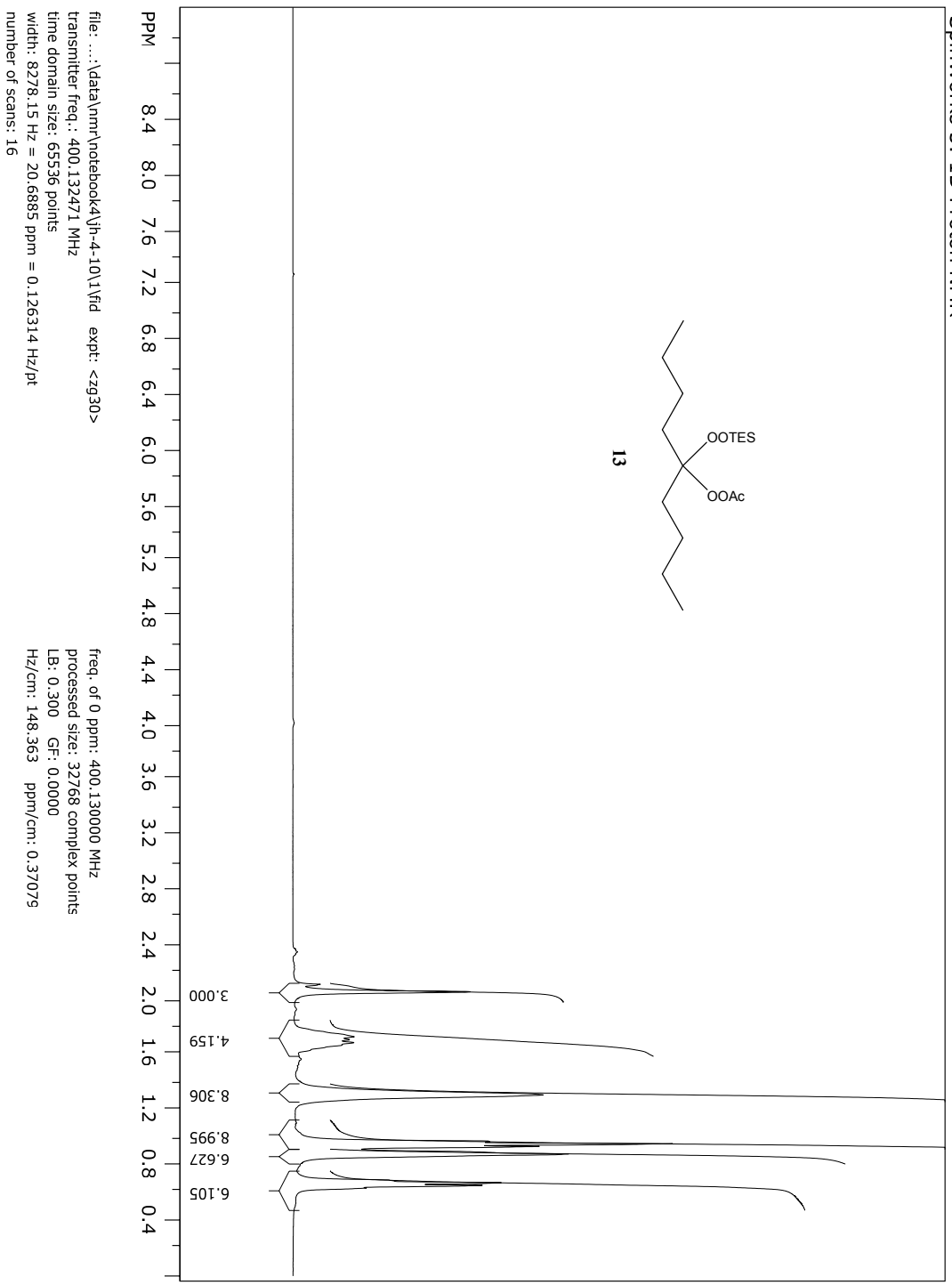
OOTES
OOAc
11
PPM
8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4
3.000
4.229
10.47
9.030
6.166
file: ...\data\nmr\notebook4\jh-4-19\1\fid expt: <zg30>
transmitter freq.: 400.132471 MHz
time domain size: 65536 points
width: 8278.15 Hz = 20.6885 ppm = 0.126314 Hz/pt
number of scans: 16
freq. of 0 ppm: 400.130000 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 151.777 ppm/cm: 0.37932

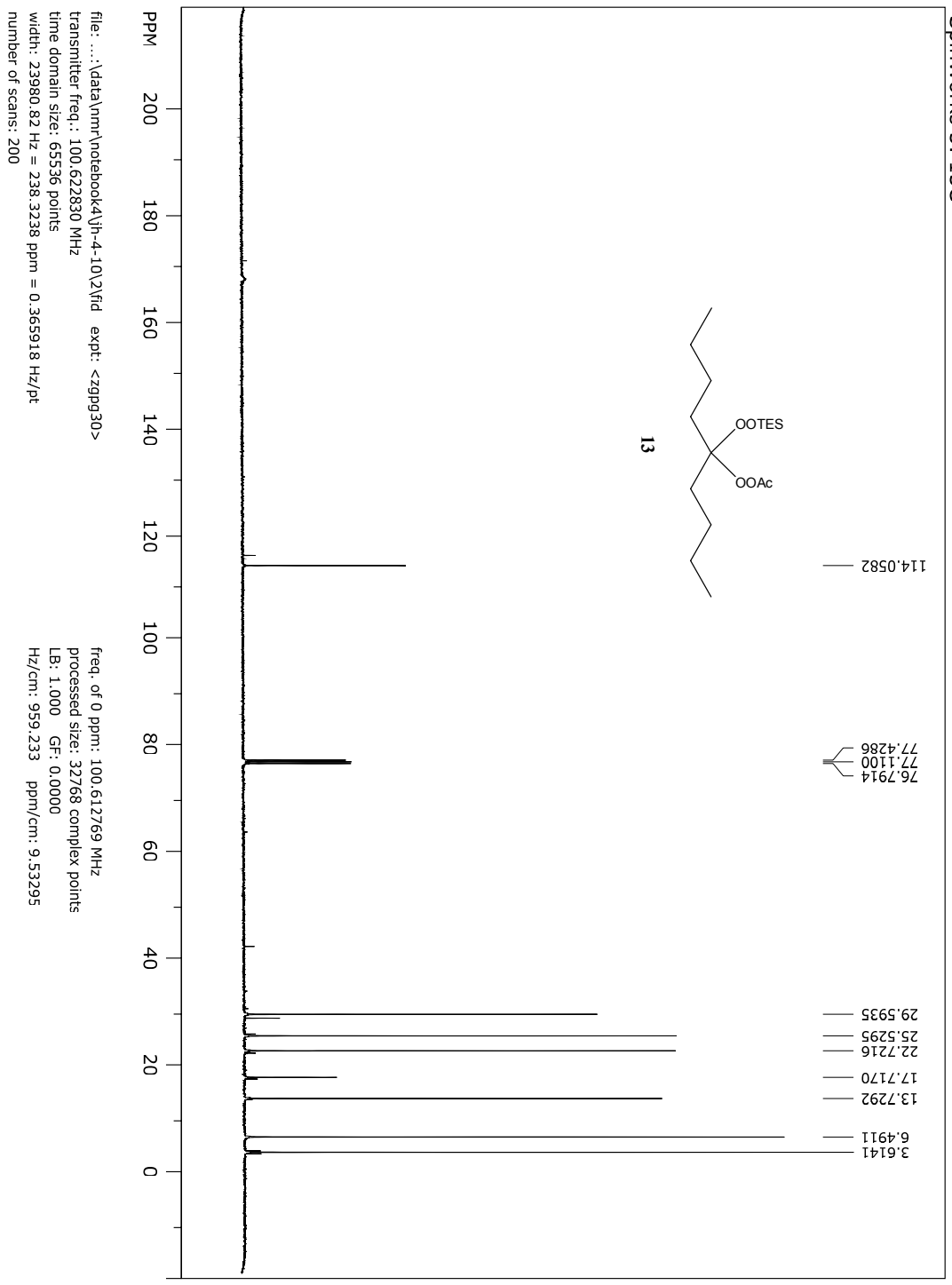
.

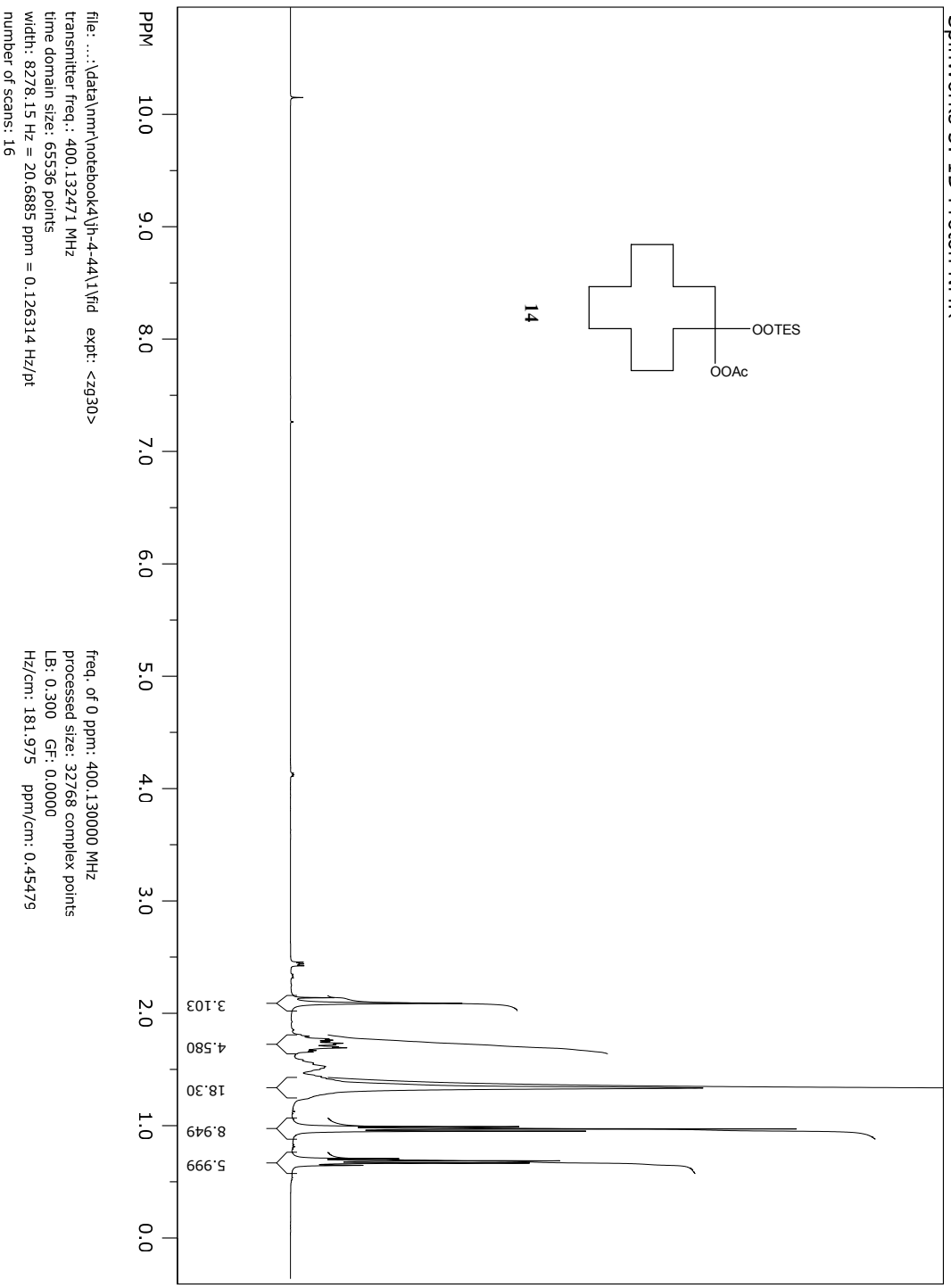

SpinWorks 3: 13C
11
OOTES
OOAc
168.0850
115.0308
77.0573
77.3758
77.6946
27.8421
27.2127
24.6628
21.9830
18.1862
6.9783
3.3991
PPM
0
20
40
60
80
100
120
140
160
180
file: ...a\nmr\notebook7\jh-4-19-233K\1\fid expt: <zgpg30>
transmitter freq.: 100.622830 MHz
time domain size: 65536 points
width: 23980.82 Hz = 238.3238 ppm = 0.365918 Hz/pt
number of scans: 608
freq. of 0 ppm: 100.612769 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 850.454 ppm/cm: 8.45190

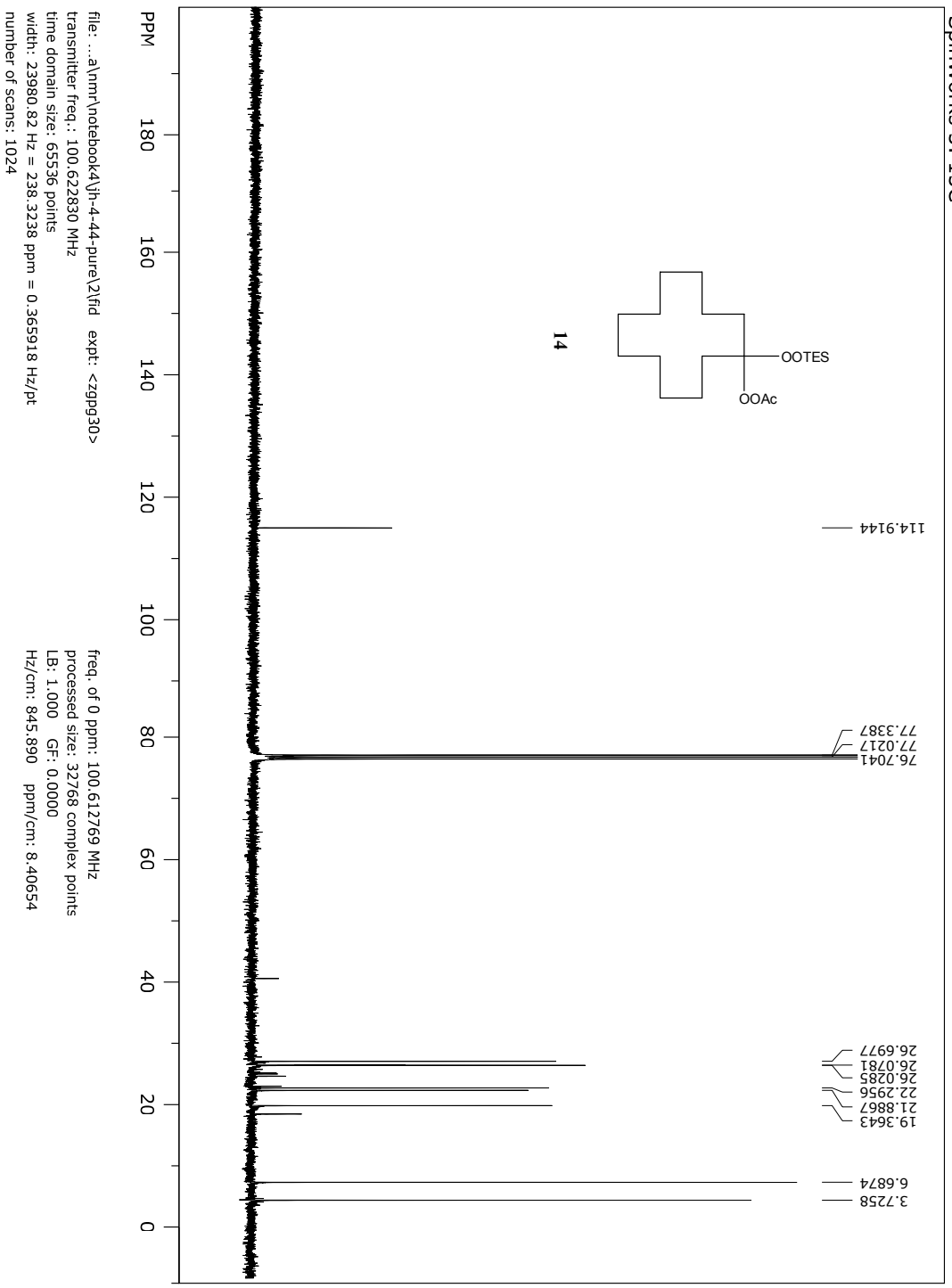

SpinWorks 3: 1D Proton NMR
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
3.106
2.110
2.059
5.089
3.085
9.116
5.998
12
OOTES
OOAc
file: E:\data\nmr\notebook4\jh-4-3\1\fid expt: <zg30>
transmitter freq.: 400.132471 MHz
time domain size: 65536 points
width: 8278.15 Hz = 20.6885 ppm = 0.126314 Hz/pt
number of scans: 16
freq. of 0 ppm: 400.130000 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 165.432 ppm/cm: 0.41344

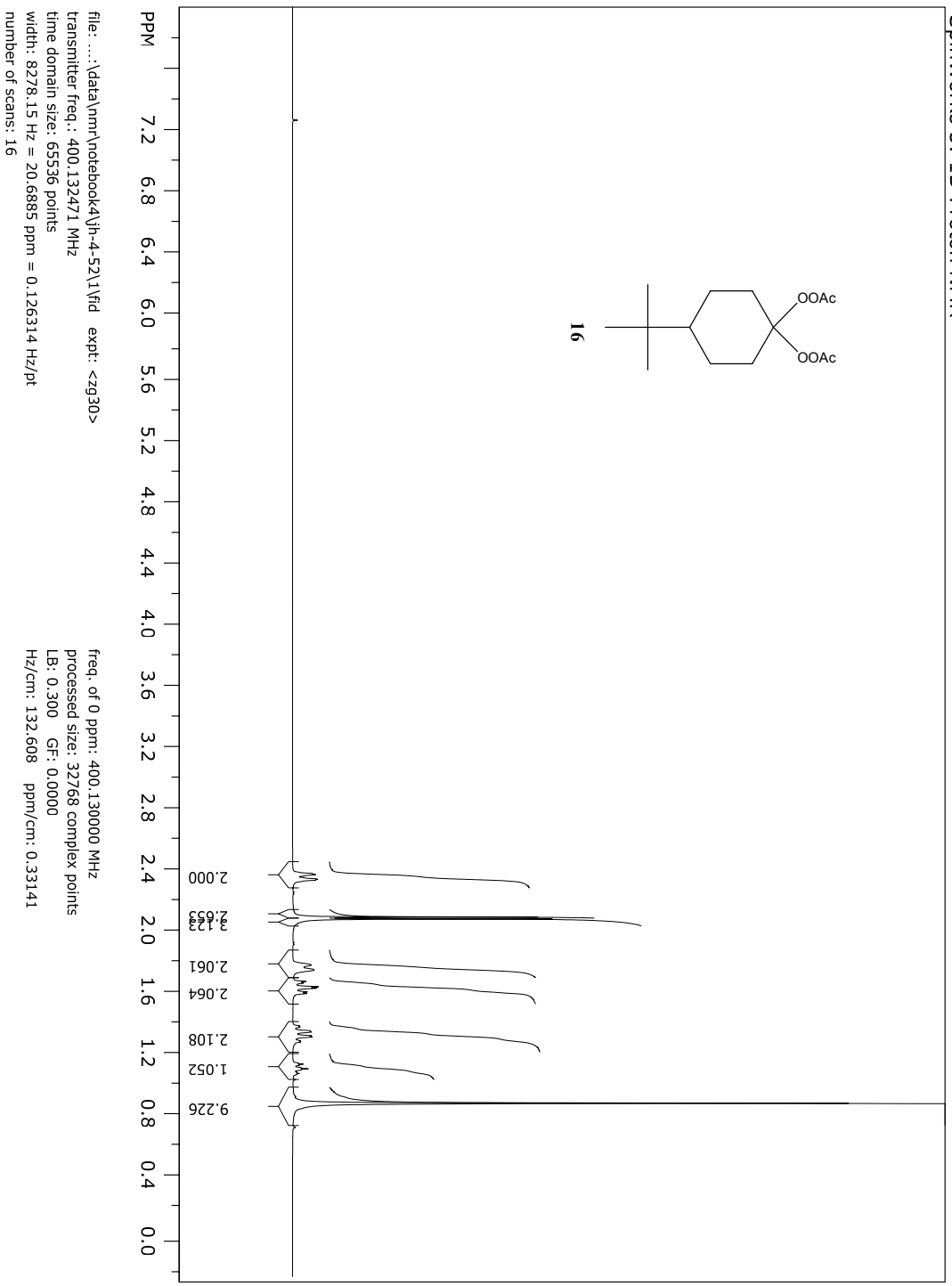

SpinWorks 3: 13C
file: E:\data\nmr\notebook4\jh-4-3\2\fid expt: <zgpg30>
transmitter freq.: 100.622830 MHz
time domain size: 65536 points
width: 23980.82 Hz = 238.3238 ppm = 0.365918 Hz/pt
number of scans: 46
freq. of 0 ppm: 100.612769 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 959.233 ppm/cm: 9.53295
PPM
200
180
160
140
120
100
80
60
40
20
0
12
OOTES
OOAc
141.2659
128.5055
128.3132
126.1018
111.9391
76.7997
77.1181
77.4360
35.5343
30.3452
18.4709
17.8161
6.6915
3.7438


SpinWorks 3: 1D Proton NMR
OOTES
OOAc
13
3.000
4.159
8.306
8.995
6.627
6.105
PPM
8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4
file: ...\data\nmr\notebook4\jh-4-10\1\fid expt: <zg30>
transmitter freq.: 400.132471 MHz
time domain size: 65536 points
width: 8278.15 Hz = 20.6885 ppm = 0.126314 Hz/pt
number of scans: 16
freq. of 0 ppm: 400.130000 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 148.363 ppm/cm: 0.37079


SpinWorks 3: 13C
13
OOTES
OOAc
114.0582
76.7914
77.1100
77.4286
29.5935
25.5295
22.7216
17.7170
13.7292
6.4911
3.6141
PPM
200
180
160
140
120
100
80
60
40
20
0
file: ...\data\nmr\notebook4\jh-4-10\2\fid expt: <zgpg30>
transmitter freq.: 100.622830 MHz
time domain size: 65536 points
width: 23980.82 Hz = 238.3238 ppm = 0.365918 Hz/pt
number of scans: 200
freq. of 0 ppm: 100.612769 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 959.233 ppm/cm: 9.53295


SpinWorks 3: 1D Proton NMR
14
OOTES
OOAc
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
3.103
4.580
18.30
8.949
5.999
file: ...\data\nmr\notebook4\jh-4-44\1\fid expt: <zg30>
transmitter freq.: 400.132471 MHz
time domain size: 65536 points
width: 8278.15 Hz = 20.6885 ppm = 0.126314 Hz/pt
number of scans: 16
freq. of 0 ppm: 400.130000 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 181.975 ppm/cm: 0.45479


SpinWorks 3: 13C
14
OOTES
OOAc
114.9144
76.7041
77.0217
77.3387
26.6977
26.0781
26.0285
22.2956
21.8867
19.3643
6.6874
3.7258
PPM
0
20
40
60
80
100
120
140
160
180
file: ...a\nmr\notebook4\jh-4-44-pure\2\fid expt: <zgpg30>
transmitter freq.: 100.622830 MHz
time domain size: 65536 points
width: 23980.82 Hz = 238.3238 ppm = 0.365918 Hz/pt
number of scans: 1024
freq. of 0 ppm: 100.612769 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 845.890 ppm/cm: 8.40654


SpinWorks 3: 1D Proton NMR
OOAc
OOAc
16
PPM
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
2.000
2.653
2.123
2.061
2.064
2.108
1.052
9.226
file: ...\data\nmr\notebook4\jh-4-52\1\fid expt: <zg30>
transmitter freq.: 400.132471 MHz
time domain size: 65536 points
width: 8278.15 Hz = 20.6885 ppm = 0.126314 Hz/pt
number of scans: 16
freq. of 0 ppm: 400.130000 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 132.608 ppm/cm: 0.33141

.

SpinWorks 3: 13C
file: ...nmr\notebook4\jh-4-52-carbon\2\fid expt: <zgpg30>
transmitter freq.: 100.622830 MHz
time domain size: 65536 points
width: 23980.82 Hz = 238.3238 ppm = 0.365918 Hz/pt
number of scans: 265
freq. of 0 ppm: 100.612769 MHz
processed size: 32768 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 881.642 ppm/cm: 8.76185
PPM
200
180
160
140
120
100
80
60
40
20
0
167.4831
167.3791
111.5112
76.8008
77.1197
77.4387
47.0530
32.2313
30.1073
27.4833
23.1630
17.4311
17.5471
OOAc
OOAc

16