Supporting Information

Regio- and Stereoselective Mono-Epoxidation of Dienes using Methyltrioxorhenium: Synthesis of Allylic Epoxides

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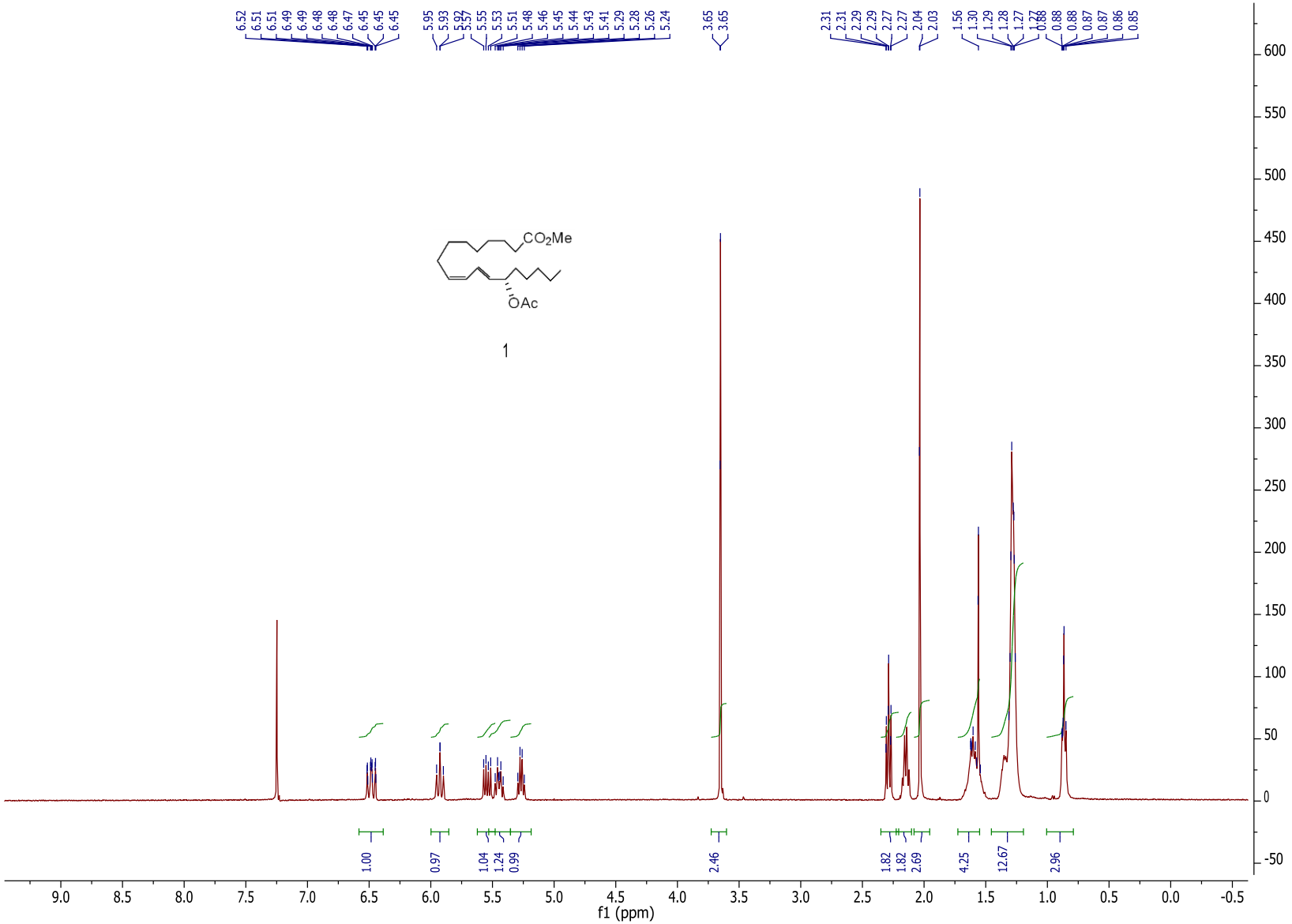
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5.93
5.92
5.57
5.55
5.53
5.51
5.48
5.46
5.45
5.44
5.43
5.41
5.29
5.28
5.26
5.24
3.65
3.65
2.31
2.31
2.29
2.29
2.27
2.27
2.04
2.03
1.56
1.30
1.29
1.28
1.27
0.88
0.88
0.87
0.87
0.86
0.85
CO2Me
OAc
1
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
1.00
0.97
1.04
1.24
0.99
2.46
1.82
1.82
2.69
4.25
12.67
2.96
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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2.5
2.0
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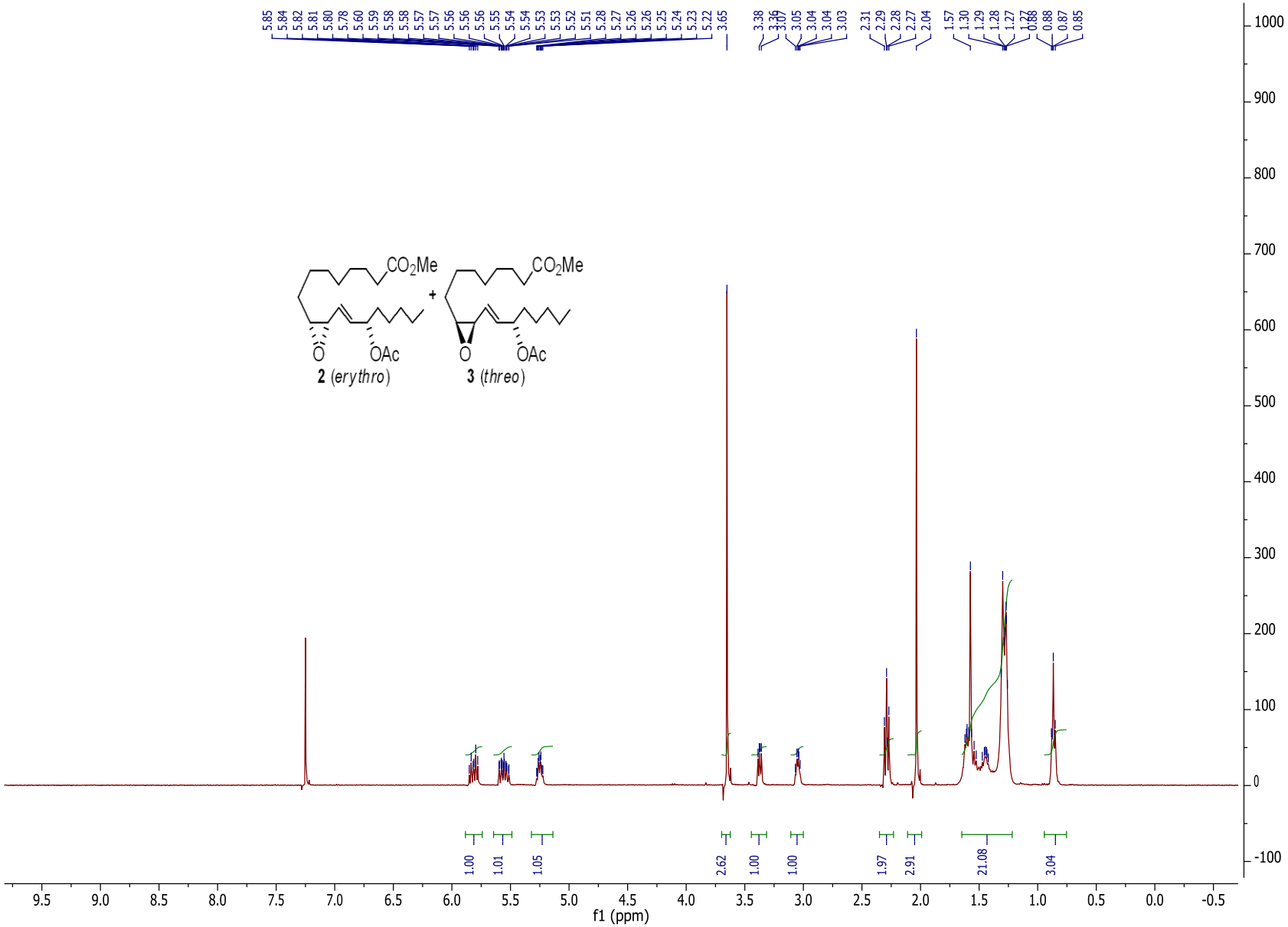
0.0
-0.5
f1 (ppm)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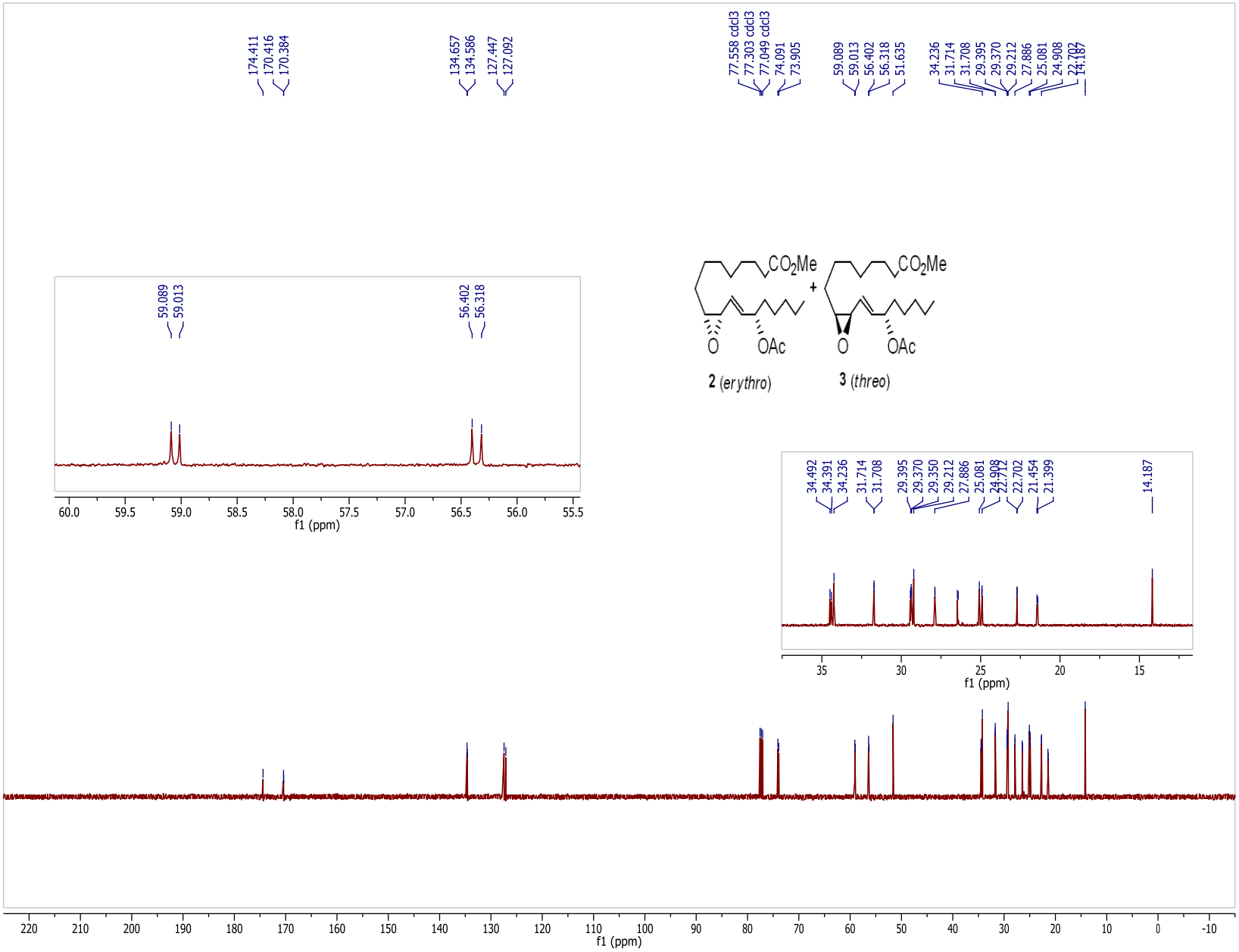
3.38 3.36 3.07 3.05 3.04 3.04 3.03
2.31 2.29 2.28 2.27 2.04
1.57 1.30 1.29 1.28 1.27 1.27 0.88 0.88 0.87 0.85
CO2Me
O
OAc
2 (erythro)
+
CO2Me
O
OAc
3 (threo)
1.00 1.01 1.05 2.62 1.00 1.00 1.97 2.91 21.08 3.04
f1 (ppm)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170.384
134.657
134.586
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127.092
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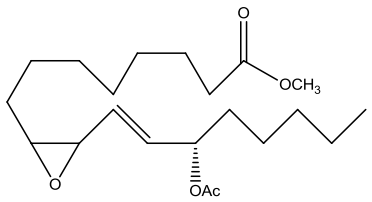
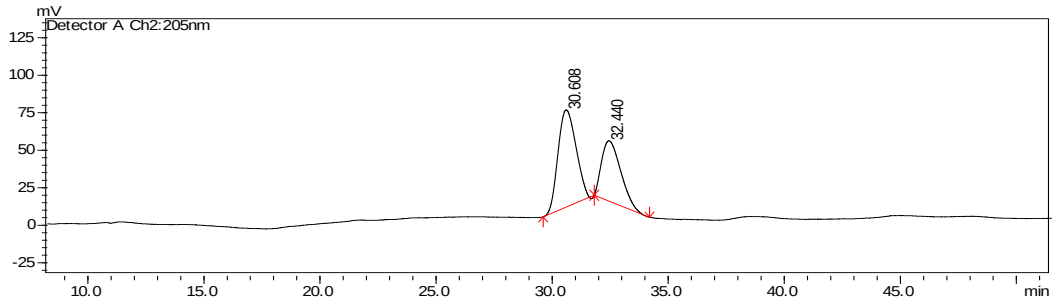
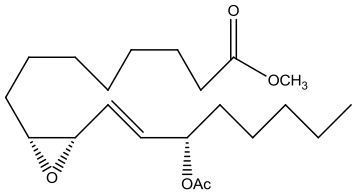
77.303 cdcl3
77.049 cdcl3
74.091
73.905
59.089
59.013
56.402
56.318
51.635
34.236
31.714
31.708
29.395
29.370
29.212
27.886
25.081
24.908
14.187
CO2Me
O
OAc
2 (erythro)
3 (threo)
f1 (ppm)

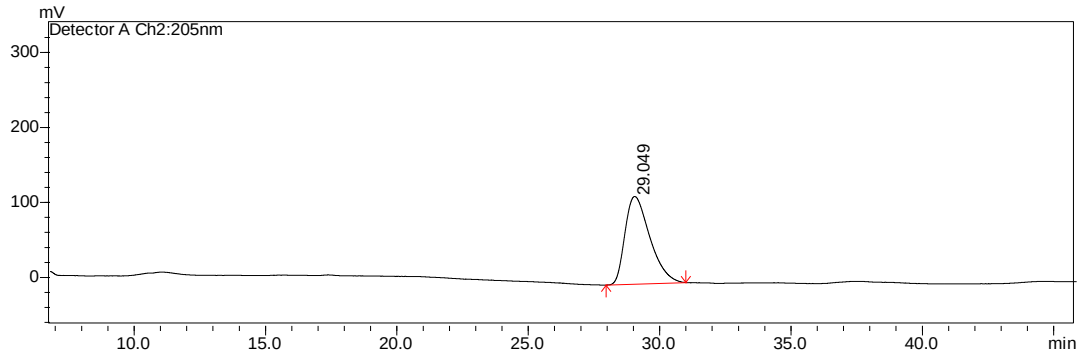




Peak	Ret. Time	Area	Height	Area %
1.	30.608	3568595	65420	58.429
2.	32.440	2539018	42270	41.571

CHIRALCEL OJ-H, 15 CM, 4.6MM, 2.7 MICRON, Hexane:IPA (99.8:0.2), 0.8 mL/min, 205.

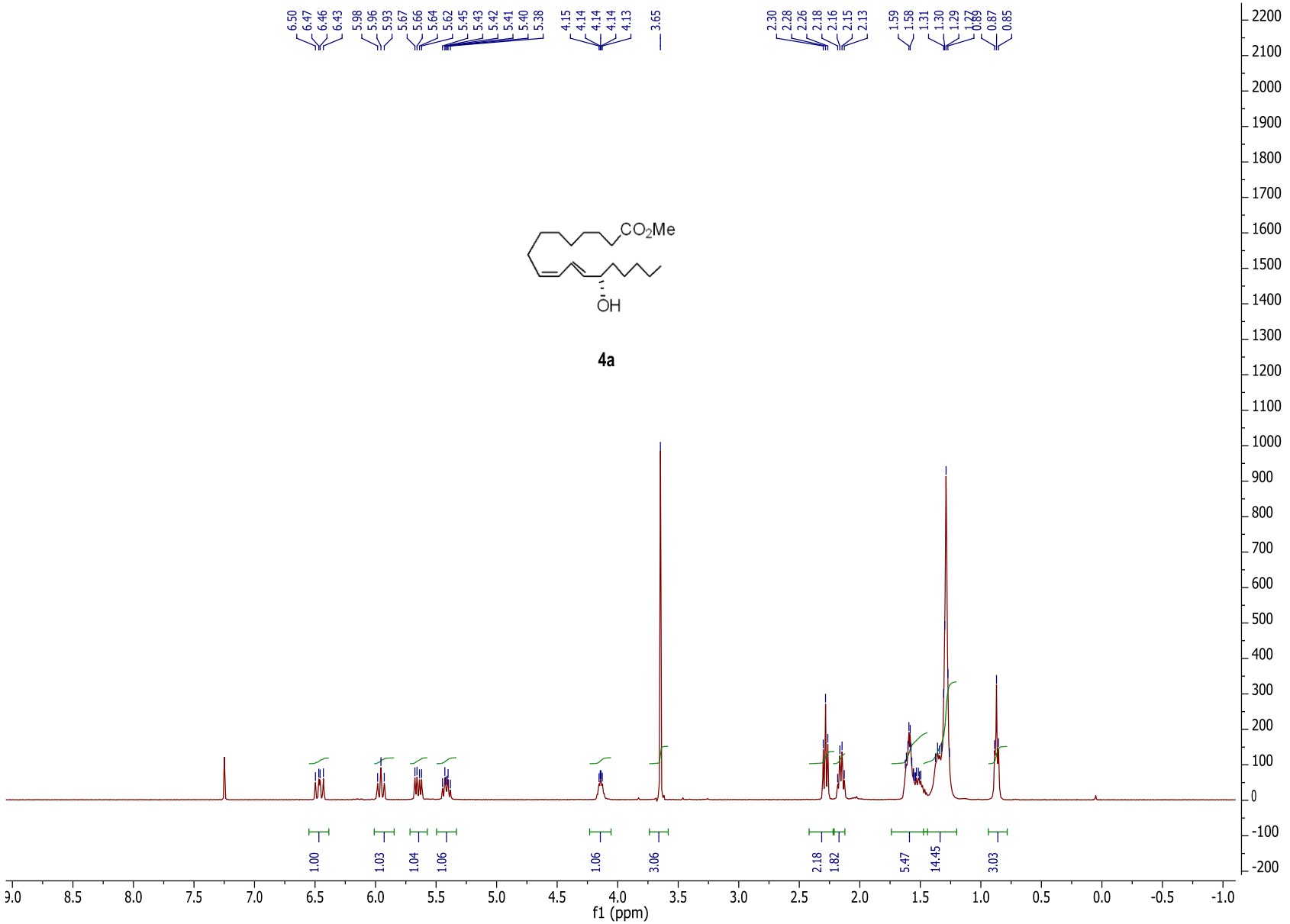




Peak	Ret. Time	Area	Height	Area %
1.	29.049	7725264	116942	100

CHIRALCEL OJ-H, 15 CM, 4.6MM, 2.7 MICRON, Hexane:IPA (99.8:0.2), 0.8 mL/min, 205.

Note: Compound obtained from chiral epoxidation as described in reference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5.66
5.64
5.62
5.45
5.43
5.42
5.41
5.40
5.38
4.15
4.14
4.14
4.14
4.13
3.65
2.30
2.28
2.26
2.18
2.16
2.15
2.13
1.59
1.58
1.31
1.30
1.29
0.89
0.87
0.85
CO2Me
OH
4a
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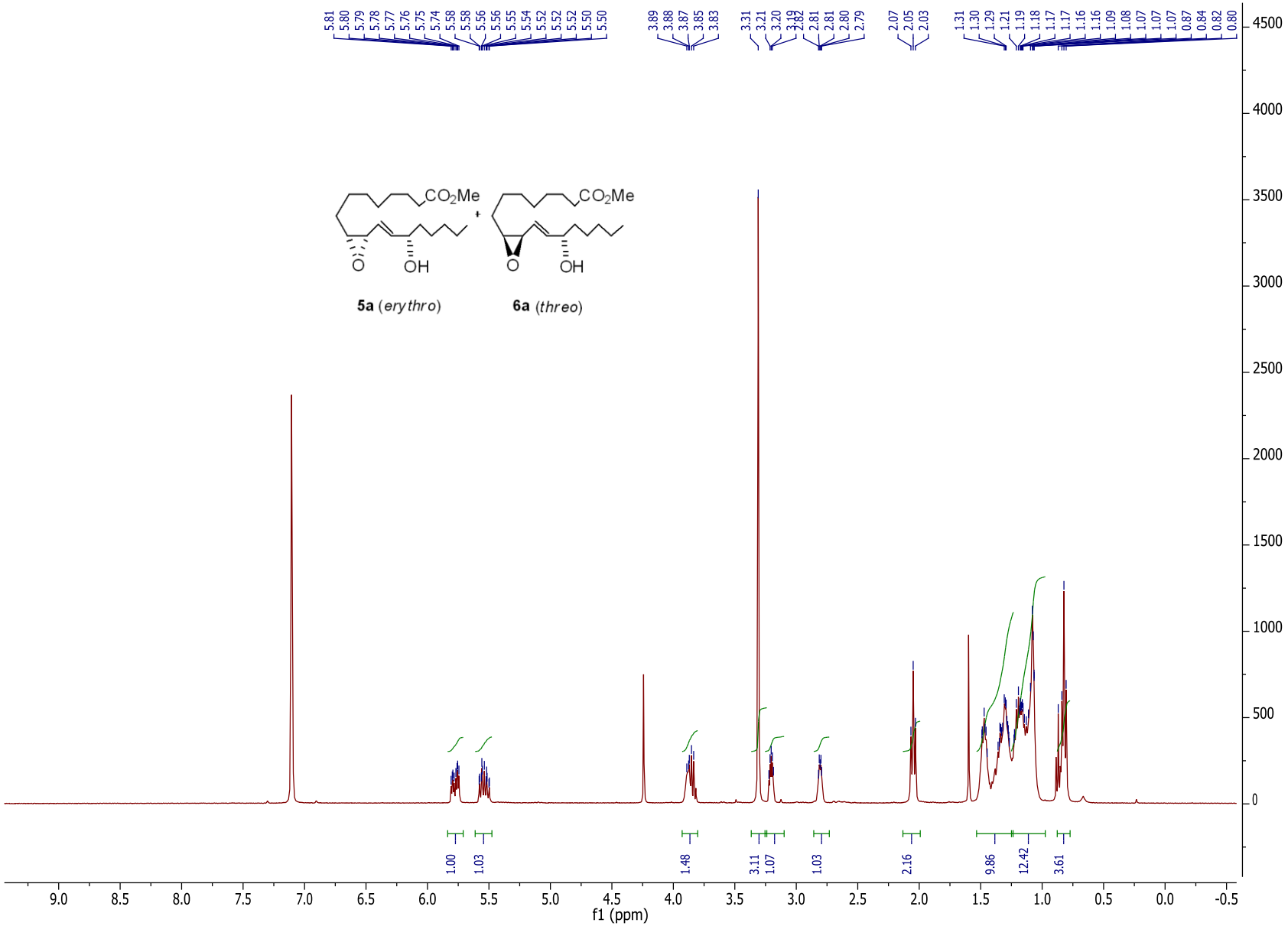
1.04
1.06
1.06
3.06
2.18
1.82
5.47
14.45
3.03
f1 (ppm)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5.58
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5.56
5.55
5.54
5.52
5.52
5.52
5.50
5.50
3.89
3.88
3.87
3.85
3.83
3.31
3.21
3.20
2.82
2.81
2.81
2.80
2.79
2.07
2.05
2.03
1.31
1.30
1.29
1.21
1.19
1.18
1.17
1.17
1.16
1.16
1.09
1.08
1.07
1.07
1.07
0.87
0.84
0.82
0.80
CO2Me
OH
O
CO2Me
OH
O
5a (erythro)
6a (threo)
4500
4000
3500
3000
2500
2000
1500
1000
500
0
1.00
1.03
1.48
3.11
1.07
1.03
2.16
9.86
12.42
3.61
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.0
1.5
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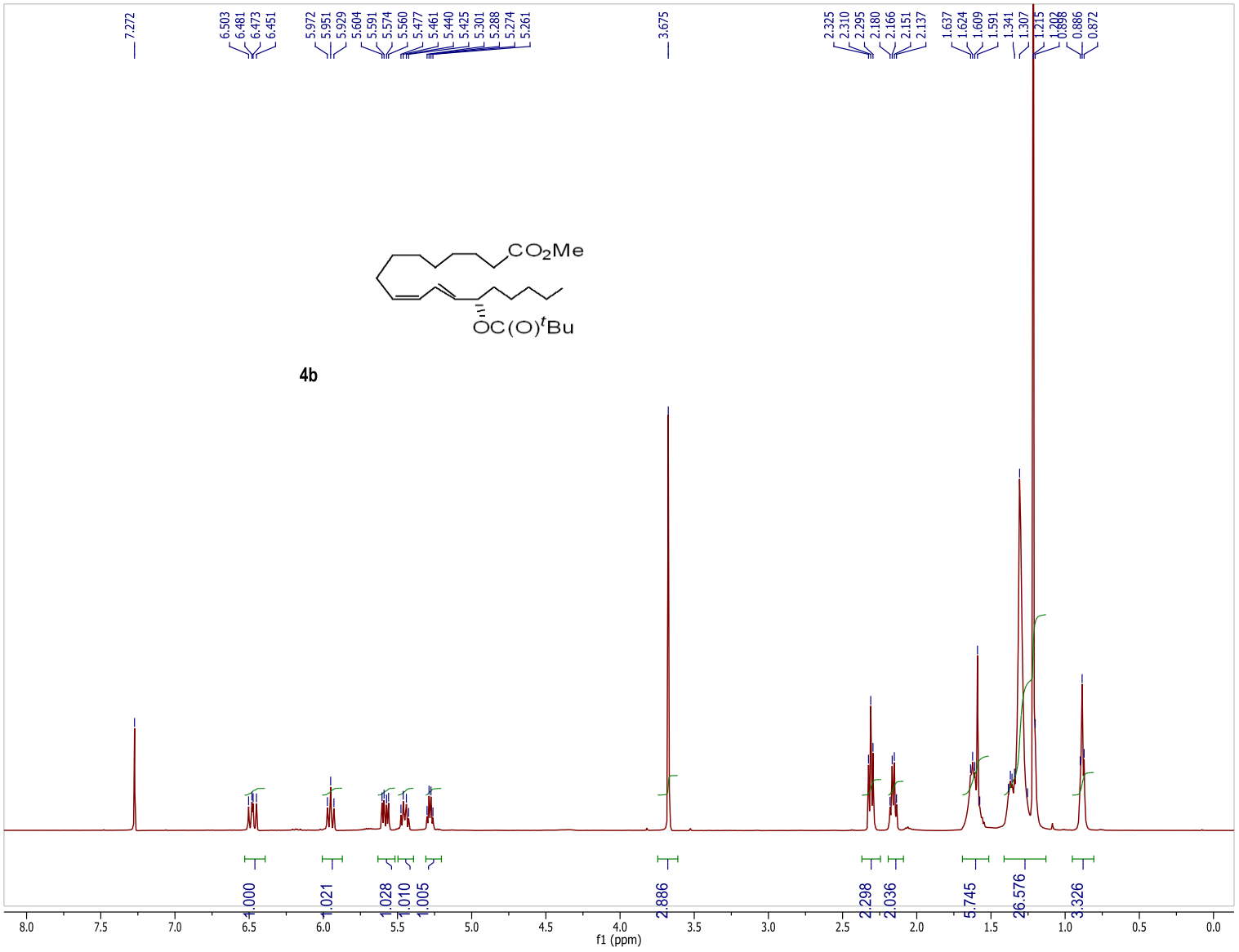
0.5
0.0
-0.5
f1 (ppm)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5.591
5.574
5.560
5.477
5.461
5.440
5.425
5.301
5.288
5.274
5.261
3.675
2.325
2.310
2.295
2.180
2.166
2.151
2.137
1.637
1.624
1.609
1.591
1.341
1.307
1.215
1.202
0.898
0.886
0.872
CO2Me
OC(O)tBu
4b
1.000
1.021
1.028
1.010
1.005
2.886
2.298
2.036
5.745
26.576
3.326
8.0
7.5
7.0
6.5
6.0
5.5
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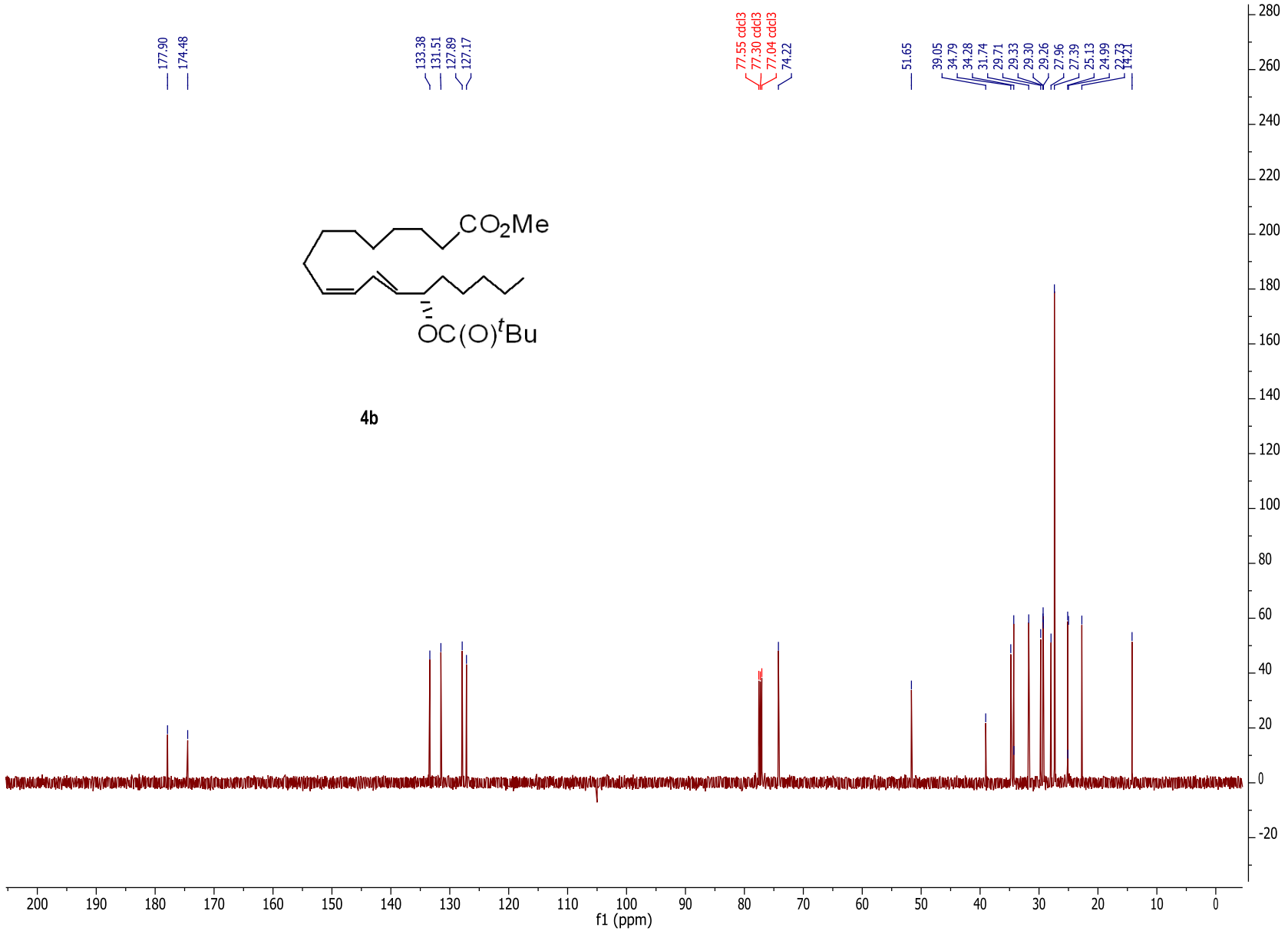
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


177.90
174.48
133.38
131.51
127.89
127.17
77.55 cdcl3
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77.04 cdcl3
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51.65
39.05
34.79
34.28
31.74
29.71
29.33
29.30
29.26
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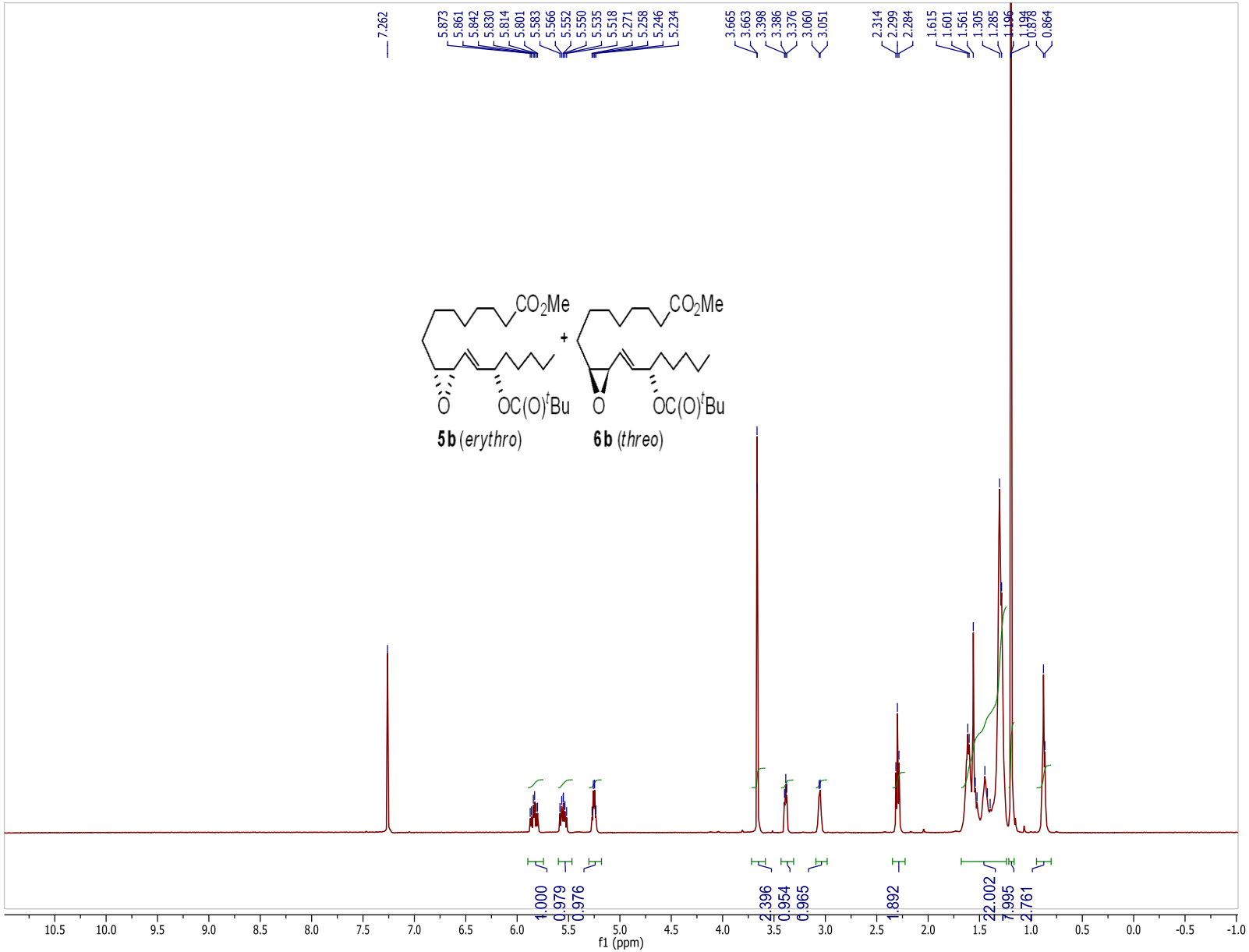
27.39
25.13
24.99
22.73
14.21
CO2Me
OC(O)tBu
4b
f1 (ppm)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5.550
5.535
5.518
5.271
5.258
5.246
5.234
3.665
3.663
3.398
3.386
3.376
3.060
3.051
2.314
2.299
2.284
1.615
1.601
1.561
1.305
1.285
1.196
0.878
0.864
CO2Me
OC(O)tBu
5b (erythro)
6b (threo)
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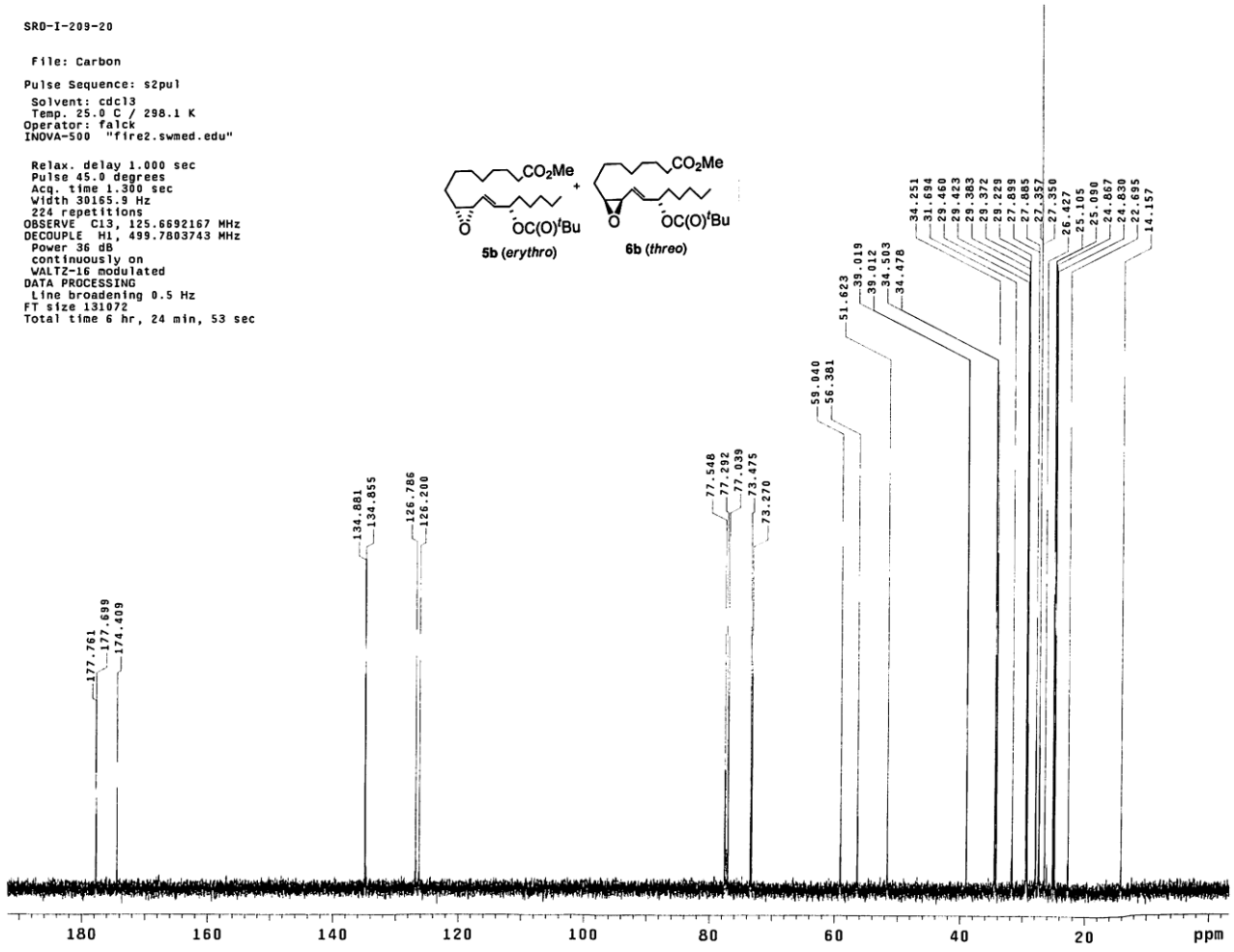
22.002
7.995
2.761
f1 (ppm)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Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: falck
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Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30165.9 Hz
224 repetitions
OBSERVE C13, 125.6692167 MHz
DECOUPLE H1, 499.7803743 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 6 hr, 24 min, 53 sec
CO2Me
OC(O)tBu
5b (erythro)
6b (threo)
177.761
177.699
174.409
134.881
134.855
126.786
126.200
77.548
77.292
77.039
73.475
73.270
59.040
56.381
51.623
39.019
39.012
34.503
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29.423
29.383
29.372
29.229
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27.865
27.357
27.350
26.427
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140
120
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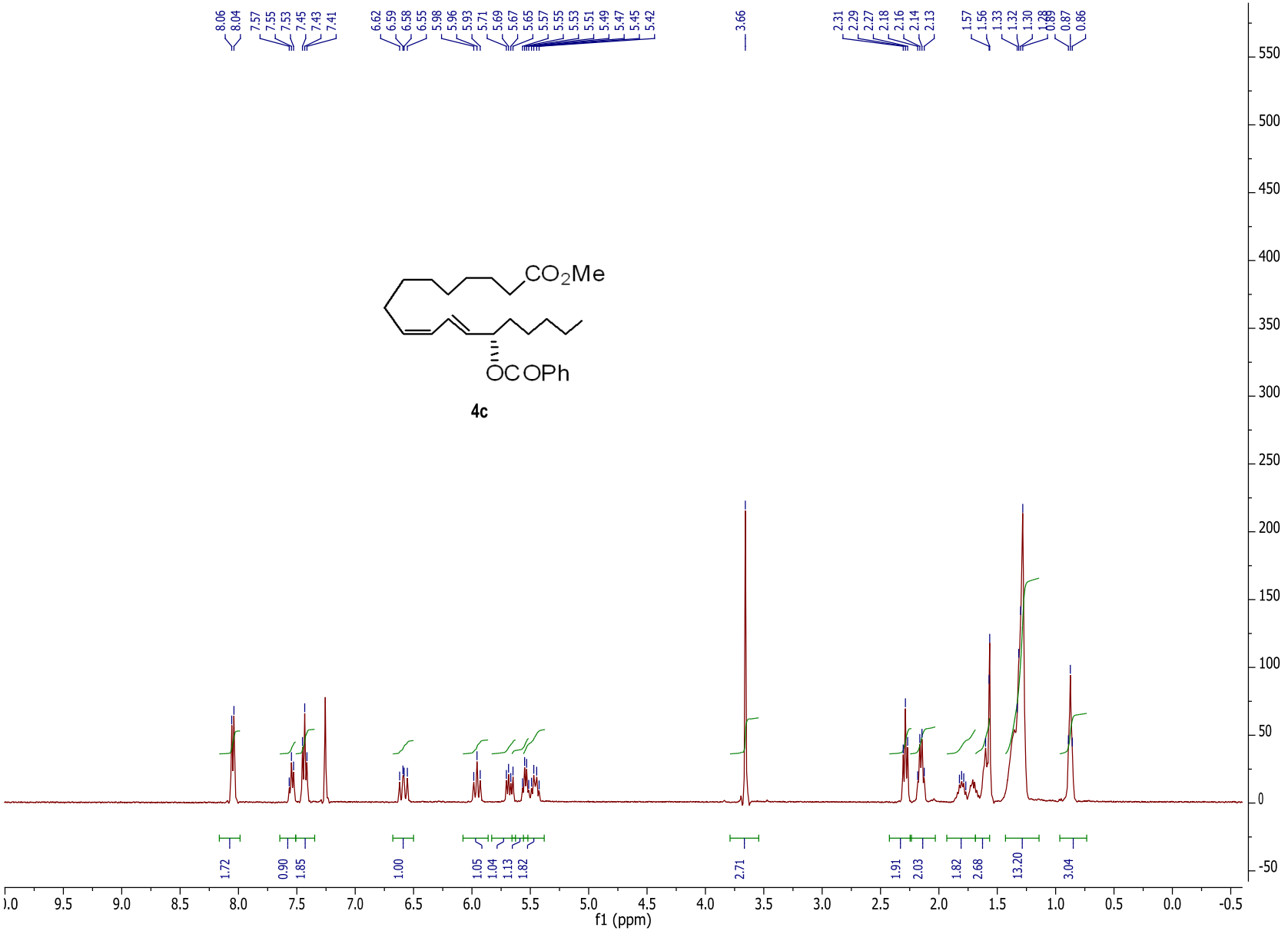
80
60
40
20
ppm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6.58
6.55
5.98
5.96
5.93
5.71
5.69
5.67
5.65
5.57
5.55
5.53
5.51
5.49
5.47
5.45
5.42
3.66
2.31
2.29
2.27
2.18
2.16
2.14
2.13
1.57
1.56
1.33
1.32
1.30
0.89
0.87
0.86
CO2Me
OCOPh
4c
1.72
0.90
1.85
1.00
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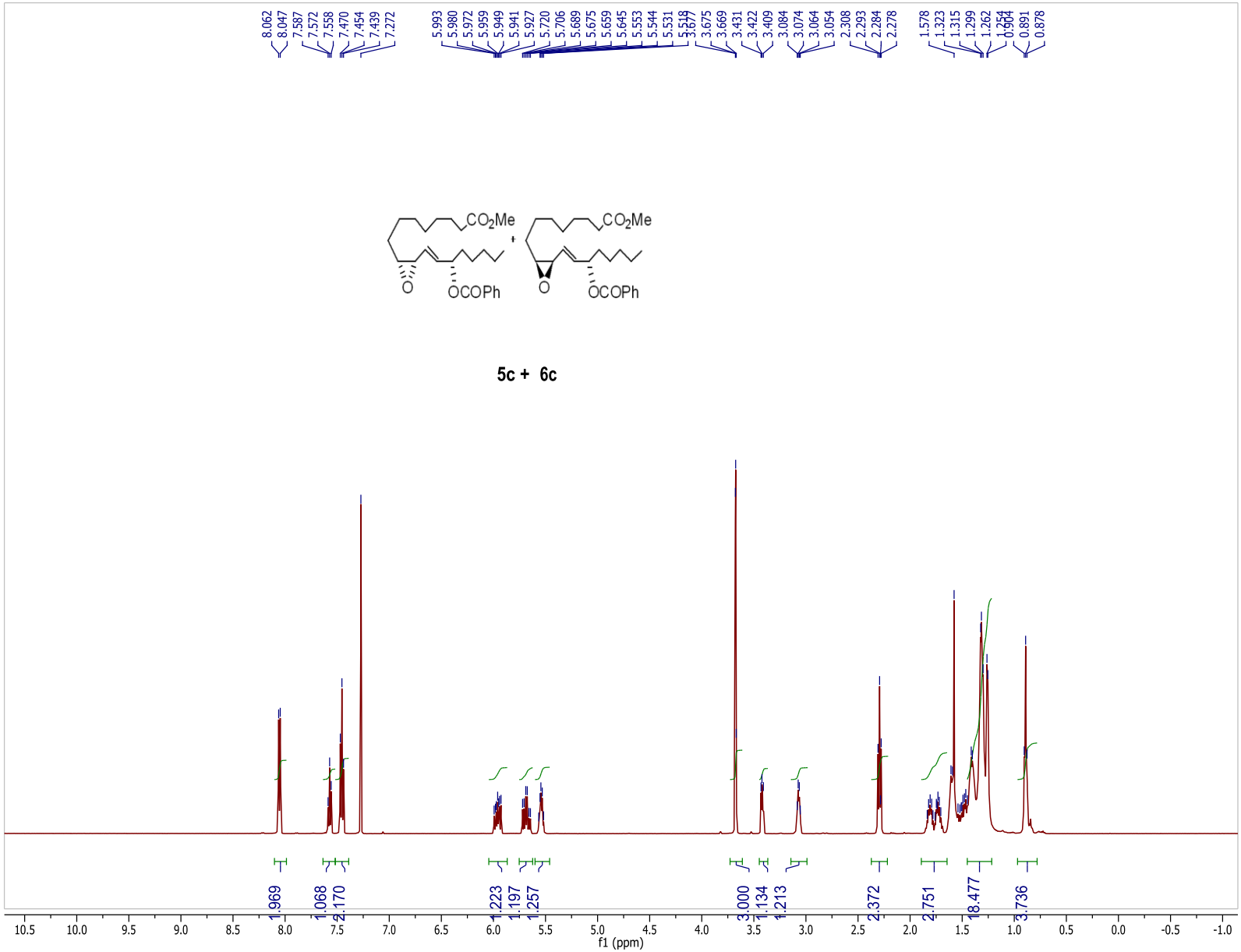
2.68
13.20
3.04
f1 (ppm)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5.959
5.949
5.941
5.927
5.720
5.706
5.689
5.675
5.659
5.645
5.553
5.544
5.531
3.675
3.669
3.431
3.422
3.409
3.084
3.074
3.064
3.054
2.308
2.293
2.284
2.278
1.578
1.323
1.315
1.299
1.262
0.891
0.878
CO2Me
OCOPh
CO2Me
OCOPh
1.969
1.068
2.170
1.223
1.197
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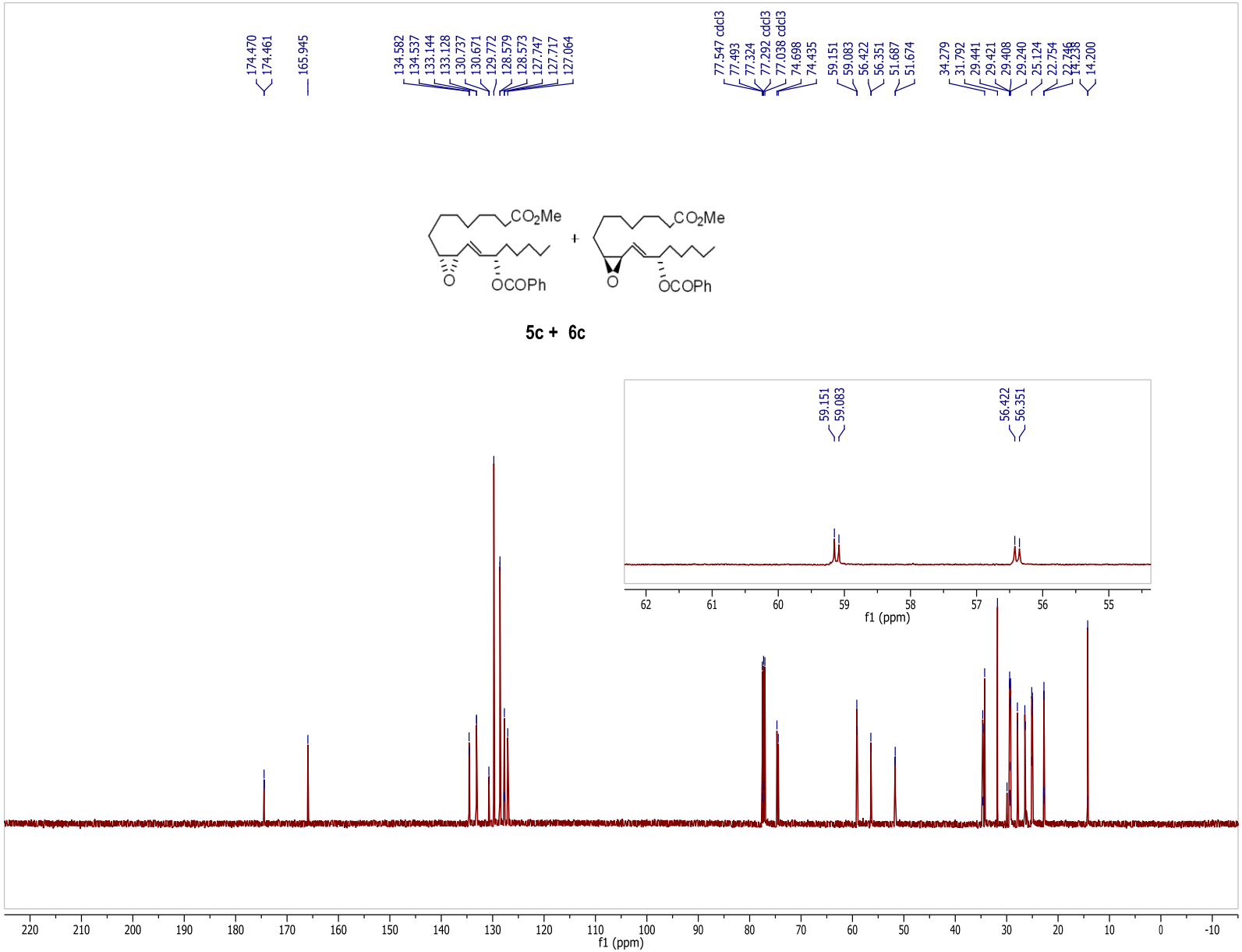
2.751
18.477
3.736
f1 (ppm)

5c + 6c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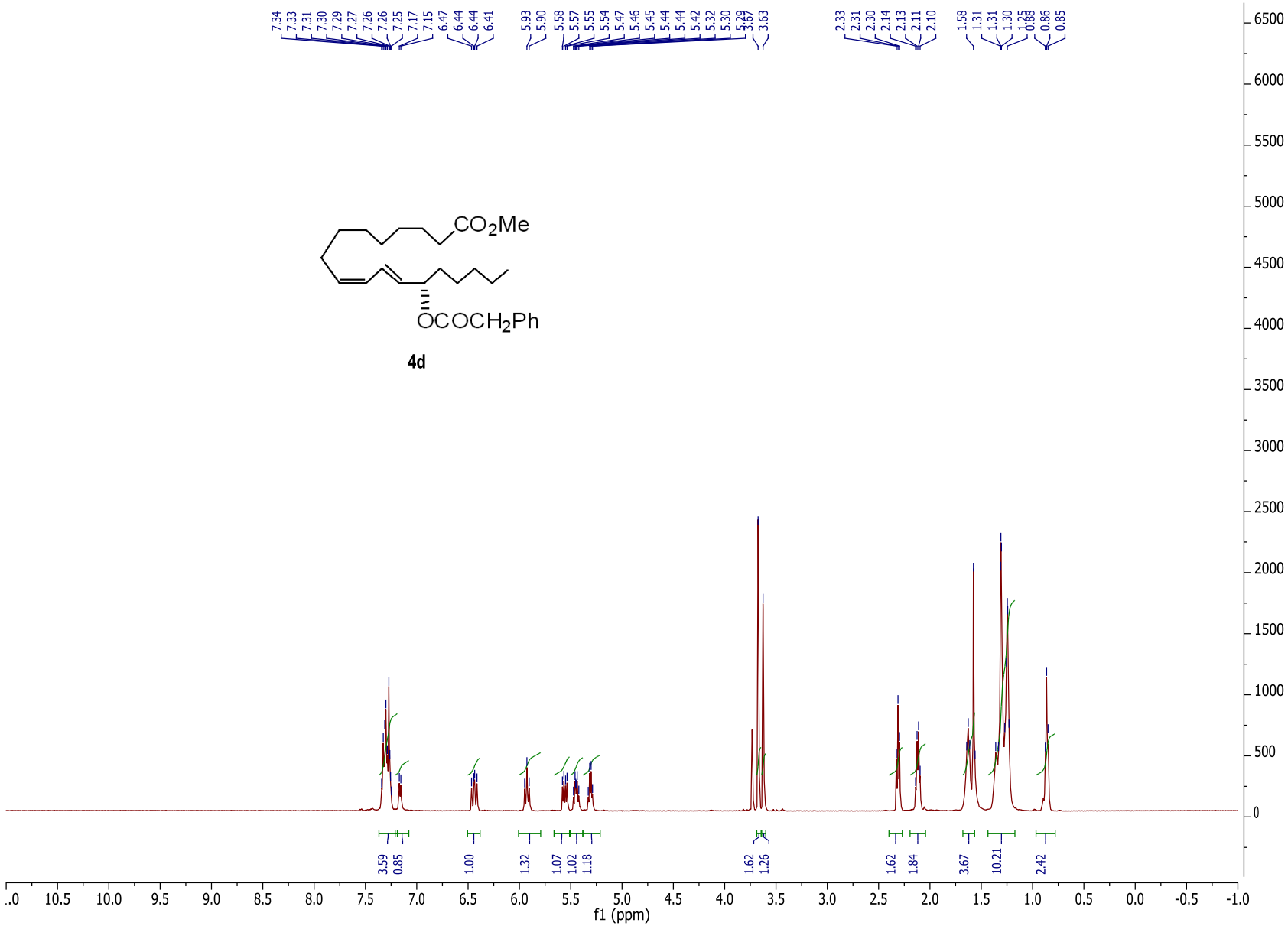
127.747
127.717
127.064
77.547 cdcl3
77.493
77.324
77.292 cdcl3
77.038 cdcl3
74.698
74.435
59.151
59.083
56.422
56.351
51.687
51.674
34.279
31.792
29.441
29.421
29.408
29.240
25.124
22.754
14.238
14.200
CO2Me
OCOPh
CO2Me
OCOPh
5c + 6c
59.151
59.083
56.422
56.351
f1 (ppm)
f1 (ppm)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6.44
6.44
6.41
5.93
5.90
5.58
5.57
5.55
5.54
5.47
5.46
5.45
5.44
5.44
5.42
5.32
5.30
3.67
3.63
2.33
2.31
2.30
2.14
2.13
2.11
2.10
1.58
1.31
1.31
1.30
0.88
0.86
0.85
CO2Me
OCOCH2Ph
4d
3.59
0.85
1.00
1.32
1.07
1.02
1.18
1.62
1.26
1.62
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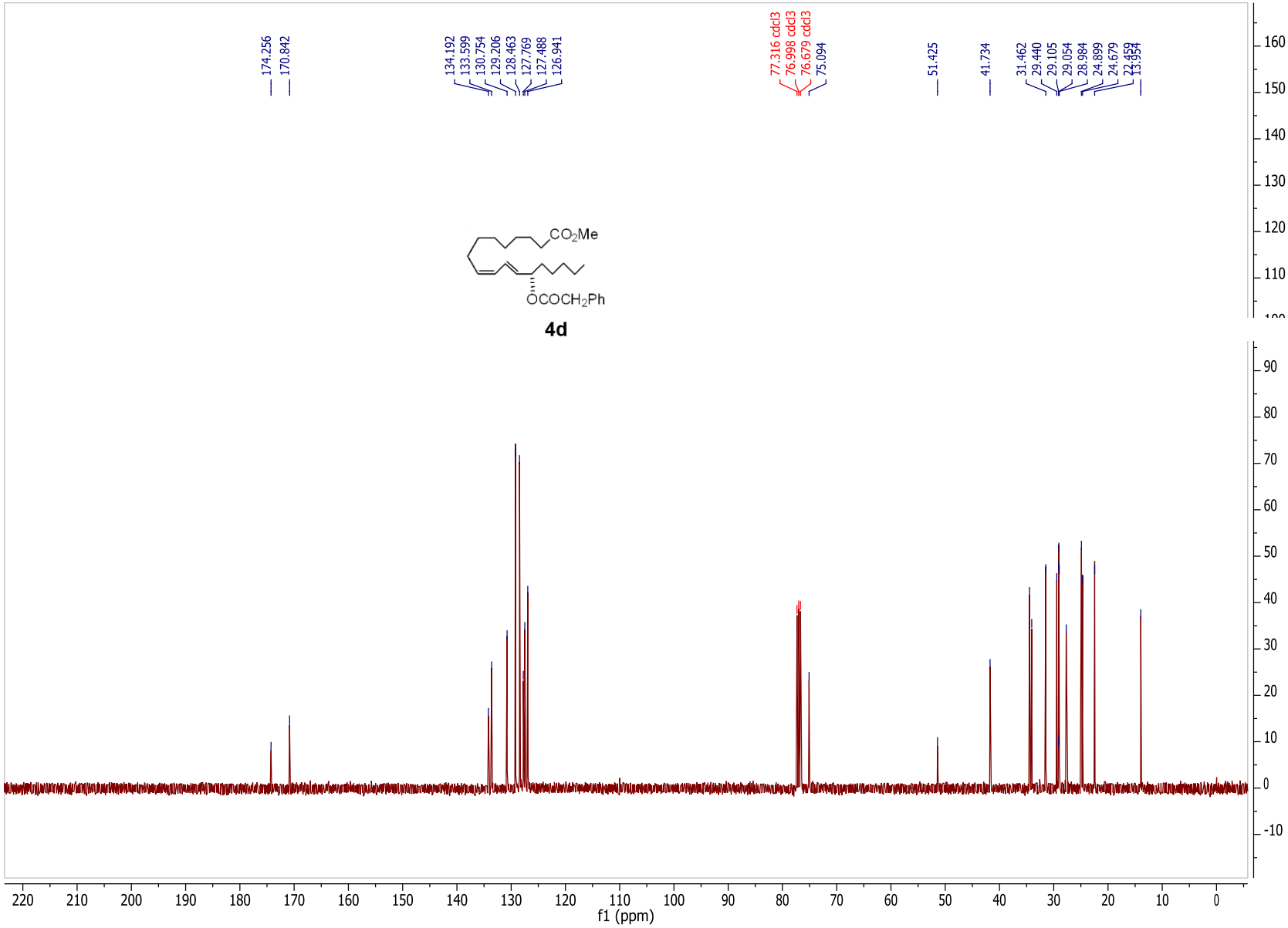
3.67
10.21
2.42
f1 (ppm)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134.192
133.599
130.754
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127.488
126.941
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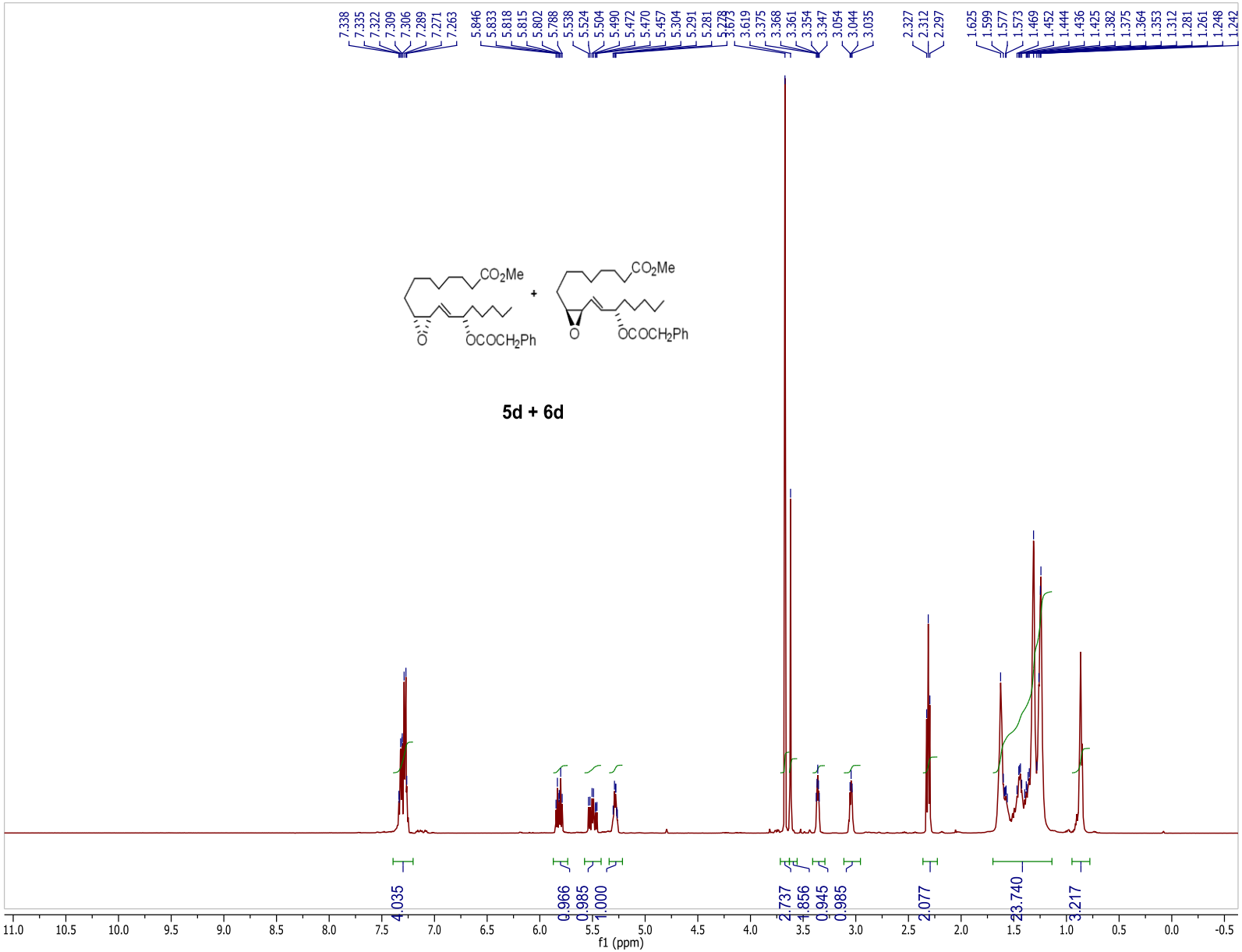
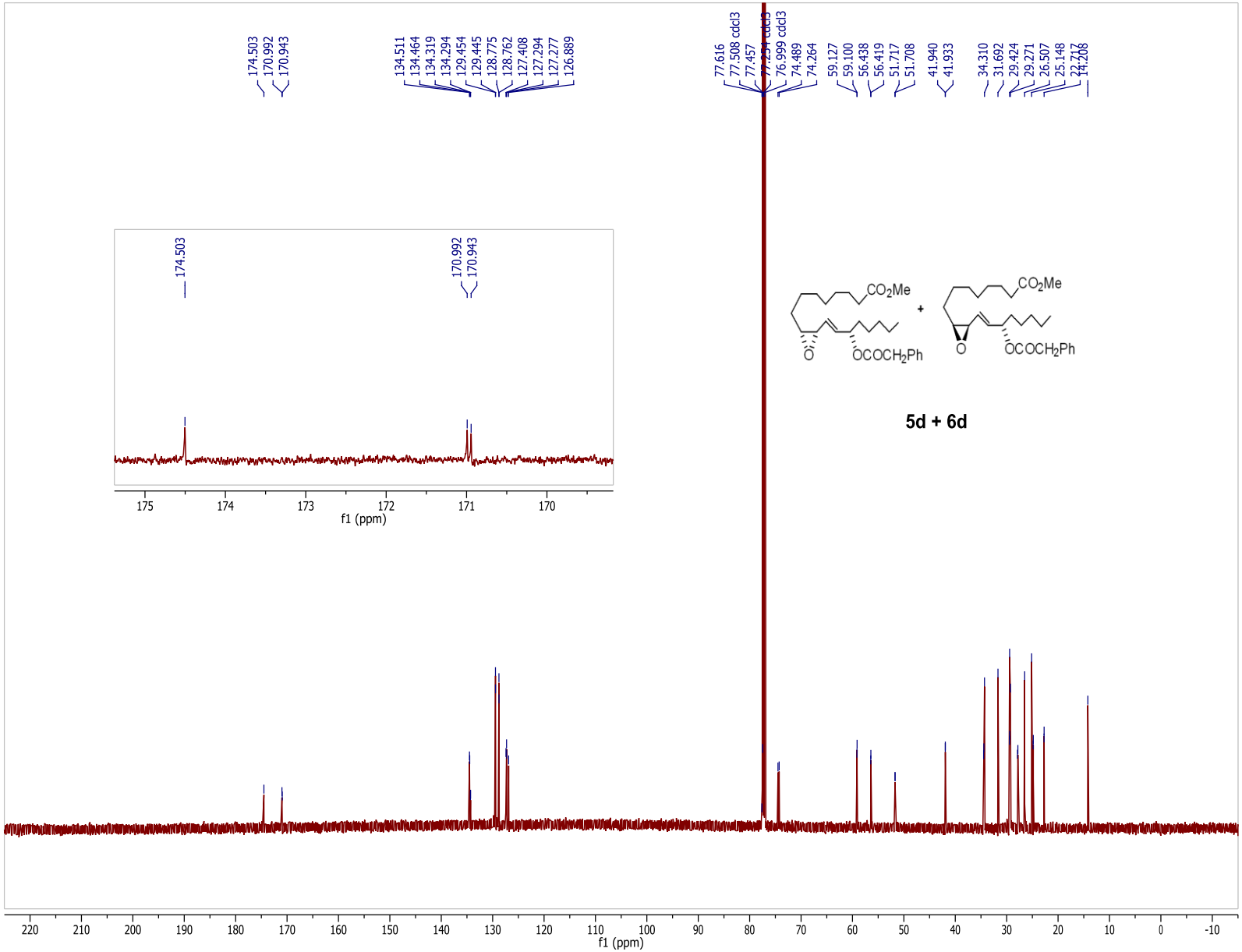
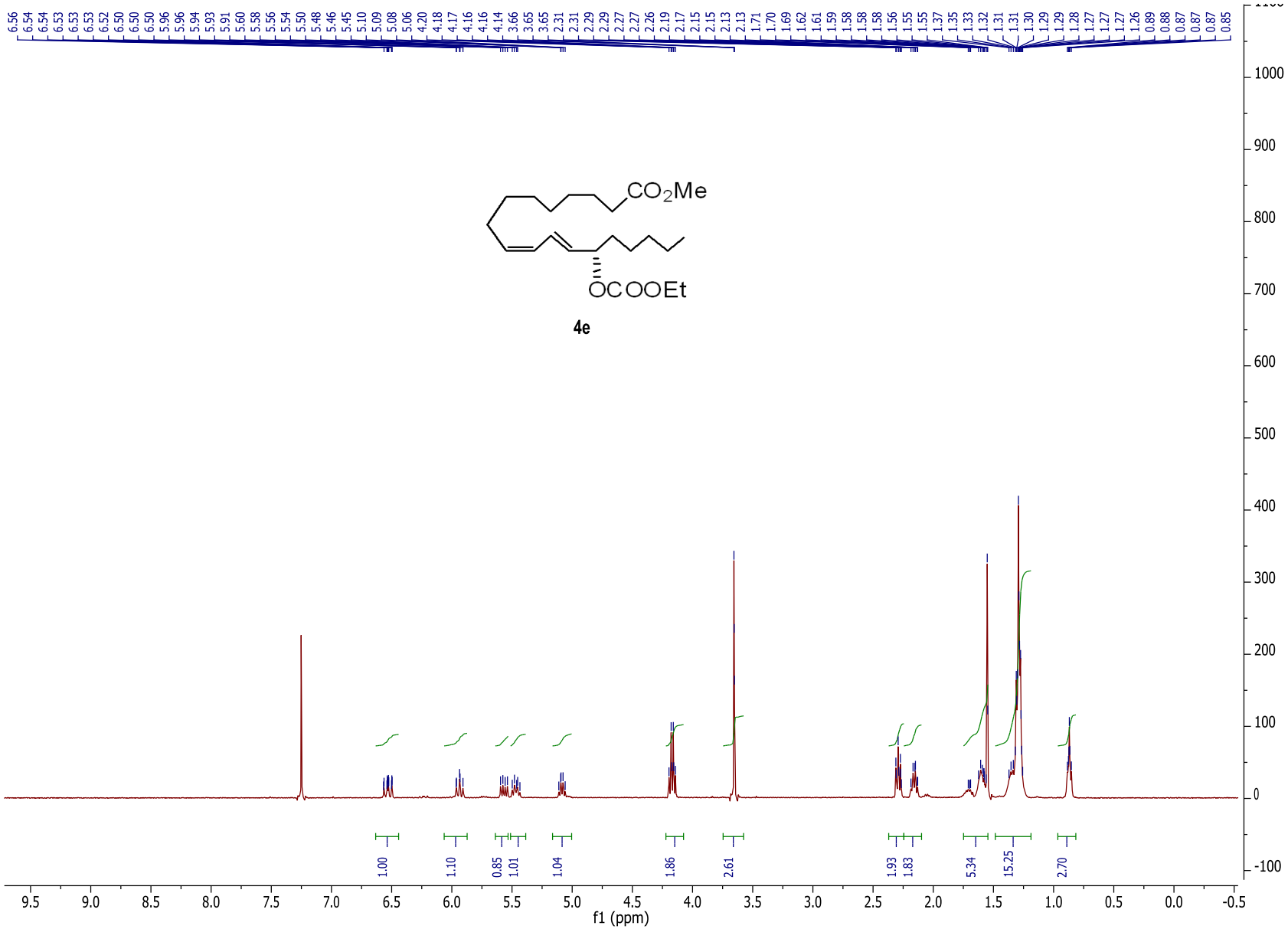
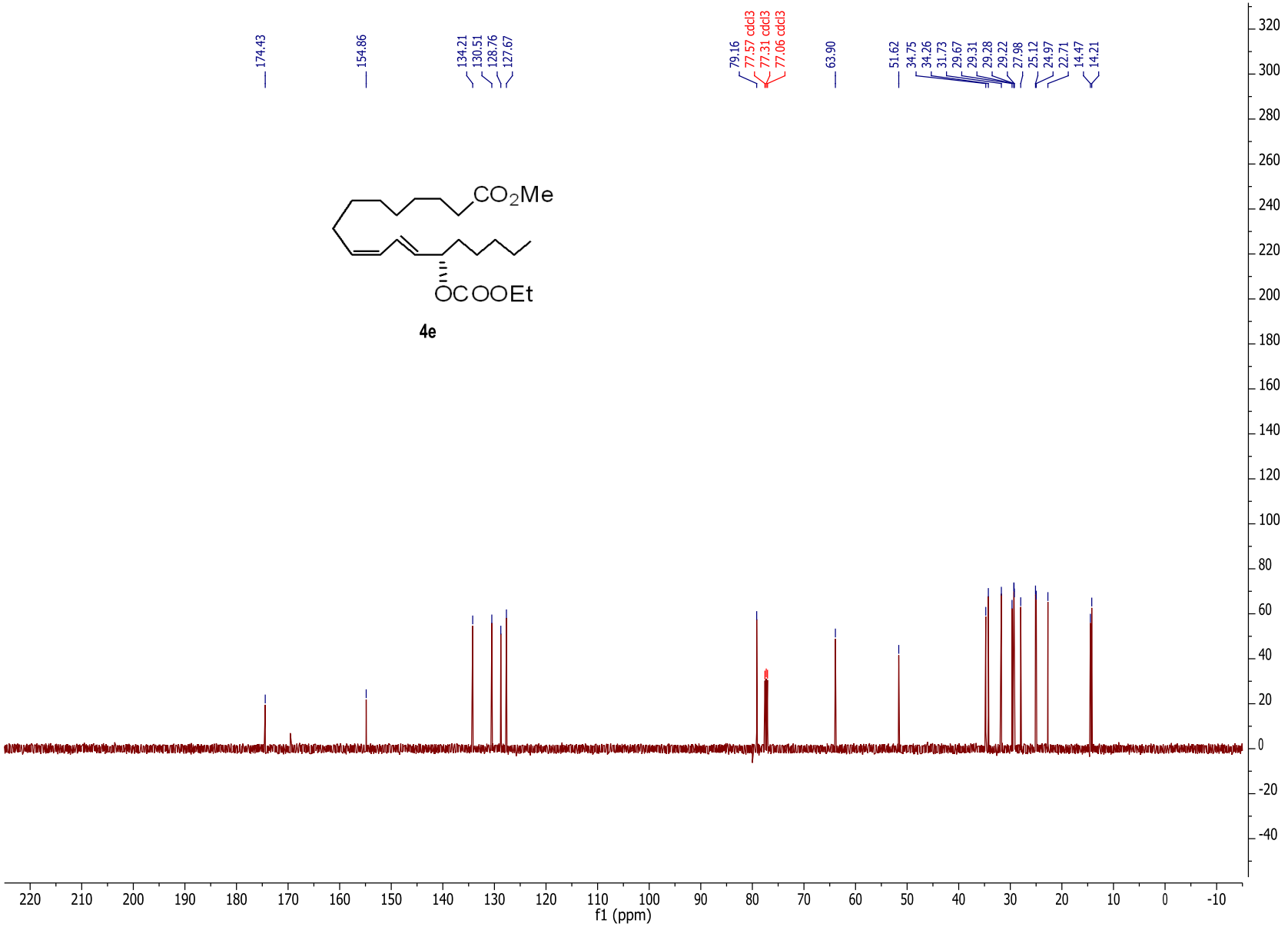
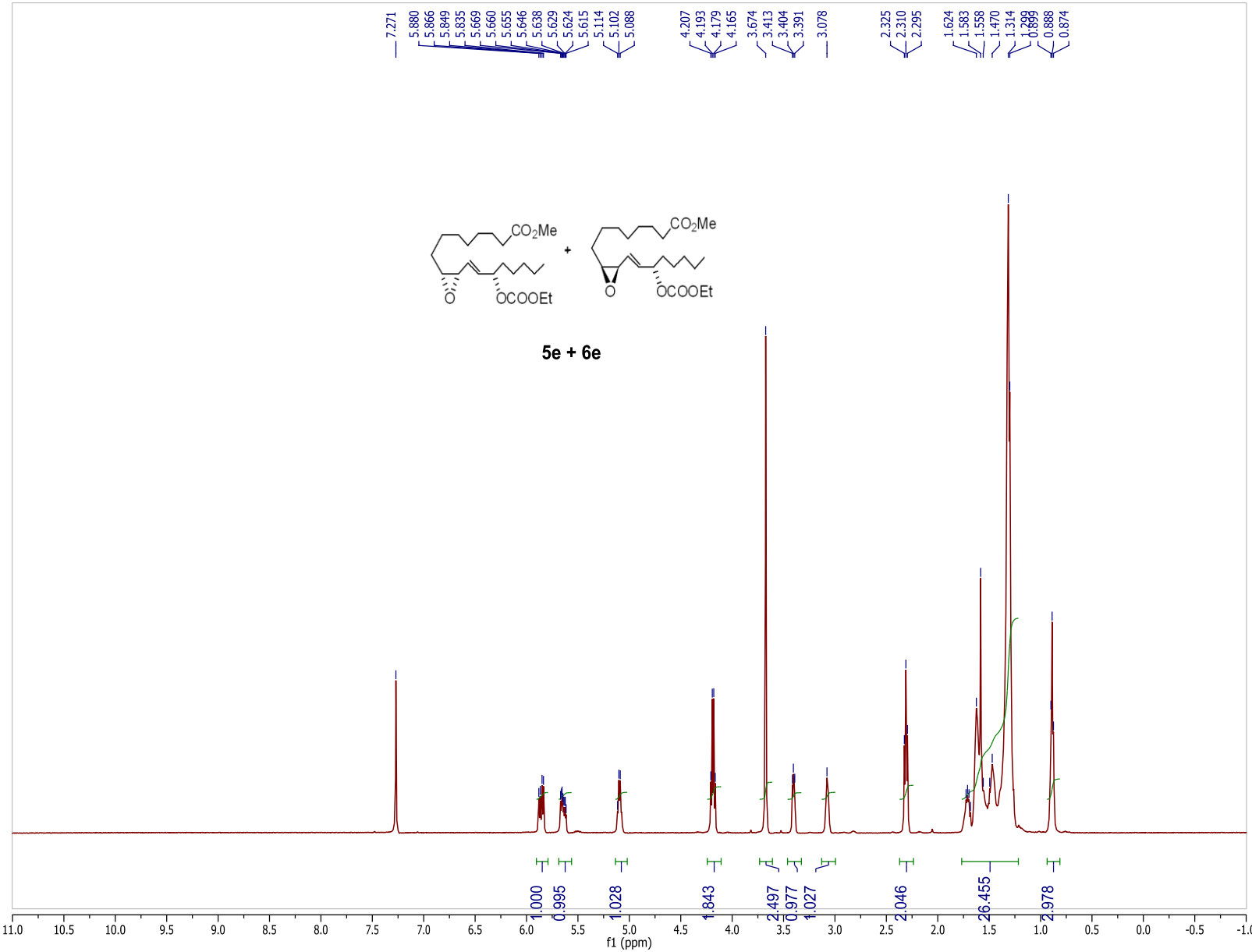
76.998 cdcl3
76.679 cdcl3
75.094
51.425
41.734
31.462
29.440
29.105
29.054
28.984
24.899
24.679
22.459
13.954
CO2Me
OCOCH2Ph
4d
f1 (ppm)

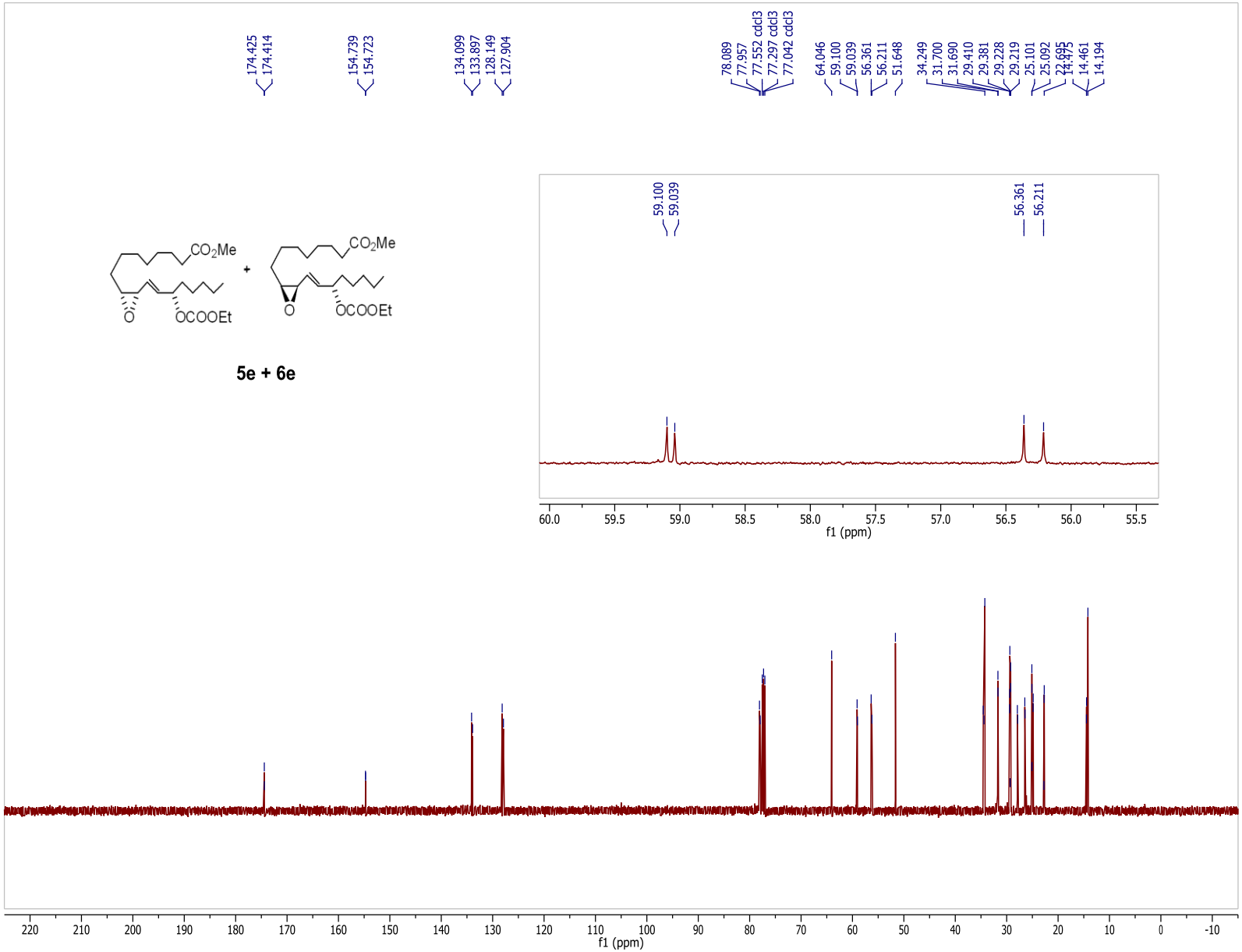

7.338
7.335
7.322
7.309
7.306
7.289
7.271
7.263
5.846
5.833
5.818
5.815
5.802
5.788
5.538
5.524
5.504
5.490
5.472
5.470
5.457
5.304
5.291
5.281
5.278
3.673
3.619
3.375
3.368
3.361
3.354
3.347
3.054
3.044
3.035
2.327
2.312
2.297
1.625
1.599
1.577
1.573
1.469
1.452
1.444
1.436
1.425
1.382
1.375
1.364
1.353
1.312
1.281
1.261
1.248
1.242
CO2Me
OCOCH2Ph
CO2Me
OCOCH2Ph
5d + 6d
4.035
0.966
0.985
1.000
2.737
1.856
0.945
0.985
2.077
3.740
3.217
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
0.0
-0.5
f1 (ppm)

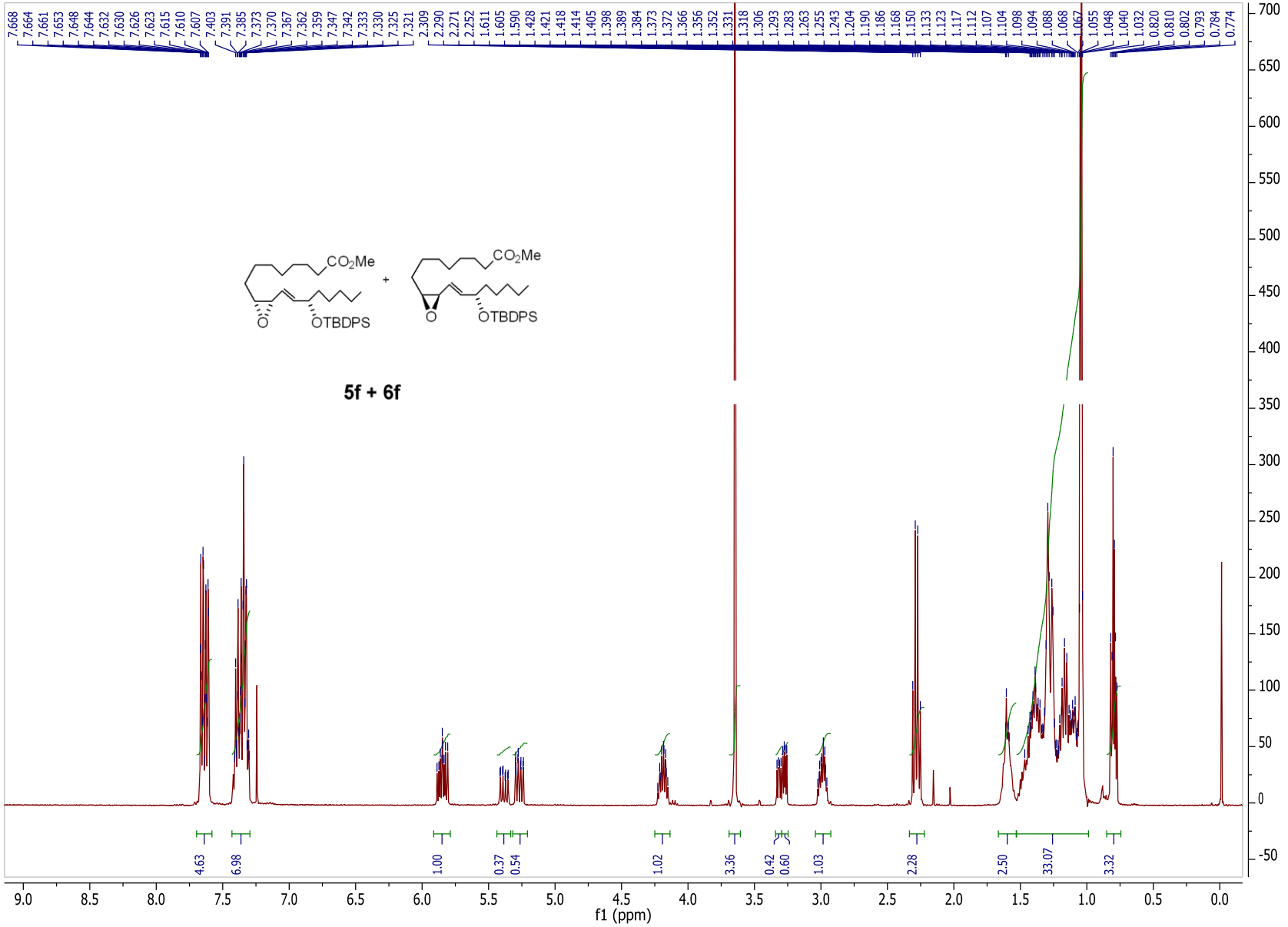

174.503
170.992
170.943
134.511
134.464
134.319
134.294
129.454
129.445
128.775
128.762
127.408
127.294
127.277
126.889
77.616
77.508 cdcl3
77.457
77.254 cdcl3
76.999 cdcl3
74.489
74.264
59.127
59.100
56.438
56.419
51.717
51.708
41.940
41.933
34.310
31.692
29.424
29.271
26.507
25.148
22.717
14.208
CO2Me
OCOCH2Ph
CO2Me
OCOCH2Ph
5d + 6d
f1 (ppm)
f1 (ppm)

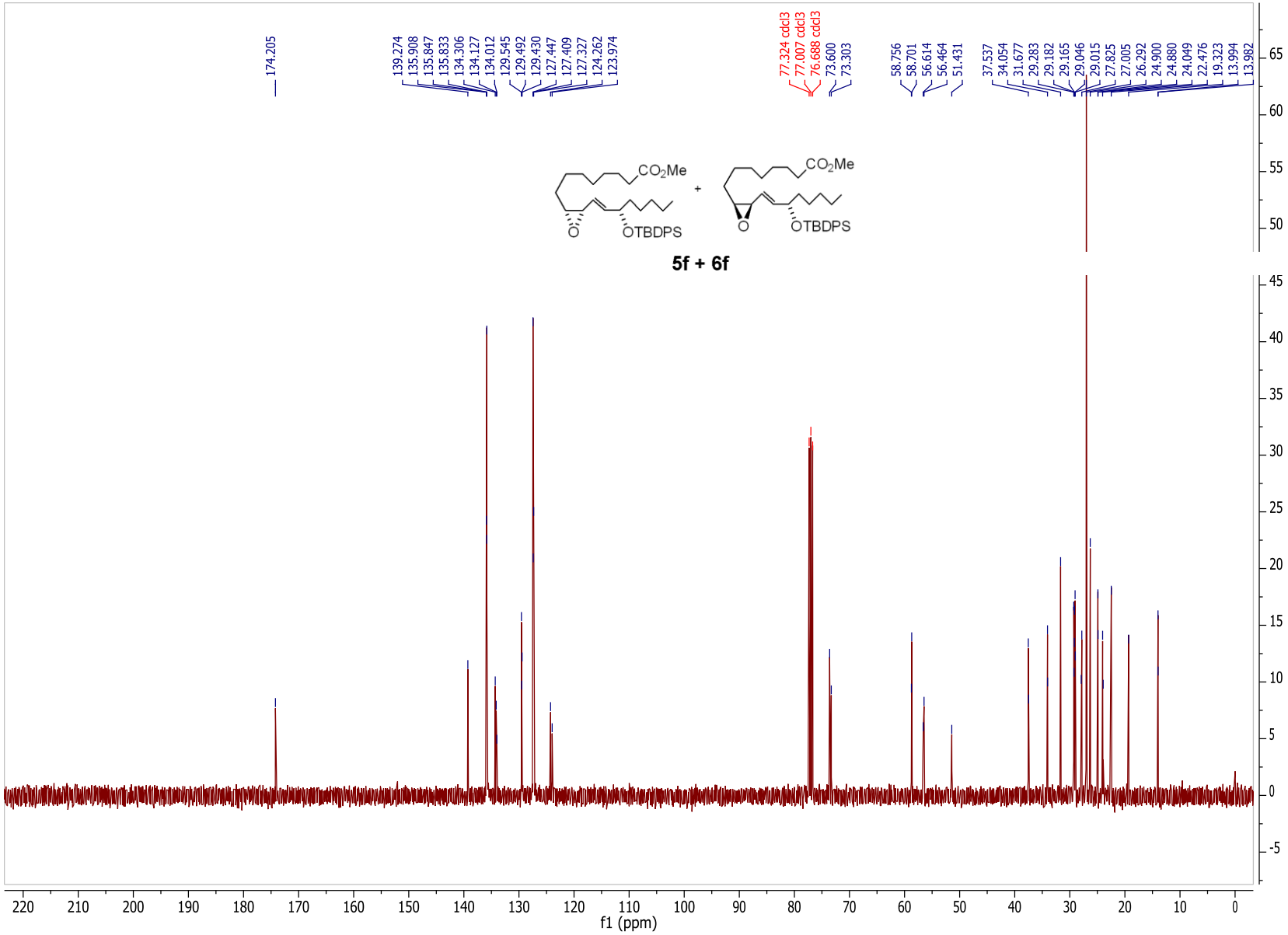

CO2Me
OCOOEt
4e
f1 (ppm)

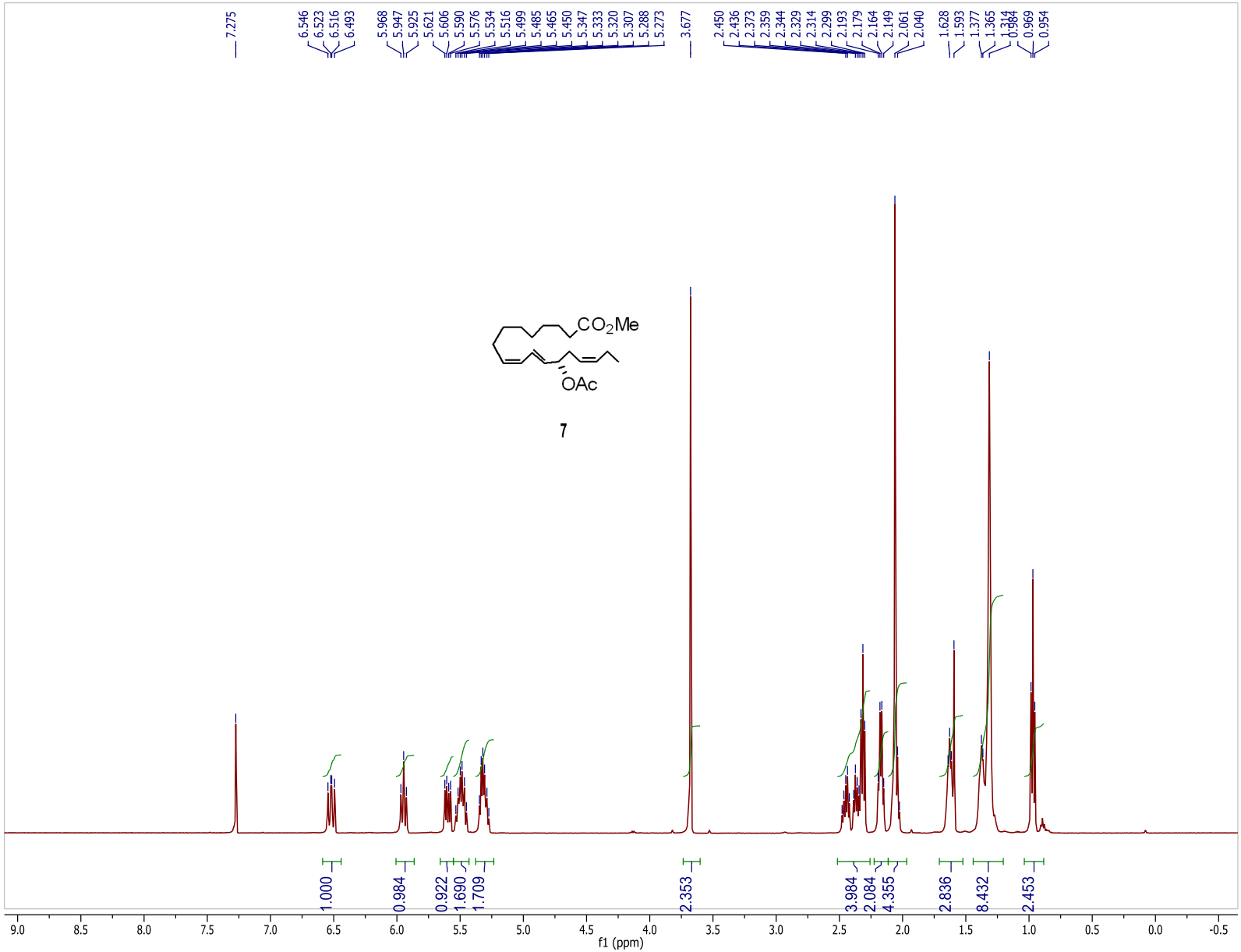

174.43
154.86
134.21
130.51
128.76
127.67
79.16
77.57 cdcl3
77.31 cdcl3
77.06 cdcl3
63.90
51.62
34.75
34.26
31.73
29.67
29.31
29.28
29.22
27.98
25.12
24.97
22.71
14.47
14.21
CO2Me
OCOOEt
4e
f1 (ppm)

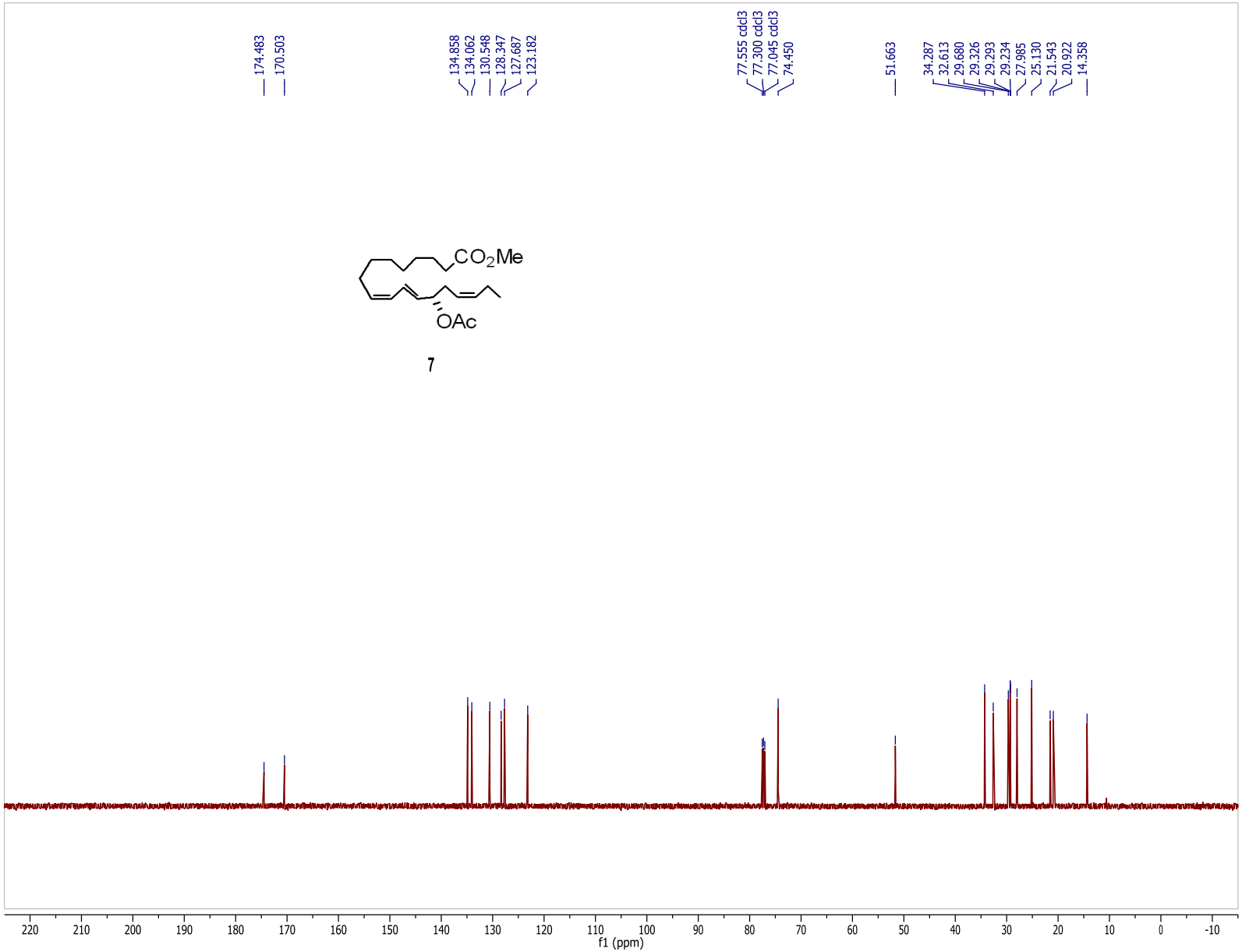

7.271
5.880
5.866
5.849
5.835
5.669
5.660
5.655
5.646
5.638
5.629
5.624
5.615
5.114
5.102
5.088
4.207
4.193
4.179
4.165
3.674
3.413
3.404
3.391
3.078
2.325
2.310
2.295
1.624
1.583
1.558
1.470
1.314
1.299
0.899
0.888
0.874
CO2Me
OCOOEt
CO2Me
OCOOEt
5e + 6e
1.000
0.995
1.028
1.843
2.497
0.977
1.027
2.046
26.455
2.978
f1 (ppm)

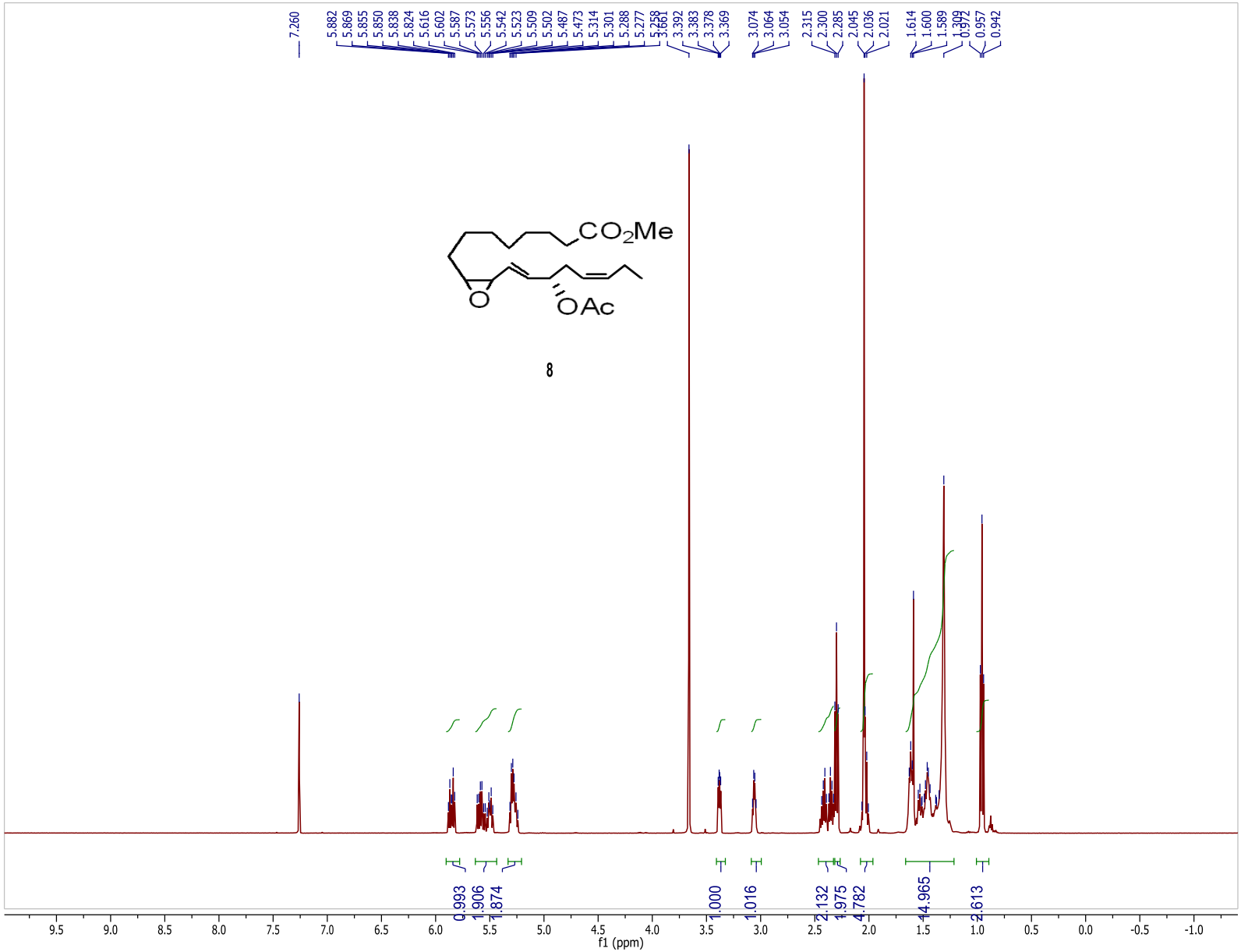

174.425
174.414
154.739
154.723
134.099
133.897
128.149
127.904
78.089
77.957
77.552 cdcl3
77.297 cdcl3
77.042 cdcl3
64.046
59.100
59.039
56.361
56.211
51.648
34.249
31.700
31.690
29.410
29.381
29.228
29.219
25.101
25.092
22.695
14.475
14.461
14.194
CO2Me
OCOOEt
CO2Me
OCOOEt
5e + 6e
59.100
59.039
56.361
56.211
60.0
59.5
59.0
58.5
58.0
57.5
57.0
56.5
56.0
55.5
f1 (ppm)
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 (ppm)

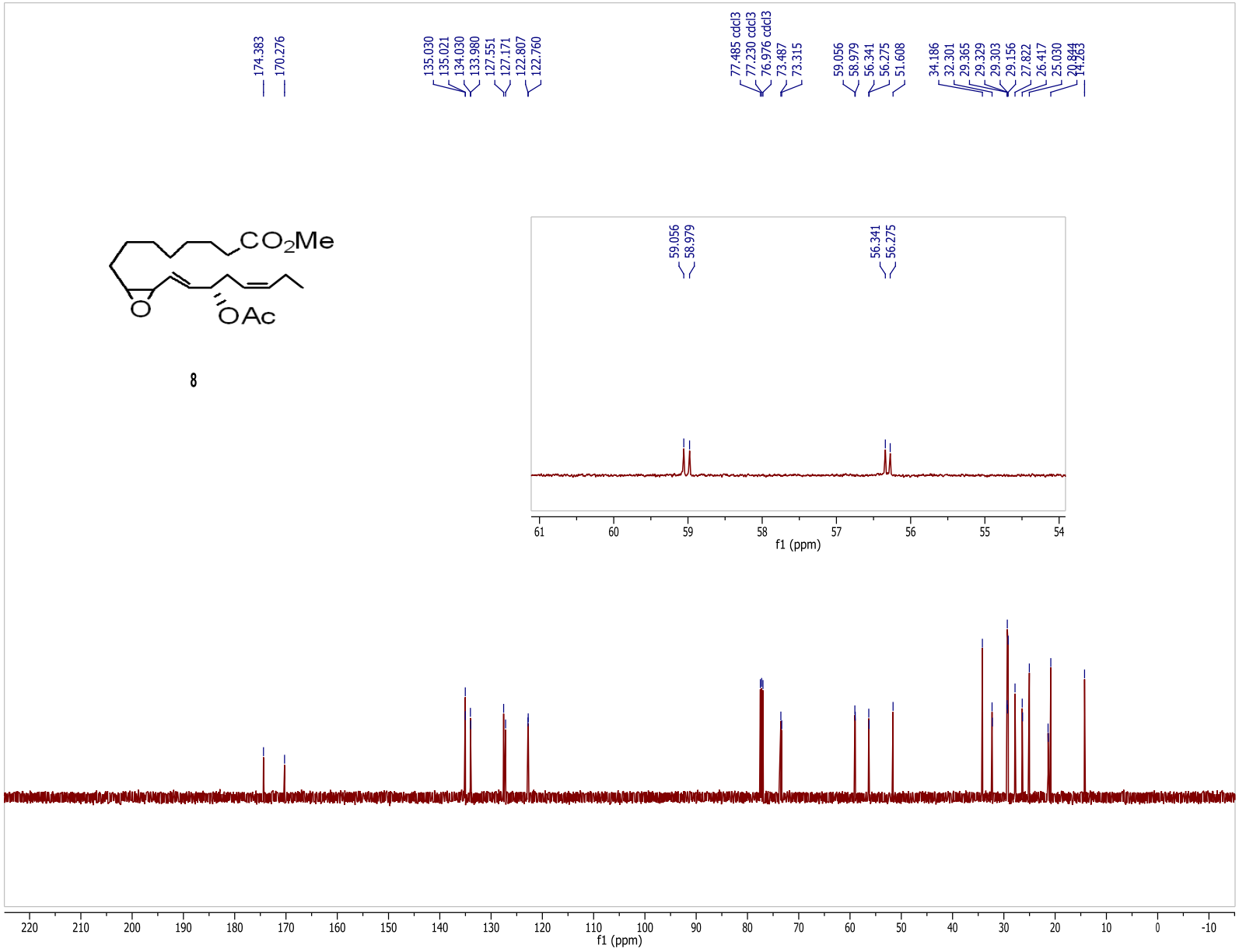

7.668 7.664 7.661 7.653 7.648 7.644 7.632 7.630 7.626 7.623 7.615 7.610 7.607 7.403 7.391 7.385 7.373 7.370 7.367 7.362 7.359 7.347 7.342 7.333 7.330 7.325 7.321 2.309 2.290 2.271 2.252 1.611 1.605 1.590 1.428 1.421 1.418 1.414 1.405 1.398 1.389 1.384 1.373 1.372 1.366 1.356 1.352 1.331 1.318 1.306 1.293 1.283 1.263 1.255 1.243 1.204 1.190 1.186 1.168 1.150 1.133 1.123 1.117 1.112 1.107 1.104 1.098 1.094 1.088 1.068 1.067 1.055 1.048 1.040 1.032 0.820 0.810 0.802 0.793 0.784 0.774
CO2Me
OTBDPS
CO2Me
OTBDPS
5f + 6f
4.63 6.98 1.00 0.37 0.54 1.02 3.36 0.42 0.60 1.03 2.28 2.50 33.07 3.32
f1 (ppm)

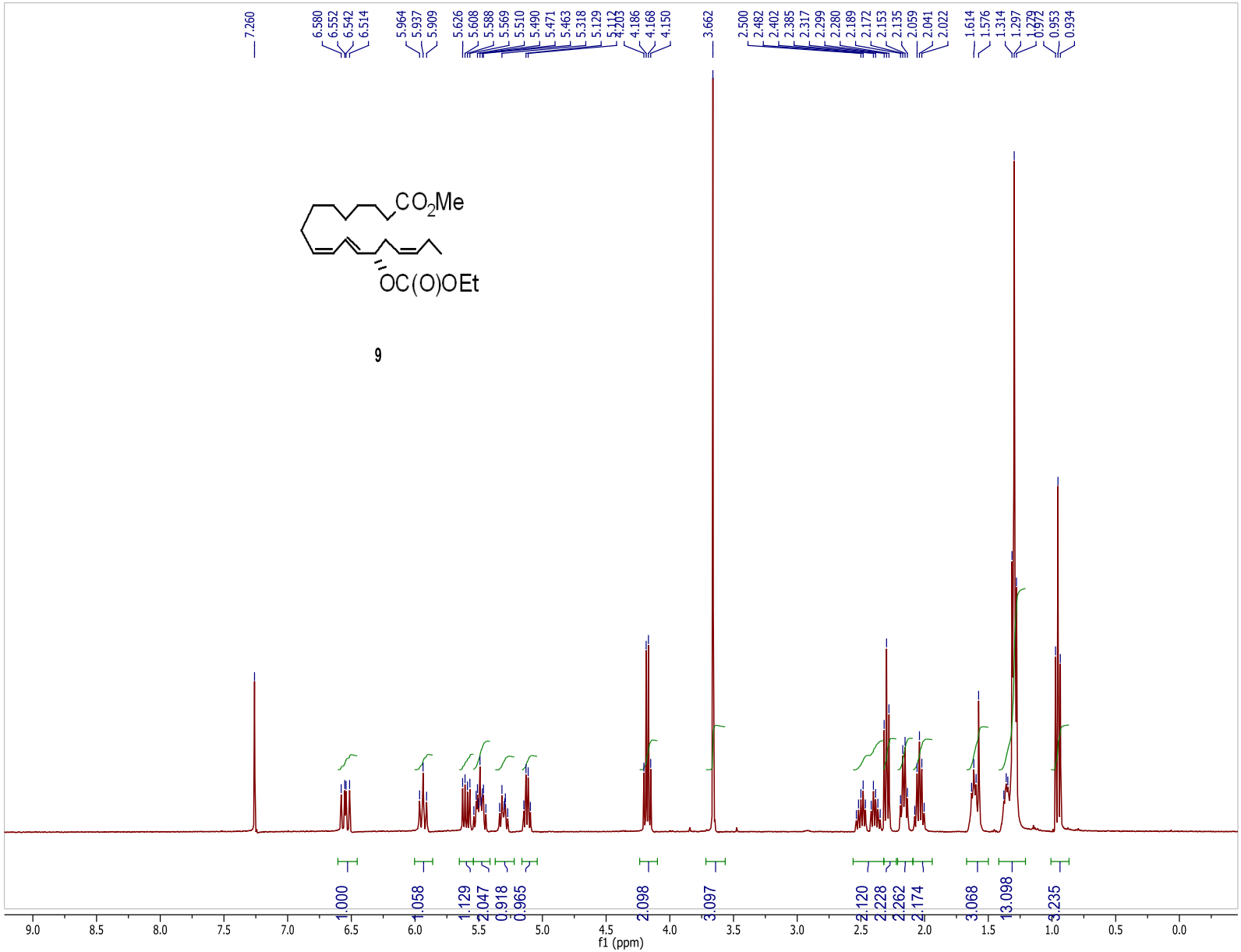

174.205
139.274
135.908
135.847
135.833
134.306
134.127
134.012
129.545
129.492
129.430
127.447
127.409
127.327
124.262
123.974
77.324 cdcl3
77.007 cdcl3
76.688 cdcl3
73.600
73.303
58.756
58.701
56.614
56.464
51.431
37.537
34.054
31.677
29.283
29.182
29.165
29.046
29.015
27.825
27.005
26.292
24.900
24.880
24.049
22.476
19.323
13.994
13.982
CO2Me
OTBDPS
CO2Me
OTBDPS
5f + 6f
f1 (ppm)

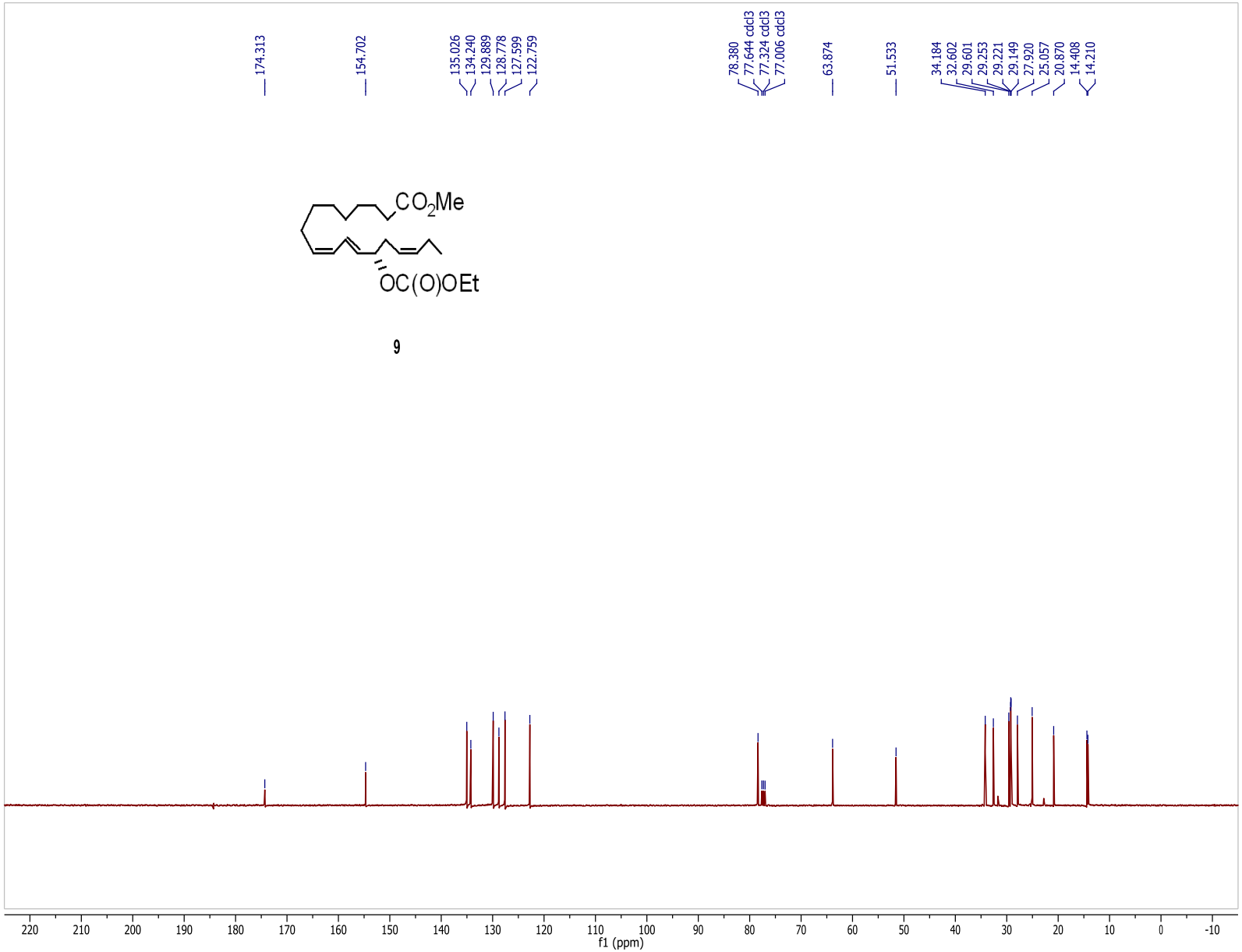

7.275
6.546
6.523
6.516
6.493
5.968
5.947
5.925
5.621
5.606
5.590
5.576
5.534
5.516
5.499
5.485
5.465
5.450
5.347
5.333
5.320
5.307
5.288
5.273
3.677
2.450
2.436
2.373
2.359
2.344
2.329
2.314
2.299
2.193
2.179
2.164
2.149
2.061
2.040
1.628
1.593
1.377
1.365
1.314
0.984
0.969
0.954
CO2Me
OAc
7
1.000
0.984
0.922
1.690
1.709
2.353
3.984
2.084
4.355
2.836
8.432
2.453
f1 (ppm)

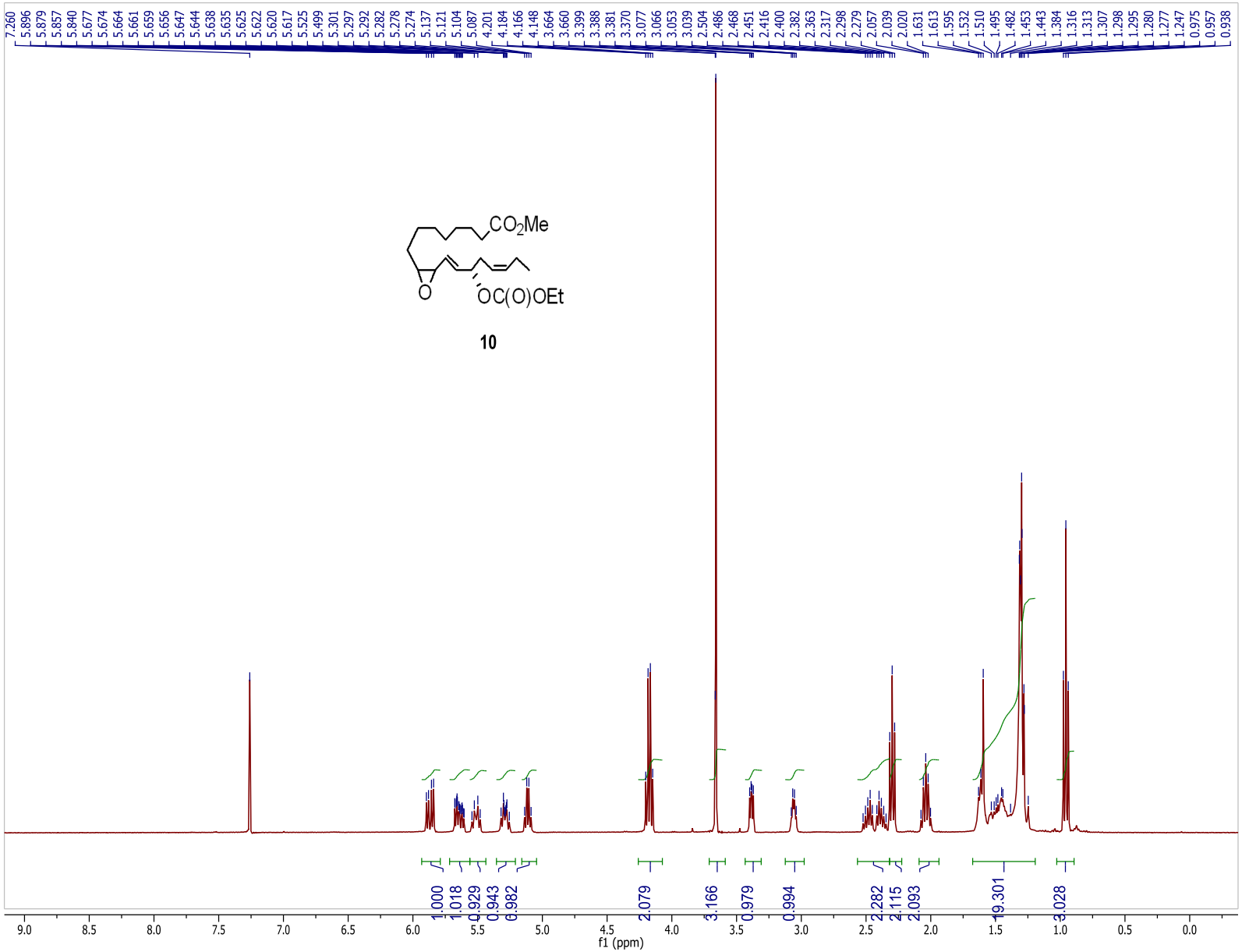

174.483
170.503
134.858
134.062
130.548
128.347
127.687
123.182
77.555 cdcl3
77.300 cdcl3
77.045 cdcl3
74.450
51.663
34.287
32.613
29.680
29.326
29.293
29.234
27.985
25.130
21.543
20.922
14.358
CO2Me
OAc
7
f1 (ppm)

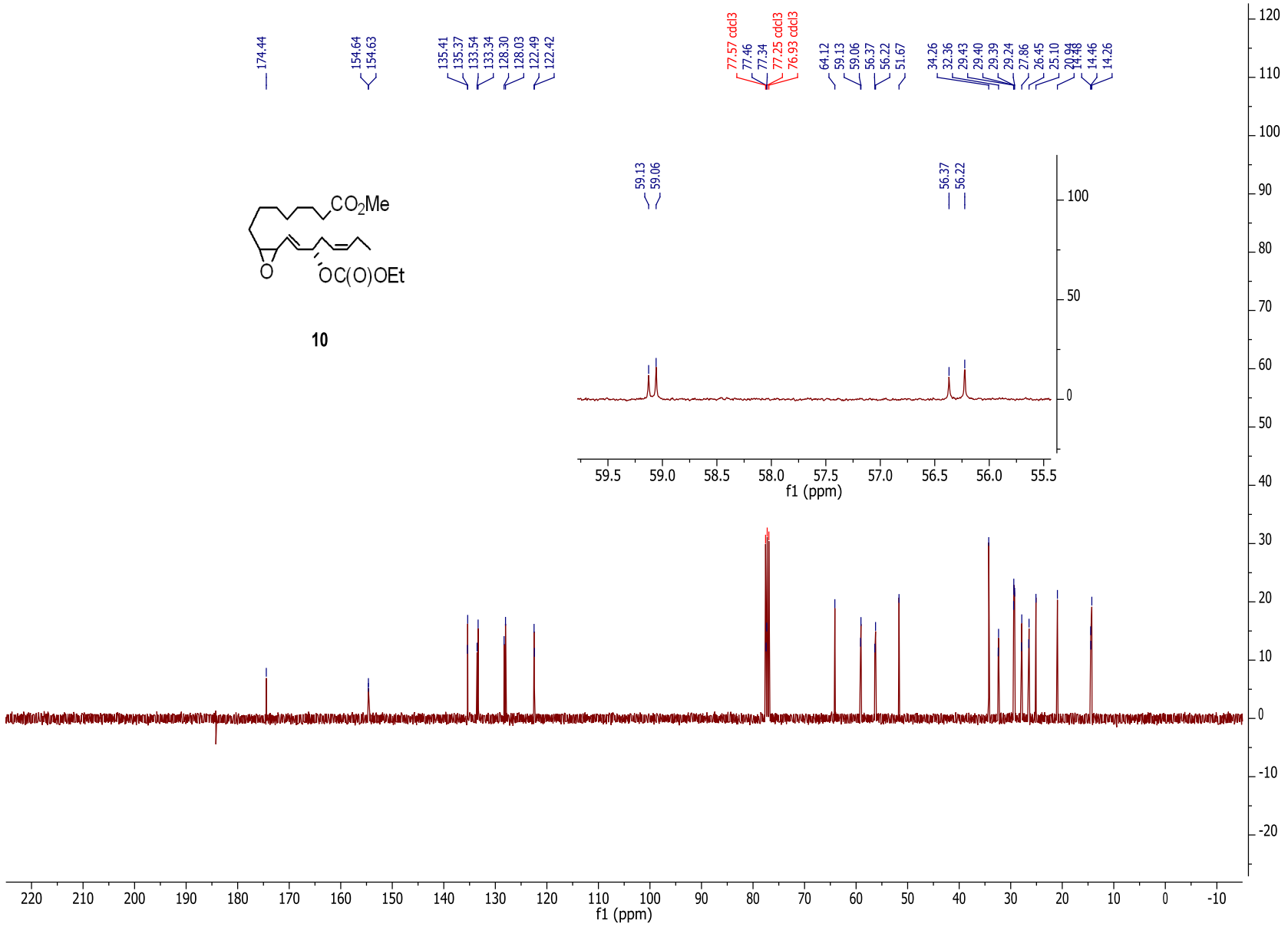

7.260
5.882
5.869
5.855
5.850
5.838
5.824
5.616
5.602
5.587
5.573
5.556
5.542
5.523
5.509
5.502
5.487
5.473
5.314
5.301
5.288
5.277
5.258
5.251
3.392
3.383
3.378
3.369
3.074
3.064
3.054
2.315
2.300
2.285
2.045
2.036
2.021
1.614
1.600
1.589
1.309
1.302
0.957
0.942
CO2Me
OAc
8
0.993
1.906
1.874
1.000
1.016
2.132
1.975
4.782
14.965
2.613
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
-0.5
-1.0
f1 (ppm)

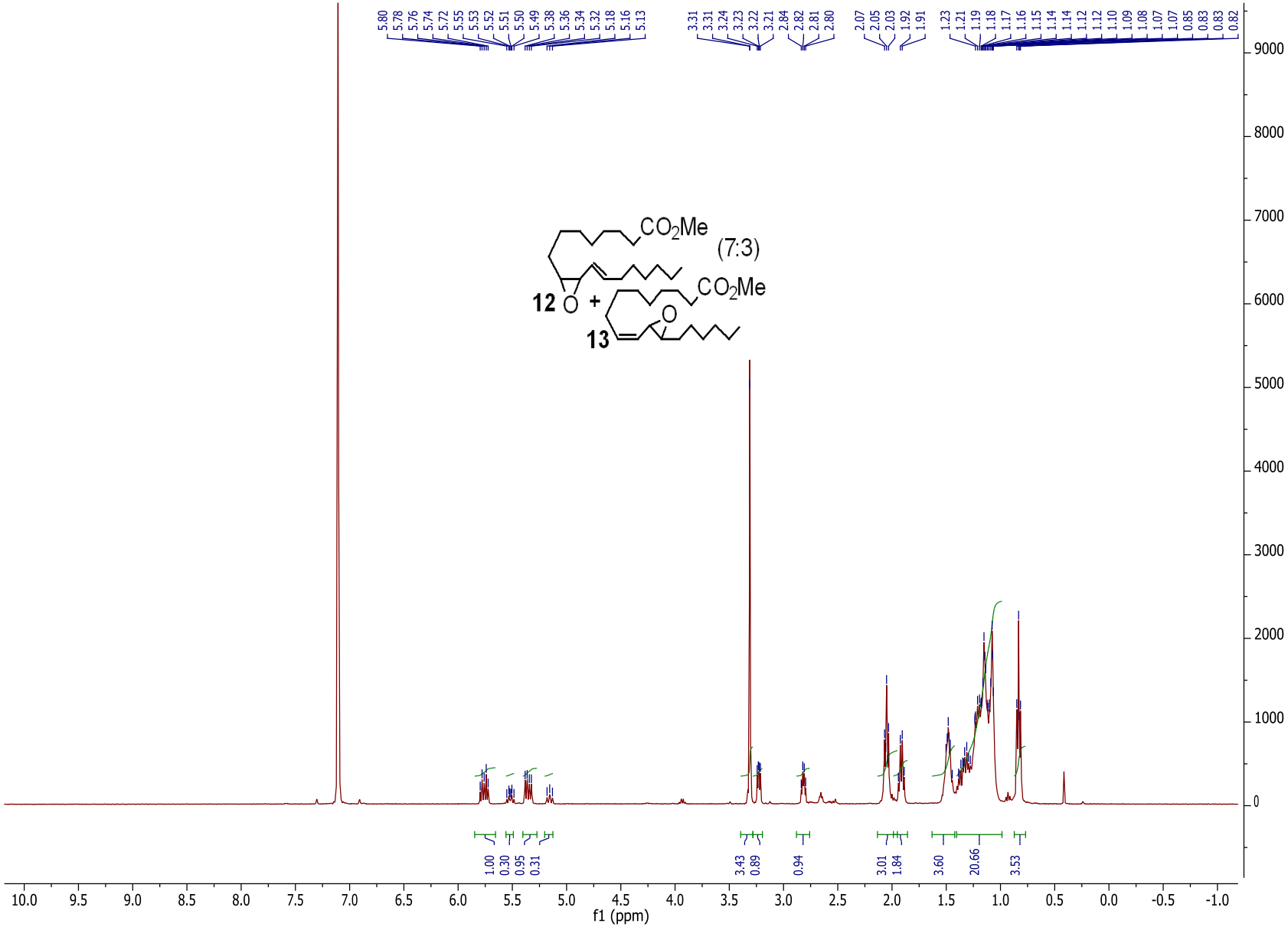

174.383
170.276
135.030
135.021
134.030
133.980
127.551
127.171
122.807
122.760
77.485 cdcl3
77.230 cdcl3
76.976 cdcl3
73.487
73.315
59.056
58.979
56.341
56.275
51.608
34.186
32.301
29.365
29.329
29.303
29.156
27.822
26.417
25.030
20.844
14.263
CO2Me
OAc
8
f1 (ppm)
f1 (ppm)

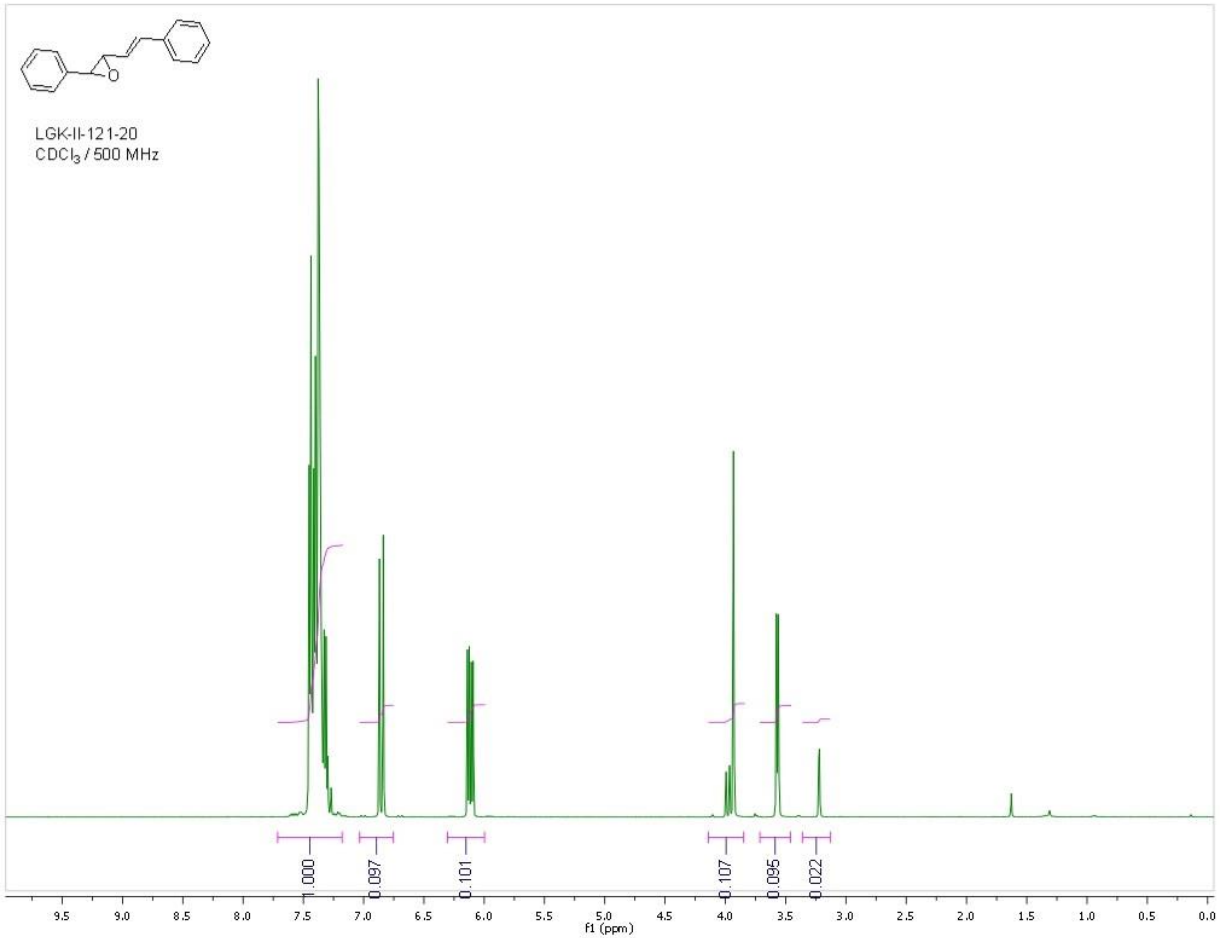

7.260
6.580
6.552
6.542
6.514
5.964
5.937
5.909
5.626
5.608
5.588
5.569
5.510
5.490
5.471
5.463
5.318
5.129
5.112
5.093
4.203
4.186
4.168
4.150
3.662
2.500
2.482
2.402
2.385
2.317
2.299
2.280
2.189
2.172
2.153
2.135
2.059
2.041
2.022
1.614
1.576
1.314
1.297
1.279
0.972
0.953
0.934
CO2Me
OC(O)OEt
9
1.000
1.058
1.129
2.047
0.918
0.965
2.098
3.097
2.120
2.228
2.262
2.174
3.068
13.098
3.235
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
f1 (ppm)

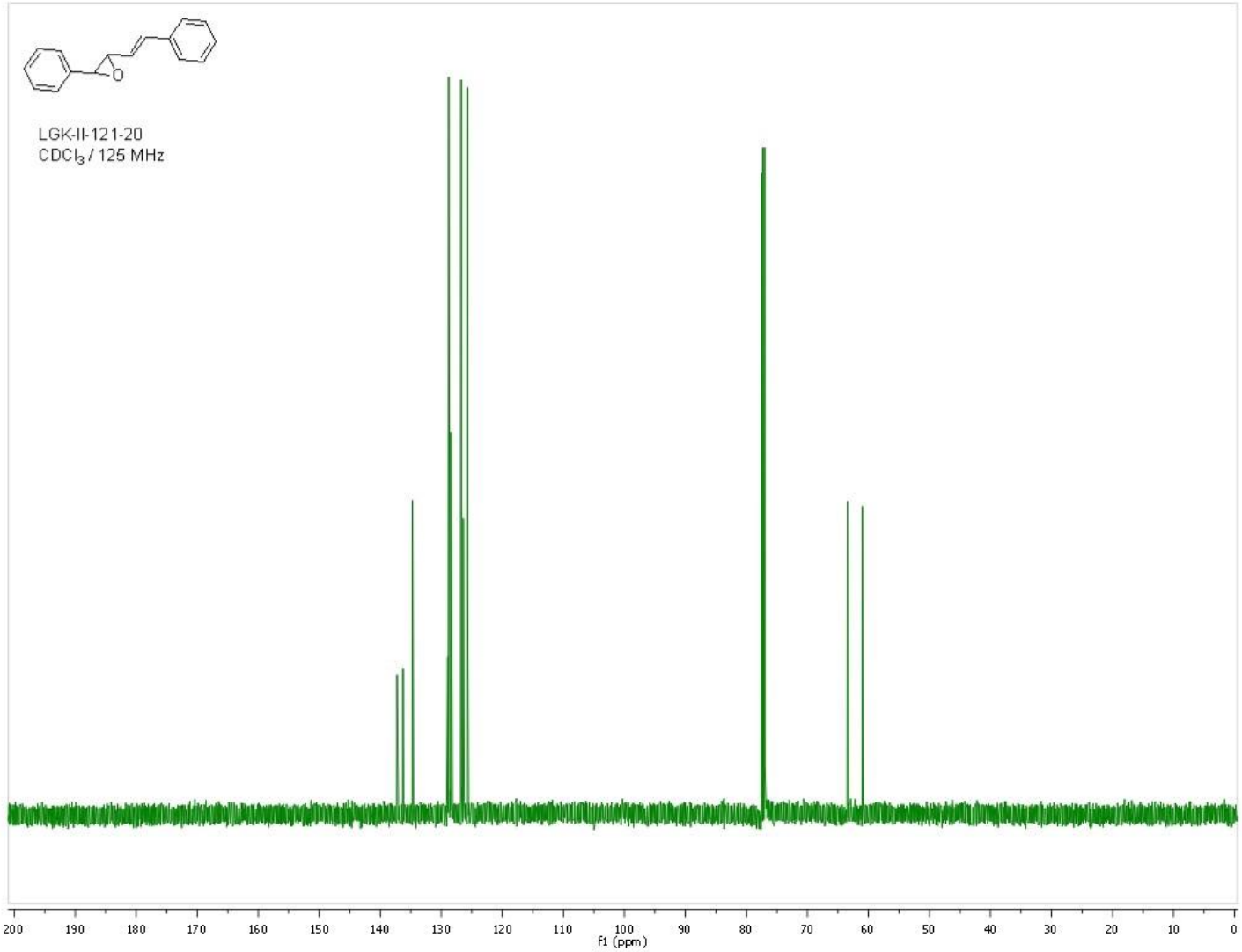

174.313
154.702
135.026
134.240
129.889
128.778
127.599
122.759
78.380
77.644 cdcl3
77.324 cdd3
77.006 cdcl3
63.874
51.533
34.184
32.602
29.601
29.253
29.221
29.149
27.920
25.057
20.870
14.408
14.210
CO2Me
OC(O)OEt
9
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

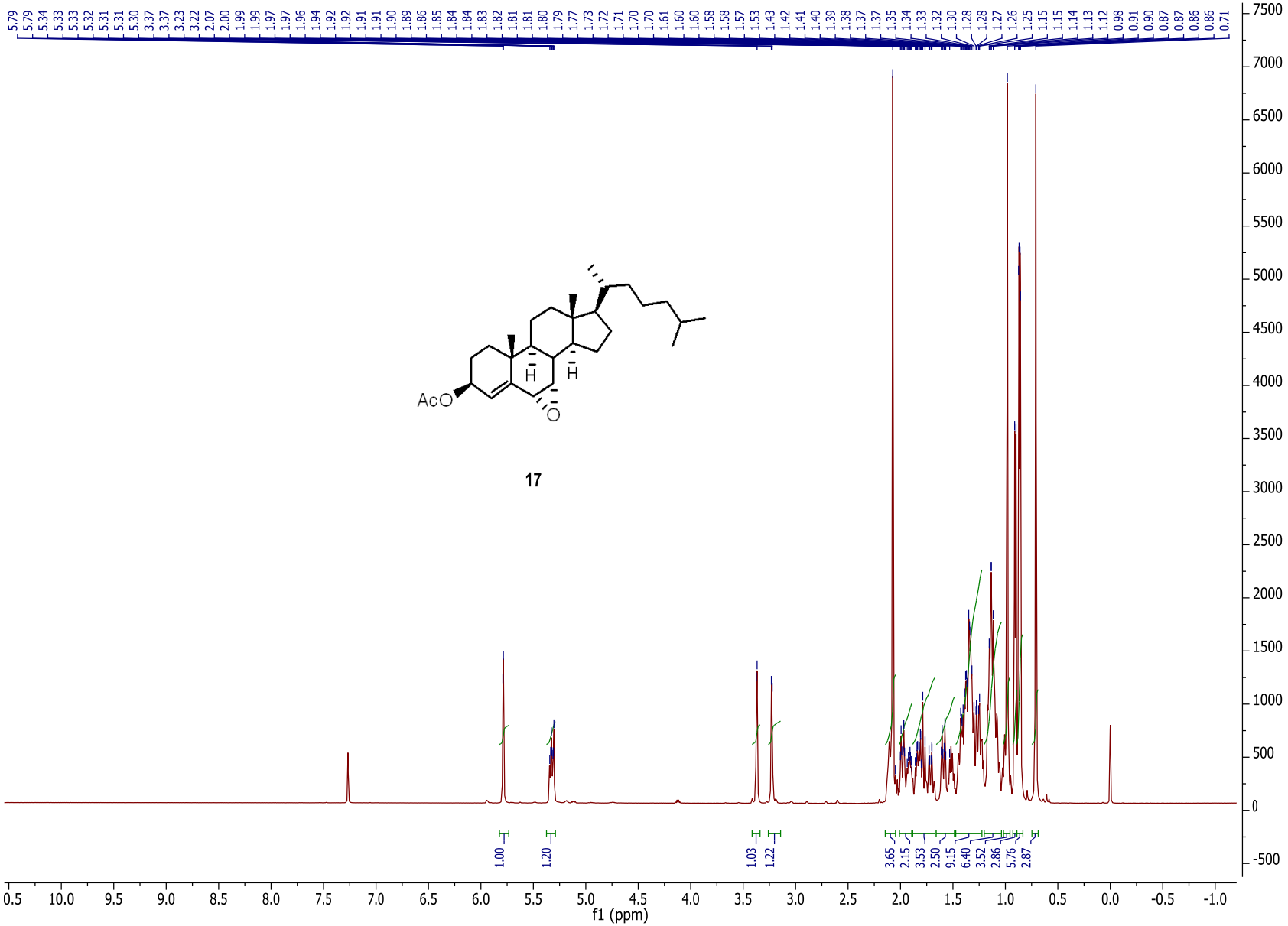

7.260
5.896
5.879
5.857
5.840
5.677
5.674
5.664
5.661
5.659
5.656
5.647
5.644
5.638
5.635
5.625
5.622
5.620
5.617
5.525
5.499
5.301
5.297
5.292
5.282
5.278
5.274
5.137
5.121
5.104
5.087
4.201
4.184
4.166
4.148
3.664
3.660
3.399
3.388
3.381
3.370
3.077
3.066
3.053
3.039
2.504
2.486
2.468
2.451
2.416
2.400
2.382
2.363
2.317
2.298
2.279
2.057
2.039
2.020
1.631
1.613
1.595
1.532
1.510
1.495
1.482
1.453
1.443
1.384
1.316
1.313
1.307
1.298
1.295
1.280
1.277
1.247
0.975
0.957
0.938
CO2Me
OC(O)OEt
10
1.000
1.018
0.929
0.943
0.982
2.079
3.166
0.979
0.994
2.282
2.115
2.093
19.301
3.028
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
f1 (ppm)

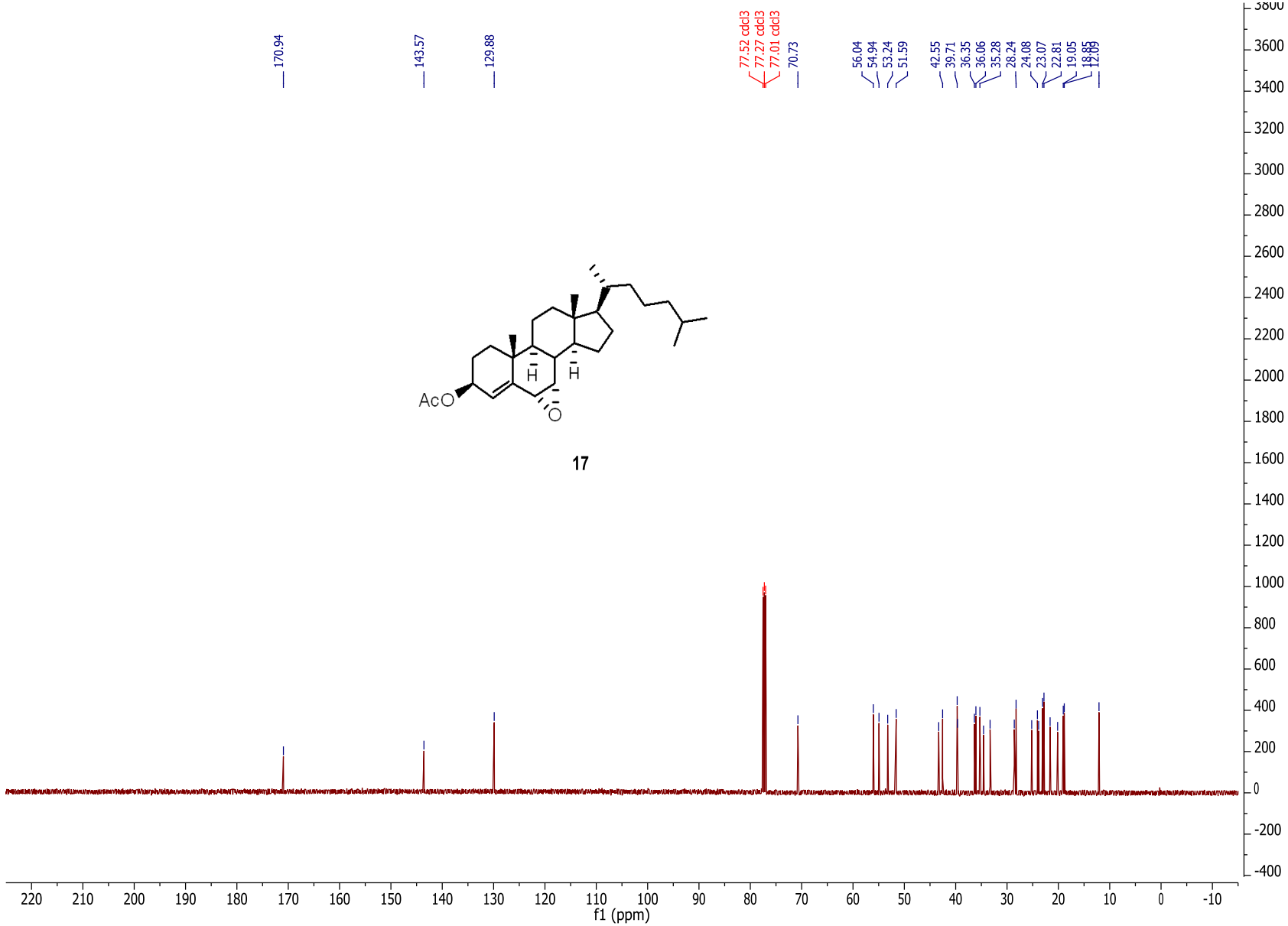

174.44
154.64
154.63
135.41
135.37
133.54
133.34
128.30
128.03
122.49
122.42
77.57 cdcl3
77.46
77.34
77.25 cdcl3
76.93 cdcl3
64.12
59.13
59.06
56.37
56.22
51.67
34.26
32.36
29.43
29.40
29.39
29.24
27.86
26.45
25.10
20.94
14.48
14.46
14.26
CO2Me
OC(O)OEt
O
10
f1 (ppm)


5.80
5.78
5.76
5.74
5.72
5.55
5.53
5.52
5.51
5.50
5.49
5.38
5.36
5.34
5.32
5.18
5.16
5.13
3.31
3.31
3.24
3.23
3.22
3.21
2.84
2.82
2.81
2.80
2.07
2.05
2.03
1.92
1.91
1.23
1.21
1.19
1.18
1.17
1.16
1.15
1.14
1.14
1.12
1.12
1.10
1.09
1.08
1.07
1.07
0.85
0.83
0.83
0.82
CO2Me
(7:3)
12
O
+
CO2Me
O
13
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
1.00
0.30
0.95
0.31
3.43
0.89
0.94
3.01
1.84
3.60
20.66
3.53
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
-0.5
-1.0
f1 (ppm)

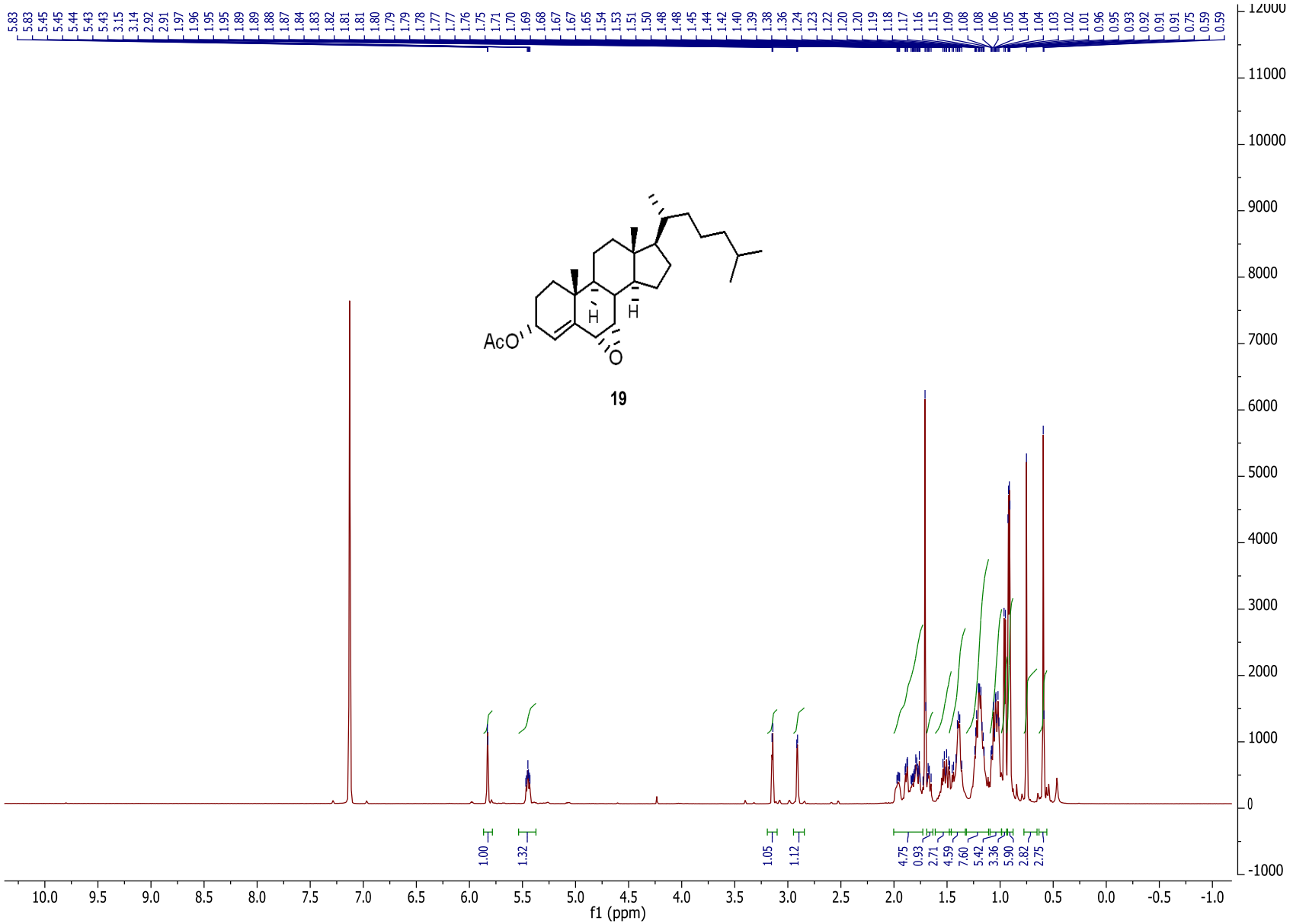

LGK-II-121-20
CDCl3 / 500 MHz
1.000
0.097
0.101
0.107
0.095
0.022
F1 (ppm)

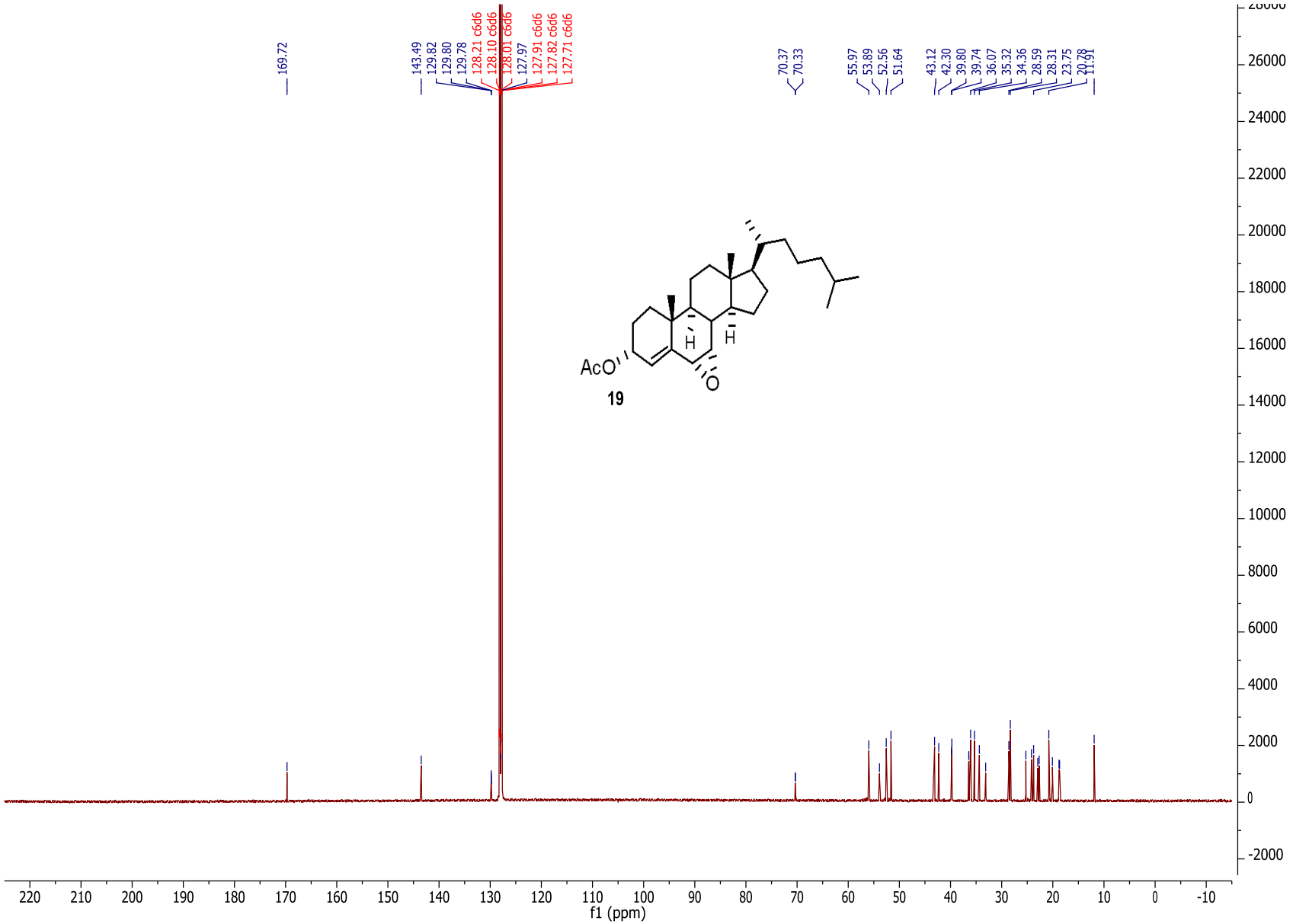

LGK-II-121-20
CDCl3 / 125 MHz
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

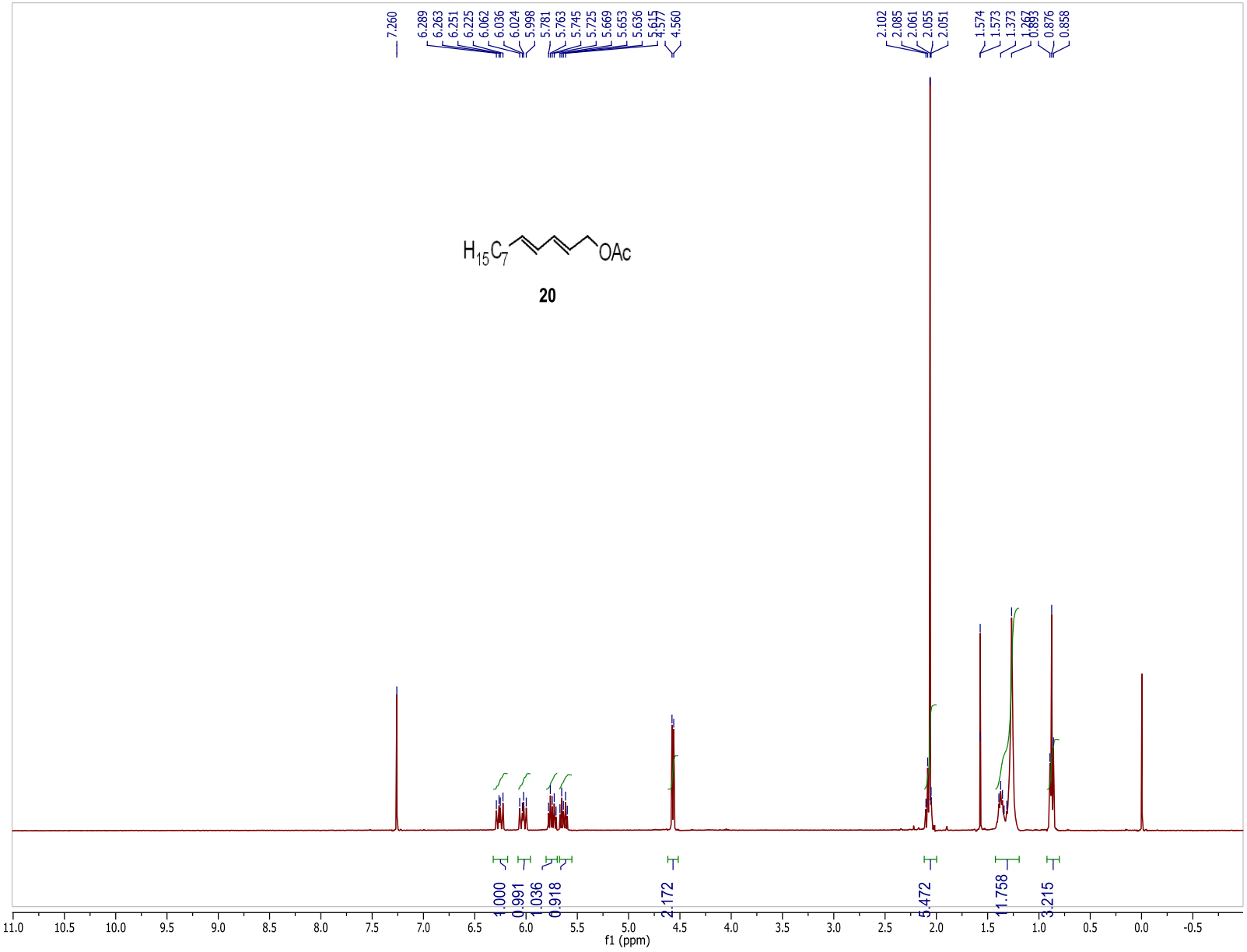

AcO
H
H
O
17
f1 (ppm)

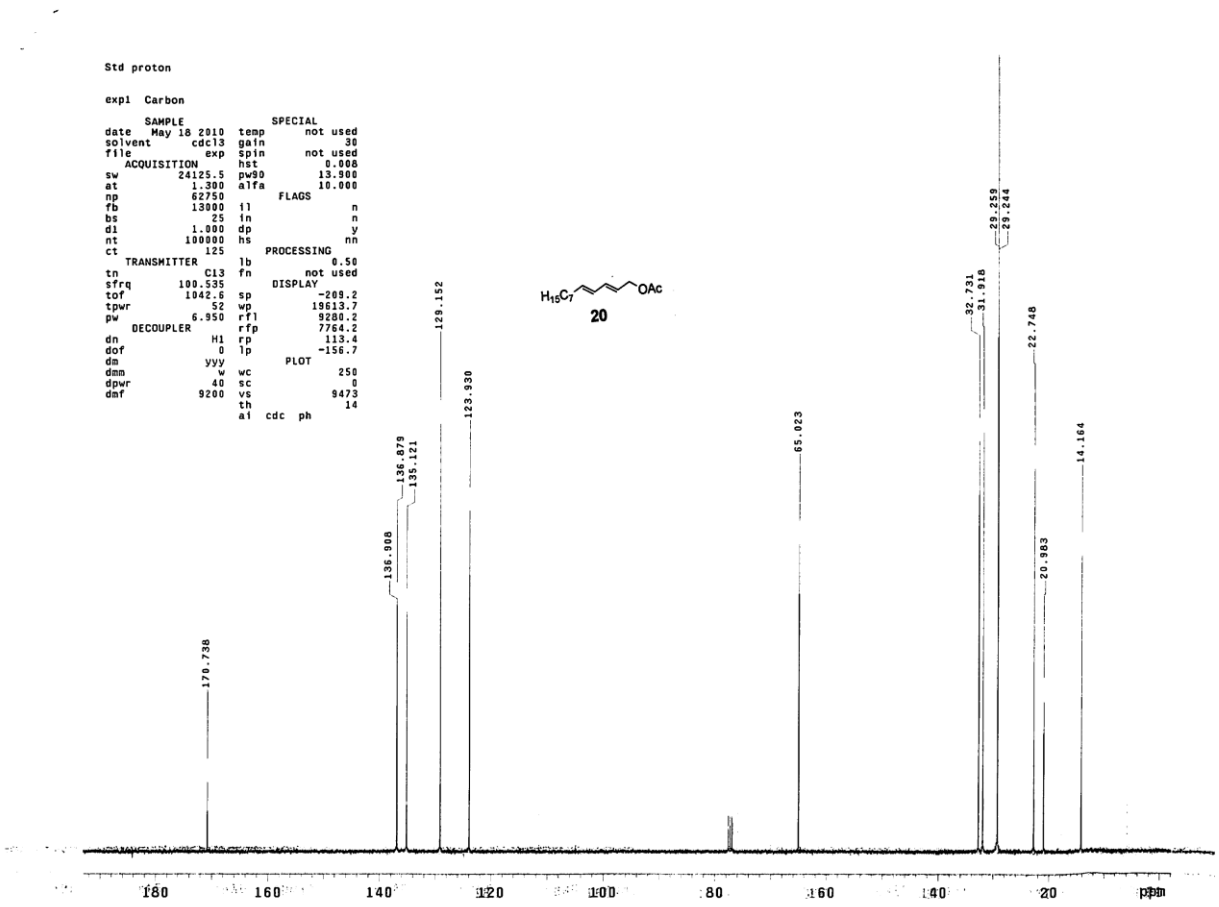

170.94
143.57
129.88
77.52 cdcl3
77.27 cdcl3
77.01 cdcl3
70.73
56.04
54.94
53.24
51.59
42.55
39.71
36.35
36.06
35.28
28.24
24.08
23.07
22.81
19.05
18.85
12.09
AcO
H
H
O
f1 (ppm)

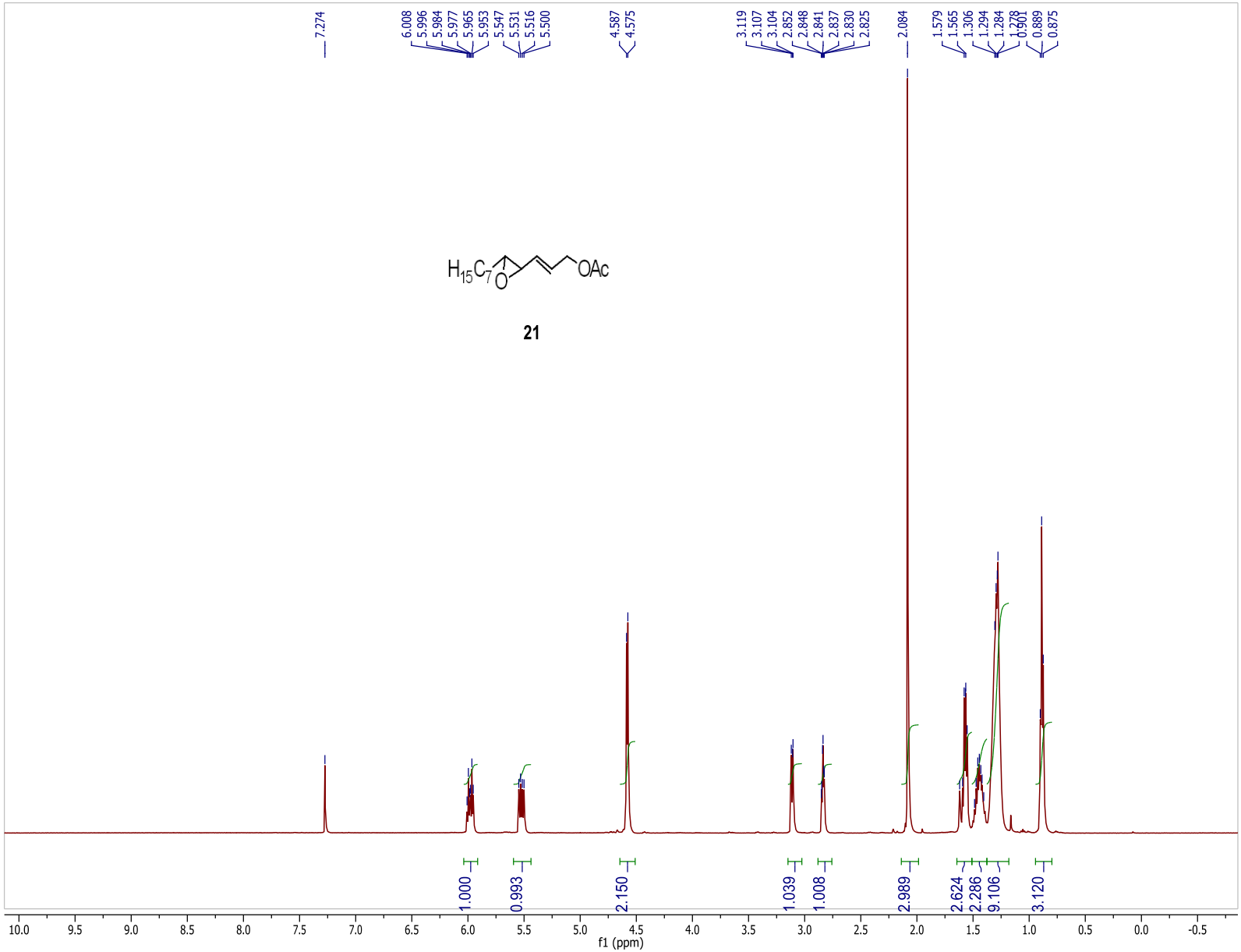
17

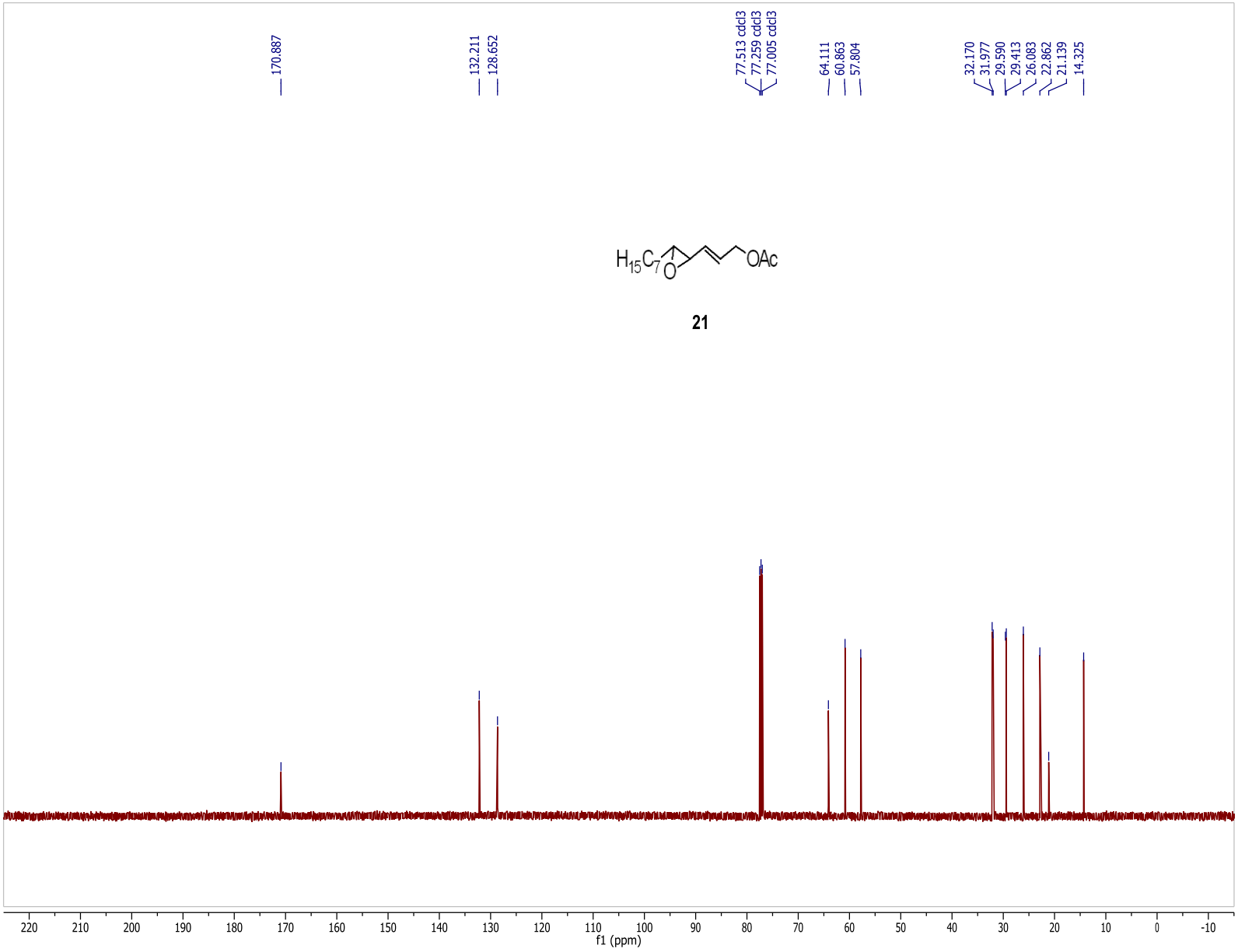

AcO
O
H
H
19
f1 (ppm)


169.72
143.49
129.82
129.80
129.78
128.21 c6d6
128.10 c6d6
128.01 c6d6
127.97
127.91 c6d6
127.82 c6d6
127.71 c6d6
70.37
70.33
55.97
53.89
52.56
51.64
43.12
42.30
39.80
39.74
36.07
35.32
34.36
28.59
28.31
23.75
20.78
11.91
AcO
O
H
H
19
f1 (ppm)


7.260
6.289
6.263
6.251
6.225
6.062
6.036
6.024
5.998
5.781
5.763
5.745
5.725
5.669
5.653
5.636
5.615
5.577
4.560
2.102
2.085
2.061
2.055
2.051
1.574
1.573
1.373
1.267
0.893
0.876
0.858
H15C7
OAc
20
1.000
0.991
1.036
0.918
2.172
5.472
11.758
3.215
f1 (ppm)


Std proton
exp1 Carbon
SAMPLE
date May 18 2010
solvent cdcl3
file exp
ACQUISITION
sw 24125.5
at 1.300
np 62750
fb 13000
bs 25
d1 1.000
nt 100800
ct 125
TRANSMITTER
tn C13
sfrq 100.535
tof 1042.6
tpwr 52
pw 6.950
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 40
dmf 9200
SPECIAL
temp not used
gain 30
spin not used
hst 0.008
pw90 13.900
alfa 10.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.50
fn not used
DISPLAY
sp -209.2
wp 19613.7
rfl 9280.2
rfp 7764.2
rp 113.4
lp -156.7
PLOT
wc 250
sc 0
vs 9473
th 14
ai cdc ph
H15C7
OAc
20
170.738
136.908
136.879
135.121
129.152
123.930
65.023
32.731
31.918
29.259
29.244
22.748
20.983
14.164
180
160
140
120
100
80
60
40
20
ppm


7.274
6.008
5.996
5.984
5.977
5.965
5.953
5.547
5.531
5.516
5.500
4.587
4.575
3.119
3.107
3.104
2.852
2.848
2.841
2.837
2.830
2.825
2.084
1.579
1.565
1.306
1.294
1.284
1.278
0.901
0.889
0.875
H15C7
O
OAc
21
1.000
0.993
2.150
1.039
1.008
2.989
2.624
2.286
9.106
3.120
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
-0.5
f1 (ppm)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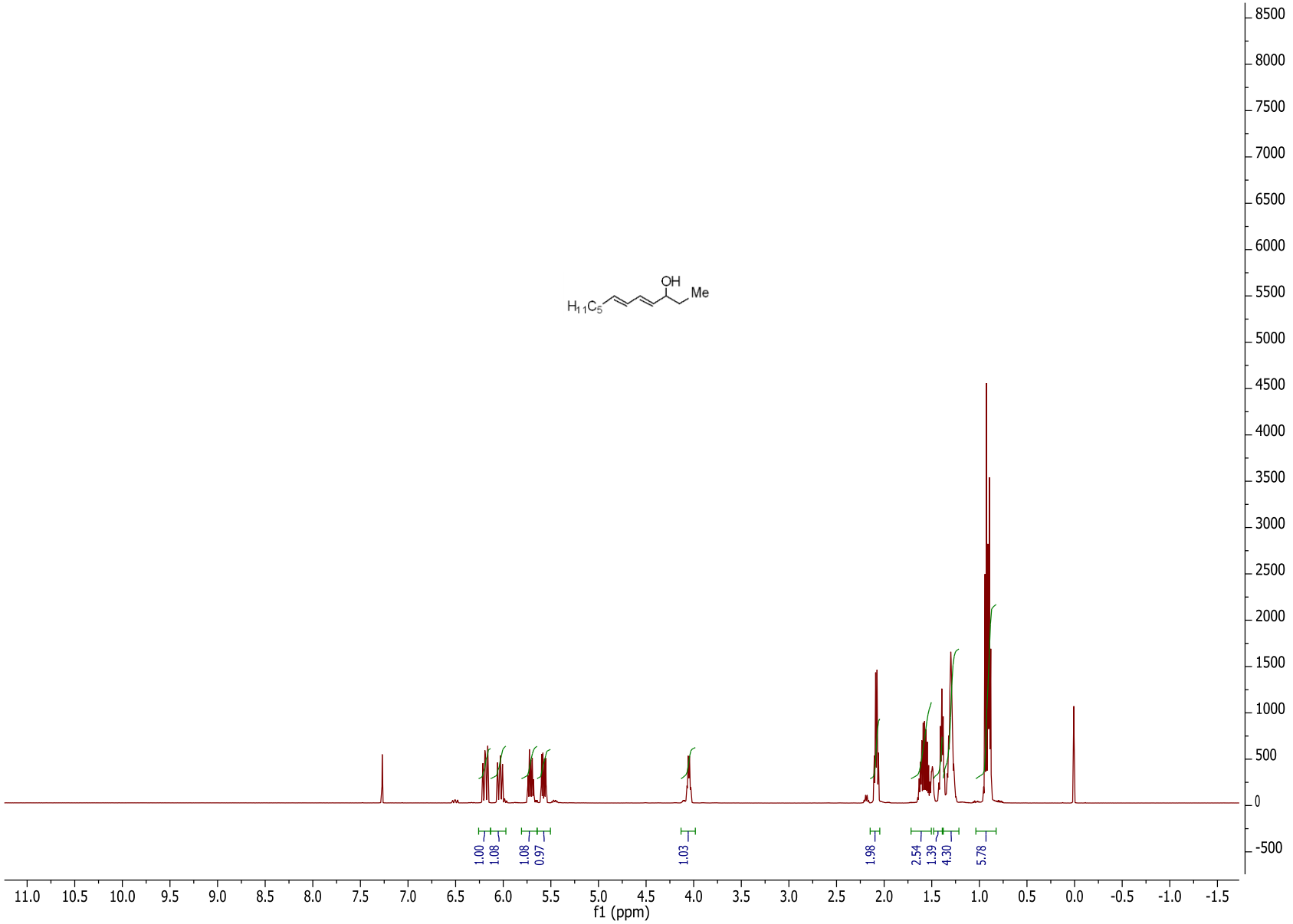
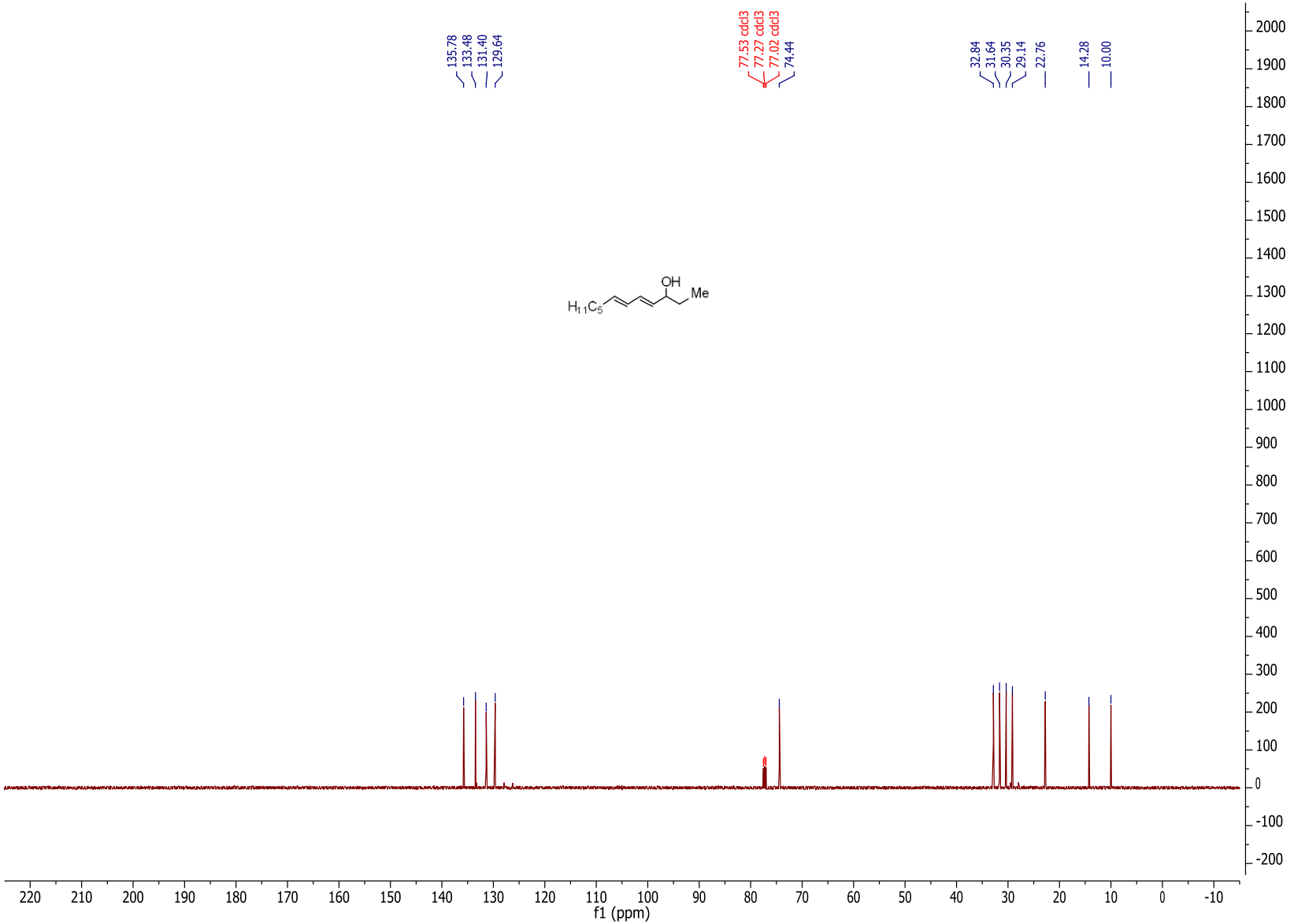
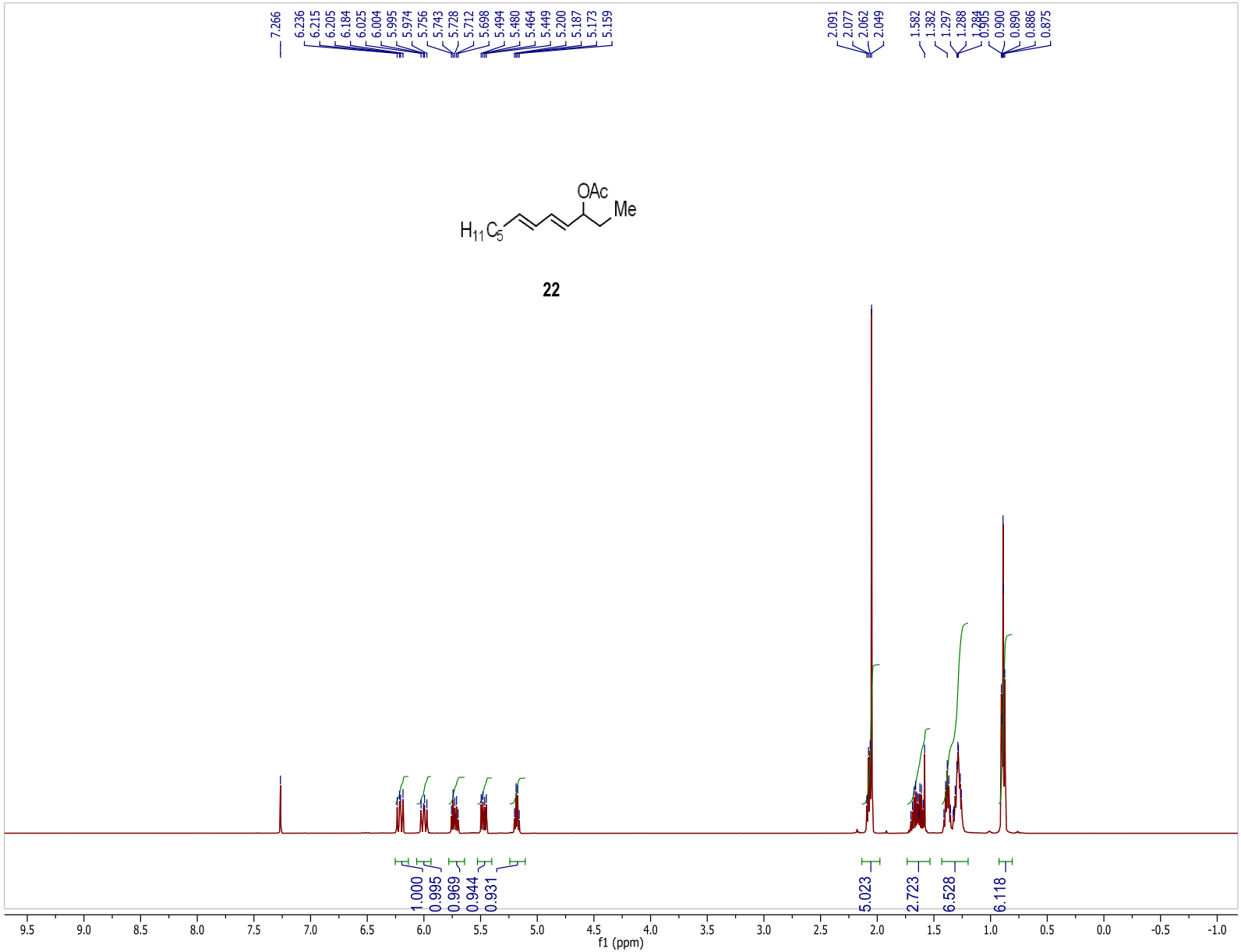
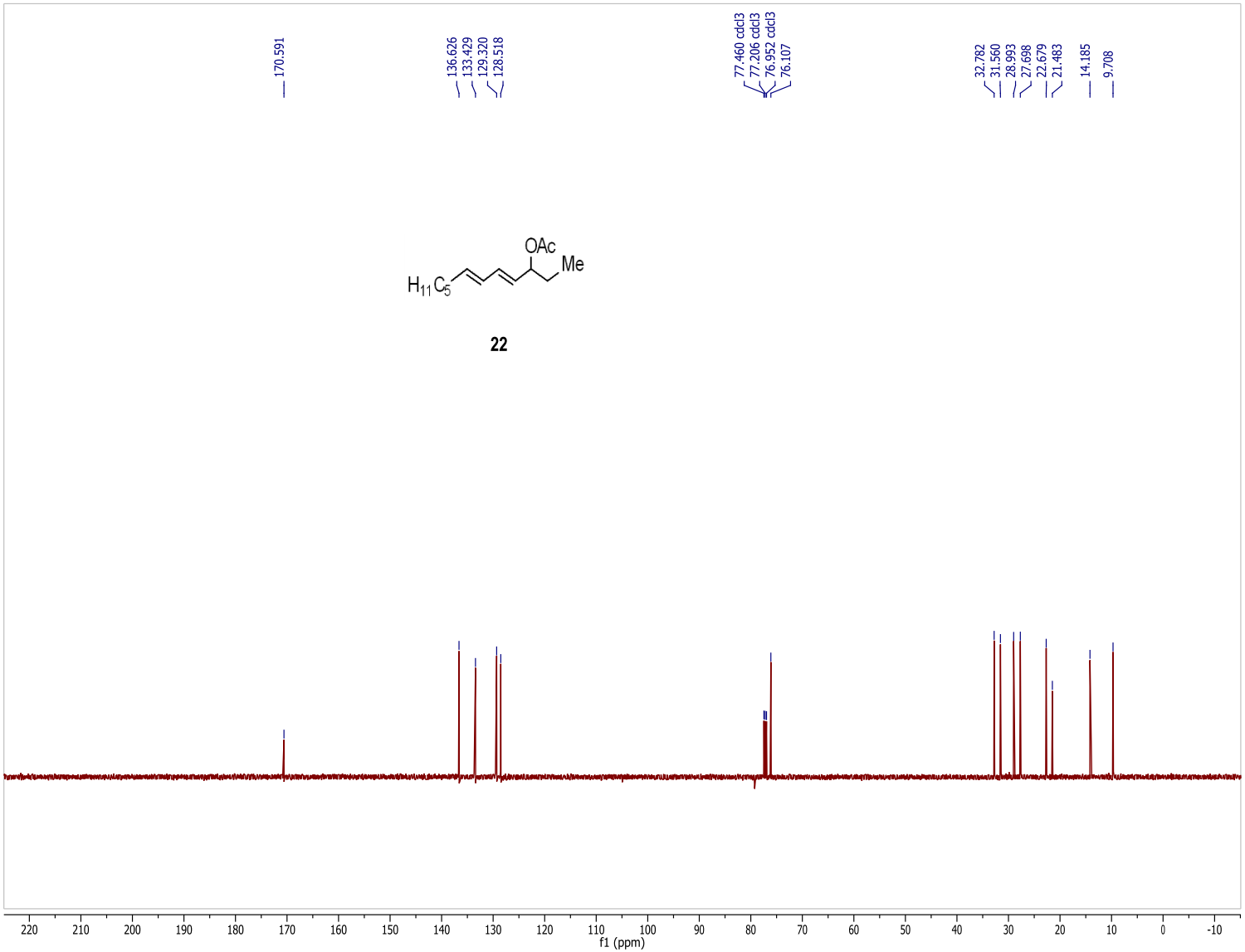
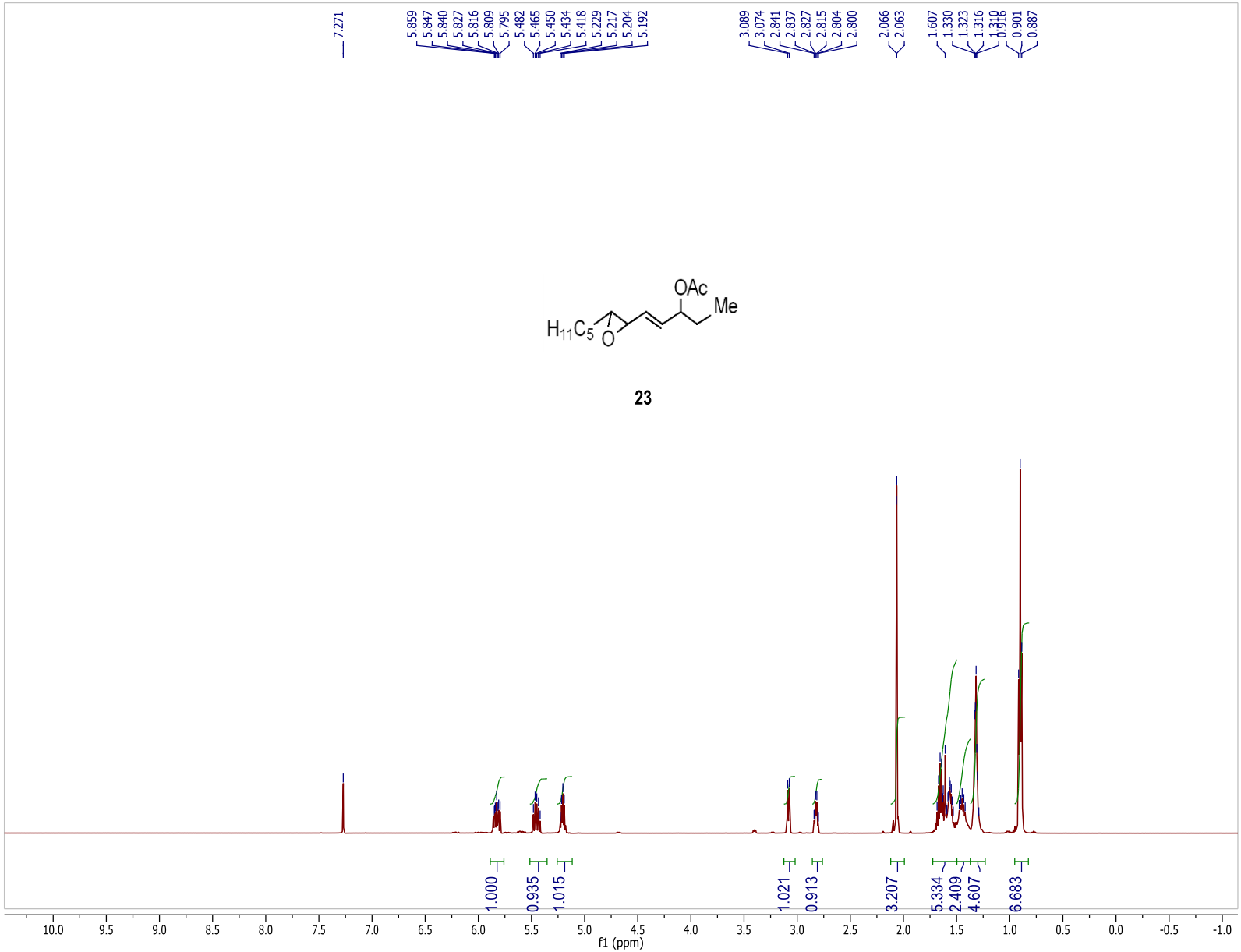
132.211
128.652
77.513 cdcl3
77.259 cdcl3
77.005 cdcl3
64.111
60.863
57.804
32.170
31.977
29.590
29.413
26.083
22.862
21.139
14.325
H15C7
O
OAc
21
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


OH
Me
H11C5
1.00
1.08
1.08
0.97
1.03
1.98
2.54
1.39
4.30
5.78
f1 (ppm)

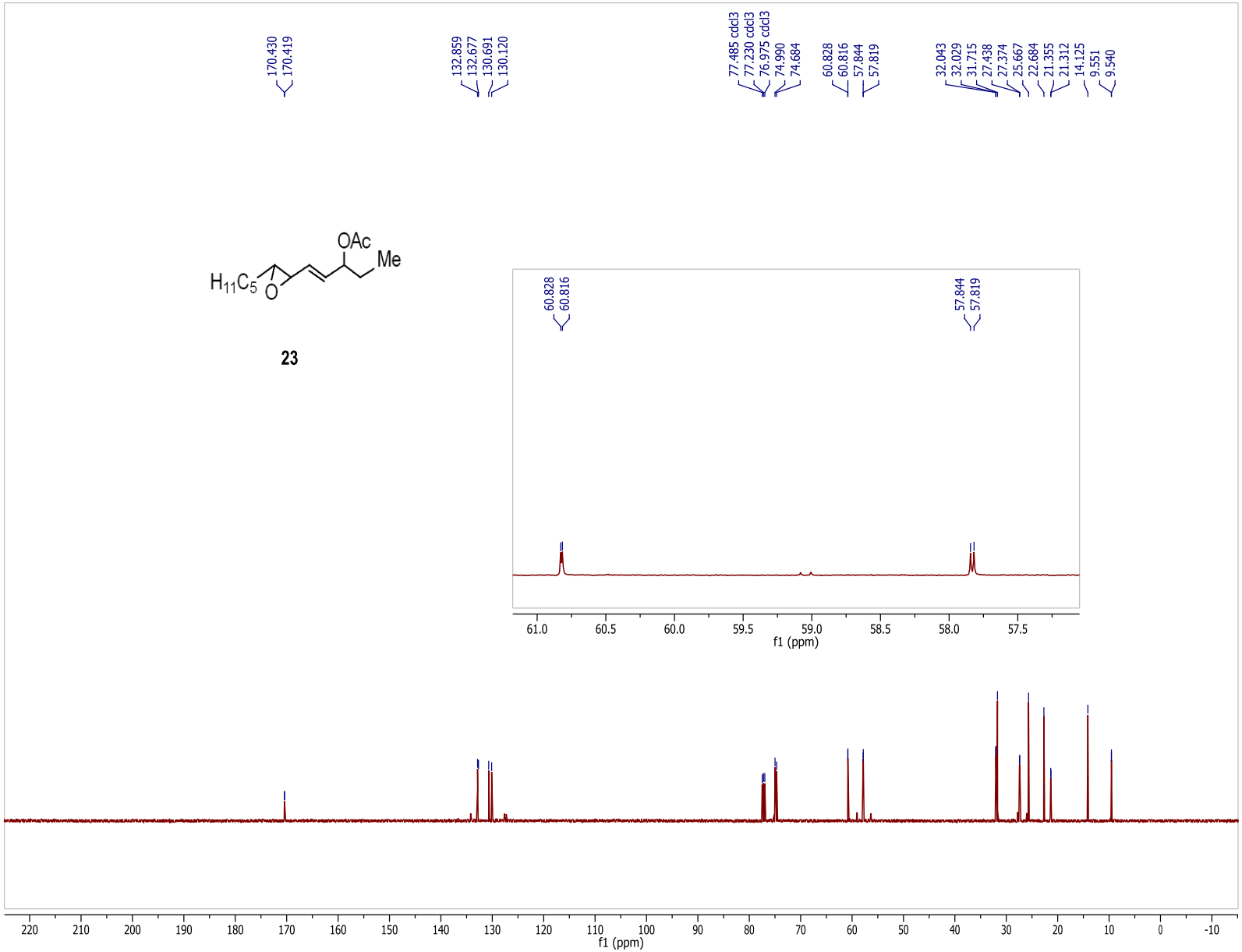

135.78
133.48
131.40
129.64
77.53 cdcl3
77.27 cdcl3
77.02 cdcl3
74.44
32.84
31.64
30.35
29.14
22.76
14.28
10.00
OH
Me
H11C5
f1 (ppm)

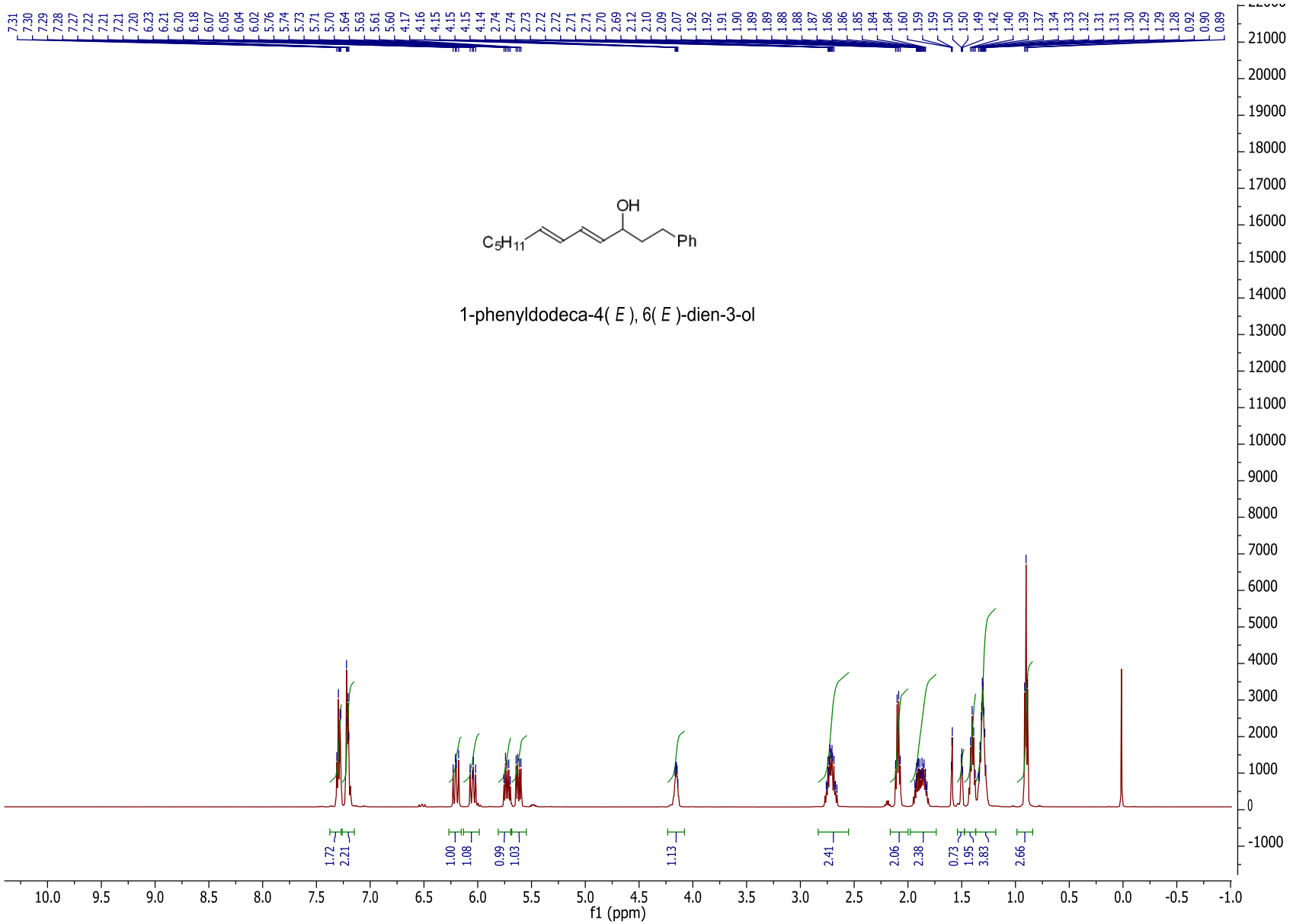

7.266
6.236
6.215
6.205
6.184
6.025
6.004
5.995
5.974
5.756
5.743
5.728
5.712
5.698
5.494
5.480
5.464
5.449
5.200
5.187
5.173
5.159
2.091
2.077
2.062
2.049
1.582
1.382
1.297
1.288
1.284
0.900
0.890
0.886
0.875
OAc
Me
H11C5
22
1.000
0.995
0.969
0.944
0.931
5.023
2.723
6.528
6.118
f1 (ppm)

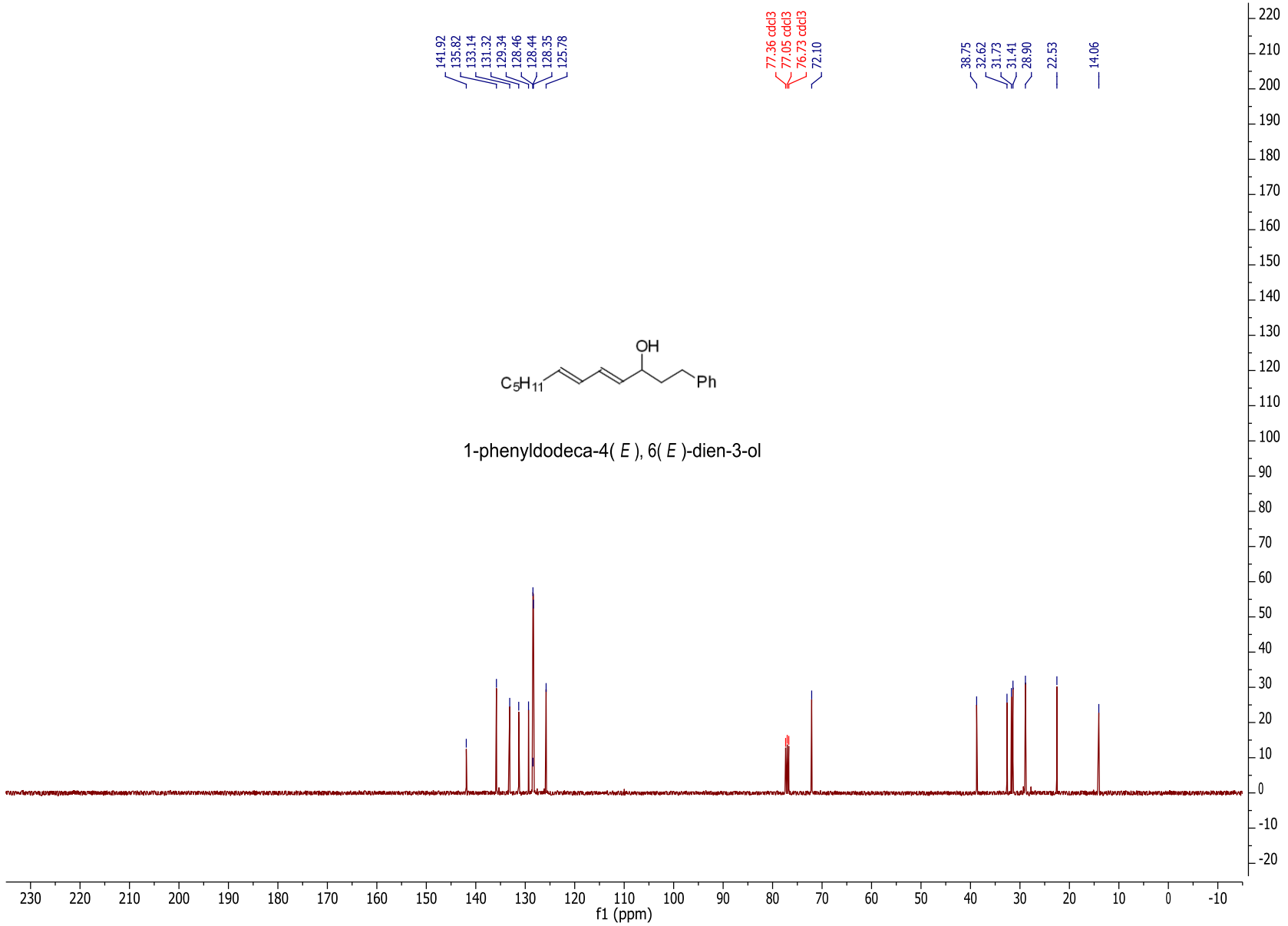

170.591
136.626
133.429
129.320
128.518
77.460 cdcl3
77.206 cdcl3
76.952 cdcl3
76.107
32.782
31.560
28.993
27.698
22.679
21.483
14.185
9.708
OAc
Me
H11C5
22
f1 (ppm)


7.271
5.859
5.847
5.840
5.827
5.816
5.809
5.795
5.482
5.465
5.450
5.434
5.418
5.229
5.217
5.204
5.192
3.089
3.074
2.841
2.837
2.827
2.815
2.804
2.800
2.066
2.063
1.607
1.330
1.323
1.316
1.310
0.916
0.901
0.887
OAc
Me
H11C5
O
1.000
0.935
1.015
1.021
0.913
3.207
5.334
2.409
4.607
6.683
f1 (ppm)

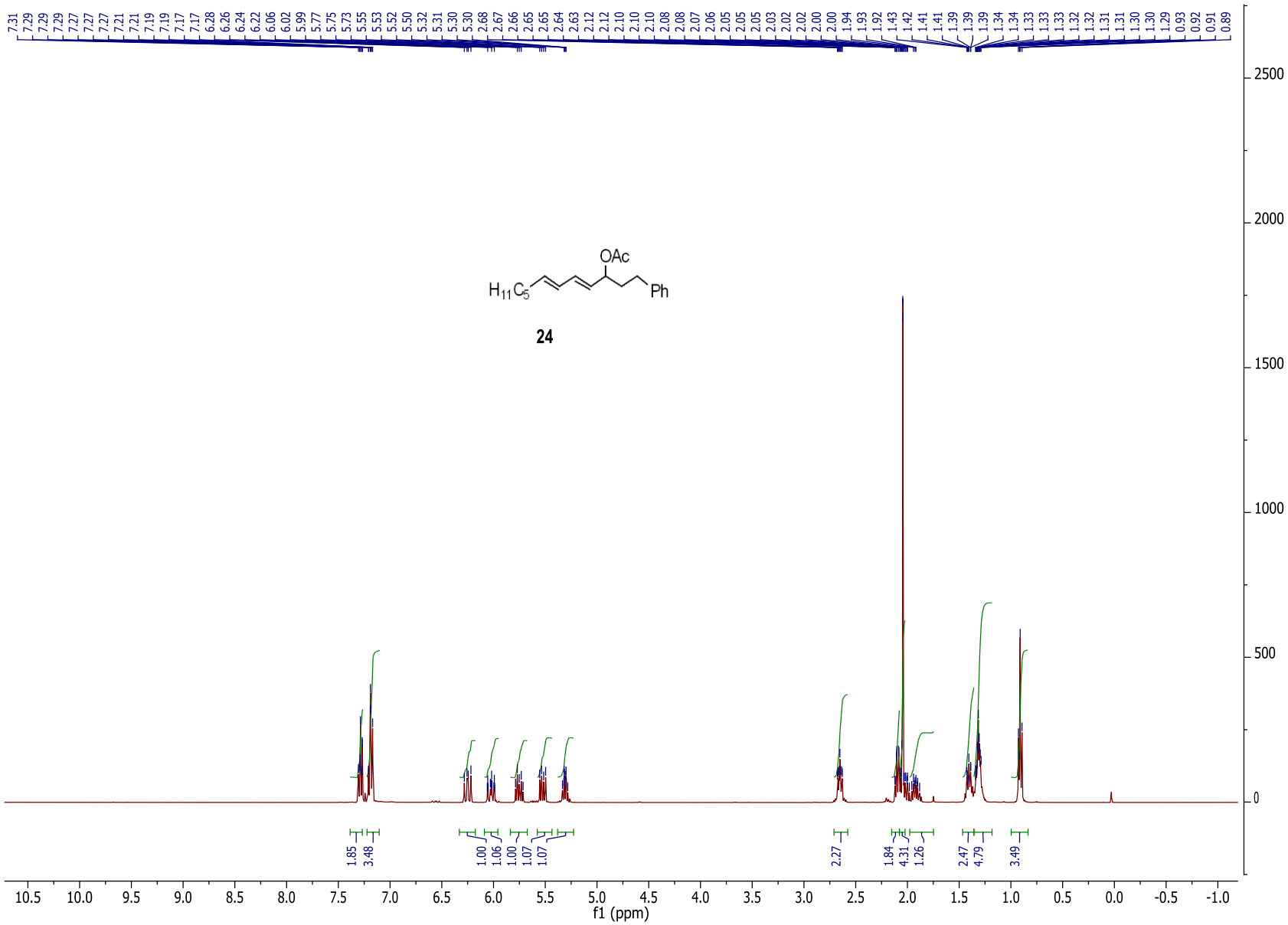
23

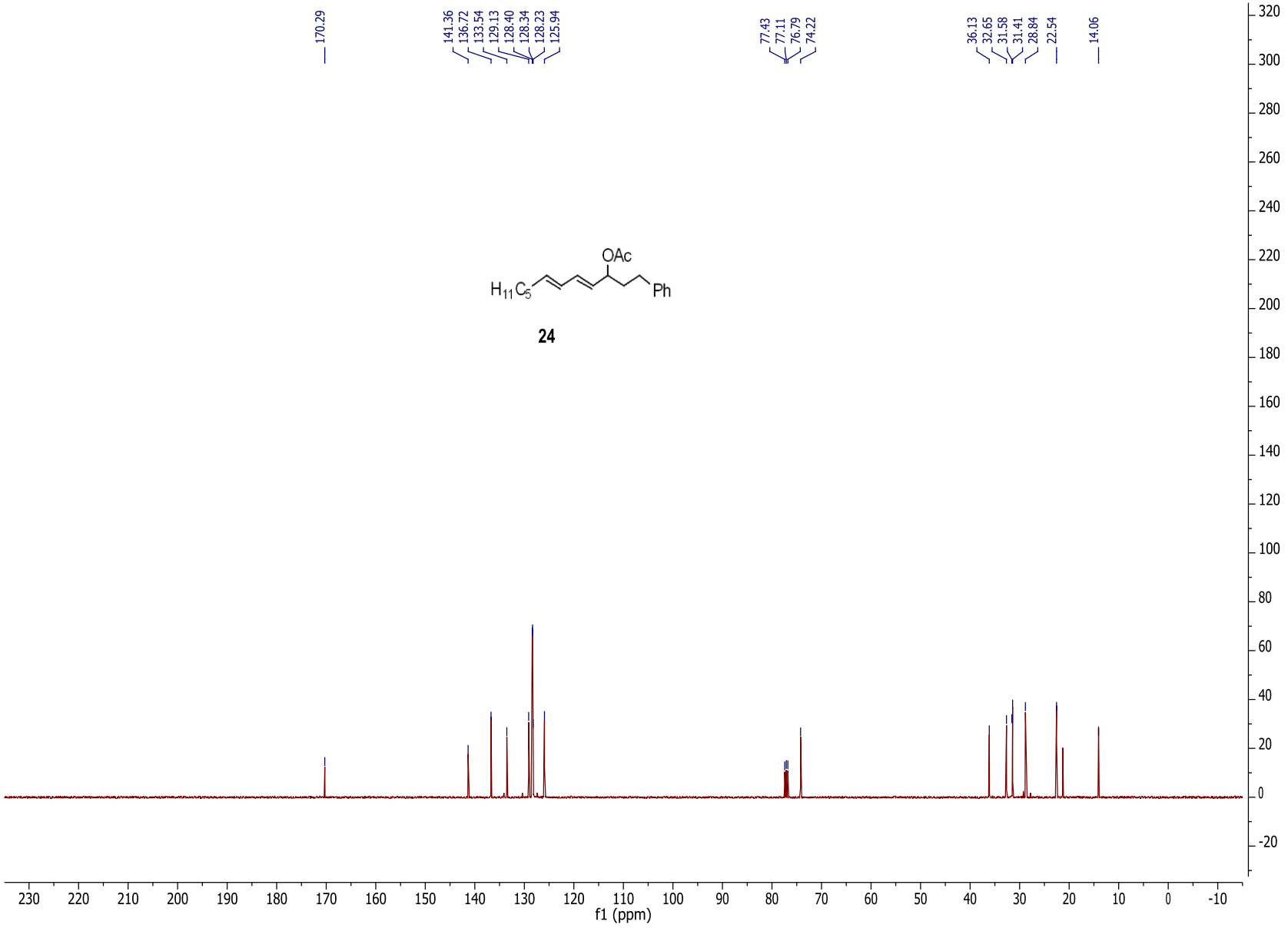

170.430
170.419
132.859
132.677
130.691
130.120
77.485 cdcl3
77.230 cdcl3
76.975 cdcl3
74.990
74.684
60.828
60.816
57.844
57.819
32.043
32.029
31.715
27.438
27.374
25.667
22.684
21.355
21.312
14.125
9.551
9.540
OAc
Me
H11C5
O
23
60.828
60.816
57.844
57.819
61.0
60.5
60.0
59.5
59.0
58.5
58.0
57.5
f1 (ppm)
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 (ppm)

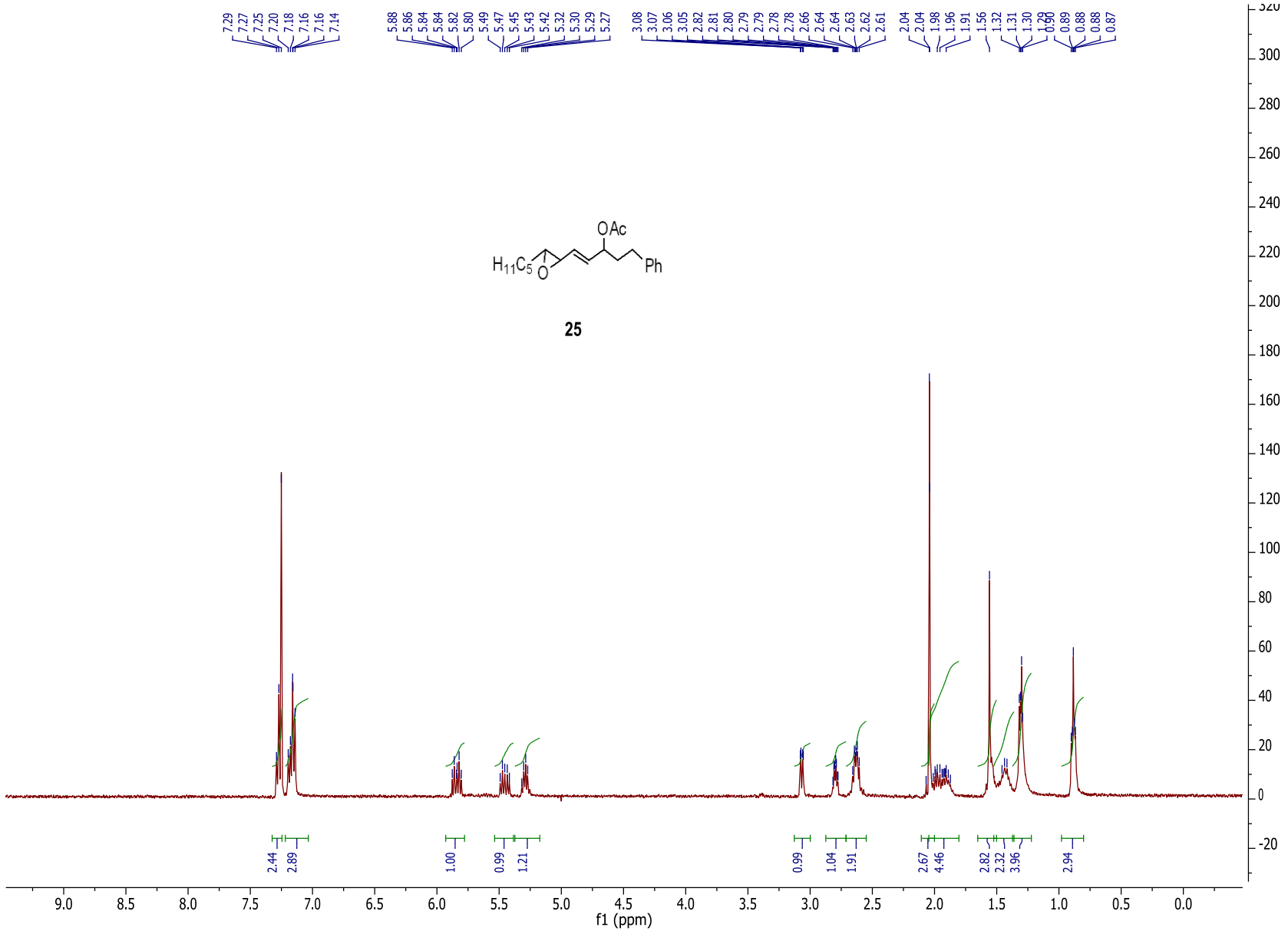

OH
C5H11
Ph
1-phenyldodeca-4(E), 6(E)-dien-3-ol
f1 (ppm)

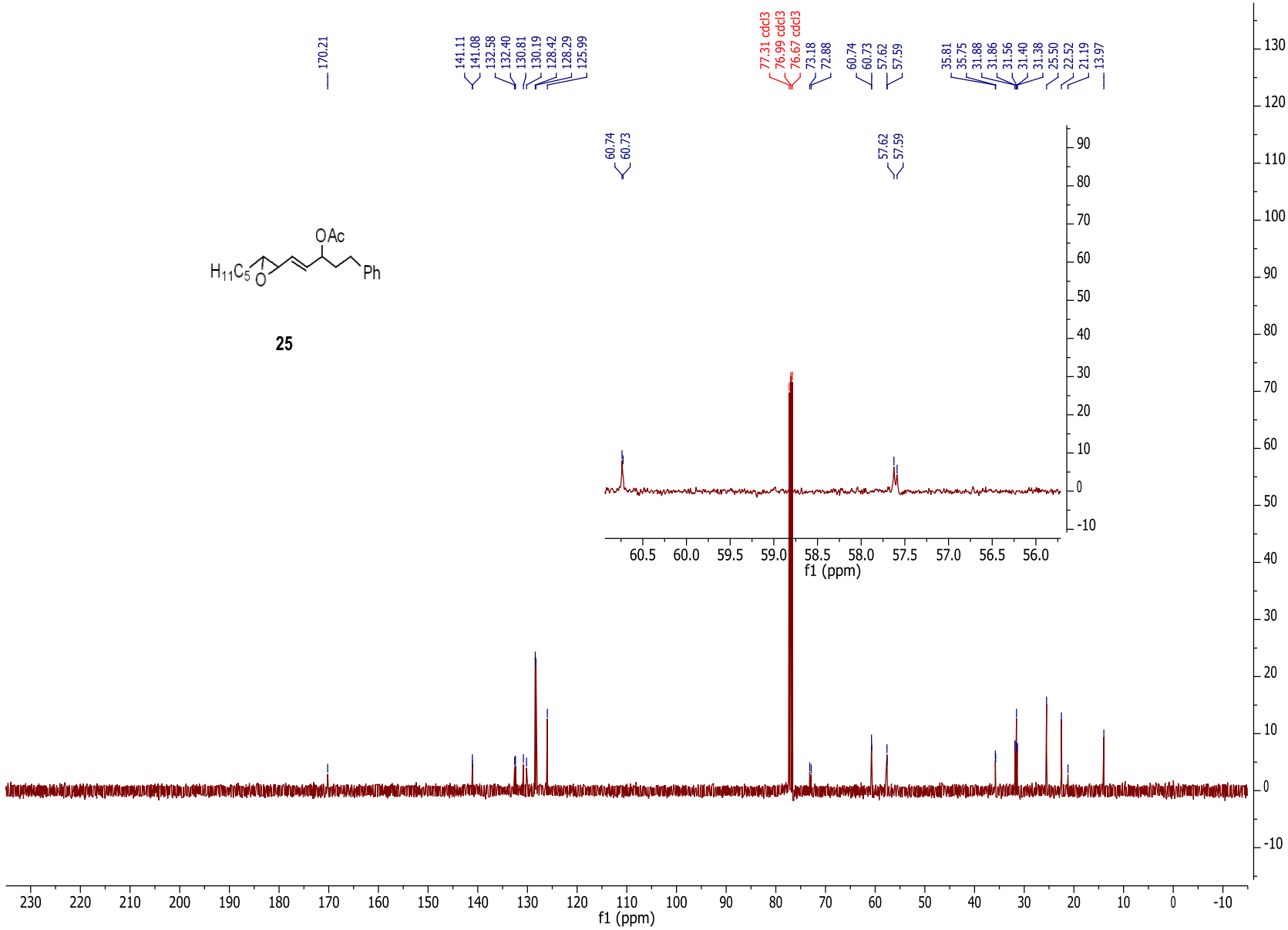


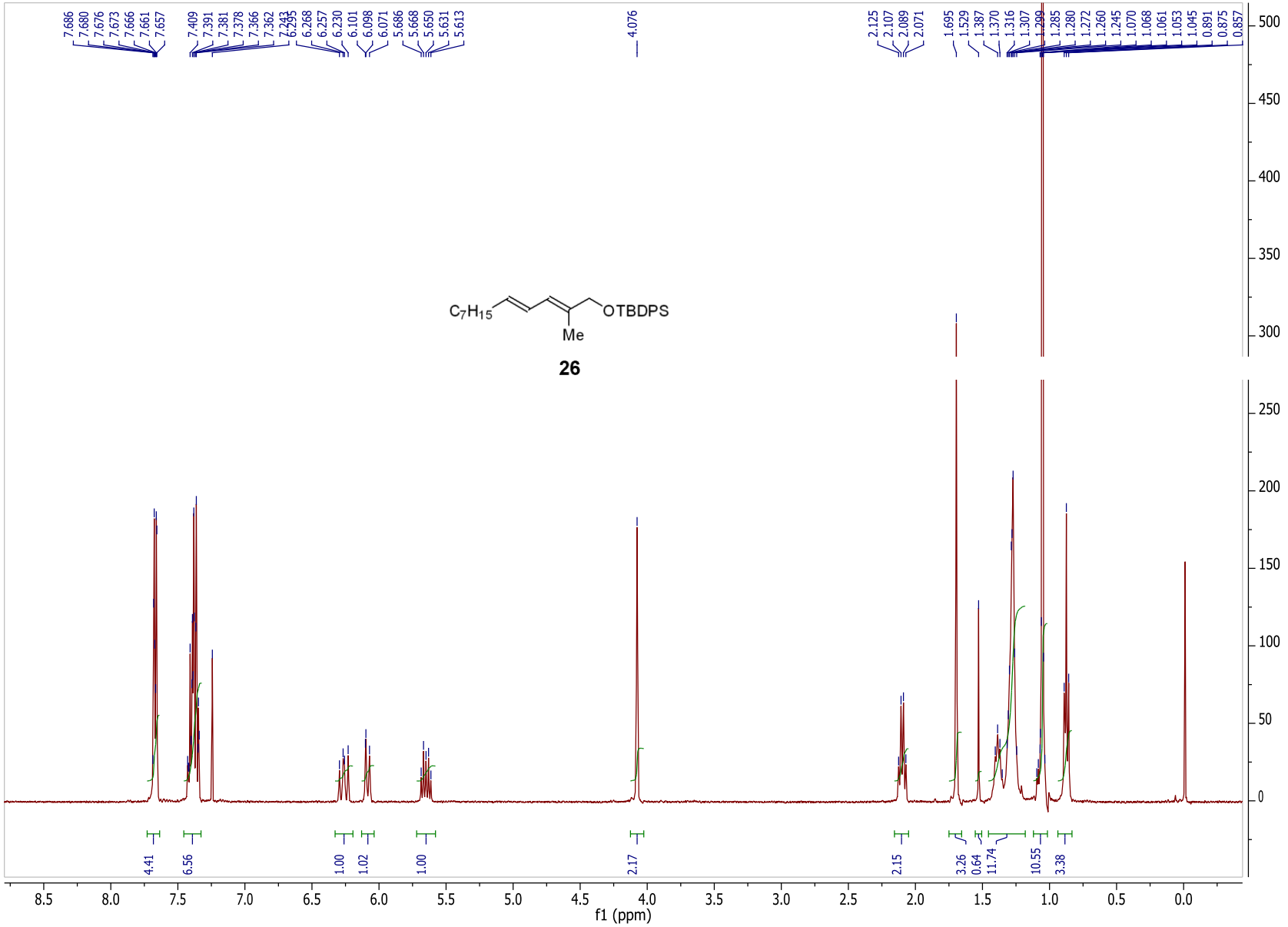
1-phenyldodeca-4(*E*), 6(*E*)-dien-3-ol


OAc
H11C5
Ph
24
f1 (ppm)


170.29
141.36
136.72
133.54
129.13
128.40
128.34
128.23
125.94
77.43
77.11
76.79
74.22
36.13
32.65
31.58
31.41
28.84
22.54
14.06
OAc
H11C5
Ph
24
f1 (ppm)


7.29 7.27 7.25 7.20 7.18 7.16 7.16 7.14
5.88 5.86 5.84 5.84 5.82 5.80 5.49 5.47 5.45 5.43 5.42 5.32 5.30 5.29 5.27
3.08 3.07 3.06 3.05 2.82 2.81 2.80 2.79 2.79 2.78 2.78 2.66 2.64 2.64 2.63 2.62 2.61
2.04 2.04 1.98 1.96 1.91 1.56 1.32 1.31 1.30 0.90 0.89 0.88 0.88 0.87
OAc
H11C5
O
Ph
25
2.44 2.89 1.00 0.99 1.21 0.99 1.04 1.91 2.67 4.46 2.82 2.32 3.96 2.94
f1 (ppm)


170.21
141.11
141.08
132.58
132.40
130.81
130.19
128.42
128.29
125.99
77.31 cdcl3
76.99 cdcl3
76.67 cdcl3
73.18
72.88
60.74
60.73
57.62
57.59
35.81
35.75
31.88
31.86
31.56
31.40
31.38
25.50
22.52
21.19
13.97
OAc
H11C5
O
Ph
25
f1 (ppm)
f1 (ppm)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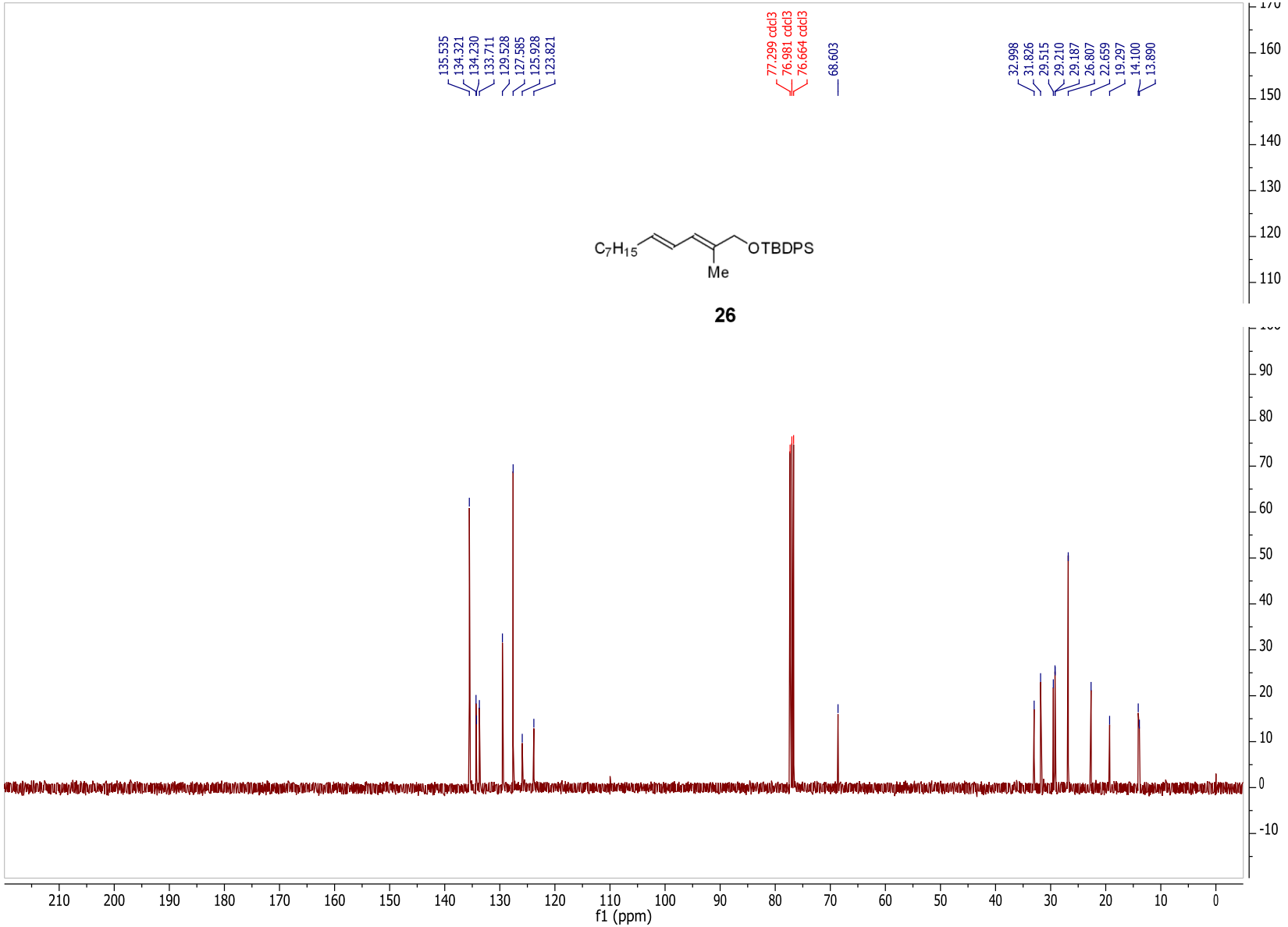
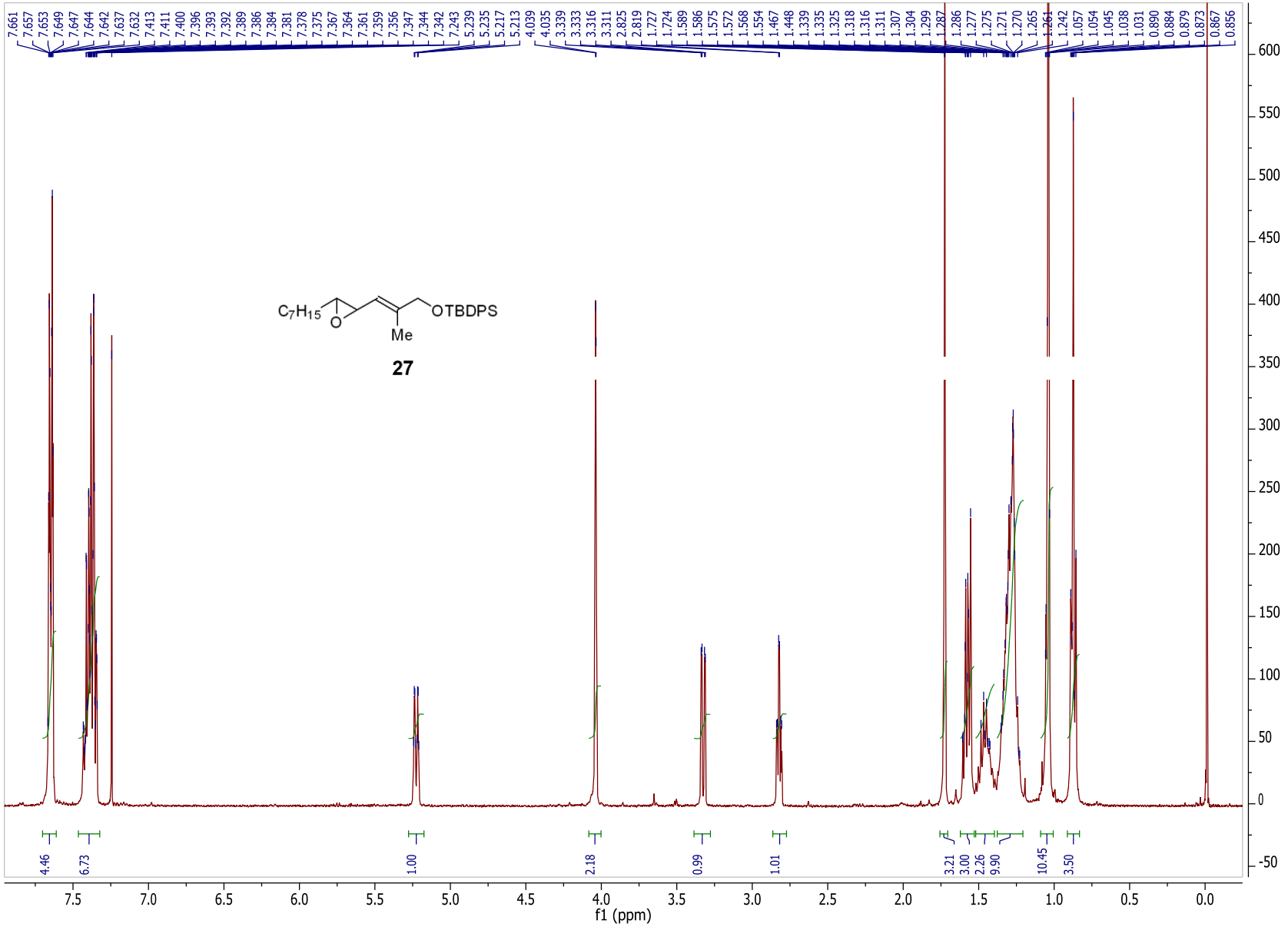
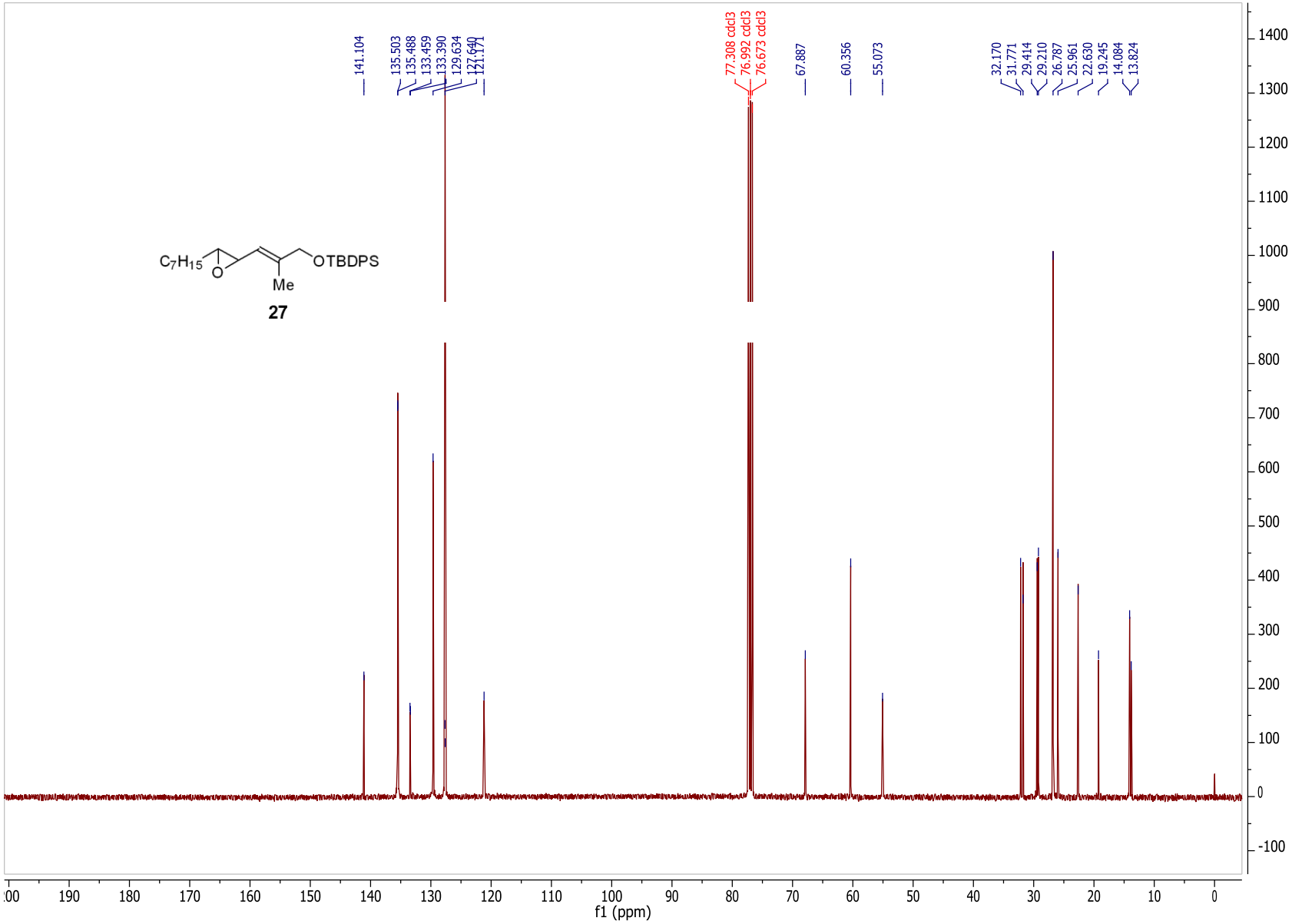
7.680
7.676
7.673
7.666
7.661
7.657
7.409
7.391
7.381
7.378
7.366
7.362
7.243
6.295
6.268
6.257
6.230
6.101
6.098
6.071
5.686
5.668
5.650
5.631
5.613
4.076
2.125
2.107
2.089
2.071
1.695
1.529
1.387
1.370
1.316
1.307
1.299
1.285
1.280
1.272
1.260
1.245
1.070
1.068
1.061
1.053
1.045
0.891
0.875
0.857
C7H15
OTBDPS
Me
26
4.41
6.56
1.00
1.02
1.00
2.17
2.15
3.26
0.64
11.74
10.55
3.38
f1 (ppm)


135.535
134.321
134.230
133.711
129.528
127.585
125.928
123.821
77.299 cdcl3
76.981 cdcl3
76.664 cdcl3
68.603
32.998
31.826
29.515
29.210
29.187
26.807
22.659
19.297
14.100
13.890
C7H15
OTBDPS
Me
26
f1 (ppm)


7.661 7.657 7.653 7.649 7.647 7.644 7.642 7.637 7.632 7.413 7.411 7.400 7.396 7.393 7.392 7.389 7.386 7.384 7.381 7.378 7.375 7.367 7.364 7.361 7.359 7.356 7.347 7.344 7.342 7.243 5.239 5.235 5.217 5.213 4.039 4.035 3.339 3.333 3.316 3.311 2.825 2.819 1.727 1.724 1.589 1.586 1.575 1.572 1.568 1.554 1.467 1.448 1.339 1.335 1.325 1.318 1.316 1.311 1.307 1.304 1.299 1.287 1.286 1.277 1.275 1.271 1.270 1.265 1.261 1.242 1.057 1.054 1.045 1.038 1.031 0.890 0.884 0.879 0.873 0.867 0.856
C7H15
O
OTBDPS
Me
27
4.46
6.73
1.00
2.18
0.99
1.01
3.21
3.00
2.26
9.90
10.45
3.50
f1 (ppm)


141.104
135.503
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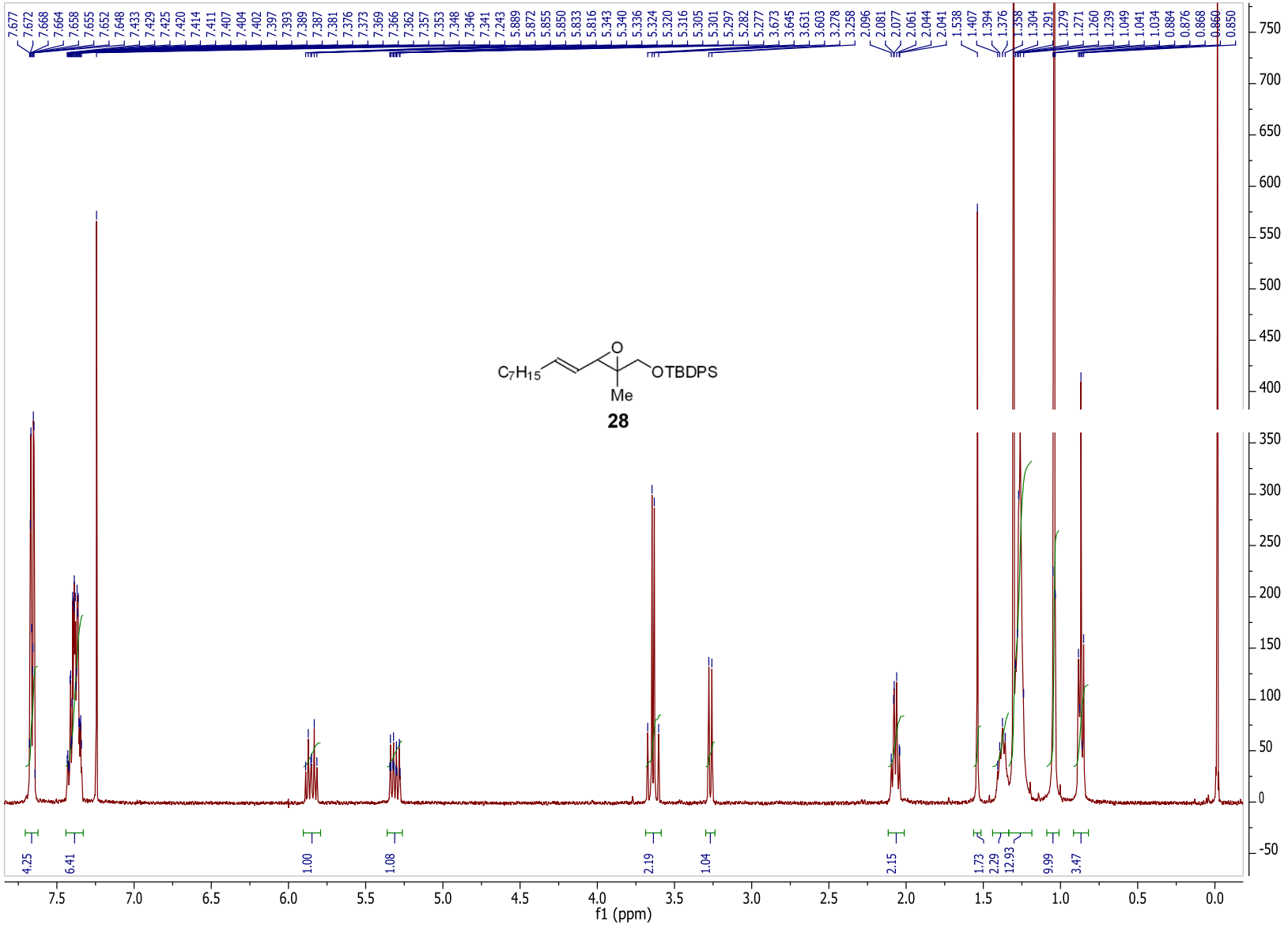
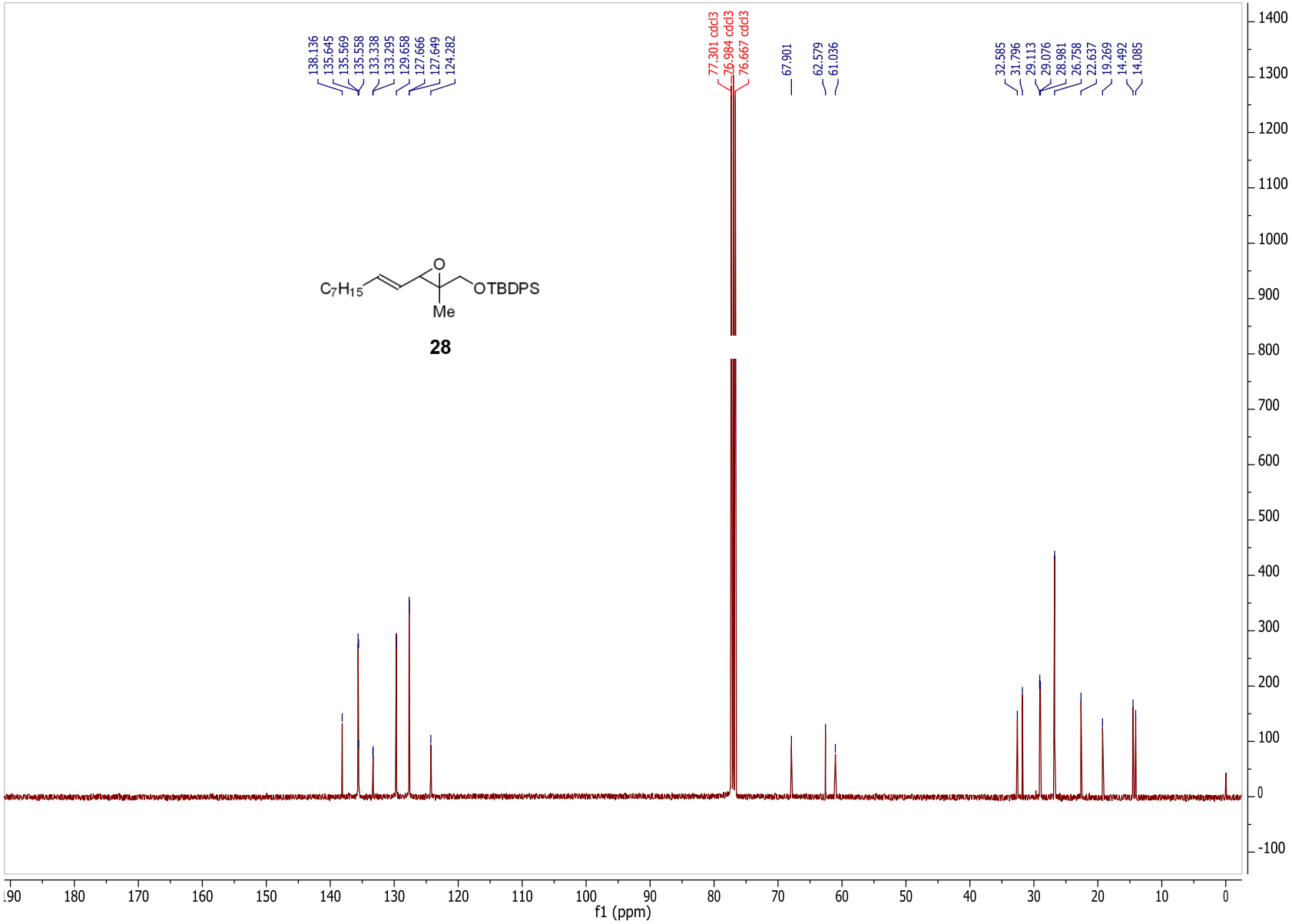
129.634
127.640
121.171
77.308 cdcl3
76.992 cdcl3
76.673 cdcl3
67.887
60.356
55.073
32.170
31.771
29.414
29.210
26.787
25.961
22.630
19.245
14.084
13.824
C7H15
O
OTBDPS
Me
27
f1 (ppm)


7.677 7.672 7.668 7.664 7.658 7.655 7.652 7.648 7.433 7.429 7.425 7.420 7.414 7.411 7.407 7.404 7.402 7.397 7.393 7.389 7.387 7.381 7.376 7.373 7.369 7.366 7.362 7.357 7.353 7.348 7.346 7.341 7.243 5.889 5.872 5.855 5.850 5.833 5.816 5.343 5.340 5.336 5.324 5.320 5.316 5.305 5.301 5.297 5.282 5.277 3.673 3.645 3.631 3.603 3.278 3.258 2.096 2.081 2.077 2.061 2.044 2.041 1.538 1.407 1.394 1.376 1.358 1.304 1.291 1.279 1.271 1.260 1.239 1.049 1.041 1.034 0.884 0.876 0.868 0.860 0.850
C7H15
O
OTBDPS
Me
28
4.25 6.41 1.00 1.08 2.19 1.04 2.15 1.73 2.29 12.93 9.99 3.47
f1 (ppm)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135.558
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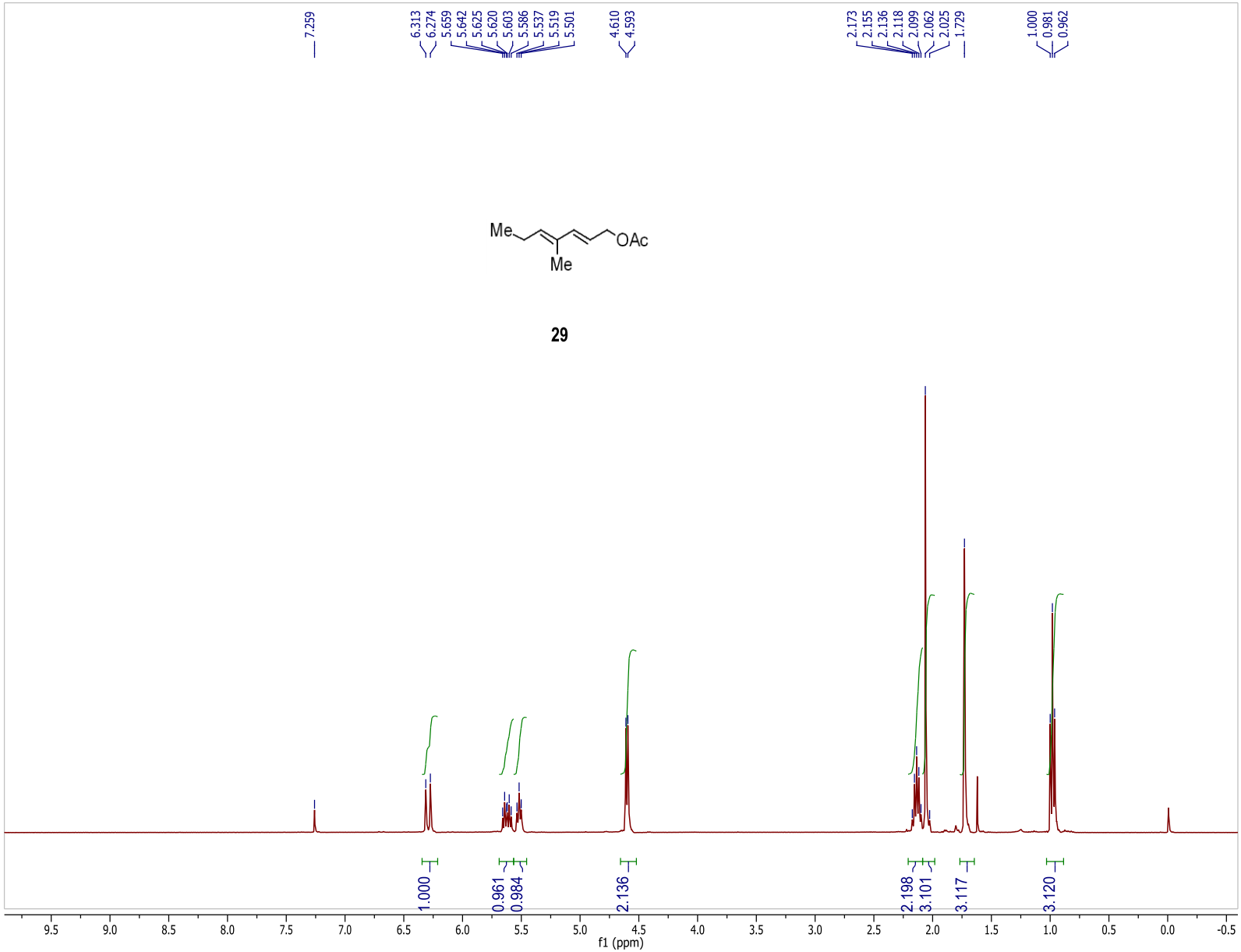
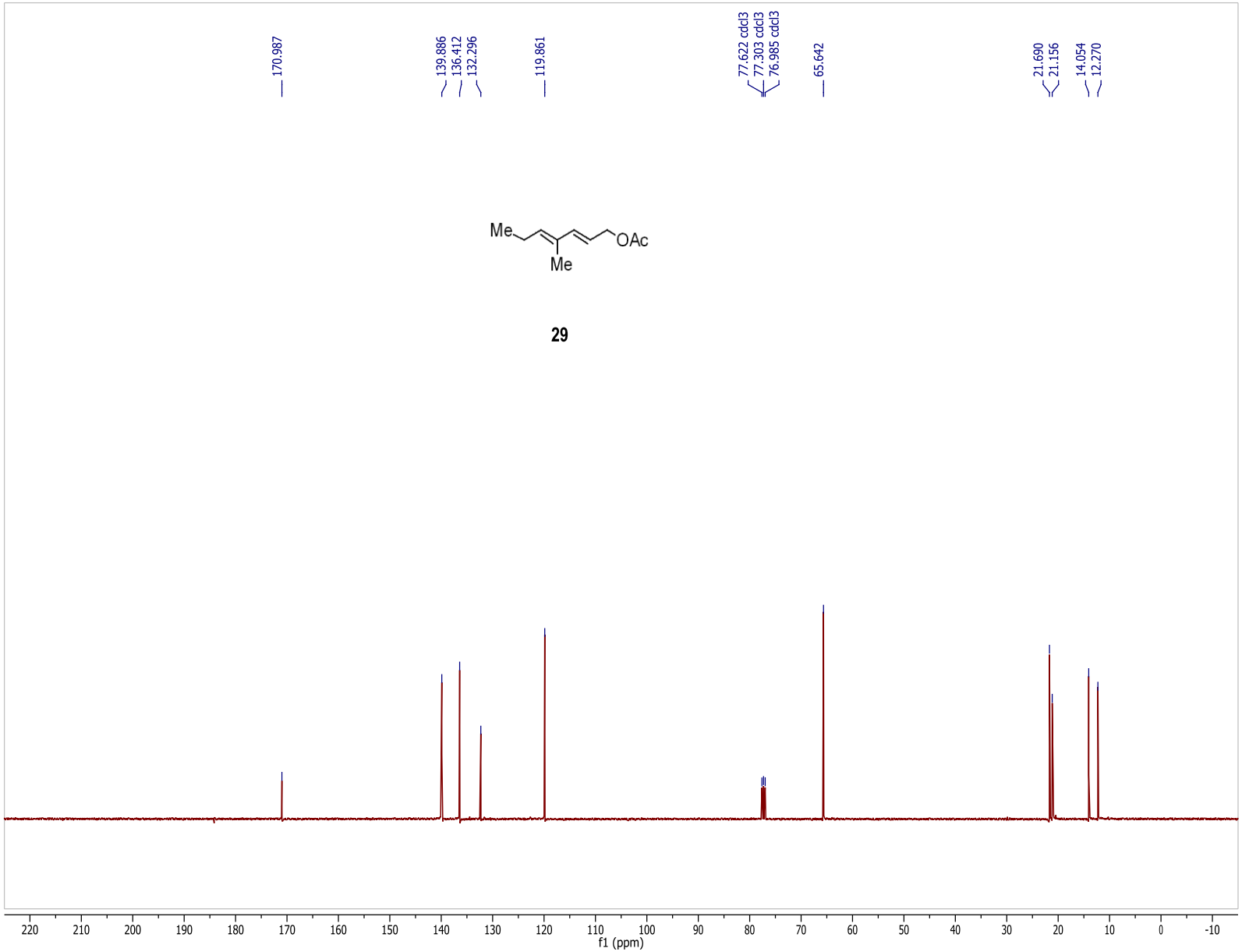
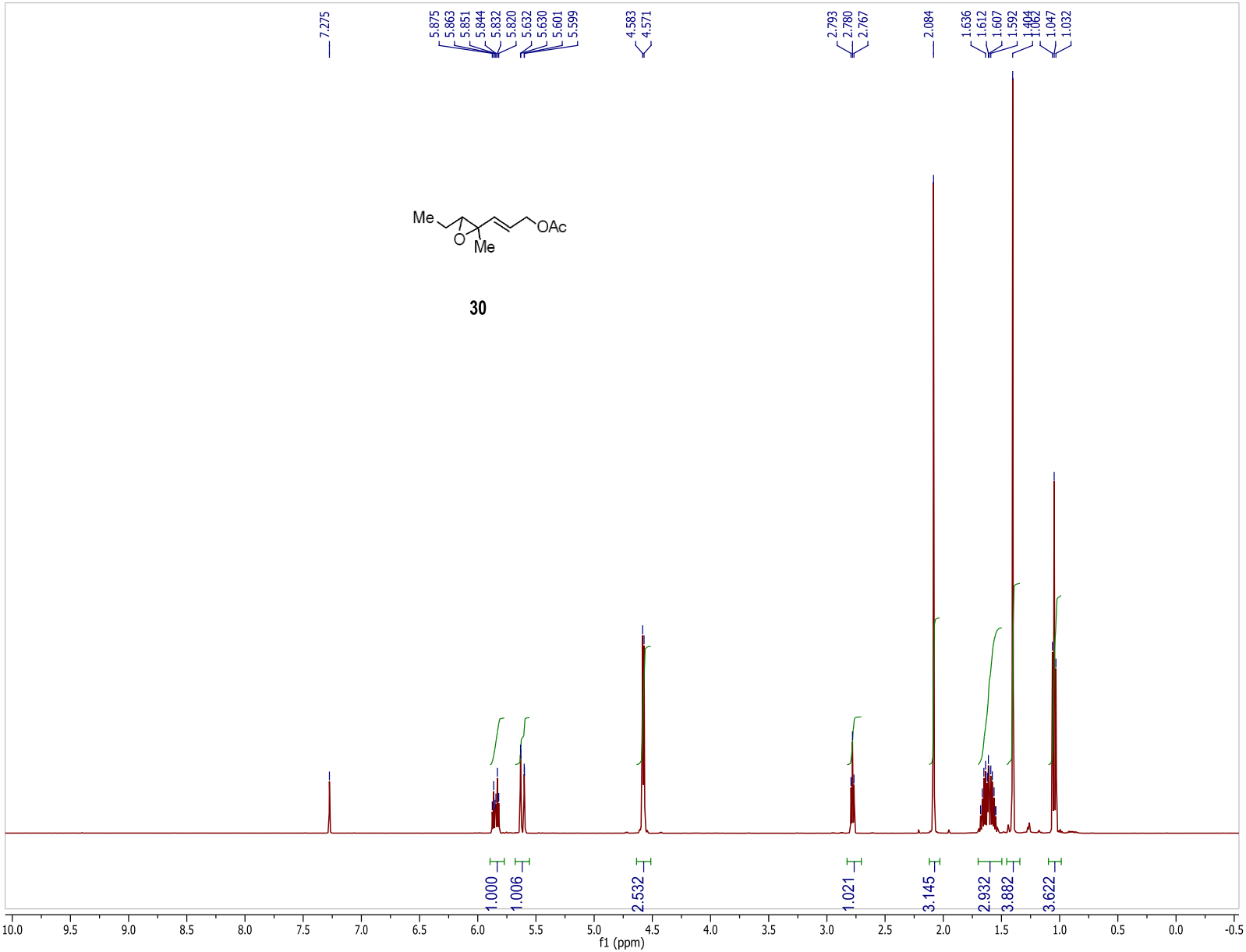
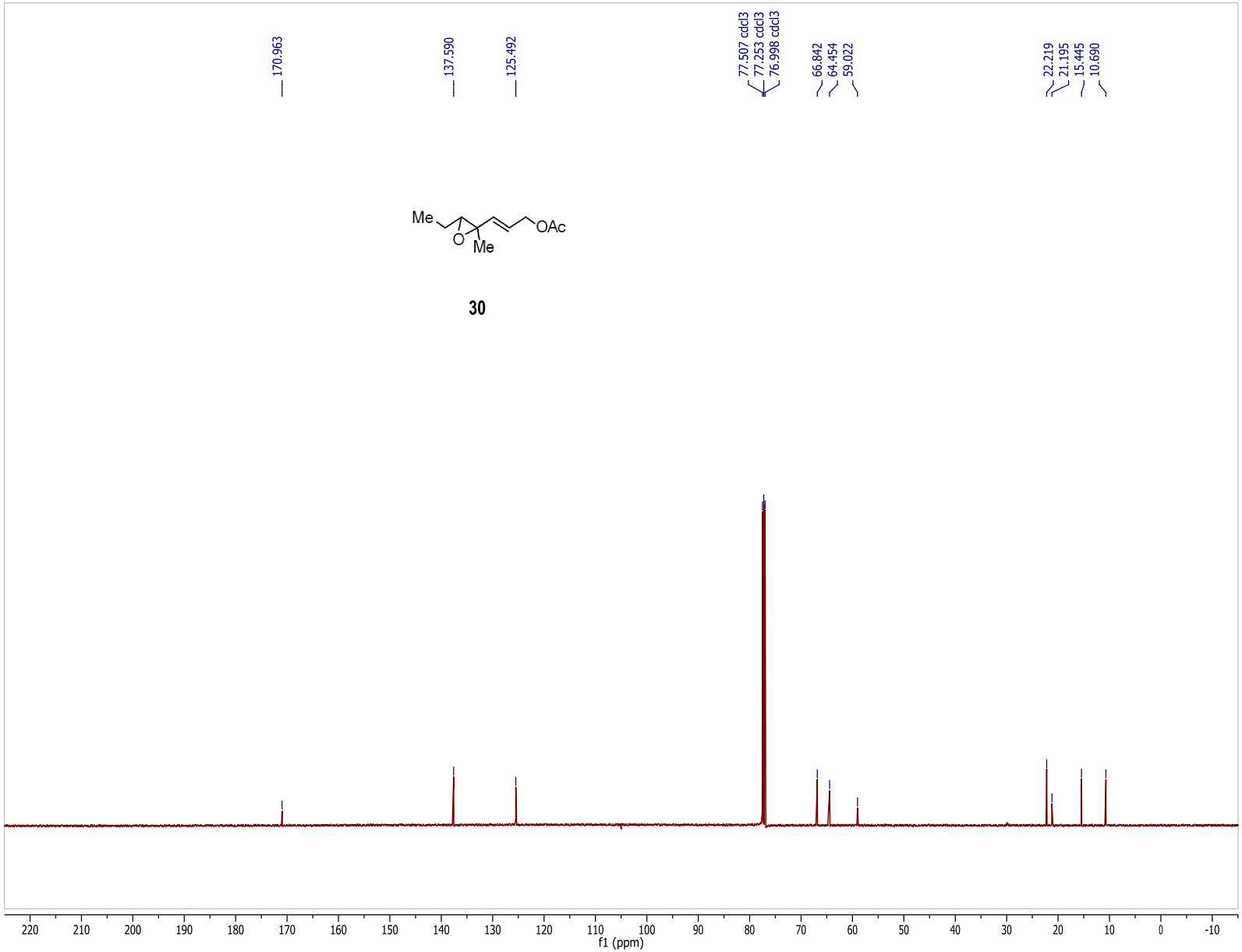
133.295
129.658
127.666
127.649
124.282
77.301 cdcl3
76.984 cdcl3
76.667 cdcl3
67.901
62.579
61.036
32.585
31.796
29.113
29.076
28.981
26.758
22.637
19.269
14.492
14.085
C7H15
O
OTBDPS
Me
28
f1 (ppm)

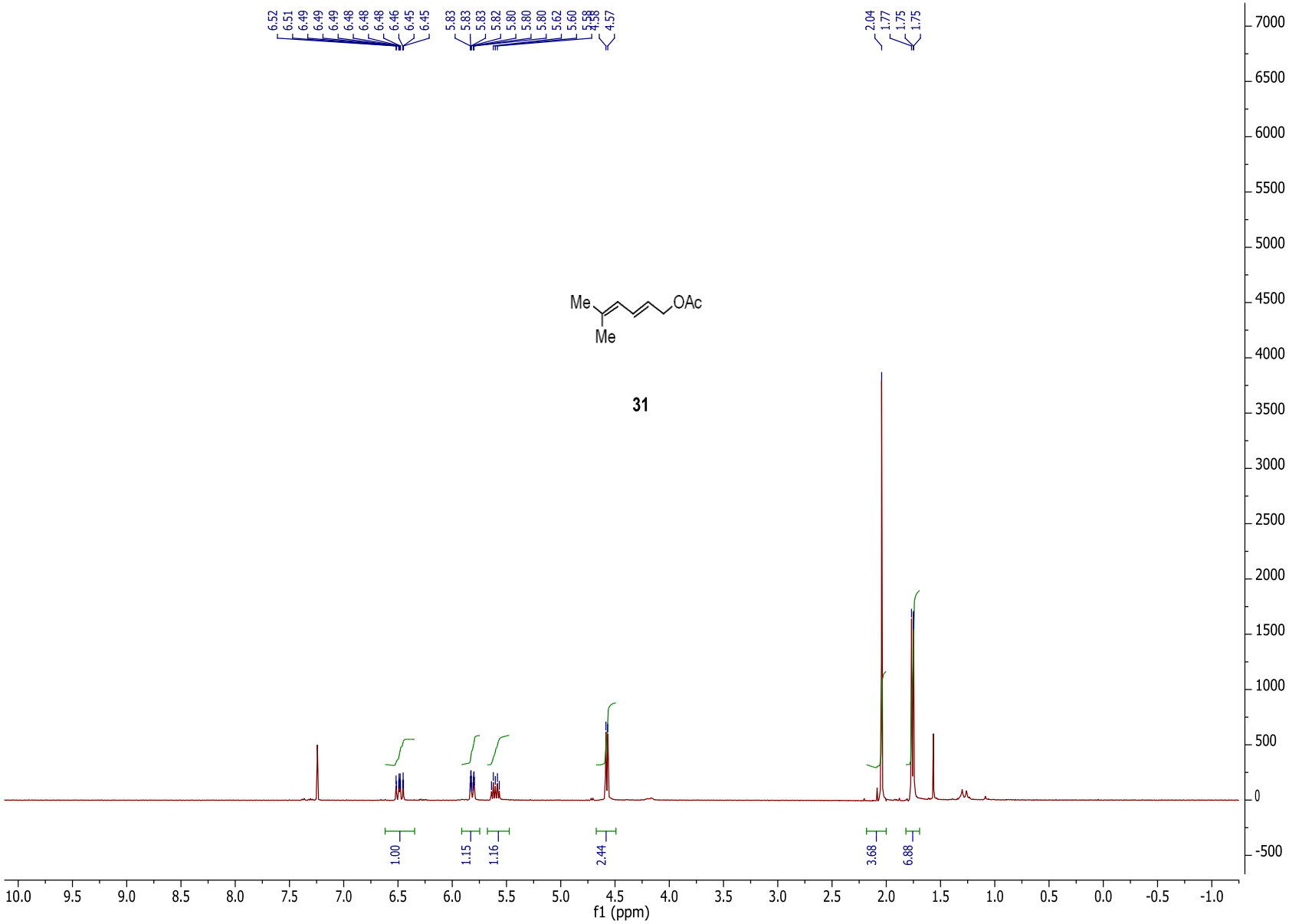

7.259
6.313
6.274
5.659
5.642
5.625
5.620
5.603
5.586
5.537
5.519
5.501
4.610
4.593
2.173
2.155
2.136
2.118
2.099
2.062
2.025
1.729
1.000
0.981
0.962
Me
OAc
Me
29
1.000
0.961
0.984
2.136
2.198
3.101
3.117
3.120
f1 (ppm)

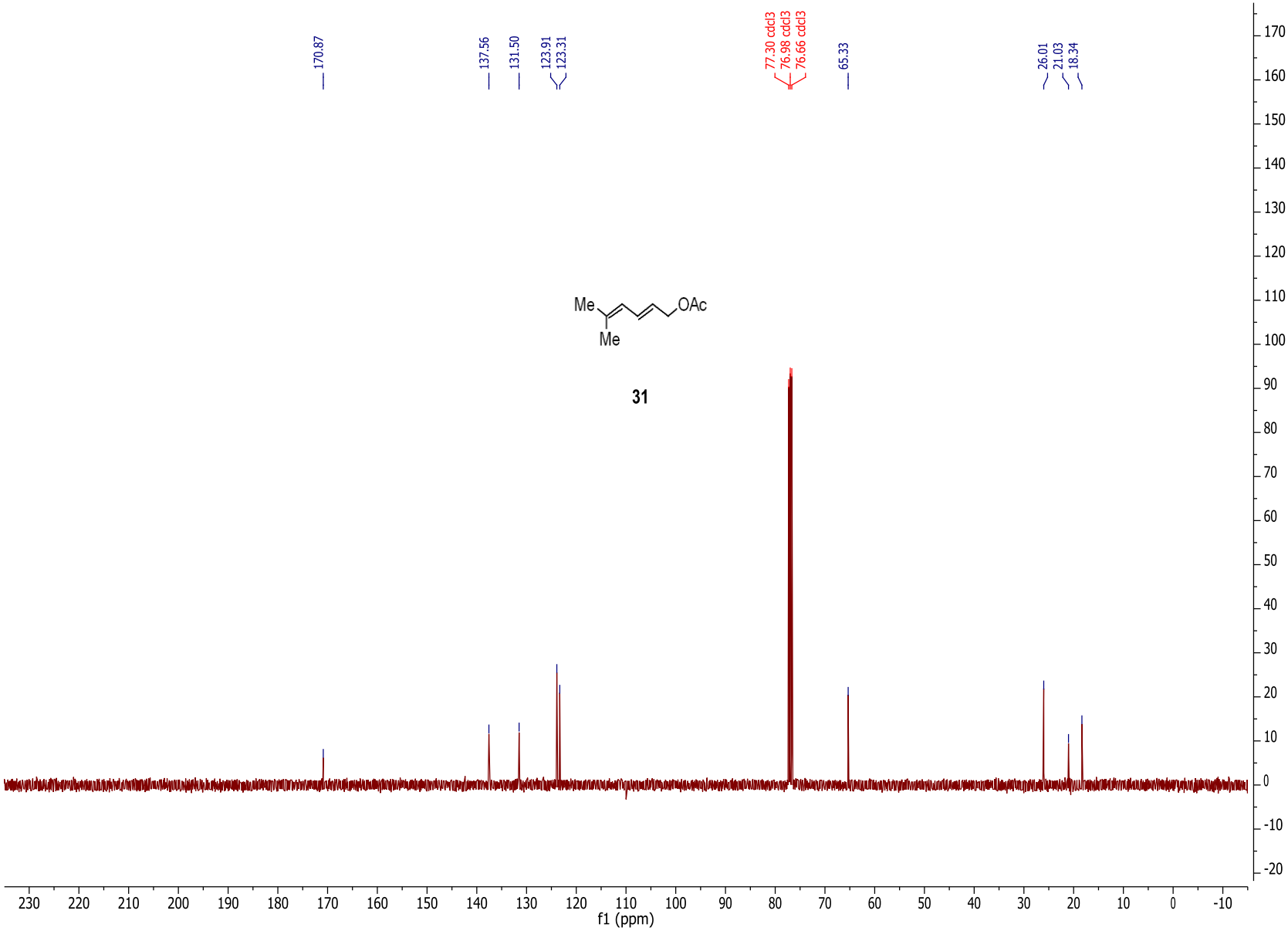

170.987
139.886
136.412
132.296
119.861
77.622 cdcl3
77.303 cdcl3
76.985 cdcl3
65.642
21.690
21.156
14.054
12.270
Me
OAc
Me
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

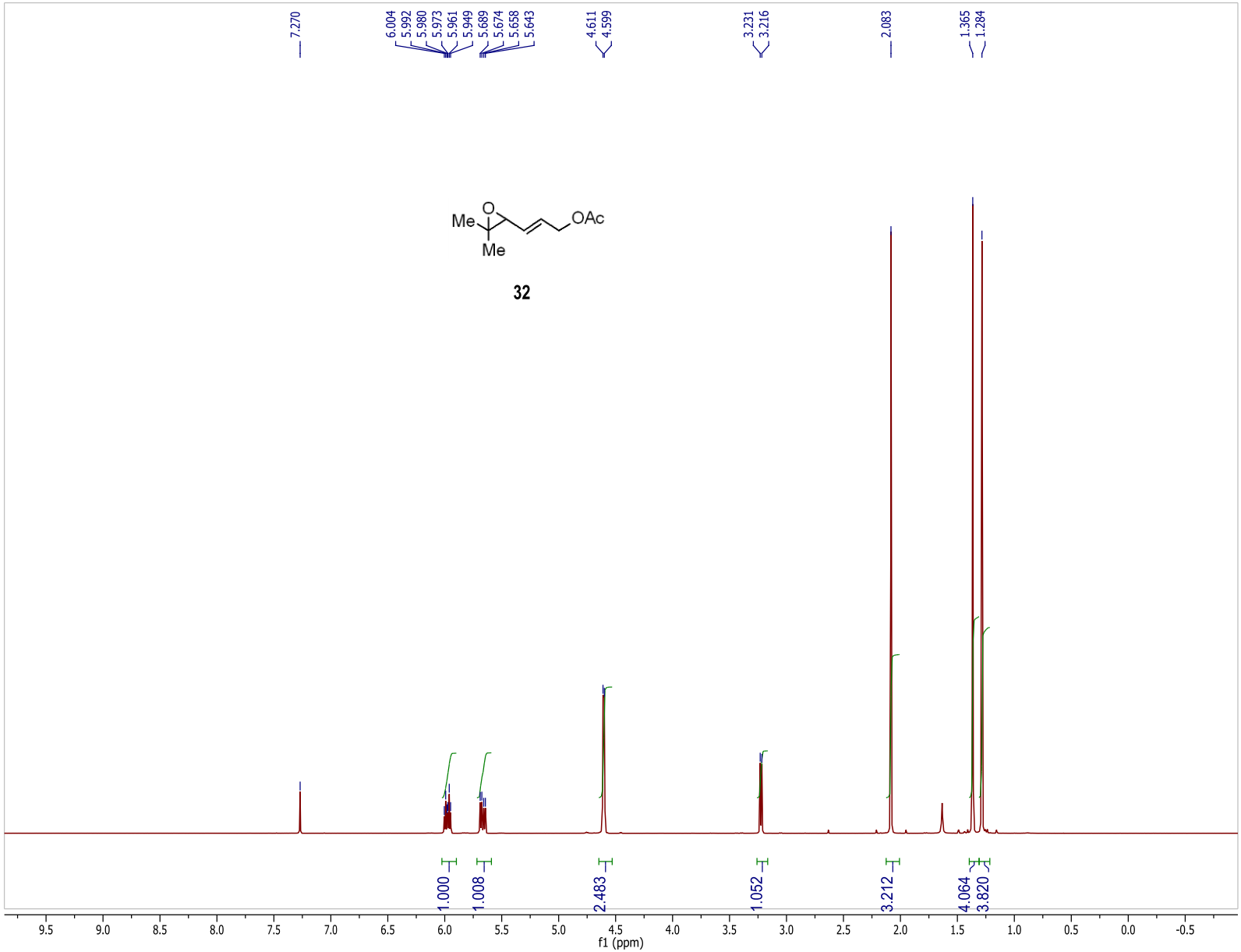
29

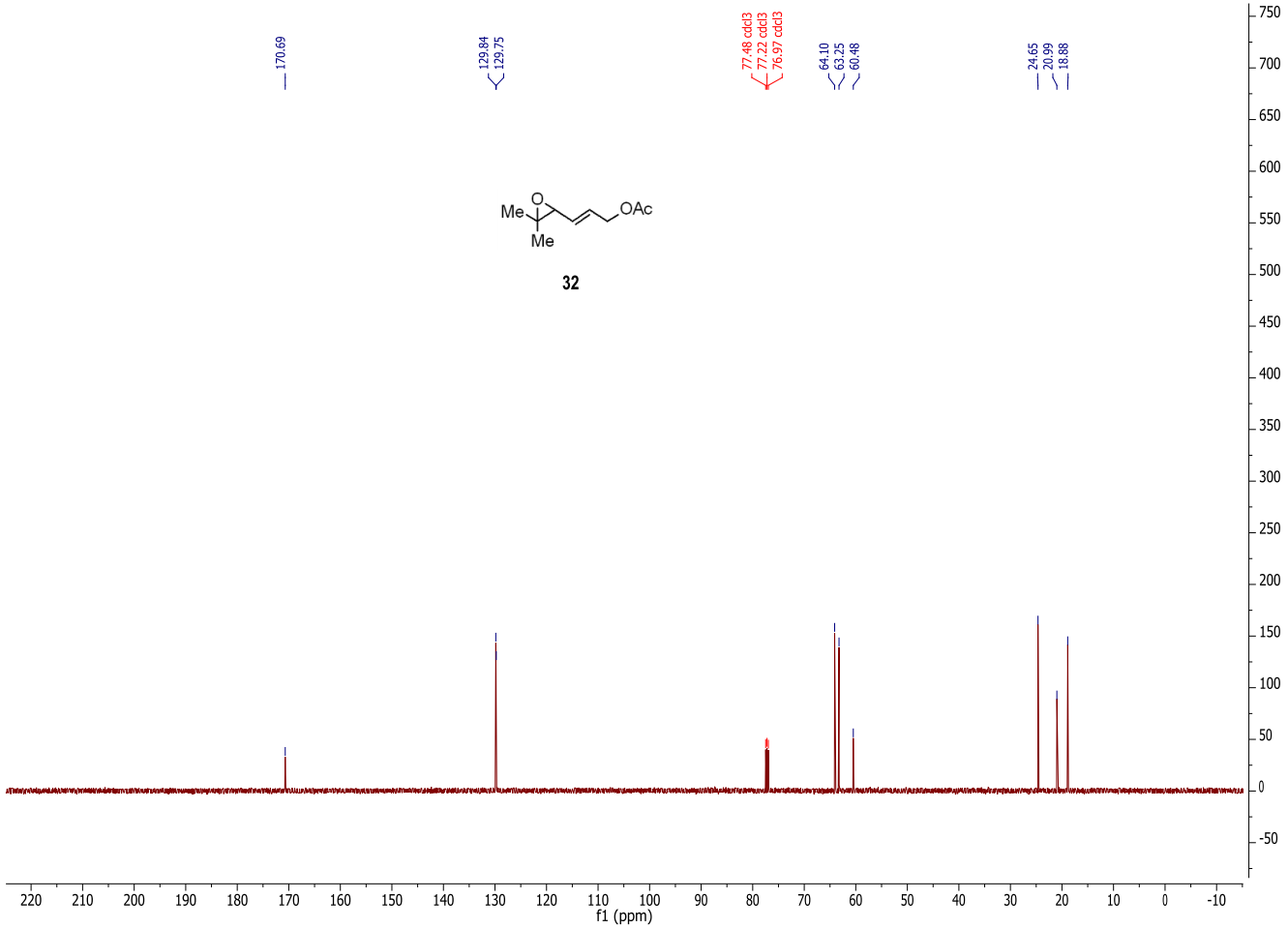

7.275
5.875
5.863
5.851
5.844
5.832
5.820
5.632
5.630
5.601
5.599
4.583
4.571
2.793
2.780
2.767
2.084
1.636
1.612
1.607
1.592
1.404
1.062
1.047
1.032
Me
O
Me
OAc
30
1.000
1.006
2.532
1.021
3.145
2.932
3.882
3.622
f1 (ppm)

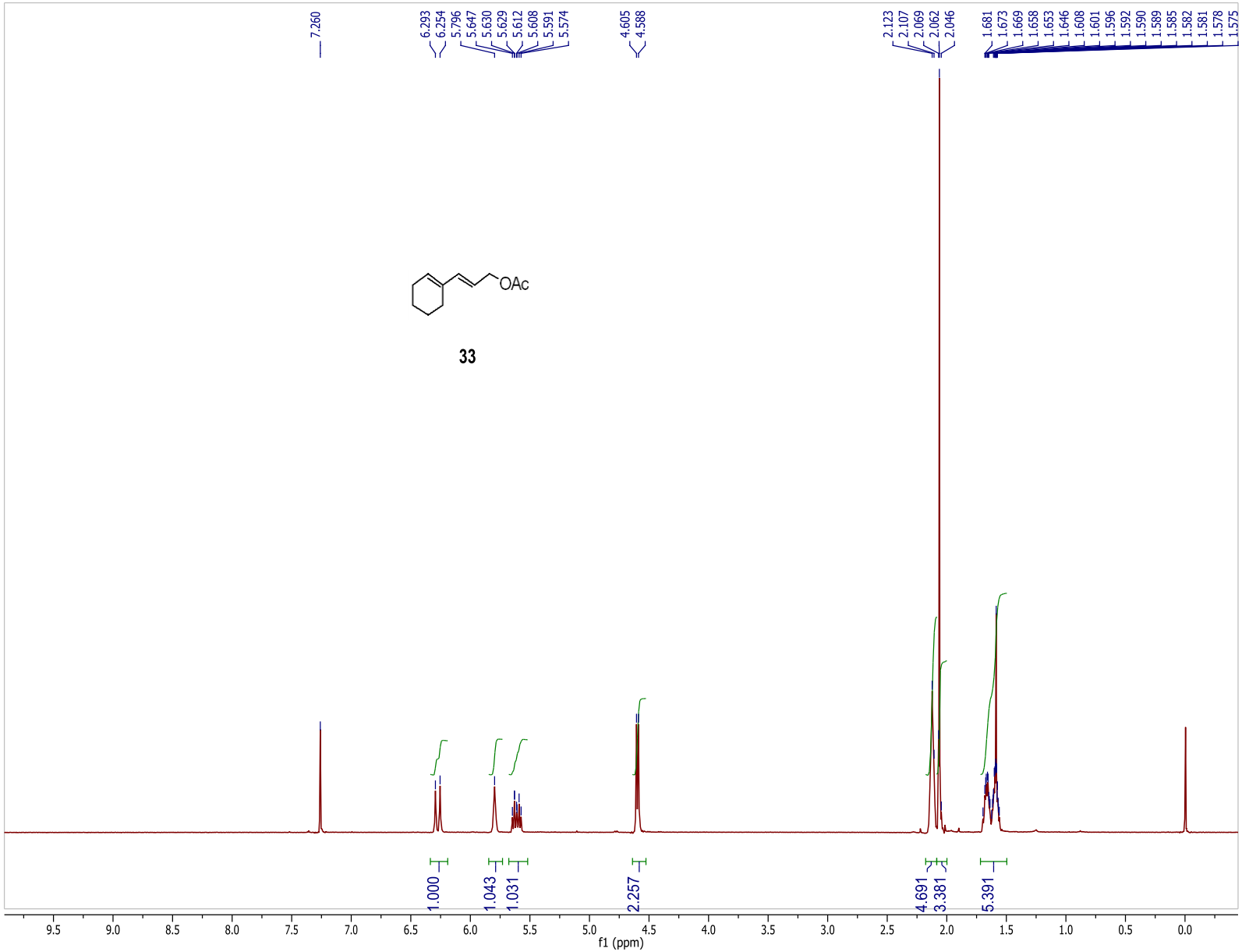

170.963
137.590
125.492
77.507 cdcl3
77.253 cdcl3
76.998 cdcl3
66.842
64.454
59.022
22.219
21.195
15.445
10.690
Me
O
Me
OAc
30
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


6.52
6.51
6.49
6.49
6.49
6.48
6.48
6.48
6.46
6.45
6.45
5.83
5.83
5.83
5.82
5.80
5.80
5.80
5.62
5.60
4.57
2.04
1.77
1.75
1.75
Me
OAc
Me
31
1.00
1.15
1.16
2.44
3.68
6.88
f1 (ppm)


170.87
137.56
131.50
123.91
123.31
77.30 cdcl3
76.98 cdcl3
76.66 cdcl3
65.33
26.01
21.03
18.34
Me
Me
OAc
31
f1 (ppm)


7.270
6.004
5.992
5.980
5.973
5.961
5.949
5.689
5.674
5.658
5.643
4.611
4.599
3.231
3.216
2.083
1.365
1.284
Me
O
OAc
Me
32
1.000
1.008
2.483
1.052
3.212
4.064
3.820
f1 (ppm)


170.69
129.84
129.75
77.48 cdcl3
77.22 cdcl3
76.97 cdcl3
64.10
63.25
60.48
24.65
20.99
18.88
Me
O
OAc
Me
32
f1 (ppm)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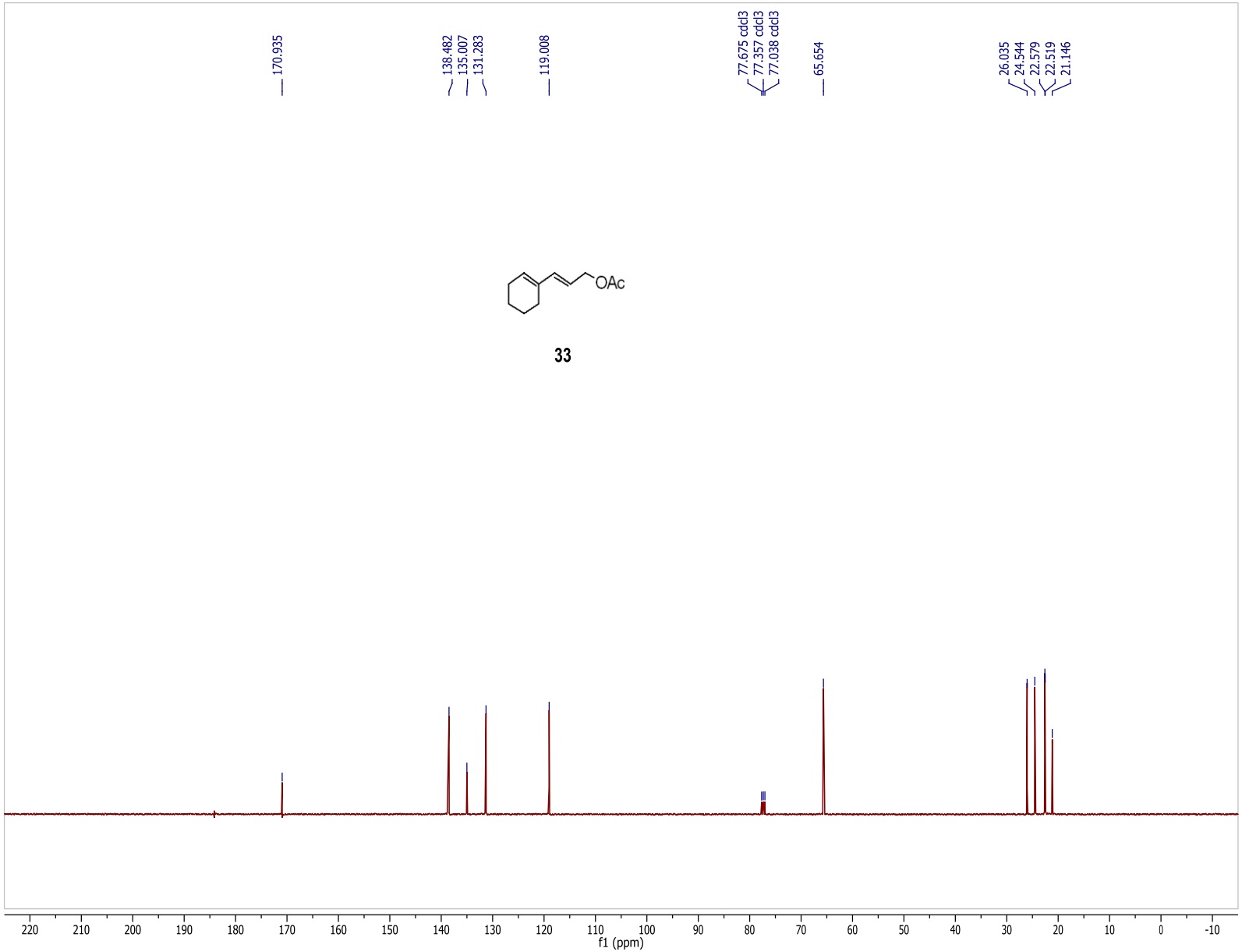
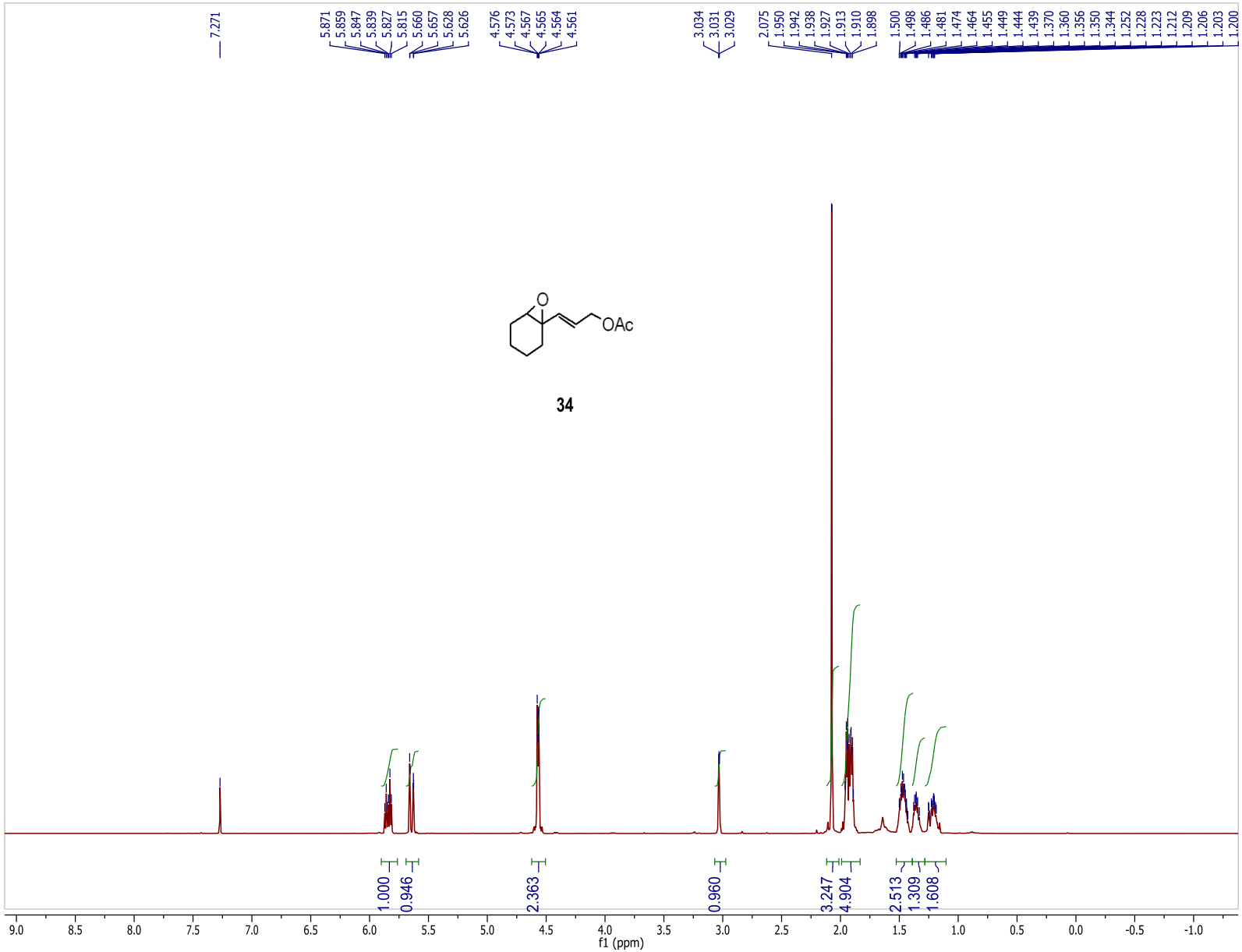
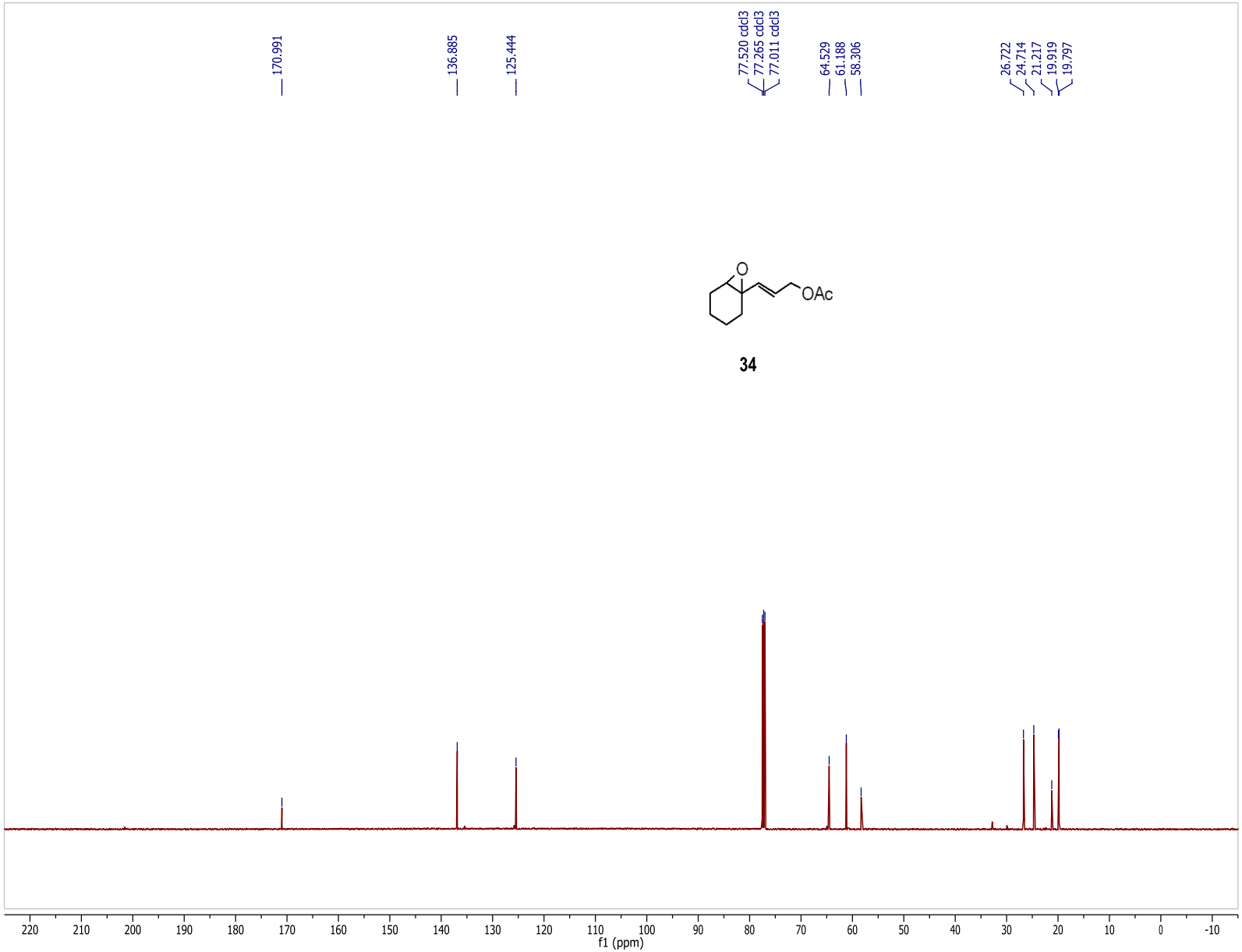
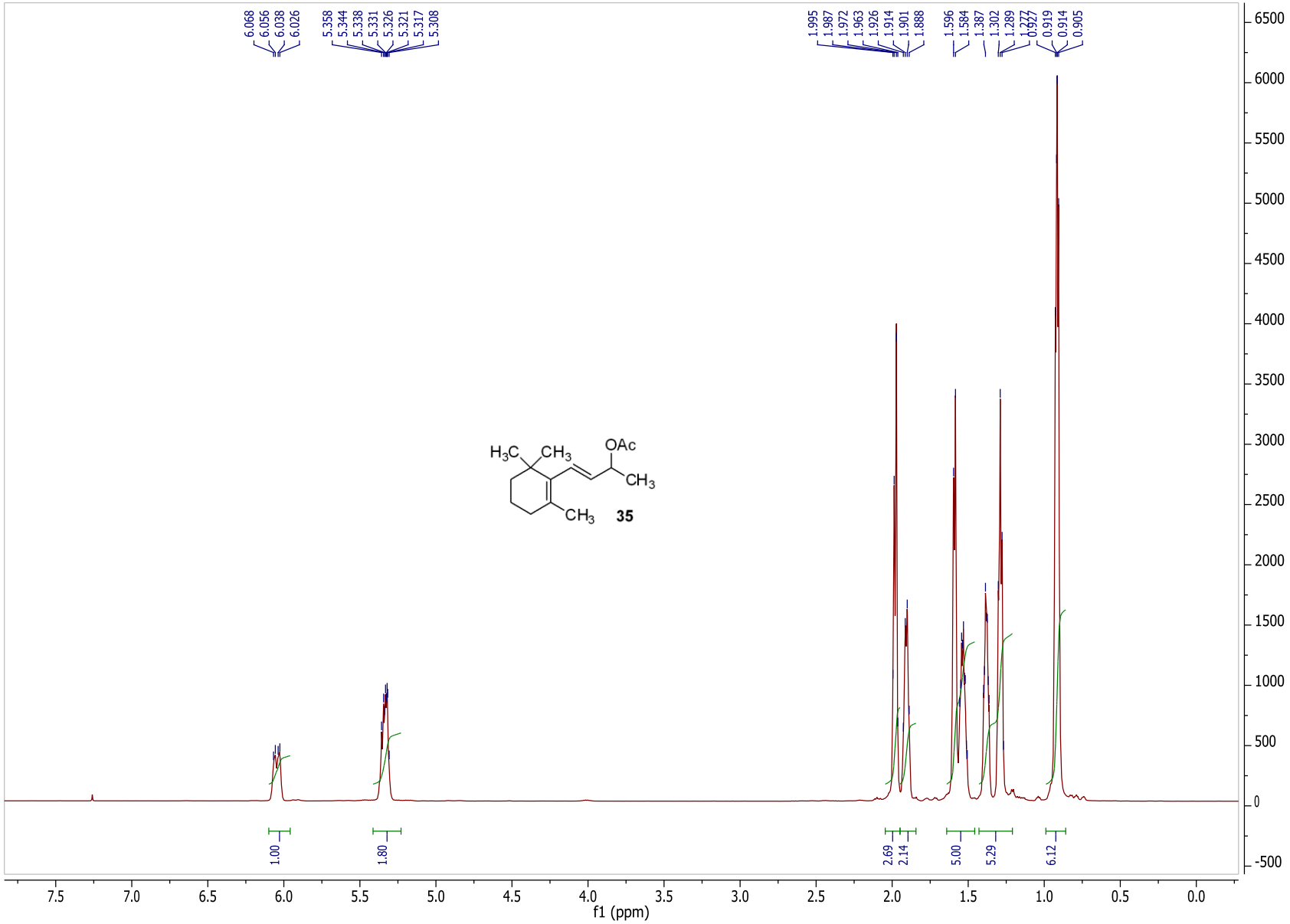
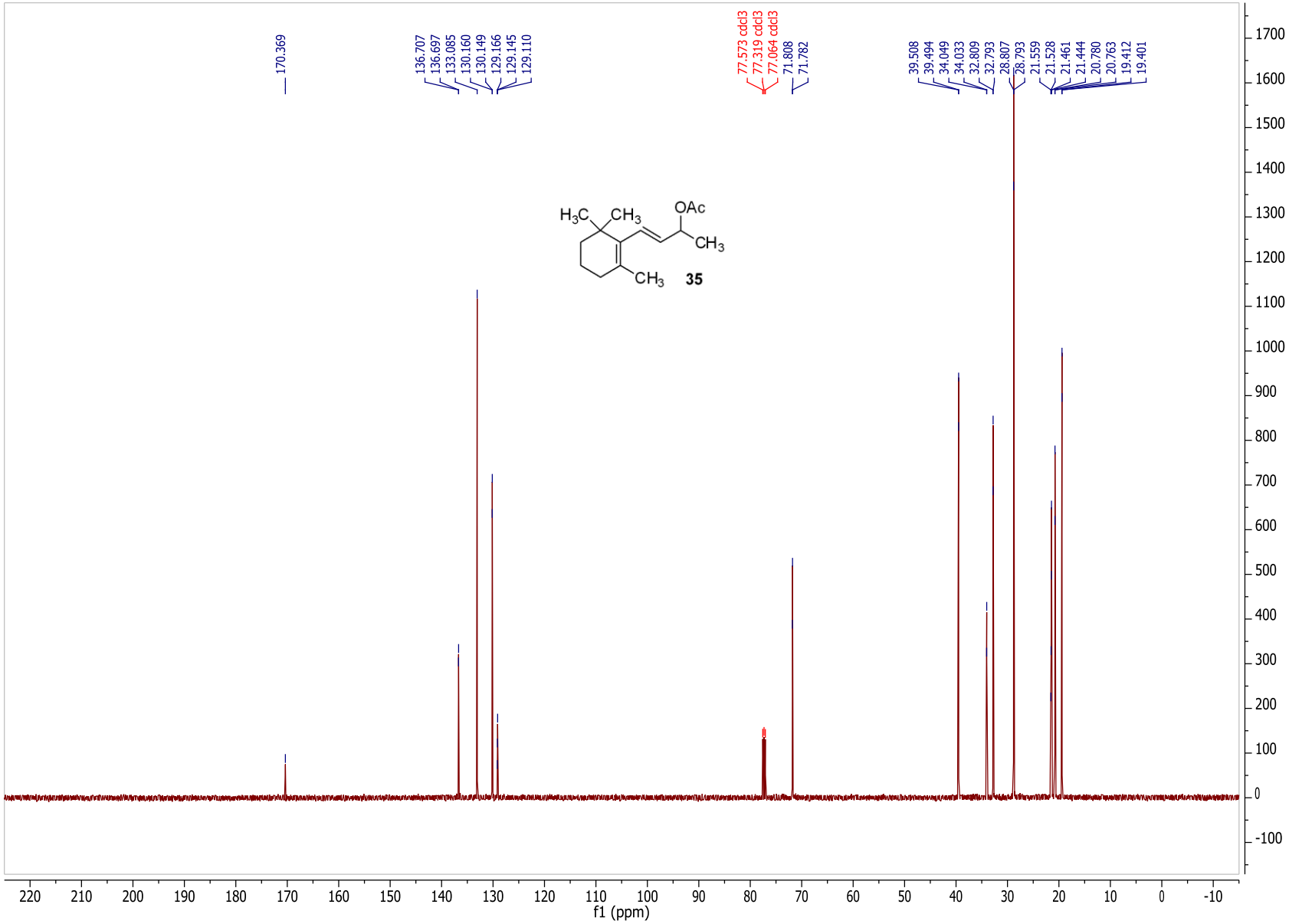
6.293
6.254
5.796
5.647
5.630
5.629
5.612
5.608
5.591
5.574
4.605
4.588
2.123
2.107
2.069
2.062
2.046
1.681
1.673
1.669
1.658
1.653
1.646
1.608
1.601
1.596
1.592
1.590
1.589
1.585
1.582
1.581
1.578
1.575
OAc
33
1.000
1.043
1.031
2.257
4.691
3.381
5.391
f1 (ppm)

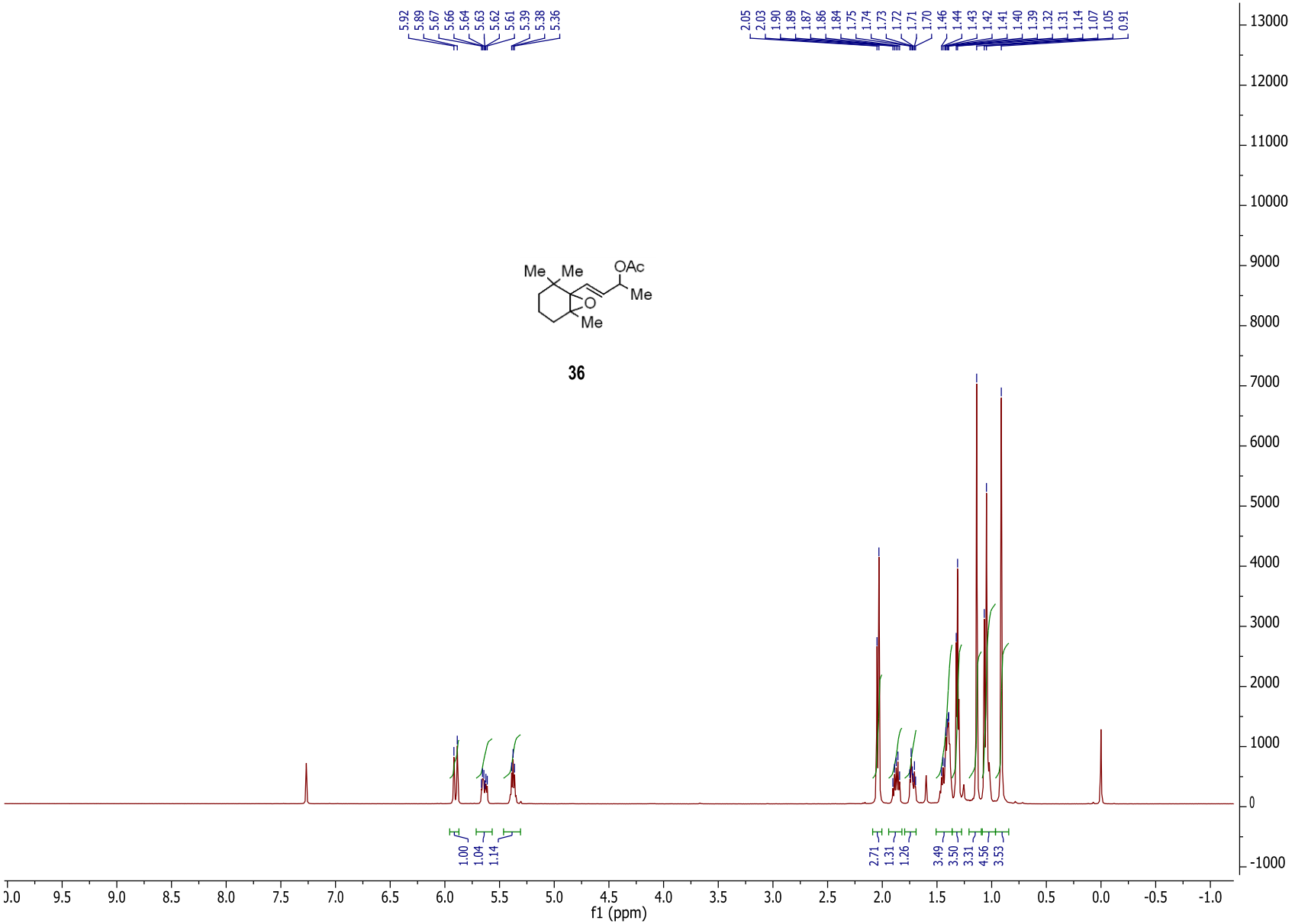

170.935
138.482
135.007
131.283
119.008
77.675 cdcl3
77.357 cdcl3
77.038 cdcl3
65.654
26.035
24.544
22.579
22.519
21.146
OAc
33
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

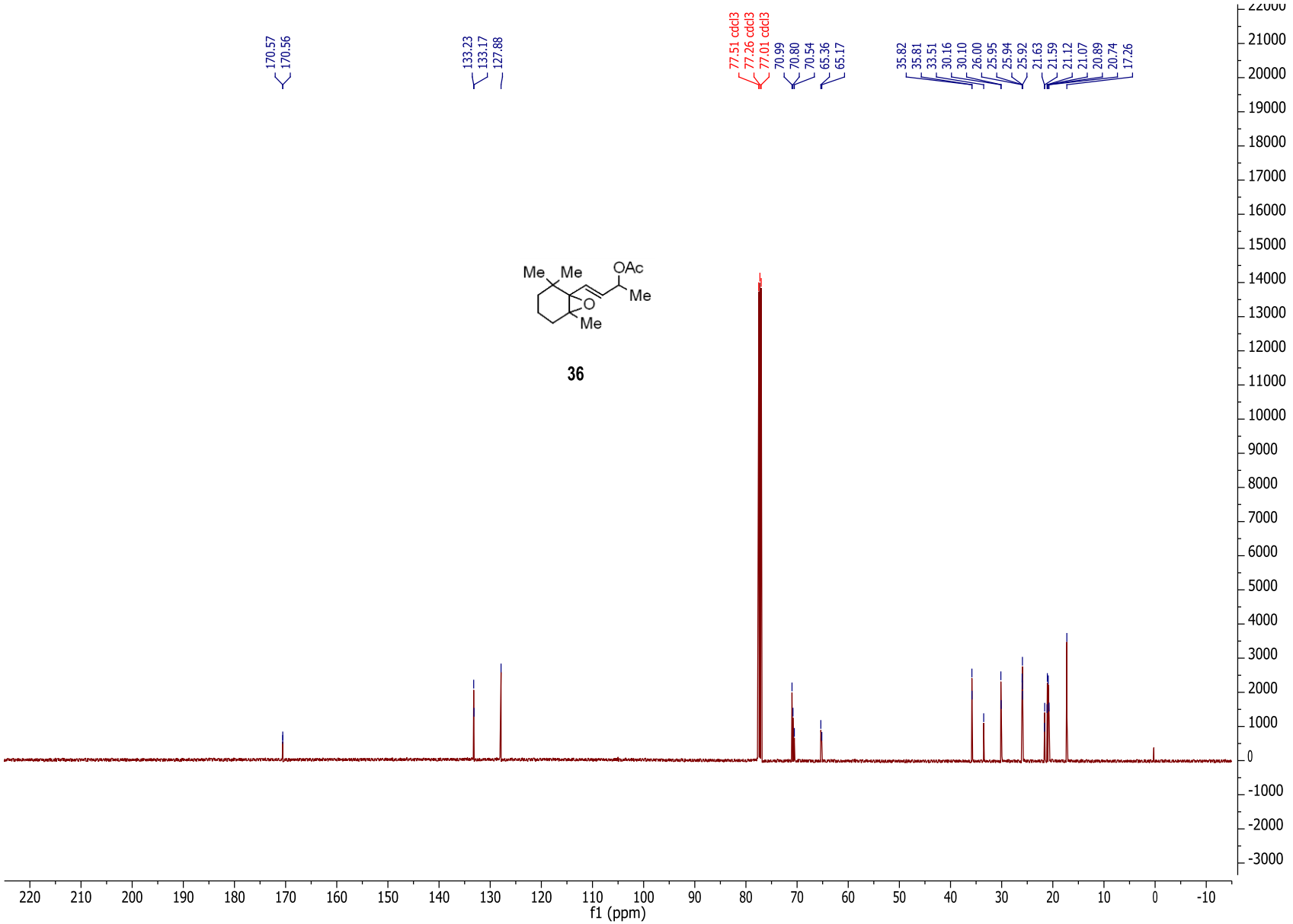

7.271
5.871
5.859
5.847
5.839
5.827
5.815
5.660
5.657
5.628
5.626
4.576
4.573
4.567
4.565
4.564
4.561
3.034
3.031
3.029
2.075
1.950
1.942
1.938
1.927
1.913
1.910
1.898
1.500
1.498
1.486
1.481
1.474
1.464
1.455
1.449
1.444
1.439
1.370
1.360
1.356
1.350
1.344
1.252
1.228
1.223
1.212
1.209
1.206
1.203
1.200
O
OAc
34
1.000
0.946
2.363
0.960
3.247
4.904
2.513
1.309
1.608
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
-0.5
-1.0
f1 (ppm)


170.991
136.885
125.444
77.520 cdcl3
77.265 cdcl3
77.011 cdcl3
64.529
61.188
58.306
26.722
24.714
21.217
19.919
19.797
O
OAc
34
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 (ppm)

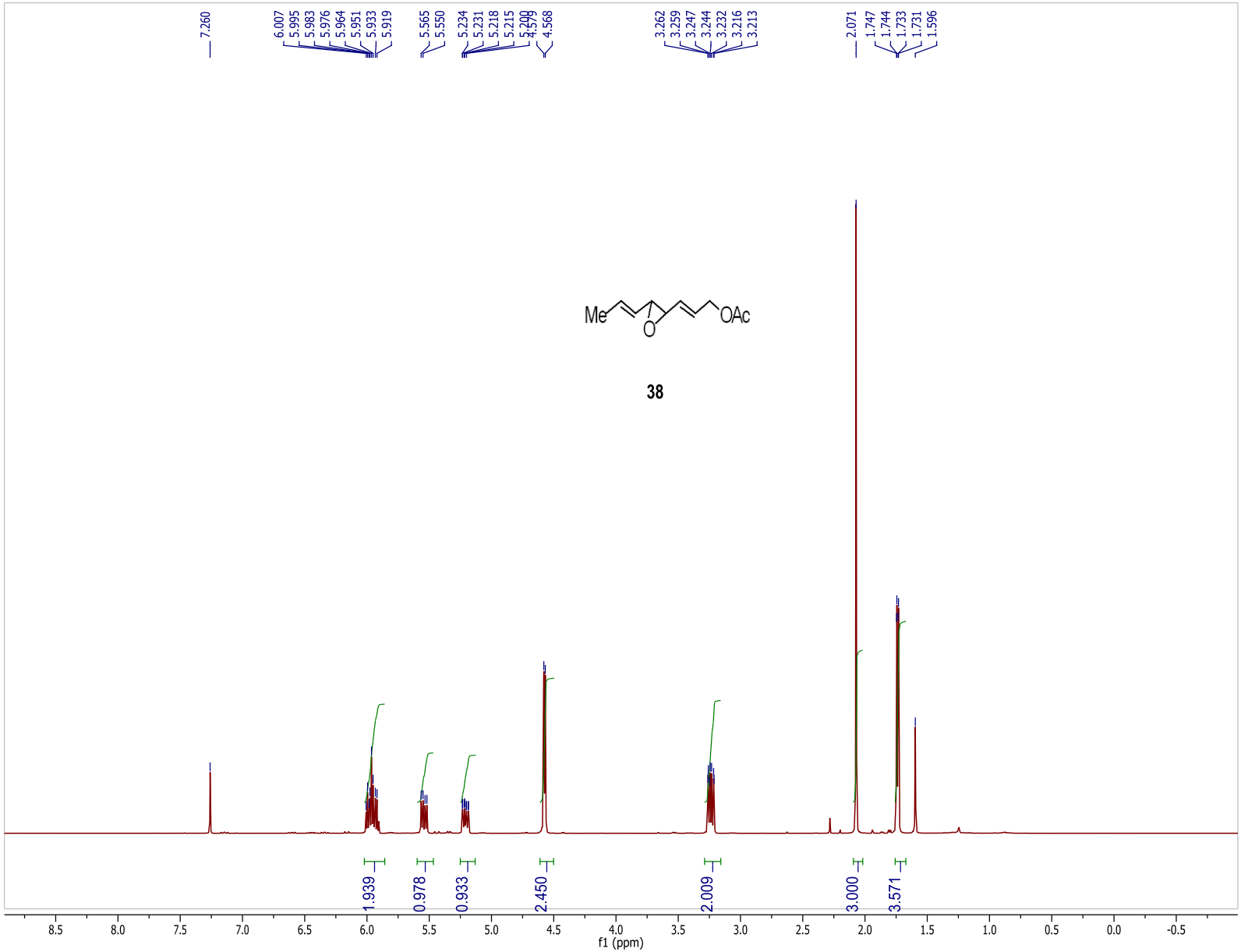

6.068
6.056
6.038
6.026
5.358
5.344
5.338
5.331
5.326
5.321
5.317
5.308
1.995
1.987
1.972
1.963
1.926
1.914
1.901
1.888
1.596
1.584
1.387
1.302
1.289
0.919
0.914
0.905
H3C
CH3
OAc
CH3
CH3
35
1.00
1.80
2.69
2.14
5.00
5.29
6.12
f1 (ppm)

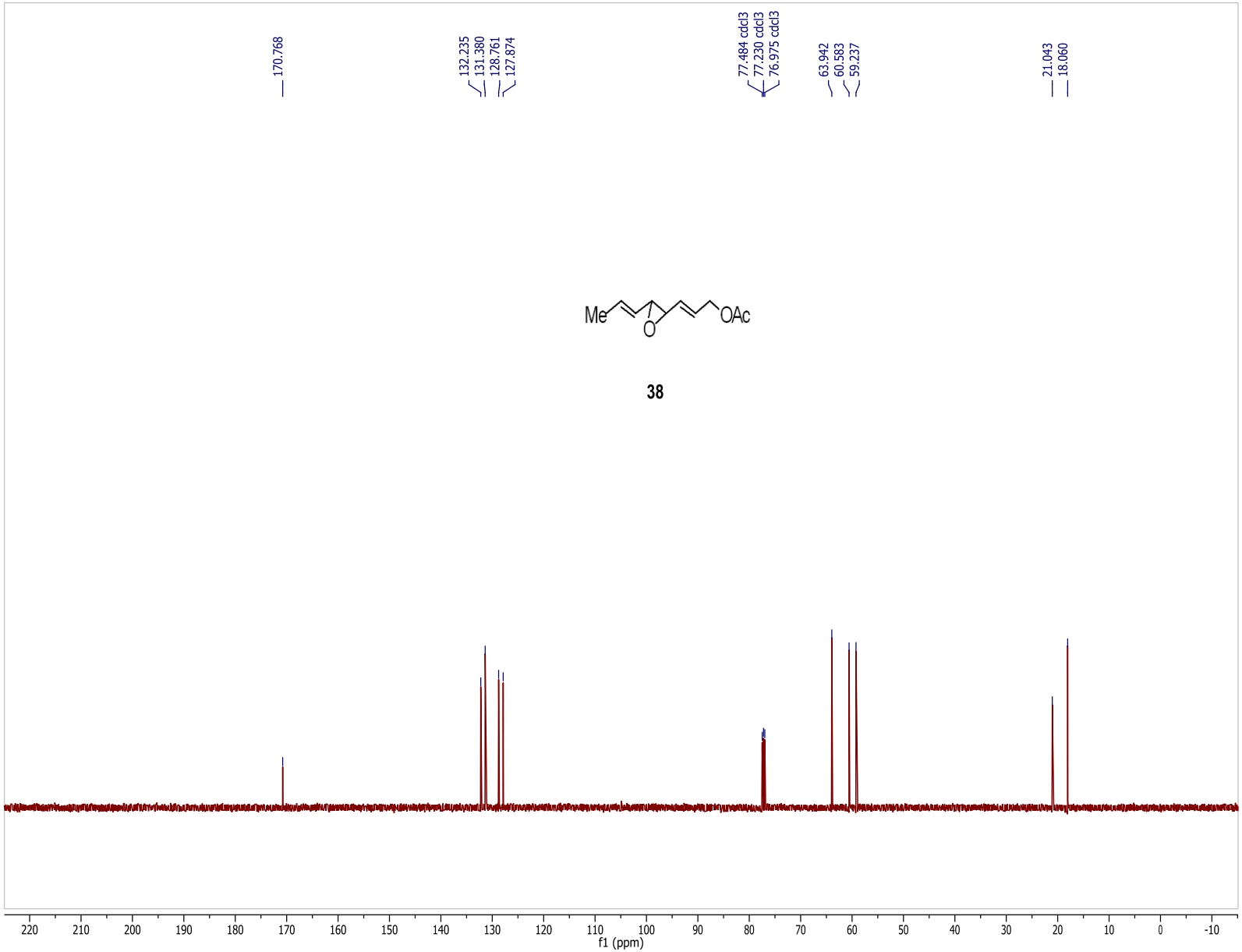

170.369
136.707
136.697
133.085
130.160
130.149
129.166
129.145
129.110
77.573 cdcl3
77.319 cdcl3
77.064 cdcl3
71.808
71.782
39.508
39.494
34.049
34.033
32.809
32.793
28.807
28.793
21.559
21.528
21.461
21.444
20.780
20.763
19.412
19.401
H3C
CH3
OAc
CH3
CH3
35
f1 (ppm)


5.92
5.89
5.67
5.66
5.64
5.63
5.62
5.61
5.39
5.38
5.36
2.05
2.03
1.90
1.89
1.87
1.86
1.84
1.75
1.74
1.73
1.72
1.71
1.70
1.46
1.44
1.43
1.42
1.41
1.40
1.39
1.32
1.31
1.14
1.07
1.05
0.91
Me
Me
OAc
Me
O
Me
36
1.00
1.04
1.14
2.71
1.31
1.26
3.49
3.50
3.31
4.56
3.53
f1 (ppm)

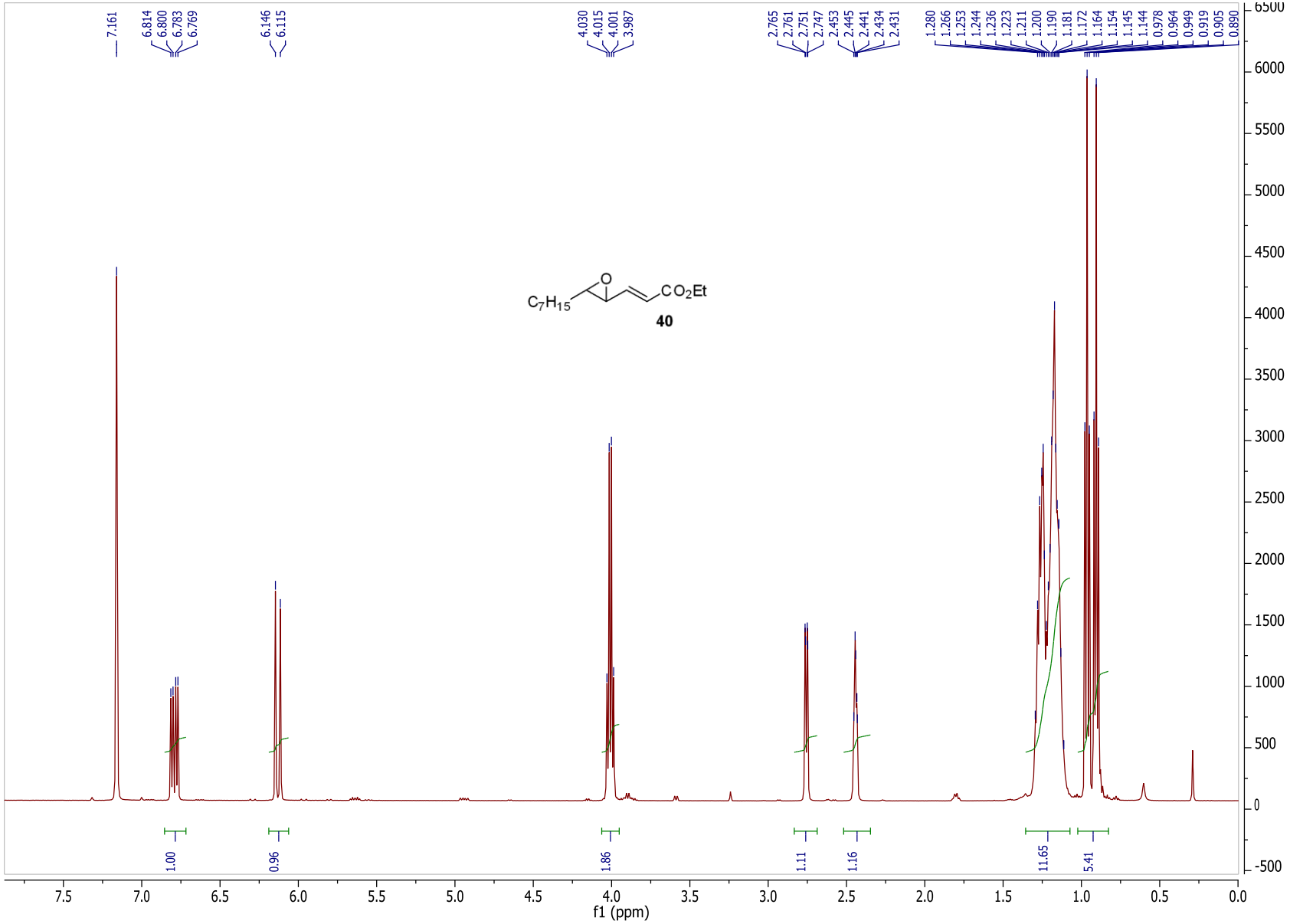

170.57
170.56
133.23
133.17
127.88
77.51 cdcl3
77.26 cdcl3
77.01 cdcl3
70.99
70.80
70.54
65.36
65.17
35.82
35.81
33.51
30.16
30.10
26.00
25.95
25.94
25.92
21.63
21.59
21.12
21.07
20.89
20.74
17.26
Me
Me
OAc
Me
O
Me
f1 (ppm)

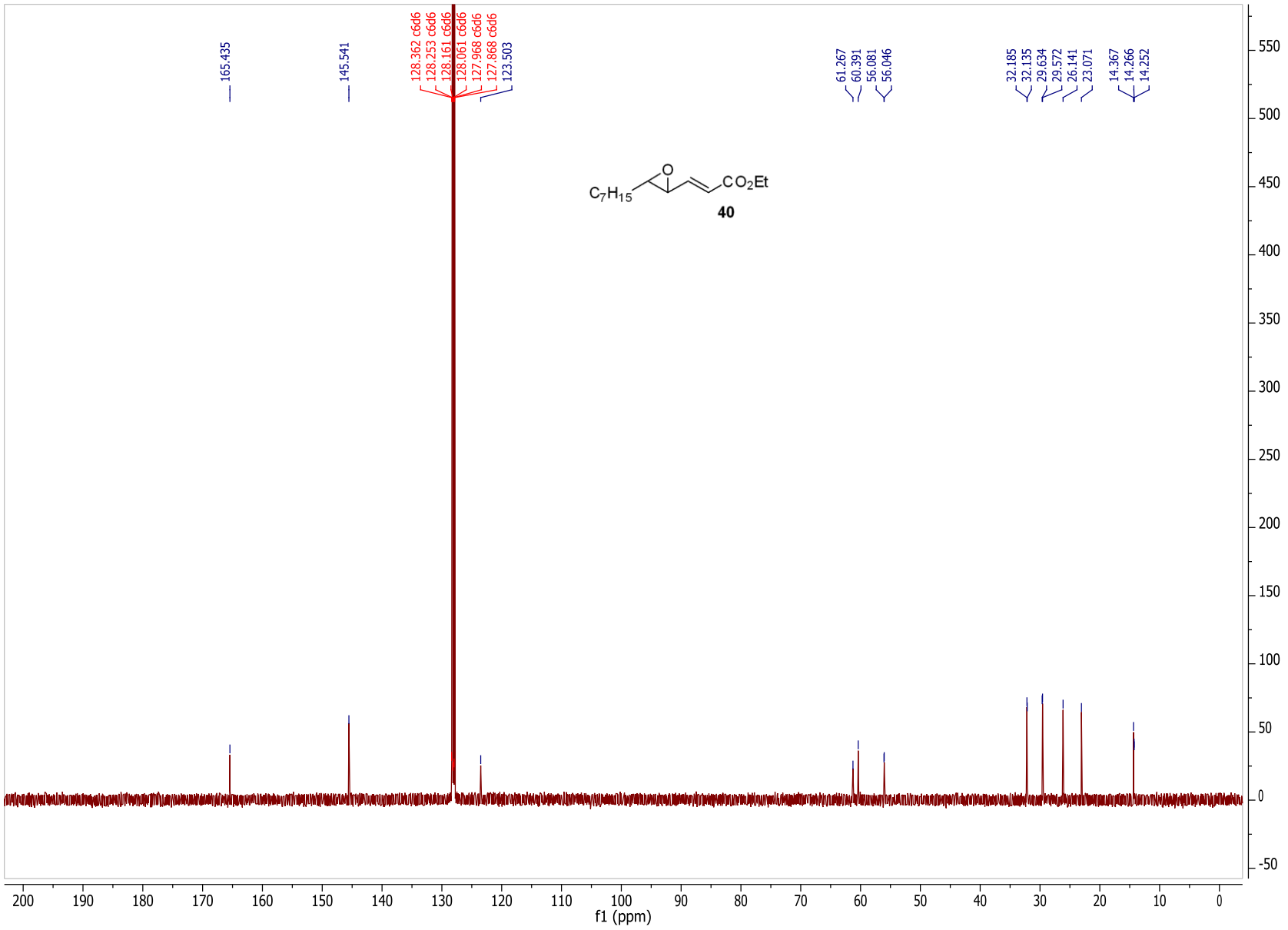
36

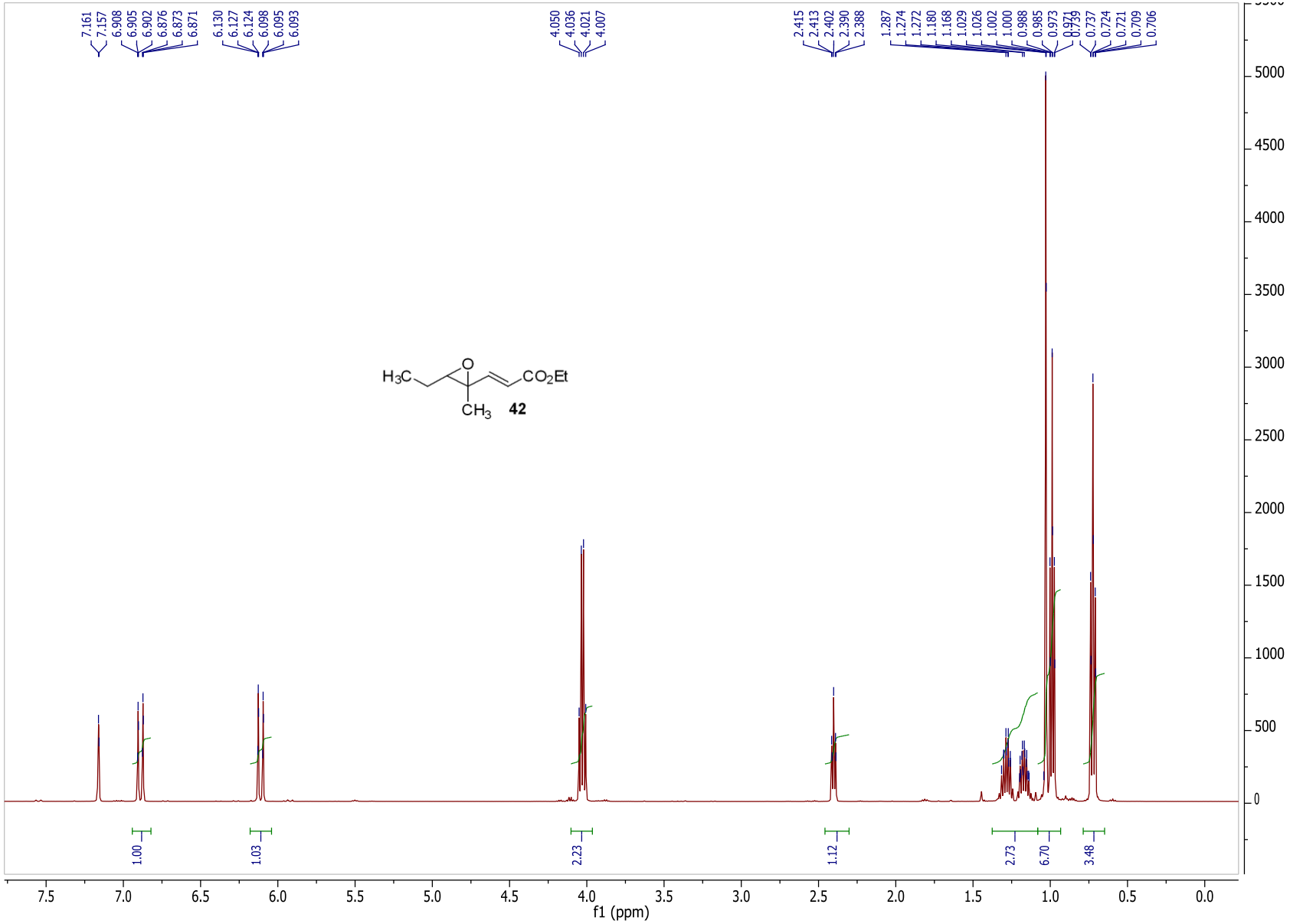

7.260
6.007
5.995
5.983
5.976
5.964
5.951
5.933
5.919
5.565
5.550
5.234
5.231
5.218
5.215
5.200
4.579
4.568
3.262
3.259
3.247
3.244
3.232
3.216
3.213
2.071
1.747
1.744
1.733
1.731
1.596
Me
O
OAc
38
1.939
0.978
0.933
2.450
2.009
3.000
3.571
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

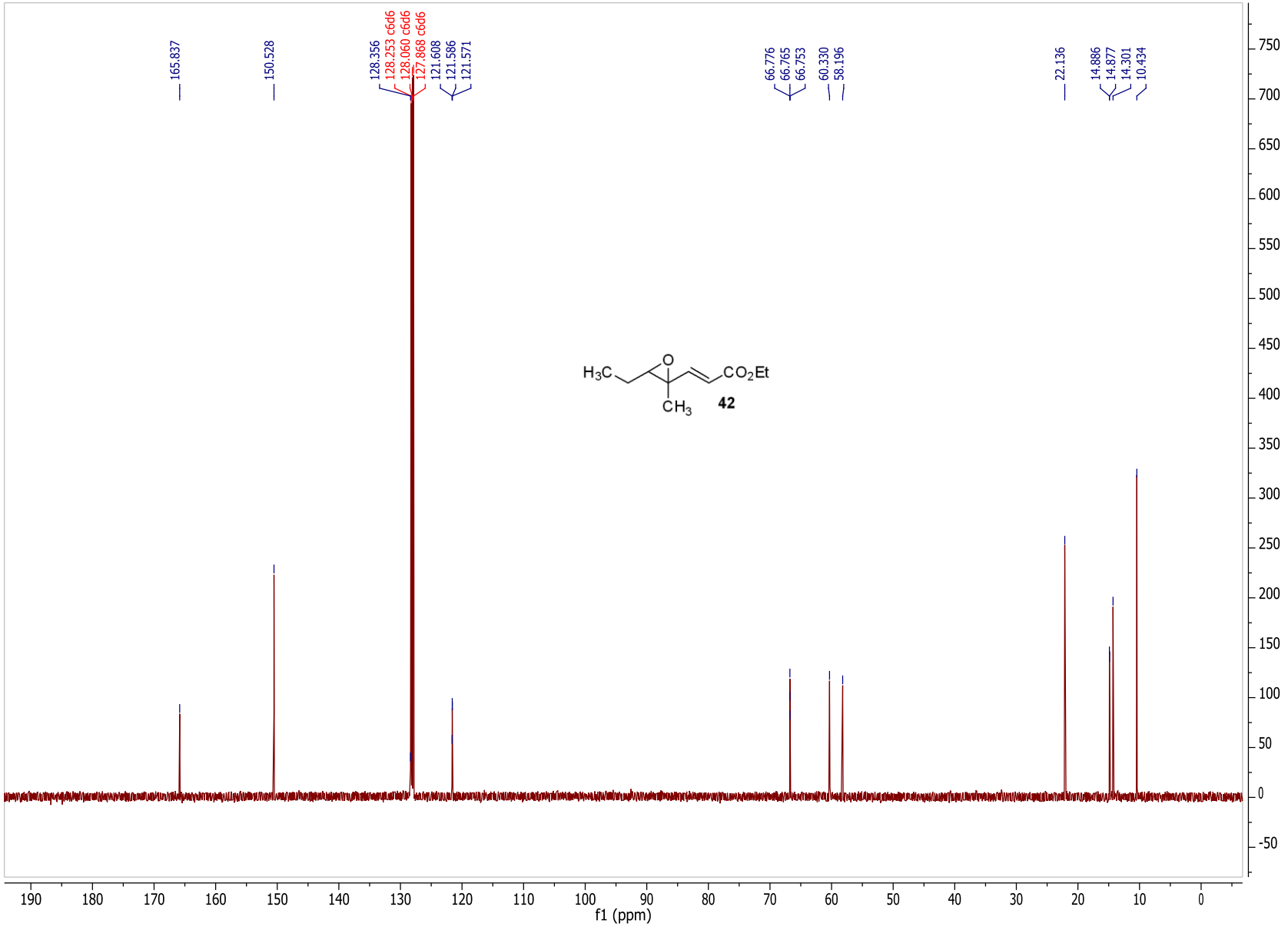

170.768
132.235
131.380
128.761
127.874
77.484 cdcl3
77.230 cdcl3
76.975 cdcl3
63.942
60.583
59.237
21.043
18.060
Me
O
OAc
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

38


7.161
6.814
6.800
6.783
6.769
6.146
6.115
4.030
4.015
4.001
3.987
2.765
2.761
2.751
2.747
2.453
2.445
2.441
2.434
2.431
1.280
1.266
1.253
1.244
1.236
1.223
1.211
1.200
1.190
1.181
1.172
1.164
1.154
1.145
1.144
0.978
0.964
0.949
0.919
0.905
0.890
C7H15
O
CO2Et
40
1.00
0.96
1.86
1.11
1.16
11.65
5.41
f1 (ppm)

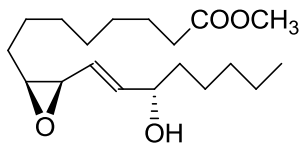

165.435
145.541
128.362 c6d6
128.253 c6d6
128.161 c6d6
128.061 c6d6
127.968 c6d6
127.868 c6d6
123.503
61.267
60.391
56.081
56.046
32.185
32.135
29.634
29.572
26.141
23.071
14.367
14.266
14.252
C7H15
O
CO2Et
40
f1 (ppm)


7.161
7.157
6.908
6.905
6.902
6.876
6.873
6.871
6.130
6.127
6.124
6.098
6.095
6.093
4.050
4.036
4.021
4.007
2.415
2.413
2.402
2.390
2.388
1.287
1.274
1.272
1.180
1.168
1.029
1.026
1.002
1.000
0.988
0.985
0.973
0.971
0.739
0.737
0.724
0.721
0.709
0.706
H3C
O
CO2Et
CH3
42
1.00
1.03
2.23
1.12
2.73
6.70
3.48
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
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
f1 (ppm)

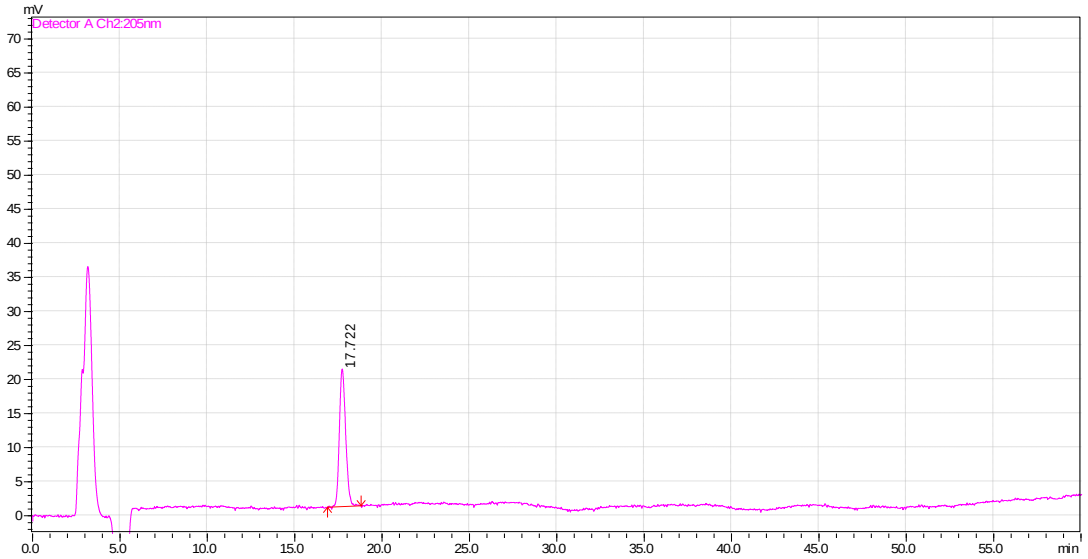

165.837
150.528
128.356
128.253 c6d6
128.060 c6d6
127.868 c6d6
121.608
121.586
121.571
66.776
66.765
66.753
60.330
58.196
22.136
14.886
14.877
14.301
10.434
H3C
O
CO2Et
CH3
42
f1 (ppm)

Stereochemistry Determination:

1. HPLC chromatogram of standard chiral epoxide.



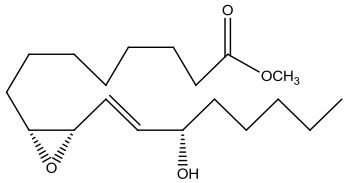
Source: Larodan Fine Chemicals,
Cat. no.: 24-1802-12b, Lot. No.: H-074

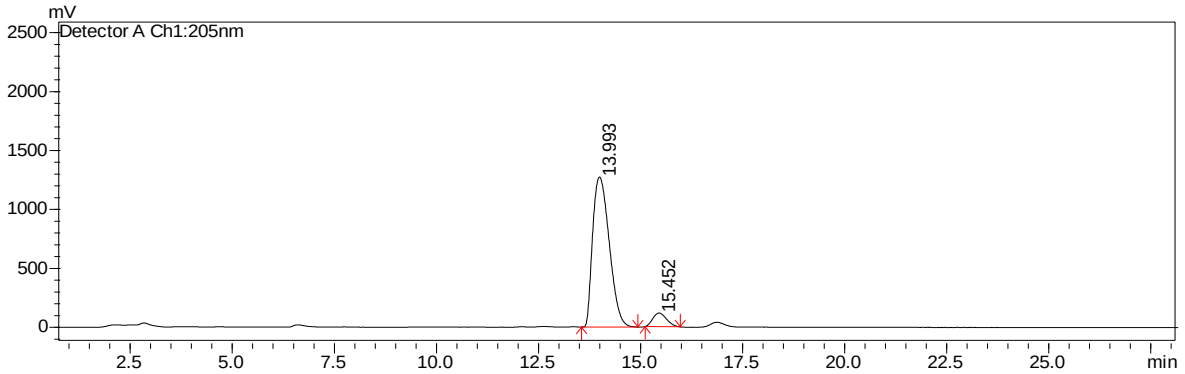


Ascestis Express, 15cm, 4.6mm, 2.7 micron; hexane/IPA :99.9/0.1, 0.75mL/min, 205nm

2. HPLC chromatogram of chiral epoxide prepared using chiral salan ligand and Ti(IV) using HPLC analysis condition above

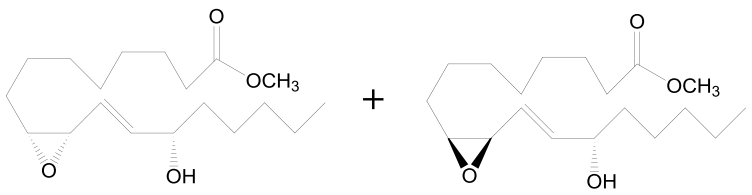
Reference: Jat, J. L.; De, S. R.; Kumar, G.; Adebesin, A. M.; Gandham, S. K.; Falck, J. R., submitted for publication.



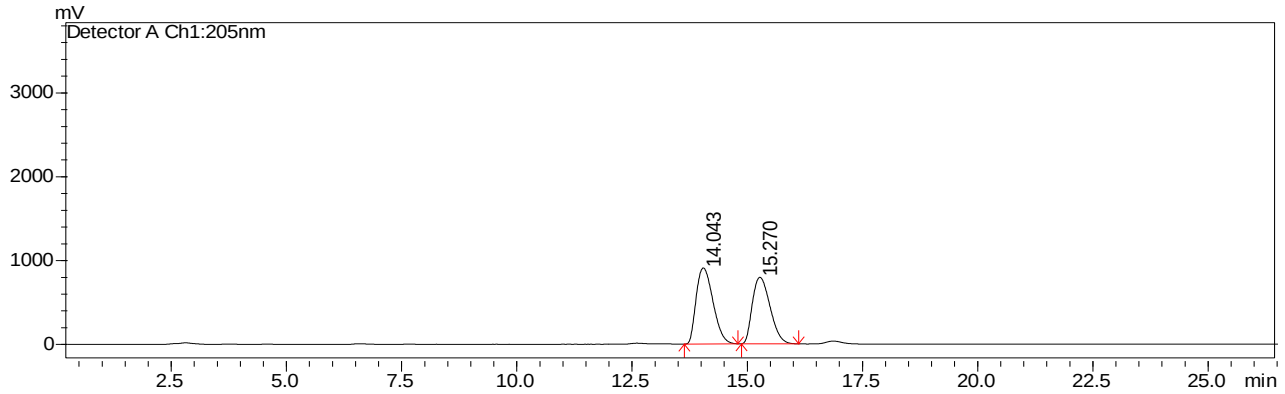


Peak	Ret. Time	Area	Height	Area %
1.	13.993	36061338	1272814	93.039
2.	15.452	2698005	115438	6.961

3. HPLC chromatogram of 1:1 mixture of chiral Ti(salan)-generated epoxide + commercial epoxide standard using HPLC analysis condition above.

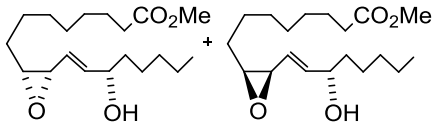


(1:1 mixture of epoxides)

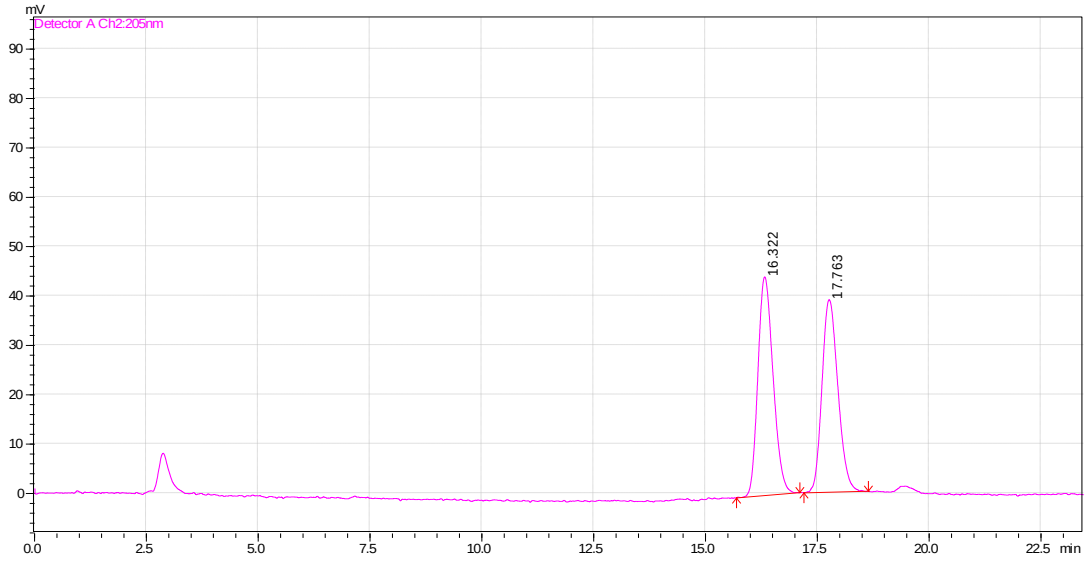


Peak	Ret. Time	Area	Height	Area %
1.	14.043	23200616	908224	52.162
2.	15.270	21276975	793732	47.838

4. HPLC chromatogram of epoxide 5a/6a from MTO-pyridine epoxidation using HPLC analysis condition above.

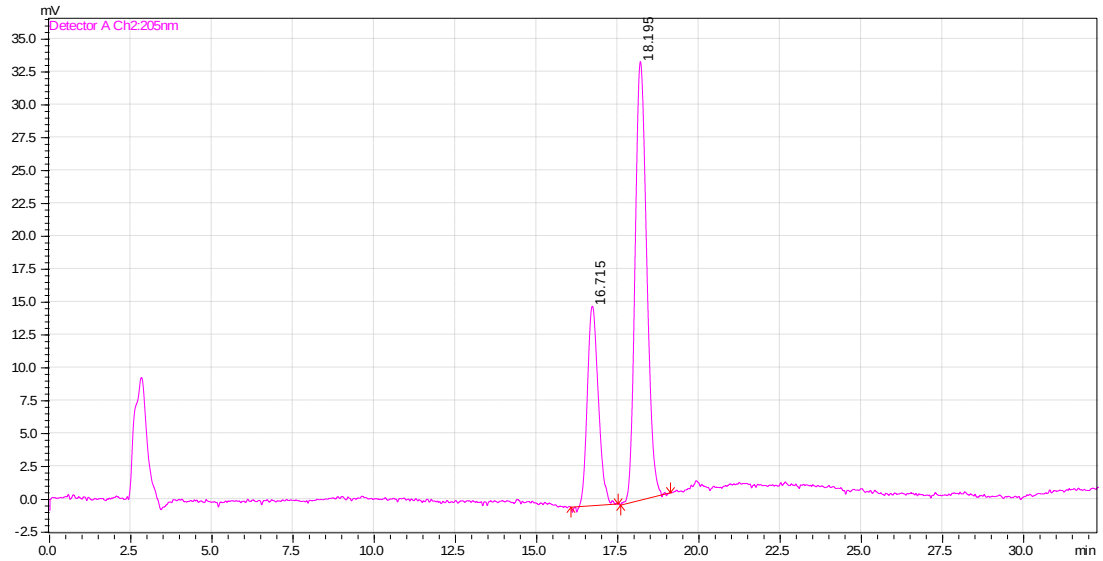


5a (*erythro*) **6a** (*threo*)



Peak Table Detector A Ch 2 205nm				
Peak #	Ret. Time	Area	Height	Area %
1	16.322	1050224	44308	52.0176
2	17.763	968752	39023	47.9824

5. HPLC chromatogram of epoxide 5a/6a from MTO-pyridine epoxidation + commercial epoxide standard using HPLC analysis condition above.



Peak Table Detector A Ch 2 205nm				
Peak #	Ret. Time	Area	Height	Area %
1	16.715	355843	15164	29.9270
2	18.195	833193	33361	70.0730