

Supporting information for:

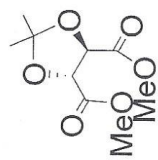
A C_2 -Symmetric Chiral Pool - Based Flexible Strategy: Synthesis of (+)- and (-)-Shikimic Acids, (+)- and (-)-4-*epi*-Shikimic Acids, and (+)- and (-)-Pinitol

Bakthavachalam Ananthan, Wan-Chun Chang, Jhe-Sain Lin, Ping-Hui Lee, Tu-Hsin Yan*

Department of Chemistry, National Chung-Hsing University, Taichung 400, Taiwan, Republic of China. E-mail: thyan@mail.nchu.edu.tw

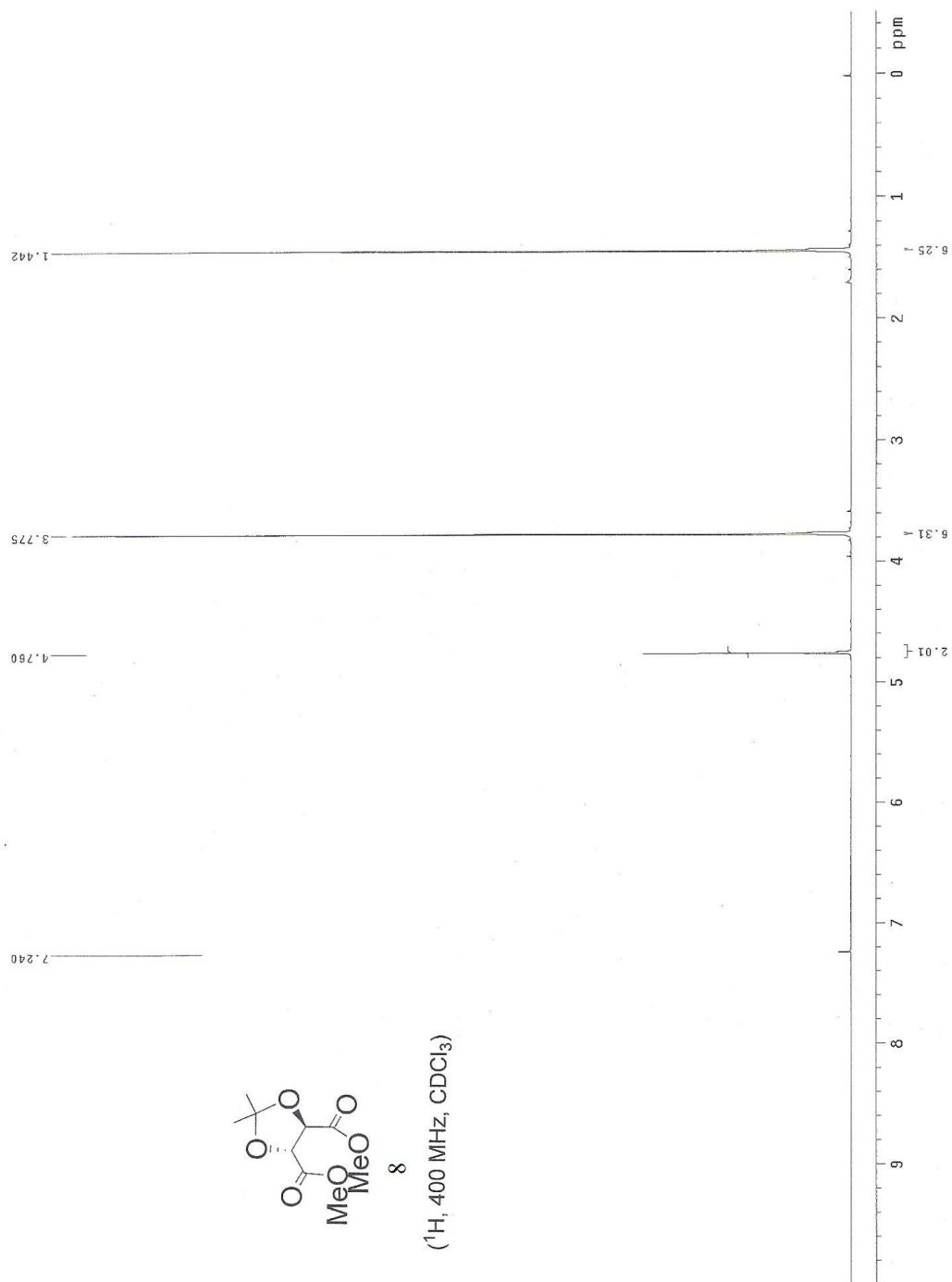
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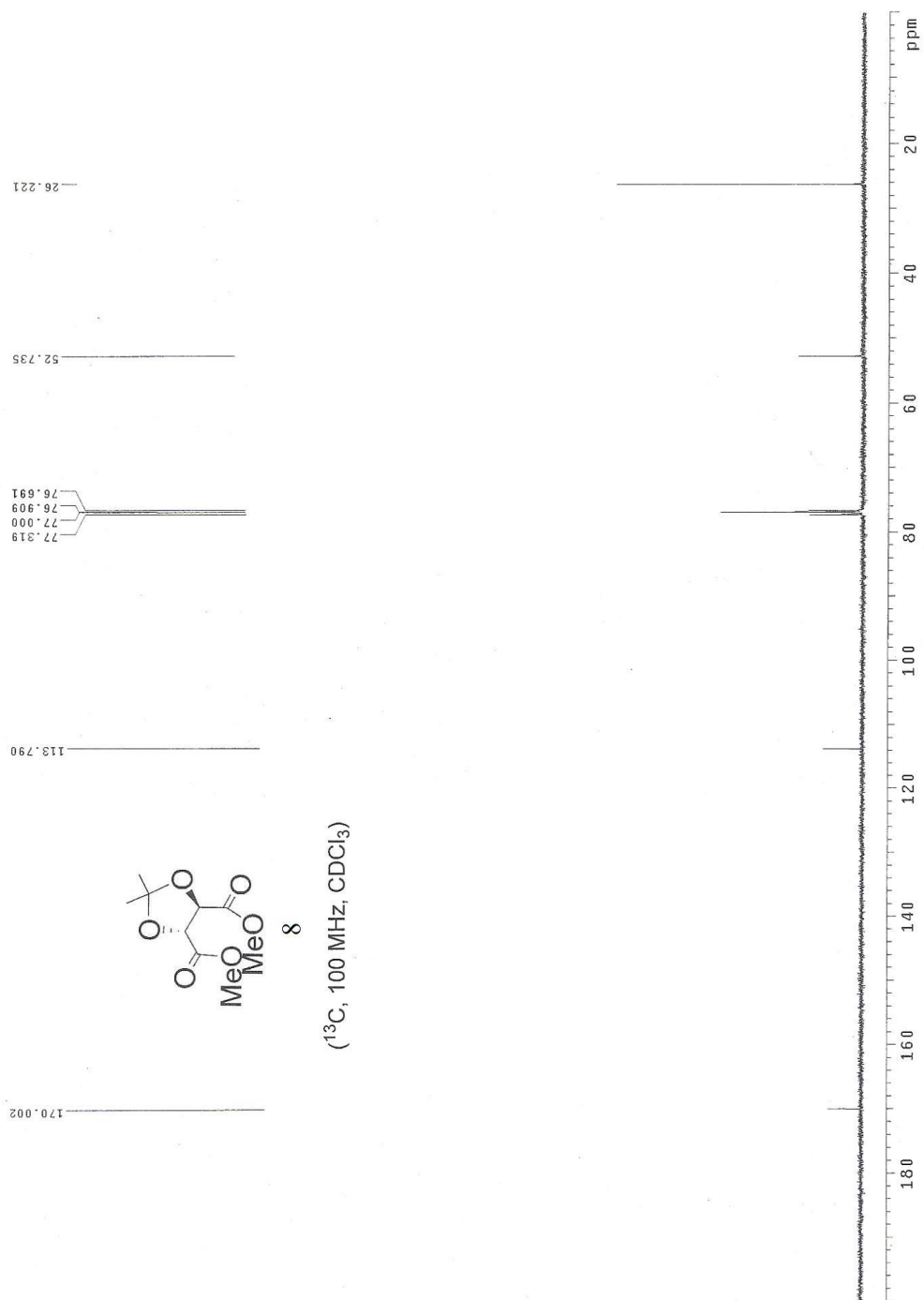
^1H and ^{13}C NMR spectra of the compounds.....	2
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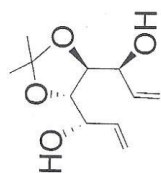


8

(¹H, 400 MHz, CDCl₃)

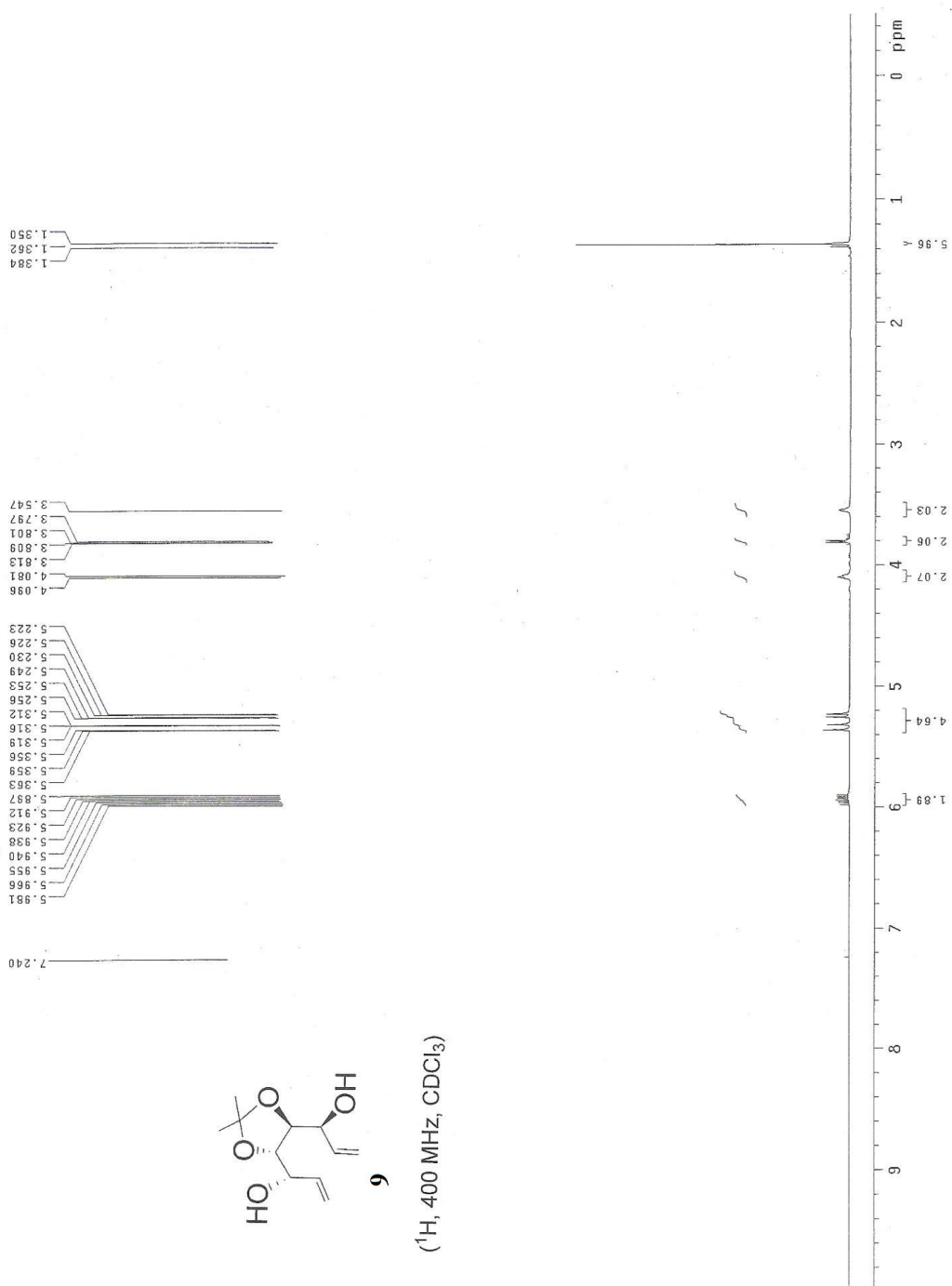


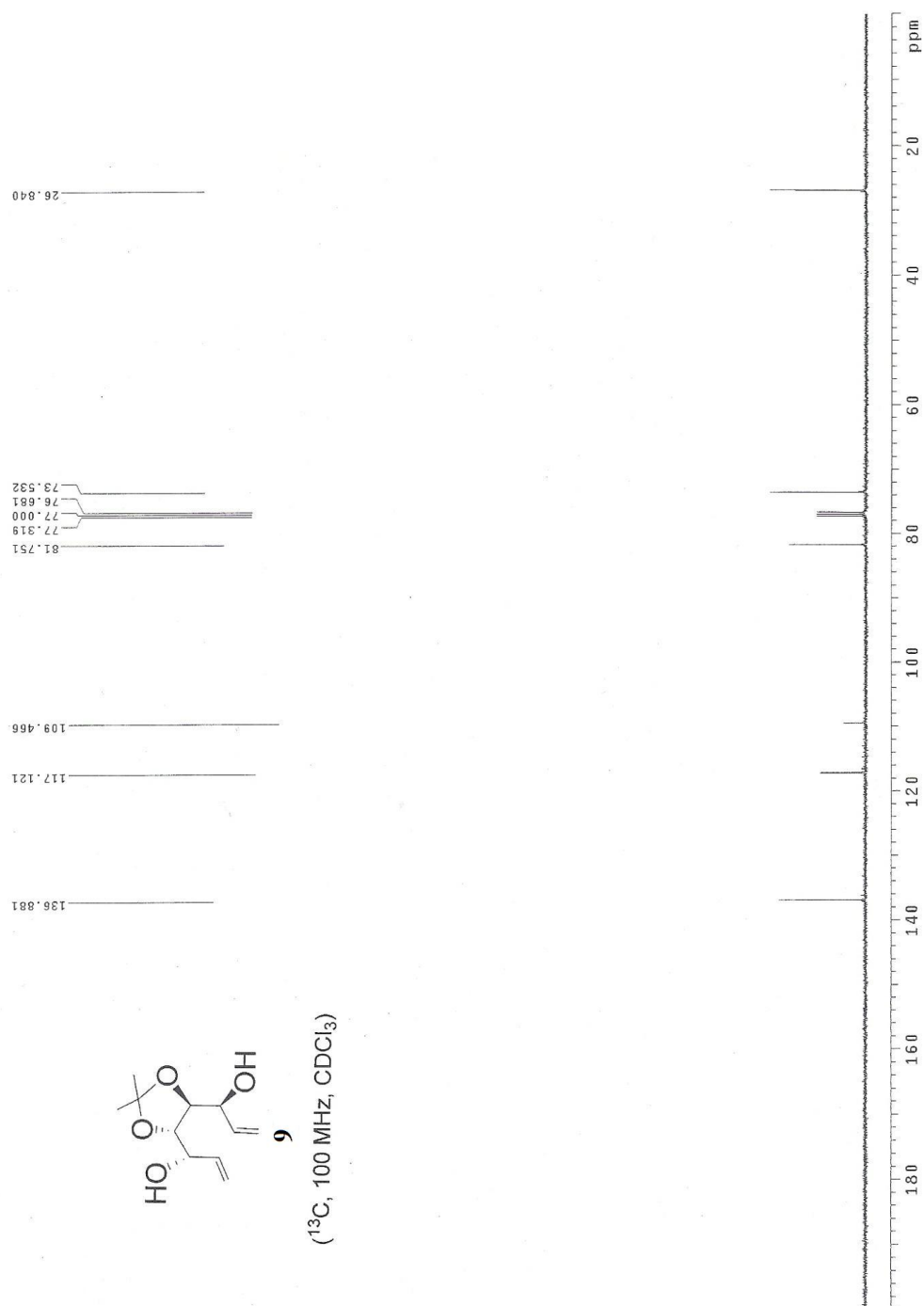


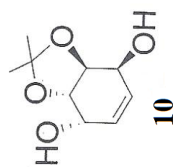


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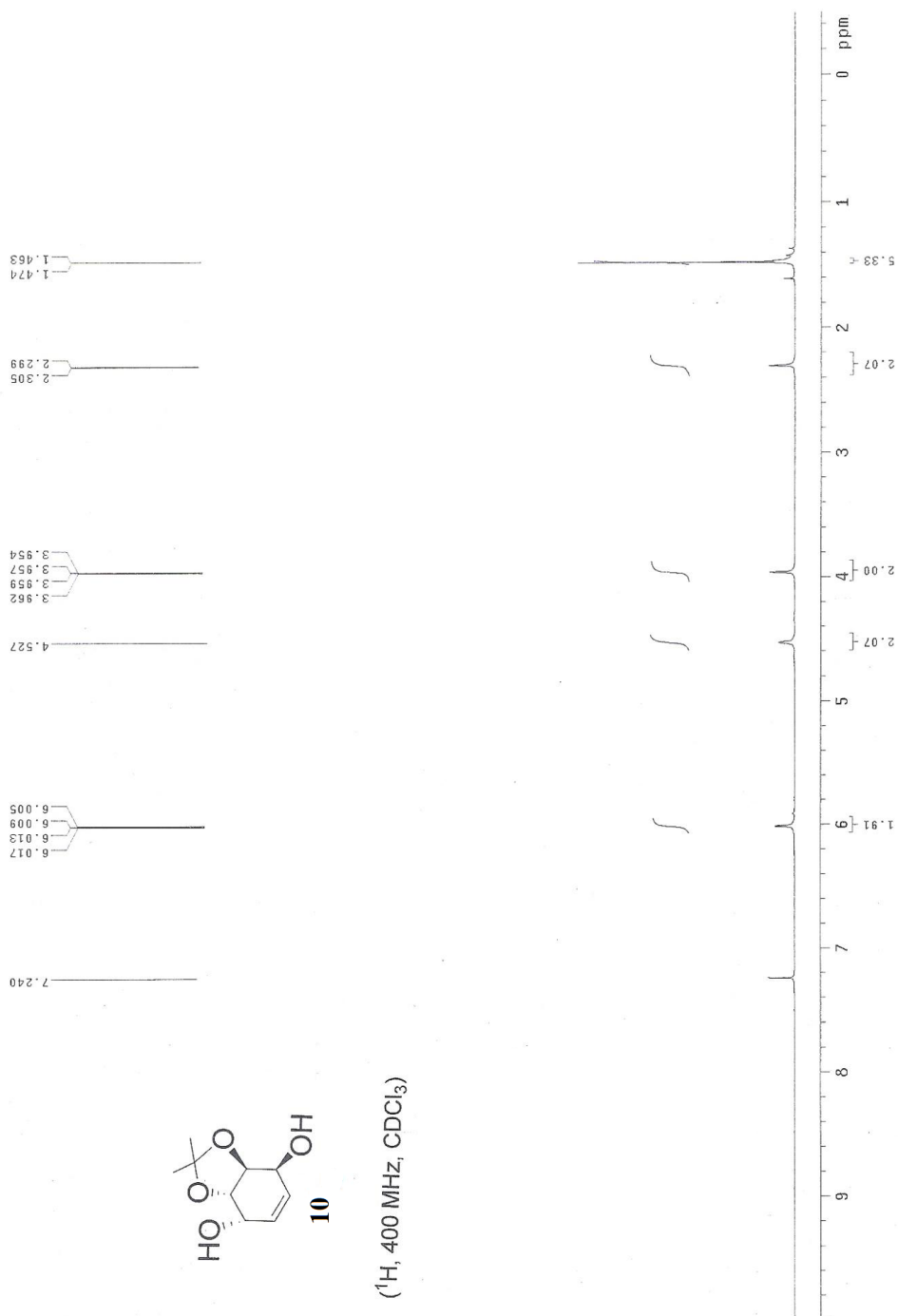
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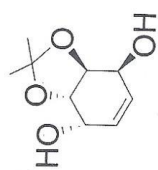






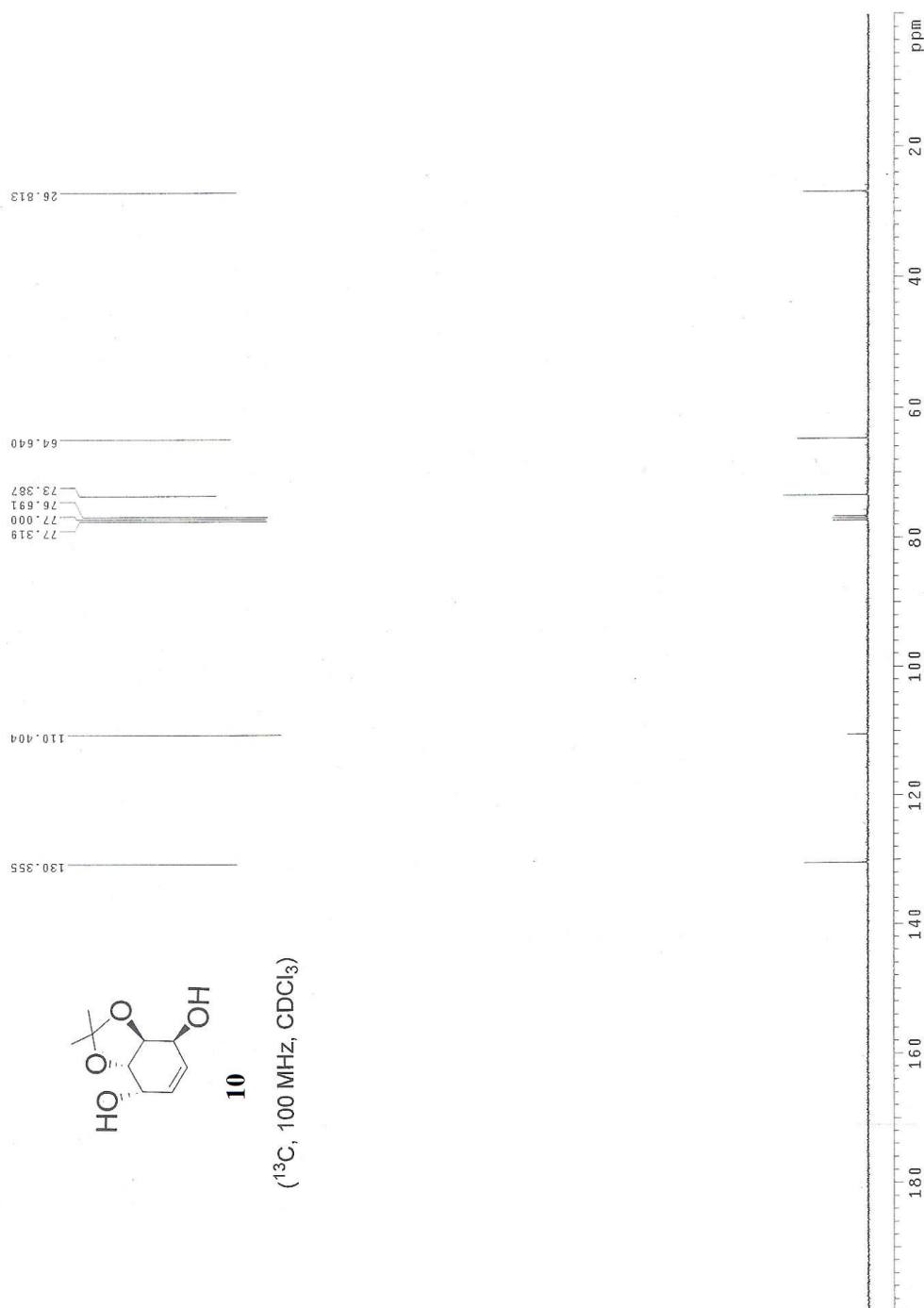
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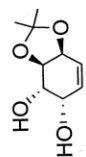




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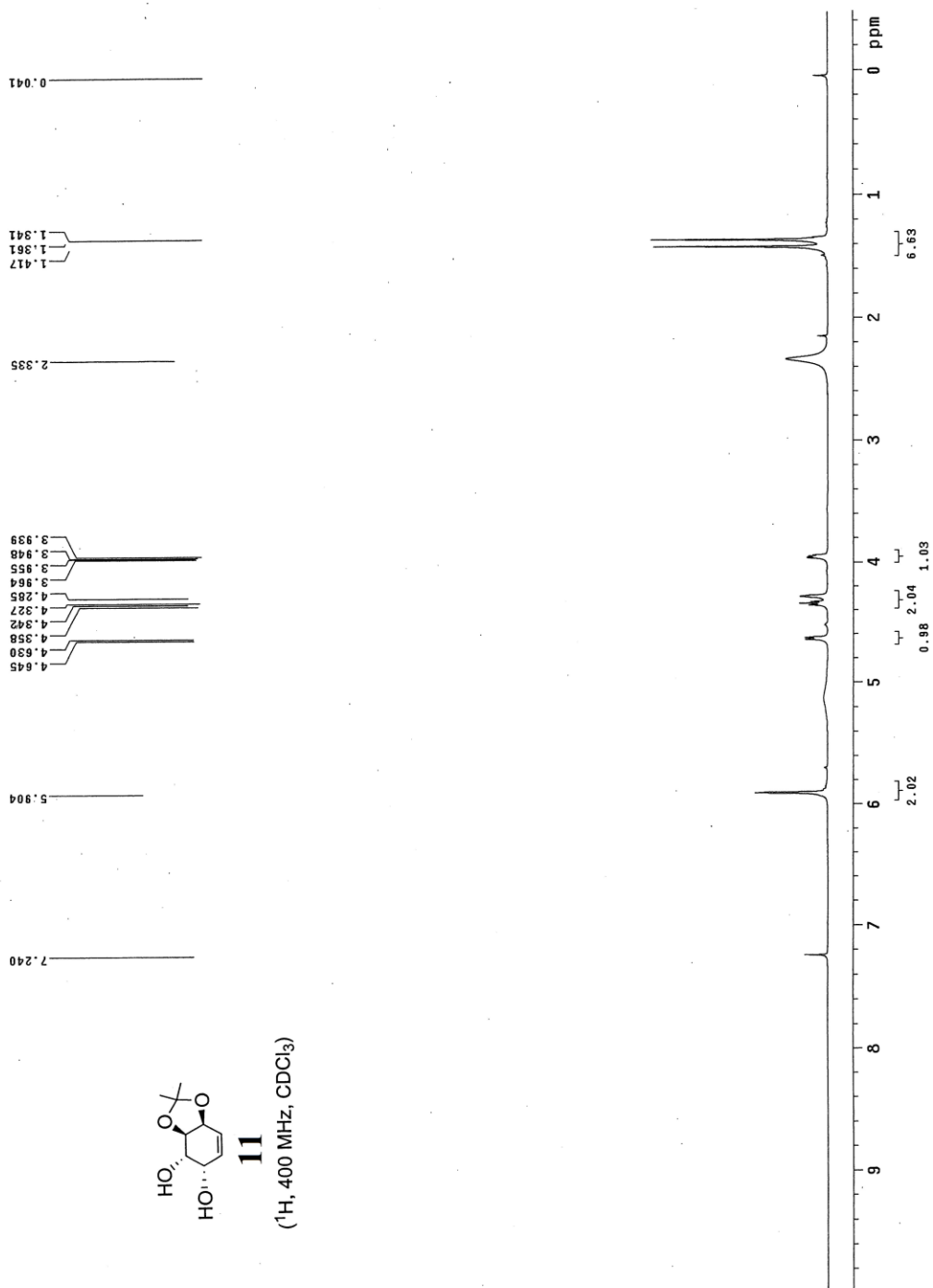
(¹³C, 100 MHz, CDCl₃)

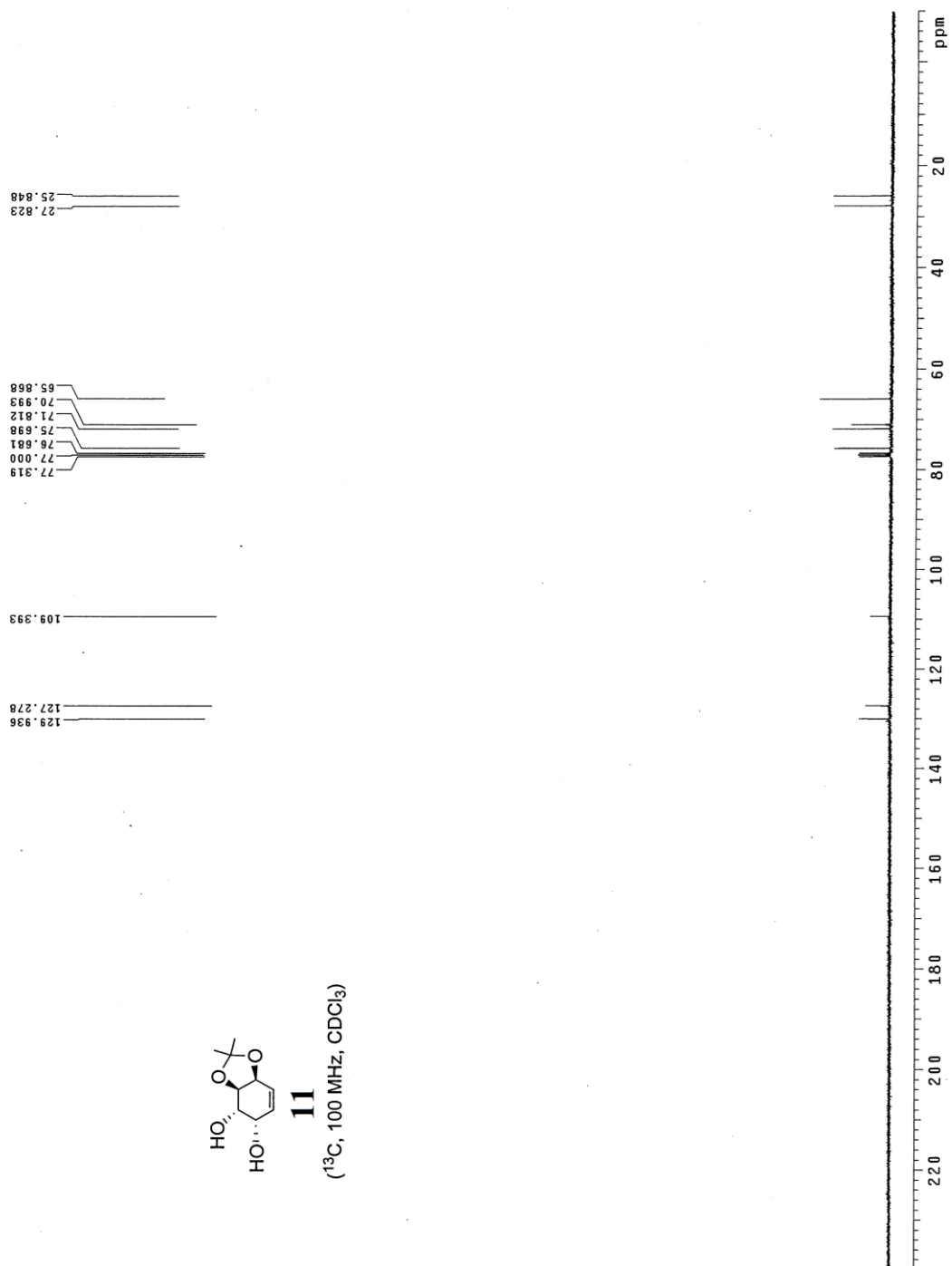
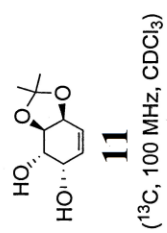




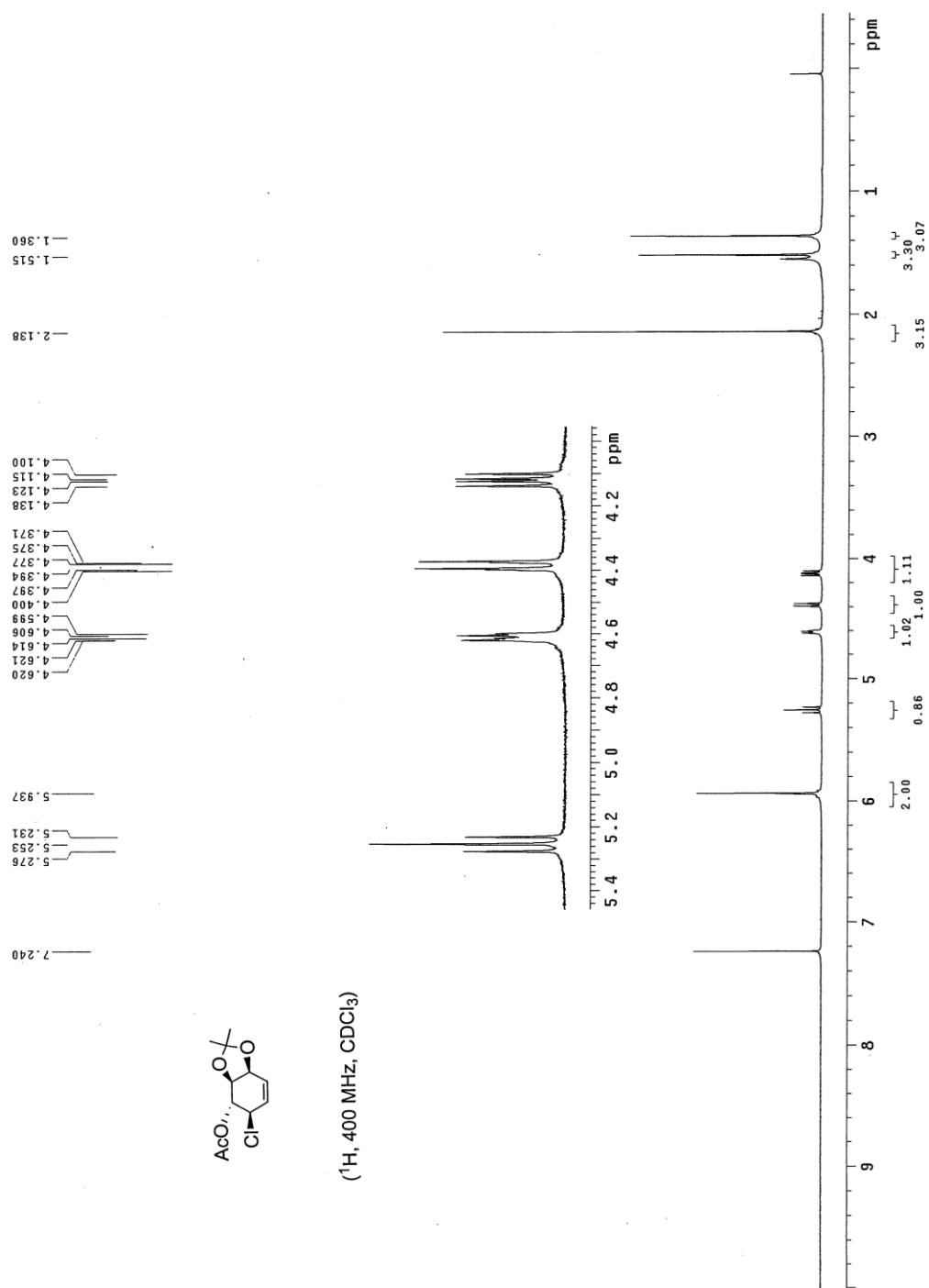
11

(¹H, 400 MHz, CDCl₃)

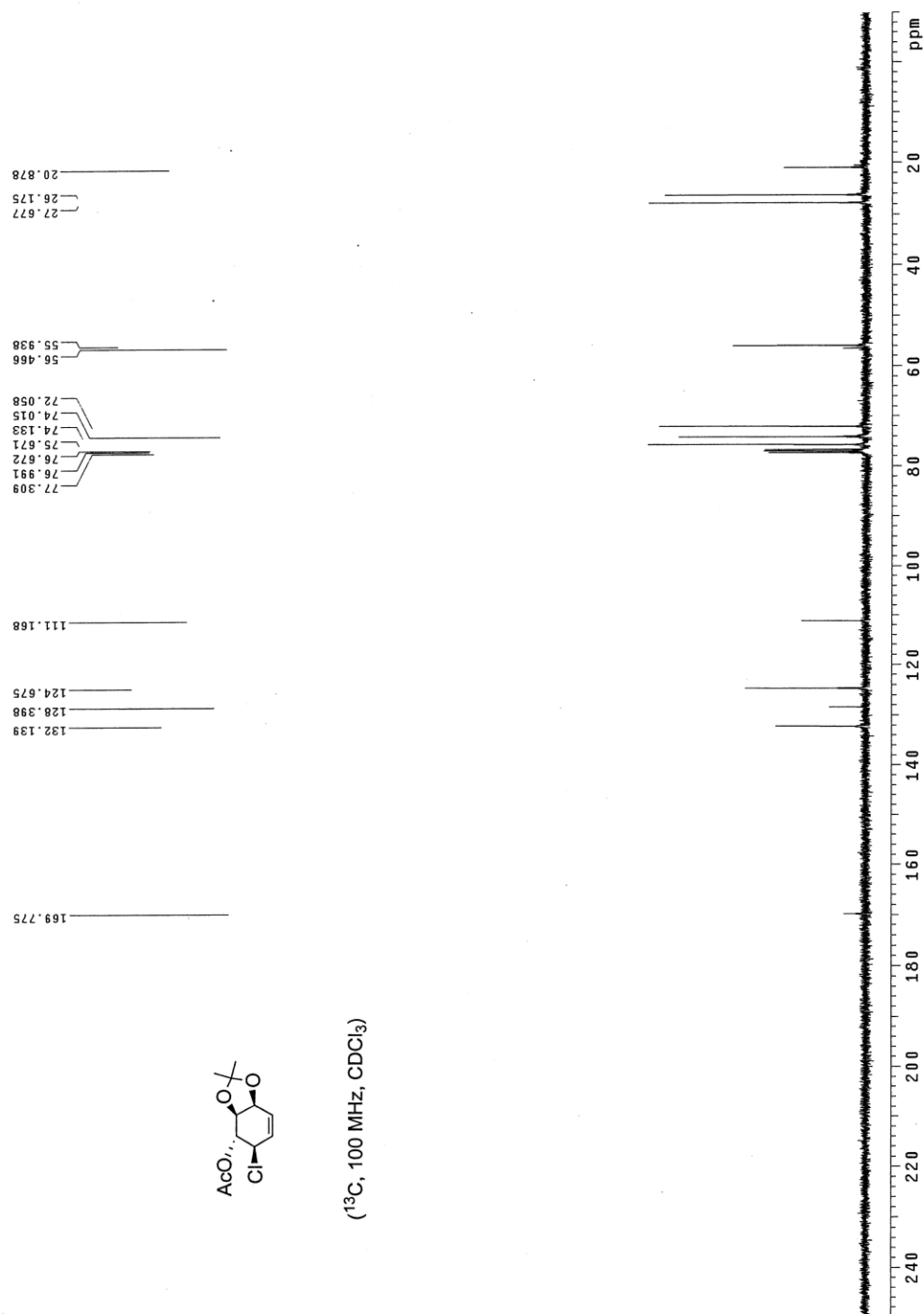




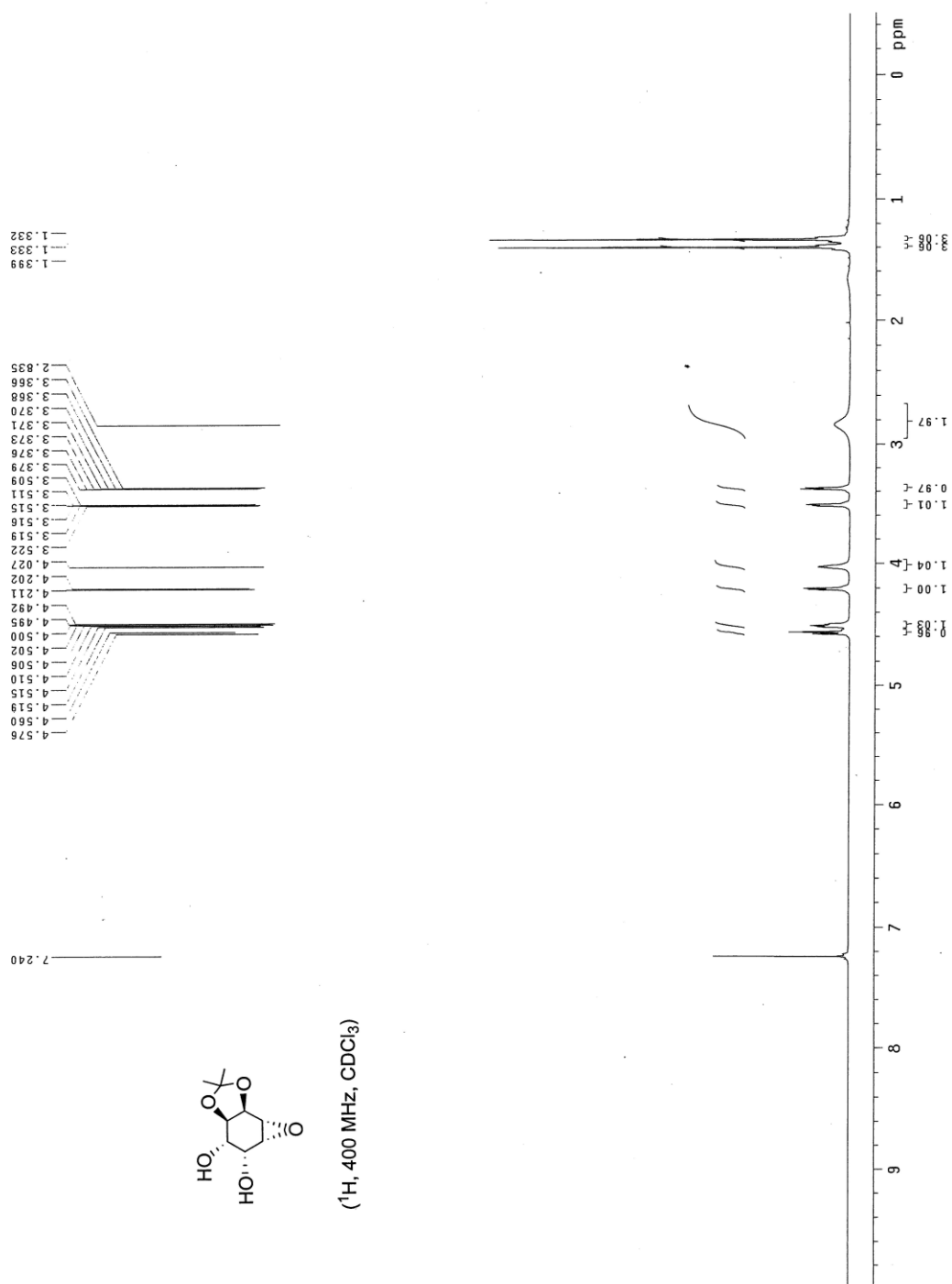
Compound No. 12



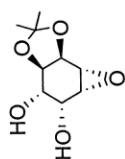
Compound No. 12



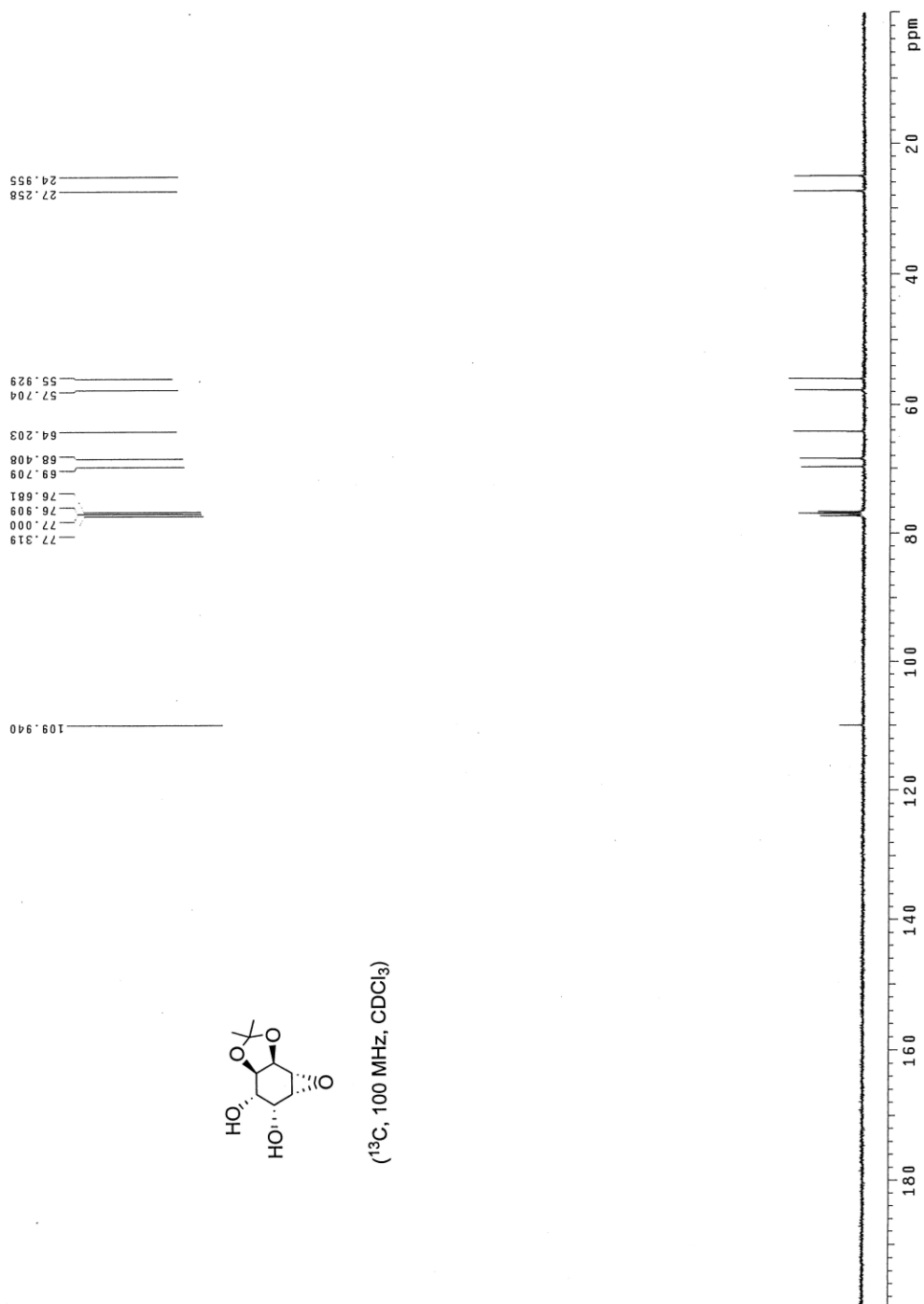
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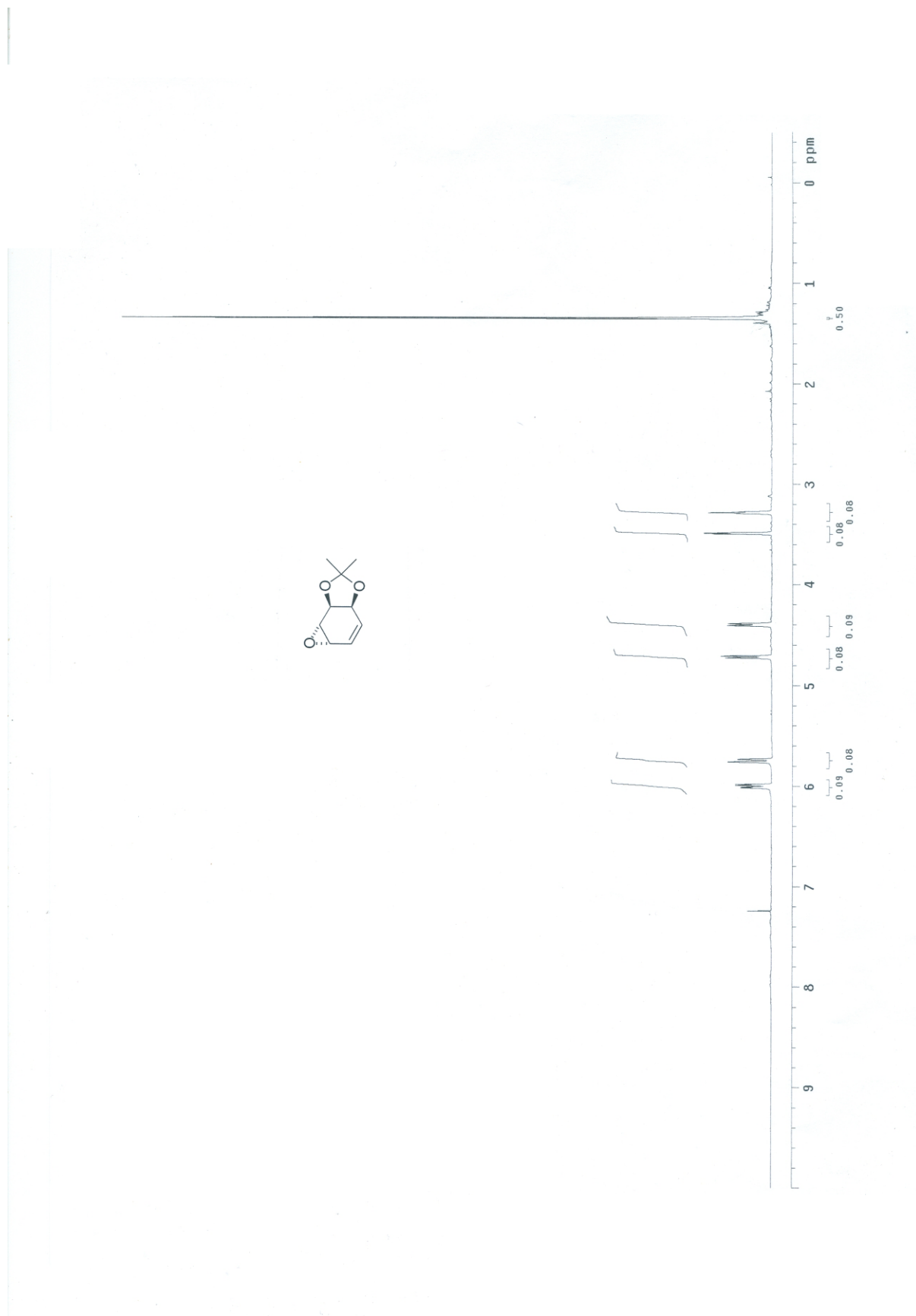


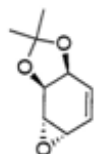
Compound No. 13



(^{13}C , 100 MHz, CDCl_3)

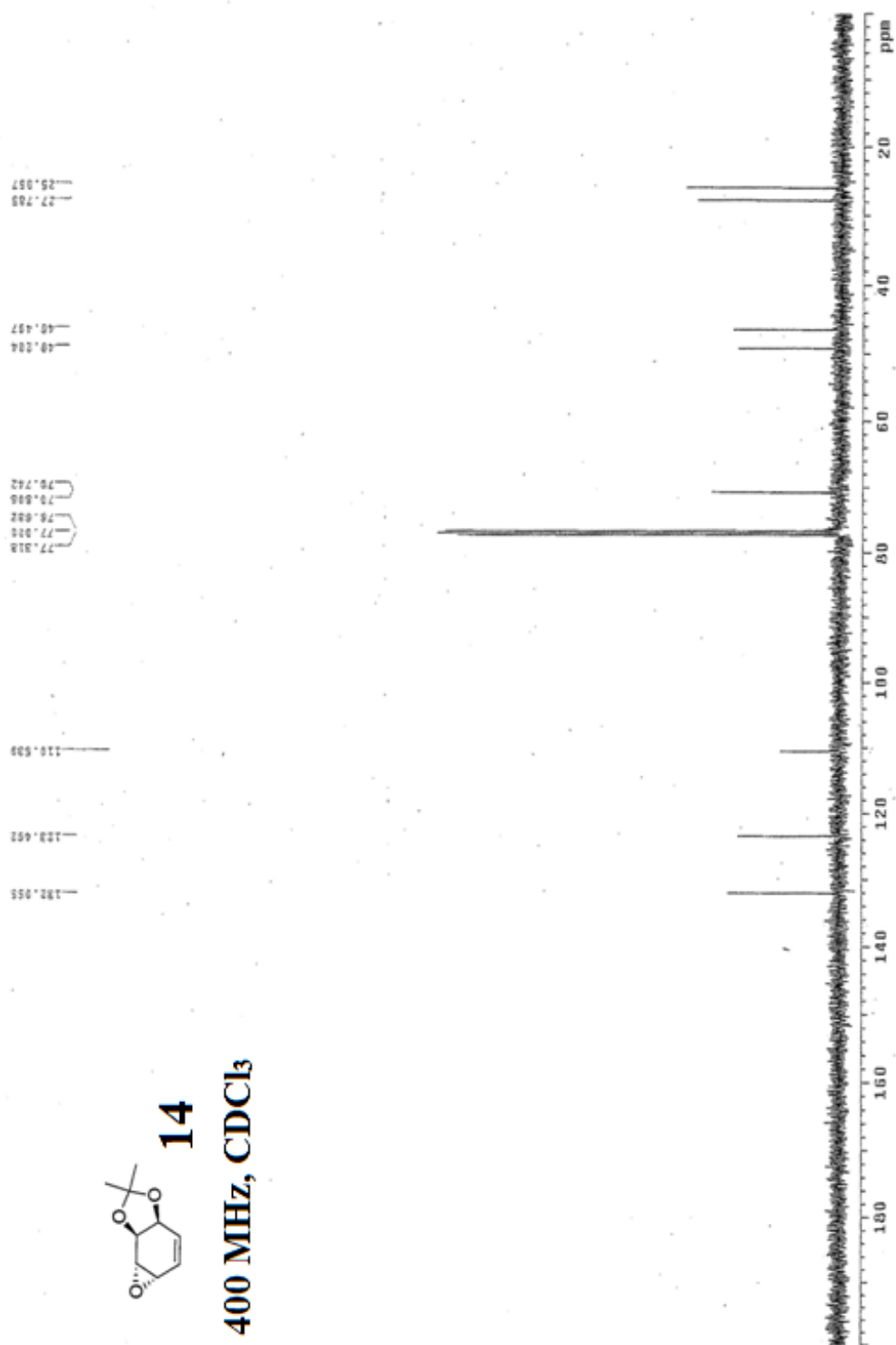






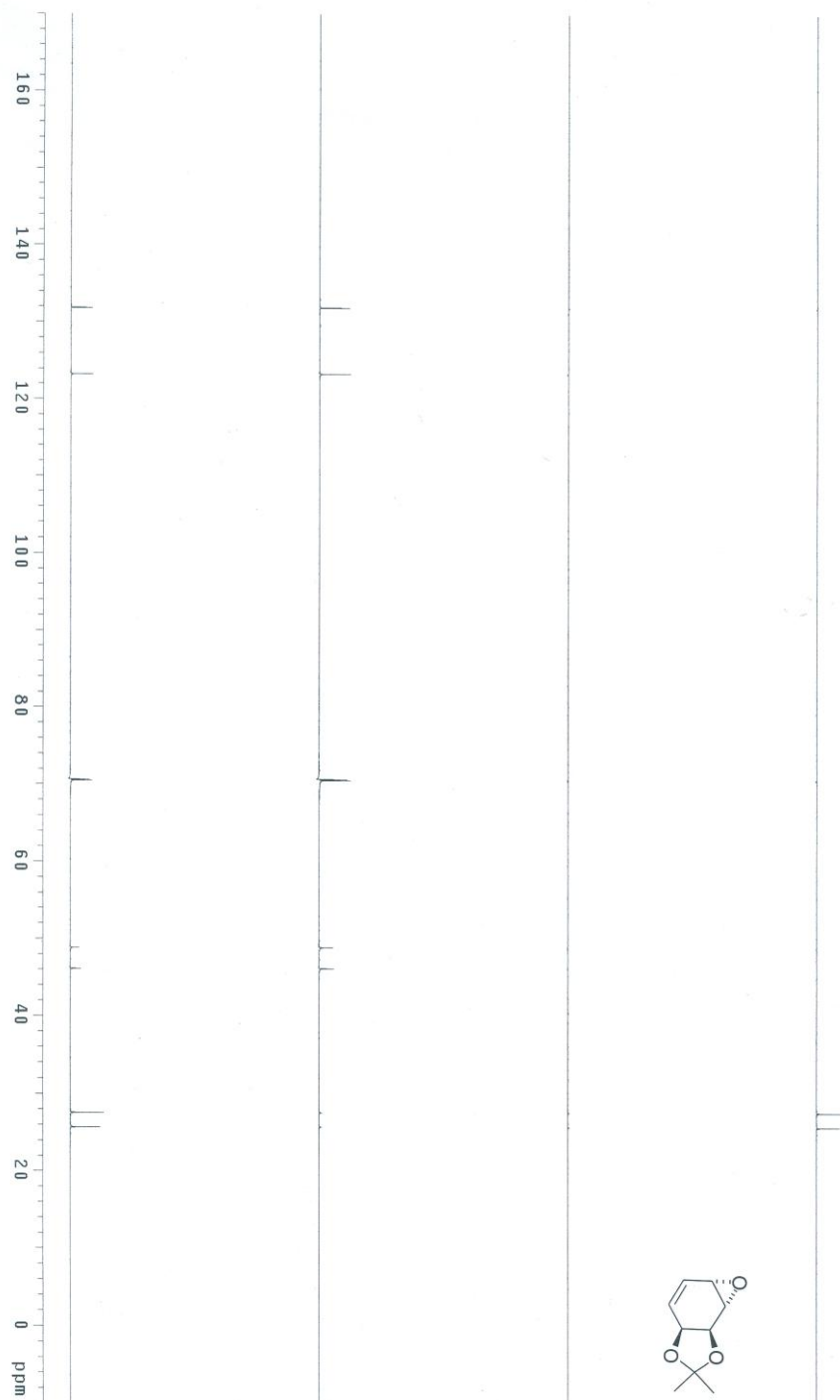
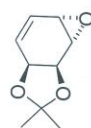
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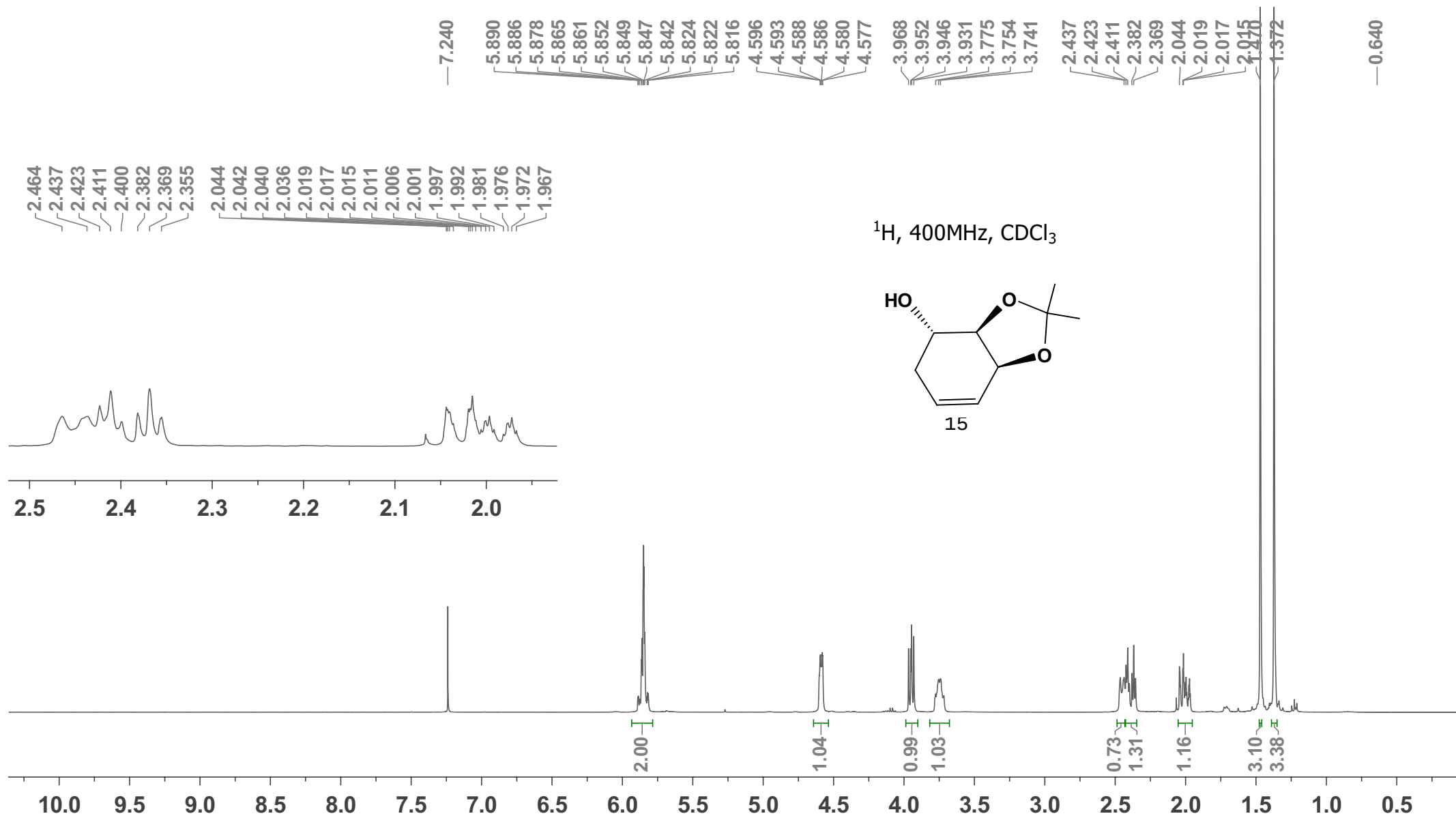
400 MHz, CDCl₃



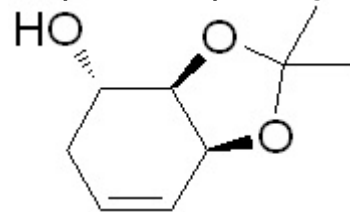
W-3257

Pulse Sequence: dept





¹³C, 100MHz, CDCl₃



15

—129.321

—124.289

—109.153

79.404

77.317

77.000

76.682

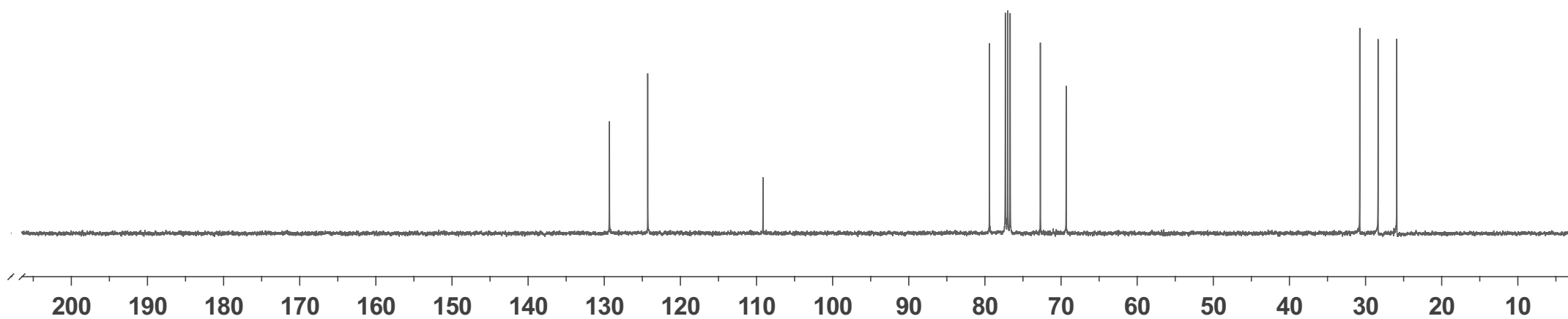
72.719

69.328

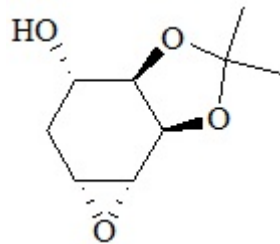
30.763

28.359

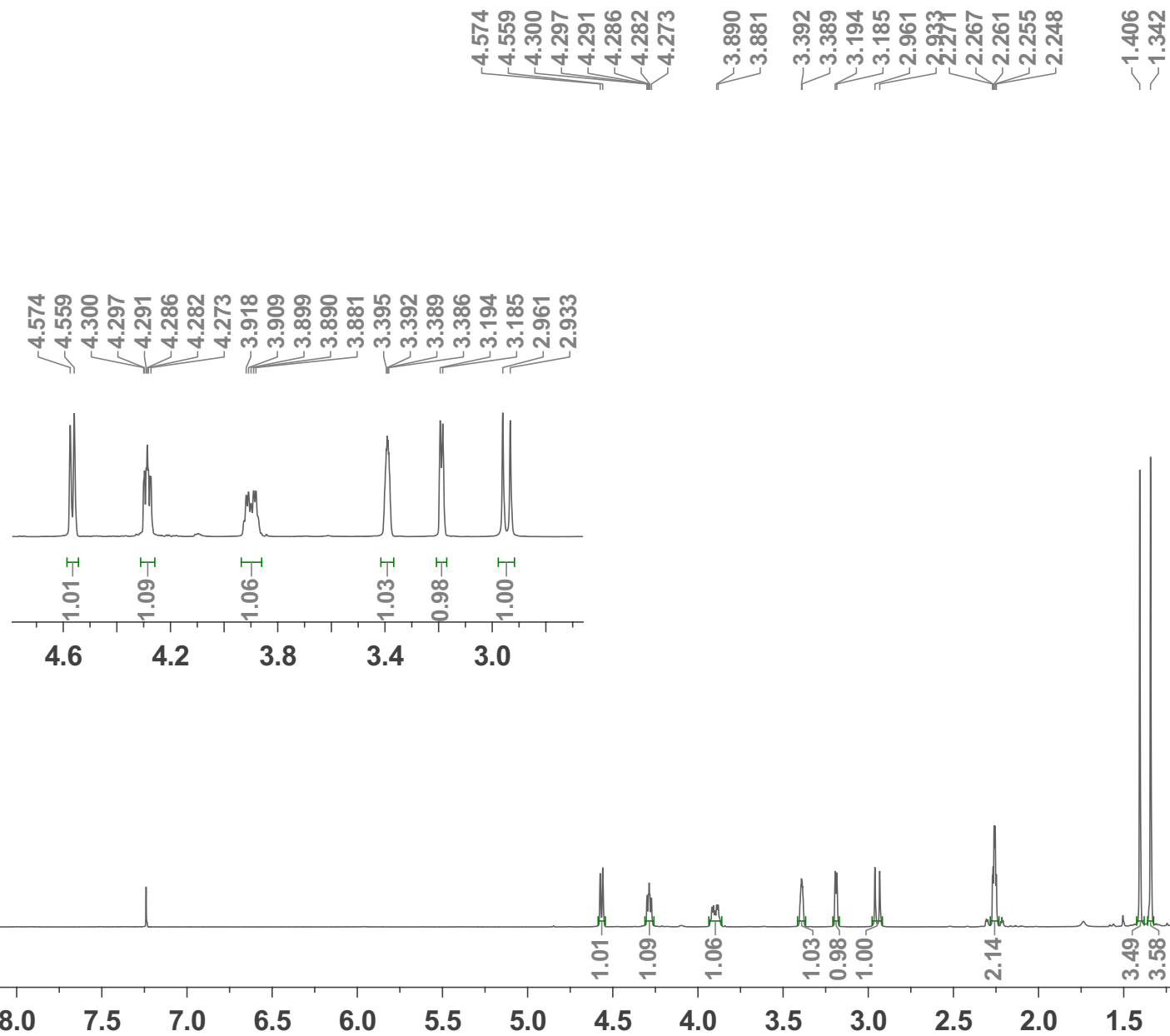
25.900

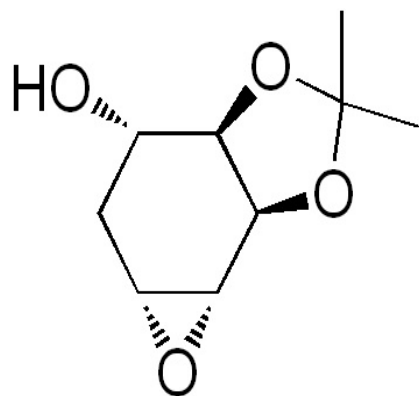


S18



16





^{13}C , CDCl_3 , 100MHz

16

109.851

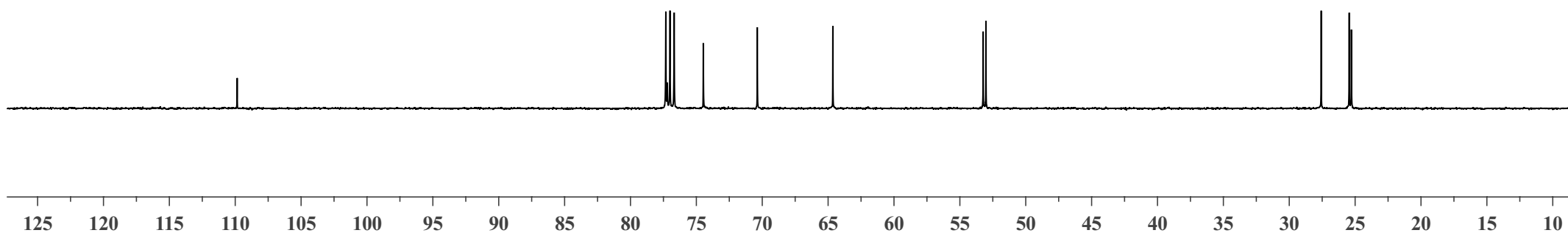
77.318
77.000
76.683
74.473

70.374

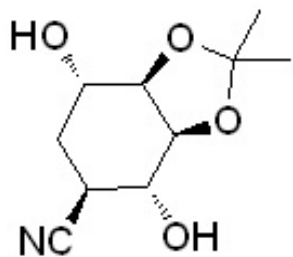
64.641

53.232
53.021

27.574
25.449
25.283

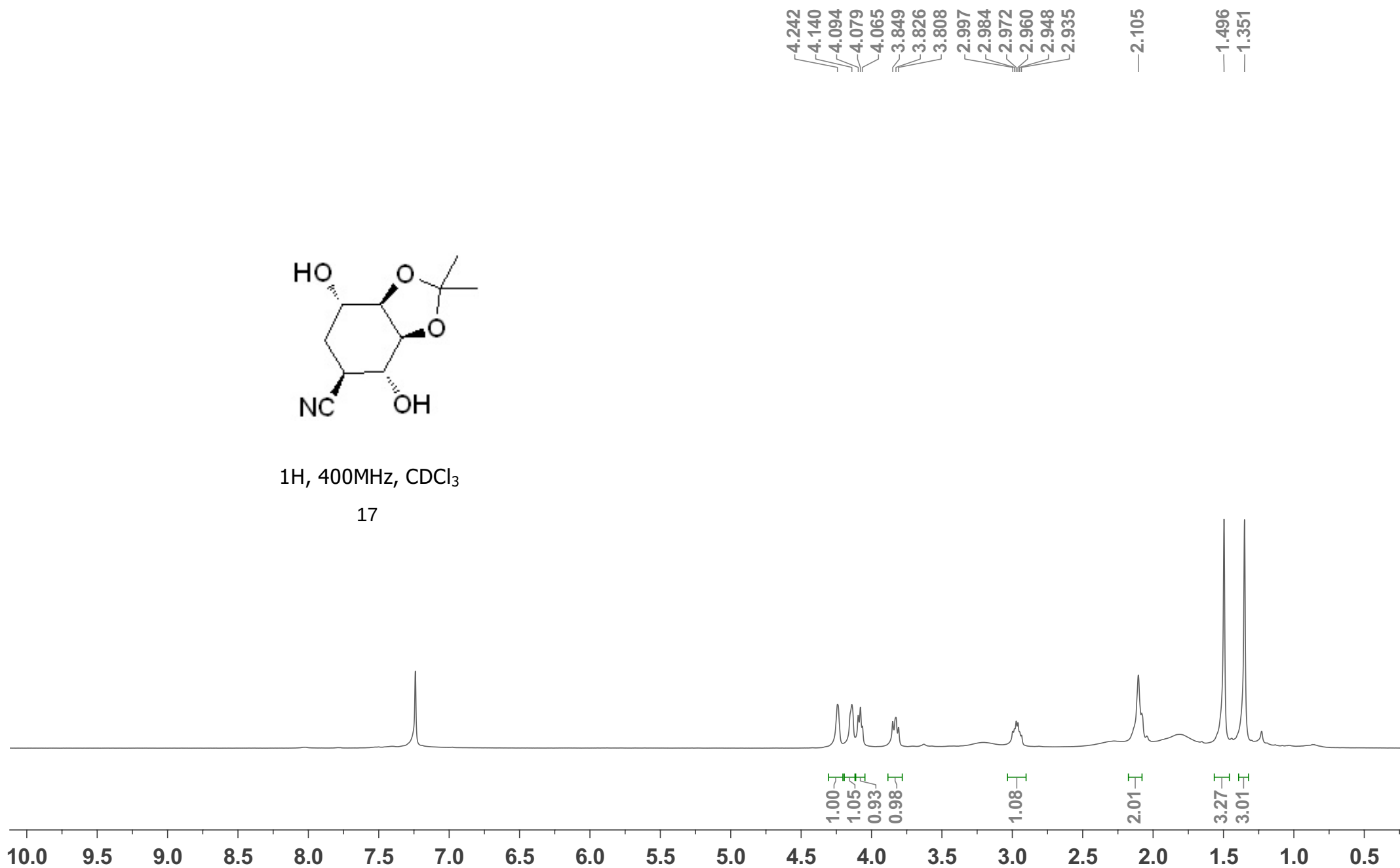


S20

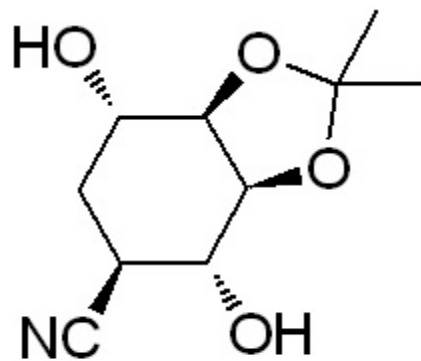


1H, 400MHz, CDCl₃

17

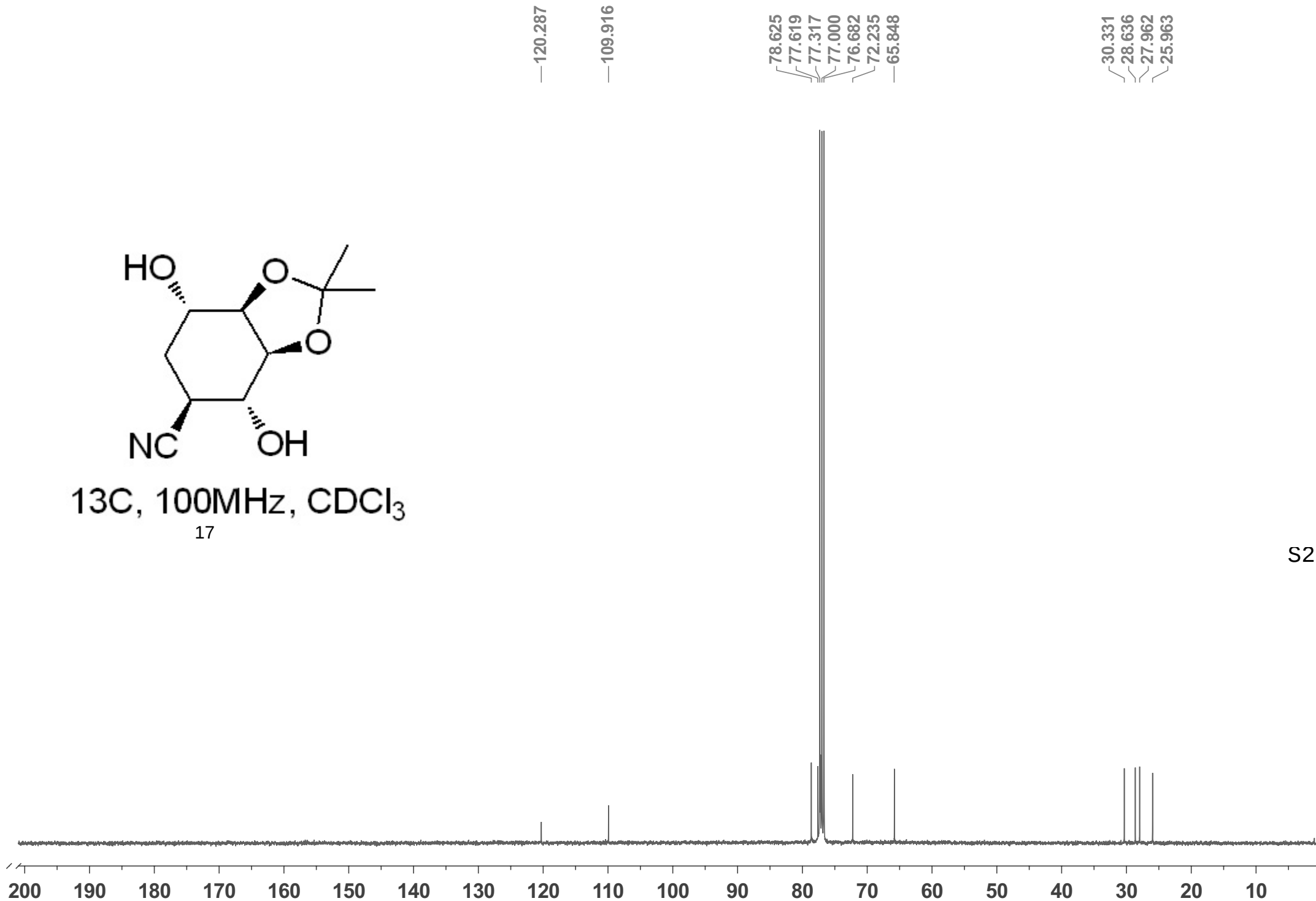


4.242
4.140
4.094
4.079
4.065
3.849
3.826
3.808
2.997
2.984
2.972
2.960
2.948
2.935
2.105
1.496
1.351

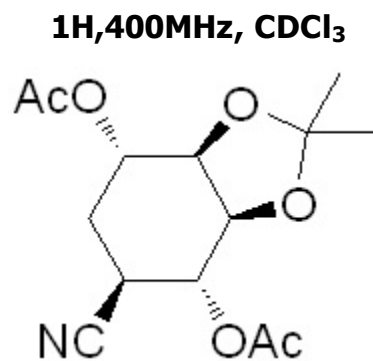


^{13}C , 100MHz, CDCl_3

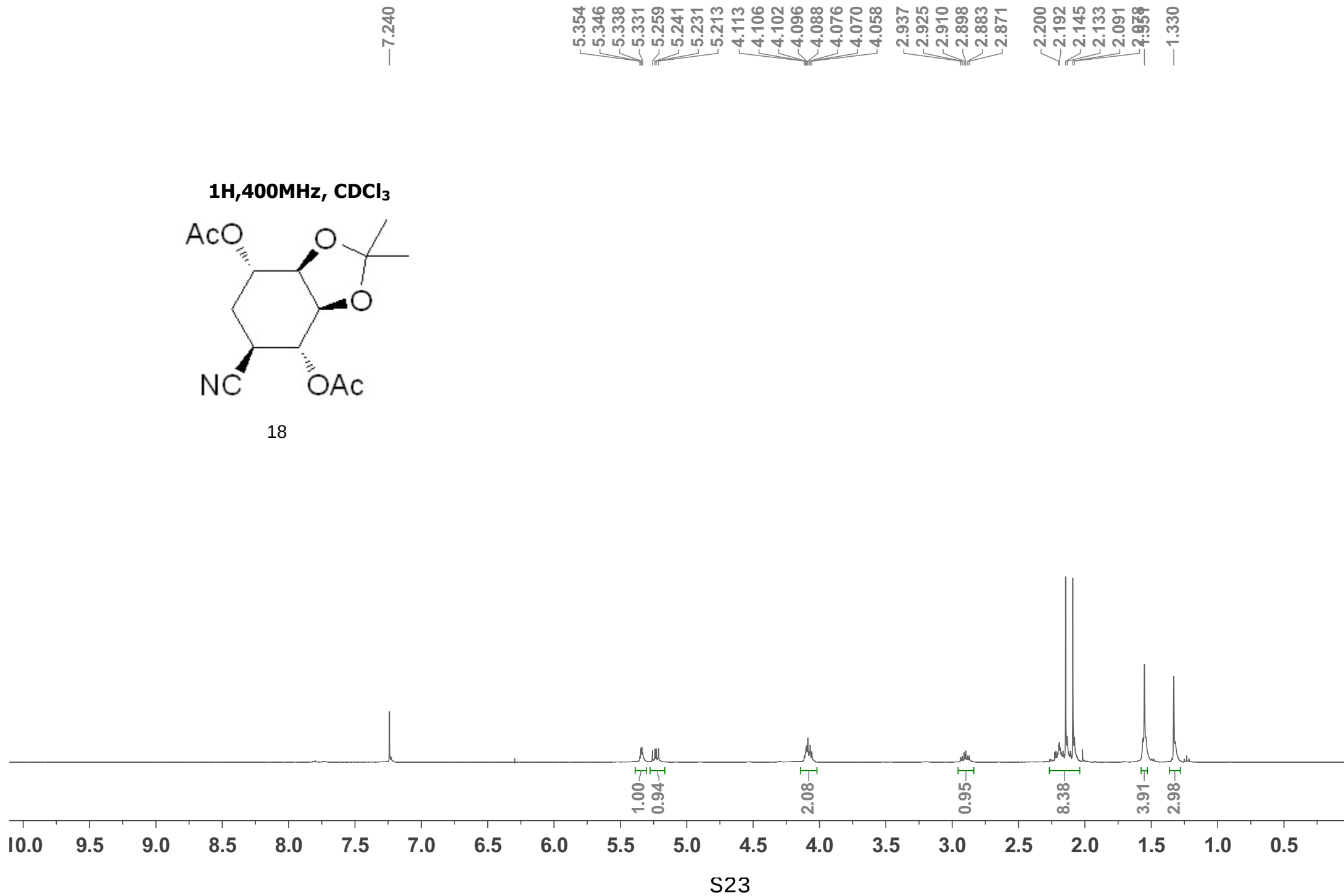
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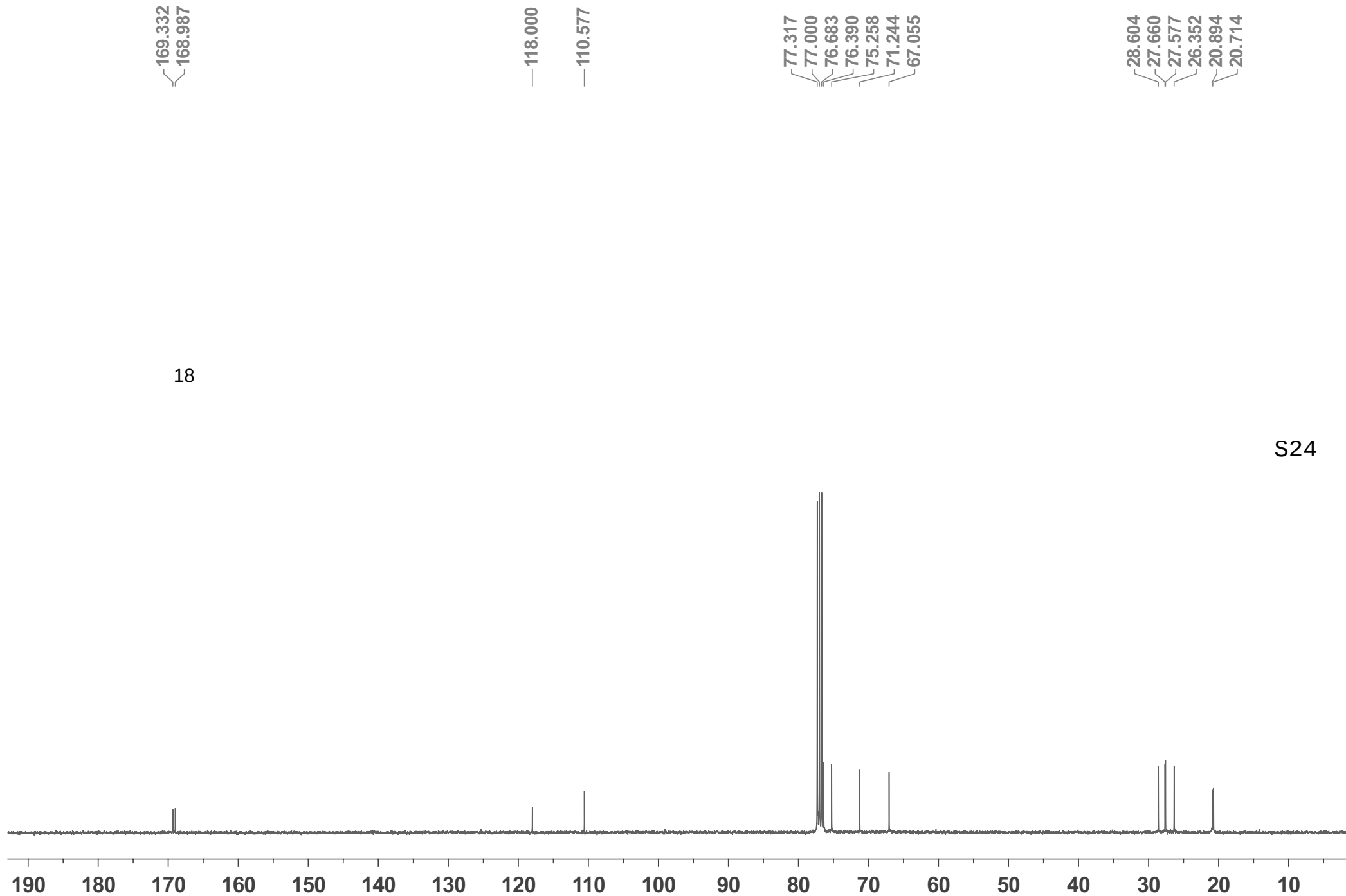


S22

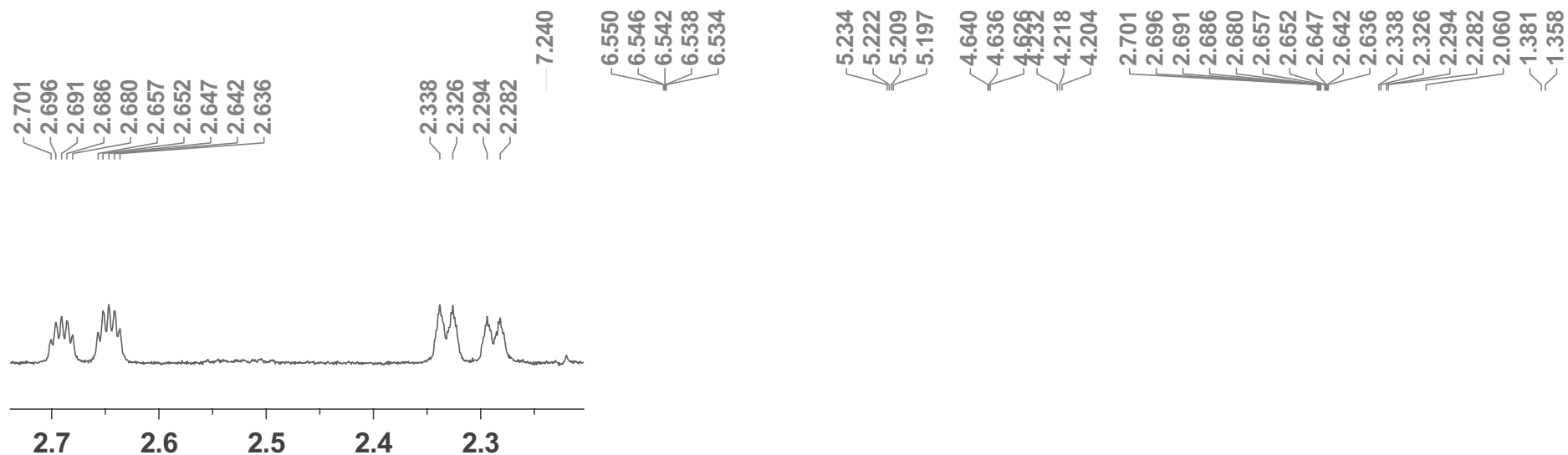


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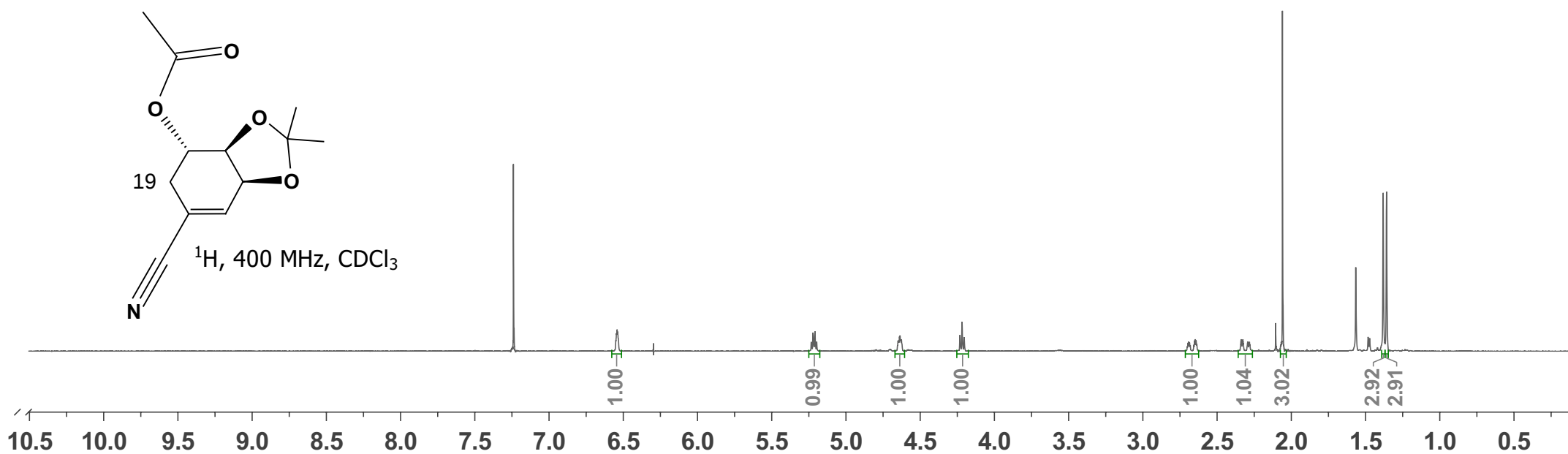


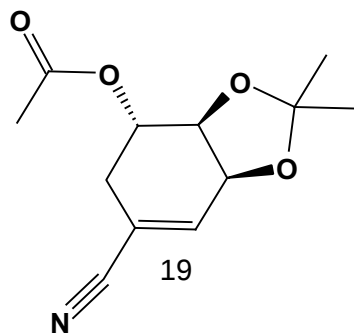


S24



S25





^{13}C , 100 MHz, CDCl_3

— 169.831

— 140.578

— 117.762

— 111.326

— 110.461

77.317

77.000

76.683

72.495

70.672

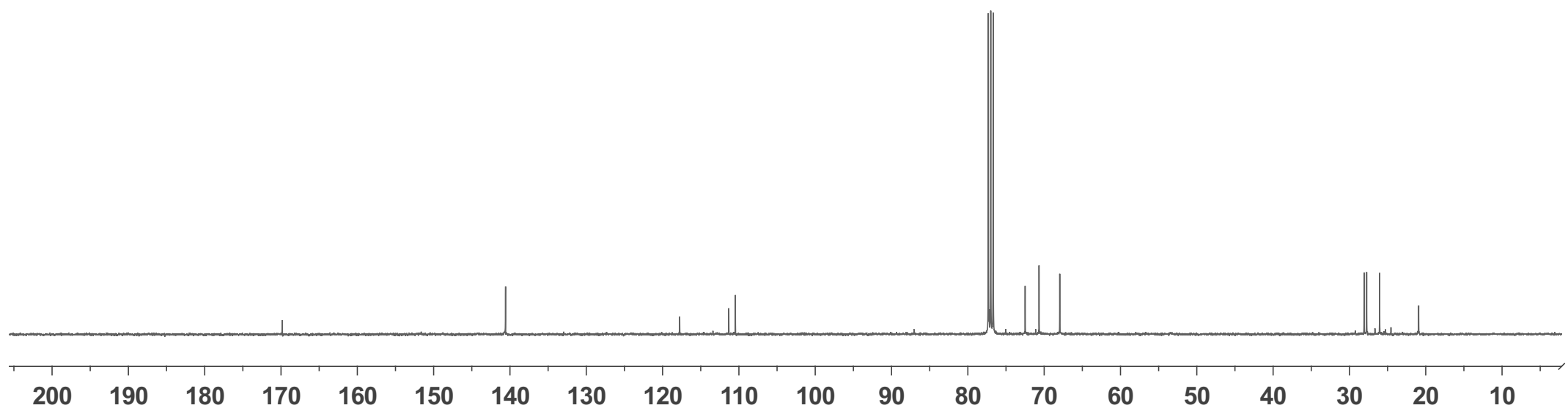
67.960

28.073

27.741

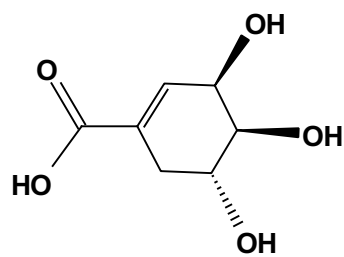
26.042

20.925

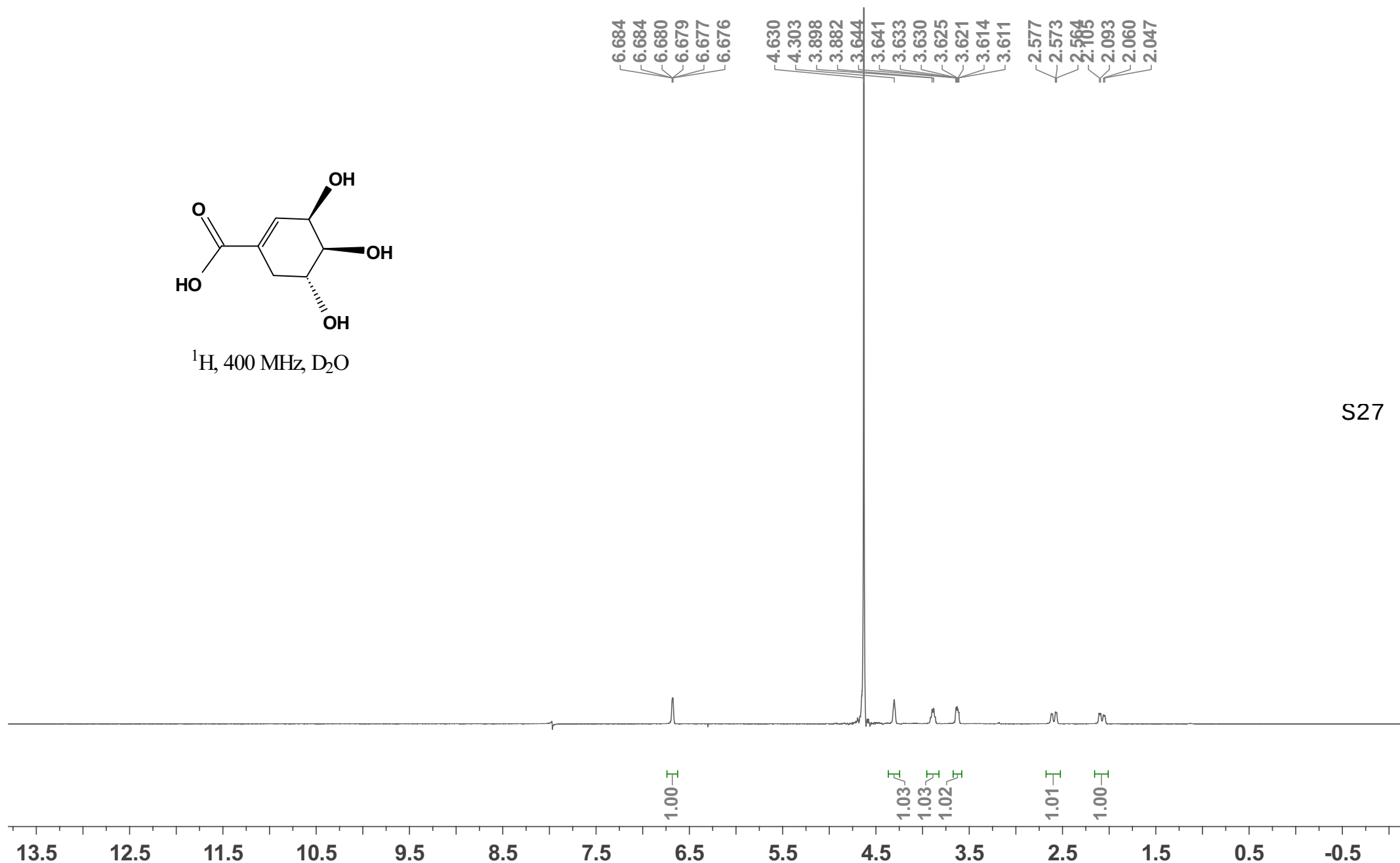


S26

For compounds 1 and 2

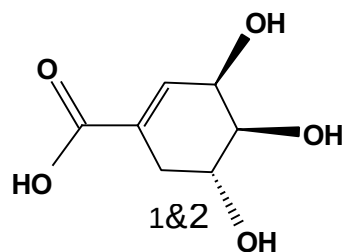


^1H , 400 MHz, D_2O

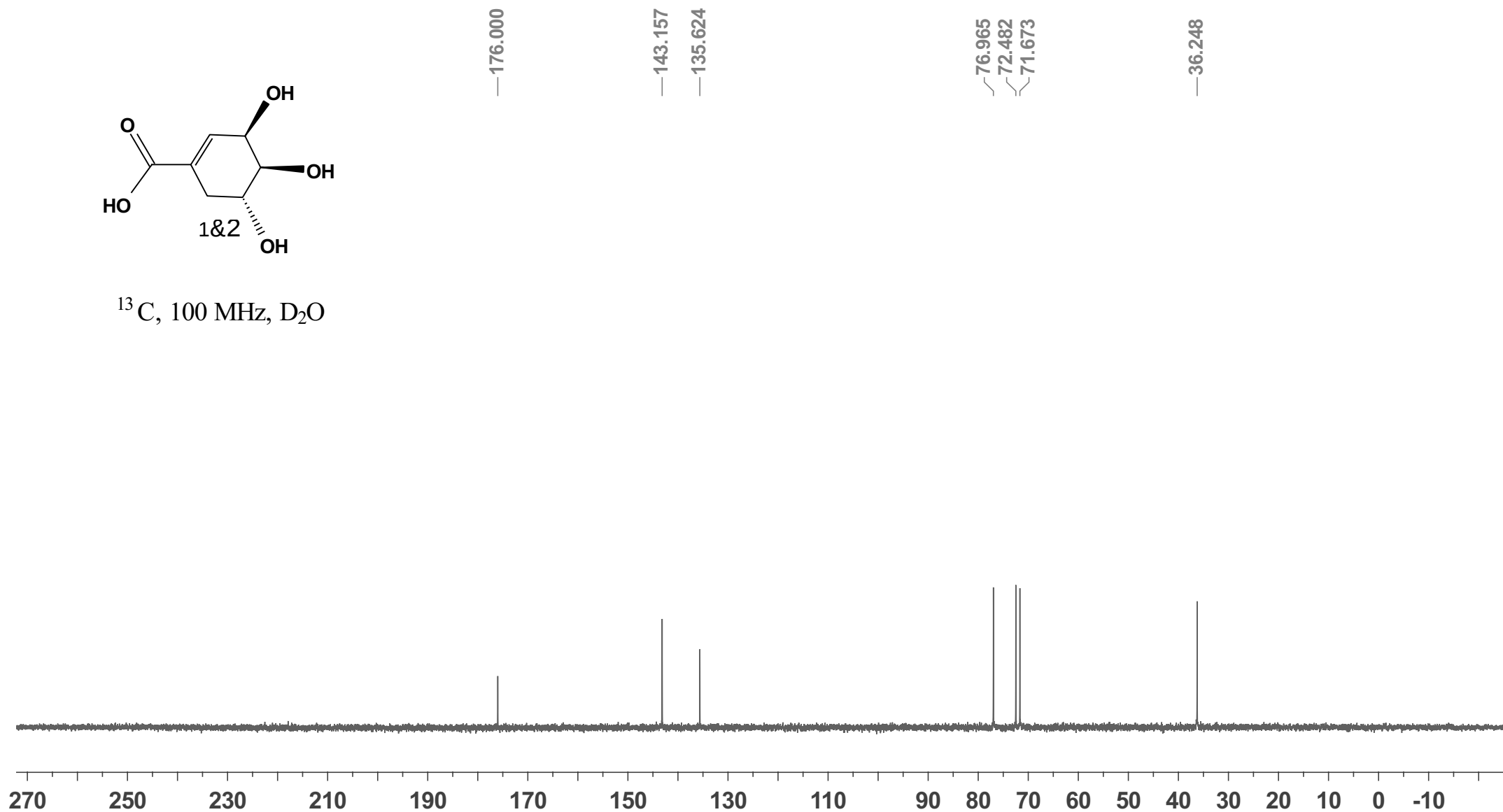


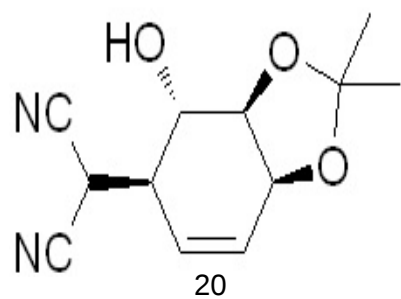
S27

For compounds 1 and 2

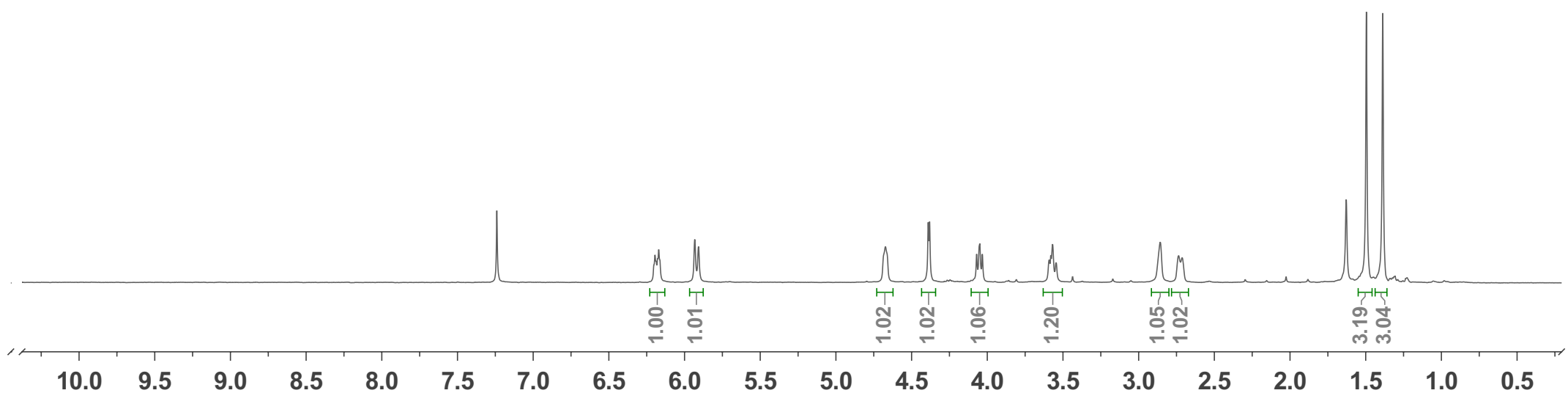


^{13}C , 100 MHz, D_2O

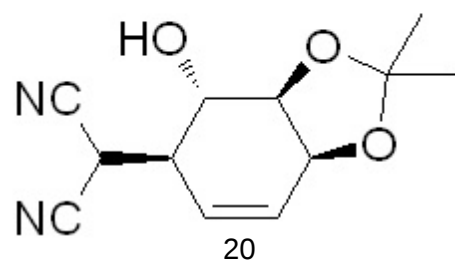




^1H , 400 MHz, CDCl_3



^{13}C , 100MHz, CDCl_3



—128.943
—125.868

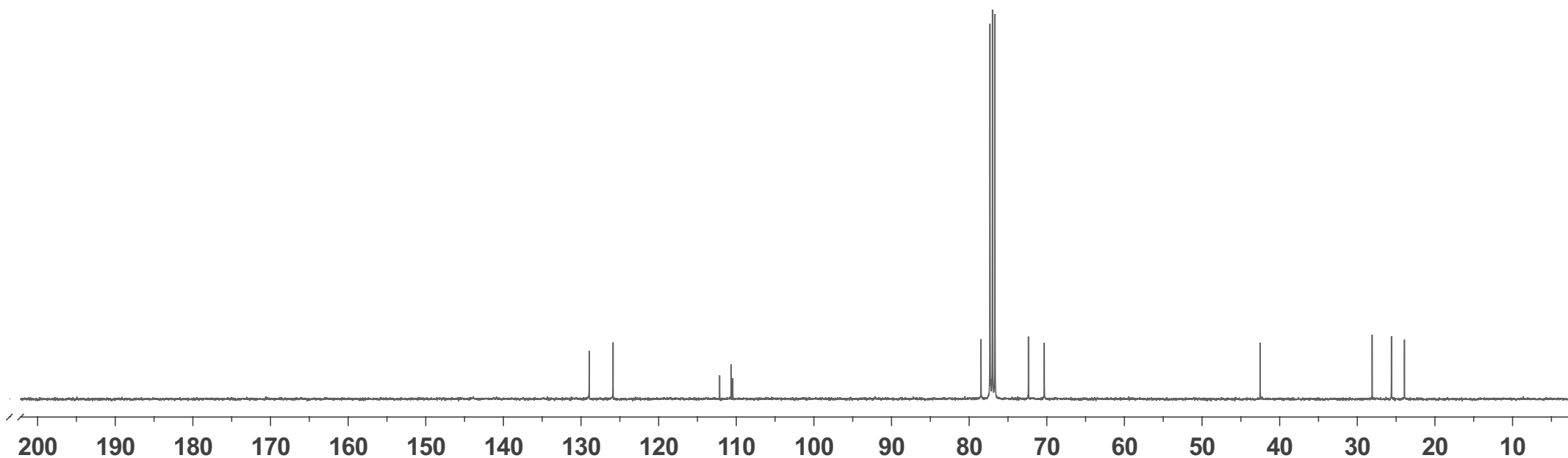
—112.142
—110.654
—110.449

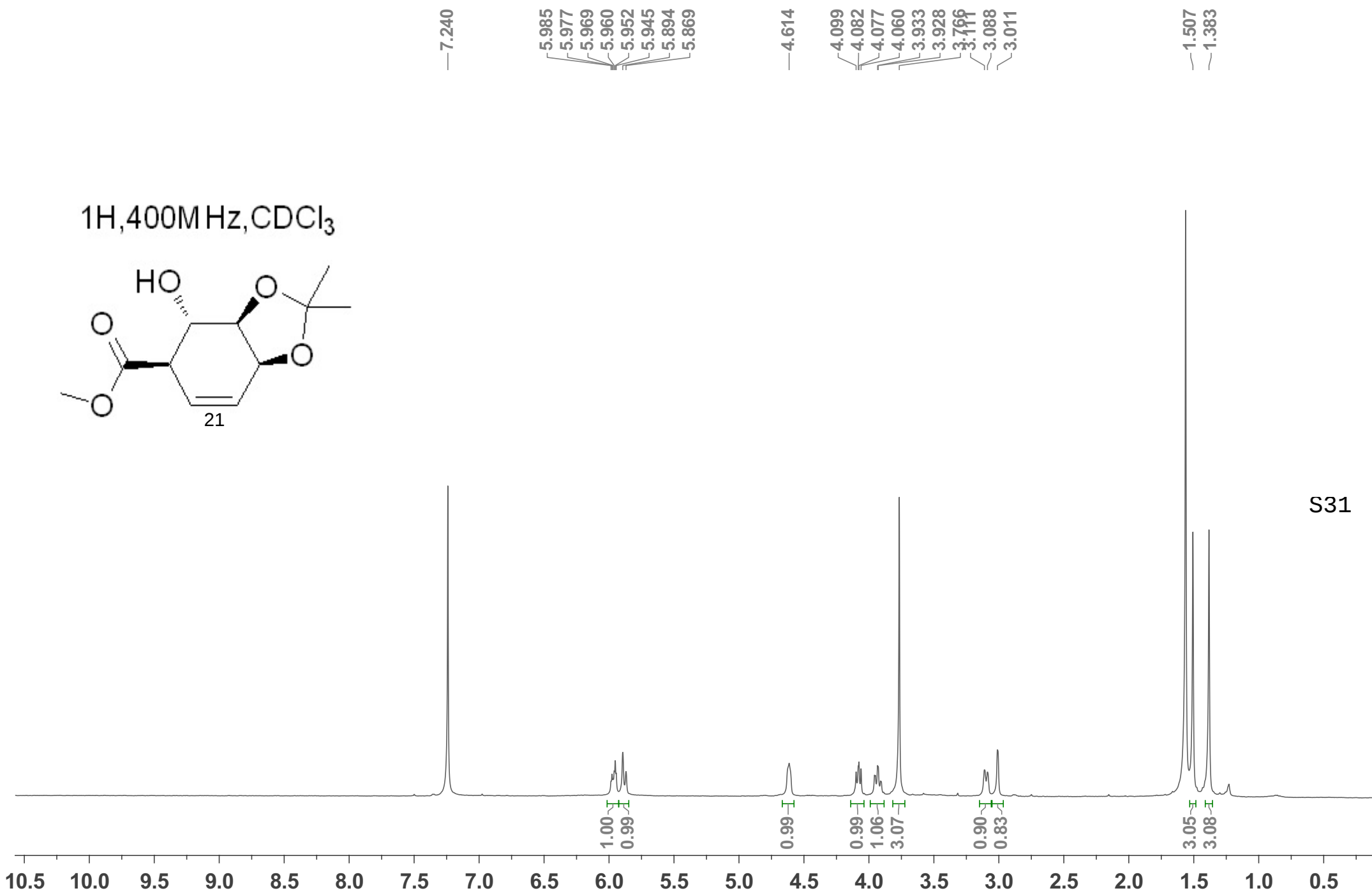
78.470
77.317
77.000
76.682
72.368
70.323

—42.517

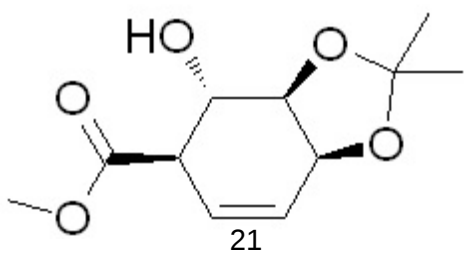
—28.089
—25.605
—23.927

S30





^{13}C , 100 MHz, CDCl_3



21

—172.507

~127.362
~125.657

—109.903

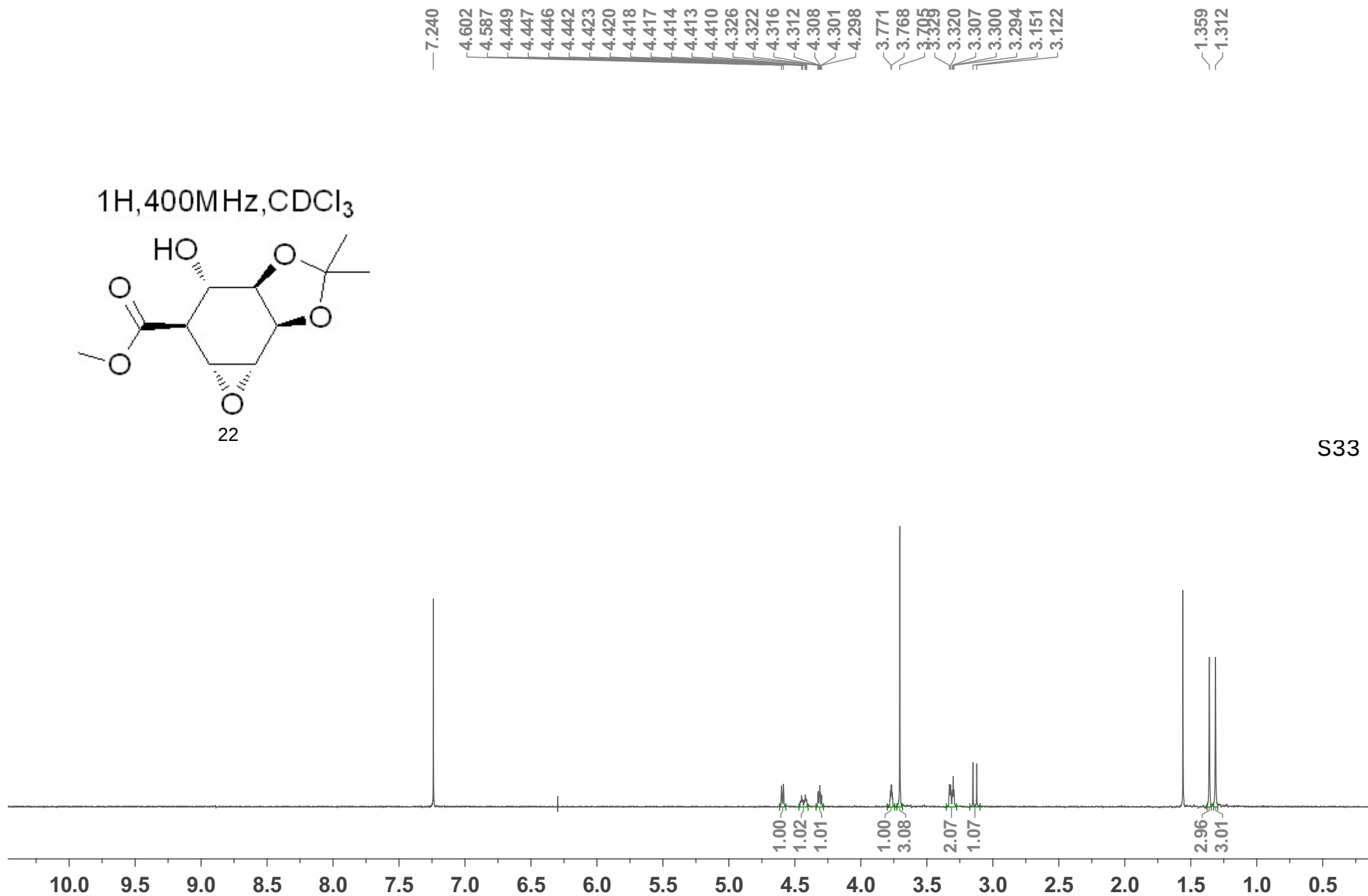
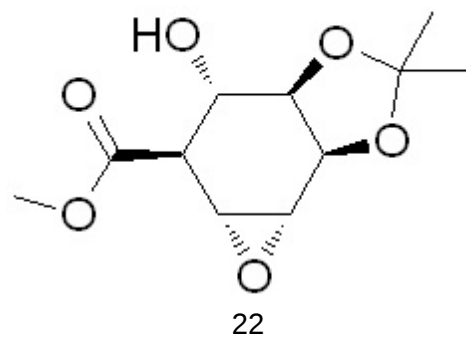
78.106
77.318
77.000
76.683
72.187
70.408

—52.461
—47.910

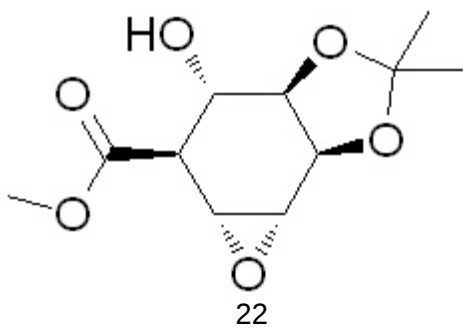
~28.142
~25.693

S32

1H, 400MHz, CDCl₃



^{13}C , 100MHz, CDCl_3



—169.645

—110.379

77.318
77.000
76.683
74.129
70.198
66.602

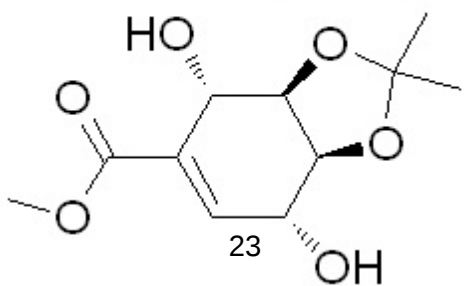
53.412
53.050
52.025

—42.480

26.575
25.371

S34

¹H, 400MHz, CDCl₃



23

7.240
7.219
7.206

4.724
4.577
4.570
4.560
4.553
4.481
4.474
4.463
4.456
4.344
3.795
3.646

3.086
2.983

1.694

1.345

S35

0.90

1.00

1.07

1.05

1.03

3.19

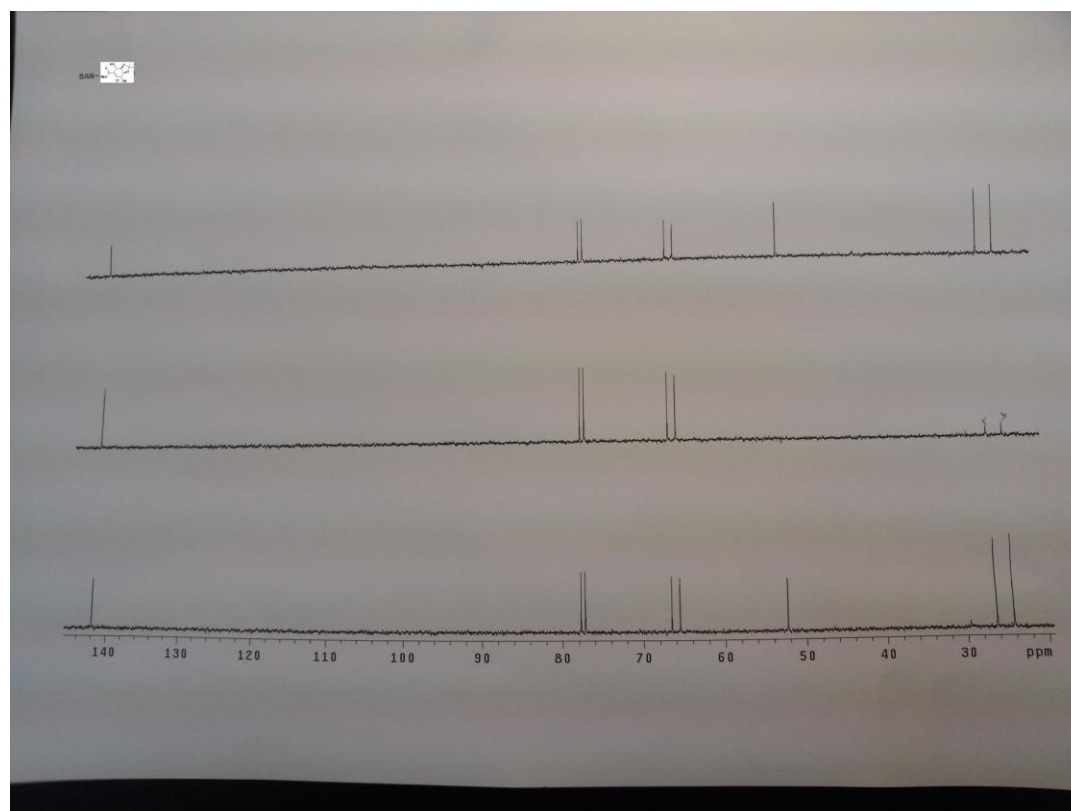
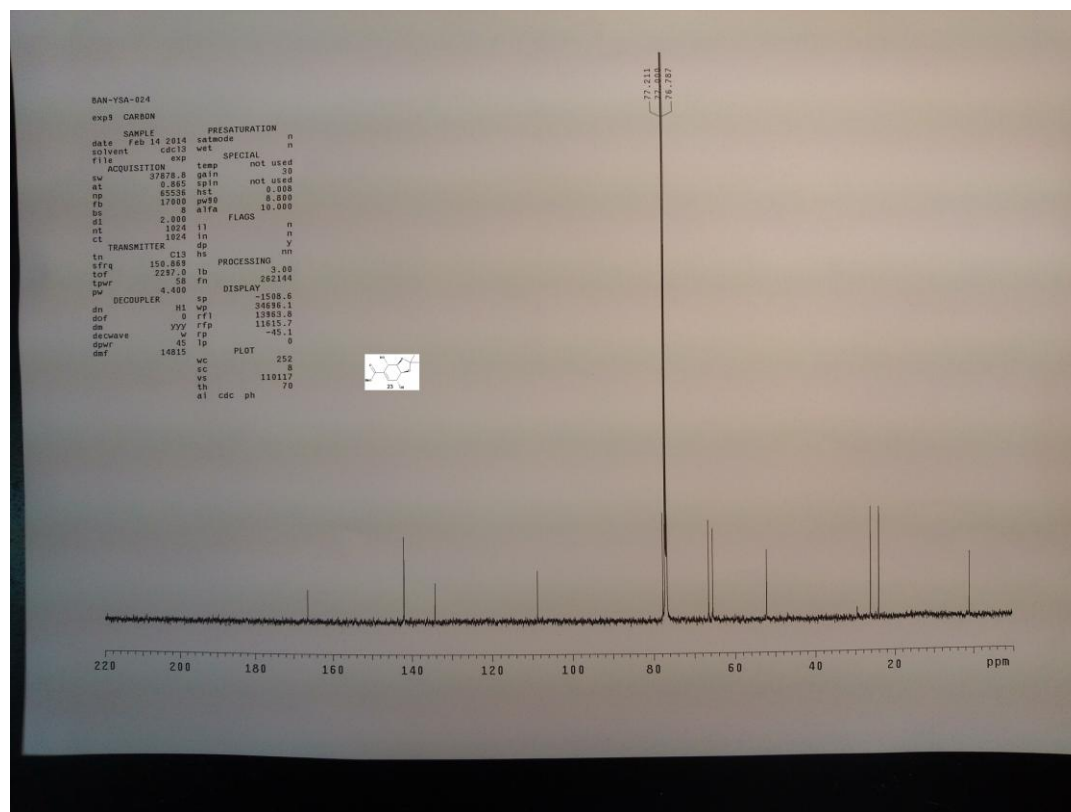
0.96

0.90

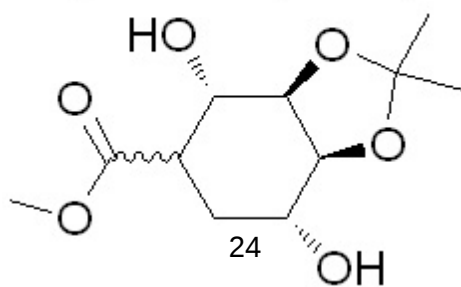
6.70

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

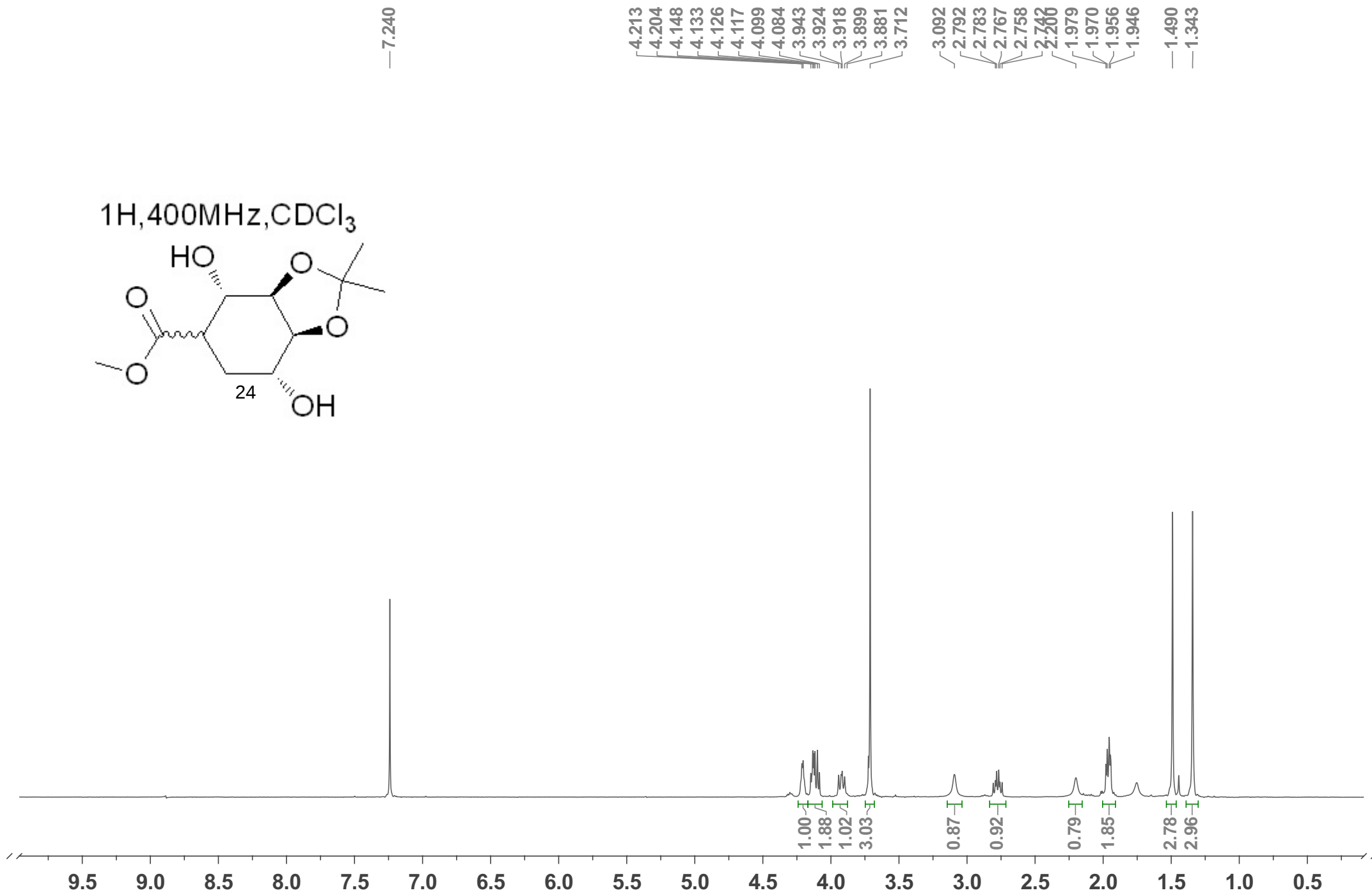
Compound No. 23 (13C, 150MHz, CDCl3)

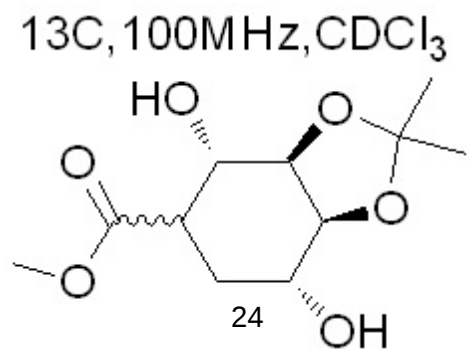


^1H , 400MHz, CDCl_3



24





—174.636

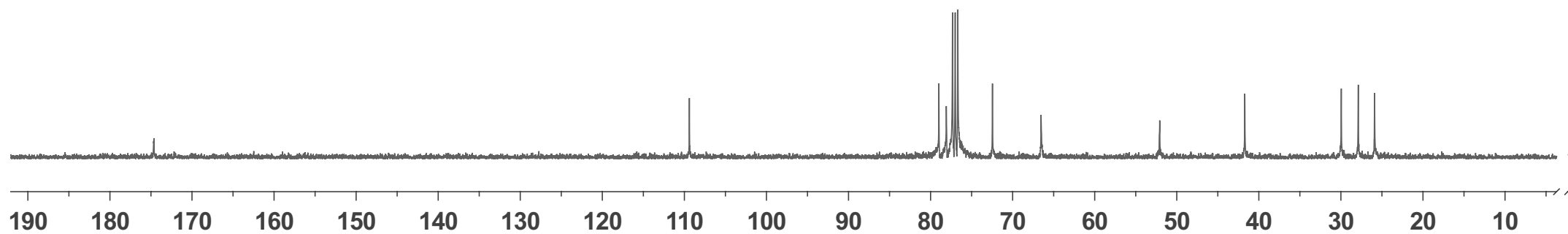
—109.392

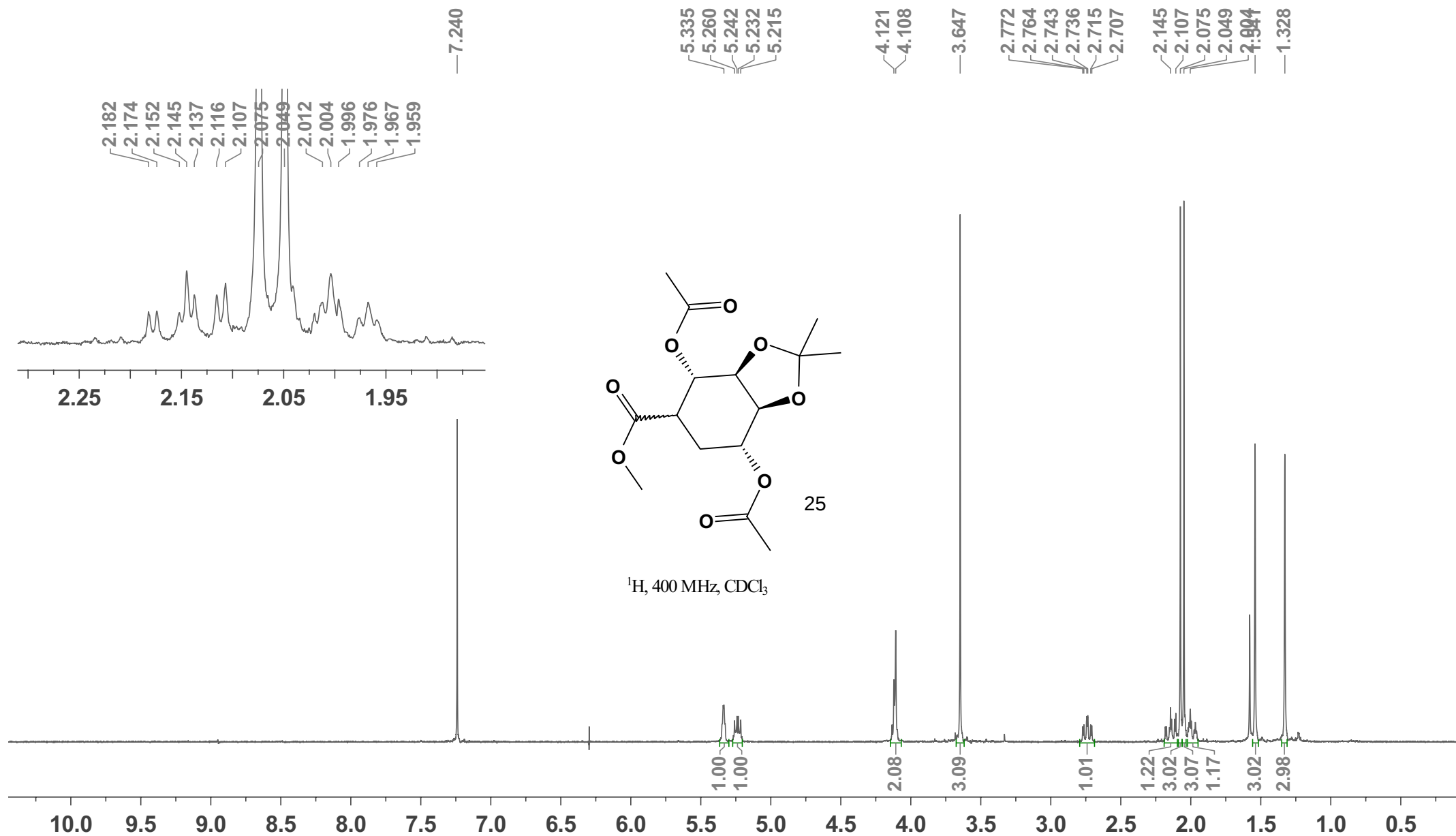
78.983
78.070
77.317
77.000
76.682
72.458
—66.531

—52.080

—41.714

29.954
—27.887
25.894





171.768
169.654
169.349

110.121

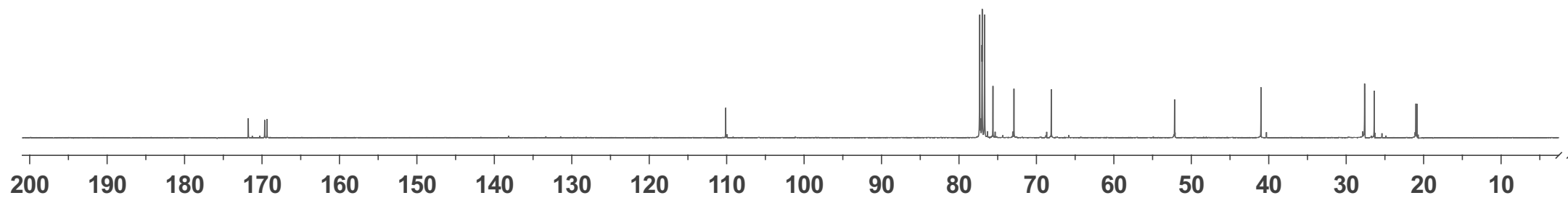
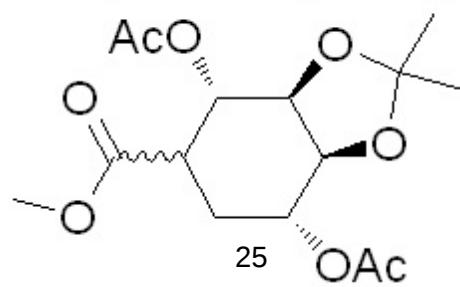
77.317
77.000
76.682
75.612
72.898
68.085
65.823

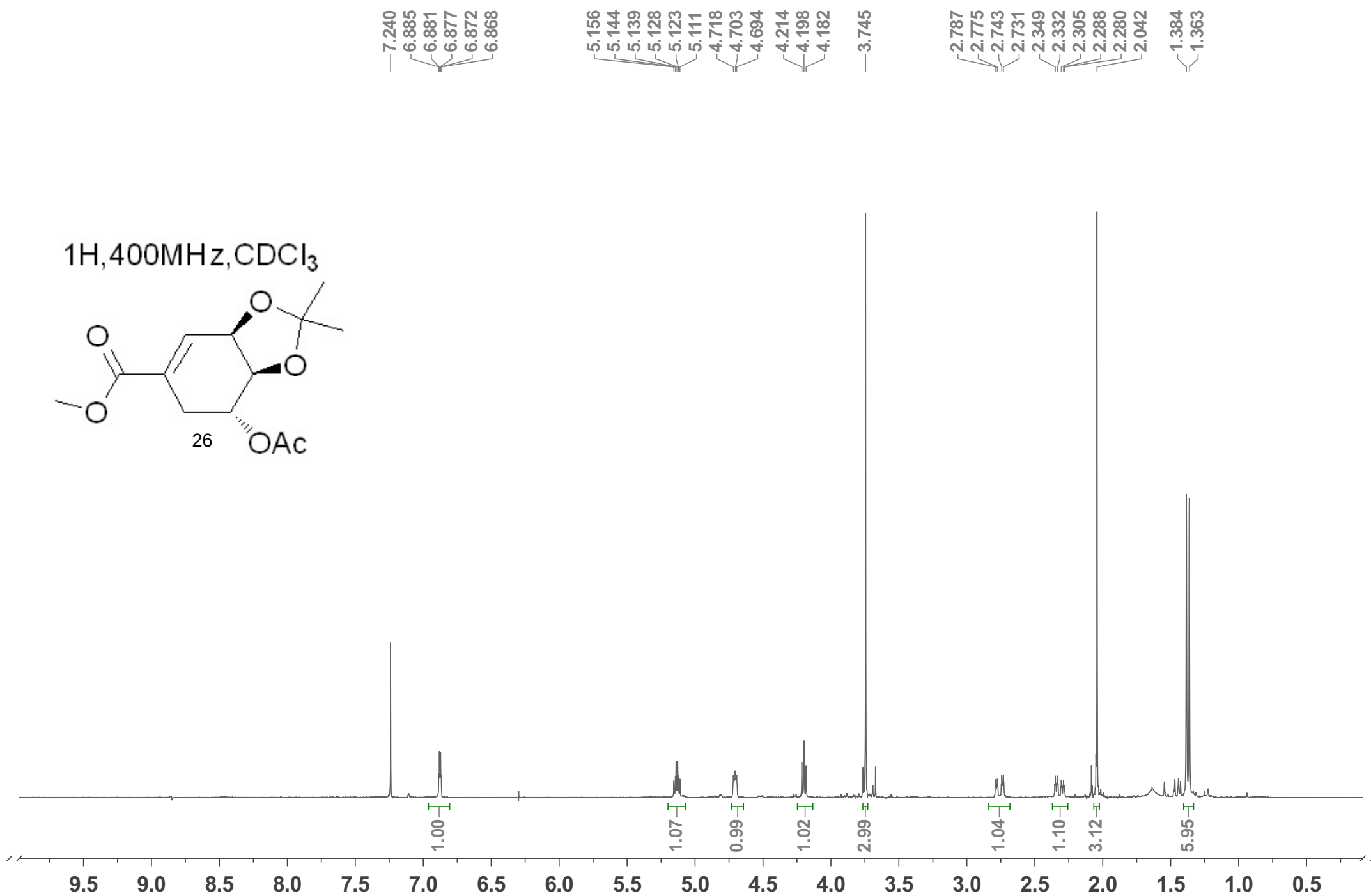
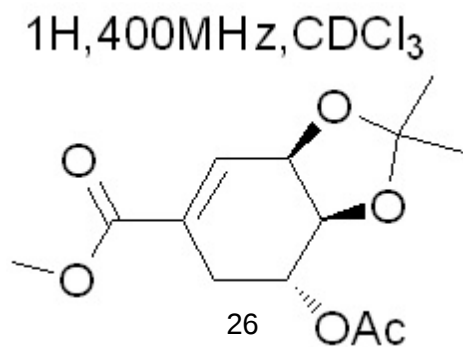
52.162

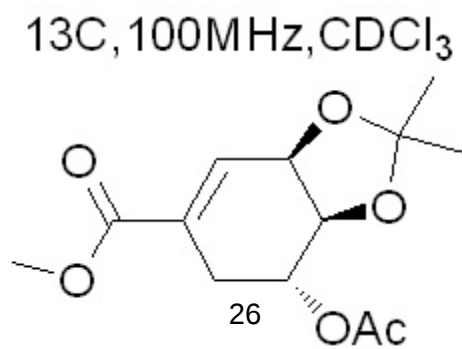
41.007

27.623
27.581
26.377
20.994
20.862

^{13}C , 100MHz, CDCl_3







—170.161
—166.395

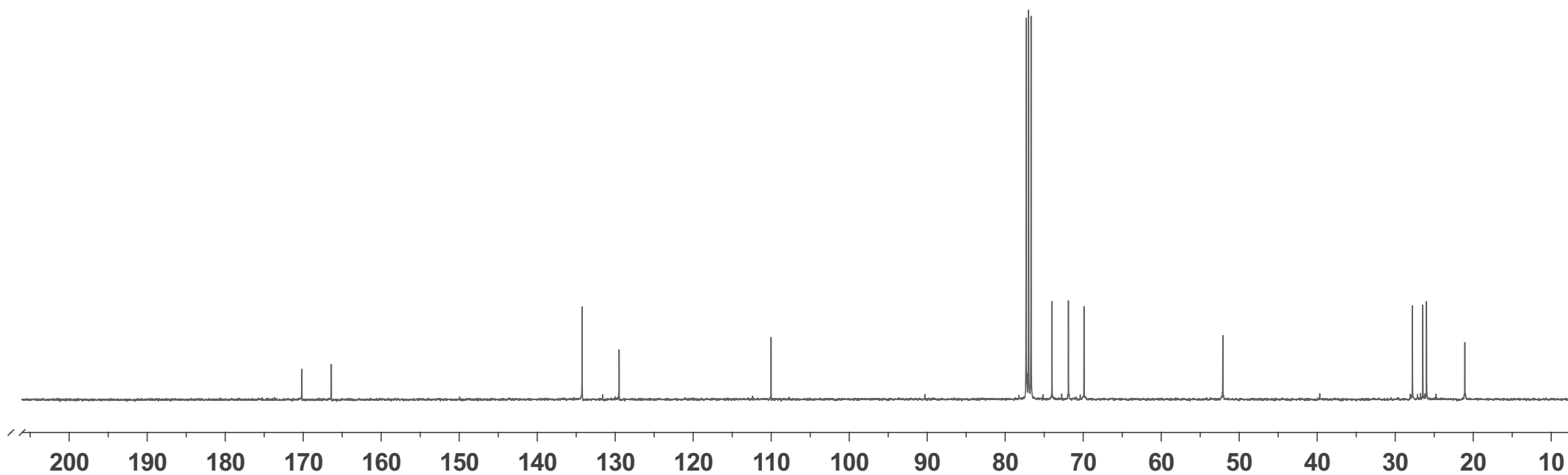
—134.242
—129.497

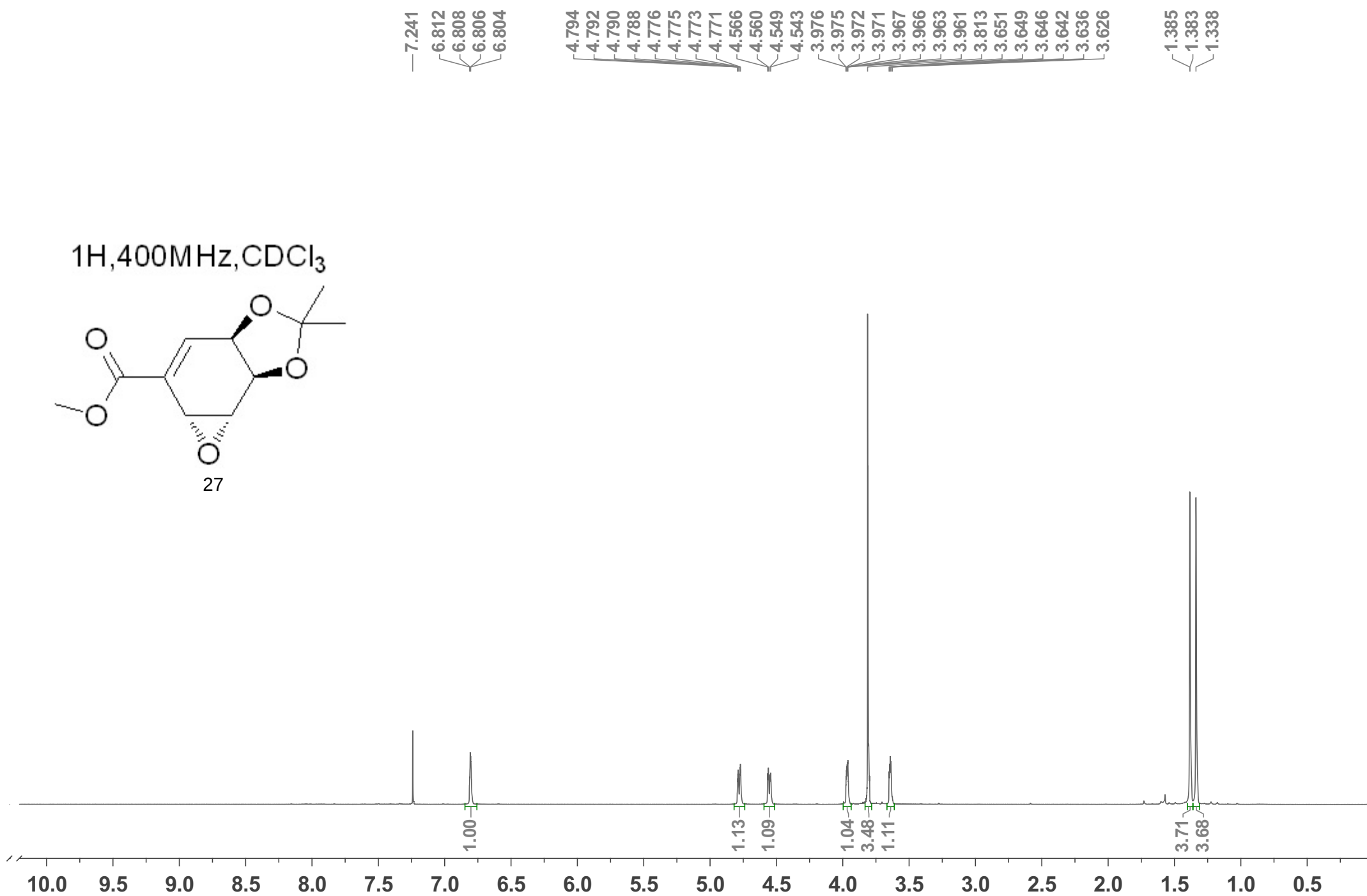
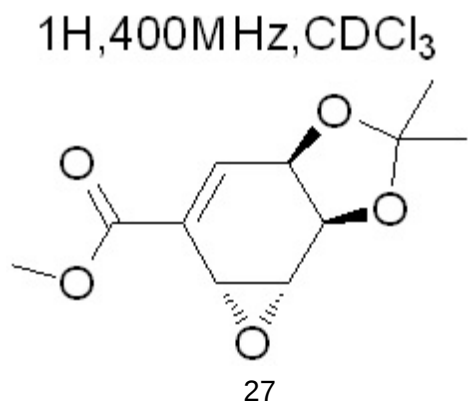
—110.017

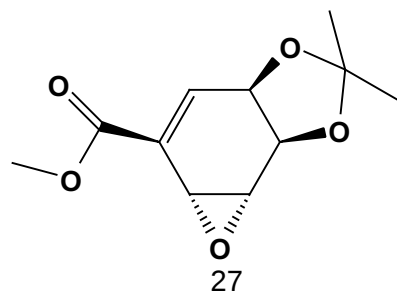
77.317
77.000
76.683
74.006
71.896
69.900

—52.099

27.795
26.459
25.986
21.072







¹³C, 100MHZ, CDCl₃

165.44

139.94

127.41

111.04

77.32

77.00

76.68

71.20

70.39

52.26

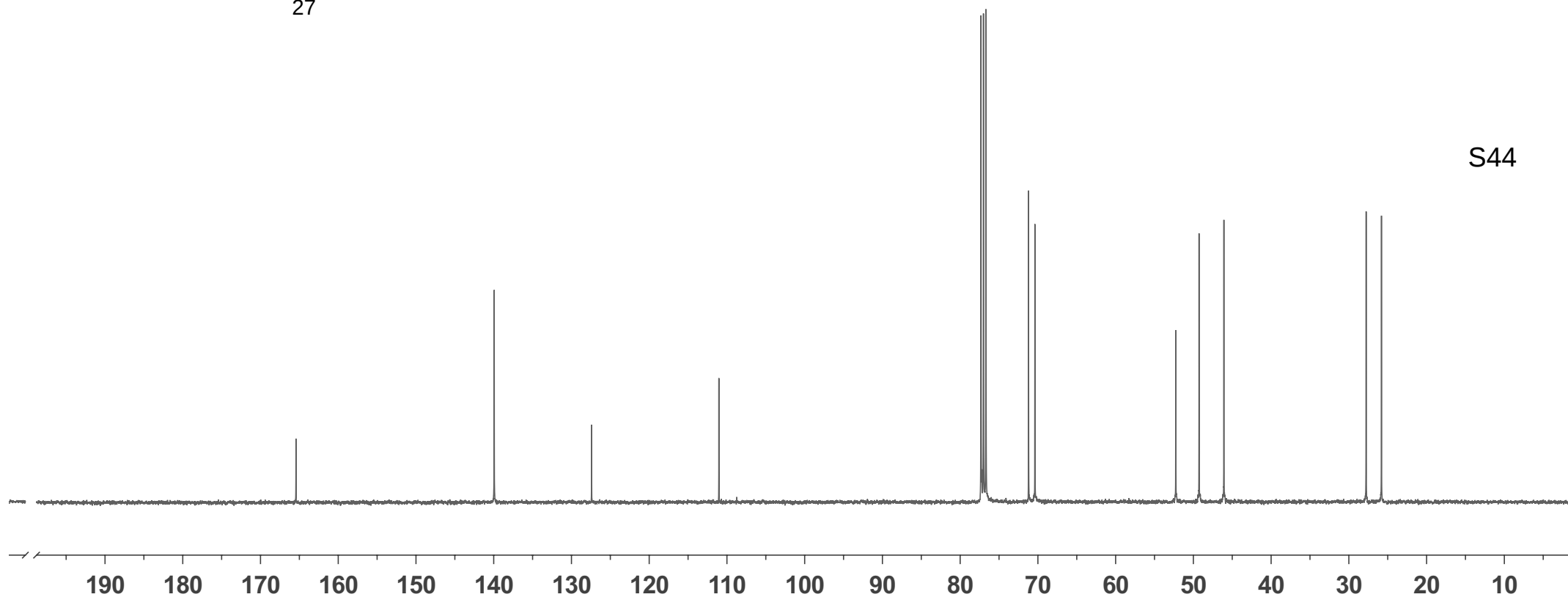
49.27

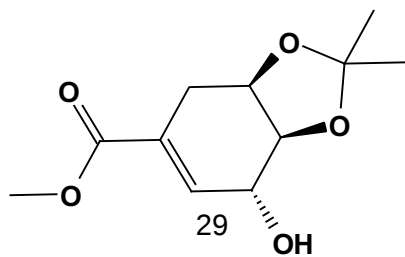
46.07

27.78

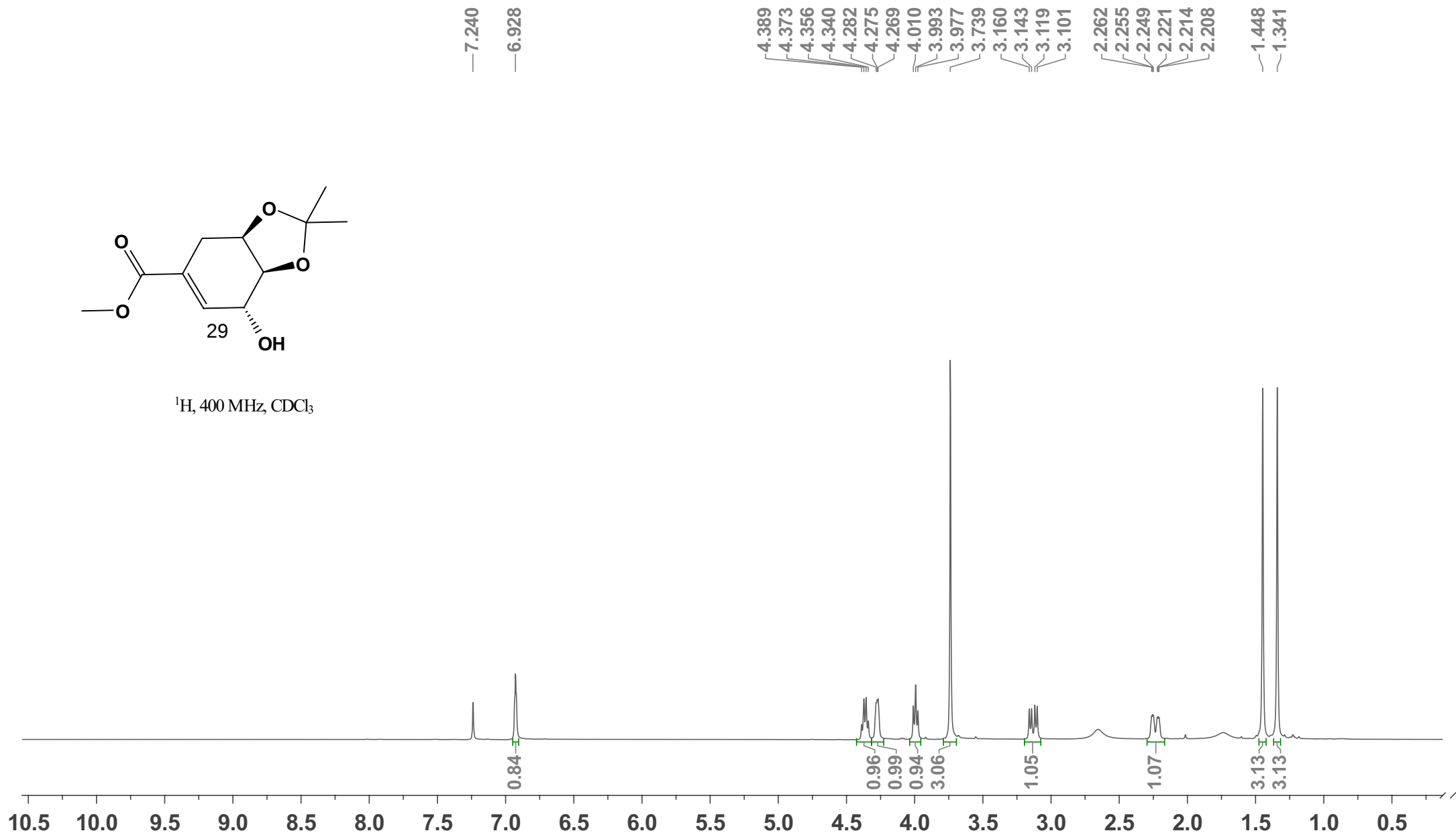
25.81

S44



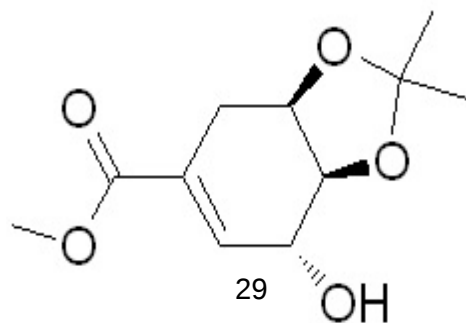


^1H , 400 MHz, CDCl_3



S45

^{13}C , 100MHz, CDCl_3



—165.991

—140.829

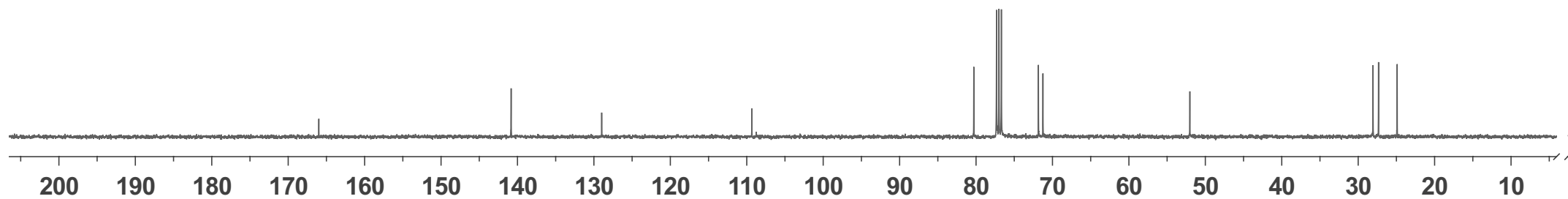
—128.980

—109.332

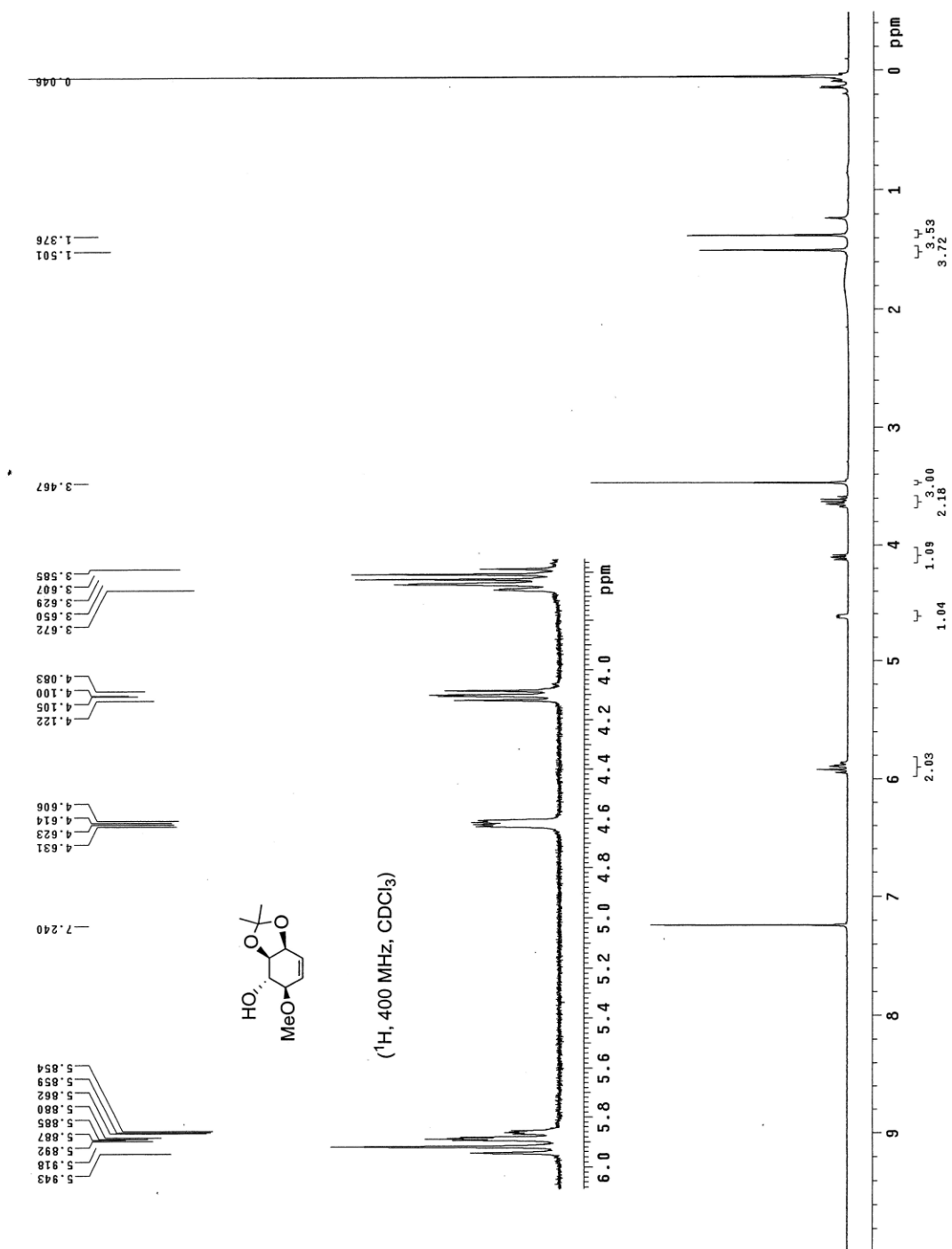
80.295
77.318
77.000
76.683
71.839
71.246

—52.021

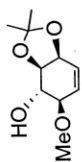
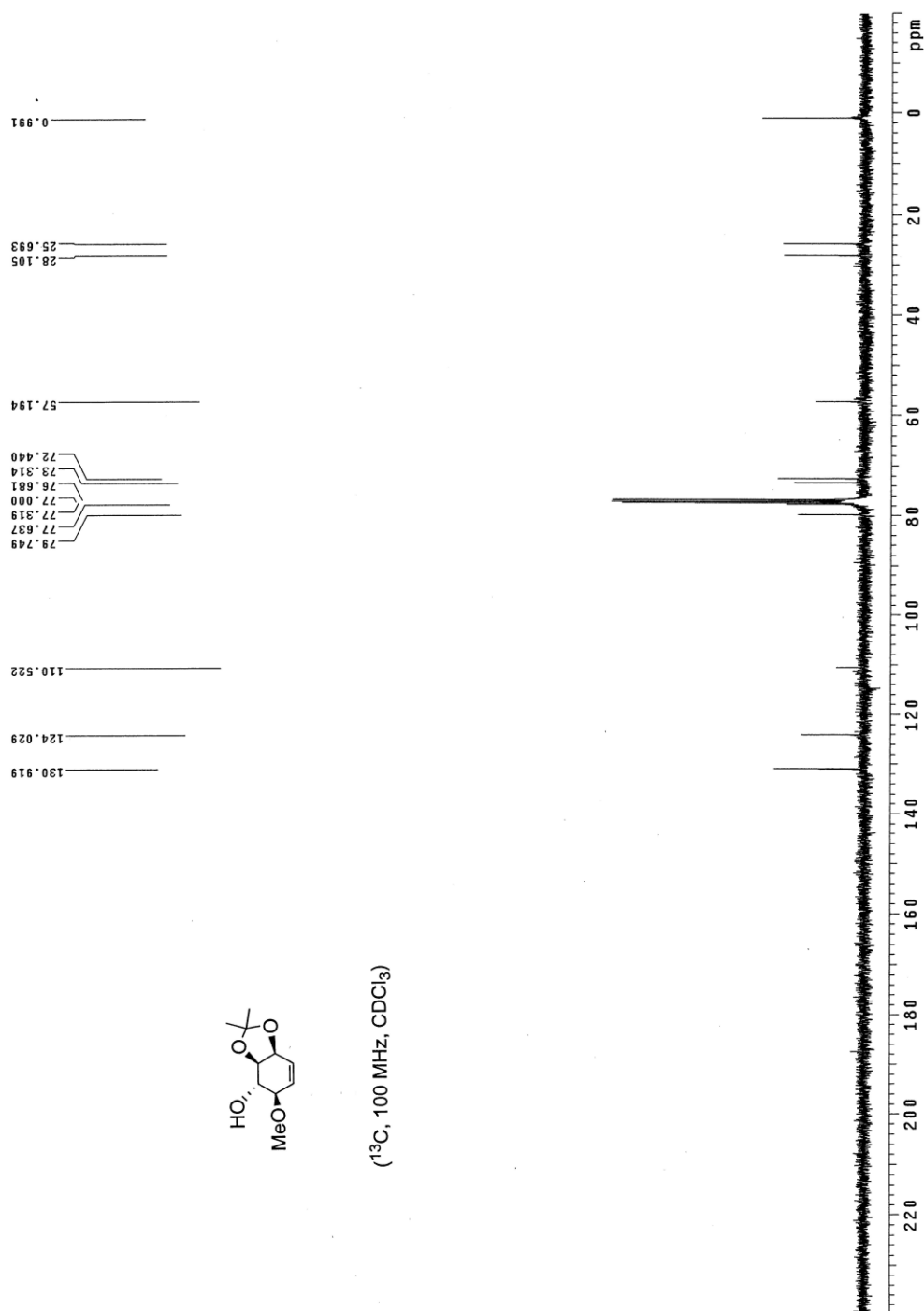
28.058
27.337
24.898



Compound No. 29 (^1H , 400MHz, CDCl_3)

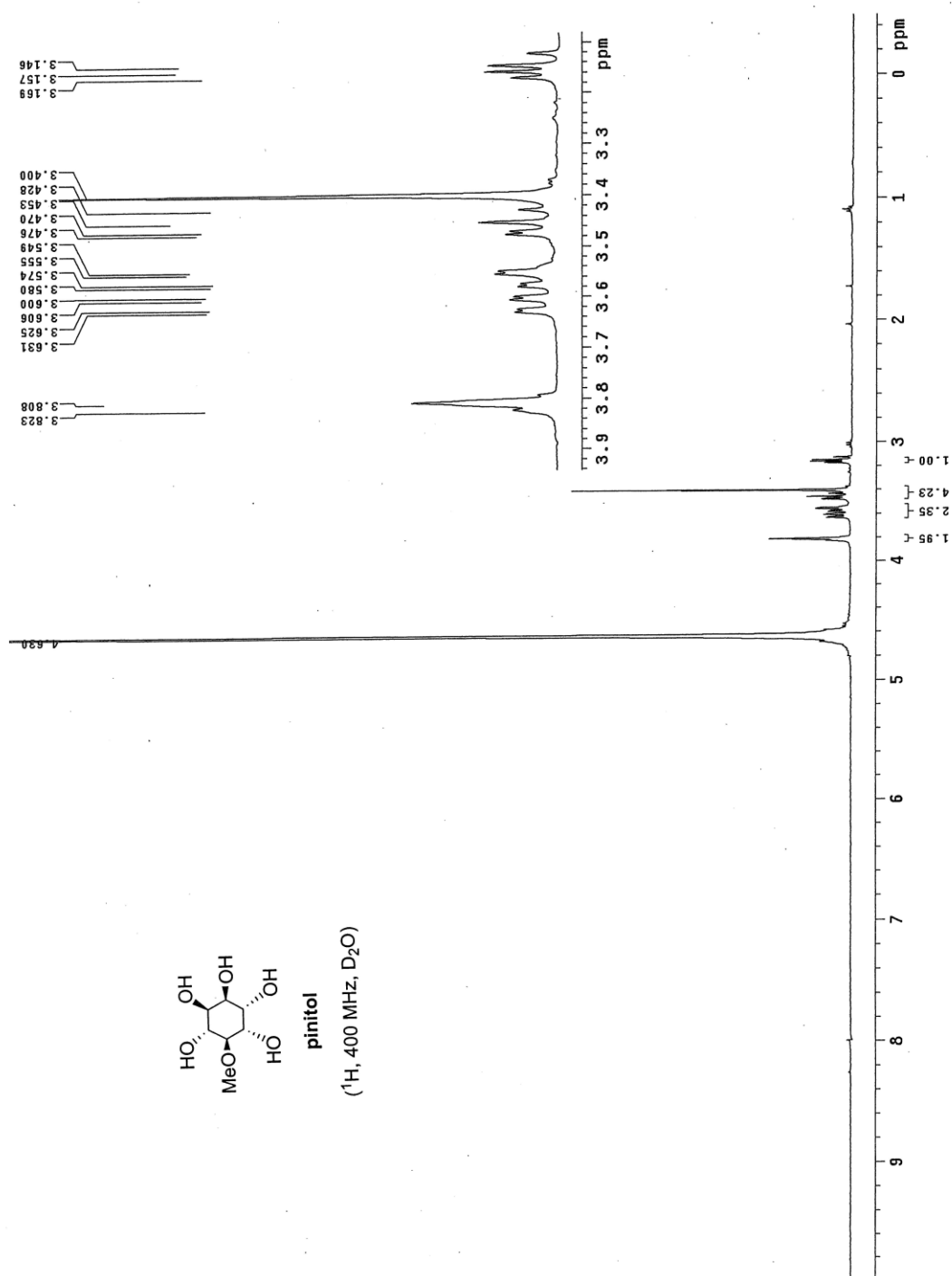


Compound No. 29 (^{13}C , 100 MHz, CDCl_3)

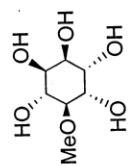
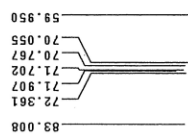


(^{13}C , 100 MHz, CDCl_3)

Compound No. 5 and 6



Compound No. 5 and 6



pinitol

(¹³C, 100 MHz, D₂O)

