

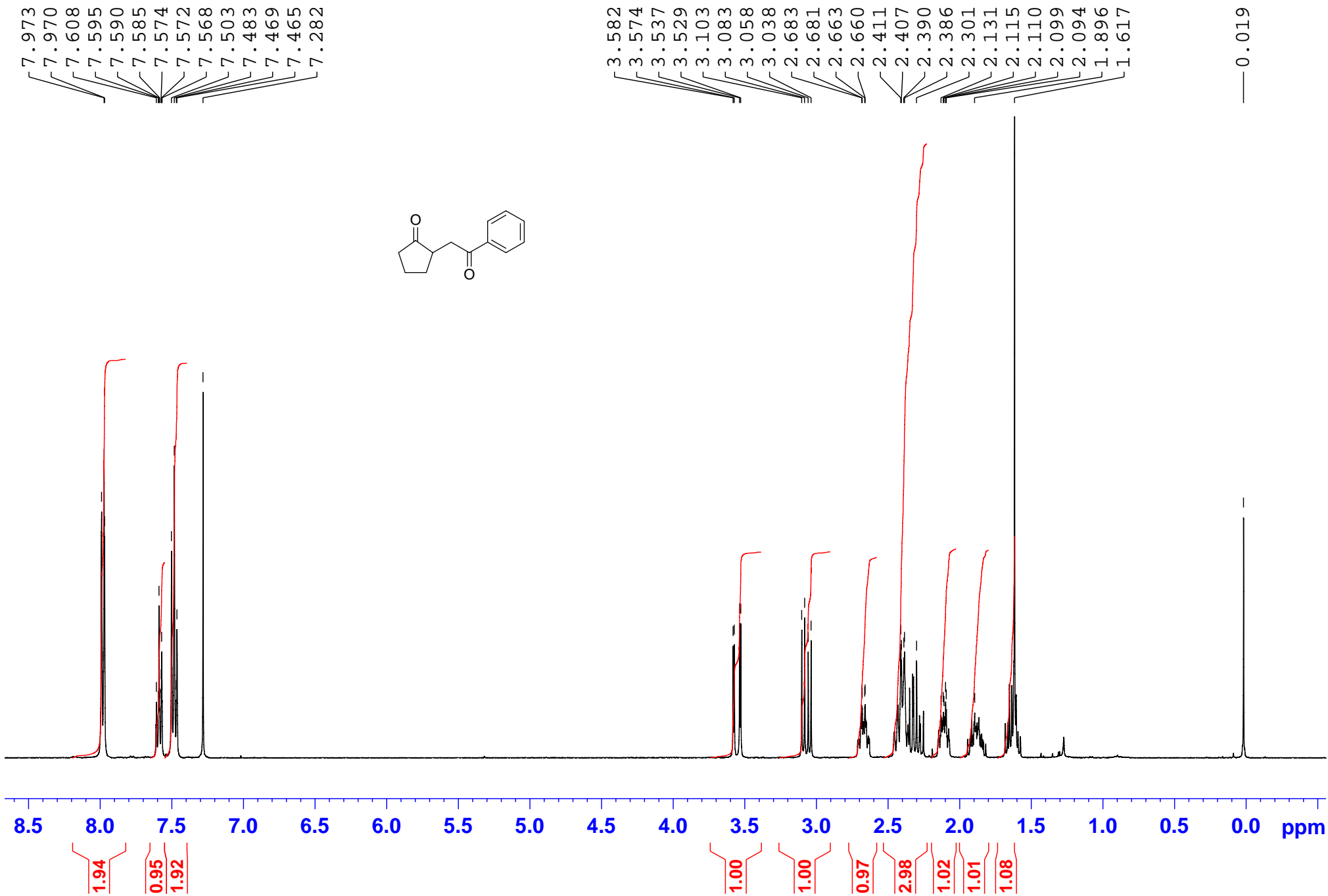
Catalyst-free Formation of 1,4-Diketones by Addition of Silyl Enolates to Oxyallyl Zwitterions *in situ*

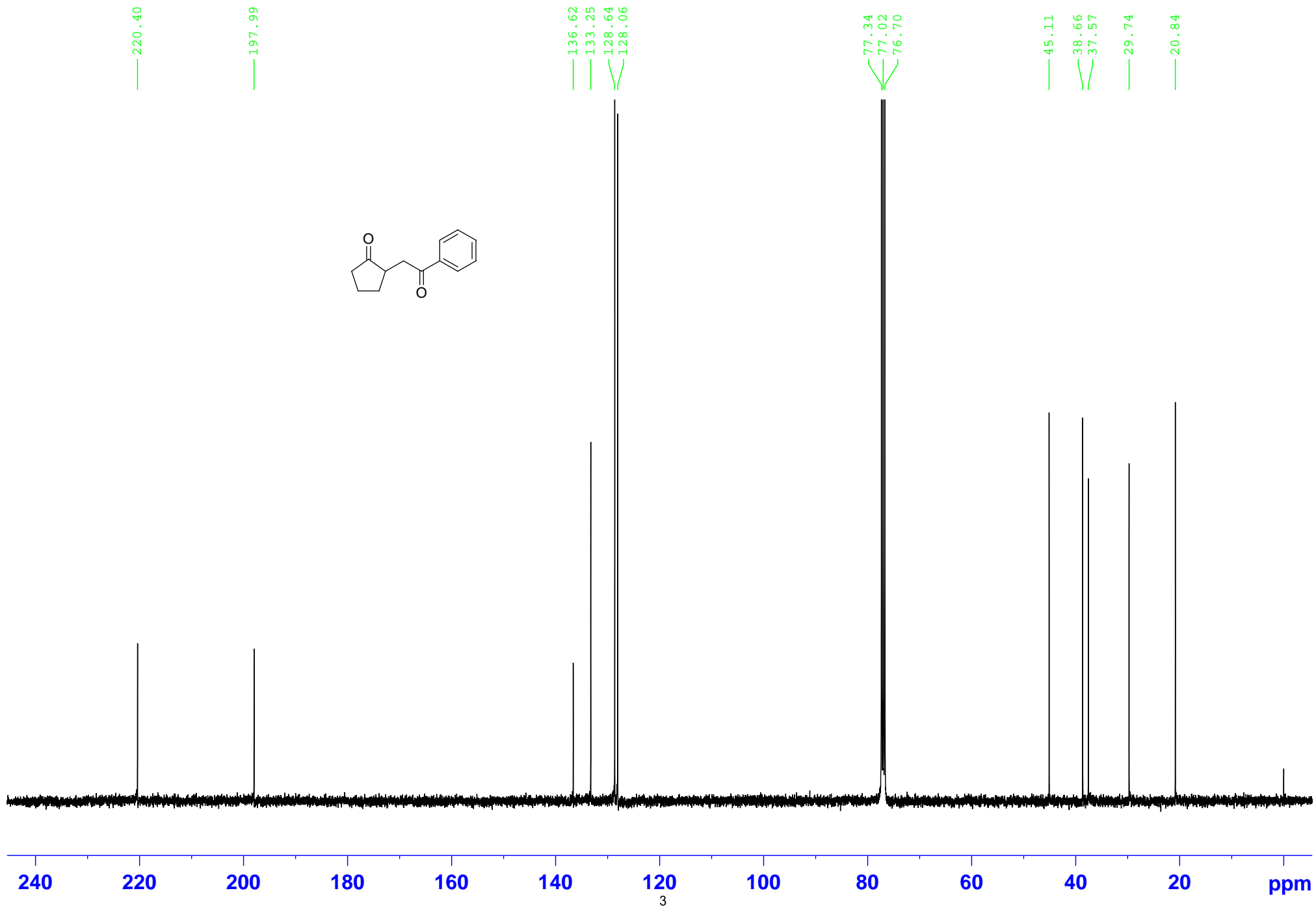
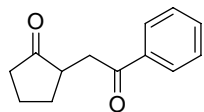
Generated from α -Haloketones

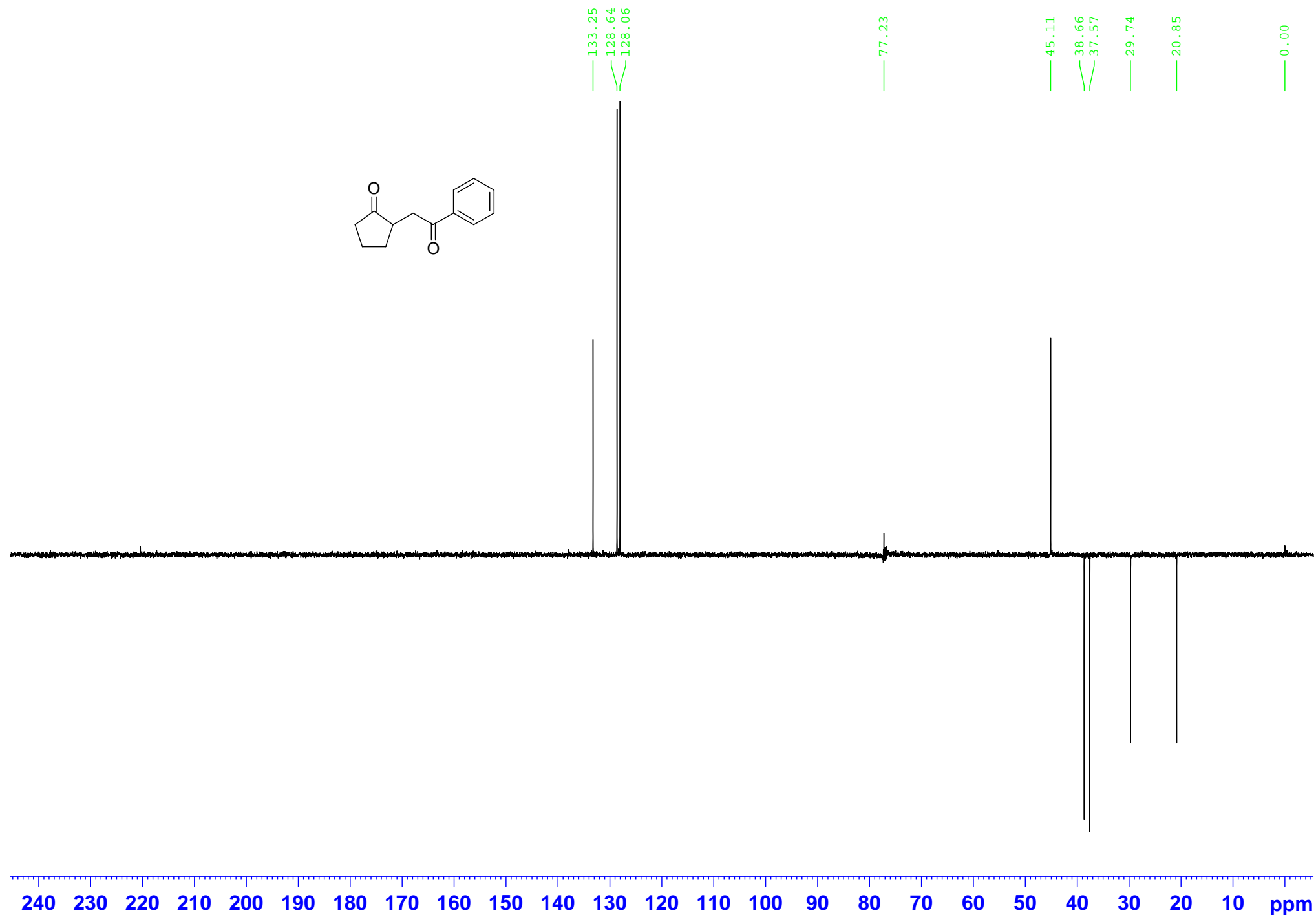
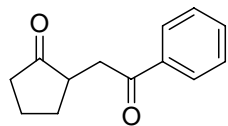
Juan Luo, Qihua Jiang, Hao Chen, and Qiang Tang*

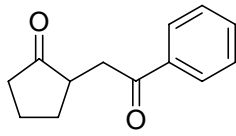
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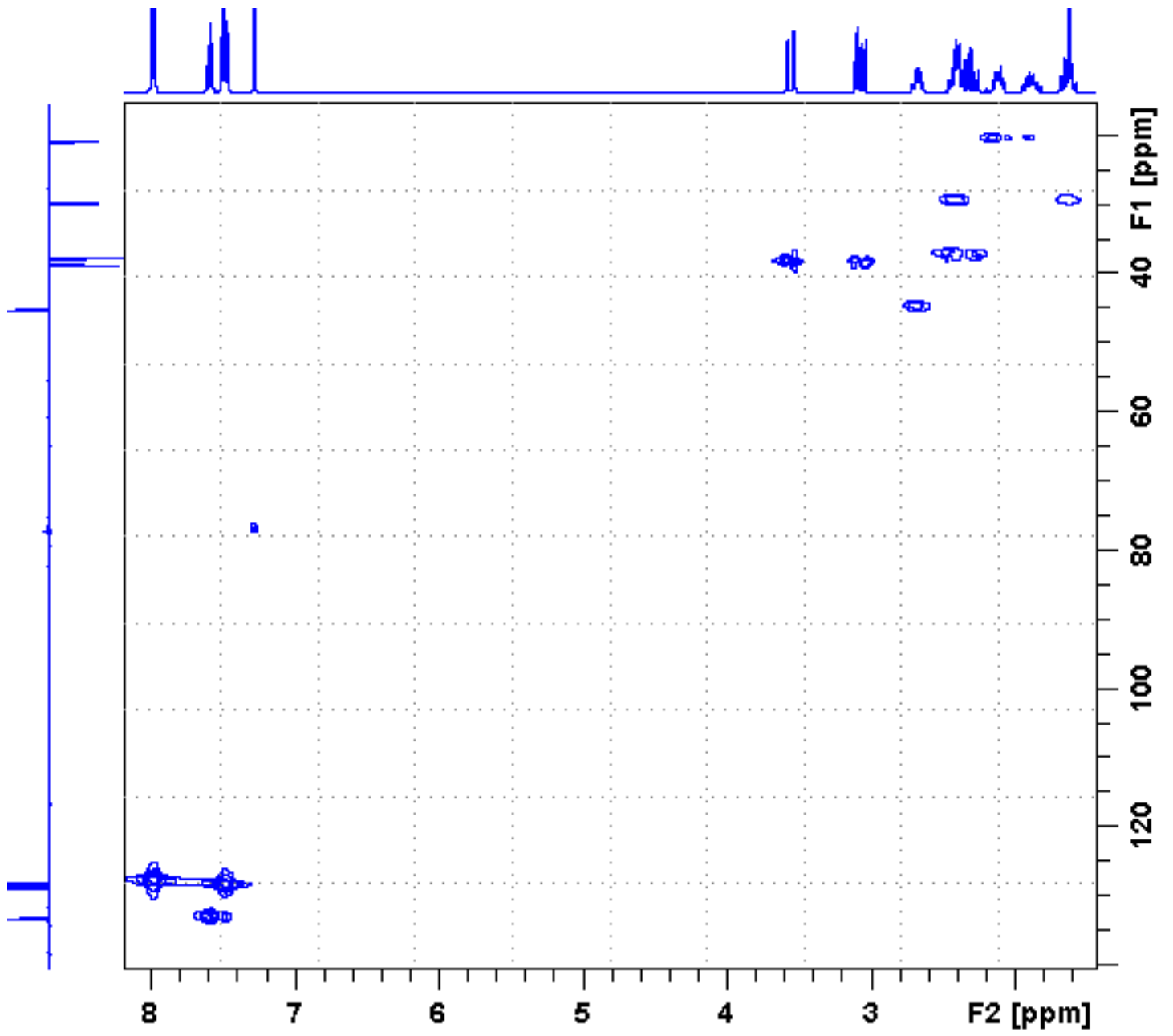


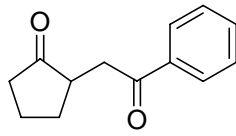




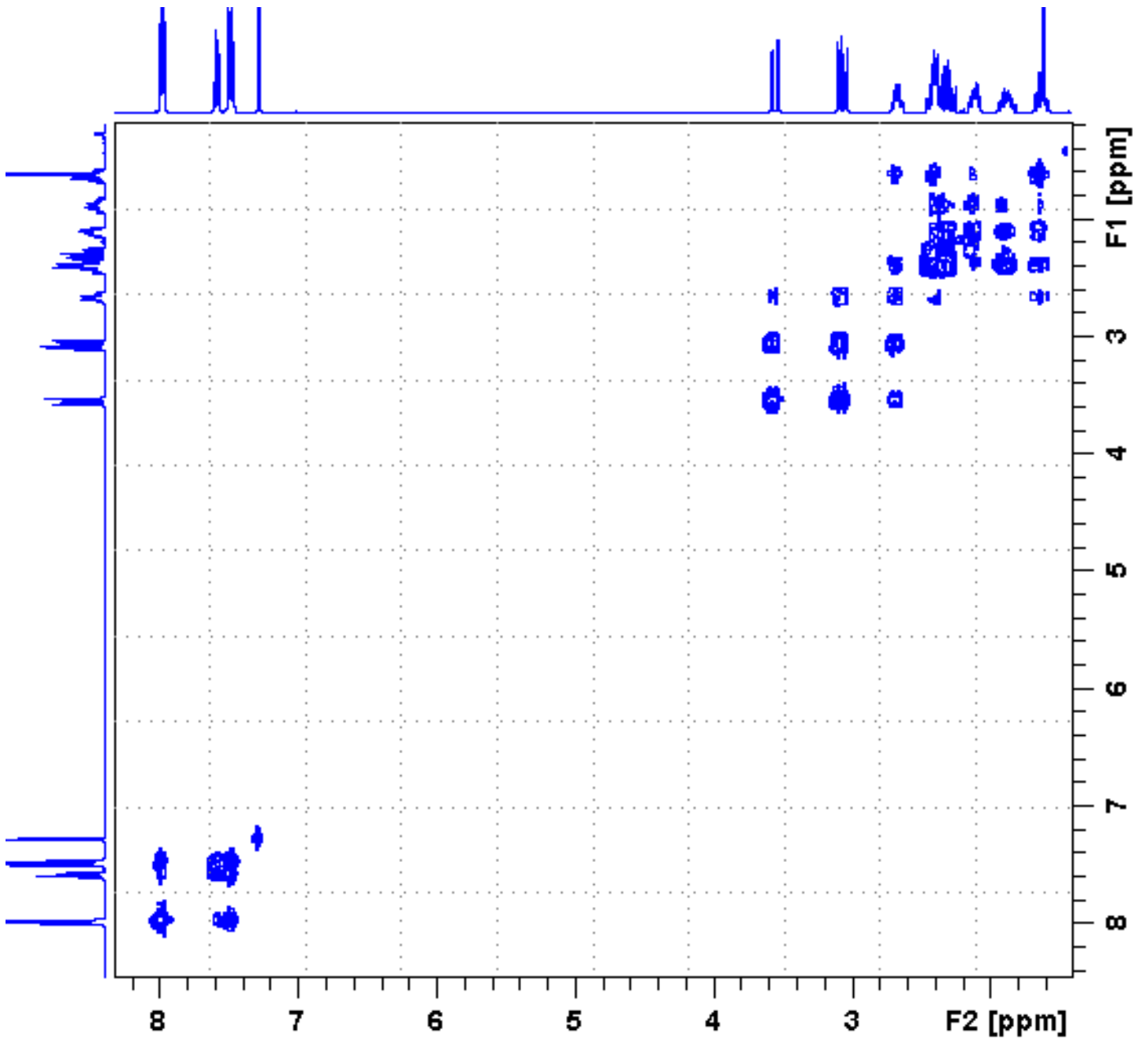


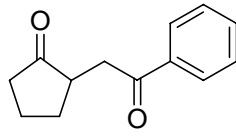
HMQC



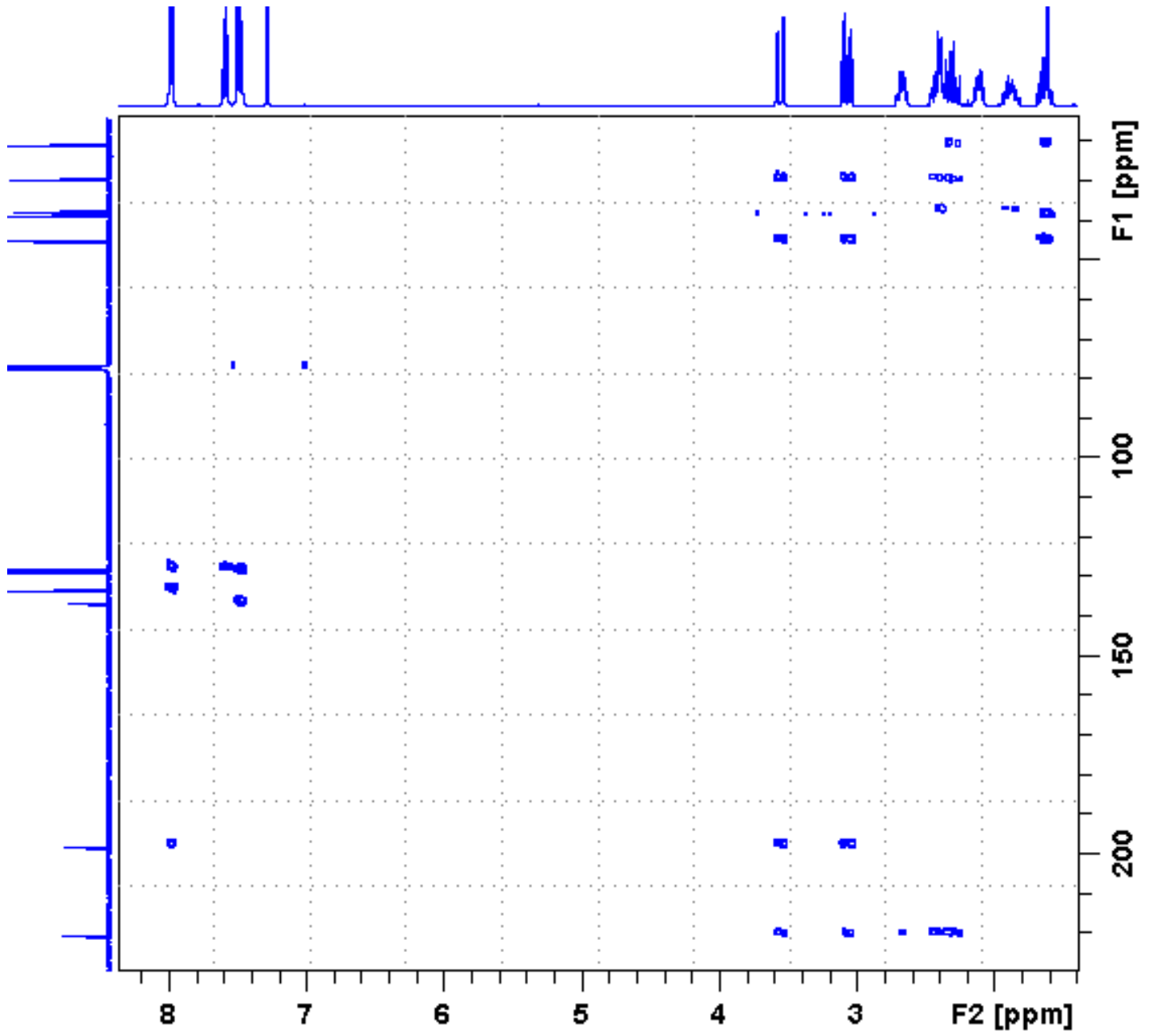


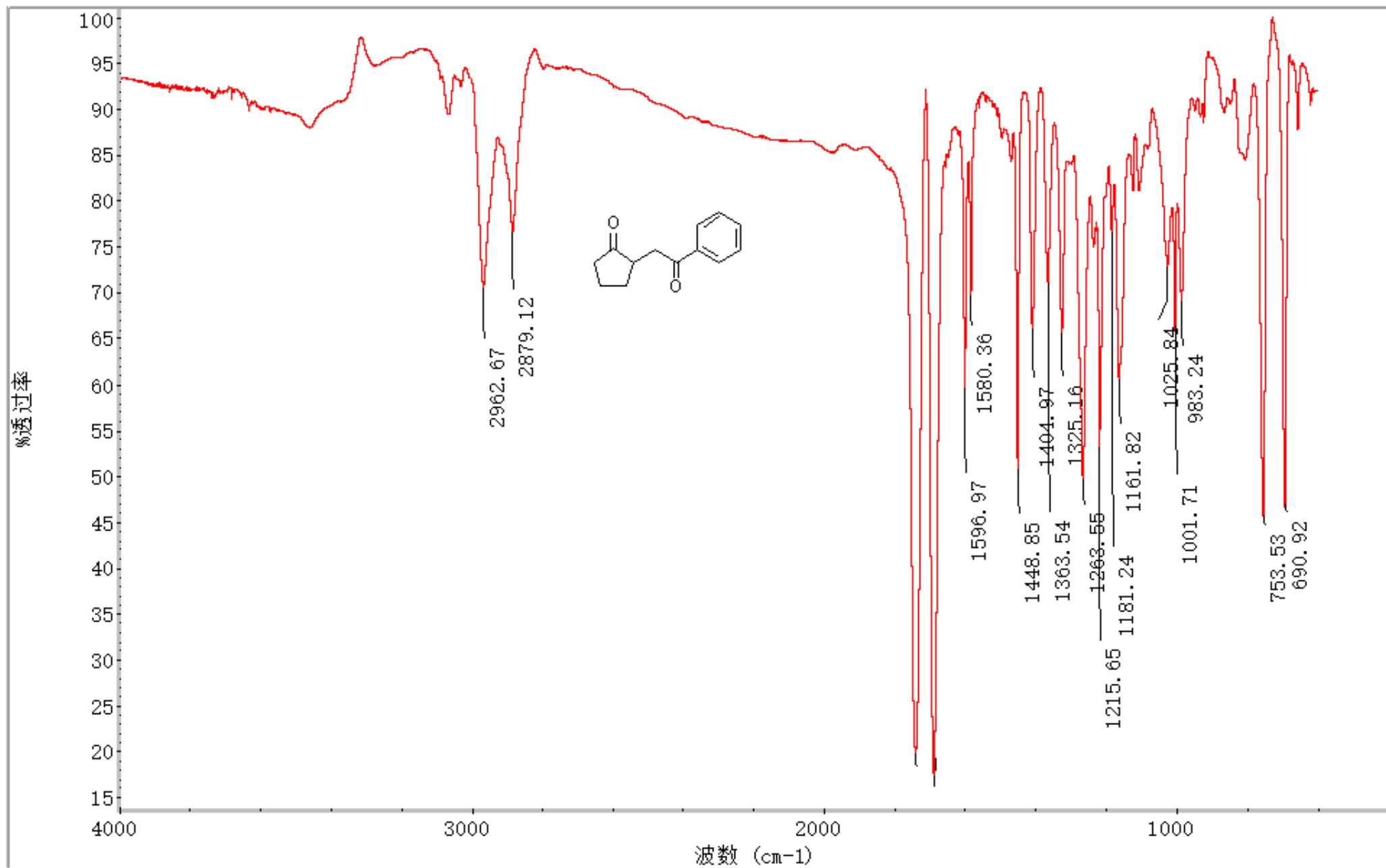
COSY





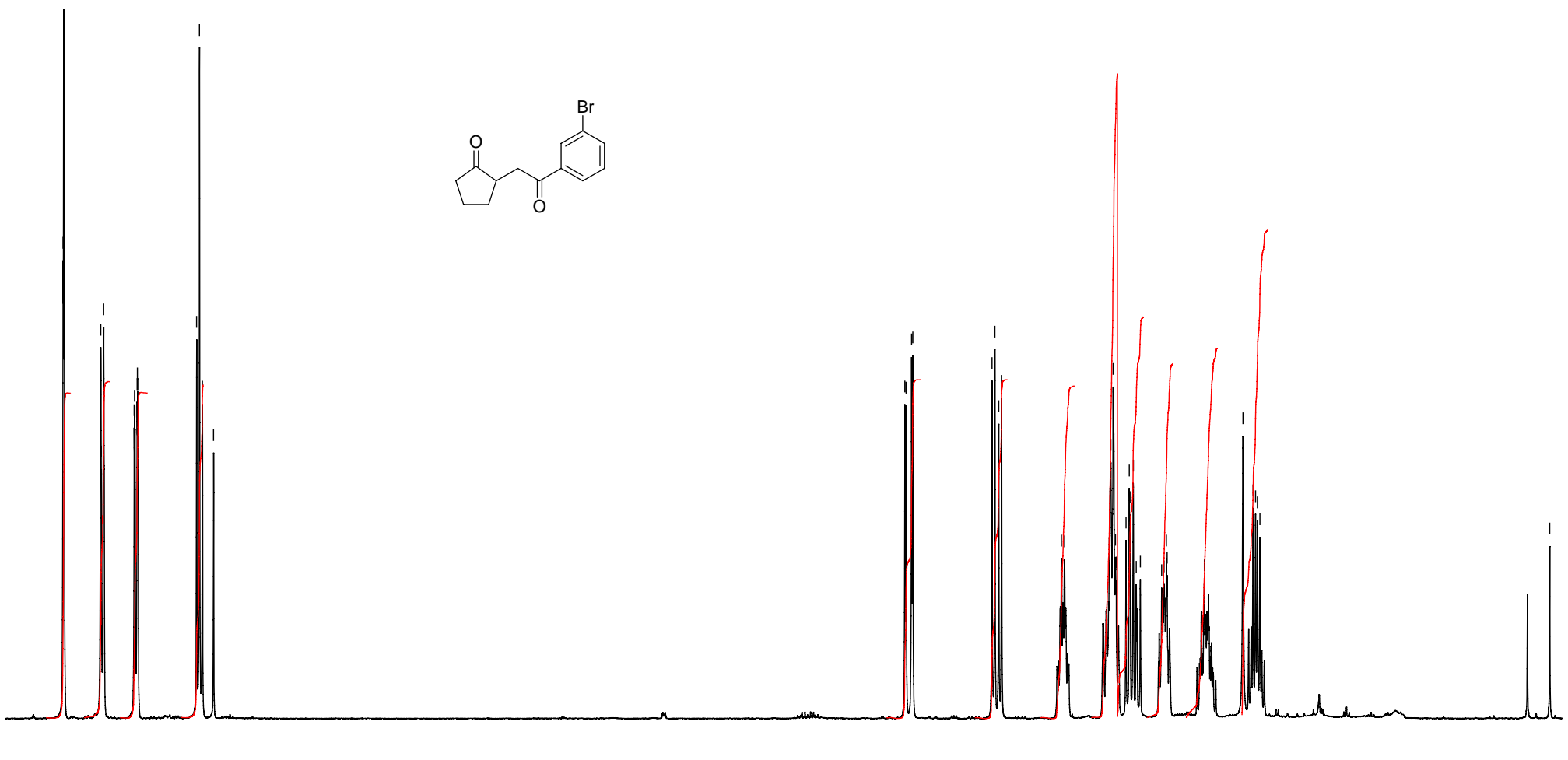
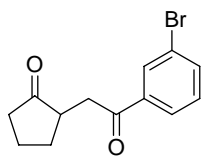
HMBC





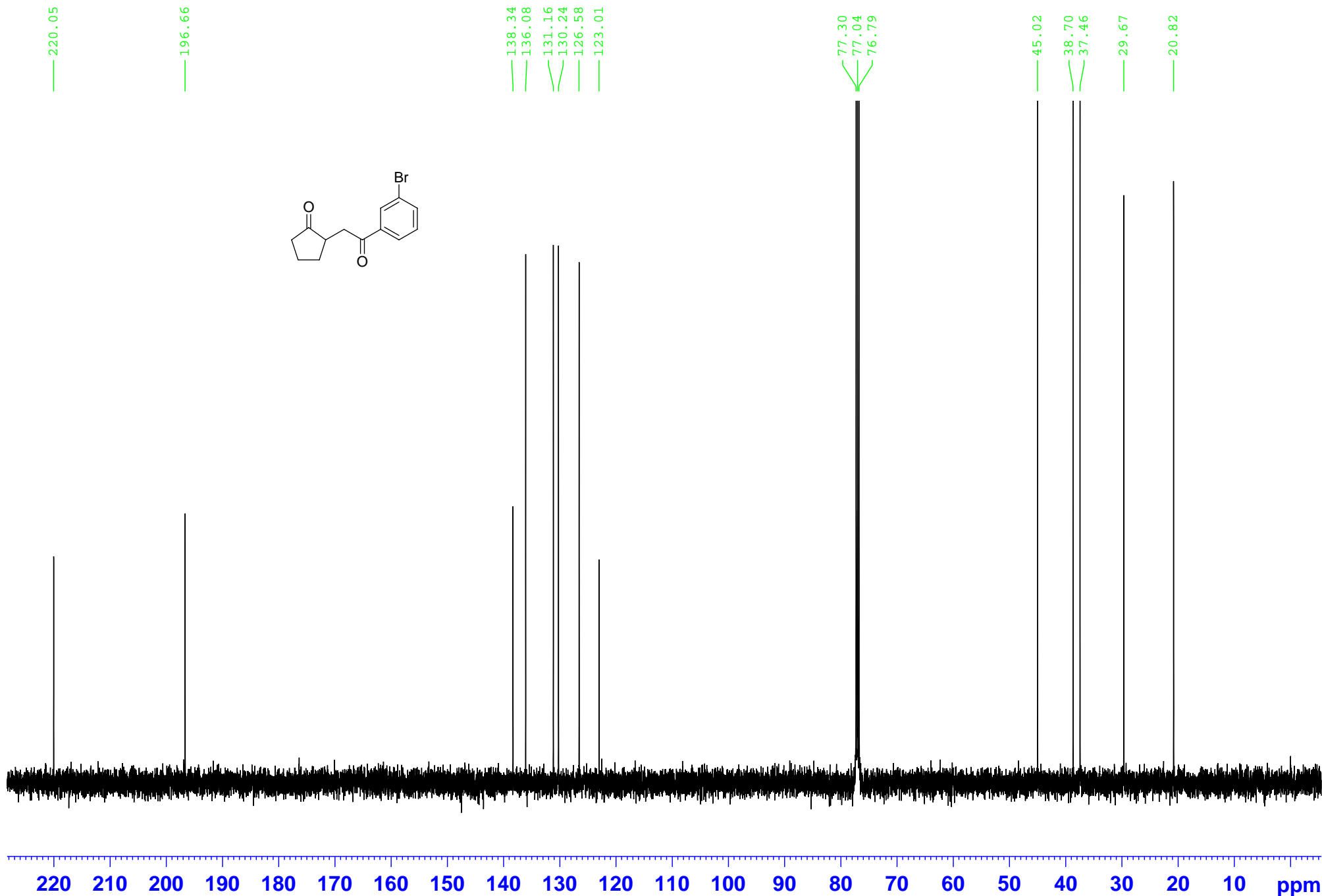
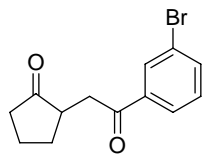
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7.703
7.701
7.699
7.687
7.685
7.683
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7.332
7.271

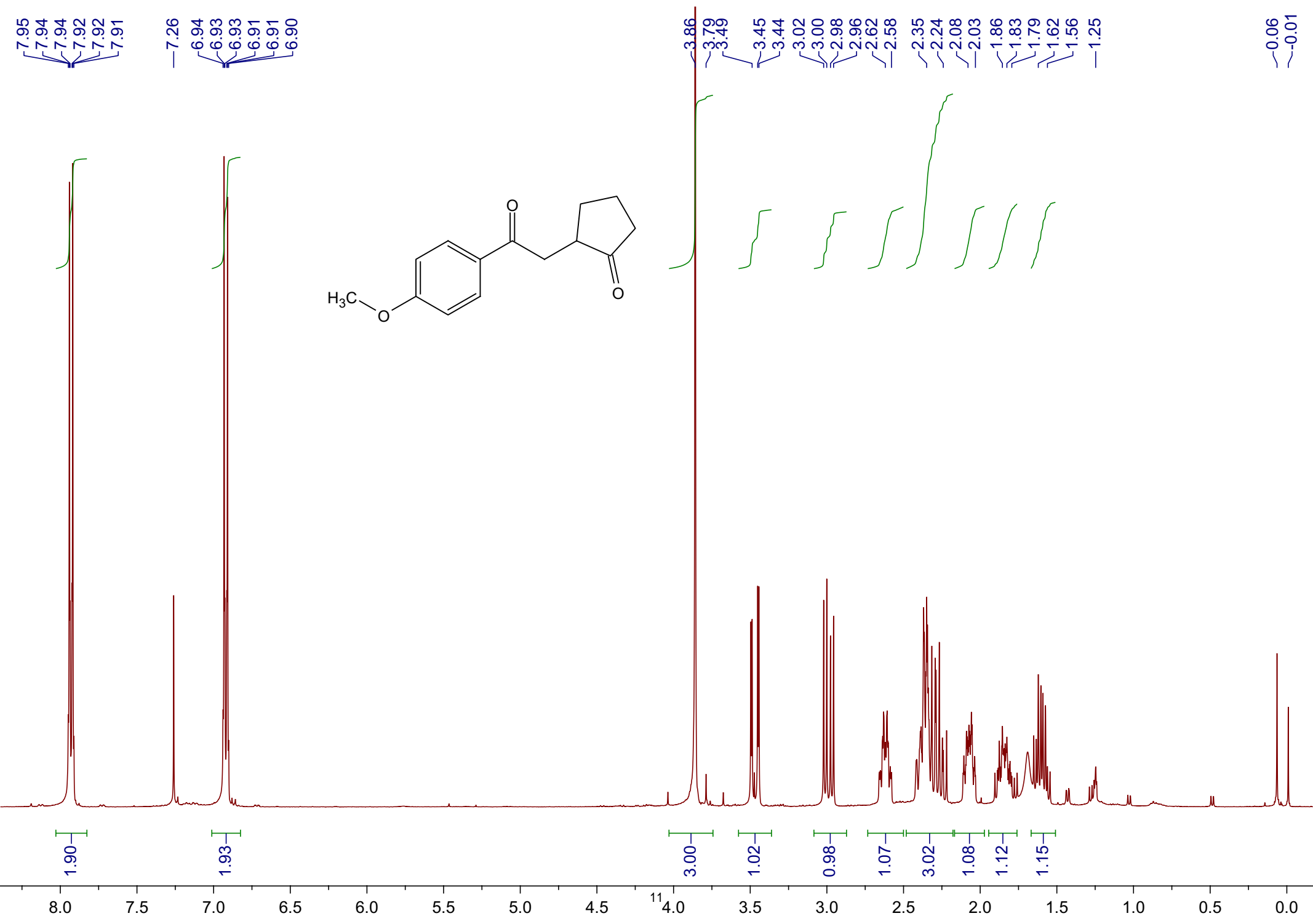
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3.473
3.466
3.035
3.019
2.999
2.983
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2.389
2.376
2.373
2.363
2.360
2.306
2.288
2.284
2.266
2.250
2.228
2.112
2.099
2.086
2.082
1.880
1.670
1.615
1.601
1.591
1.577

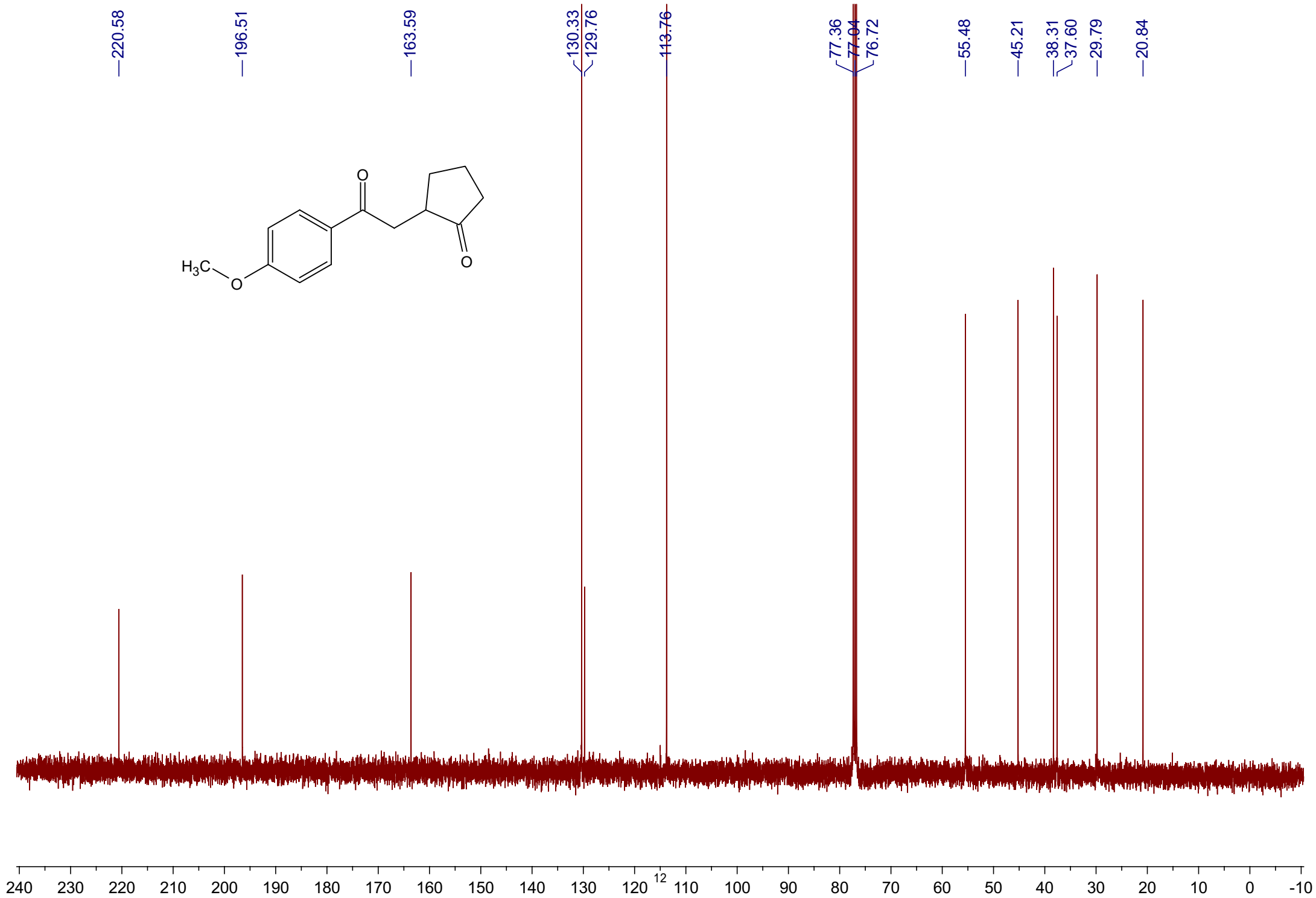
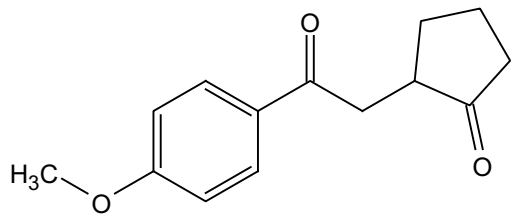


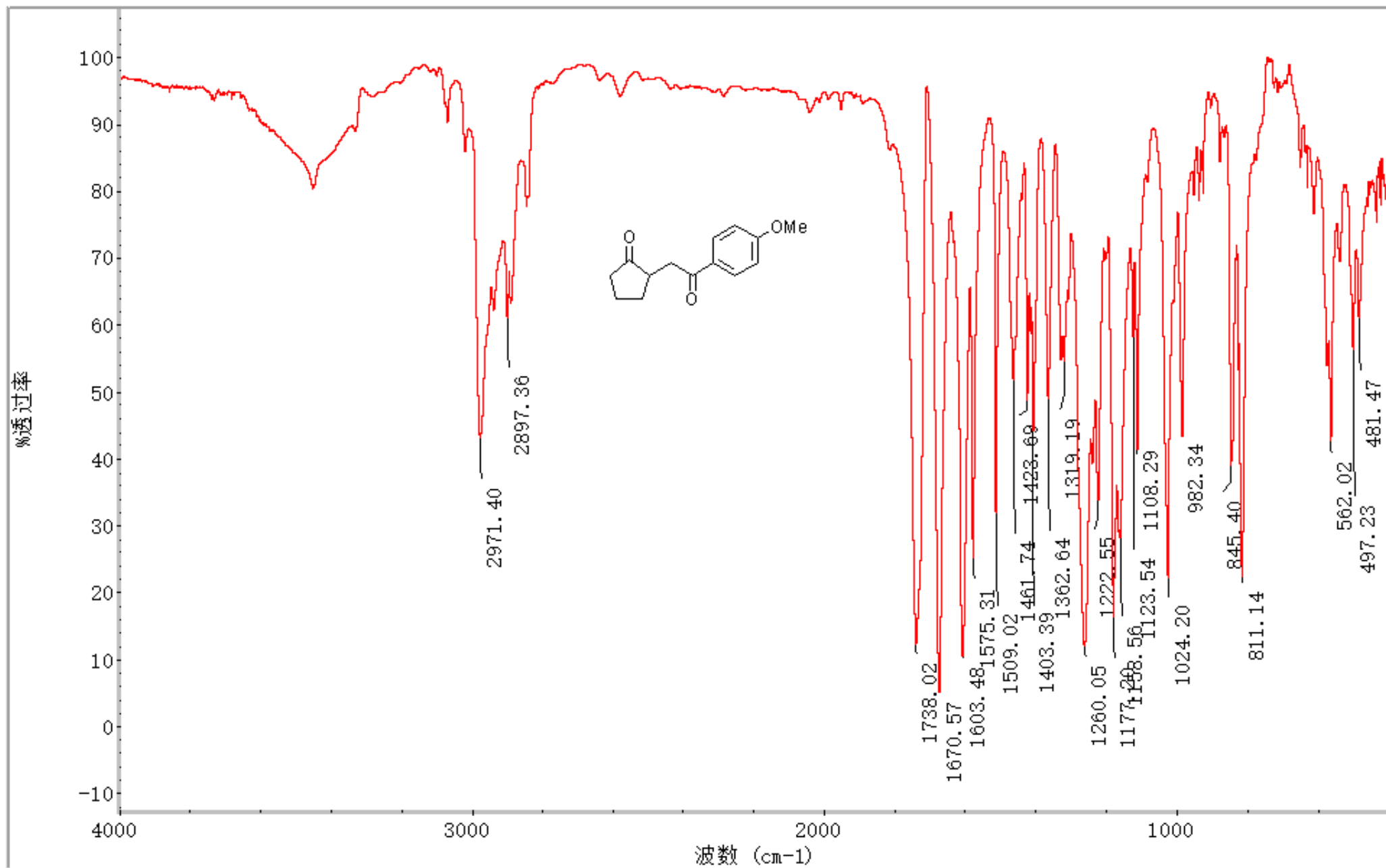
1.00
1.03
1.00
1.02

1.04
1.04
1.02
2.08
1.23
1.09
1.13
1.50



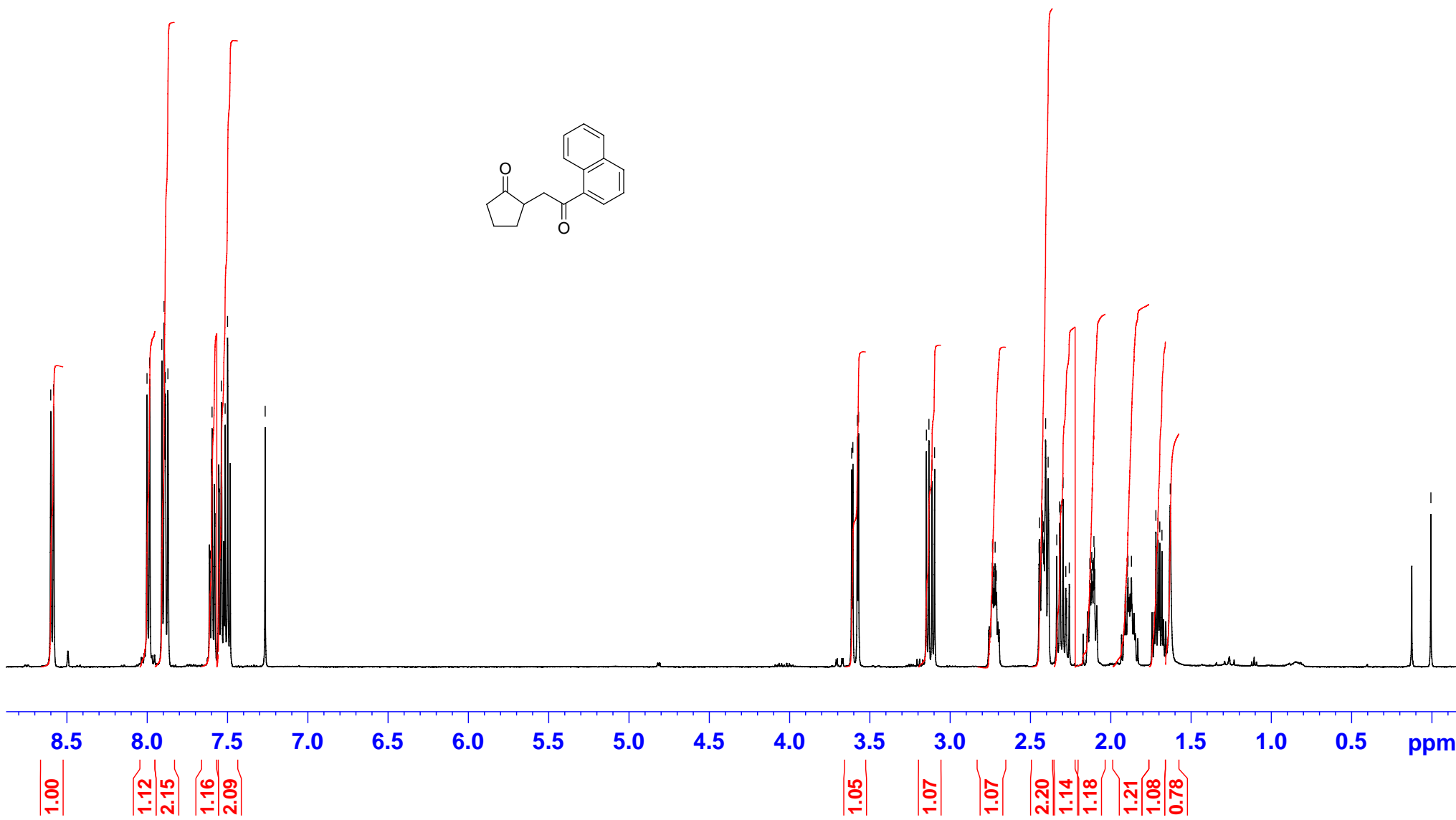
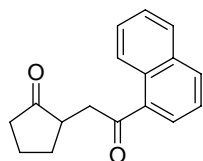


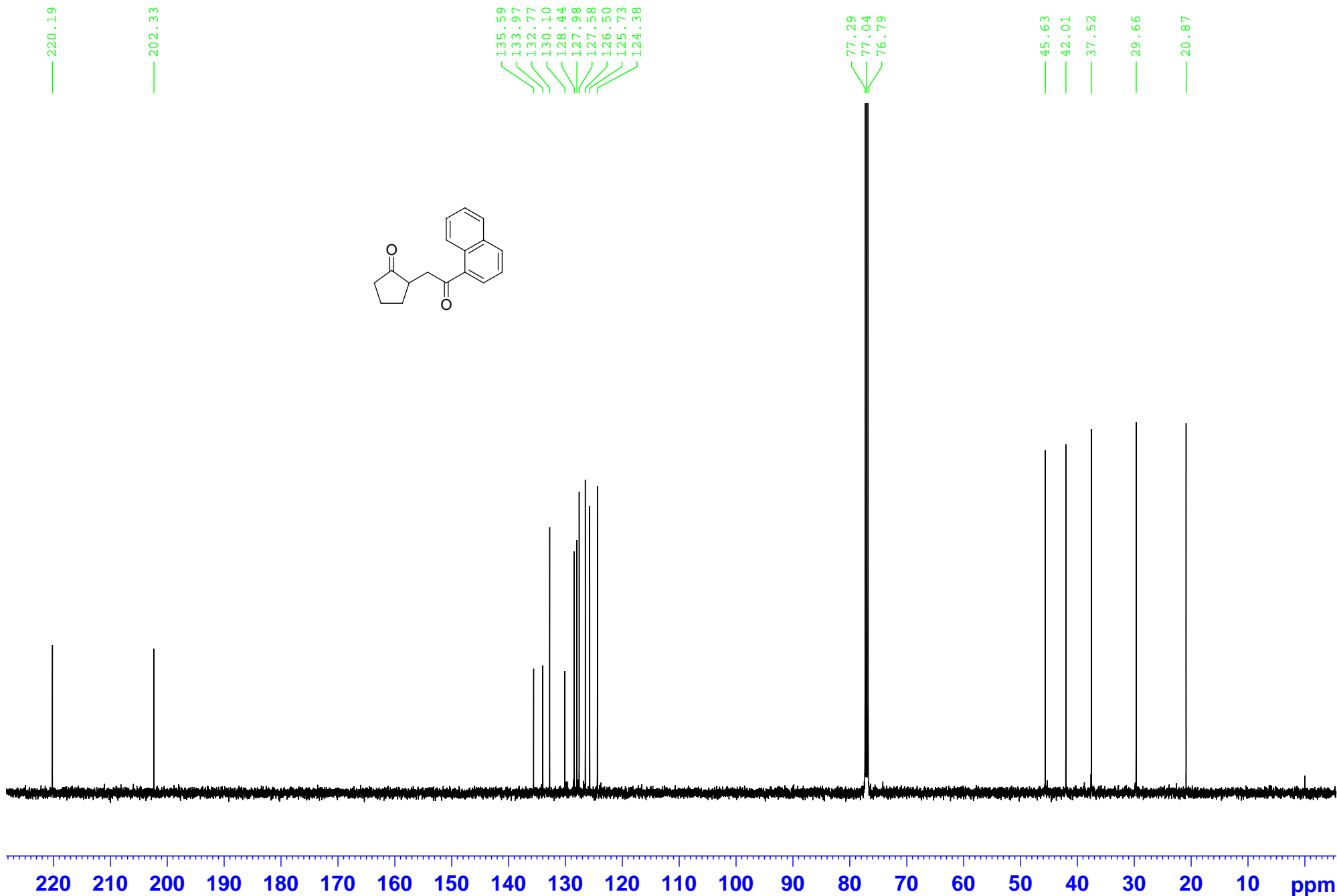
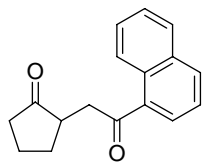


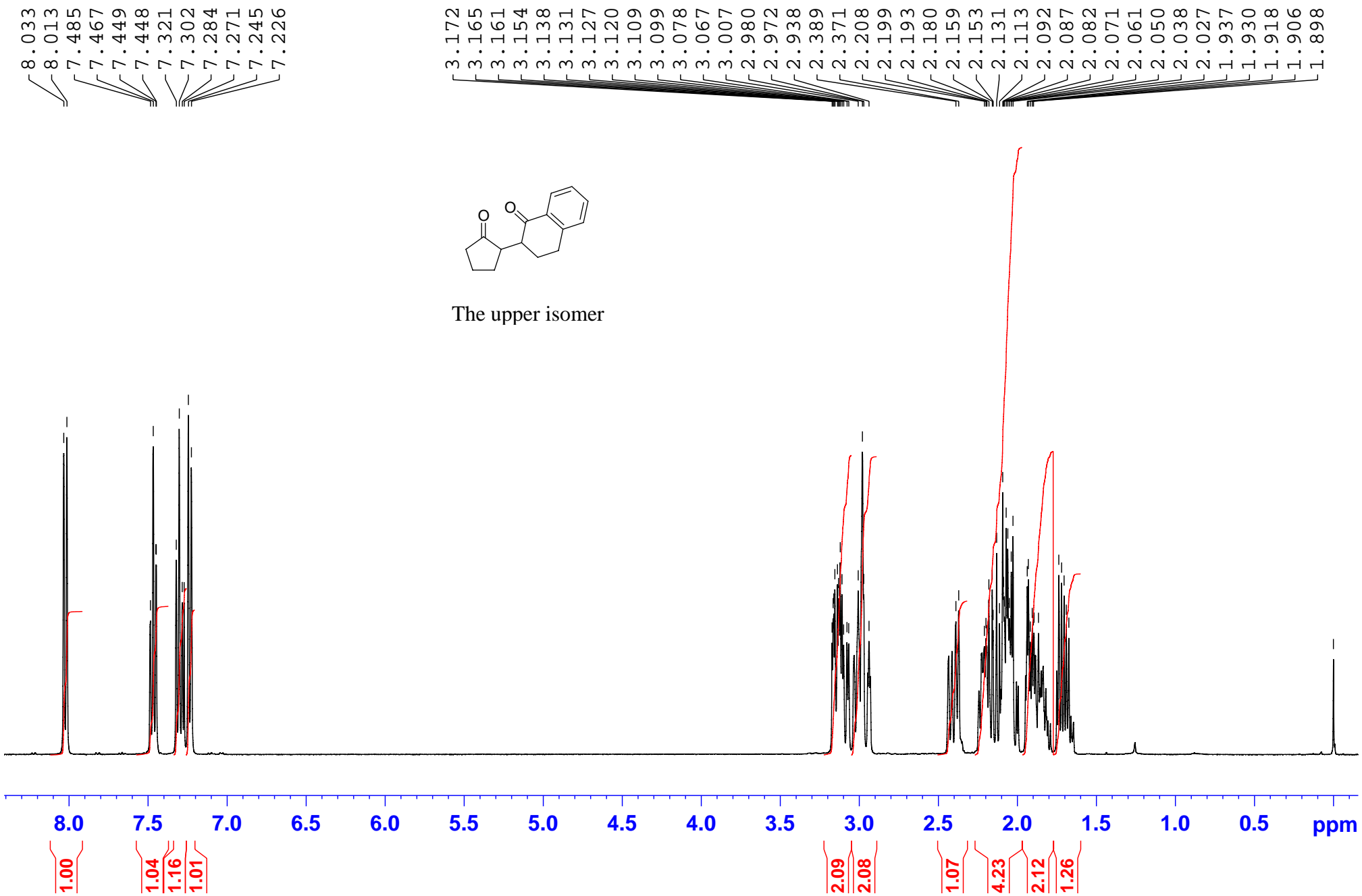


8.601
8.584
8.002
7.986
7.910
7.895
7.889
7.872
7.597
7.539
7.515
7.500
7.266

3.614
3.607
3.579
3.571
3.149
3.133
3.113
3.098
2.737
2.729
2.721
2.713
2.447
2.444
2.431
2.428
2.421
2.416
2.407
2.391
2.337
2.319
2.315
2.297
2.281
2.259
2.131
2.127
2.123
2.119
2.115
2.109
2.105
2.102
1.897
1.893
1.872







220.66

198.59

144.13

133.41

132.43

128.77

127.38

126.61

49.68

47.76

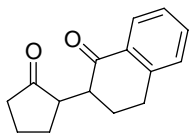
38.54

29.65

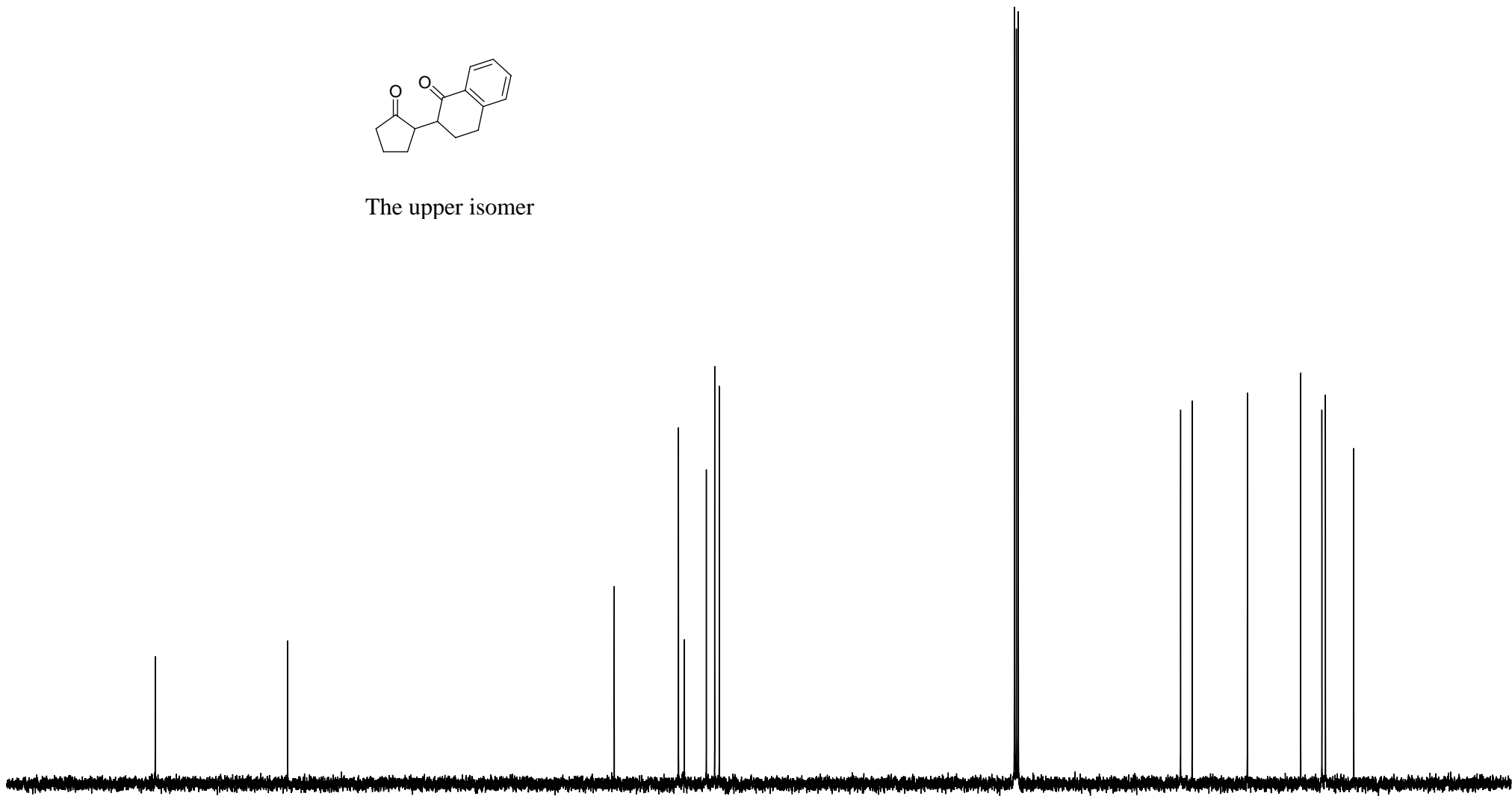
26.11

25.52

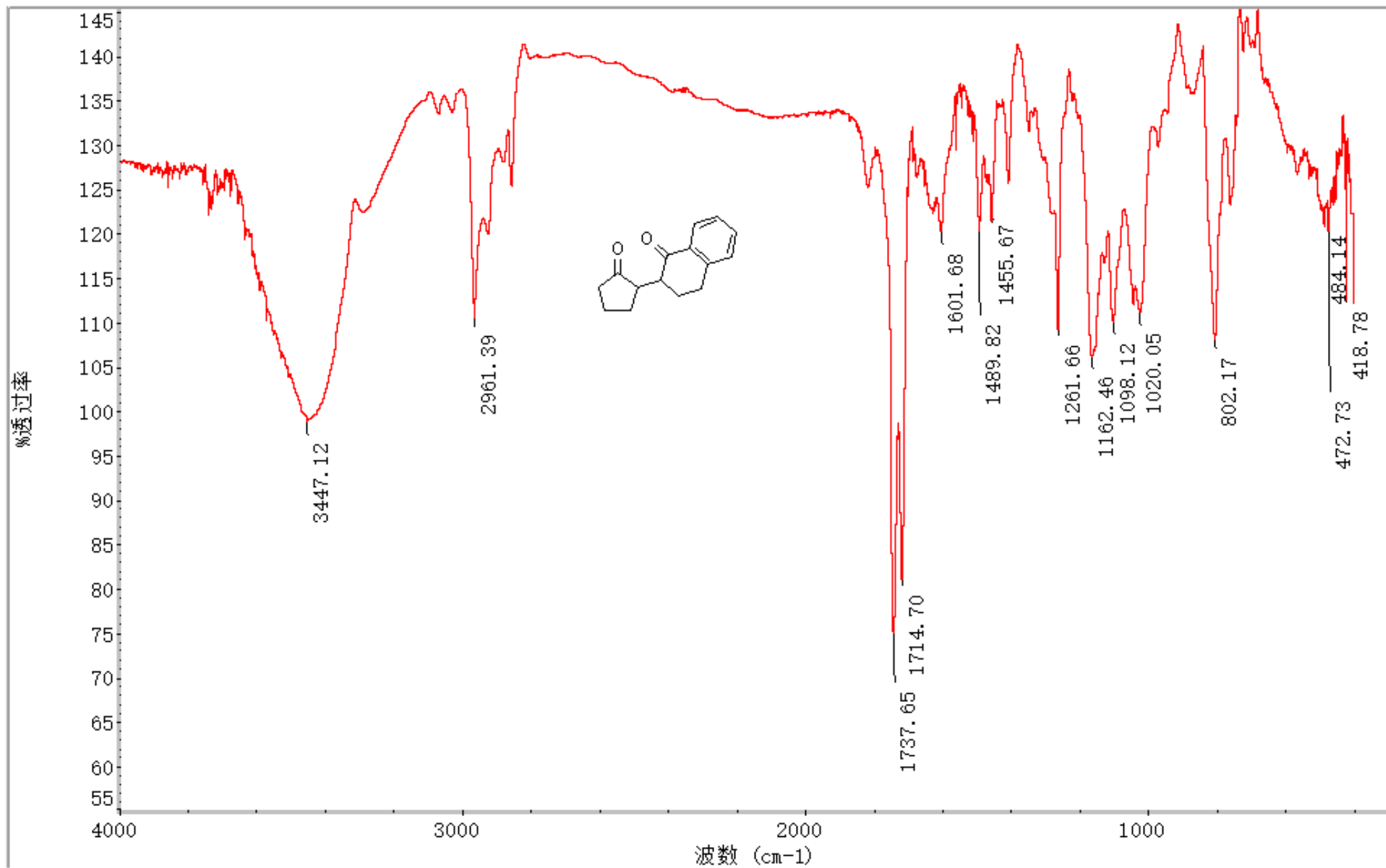
20.80

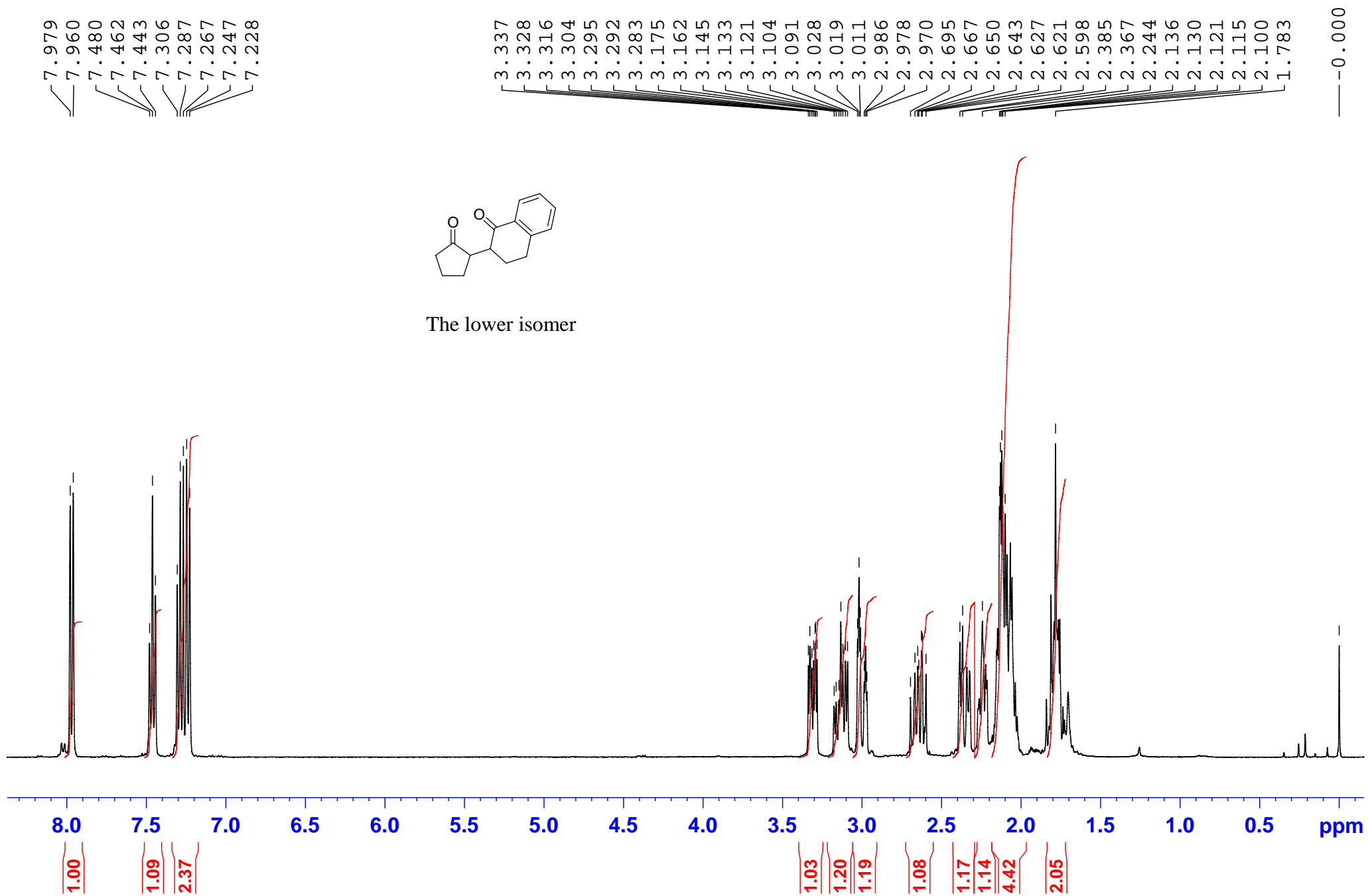


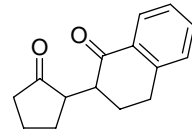
The upper isomer



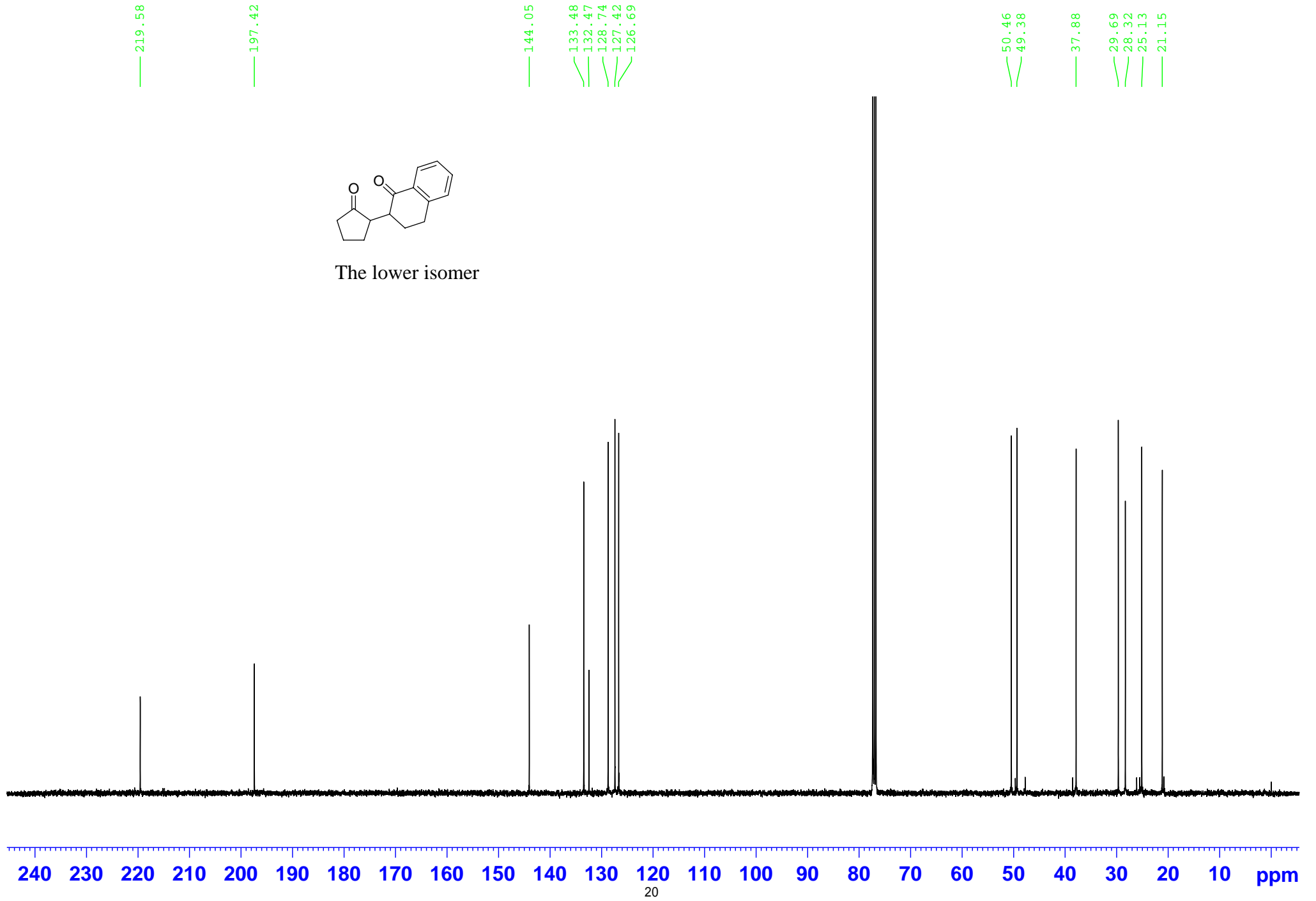
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

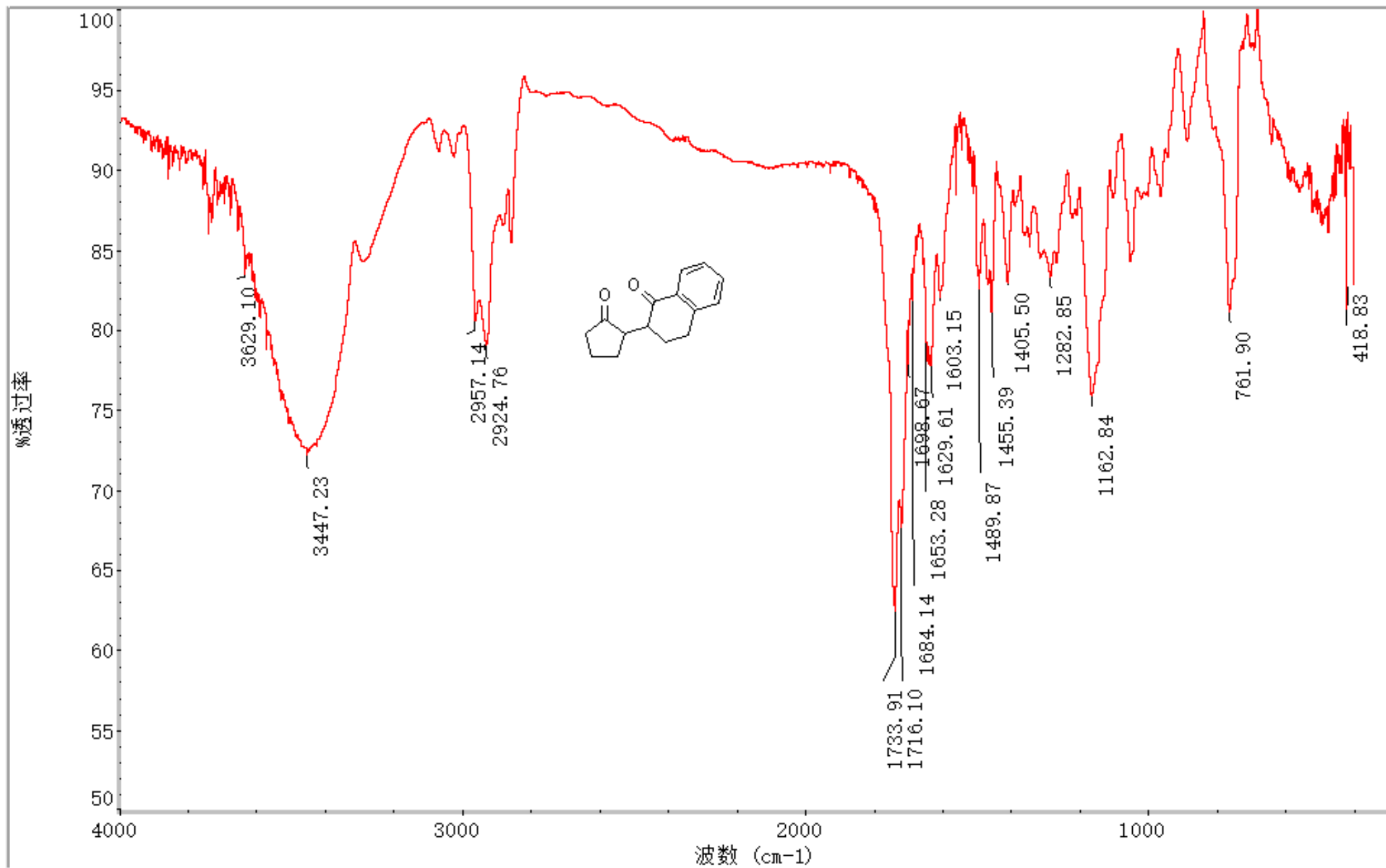


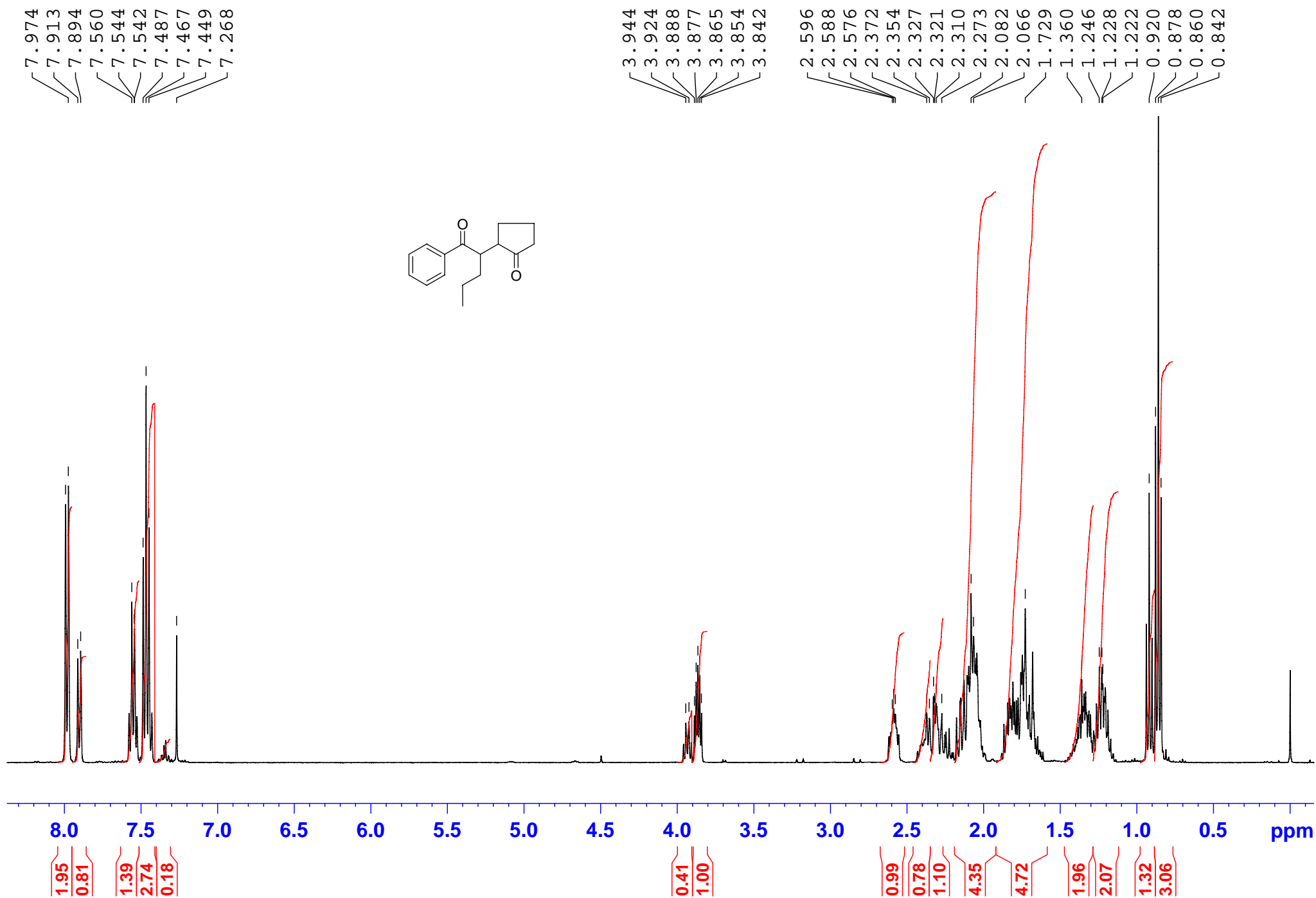


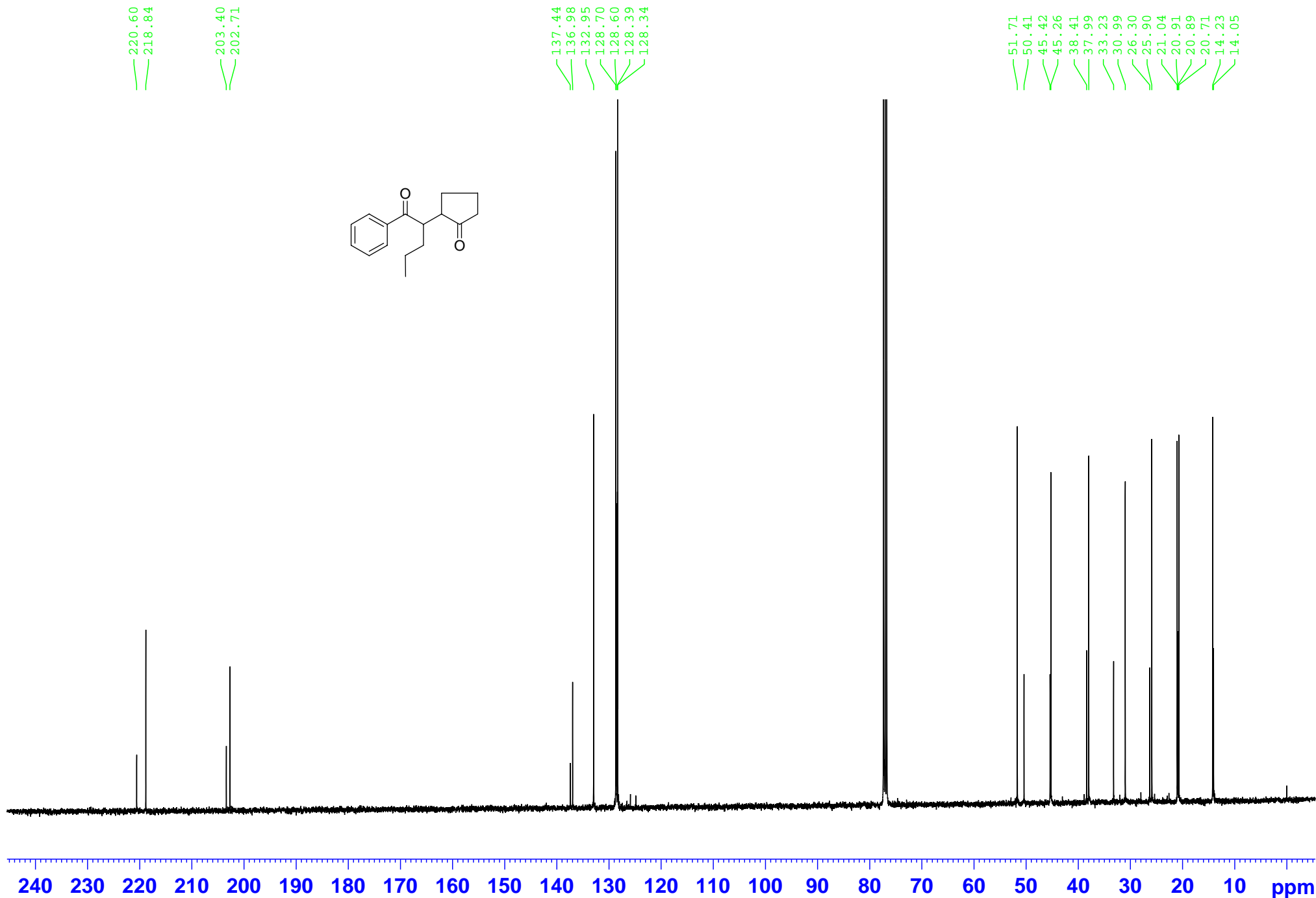
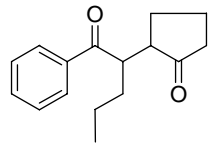


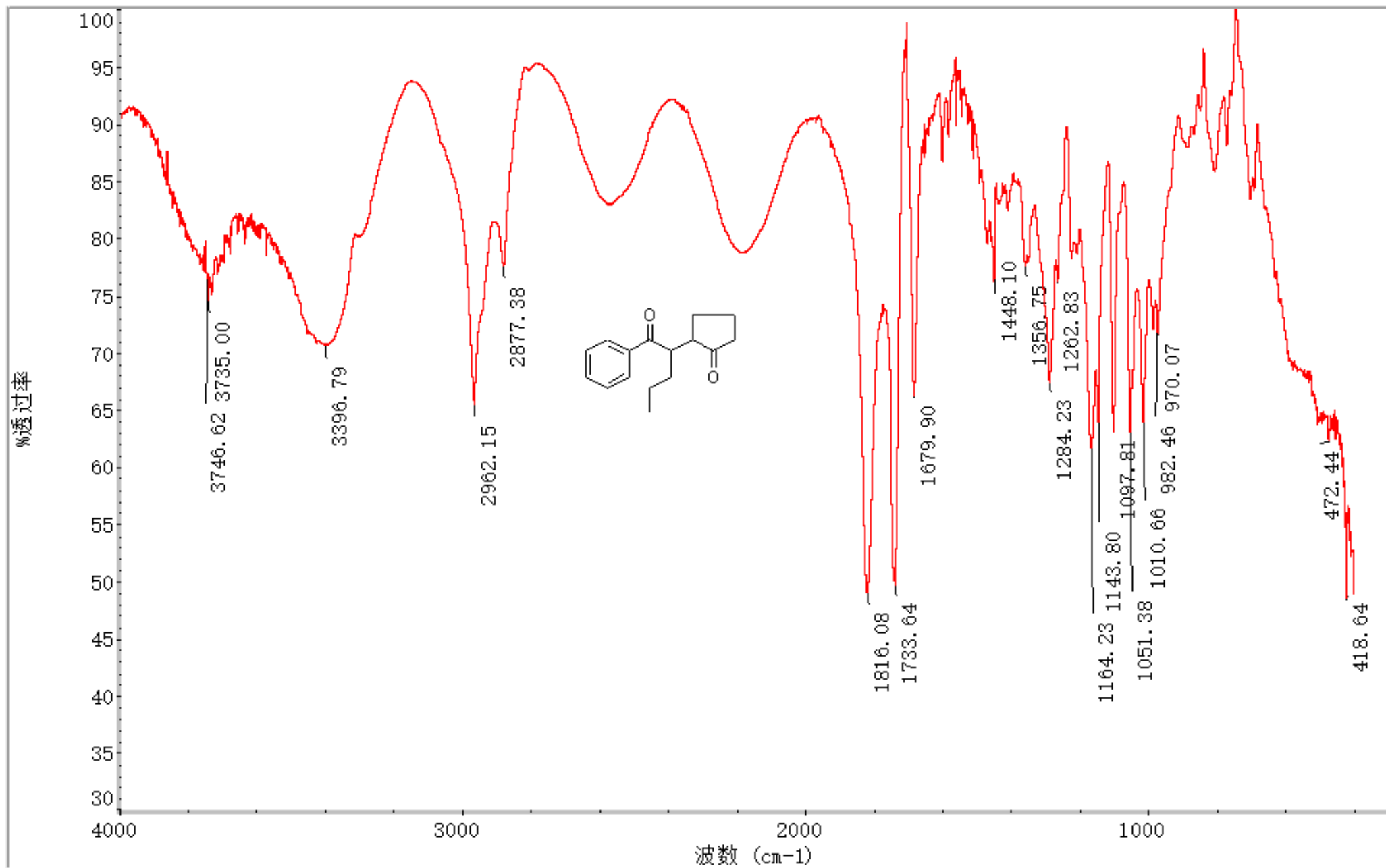
The lower isomer

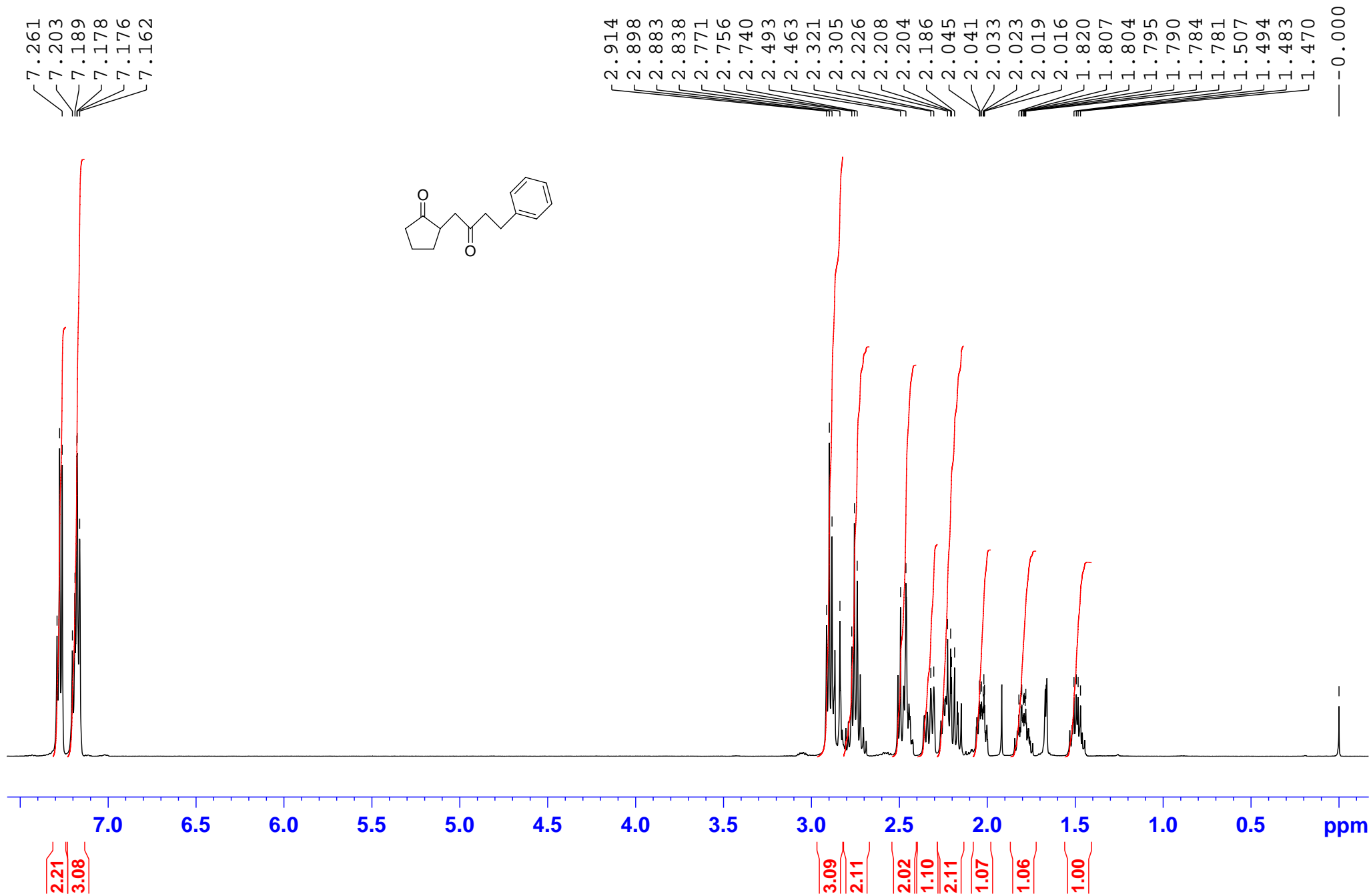


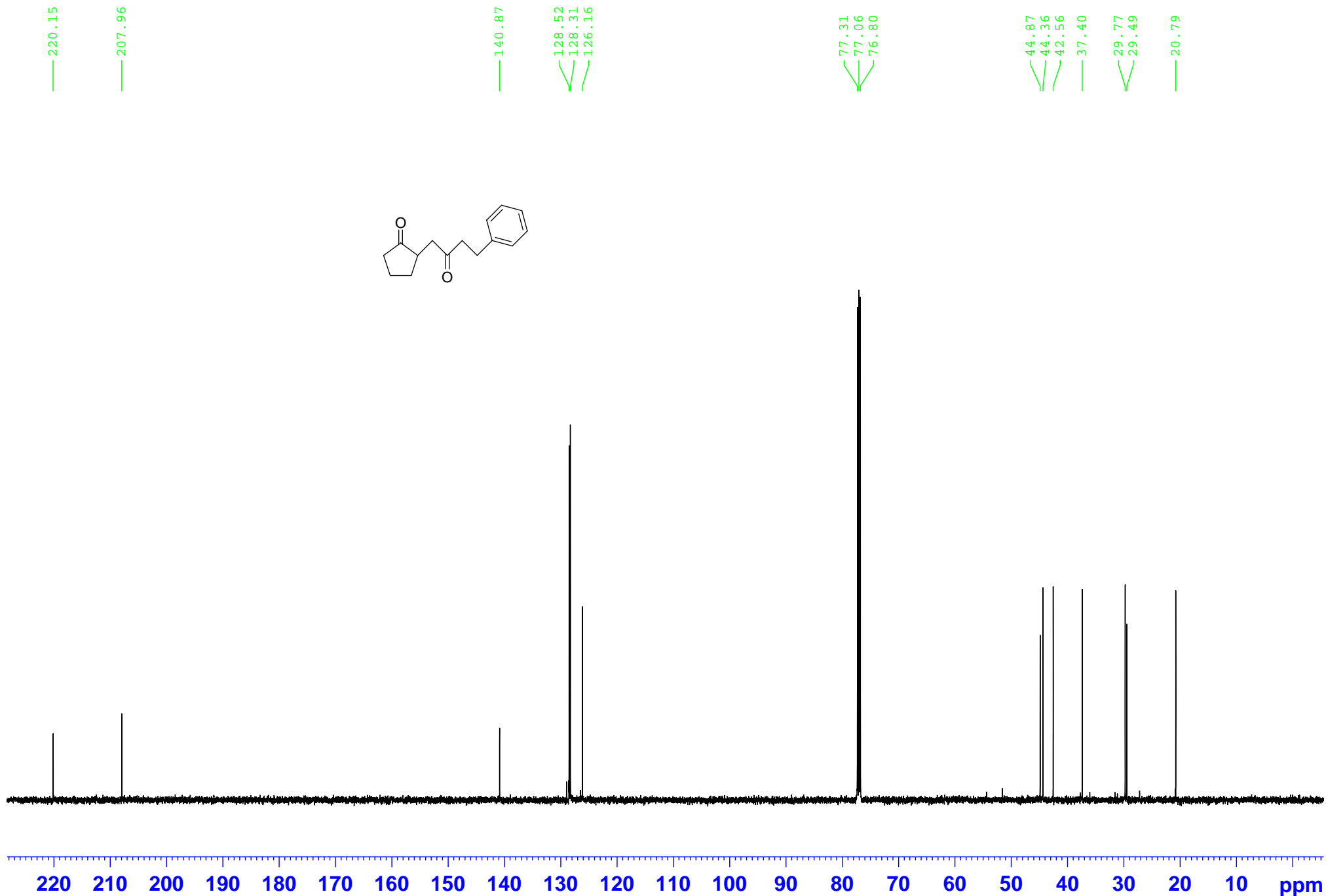
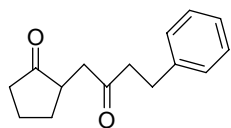




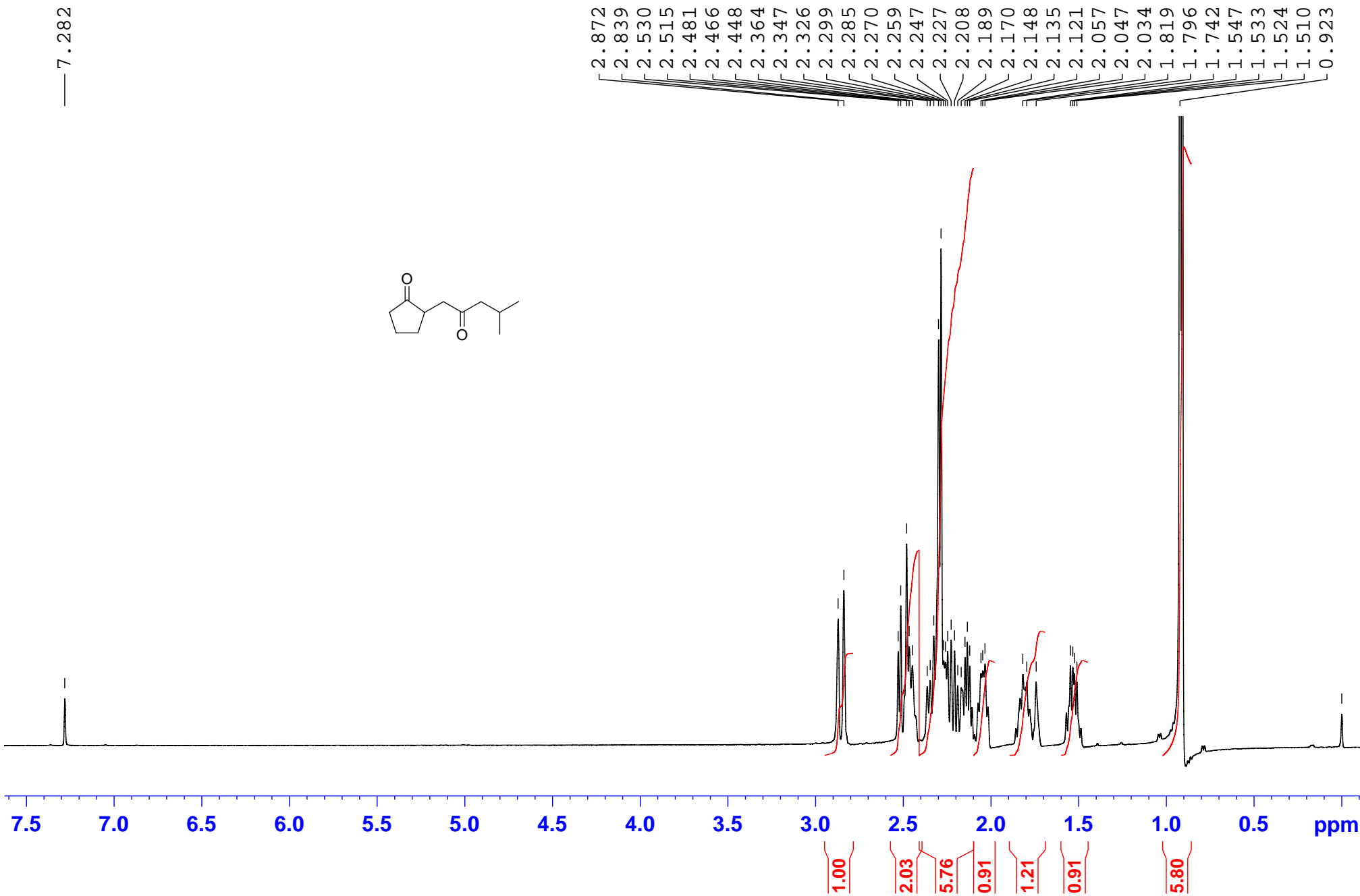
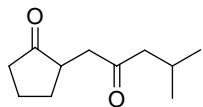


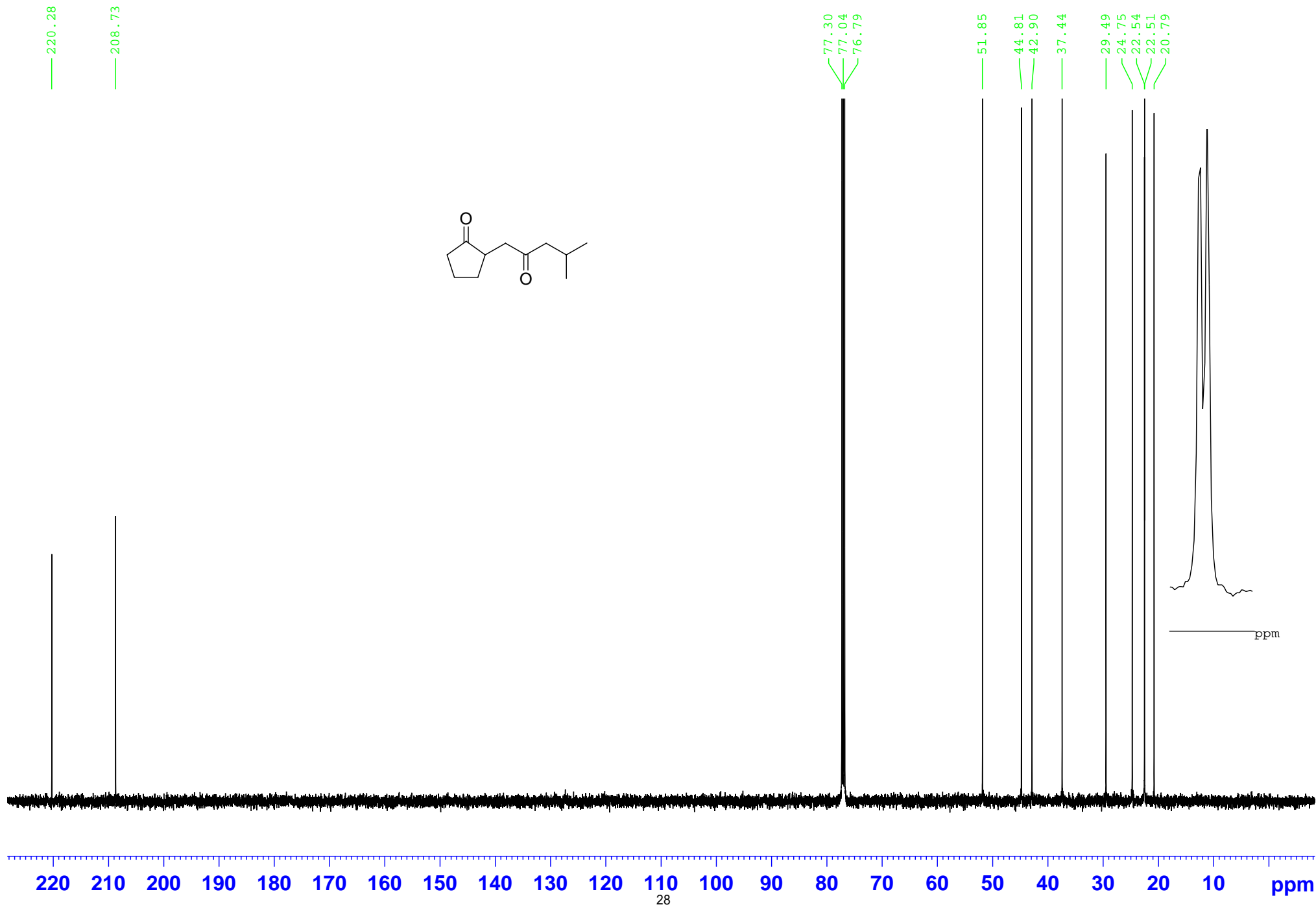


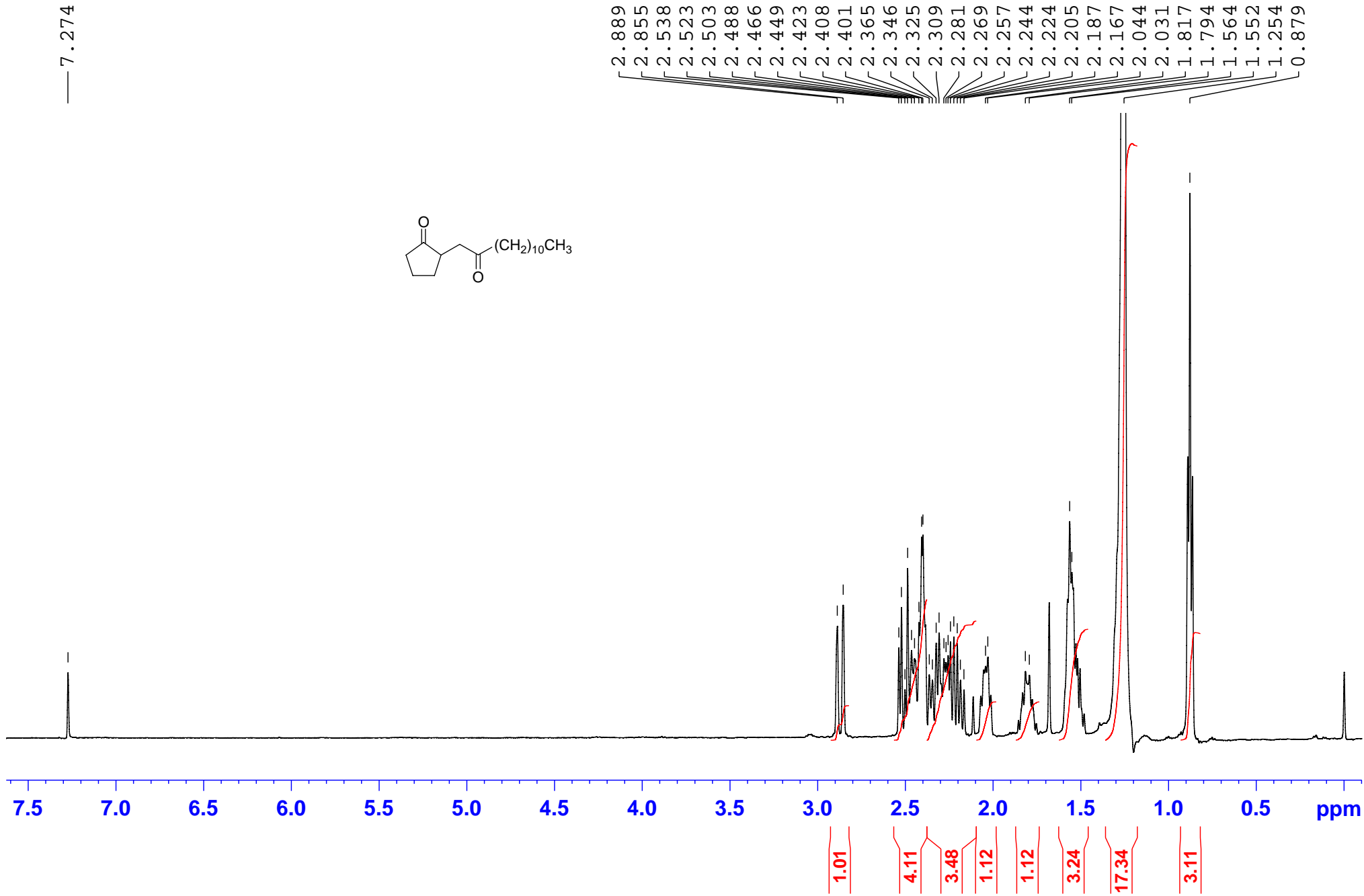


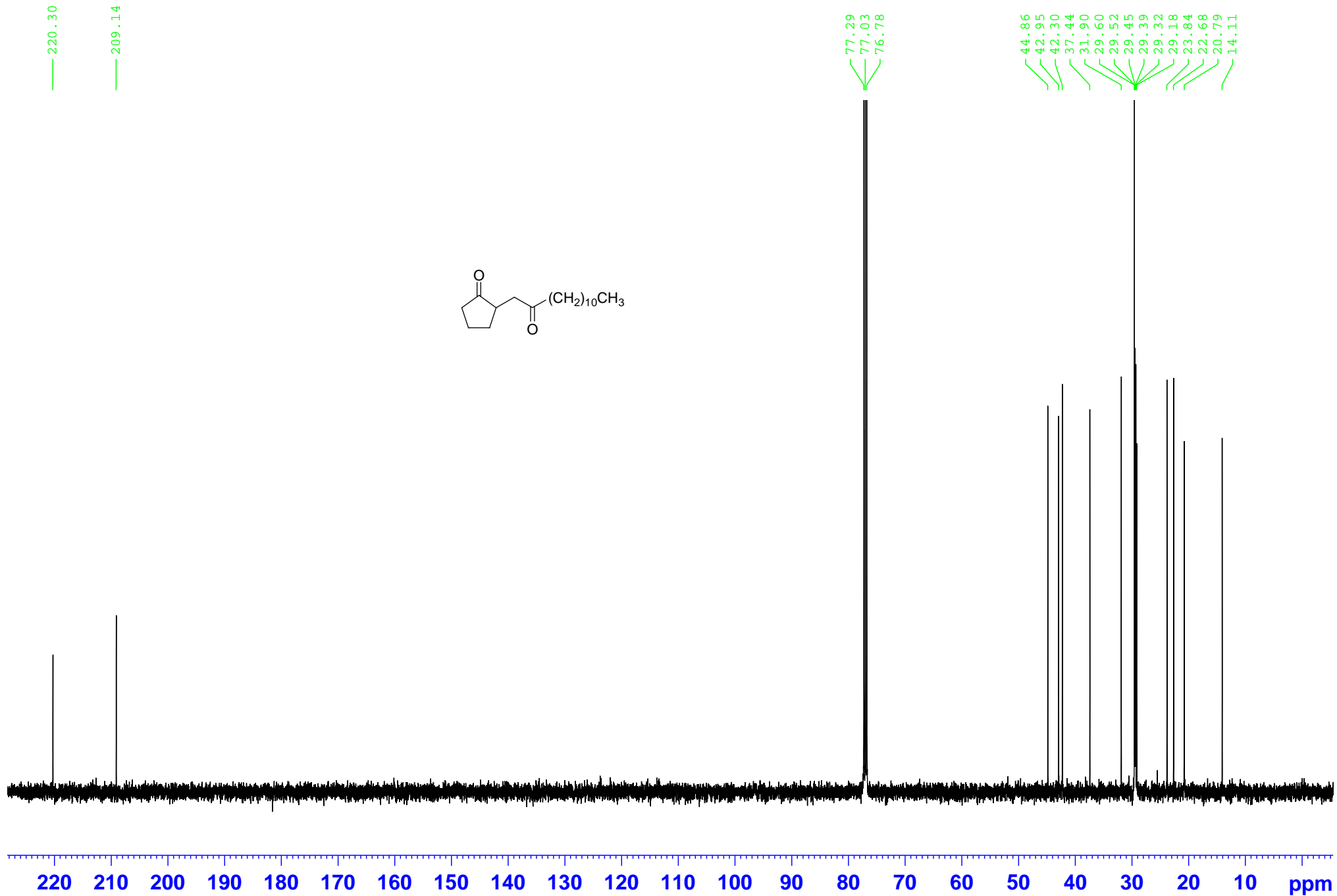


— 7.282

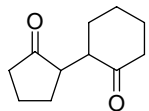




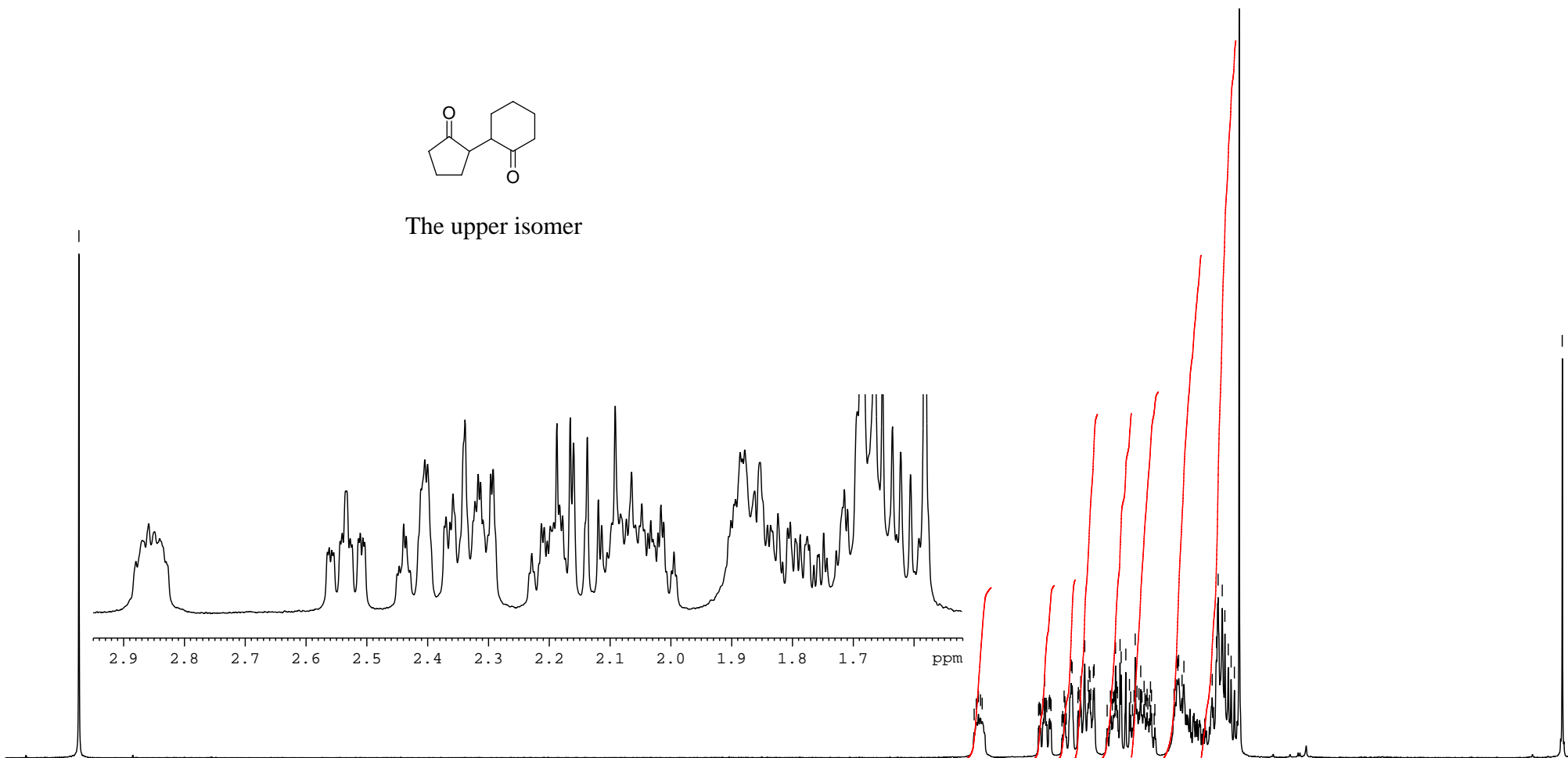




7.264
 2.859
 2.849
 2.535
 2.439
 2.405
 2.400
 2.372
 2.370
 2.363
 2.358
 2.338
 2.322
 2.317
 2.313
 2.309
 2.296
 2.292
 2.213
 2.208
 2.198
 2.192
 2.187
 2.183
 2.178
 2.166
 2.160
 2.137
 2.119
 2.114
 2.097
 2.091
 2.083
 2.073
 2.065
 2.058
 2.048
 2.043
 2.037
 2.033
 2.021
 2.016
 2.012
 1.901
 1.893
 1.886
 1.882
 1.878
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 1.685
 1.665
 1.652
 1.636
 1.622
 1.606
 -0.000



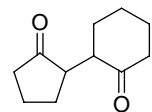
The upper isomer



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
 ppm

1.00
 1.01
 1.05
 2.01
 2.02
 2.14
 2.94
 4.20

220.71
211.07



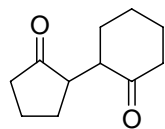
The upper isomer

77.34
77.02
76.71

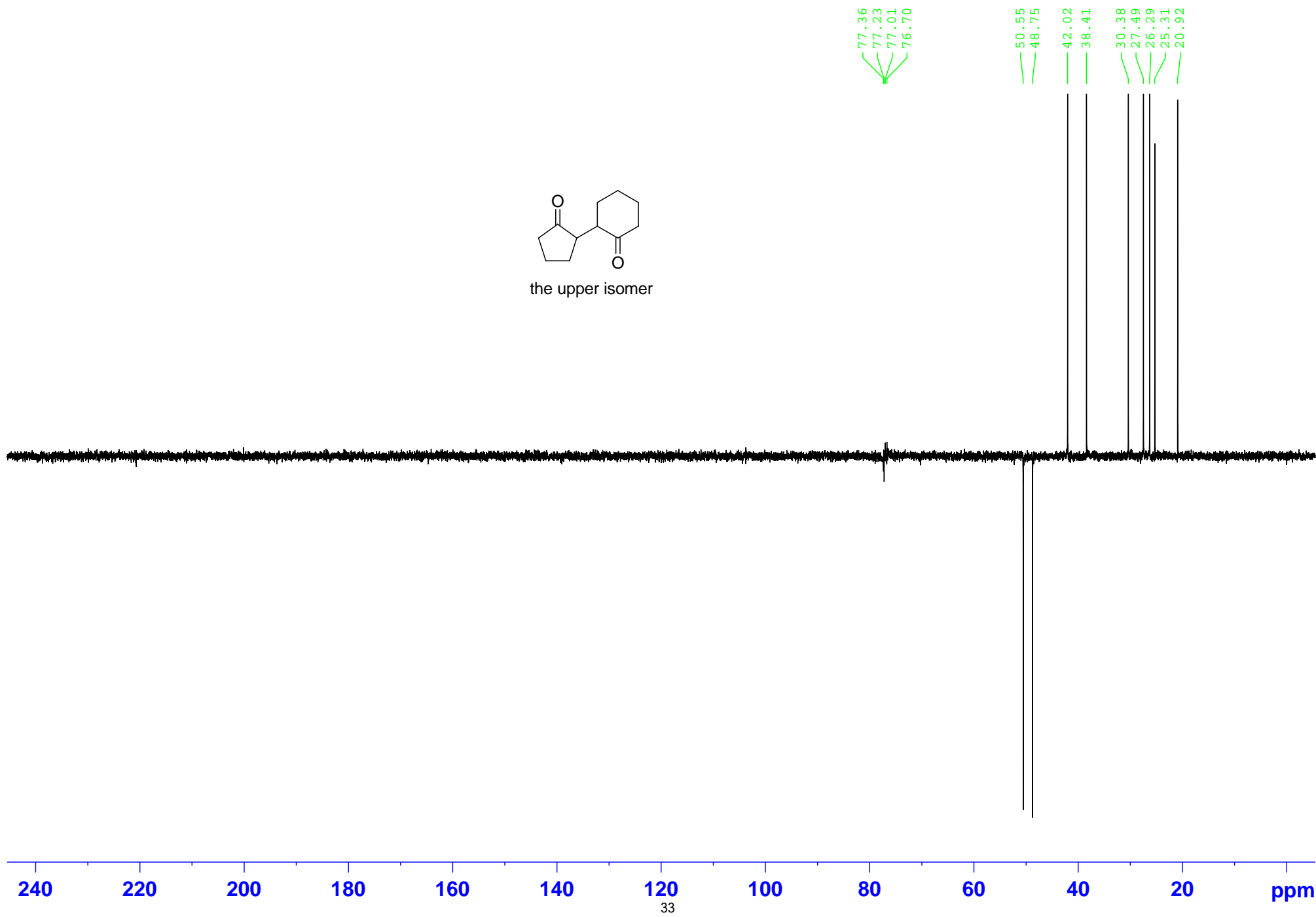
50.56
48.75
42.02
38.41

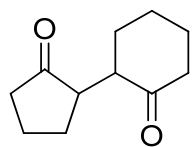
30.38
27.48
26.29
25.31
20.92



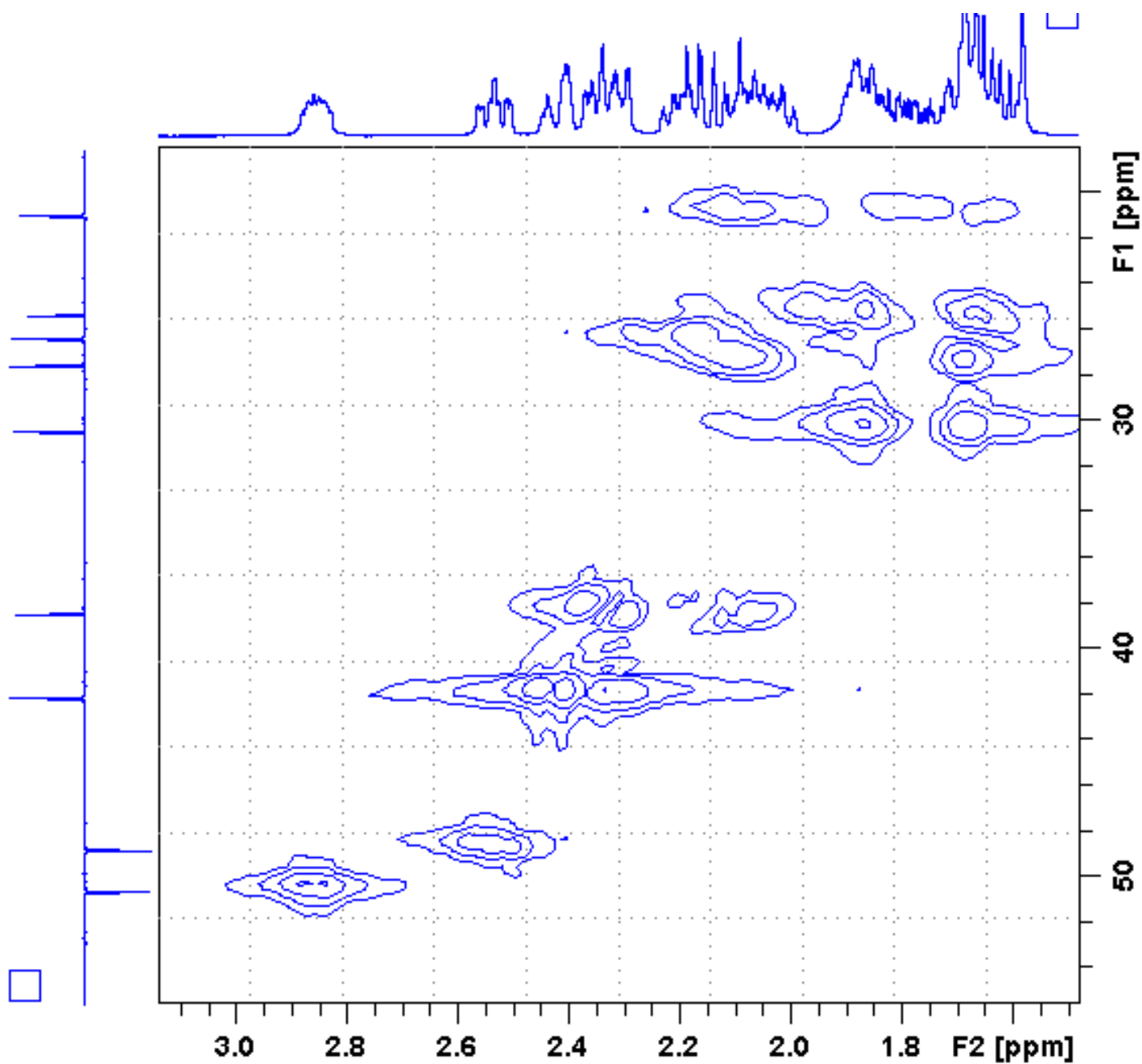


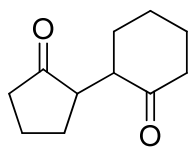
the upper isomer



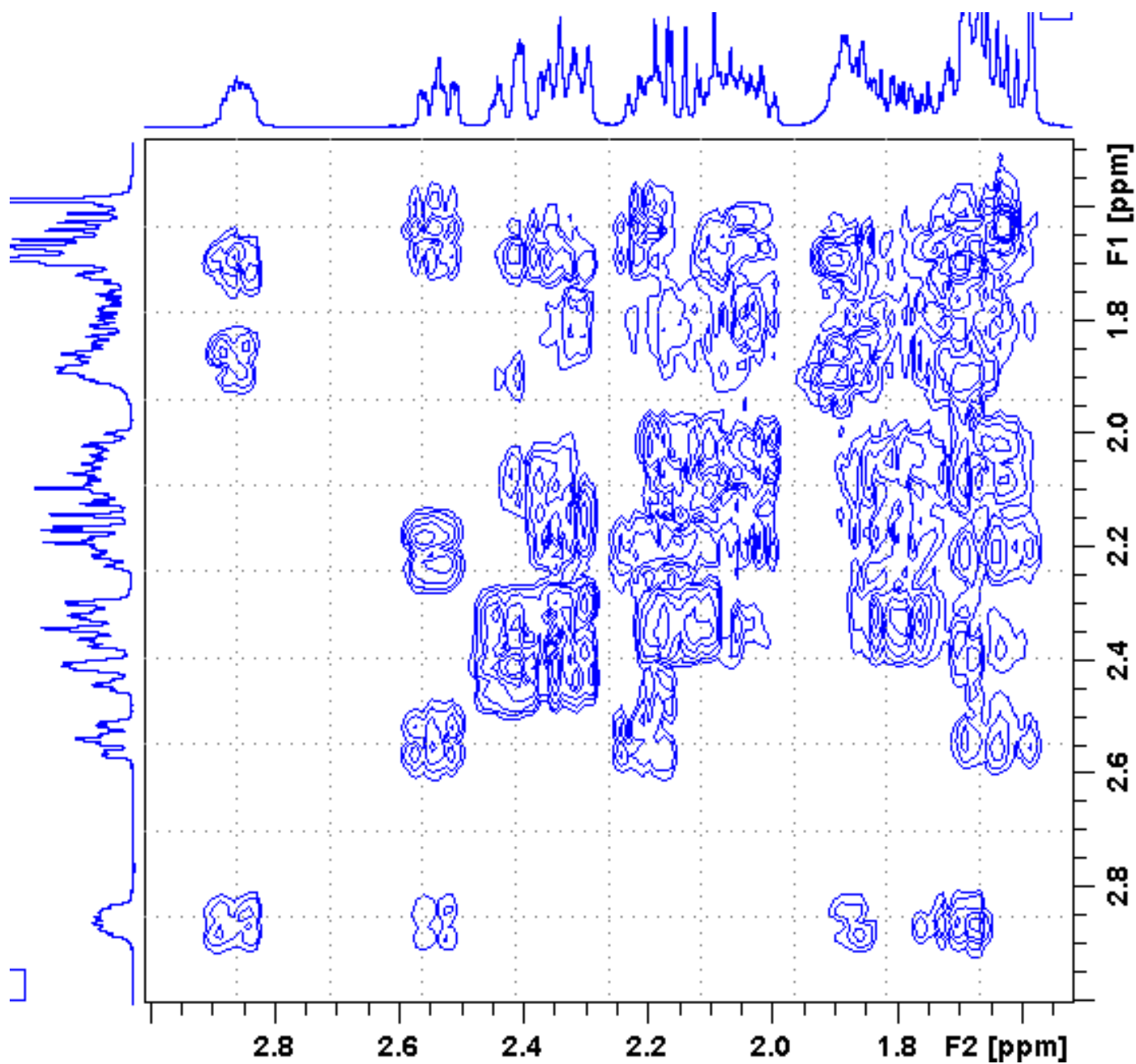


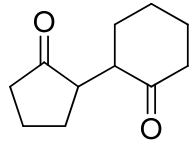
HMQC, The upper isomer



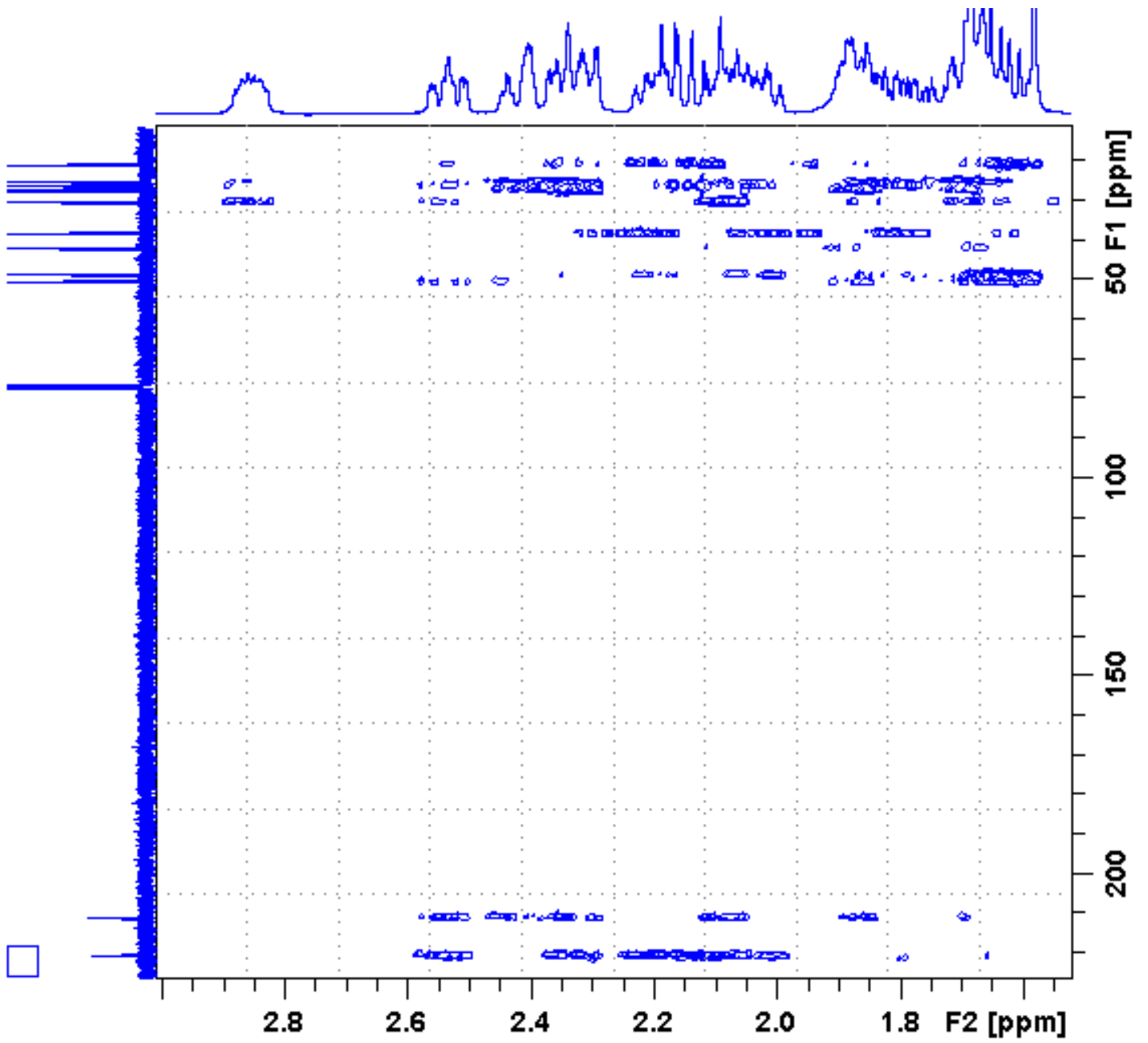


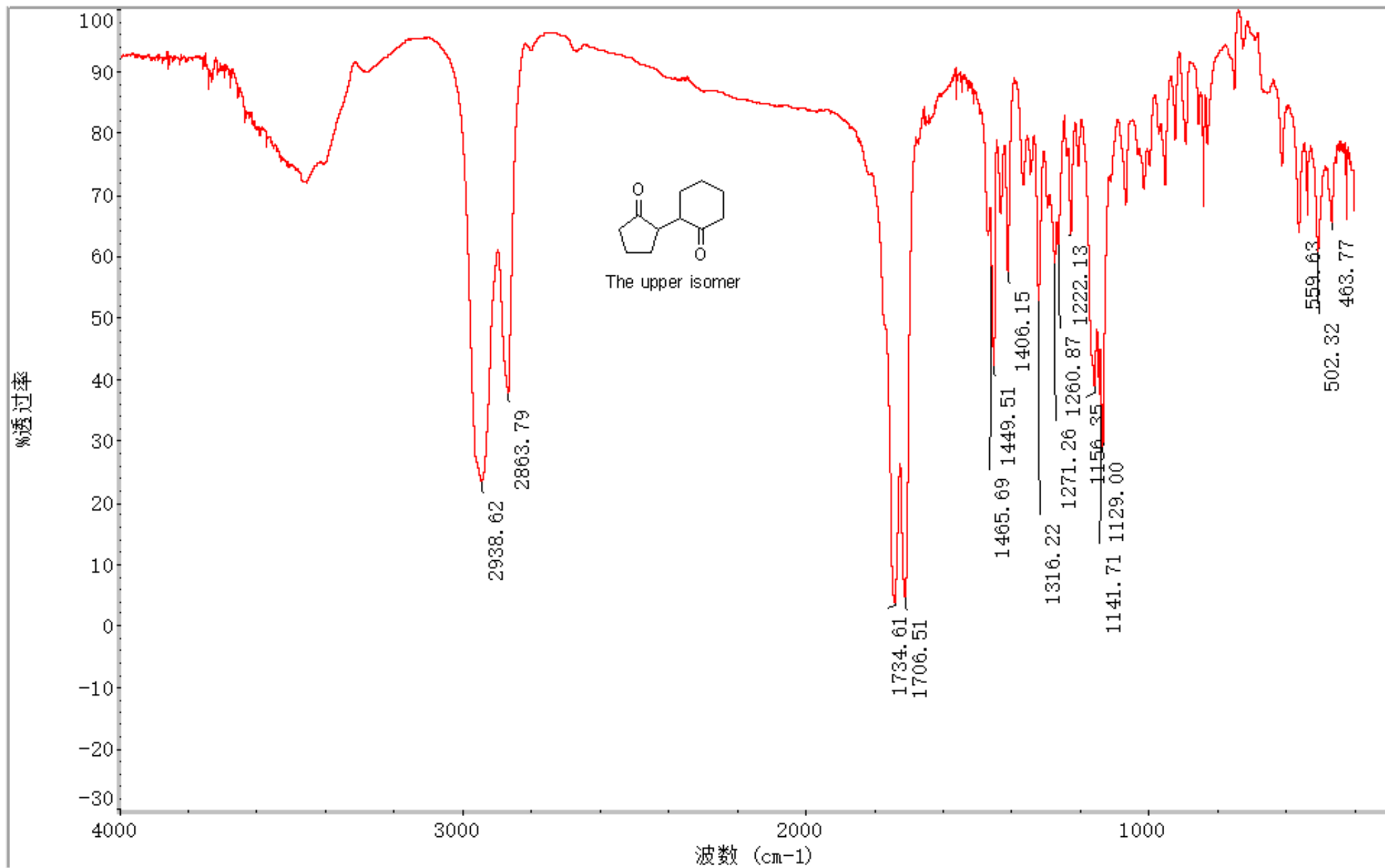
COSY; The upper isomer



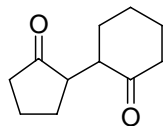


HMBC; The upper isomer

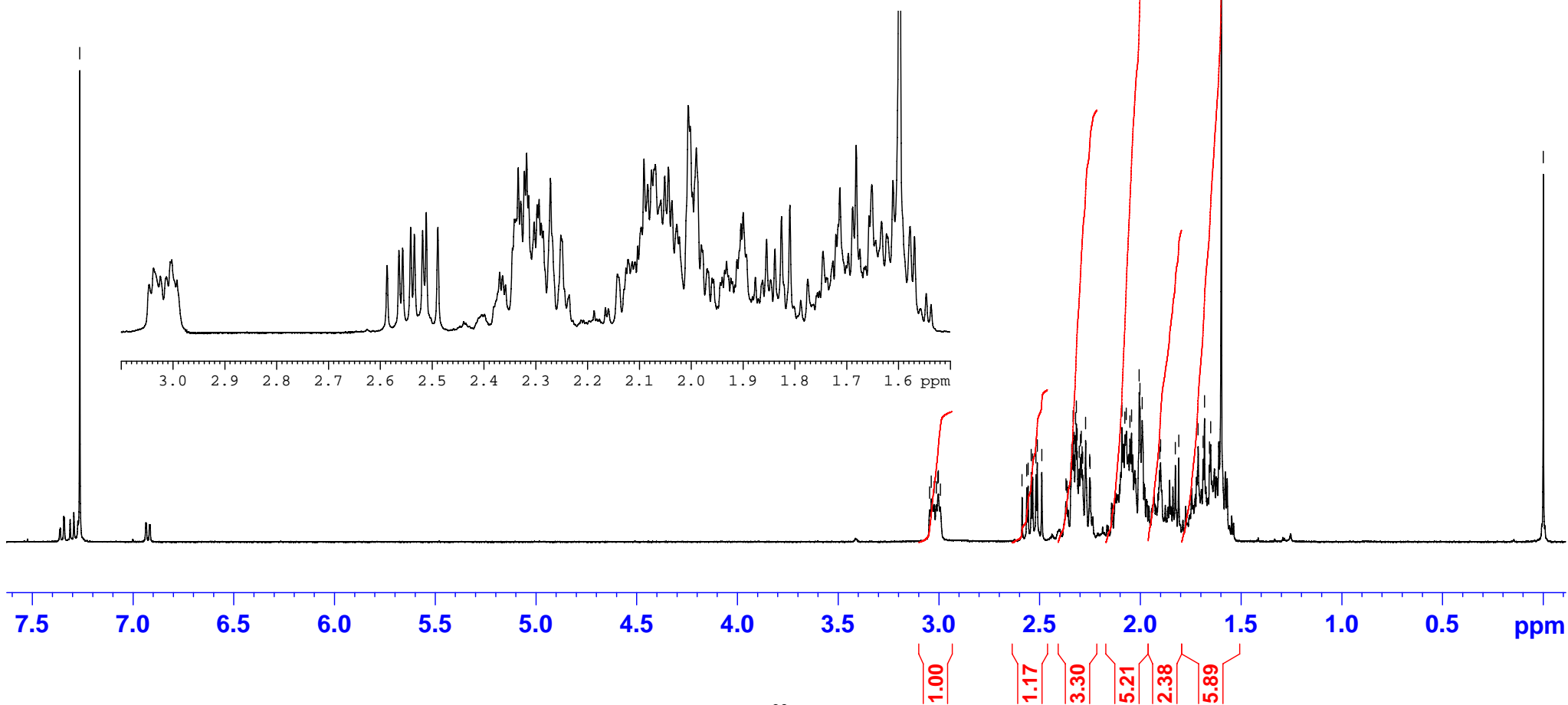


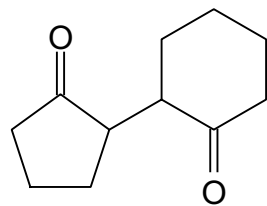


— 7.265



the lower isomer





the lower isomer

—220.36

—210.01

77.42
77.10
76.78

51.27
49.95

—38.03

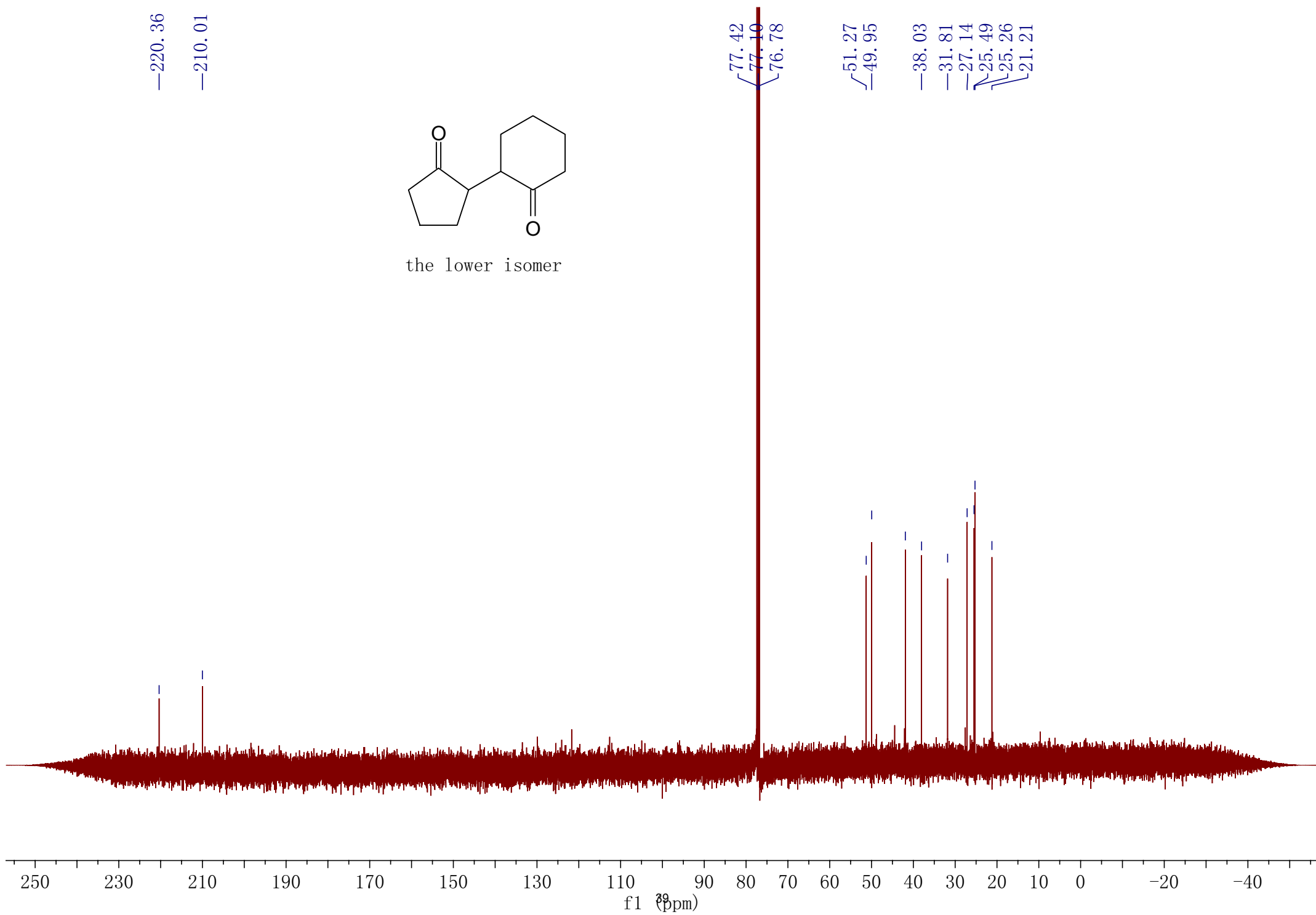
—31.81

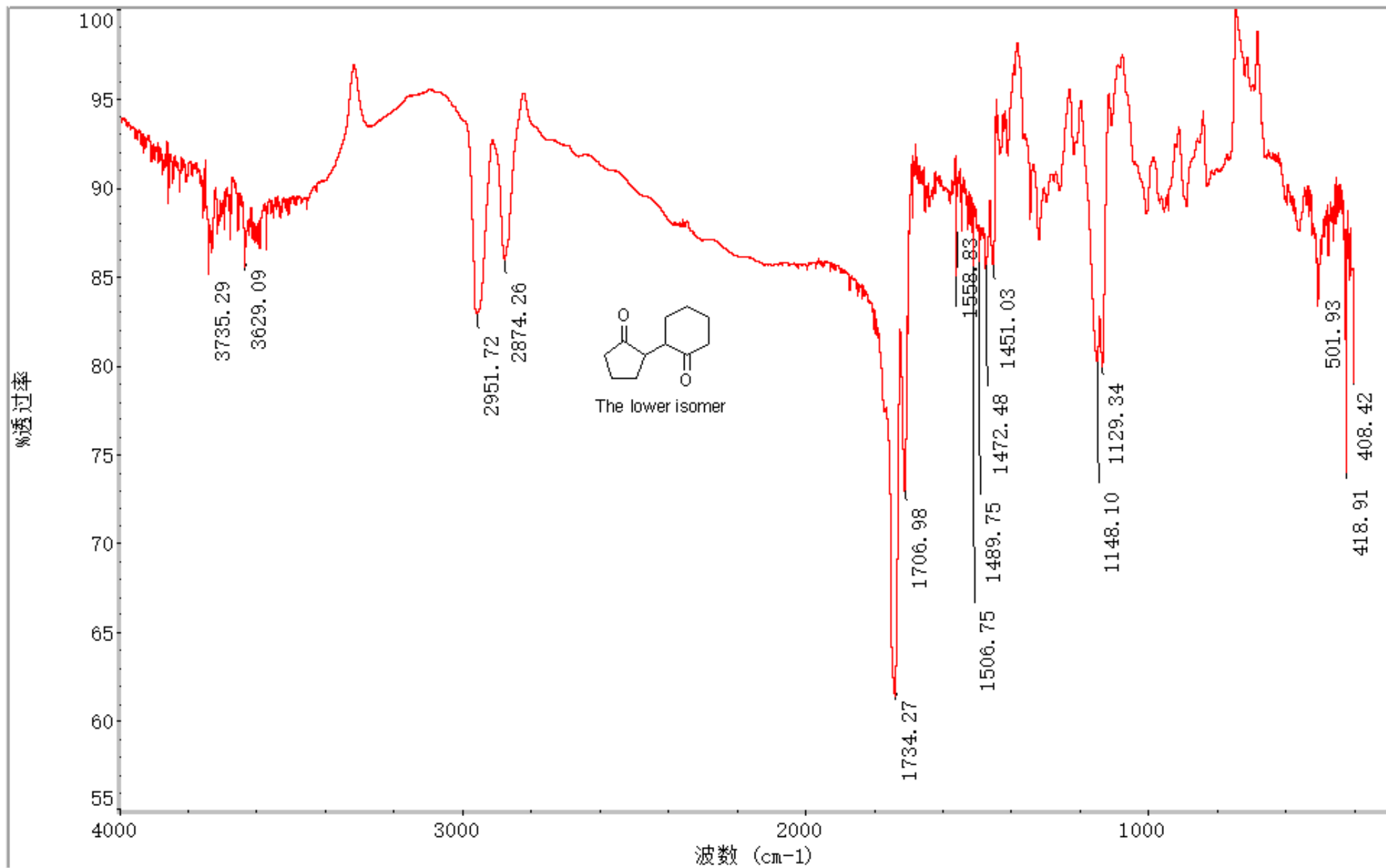
27.14

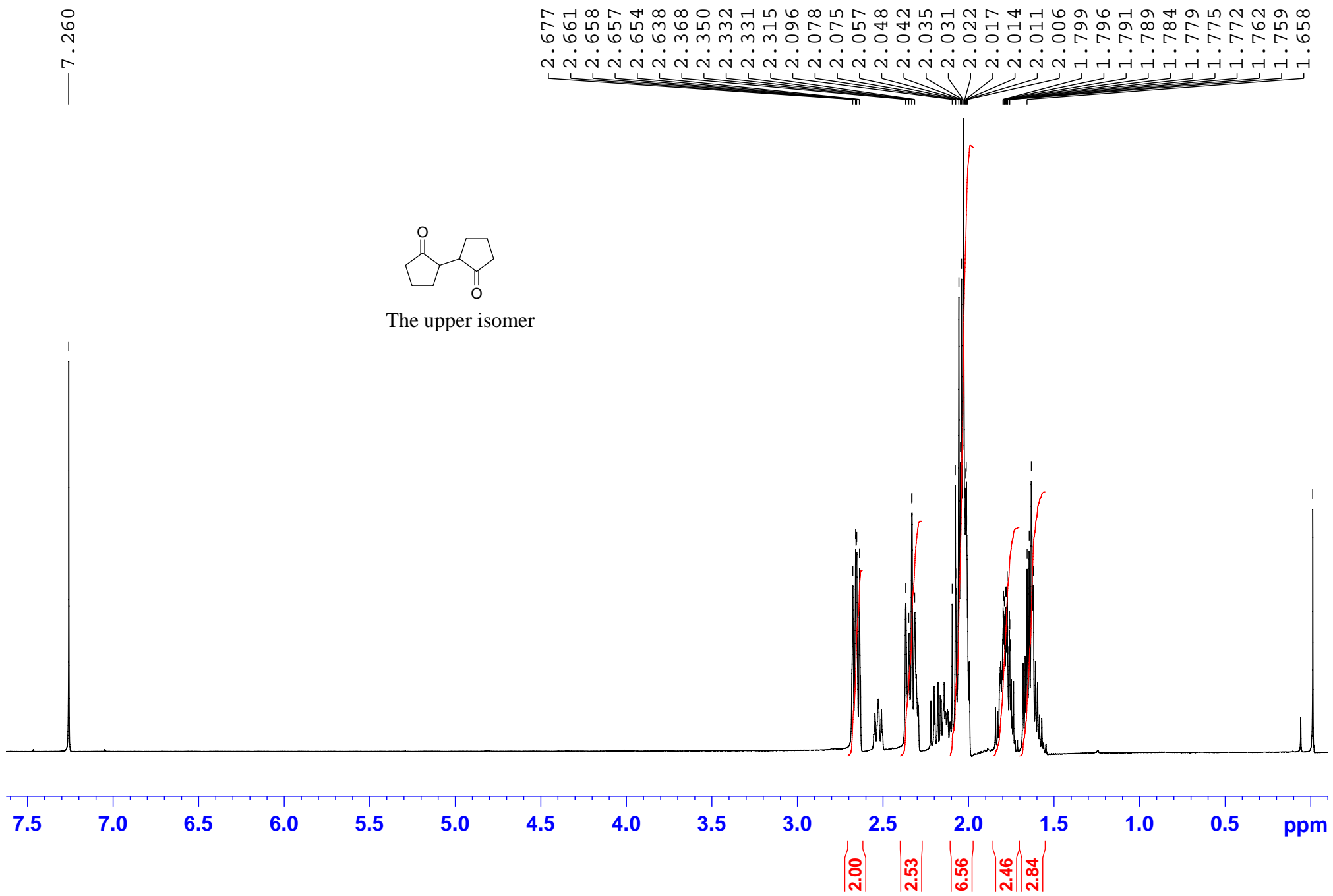
25.49

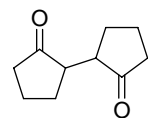
25.26

21.21

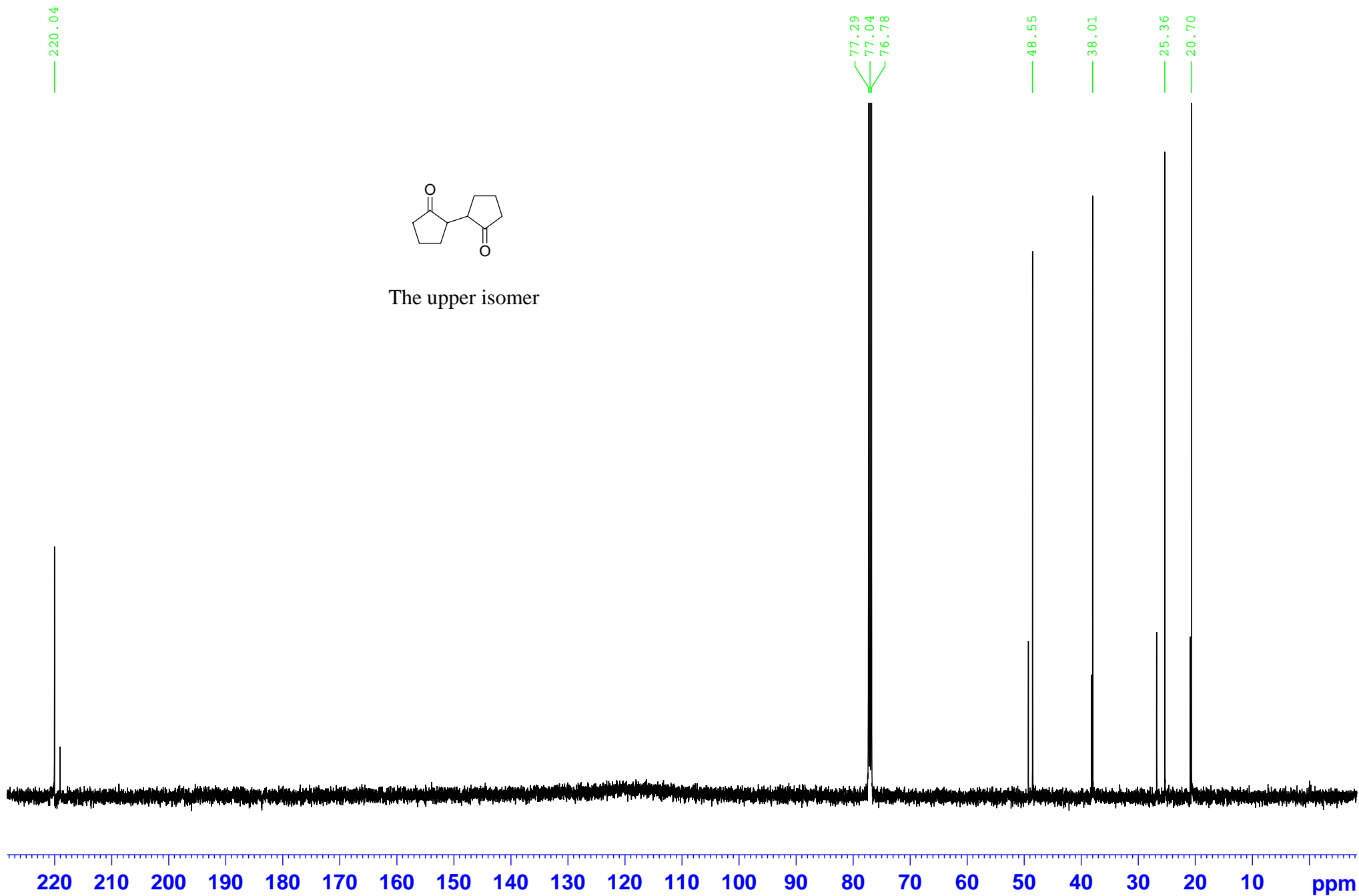


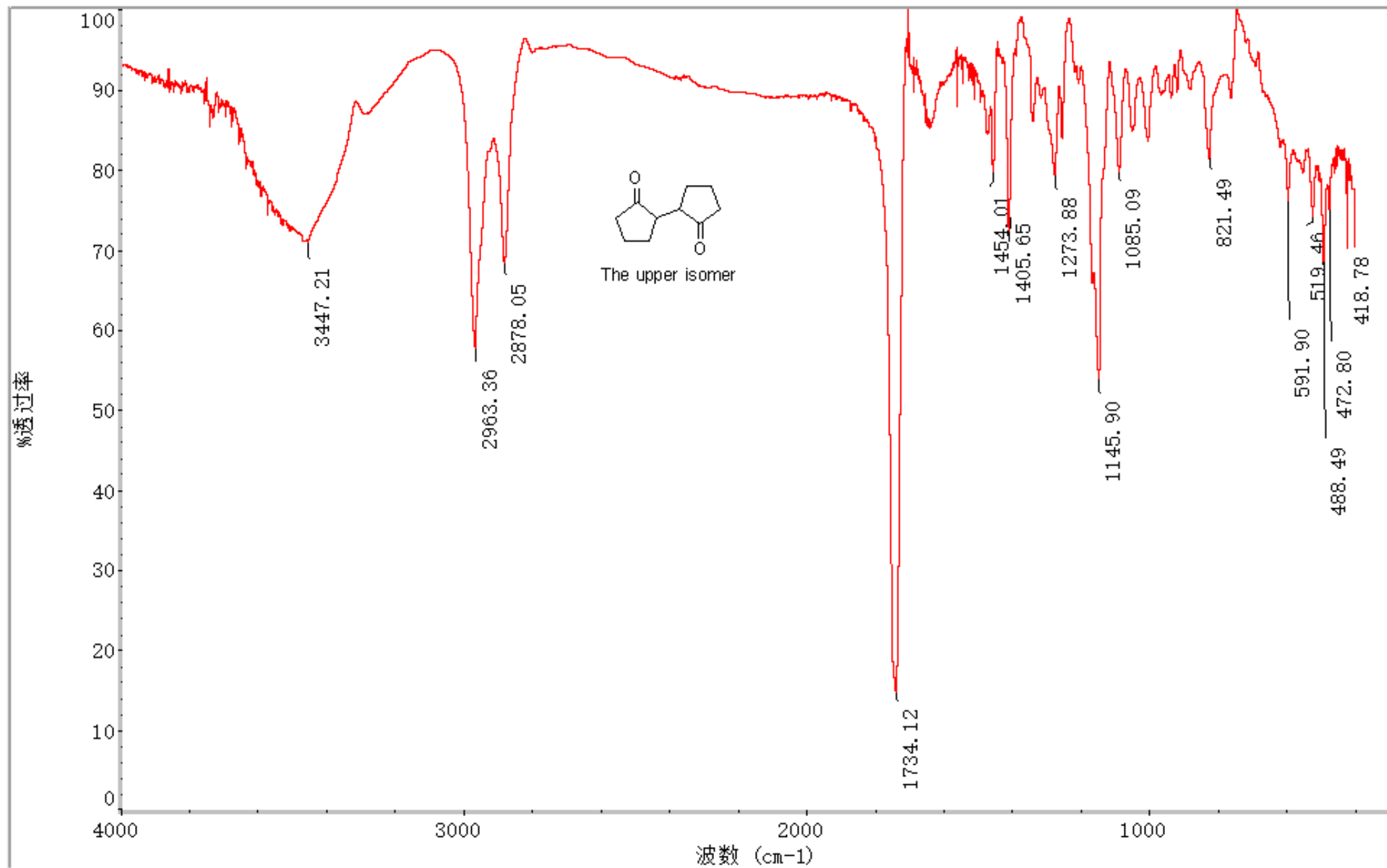


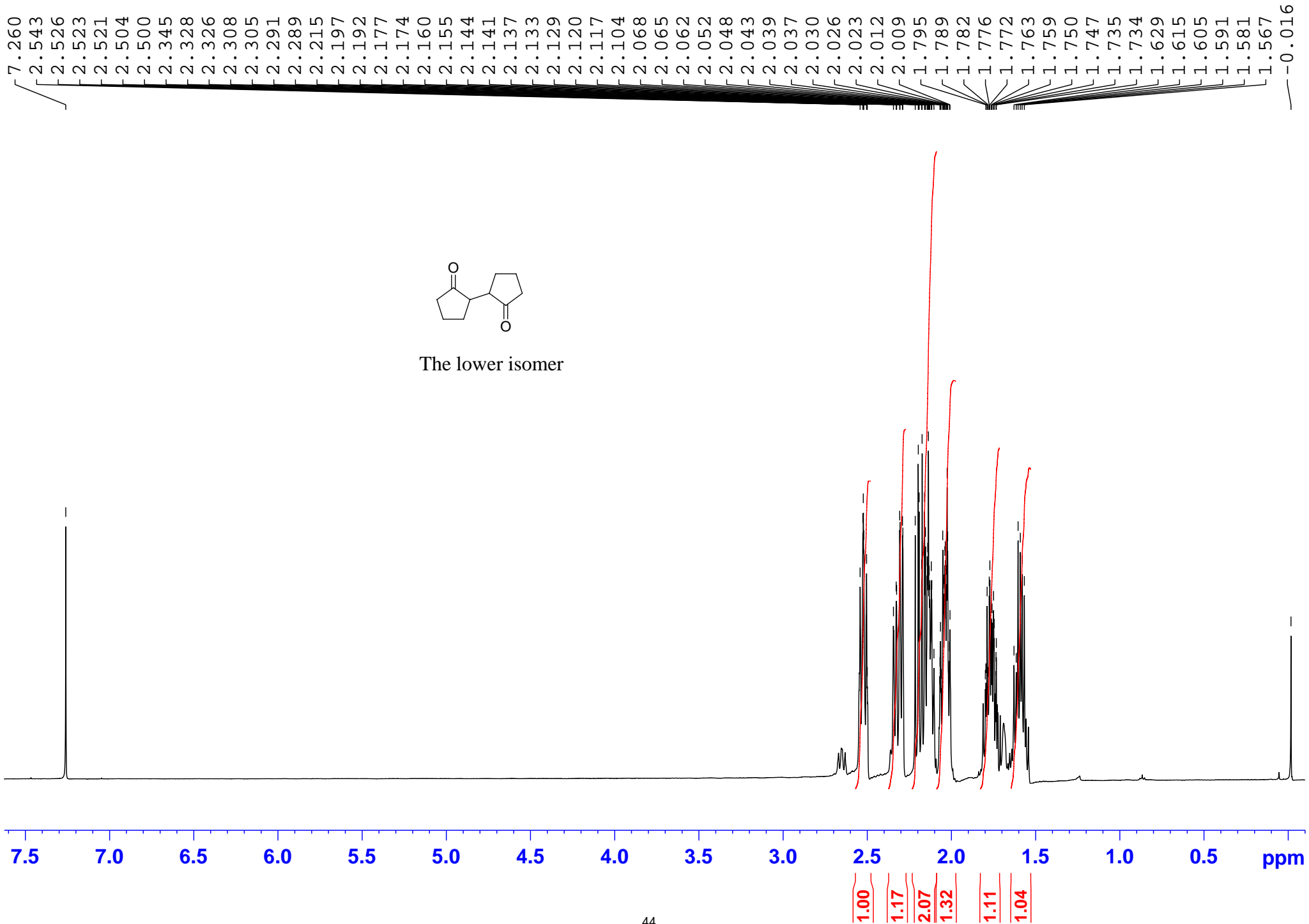




The upper isomer







219.08

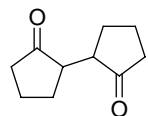
77.31
77.05
76.80

49.28

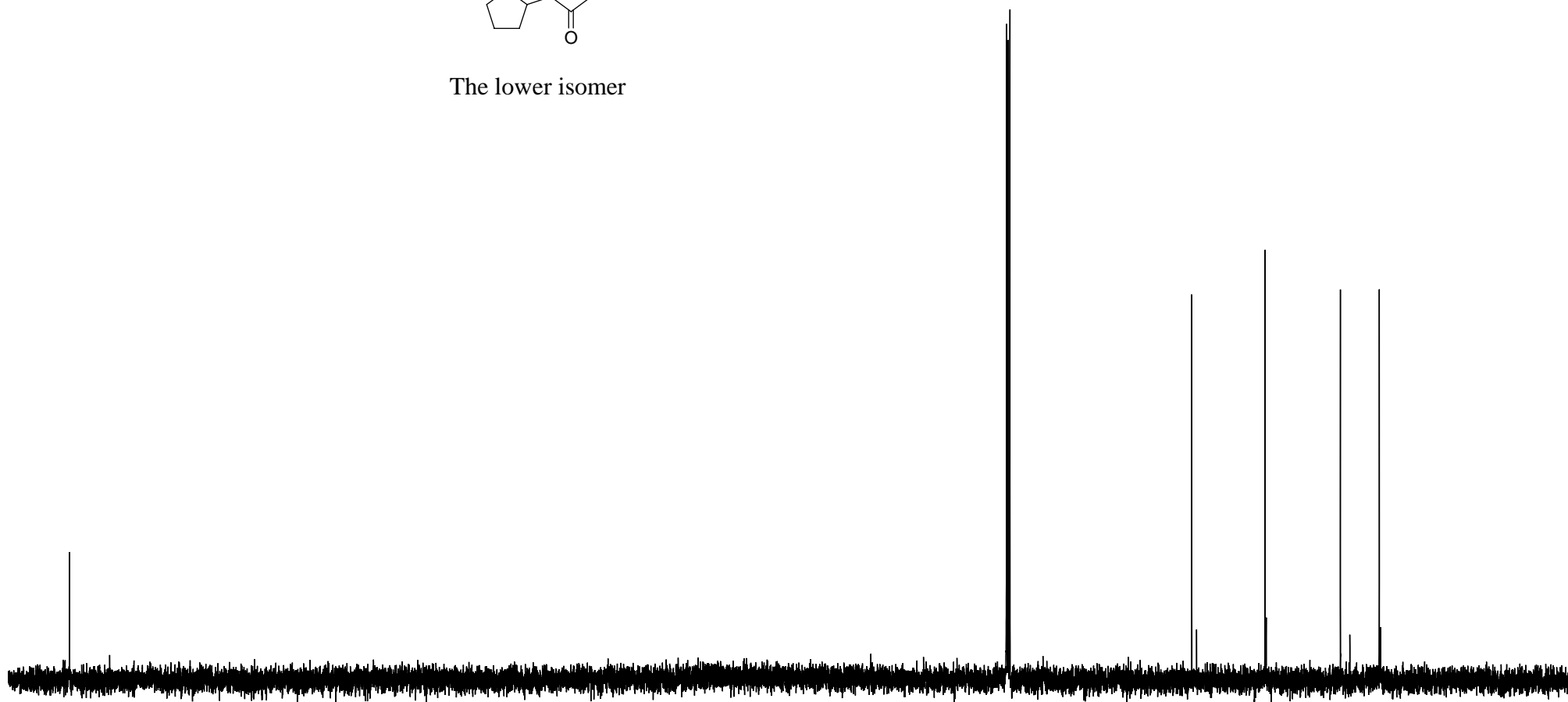
38.20

26.79

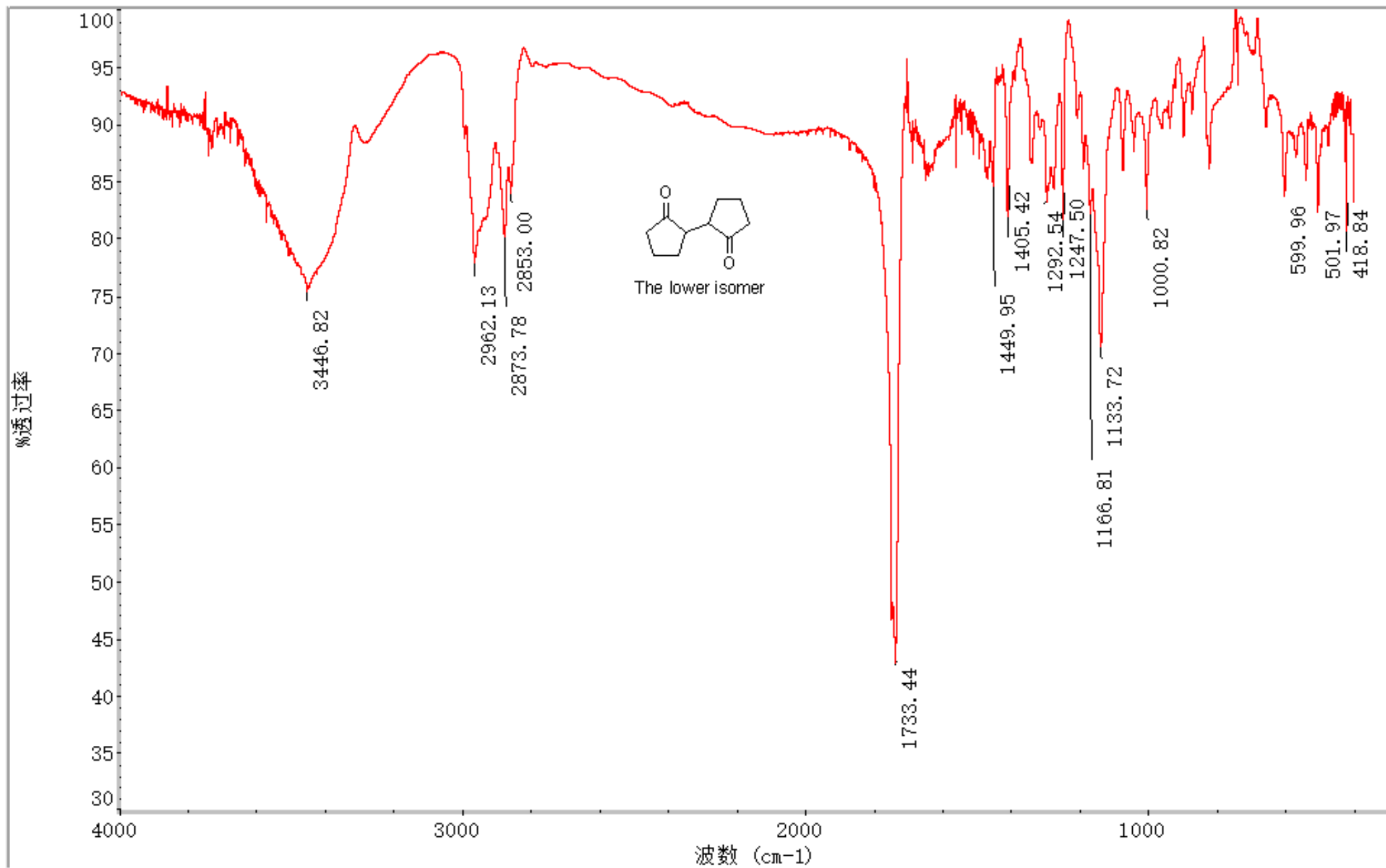
20.90

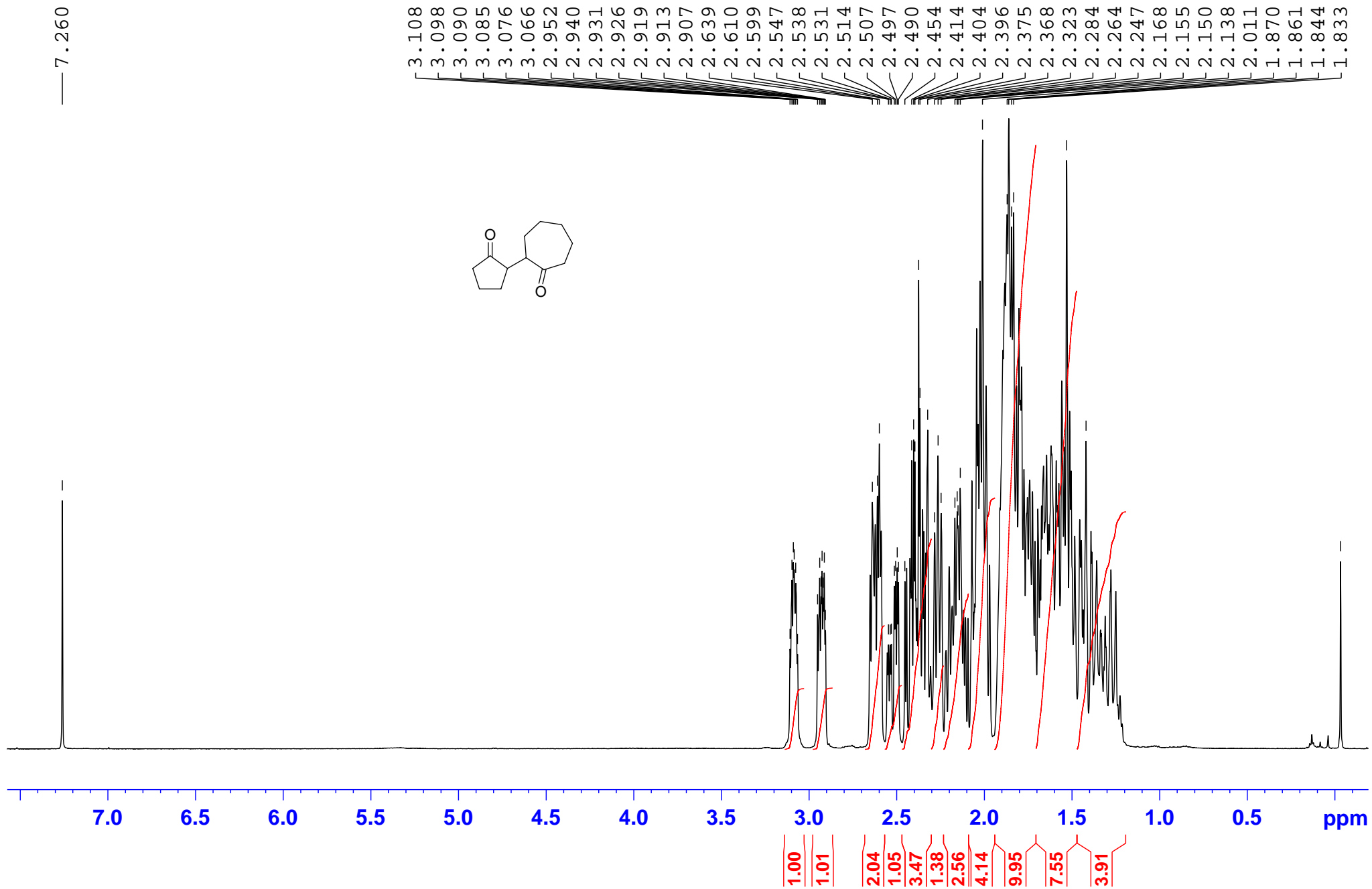


The lower isomer

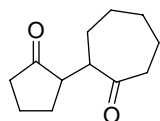


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm





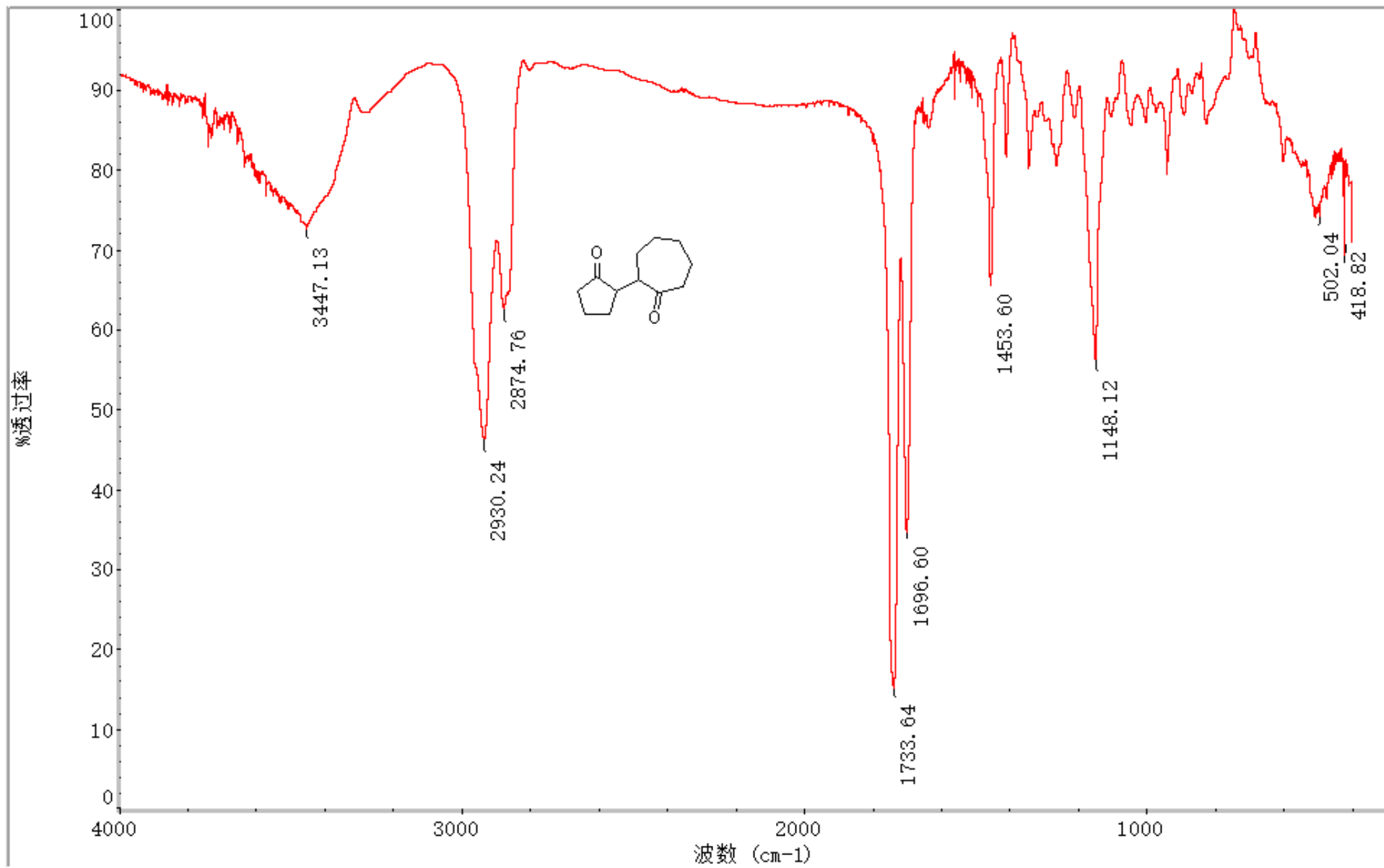
220.06
220.02
214.58
213.75

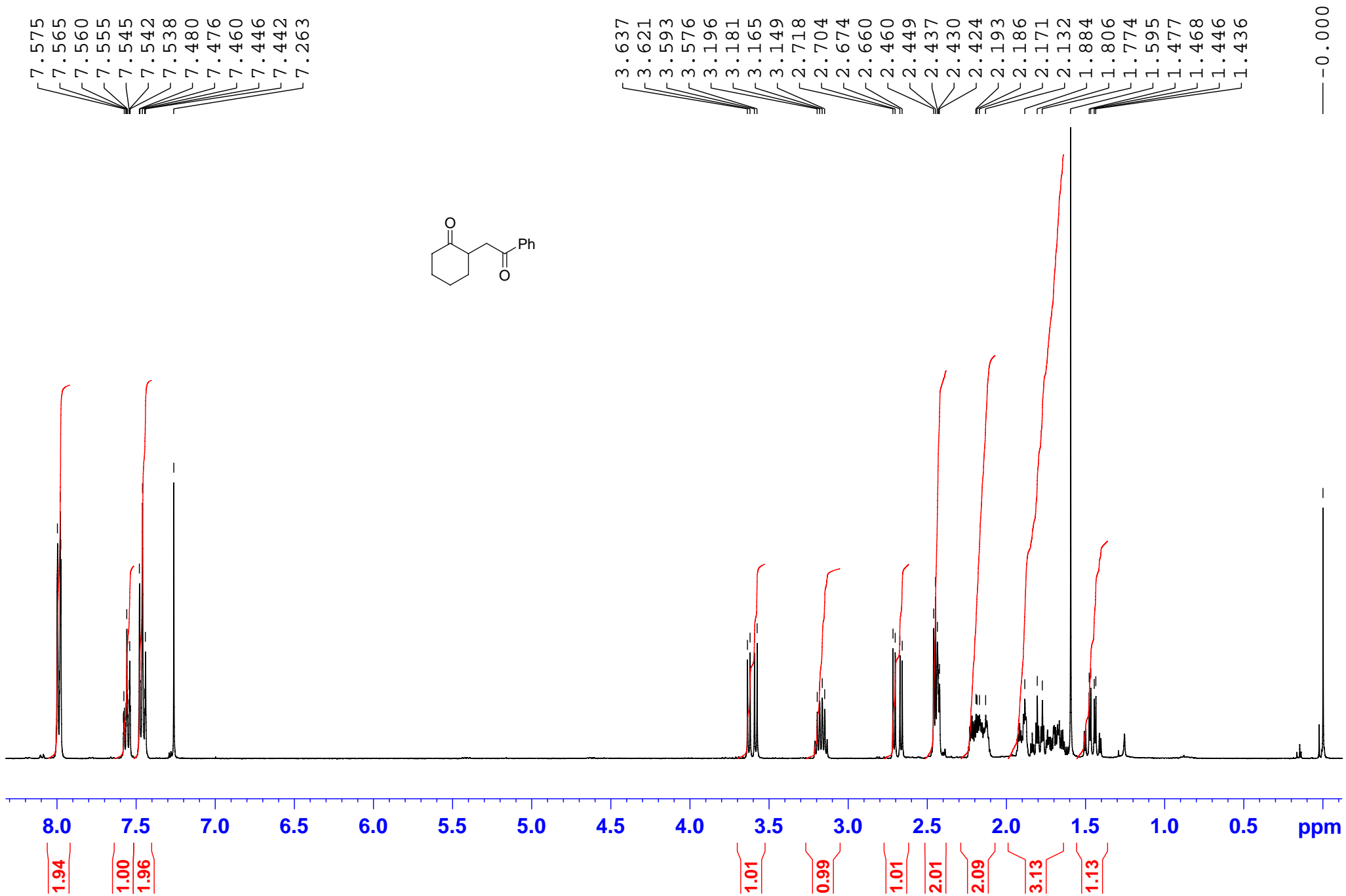


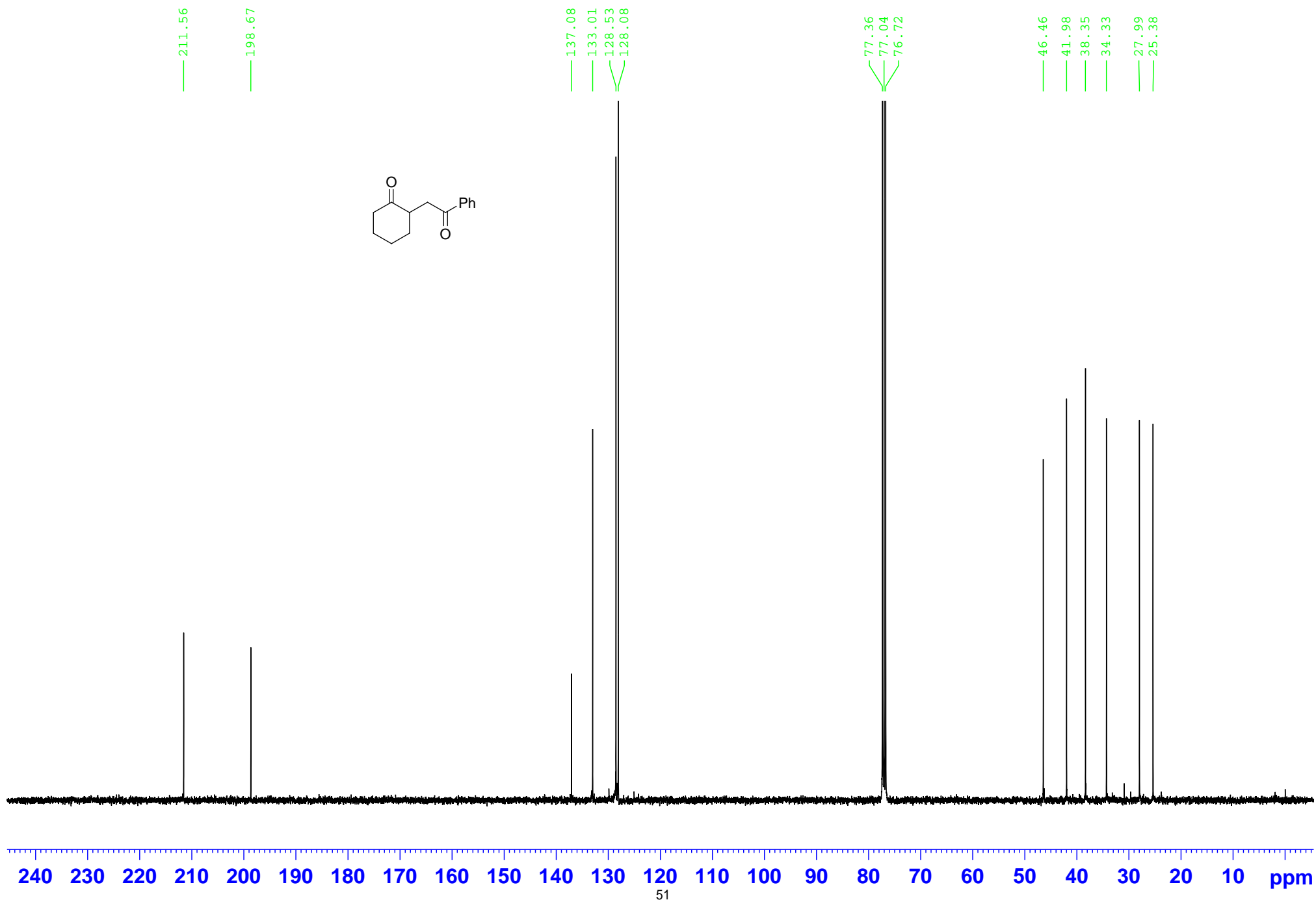
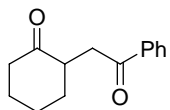
77.39
77.07
76.75

52.47
52.29
51.73
51.28
43.91
43.78
37.99
37.94
30.16
29.84
29.74
29.28
29.17
28.83
26.38
25.71
23.90
23.69
21.04
20.78

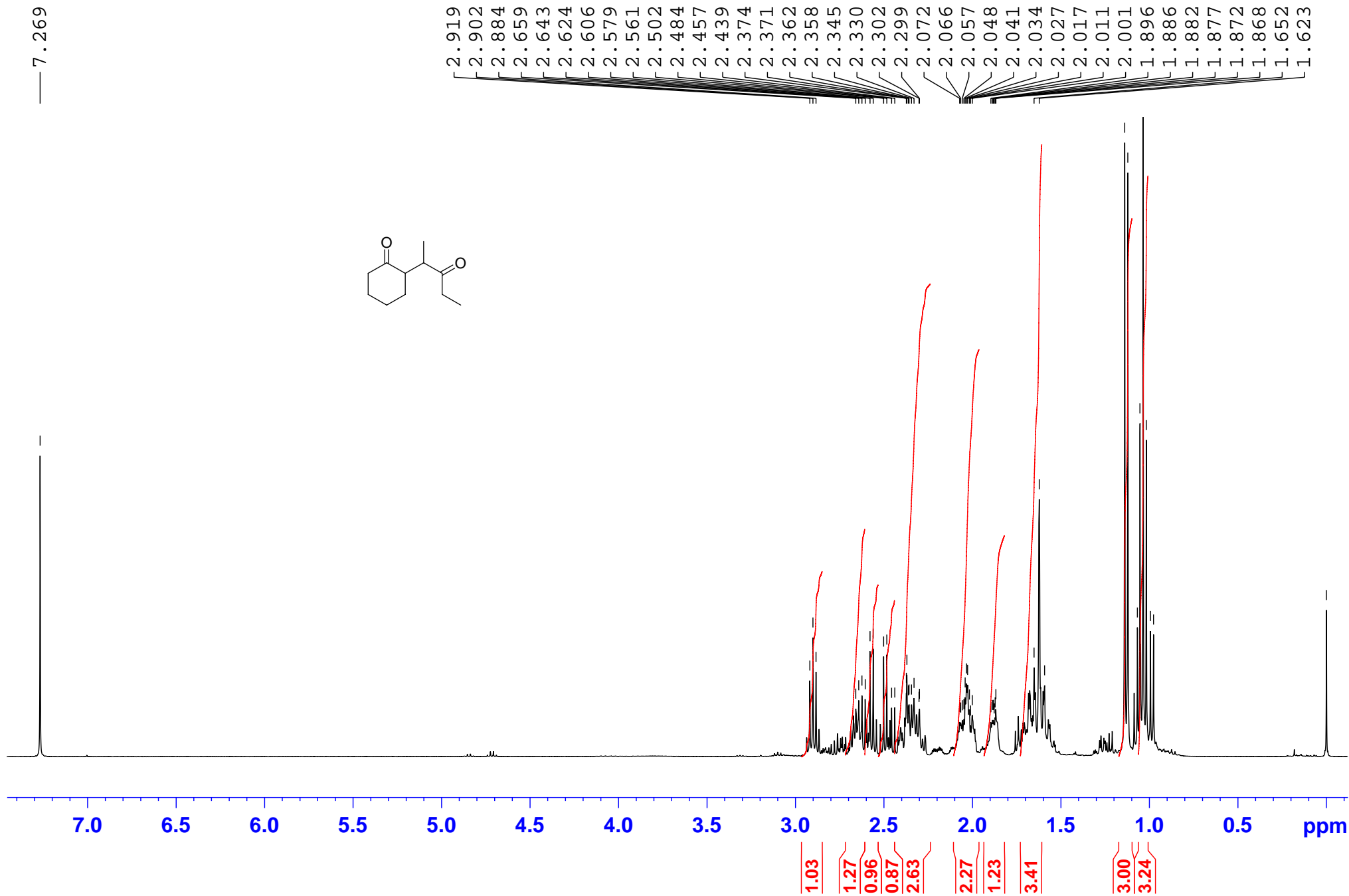
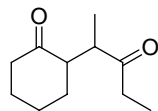








— 7.269



214.43
211.74

77.34
77.02
76.71

53.82

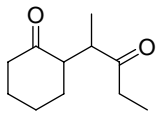
44.88
42.28

35.41
30.88

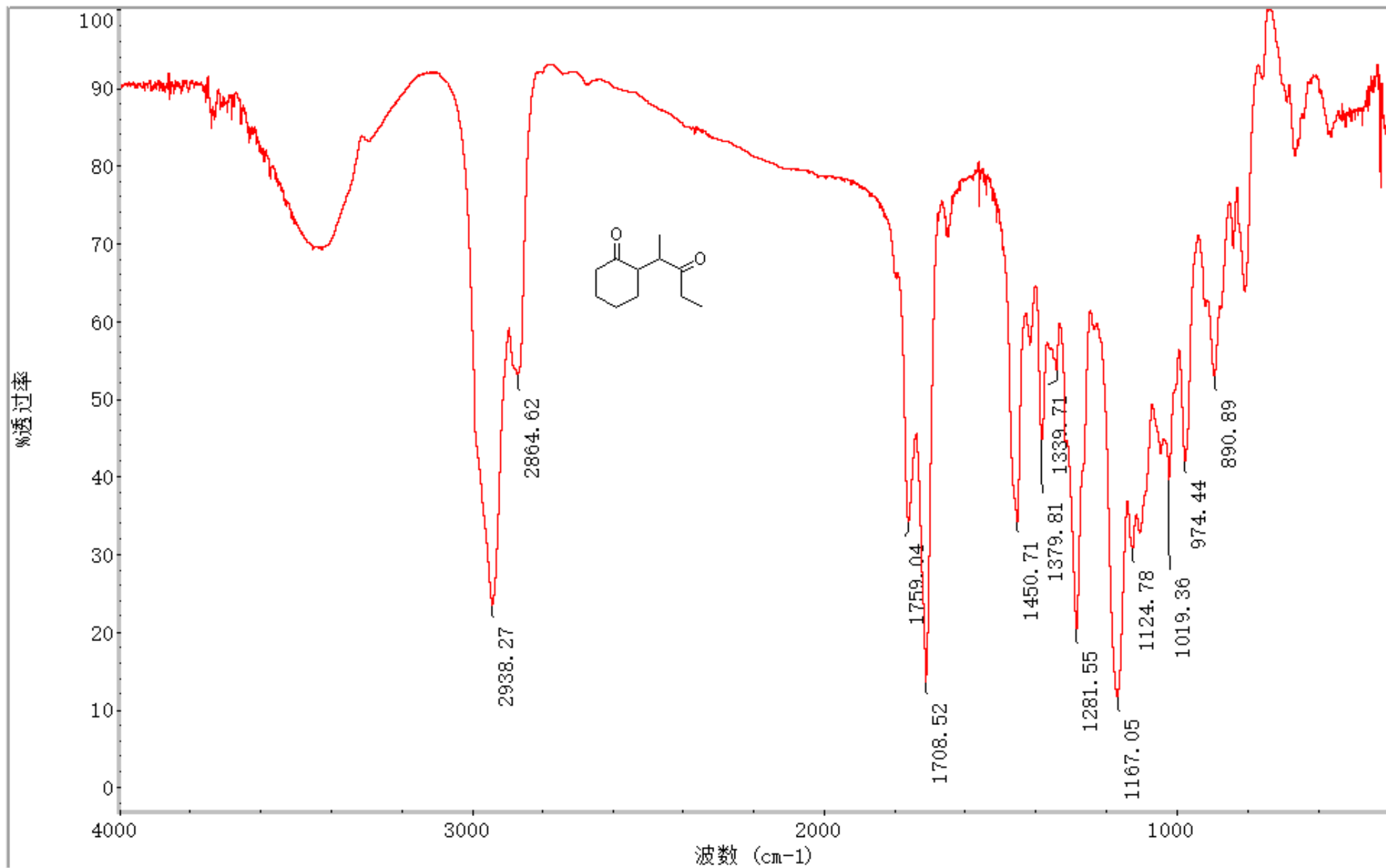
27.70
25.14

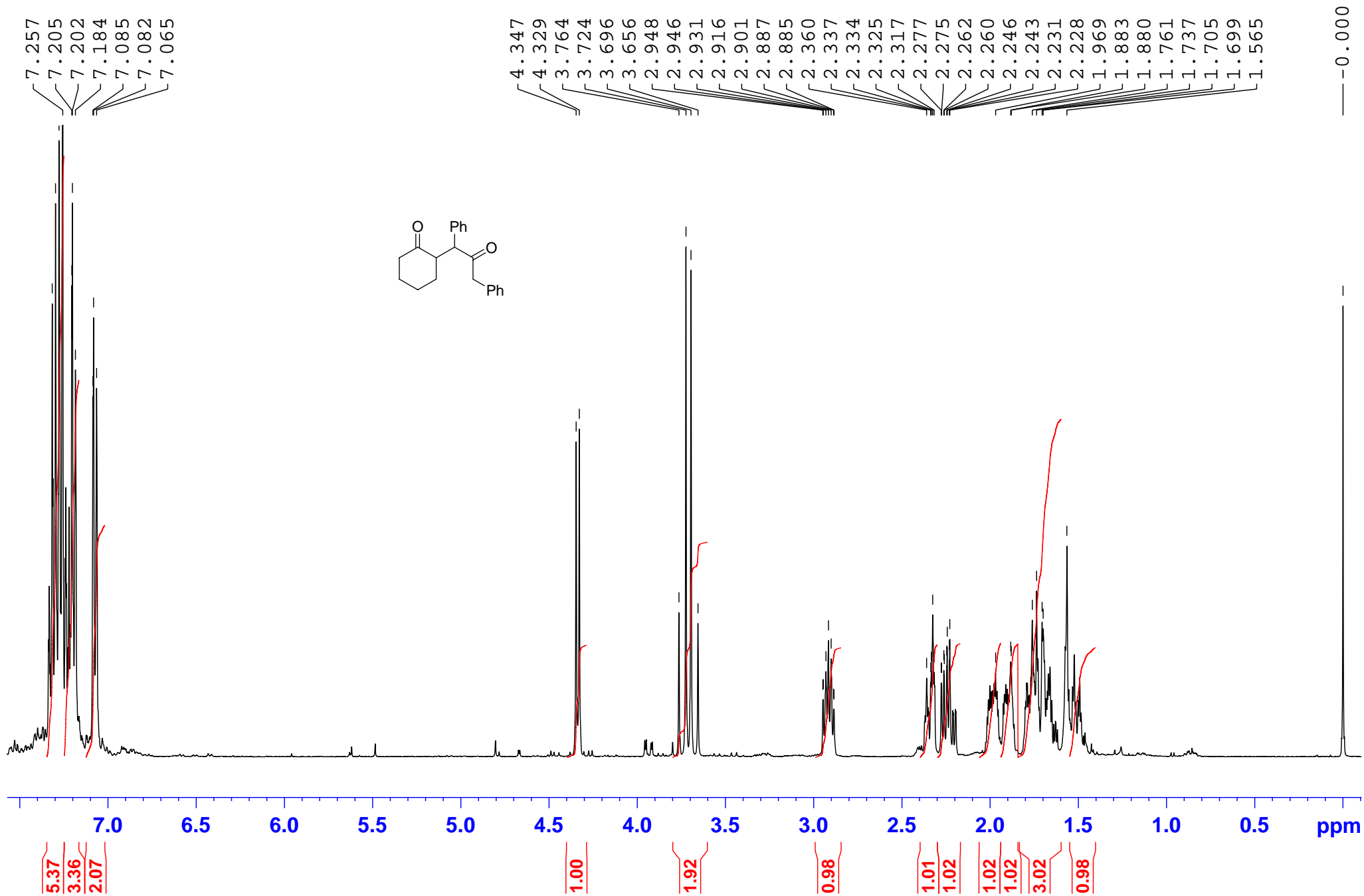
14.81

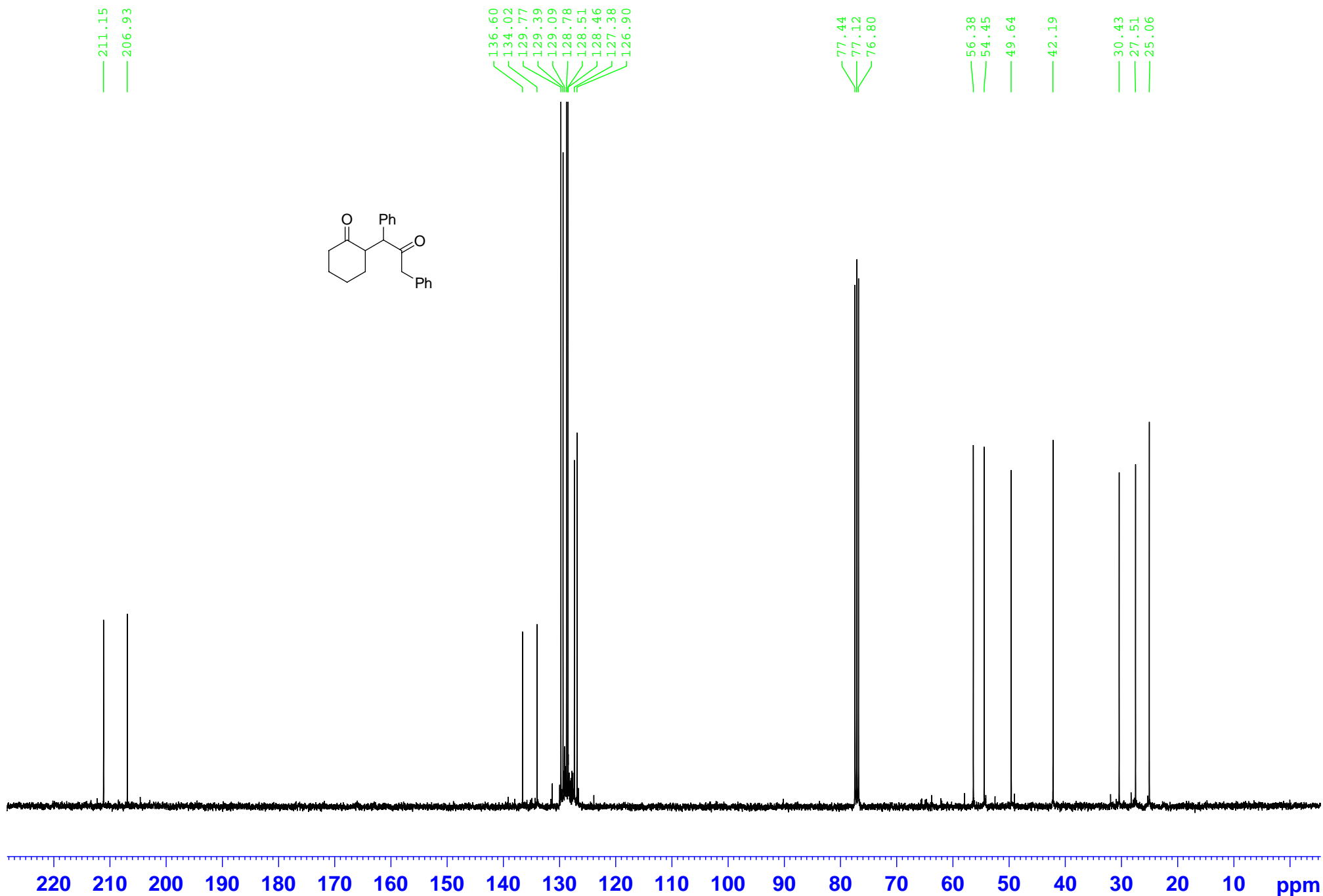
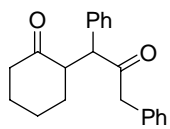
7.59

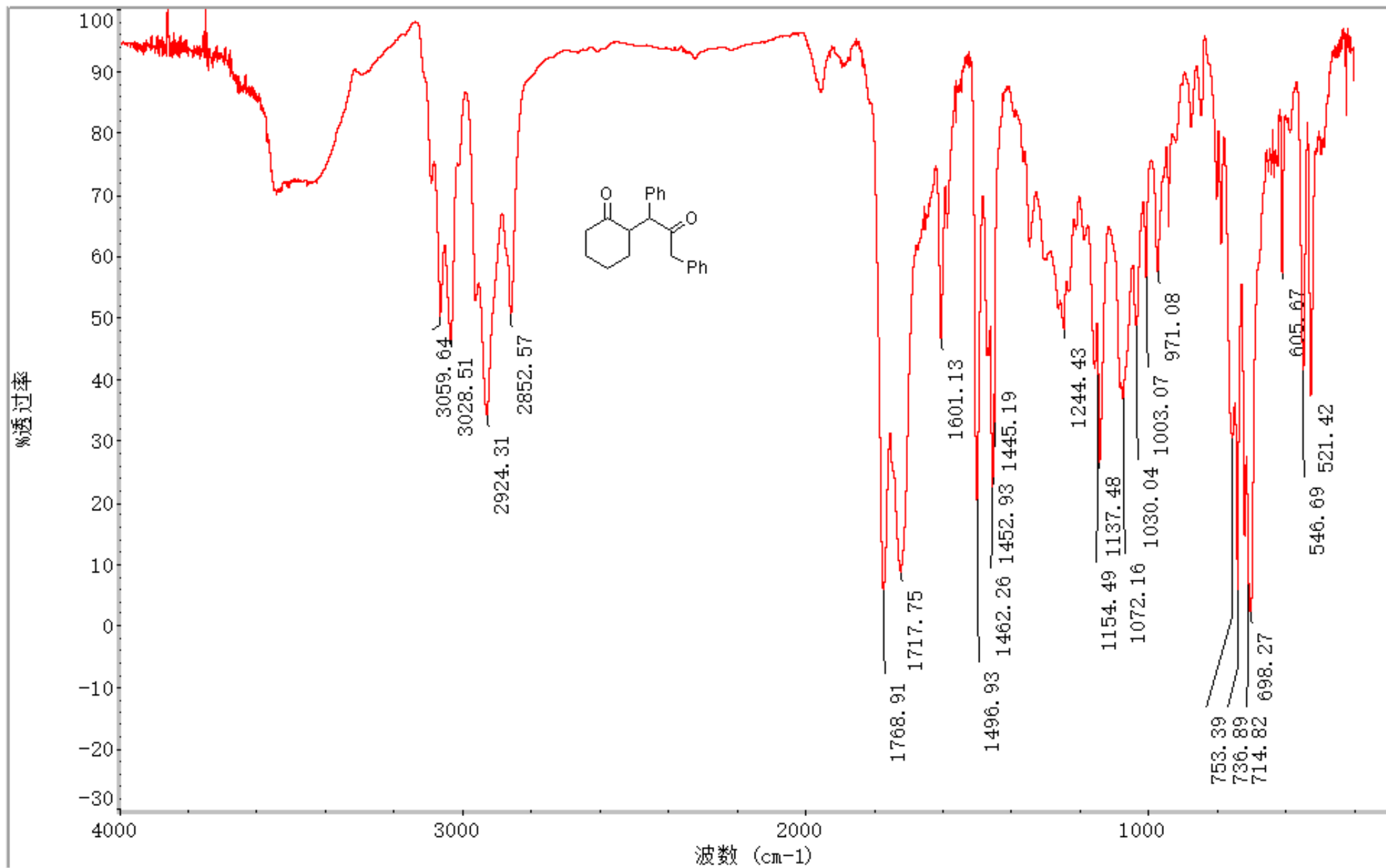


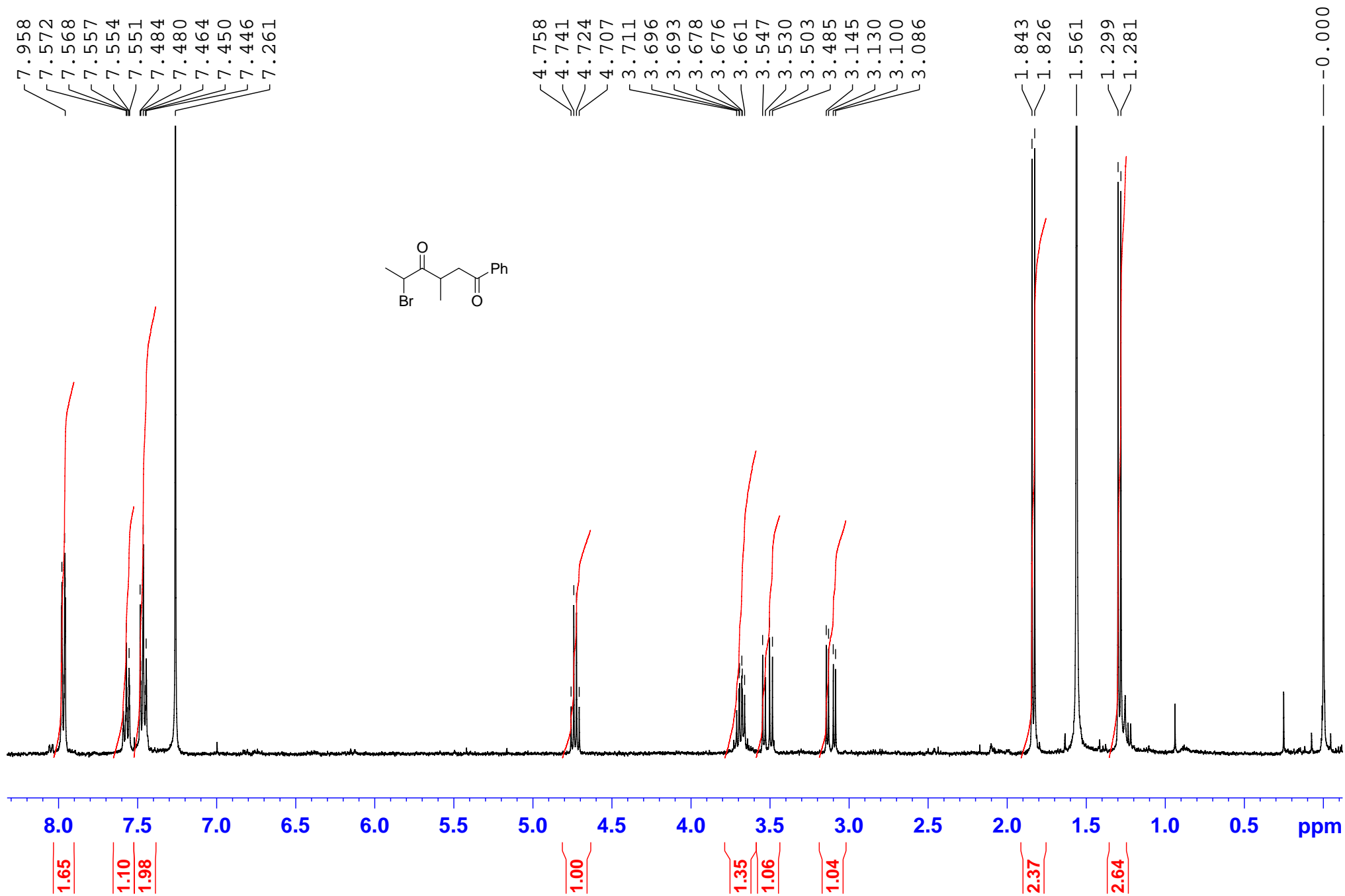
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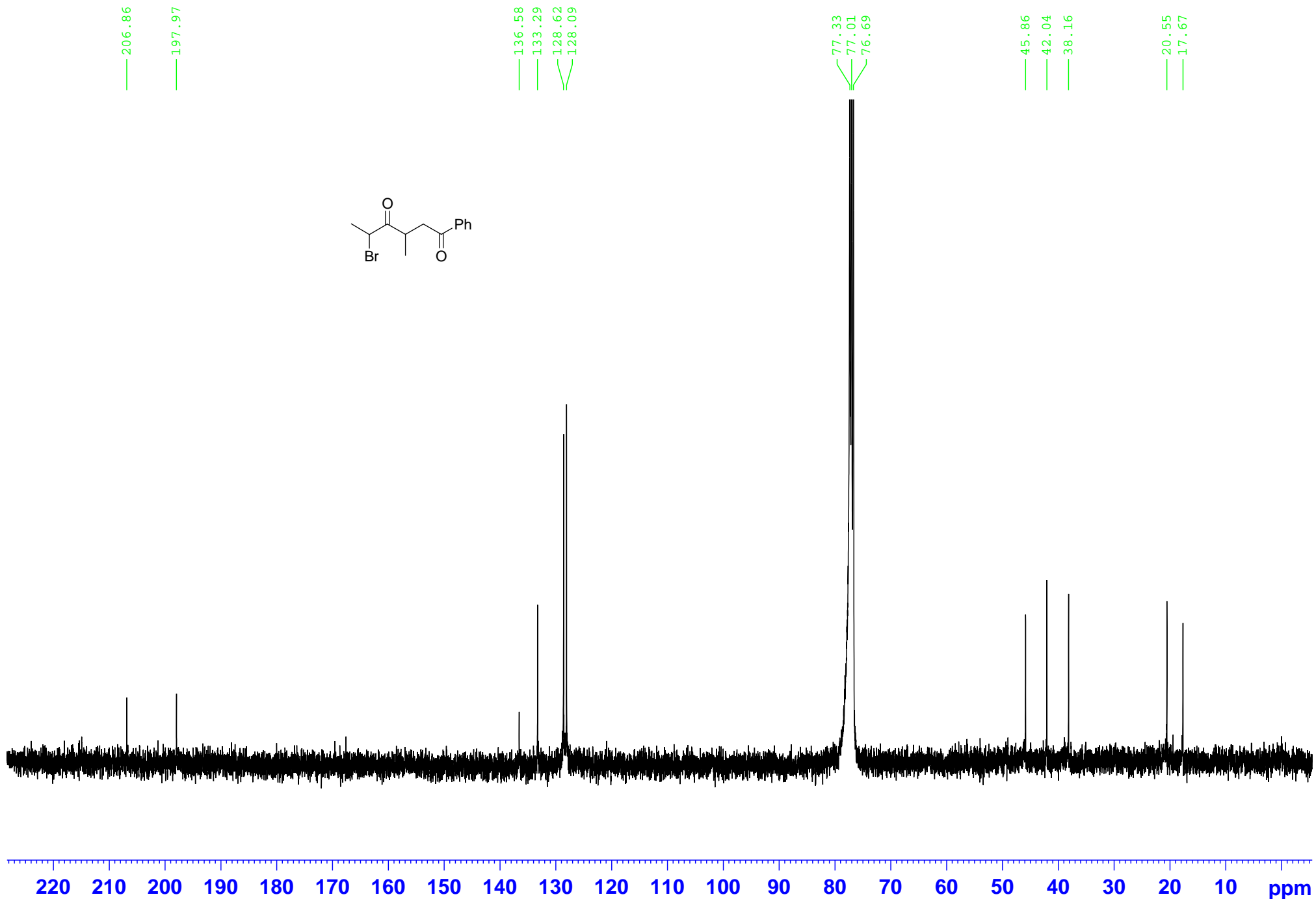
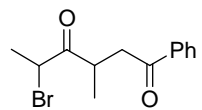


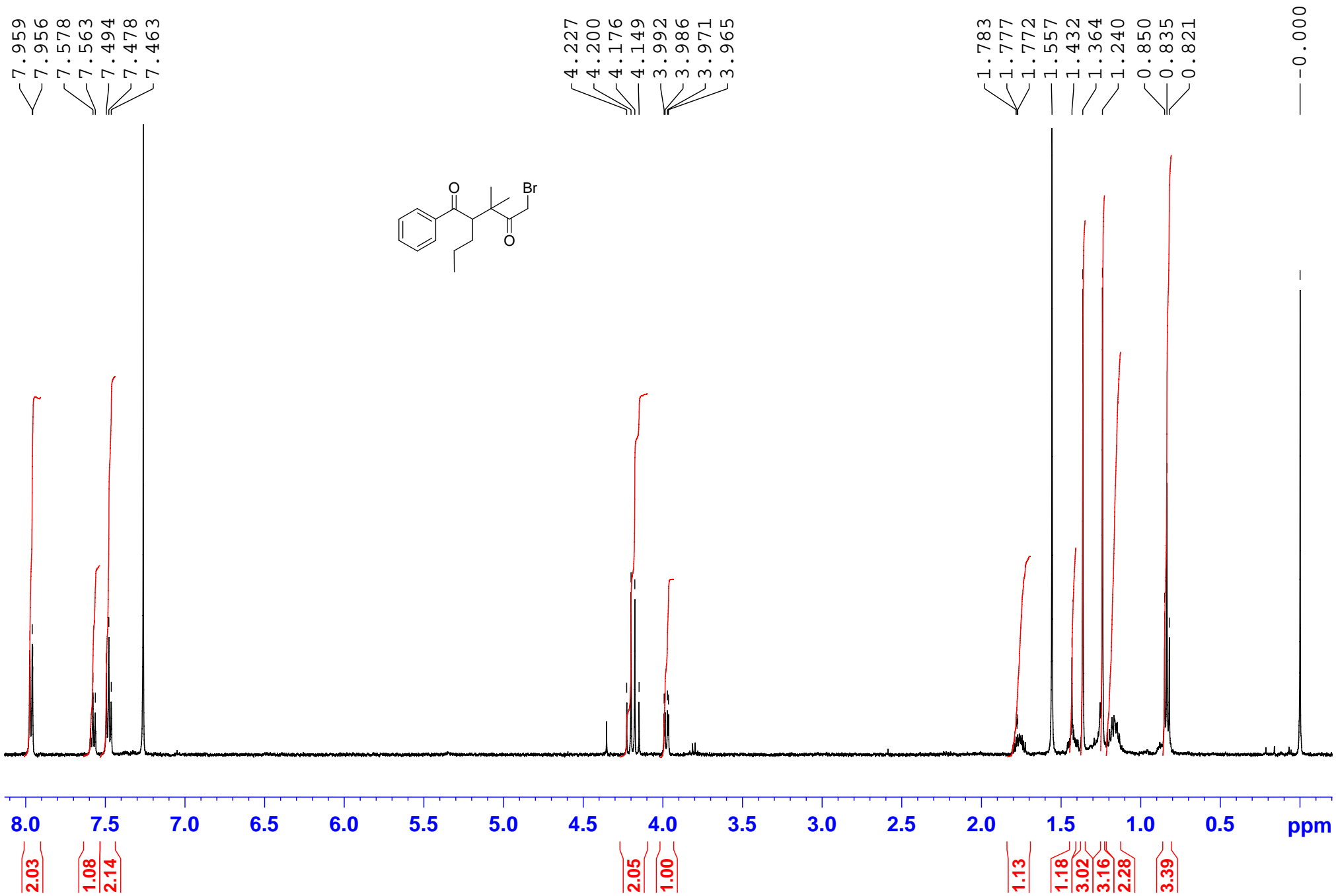












205.50
204.63

139.08
133.24
128.75
128.33

77.28
77.02
76.77

51.57
50.37

32.91
31.92
24.31
22.35
21.90
14.29

