

Electronic Supplementary Information for

The α -alkylation of ketones with alcohols in pure water catalyzed by a water-soluble Cp*Ir complex bearing a functional ligand

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^b State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian 116024, P. R. China

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Copies of ¹H NMR and ¹³C NMR spectra of products

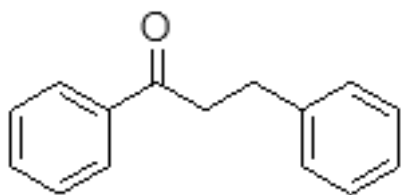
S2-S62

1,3-diphenylpropan-1-one
 e Proton CDCl₃

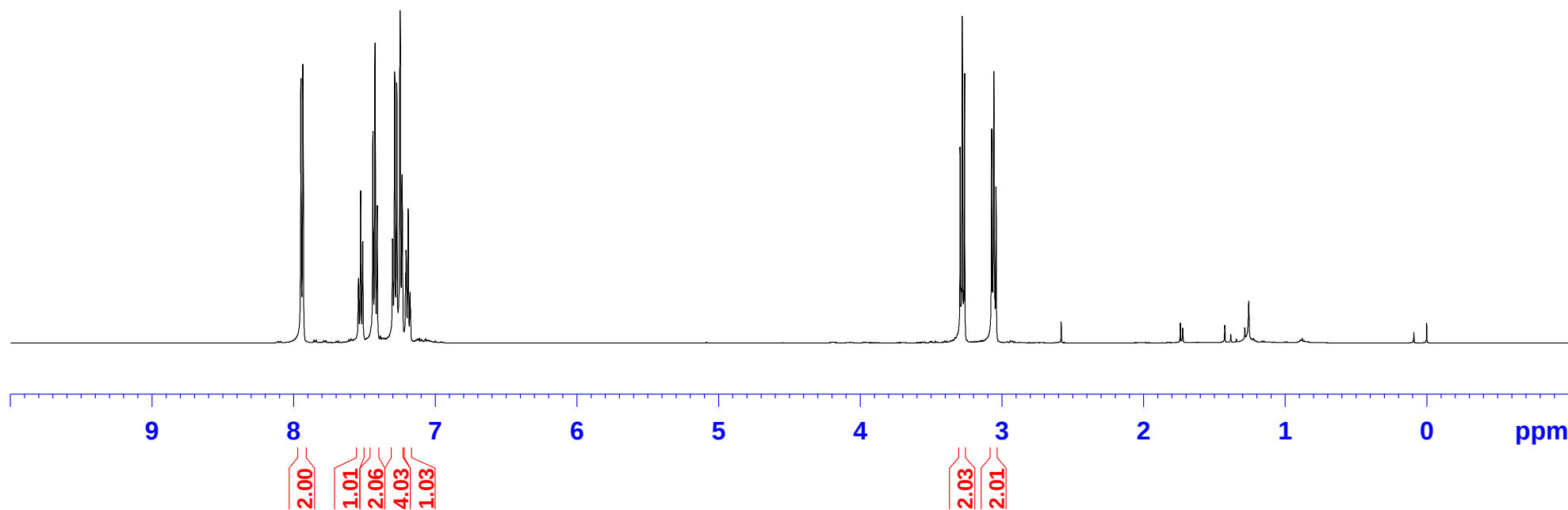
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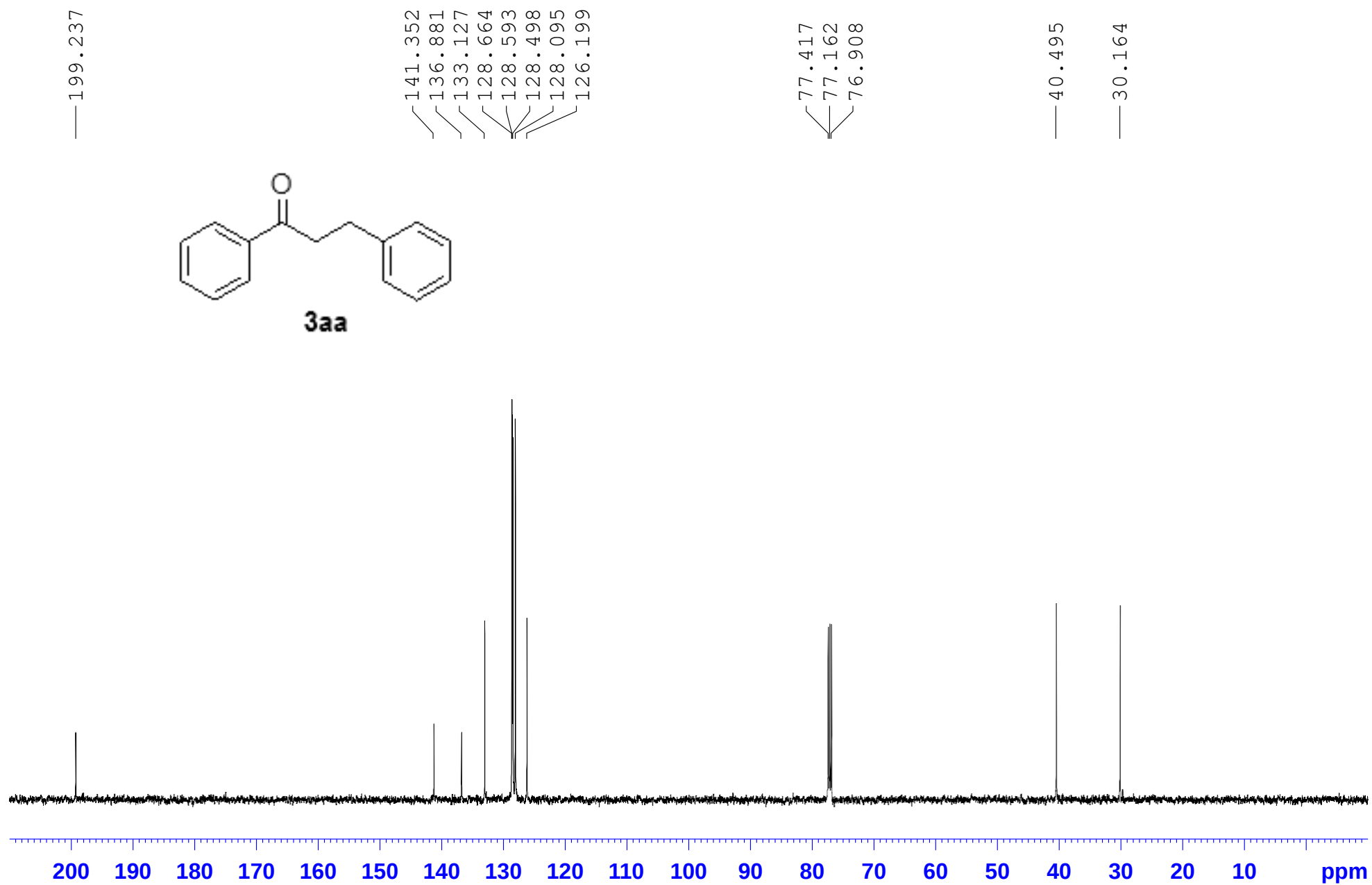
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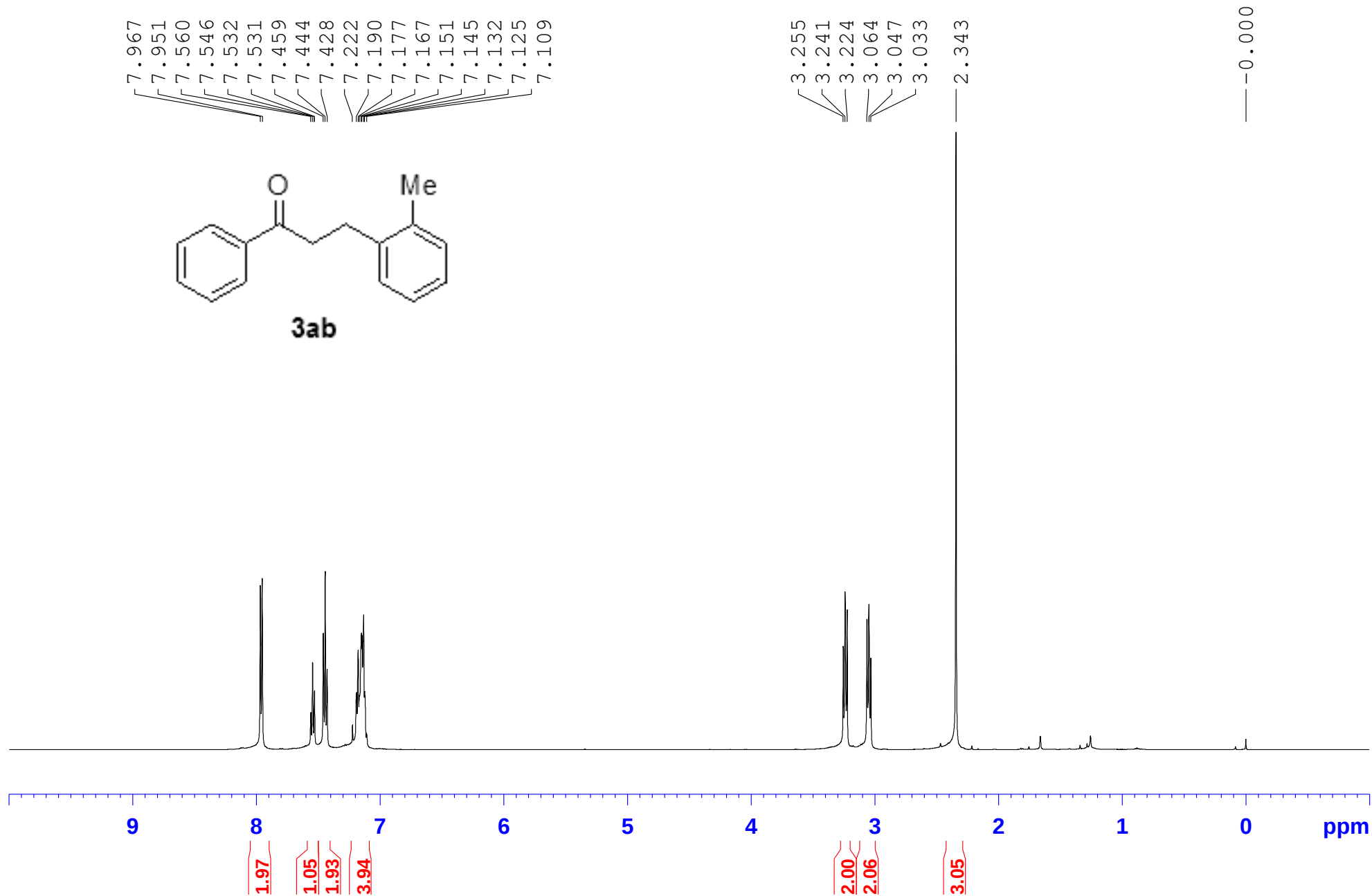
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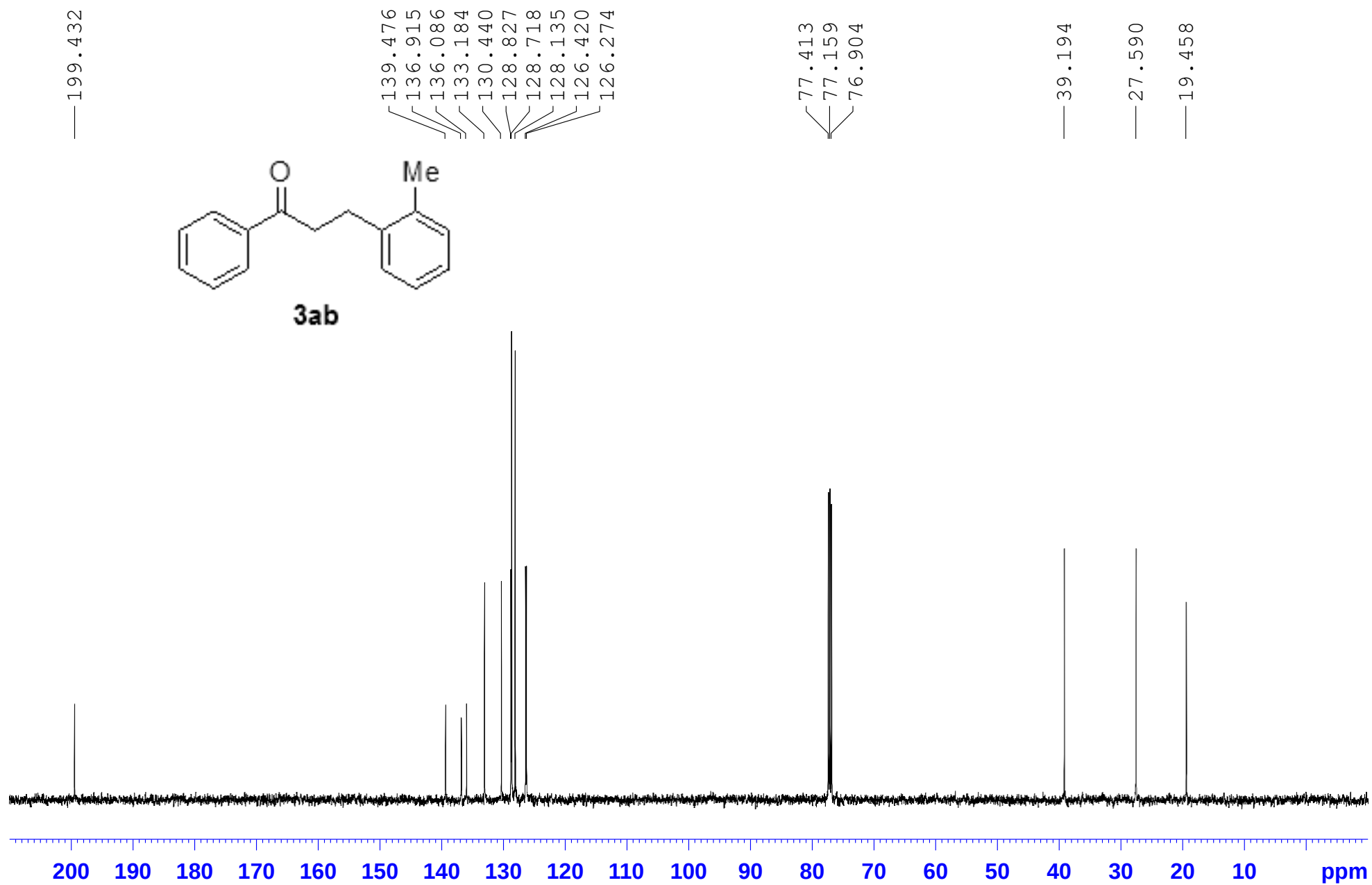
1,3-diphenylpropan-1-one
e C13CPD CDC13



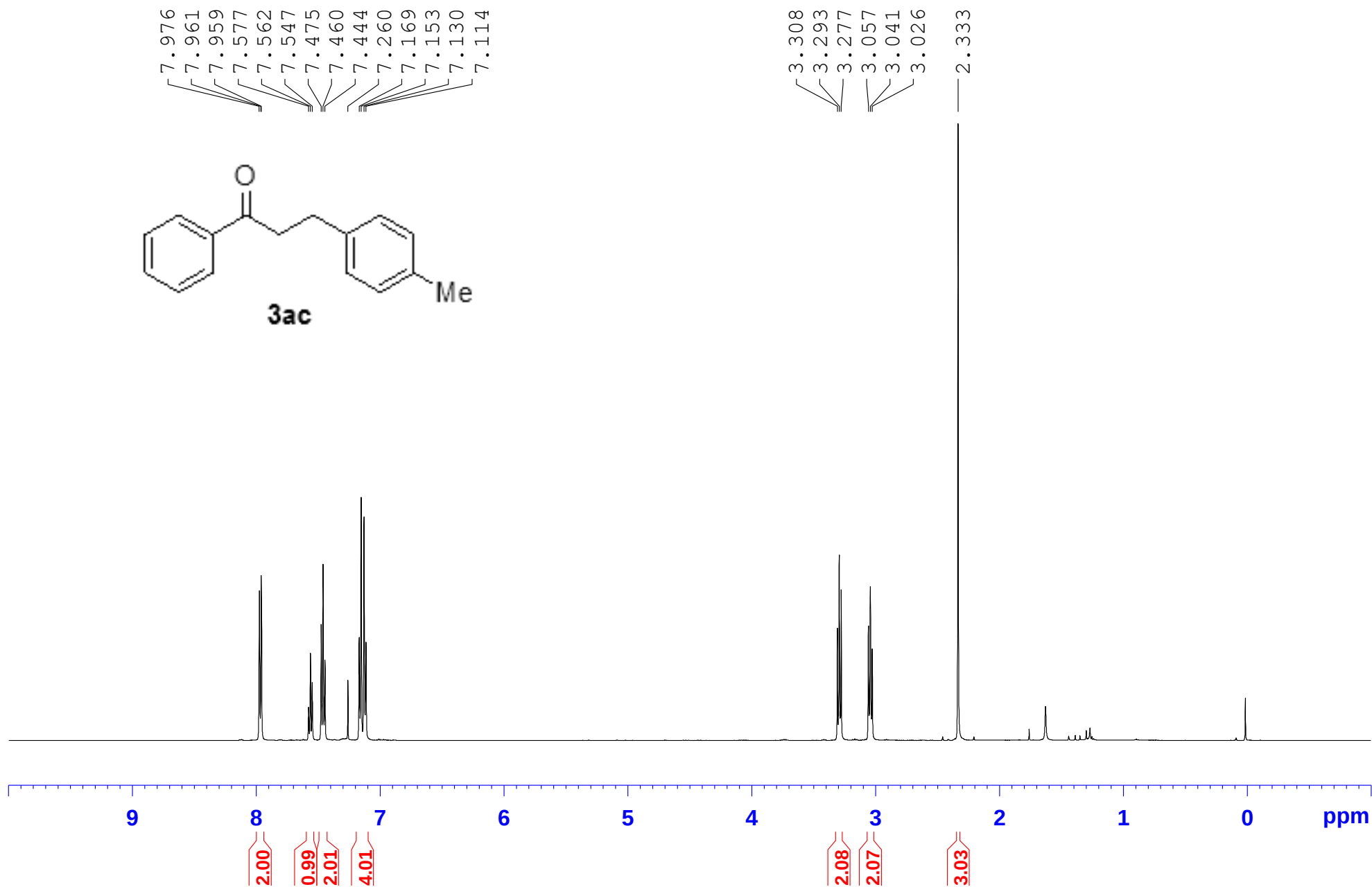
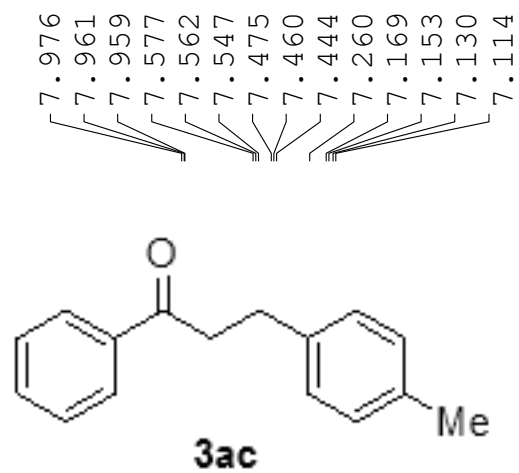
1-phenyl-3-(o-tolyl)propan-1-one
e Proton CDCl₃



1-phenyl-3-(o-tolyl)propan-1-on
e C13CPD CDC13



1-phenyl-3-p-tolylpropan-1-on
e Proton CDCl₃



1-phenyl-3-p-tolylpropan-1-on
e C13CPD CDC13

— 199.471

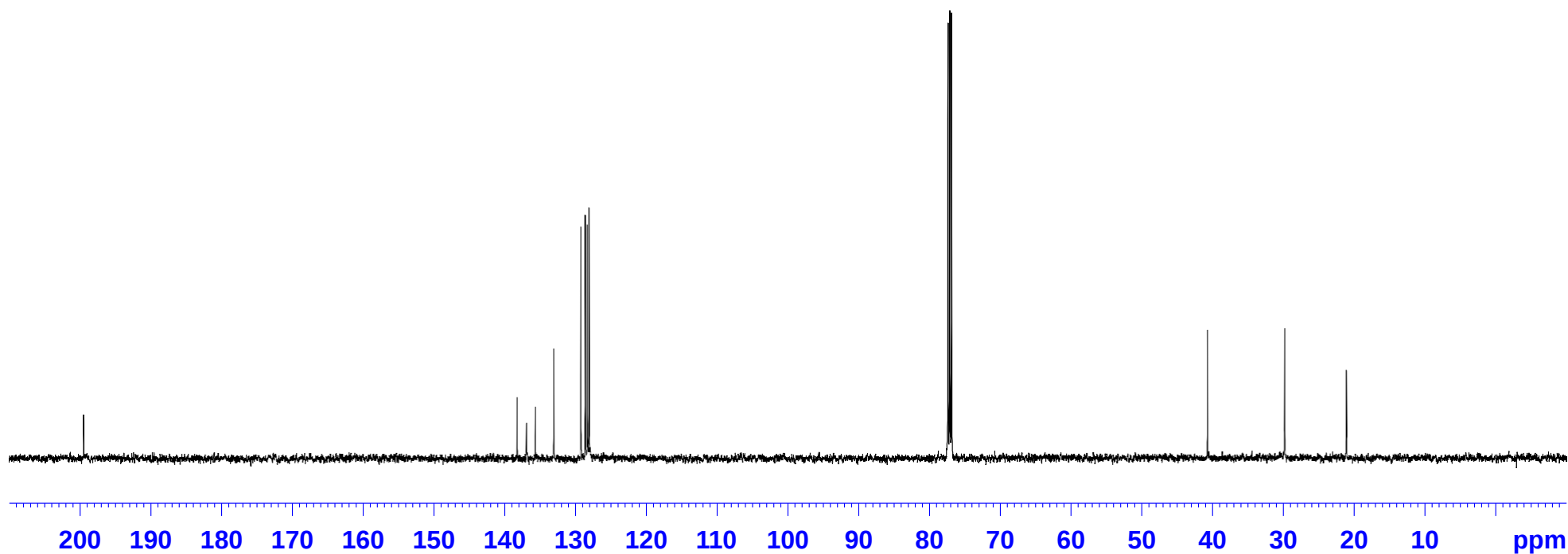
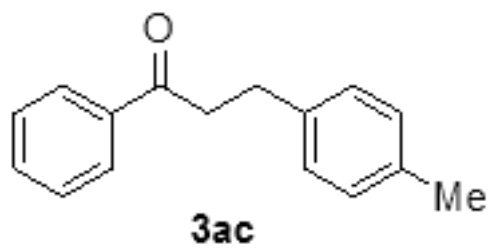
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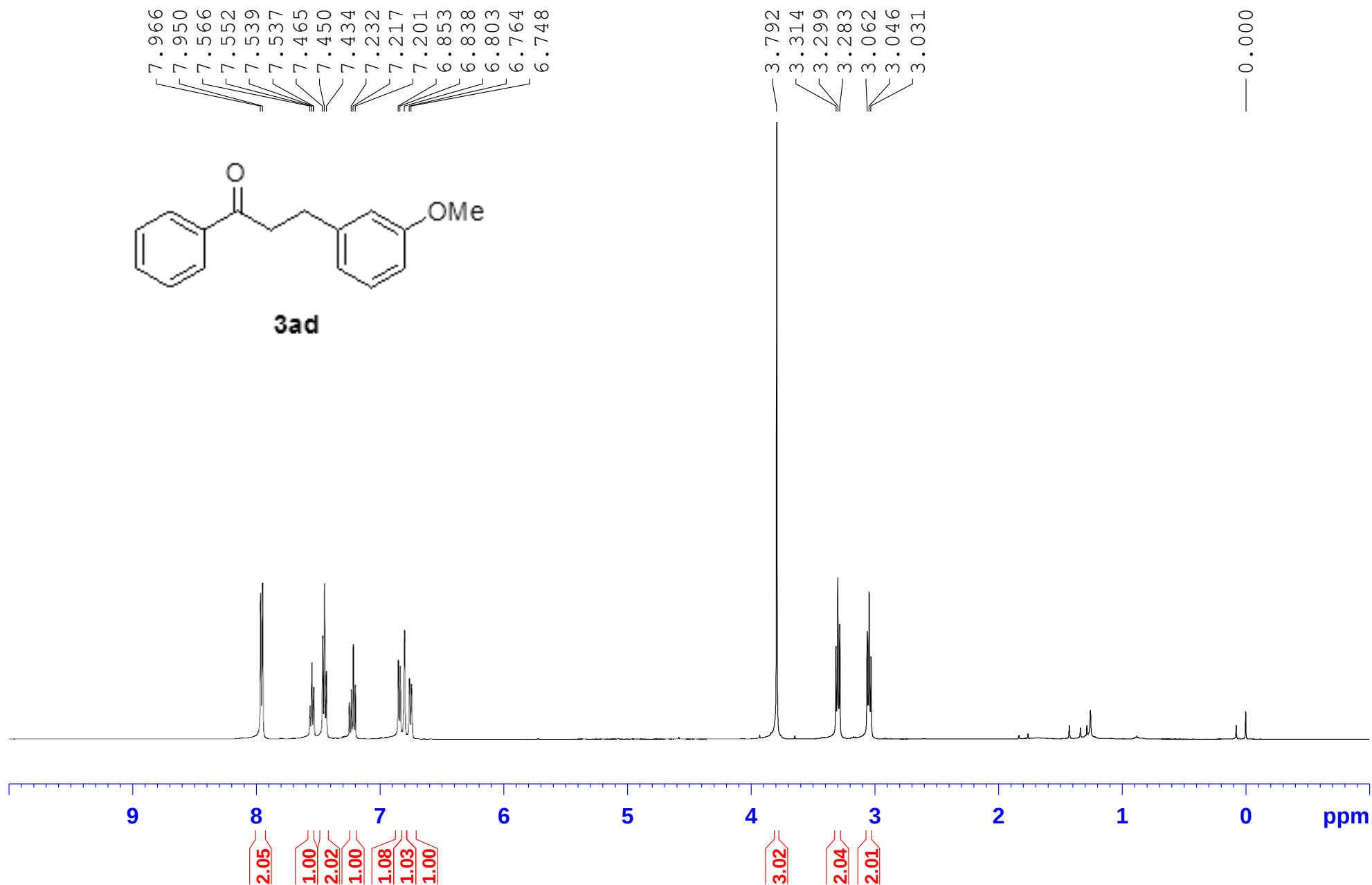
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— 29.842

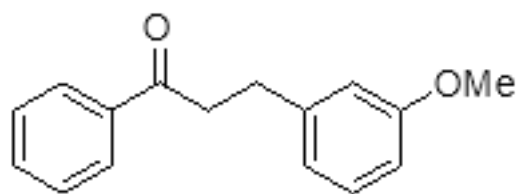
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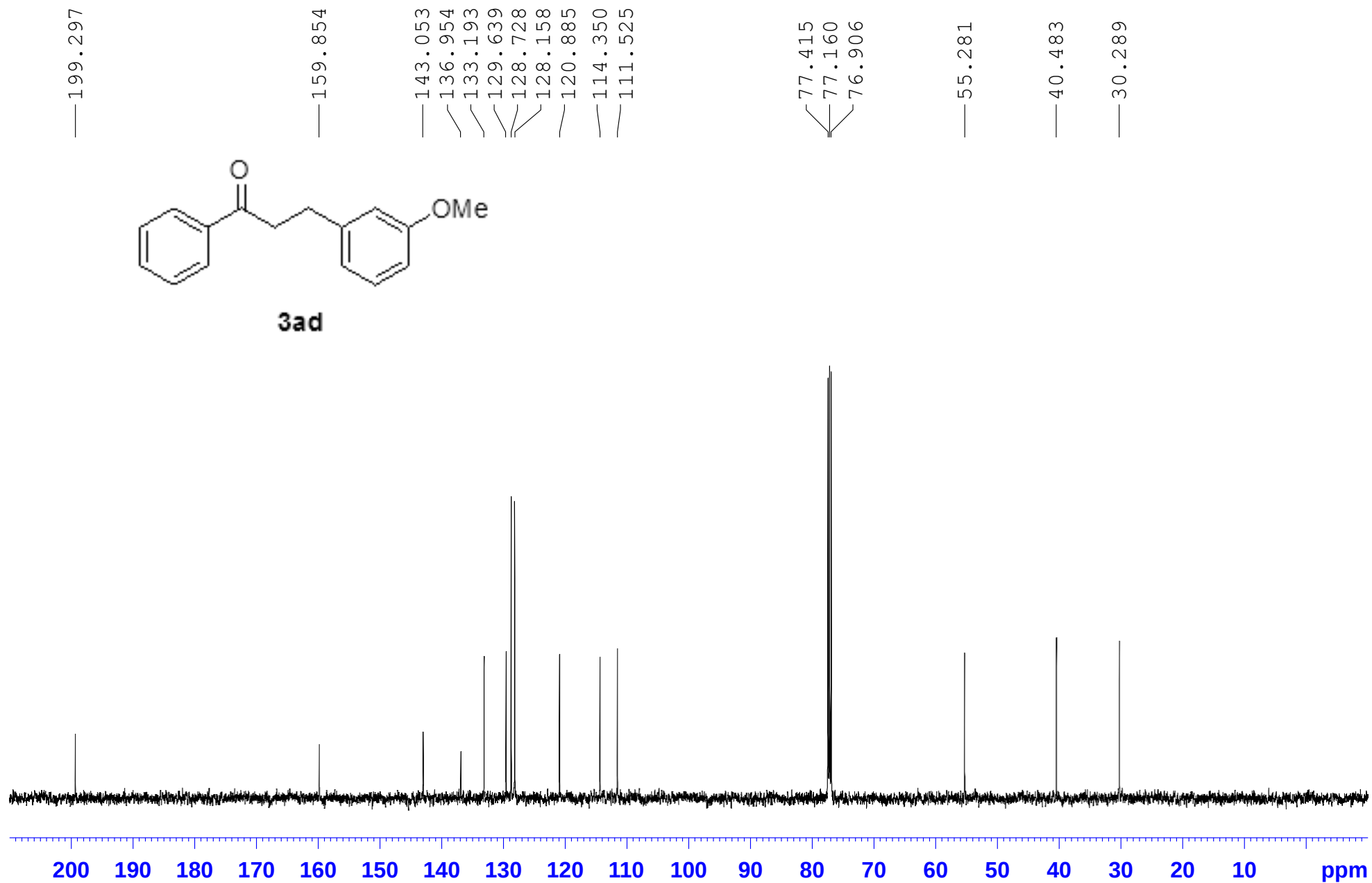
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 e Proton CDC13



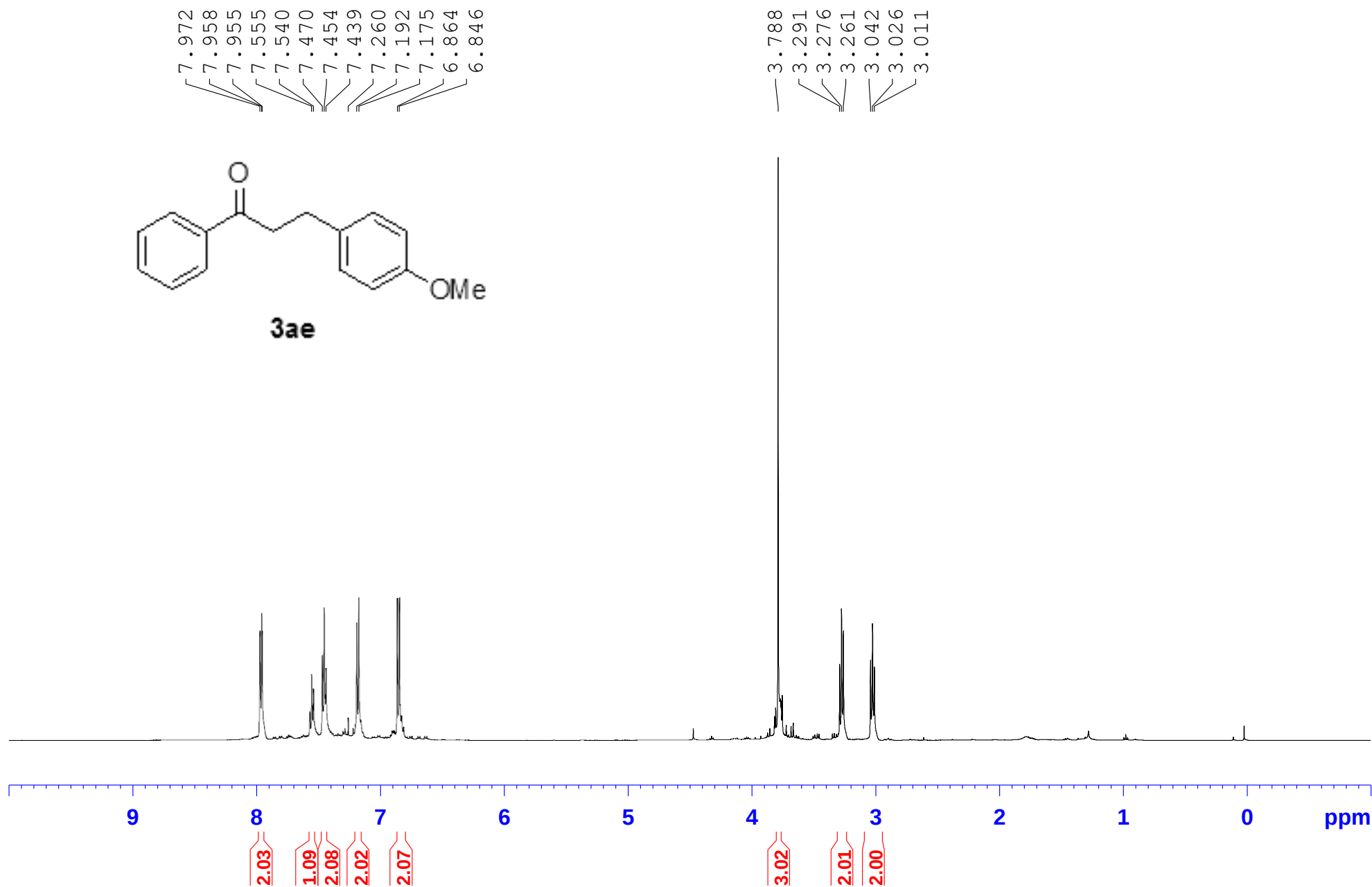
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 e C13CPD CDC13



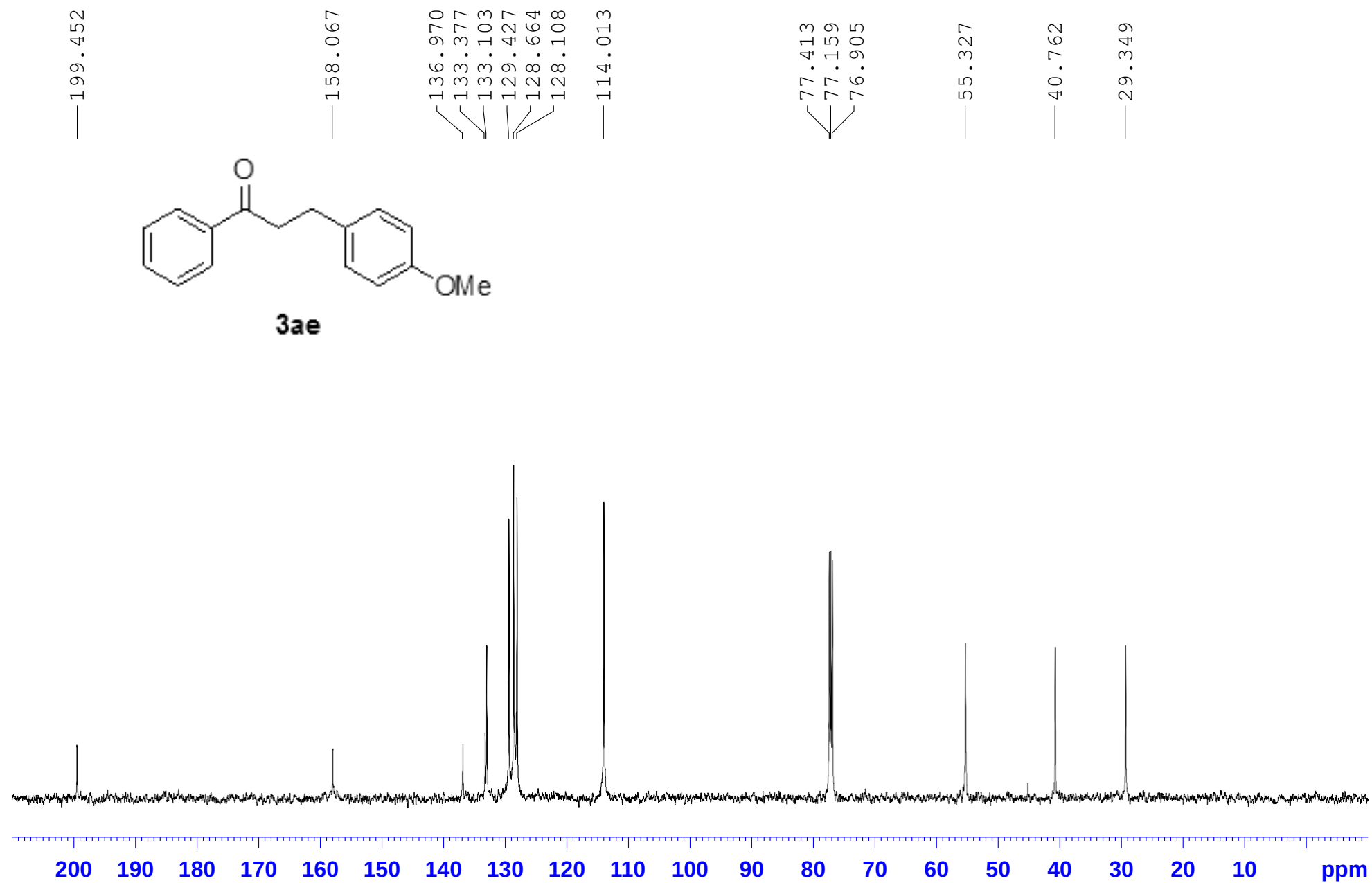
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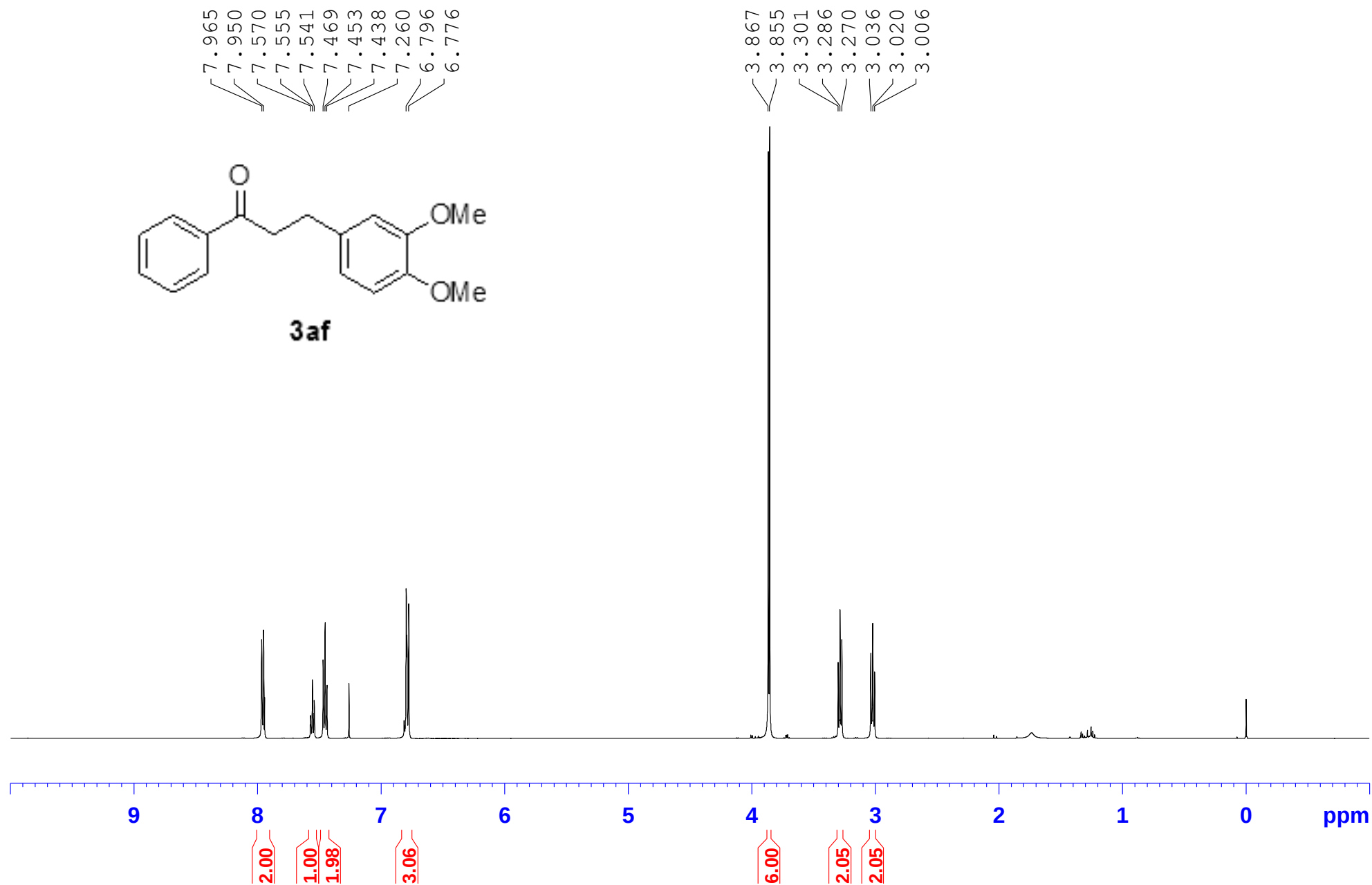
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 e Proton CDCl₃



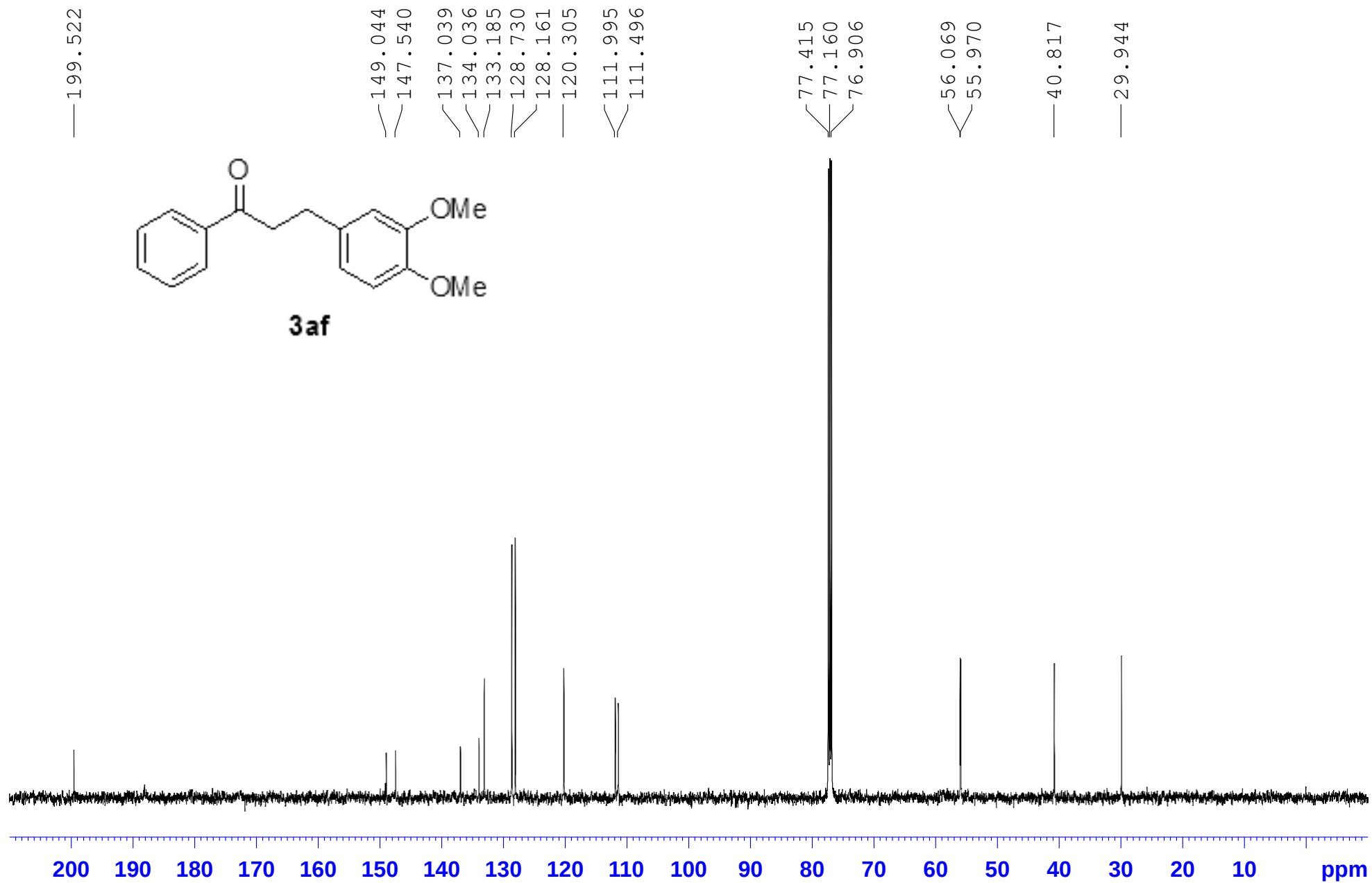
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3-(3,4-dimethoxyphenyl)-1-phenylpropan-1-one
 e Proton CDCl₃



3-(3,4-dimethoxyphenyl)-1-phenylpropan-1-one
 e C13CPD CDC13

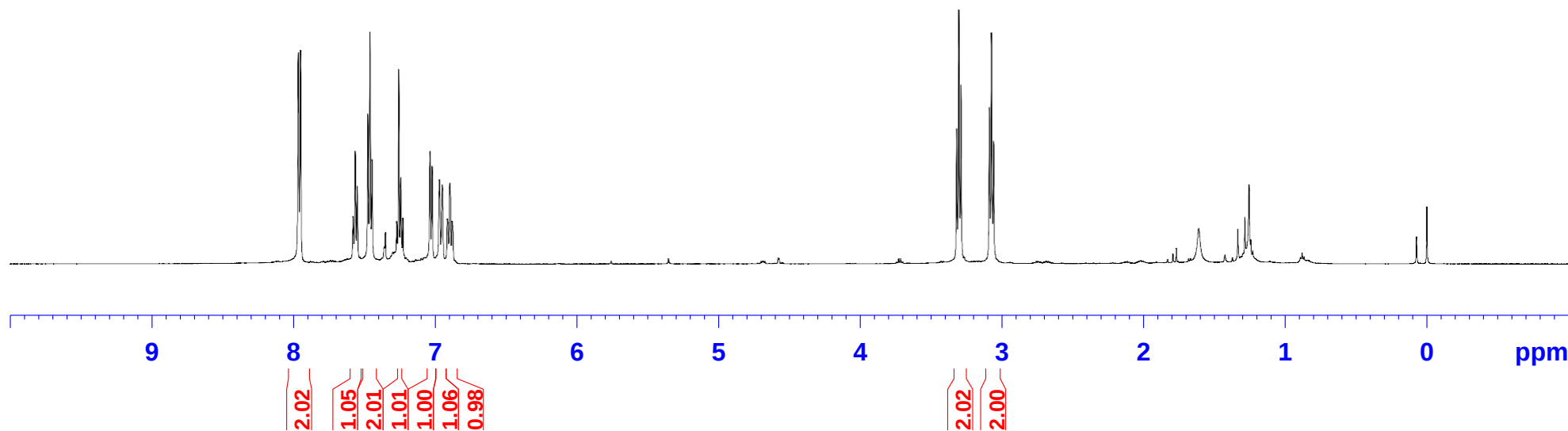
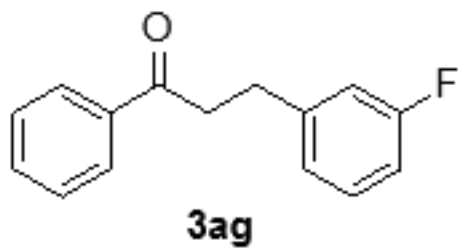


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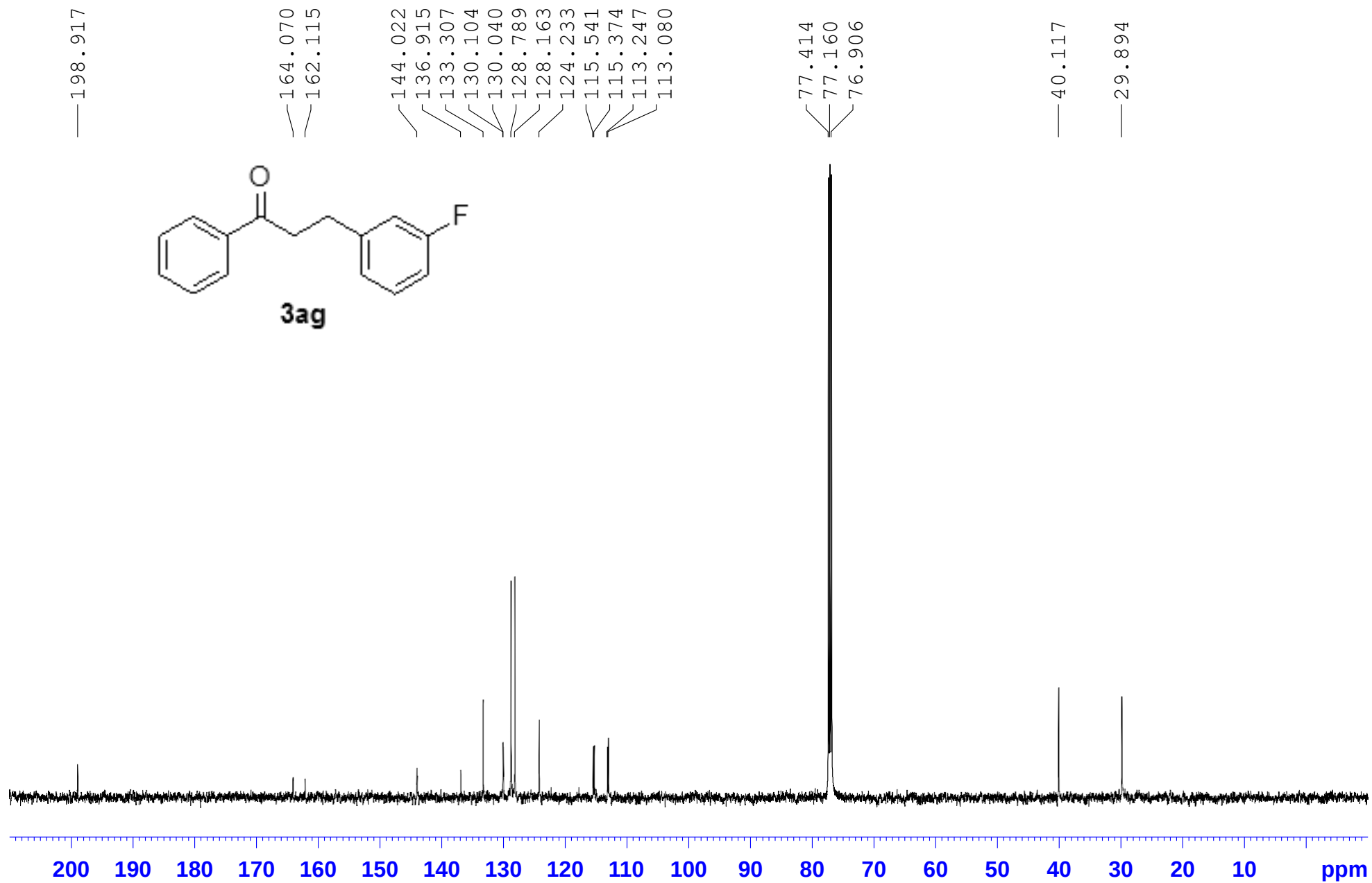
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 7.564
 7.550
 7.475
 7.460
 7.444
 7.271
 7.257
 7.243
 7.228
 7.037
 7.021
 6.970
 6.949
 6.914
 6.910
 6.897
 6.880
 6.876

3.319
 3.304
 3.288
 3.088
 3.073
 3.058

— 0.000



3-(3-fluorophenyl)-1-phenylpropan-1-one
 e C13CPD CDCl3

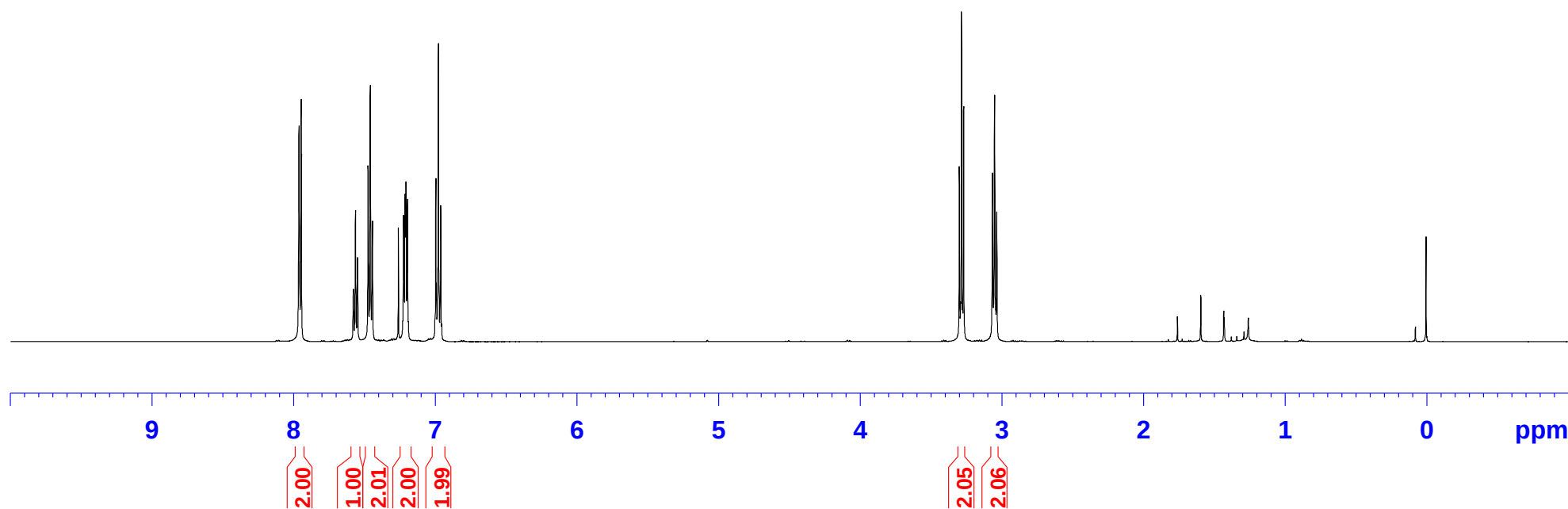
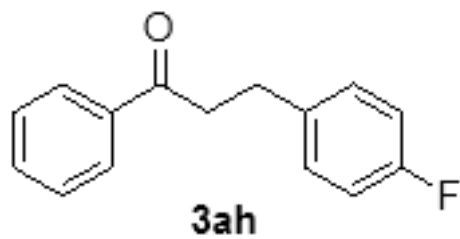


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 e Proton CDCl₃

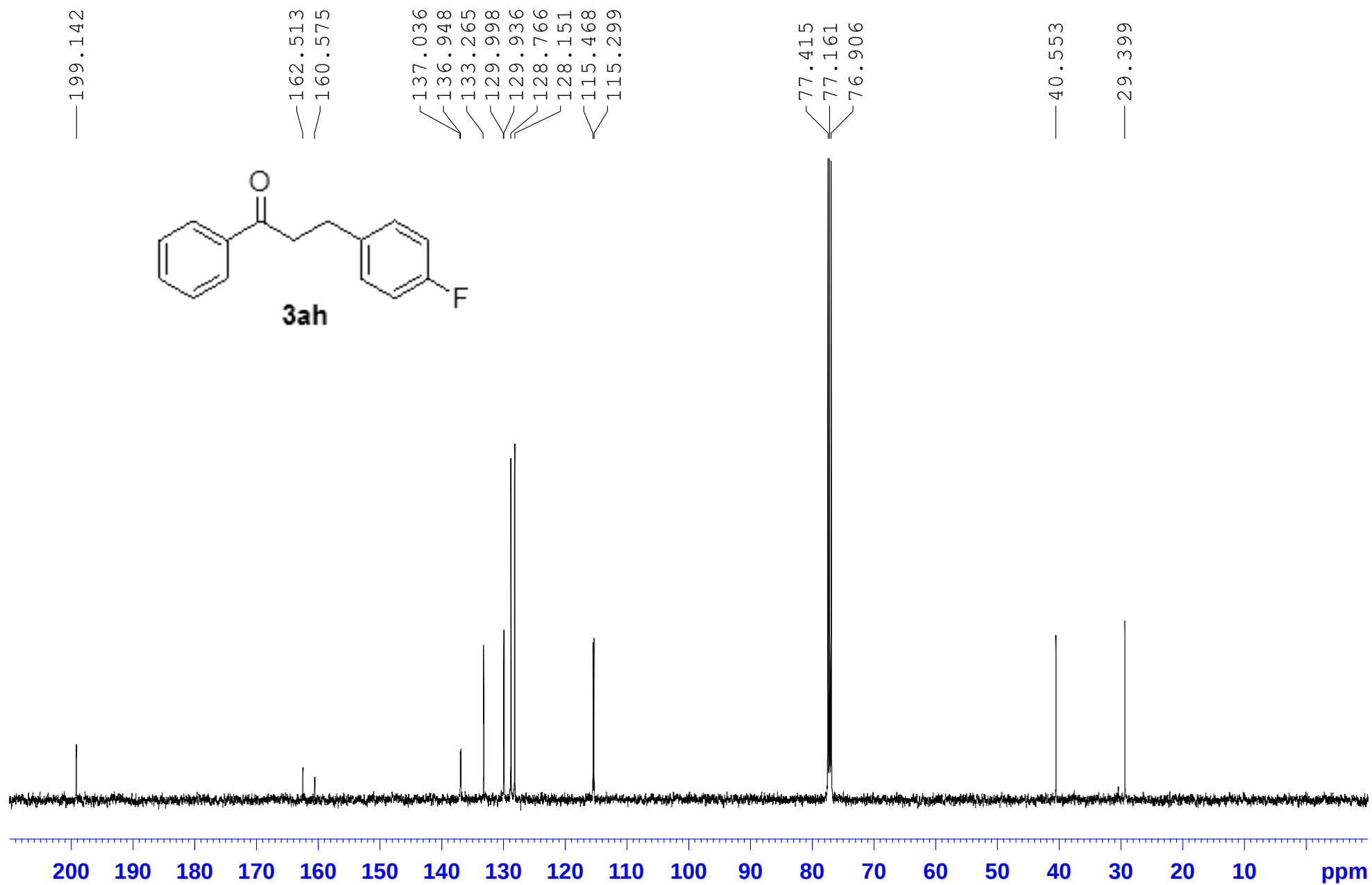
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 7.946
 7.578
 7.563
 7.548
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 7.458
 7.443
 7.260
 7.224
 7.213
 7.207
 7.196
 6.995
 6.978
 6.961

3.300
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 3.269
 3.066
 3.050
 3.035

— 0.005



3-(4-fluorophenyl)-1-phenylpropan-1-one
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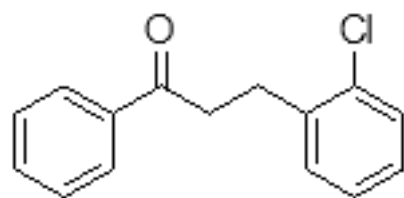


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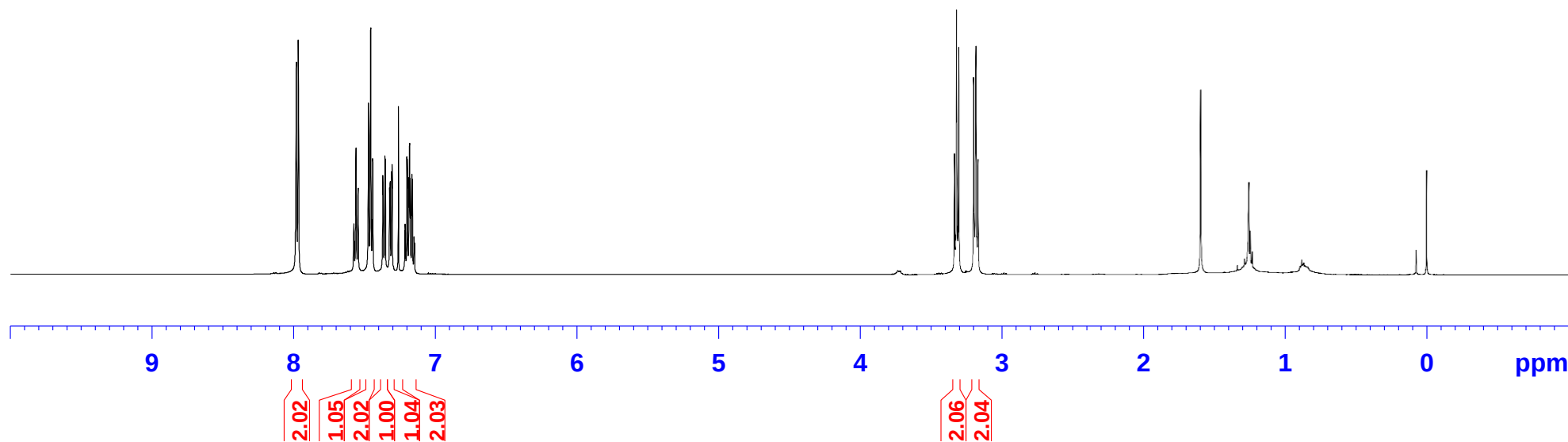
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7.368
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7.319
7.308
7.304
7.260
7.214
7.211
7.199
7.197
7.185
7.181
7.176
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7.161
7.150
7.146

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3.198
3.182
3.168

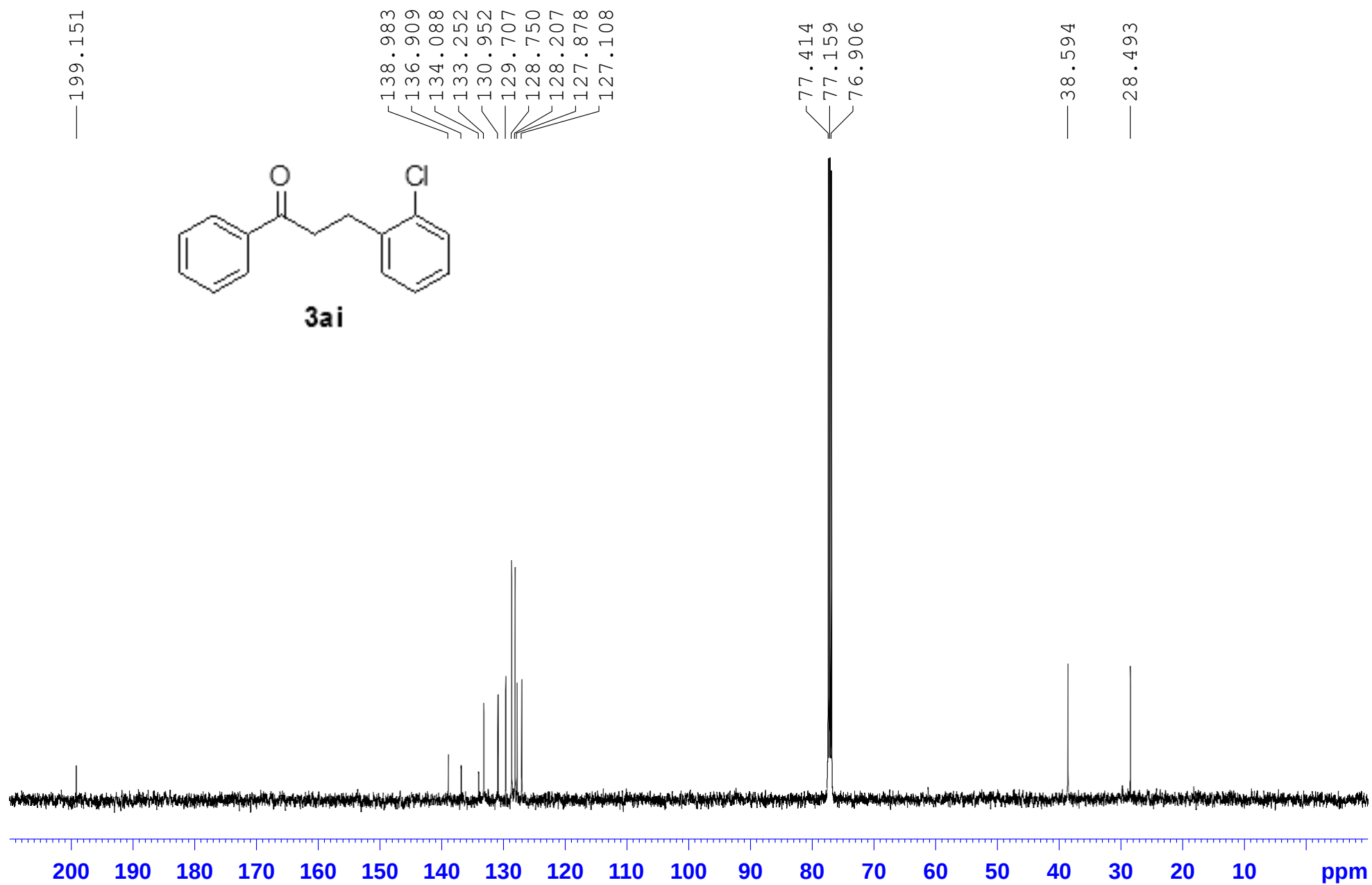
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3ai



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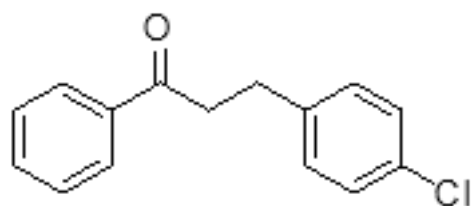


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e Proton CDCl₃

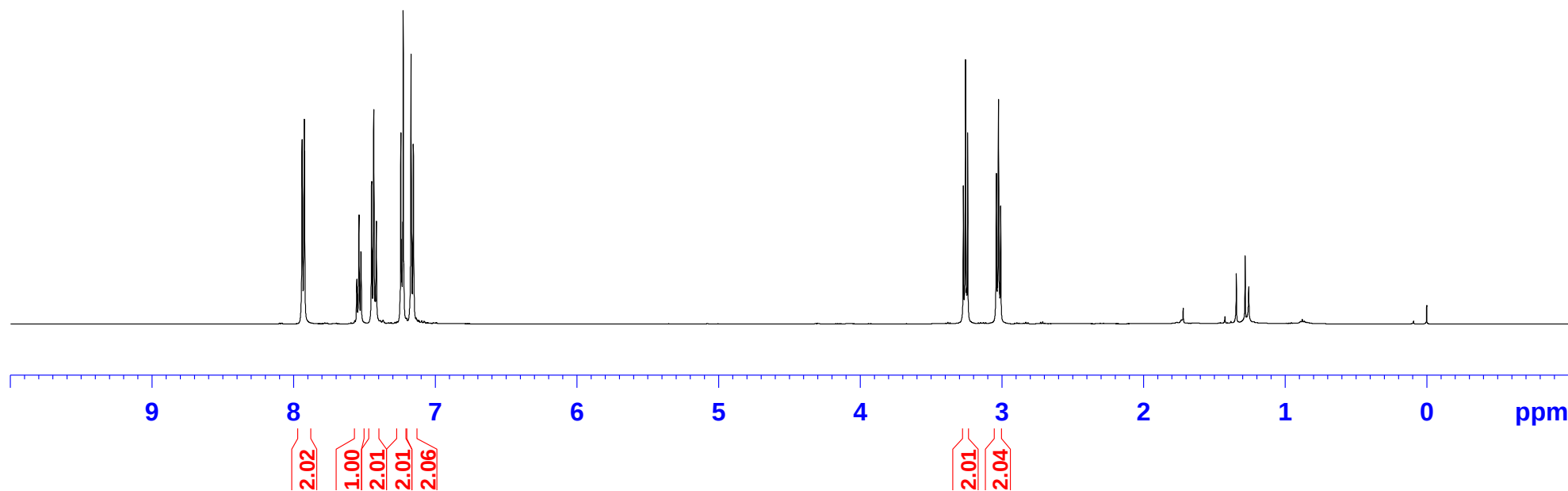
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7.222
7.171
7.155

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3.257
3.241
3.039
3.024
3.009

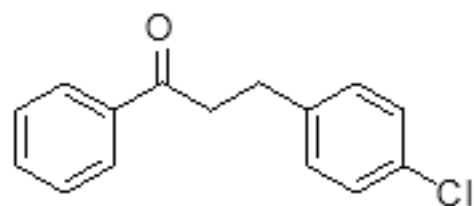
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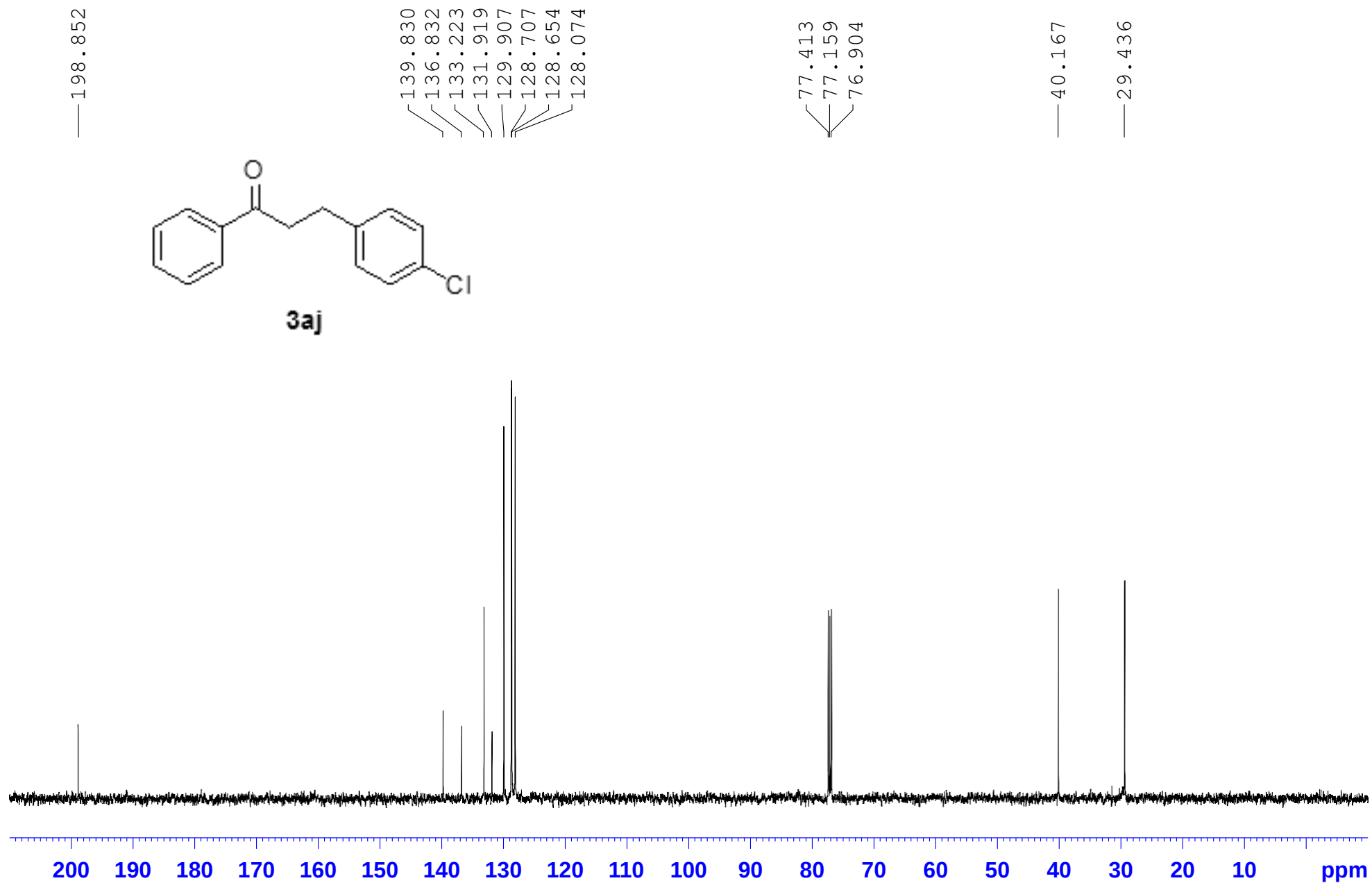
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3-(4-chlorophenyl)-1-phenylpropan-1-one
 e C13CPD CDC13



3aj

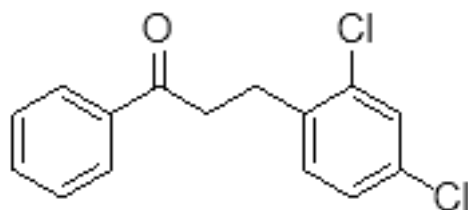


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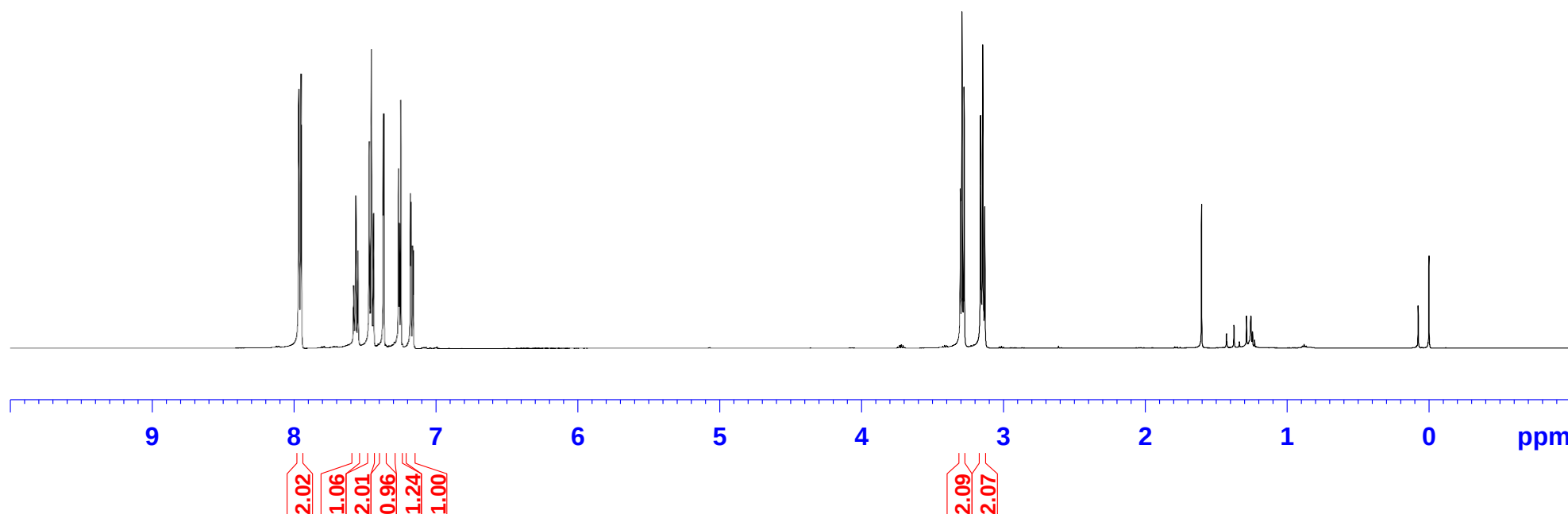
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 7.547
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 7.455
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 7.264
 7.258
 7.248
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 7.160

3.306
 3.298
 3.292
 3.282
 3.276
 3.161
 3.146
 3.131

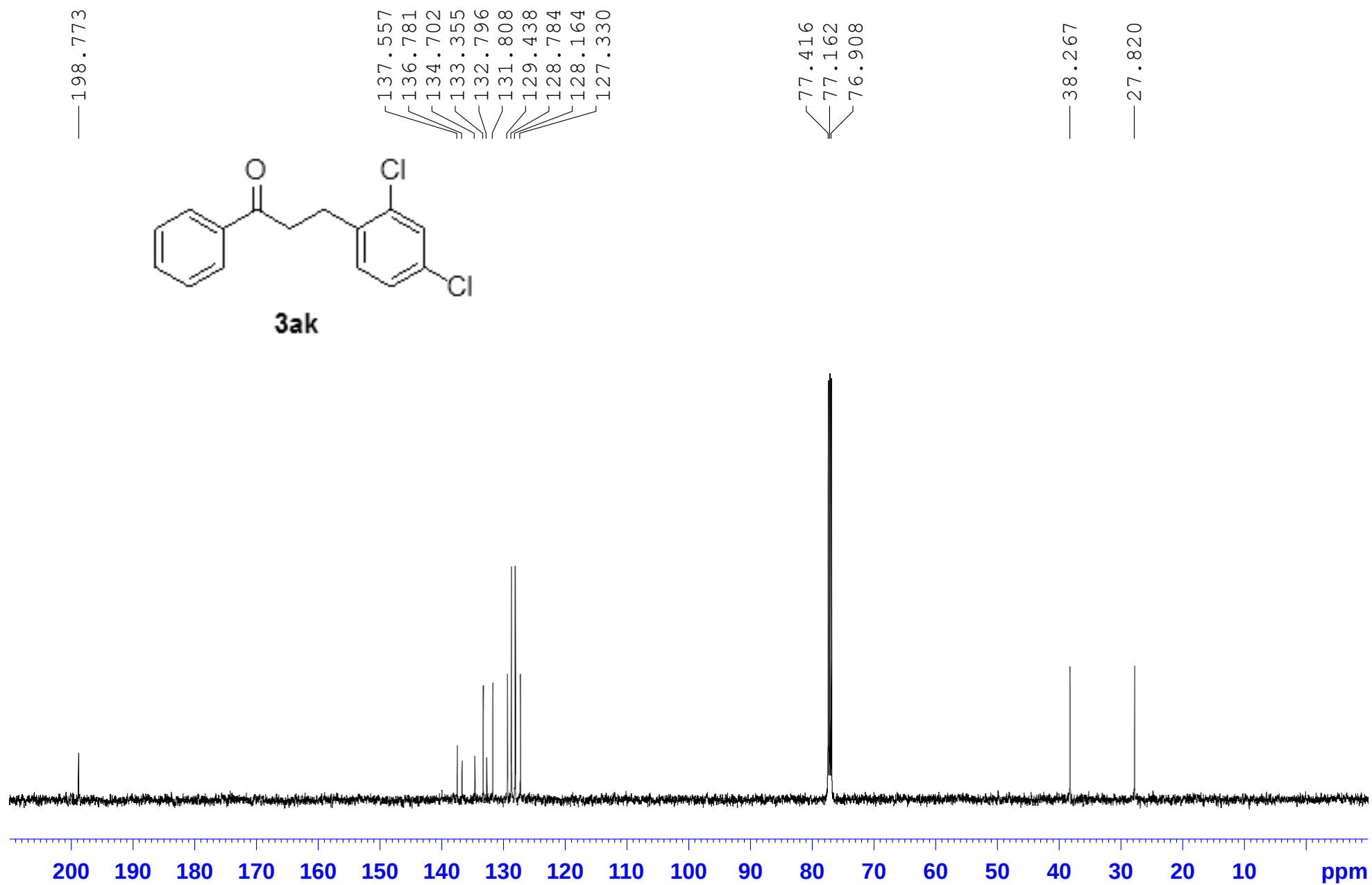
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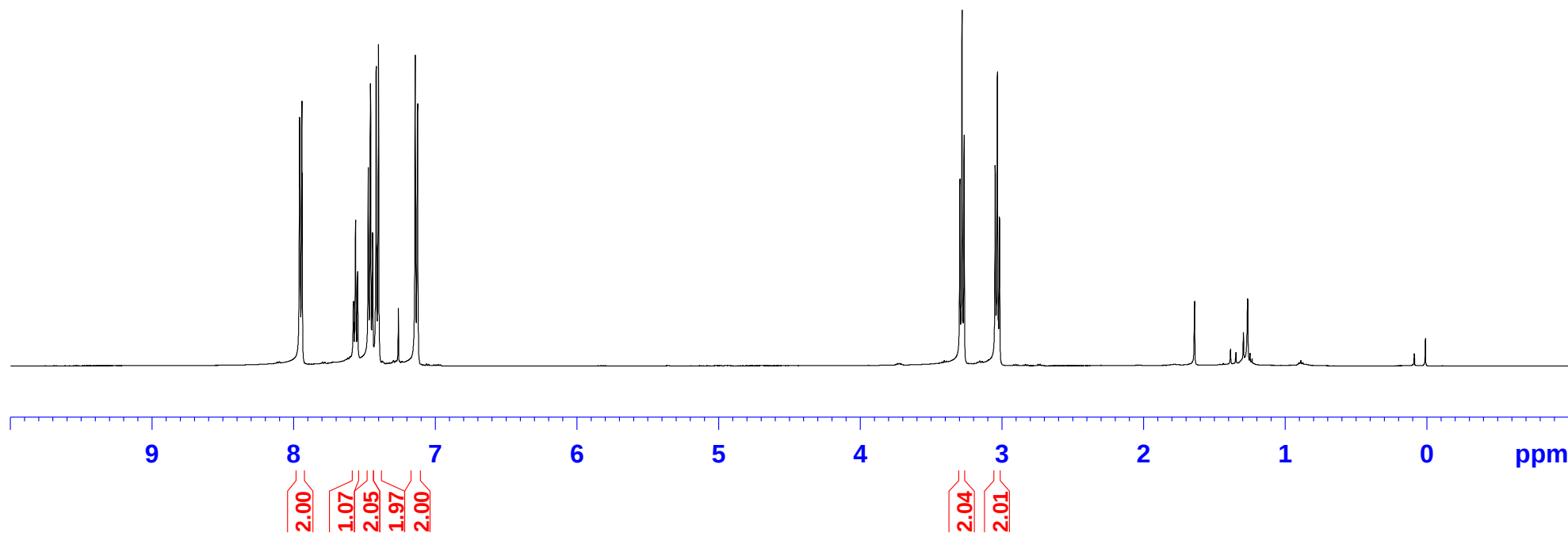
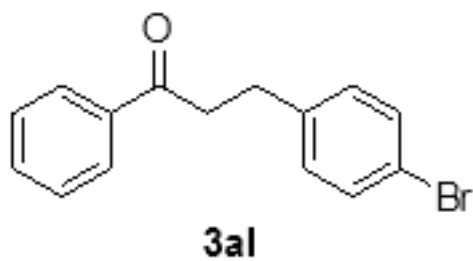
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e C13CPD CDCl3



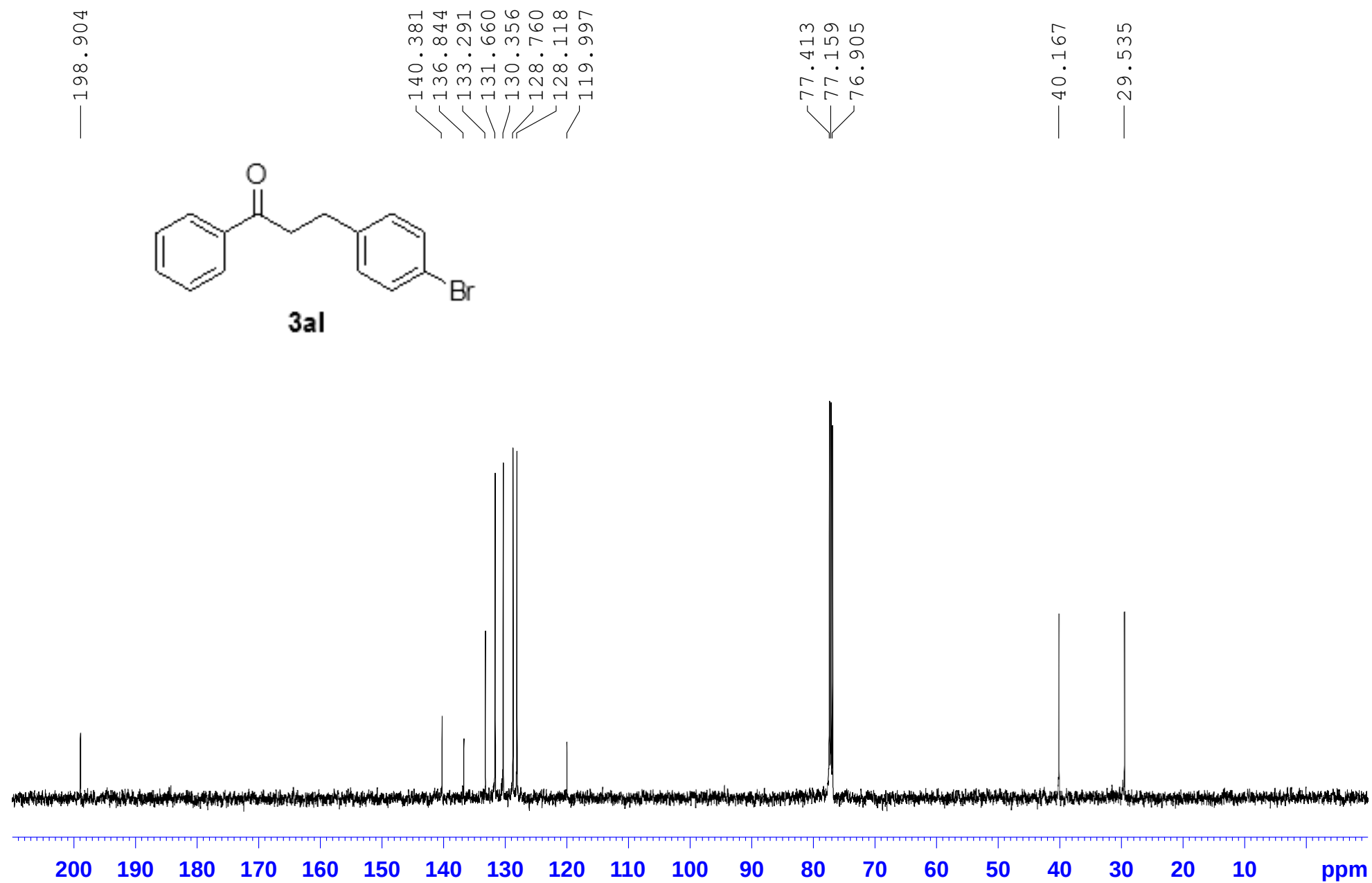
3-(4-bromophenyl)-1-phenylpropan-1-one
e Proton CDCl₃

7.958
7.942
7.939
7.577
7.563
7.548
7.473
7.457
7.442
7.417
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7.141
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3.273
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3.031
3.016



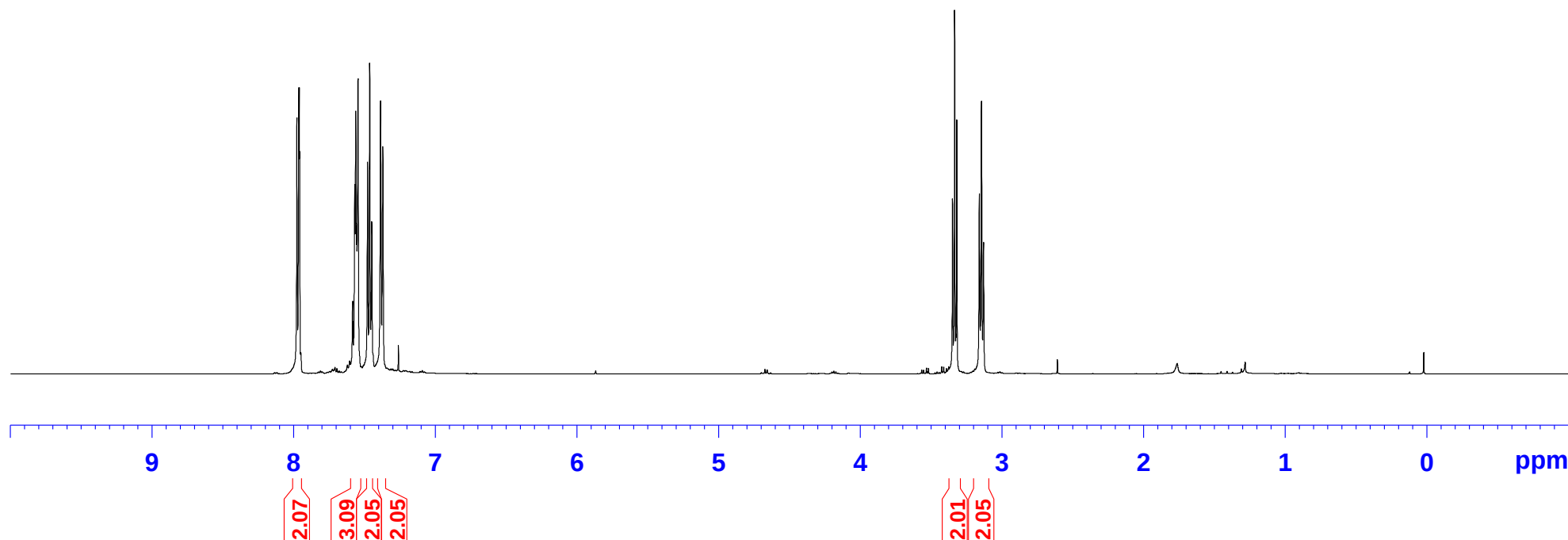
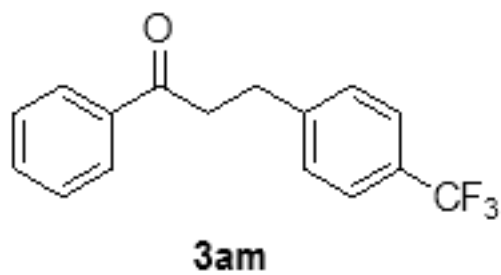
3-(4-bromophenyl)-1-phenylpropan-1-one
e C13CPD CDC13



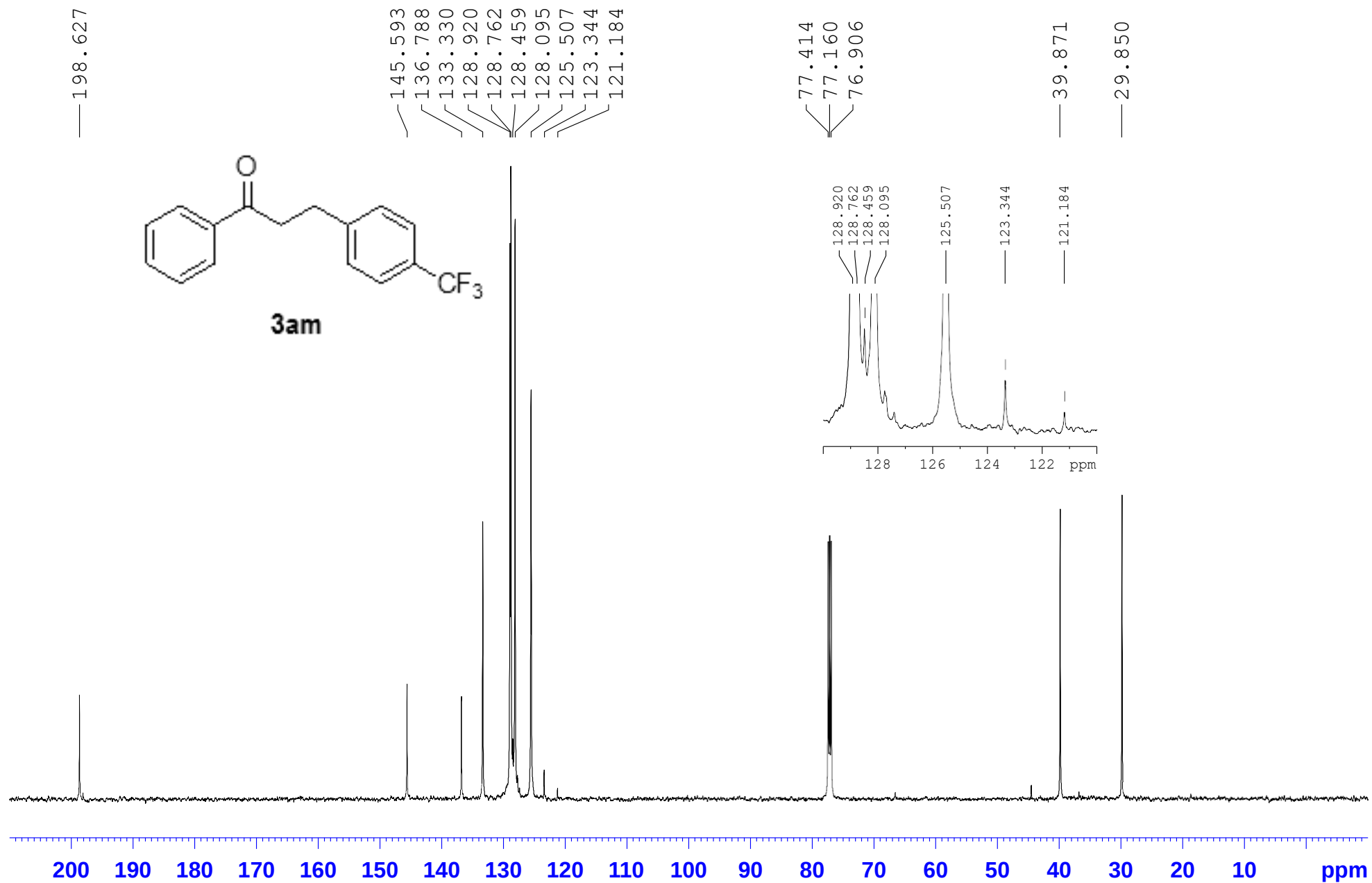
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 e Proton CDCl₃

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7.569
7.562
7.554
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7.546
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7.463
7.448
7.386
7.370
7.260

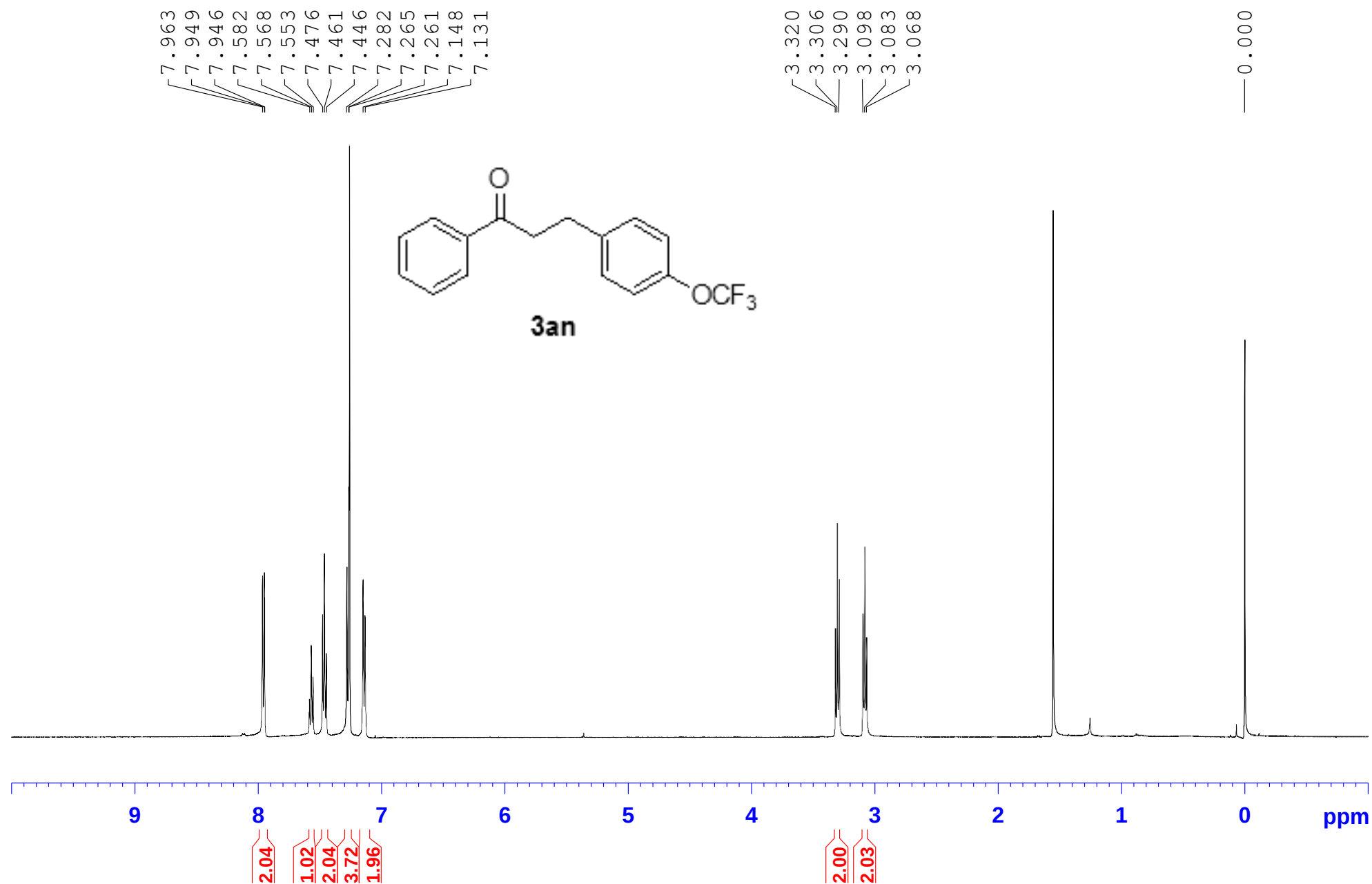
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3.333
3.325
3.318
3.159
3.143
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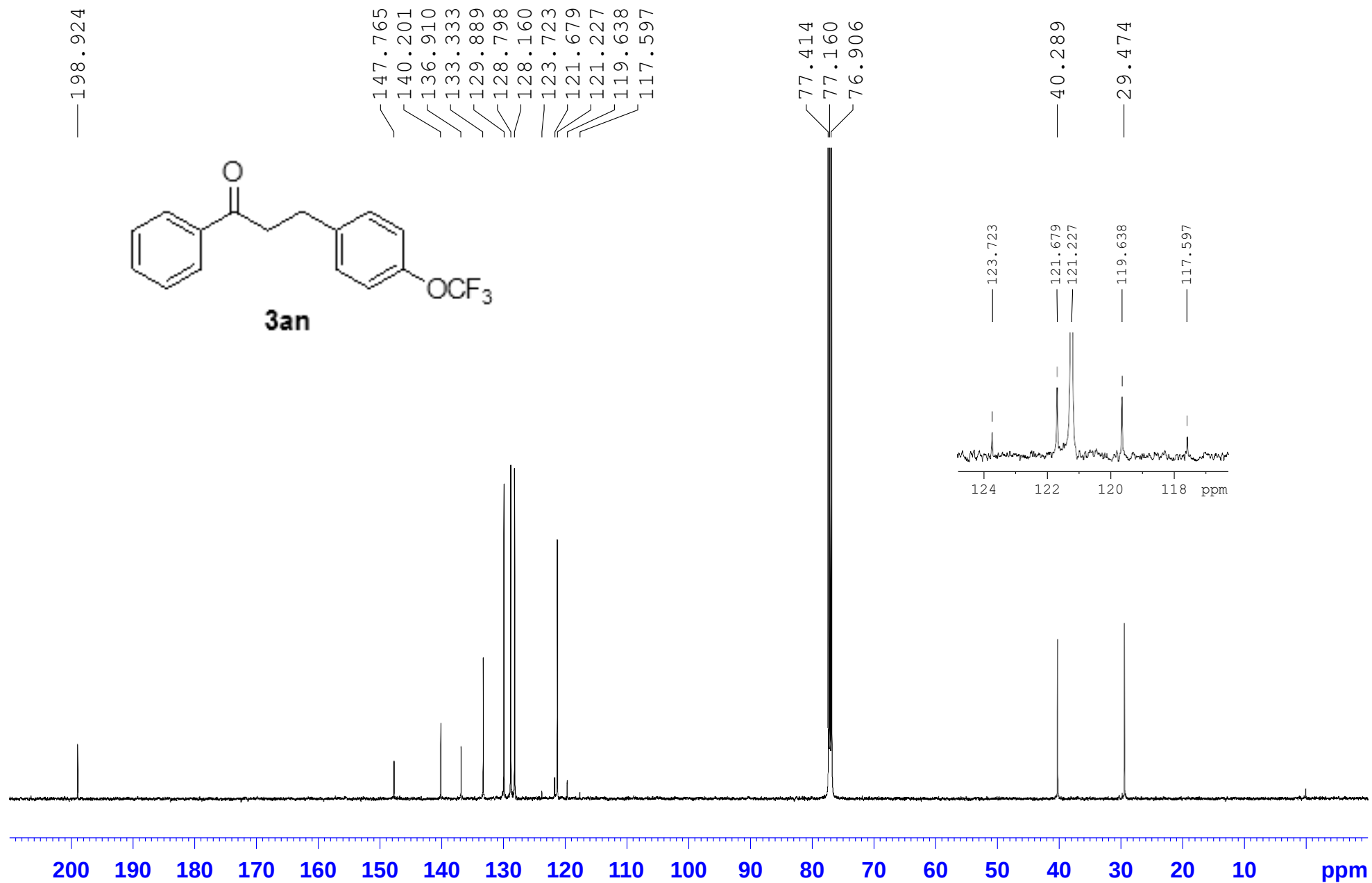
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 e C13CPD CDC13



1-phenyl-3-[4-(trifluoromethoxy)phenyl]propan-1-one
 e Proton CDC13



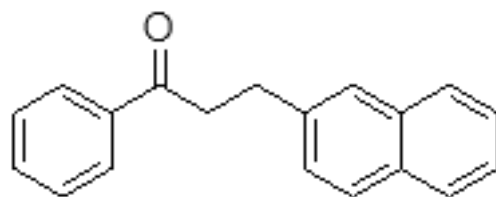
1-phenyl-3-[4-(trifluoromethoxy)phenyl]propan-1-one
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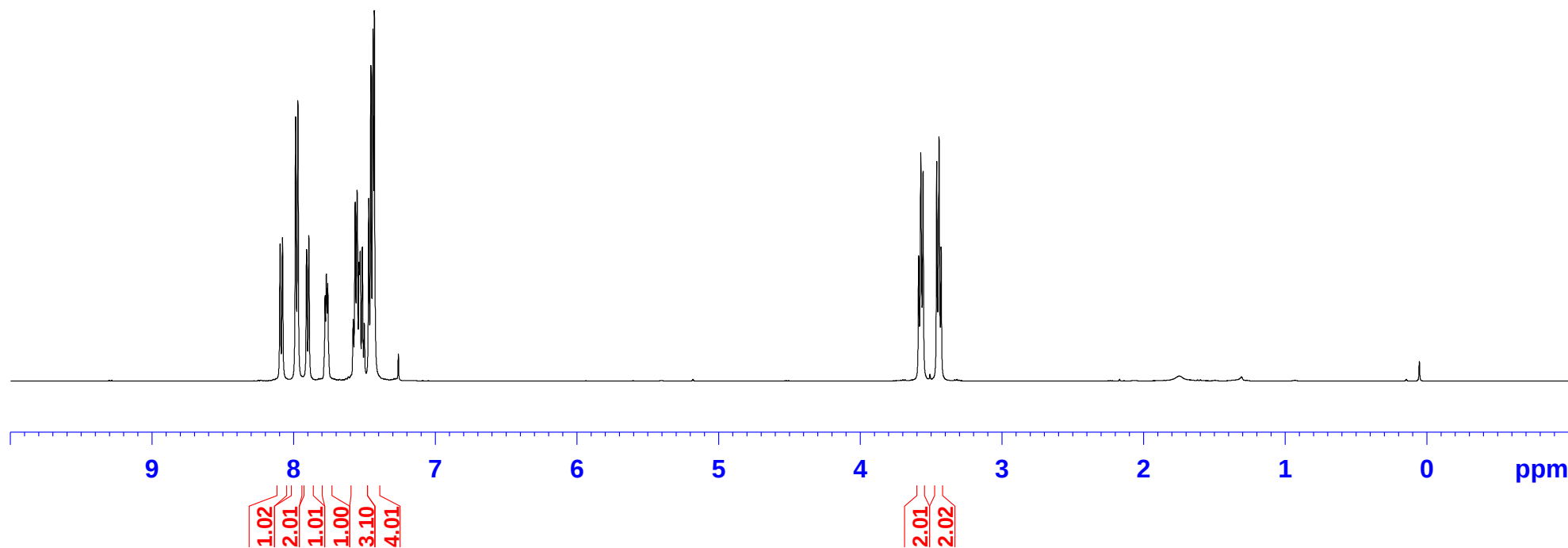
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 7.970
 7.908
 7.893
 7.778
 7.769
 7.759
 7.579
 7.566
 7.552
 7.538
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 7.515
 7.501
 7.469
 7.454
 7.439
 7.430
 7.260

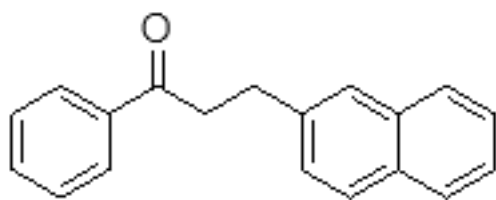
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 3.556
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 3.443
 3.429



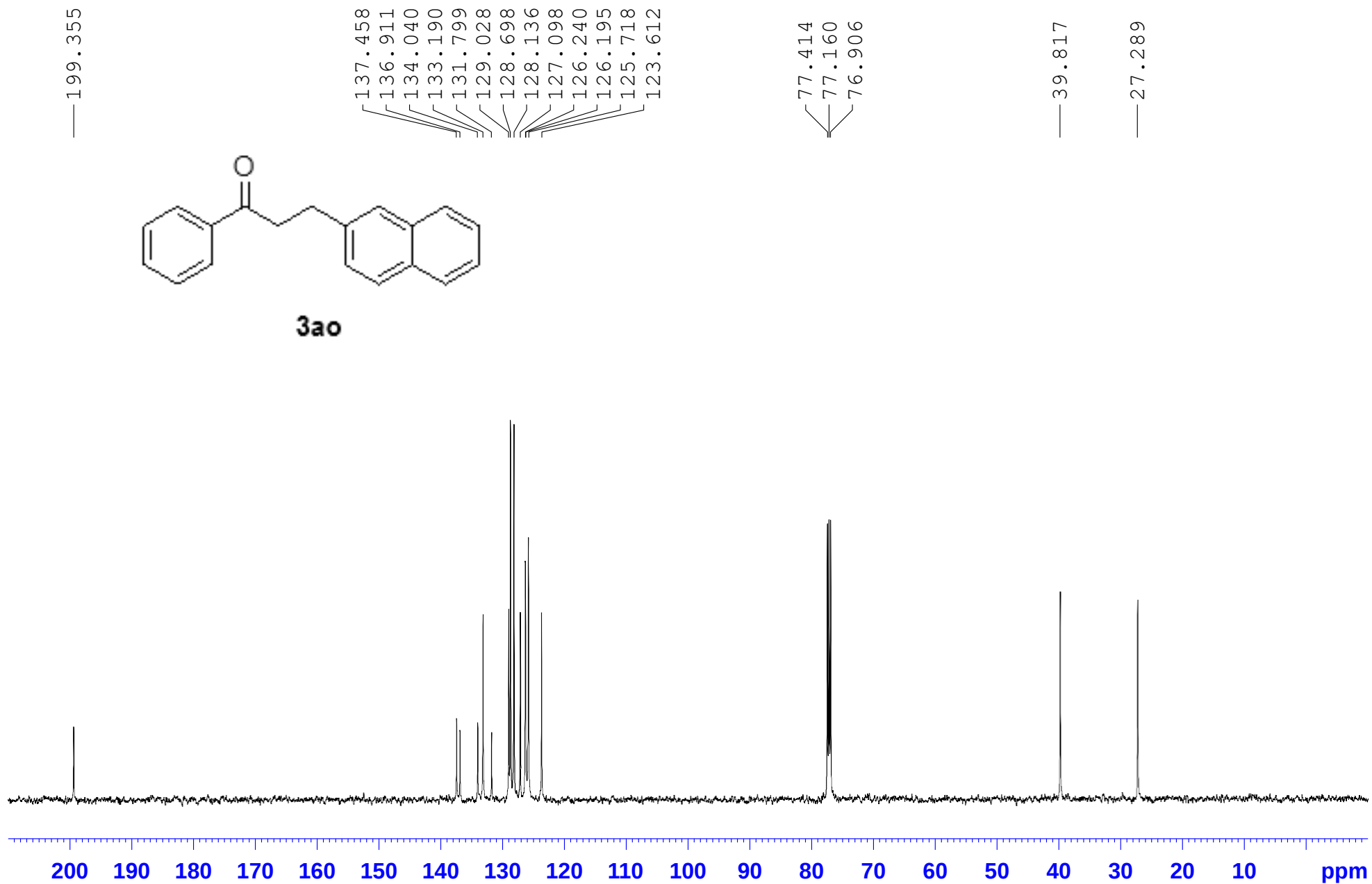
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3-(naphthalen-1-yl)-1-phenylpropan-1-one
 e C13CPD CDC13



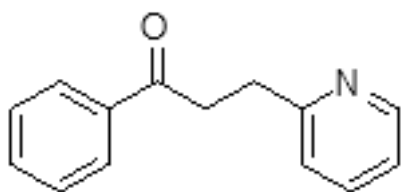
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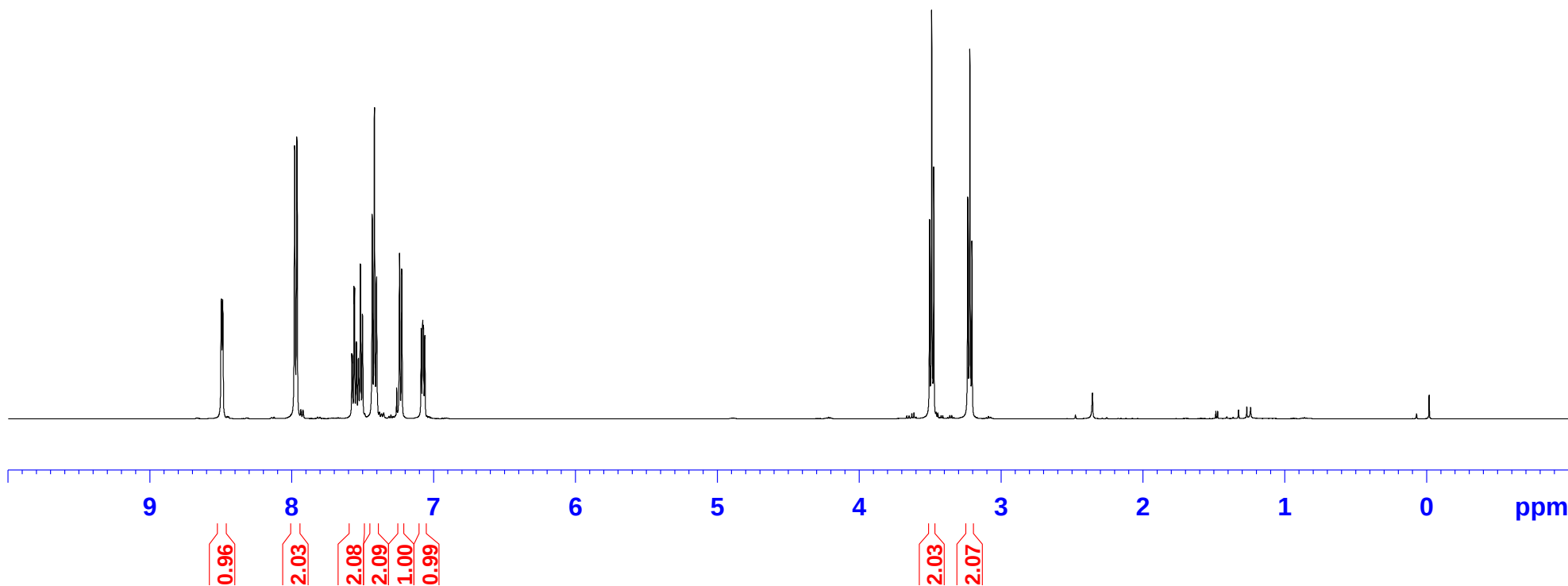
1-phenyl-3-(pyridin-2-yl)propan-1-one
 e Proton CDCl₃

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 8.485
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 7.964
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 7.573
 7.561
 7.558
 7.546
 7.542
 7.531
 7.516
 7.501
 7.433
 7.417
 7.402
 7.260
 7.239
 7.224
 7.086
 7.076
 7.072
 7.062

3.503
 3.488
 3.474
 3.234
 3.219
 3.205



3ap



1-phenyl-3-(pyridin-2-yl)propan-1-one
 e C13CPD CDCl3

— 199.317

— 160.764

— 149.281

136.956

136.393

133.037

128.589

128.127

123.392

121.269

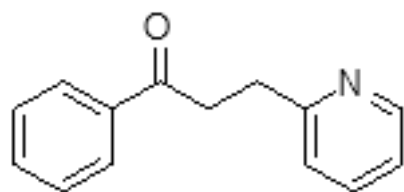
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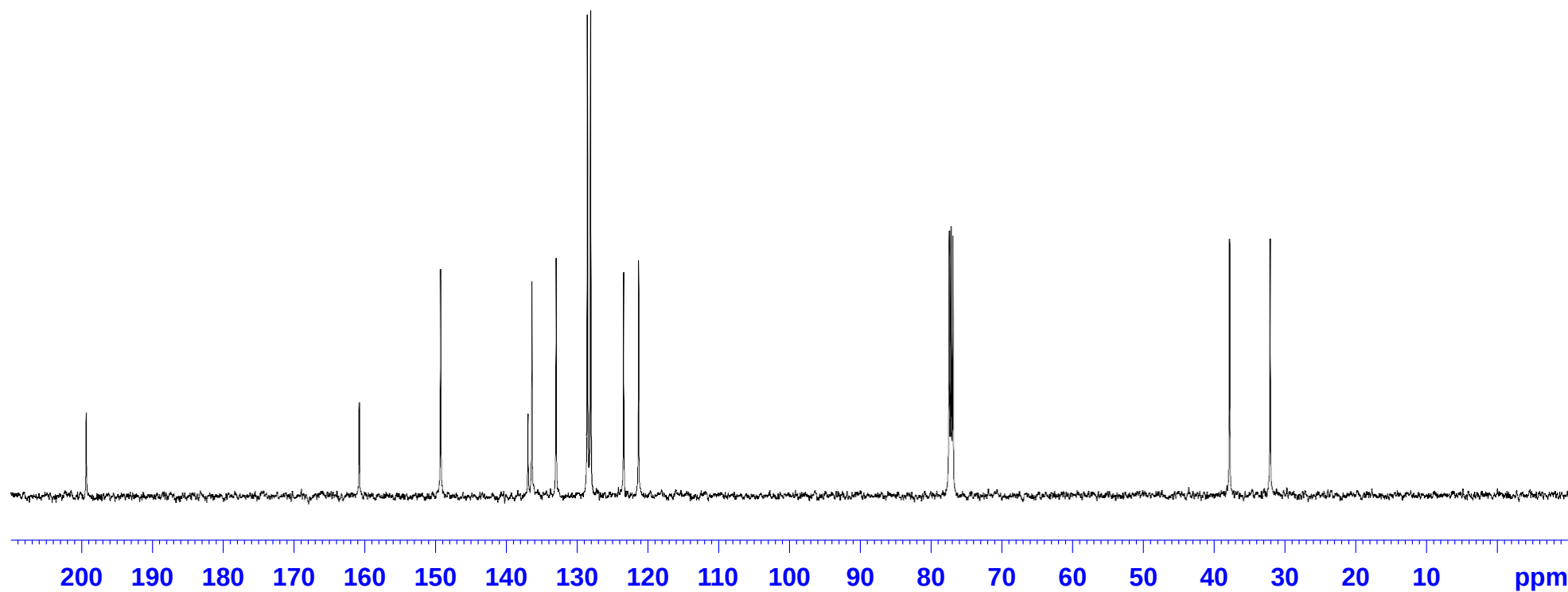
76.906

— 37.848

— 32.124



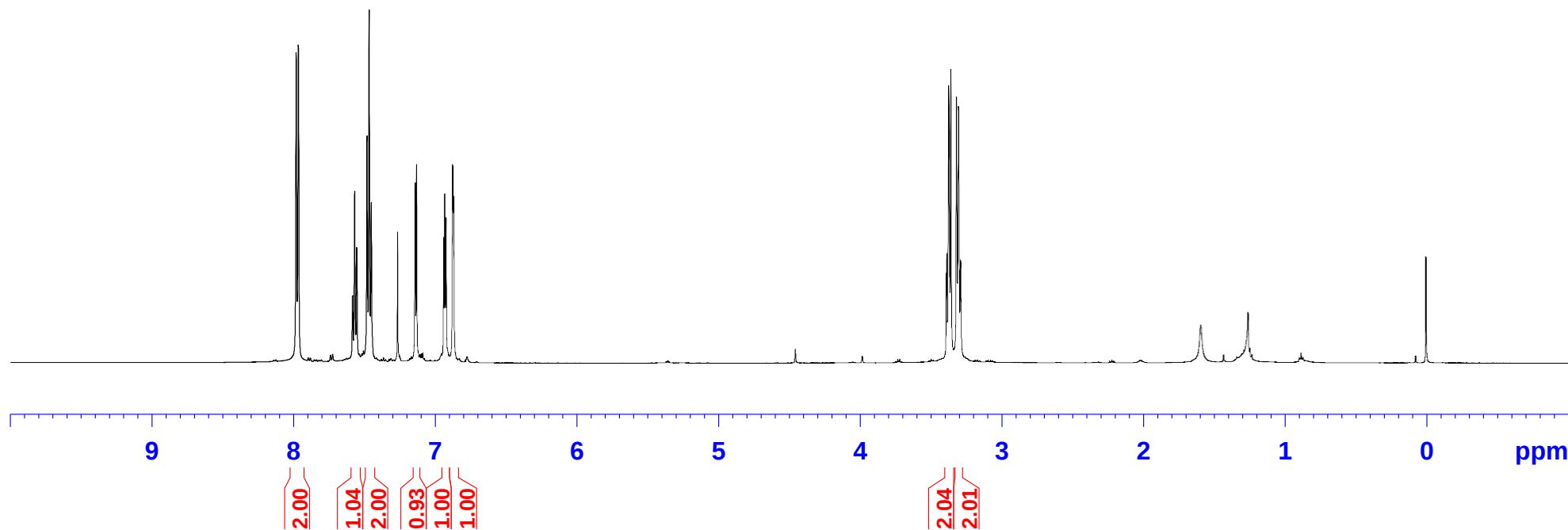
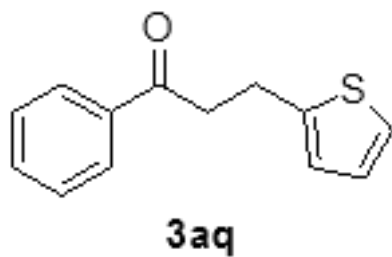
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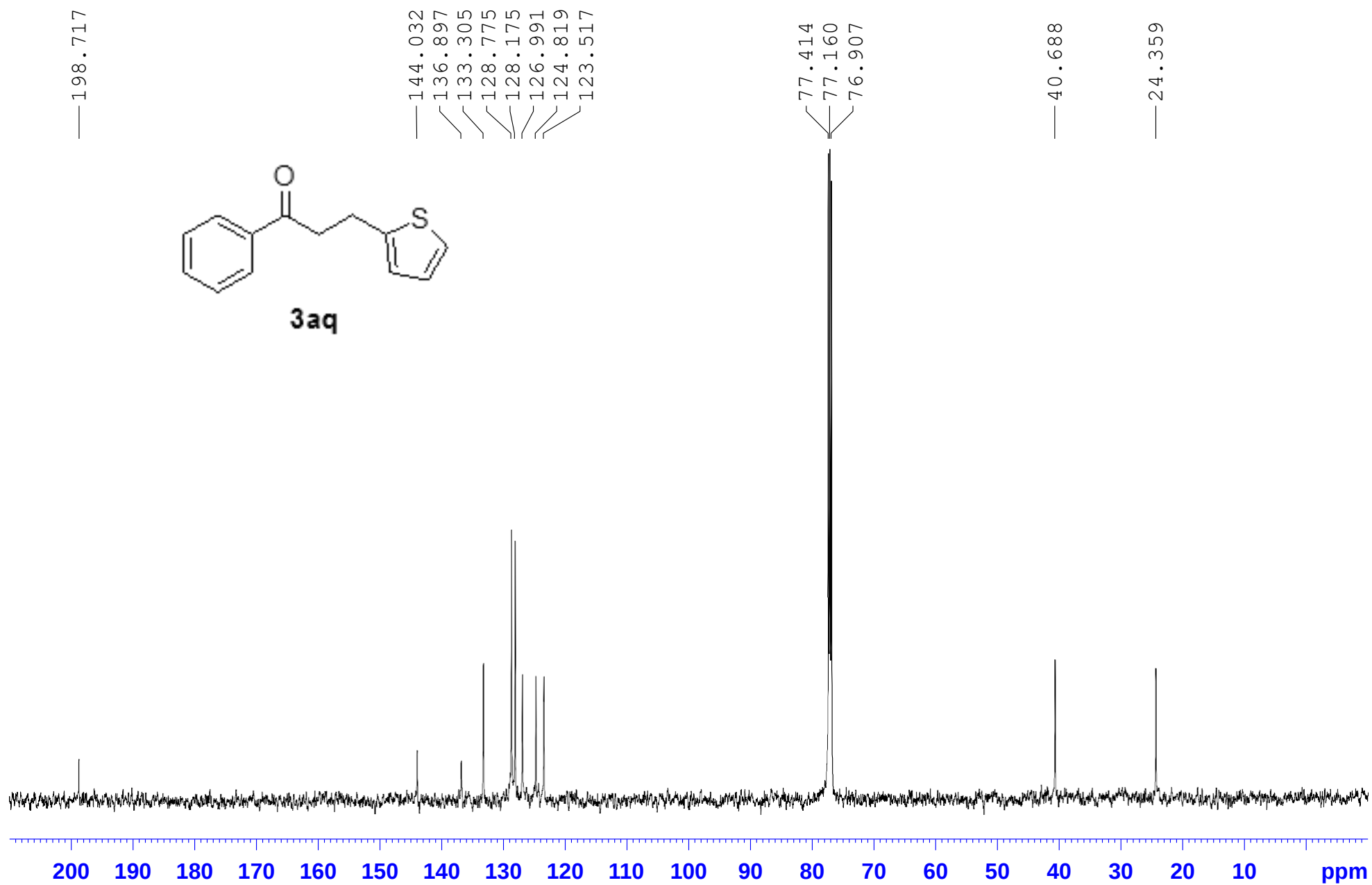
1-phenyl-3-(thiophen-2-yl)propan-1-one
 e Proton CDCl₃

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 7.260
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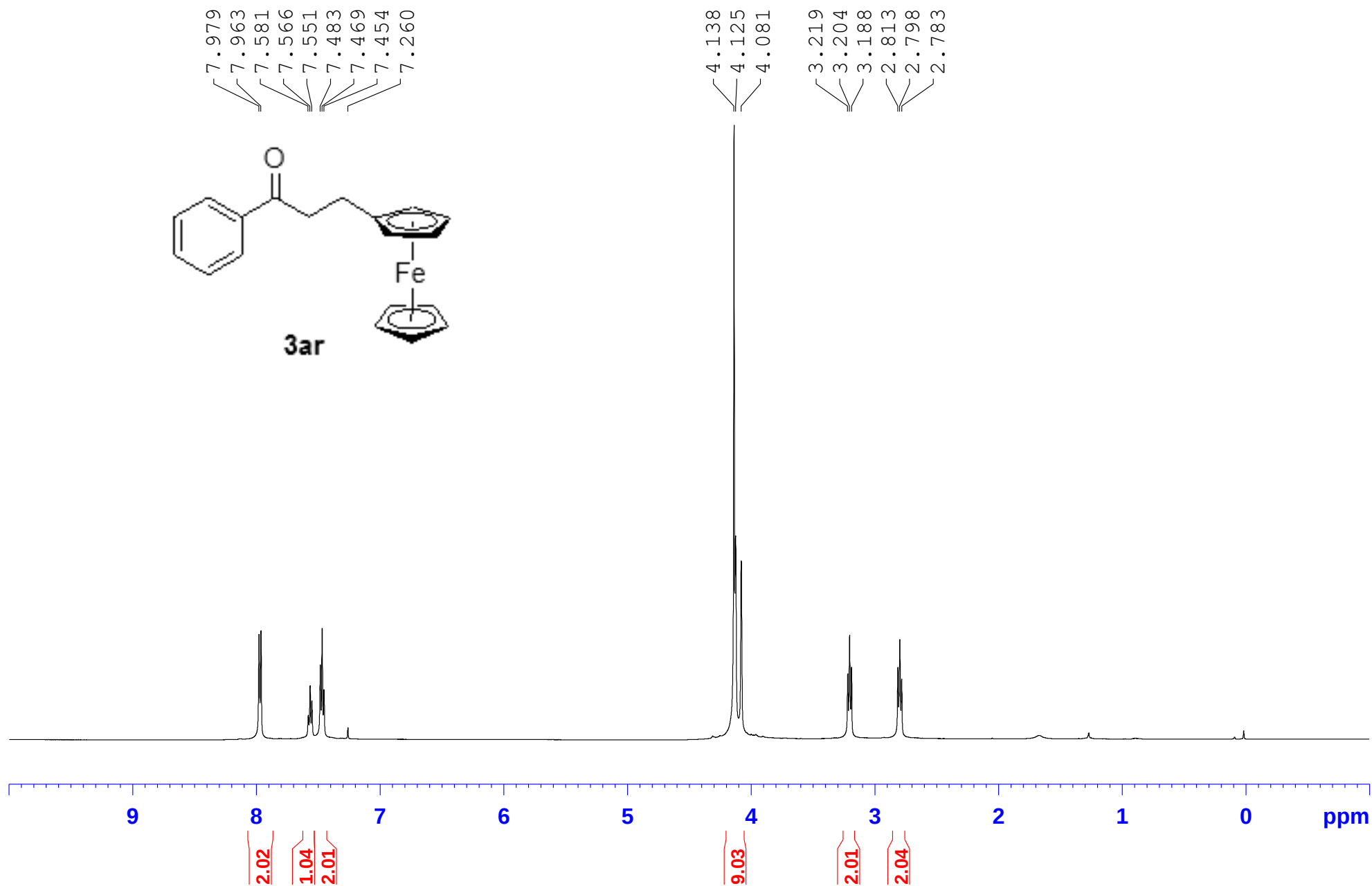
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 3.303
 3.289



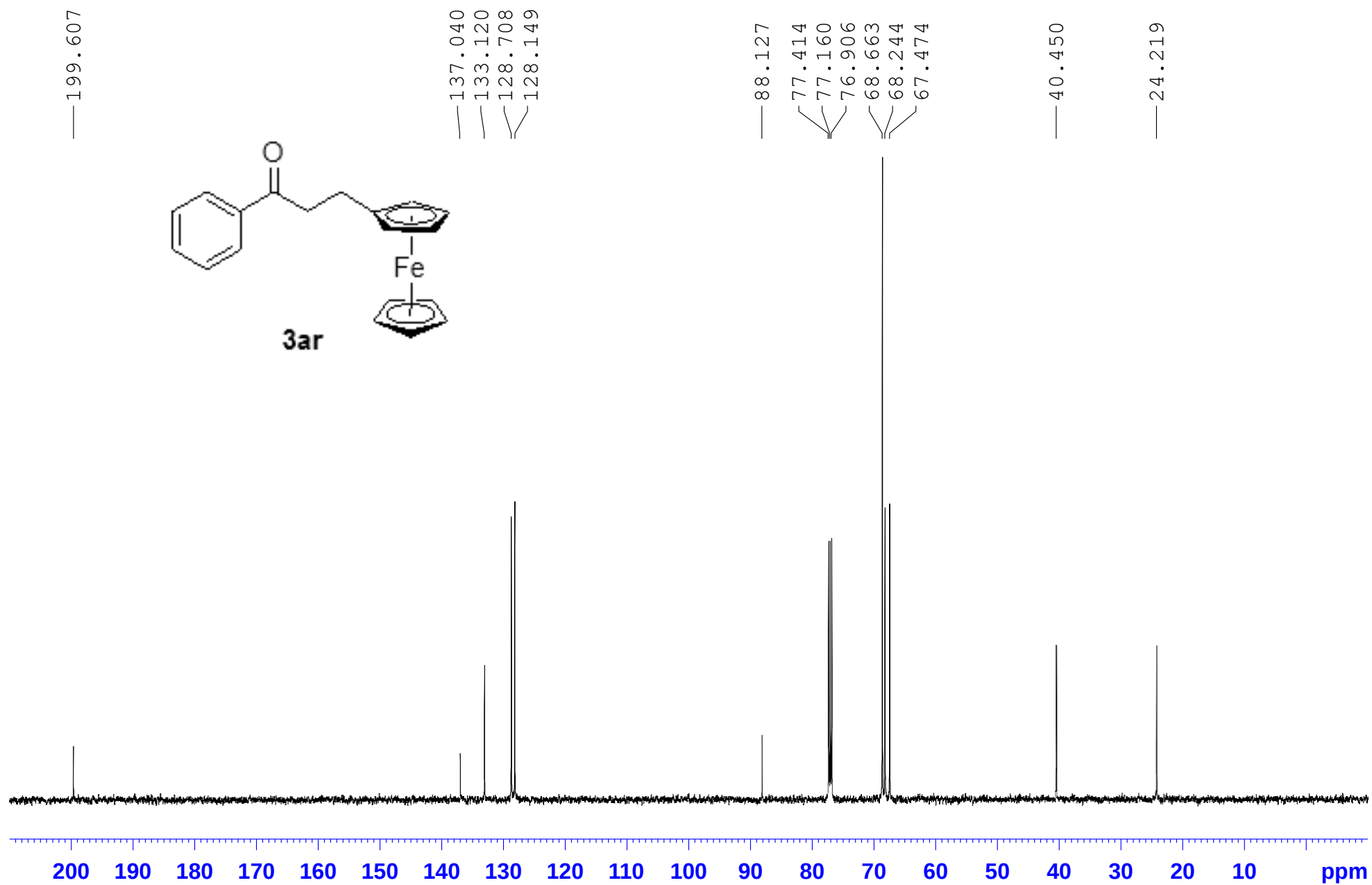
1-phenyl-3-(thiophen-2-yl)propan-1-one
e C13CPD CDC13



3-Ferrocenyl-1-phenylpropan-1-one
 e Proton CDCl₃

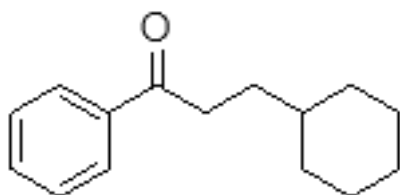


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 e C13CPD CDCl3



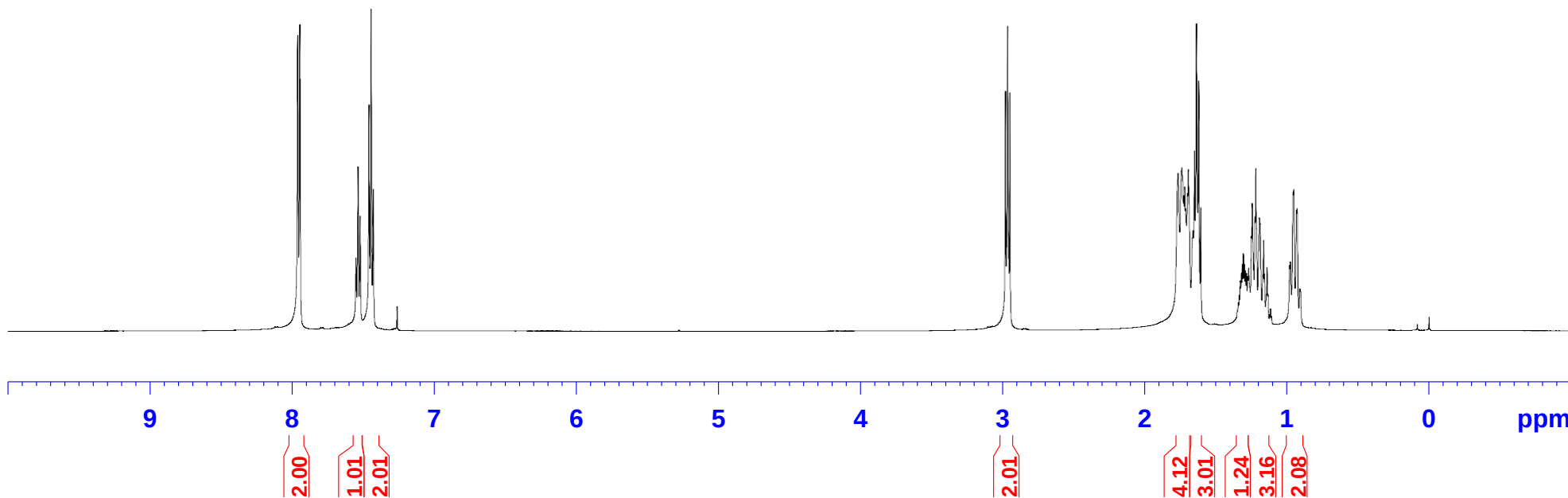
3-cyclohexyl-1-phenylpropan-1-one
 e Proton CDCl₃

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 7.945
 7.943
 7.550
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 7.520
 7.458
 7.443
 7.428
 7.260

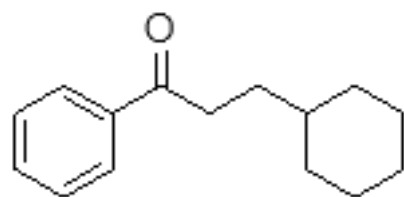


3as

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 1.636
 1.620
 1.306
 1.249
 1.243
 1.224
 1.218
 1.192
 1.188
 1.163
 1.139
 0.980
 0.975
 0.955
 0.950
 0.931
 0.927
 0.908
 0.903



3-cyclohexyl-1-phenylpropan-1-one
e C13CPD CDC13



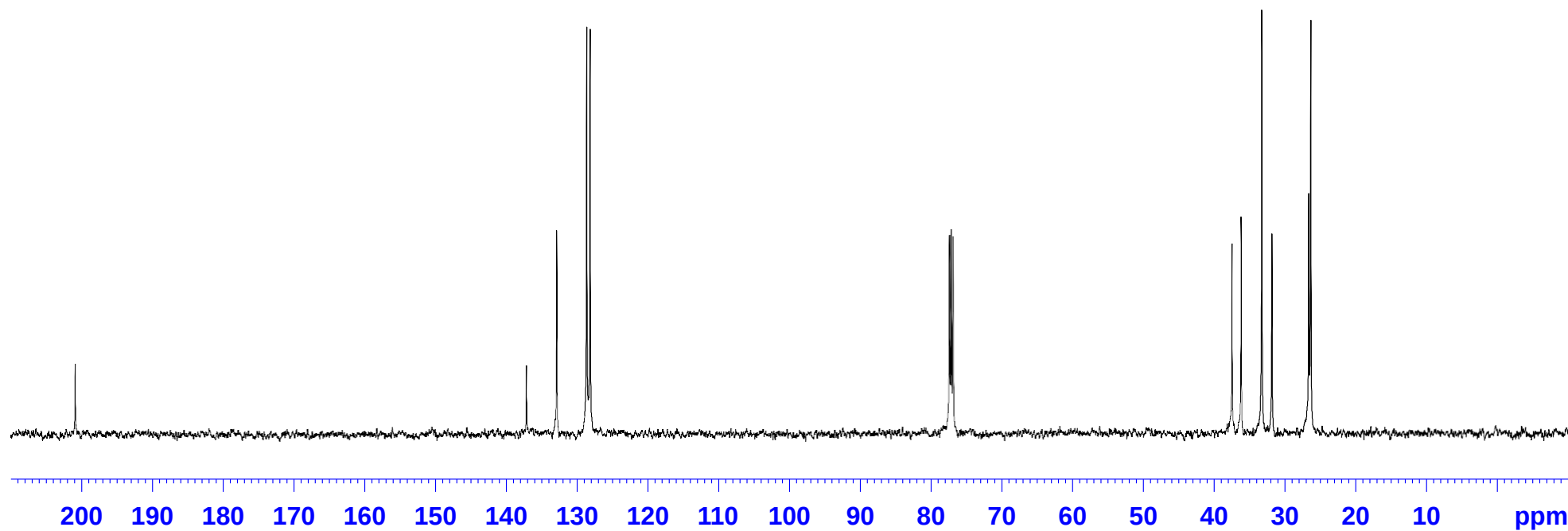
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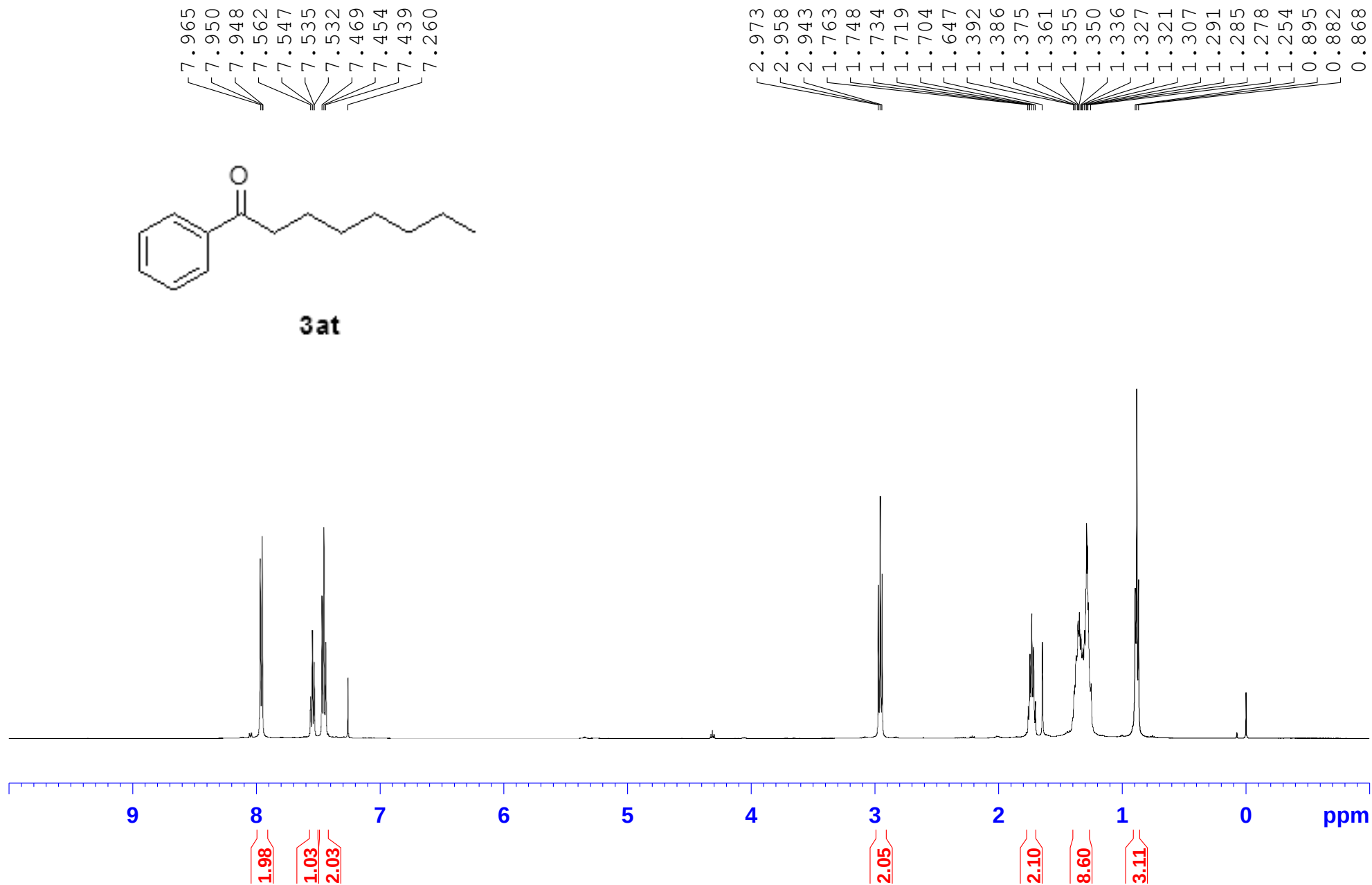
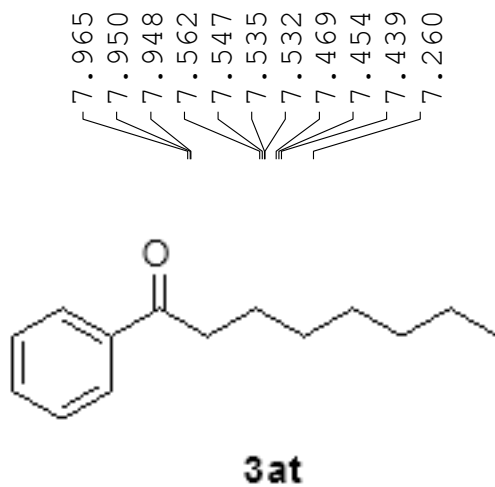
— 137.183
— 132.908
— 128.619
— 128.141

77.413
77.159
76.905

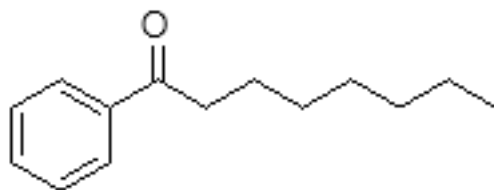
37.530
36.240
33.298
31.873
26.667
26.380



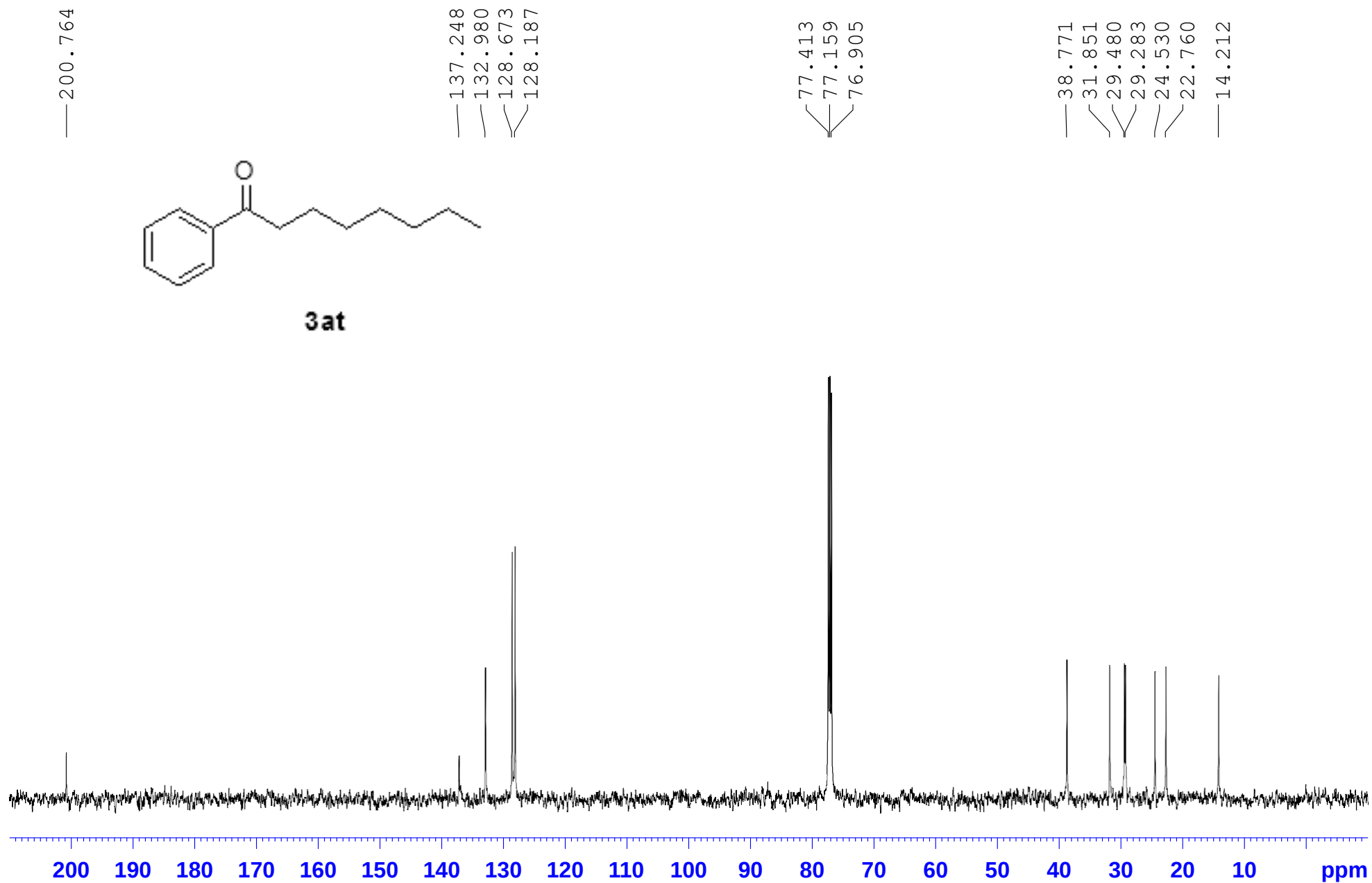
1-phenyloctan-1-on
e Proton CDCl₃



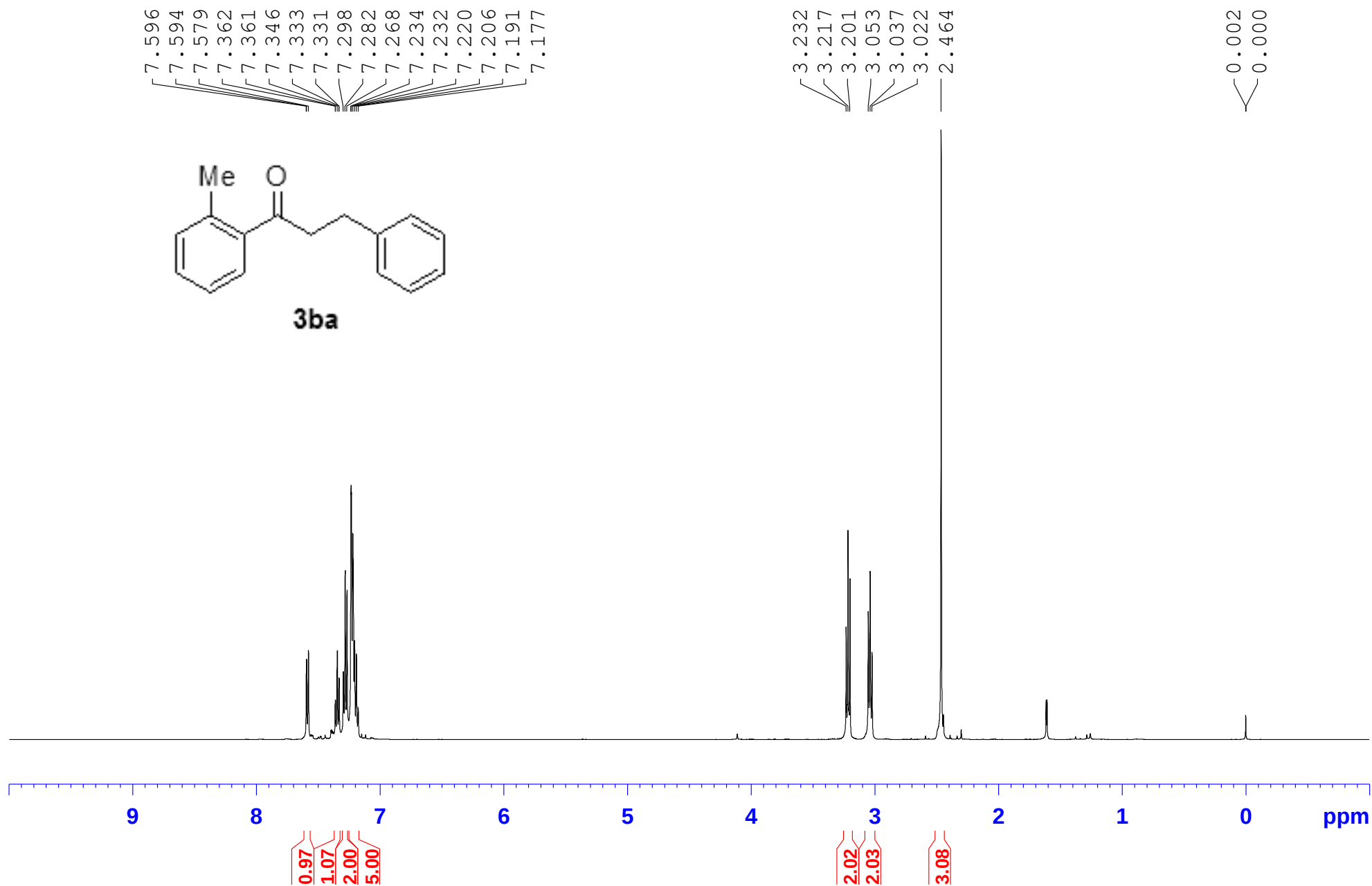
1-phenyloctan-1-one
e C13CPD CDC13



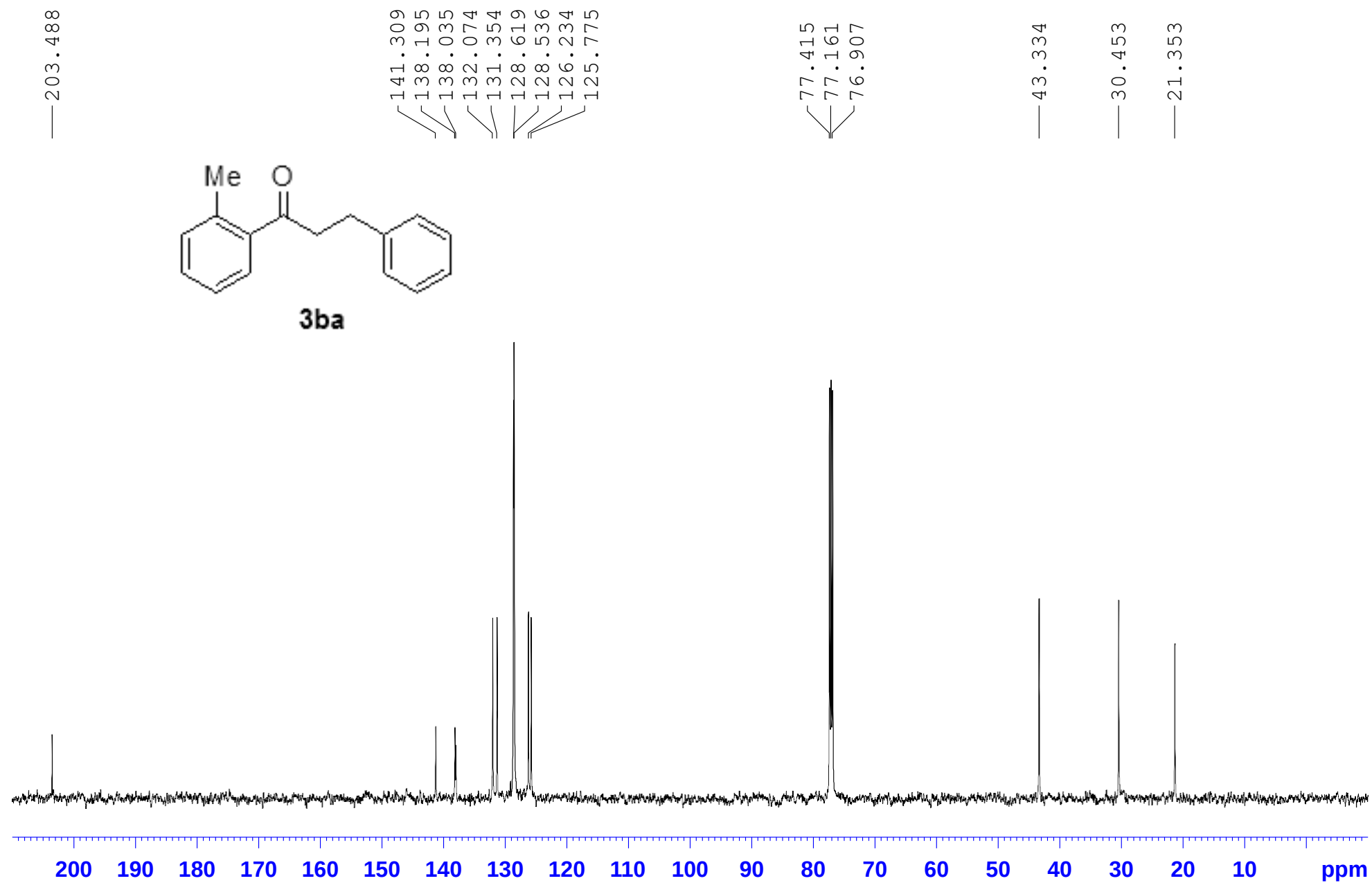
3at



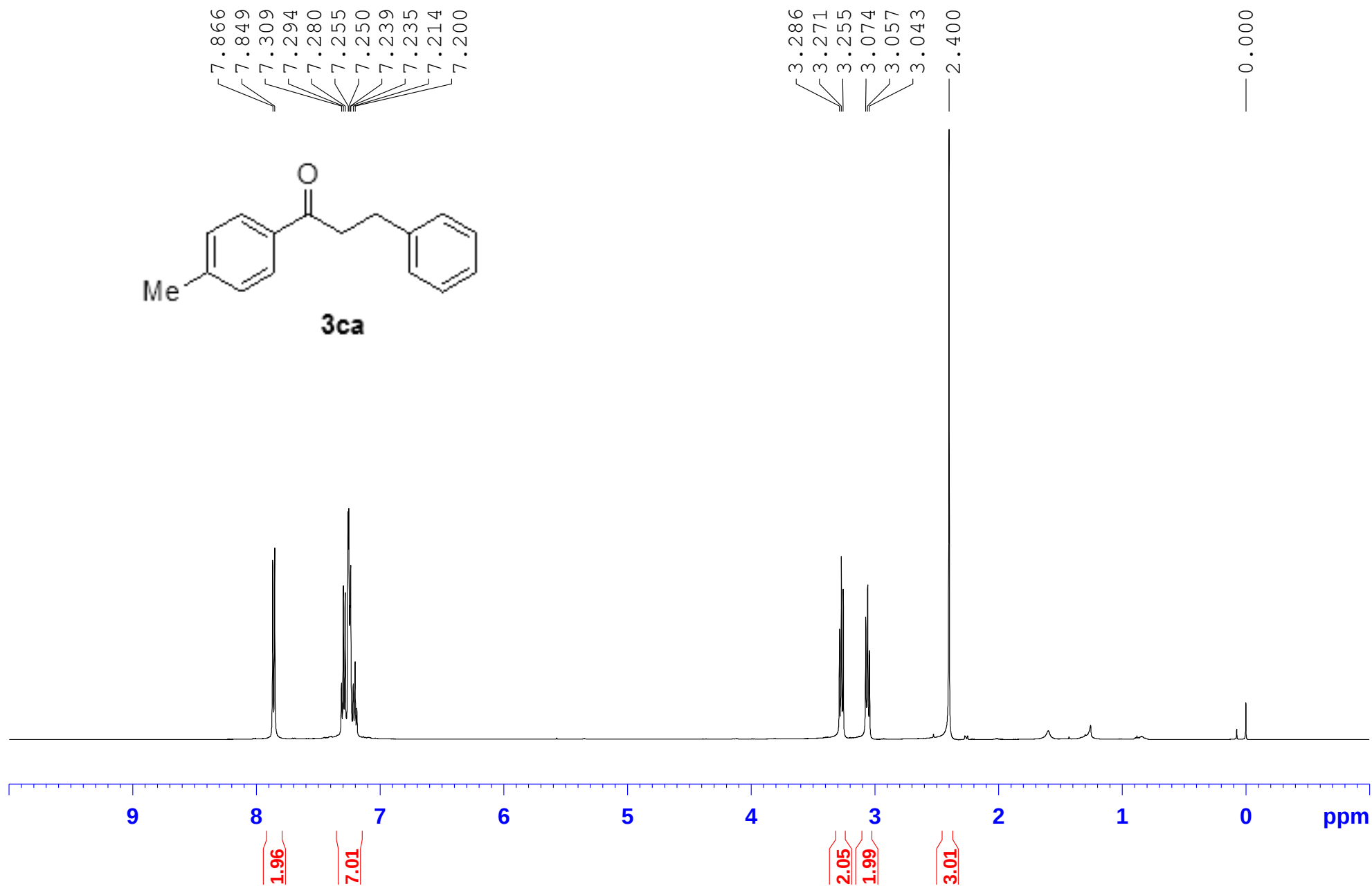
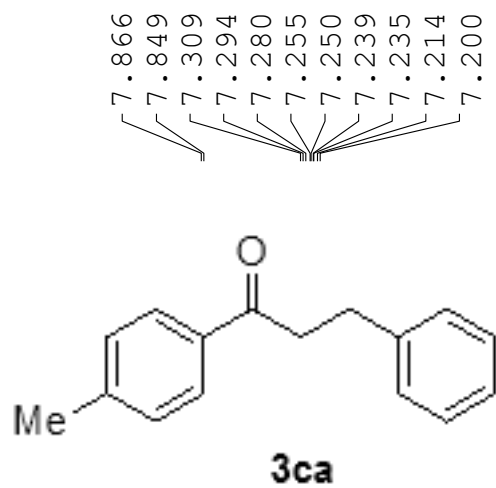
3-phenyl-1-o-tolylpropan-1-on
e Proton CDCl3



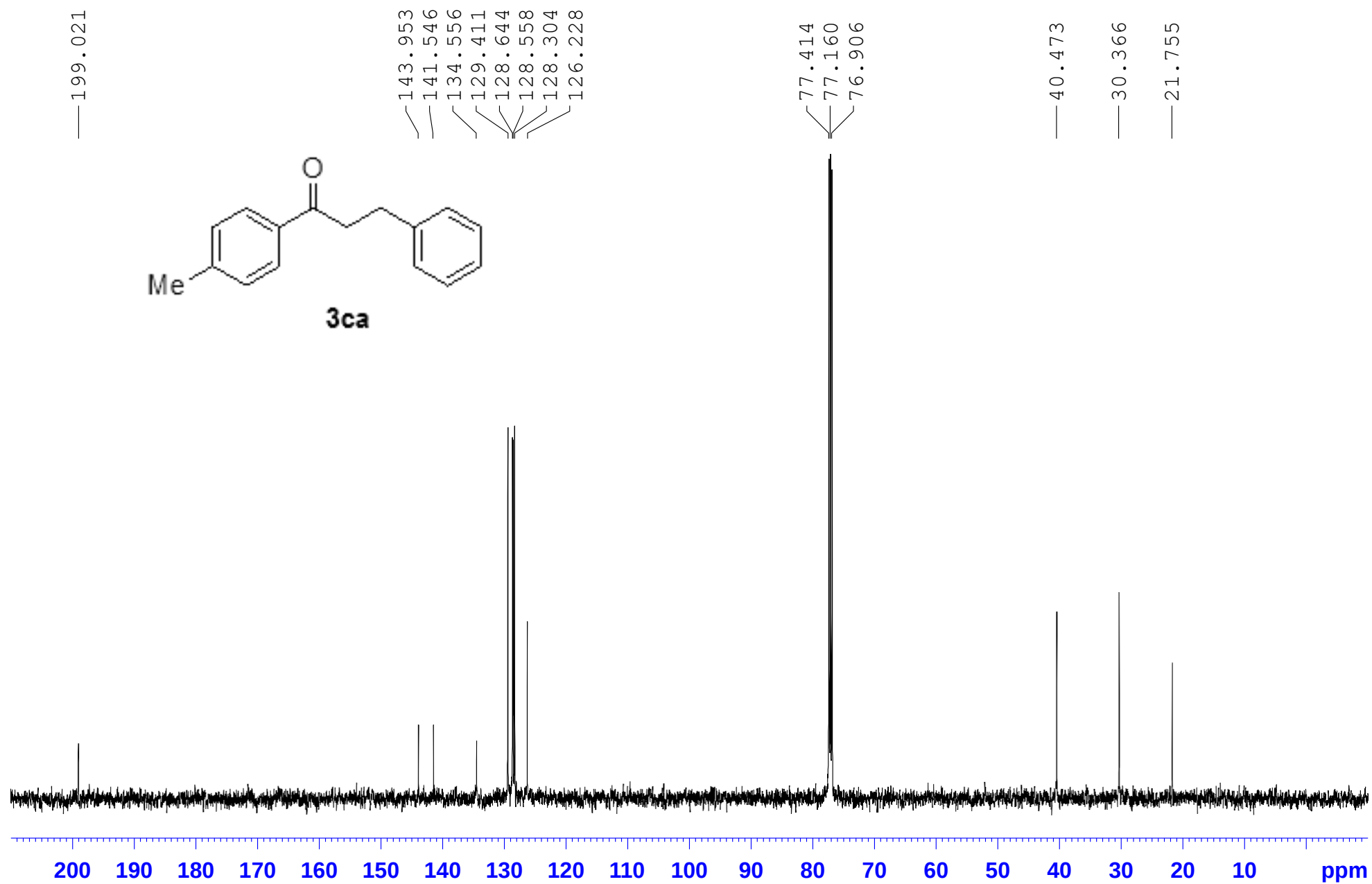
3-phenyl-1-o-tolylpropan-1-on
 e C13CPD CDC13



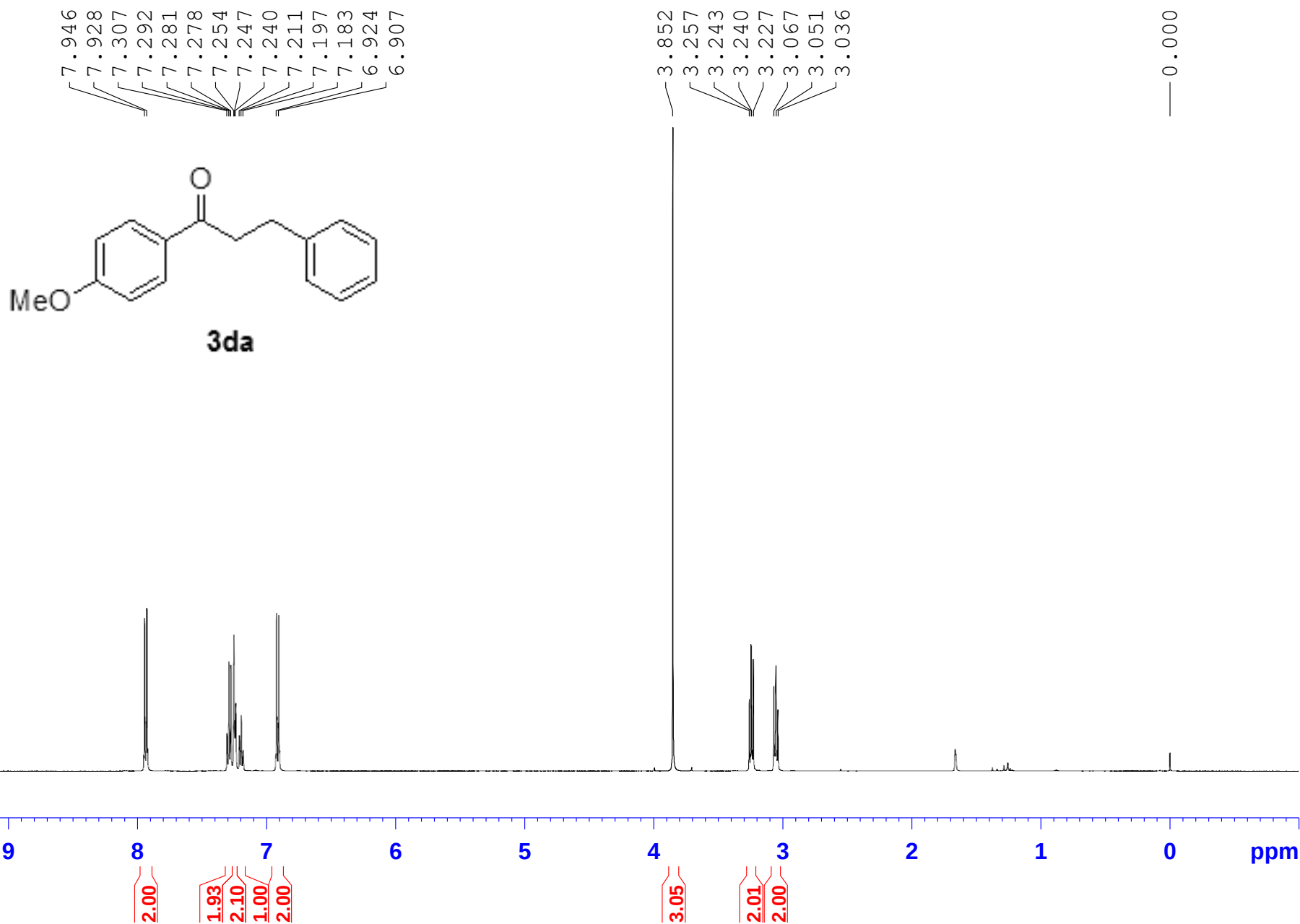
3-phenyl-1-p-tolylpropan-1-on
e Proton CDC13



3-phenyl-1-p-tolylpropan-1-one
e C13CPD CDC13



1-(4-methoxyphenyl)-3-phenylpropan-1-one
 e Proton CDCl₃



1-(4-methoxyphenyl)-3-phenylpropan-1-one
e C13CPD CDC13

— 197.938

— 163.562

— 141.582

130.418

130.083

128.615

128.542

126.194

— 113.841

77.413

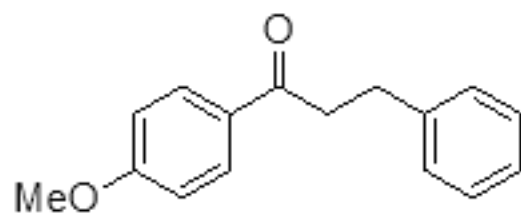
77.159

76.905

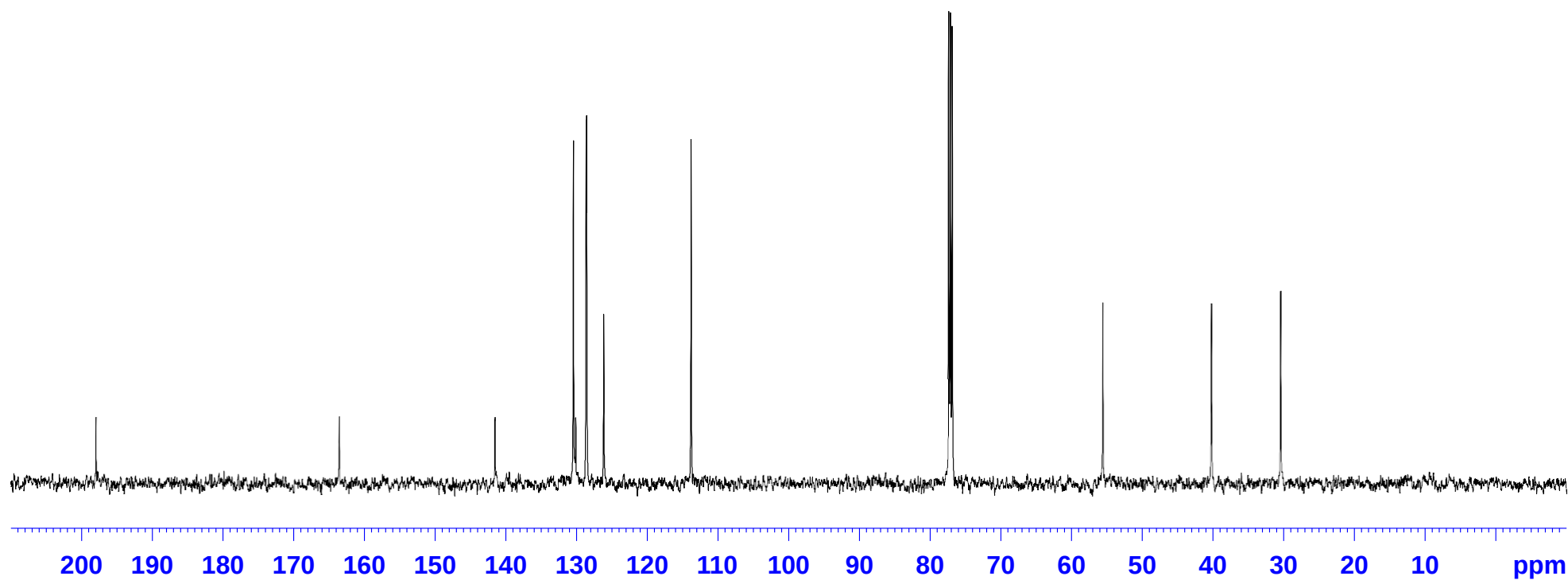
— 55.571

— 40.226

— 30.446



3da

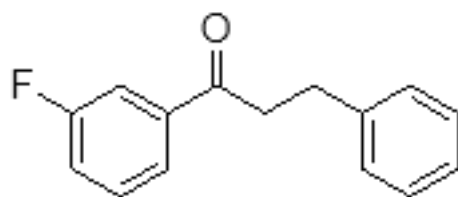


1-(3-fluorophenyl)-3-phenylpropan-1-one
 e Proton CDCl₃

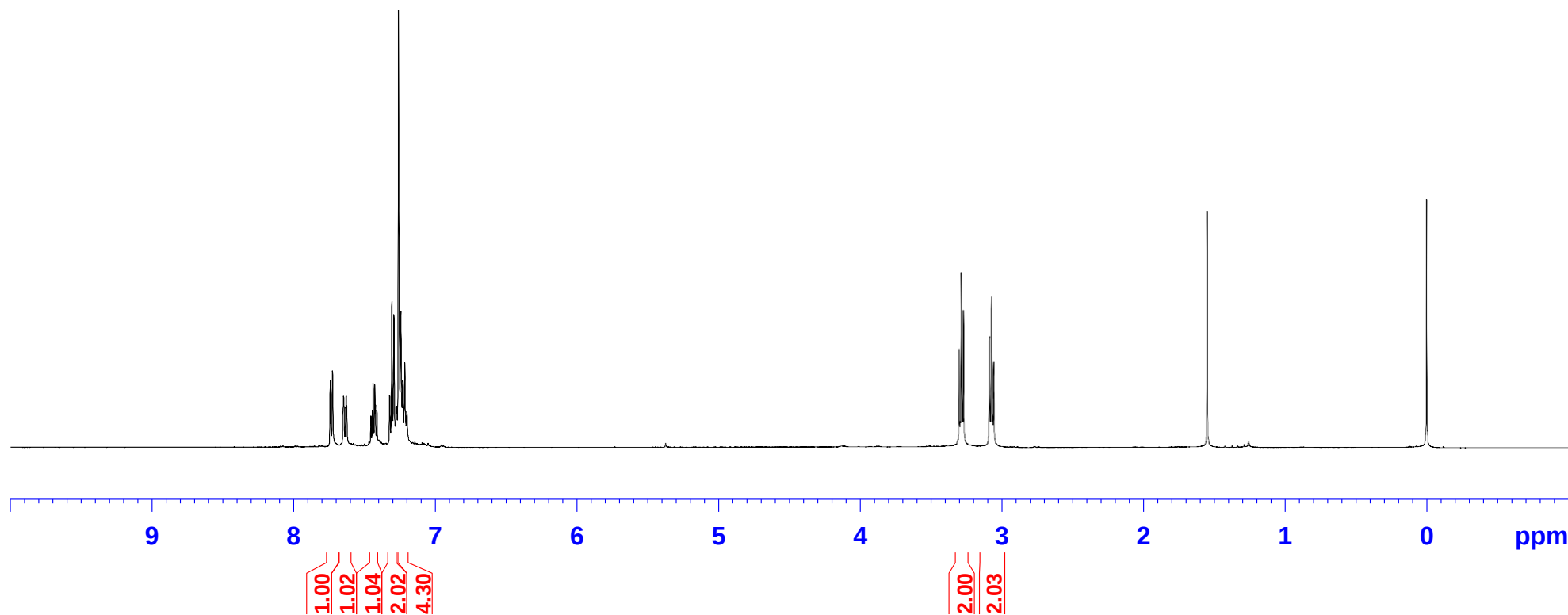
7.741
7.725
7.652
7.648
7.644
7.633
7.629
7.625
7.454
7.443
7.438
7.427
7.423
7.411
7.322
7.306
7.292
7.260
7.243
7.229
7.215
7.201

3.301
3.286
3.270
3.087
3.072
3.057

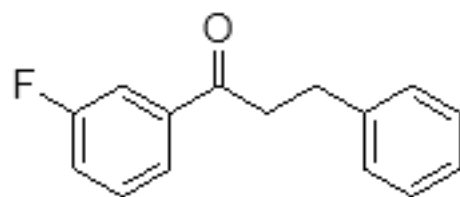
— 0.002



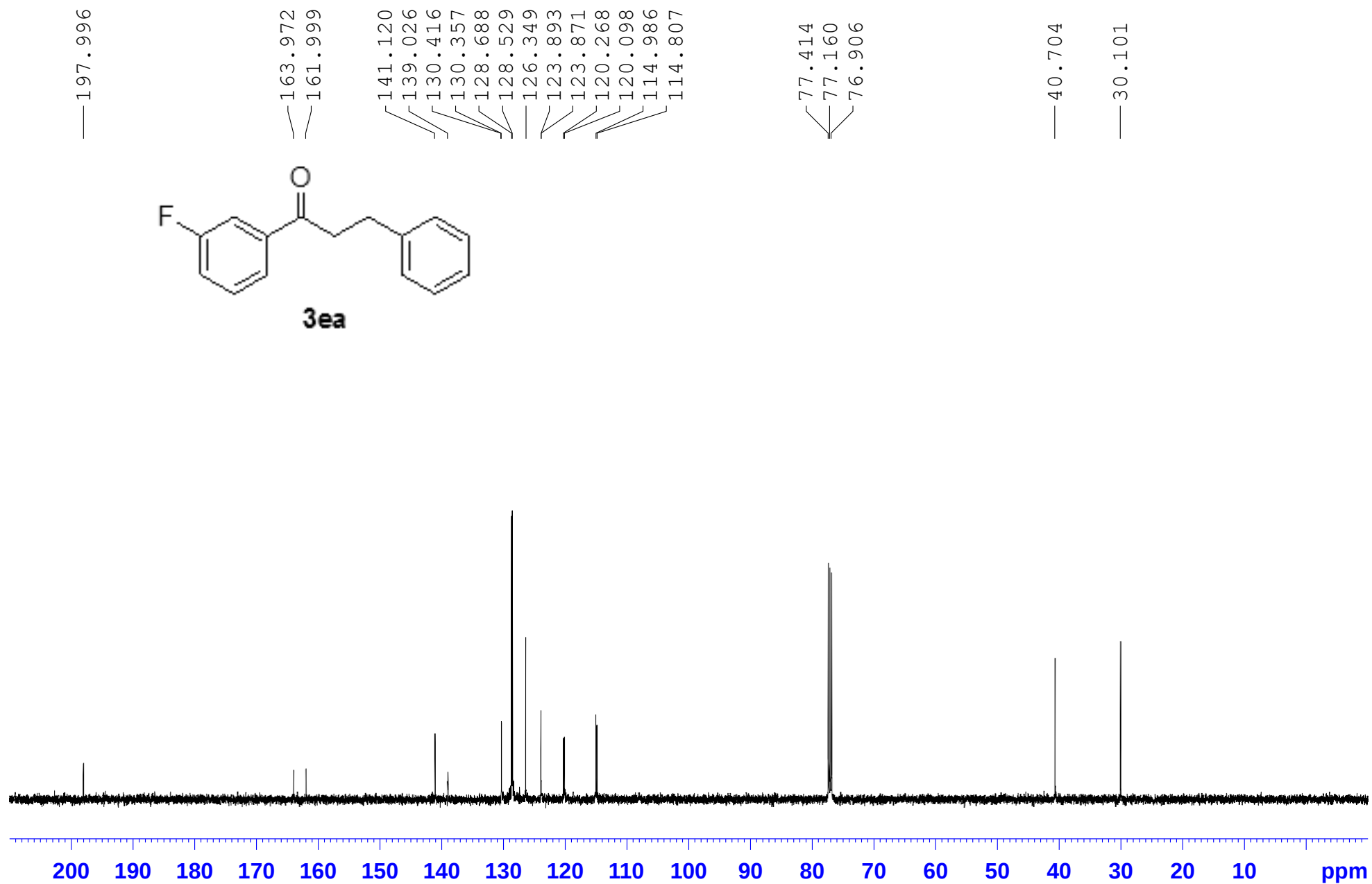
3ea



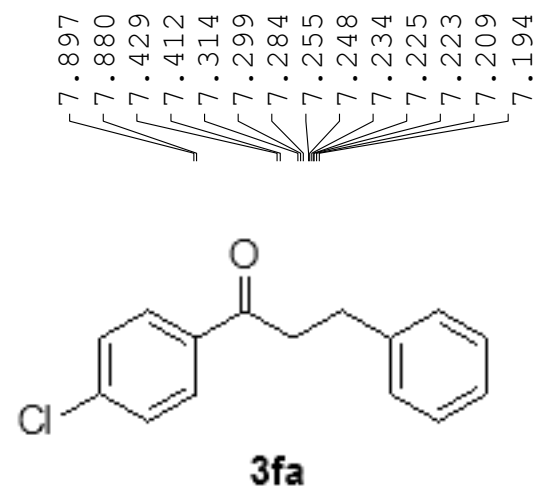
1-(3-fluorophenyl)-3-phenylpropan-1-one
 e C13CPD CDC13



3ea

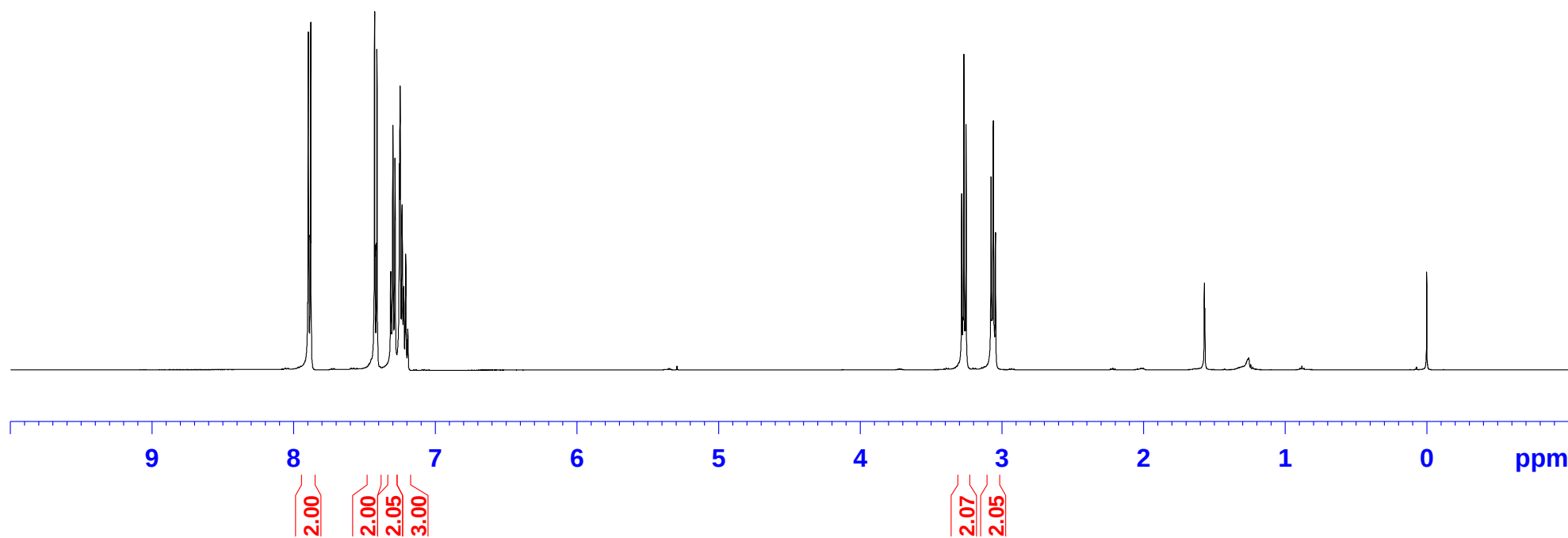


1-(4-chlorophenyl)-3-phenylpropan-1-one
e Proton CDCl₃

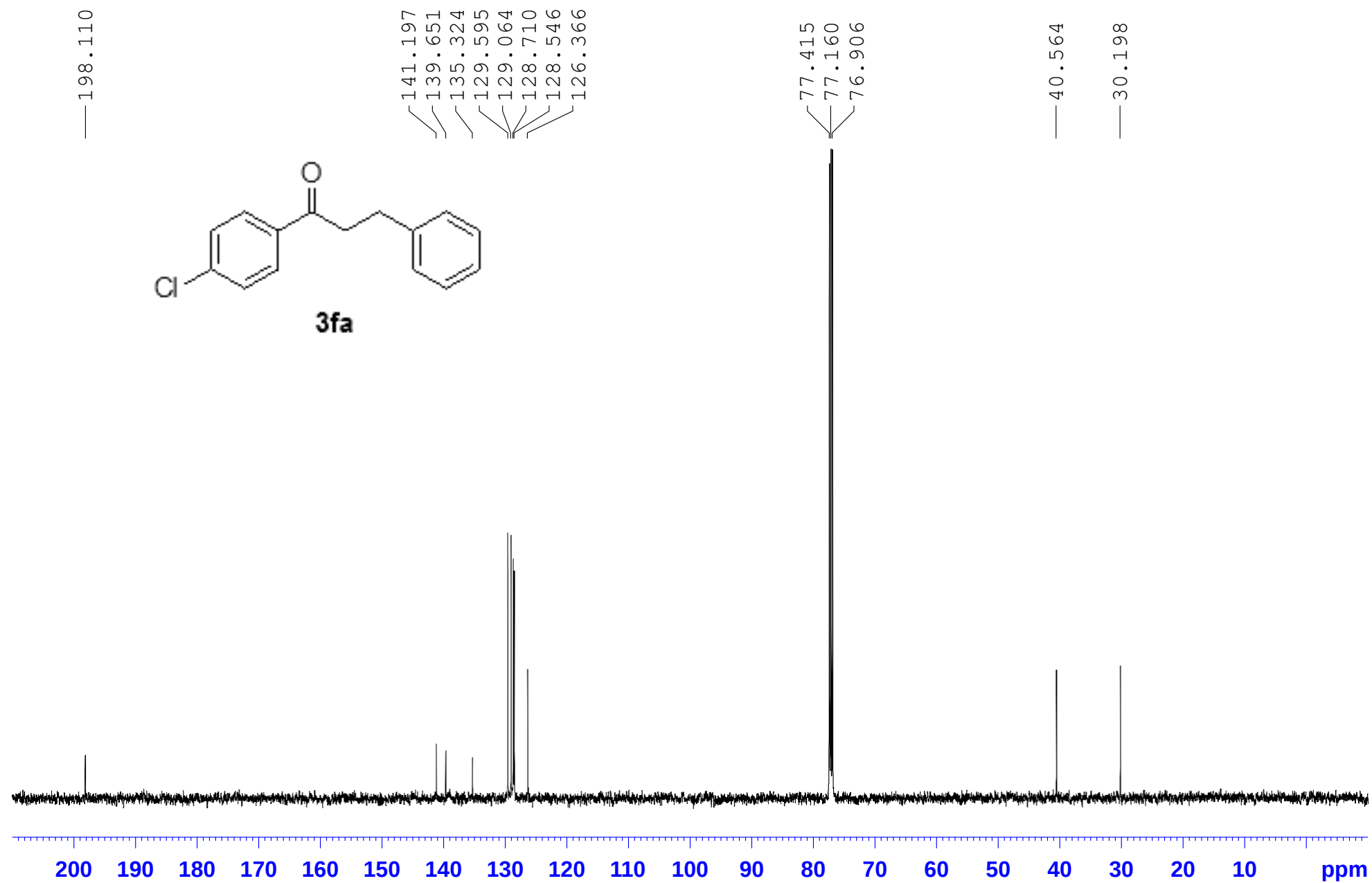


3.283
3.268
3.252
3.076
3.060
3.045

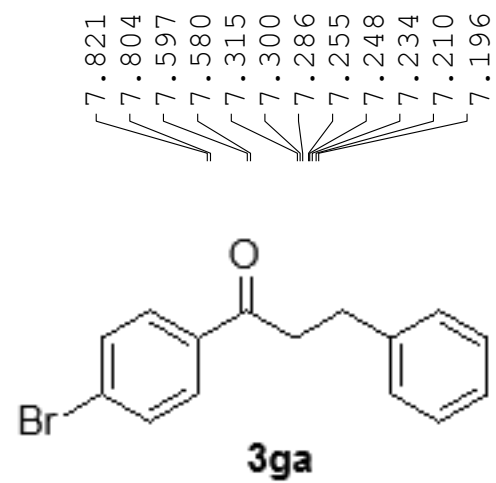
— 0.000



1-(4-chlorophenyl)-3-phenylpropan-1-one
e C13CPD CDC13

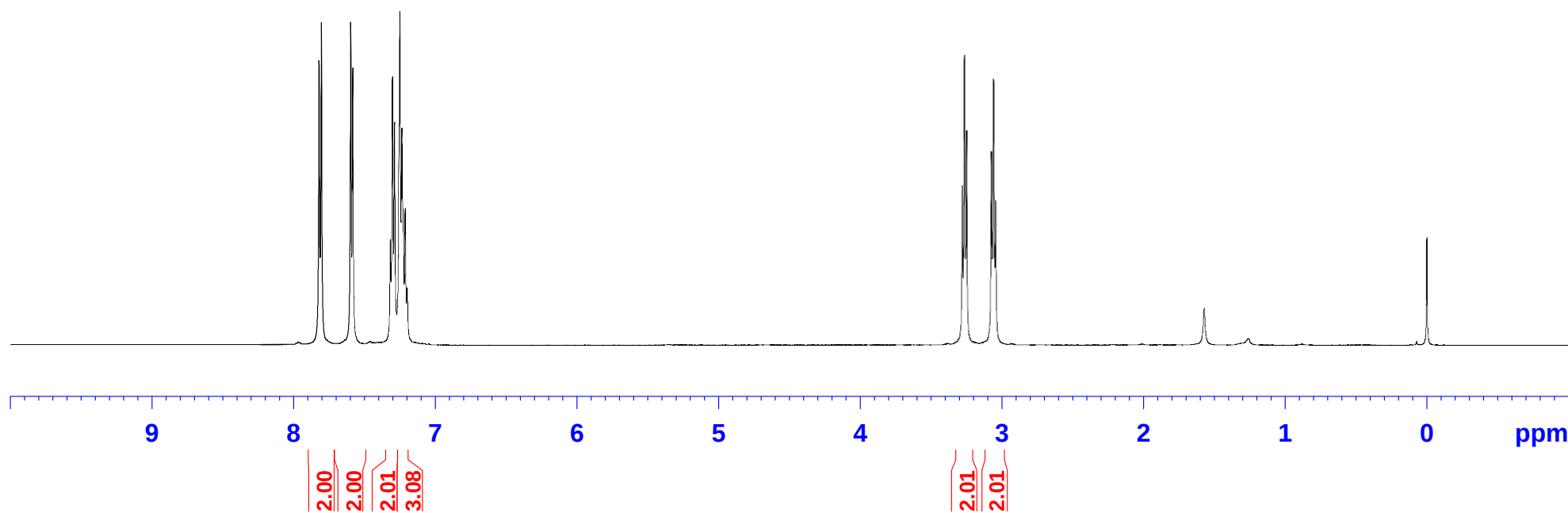


1-(4-bromophenyl)-3-phenylpropan-1-one
 e Proton CDCl₃

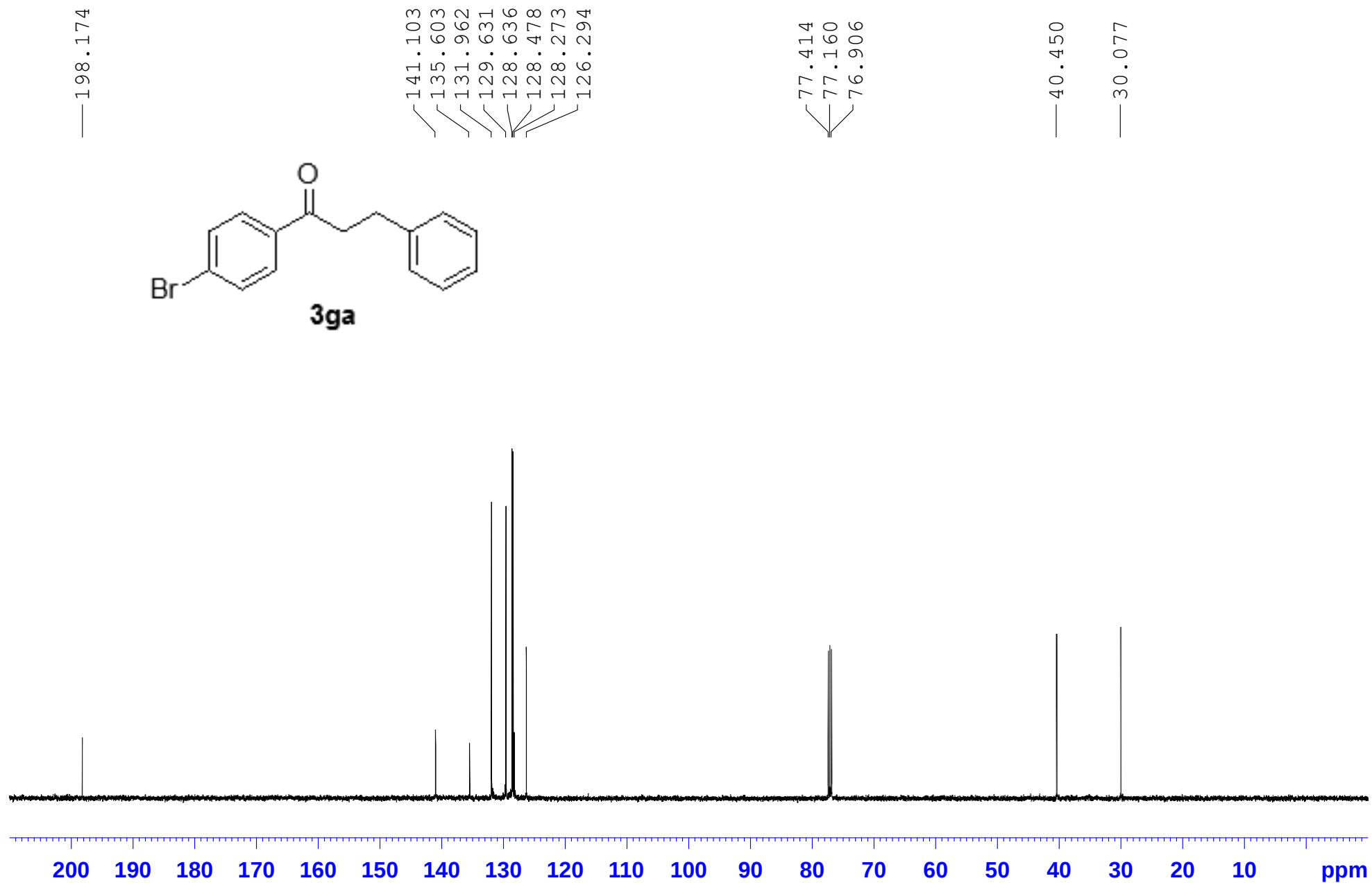
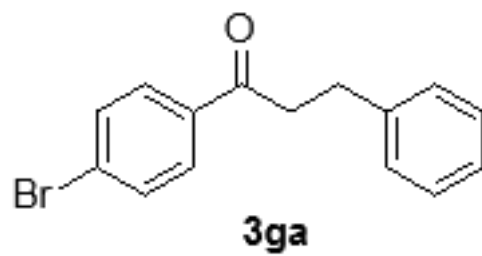


3.278
3.264
3.248
3.074
3.058
3.043

— 0.000



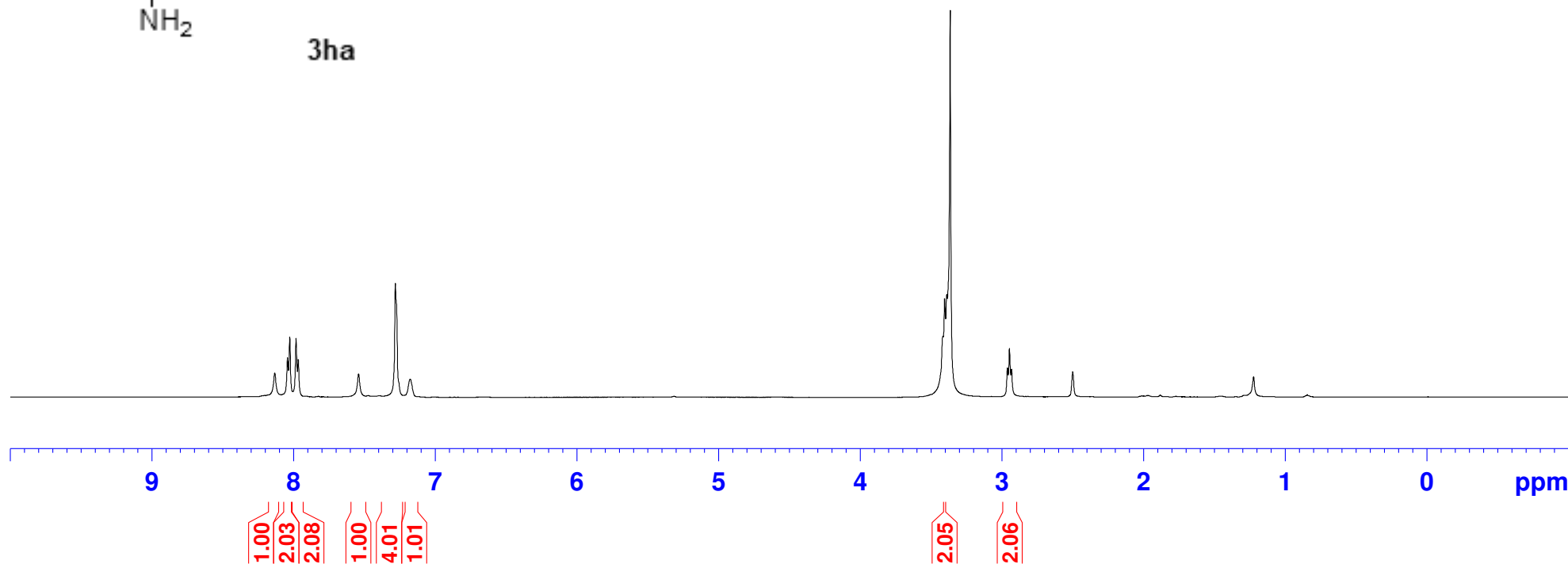
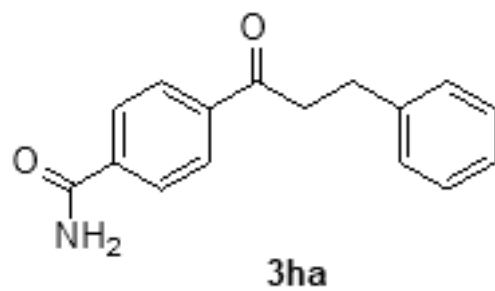
1-(4-bromophenyl)-3-phenylpropan-1-on
e C13CPD CDC13



4-(1-Oxo-3-phenylpropyl)benzamide
Proton DMSO

8.133
8.043
8.027
7.983
7.967
7.541
7.282
7.175

3.416
3.404
3.389
2.961
2.946
2.932
2.500



4-(1-Oxo-3-phenylpropyl)benzamide
C13CPD DMSO

—199.078

—167.221

141.218

138.578

138.133

128.481

128.357

127.952

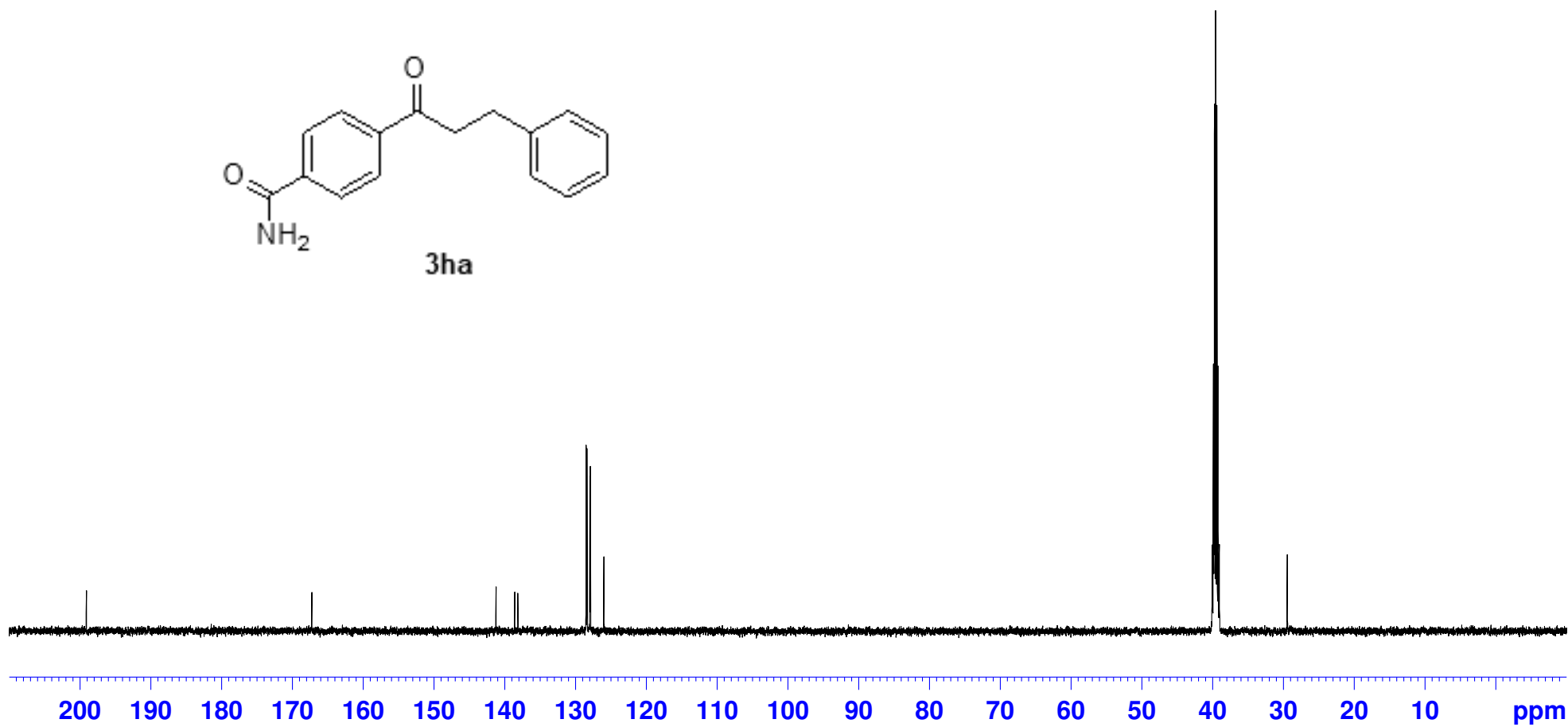
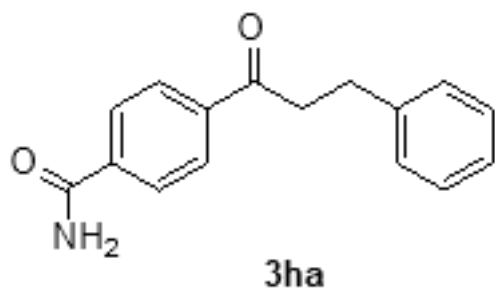
127.875

125.971

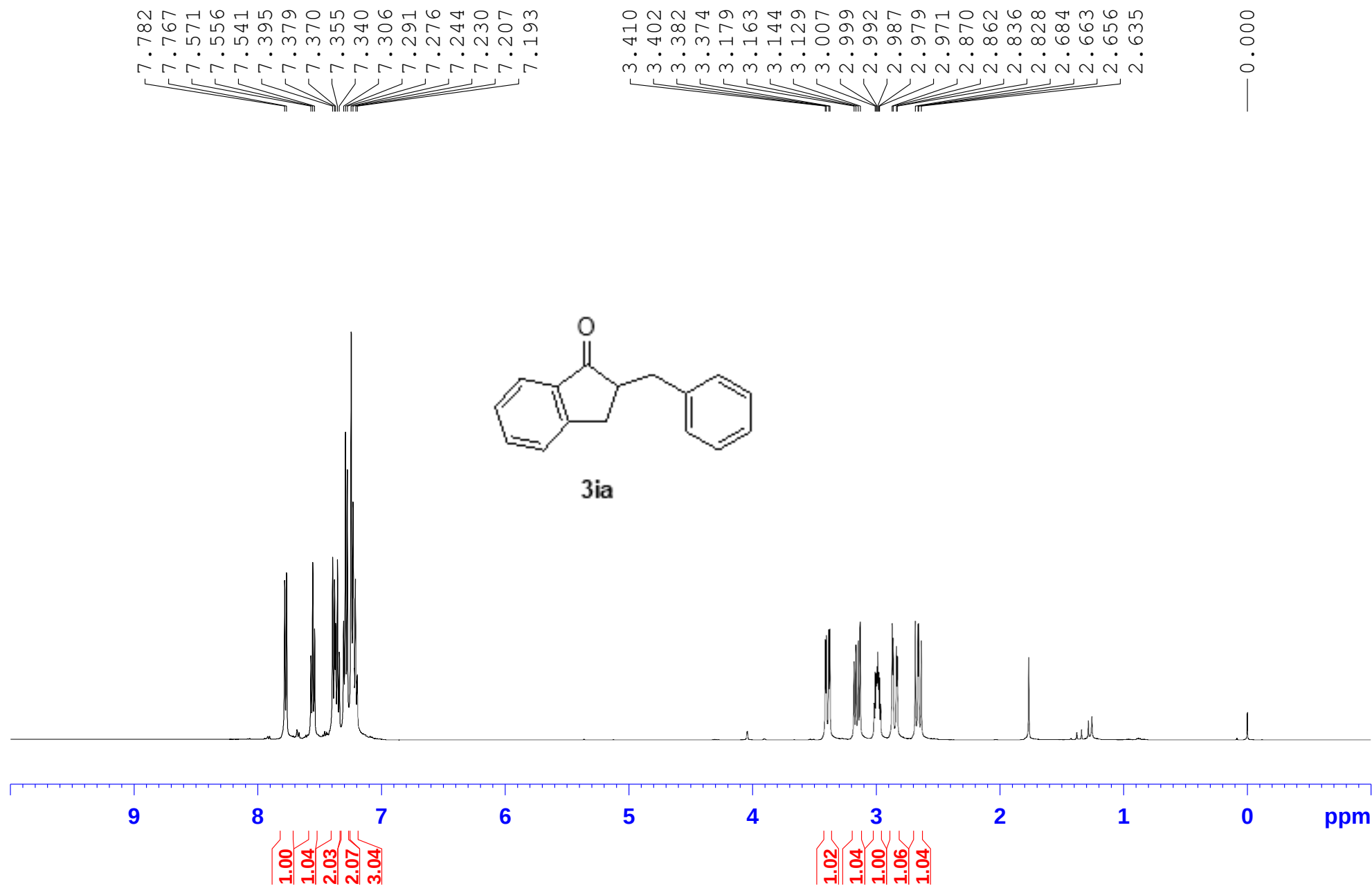
39.834

39.600

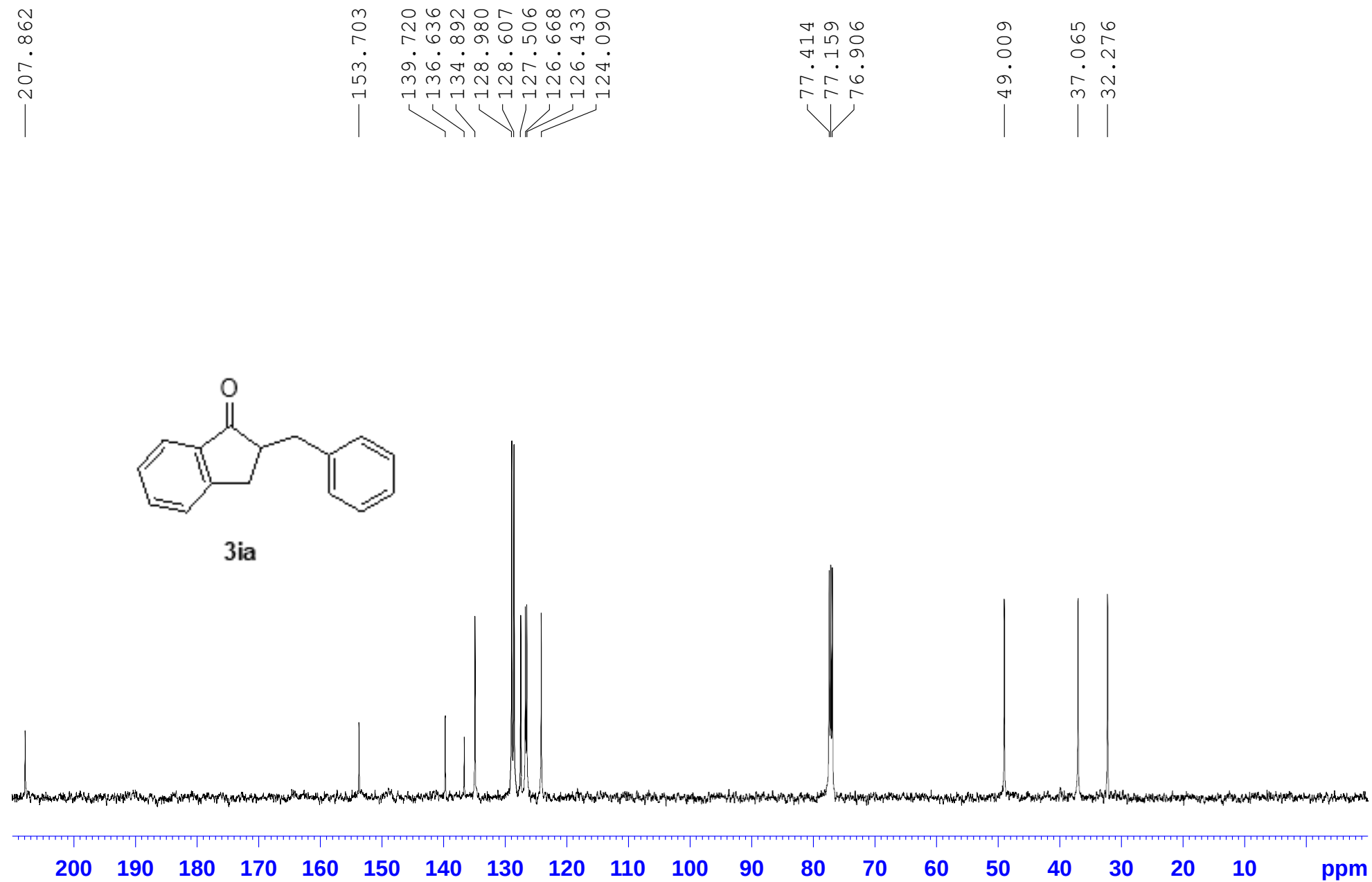
—29.492



2-benzyl-2,3-dihydroinden-1-one
 e Proton CDCl₃



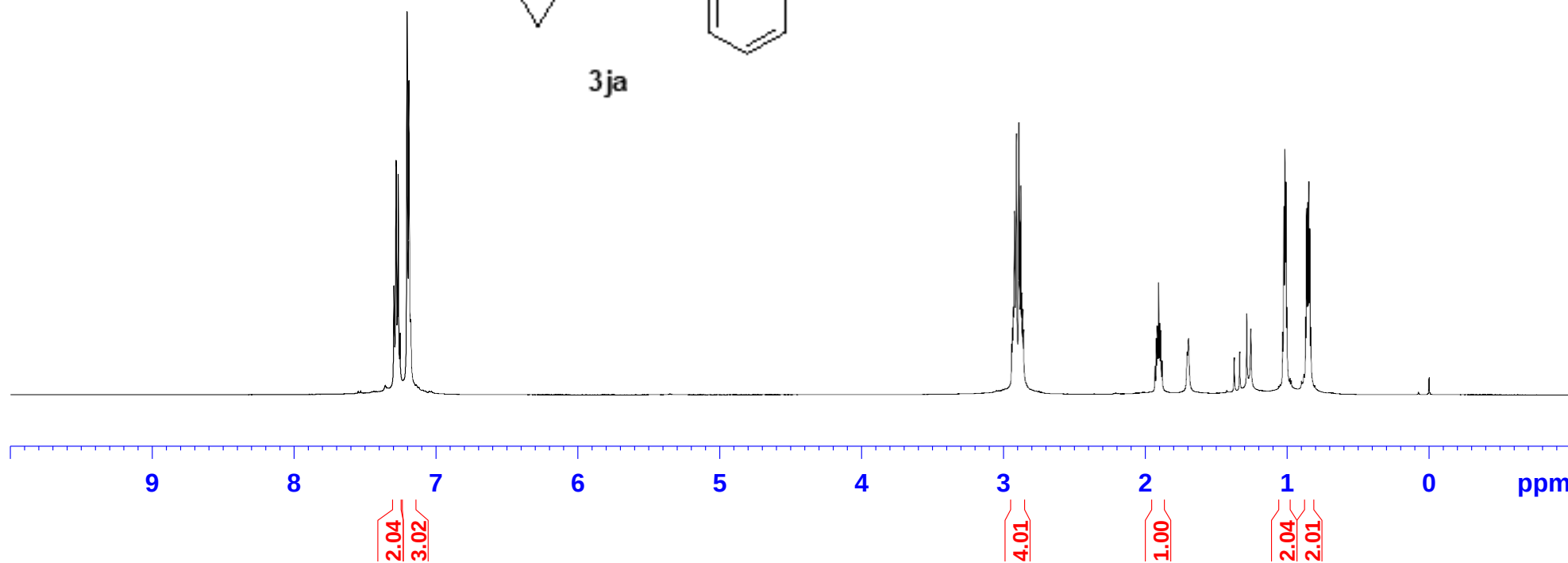
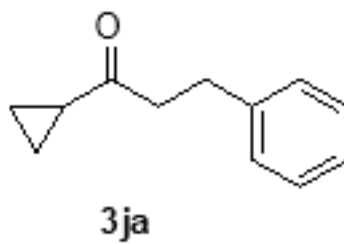
2-benzyl-2,3-dihydroinden-1-one
e C13CPD CDC13



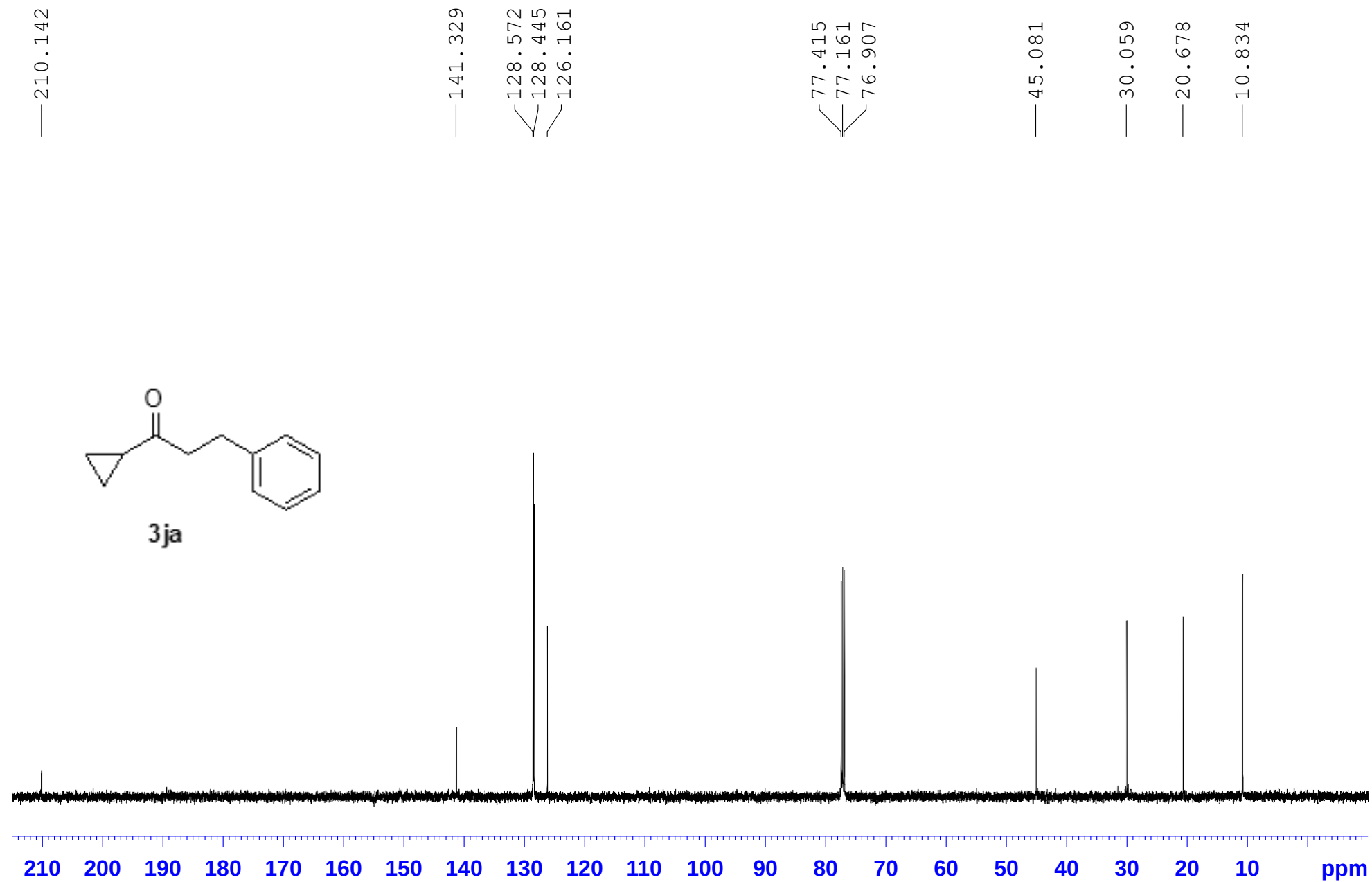
1-cyclopropyl-3-phenylpropan-1-one
 e Proton CDCl₃

7.293
 7.278
 7.263
 7.201
 7.187

2.921
 2.908
 2.890
 2.876
 1.931
 1.922
 1.915
 1.906
 1.897
 1.890
 1.881
 1.023
 1.016
 1.008
 0.863
 0.856
 0.847
 0.840
 0.000

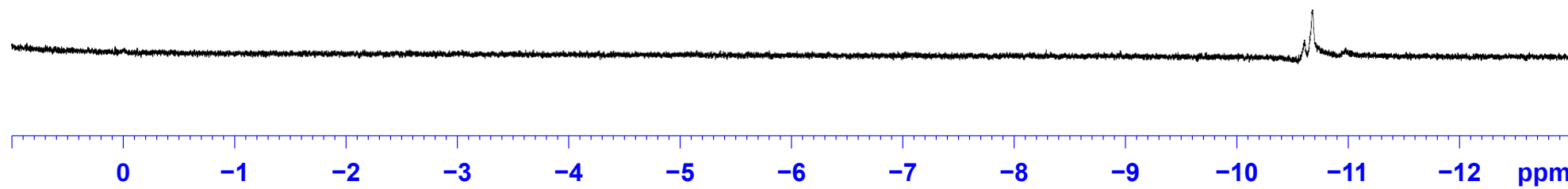


1-cyclopropyl-3-phenylpropan-1-one
e C13CPD CDC13

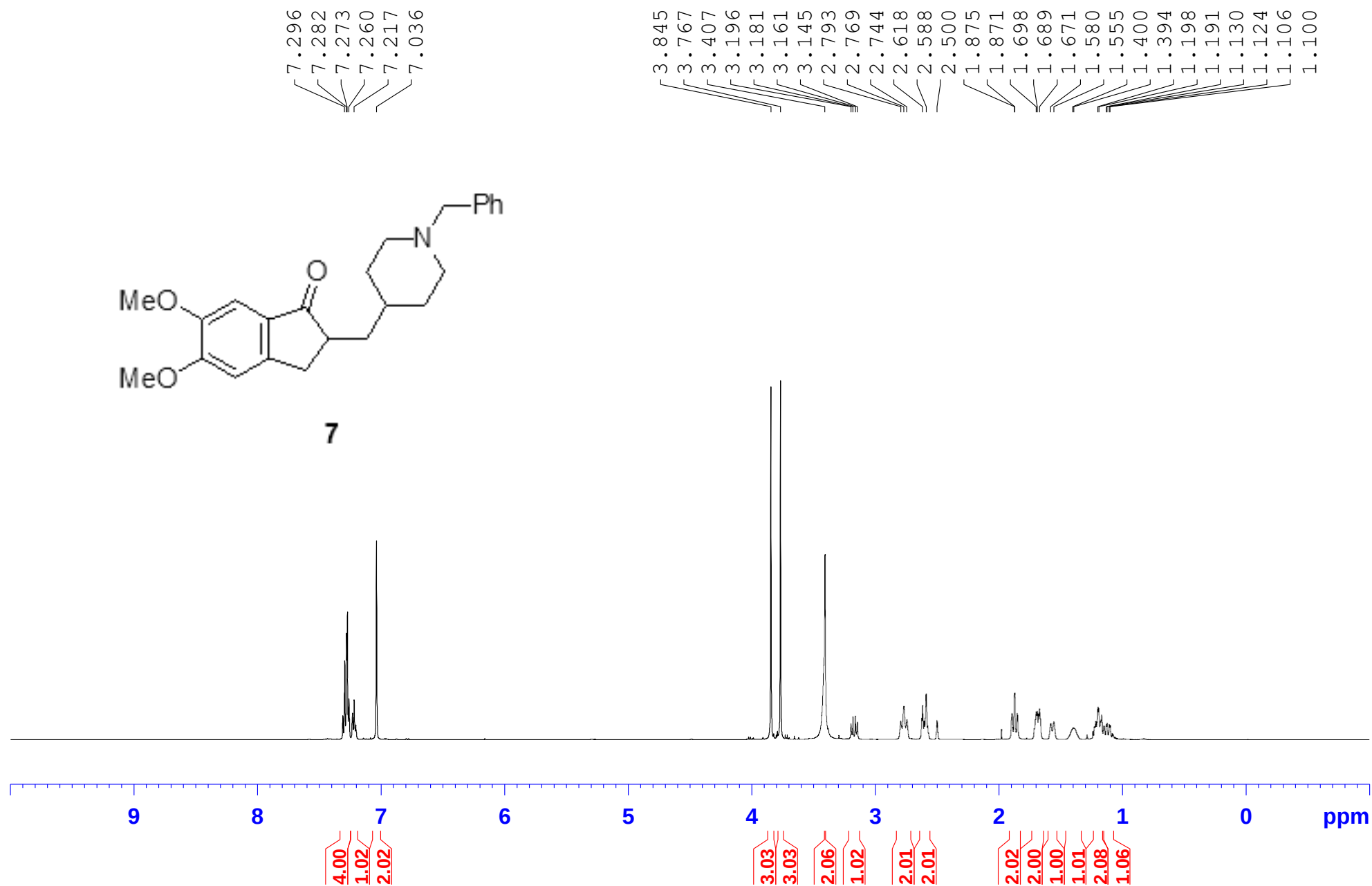


[Ir-H]
Proton D2O

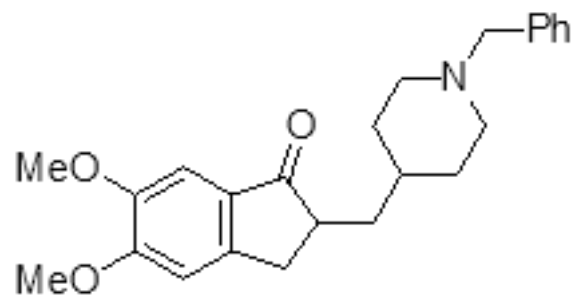
— -10.679



2-((1-benzylpiperidin-4-yl)methyl)-5,6-dimethoxy-2,3-dihydroinden-1-one
 e Proton DMSO-d₆



2-((1-benzylpiperidin-4-yl)methyl)-5,6-dimethoxy-2,3-dihydroinden-1-one
 e C13CPD DMSO-d6



7

