

Supporting Information for

**α -Alkylation of Ketones with Primary Alcohols Catalyzed by a Cp*Ir Complex
Bearing a Functional Bipyridonate Ligand**

Feng Li,* Juan Ma and Nana Wang

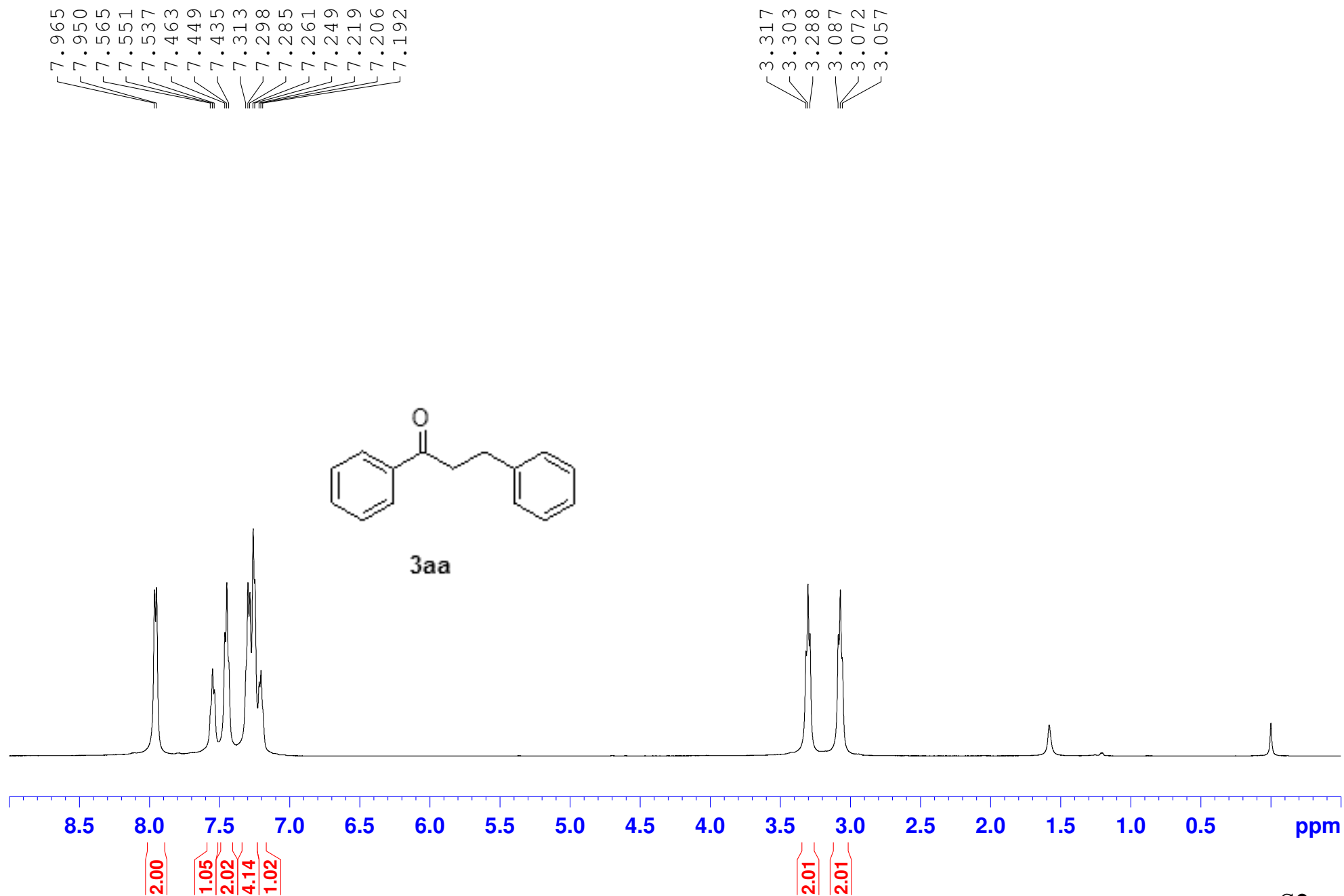
* E-mail: fengli@njust.edu.cn

Key Laboratory for Soft Chemistry and Functional Materials, Ministry of Education, Nanjing
University of Science and Technology, People's Republic of China

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The ^1H NMR and ^{13}C NMR spectra of all products	S2-S73
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1,3-diphenylpropan-1-one
Proton CDCl₃



1,3-diphenylpropan-1-one
C13CPD CDCl3

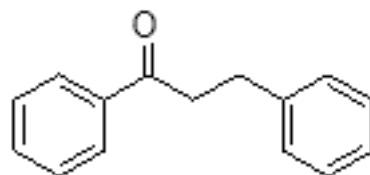
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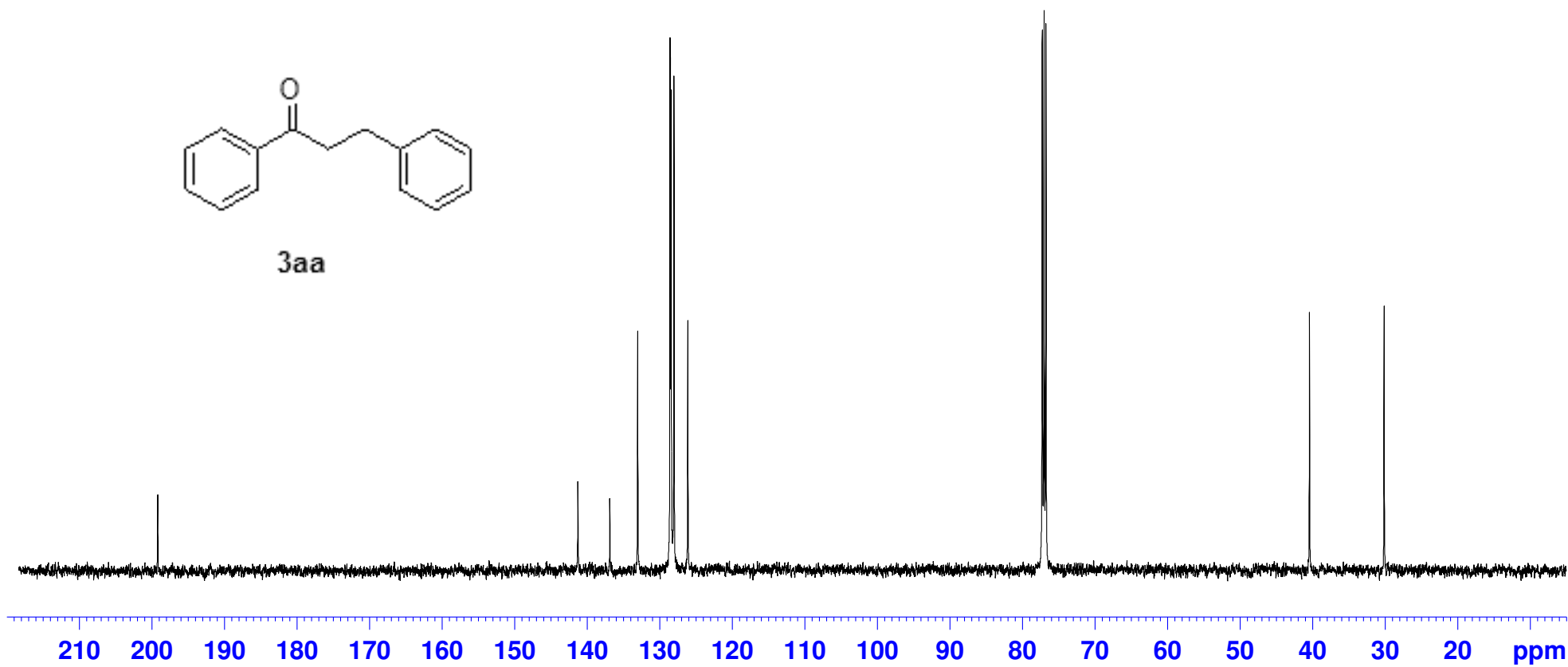
— 77.000

— 40.411

— 30.119



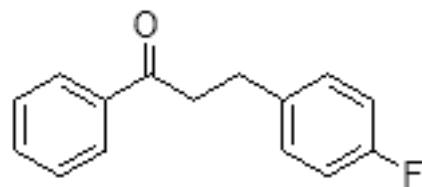
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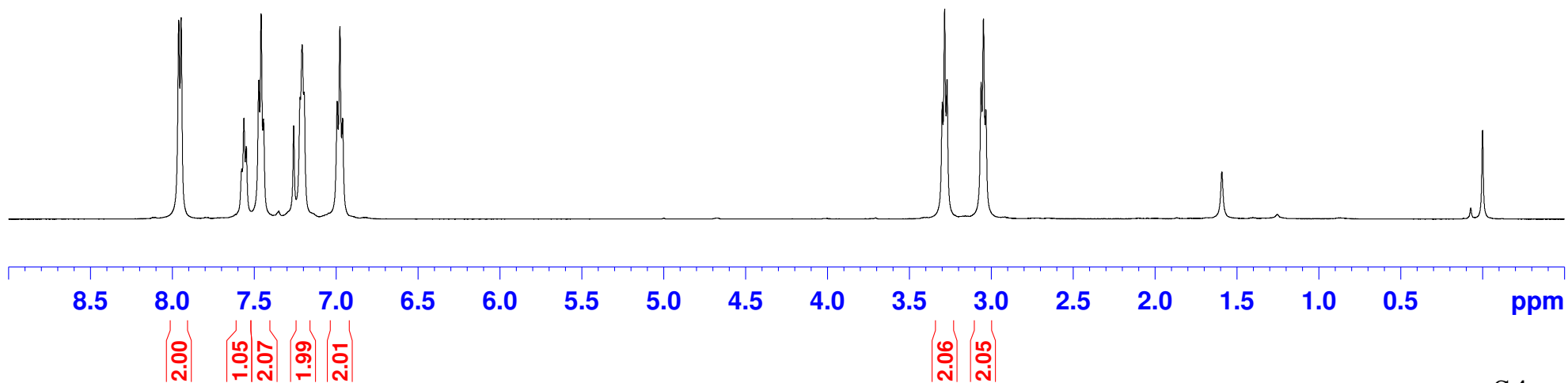
3-(4-fluorophenyl)-1-phenylpropan-1-one
Proton CDCl₃

7.962
7.947
7.577
7.564
7.550
7.473
7.458
7.444
7.259
7.221
7.208
7.197
6.994
6.977
6.961

3.299
3.285
3.270
3.062
3.048
3.033



3ab



3-(4-fluorophenyl)-1-phenylpropan-1-one
C13CPD CDCl3

— 198.976

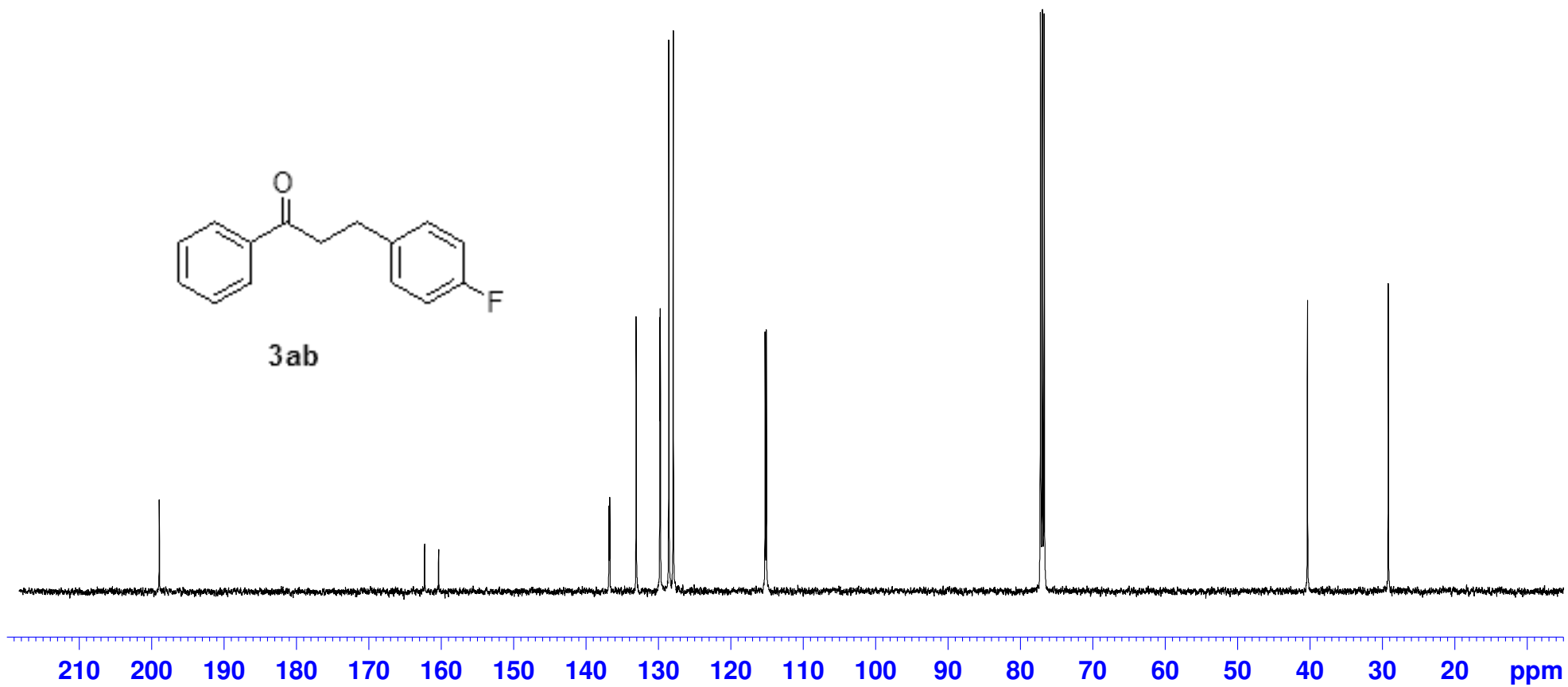
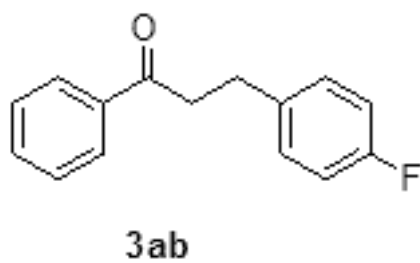
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— 160.388

— 136.843
— 136.748
— 133.103
— 129.827
— 129.766
— 128.595
— 127.975
— 115.290
— 115.124

— 77.000

— 40.380

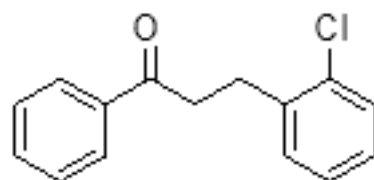
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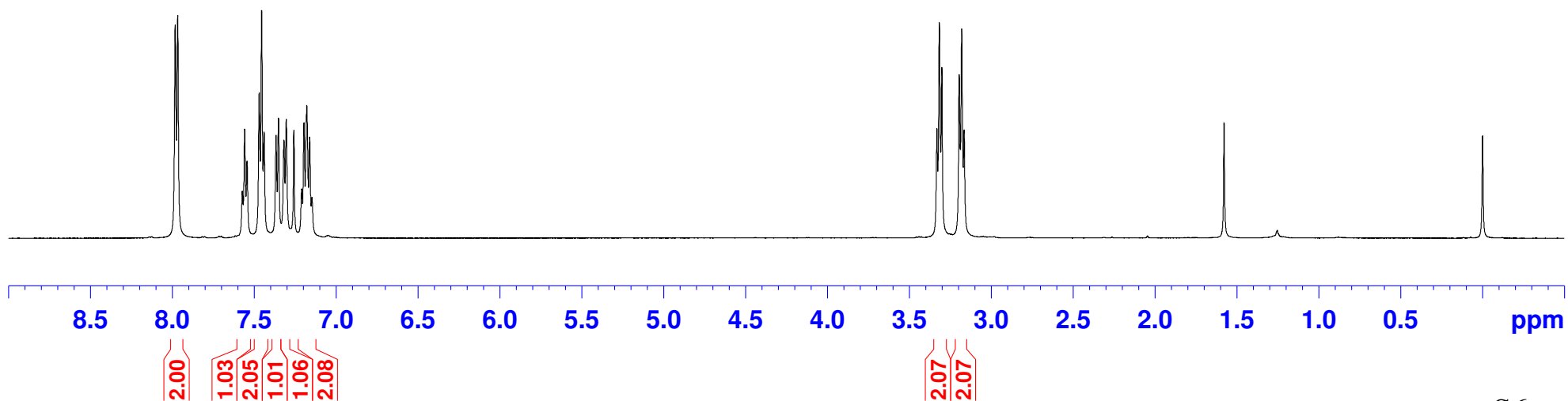
3-(2-chlorophenyl)-1-phenylpropan-1-one
Proton CDCl₃

7.981
7.965
7.573
7.559
7.545
7.471
7.455
7.441
7.368
7.353
7.319
7.305
7.258
7.211
7.197
7.180
7.163
7.148

3.332
3.317
3.302
3.196
3.181
3.166



3ac



3-(2-chlorophenyl)-1-phenylpropan-1-one
C13CPD CDCl3

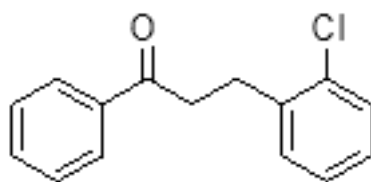
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130.776
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127.703
126.934

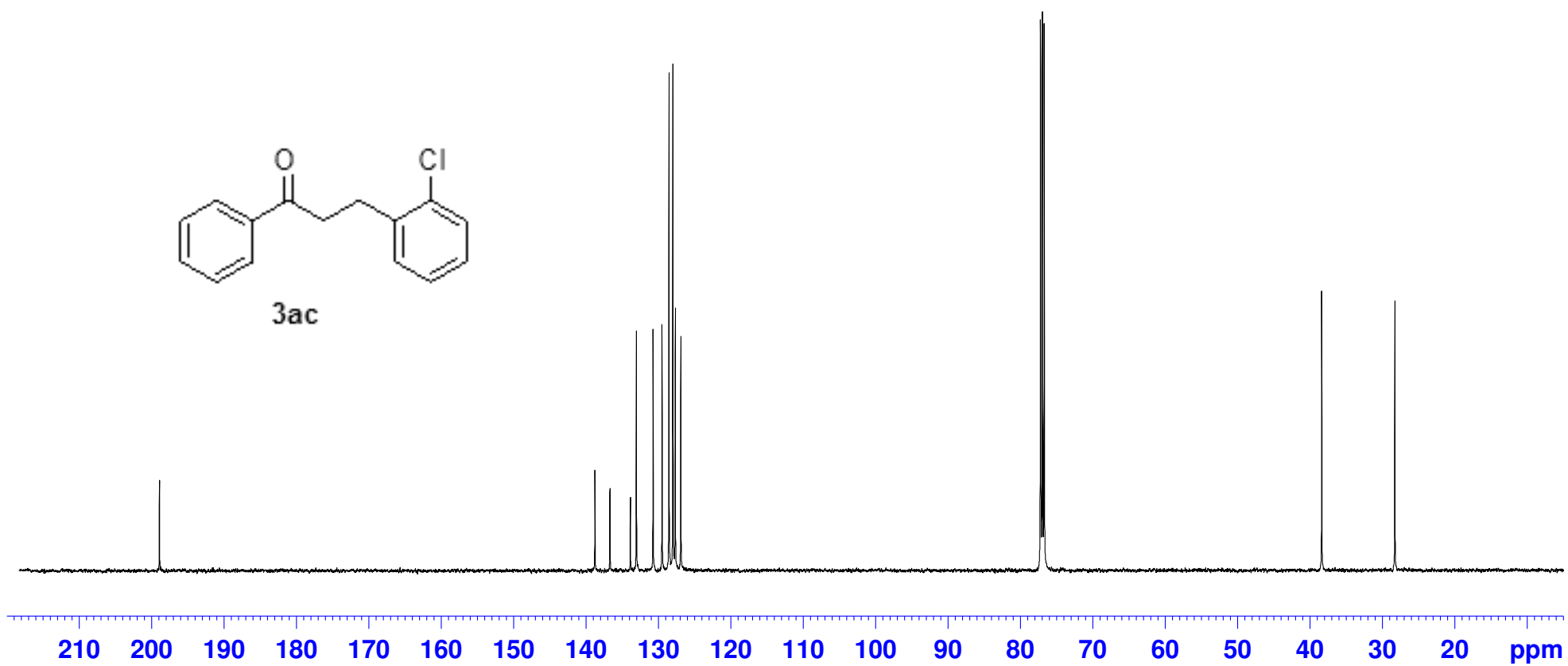
— 77.000

— 38.412

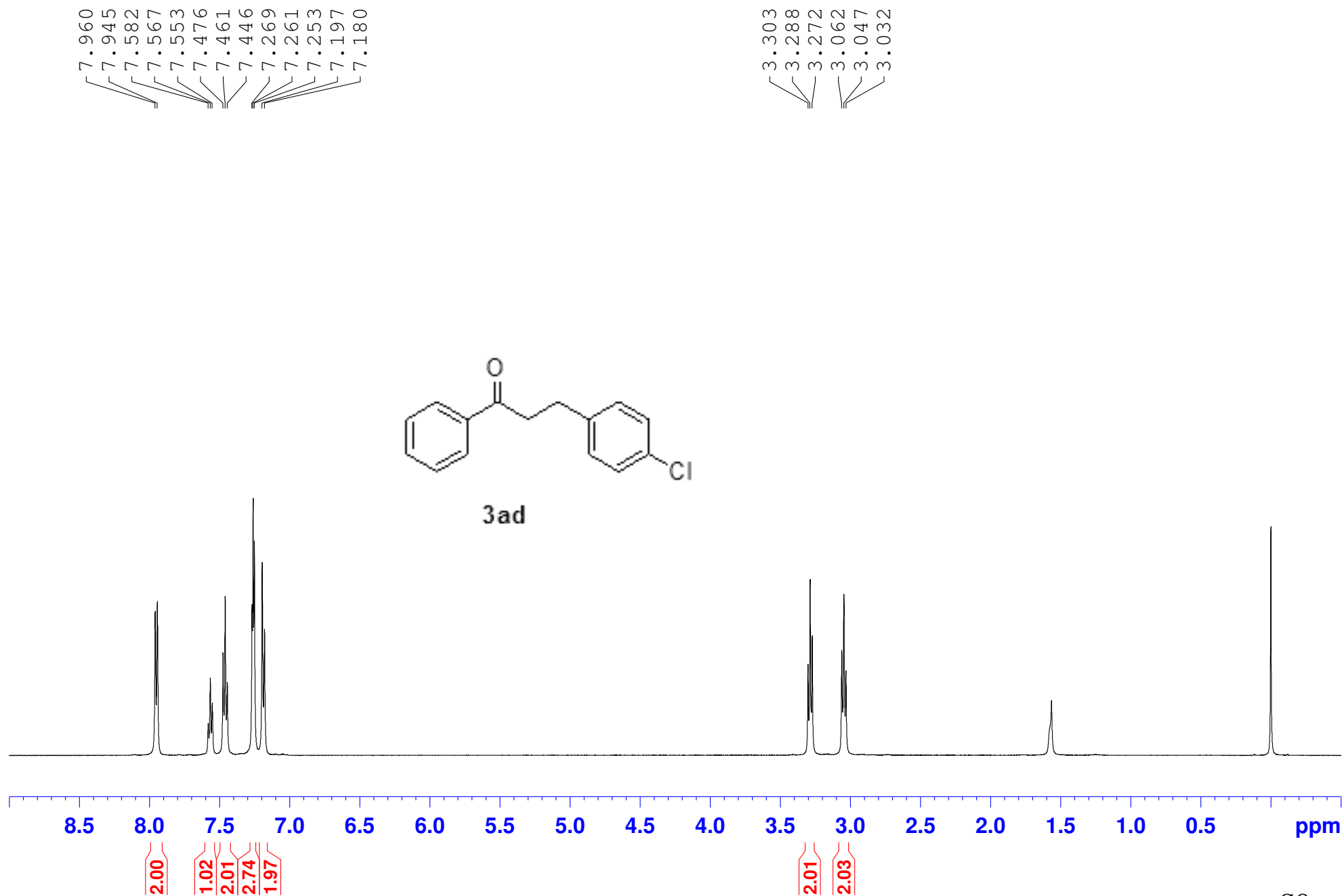
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3ac



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



3-(4-chlorophenyl)-1-phenylpropan-1-one
C13CPD CDCl3

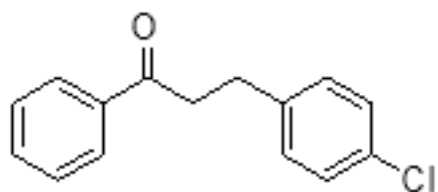
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128.556
127.972

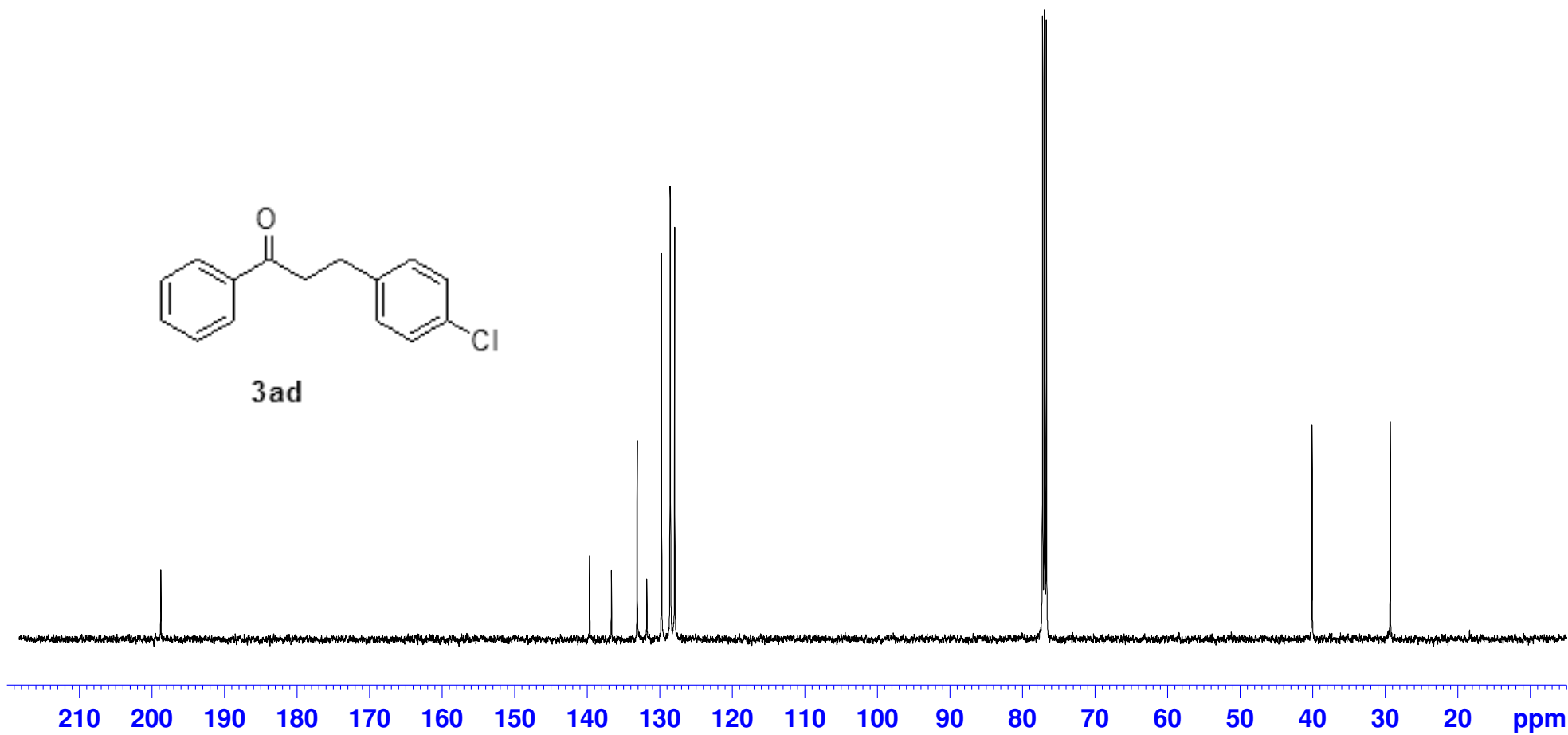
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—40.104

—29.329



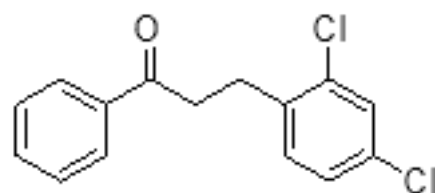
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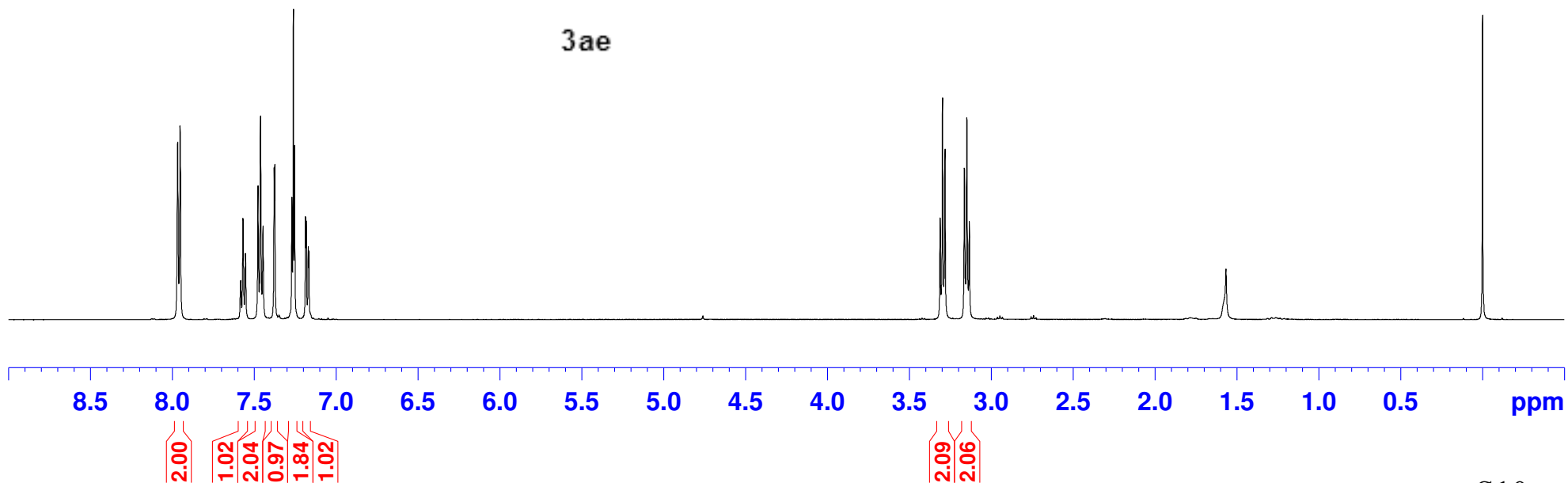
3-(2,4-dichlorophenyl)-1-phenylpropan-1-one
Proton CDCl₃

7.968
7.954
7.584
7.569
7.554
7.478
7.462
7.447
7.379
7.375
7.271
7.262
7.254
7.187
7.183
7.171
7.167

3.312
3.298
3.282
3.164
3.149
3.134



3ae



3-(2,4-dichlorophenyl)-1-phenylpropan-1-one
C13CPD CDCl3

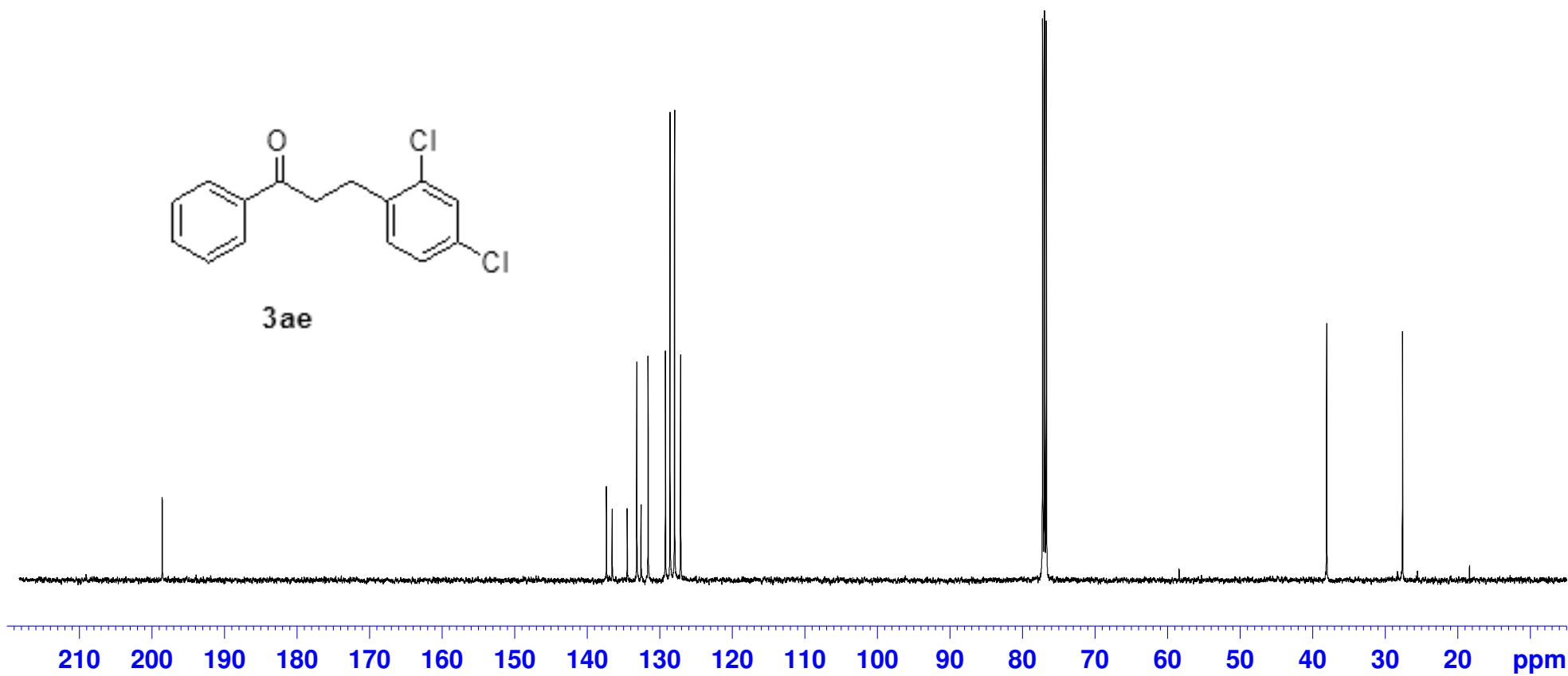
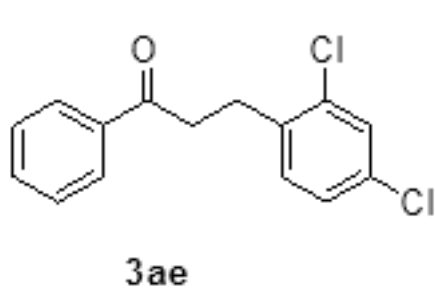
—198.610

137.380
136.593
134.523
133.193
132.616
131.640
129.260
128.614
127.992
127.157

—77.000

—38.093

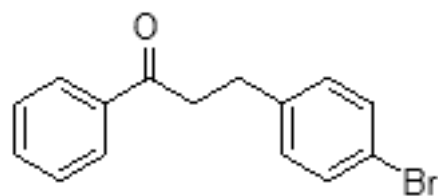
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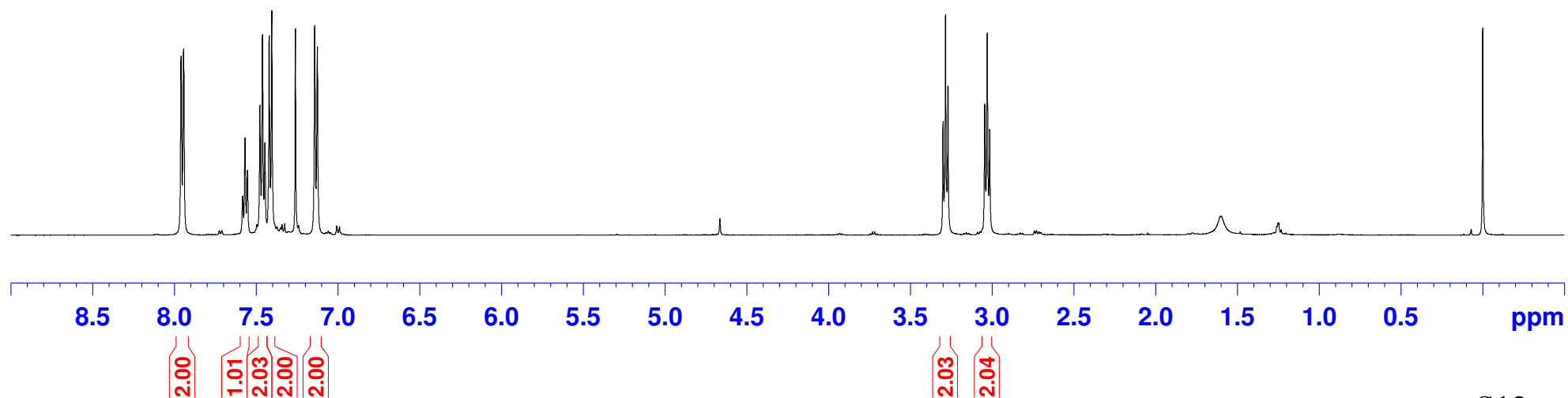
3-(4-bromophenyl)-1-phenylpropan-1-one
Proton CDCl₃

7.957
7.942
7.581
7.567
7.552
7.476
7.460
7.445
7.419
7.403
7.261
7.143
7.127

3.301
3.286
3.270
3.045
3.030
3.015



3af



3-(4-bromophenyl)-1-phenylpropan-1-one
C13CPD CDCl3

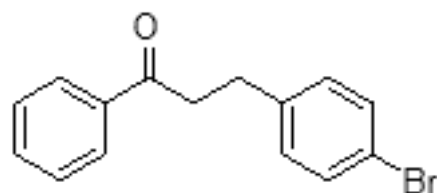
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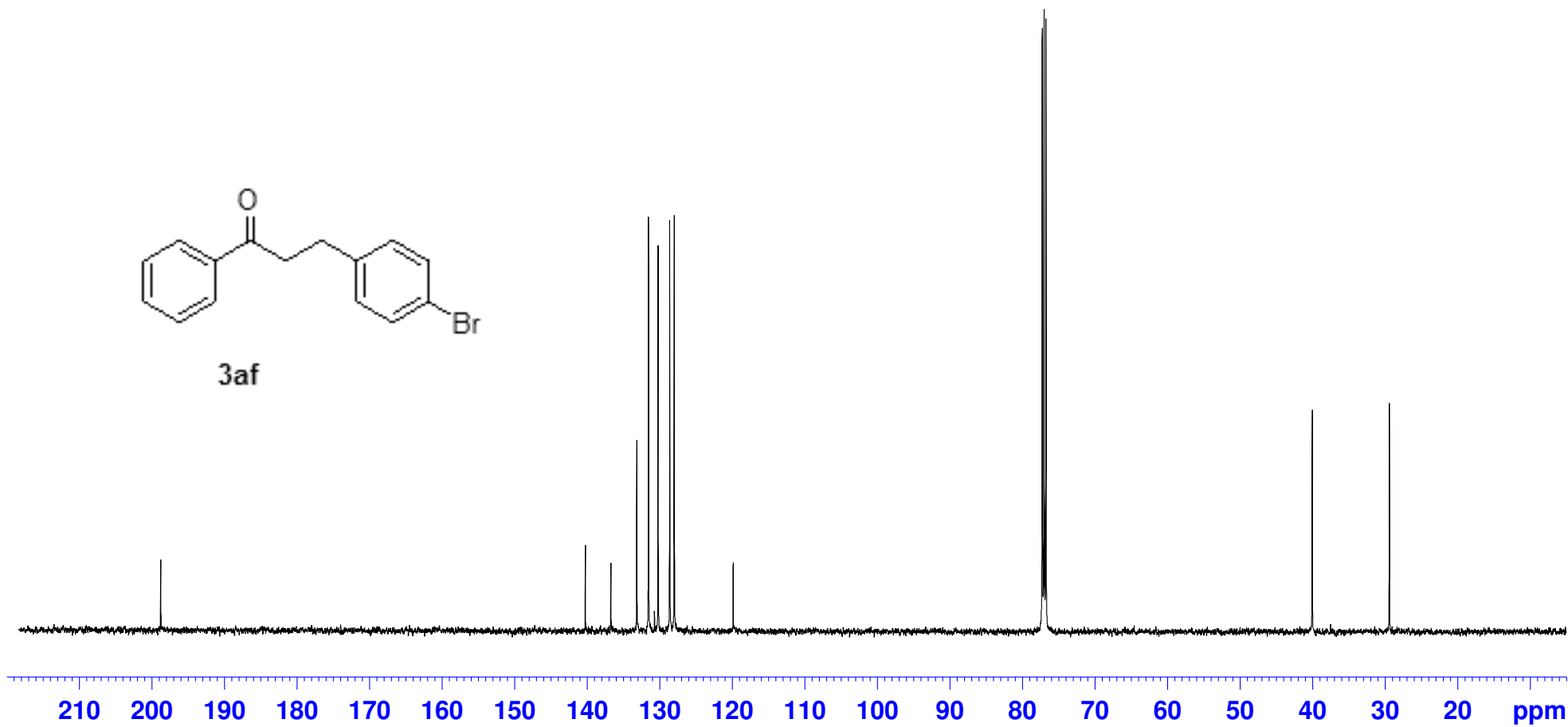
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—40.029

—29.403



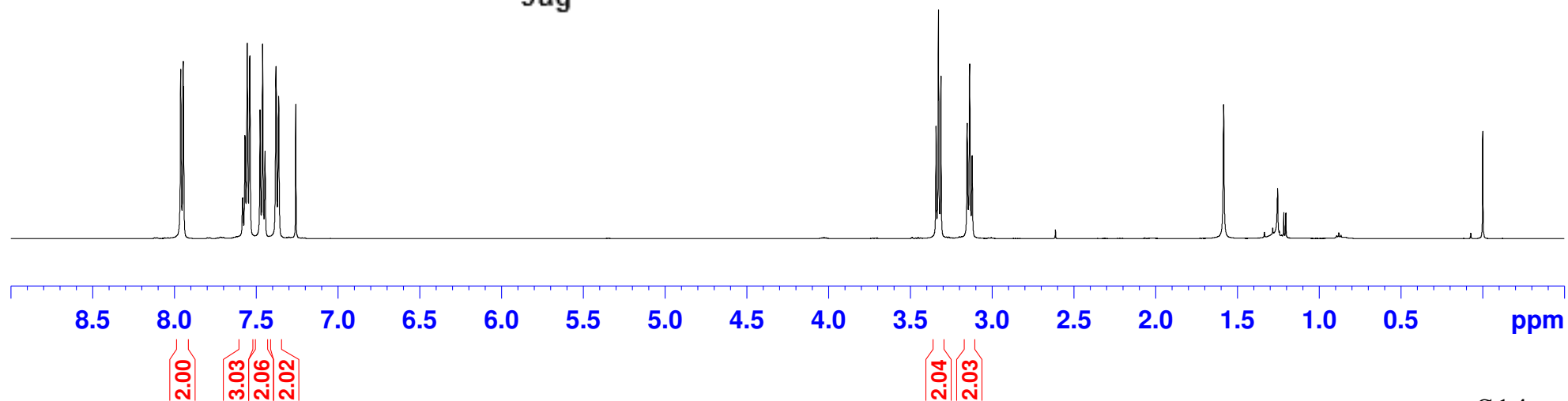
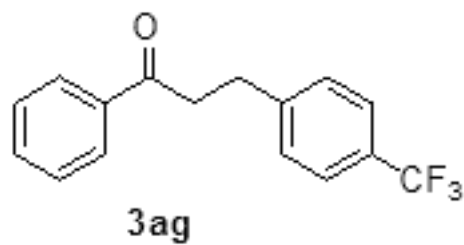
3af



1-phenyl-3-(4-(trifluoromethyl)phenyl)propan-1-one
Proton CDCl₃

7.962
7.947
7.945
7.584
7.569
7.555
7.540
7.477
7.462
7.447
7.380
7.364
7.259

3.343
3.329
3.313
3.153
3.138
3.123



1-phenyl-3-(4-(trifluoromethyl)phenyl)propan-1-one
C13CPD CDCl3

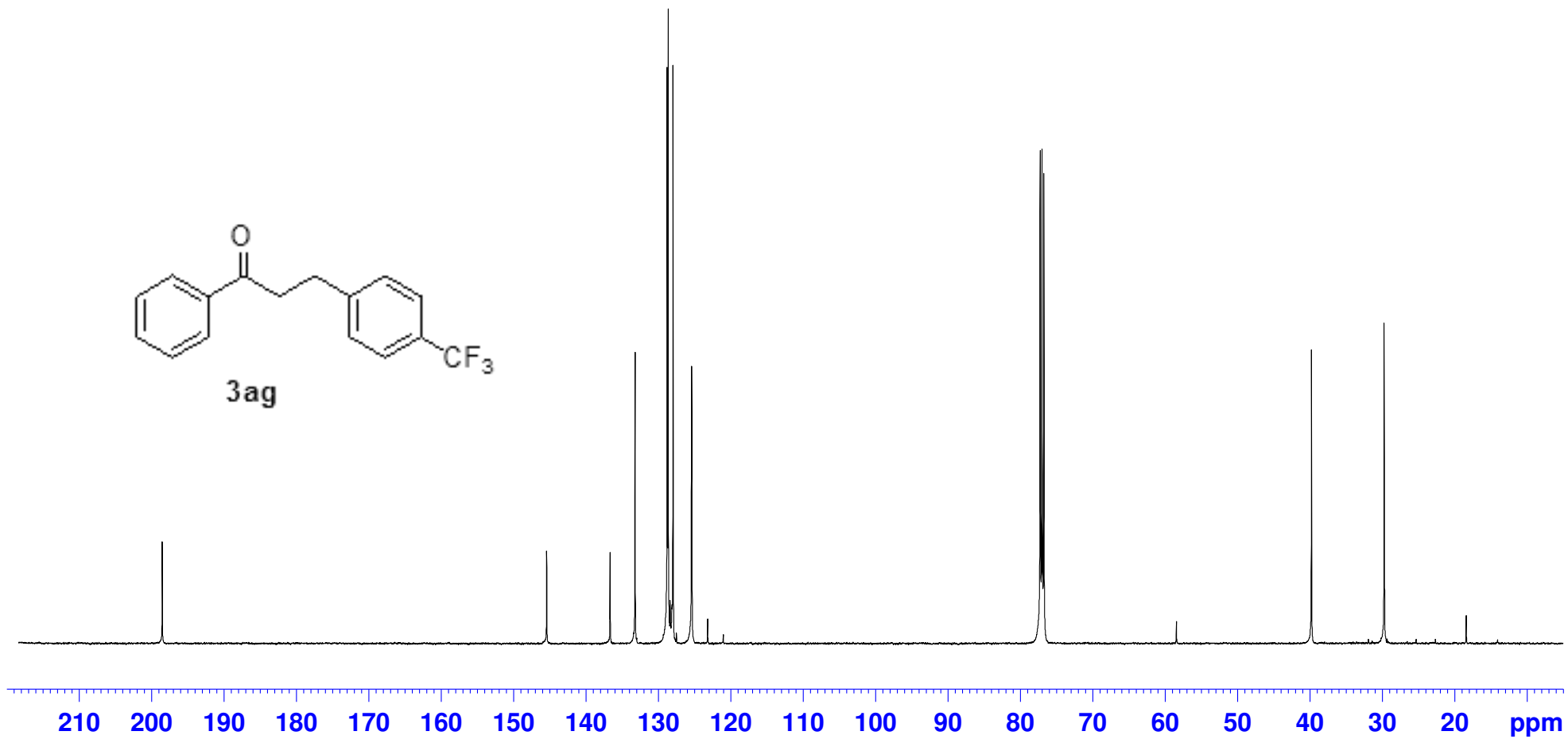
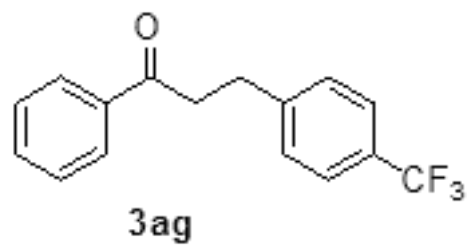
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128.643
128.373
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125.385
125.352
123.185
121.022

—77.000

—39.779

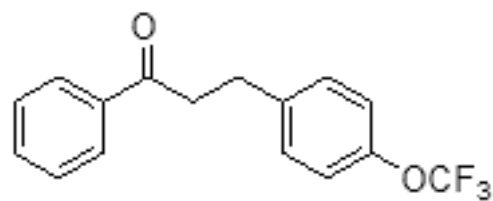
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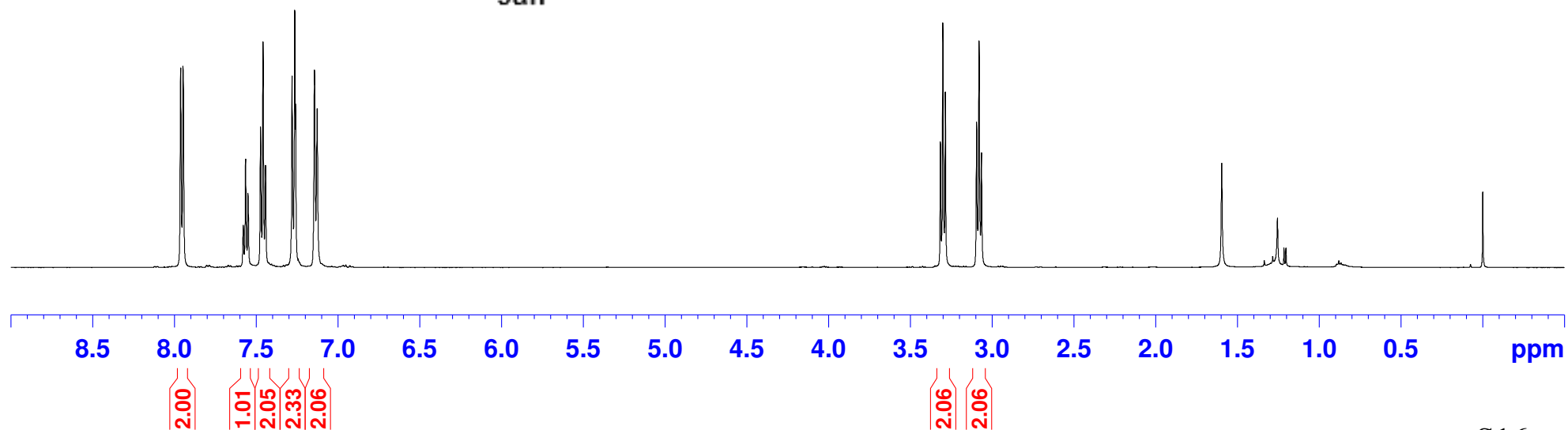
1-phenyl-3-(4-(trifluoromethoxy)phenyl)propan-1-one
Proton CDCl₃

7.960
7.946
7.944
7.578
7.563
7.549
7.472
7.457
7.441
7.279
7.262
7.258
7.144
7.128

3.317
3.302
3.287
3.095
3.080
3.065



3ah



1-phenyl-3-(4-(trifluoromethoxy)phenyl)propan-1-one
C13CPD CDCl3

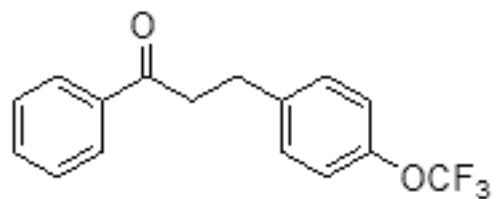
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147.600
140.038
136.759
133.140
129.715
128.614
127.979
123.560
121.521
121.033
119.479
117.437

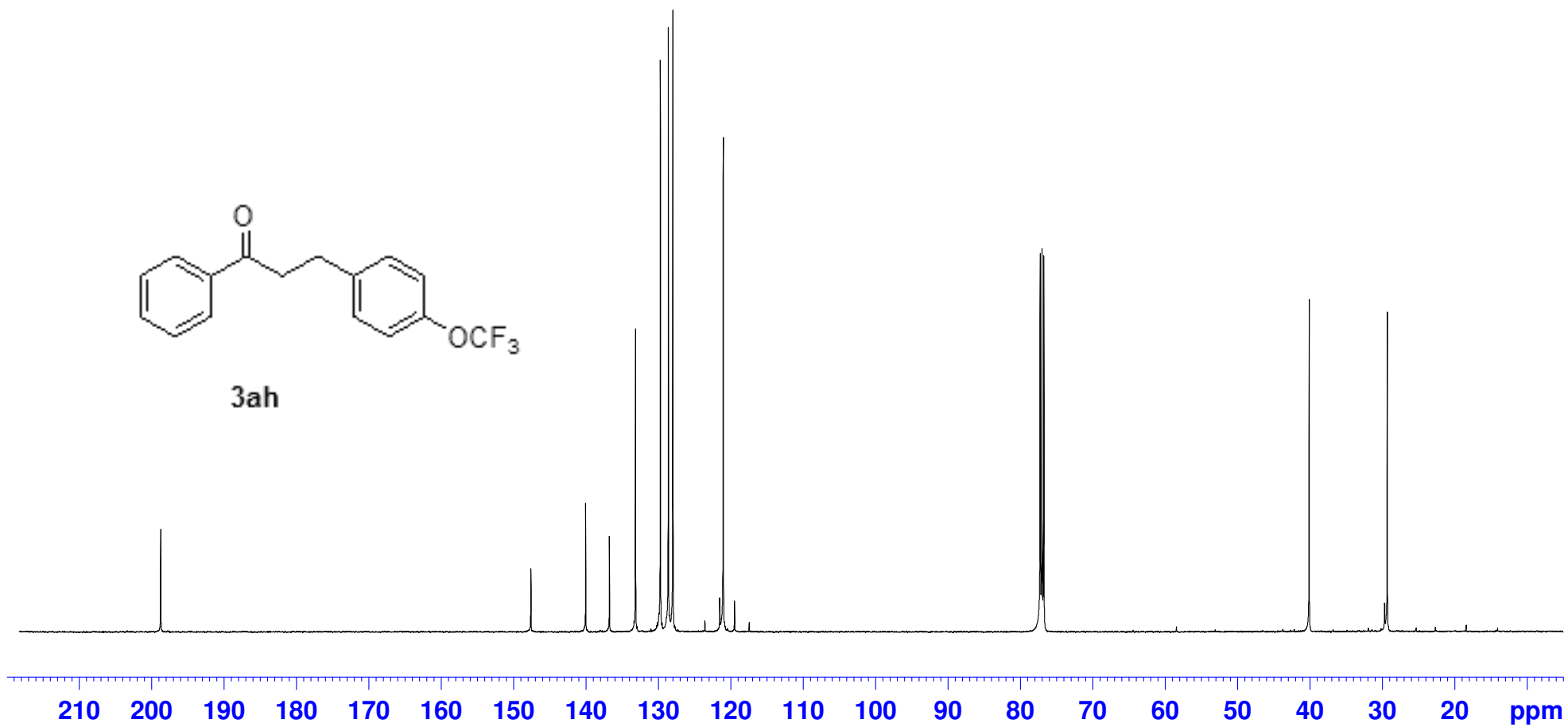
—77.000

—40.090

—29.301



3ah

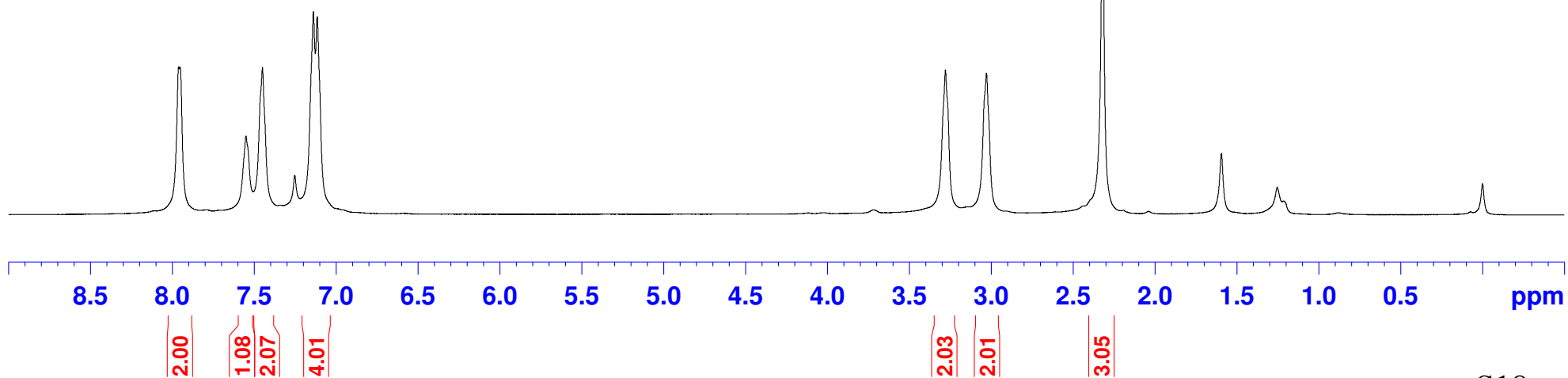
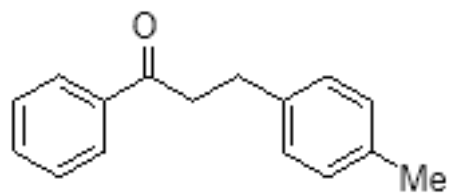


1-phenyl-3-p-tolylpropan-1-one
Proton CDCl₃

7.962
7.949
7.563
7.549
7.535
7.463
7.449
7.433
7.252
7.154
7.140
7.116

3.294
3.281
3.266
3.043
3.030
3.014

— 2.321



1-phenyl-3-p-tolylpropan-1-one
C13CPD CDCl3

— 199.313

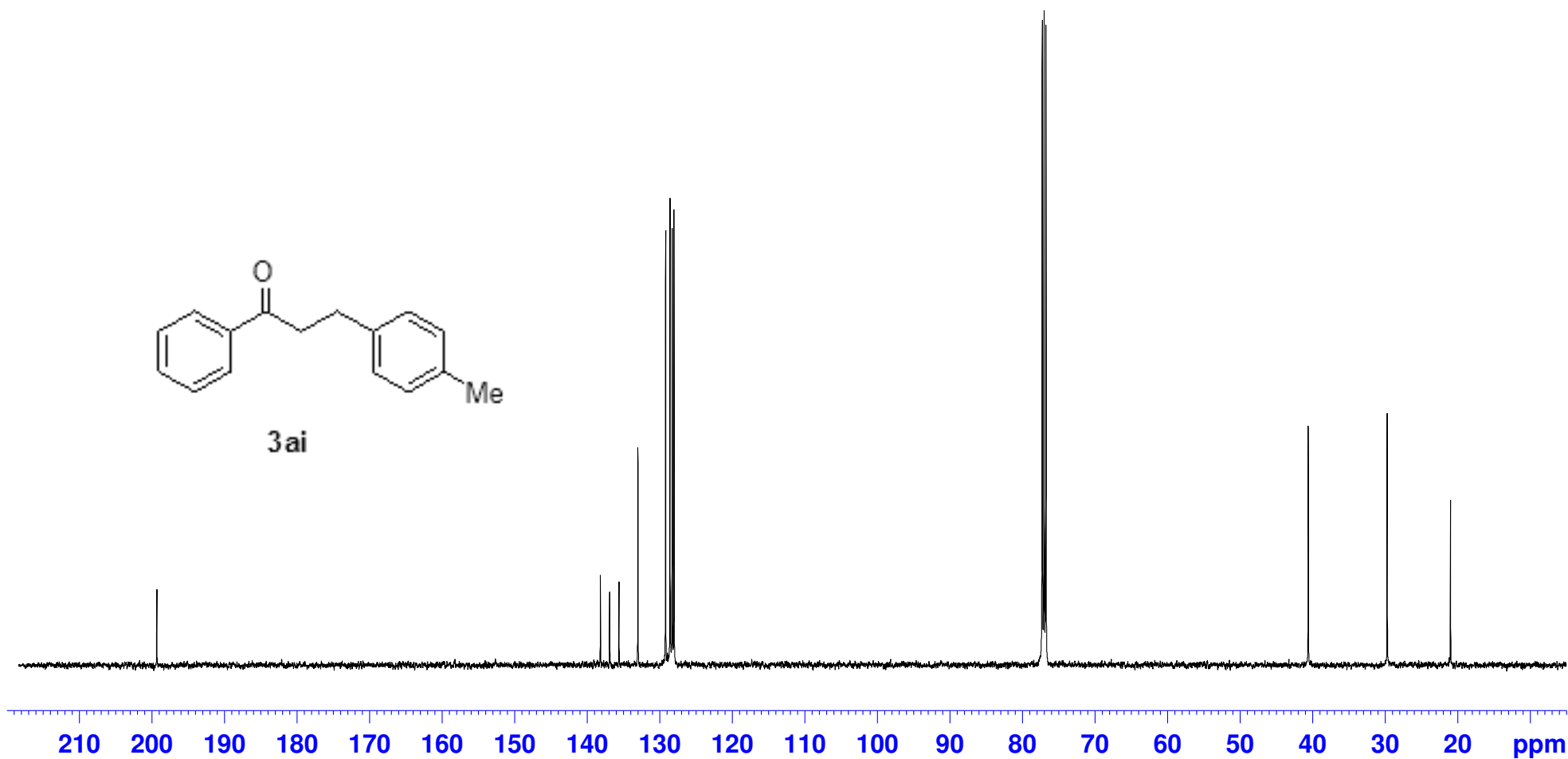
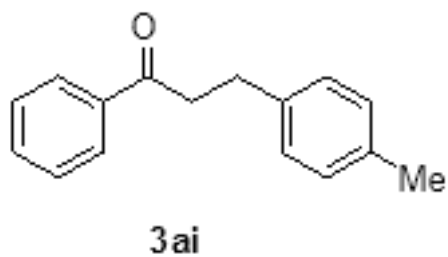
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135.596
132.990
129.177
128.563
128.267
128.018

— 77.000

— 40.579

— 29.699

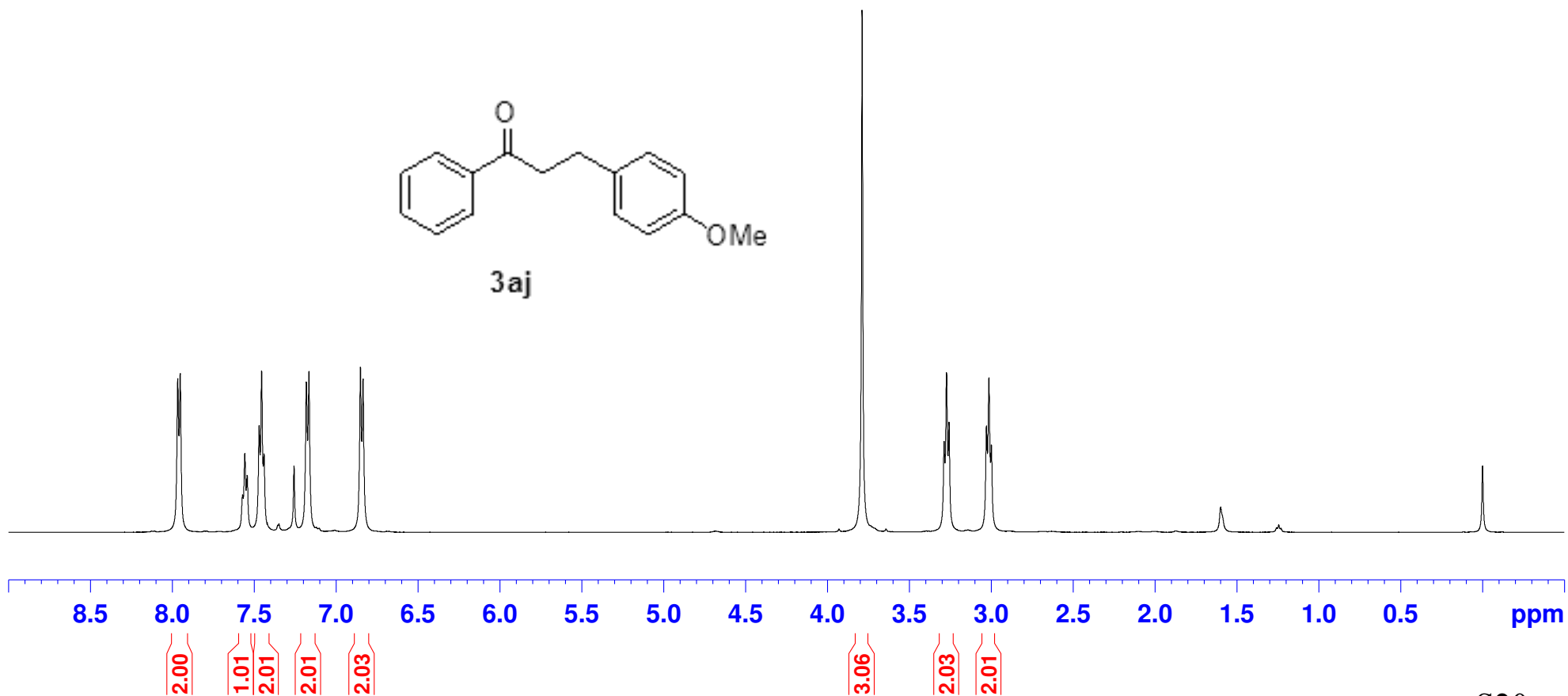
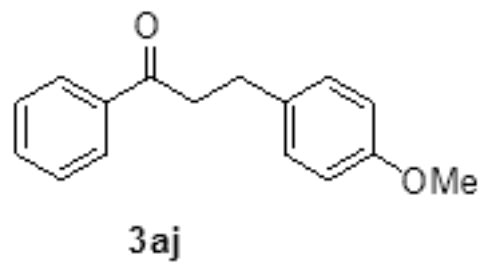
— 20.970



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

7.965
7.950
7.570
7.556
7.542
7.468
7.453
7.439
7.258
7.183
7.167
6.852
6.836

3.789
3.288
3.273
3.258
3.029
3.014
2.999



3-(4-methoxyphenyl)-1-phenylpropan-1-one
C13CPD CDCl3

—199.345

—157.928

136.828

133.254

132.988

129.306

128.546

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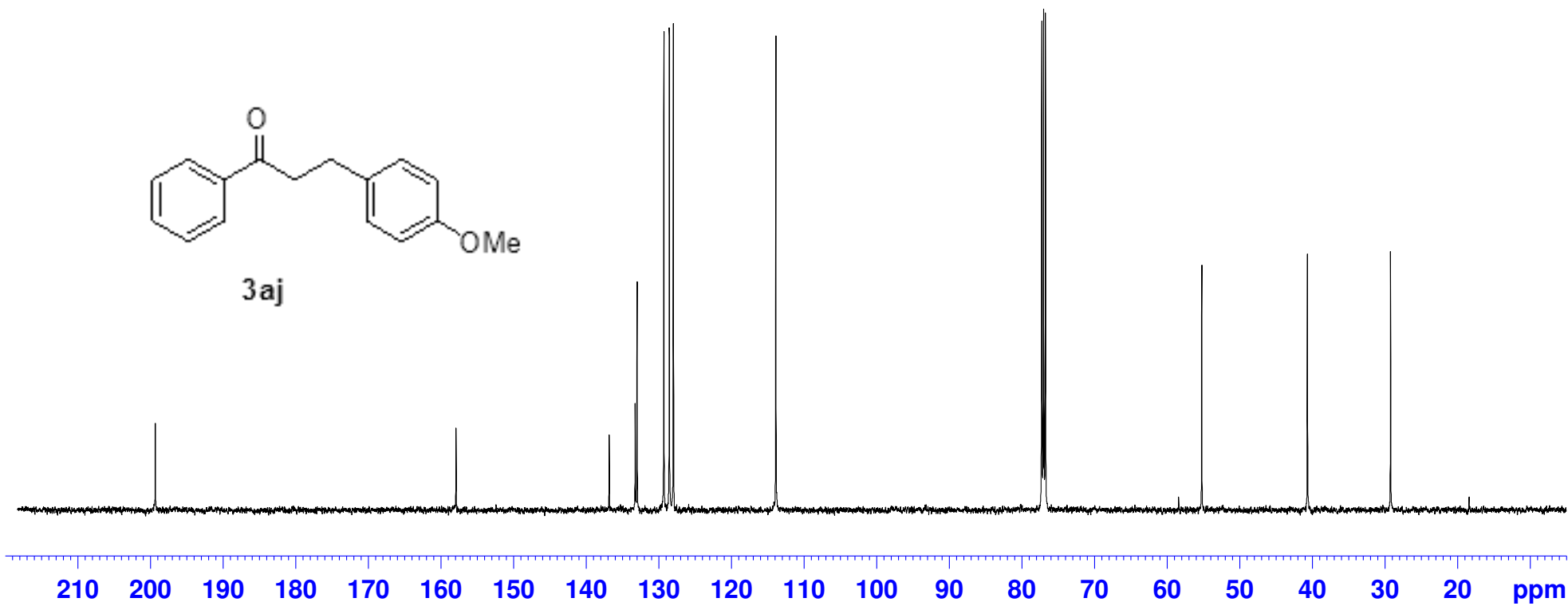
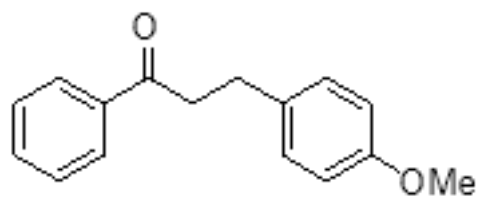
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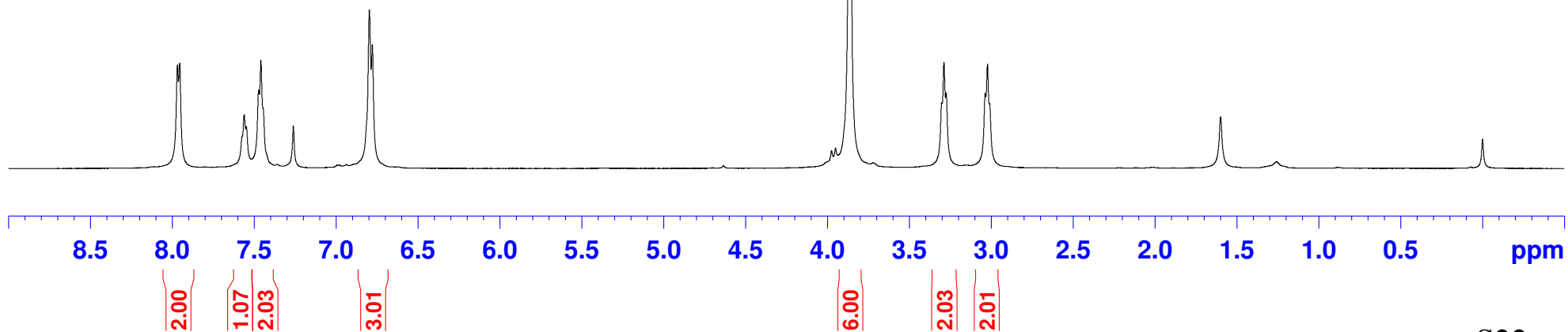
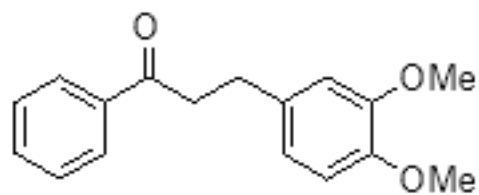
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3-(3,4-dimethoxyphenyl)-1-phenylpropan-1-one
Proton CDCl₃

7.967
7.953
7.573
7.559
7.546
7.471
7.457
7.444
7.262
6.798
6.779

3.869
3.860
3.303
3.289
3.275
3.038
3.023
3.010



3-(3,4-dimethoxyphenyl)-1-phenylpropan-1-one
C13CPD CDCl3

—199.316

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147.356

136.856
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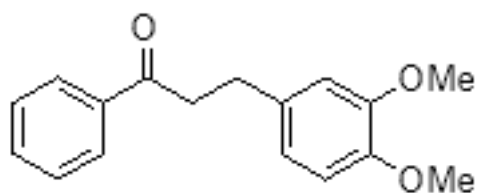
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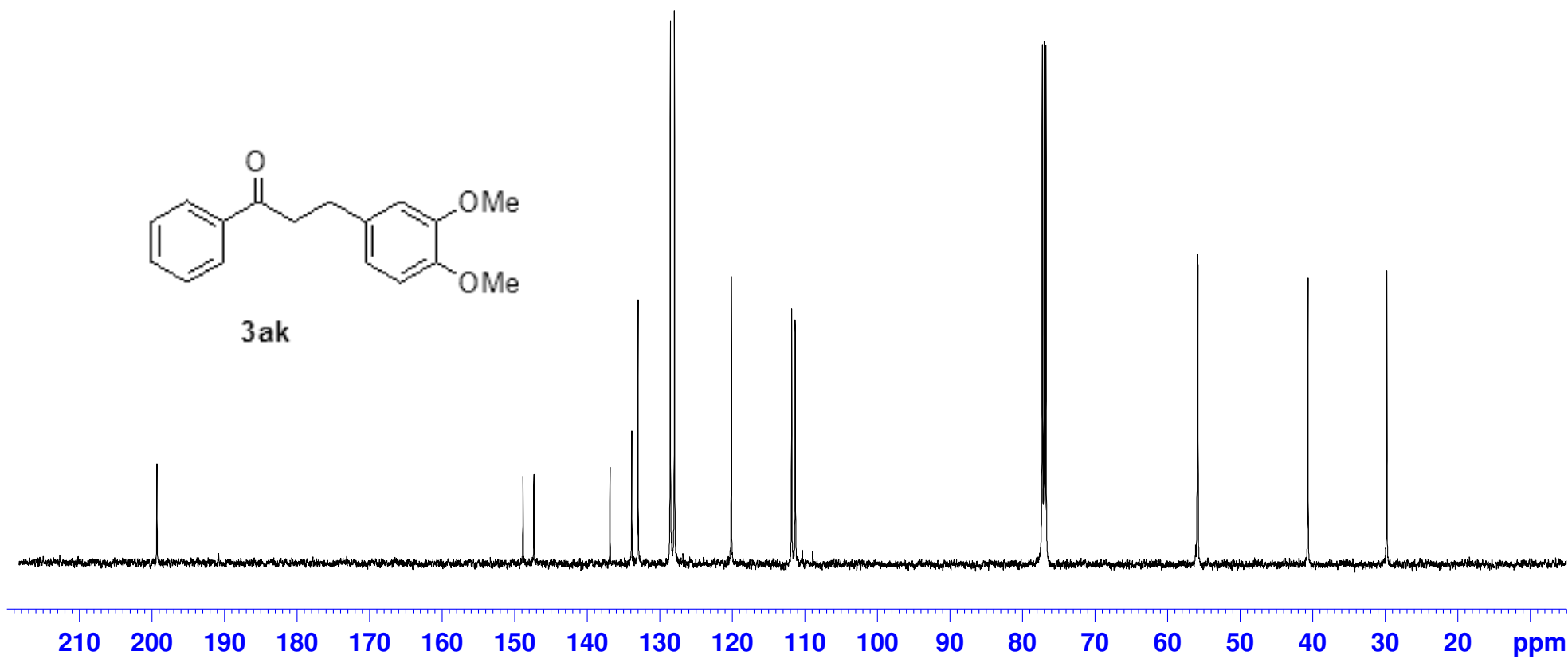
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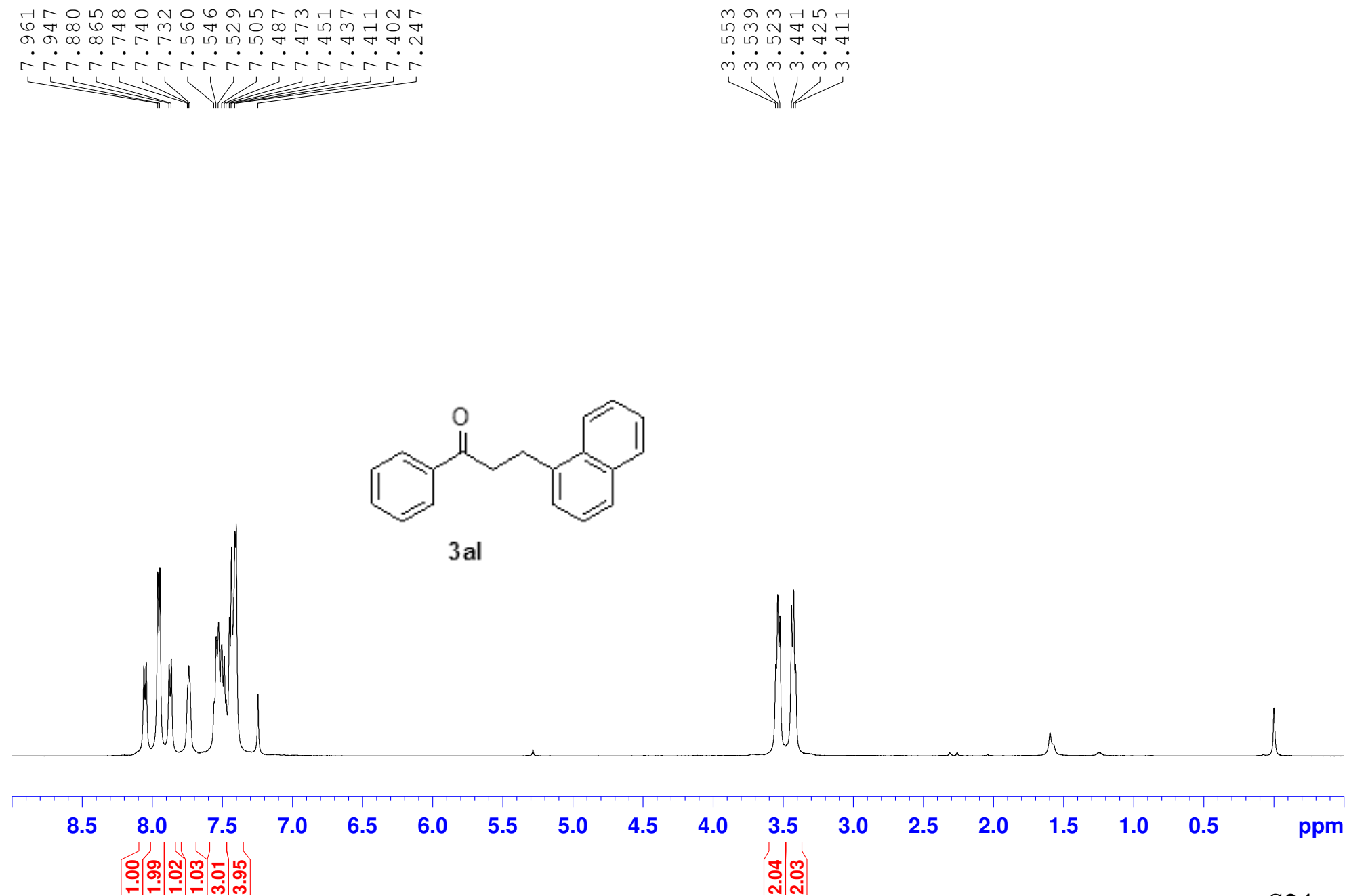
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3ak



3-(naphthalen-1-yl)-1-phenylpropan-1-one
Proton CDCl₃



3-(naphthalen-1-yl)-1-phenylpropan-1-one
C13CPD CDCl3

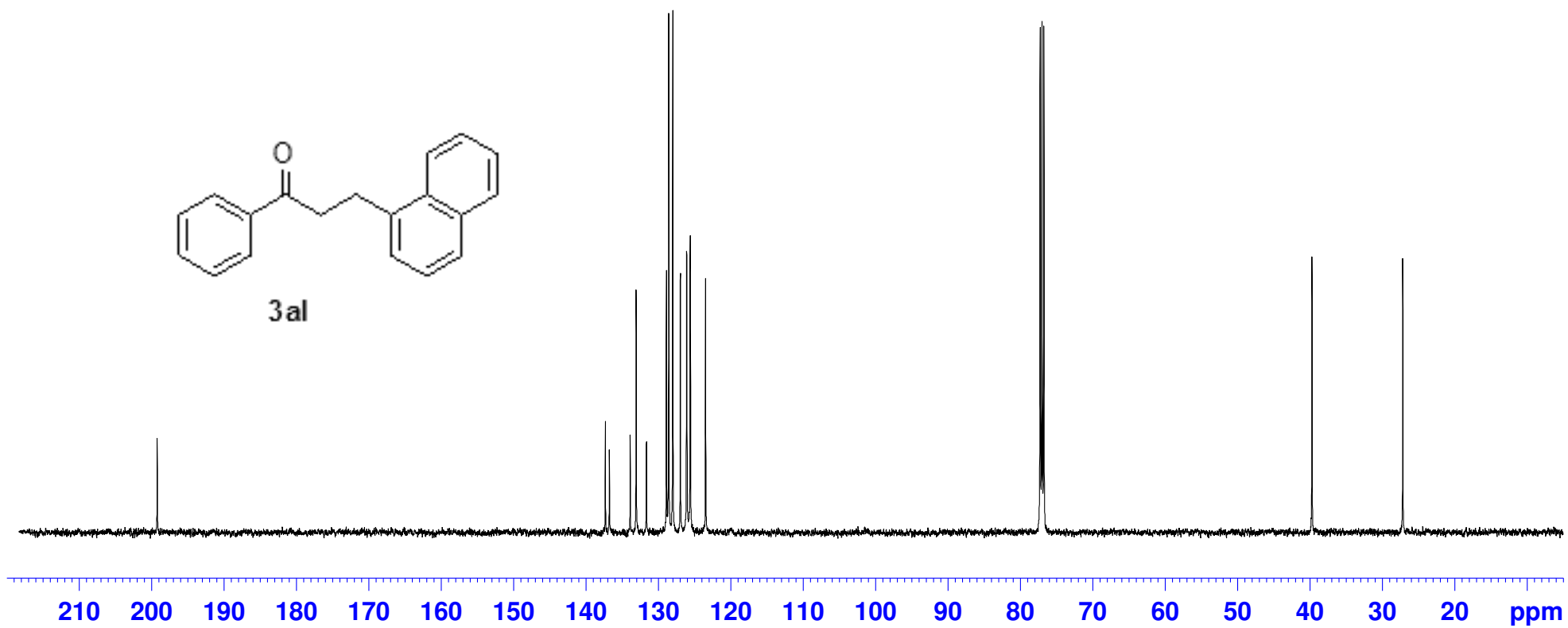
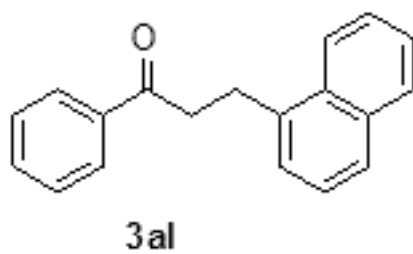
— 199.239

137.317
136.767
133.893
133.066
131.647
128.888
128.568
128.004
126.959
126.112
126.053
125.611
125.571
123.472

— 77.000

— 39.695

— 27.158

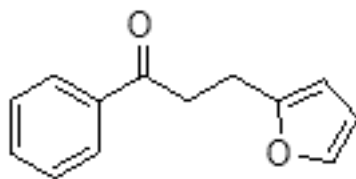


3-(furan-2-yl)-1-phenylpropan-1-one
Proton CDCl₃

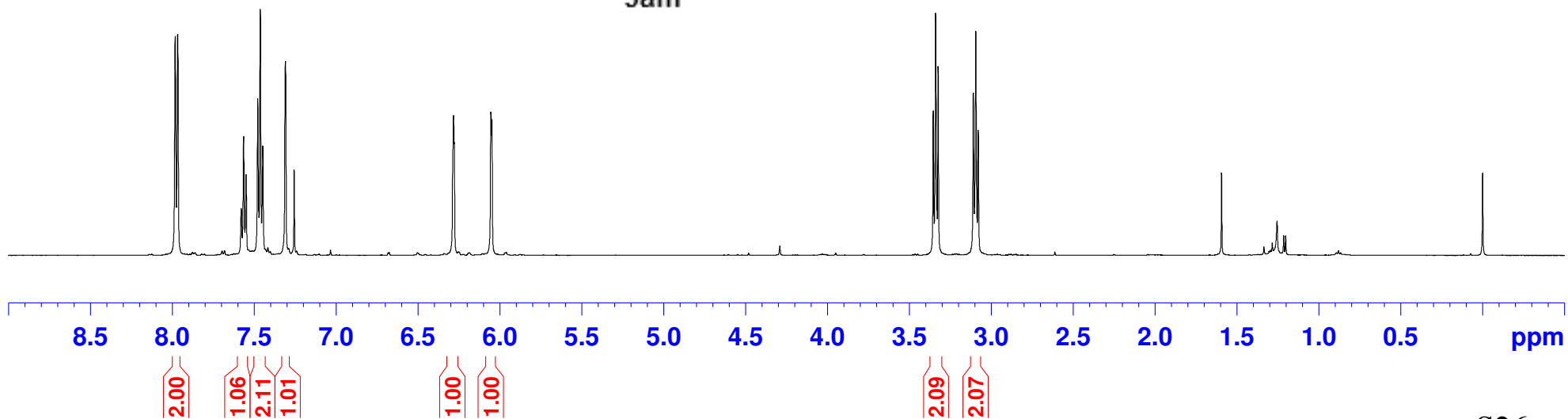
7.983
7.968
7.580
7.566
7.551
7.479
7.464
7.449
7.310
7.257

6.288
6.284
6.280
6.056
6.050

3.354
3.340
3.325
3.110
3.095
3.080



3am



3-(furan-2-yl)-1-phenylpropan-1-one
C13CPD CDCl3

—198.605

—154.712

—141.054

—136.689

—133.096

—128.576

—127.985

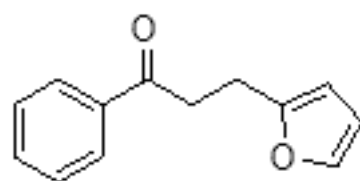
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—105.273

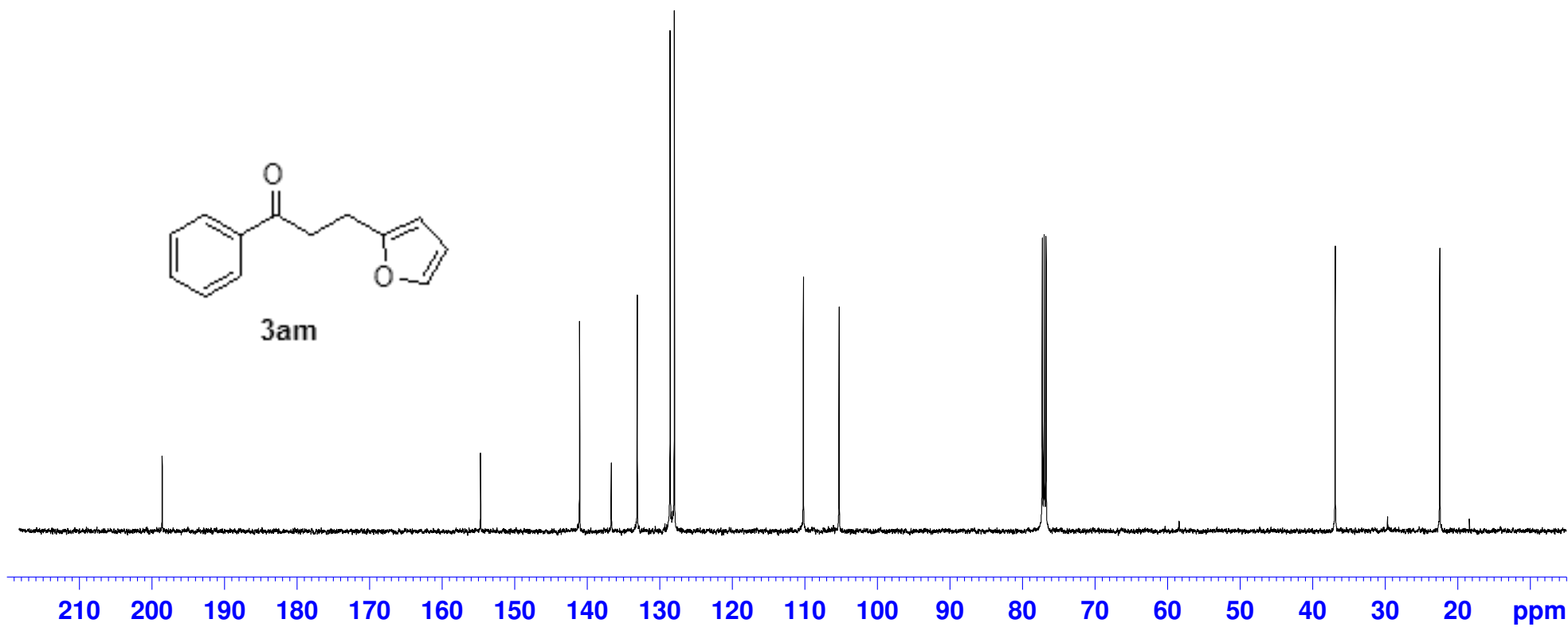
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—36.879

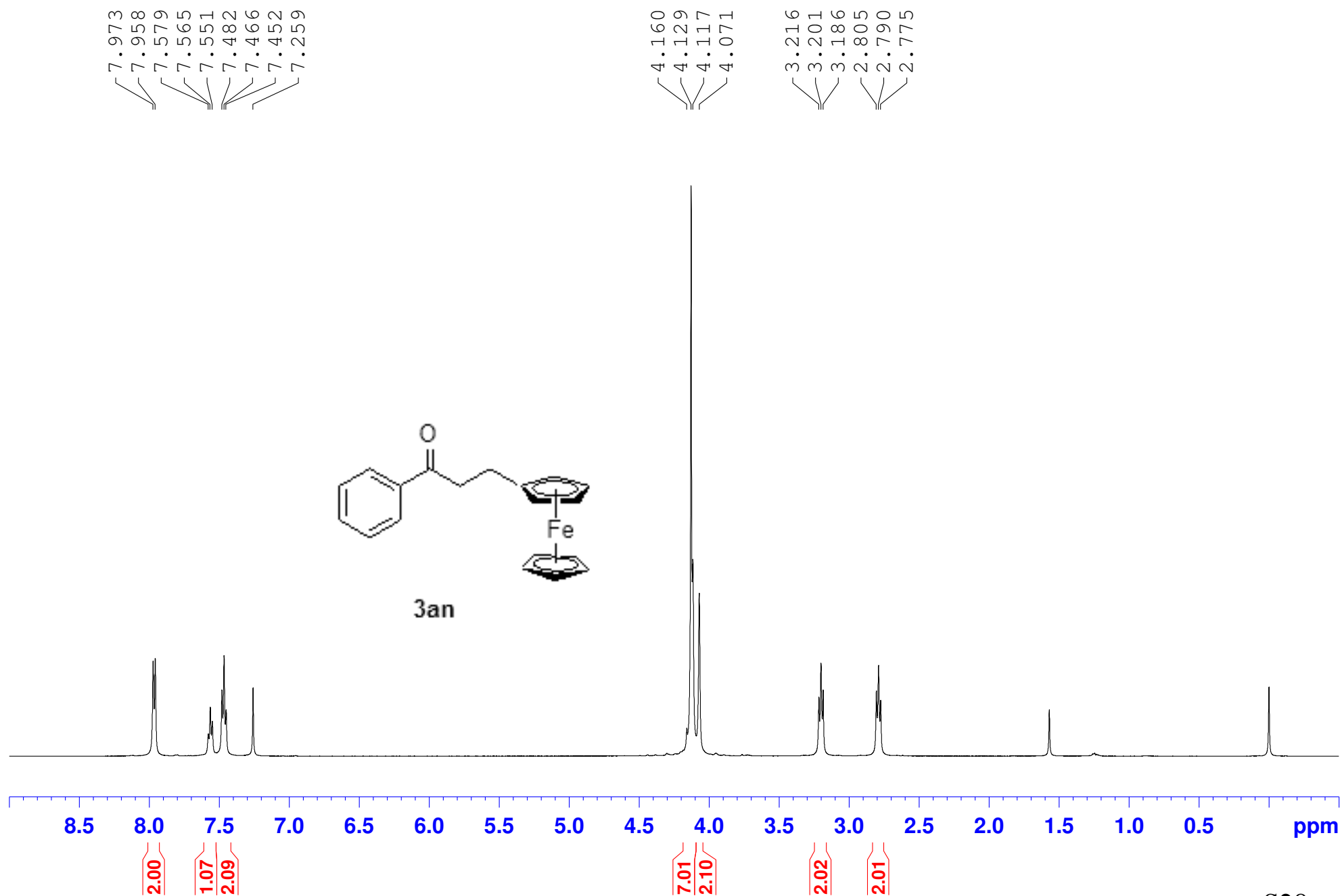
—22.460



3am



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



3-Ferrocenyl-1-phenylpropan-1-one
C13CPD CDC13

— 199.498

— 136.880
— 133.003
— 128.579
— 128.016

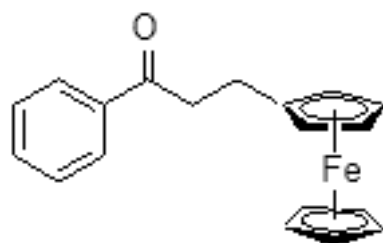
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— 77.000

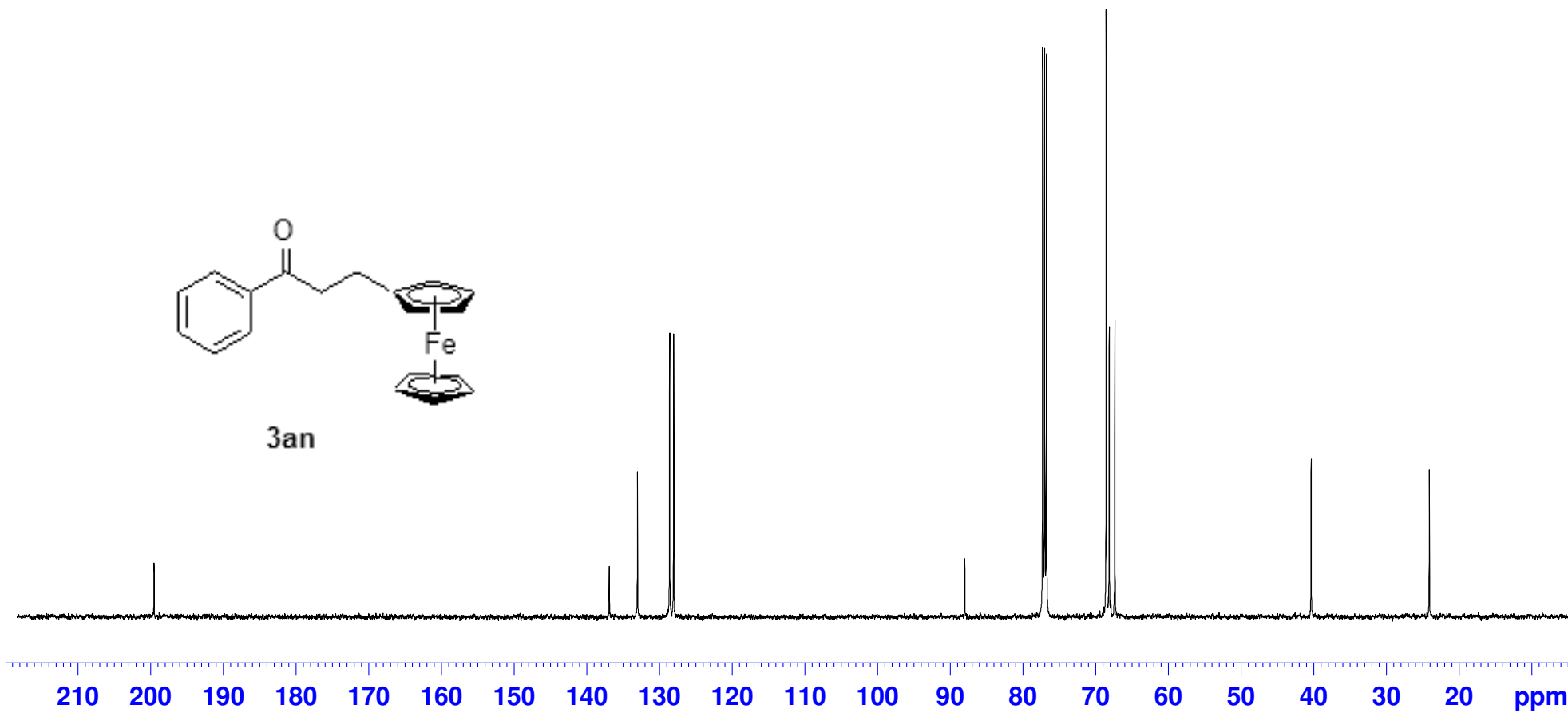
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68.108
67.335

— 40.330

— 24.072



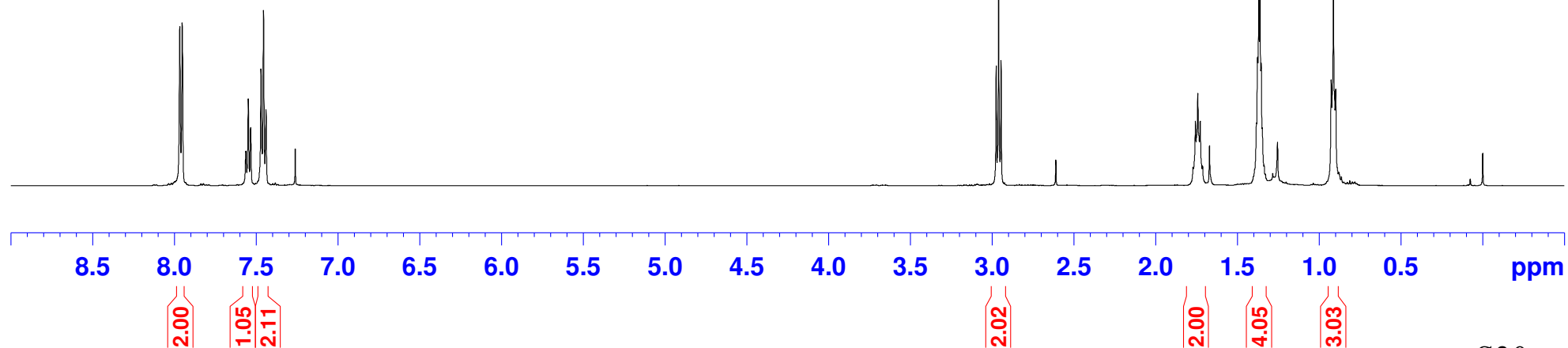
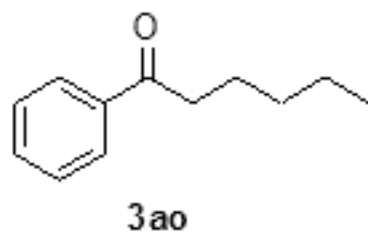
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1-phenylhexan-1-one
Proton CDCl₃

7.968
7.953
7.564
7.549
7.535
7.471
7.456
7.441
7.262

2.975
2.961
2.946
1.772
1.757
1.742
1.728
1.713
1.384
1.377
1.370
1.362
1.355
1.348
0.927
0.913
0.899



1-phenylhexan-1-one
C13CPD CDC13

— 200.526

— 137.048

— 132.789

— 128.481

— 127.989

— 77.000

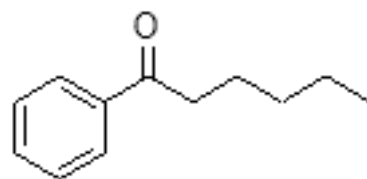
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— 31.494

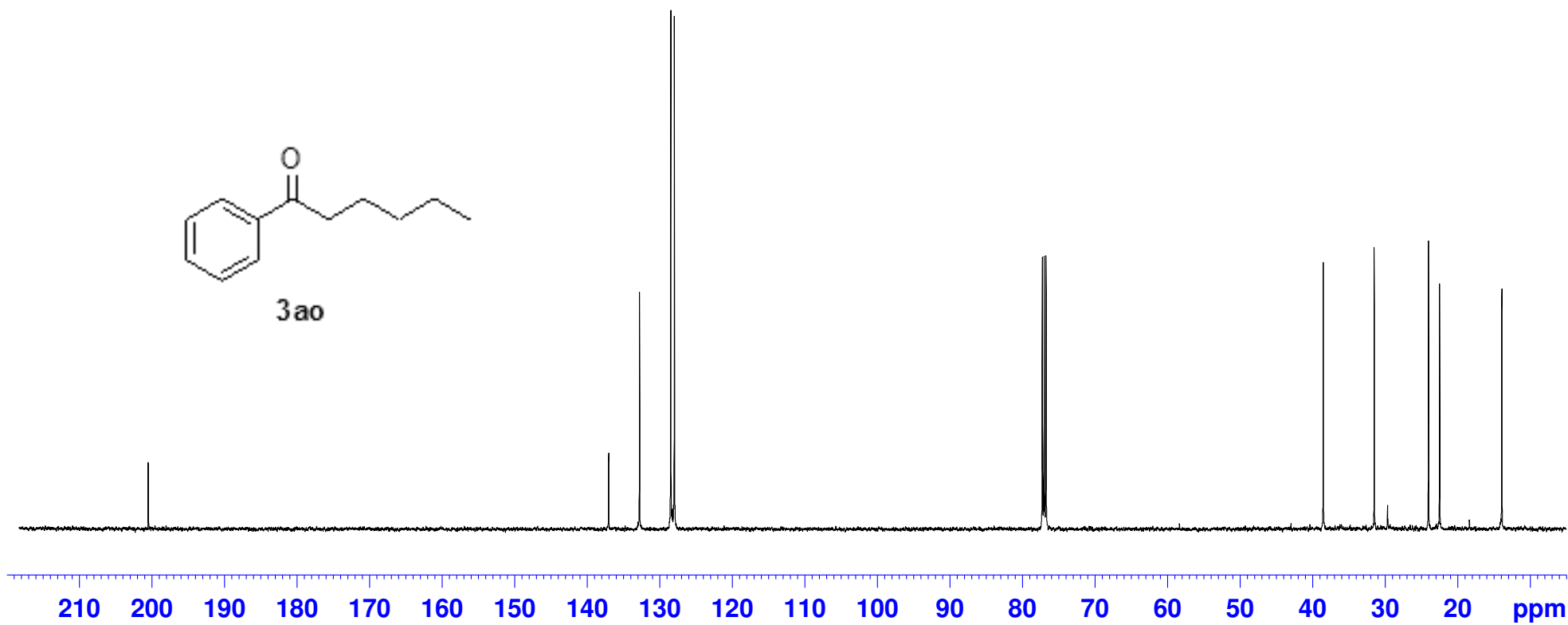
— 24.011

— 22.478

— 13.897



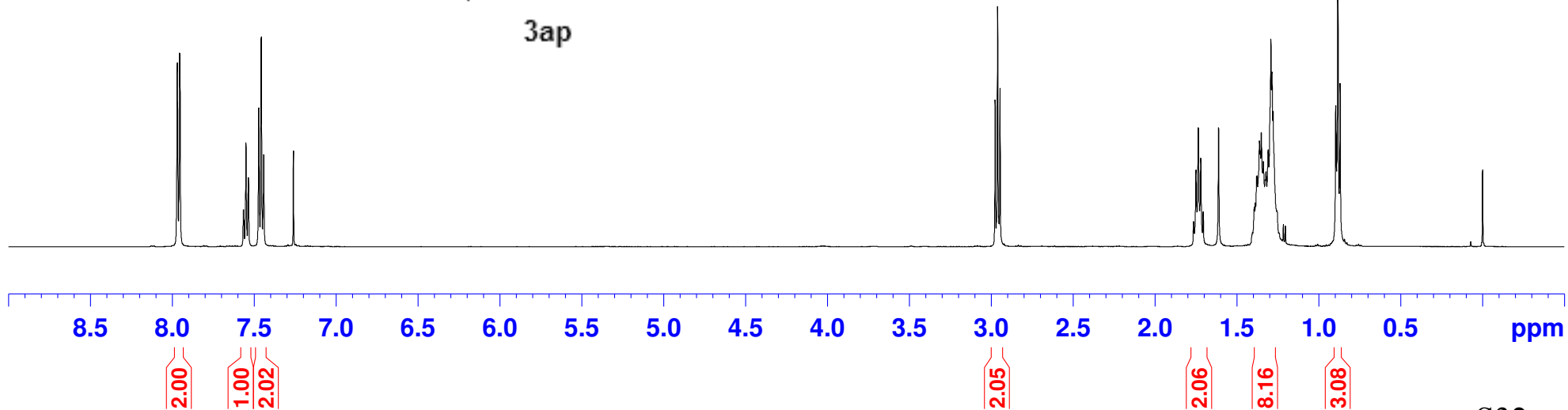
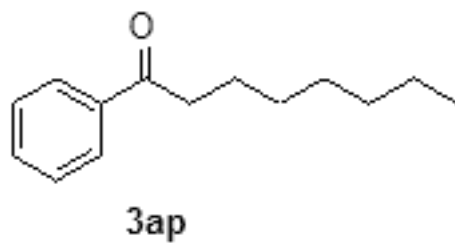
3ao



1-phenyloctan-1-one
Proton CDCl₃

7.968
7.953
7.566
7.551
7.537
7.473
7.458
7.443
7.262

2.976
2.962
2.947
1.765
1.750
1.736
1.721
1.706
1.377
1.363
1.357
1.351
1.339
1.329
1.322
1.309
1.293
1.287
1.279
0.897
0.884
0.870



1-phenyloctan-1-one
C13CPD CDC13

— 200.597

— 137.064

— 132.814

— 128.502

— 128.014

— 77.000

— 38.599

— 31.681

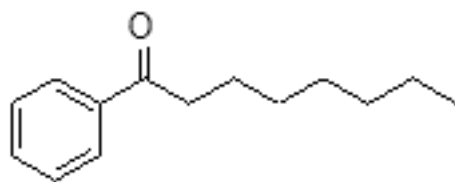
— 29.308

— 29.114

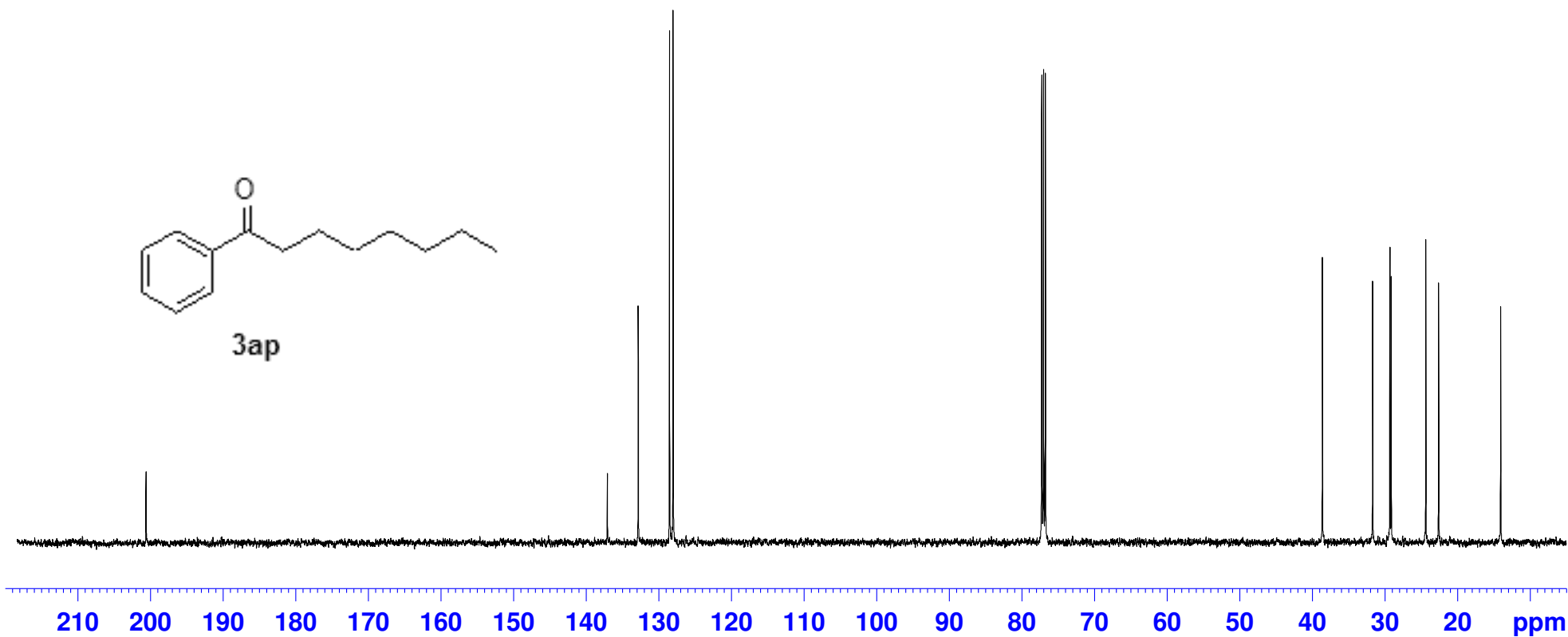
— 24.355

— 22.590

— 14.047



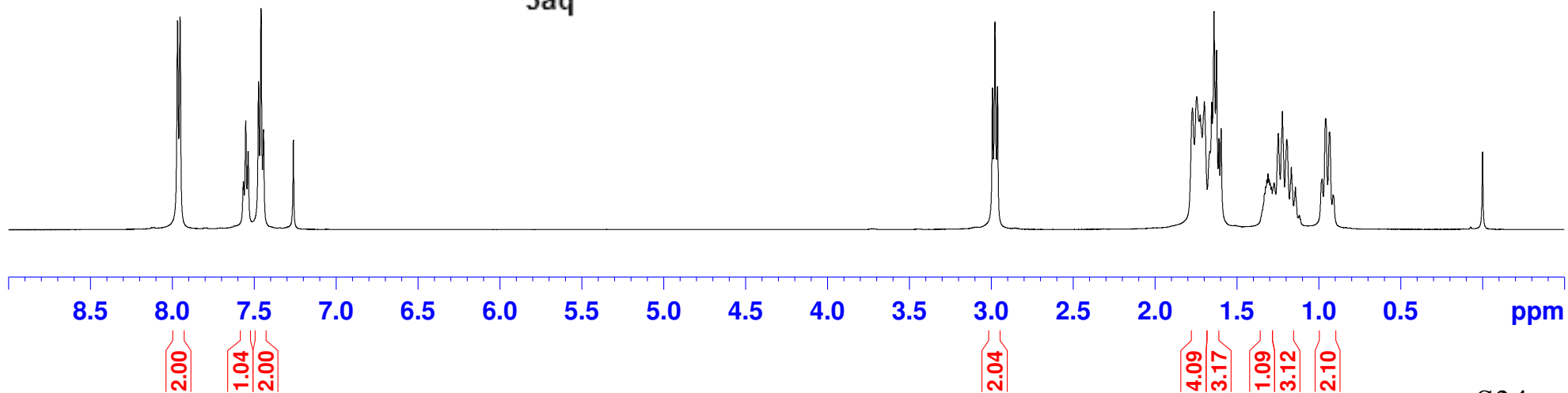
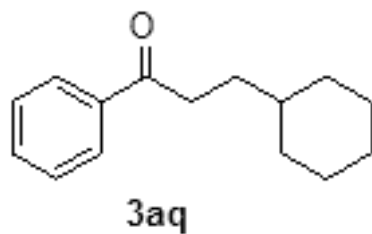
3ap



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

7.969
7.954
7.567
7.552
7.538
7.474
7.459
7.444
7.262

2.993
2.977
2.962
1.771
1.745
1.724
1.699
1.654
1.640
1.624
1.324
1.317
1.311
1.304
1.296
1.247
1.222
1.196
1.168
0.980
0.958
0.935
0.912



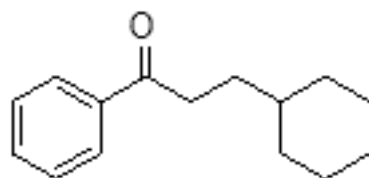
3-cyclohexyl-1-phenylpropan-1-one
C13CPD CDCl3

— 200.822

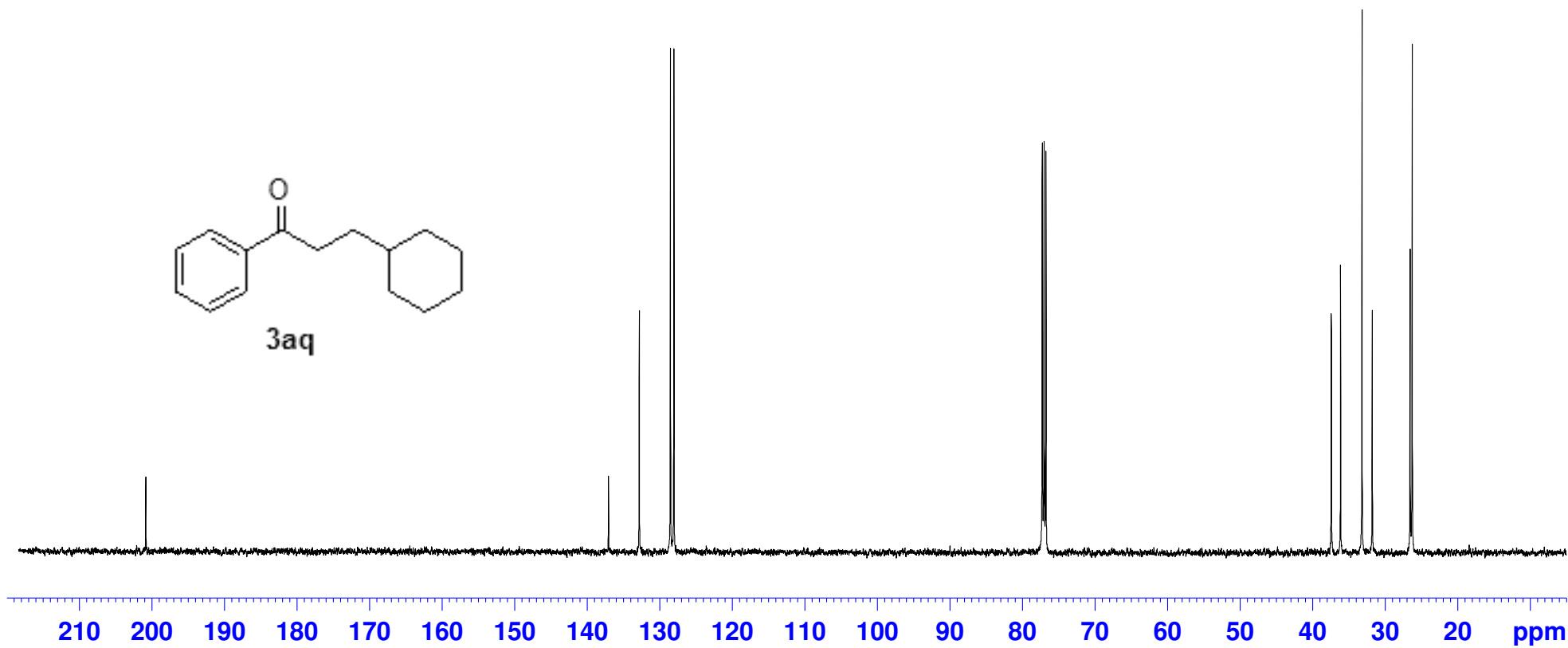
— 137.051
— 132.797
— 128.503
— 128.024

— 77.000

— 37.404
— 36.127
— 33.167
— 31.753
— 26.535
— 26.252



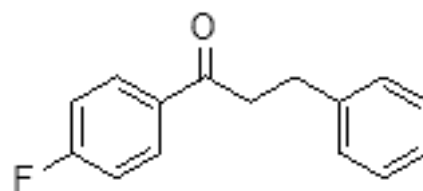
3aq



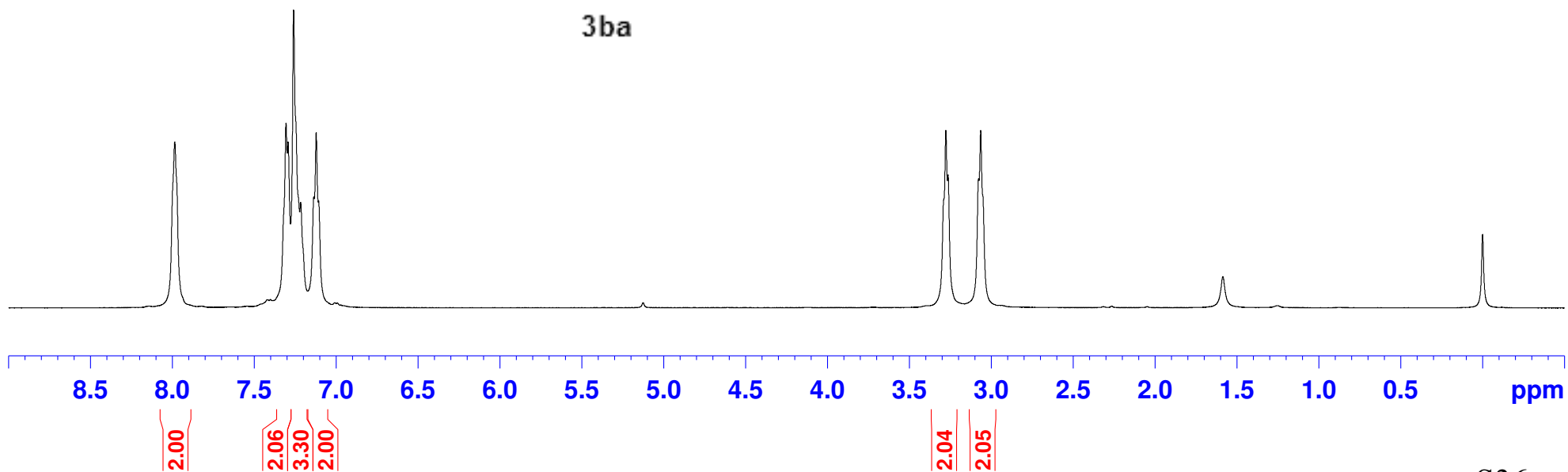
1-(4-fluorophenyl)-3-phenylpropan-1-one
Proton CDCl₃

7.995
7.984
7.971
7.319
7.304
7.290
7.257
7.243
7.229
7.214
7.199
7.135
7.120
7.105

3.292
3.279
3.265
3.079
3.066
3.052



3ba



1-(4-fluorophenyl)-3-phenylpropan-1-one
C13CPD CDCl3

— 197.558

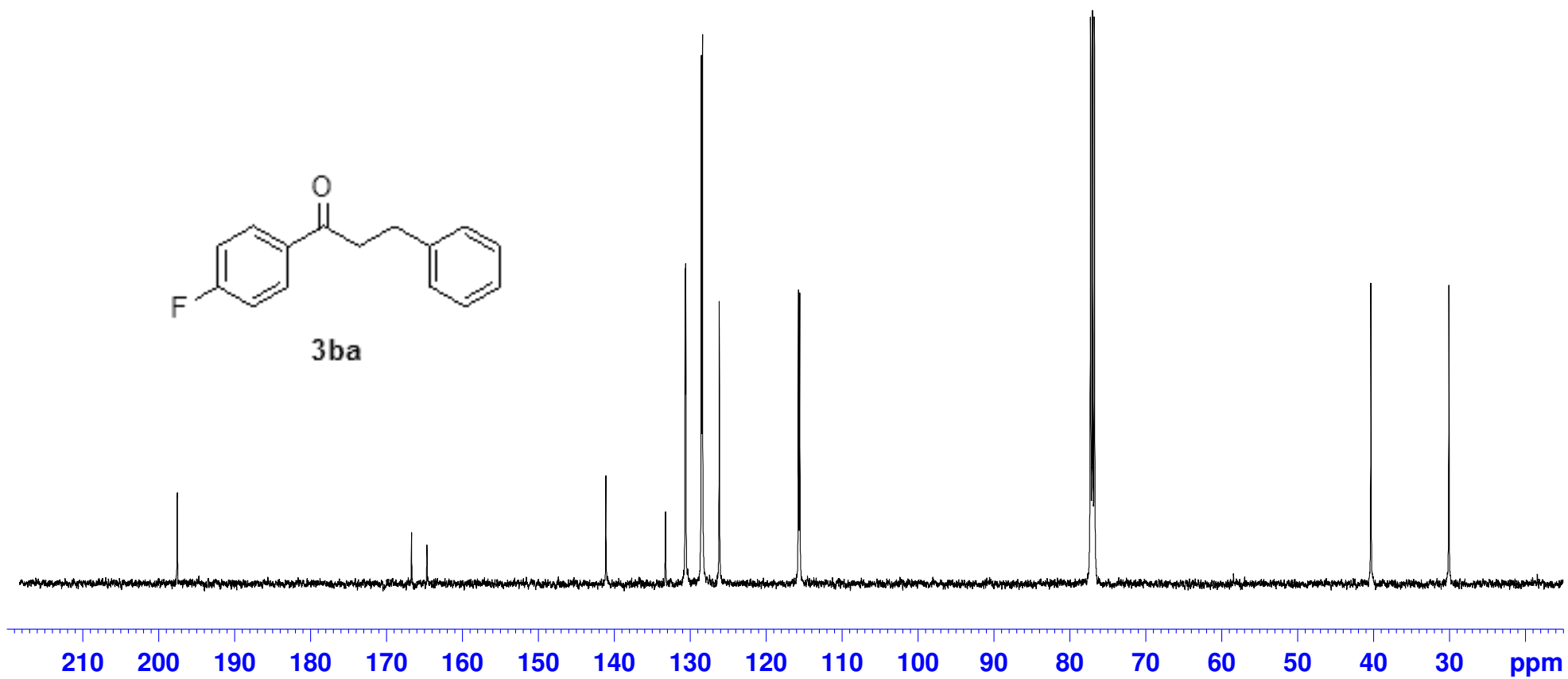
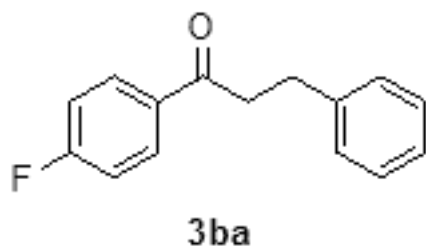
— 166.691
— 164.666

— 141.095
— 133.243
— 130.648
— 130.577
— 128.518
— 128.375
— 126.159
— 115.737
— 115.558

— 77.000

— 40.328

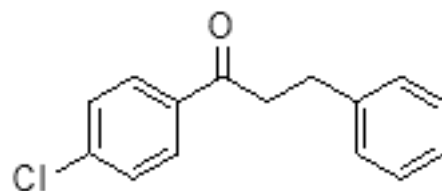
— 30.050



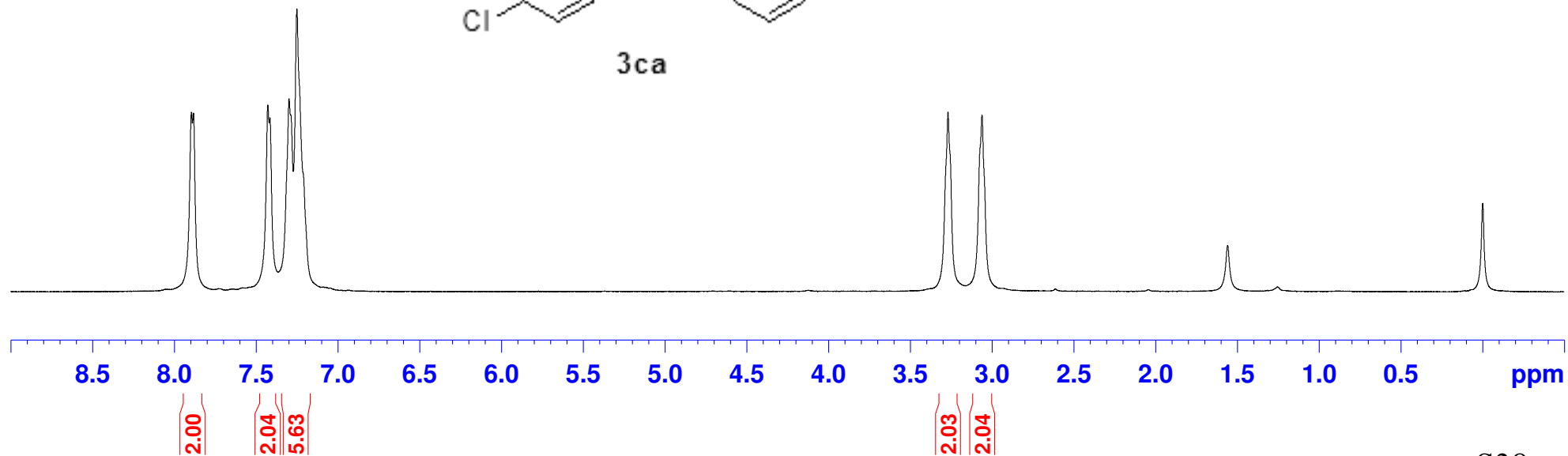
1-(4-chlorophenyl)-3-phenylpropan-1-one
Proton CDCl₃

7.898
7.885
7.430
7.417
7.300
7.288
7.252
7.237
7.212

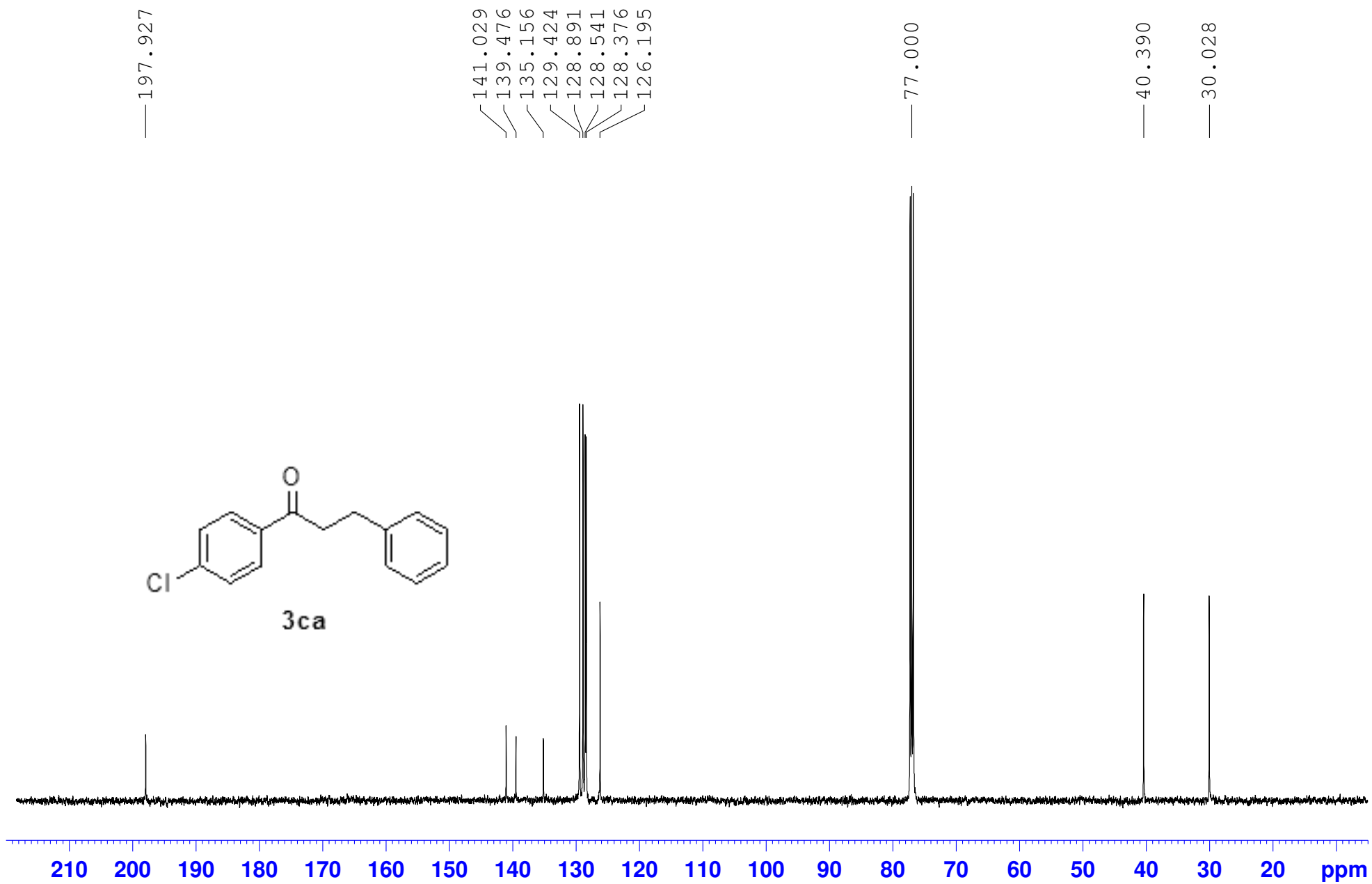
3.284
3.270
3.257
3.075
3.062
3.049



3ca



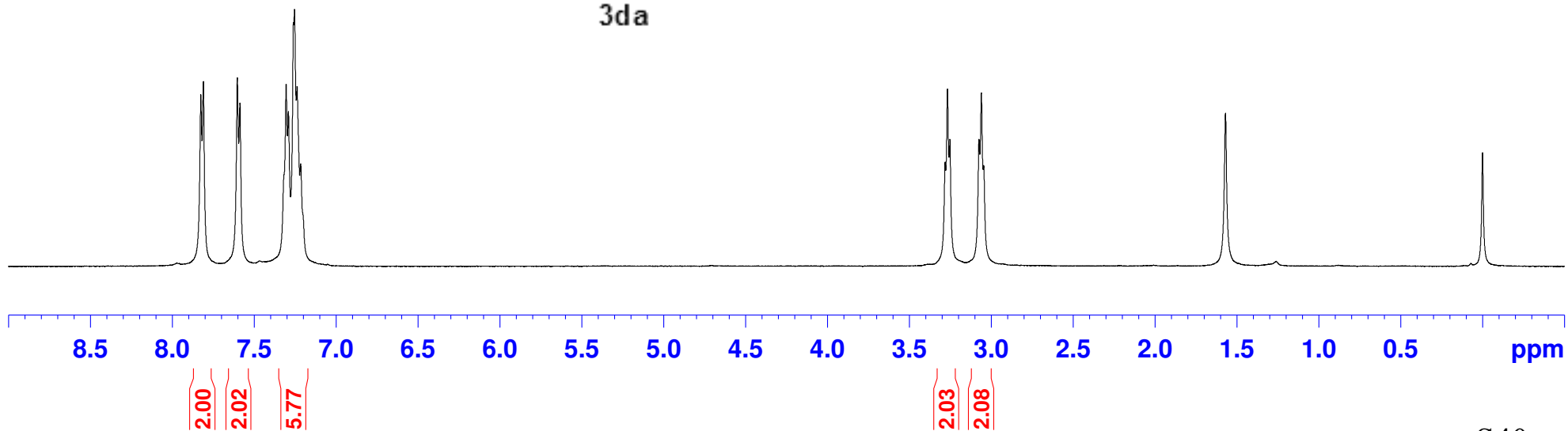
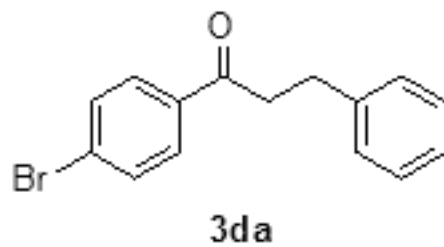
1-(4-chlorophenyl)-3-phenylpropan-1-one
C13CPD CDCl3



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

7.824
7.809
7.601
7.586
7.303
7.289
7.259
7.252
7.237
7.215

3.282
3.268
3.253
3.075
3.061
3.046



1-(4-bromophenyl)-3-phenylpropan-1-one
C13CPD CDCl3

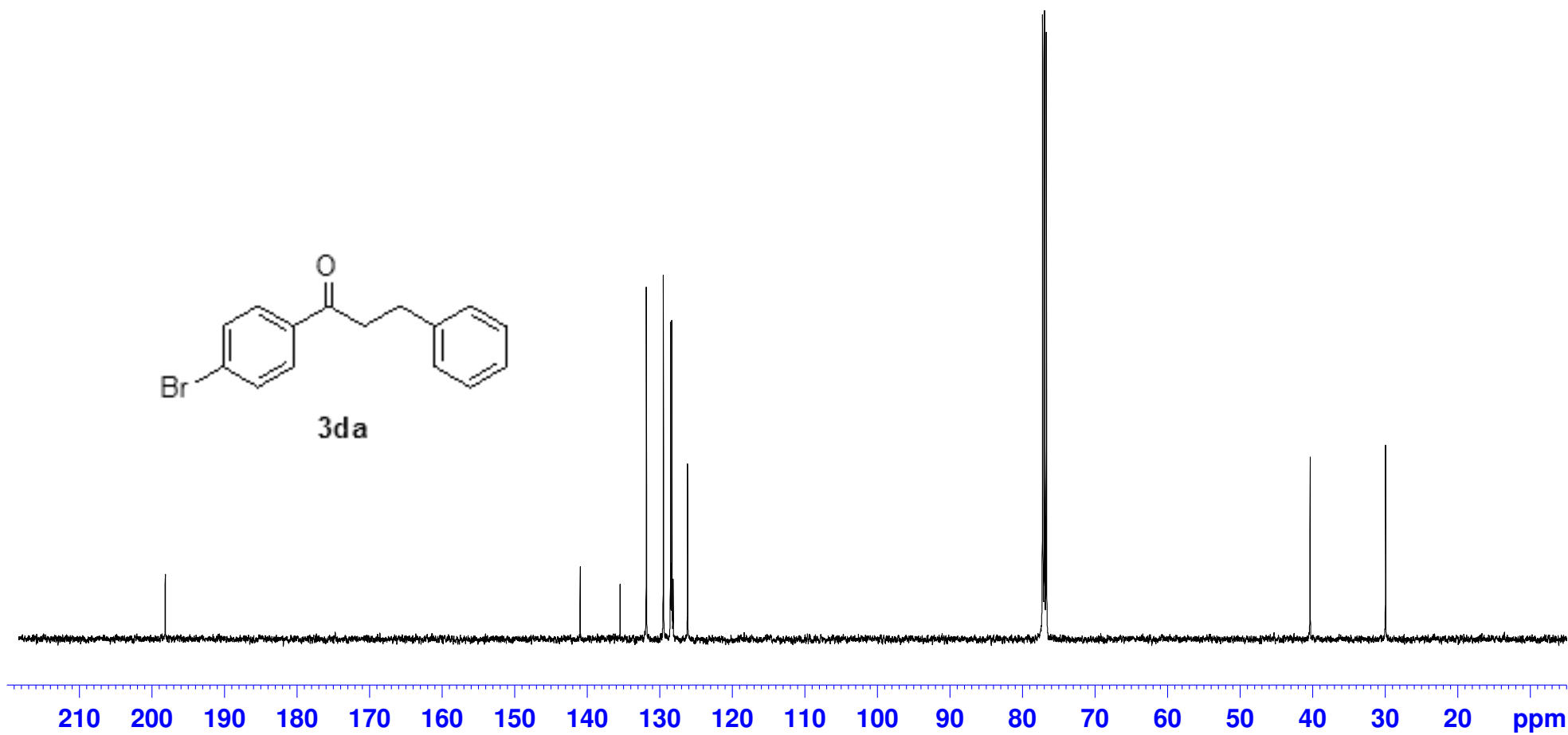
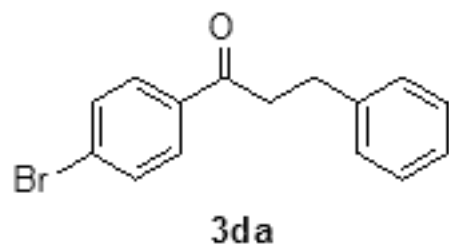
— 198.135

140.994
135.502
131.884
129.531
128.539
128.374
128.198
126.199

— 77.000

— 40.382

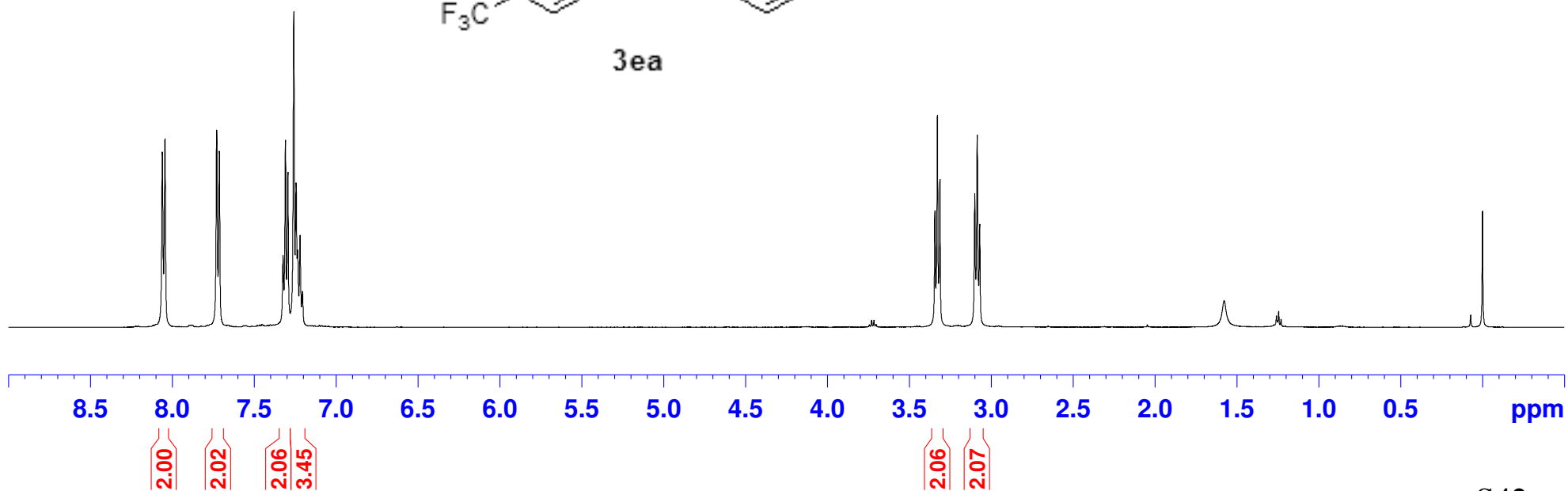
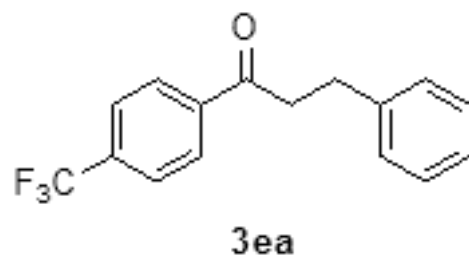
— 29.982



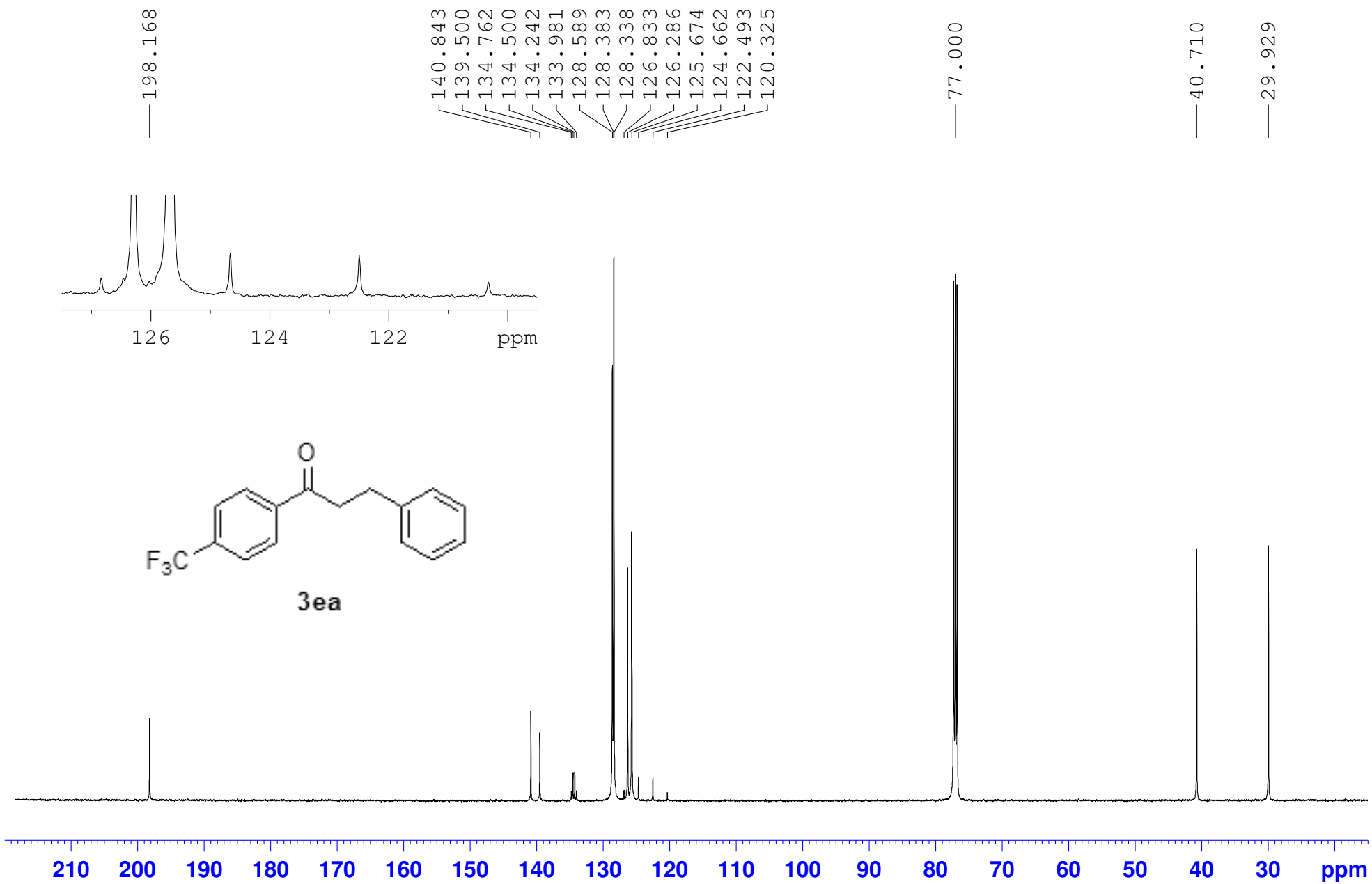
3-phenyl-1-(4-(trifluoromethyl)phenyl)propan-1-one
Proton CDCl₃

8.059
8.043
7.728
7.711
7.325
7.310
7.295
7.245
7.236
7.221
7.206

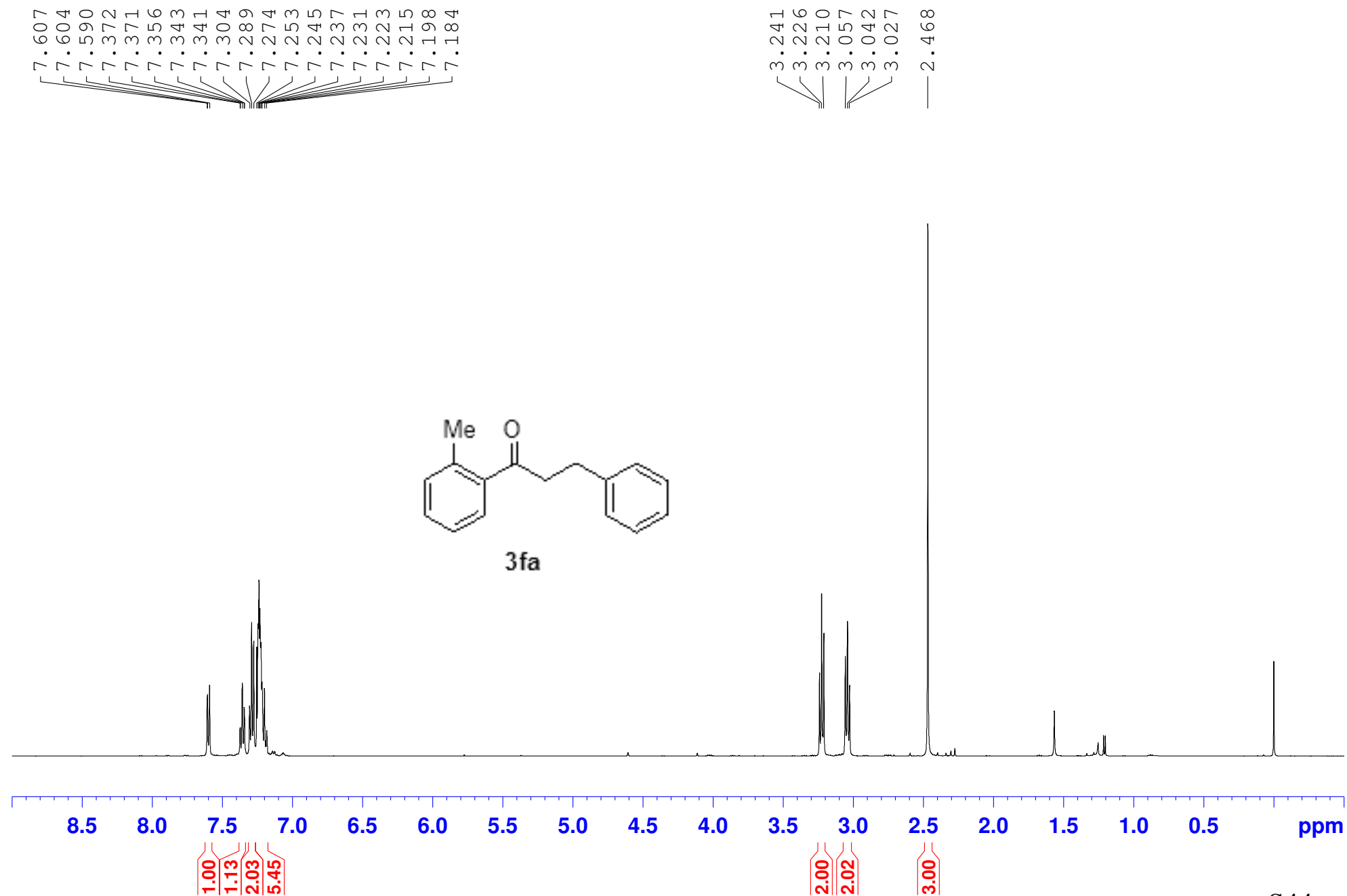
3.344
3.329
3.314
3.101
3.086
3.071



3-phenyl-1-(4-(trifluoromethyl)phenyl)propan-1-one
C13CPD CDC13



3-phenyl-1-o-tolylpropan-1-one
Proton CDCl₃



3-phenyl-1-o-tolylpropan-1-one
C13CPD CDC13

— 203.319

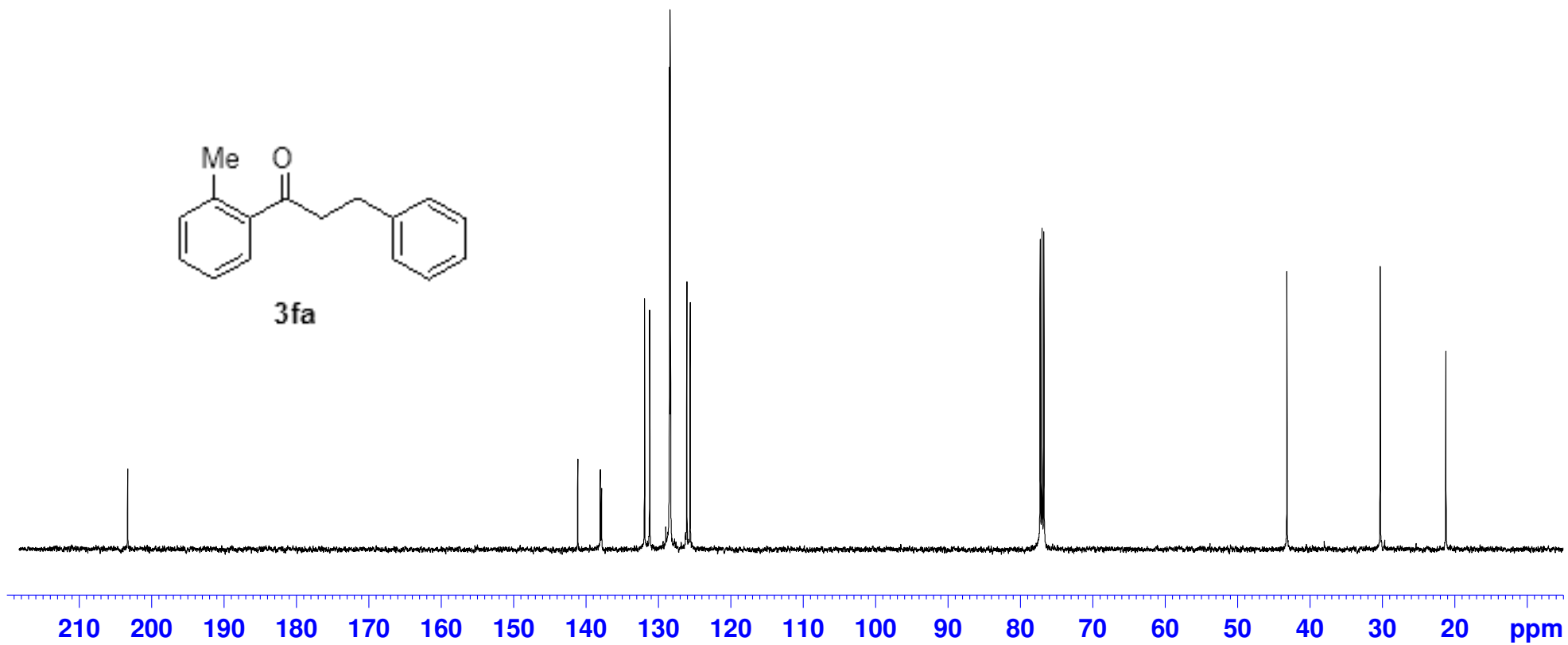
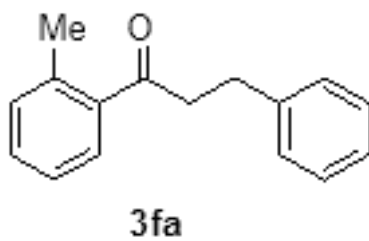
141.144
138.036
137.855
131.913
131.194
128.459
128.375
128.325
126.071
125.614

— 77.000

— 43.166

— 30.285

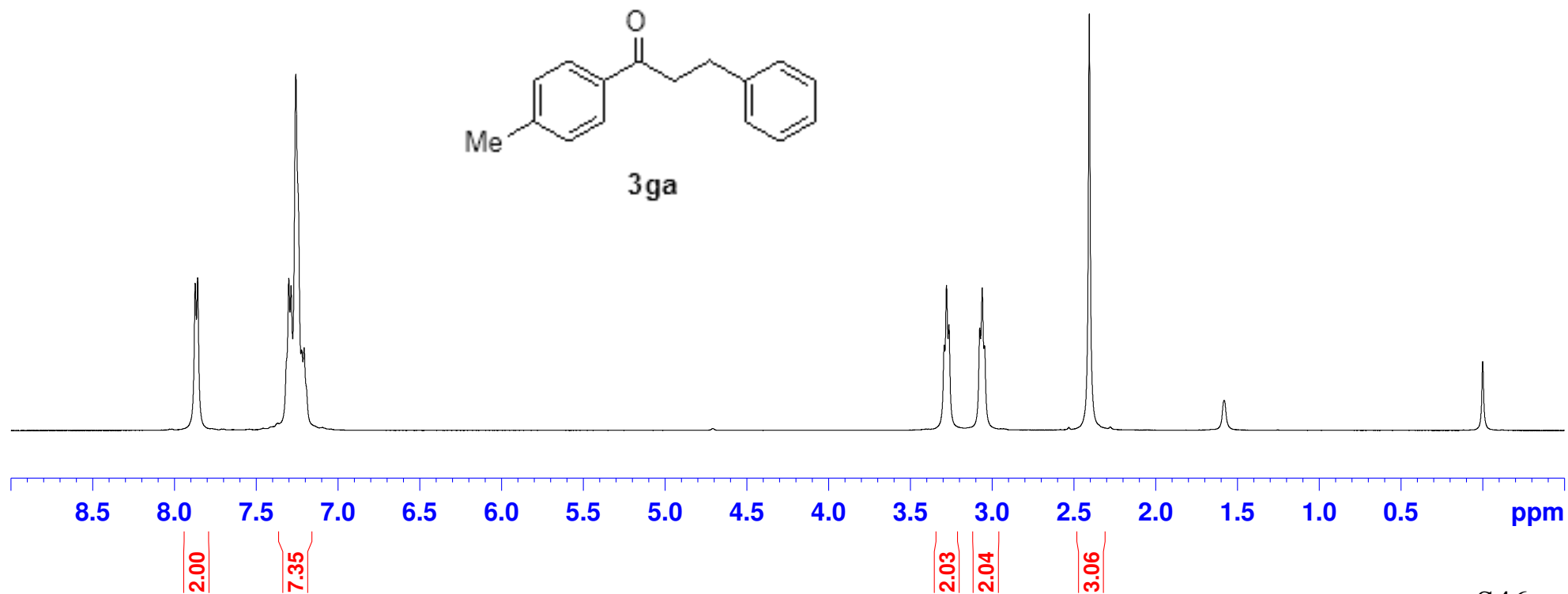
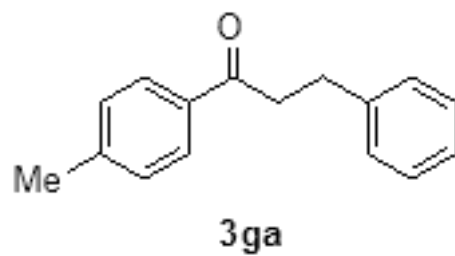
— 21.200



3-phenyl-1-p-tolylpropan-1-one
Proton CDCl₃

7.871
7.856
7.301
7.287
7.258
7.223
7.208

3.293
3.279
3.264
3.076
3.061
3.047
— 2.406



3-phenyl-1-(p-tolyl)propan-1-one
C13CPD CDC13

— 198.847

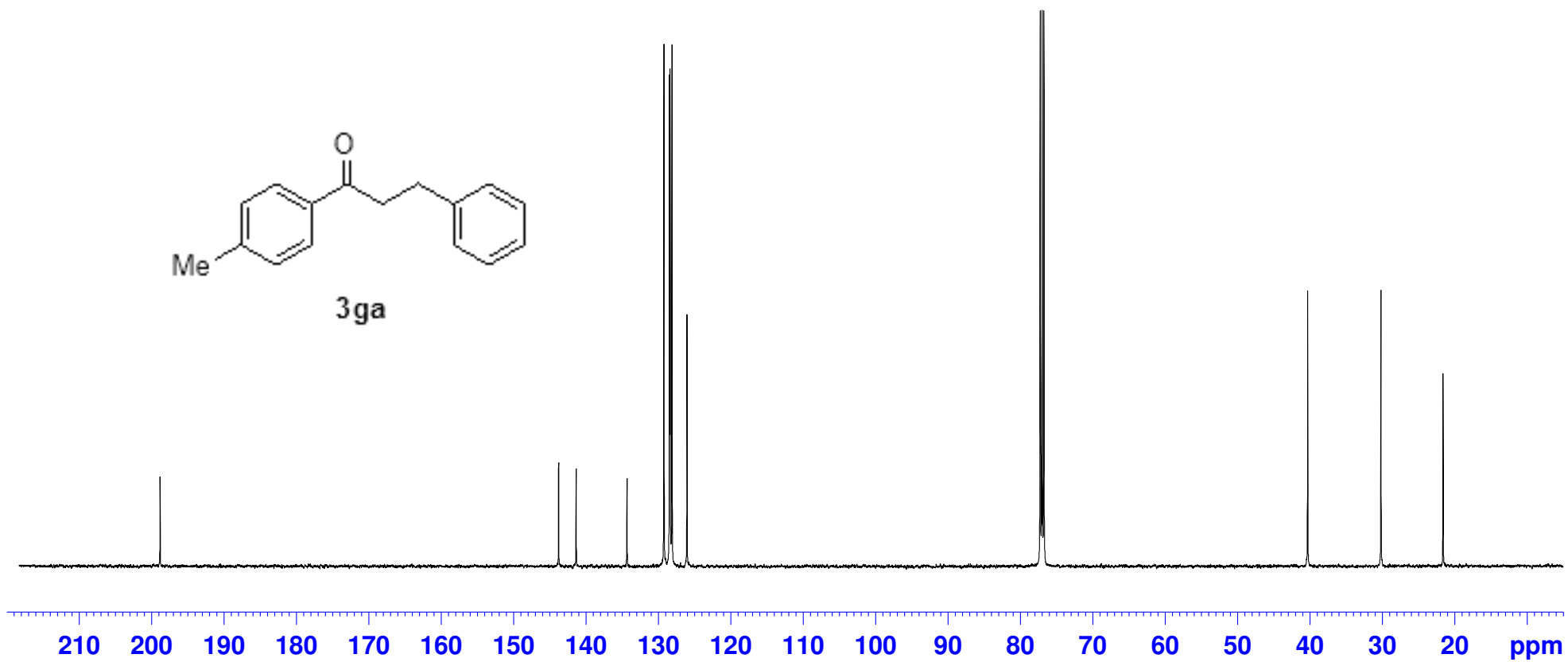
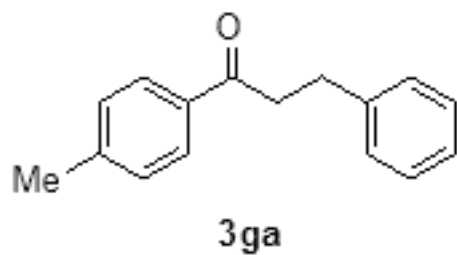
143.792
141.364
134.344
129.239
128.472
128.386
128.126
126.056

— 77.000

— 40.307

— 30.172

— 21.597

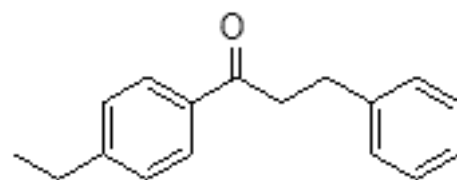


1-(4-ethylphenyl)-3-phenylpropan-1-one
Proton CDCl₃

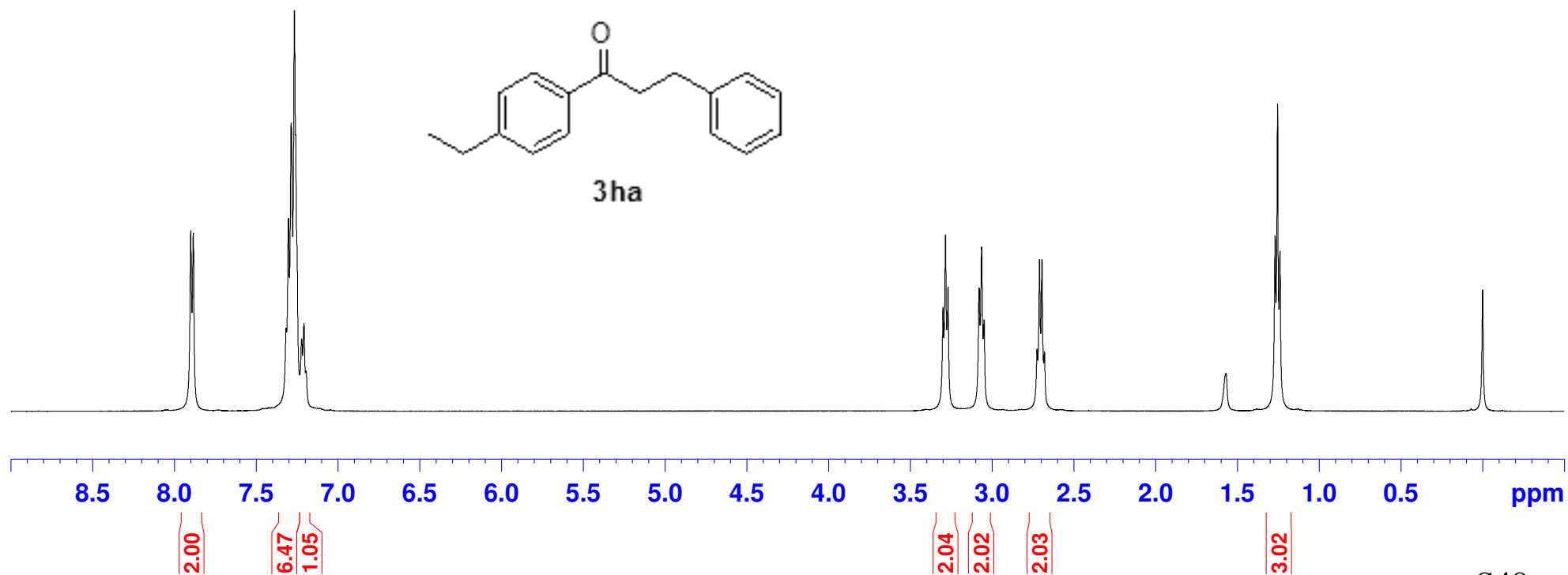
7.901
7.885
7.318
7.303
7.287
7.267
7.223
7.209
7.196

3.300
3.285
3.270
3.080
3.064
3.049
2.725
2.710
2.695
2.680

1.270
1.255
1.240



3ha



1-(4-ethylphenyl)-3-phenylpropan-1-one
C13CPD CDCl3

— 198.868

— 149.976

— 141.381

— 134.557

— 128.476

— 128.395

— 128.238

— 128.064

— 126.057

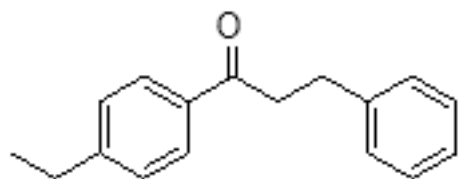
— 77.000

— 40.331

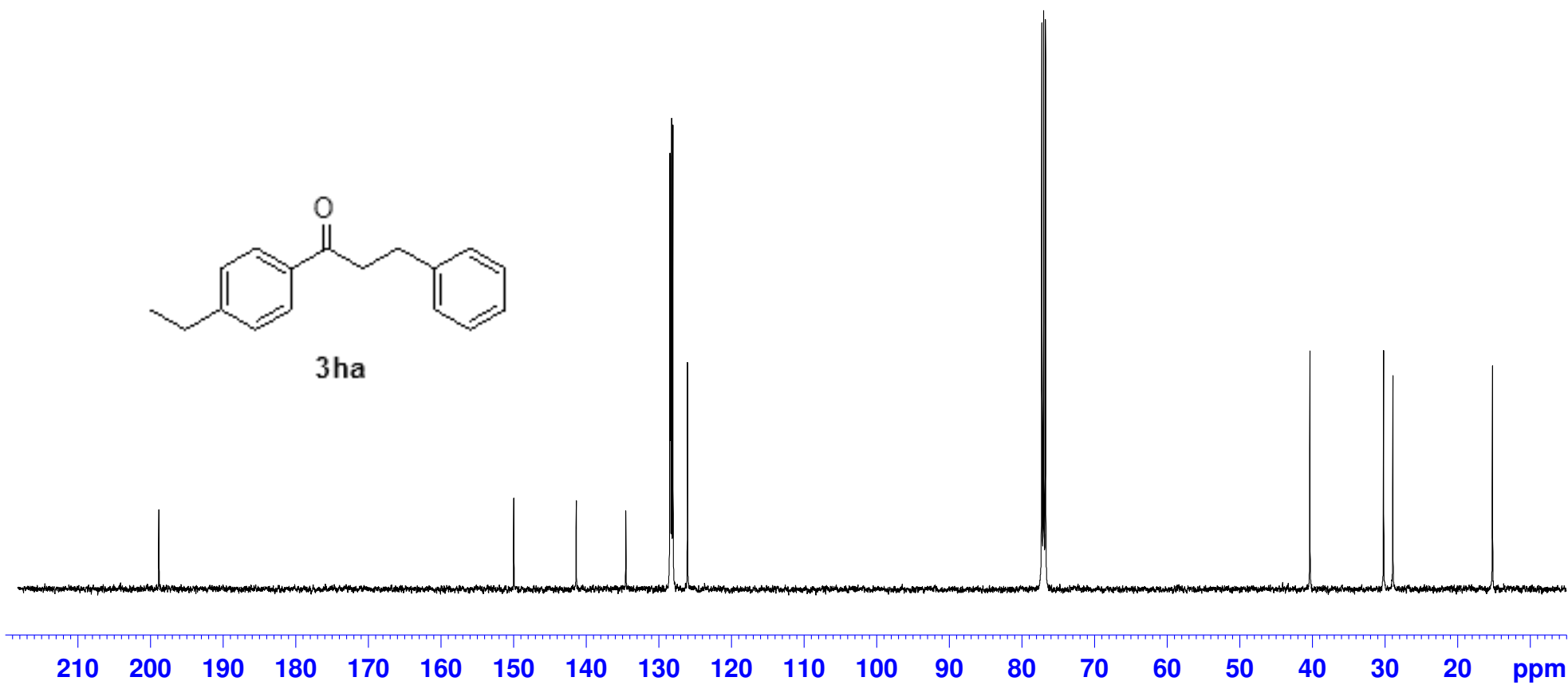
— 30.173

— 28.898

— 15.176



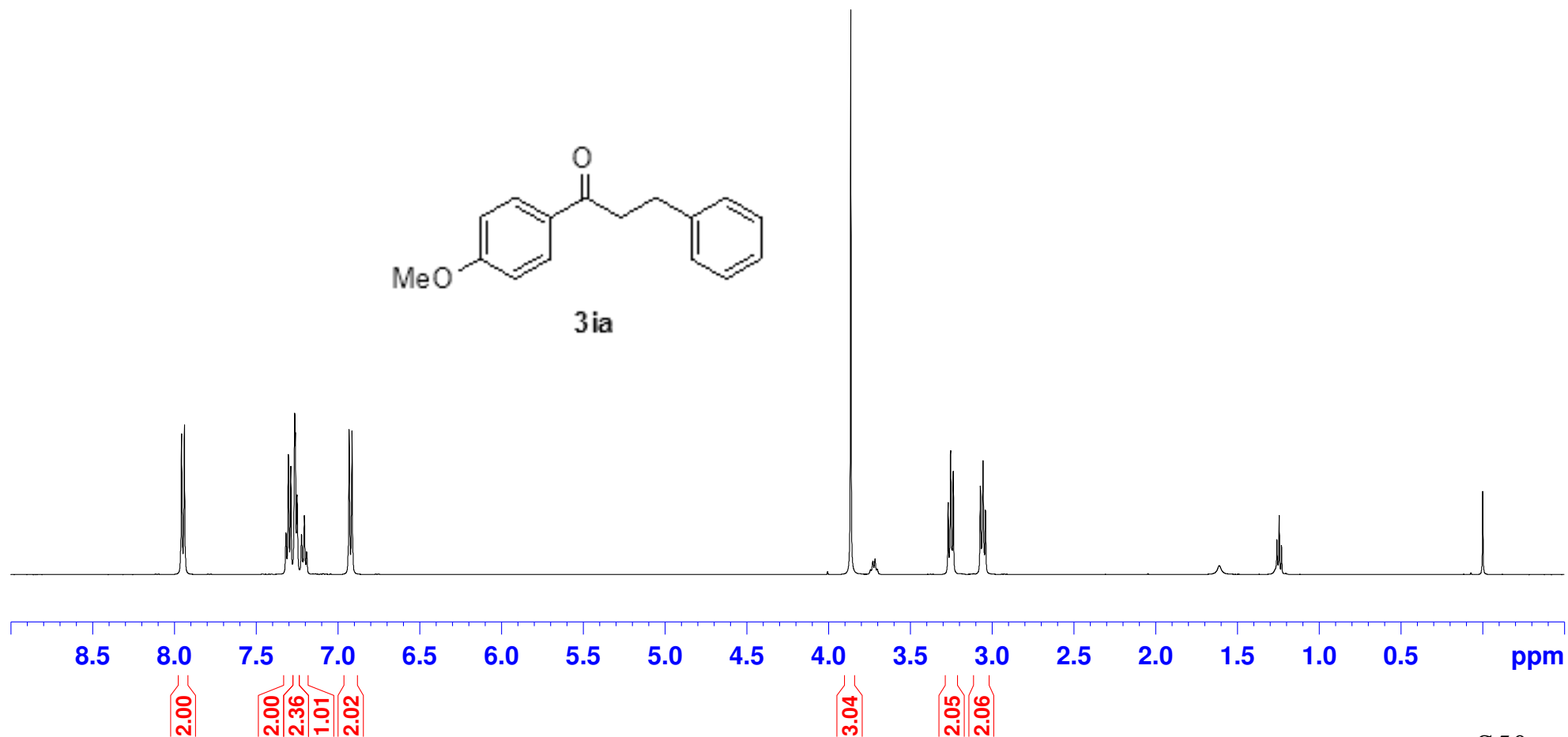
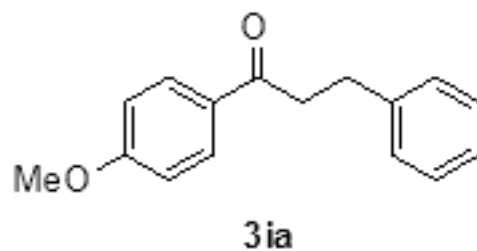
3ha



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

7.955
7.937
7.317
7.301
7.287
7.262
7.259
7.248
7.221
7.207
7.192
6.933
6.915

3.865
3.269
3.254
3.238
3.072
3.056
3.041



1-(4-methoxyphenyl)-3-phenylpropan-1-one
C13CPD CDCl3

— 197.771

— 163.404

— 141.429

130.261

129.929

128.463

128.383

126.039

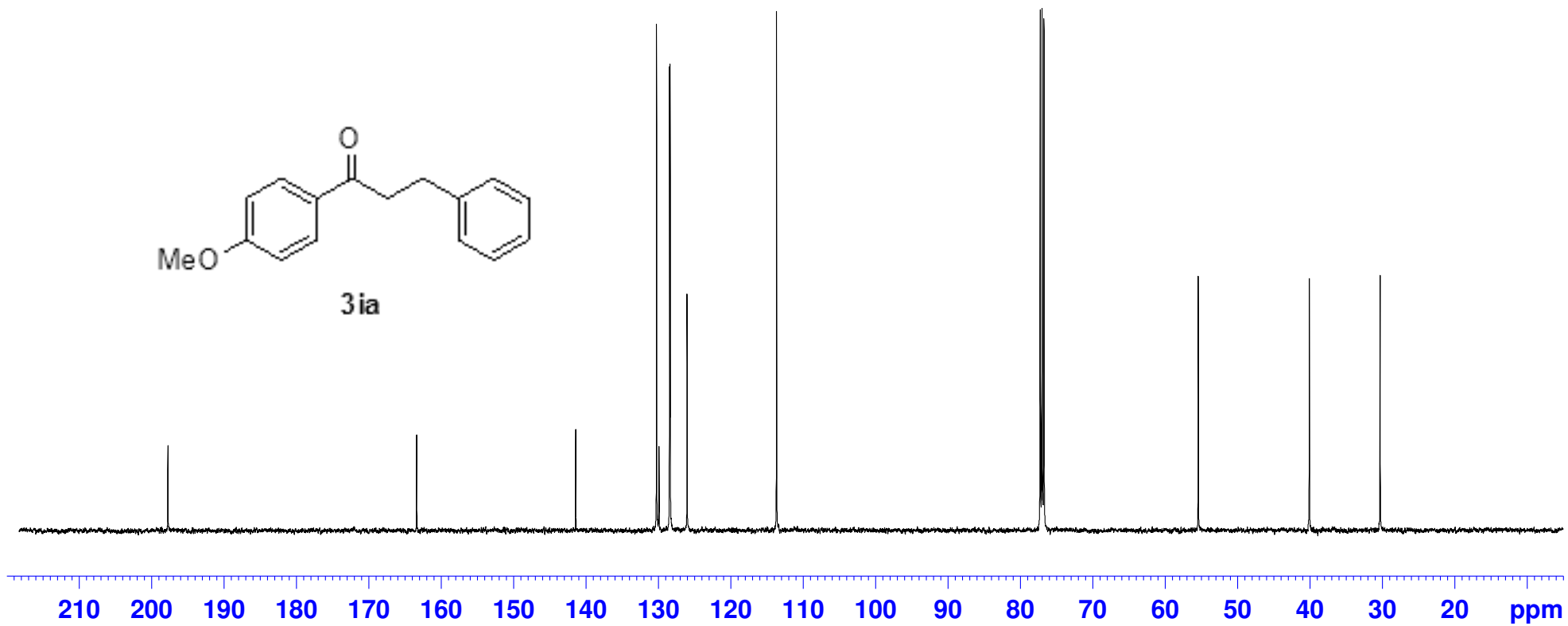
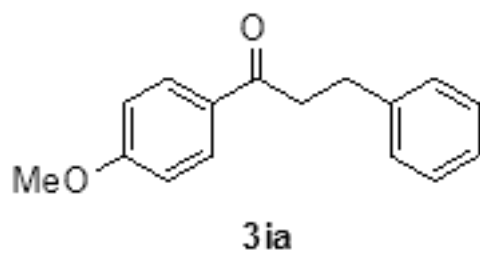
— 113.683

— 77.000

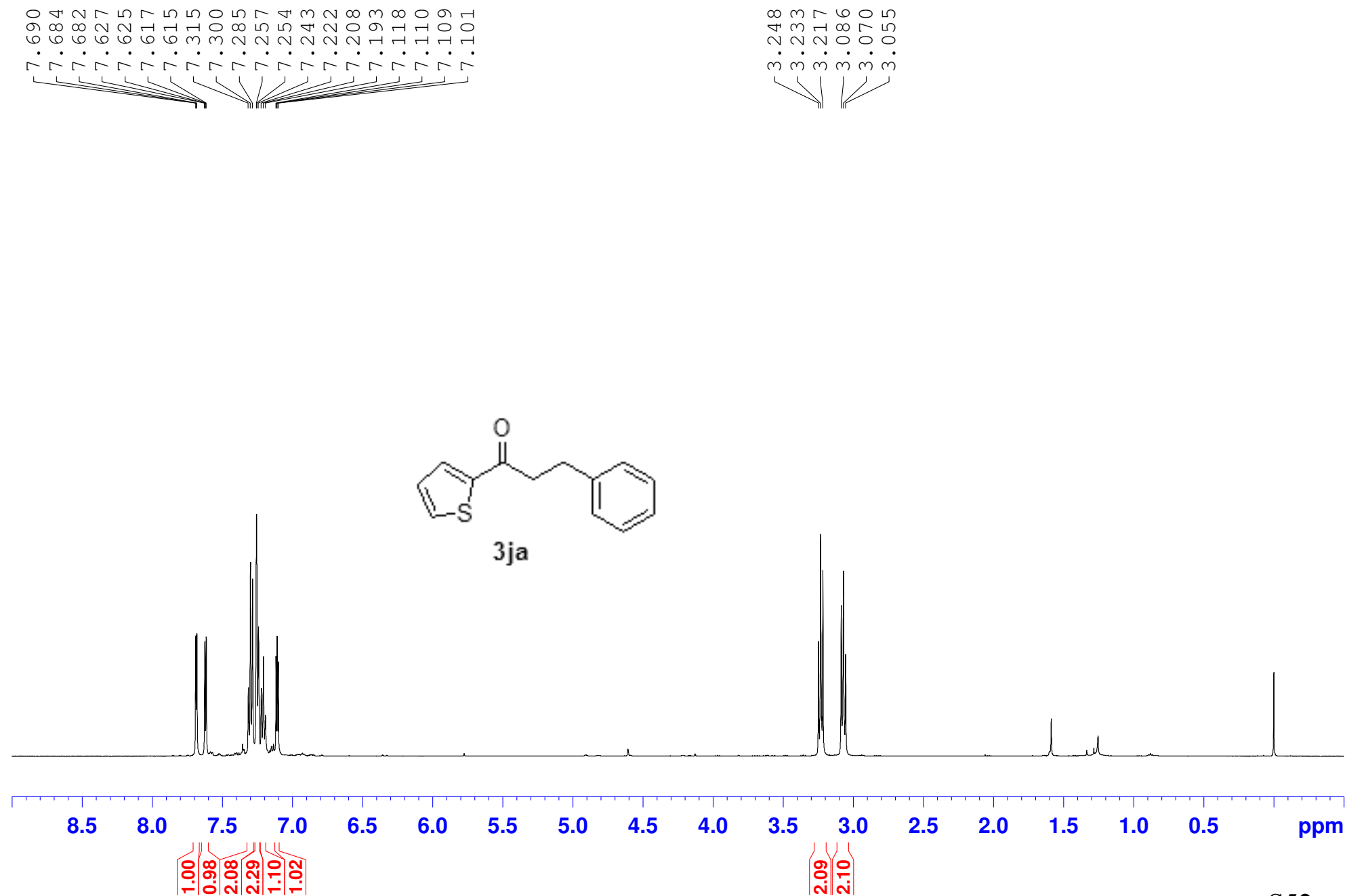
— 55.416

— 40.072

— 30.288



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



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

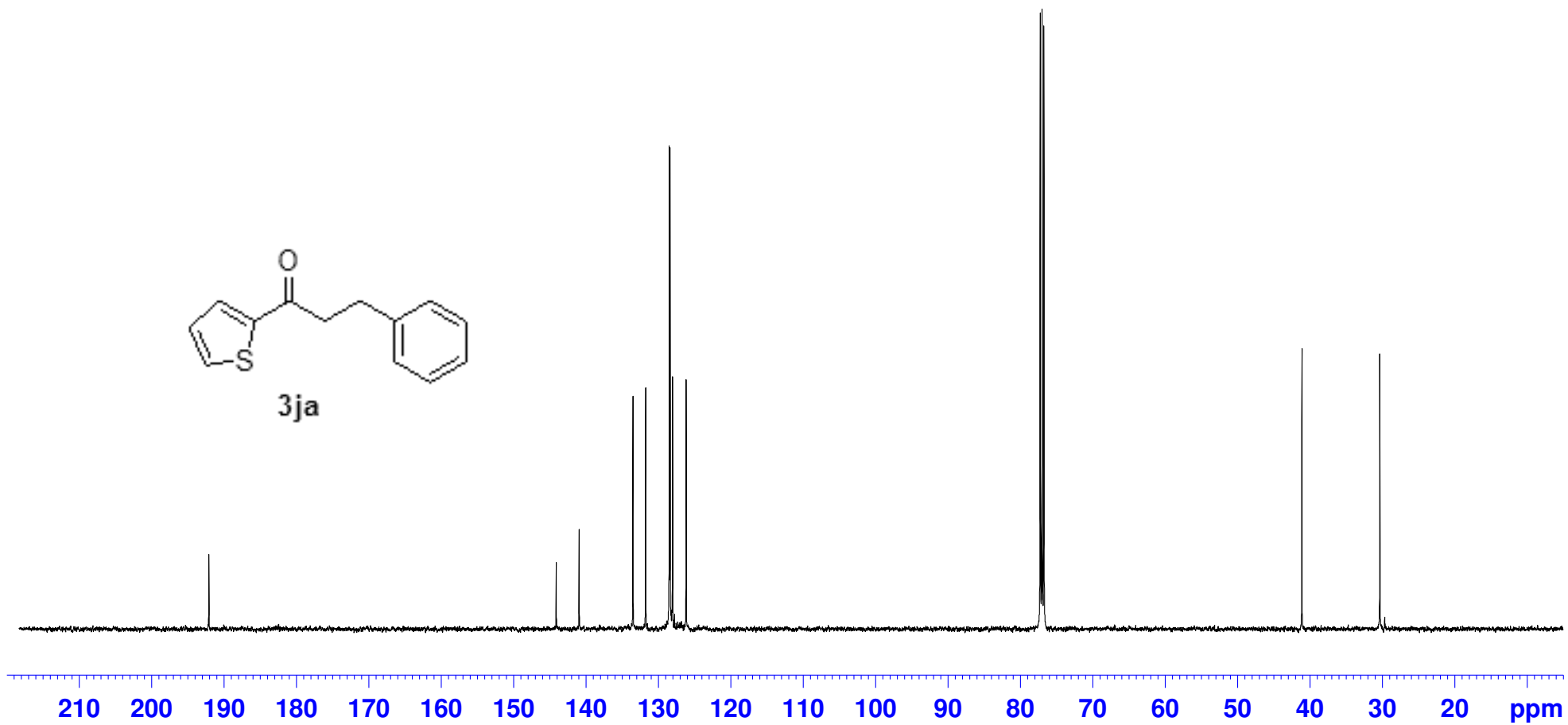
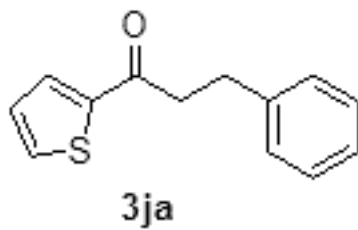
— 192.103

144.122
140.952
133.512
131.763
128.506
128.382
128.045
126.169

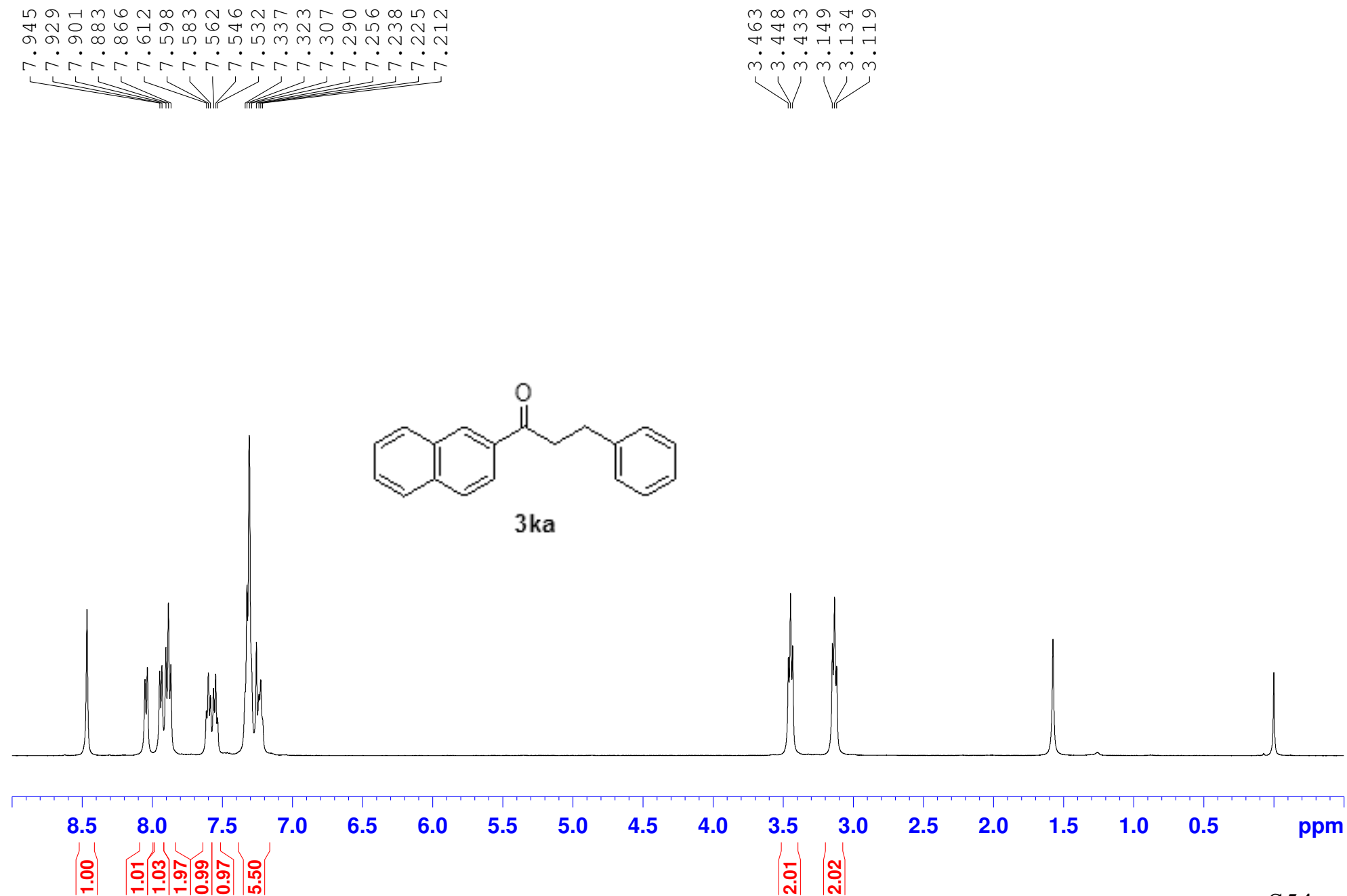
— 77.000

— 41.097

— 30.334



1-(naphthalen-2-yl)-3-phenylpropan-1-one
Proton CDCl₃



1-(naphthalen-2-yl)-3-phenylpropan-1-one
C13CPD CDC13

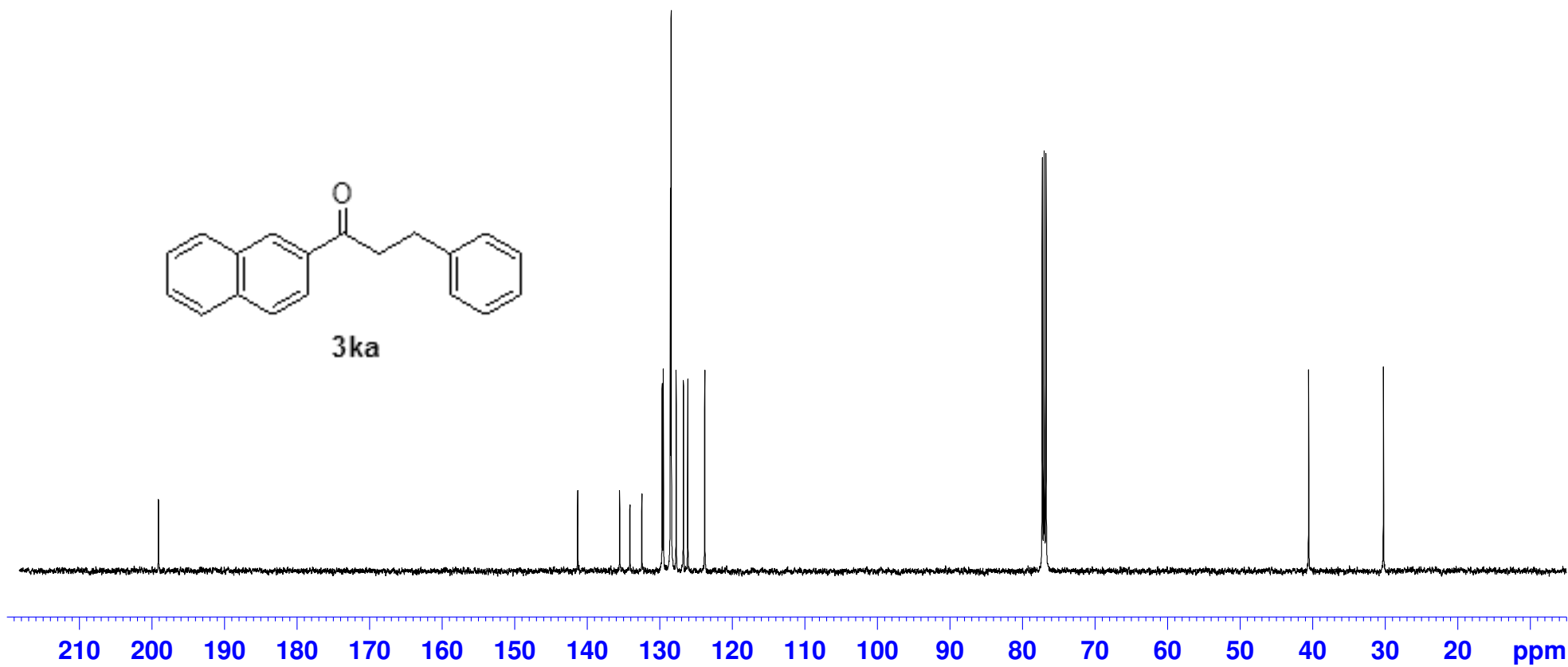
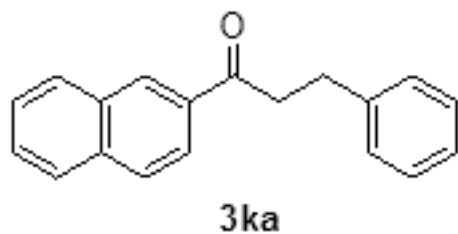
— 199.114

141.312
135.527
134.112
132.470
129.657
129.502
128.526
128.427
127.733
126.732
126.131
123.795

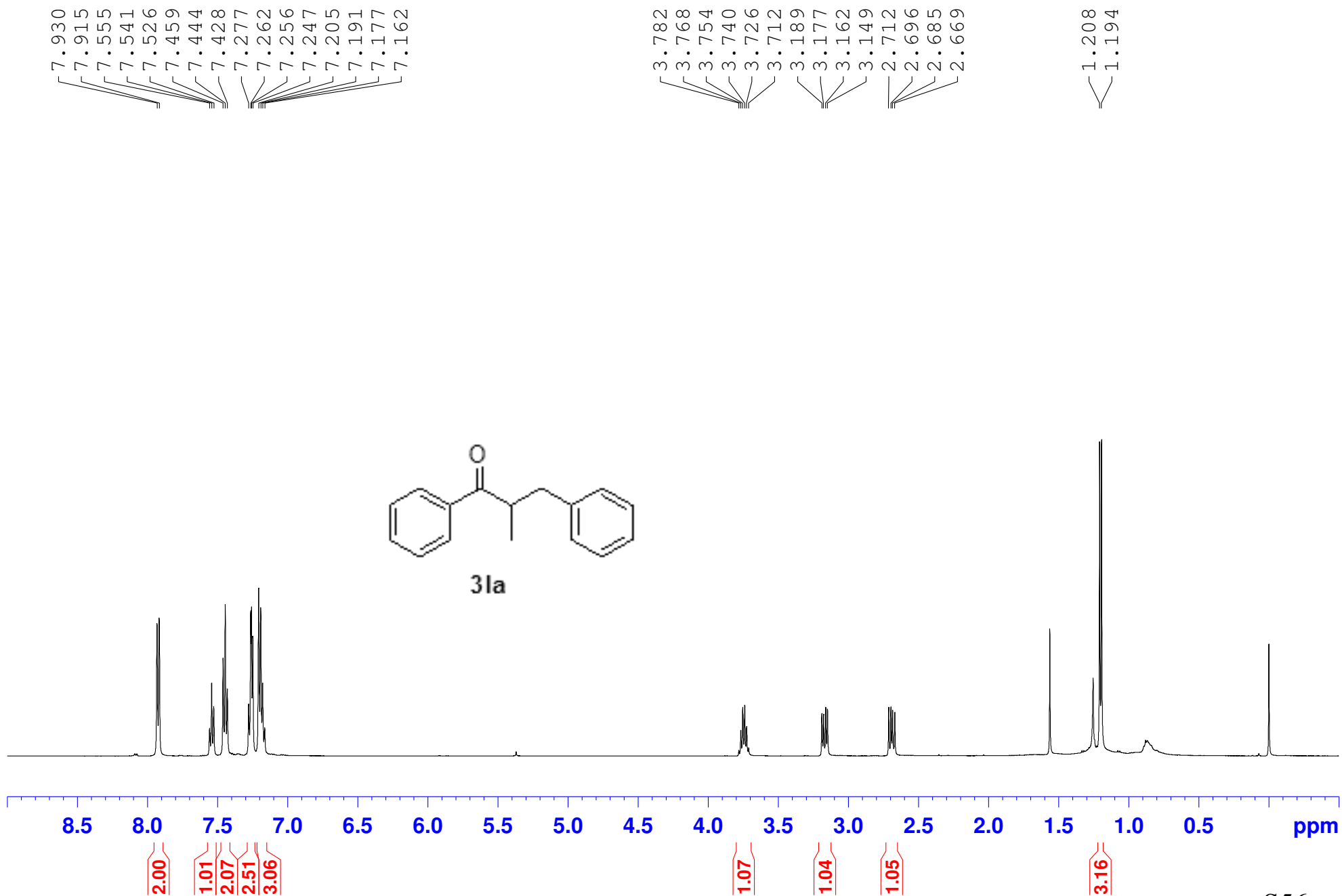
— 77.000

— 40.529

— 30.222



2-methyl-1,3-diphenylpropan-1-one
Proton CDCl₃



2-methyl-1,3-diphenylpropan-1-one
C13CPD CDC13

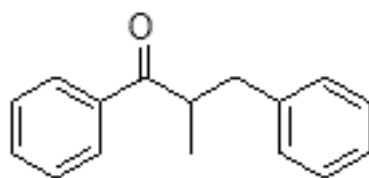
— 203.694

139.924
136.459
132.868
129.055
128.596
128.343
128.249
126.164

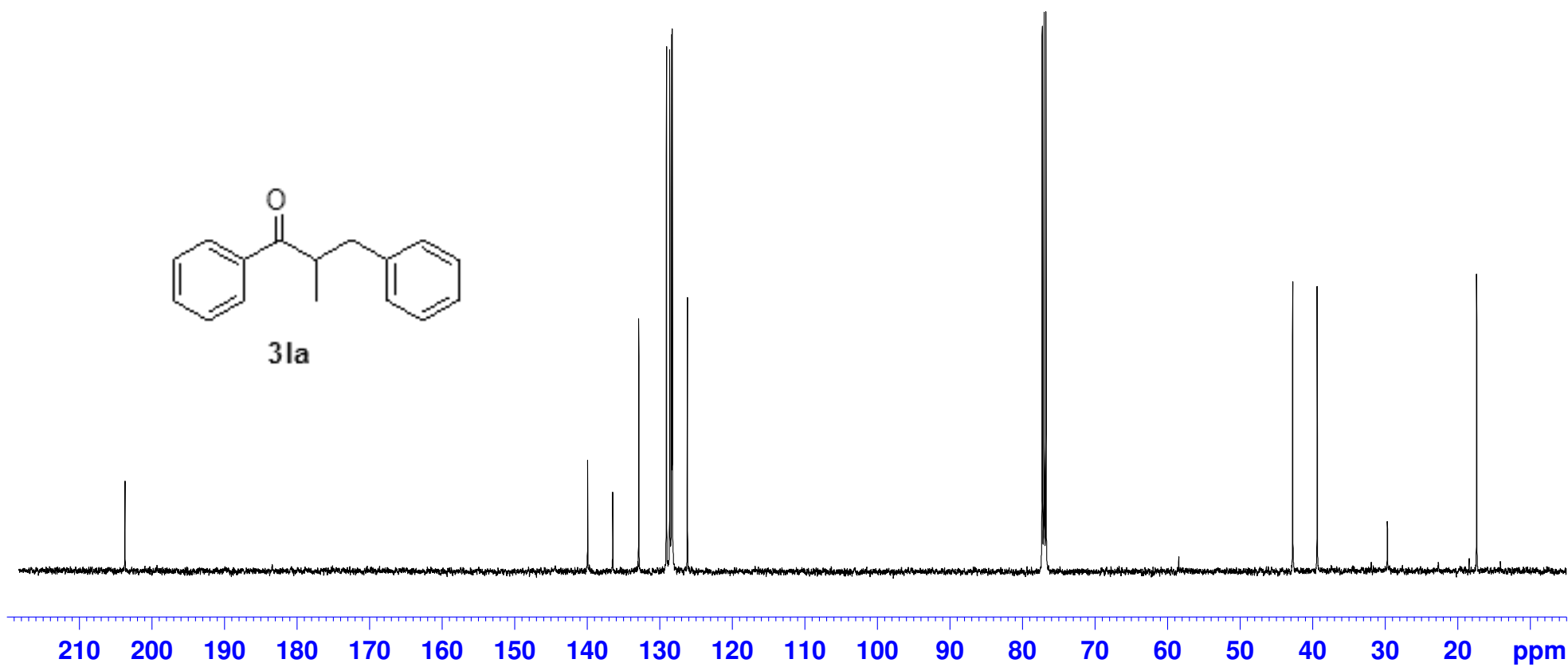
— 77.000

— 42.731
— 39.352

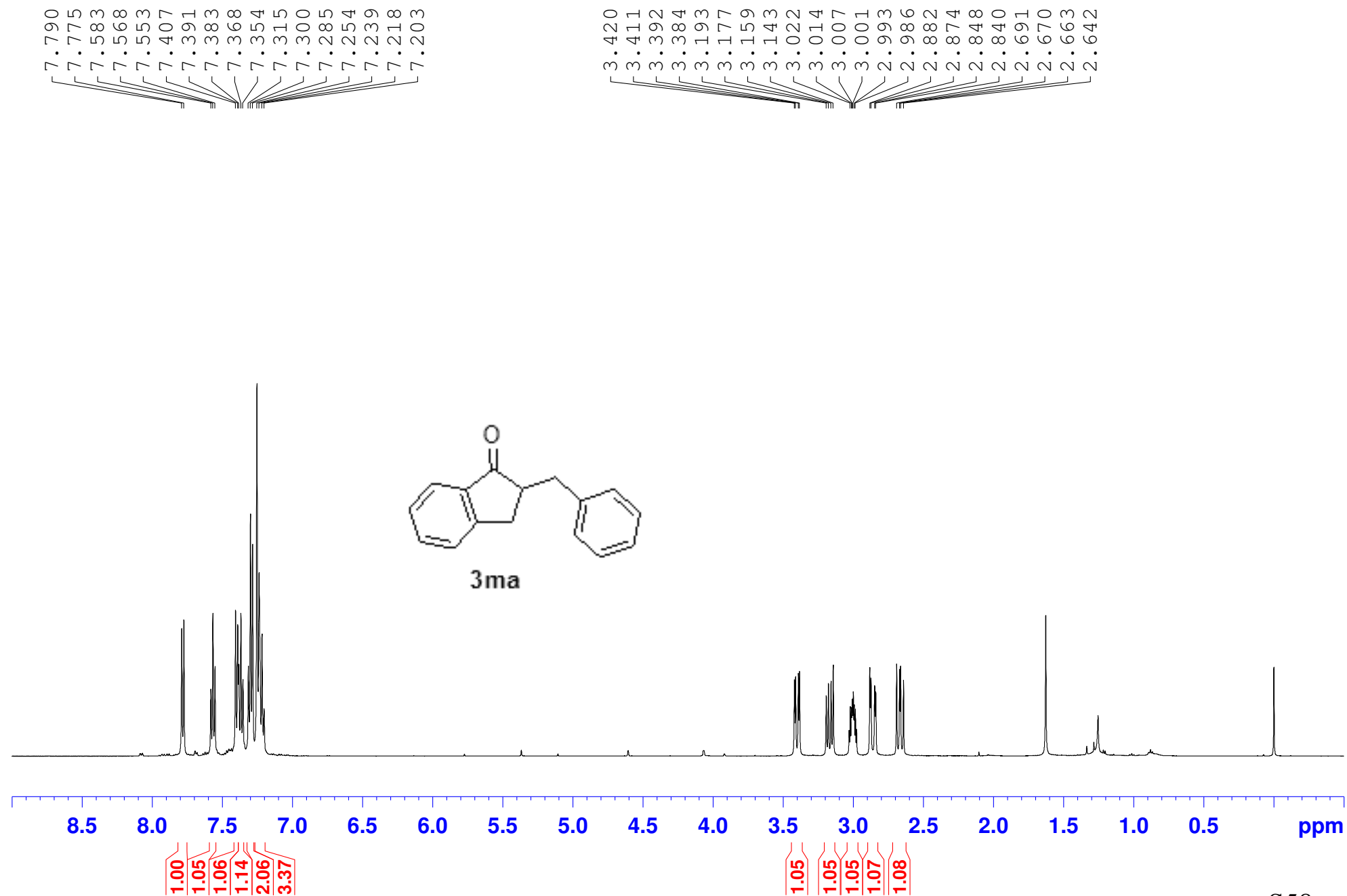
— 17.368



3la



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



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

—207.733

—153.578

139.604

136.517

134.761

128.859

128.484

127.383

126.540

126.309

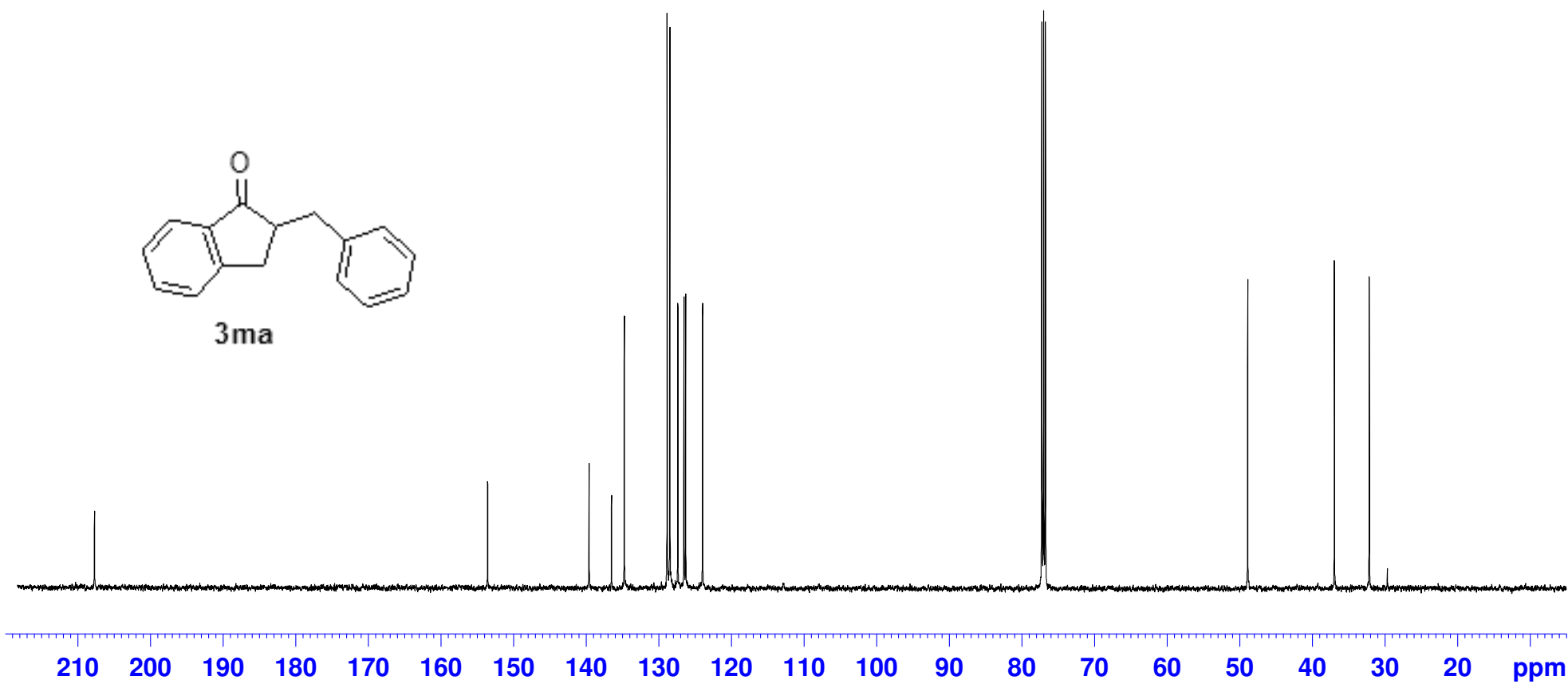
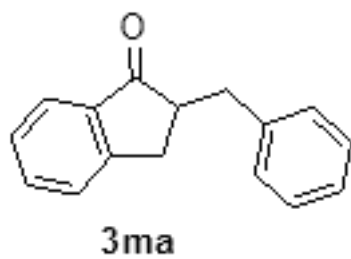
123.979

—77.000

—48.891

—36.952

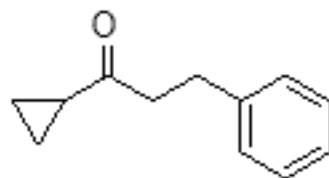
—32.152



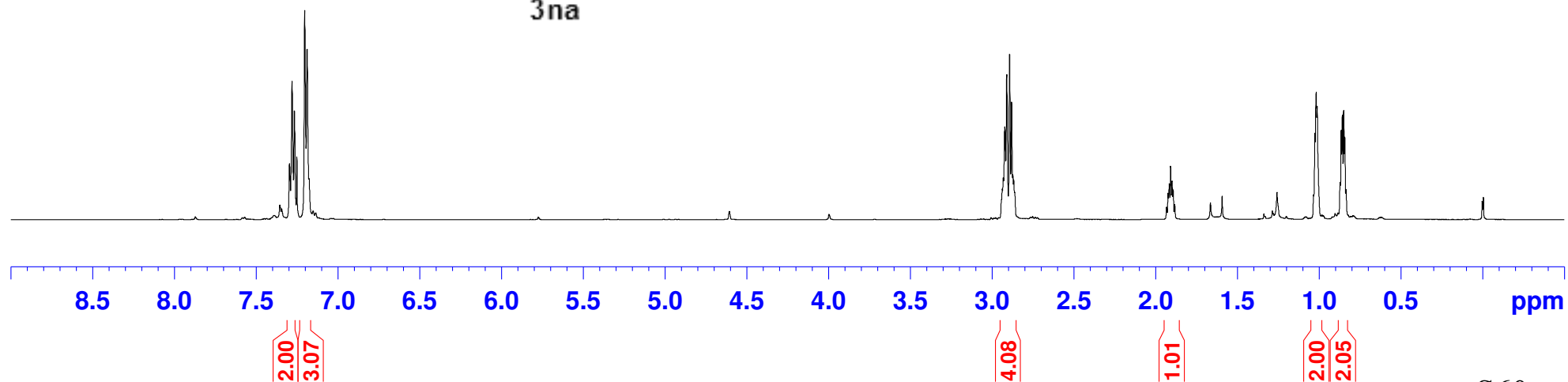
1-cyclopropyl-3-phenylpropan-1-one
Proton CDCl₃

7.297
7.281
7.267
7.252
7.204
7.189
7.178

2.938
2.932
2.923
2.911
2.893
2.881
2.873
2.868
2.862
1.934
1.925
1.917
1.909
1.900
1.894
1.884
1.035
1.027
1.018
1.012
0.872
0.866
0.858
0.850
0.844
0.836



3na



1-cyclopropyl-3-phenylpropan-1-one
C13CPD CDCl3

— 209.948

— 141.167

— 128.410

— 128.282

— 125.996

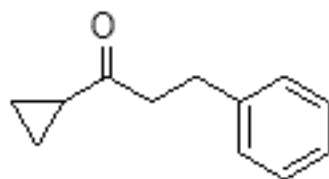
— 77.000

— 44.926

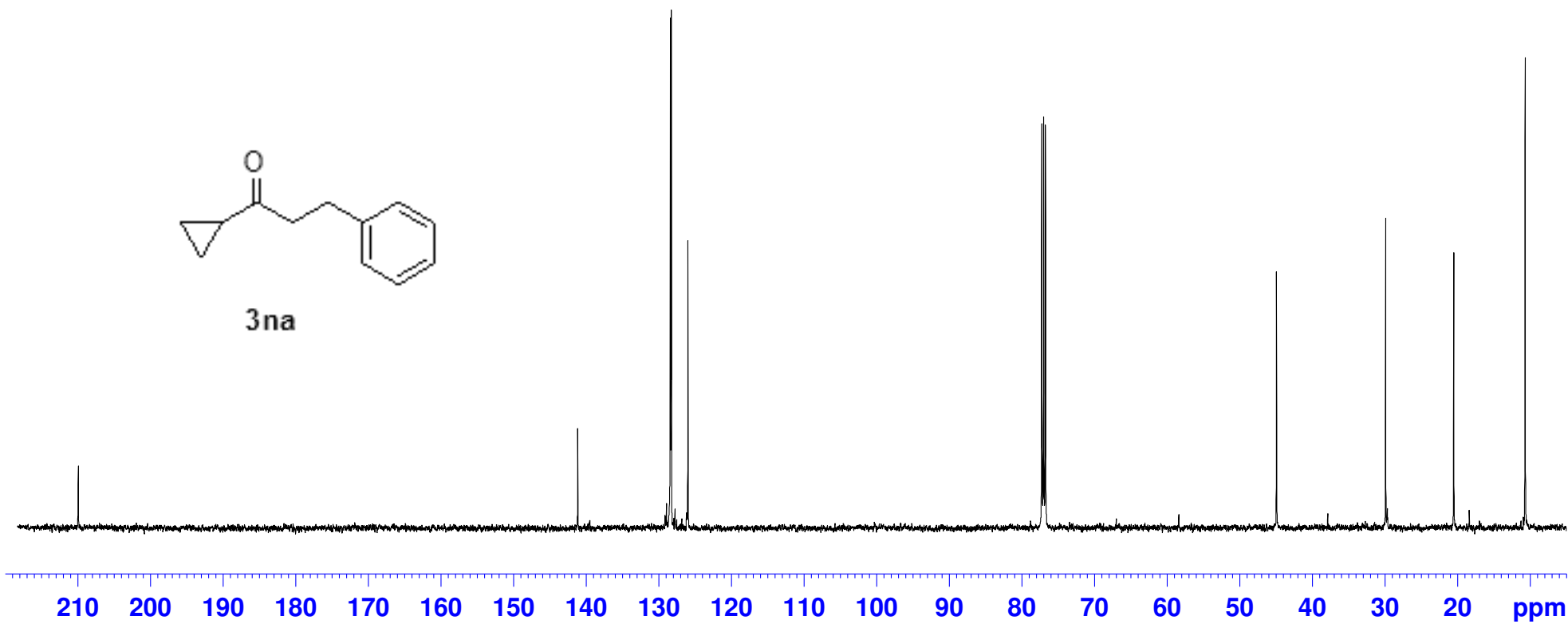
— 29.888

— 20.510

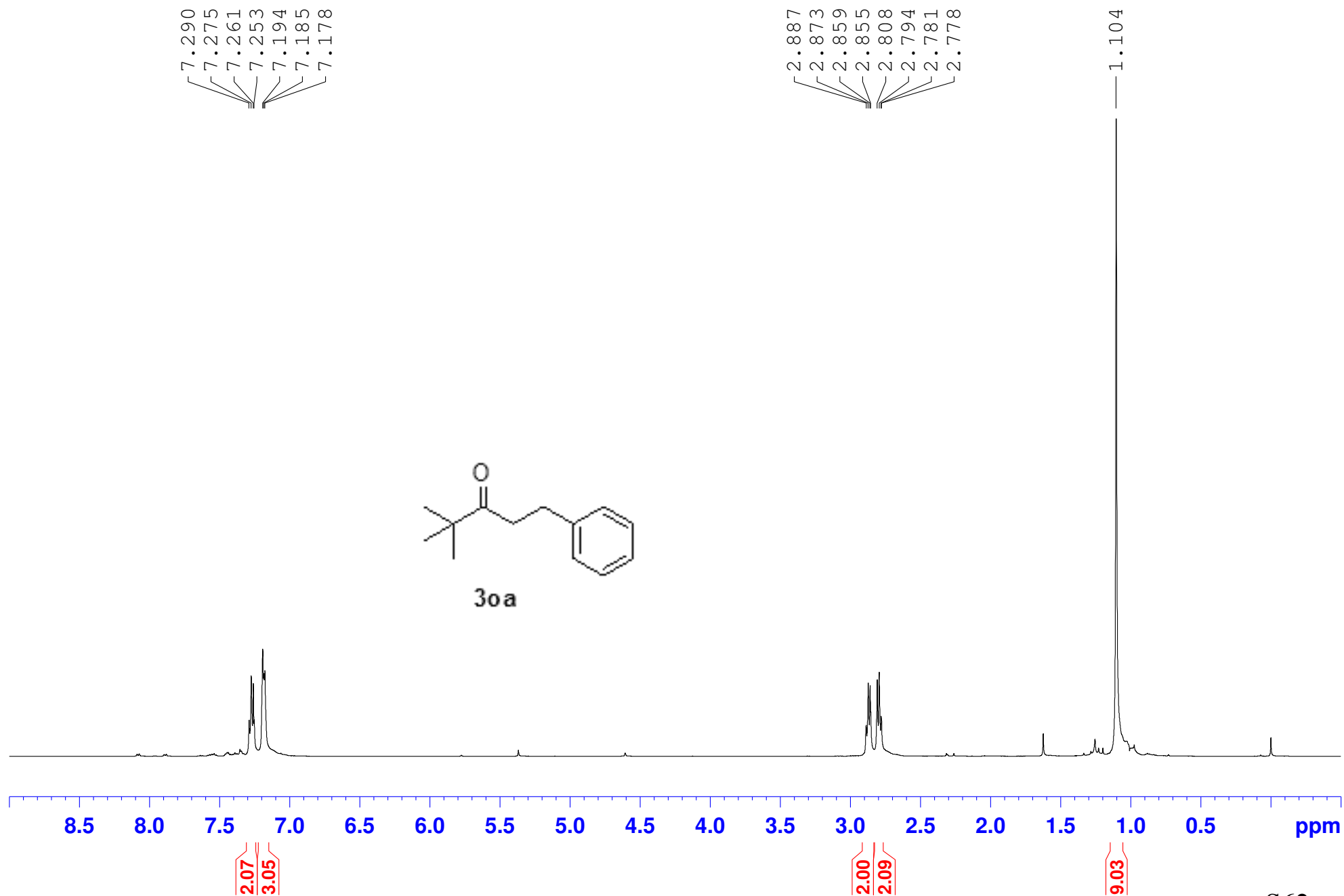
— 10.676



3na



4,4-dimethyl-1-phenylpentan-3-one
Proton CDCl₃



4,4-dimethyl-1-phenylpentan-3-one
C13CPD CDCl3

—214.825

—141.530

—128.368

—128.333

—125.944

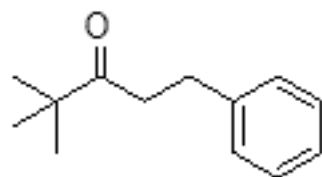
—77.000

—44.009

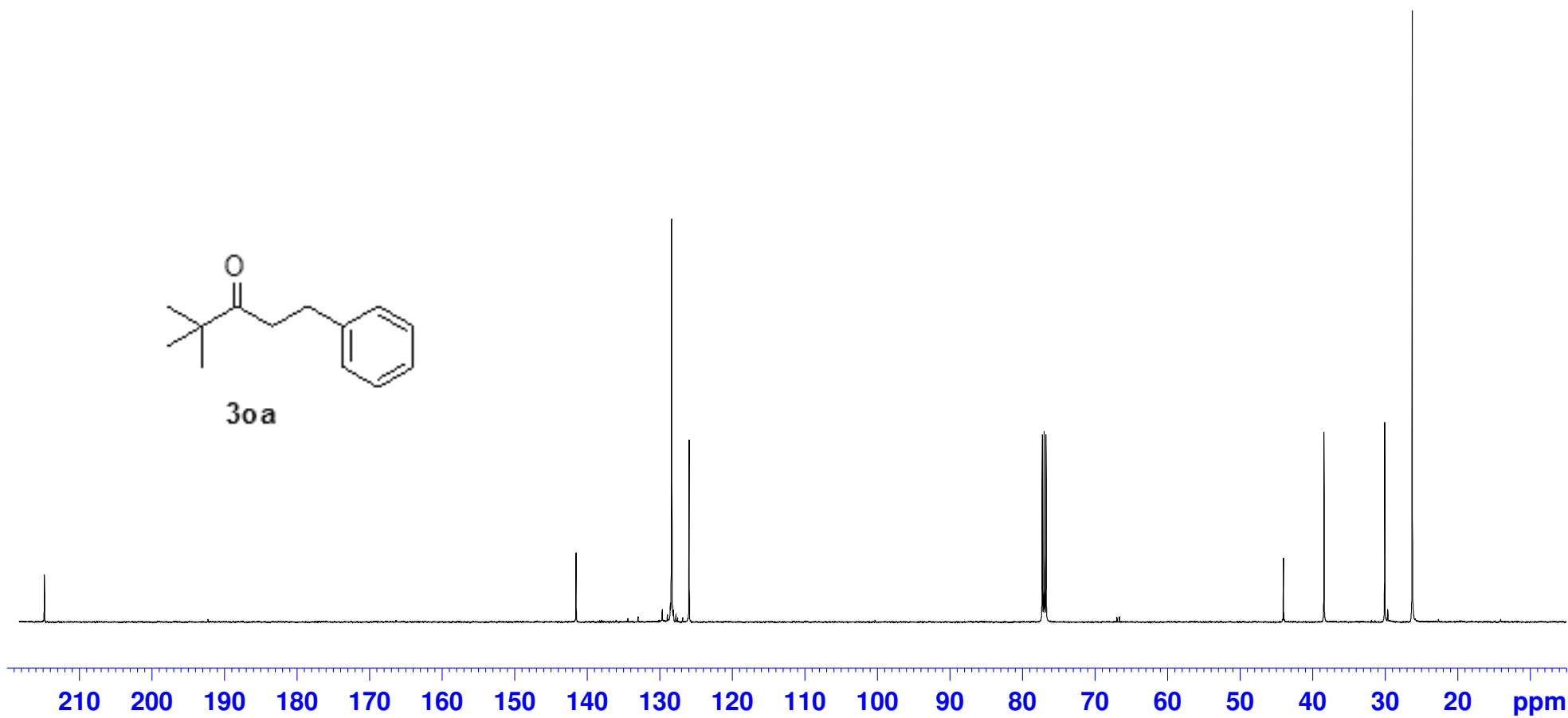
—38.417

—30.046

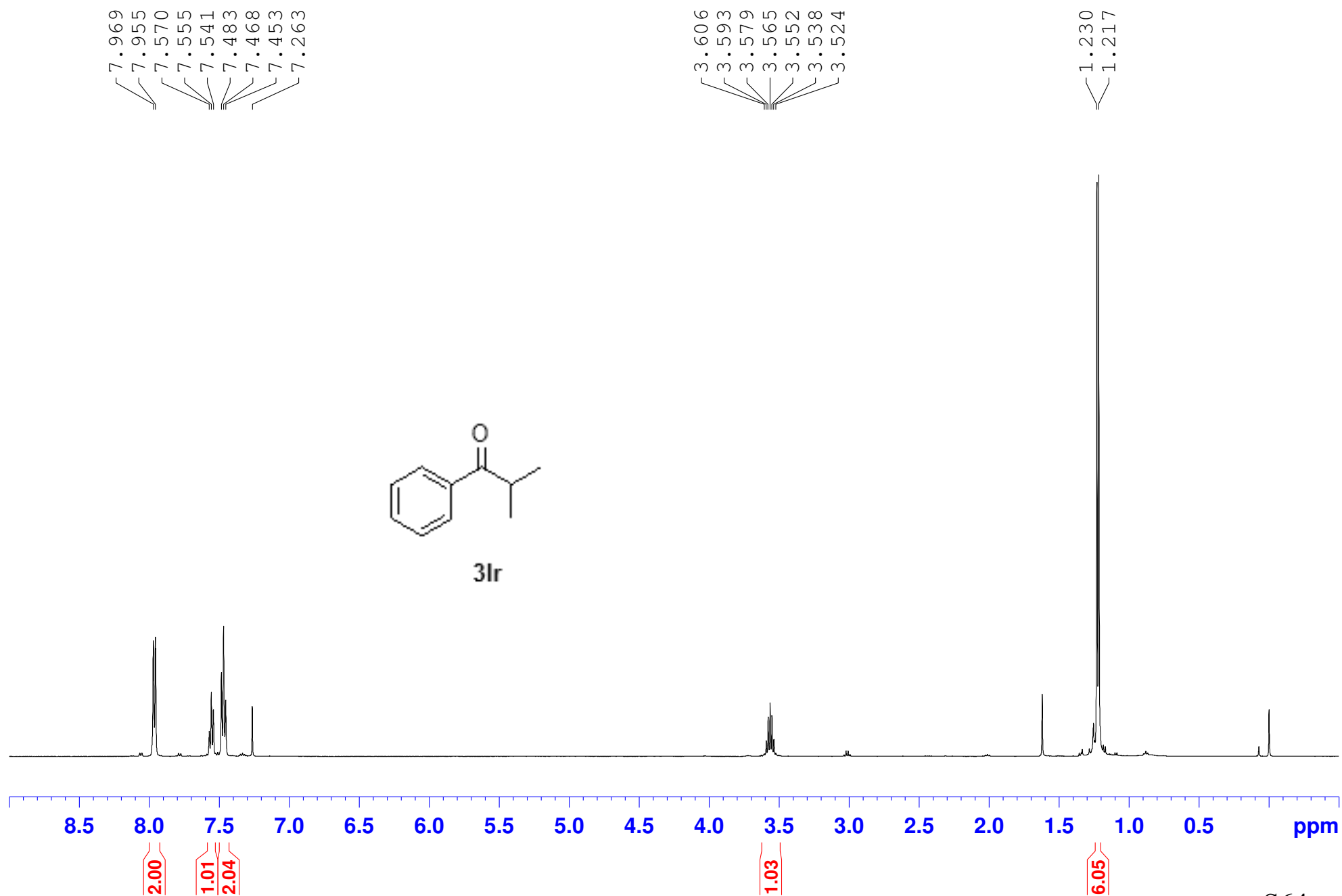
—26.253



30a



2-methyl-1-phenylpropan-1-one
Proton CDCl₃



2-methyl-1-phenylpropan-1-one
C13CPD CDC13

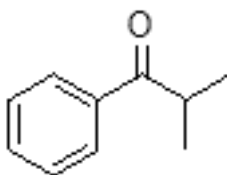
— 204.465

— 136.195
— 132.743
— 128.564
— 128.275

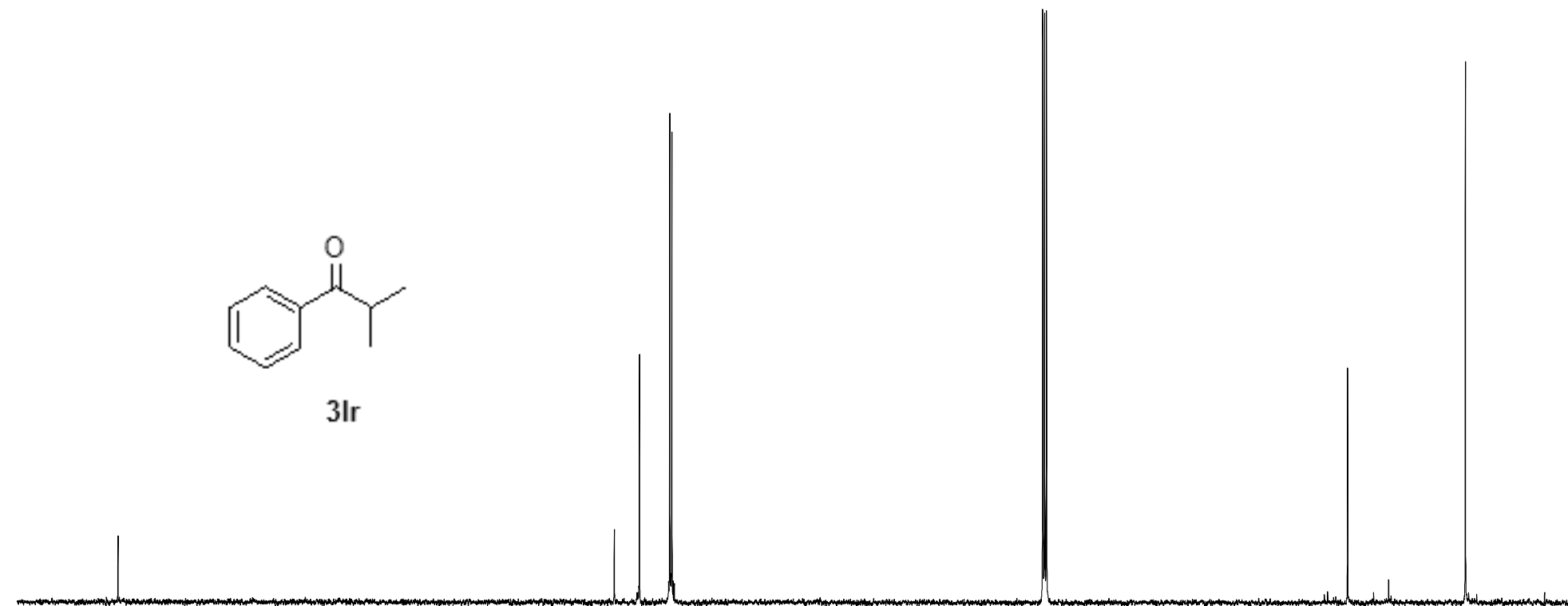
— 77.000

— 35.315

— 19.111



3Ir



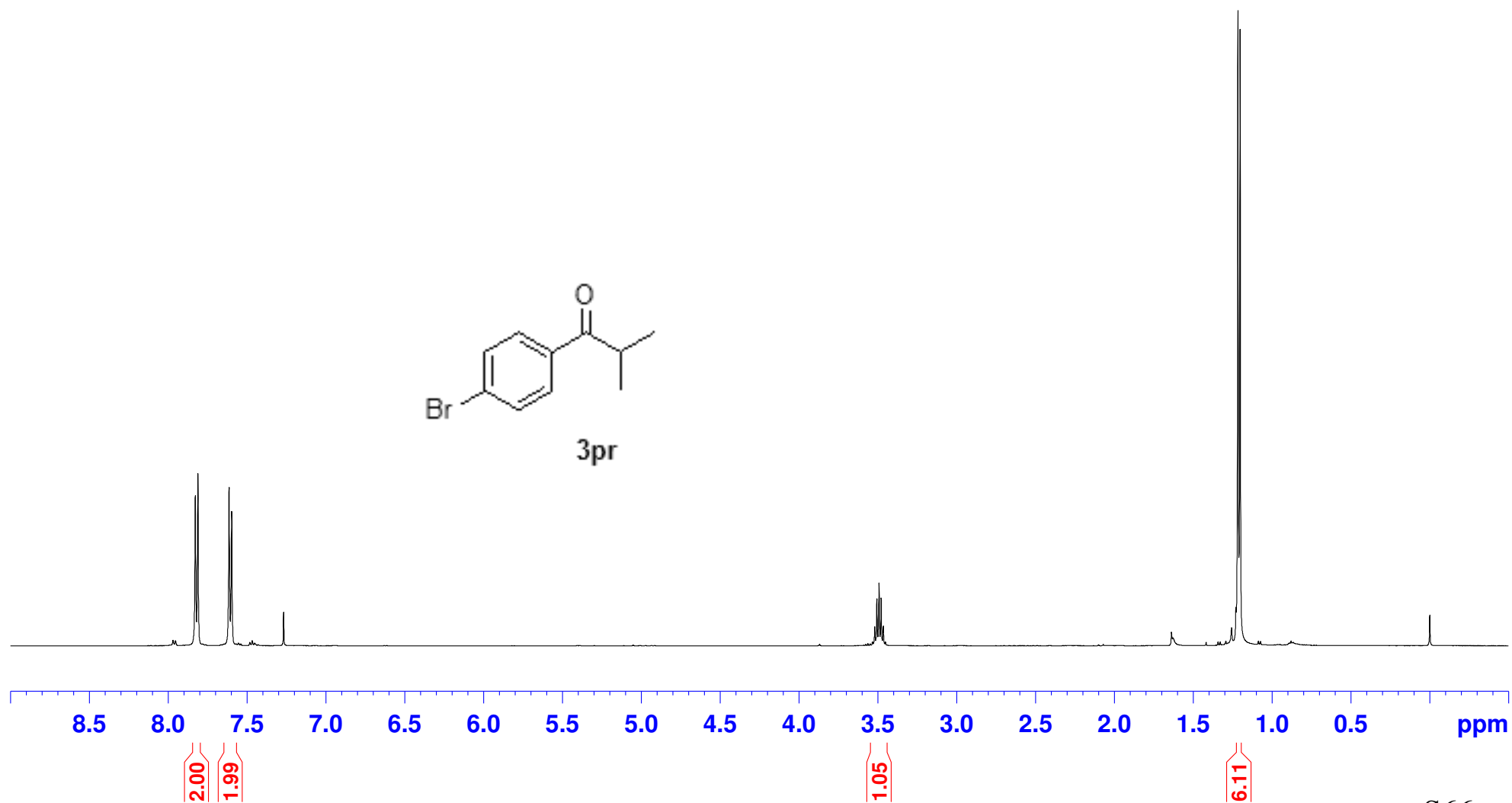
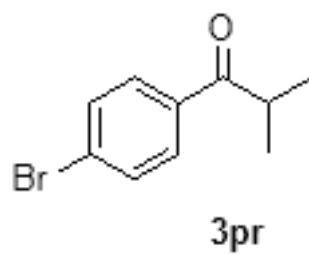
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

1-(4-bromophenyl)-2-methylpropan-1-one
Proton CDCl₃

7.827
7.810
7.612
7.596
7.266

3.534
3.520
3.507
3.493
3.479
3.466
3.452

1.217
1.203



1-(4-bromophenyl)-2-methylpropan-1-one
C13CPD CDC13

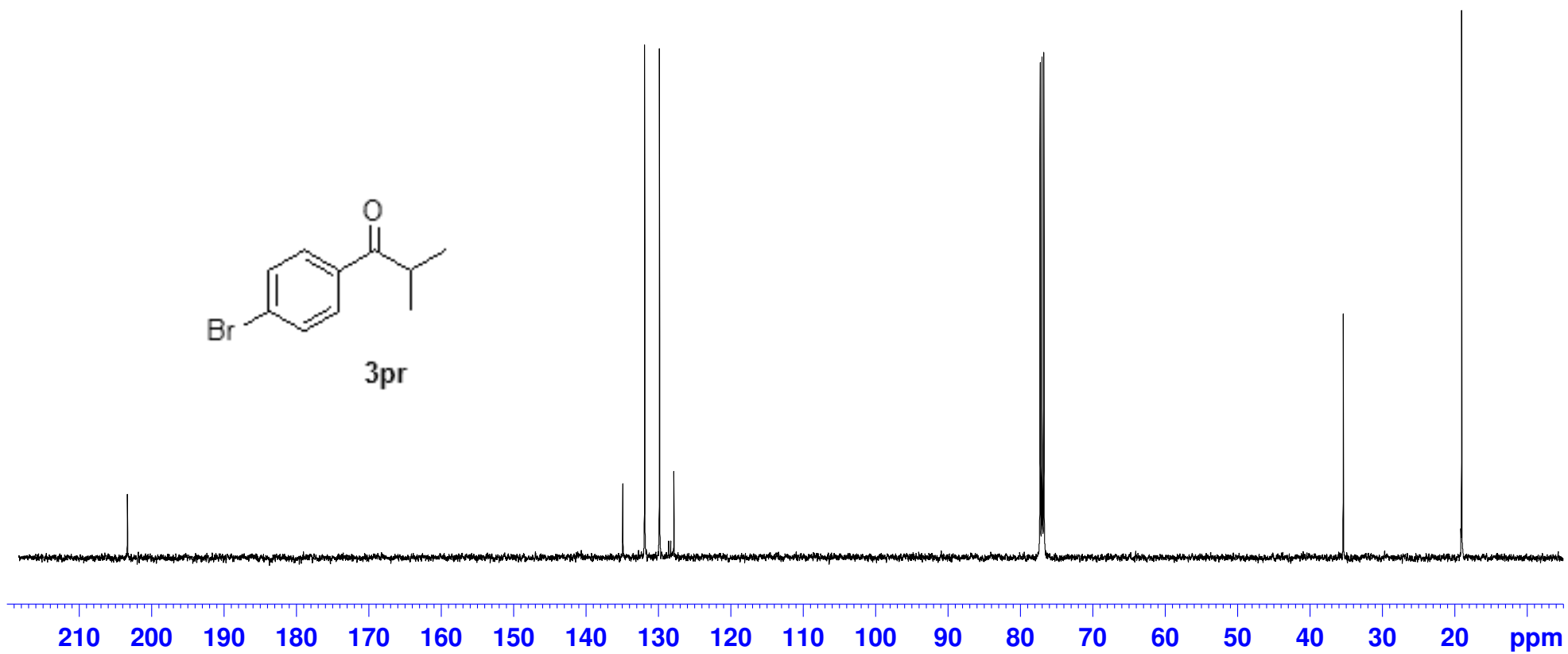
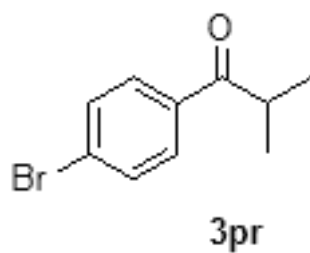
— 203.346

— 134.908
— 131.895
— 129.846
— 127.852

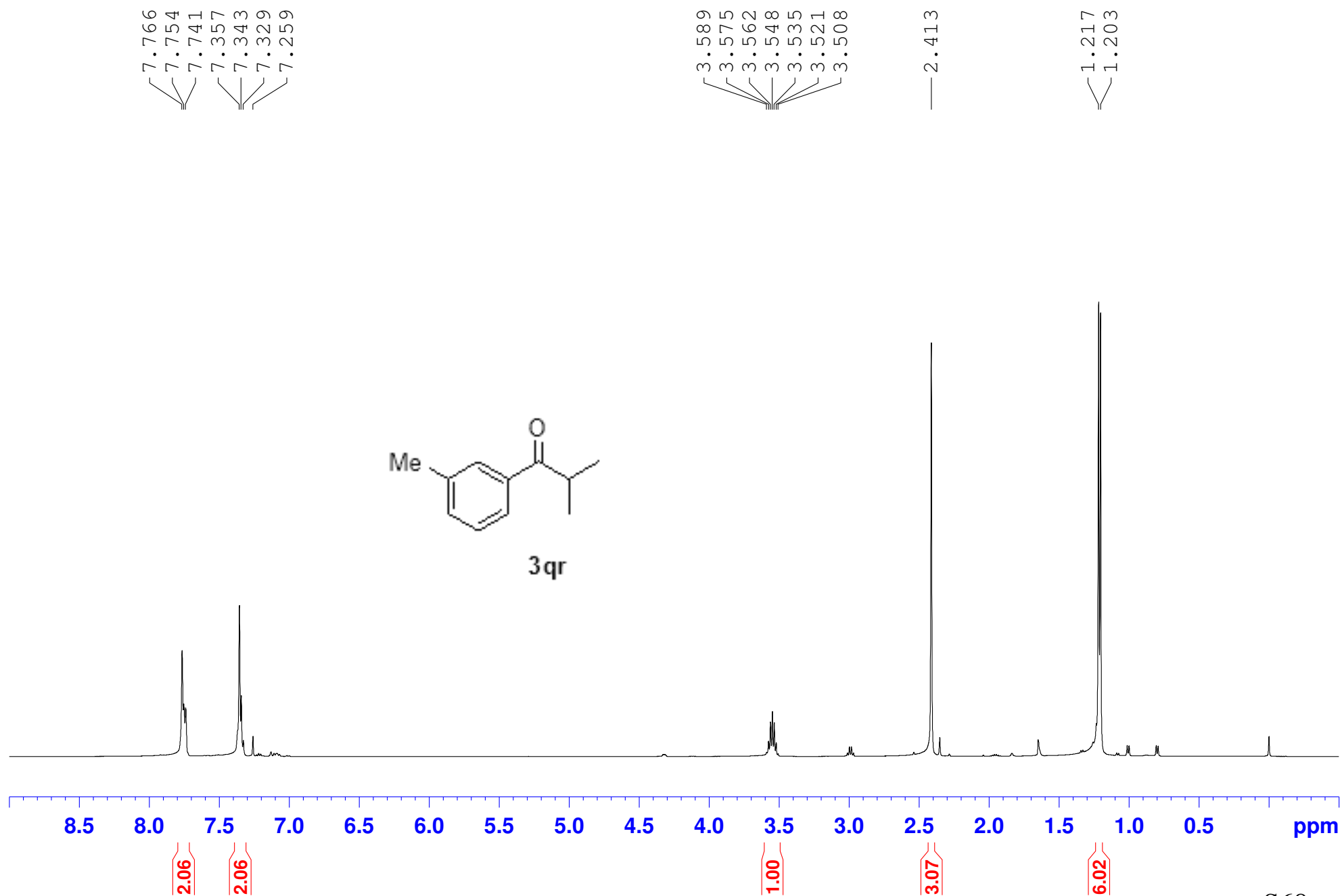
— 77.000

— 35.384

— 19.024



2-methyl-1-m-tolylpropan-1-one
Proton CDCl₃



2-methyl-1-m-tolylpropan-1-one
C13CPD CDC13

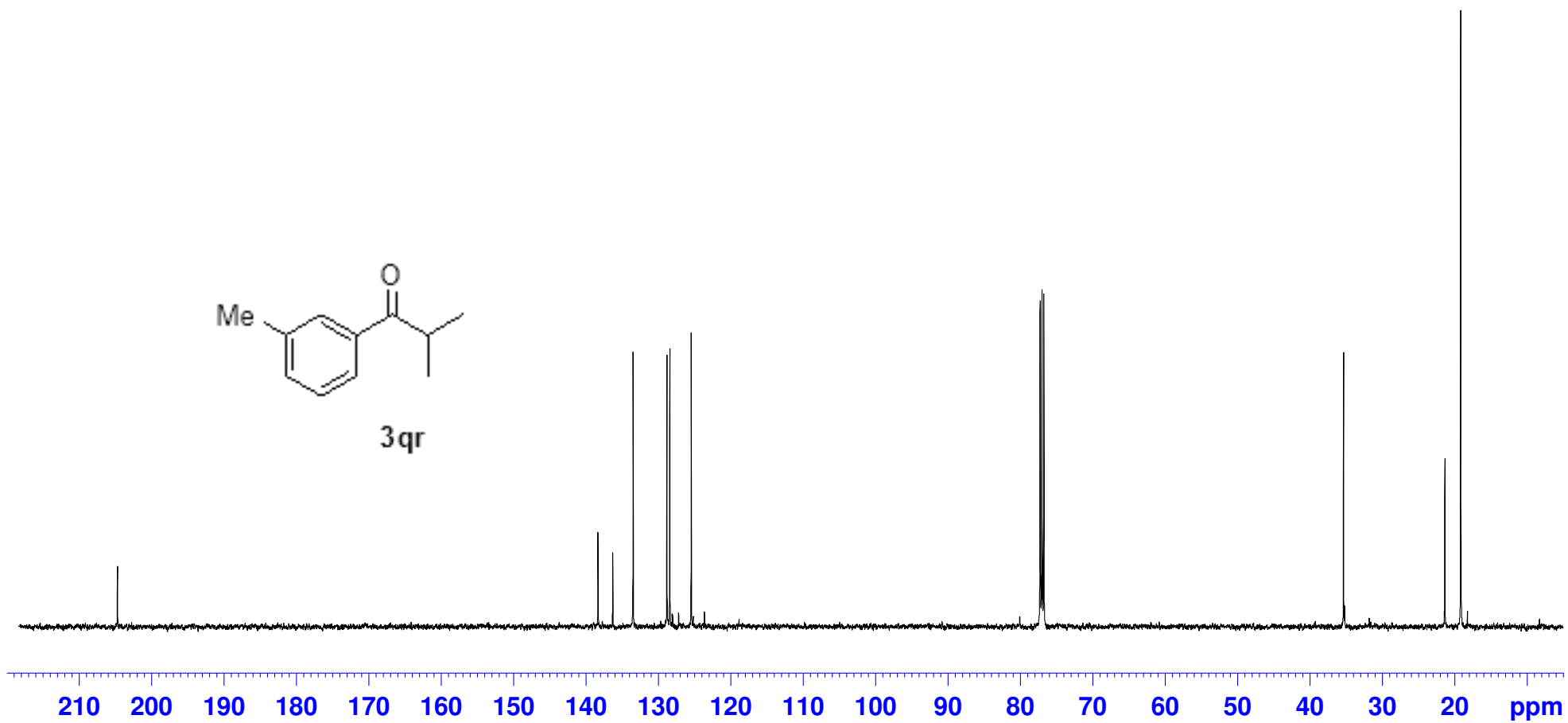
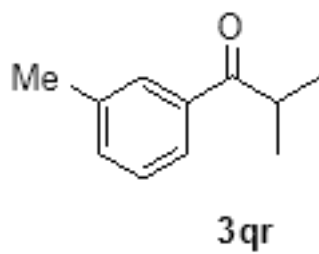
— 204.708

138.341
136.301
133.484
128.813
128.415
125.457

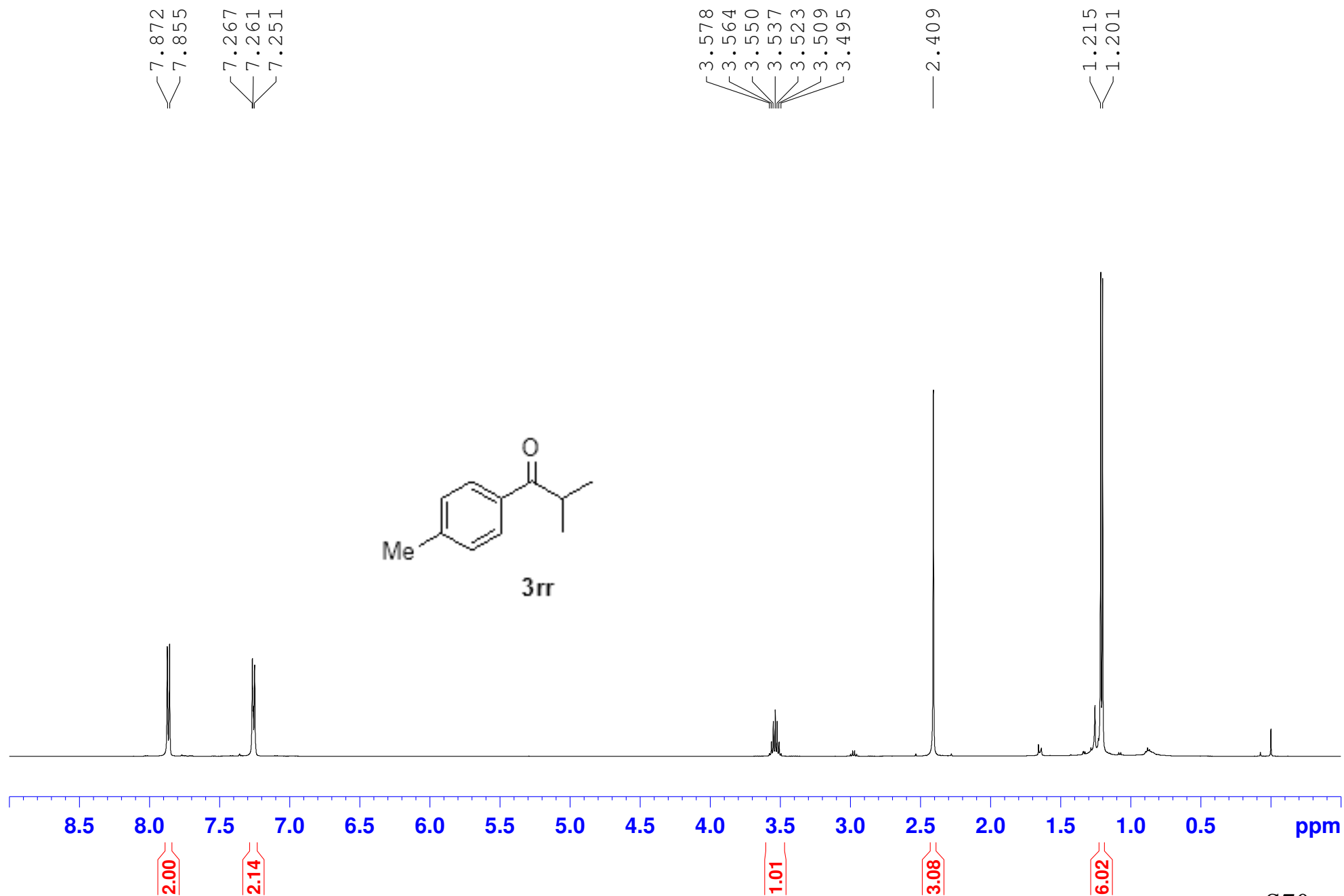
— 77.000

— 35.341

21.347
19.151



2-methyl-1-p-tolylpropan-1-one
Proton CDCl₃



2-methyl-1-p-tolylpropan-1-one
C13CPD CDC13

— 204.061

— 143.427

— 133.659

— 129.225

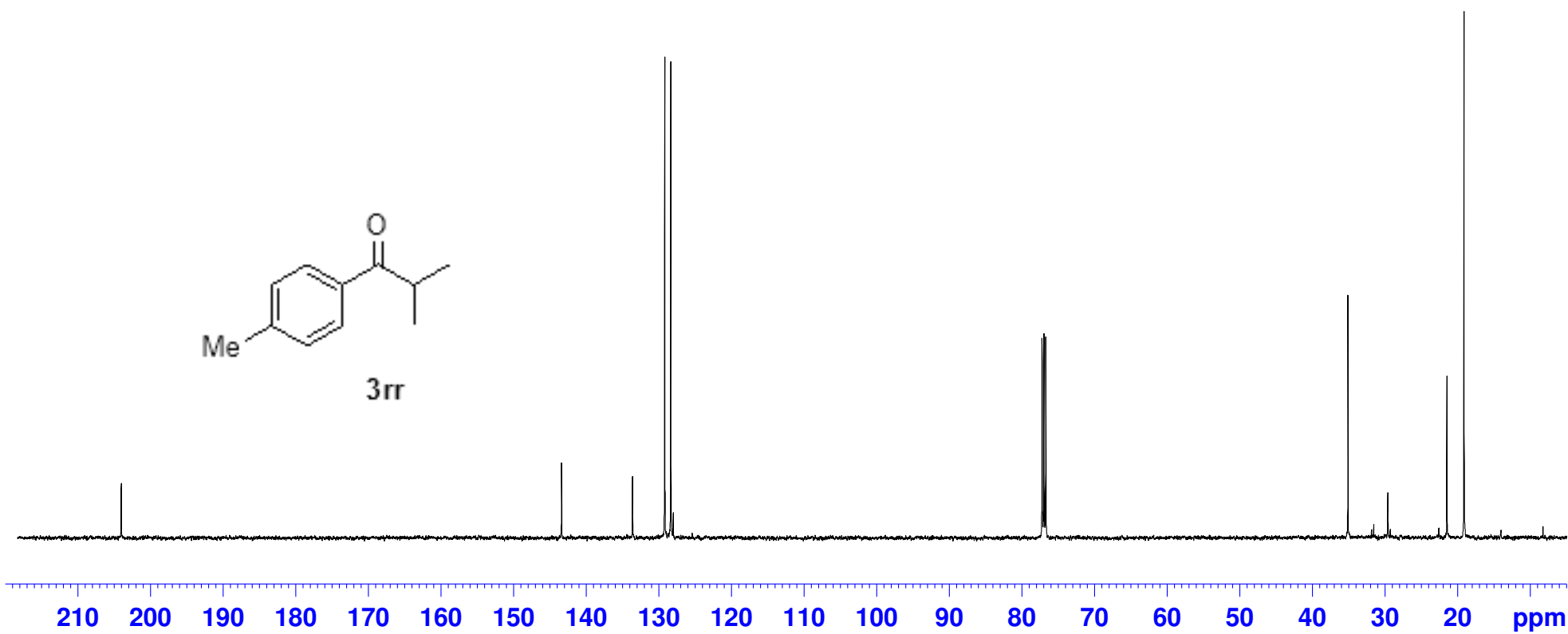
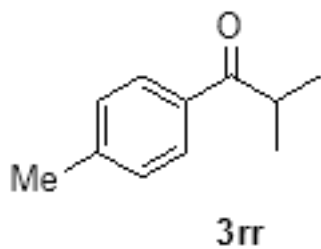
— 128.388

— 77.000

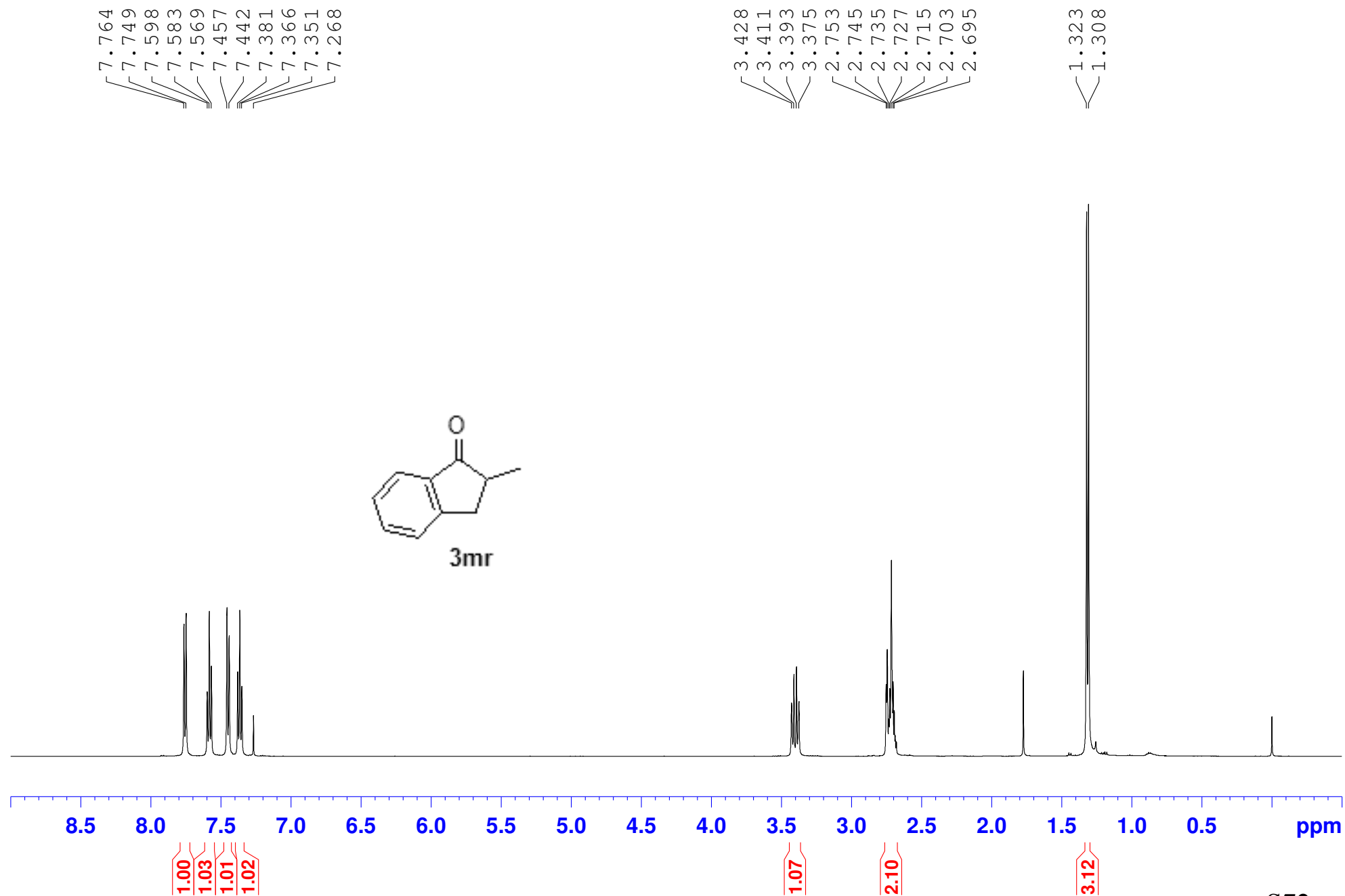
— 35.139

— 21.510

— 19.152



2-methyl-2,3-dihydroinden-1-one
Proton CDCl₃



2-methyl-2,3-dihydroinden-1-one
C13CPD CDC13

—209.380

—153.421

—136.340

—134.625

—127.313

—126.497

—123.941

—77.000

—41.951

—34.929

—16.234

