

Supporting Information for

**Use of a Cyclometalated Iridium(III) Complex Containing a
N⁺C⁻N⁻-Coordinating Terdentate Ligand as Catalyst for the
 α -Alkylation of Ketones and *N*-alkylation of Amines with Alcohols**

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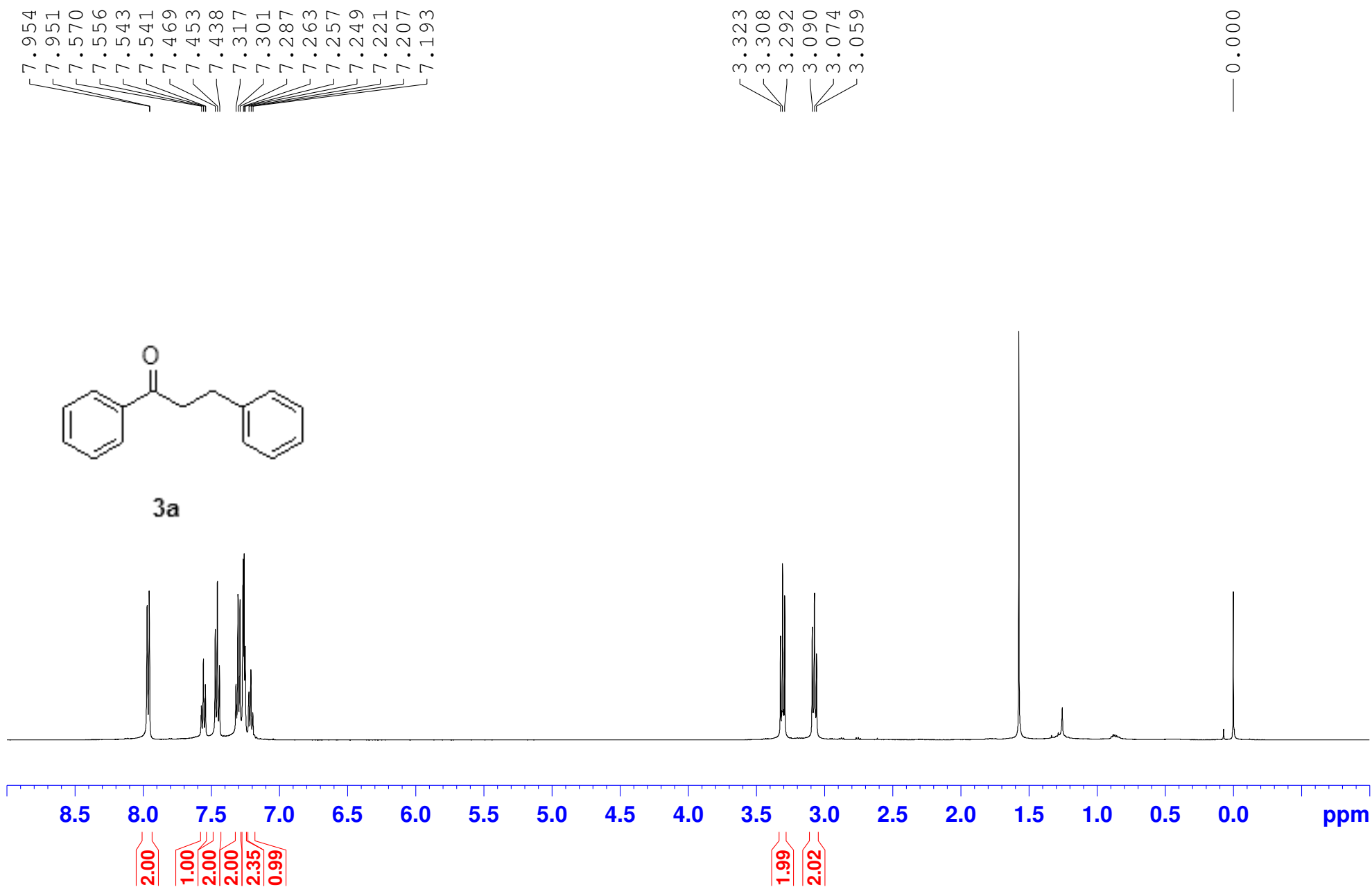
[†]School of Chemical Engineering, Nanjing University of Science & Technology,
Nanjing 210094, P. R. China

[‡]Jiangsu Key Laboratory for Nano Technology, College of Engineering and Applied
Science, Nanjing University, Nanjing 210093, P. R. China

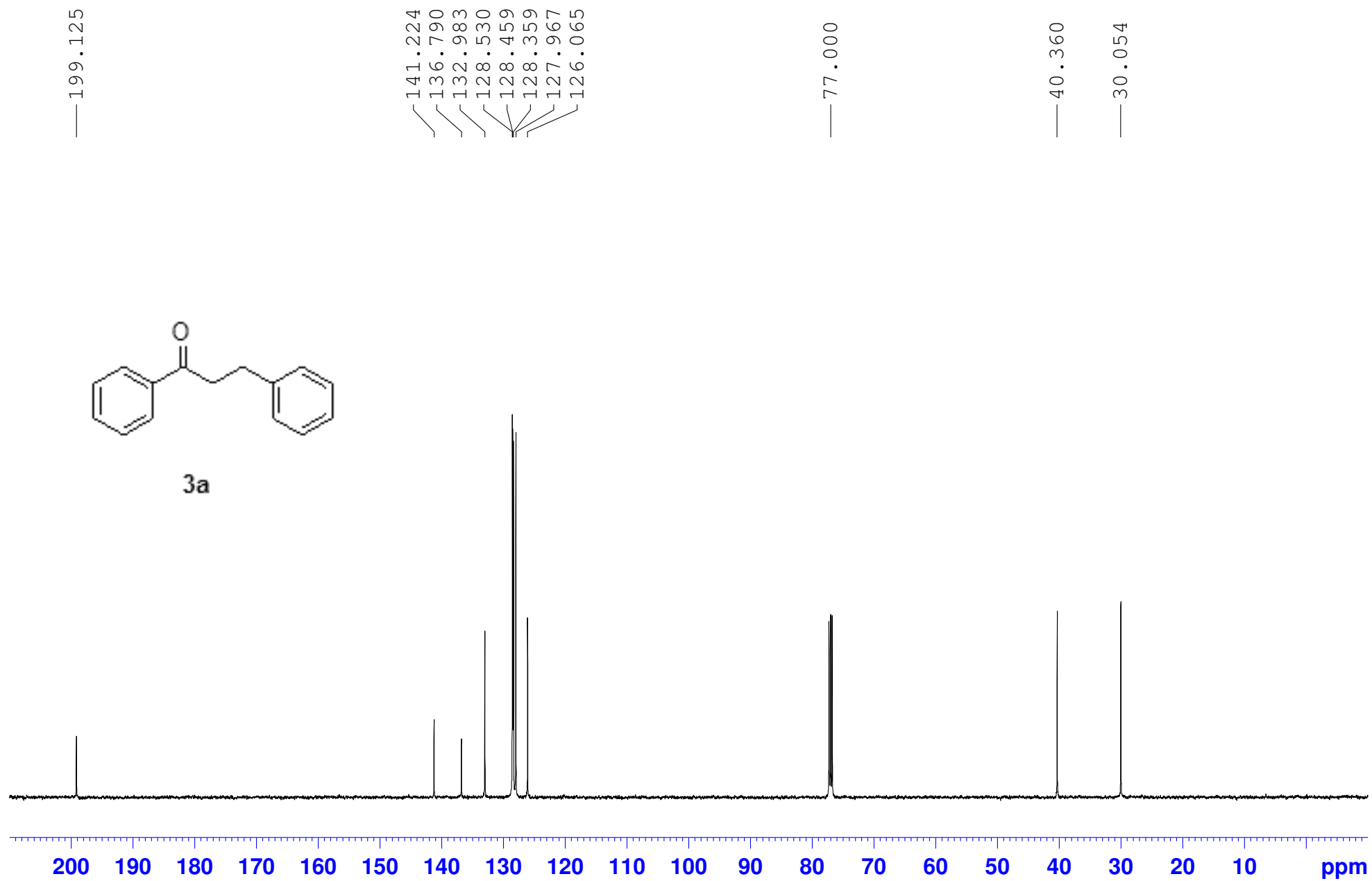
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Copies of ¹ H NMR and ¹³ C NMR spectra of products	S2-S105
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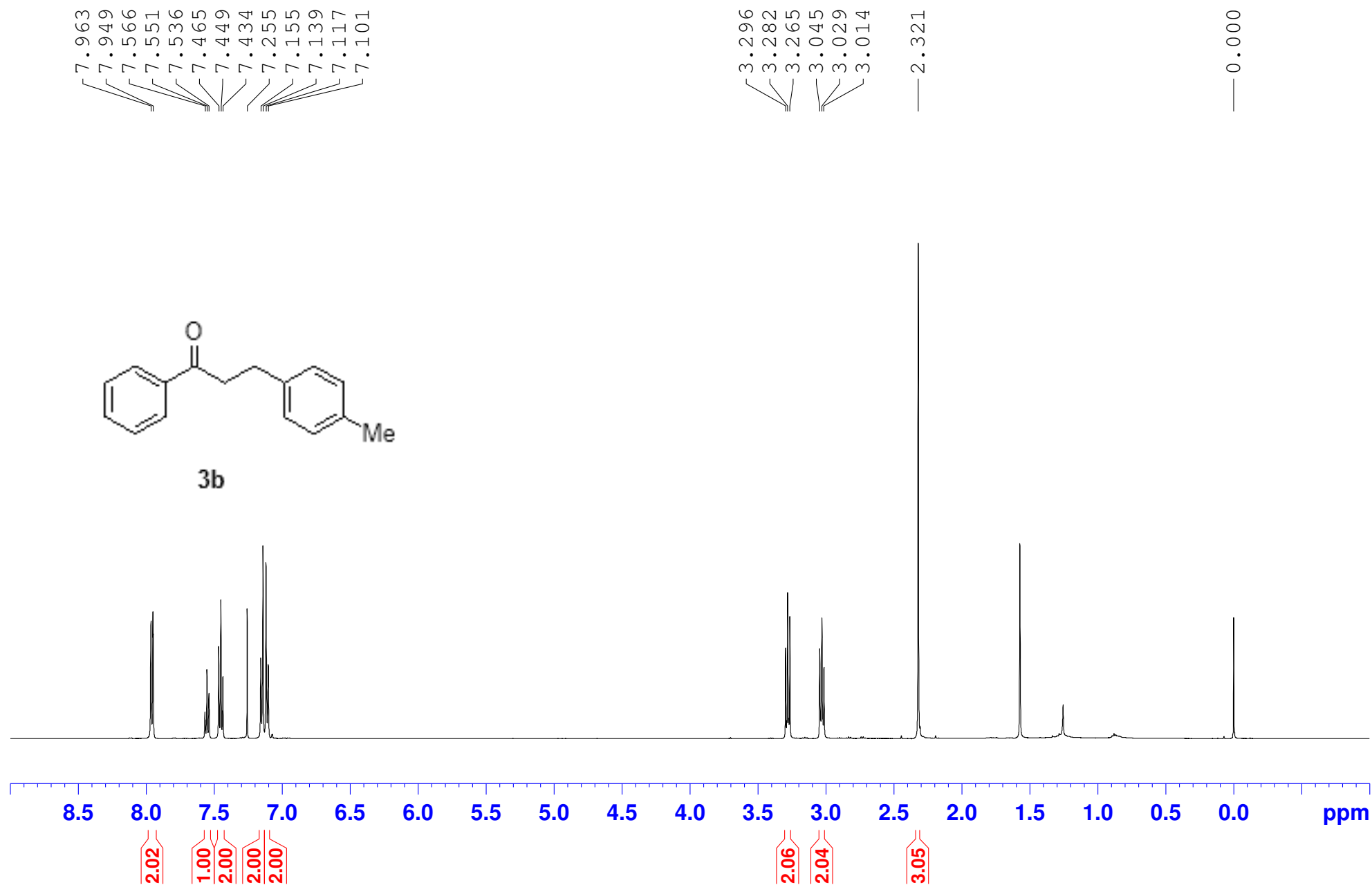
1,3-Diphenylpropan-1-one
Proton CDCl₃



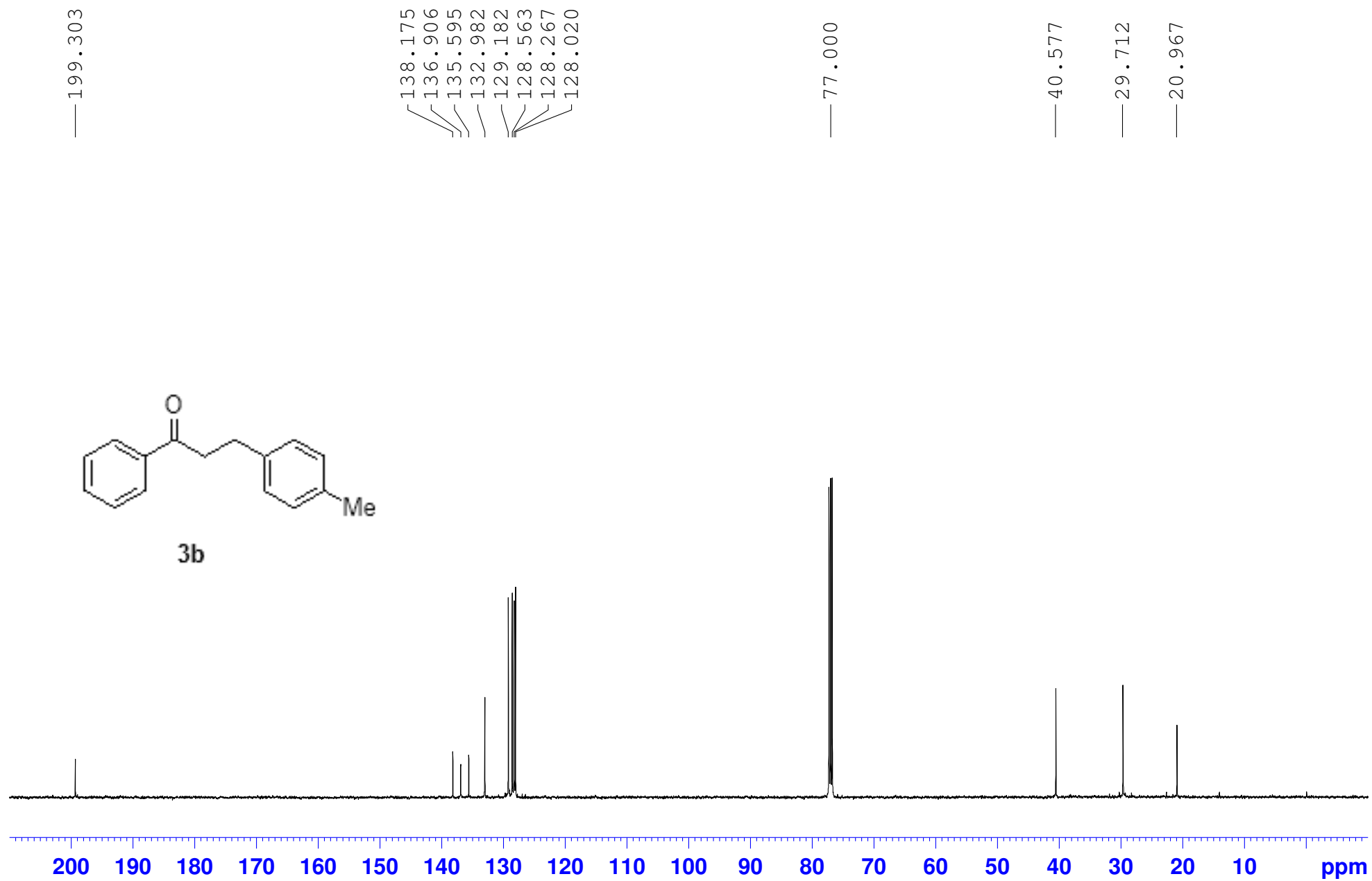
1,3-diphenylpropan-1-one
C13CPD CDCl3



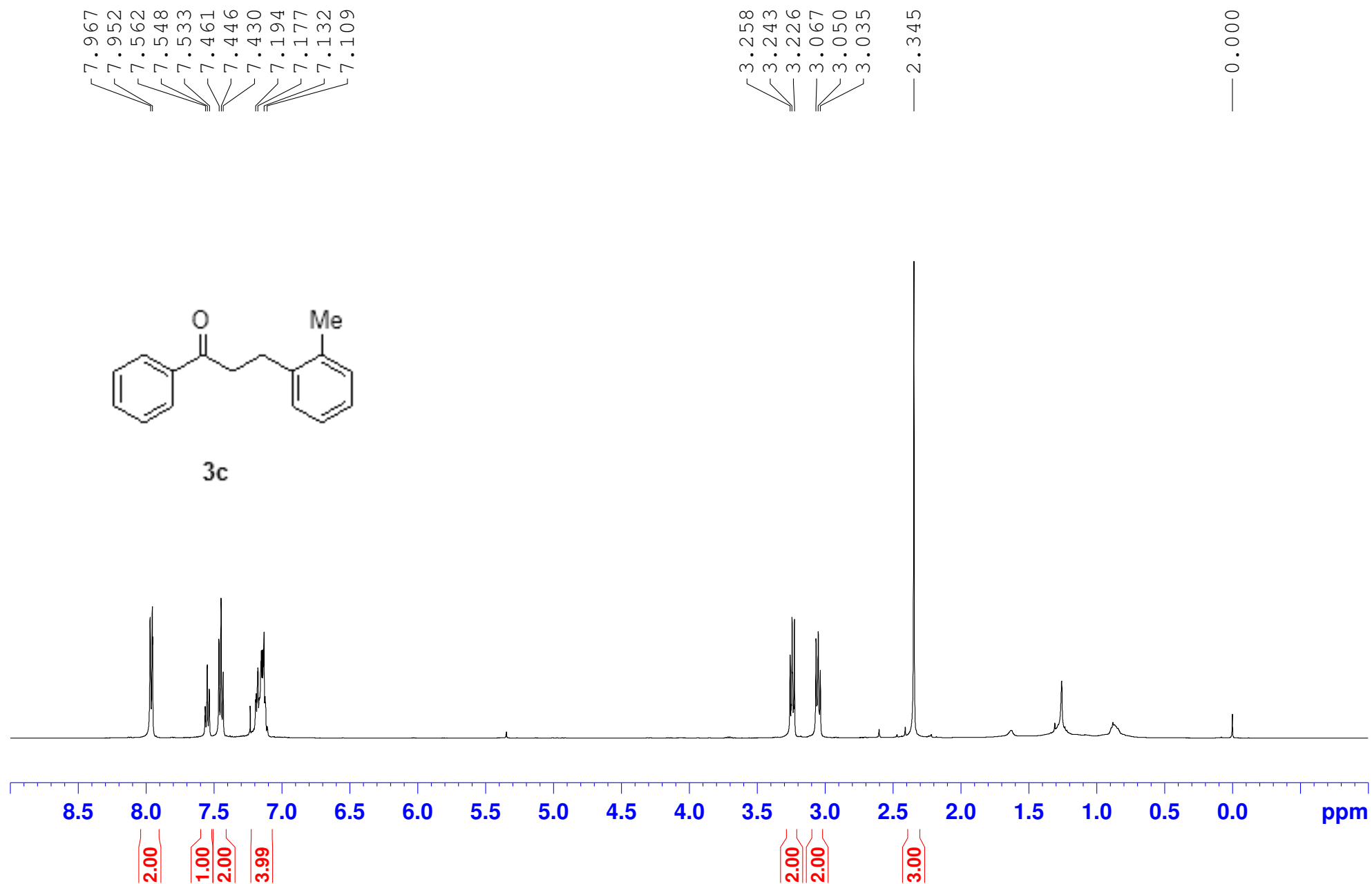
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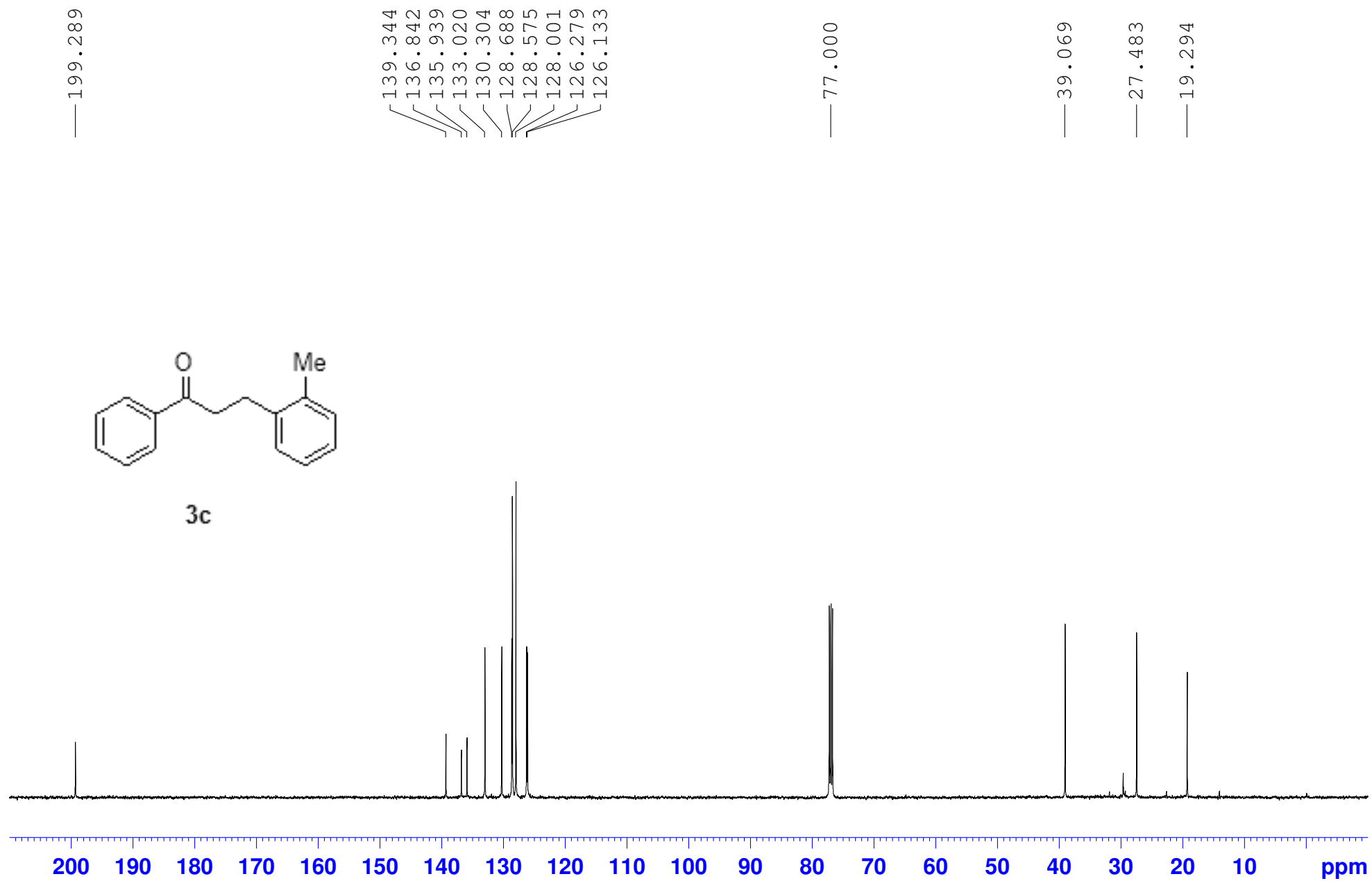
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C13CPD CDC13



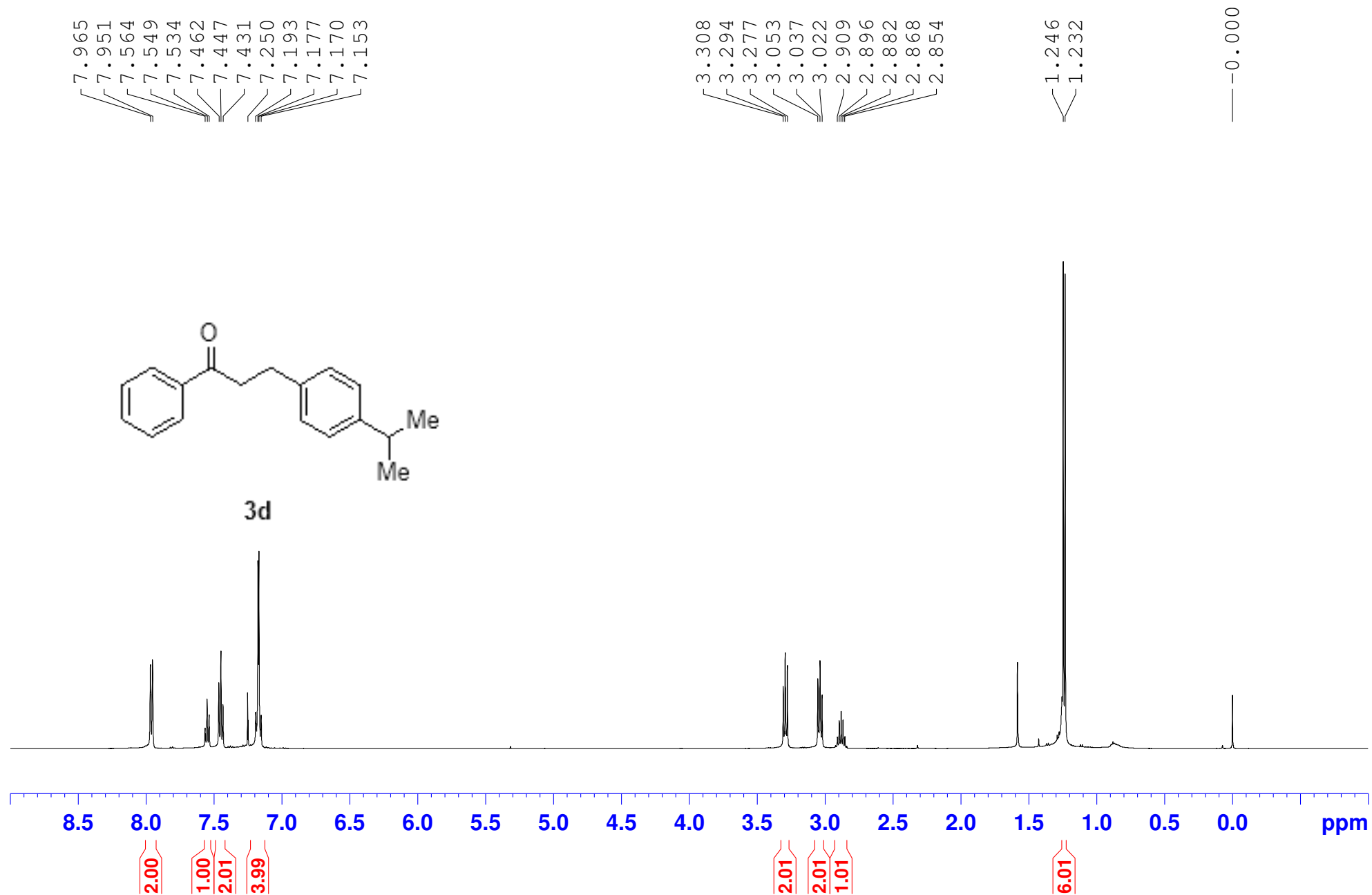
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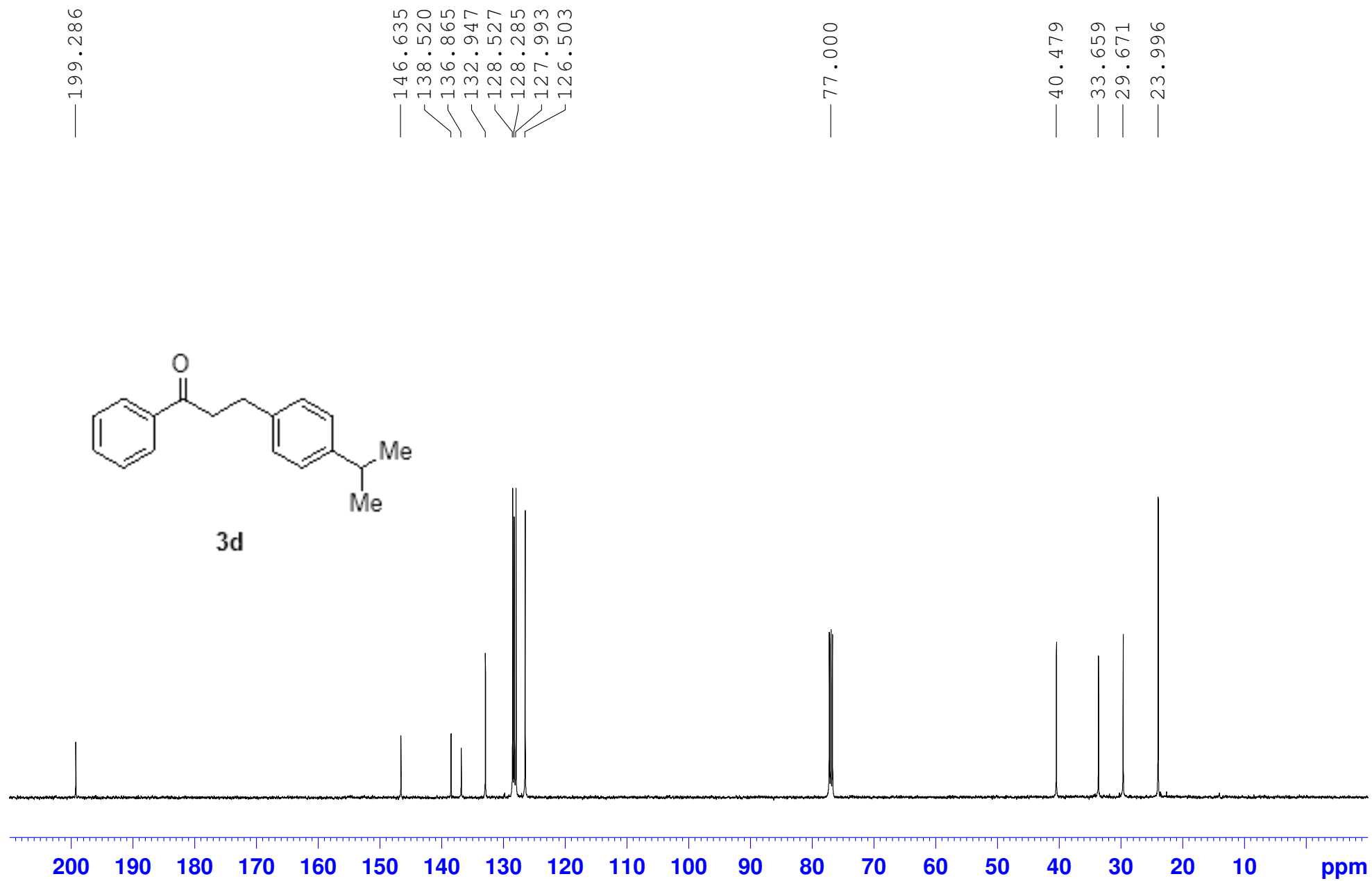
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C13CPD CDC13



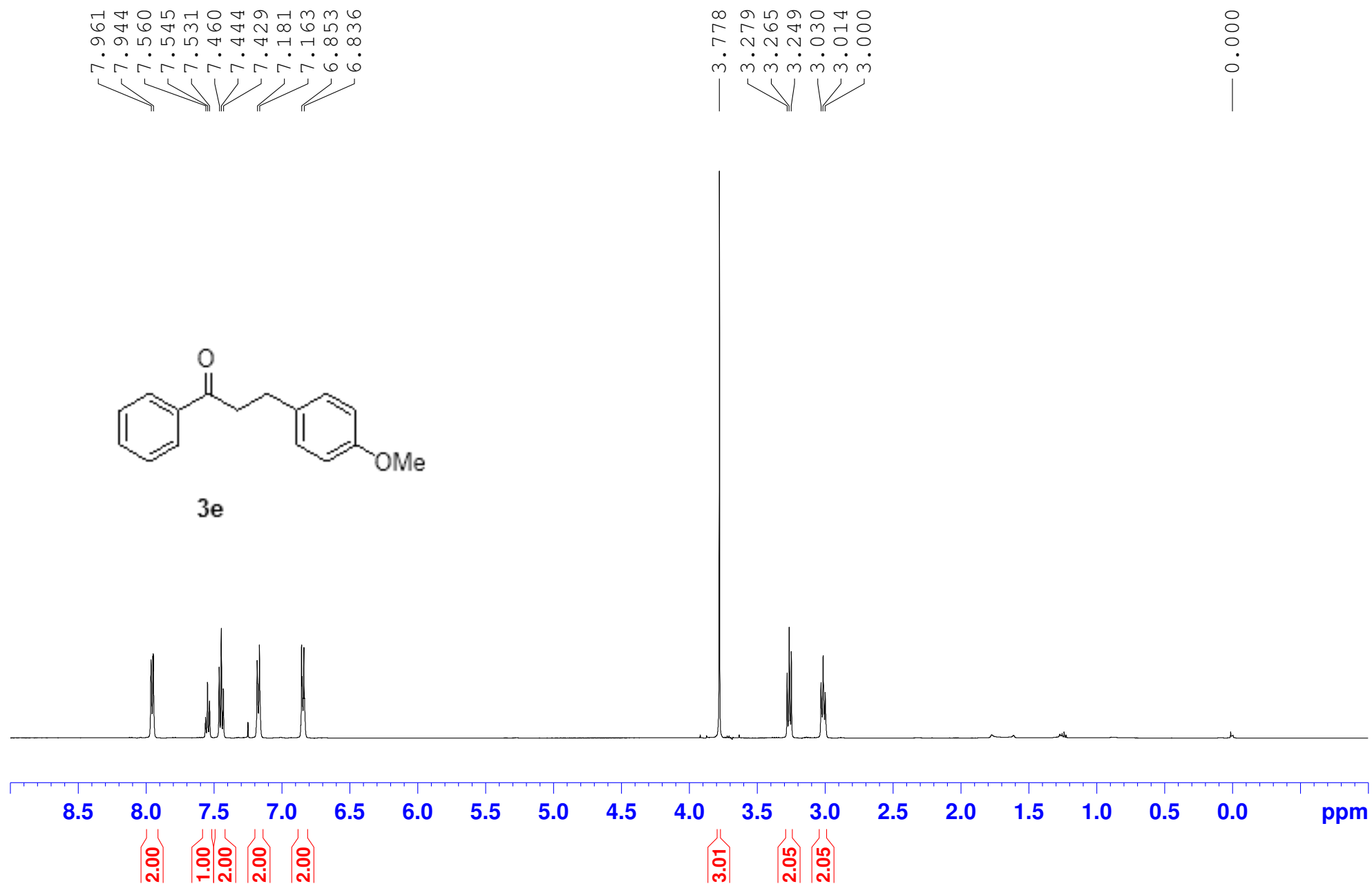
3-(4-Isopropylphenyl)-1-phenylpropan-1-one
Proton CDCl₃



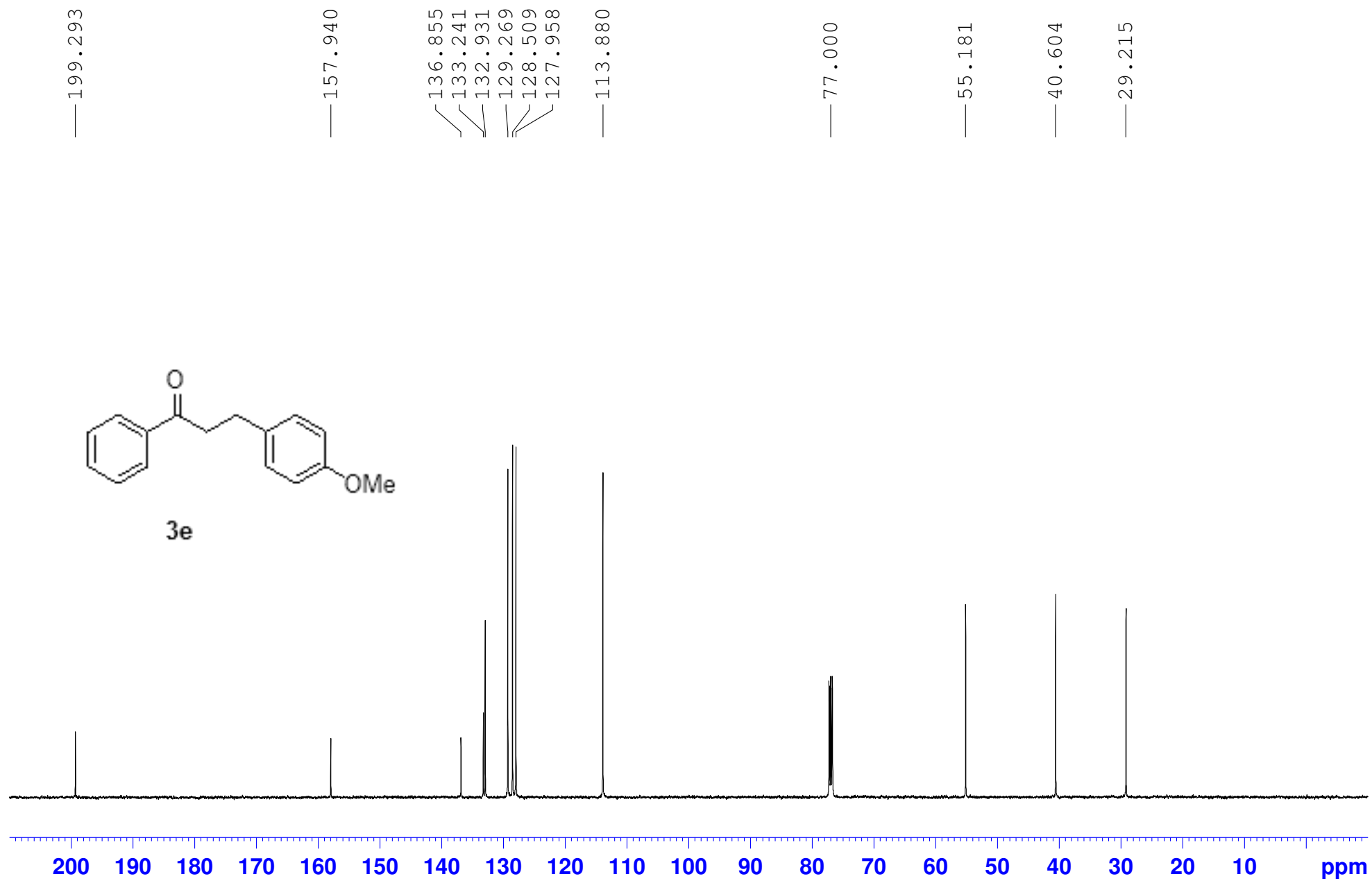
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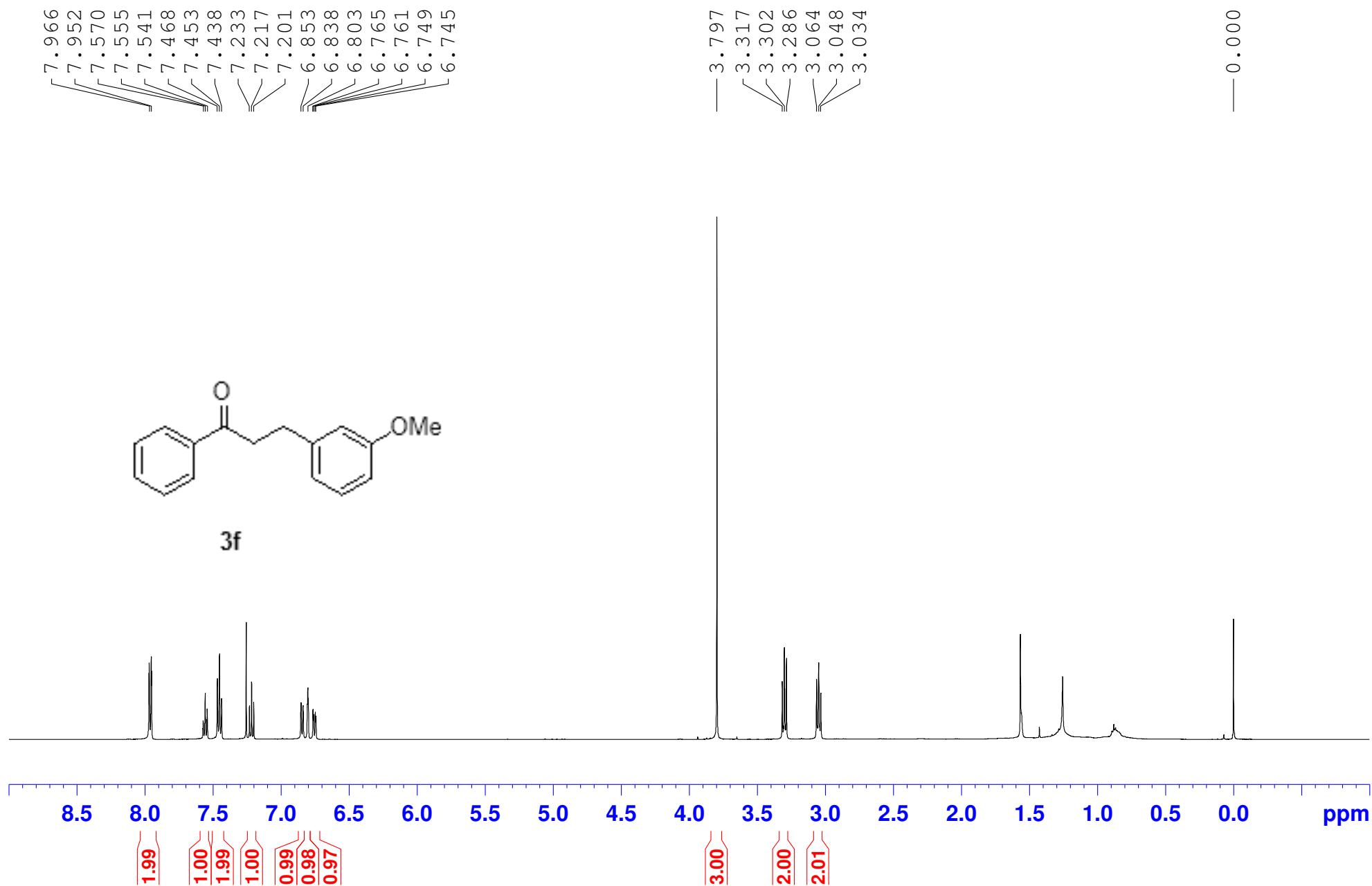
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Proton CDCl₃



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



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



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

— 198.987

— 159.661

— 142.816

— 136.768

— 132.910

— 129.386

— 128.472

— 127.908

— 120.646

— 114.151

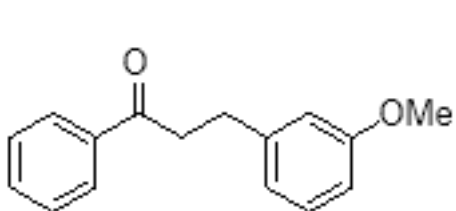
— 111.311

— 77.000

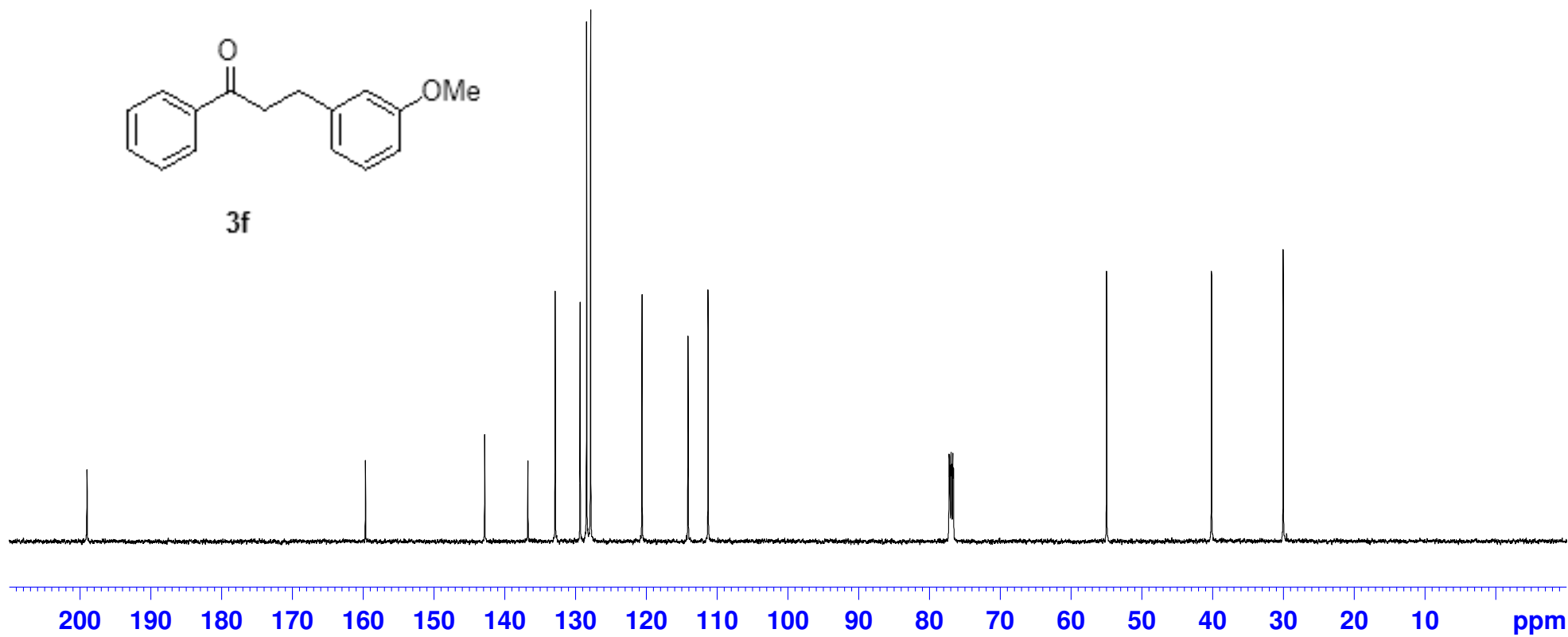
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— 40.187

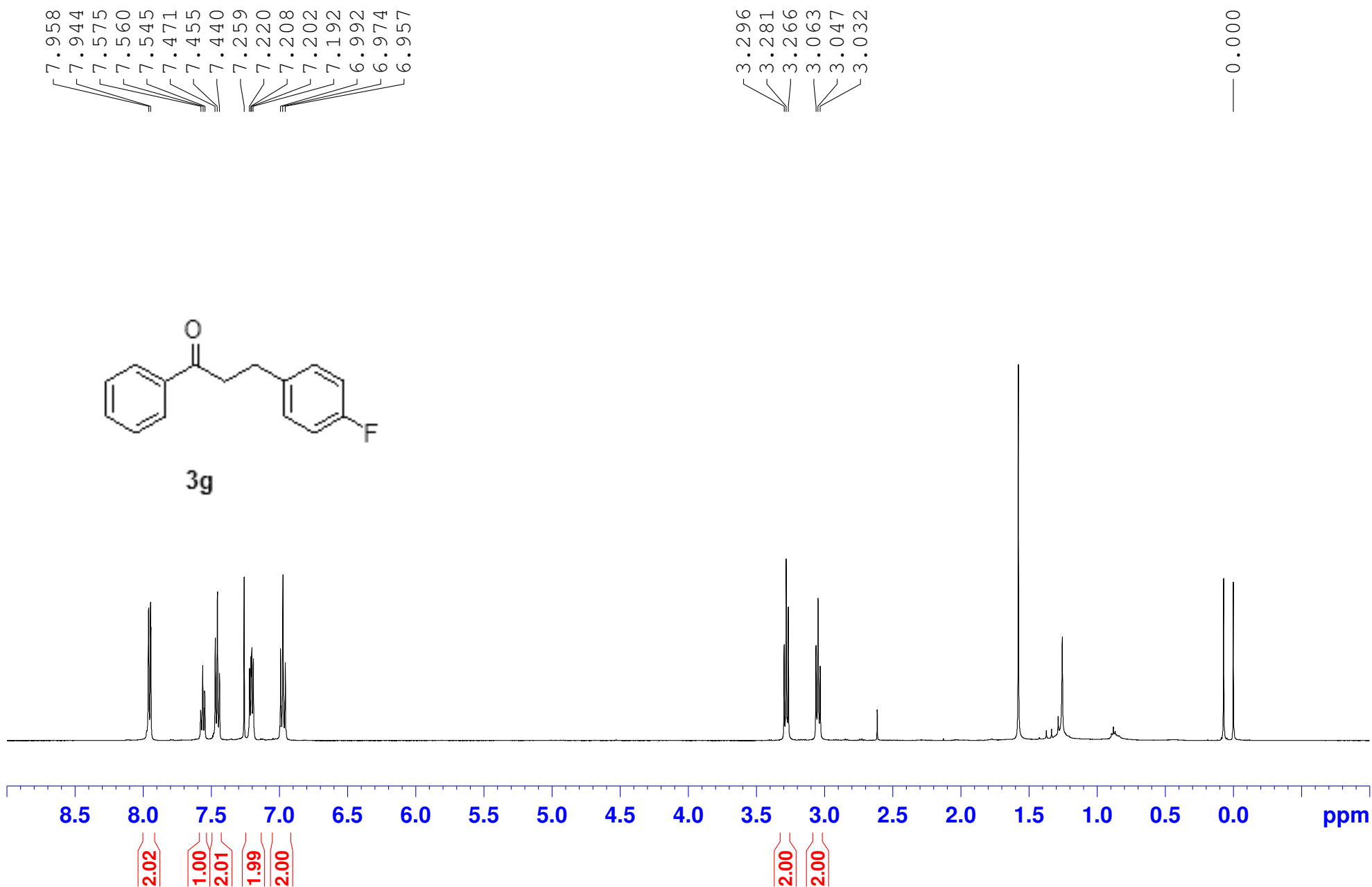
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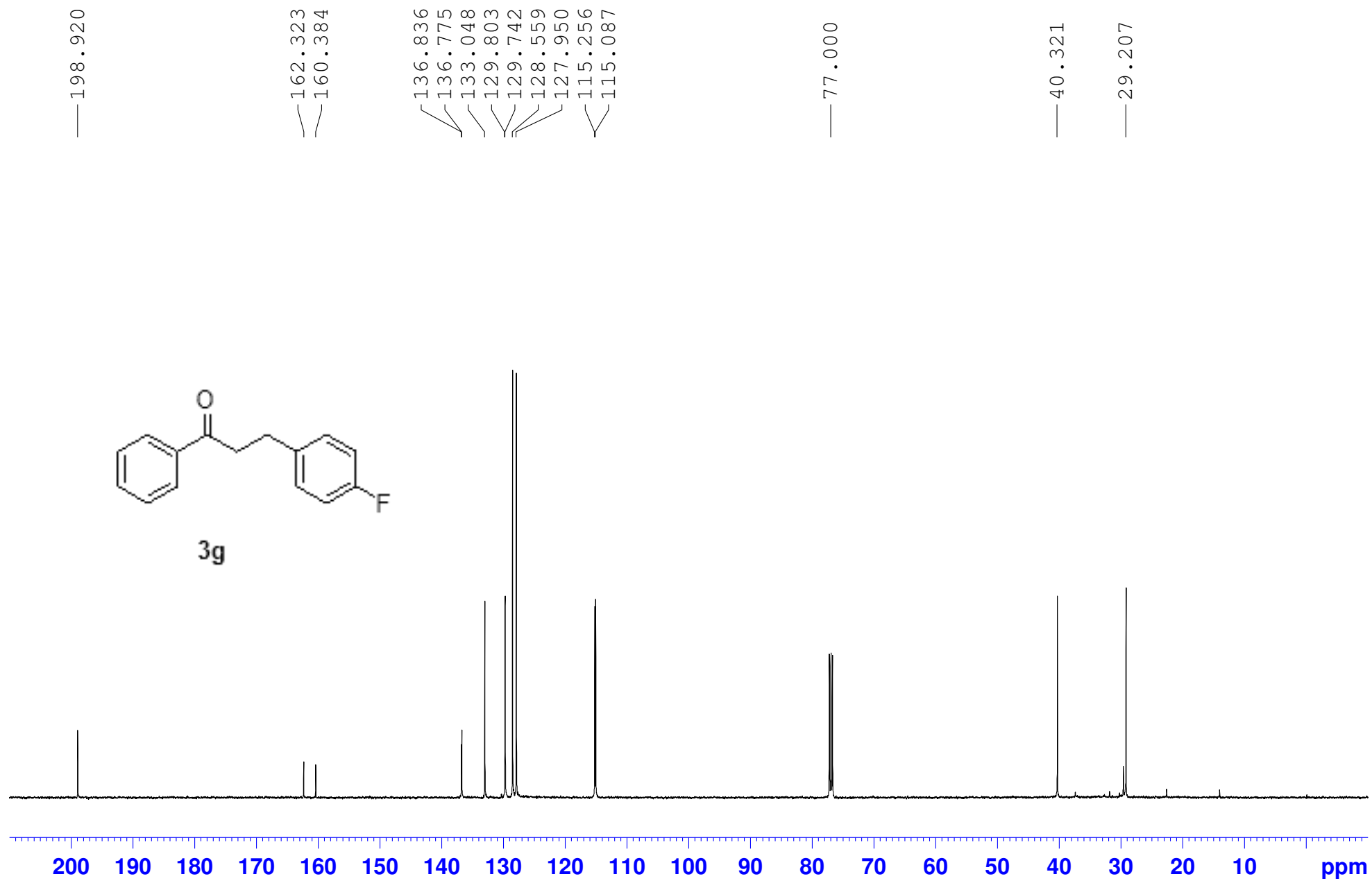
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3-(4-fluorophenyl)-1-phenylpropan-1-one
Proton CDCl₃



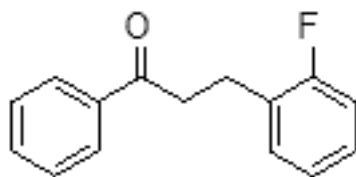
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 C13CPD CDCl3



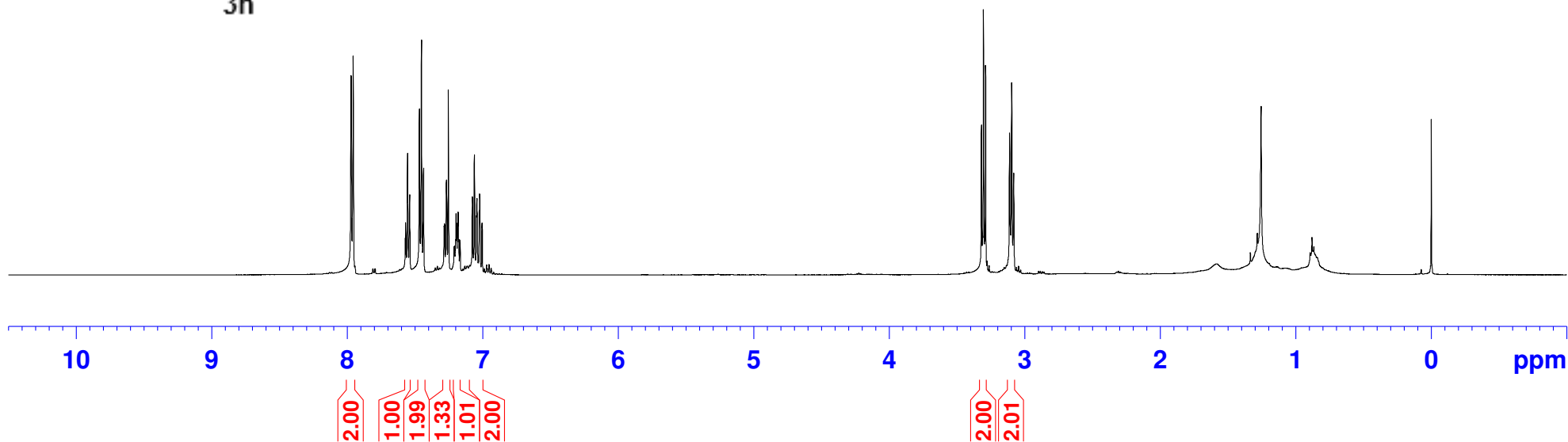
3-(2-fluorophenyl)-1-phenylpropan-1-one
Proton CDCl₃

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7.955
7.567
7.552
7.537
7.465
7.450
7.435
7.285
7.282
7.270
7.267
7.255
7.212
7.209
7.202
7.197
7.194
7.186
7.182
7.178
7.171
7.167
7.078
7.076
7.063
7.061
7.048
7.046
7.043
7.023
7.006

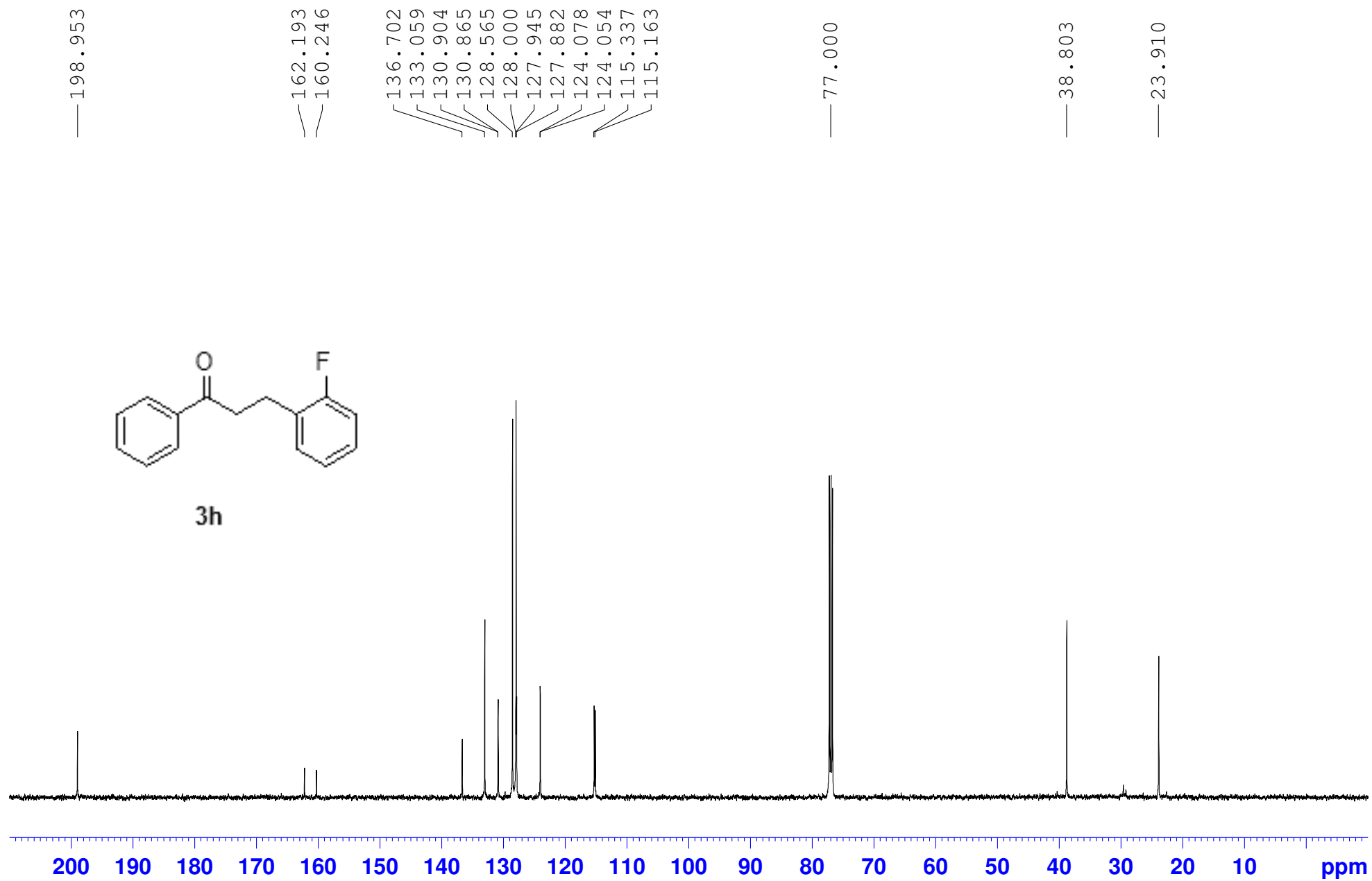
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3.305
3.289
3.112
3.097
3.082



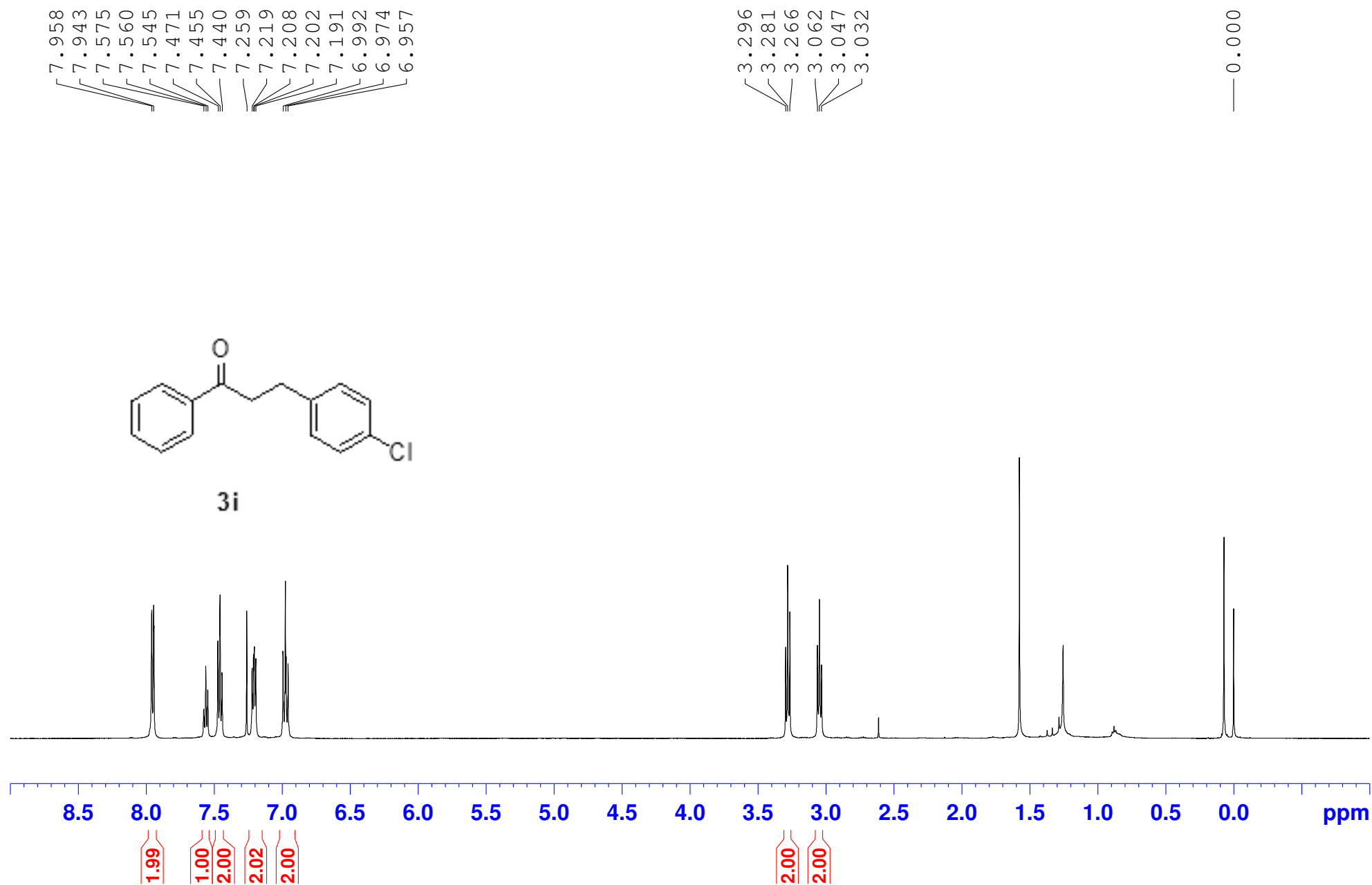
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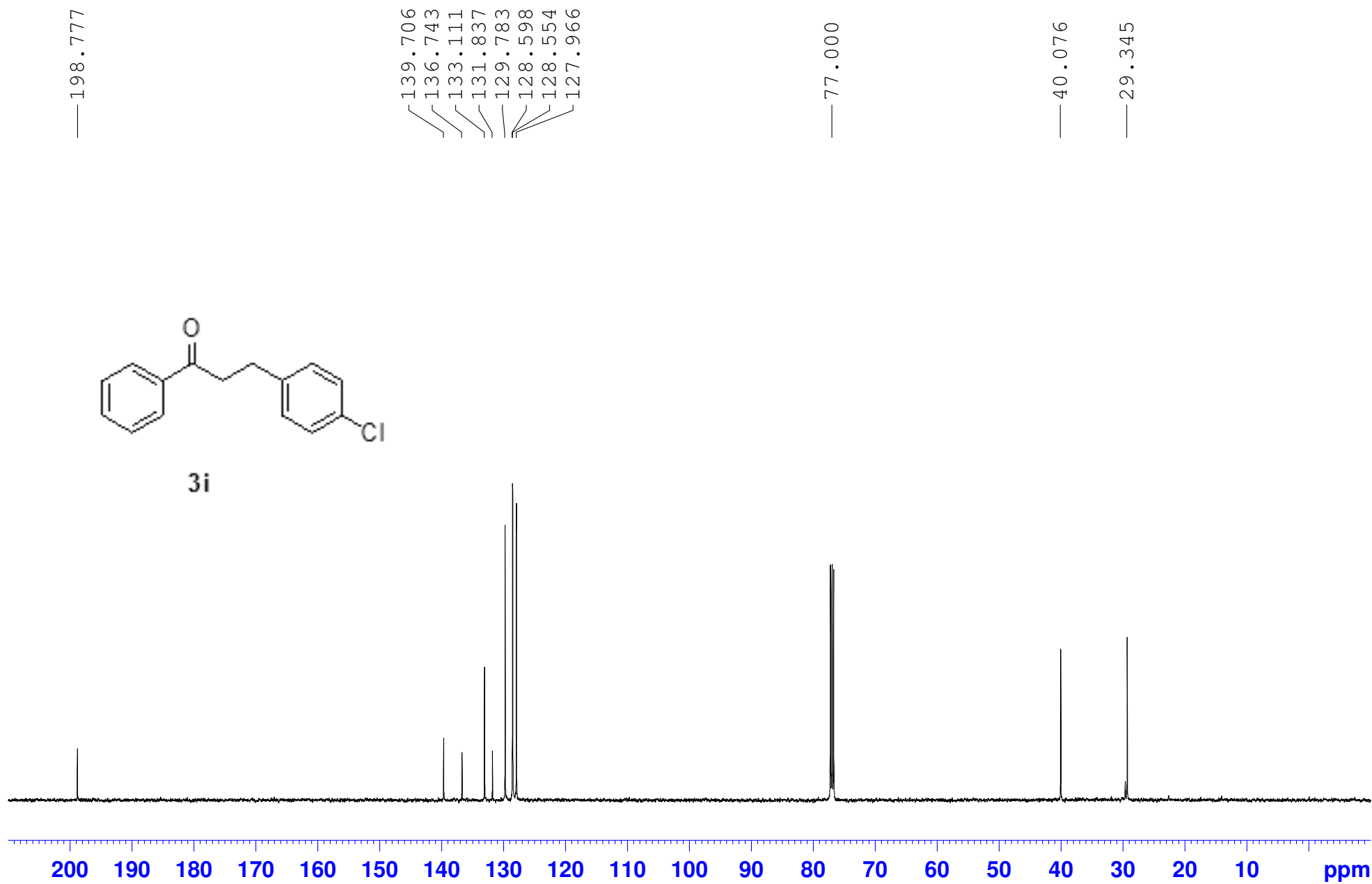
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 C13CPD CDC13



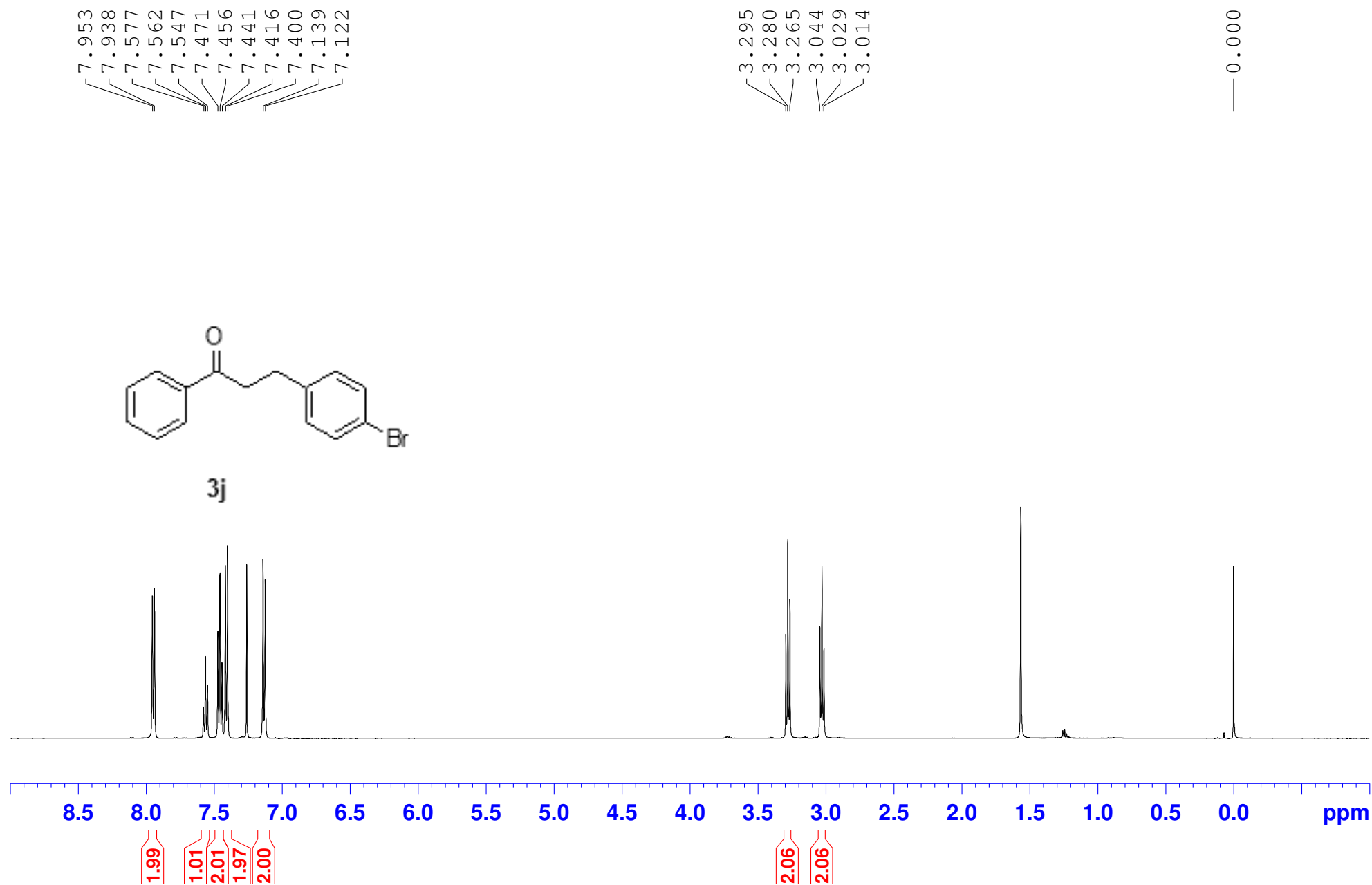
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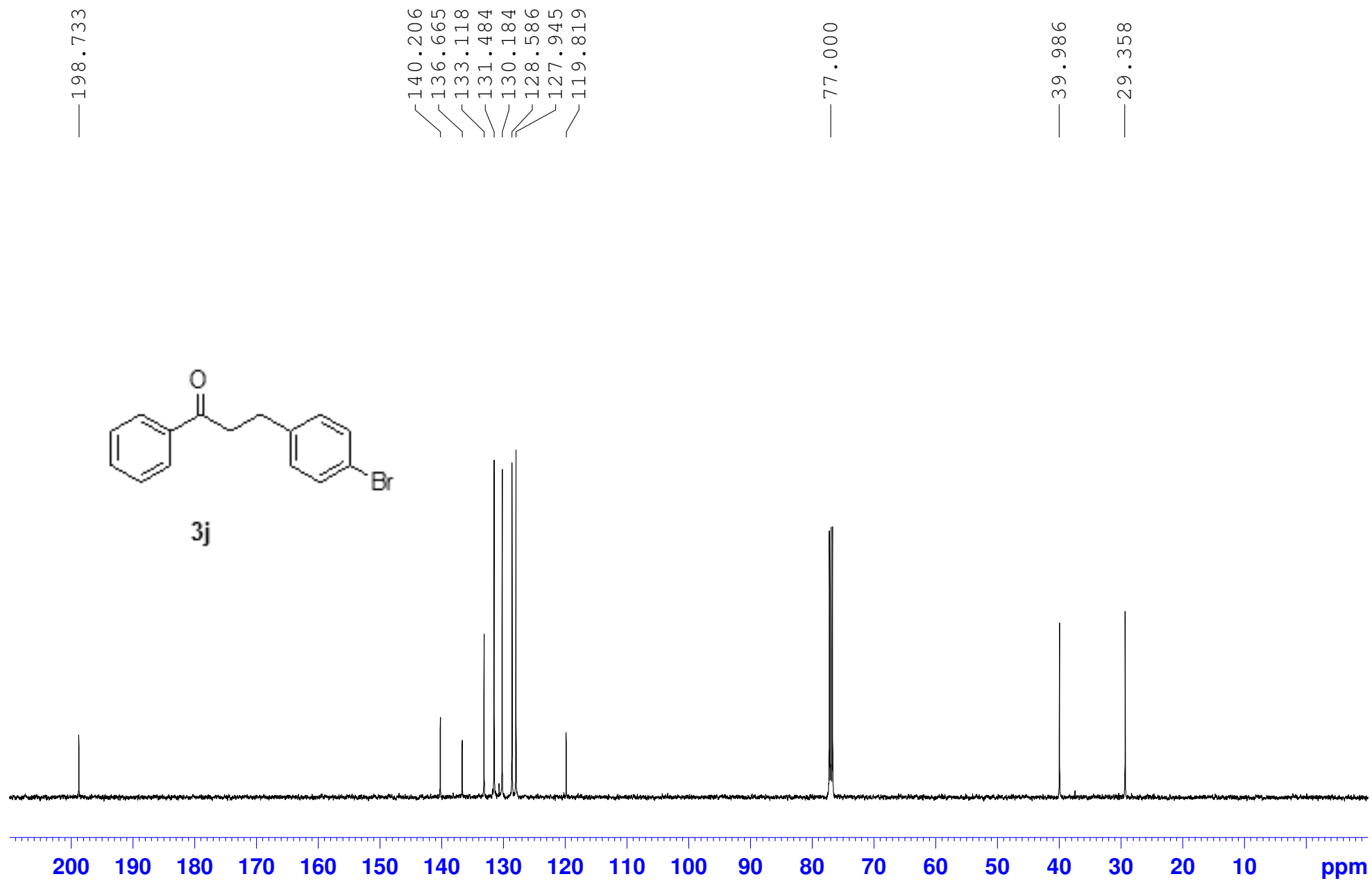
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 C13CPD CDC13



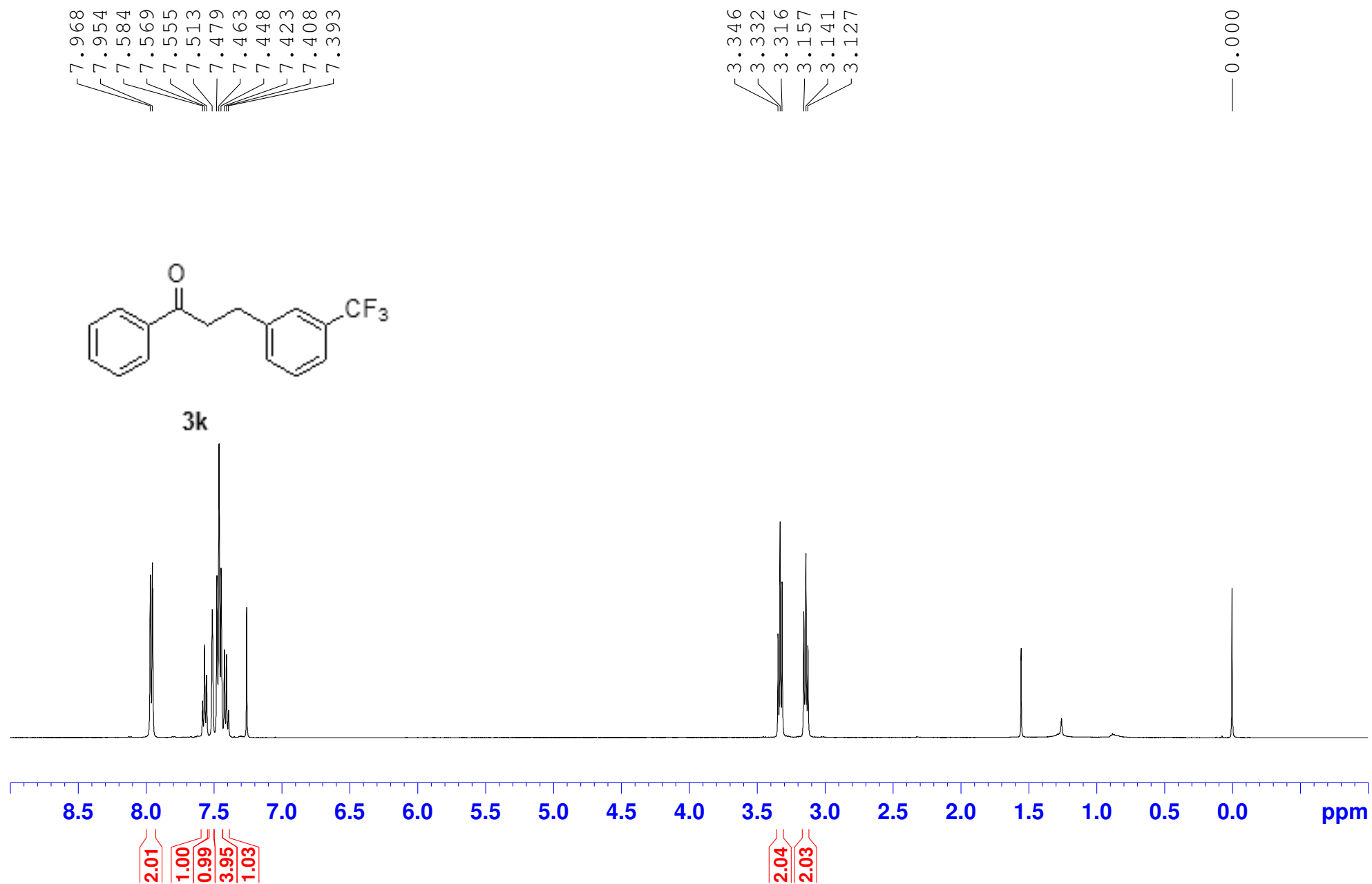
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Proton CDCl₃



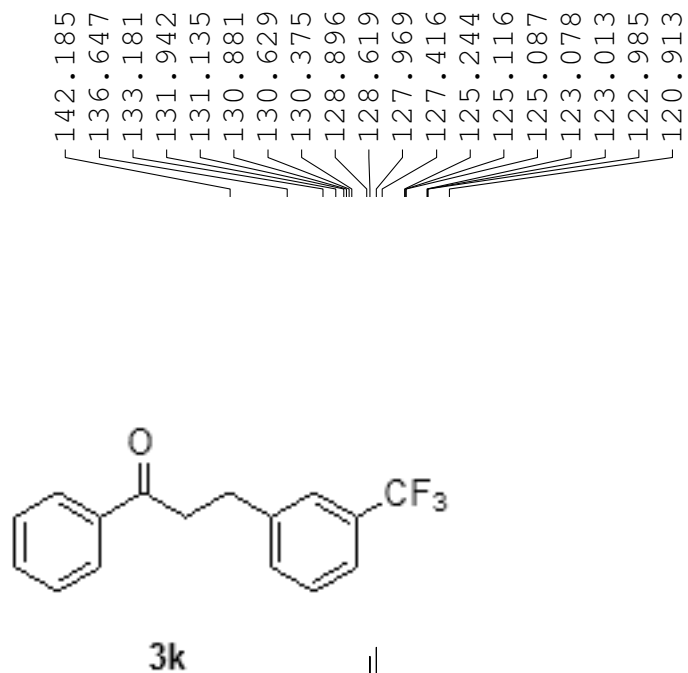
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C13CPD CDC13



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



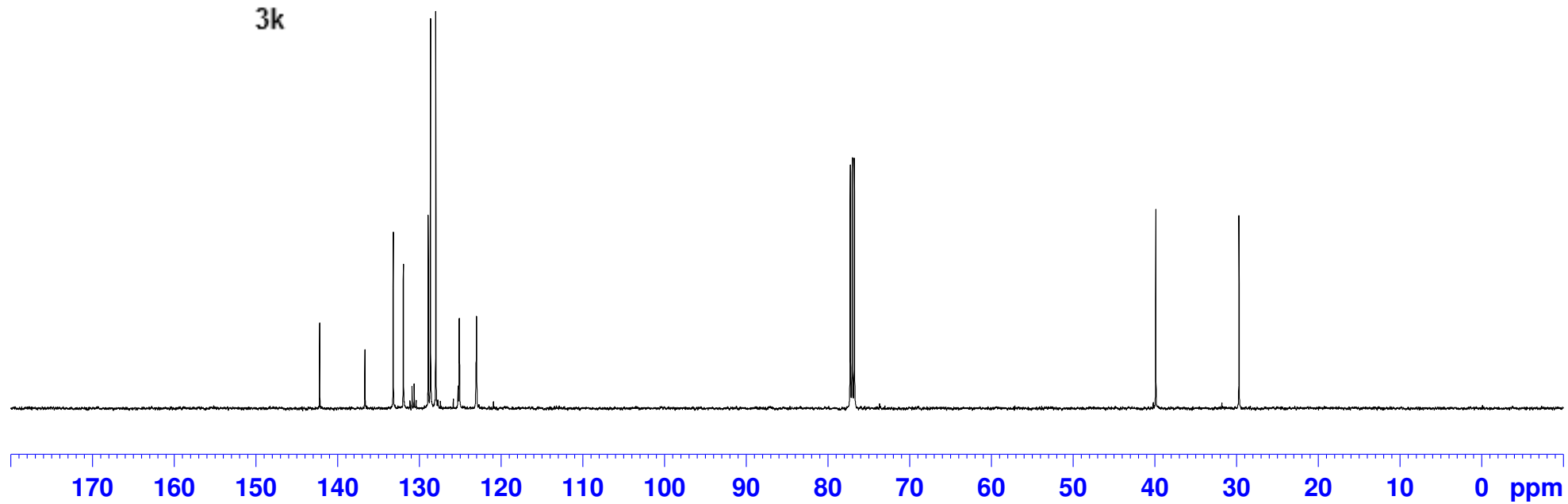
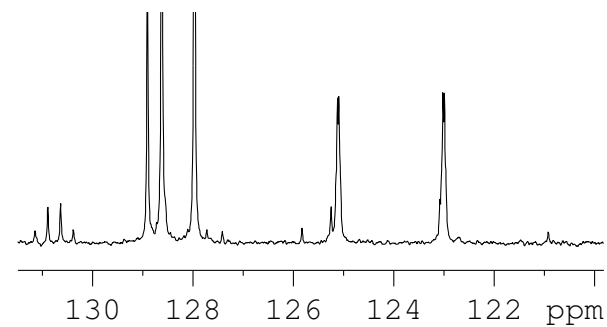
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C13CPD CDC13



— 77.000

— 39.911

— 29.730

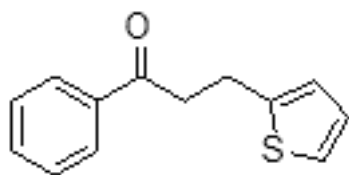


3-(Thiophen-2-yl)-1-phenylpropan-1-one
Proton CDCl₃

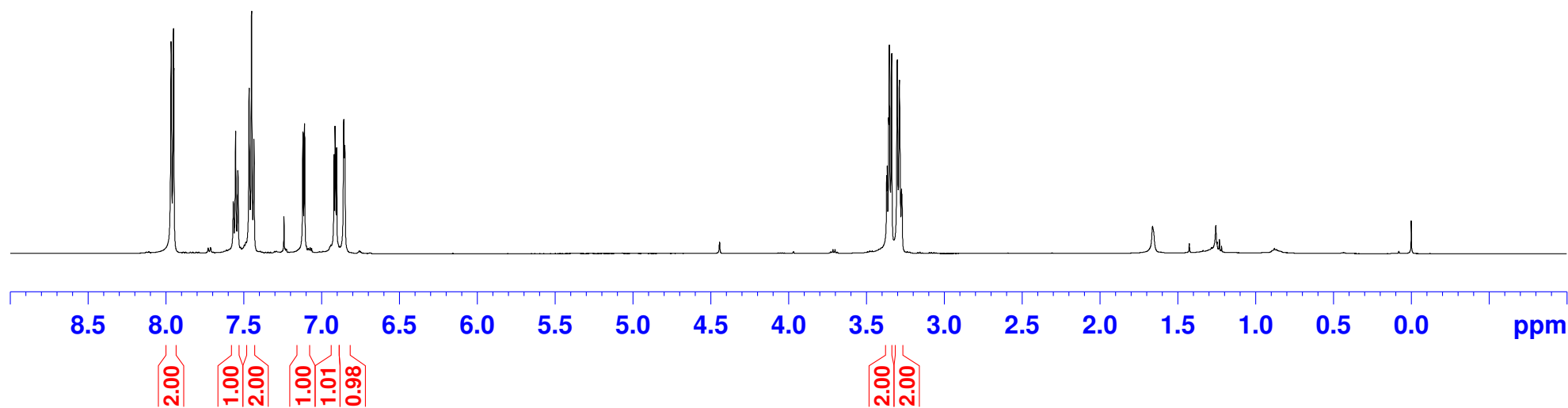
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7.952
7.567
7.552
7.537
7.466
7.450
7.435
7.242
7.121
7.119
7.111
7.109
6.920
6.913
6.903
6.857
6.852

3.366
3.353
3.338
3.302
3.288
3.274

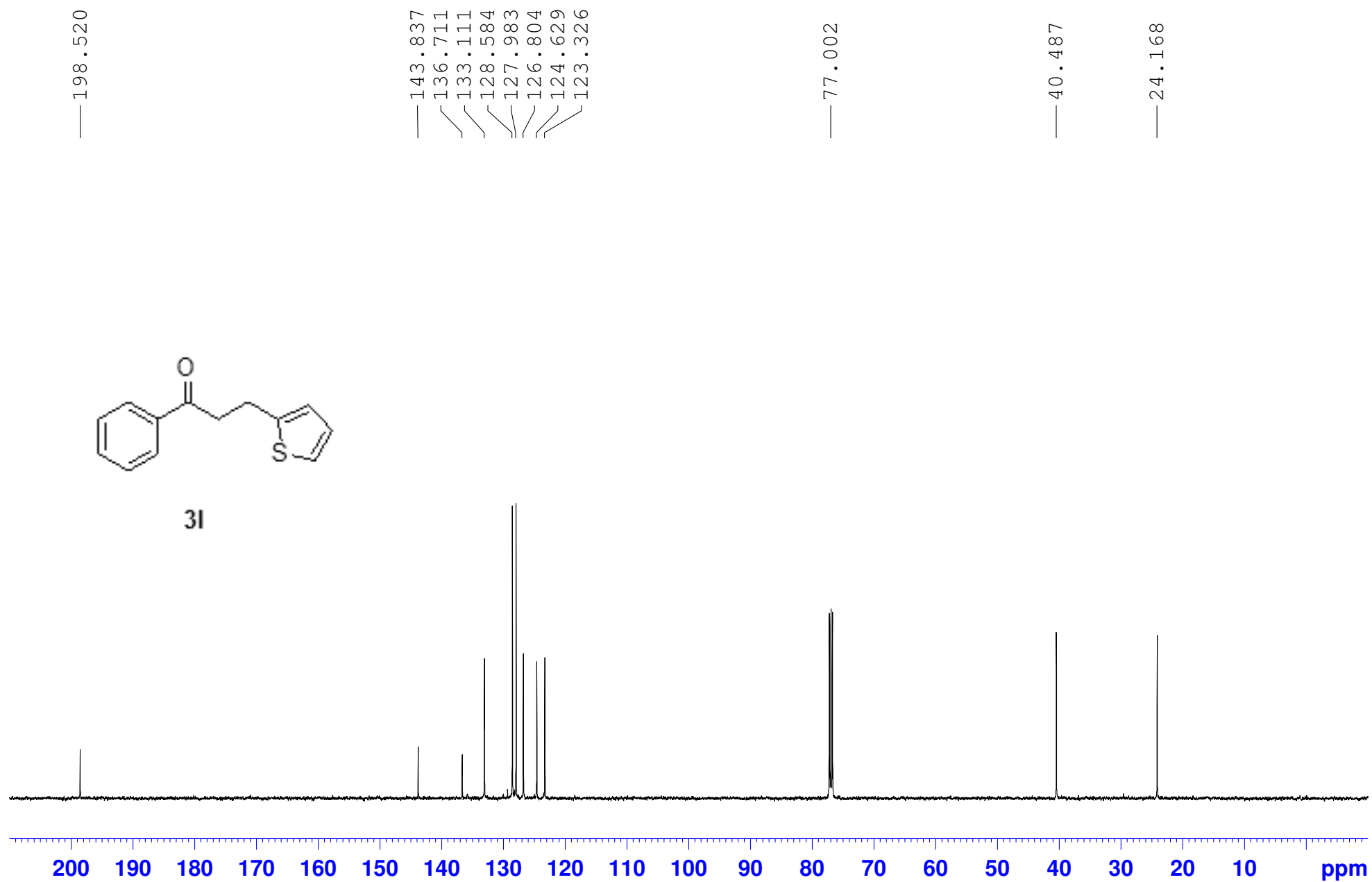
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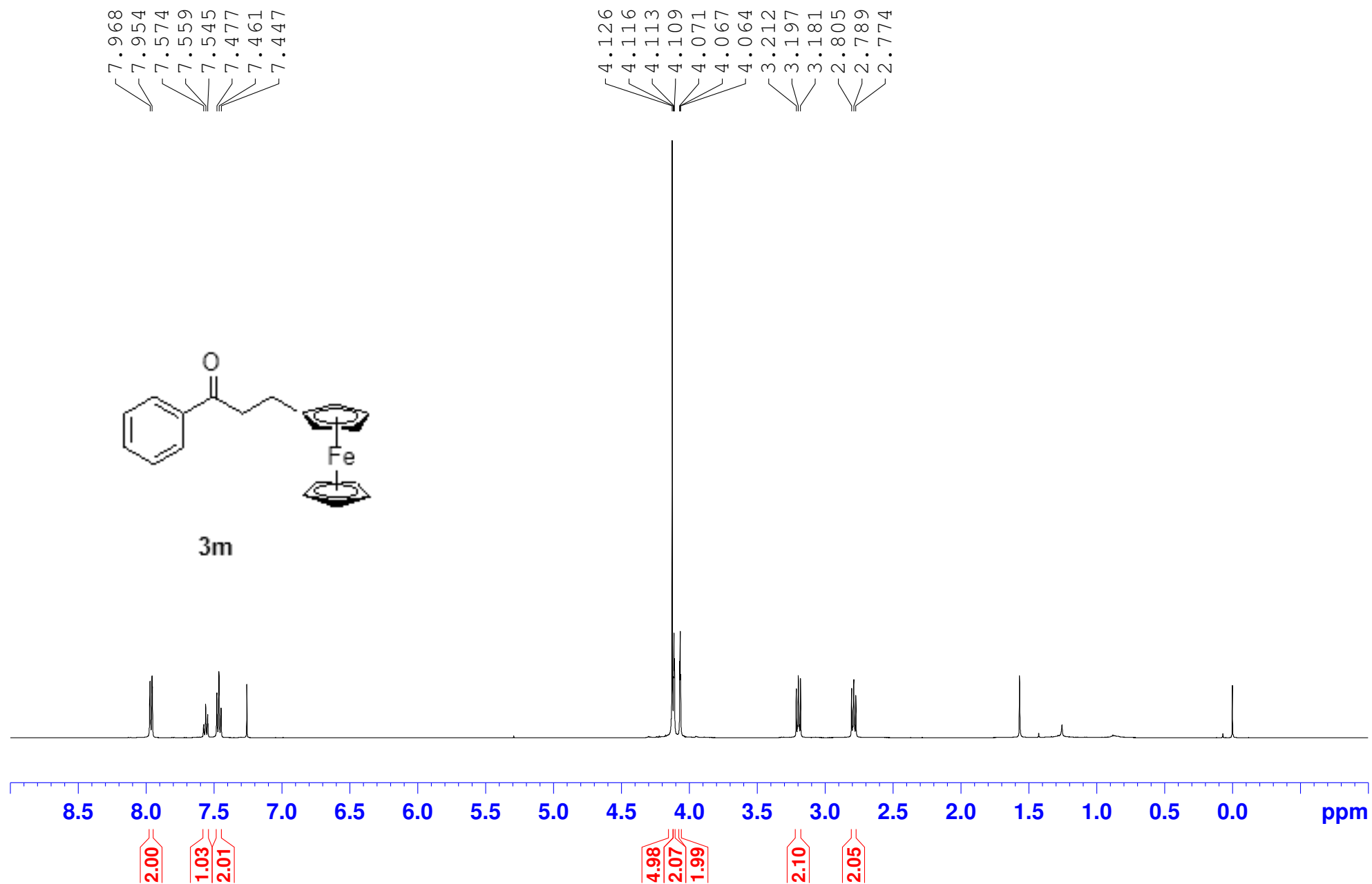
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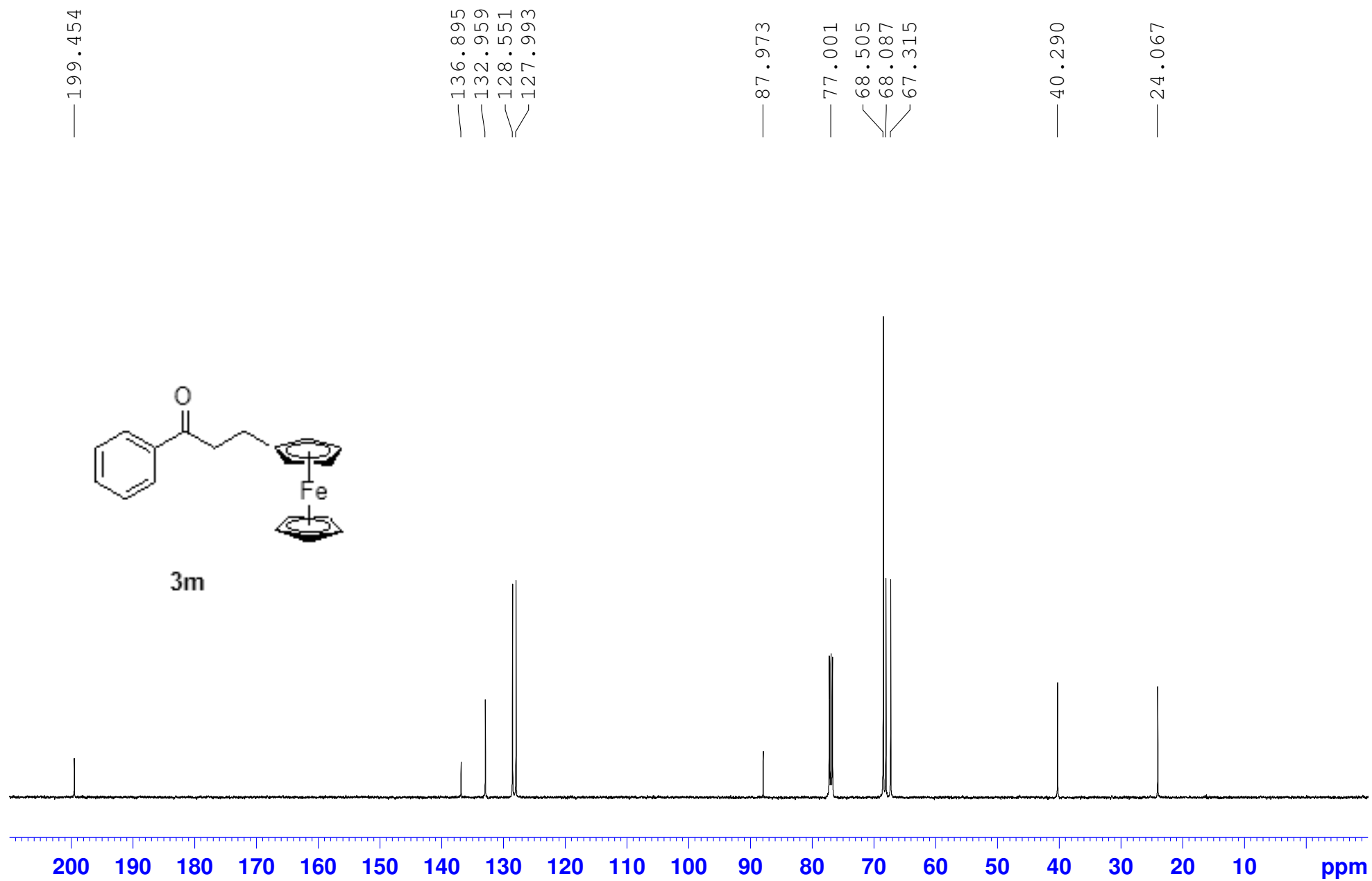
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C13CPD CDC13



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



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

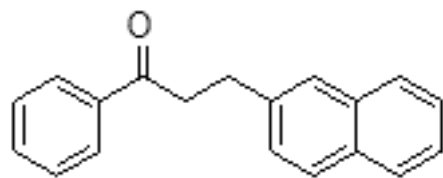


3-(Naphthalen-2-yl)-1-phenylpropan-1-one
Proton CDCl₃

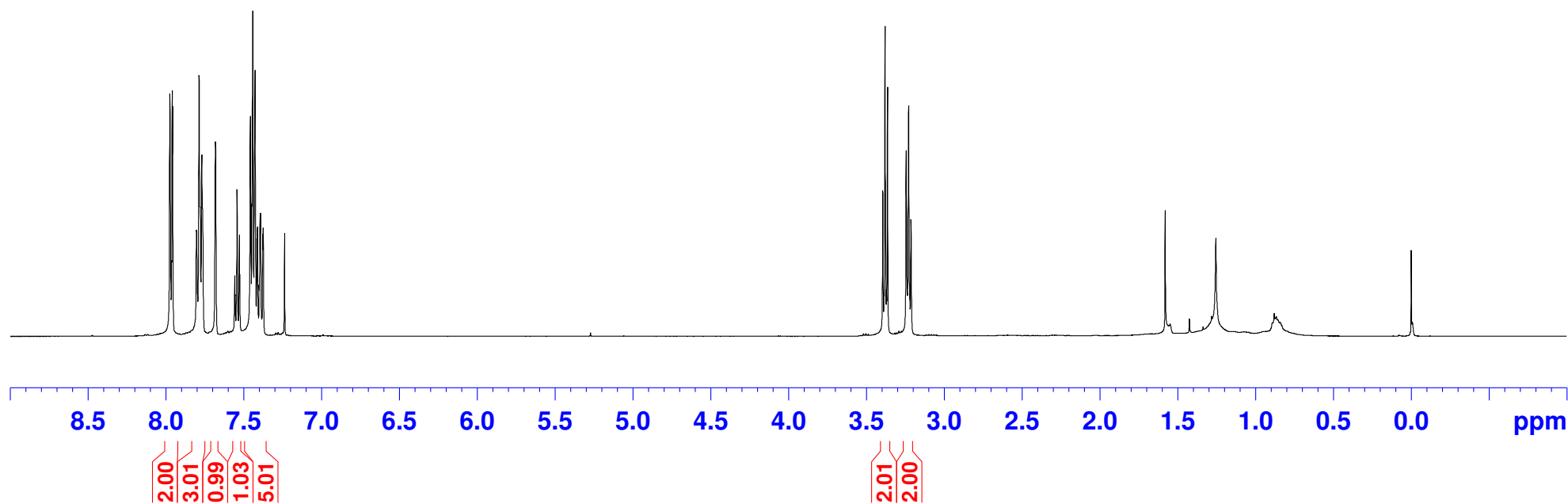
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7.804
7.787
7.770
7.682
7.558
7.543
7.528
7.458
7.442
7.427
7.412
7.392
7.375
7.237

3.395
3.380
3.364
3.244
3.229
3.214

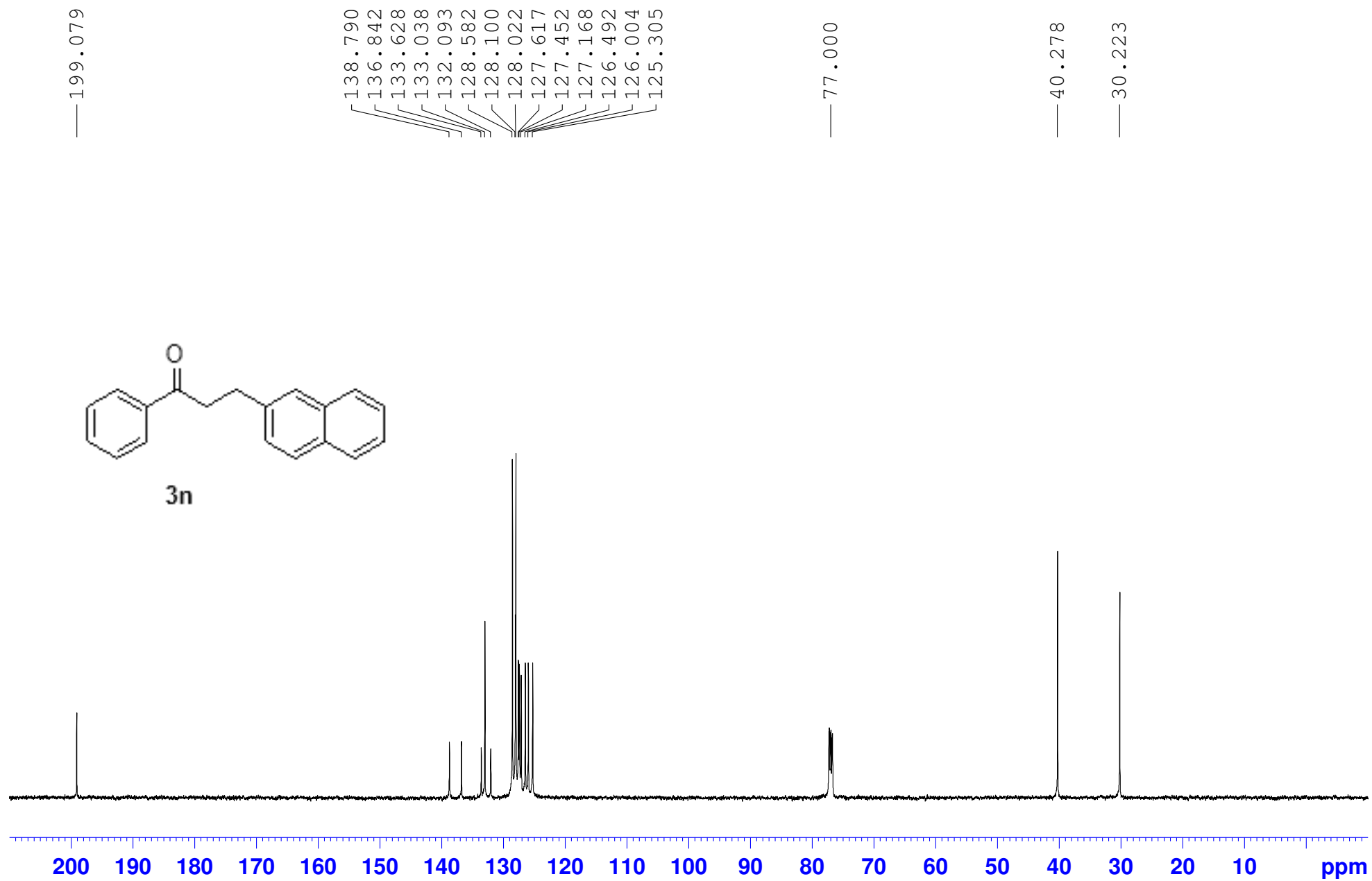
— 0.000



3n



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



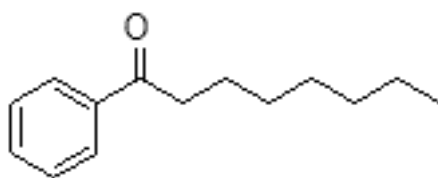
1-Phenyloctan-1-one
Proton CDCl₃

7.966
7.952
7.560
7.545
7.531
7.468
7.452
7.437

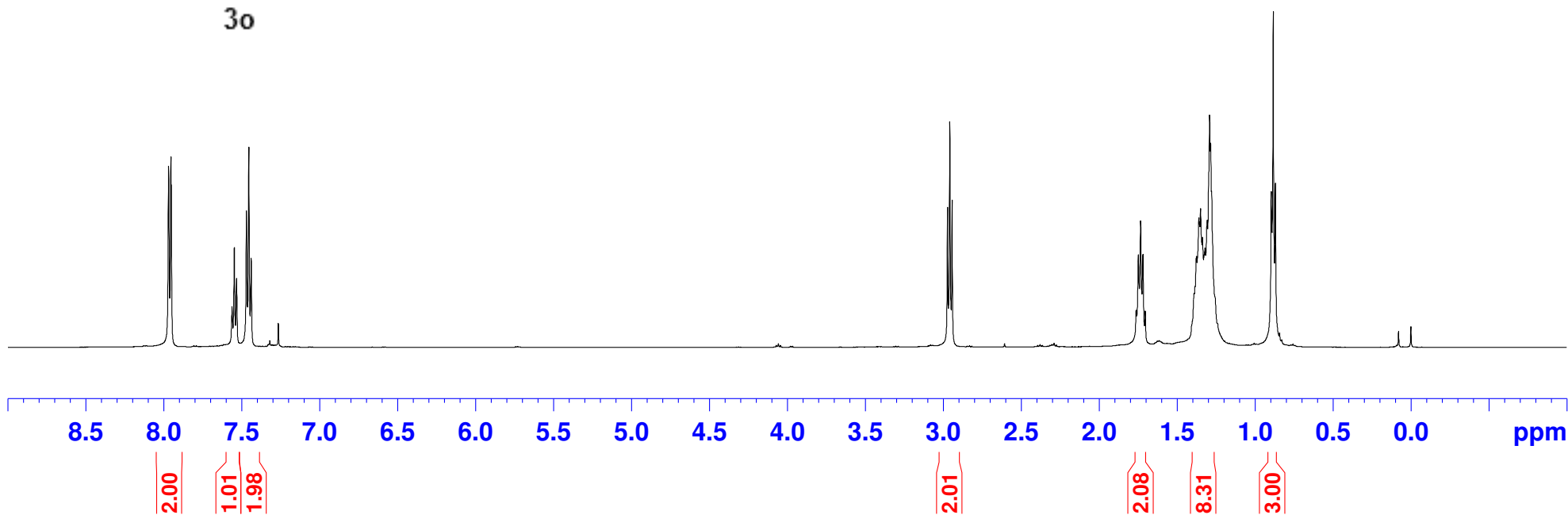
2.973
2.958
2.943

1.763
1.748
1.734
1.719
1.704
1.375
1.349
1.291
1.286
0.896
0.883
0.869

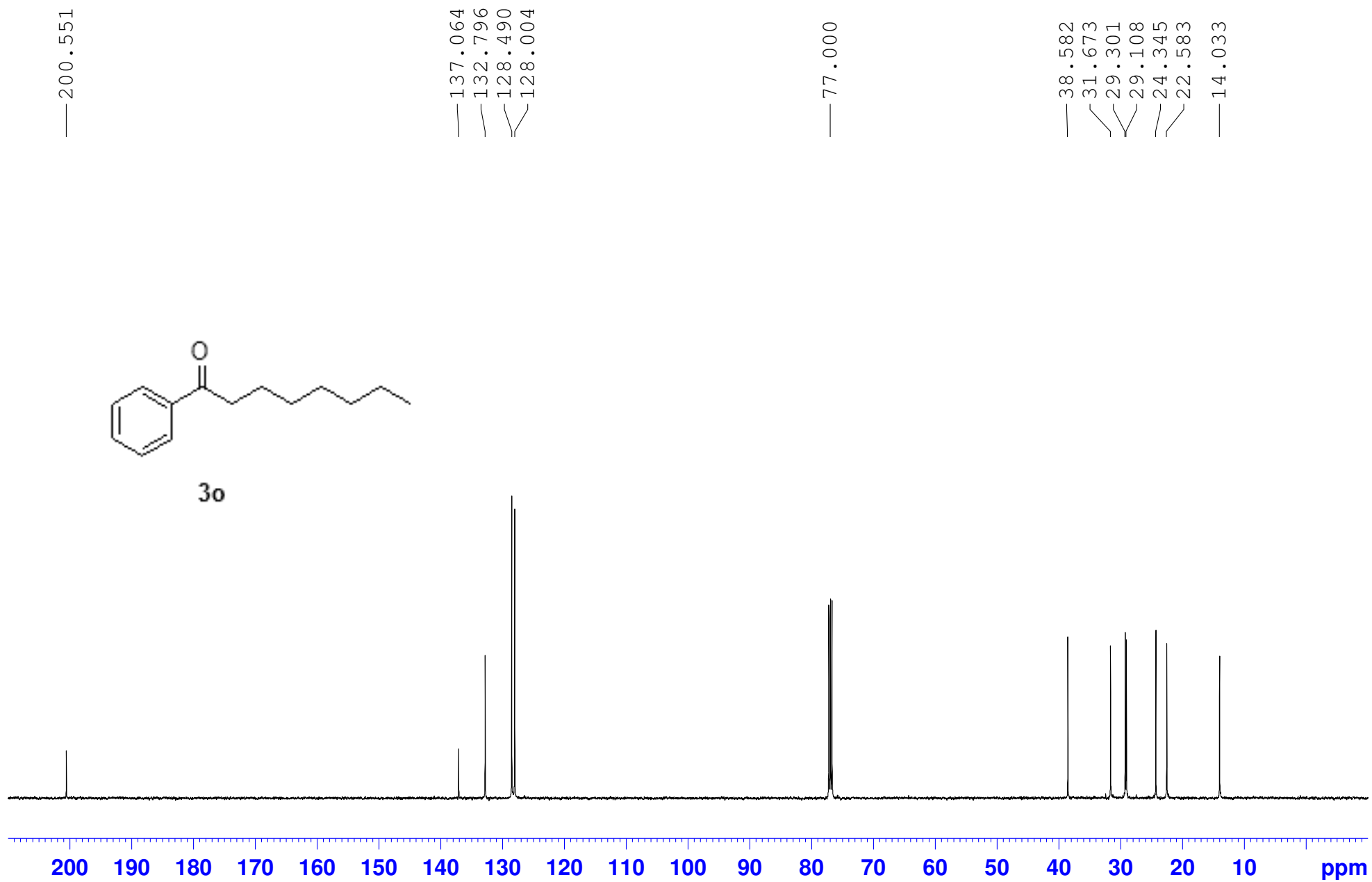
— 0.000



3o



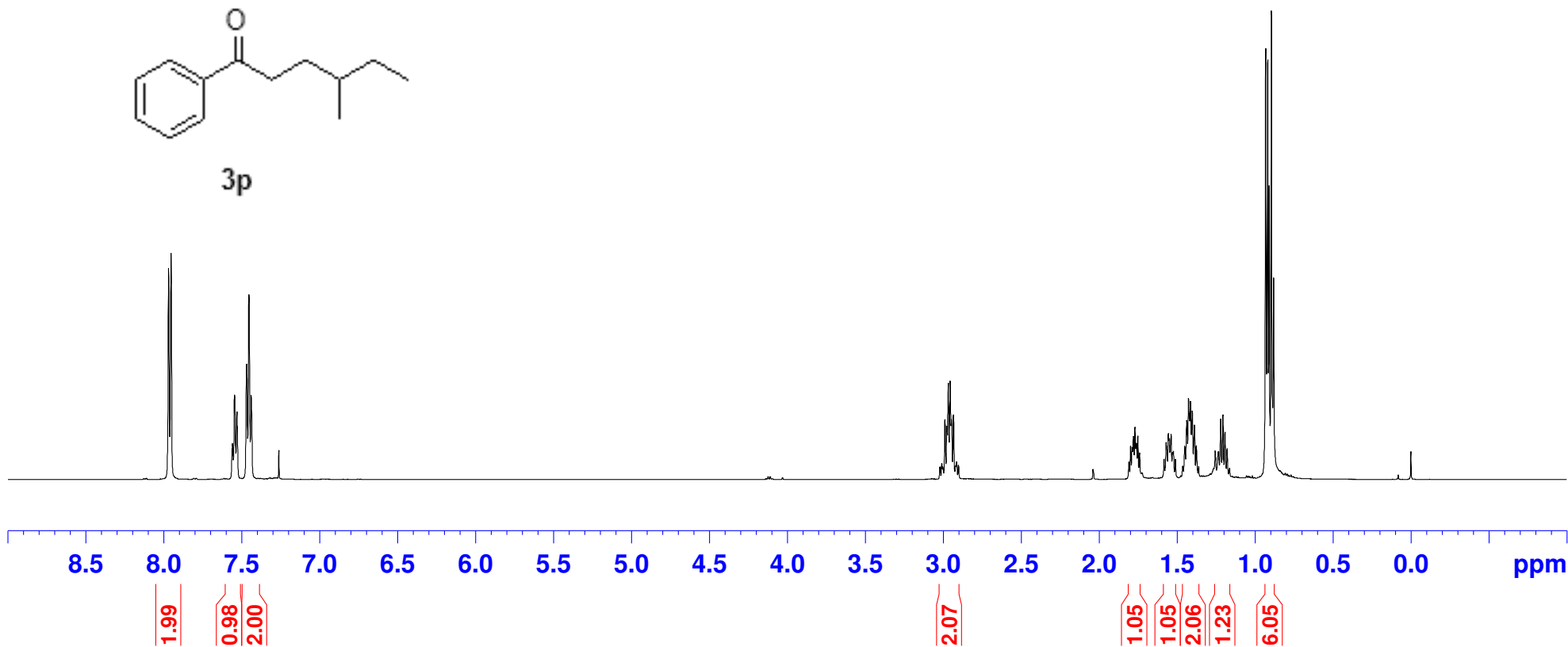
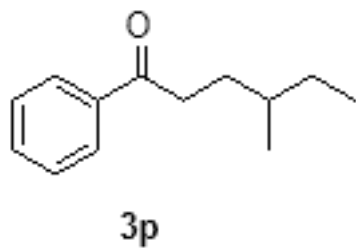
1-Phenyloctan-1-one
C13CPD CDC13



4-Methyl-1-phenylhexan-1-one
Proton CDCl₃

7.969
7.953
7.560
7.546
7.531
7.469
7.454
7.439

3.021
2.967
2.955
2.902
1.809
1.798
1.770
1.752
1.740
1.583
1.556
1.539
1.511
1.464
1.426
1.414
1.362
1.255
1.220
1.206
1.164
0.932
0.919
0.909
0.895
0.880
0.000



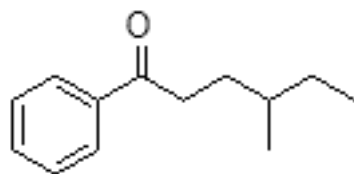
4-Methyl-1-phenylhexan-1-one
C13CPD CDCl3

— 200.786

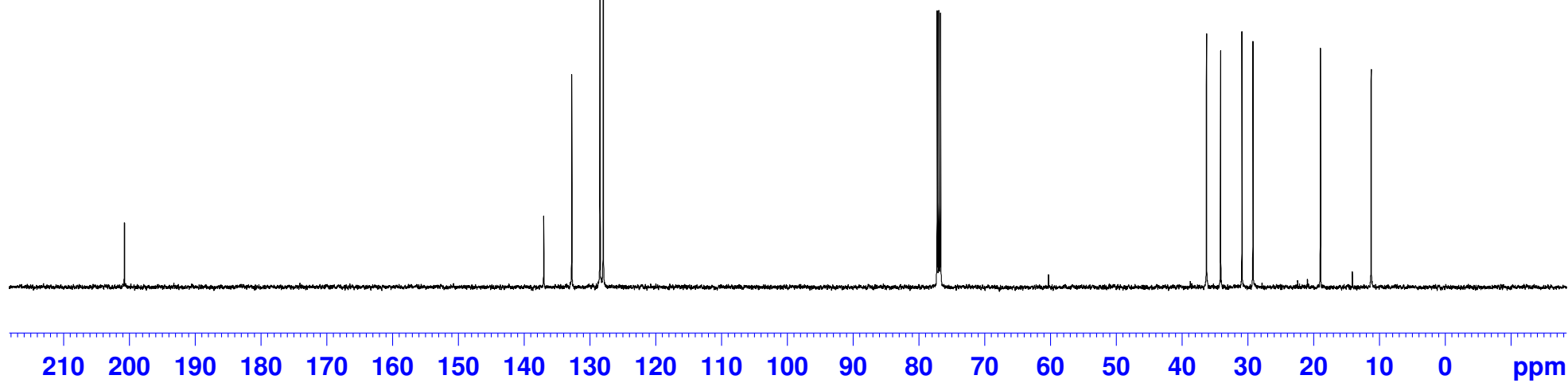
— 137.052
— 132.794
— 128.495
— 128.003

— 77.000

— 36.326
— 34.176
— 30.928
— 29.257
— 19.000
— 11.291



3p

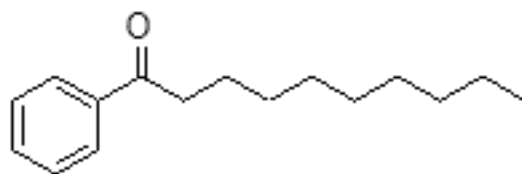


1-Phenyldecan-1-one
Proton CDCl₃

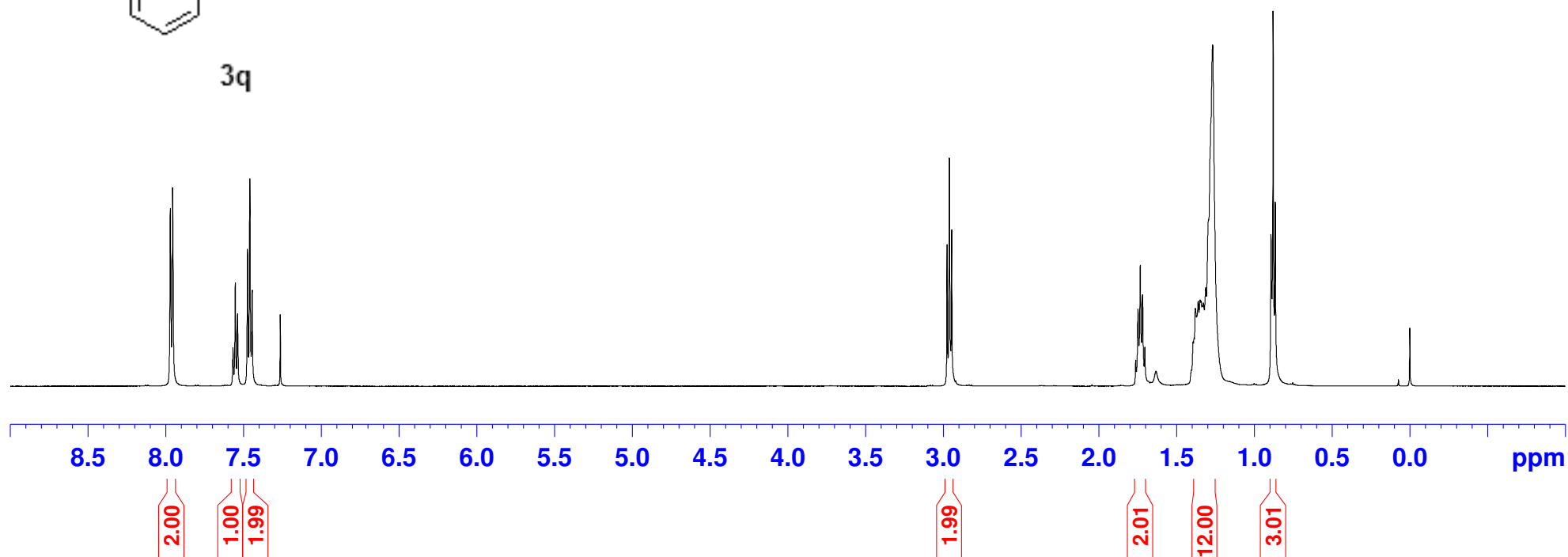
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7.954
7.565
7.550
7.536
7.472
7.457
7.442

2.975
2.961
2.946

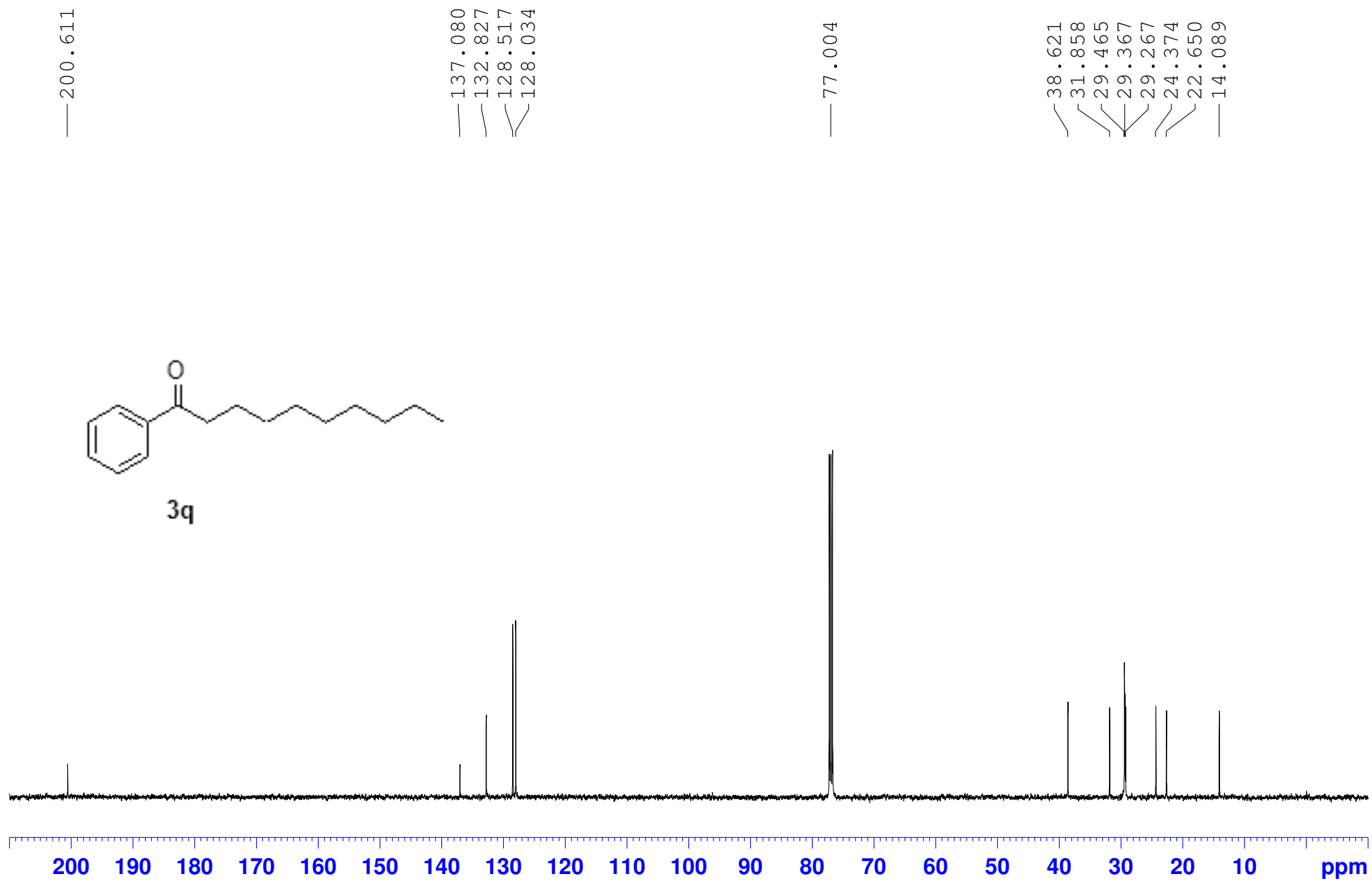
1.748
1.733
1.719
1.379
1.361
1.268
0.893
0.879
0.865



3q



1-Phenyldecan-1-one
C13CPD-1 CDC13

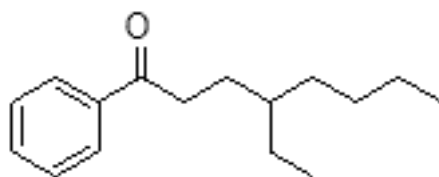


4-Ethyl-1-phenyl-1-octanone
Proton CDCl₃

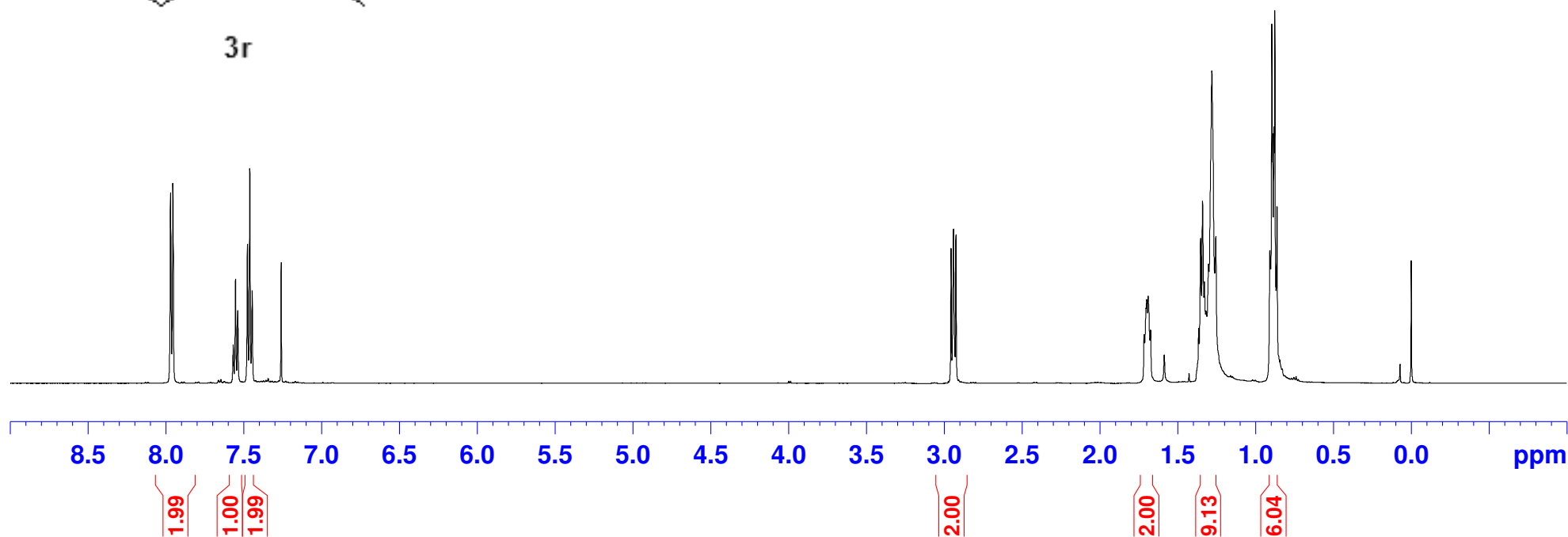
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7.956
7.568
7.553
7.539
7.477
7.461
7.446

2.956
2.941
2.925

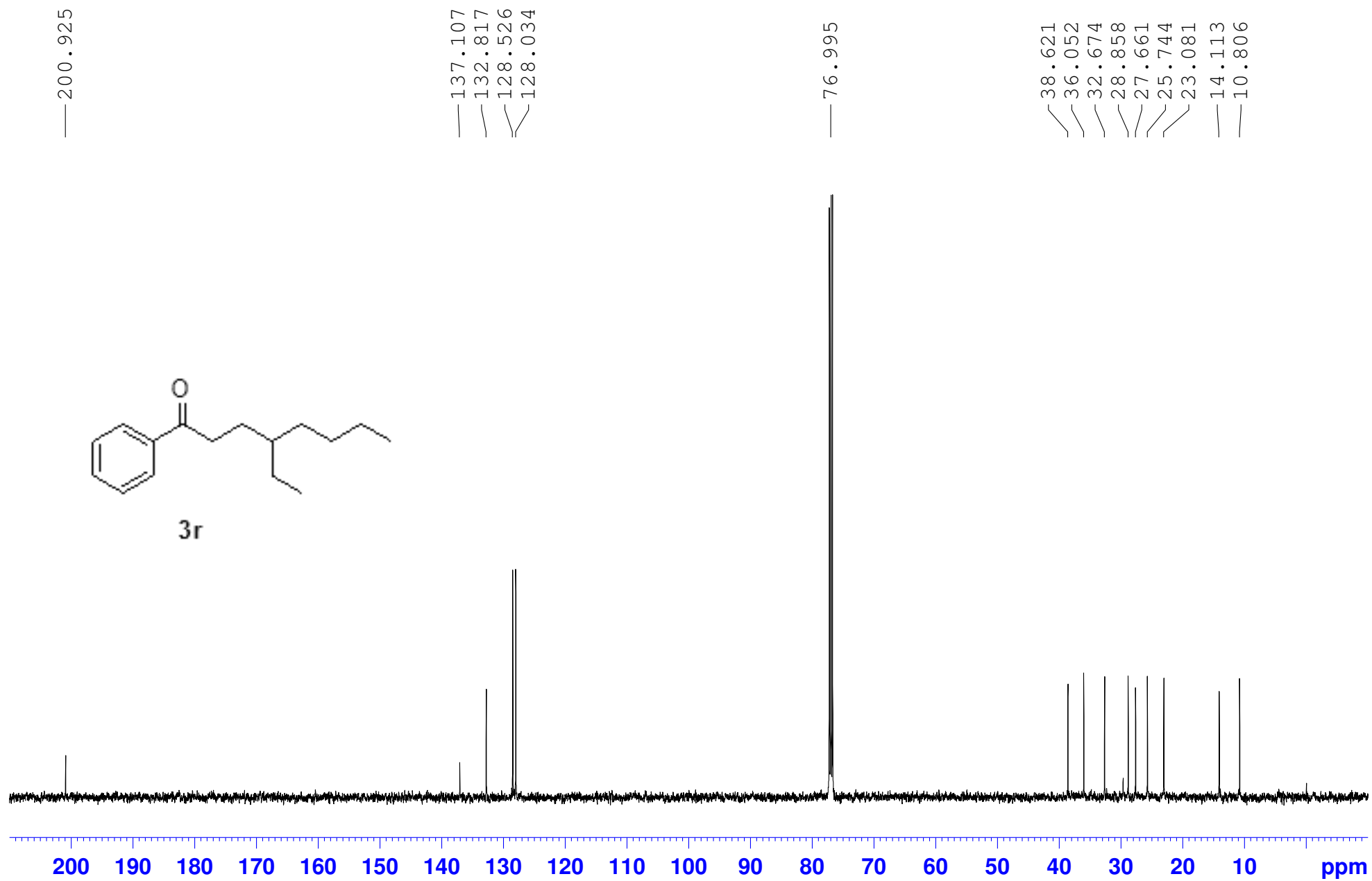
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1.674
1.352
1.281
1.255
0.908
0.876
0.862



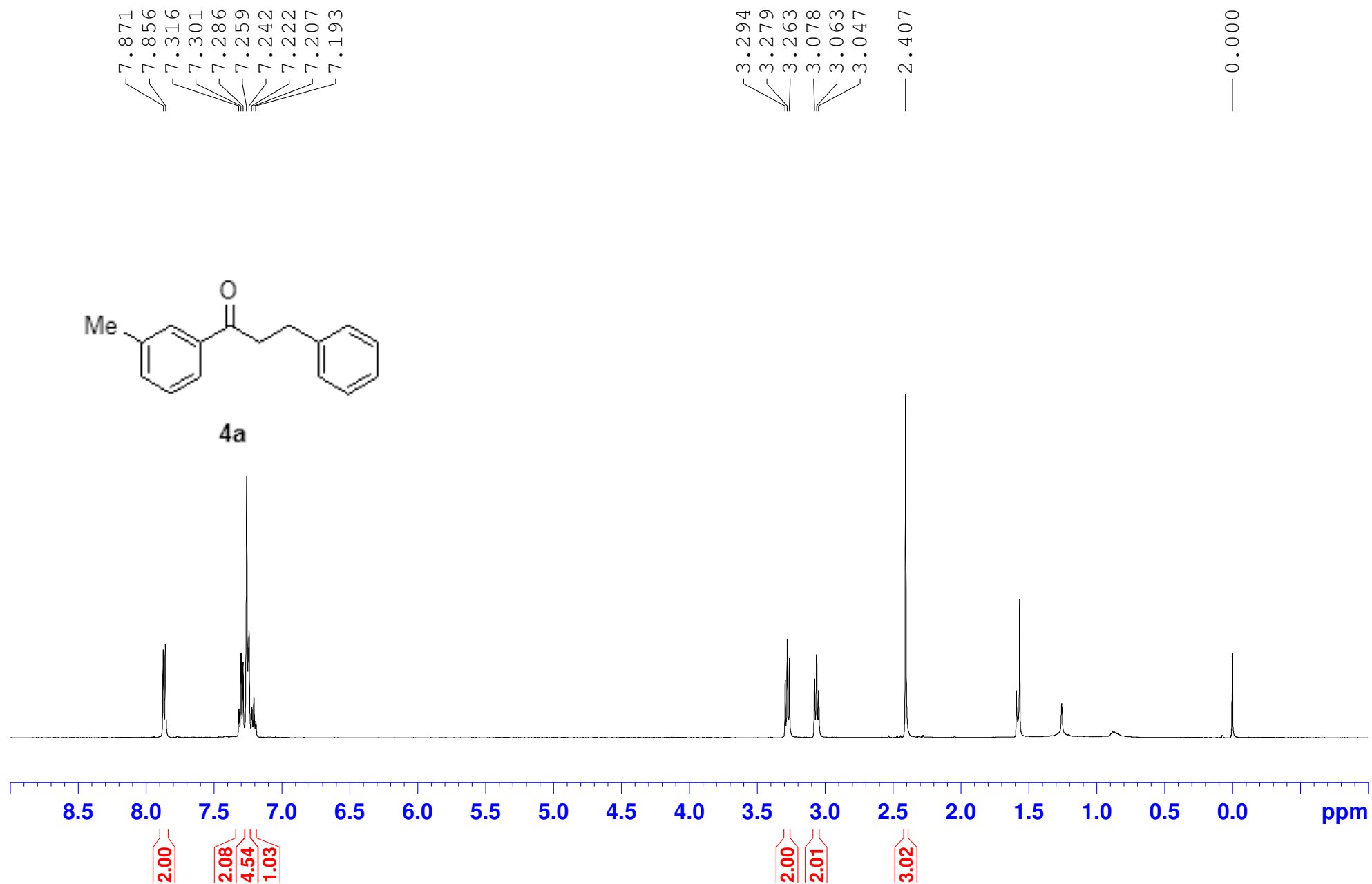
3r



4-Ethyl-1-phenyl-1-octanone
C13CPD-1 CDCl₃



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



3-Phenyl-1-m-tolylpropan-1-one
C13CPD CDC13

— 199.336

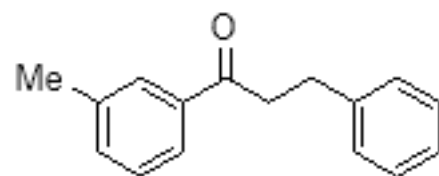
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133.730
128.528
128.454
128.405
128.371
126.049
125.198

— 77.000

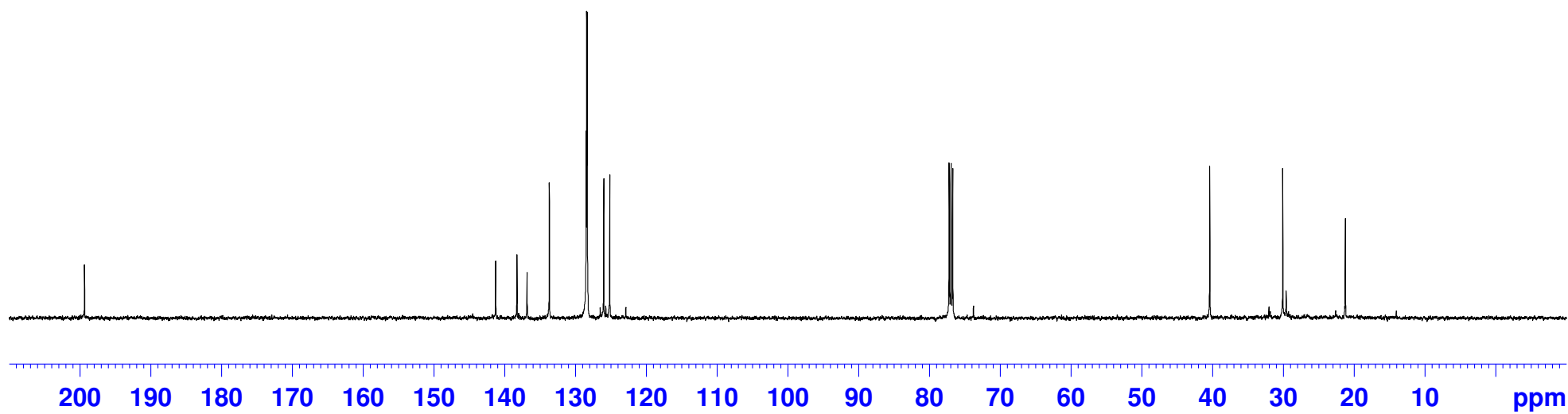
— 40.437

— 30.121

— 21.277



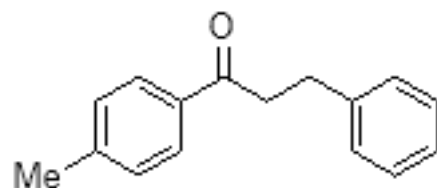
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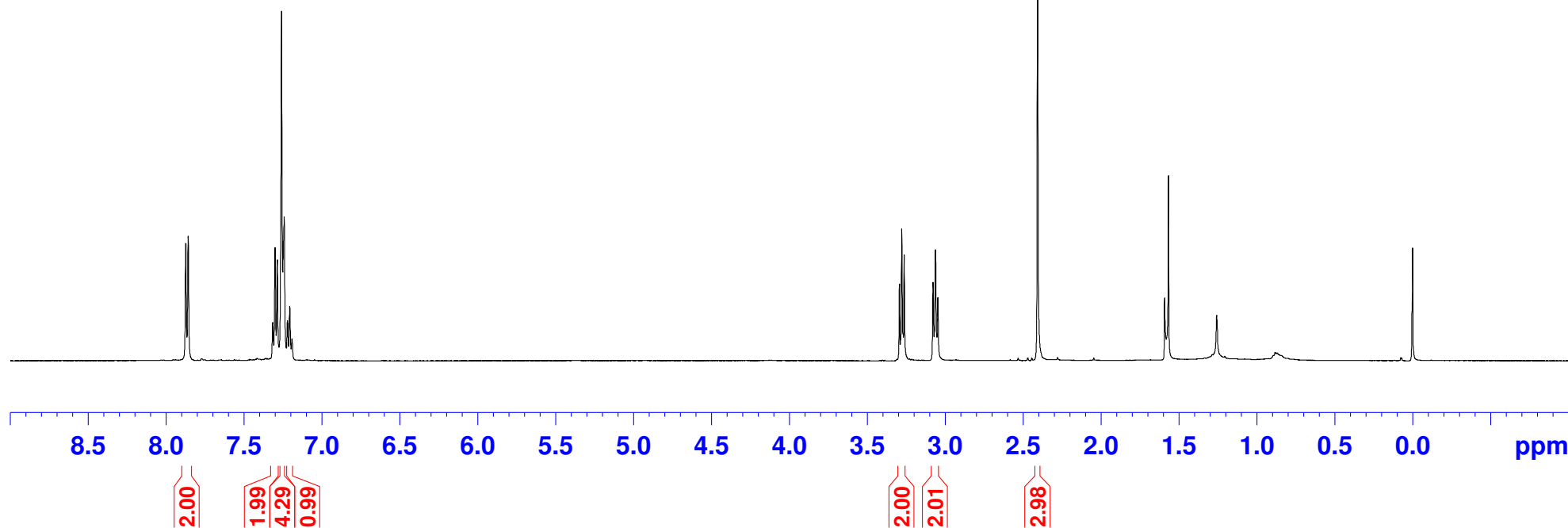
3-phenyl-1-p-tolylpropan-1-one
Proton CDCl₃

7.871
7.856
7.316
7.301
7.286
7.259
7.242
7.222
7.207
7.193

3.294
3.279
3.263
3.078
3.063
3.047
— 2.407
— 0.000



4b



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

— 198.828

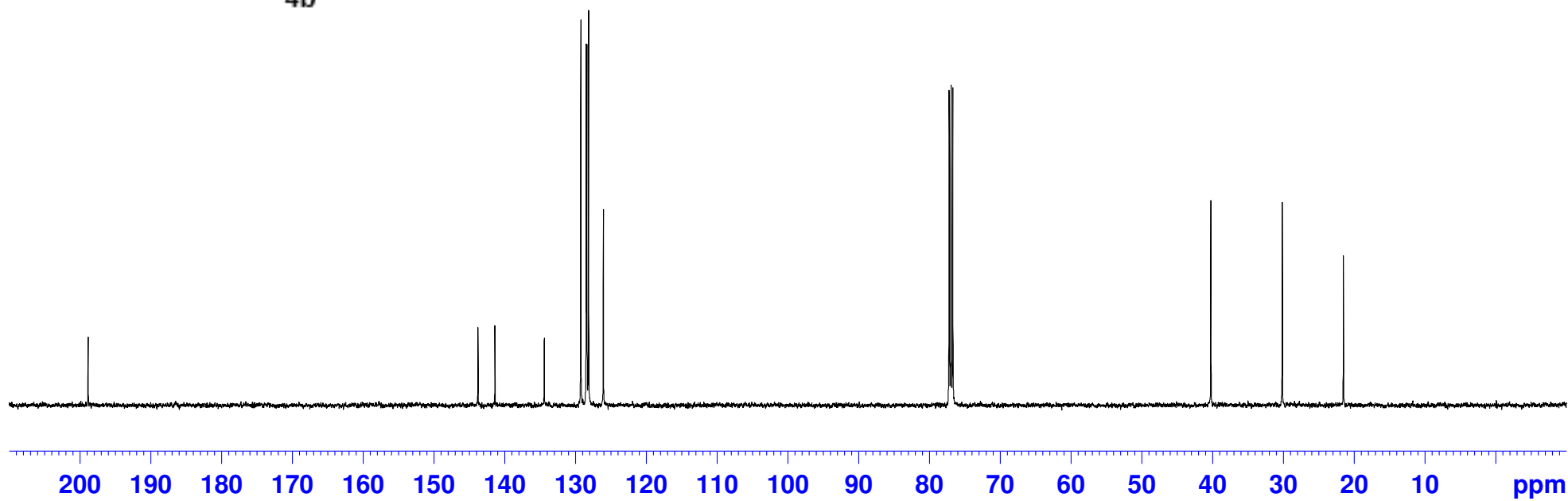
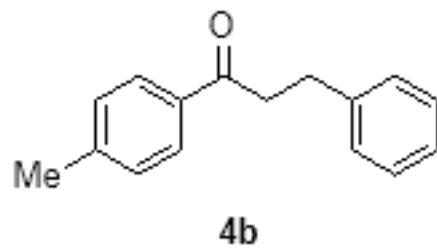
143.759
141.365
134.391
129.229
128.462
128.375
128.125
126.046

— 76.997

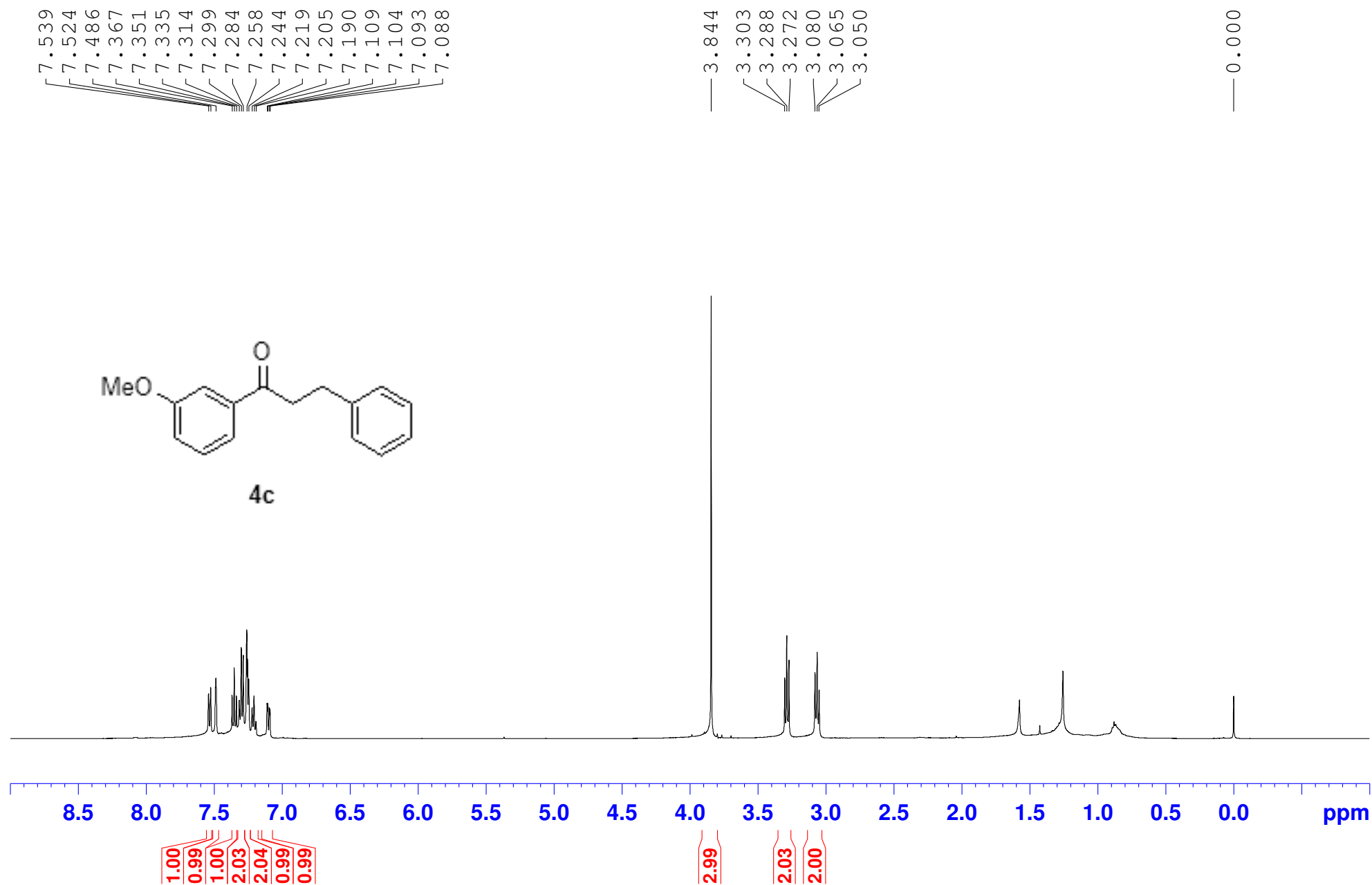
— 40.279

— 30.191

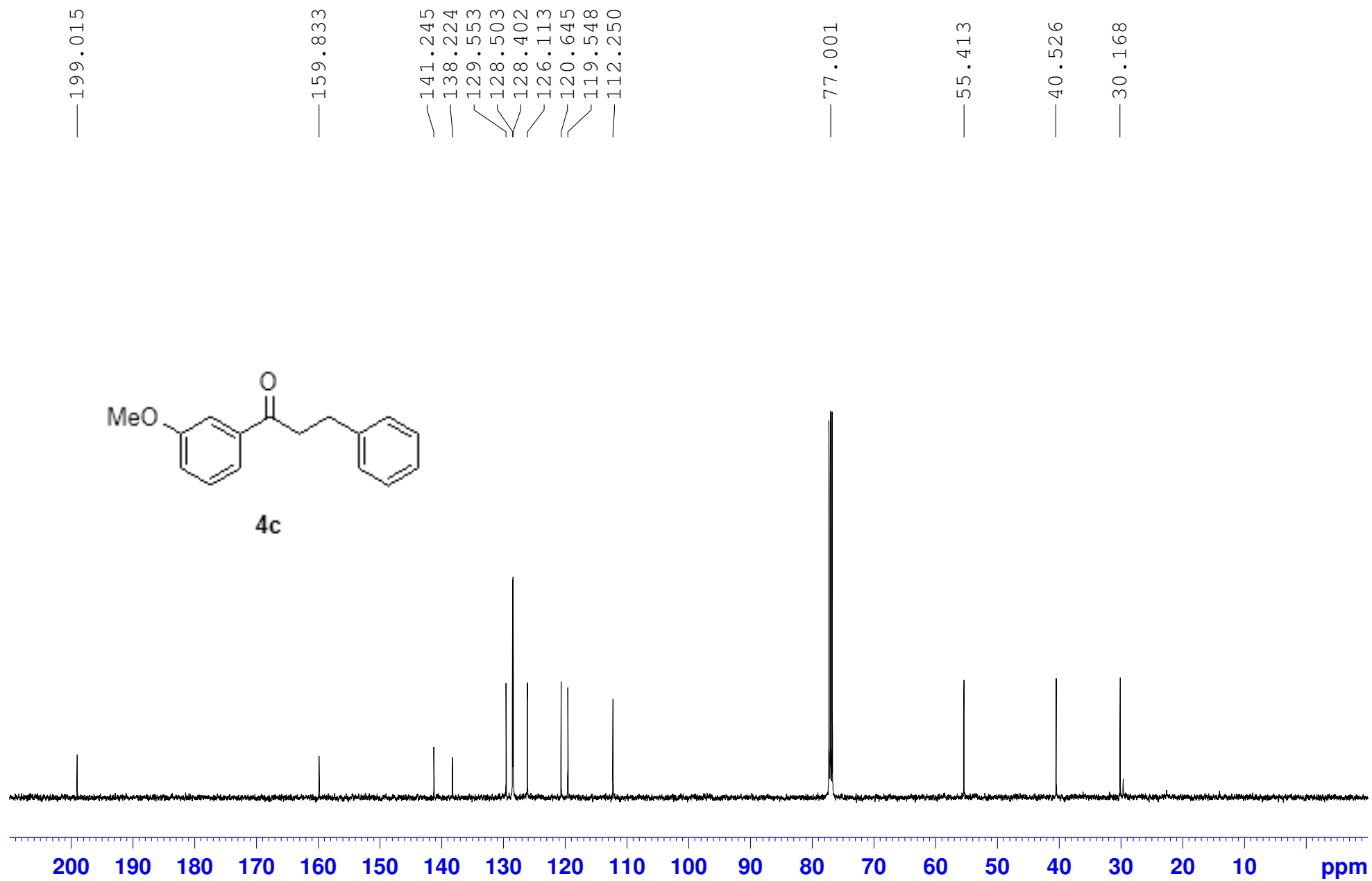
— 21.563



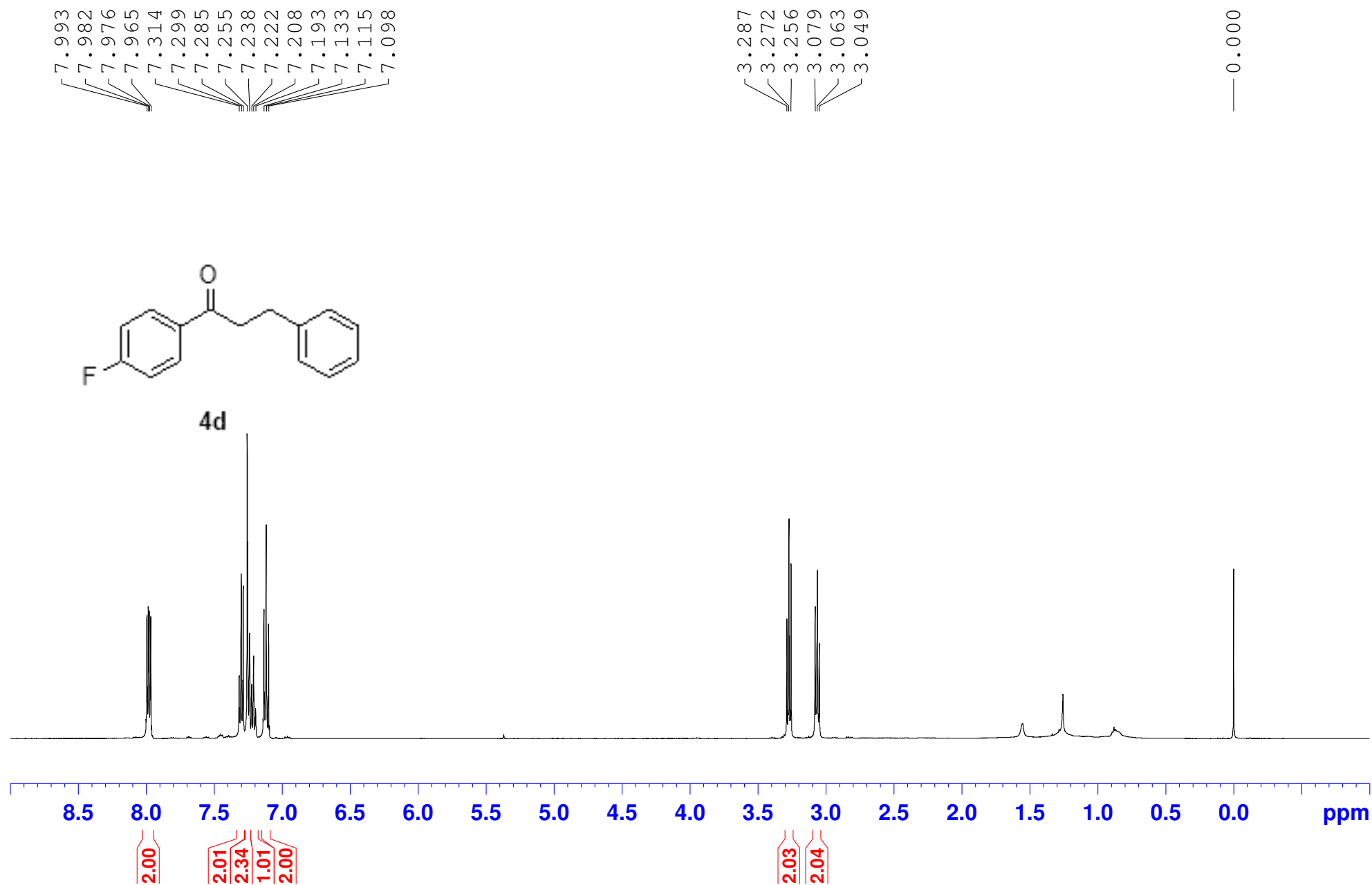
1-(3-Methoxyphenyl)-3-phenylpropan-1-one
Proton CDCl₃



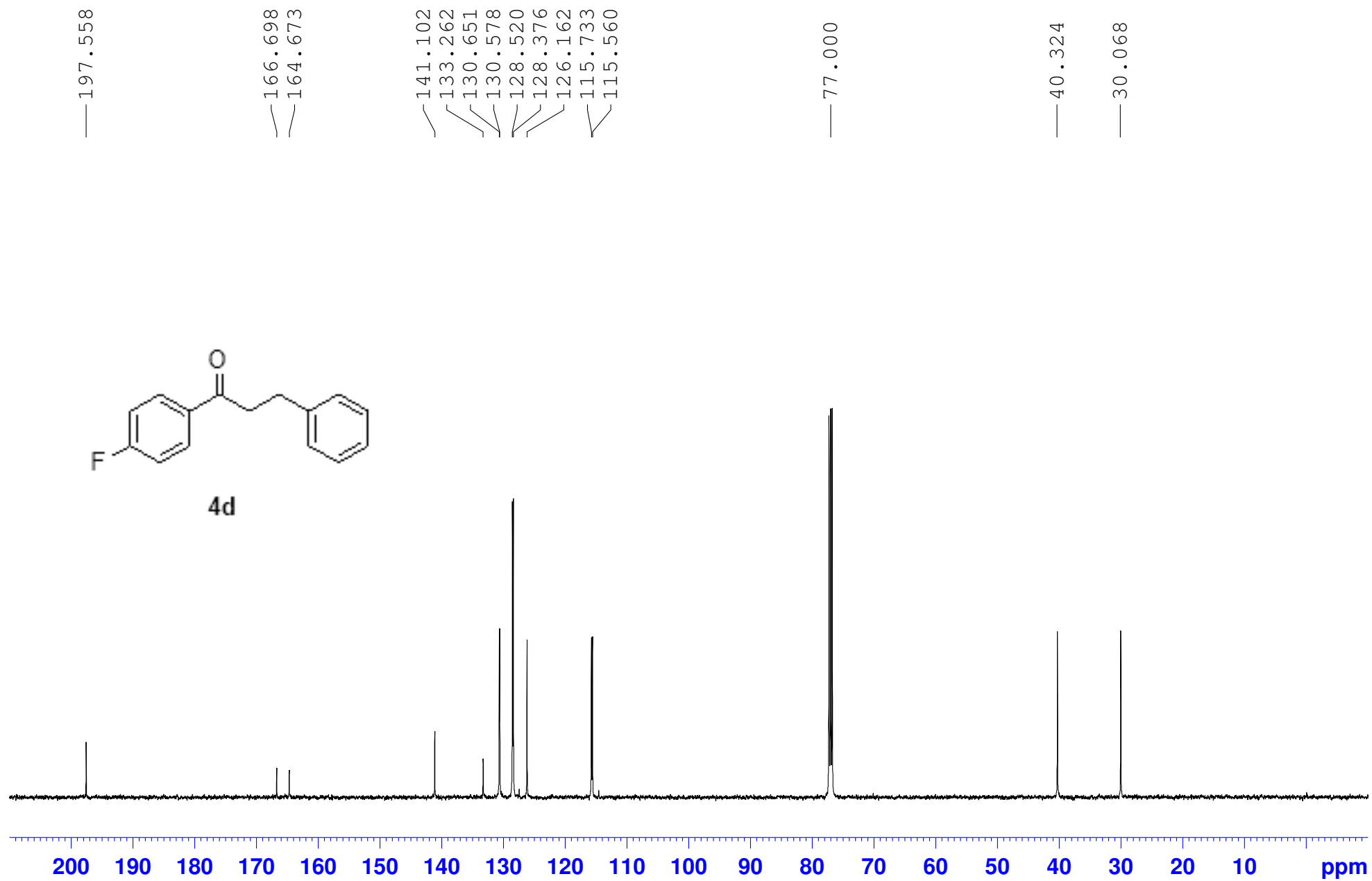
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C13CPD CDC13



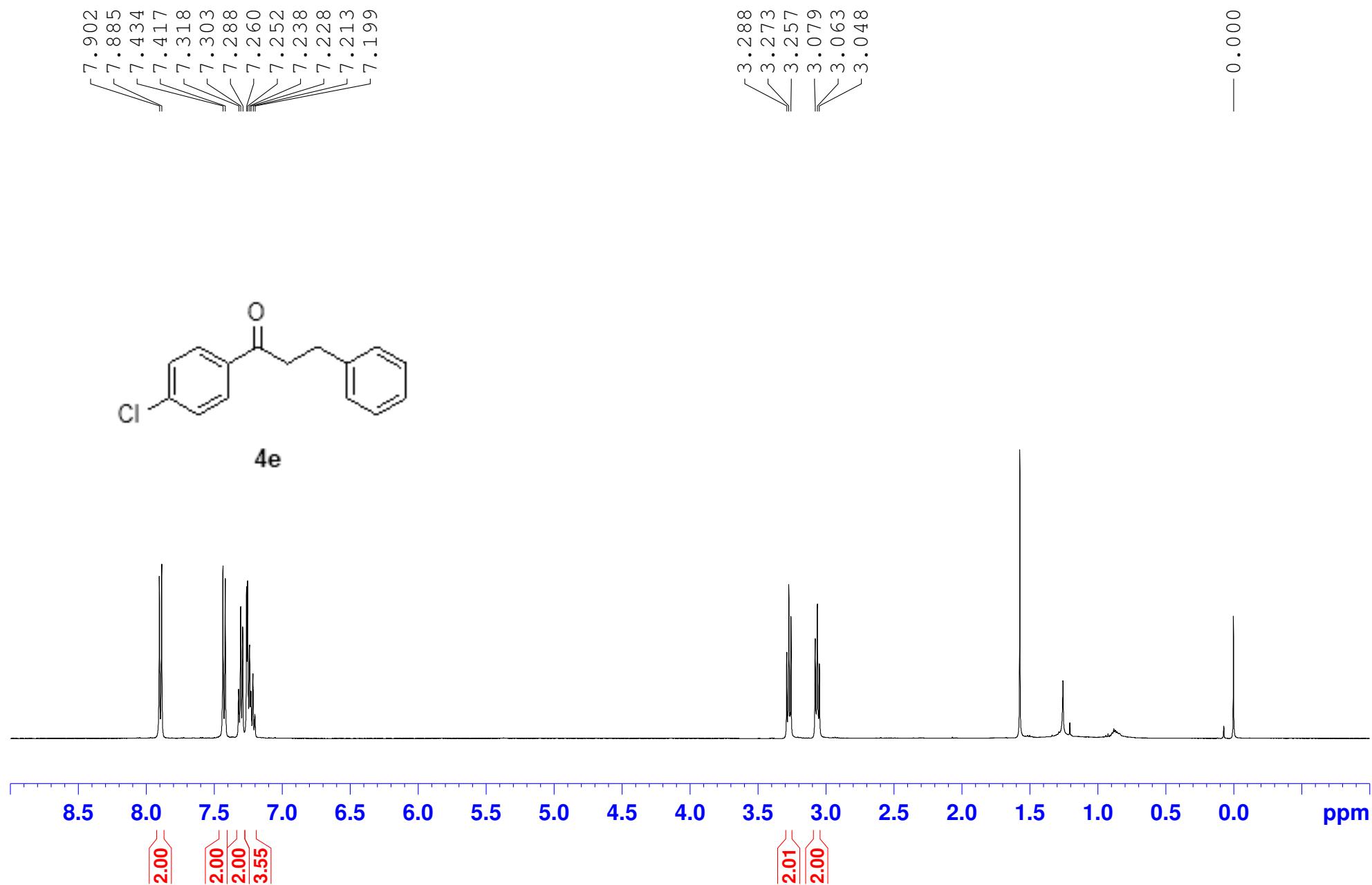
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Proton CDCl₃



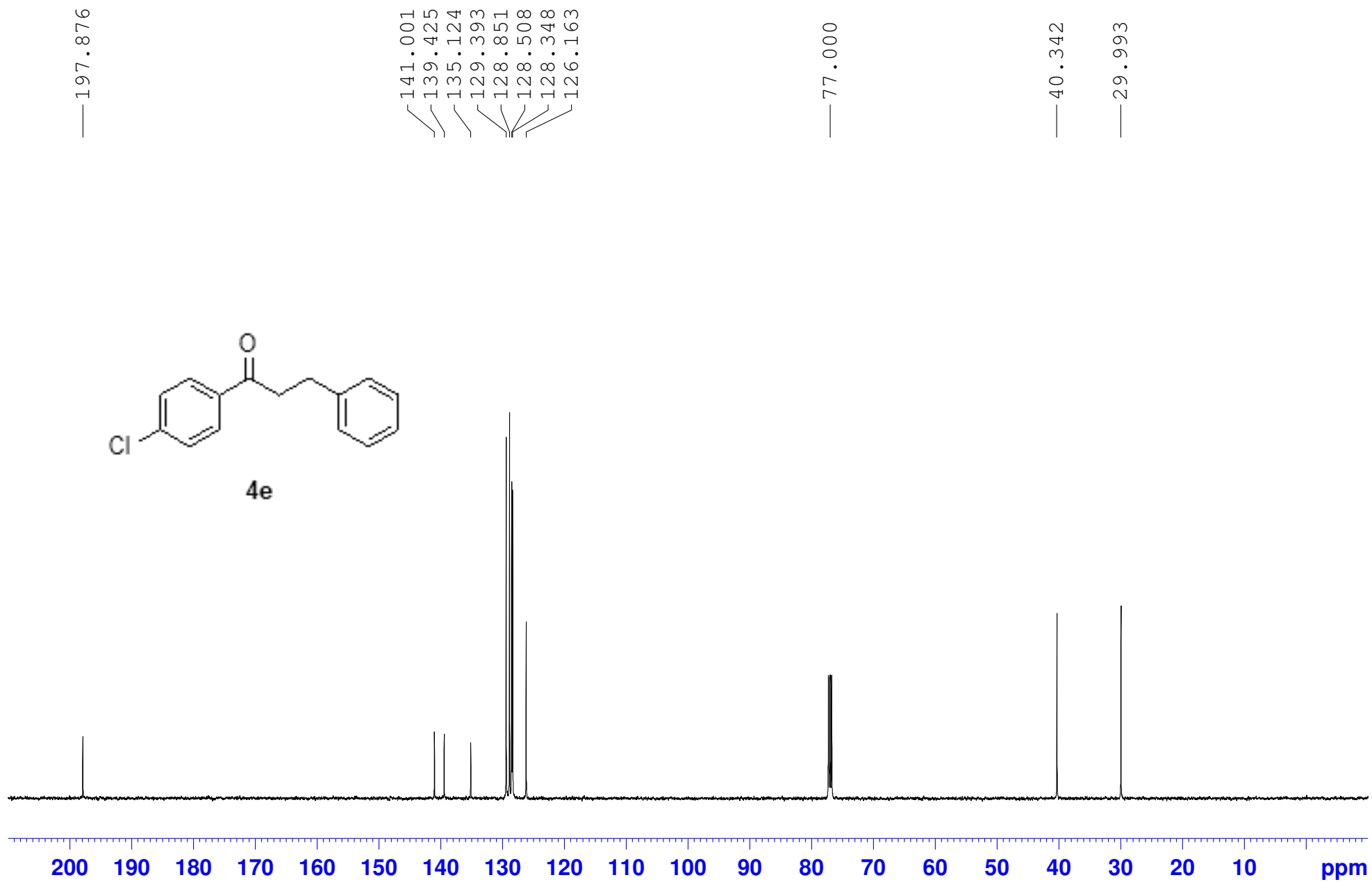
1-(4-Fluorophenyl)-3-phenylpropan-1-one
C13CPD CDCl3



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



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

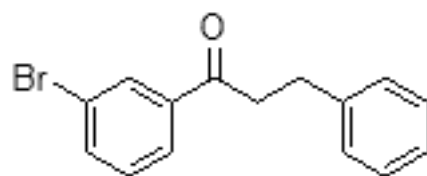


1-(3-Bromophenyl)-3-phenylpropan-1-one
Proton CDCl₃

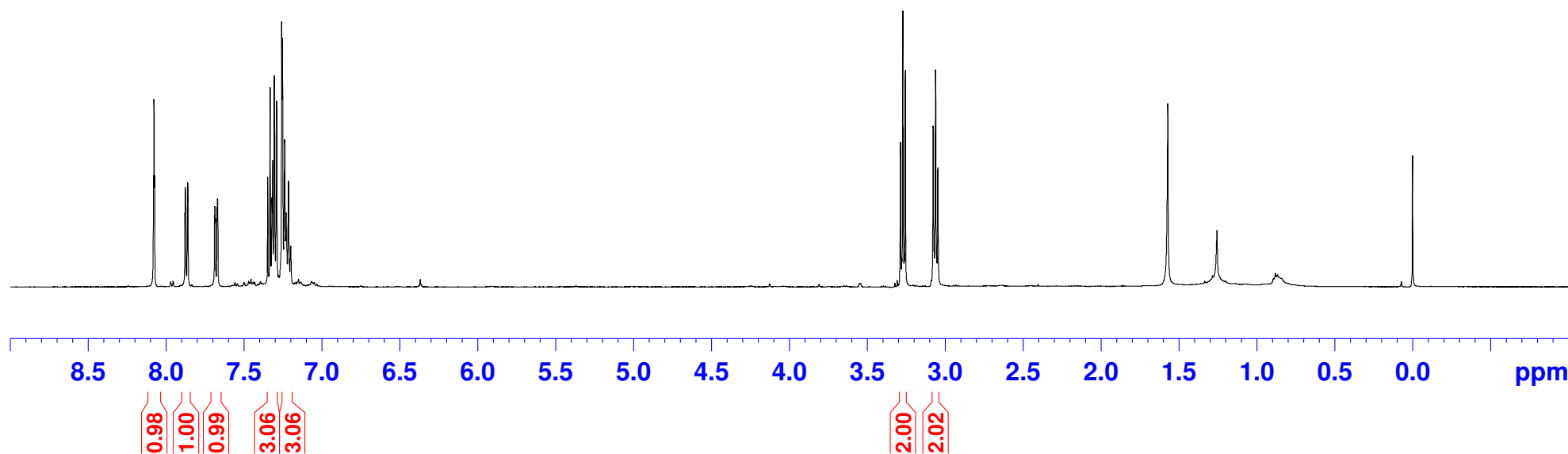
8.079
8.075
8.072
7.874
7.859
7.687
7.665
7.345
7.303
7.288
7.256
7.251
7.197

3.286
3.272
3.256
3.077
3.062
3.047

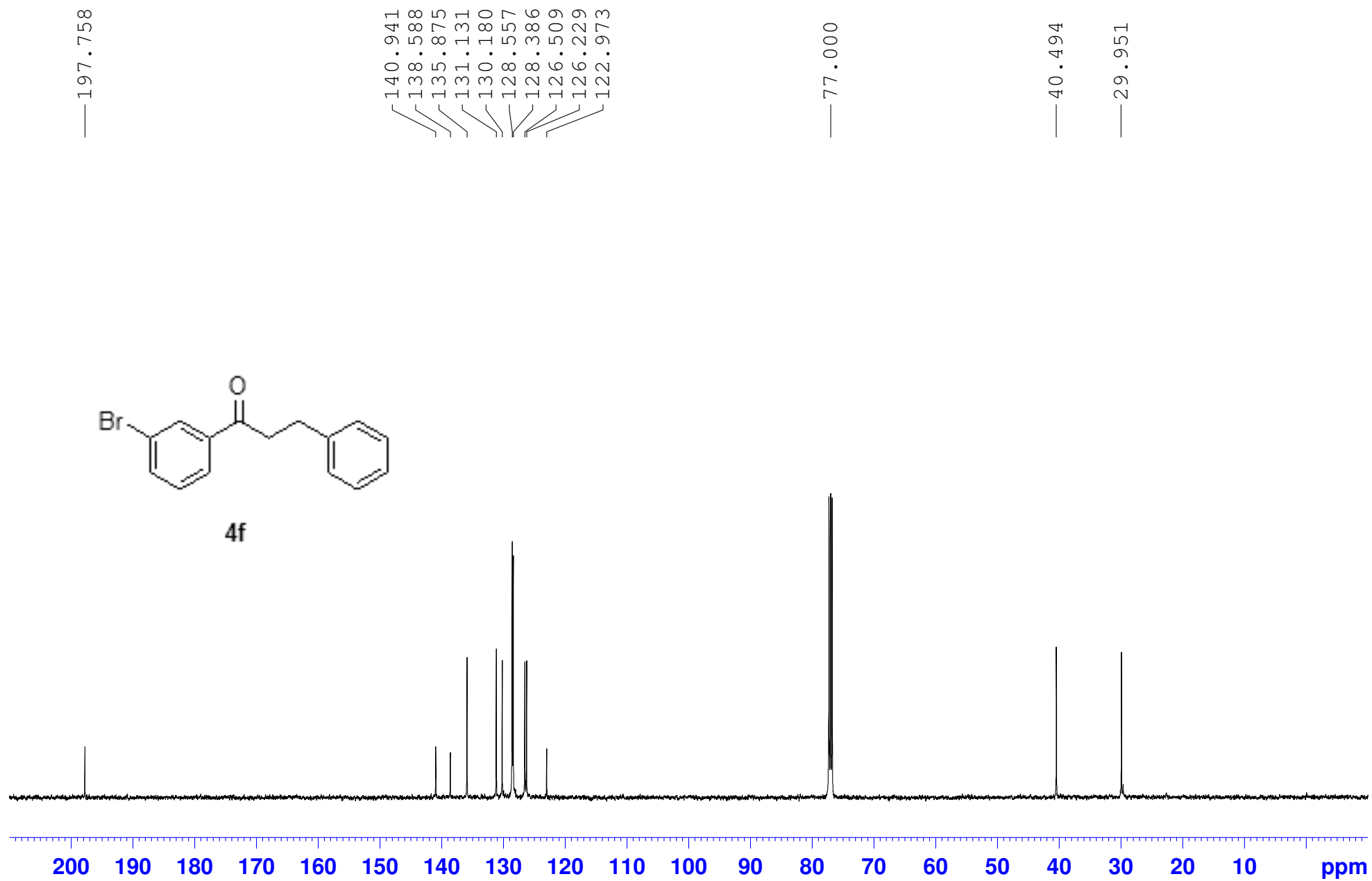
— 0.000



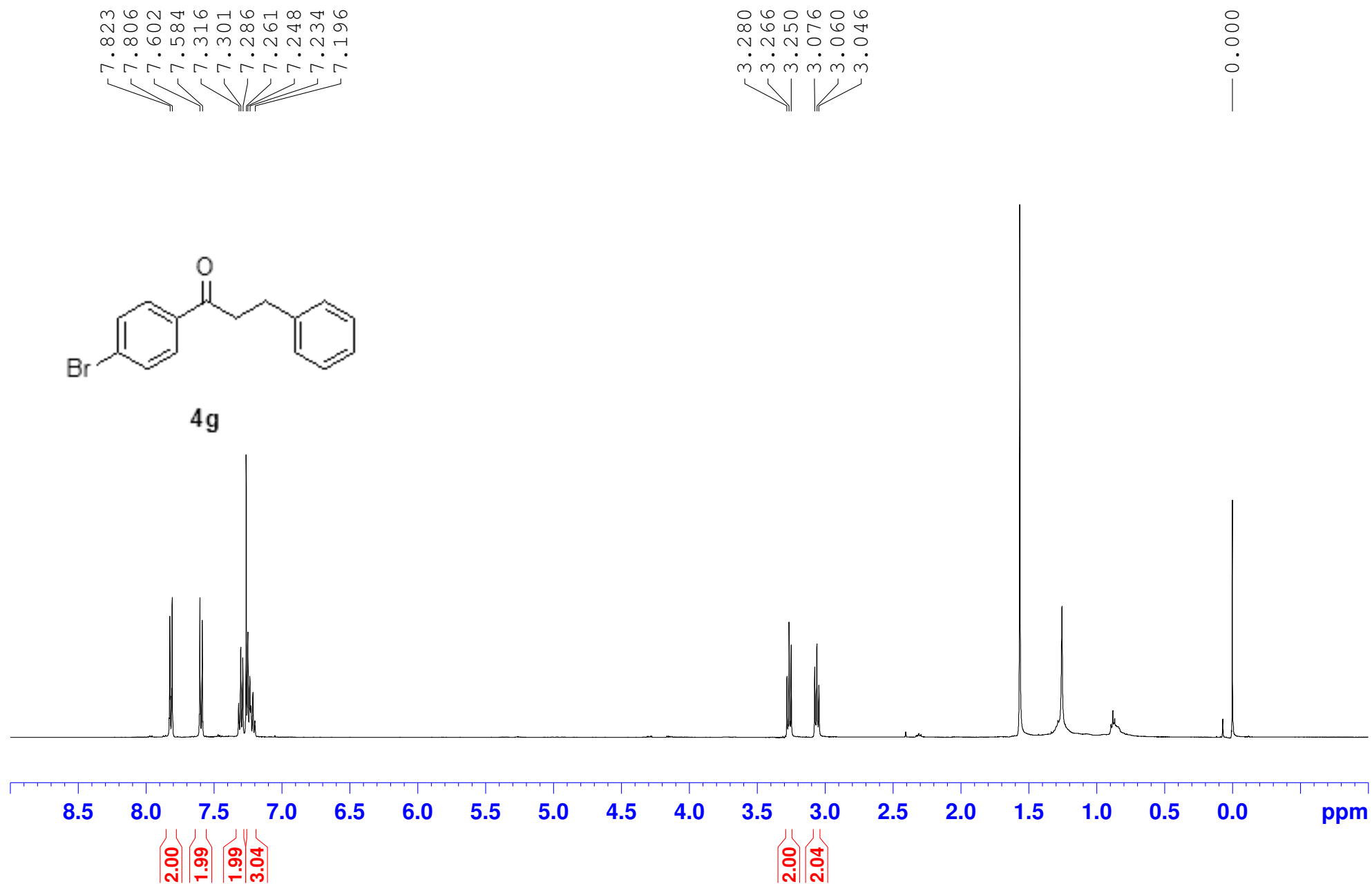
4f



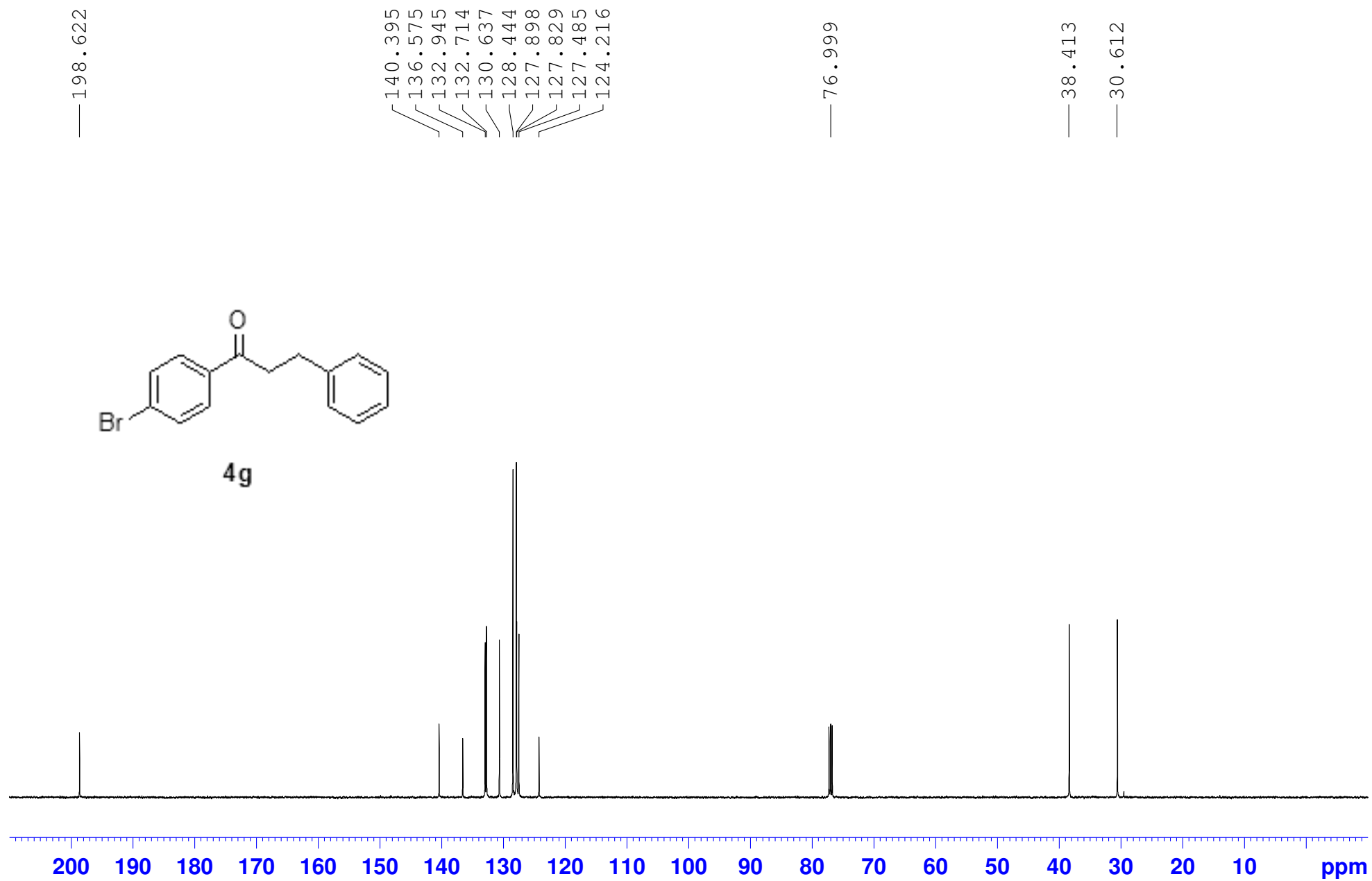
1-(3-Bromophenyl)-3-phenylpropan-1-one
C13CPD CDCl3



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



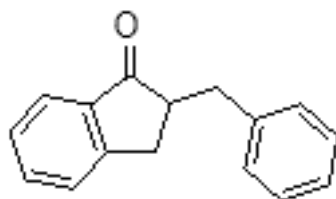
1-(4-Bromophenyl)-3-phenylpropan-1-one
C13CPD CDCl3



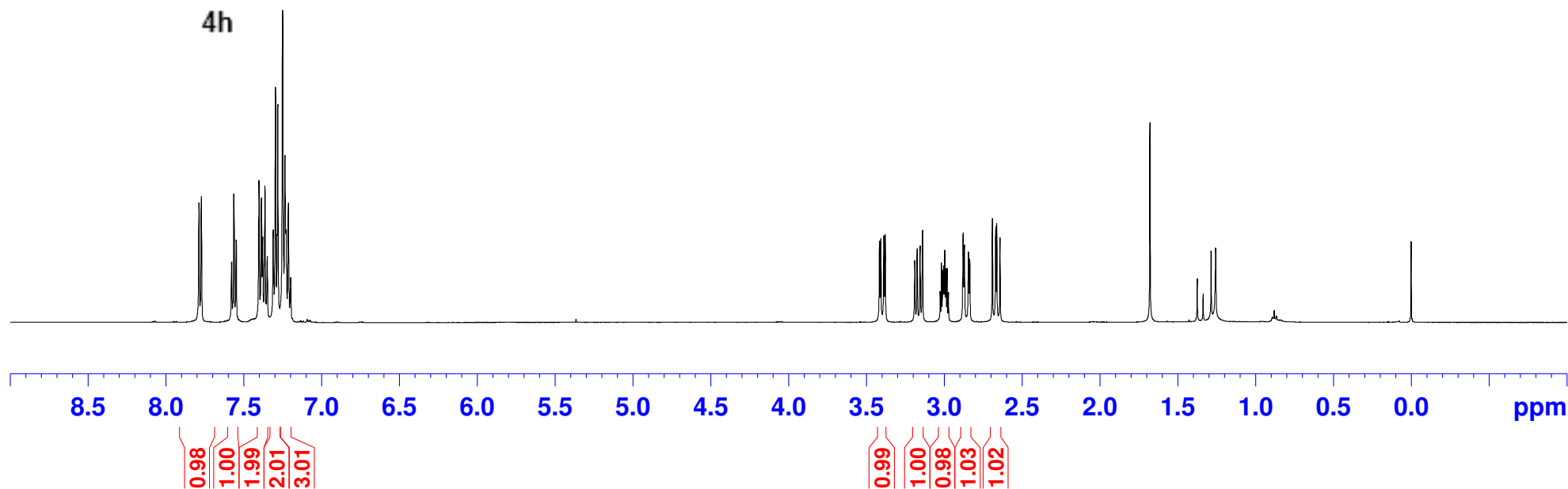
2-Benzyl-indan-1-one
Proton CDCl₃

7.788
7.773
7.580
7.564
7.550
7.402
7.364
7.348
7.311
7.296
7.281
7.250
7.235
7.199

3.416
3.407
3.388
3.379
3.026
2.997
2.973
2.878
2.870
2.844
2.836
2.690
2.669
2.662
2.642



4h



2-Benzyl-indan-1-one
C13CPD-1 CDC13

— 207.776

— 153.596

139.612

136.528

134.778

128.870

128.493

127.396

126.550

126.318

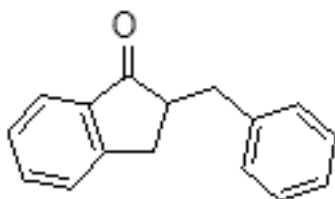
123.997

— 77.001

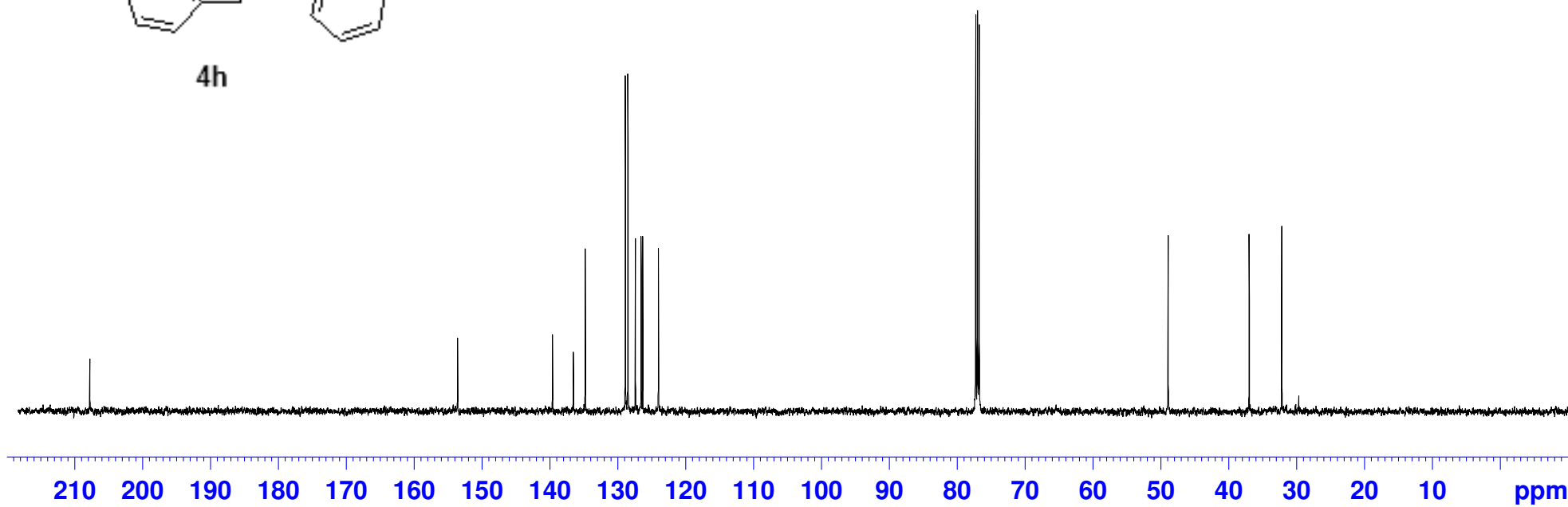
— 48.904

— 36.965

— 32.165



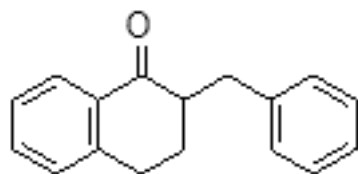
4h



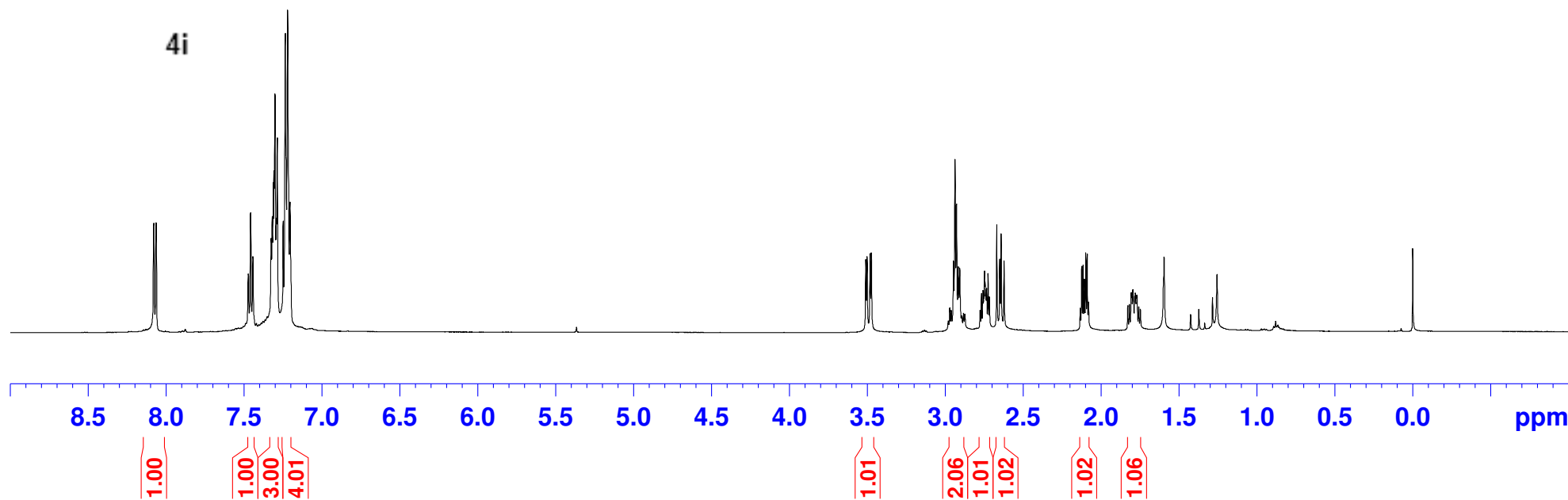
2-Benzyltetralin-1-one
Proton CDCl₃

8.077
8.061
7.471
7.455
7.441
7.323
7.301
7.287
7.249
7.220
7.205

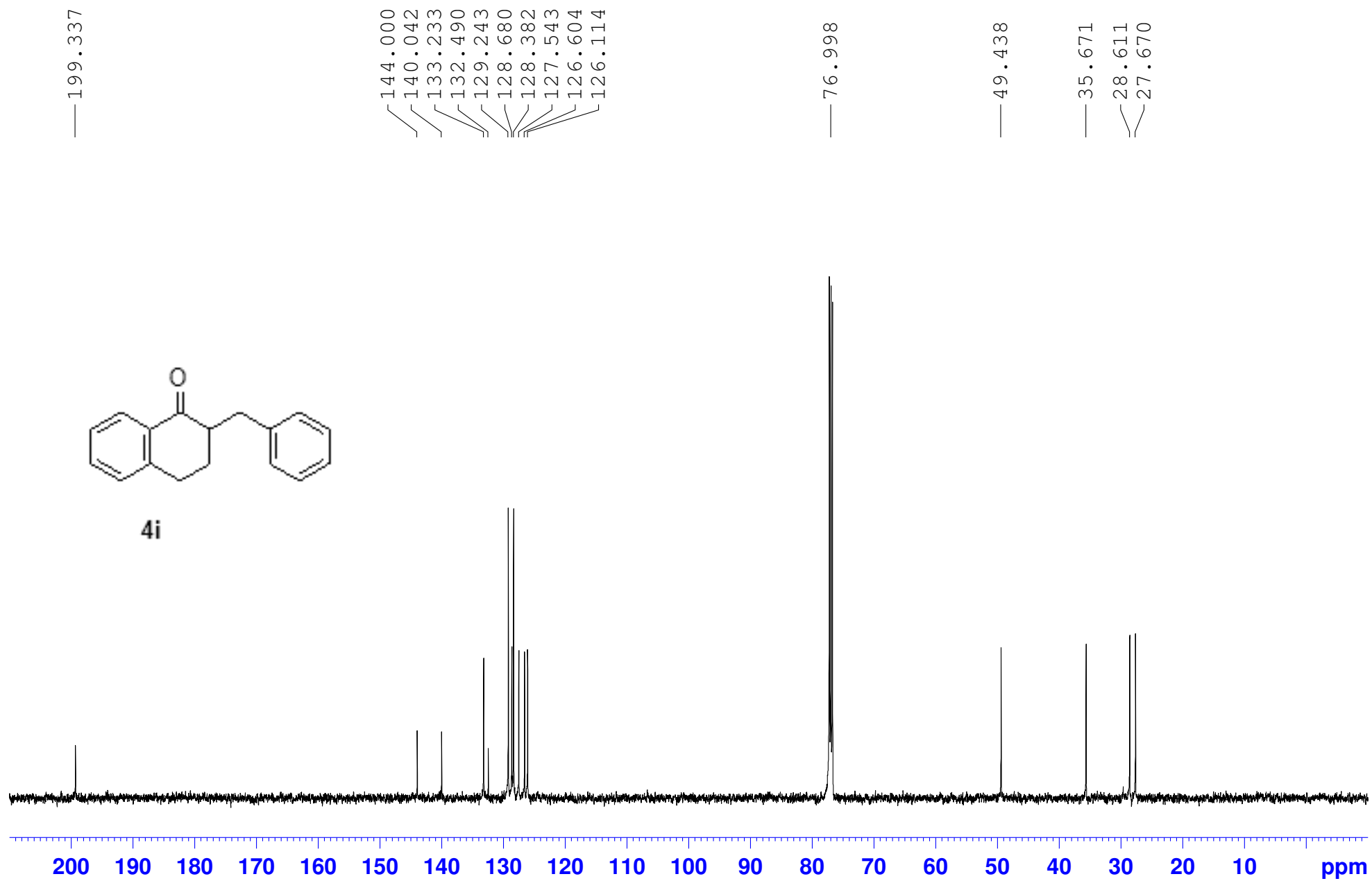
3.510
3.501
3.482
3.474
2.970
2.937
2.882
2.776
2.748
2.716
2.669
2.650
2.641
2.622
2.133
2.098
2.080
1.828
1.795
1.747



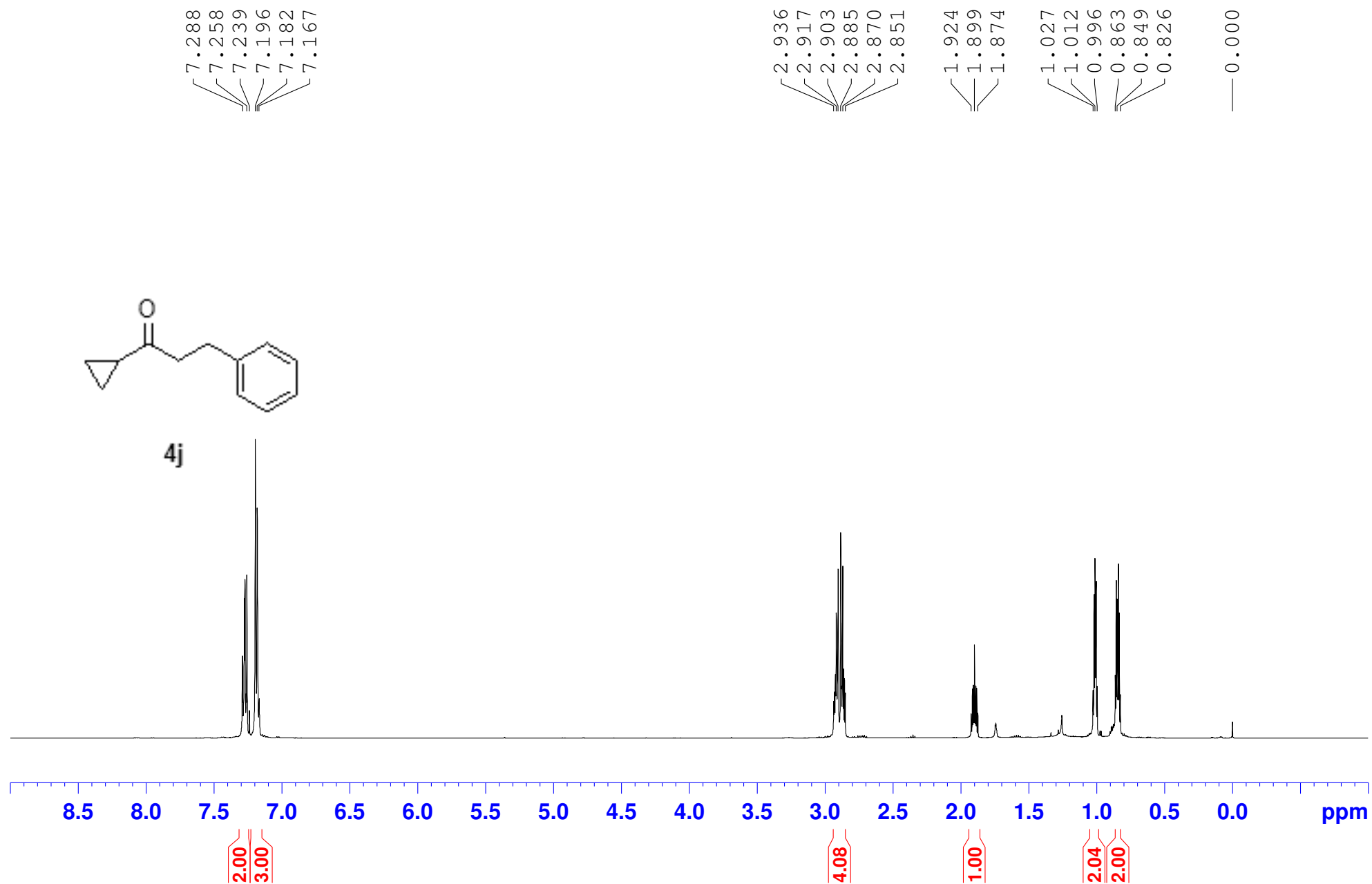
4i



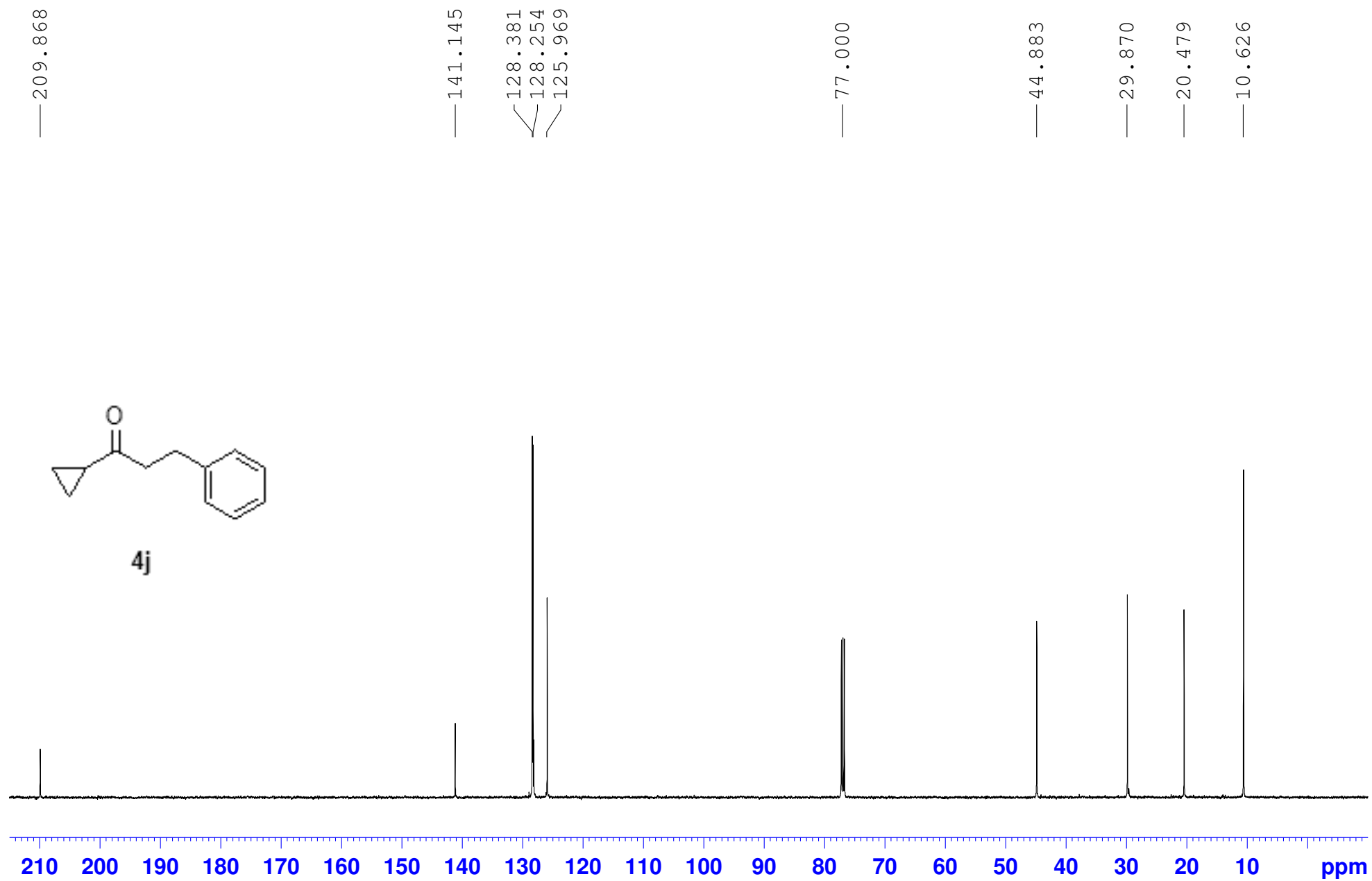
2-Benzyltetralin-1-one
C13CPD-1 CDC13



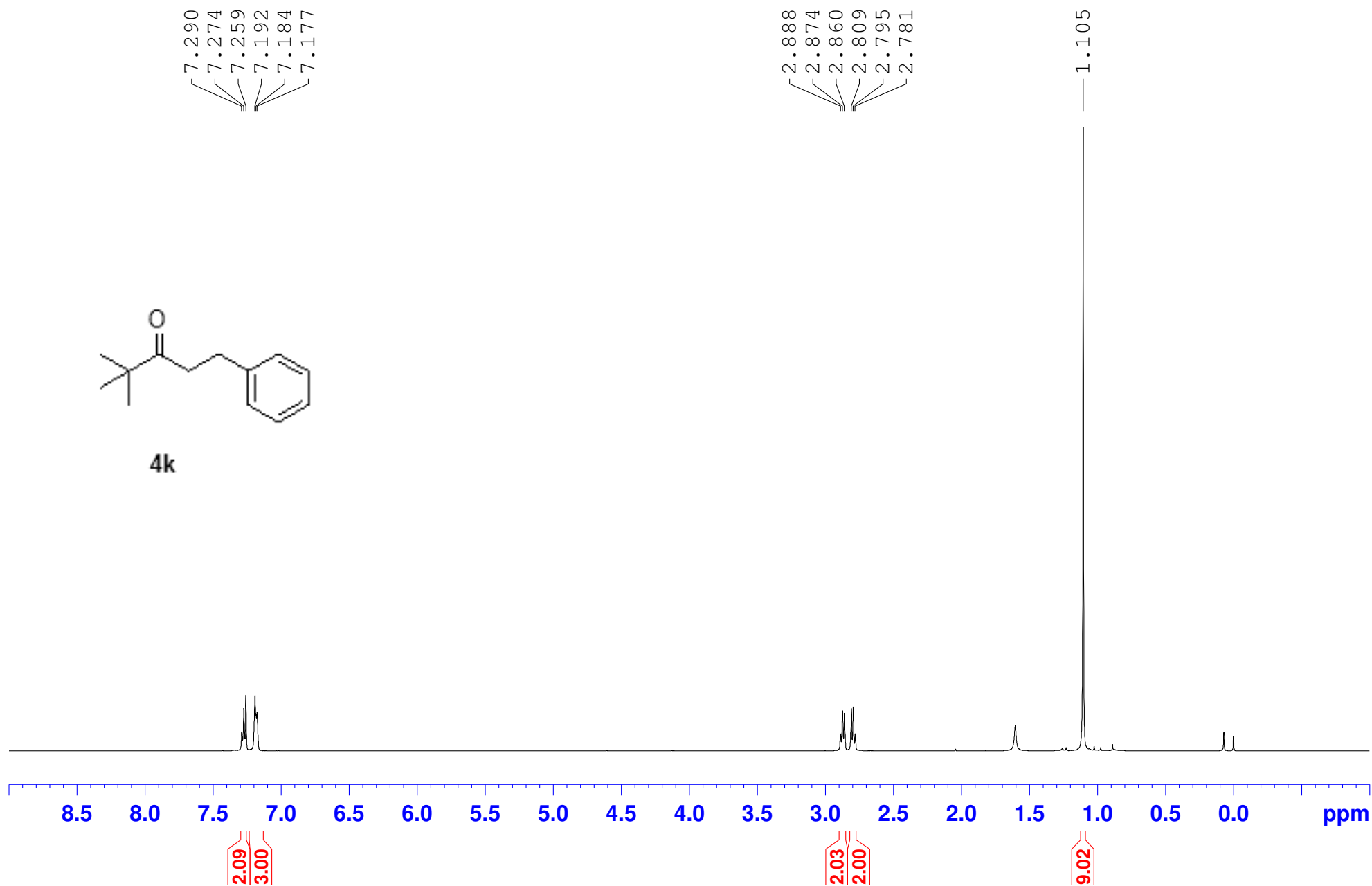
1-Cyclopropyl-3-phenylpropan-1-one
Proton CDCl₃



1-Cyclopropyl-3-phenylpropan-1-one
C13CPD CDCl3



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



4,4-Dimethyl-1-phenylpentan-3-one
C13CPD CDC13

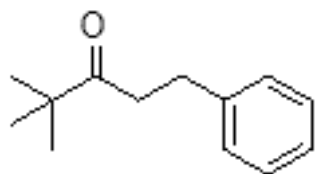
— 214.919

— 141.584

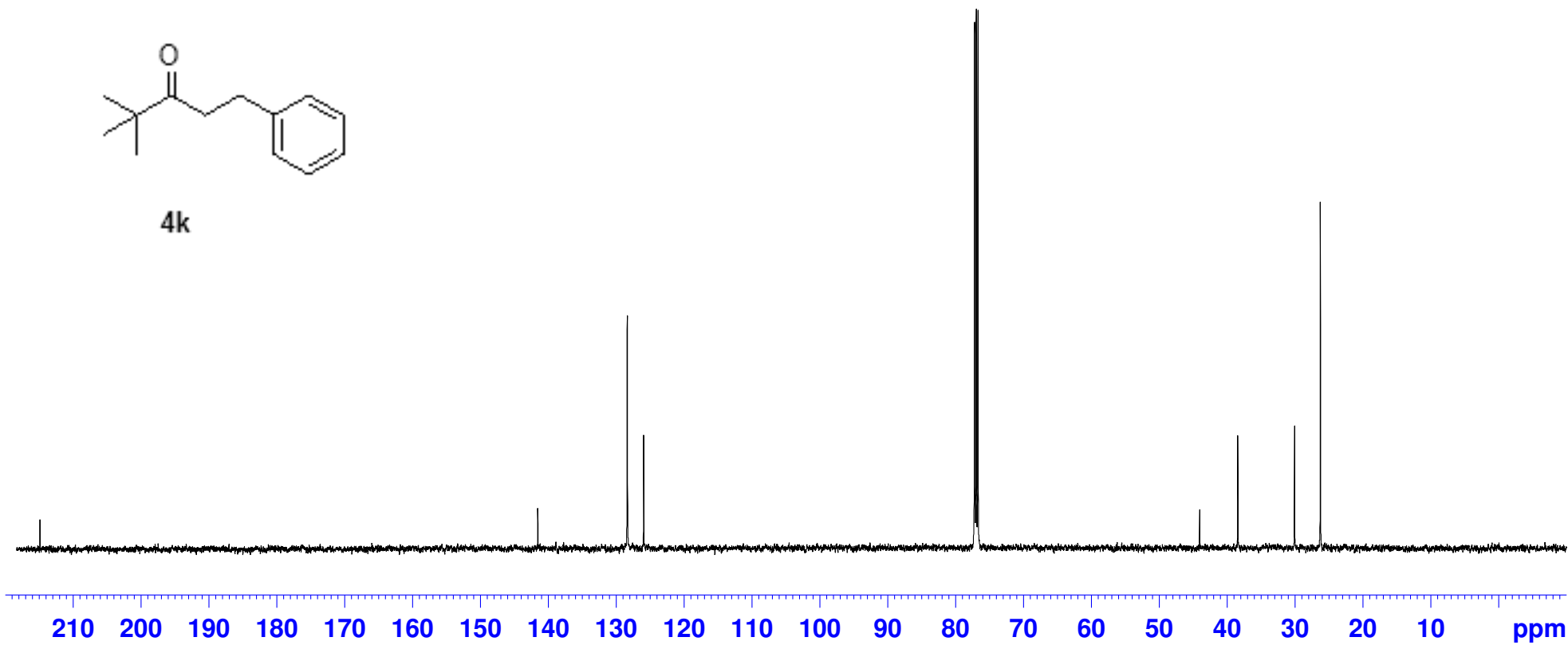
128.415
128.375
125.989

— 77.001

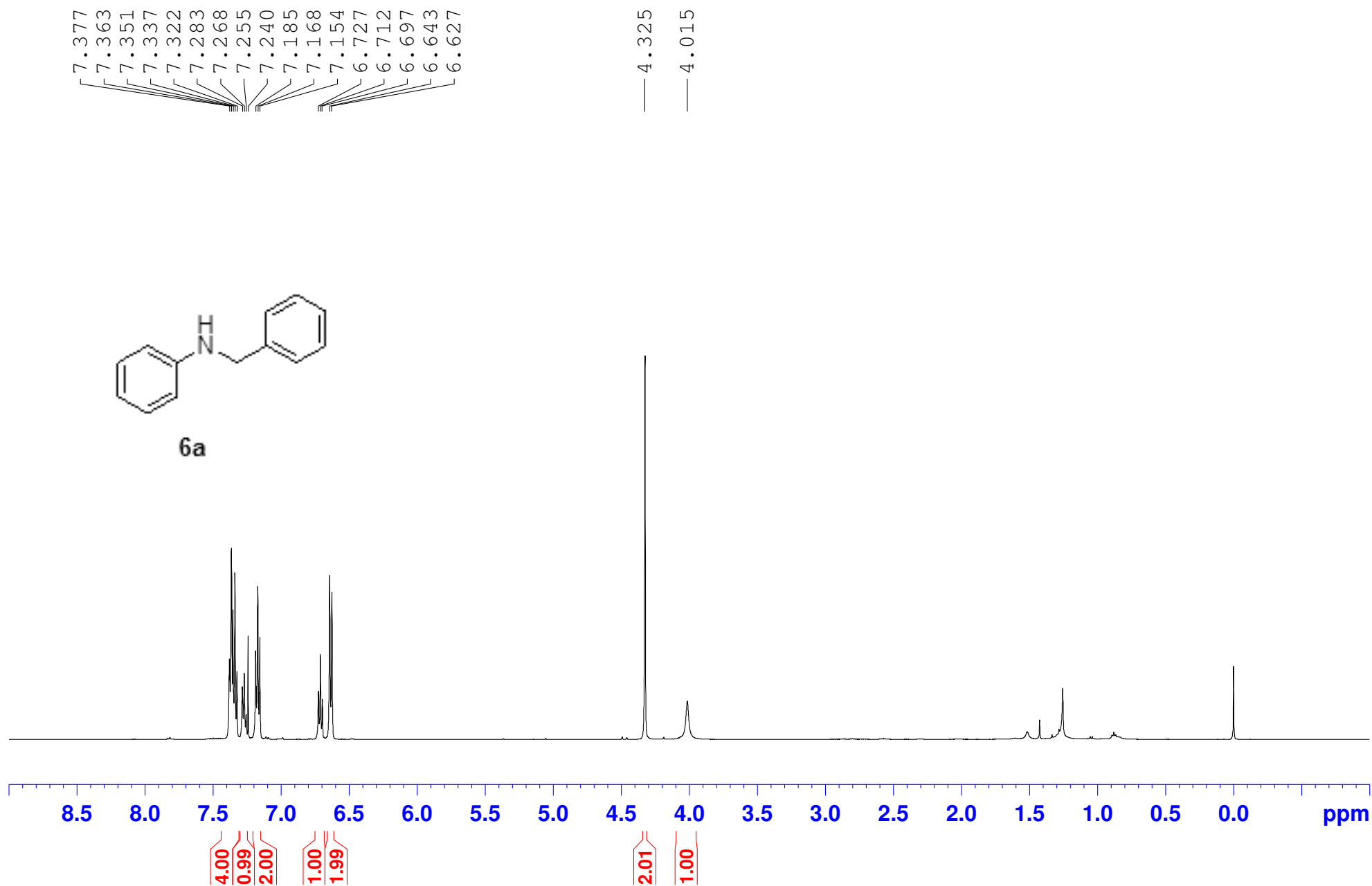
— 44.069
— 38.463
— 30.095
— 26.300



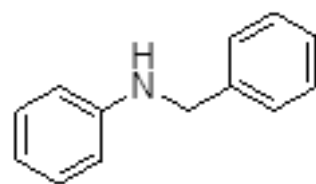
4k



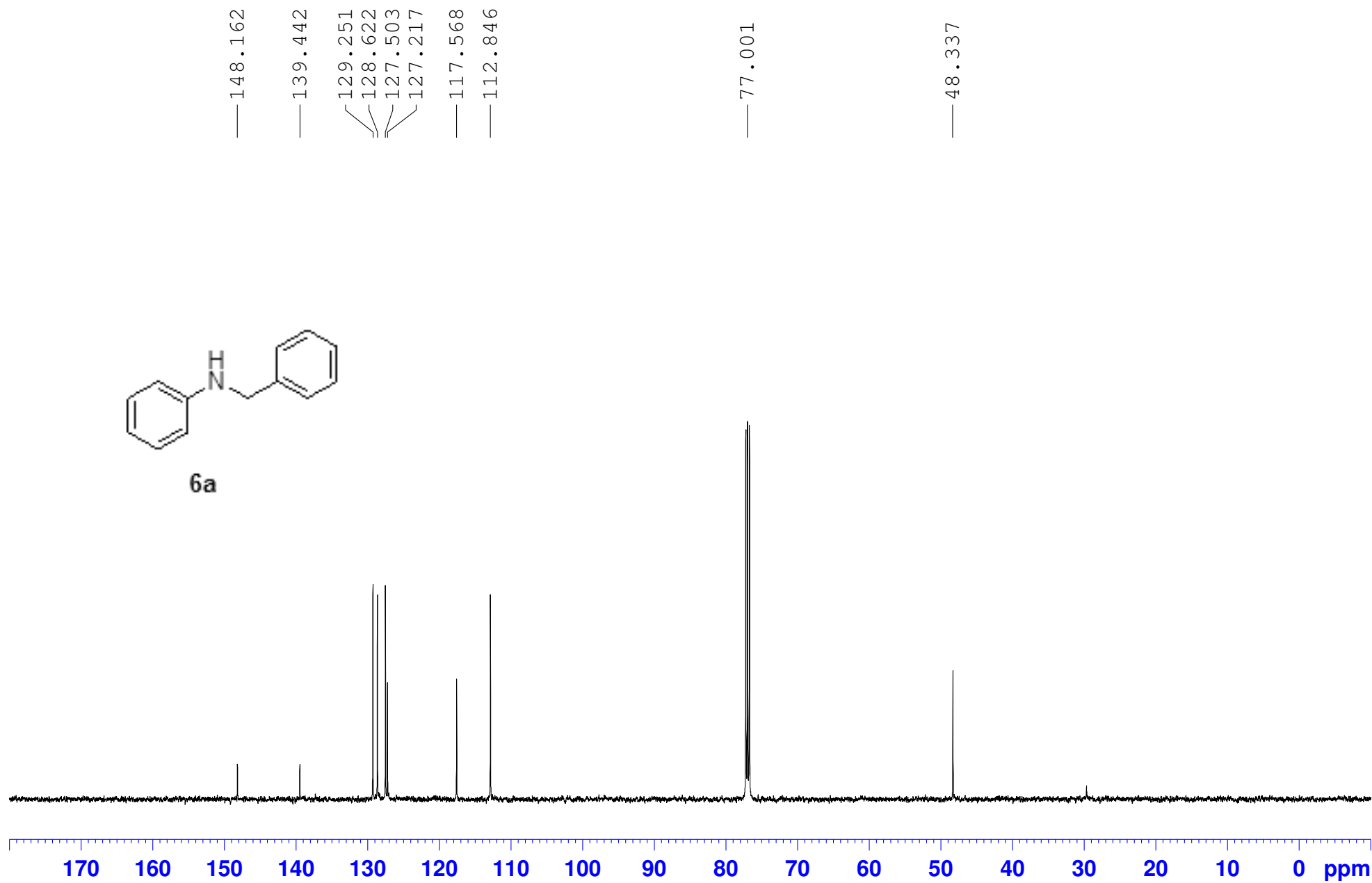
N-benzylaniline
Proton CDCl₃



N-benzylaniline
C13CPD CDC13



6a



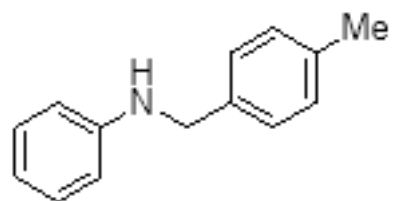
N-(4-methylbenzyl)aniline
Proton CDCl₃

7.266
7.252
7.184
7.168
7.167
7.156
7.153
7.141
6.721
6.707
6.692
6.642
6.626

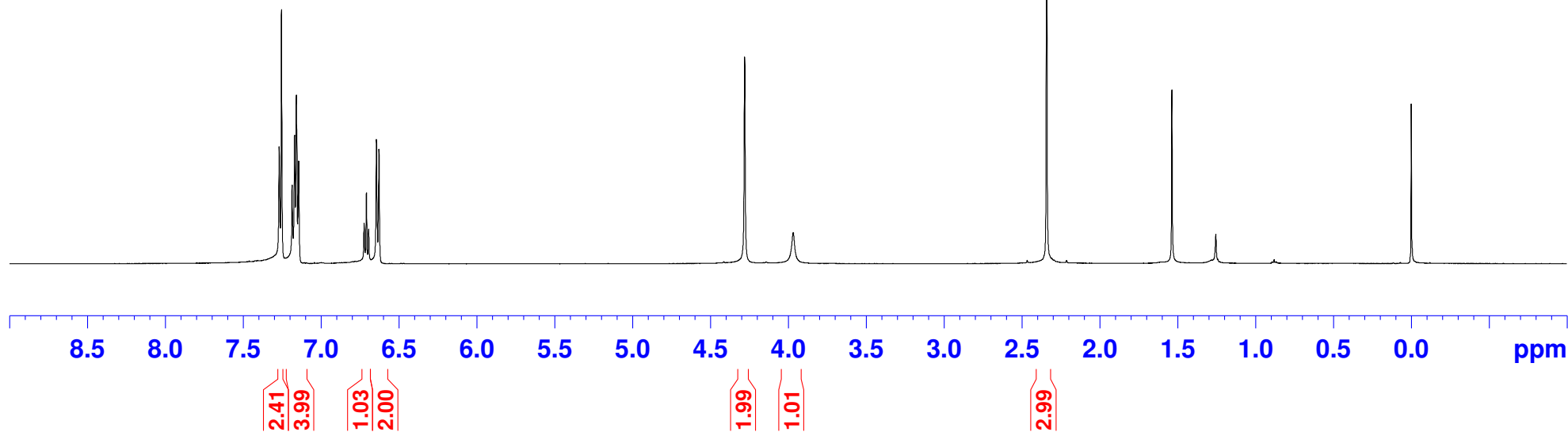
— 4.280

— 3.969

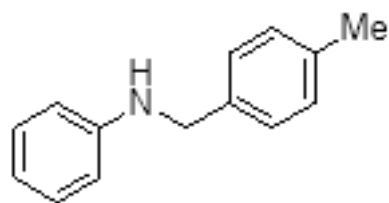
— 2.341



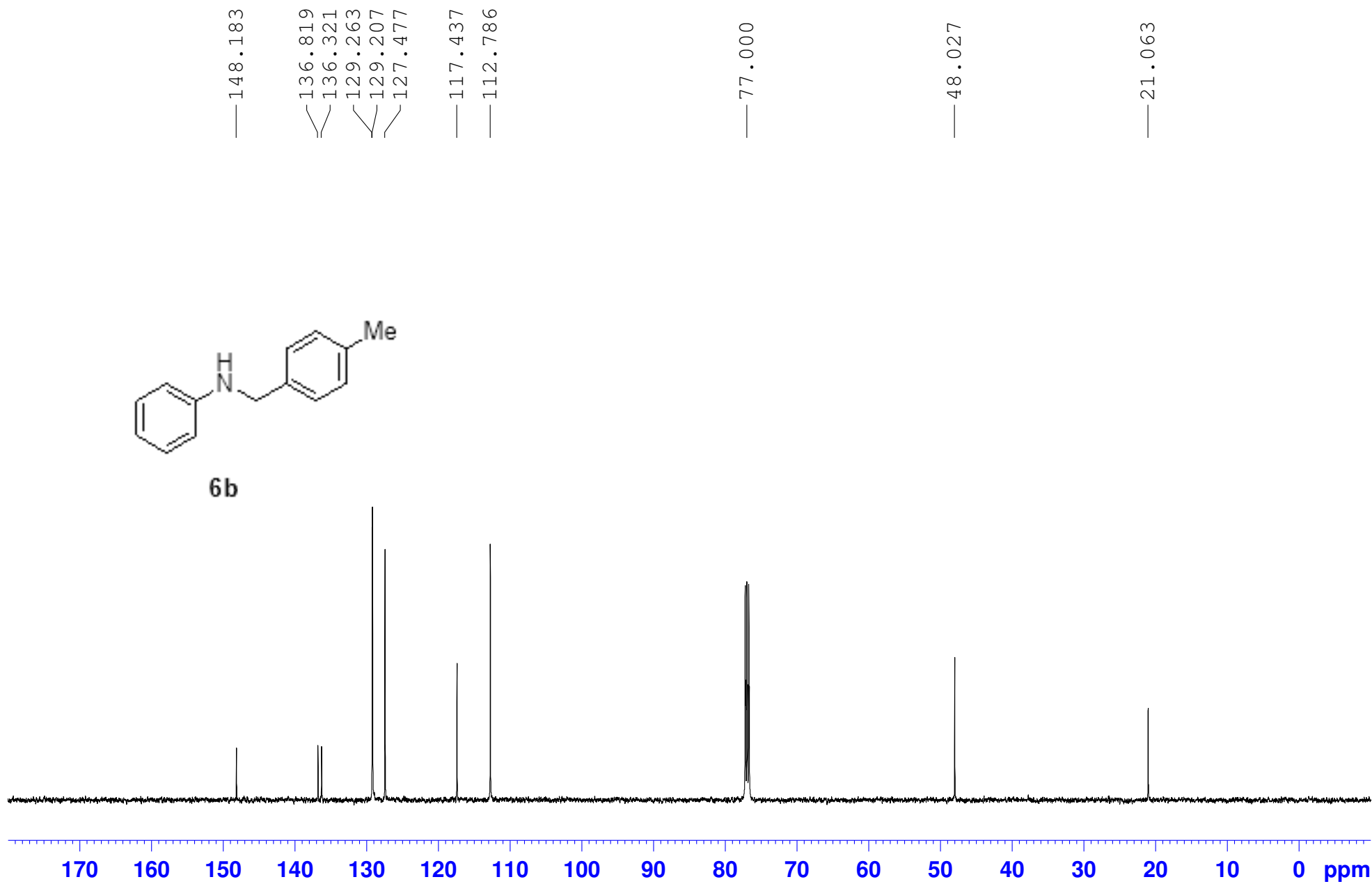
6b



N-(4-methylbenzyl)aniline
C13CPD CDCl3



6b

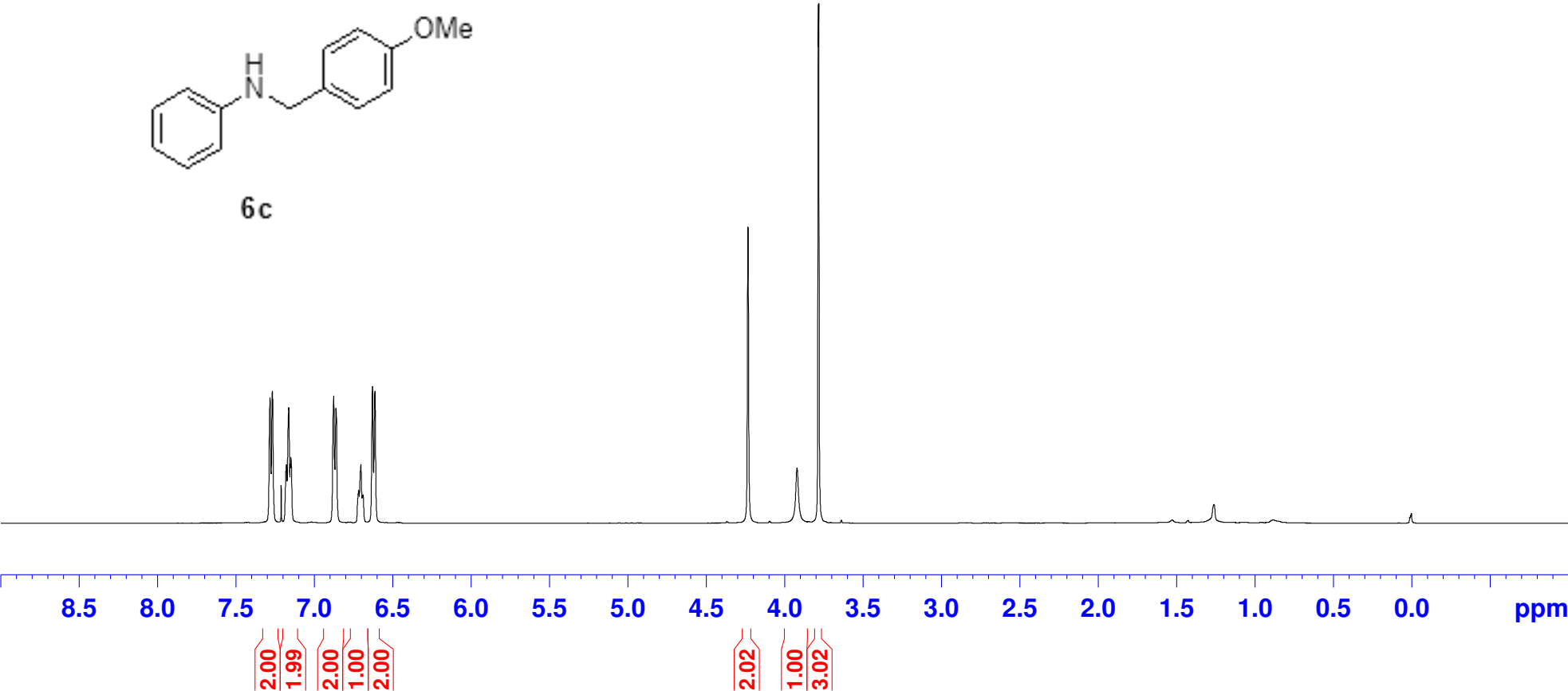
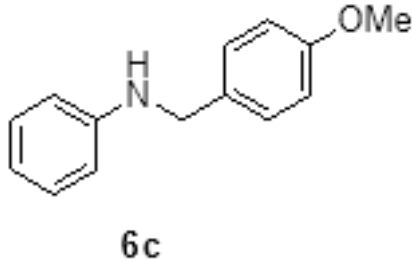


N-(4-methoxybenzyl) aniline
Proton CDCl3

7.283
7.268
7.182
7.164
7.147
6.876
6.862
6.718
6.703
6.689
6.630
6.615

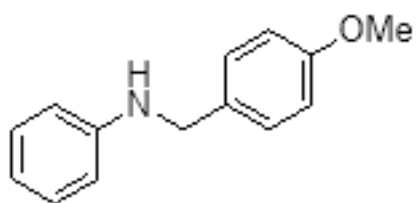
4.234
3.921
3.785

0.000

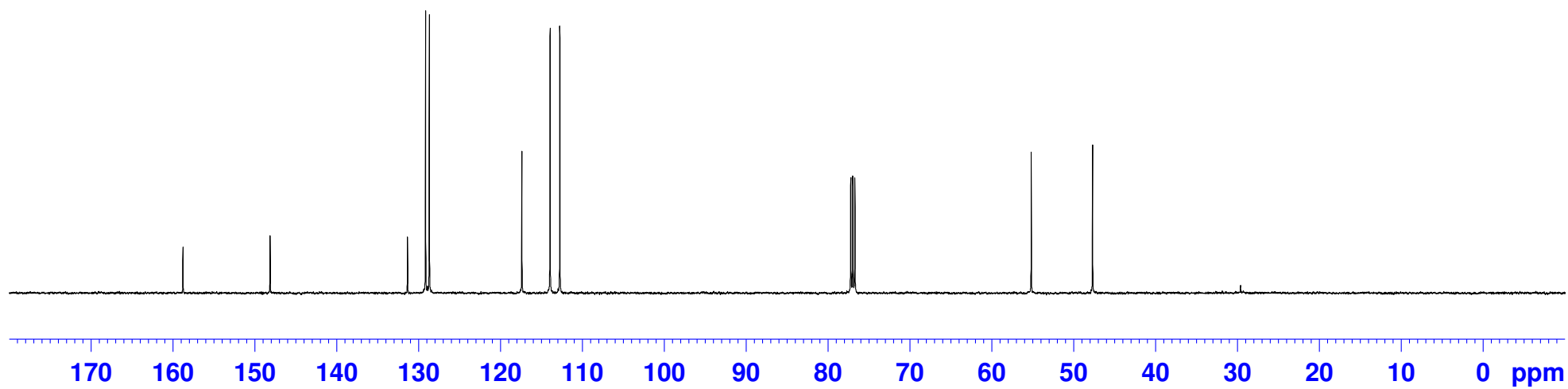


N-(4-methoxybenzyl) aniline
C13CPD CDC13

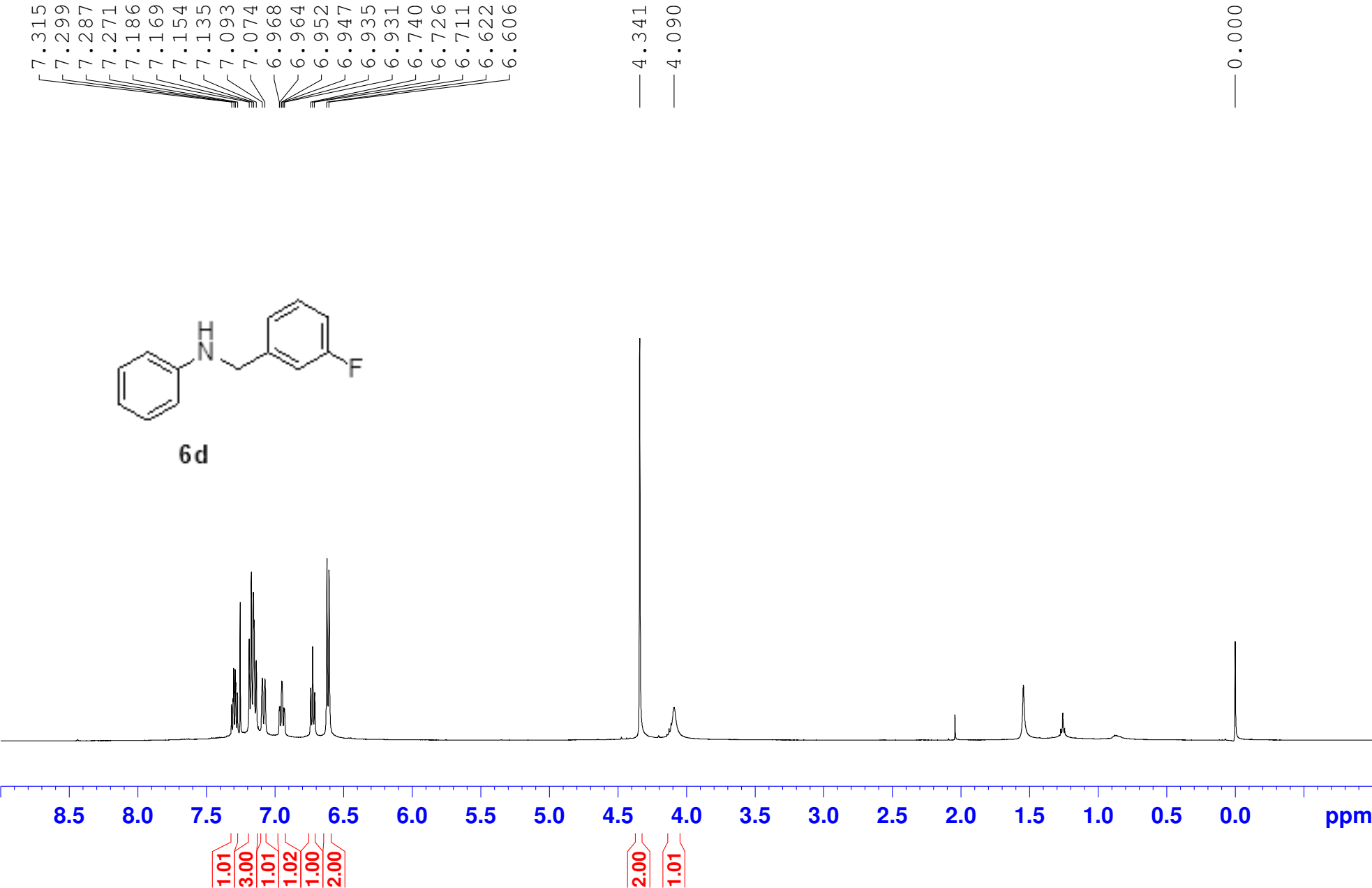
— 158.813
— 148.169
— 131.386
— 129.178
— 128.725
— 117.422
— 113.975
— 112.784
— 77.000
— 55.211
— 47.717



6c



N-(3-fluorobenzyl) aniline
Proton CDCl3



N-(3-fluorobenzyl) aniline
C13CPD CDC13

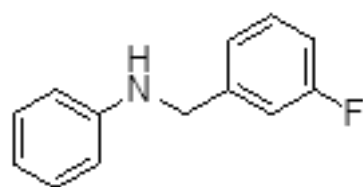
164.073
162.116

147.782
142.350
142.298

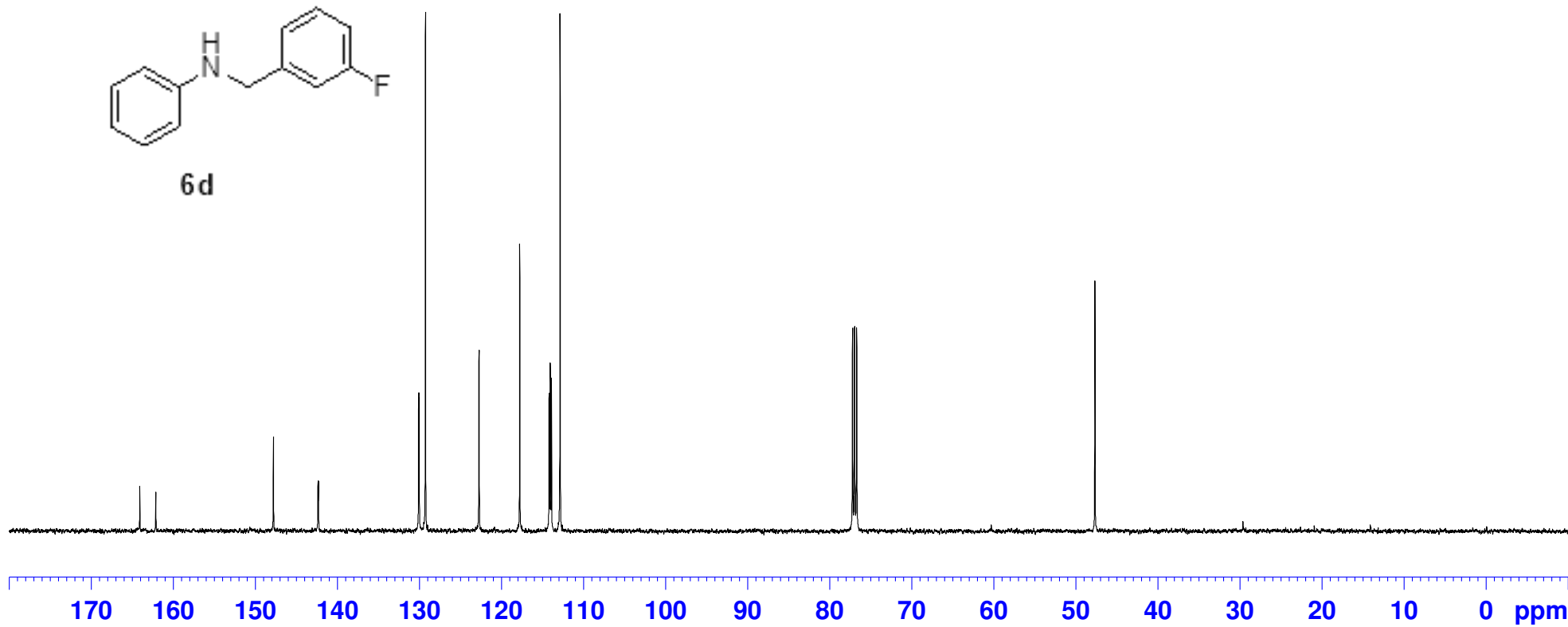
130.077
130.013
129.249
122.712
117.759
114.180
114.055
114.009
113.887
112.842

77.000

47.706



6d

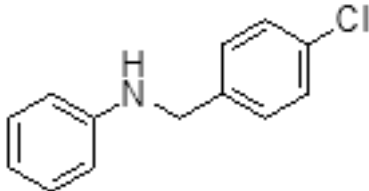


N-(4-chlorobenzyl) aniline
Proton CDCl3

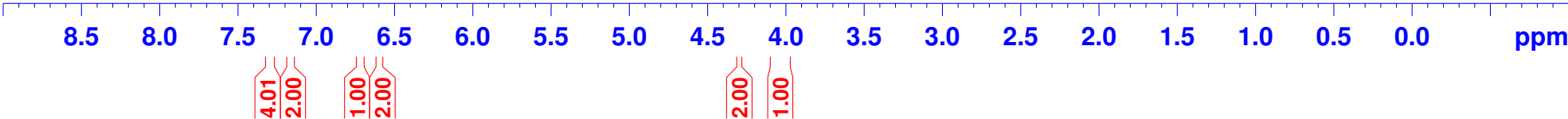
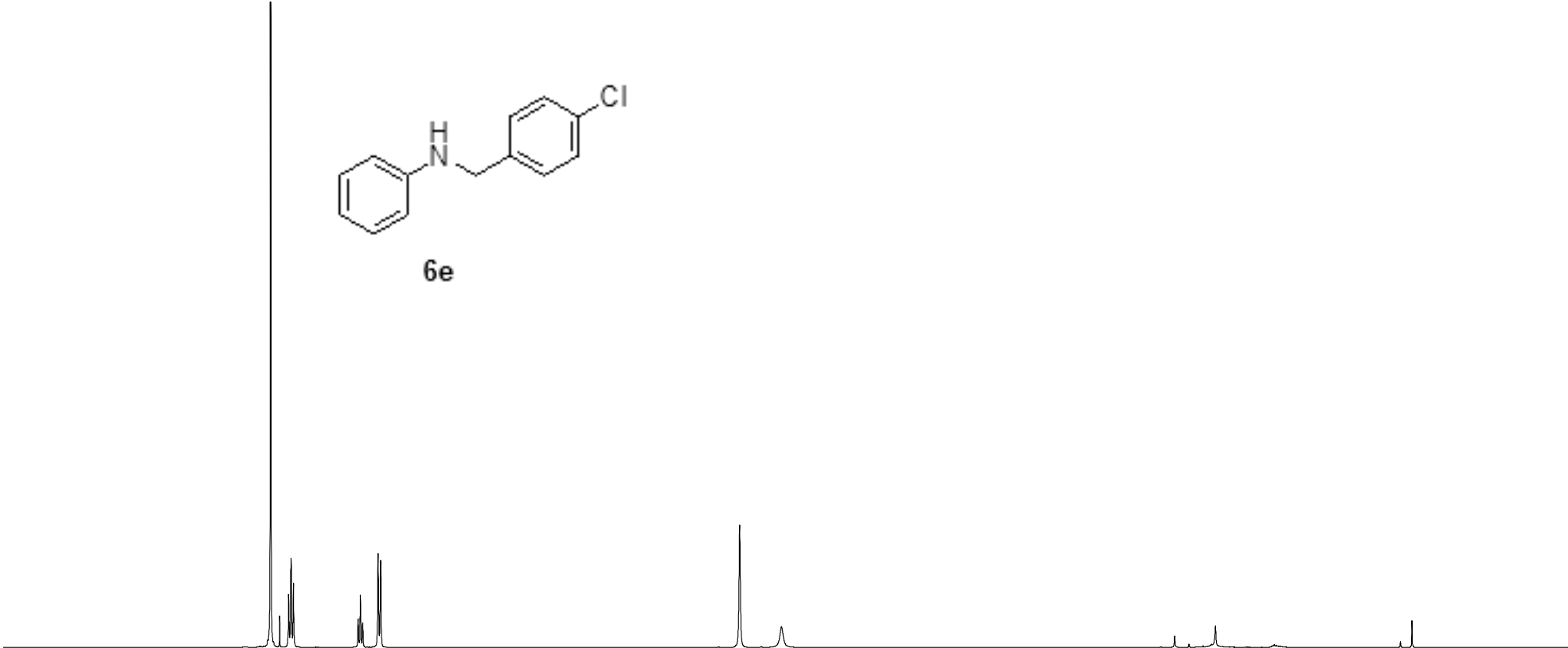
7.290
7.177
7.160
7.145
6.733
6.718
6.703
6.604
6.589

4.295
4.027

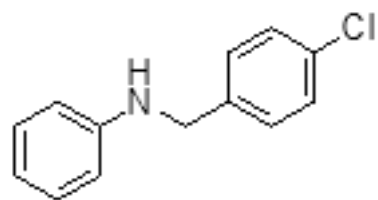
0.000



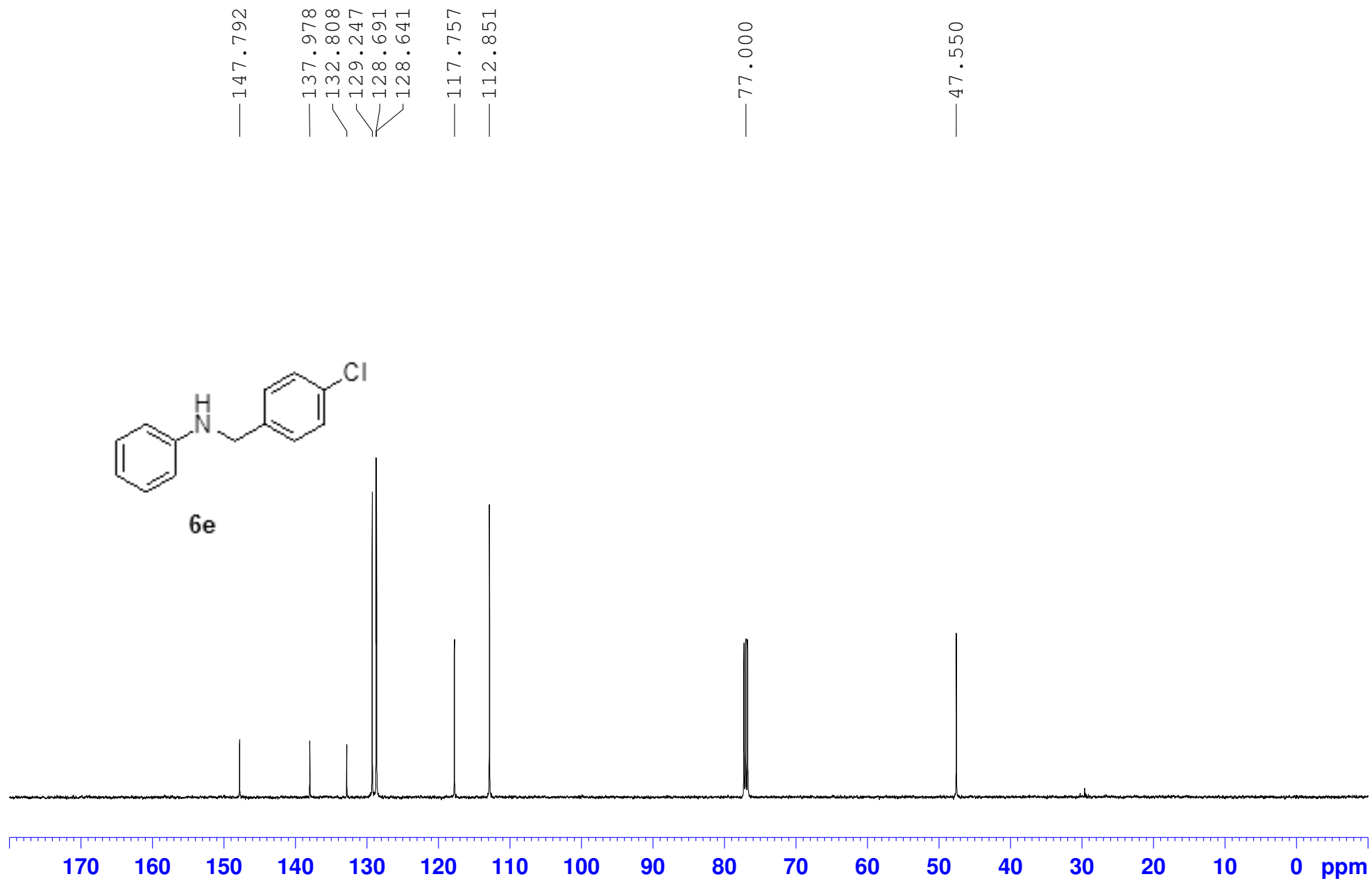
6e



N-(4-chlorobenzyl) aniline
C13CPD CDC13



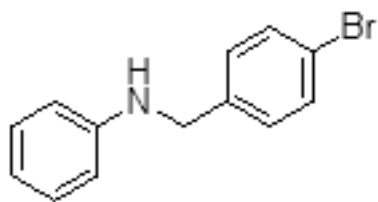
6e



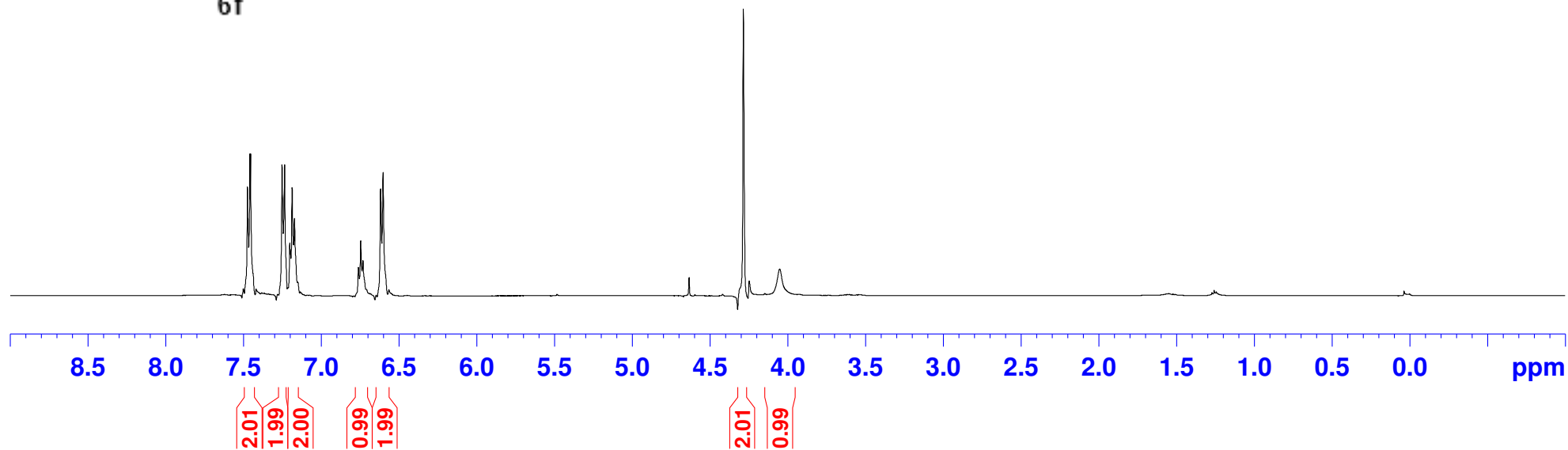
N-(4-Bromobenzyl)aniline
Proton CDCl₃

7.472
7.455
7.253
7.236
7.203
7.187
7.172
6.761
6.747
6.732
6.619
6.603

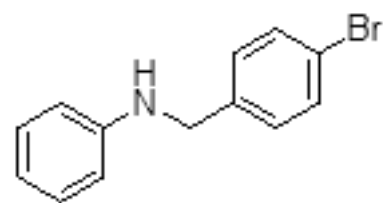
4.286
4.052



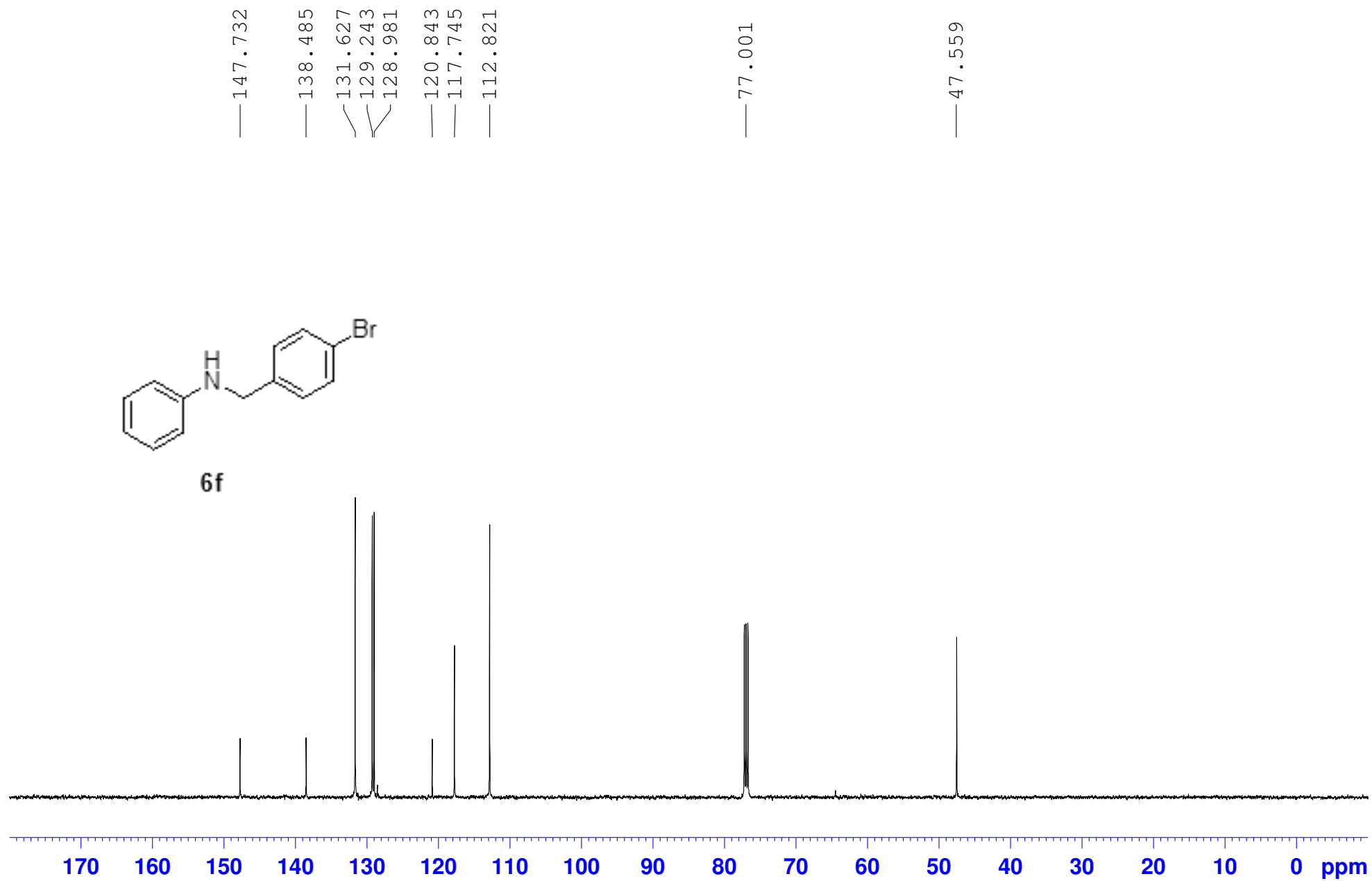
6f



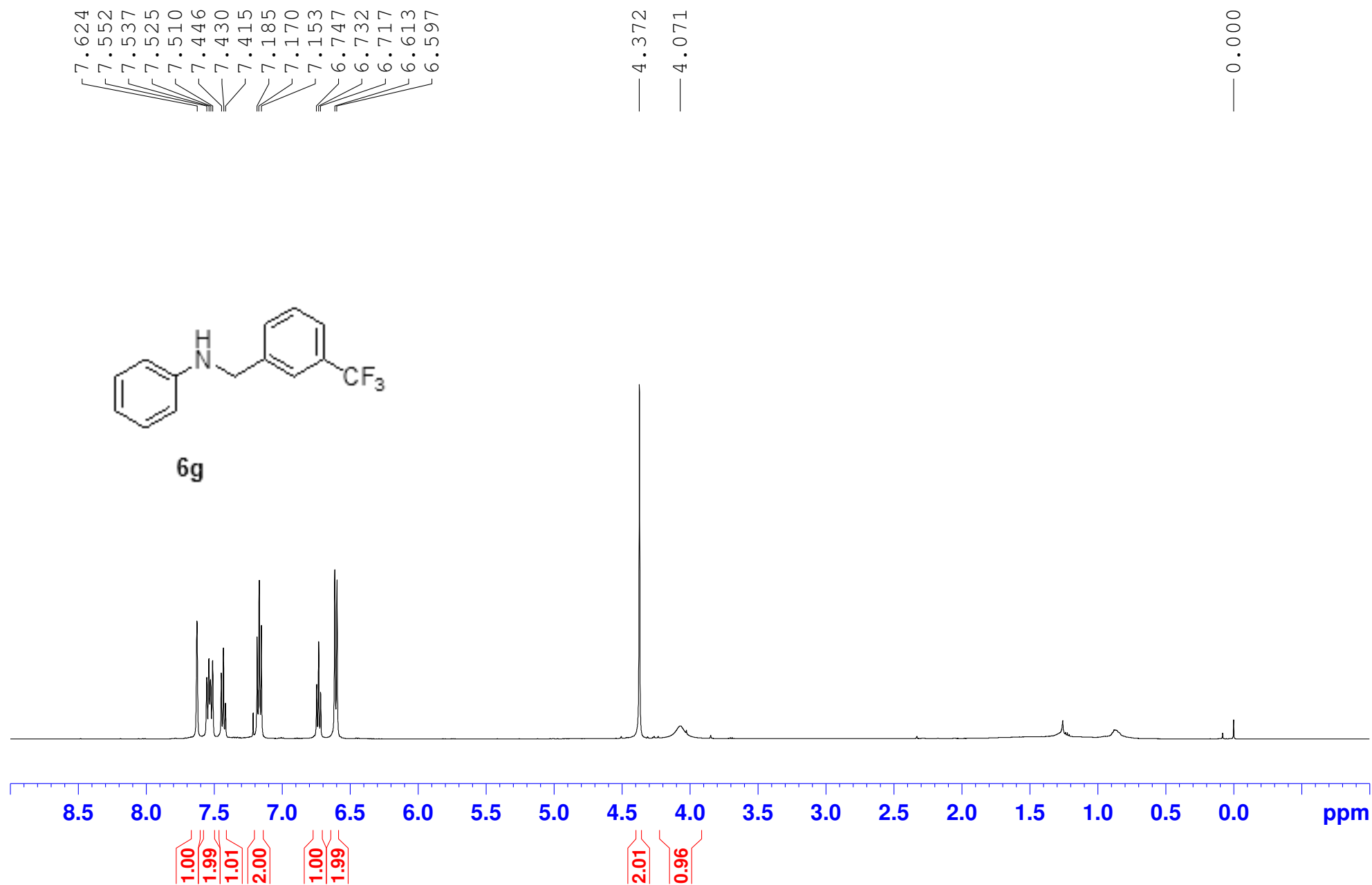
N-(4-Bromobenzyl)aniline
C13CPD CDC13



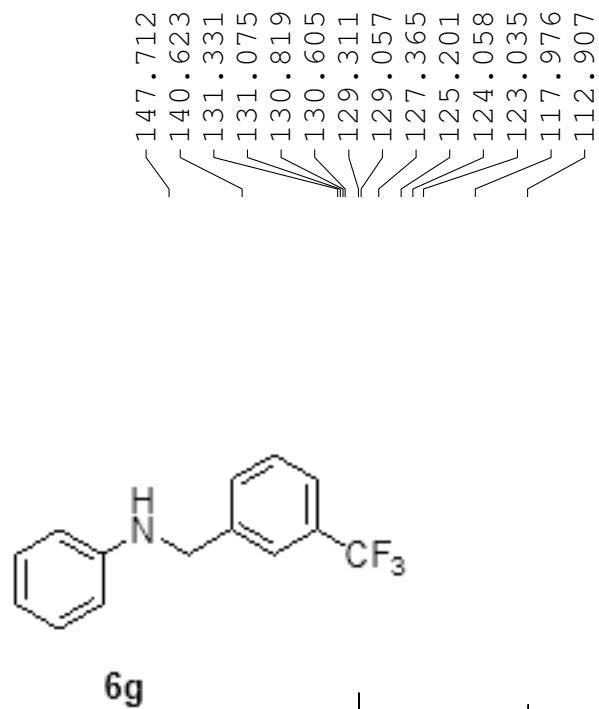
6f



N-(3-Trifluoromethylbenzyl)aniline
Proton CDCl₃

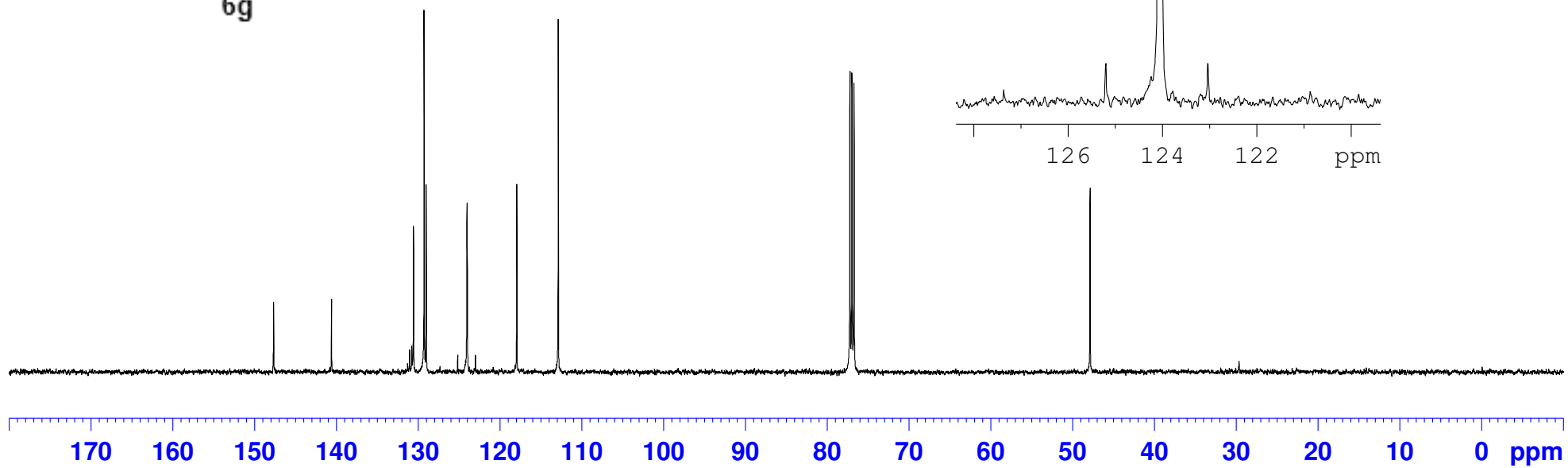
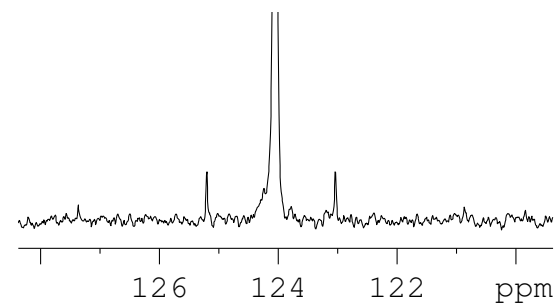
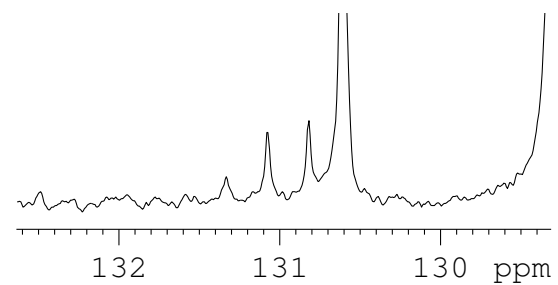


N-(3-Trifluoromethylbenzyl)aniline
C13CPD CDCl3

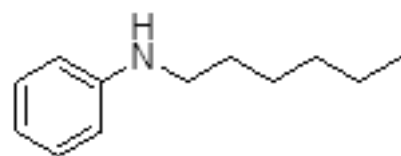


— 76.999

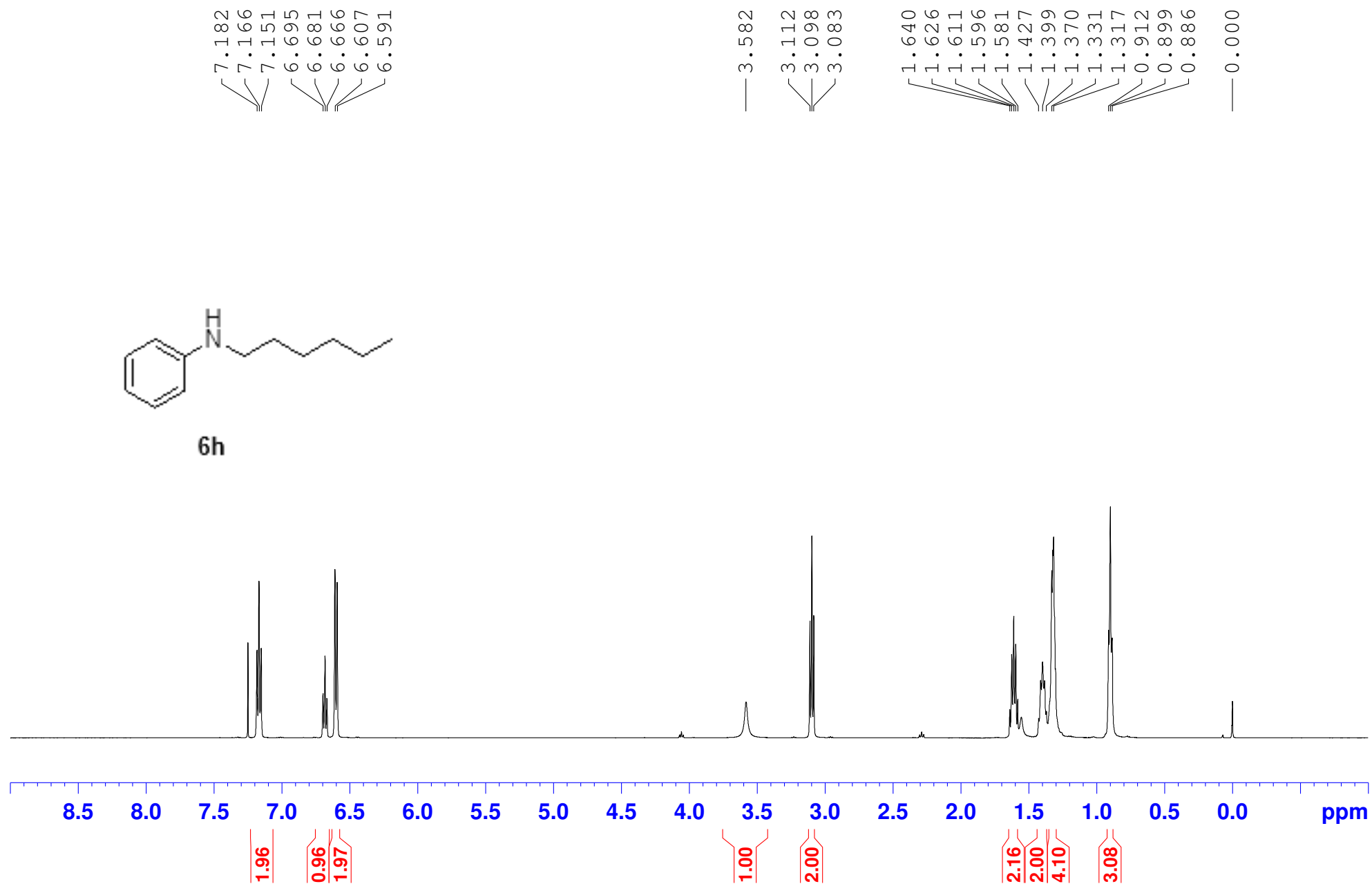
— 47.891



N-hexylaniline
Proton CDCl₃

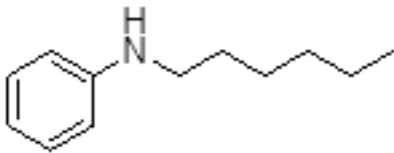


6h

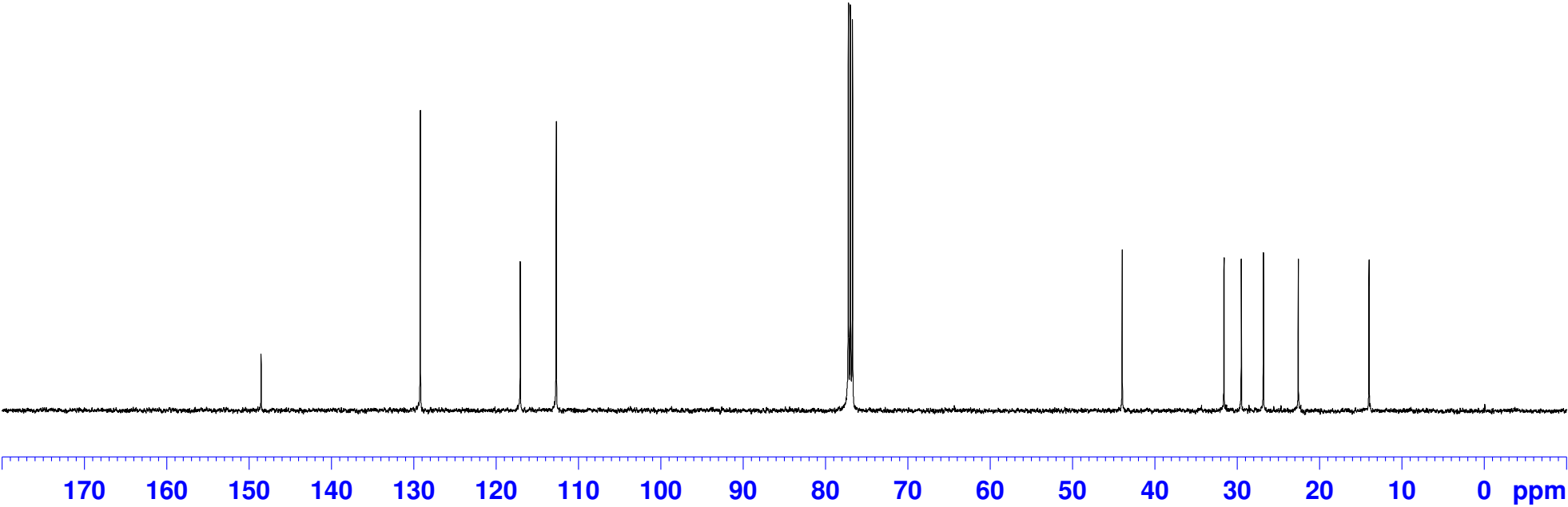


N-hexylaniline
C13CPD CDC13

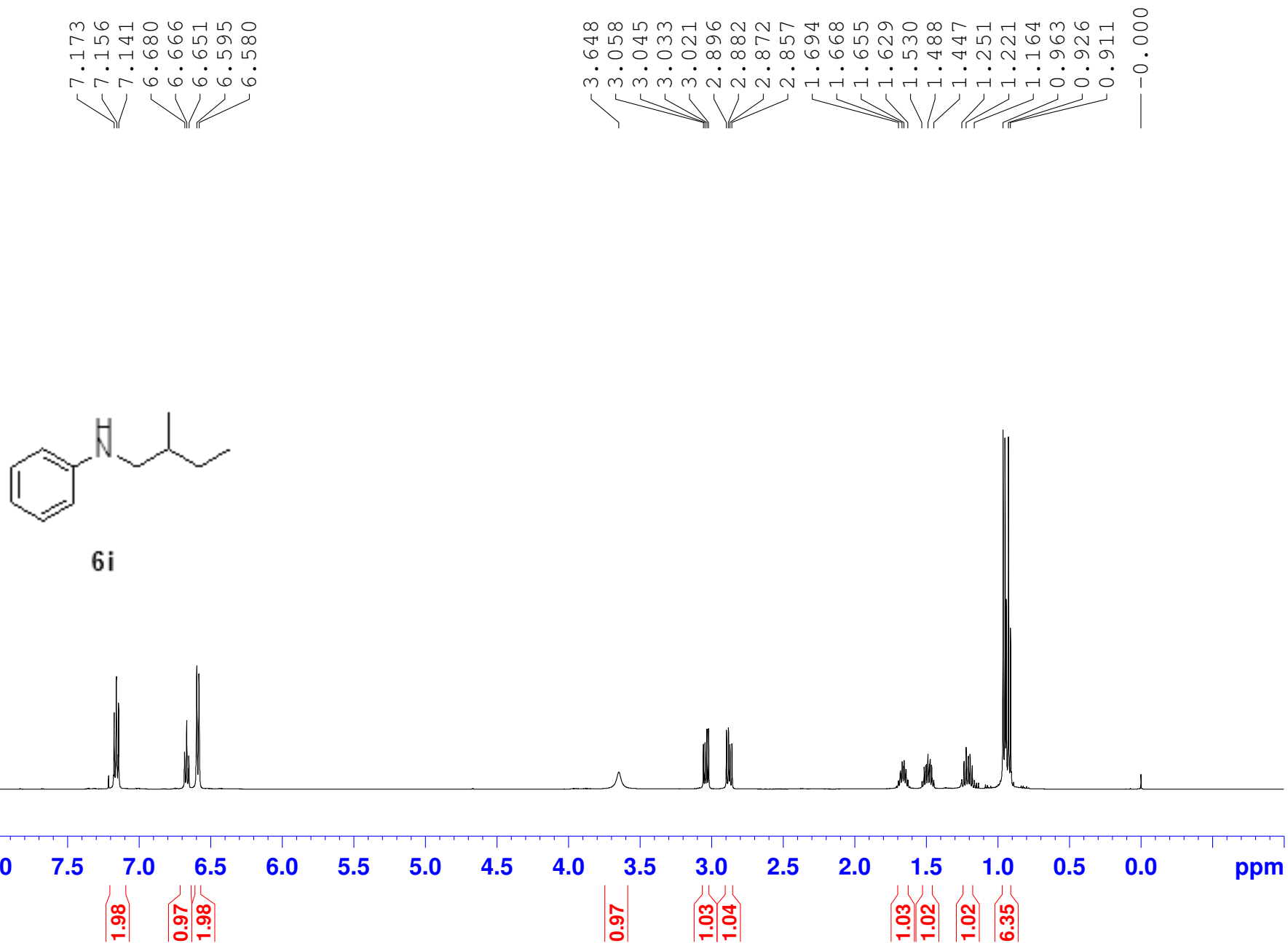
—148.518
—129.187
—117.049
—112.669
—77.000
—43.992
—31.633
—29.532
—26.839
—22.608
—14.019



6h

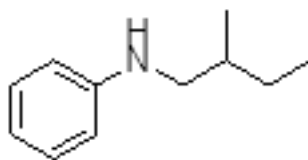


N-(2-methylbutyl)aniline
Proton CDCl₃

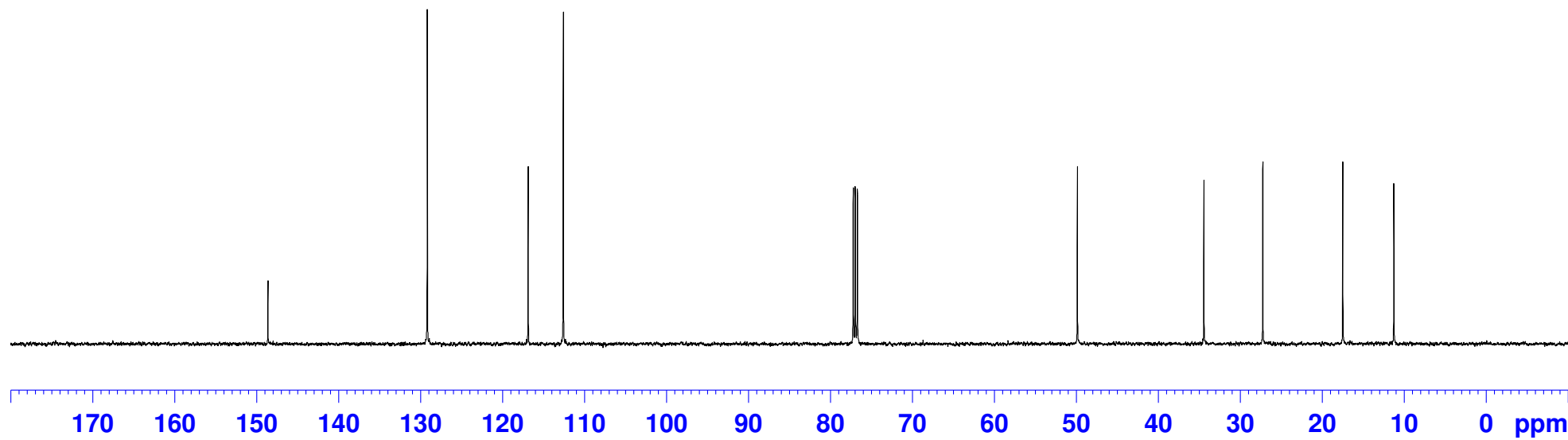


N-(2-methylbutyl)aniline
C13CPD CDCl3

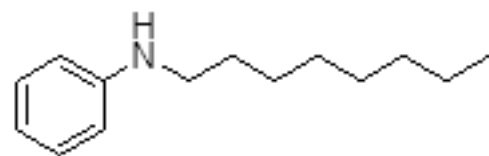
—148.611
—129.171
—116.869
—112.574
—76.999
—49.904
—34.467
—27.281
—17.521
—11.291



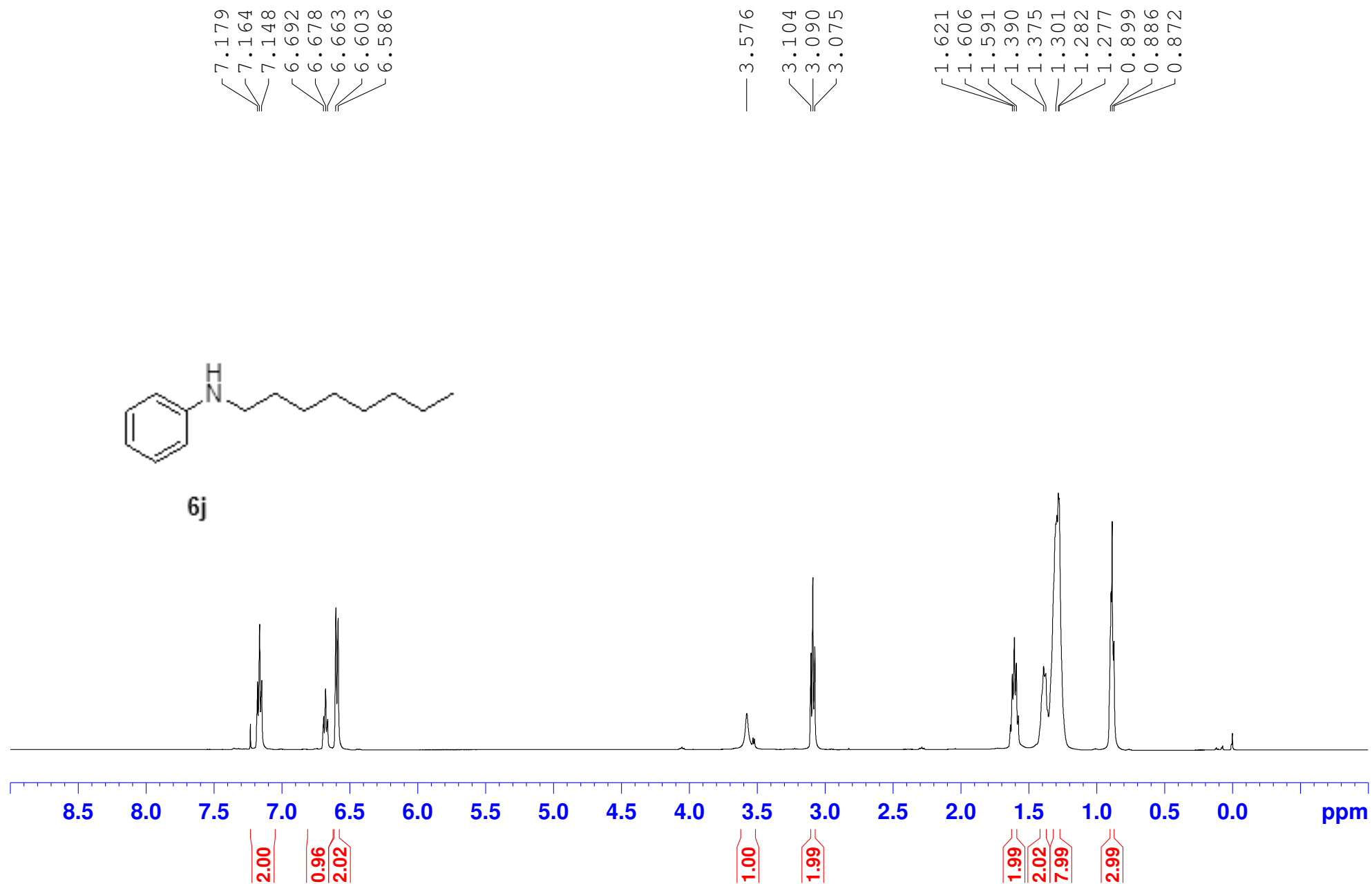
6i



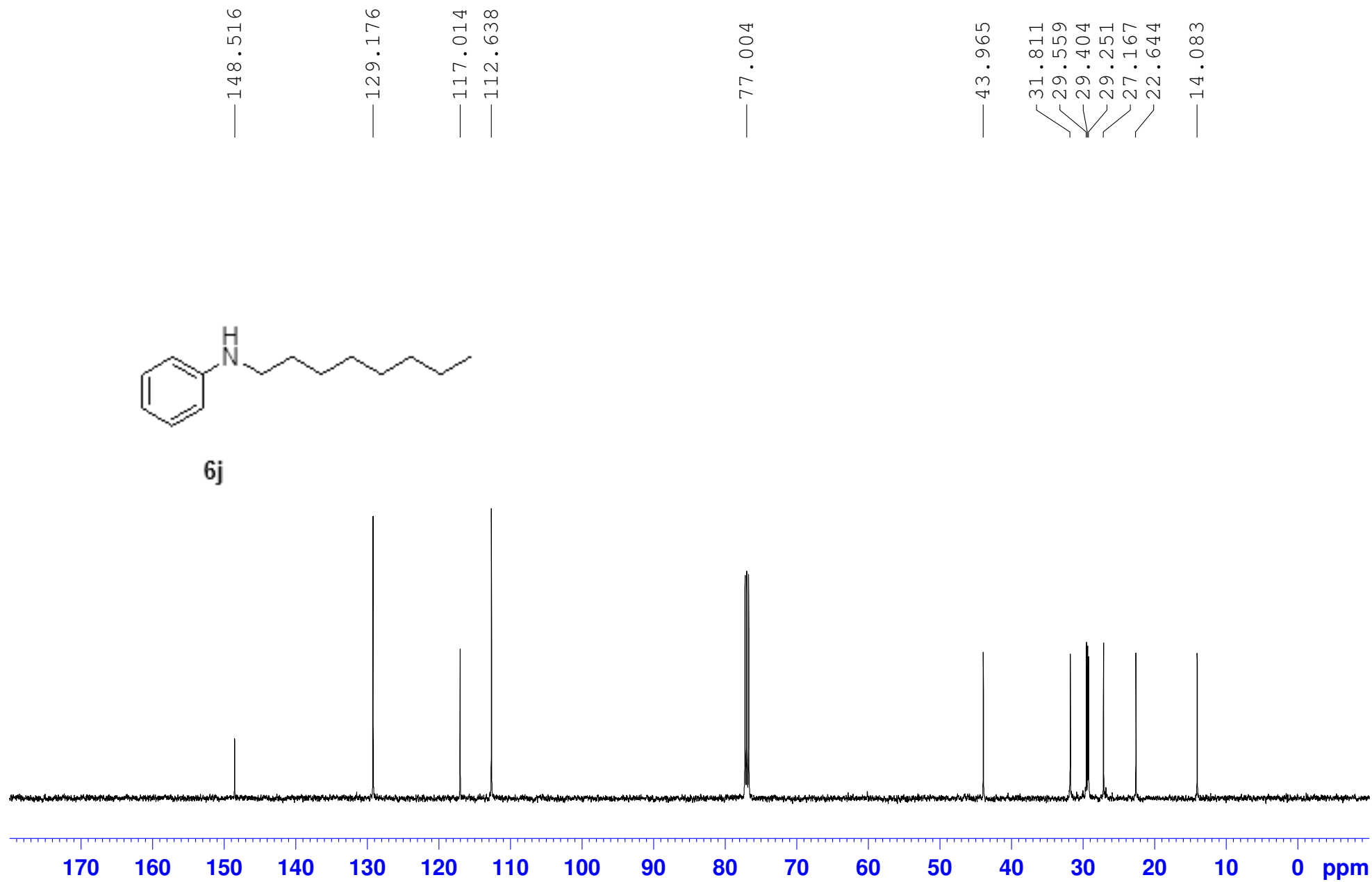
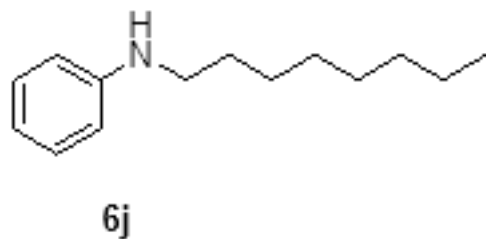
N-octylaniline
Proton CDCl₃



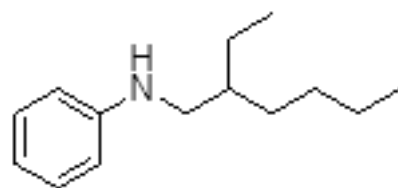
6j



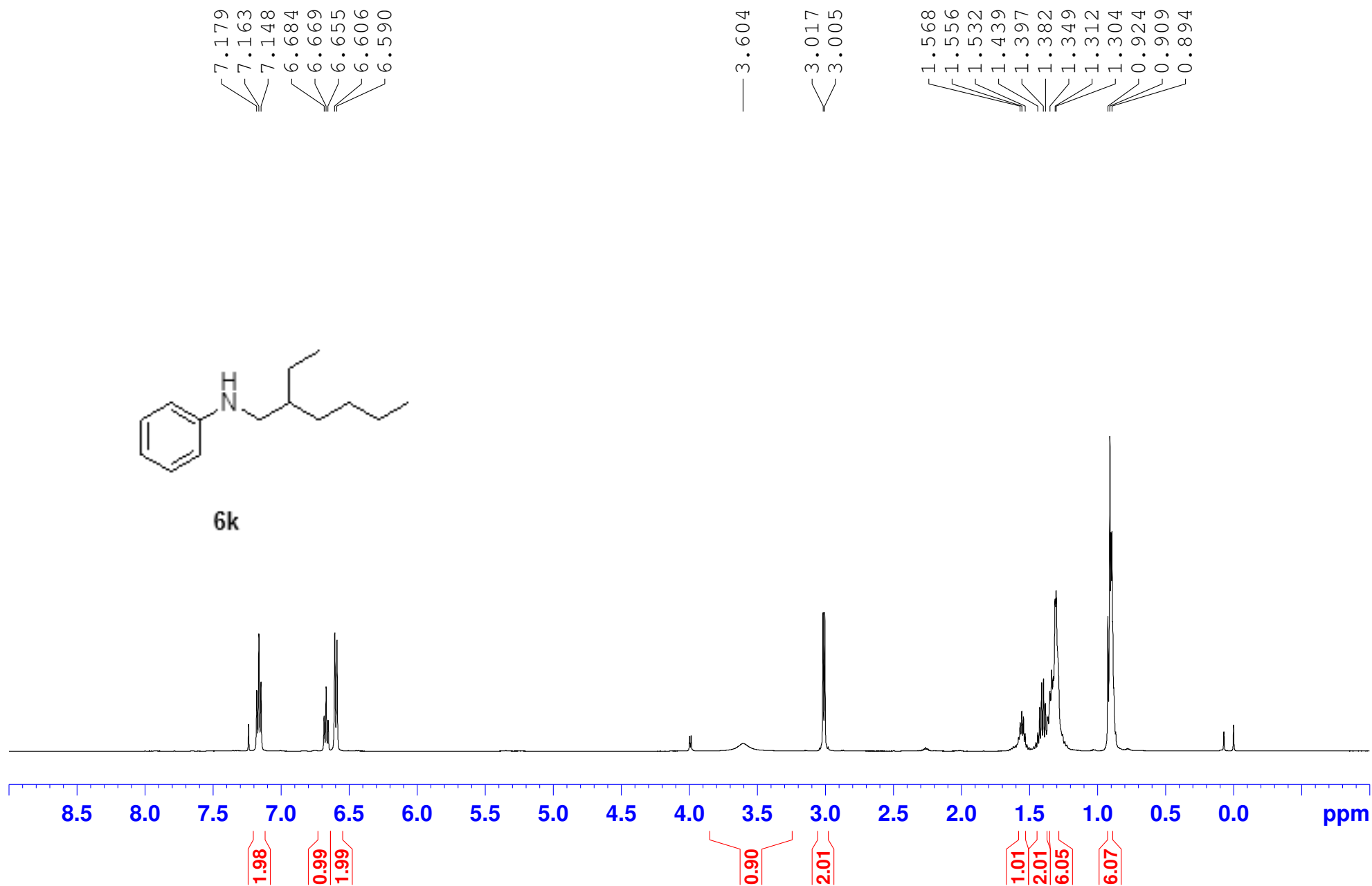
N-octylaniline
C13CPD-1 CDC13



N-(2-ethylhexyl) aniline
Proton CDCl₃



6k



N-(2-ethylhexyl) aniline
C13CPD-1 CDCl₃

—148.697

—129.179

—116.848

—112.555

—77.000

—46.972

—39.054

—31.290

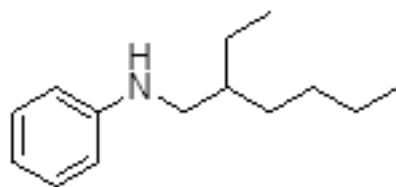
—28.956

—24.454

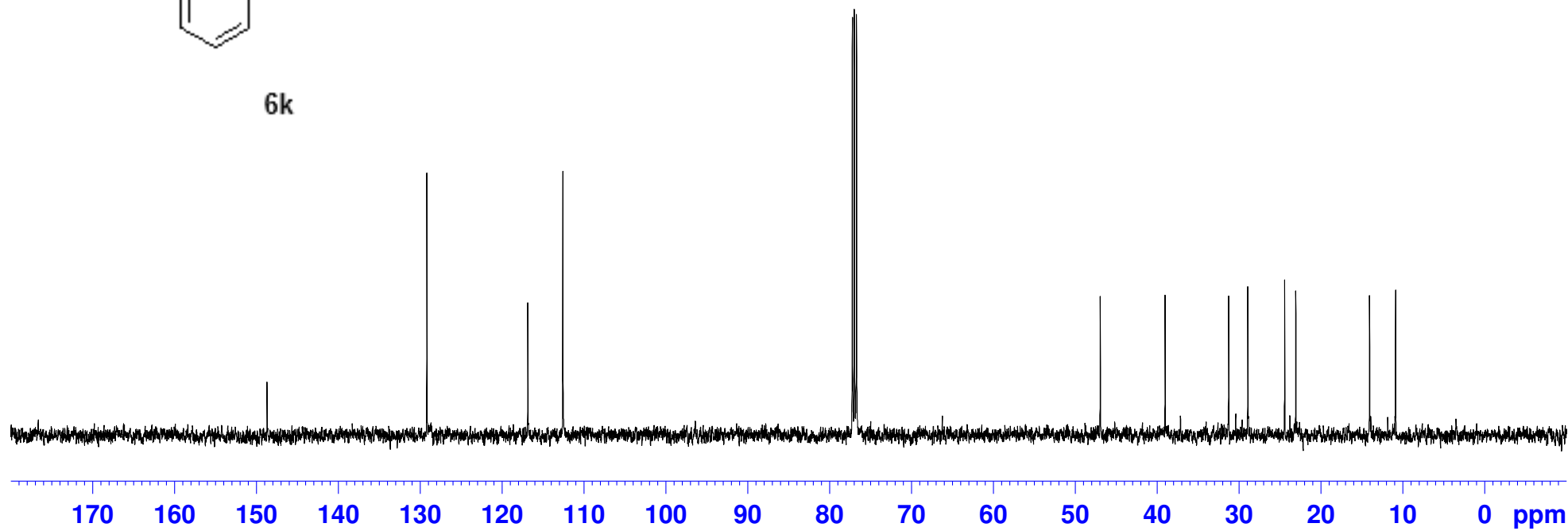
—23.087

—14.084

—10.902



6k



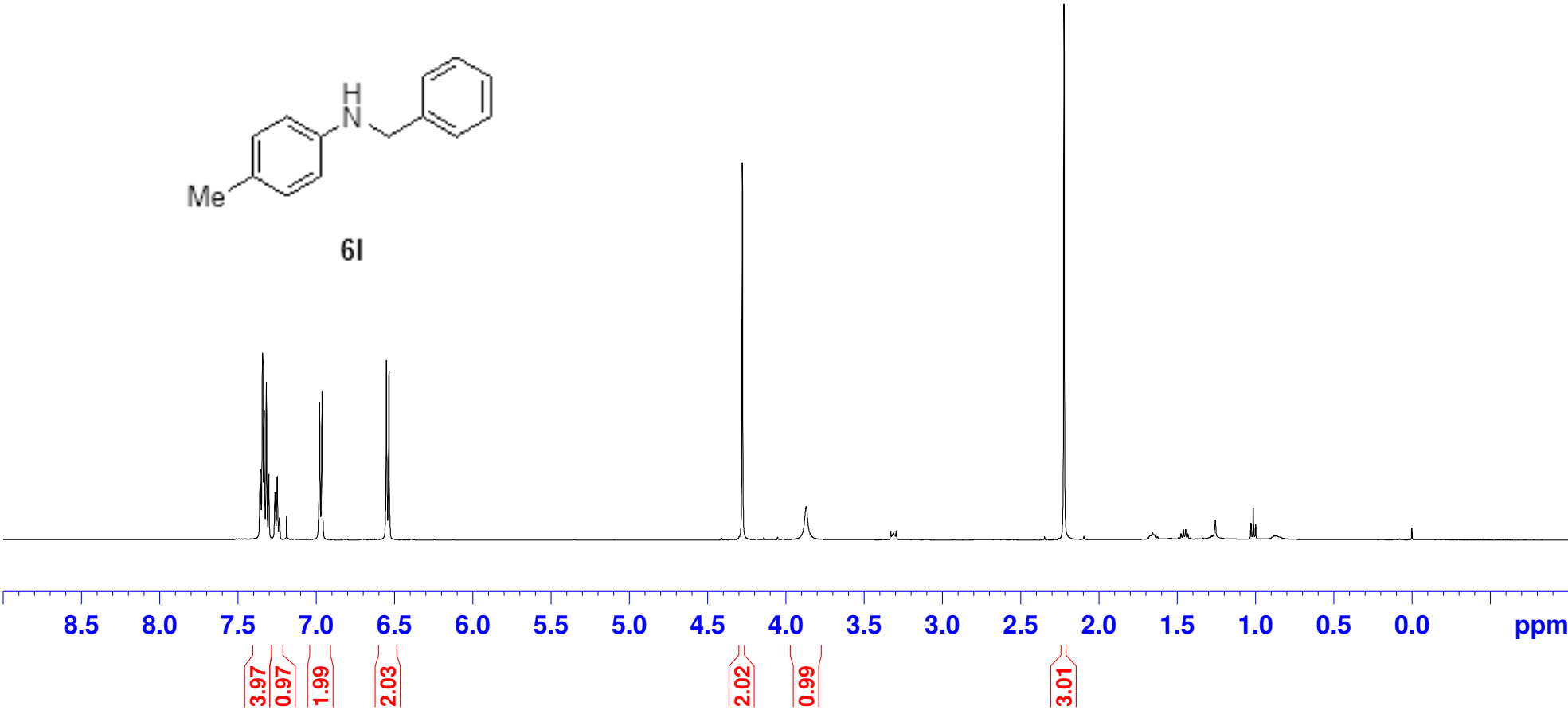
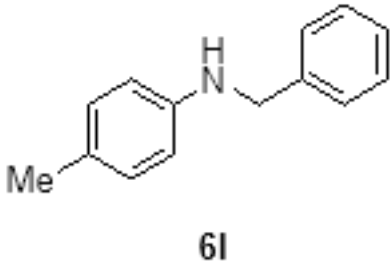
N-benzyl-4-methylaniline
Proton CDCl3

7.355
7.340
7.331
7.316
7.301
7.261
7.247
7.233
6.977
6.960
6.550
6.533

4.278
3.870

2.223

0.000



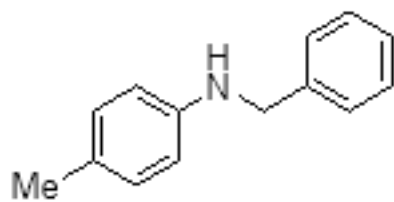
N-benzyl-4-methylaniline
C13CPD CDC13

— 145.889
— 139.629
129.703
128.553
127.451
127.104
126.687
— 112.944

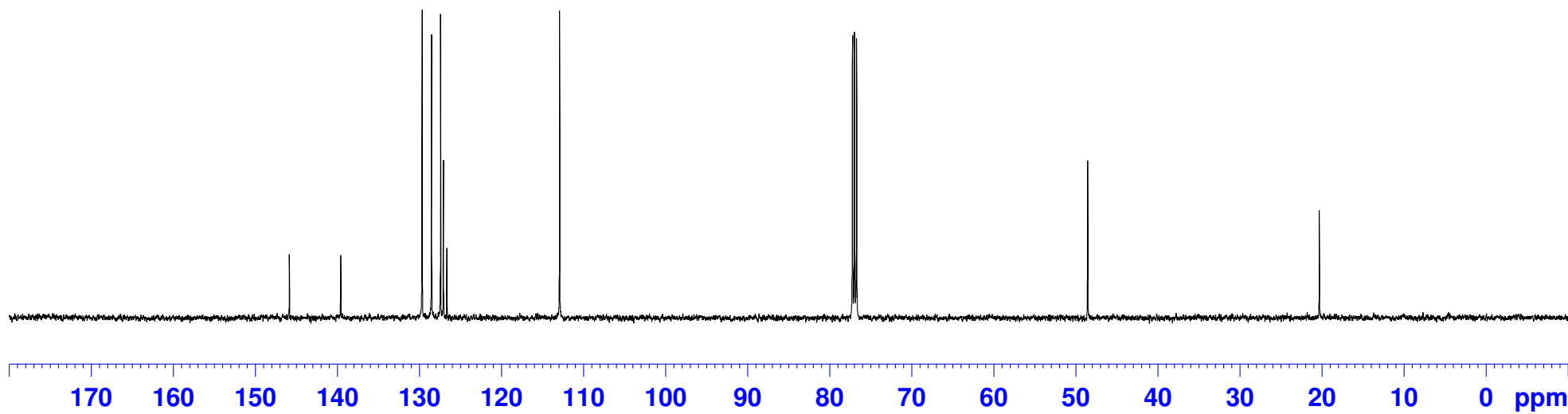
— 77.000

— 48.587

— 20.356



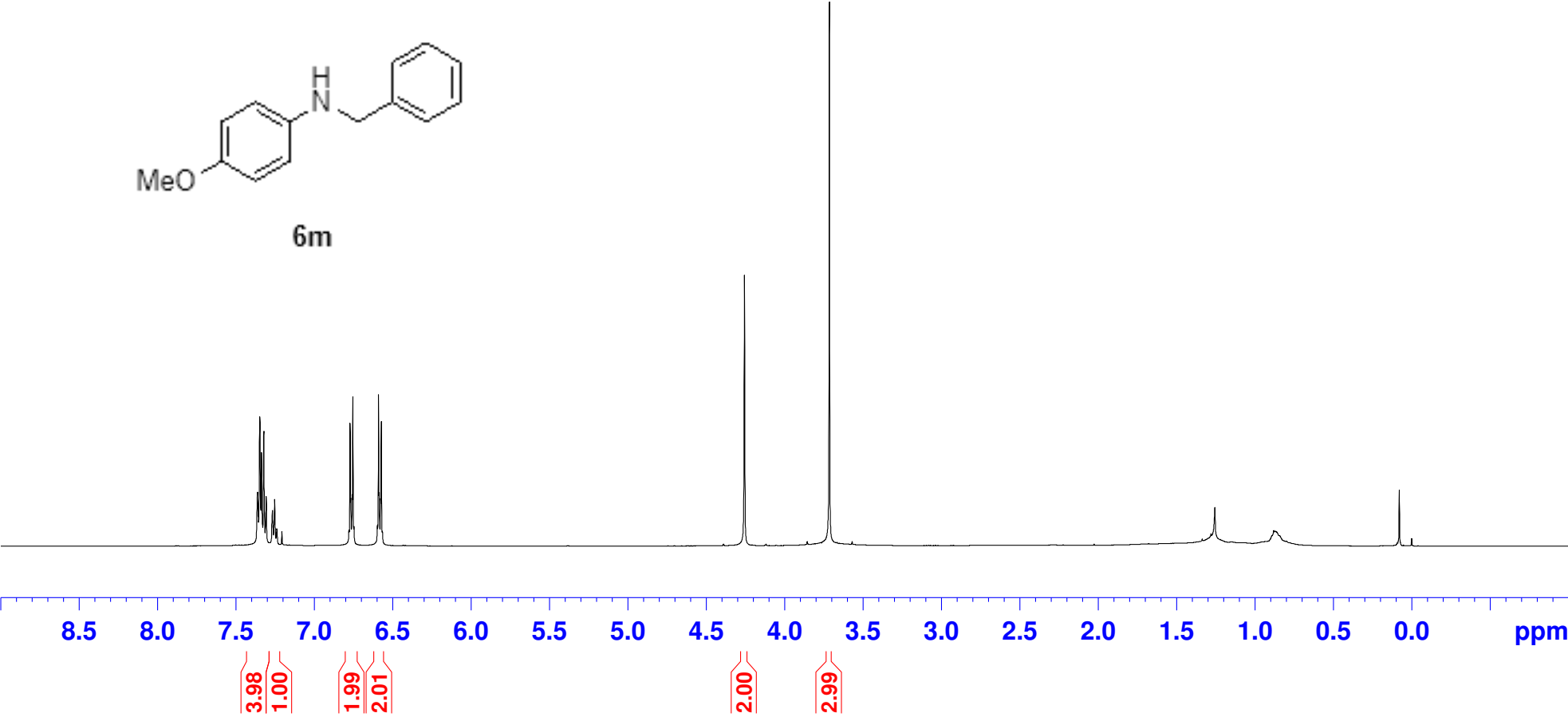
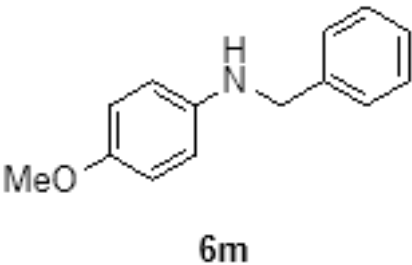
6I



N-benzyl-4-methoxyaniline
Proton CDCl3

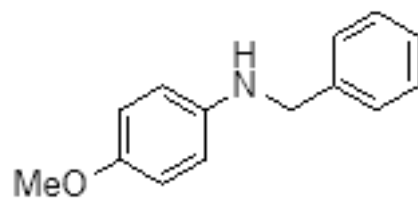
7.359
7.345
7.335
7.320
7.305
7.265
7.251
7.237
6.769
6.752
6.591
6.573

4.256
3.715

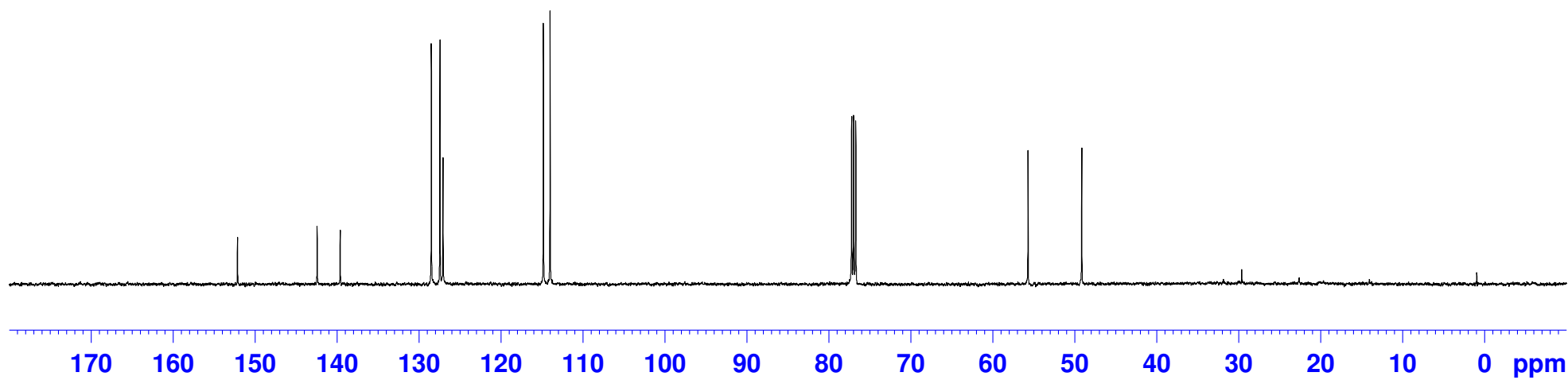


N-benzyl-4-methoxyaniline
C13CPD CDC13

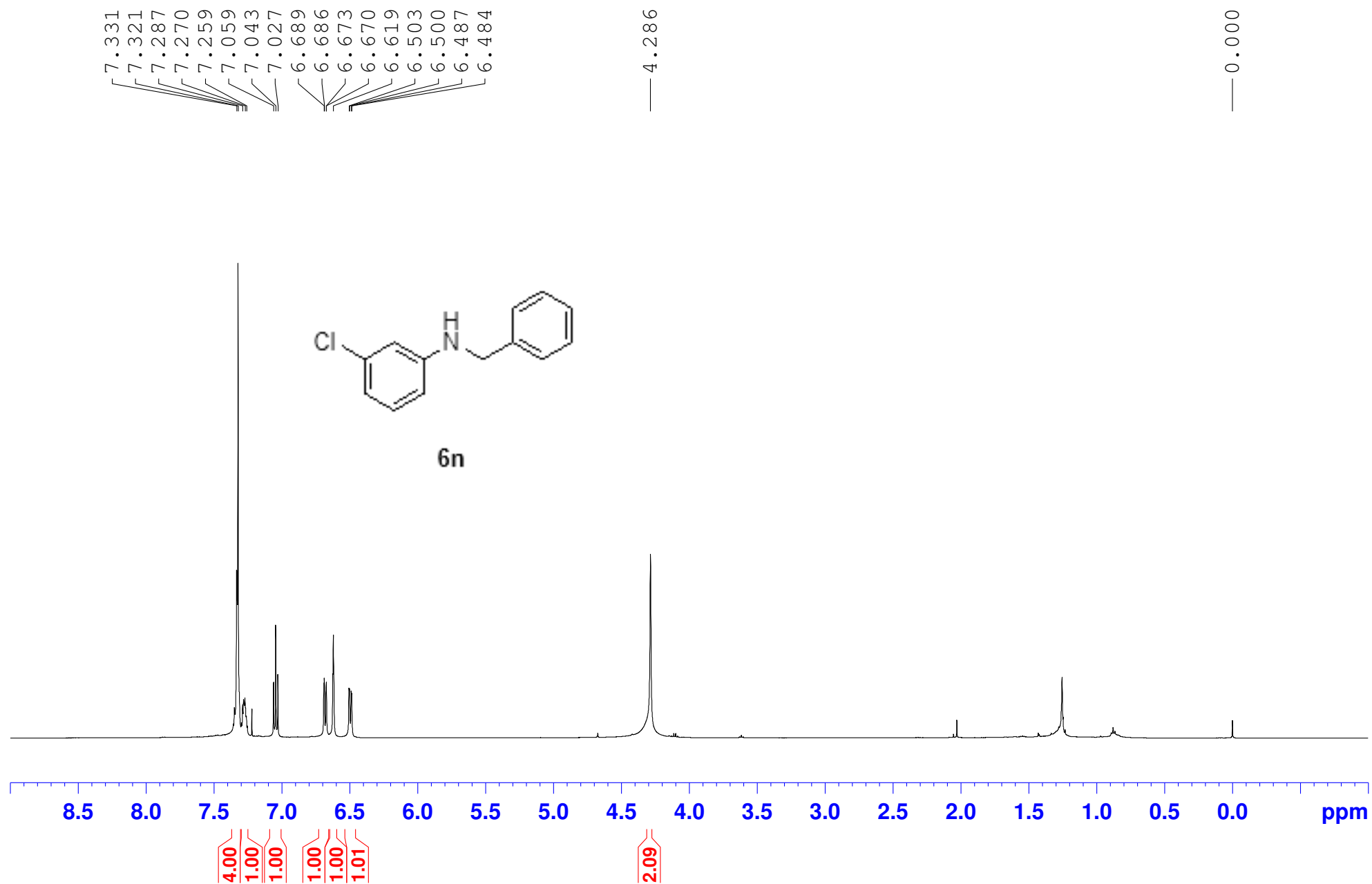
— 152.130
— 142.410
— 139.649
— 128.529
— 127.481
— 127.100
— 114.857
— 114.047
— 77.000
— 55.732
— 49.173



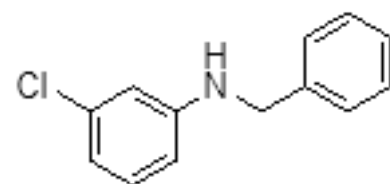
6m



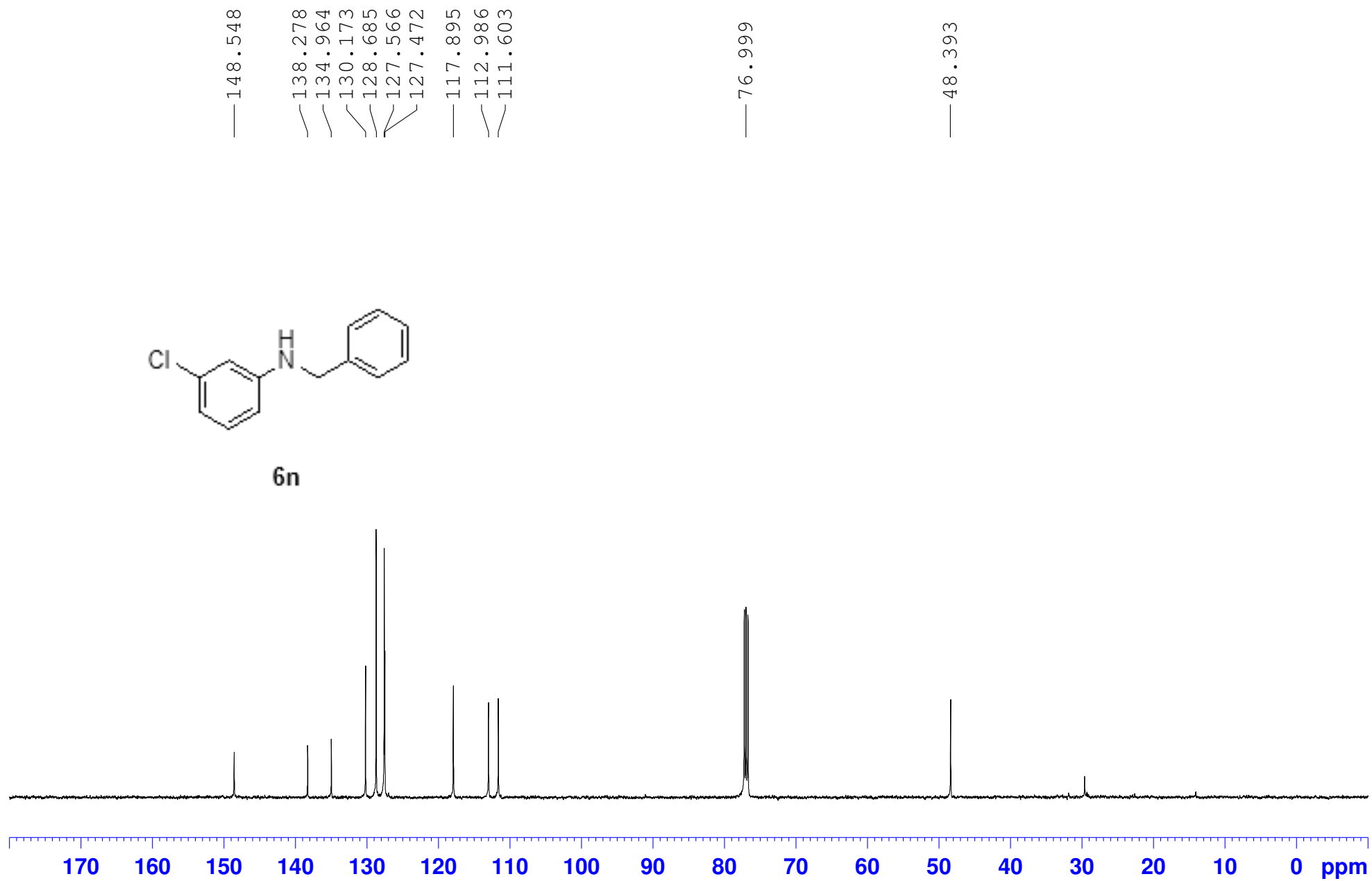
N-benzyl-3-chloroaniline
Proton CDCl₃



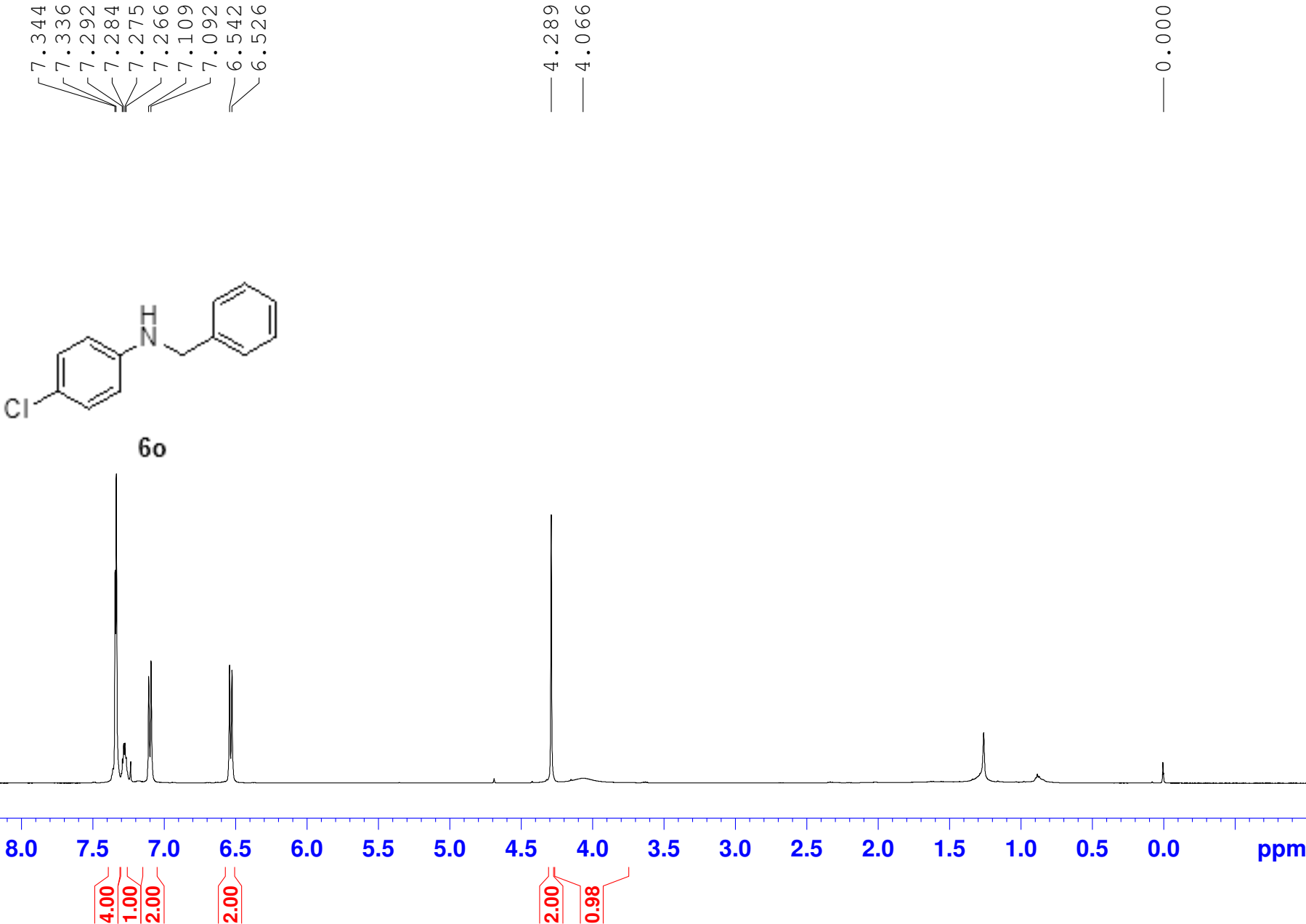
N-benzyl-3-chloroaniline
C13CPD CDC13



6n



N-benzyl-4-chloroaniline
Proton CDCl3

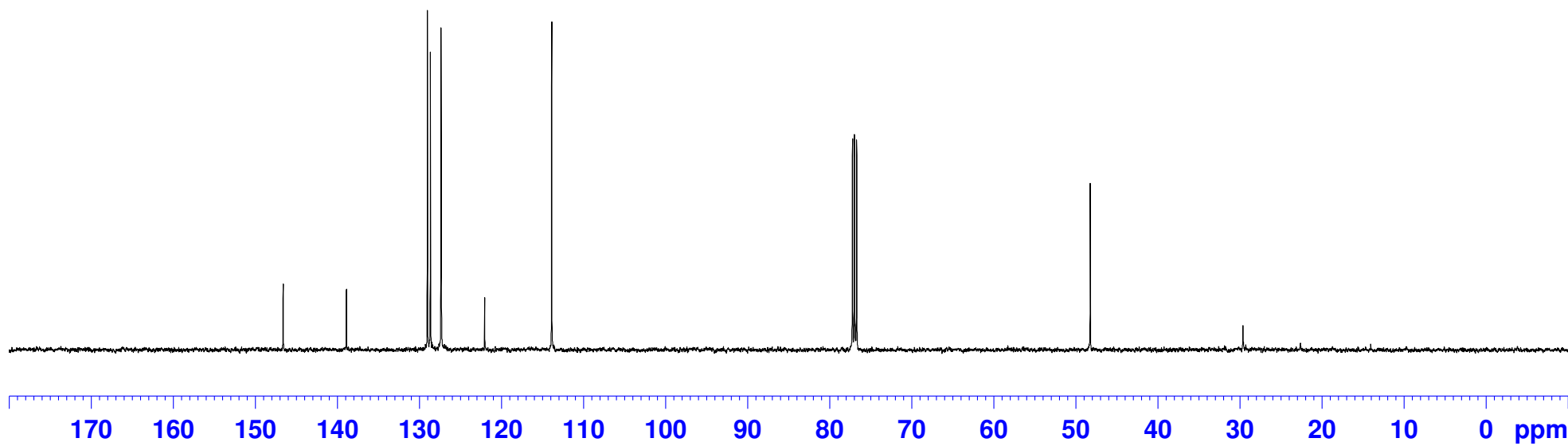
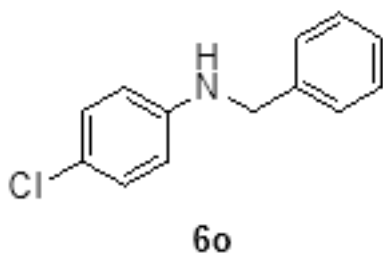


N-benzyl-4-chloroaniline
C13CPD CDC13

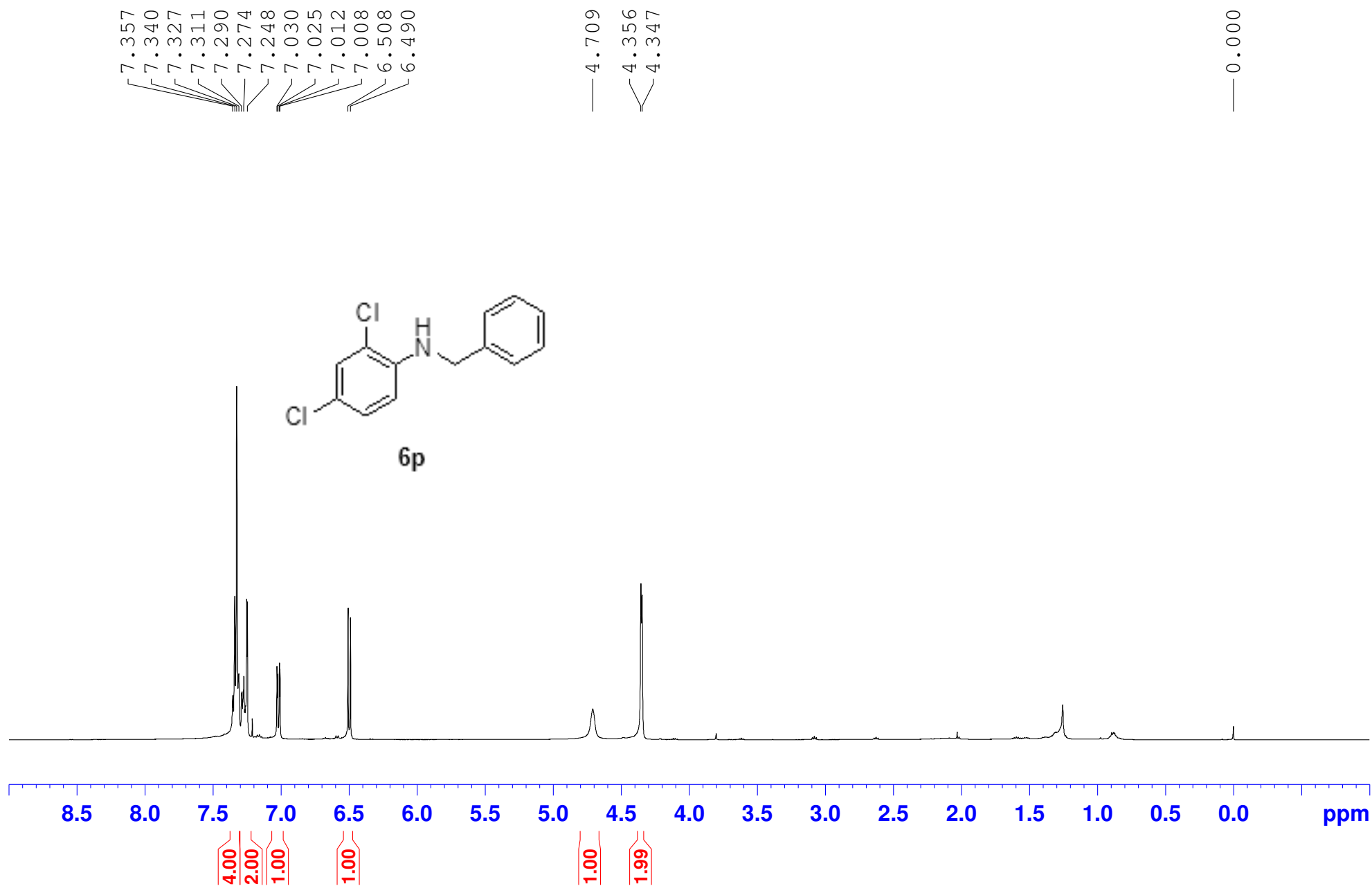
—146.600
—138.888
129.017
128.654
127.362
127.322
122.033
—113.870

—76.999

—48.279



N-benzyl-2,4-dichloroaniline
Proton CDCl₃

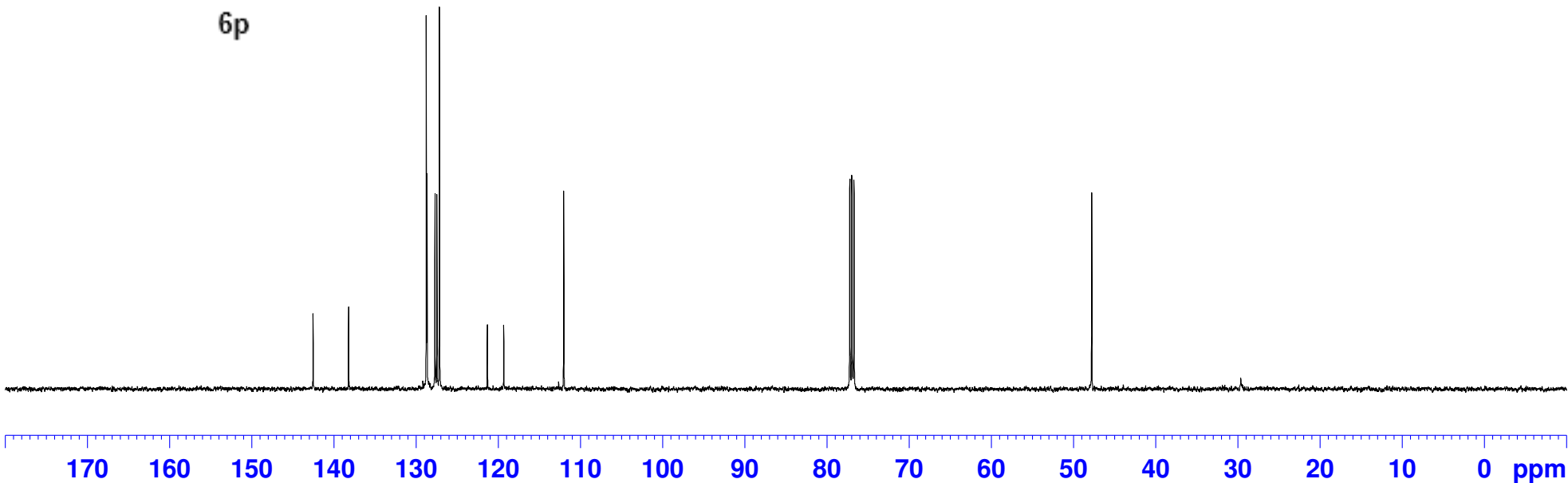
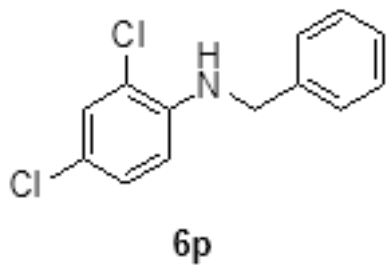


N-benzyl-2,4-dichloroaniline
C13CPD CDC13

142.518
138.198
128.745
128.651
127.692
127.455
127.140
121.311
119.320
112.020

77.000

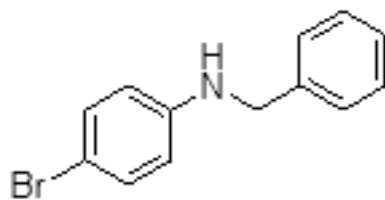
47.812



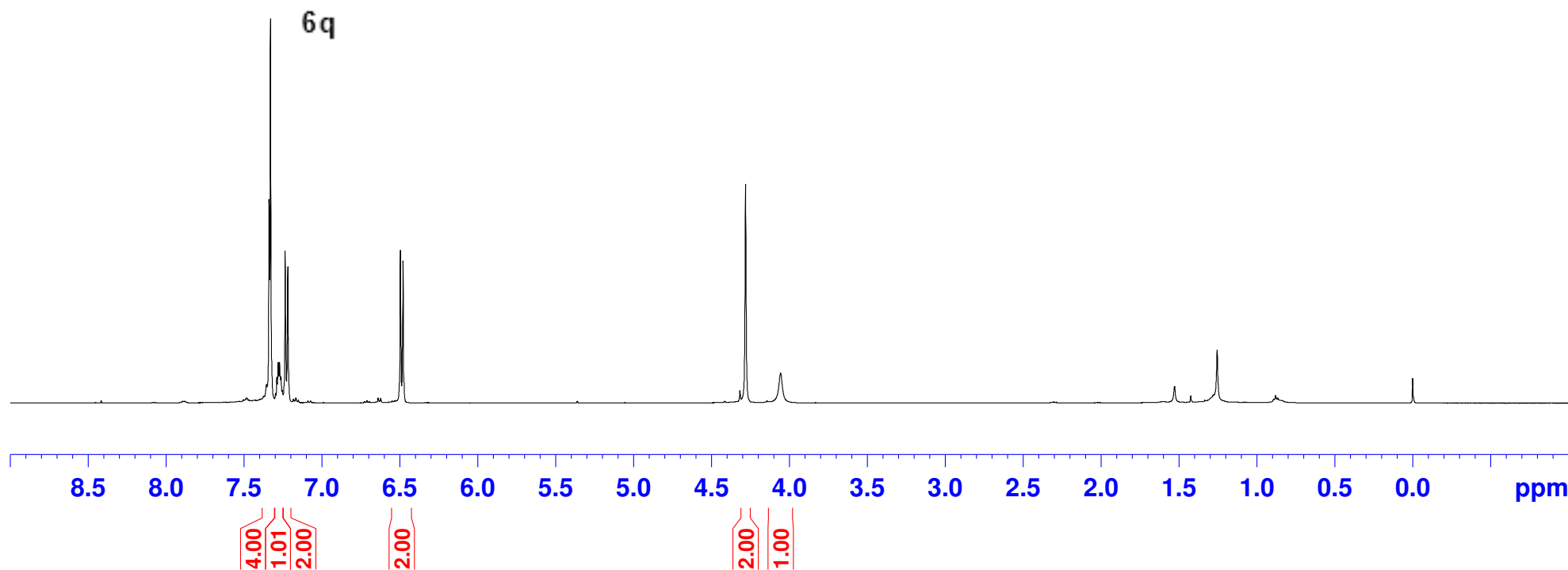
N-benzyl-4-bromoaniline
Proton CDCl₃

7.337
7.328
7.287
7.278
7.270
7.261
7.234
7.217
6.494
6.477

4.282
4.057



6q



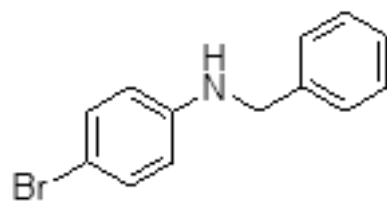
N-benzyl-4-bromoaniline
C13CPD CDC13

—147.022
—138.832
—131.903
—128.676
—127.360

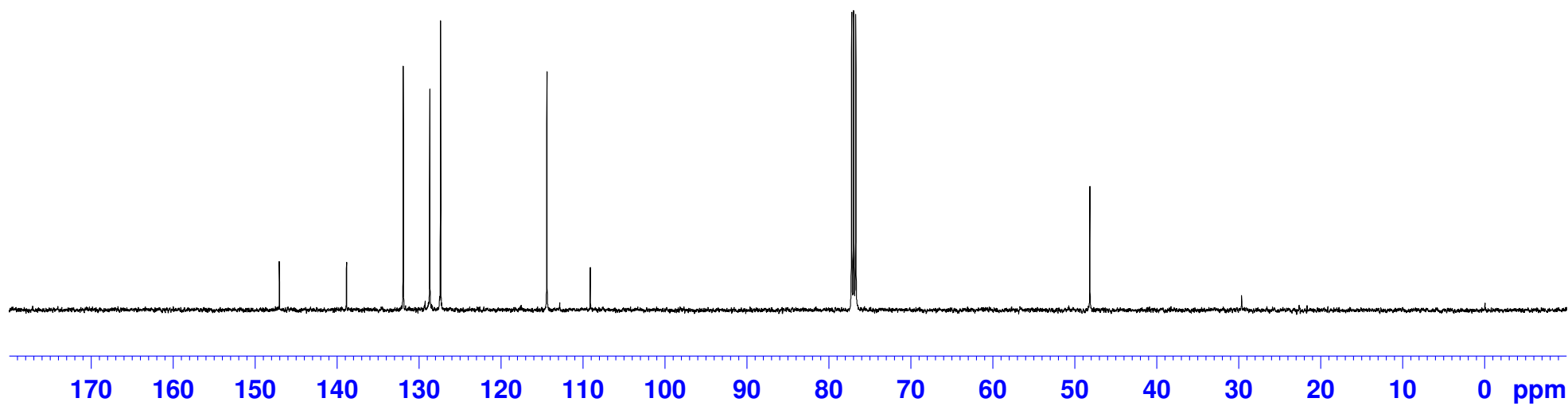
—114.386
—109.085

—77.001

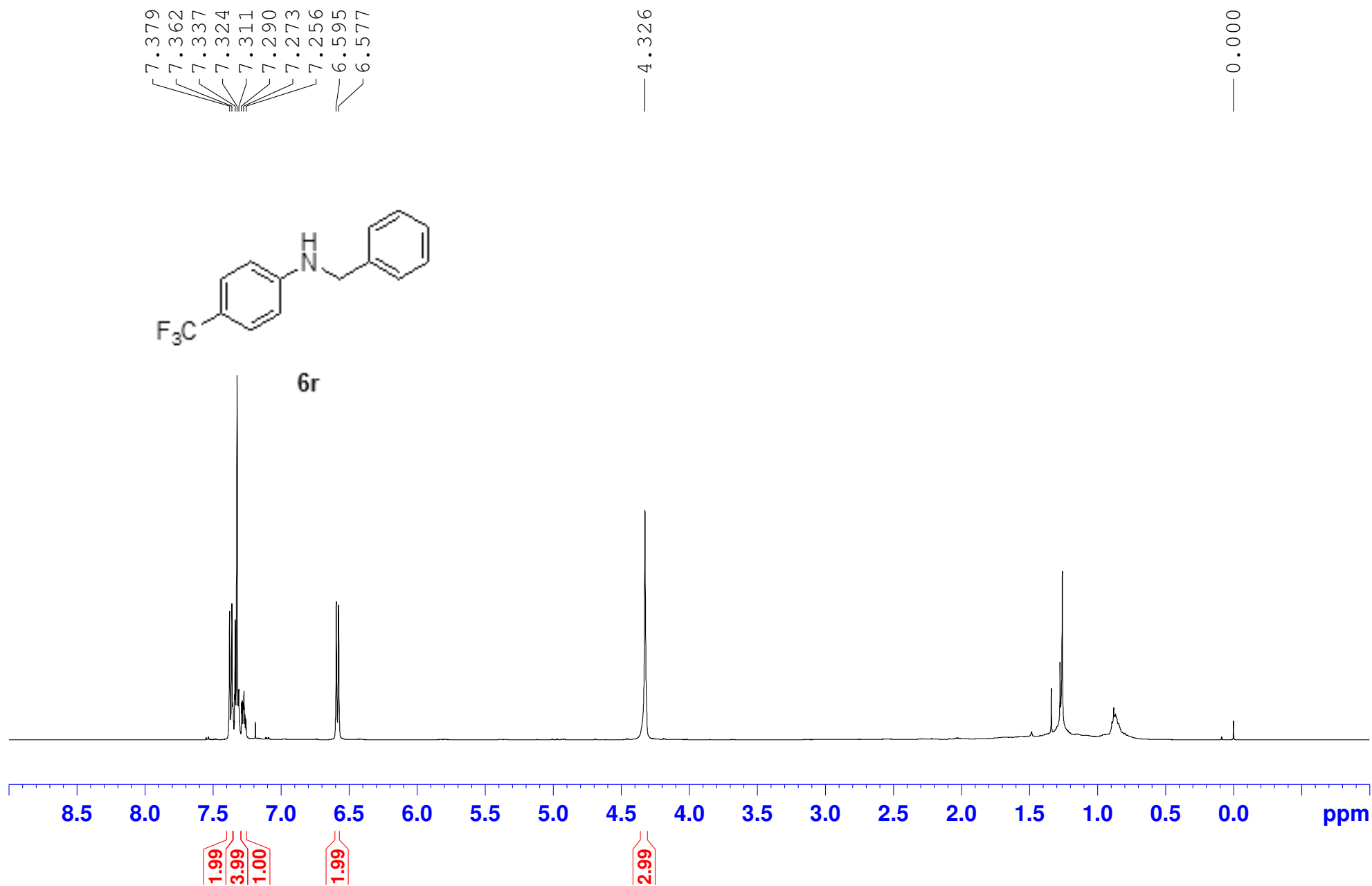
—48.195



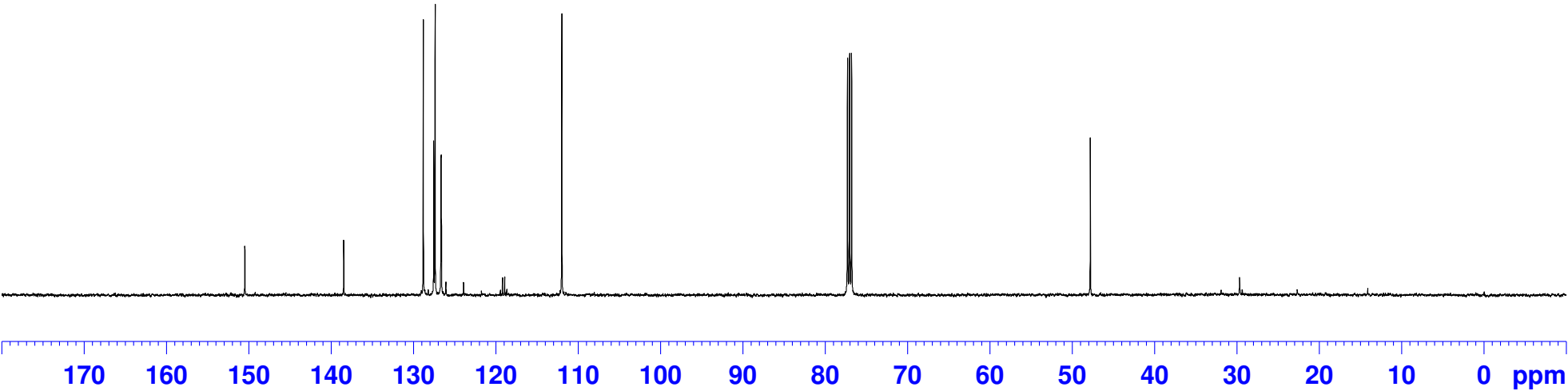
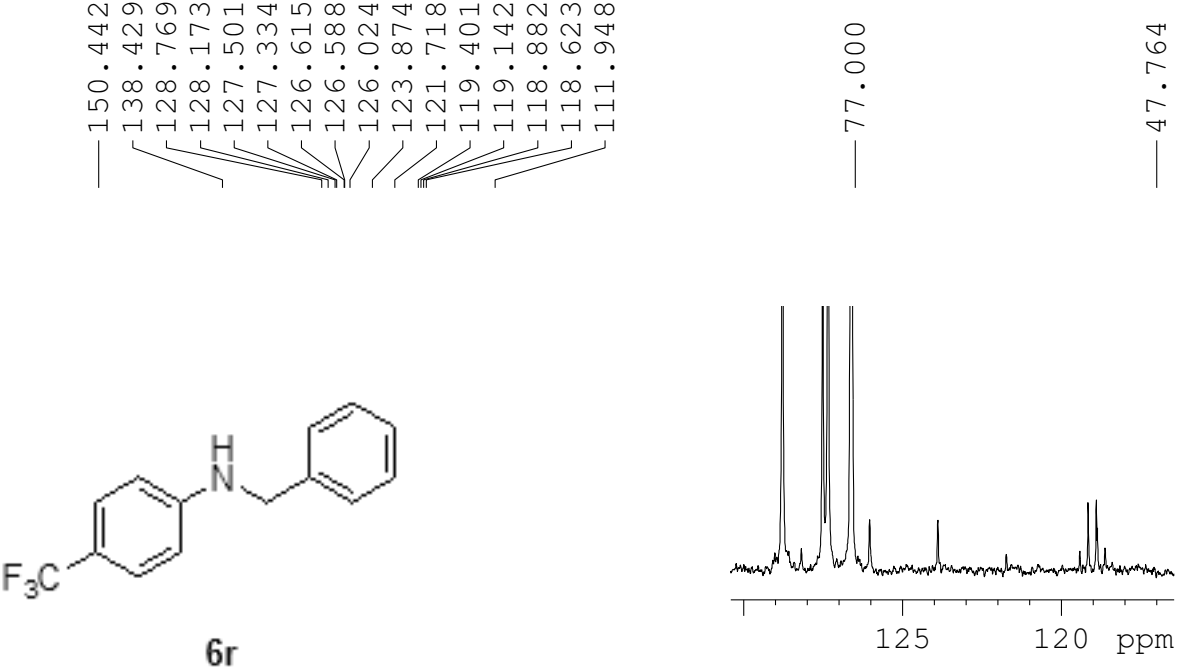
6q



N-benzyl-4-trifluoromethylaniline
Proton CDCl₃



N-benzyl-4-trifluoromethylaniline
C13CPD CDCl3

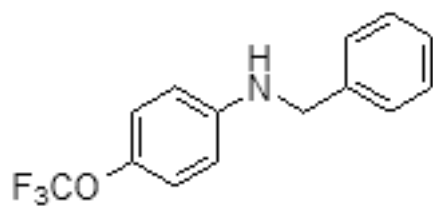


N-benzyl-4-trifluoromethoxyaniline
Proton CDCl₃

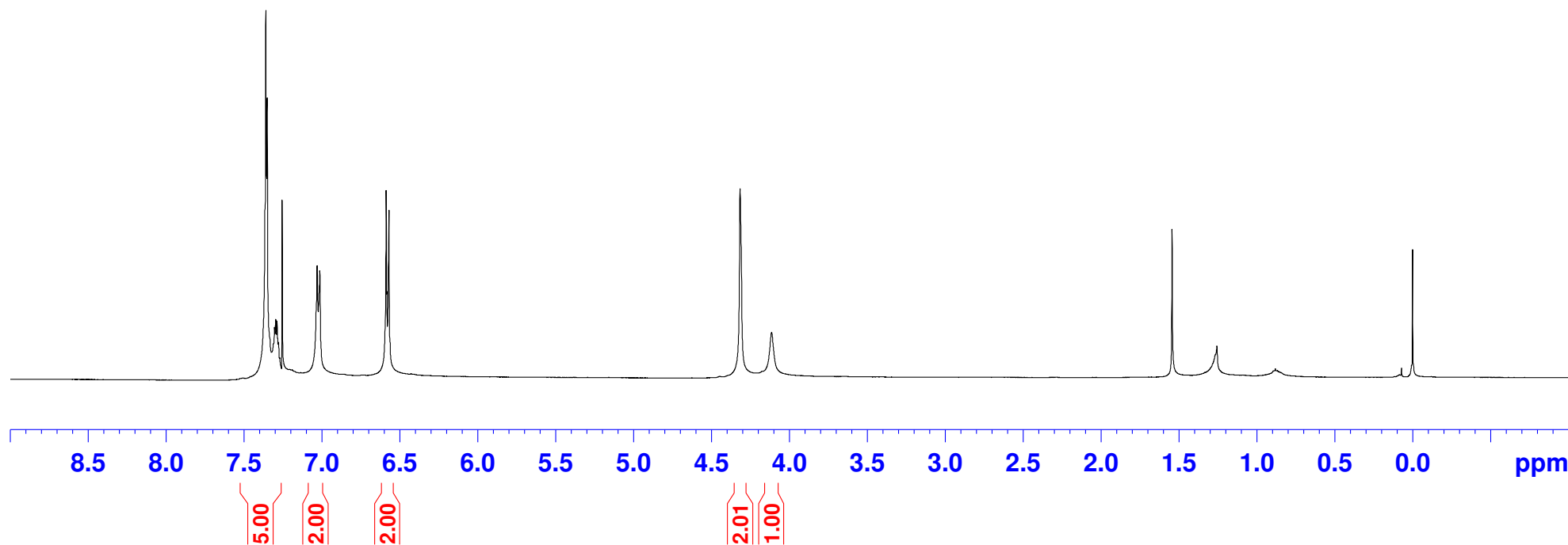
7.365
7.360
7.351
7.336
7.305
7.296
7.288
7.030
7.014
6.588
6.570

4.316
4.114

0.000



6s

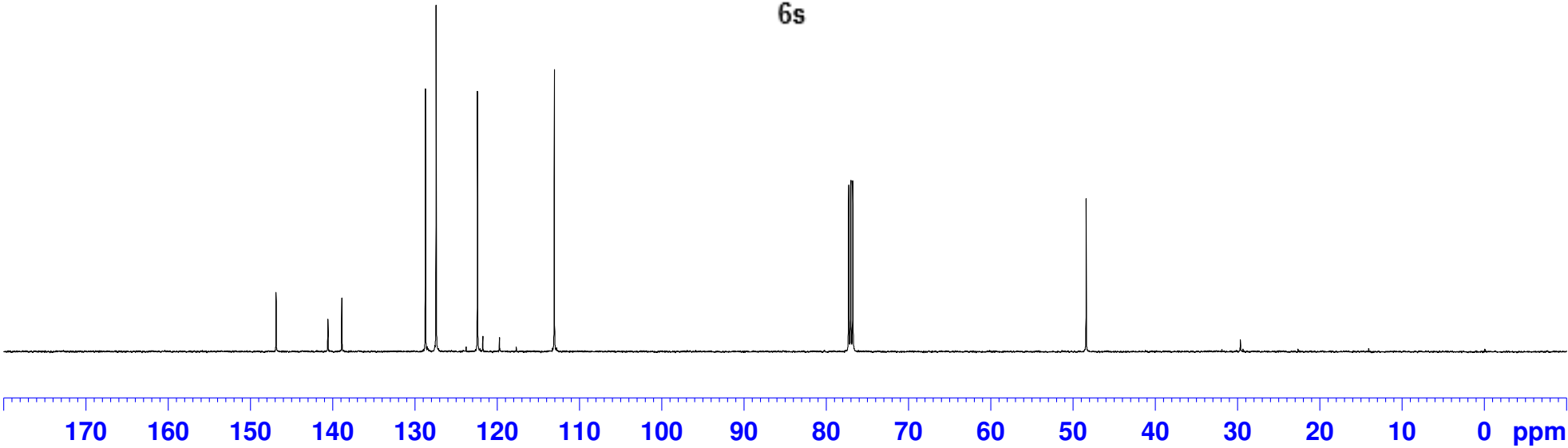
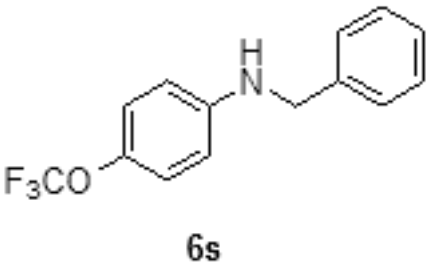
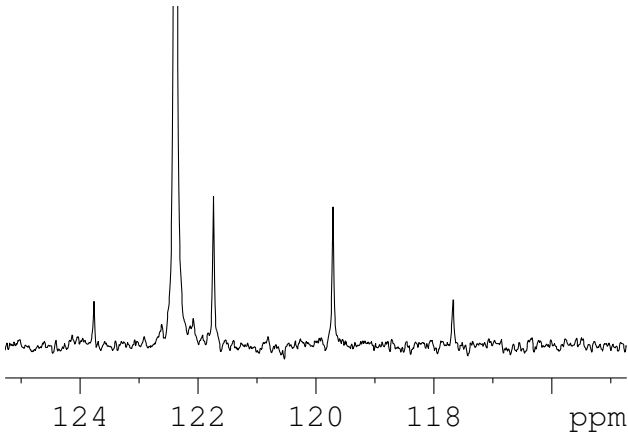


N-benzyl-4-trifluoromethoxyaniline
C13CPD CDC13

146.866
140.560
138.874
128.710
127.413
123.760
122.377
121.731
119.701
117.671
113.039

77.000

48.437

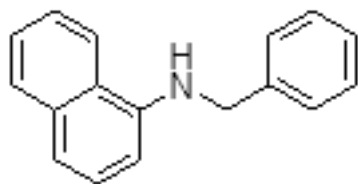


N-benzyl-naphthalen-1-amine
Proton CDCl₃

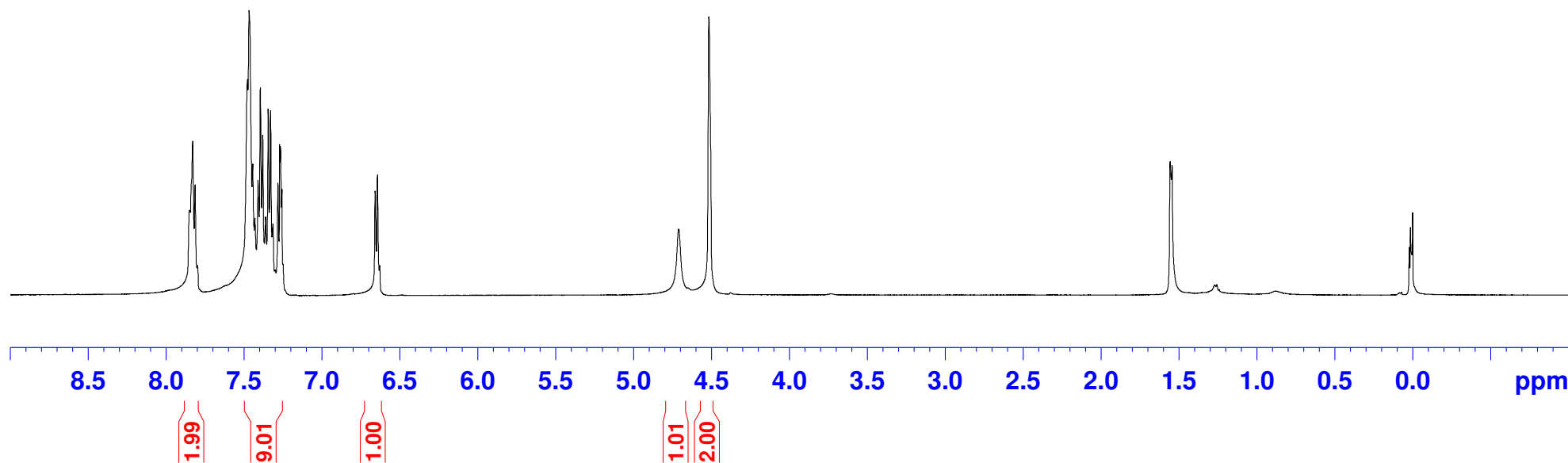
7.848
7.827
7.811
7.477
7.465
7.462
7.428
7.393
7.378
7.343
7.327
7.280
7.264
7.254
6.656
6.641

— 4.711
— 4.517

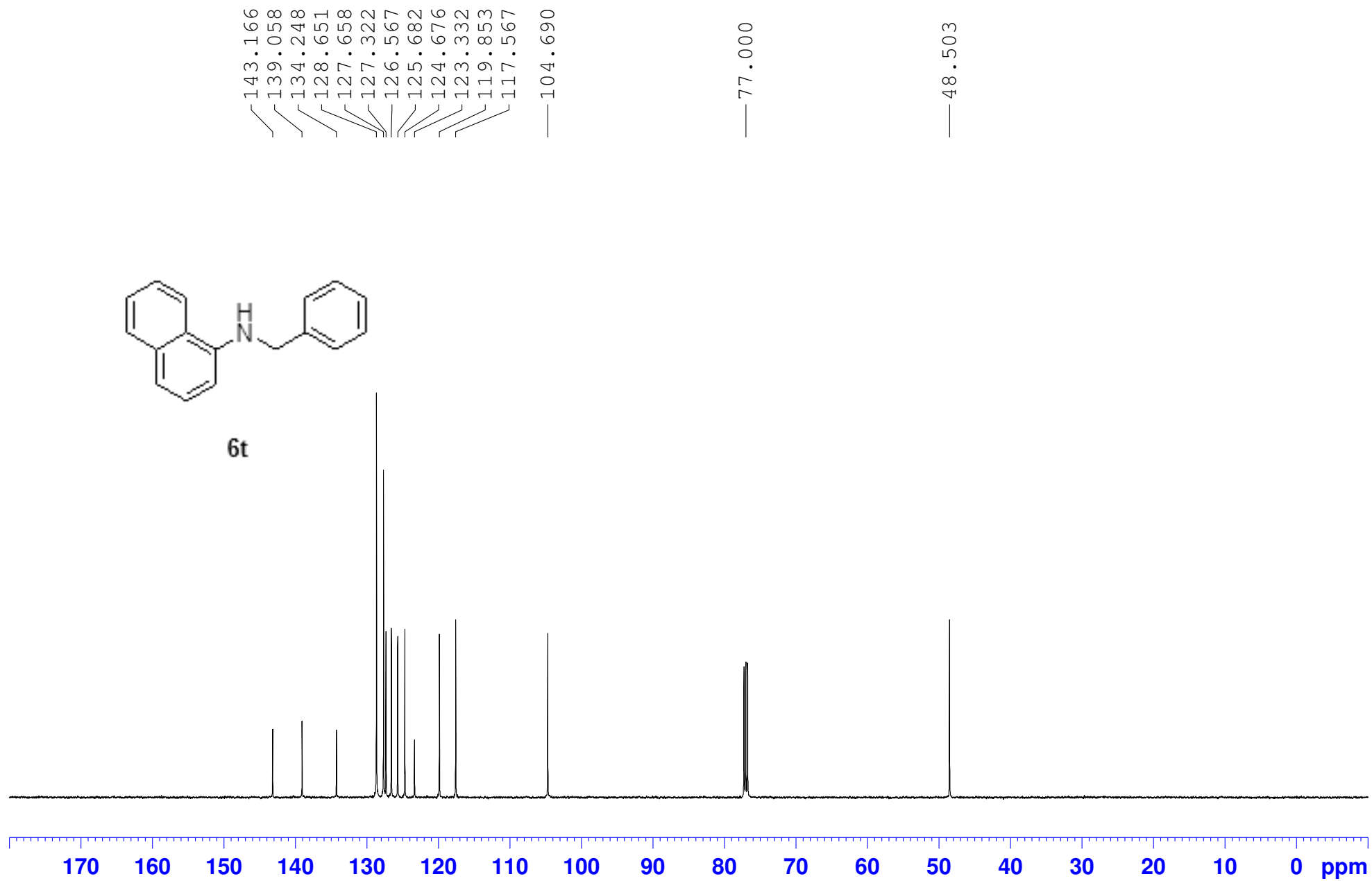
— 0.000



6t



N-benzyl-naphthalen-1-amine
C13CPD CDC13



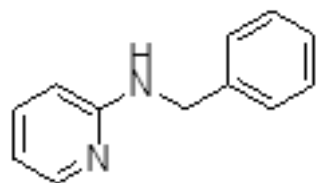
2-Benzylaminopyridine
Proton CDCl₃

8.068
8.058
7.383
7.299
7.262
7.248
7.231
6.568
6.557
6.554
6.544
6.348
6.331

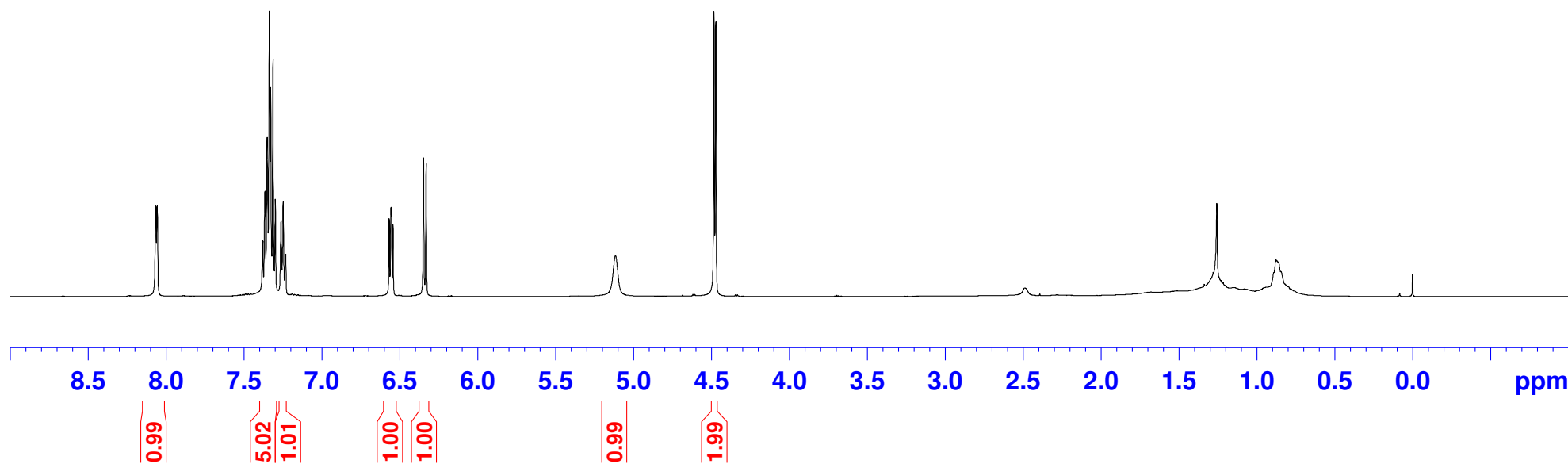
5.116

4.484
4.472

0.000



6u



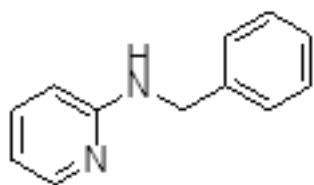
2-Benzylaminopyridine
C13CPD CDCl3

—158.610
—148.101
—139.125
—137.379
—128.536
—127.309
—127.124

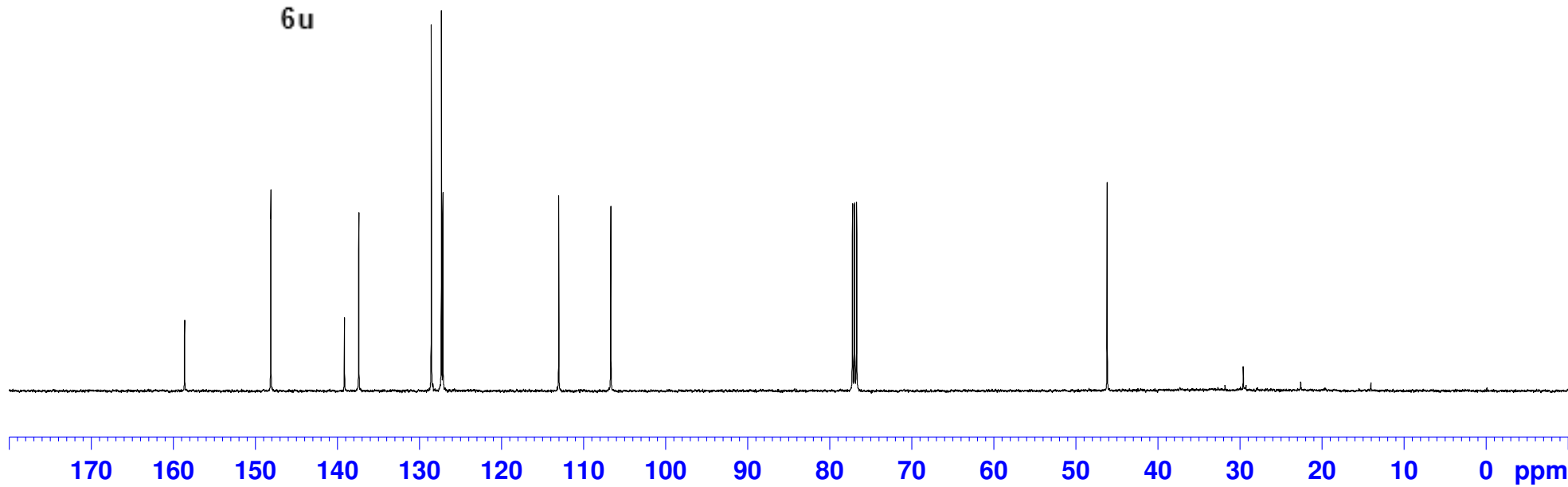
—113.004
—106.663

—77.000

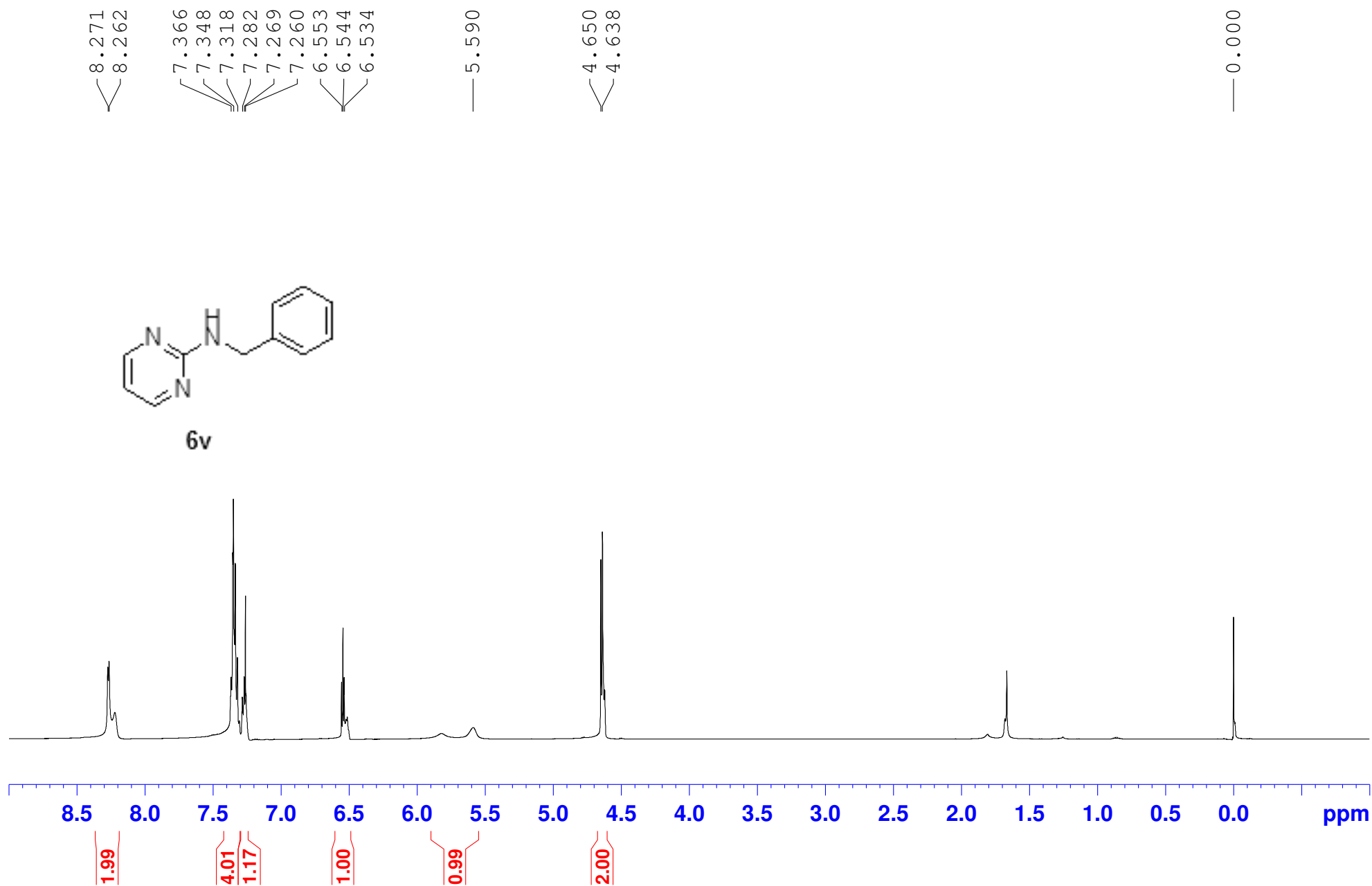
—46.215



6u



N-Benzyl-(2-pyrimidyl) amine
Proton CDCl₃



N-Benzyl-(2-pyrimidyl) amine
C13CPD CDC13

—162.305
—158.017

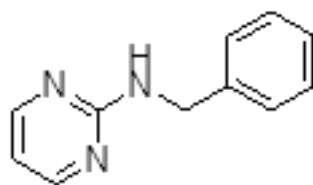
—139.067

128.558
127.500
127.192

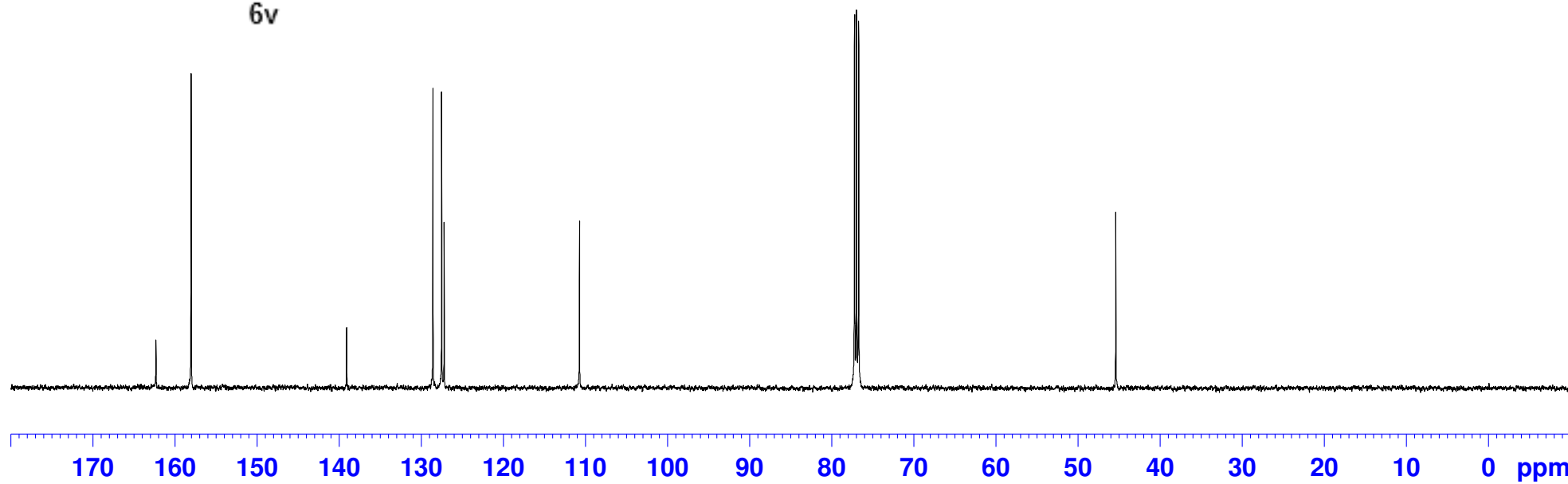
—110.709

—77.000

—45.424



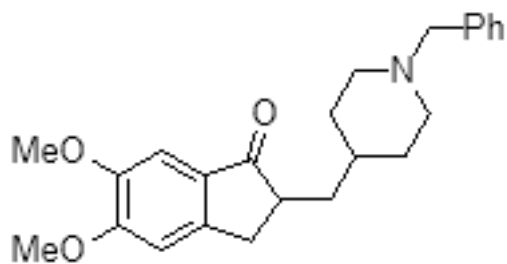
6v



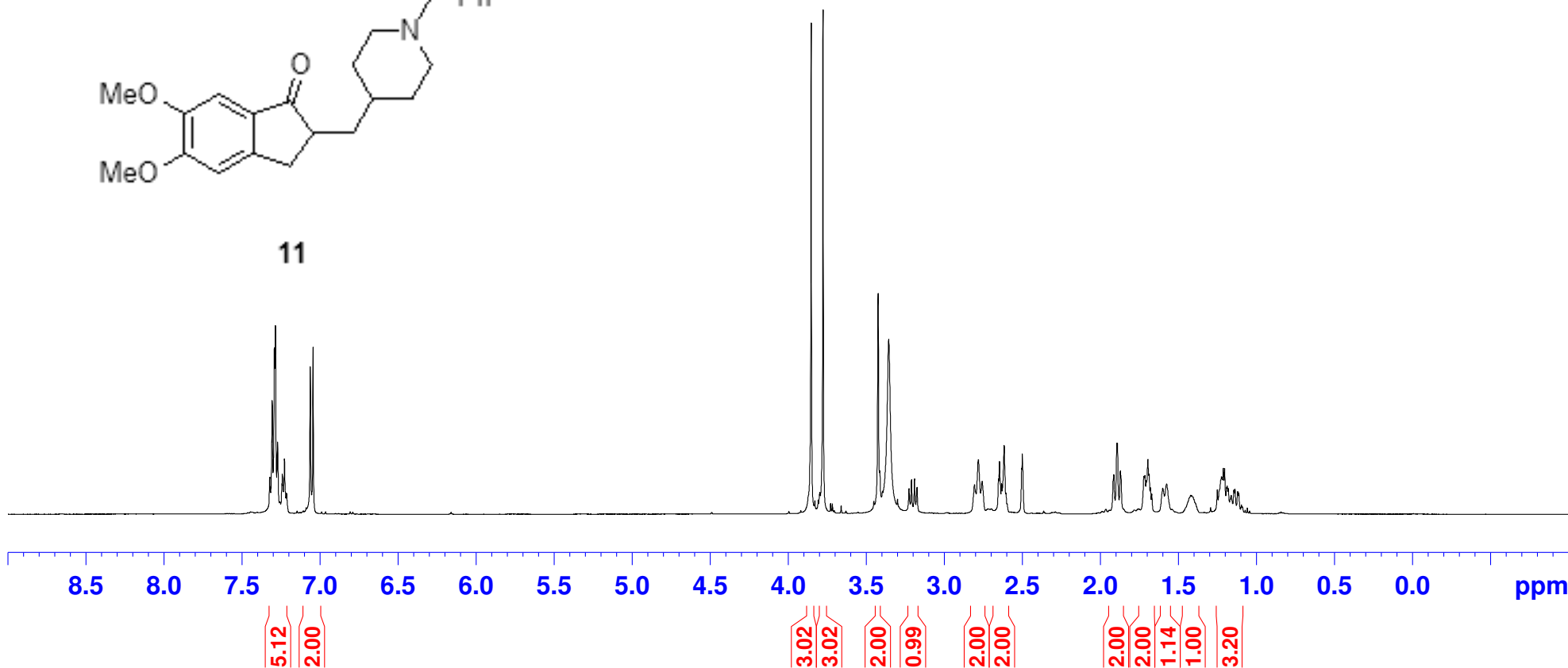
donepezil
 PROTON DMSO-d6

7.319
 7.212
 7.063
 7.045

3.853
 3.777
 3.424
 3.226
 3.210
 3.191
 3.174
 2.806
 2.781
 2.757
 2.646
 2.616
 1.913
 1.871
 1.720
 1.670
 1.600
 1.575



11



Donepezil
C13CPD DMSO

— 206.496

— 155.182

— 149.064

— 148.619

— 138.618

— 128.675

— 128.380

— 128.024

— 126.694

— 108.105

— 103.918

— 62.455

— 55.850

— 55.536

— 53.230

— 44.730

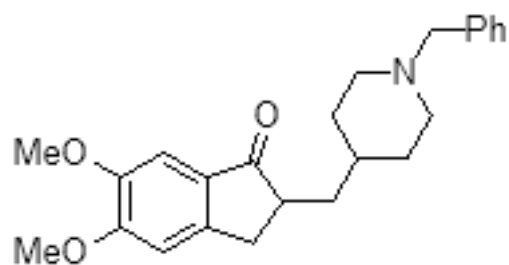
— 39.500

— 38.189

— 33.839

— 32.626

— 31.390



11

