

Electronic Supplementary Information for

**Combination of gold and iridium catalysts for the synthesis of *N*-alkylated
amides from nitriles and alcohols**

Feng Li,^{*a} Juan Ma,^a Lei Lu,^a Xiaofeng Bao^b and Wanying Tang^a

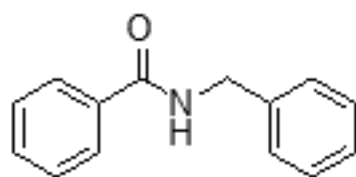
^a Key Laboratory for Soft Chemistry and Functional Materials, Ministry of Education, Nanjing University of Science and Technology, Nanjing 210094, P. R. China

^b Department of Biochemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, P. R. China

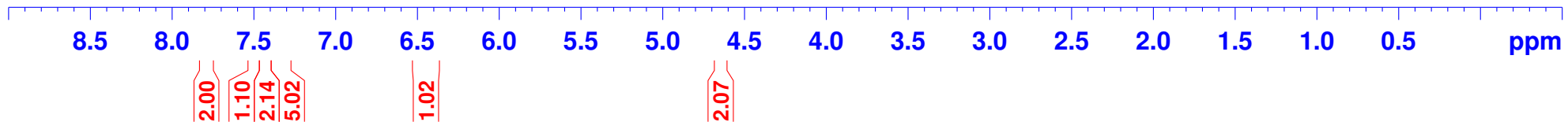
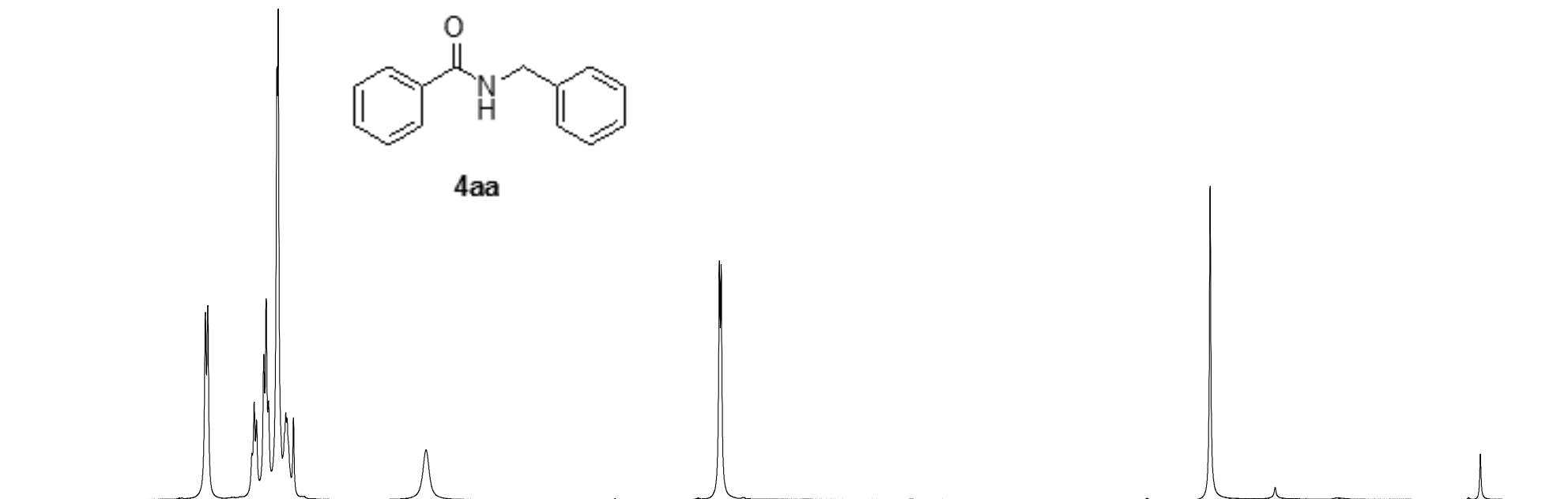
N-benzylbenzamide
Proton CDCl₃

7.797
7.783
7.512
7.499
7.484
7.440
7.425
7.411
7.360
7.352
7.305
7.297
7.258
6.448

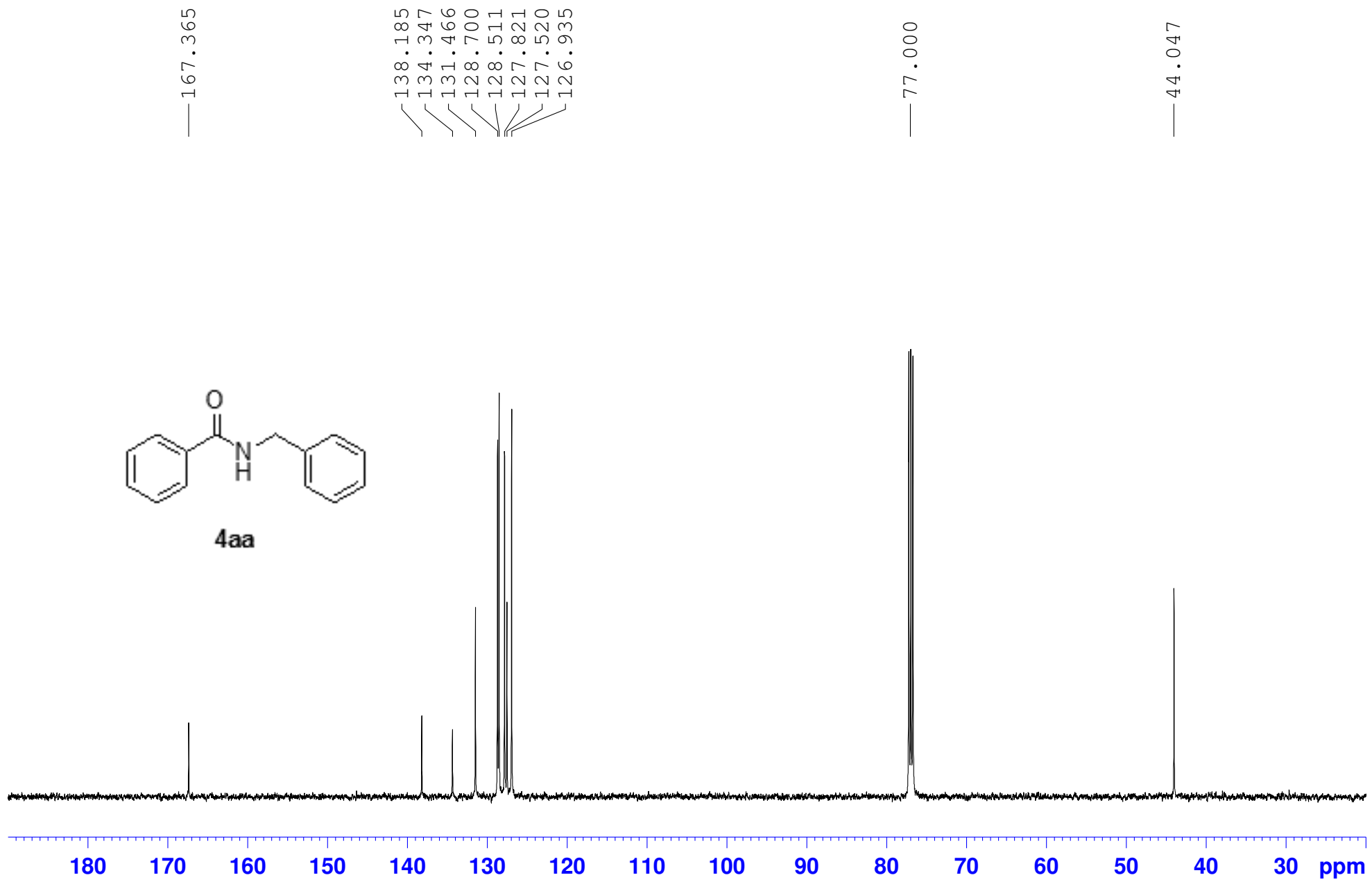
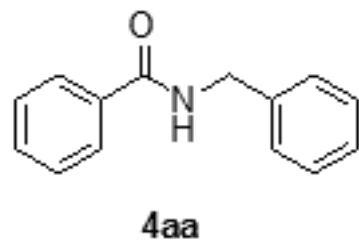
4.654
4.643



4aa



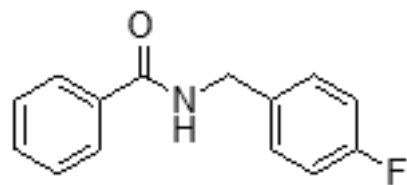
N-benzylbenzamide
C13CPD CDC13



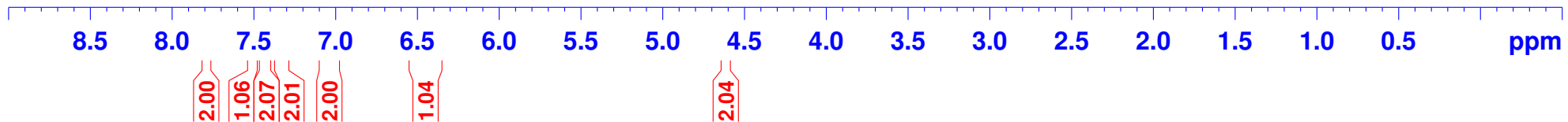
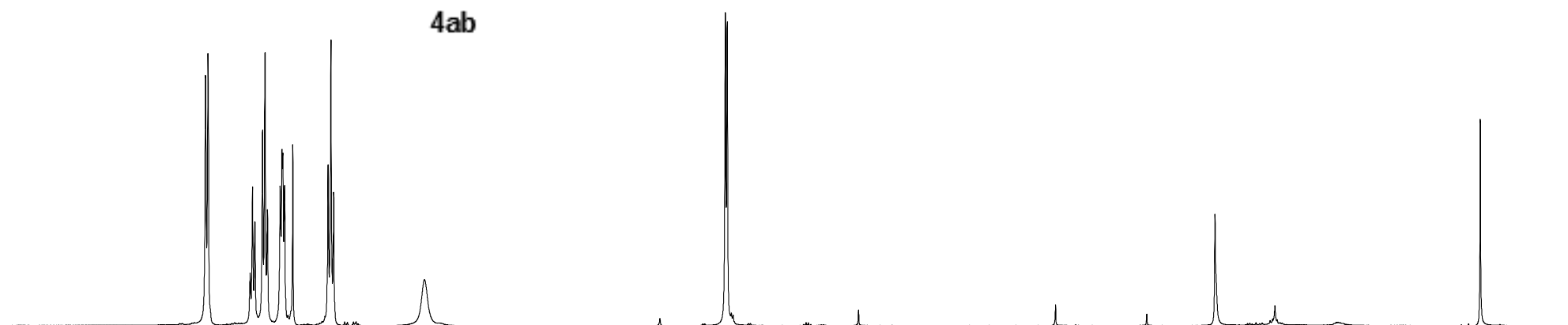
N-(4-fluorobenzyl)benzamide
Proton CDCl₃

7.794
7.779
7.521
7.506
7.492
7.445
7.430
7.415
7.337
7.326
7.321
7.310
7.260
7.047
7.029
7.012
6.457

4.617
4.606



4ab



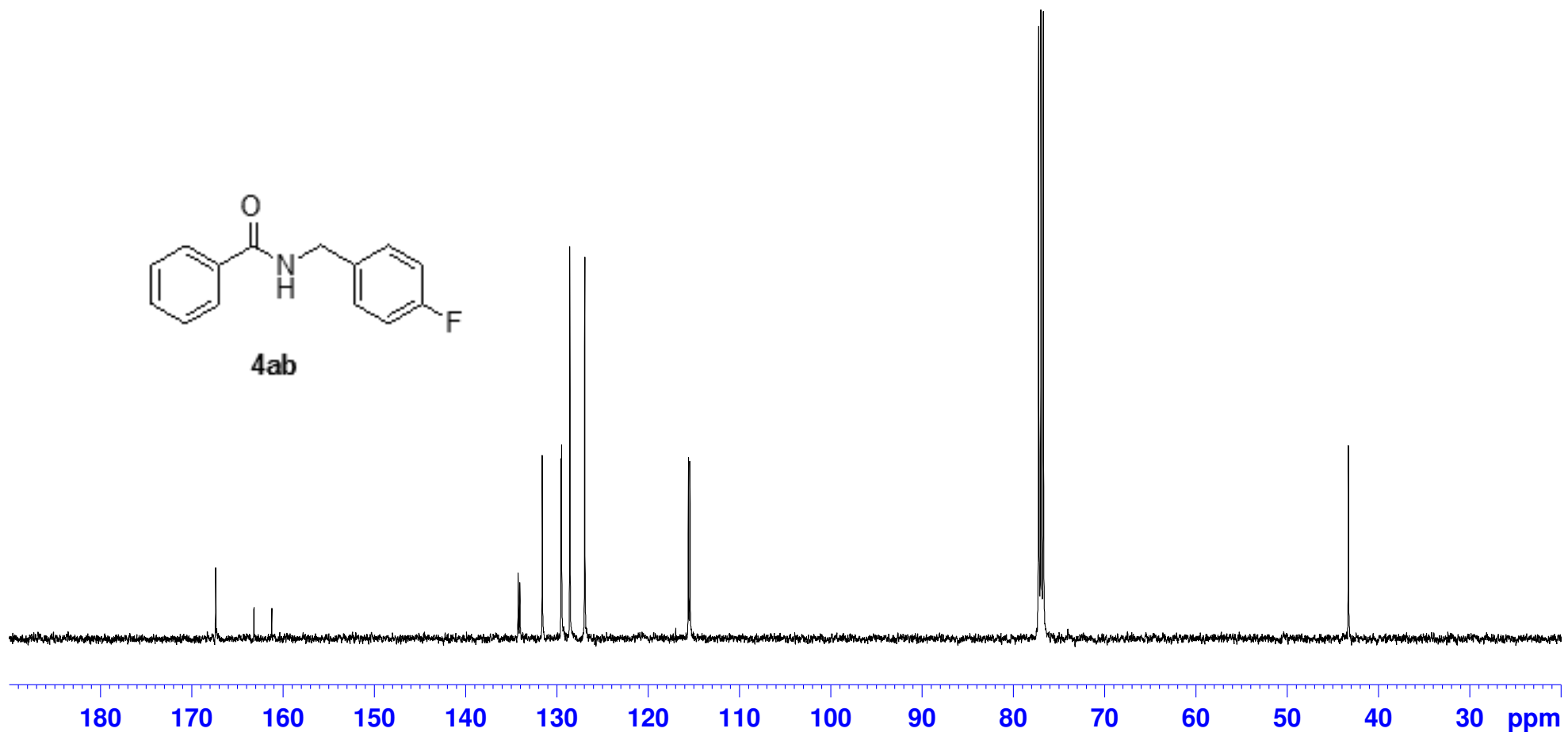
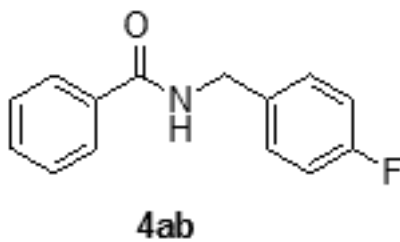
N-(4-fluorobenzyl)benzamide
C13CPD CDCl3

— 167.368
— 163.174
— 161.221

134.230
134.045
131.586
129.537
129.472
128.570
126.938
115.625
115.453

— 77.000

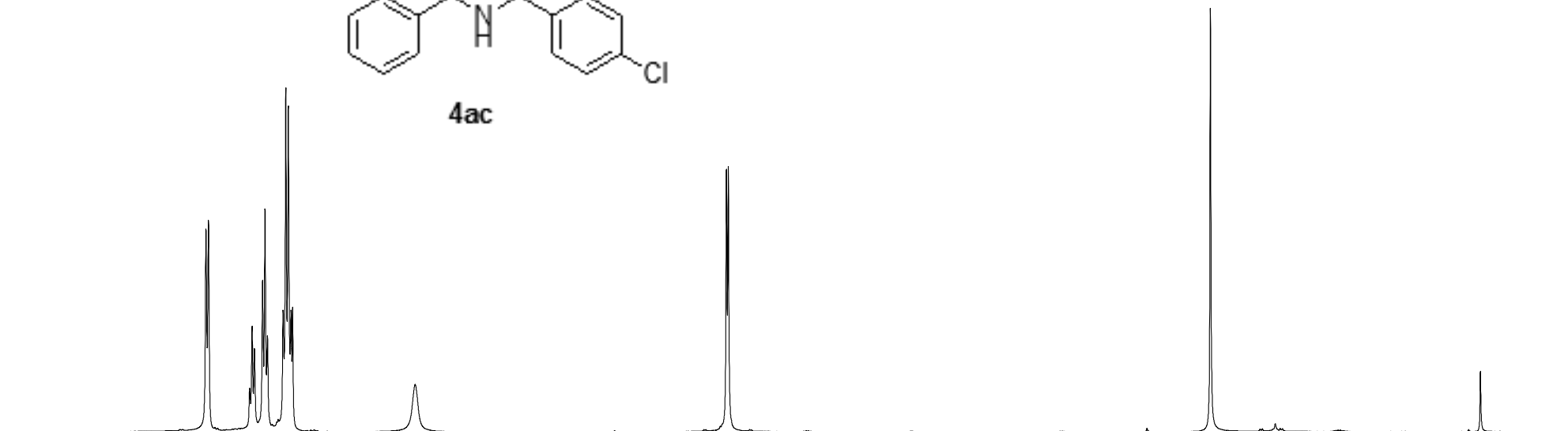
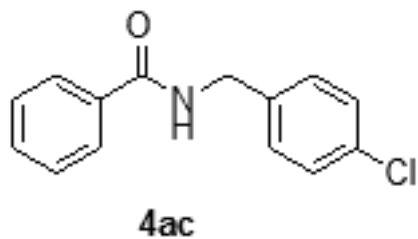
— 43.312



N-(4-chlorobenzyl)benzamide
Proton CDCl₃

7.791
7.776
7.524
7.509
7.495
7.445
7.430
7.415
7.320
7.303
7.288
7.271
7.261
6.514

4.611
4.599



8.5

8.0

7.5

7.0

6.5

6.0

5.5

5.0

4.5

4.0

3.5

3.0

2.5

2.0

1.5

1.0

0.5

ppm

2.00

1.09

2.07

4.01

1.00

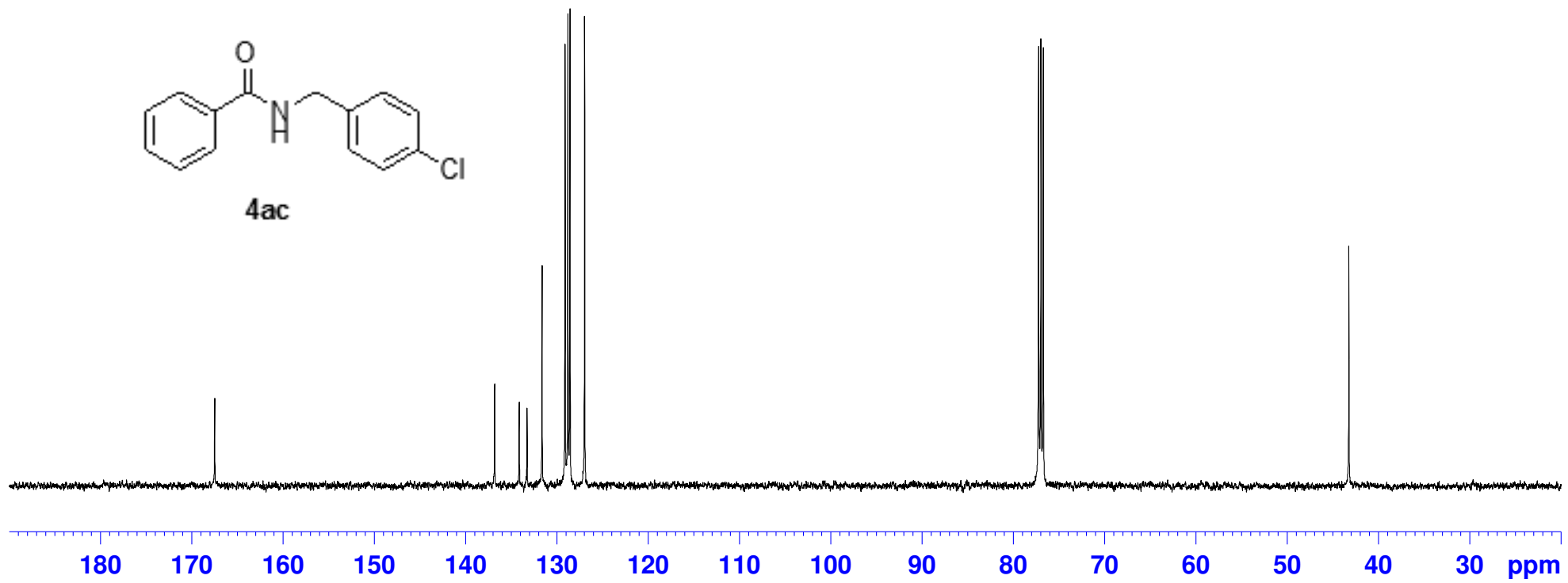
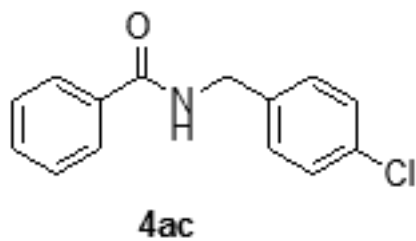
2.09

N-(4-chlorobenzyl)benzamide
C13CPD CDCl3

—167.471

136.808
134.112
133.253
131.607
129.085
128.774
128.548
126.946

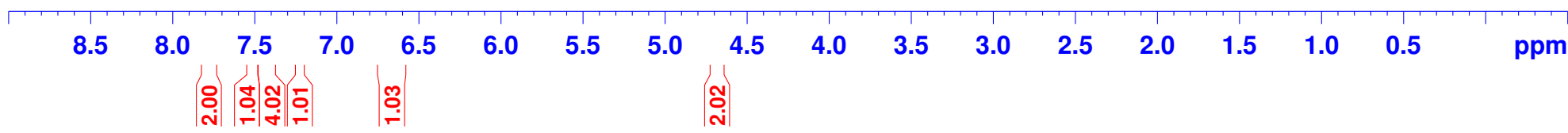
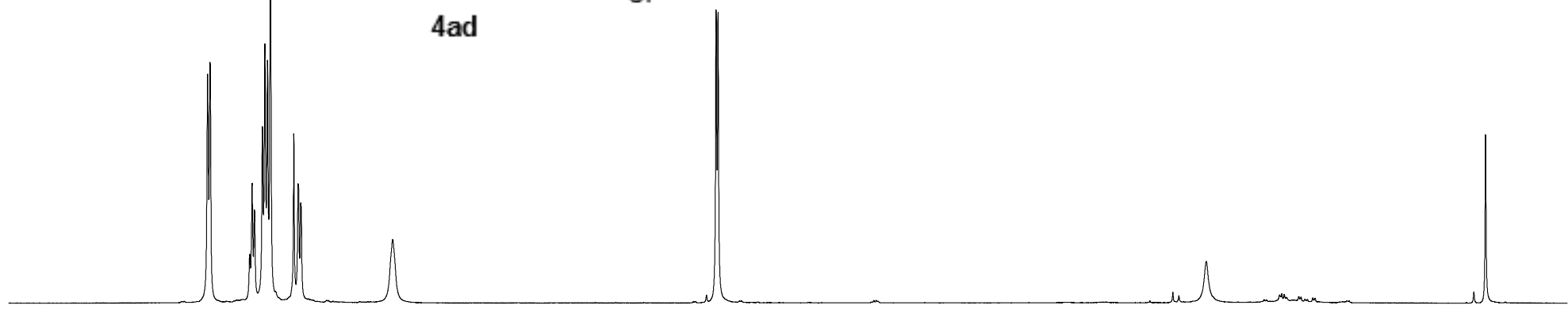
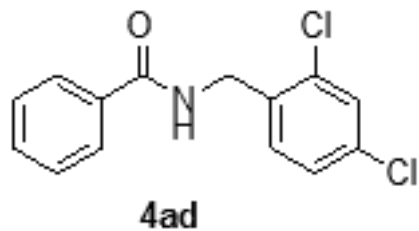
—43.267



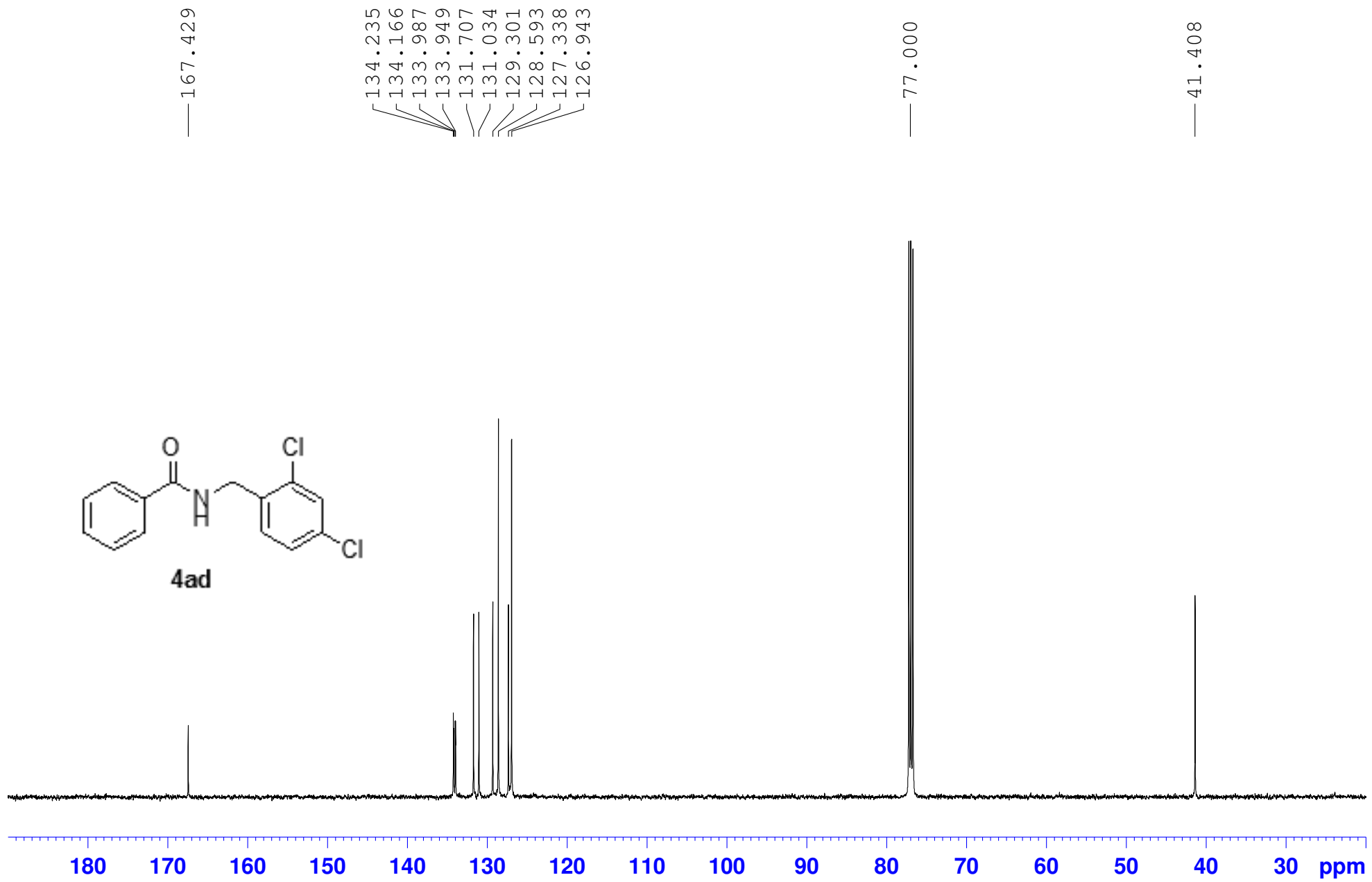
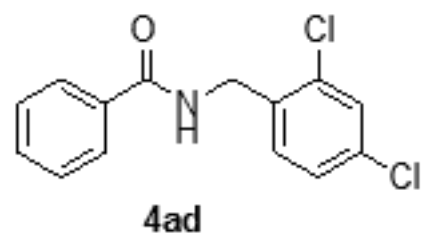
N-(2,4-dichlorobenzyl)benzamide
Proton CDCl₃

7.786
7.770
7.529
7.514
7.500
7.451
7.436
7.420
7.403
7.263
7.237
7.234
7.220
7.218
6.660

4.689
4.677



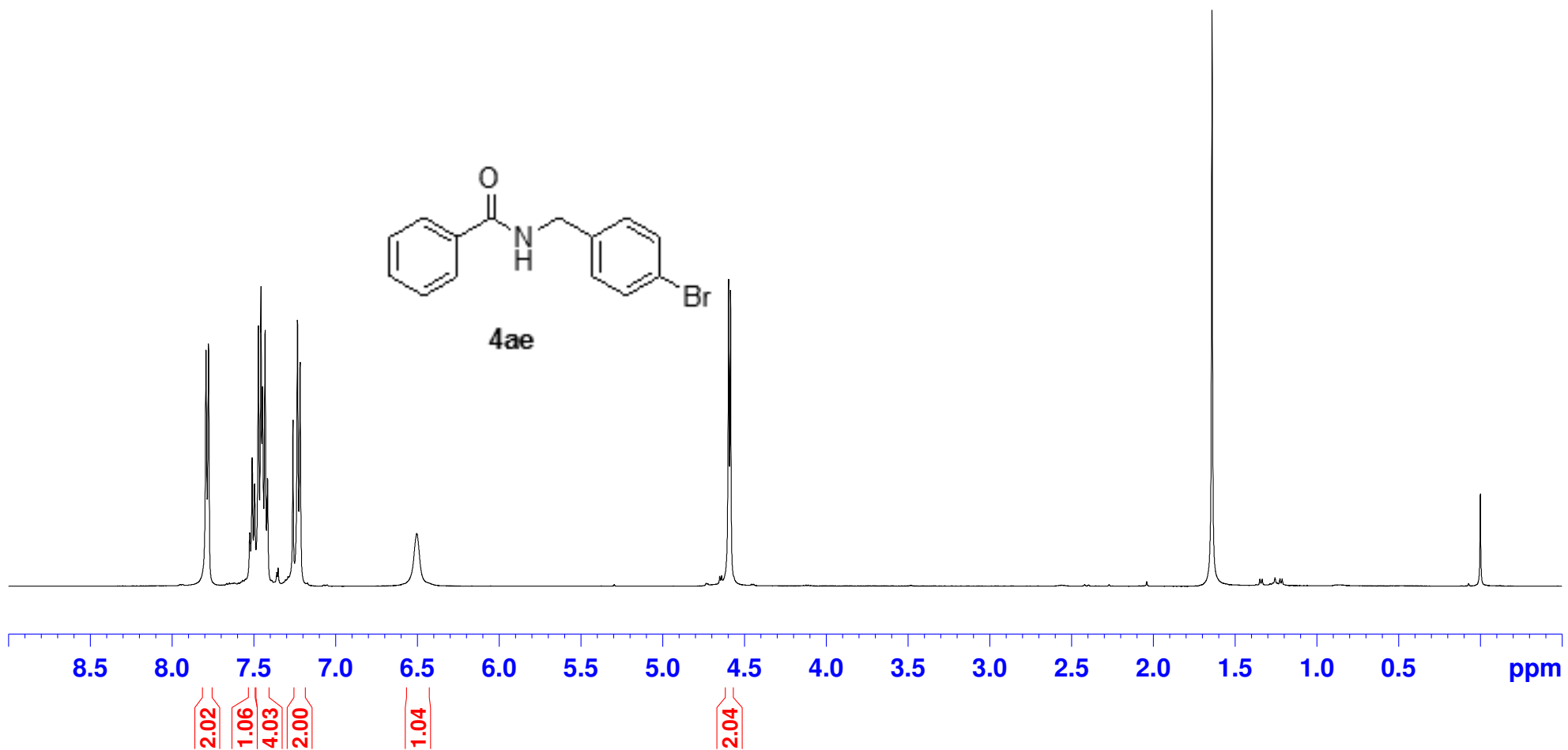
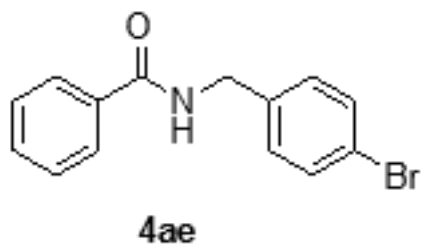
N-(2,4-dichlorobenzyl)benzamide
C13CPD CDC13



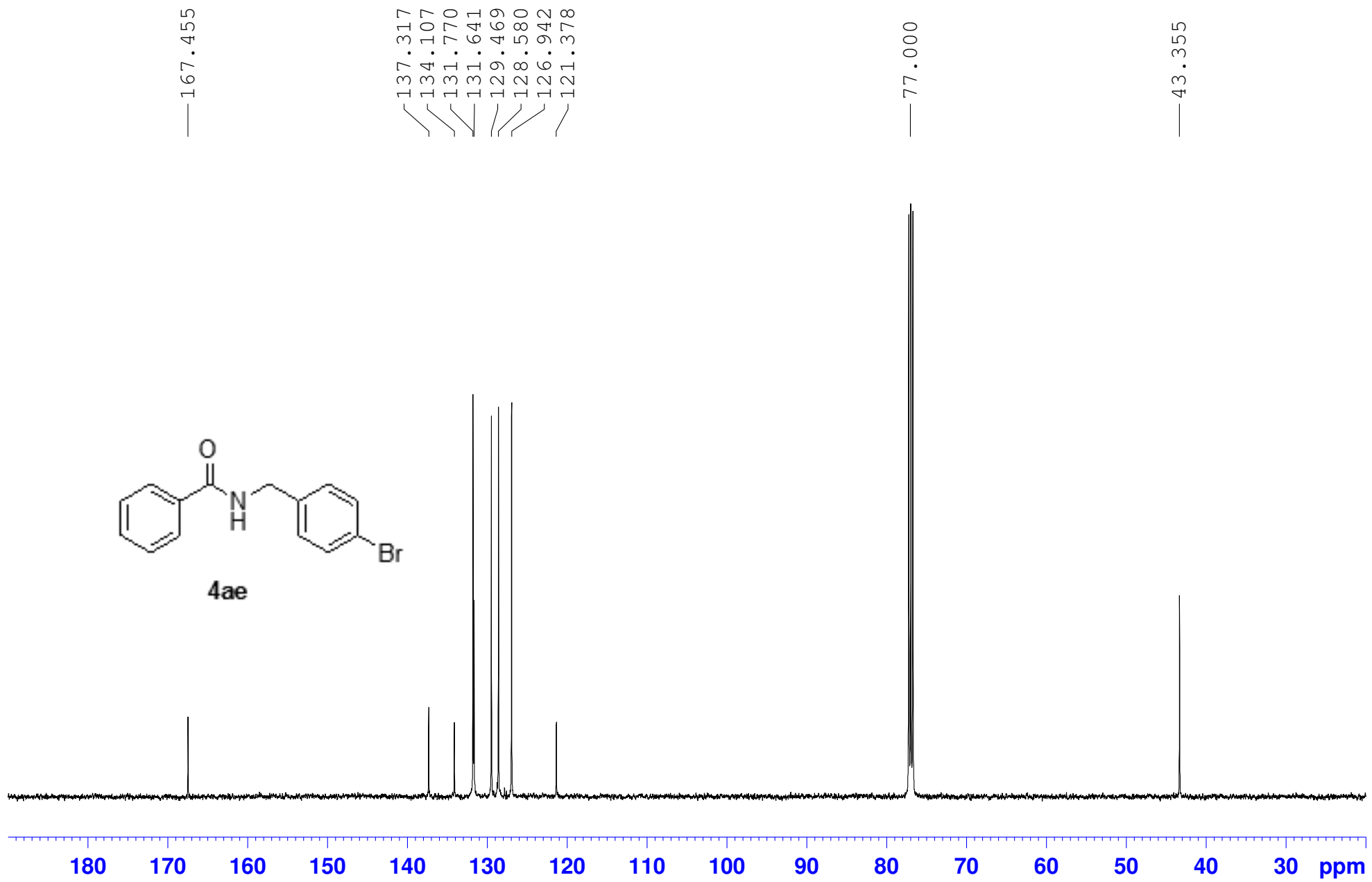
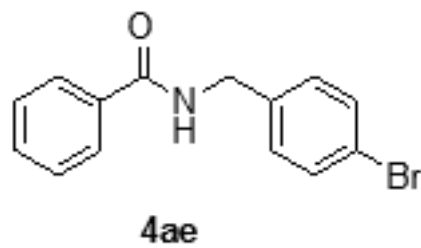
N-(4-bromobenzyl)benzamide
Proton CDCl₃

7.791
7.776
7.526
7.511
7.496
7.473
7.457
7.447
7.432
7.417
7.261
7.234
7.218
6.504

4.598
4.586



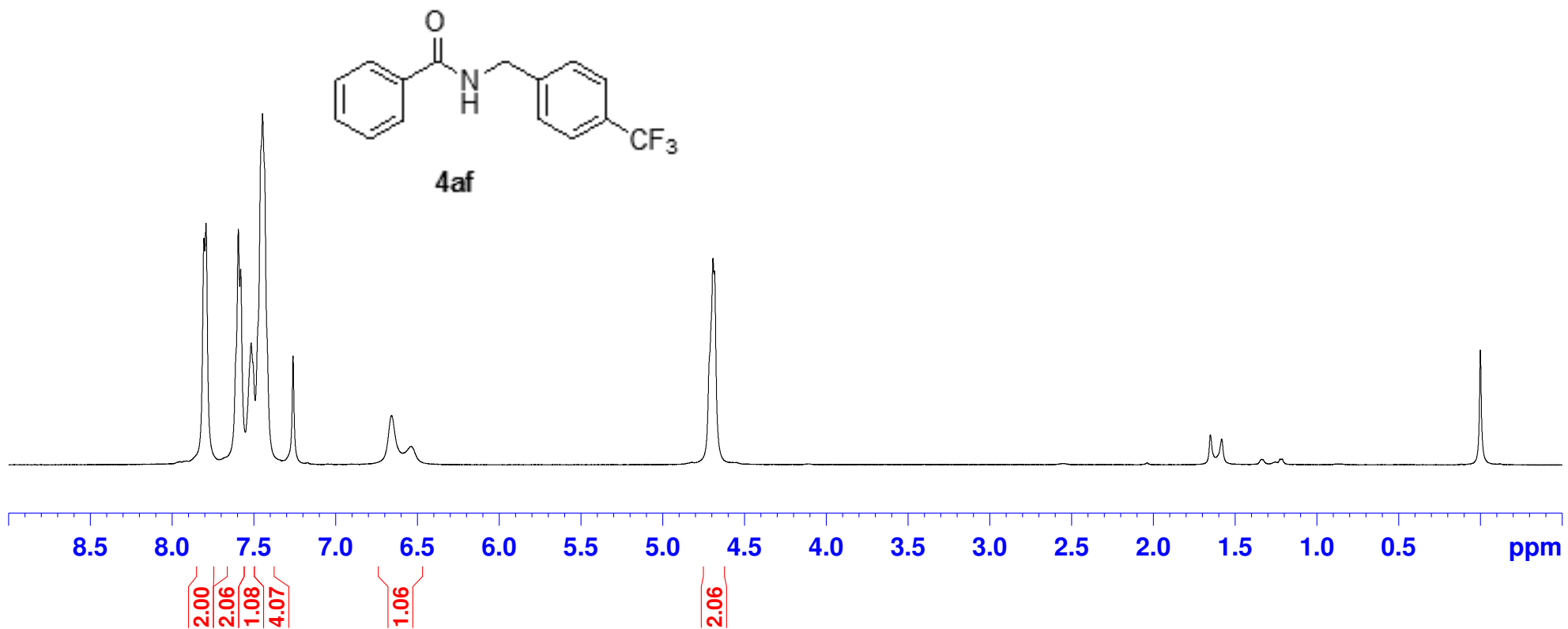
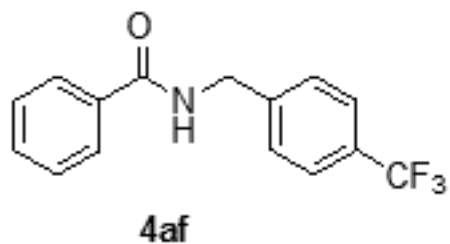
N-(4-bromobenzyl)benzamide
C13CPD CDCl3



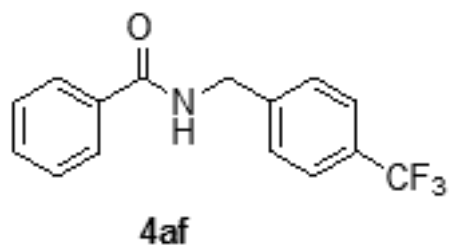
N-(4-(trifluoromethyl)benzyl)benzamide
Proton CDCl₃

7.806
7.793
7.611
7.596
7.582
7.527
7.518
7.507
7.477
7.459
7.447
7.435
7.419
7.261
6.660
6.541

4.716
4.693
4.683



N-(4-(trifluoromethyl)benzyl)benzamide
C13CPD CDCl3

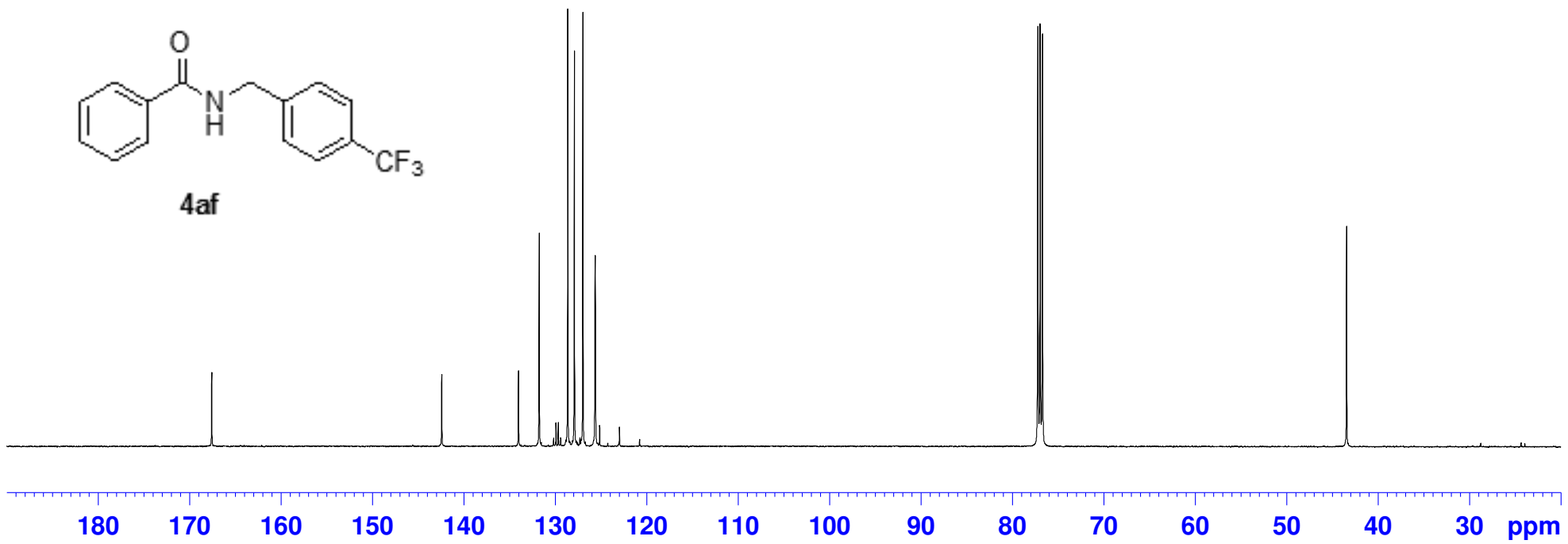


—167.571

142.411
134.018
131.749
130.173
129.914
129.658
129.401
128.628
127.898
127.302
126.968
125.661
125.634
125.606
125.576
125.140
122.977
120.812

—77.000

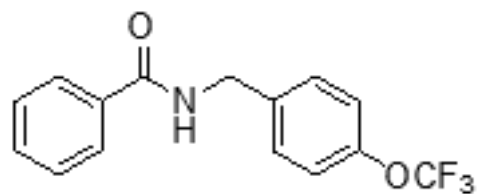
—43.475



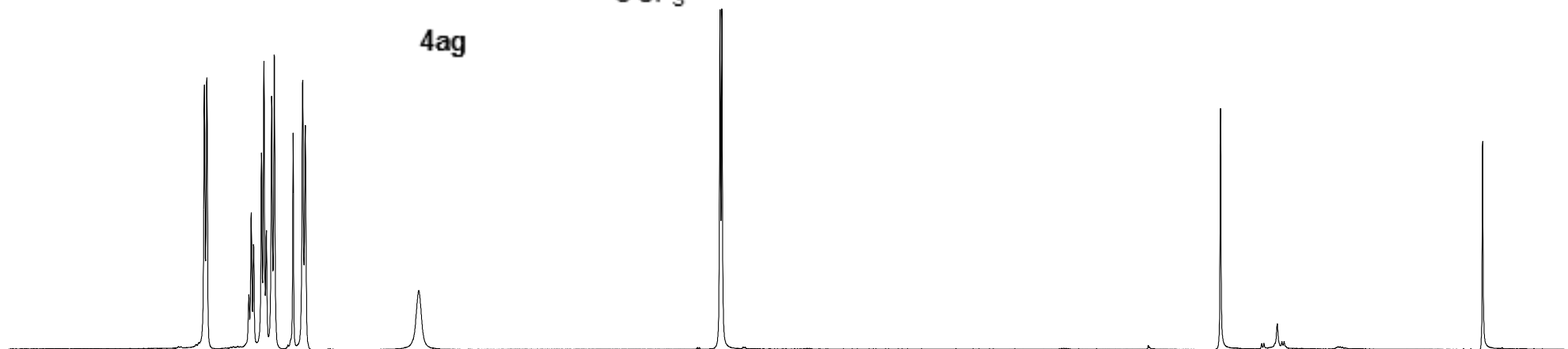
N-(4-(trifluoromethoxy)benzyl)benzamide
Proton CDCl₃

7.803
7.788
7.531
7.517
7.502
7.454
7.439
7.424
7.392
7.375
7.261
7.203
7.186
6.496

4.657
4.645



4ag



8.5

8.0

7.5

7.0

6.5

6.0

5.5

5.0

4.5

4.0

3.5

3.0

2.5

2.0

1.5

1.0

0.5

ppm

2.00

1.06

2.05

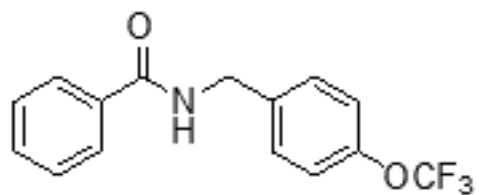
2.00

2.00

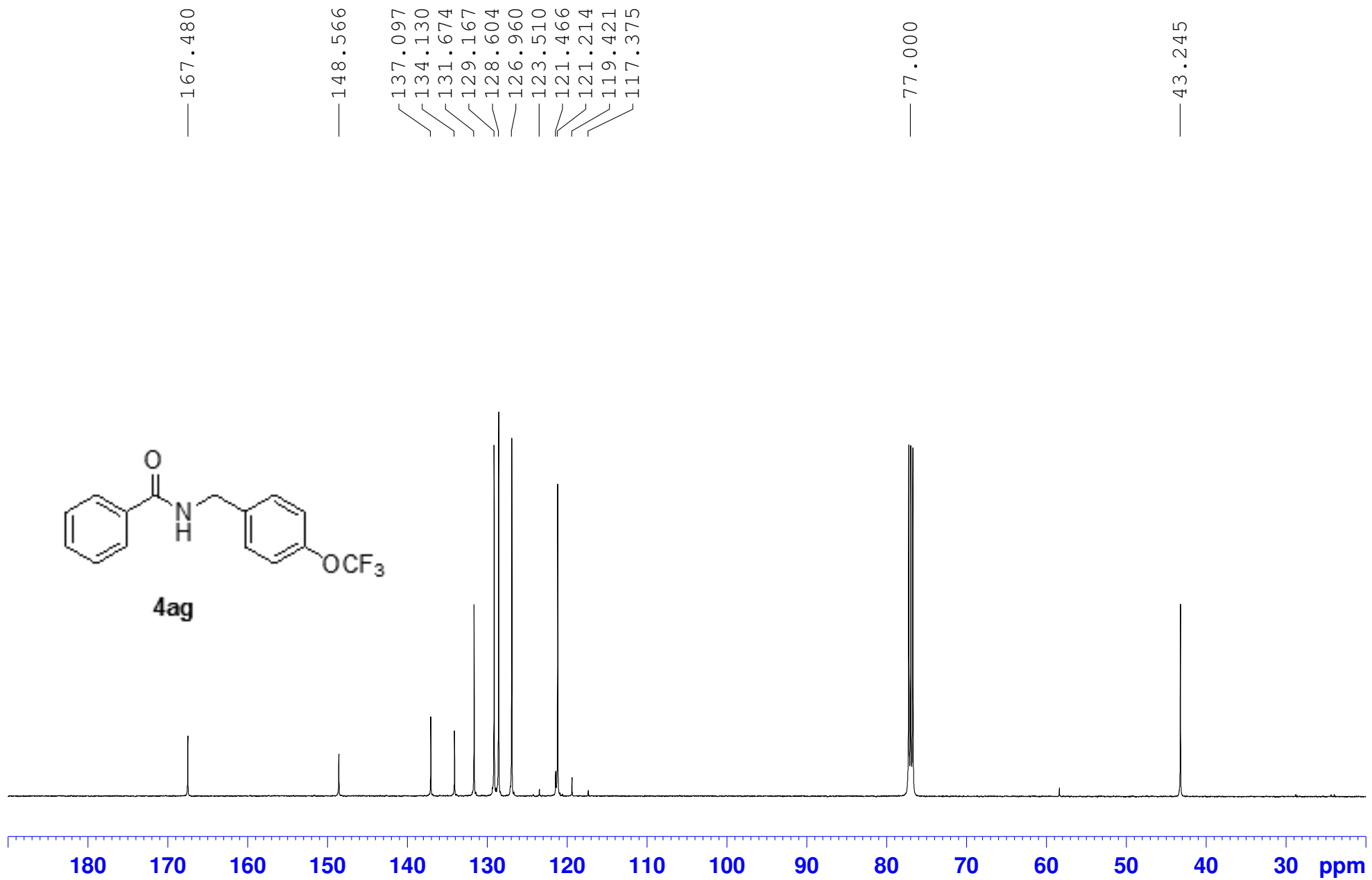
1.03

2.10

N-(4-(trifluoromethoxy)benzyl)benzamide
C13CPD CDCl3



4ag

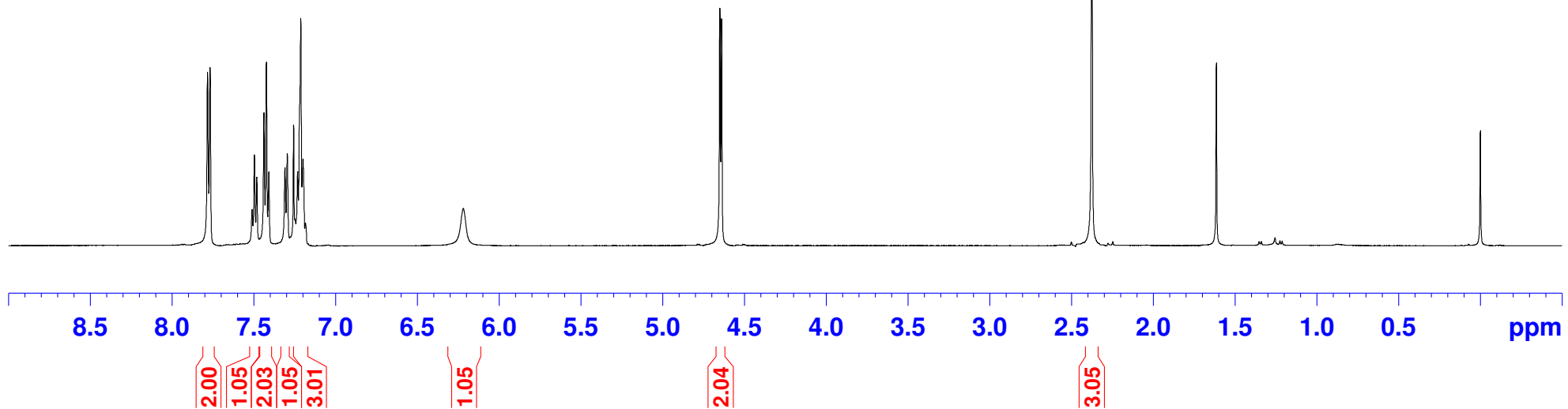
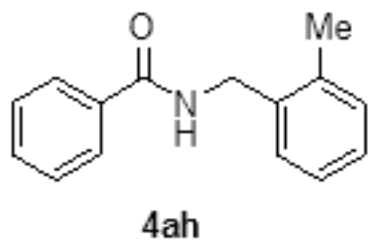


N-(2-methylbenzyl)benzamide
Proton CDCl₃

7.784
7.769
7.512
7.497
7.483
7.439
7.424
7.409
7.310
7.296
7.257
7.250
7.233
7.214
7.200
7.186
6.220

4.651
4.640

2.376



N-(2-methylbenzyl)benzamide
C13CPD CDCl3

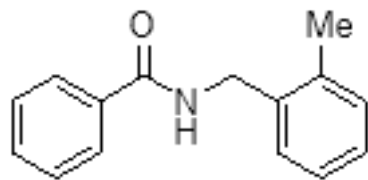
— 167.194

136.566
135.726
134.326
131.475
130.589
128.650
128.542
127.862
126.895
126.241

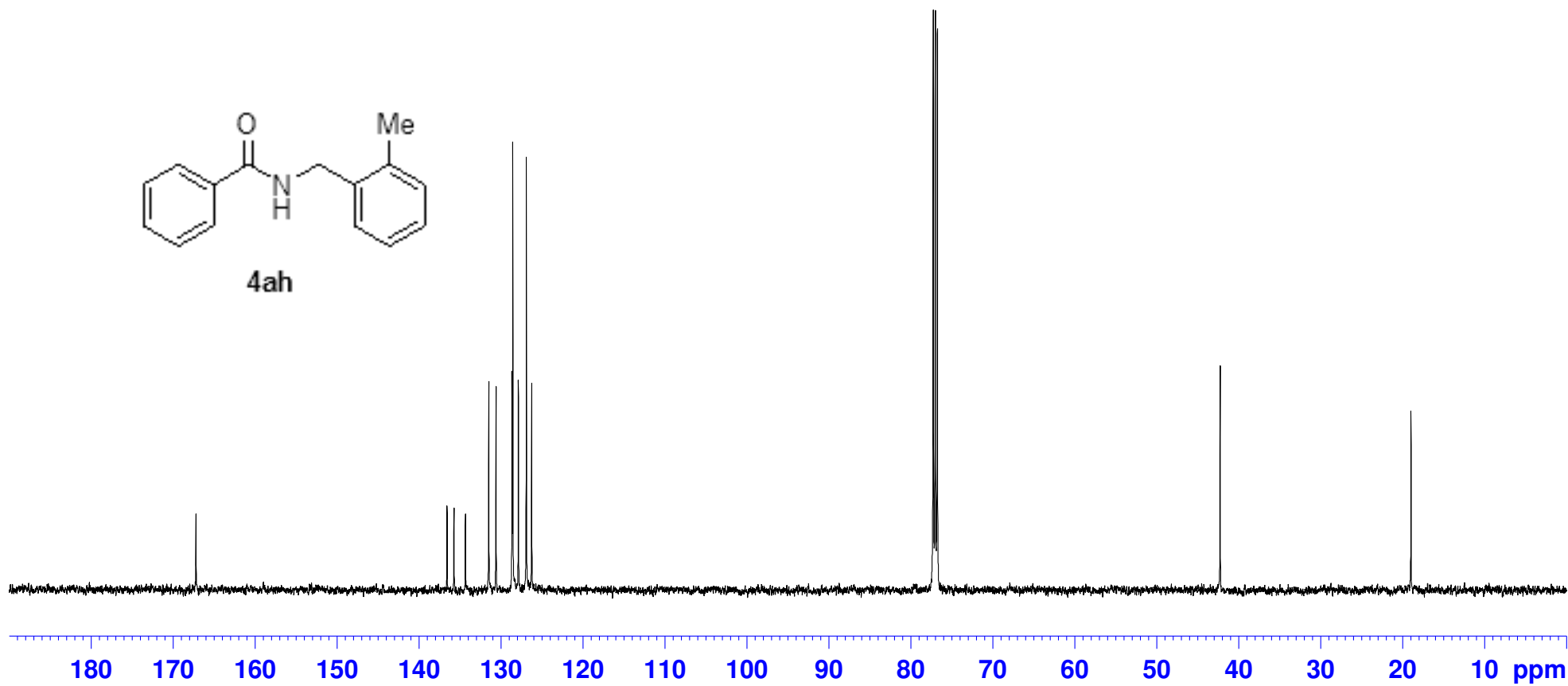
— 77.000

— 42.298

— 19.006



4ah

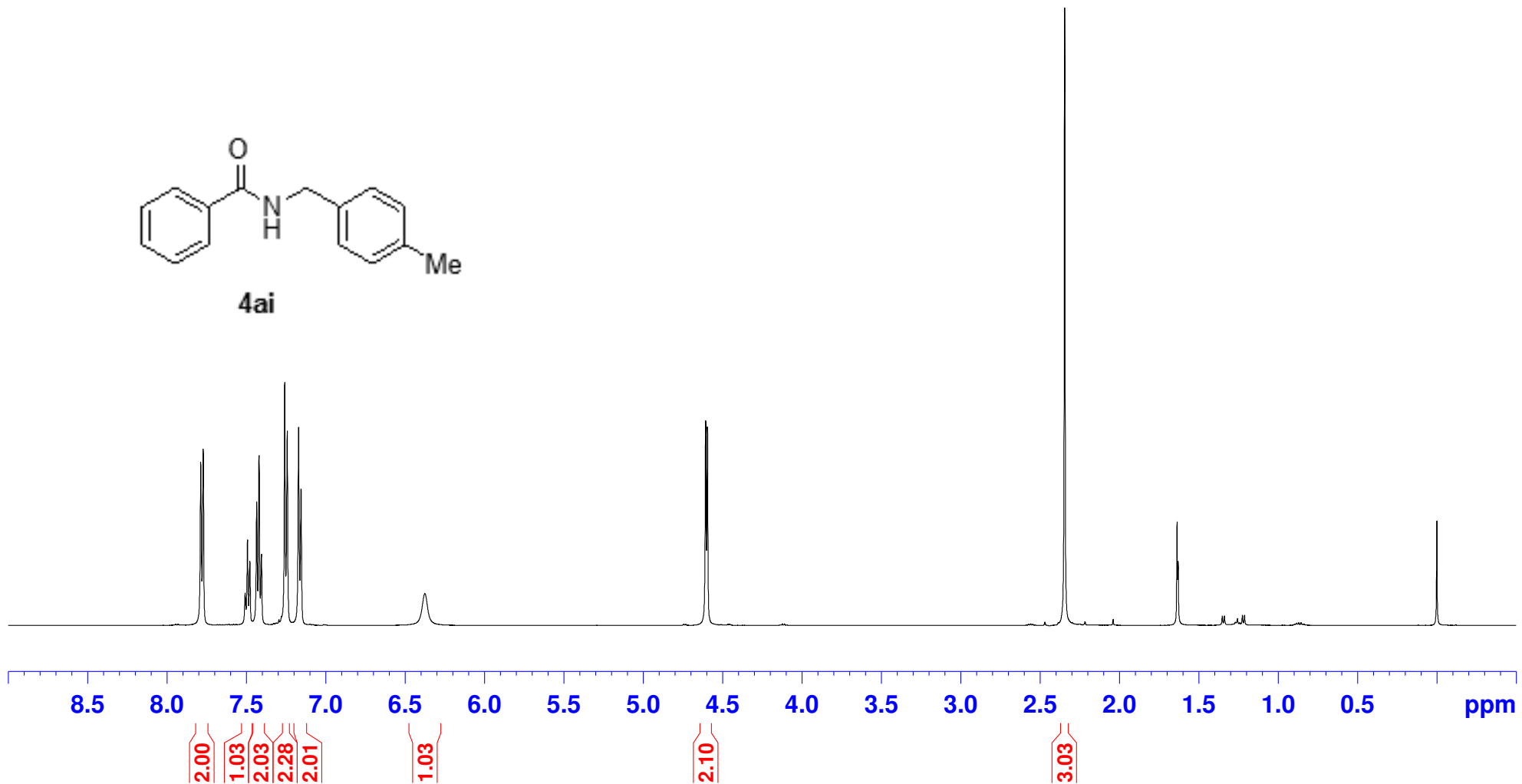
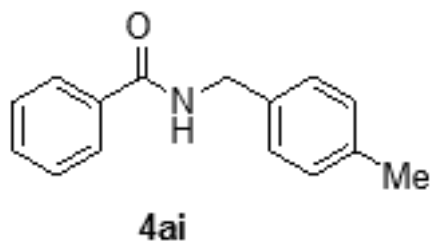


N-(4-methylbenzyl)benzamide
Proton CDCl₃

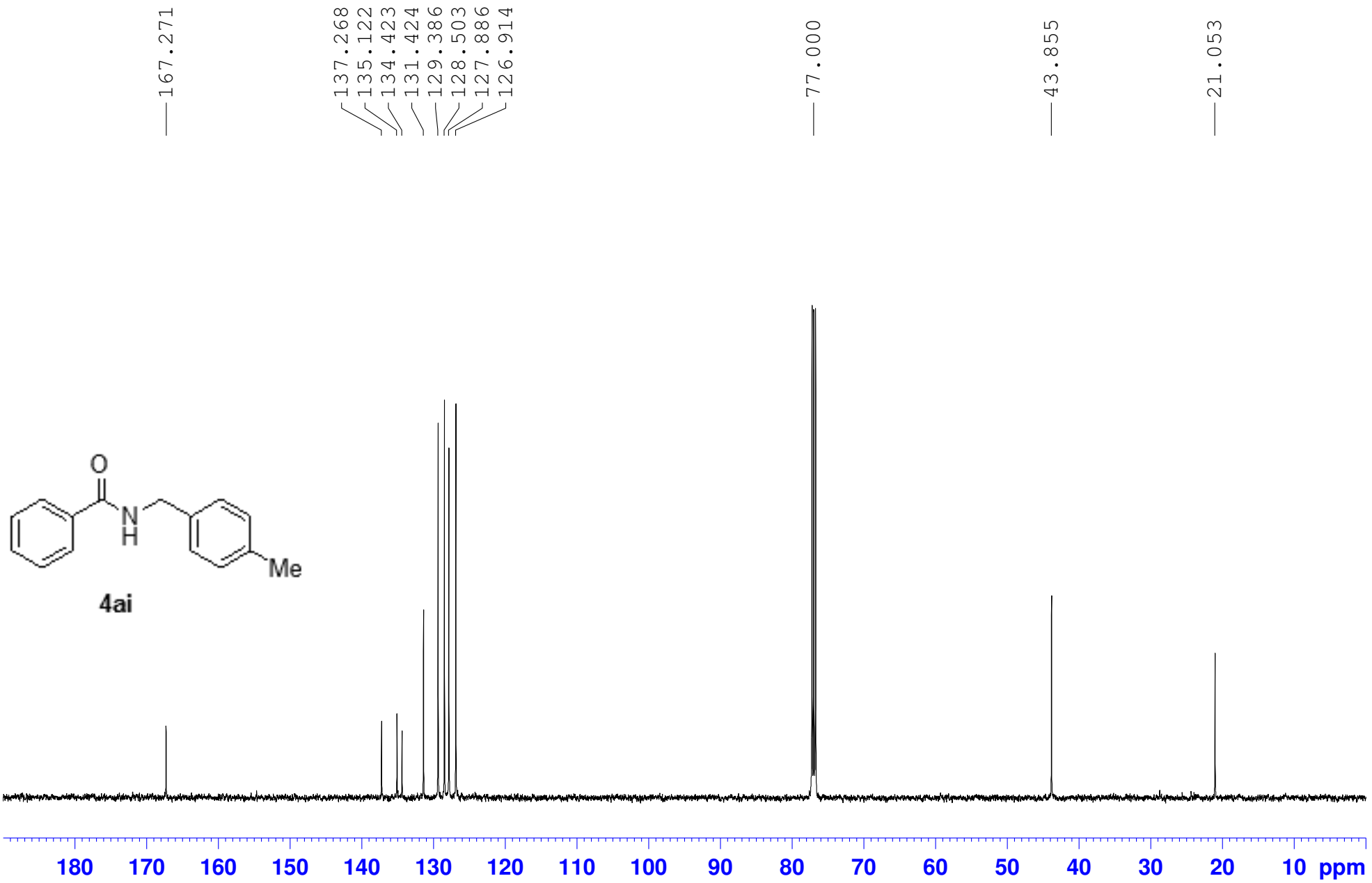
7.786
7.771
7.506
7.491
7.476
7.434
7.418
7.403
7.257
7.241
7.169
7.154
— 6.377

4.607
4.596

— 2.345



N-(4-methylbenzyl)benzamide
C13CPD CDC13

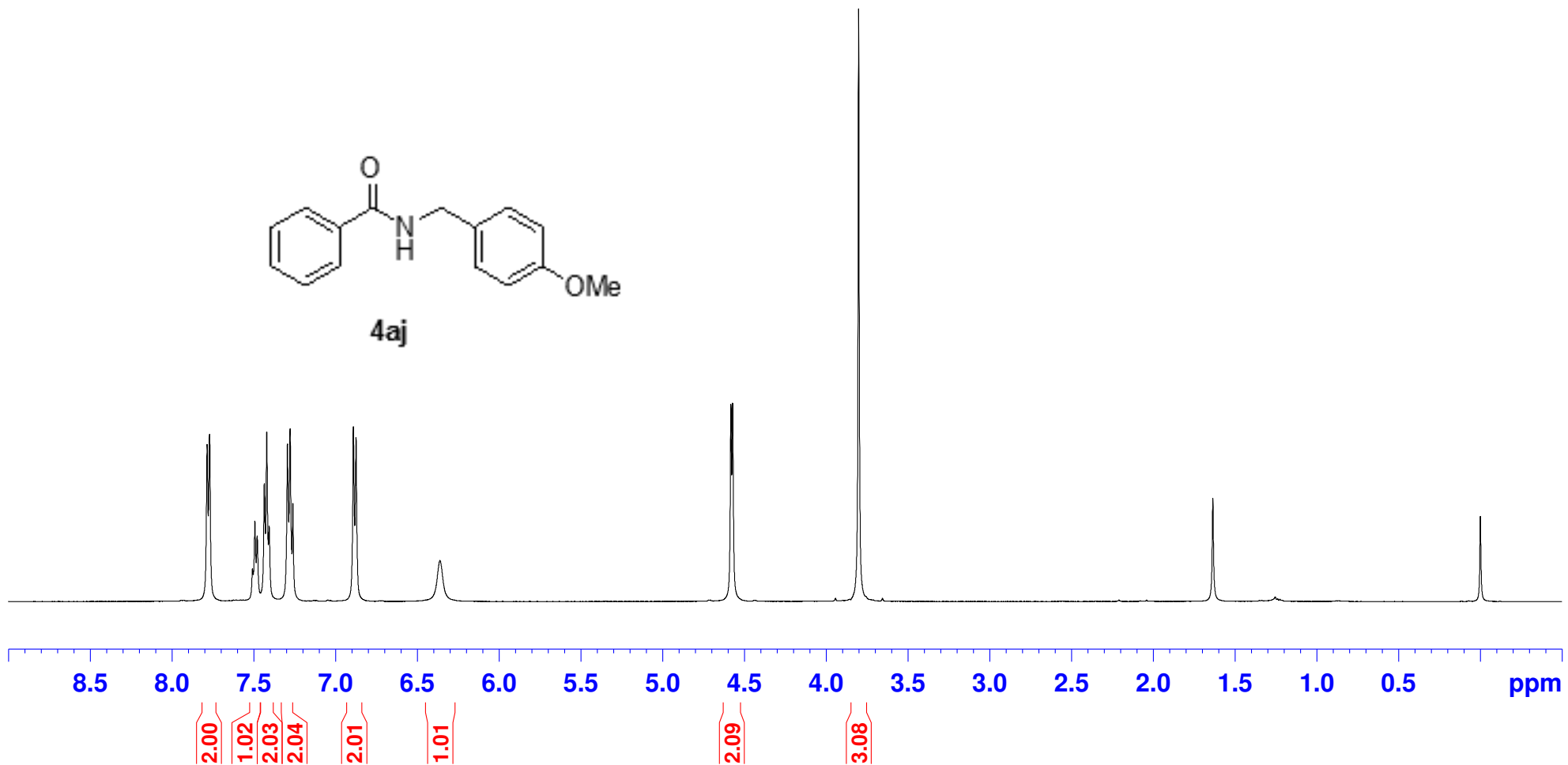
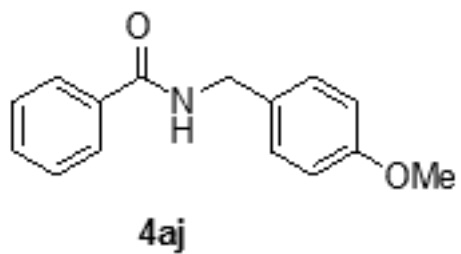


N-(4-methoxybenzyl)benzamide
Proton CDCl₃

7.784
7.769
7.506
7.492
7.478
7.434
7.419
7.404
7.293
7.276
7.260
6.892
6.876
6.363

4.583
4.573

3.802



N-(4-methoxybenzyl)benzamide
C13CPD CDC13

— 167.250

— 159.038

134.407

131.403

130.264

129.210

128.478

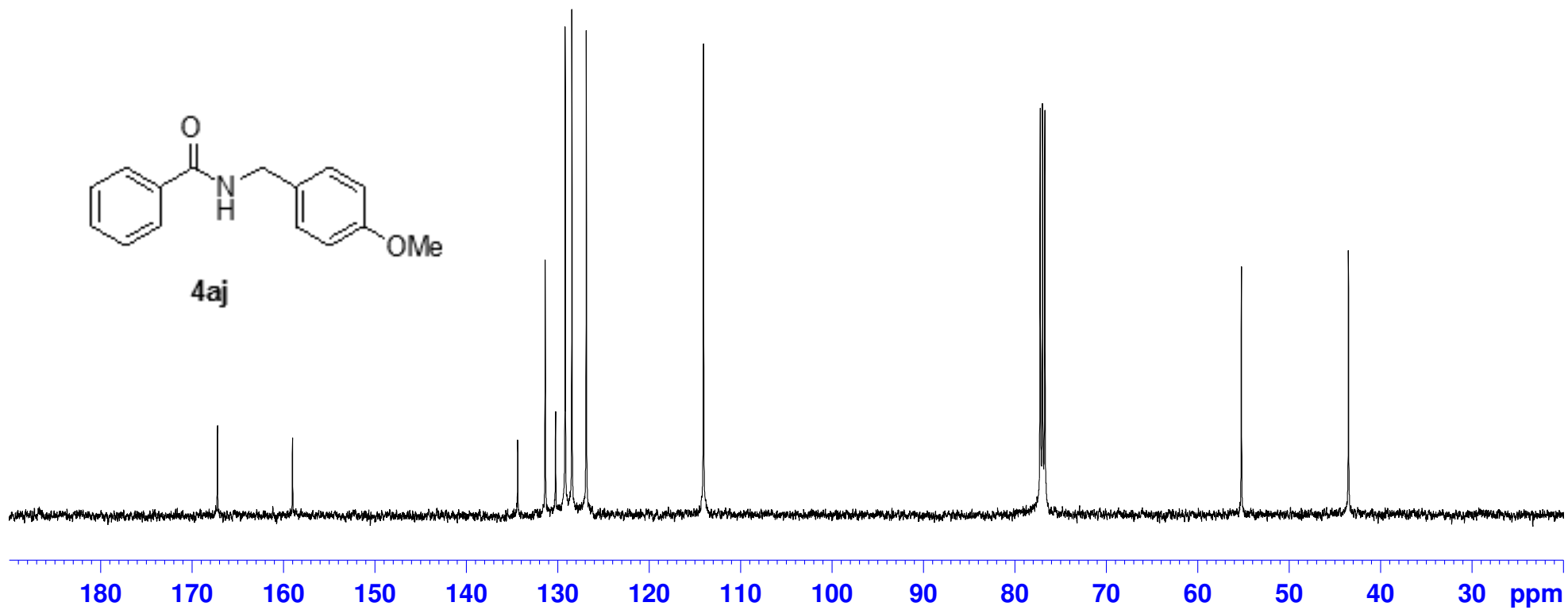
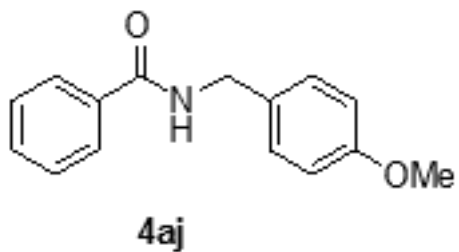
126.908

— 114.091

— 77.000

— 55.249

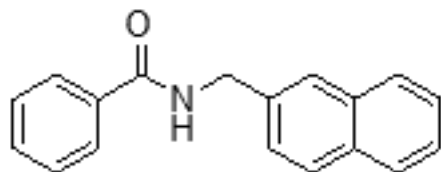
— 43.534



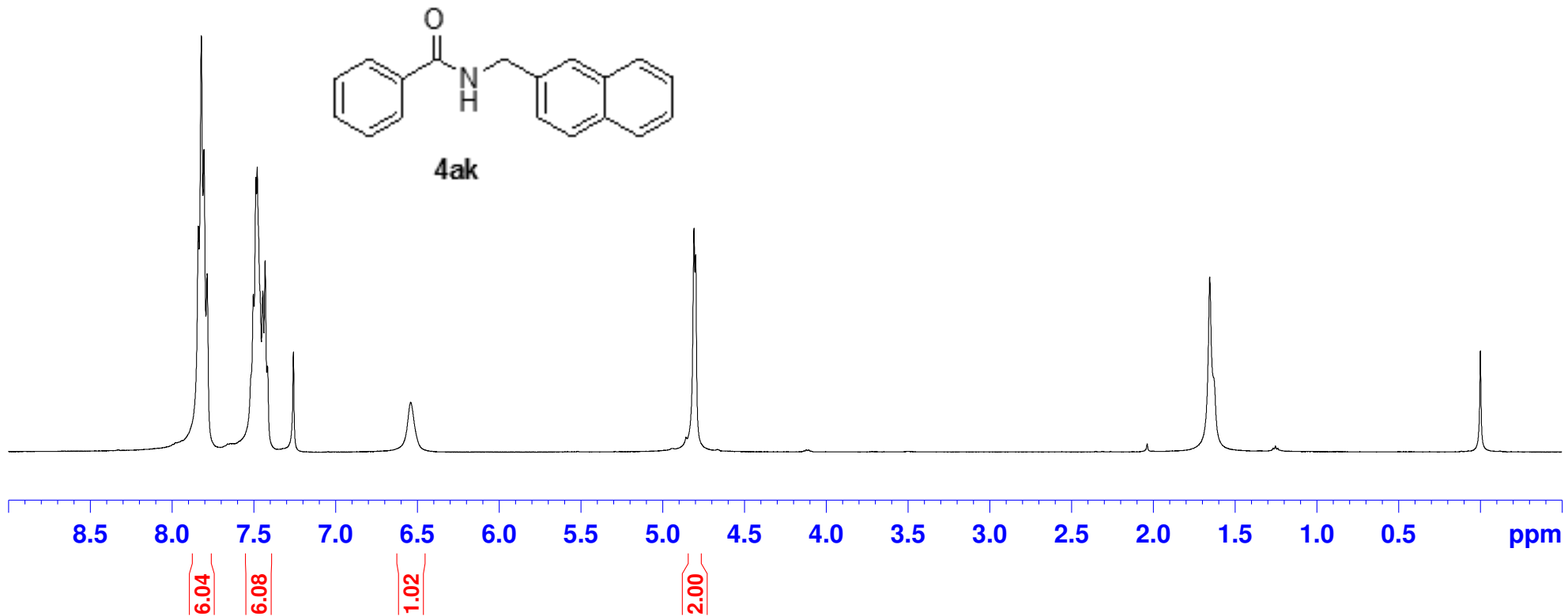
N-(naphthalen-2-ylmethyl)benzamide
Proton CDCl₃

7.838
7.820
7.803
7.784
7.501
7.486
7.478
7.444
7.429
7.415
7.256
— 6.541

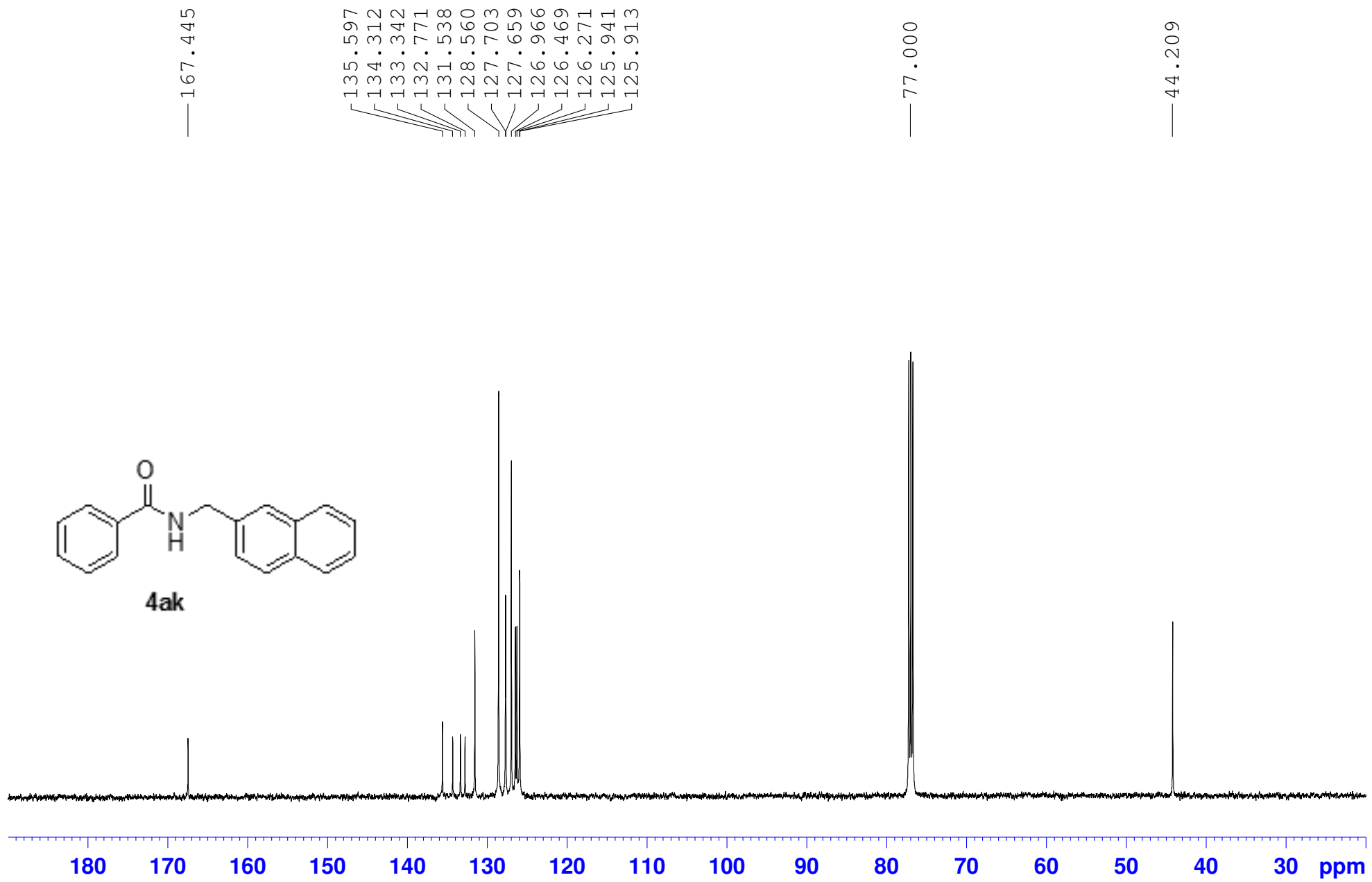
4.809
4.799



4ak



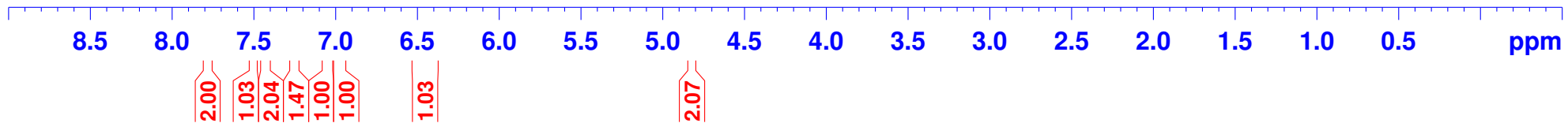
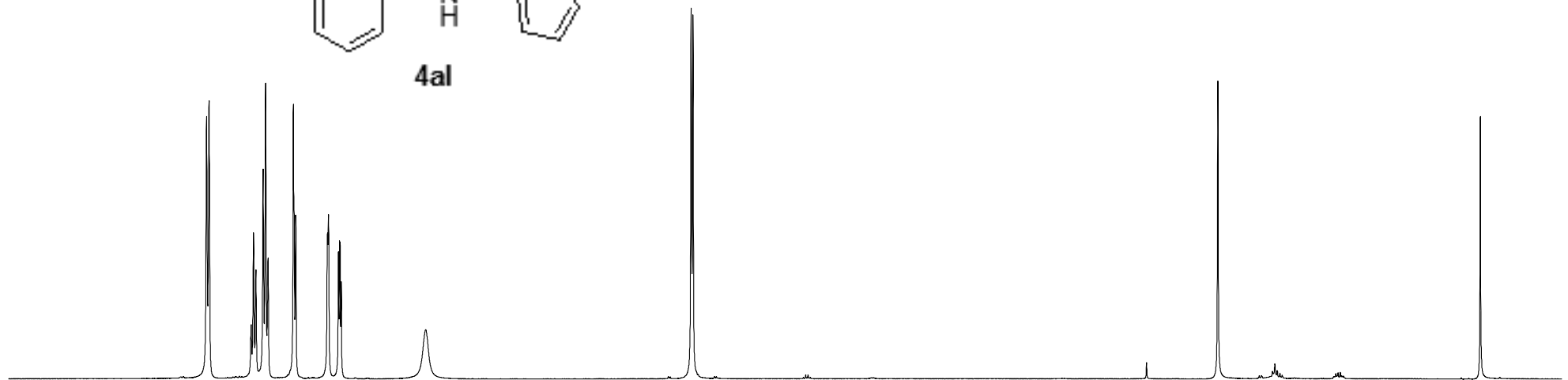
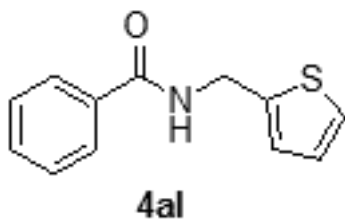
N-(naphthalen-2-ylmethyl)benzamide
C13CPD CDC13



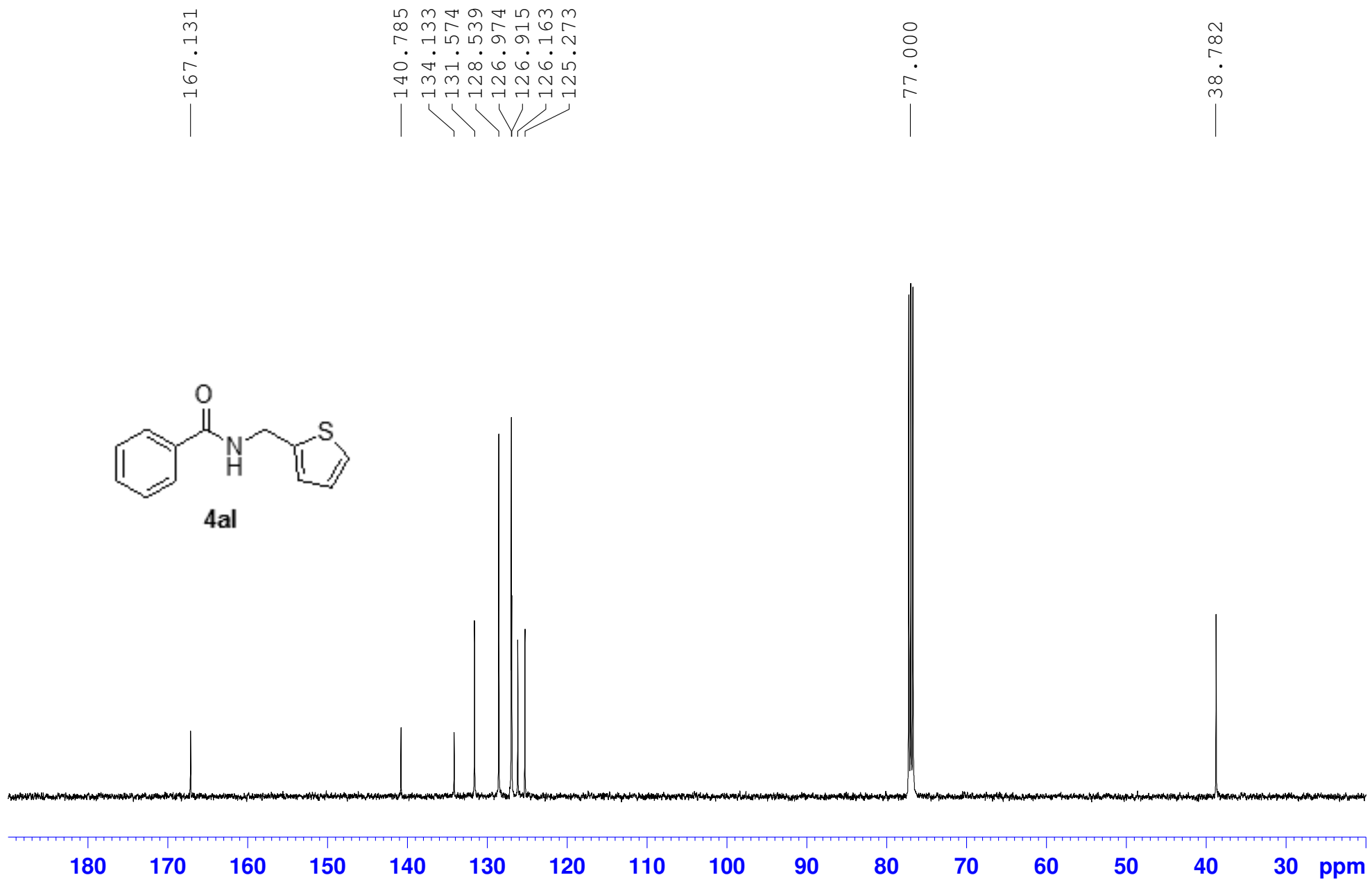
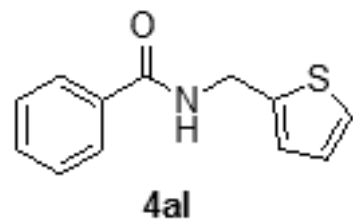
N-(thiophen-2-ylmethyl)benzamide
Proton CDCl₃

7.790
7.775
7.517
7.503
7.488
7.444
7.428
7.414
7.259
7.256
7.245
7.050
7.044
6.983
6.976
6.973
6.966
6.450

4.827
4.815



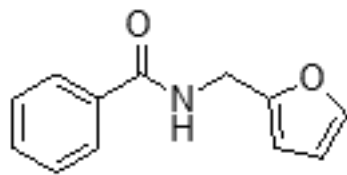
N-(thiophen-2-ylmethyl)benzamide
C13CPD CDCl3



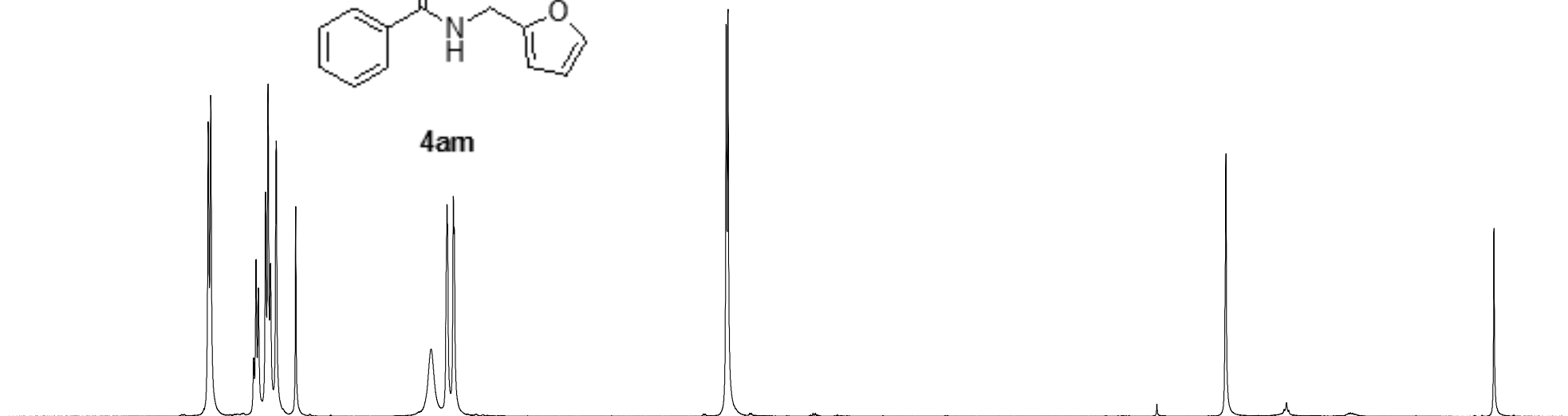
N-(furan-2-ylmethyl)benzamide
Proton CDCl₃

7.792
7.777
7.516
7.502
7.487
7.444
7.429
7.414
7.379
7.261
6.441
6.344
6.306
6.301

4.652
4.642



4am



8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

2.00
1.03
2.06
1.01

1.01
1.01
1.09

2.08

N-(furan-2-ylmethyl)benzamide
C13CPD CDC13

— 167.188

— 151.175

— 142.242

— 134.141

— 131.552

— 128.515

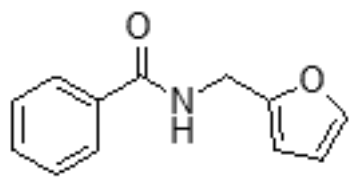
— 126.966

— 110.474

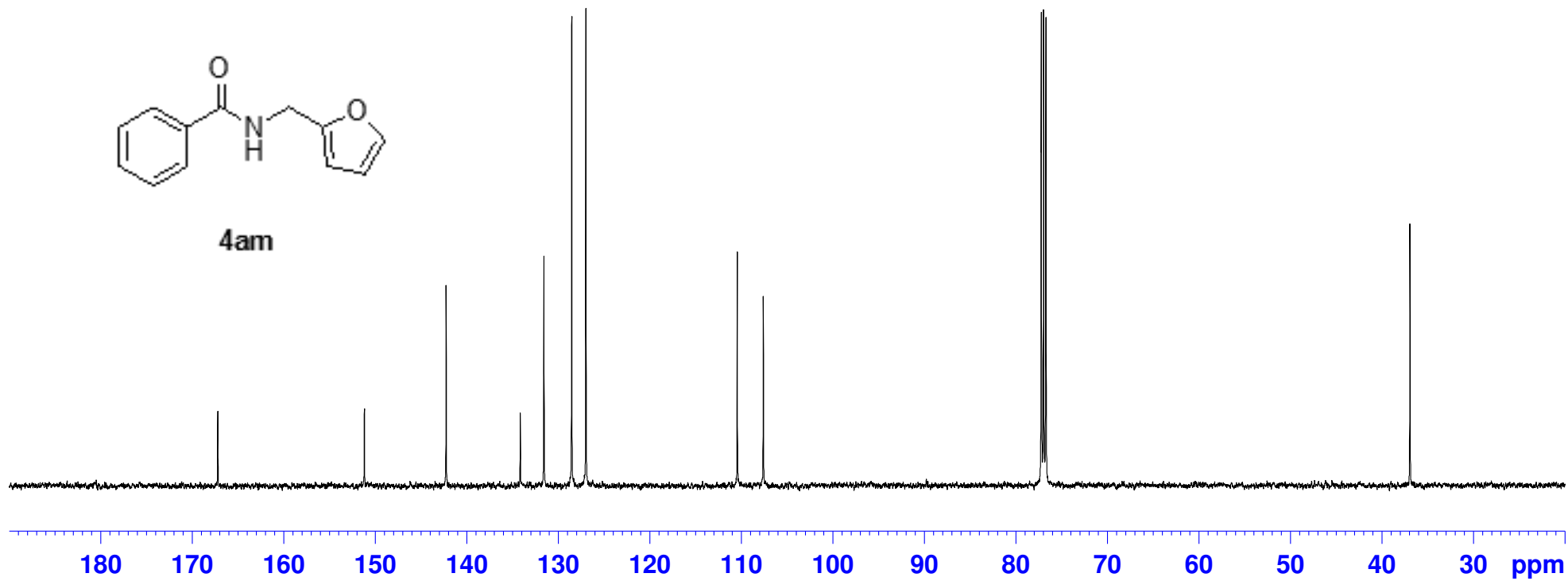
— 107.626

— 77.000

— 36.966



4am

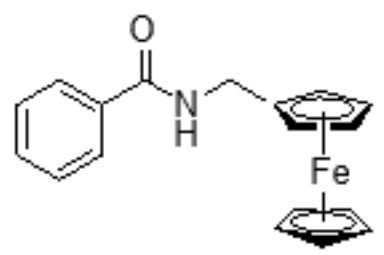


N-(Ferrocenemethyl)benzamide
Proton CDCl₃

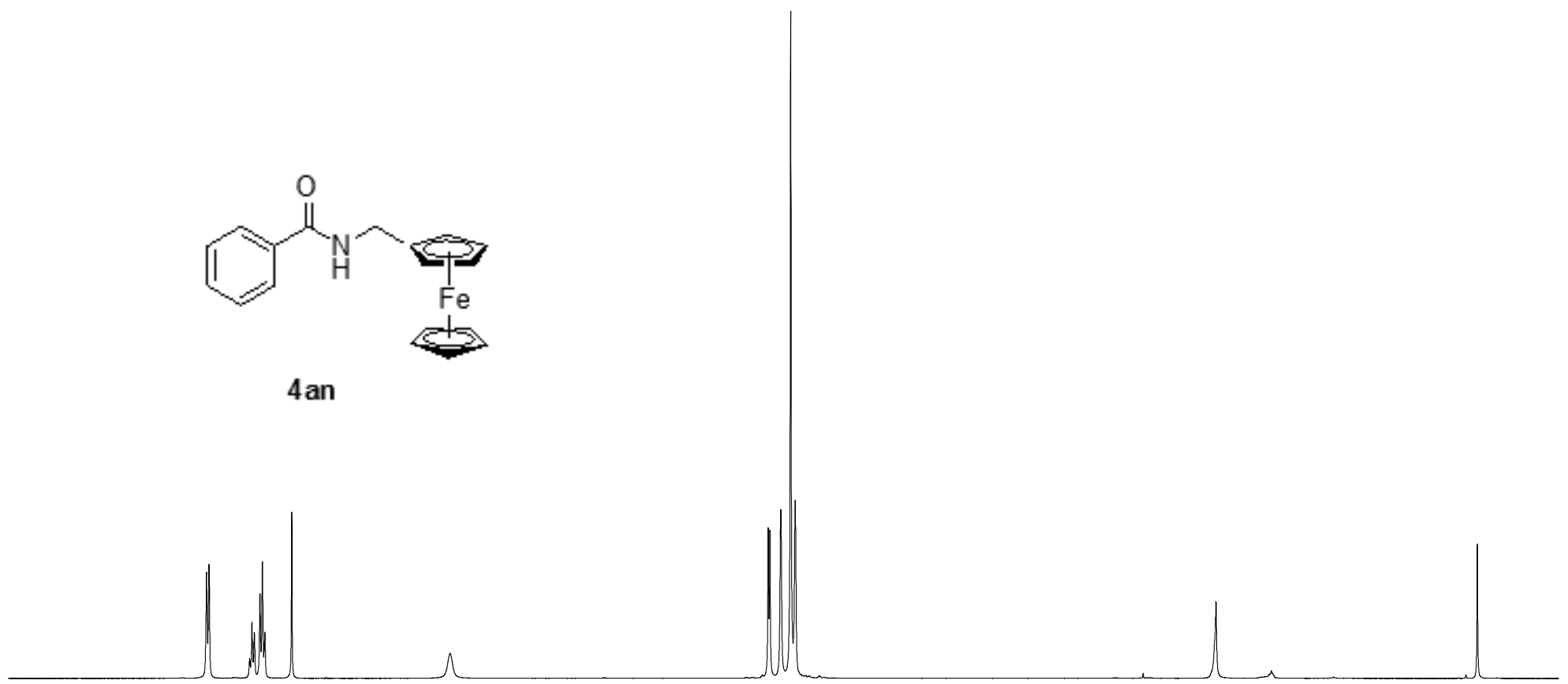
7.785
7.770
7.521
7.507
7.492
7.458
7.442
7.428
7.263

— 6.295

4.346
4.335
4.269
4.208
4.180



4an



8.5

8.0

7.5

7.0

6.5

6.0

5.5

5.0

4.5

4.0

3.5

3.0

2.5

2.0

1.5

1.0

0.5

ppm

2.00

1.03

2.01

1.06

2.05

2.08

4.96

2.03

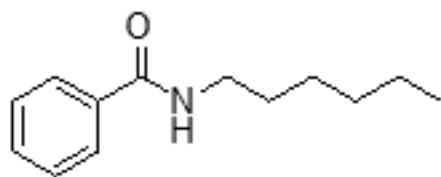
N-hexylbenzamide
Proton CDCl₃

7.765
7.750
7.502
7.487
7.473
7.439
7.424
7.409
7.263

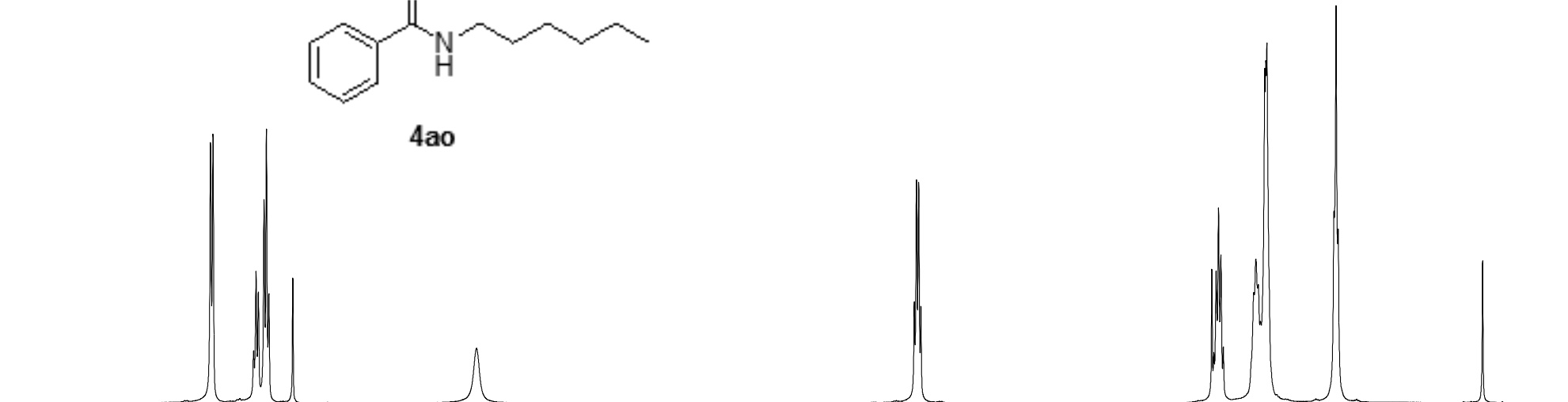
6.143

3.470
3.457
3.444
3.430

1.642
1.627
1.613
1.598
1.583
1.397
1.385
1.370
1.357
1.331
1.324
1.317
0.908
0.895
0.882



4ao



8.5

8.0

7.5

7.0

6.5

6.0

5.5

5.0

4.5

4.0

3.5

3.0

2.5

2.0

1.5

1.0

0.5

ppm

2.00

1.04

2.00

1.04

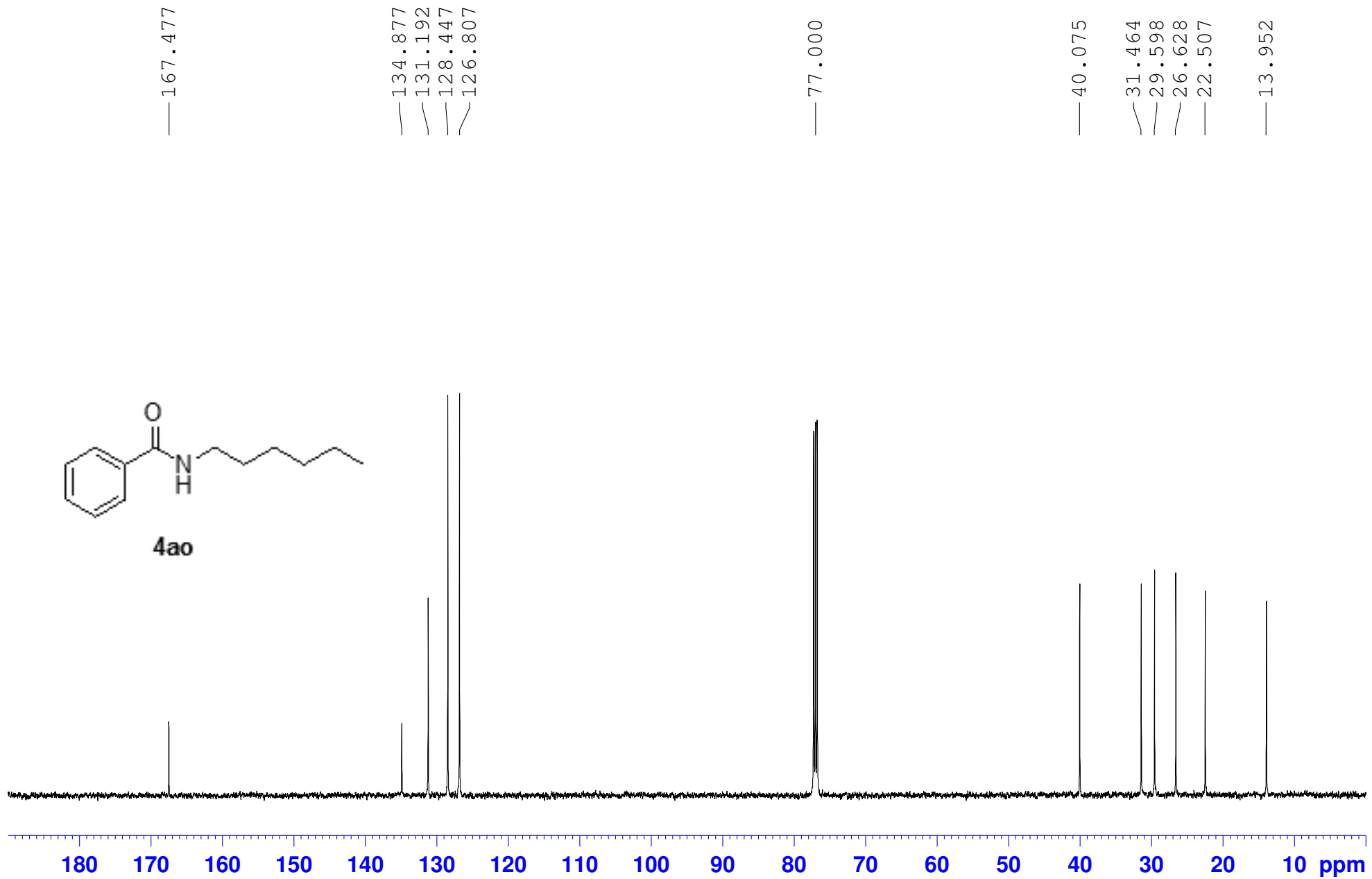
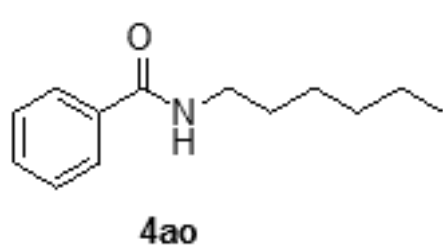
2.07

2.08

6.14

3.06

N-hexylbenzamide
C13CPD CDC13



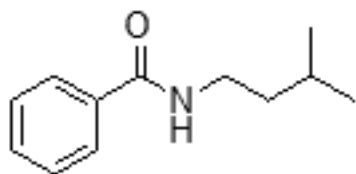
N-isopentylbenzamide
Proton CDCl₃

7.761
7.746
7.501
7.487
7.472
7.437
7.422
7.407
7.263

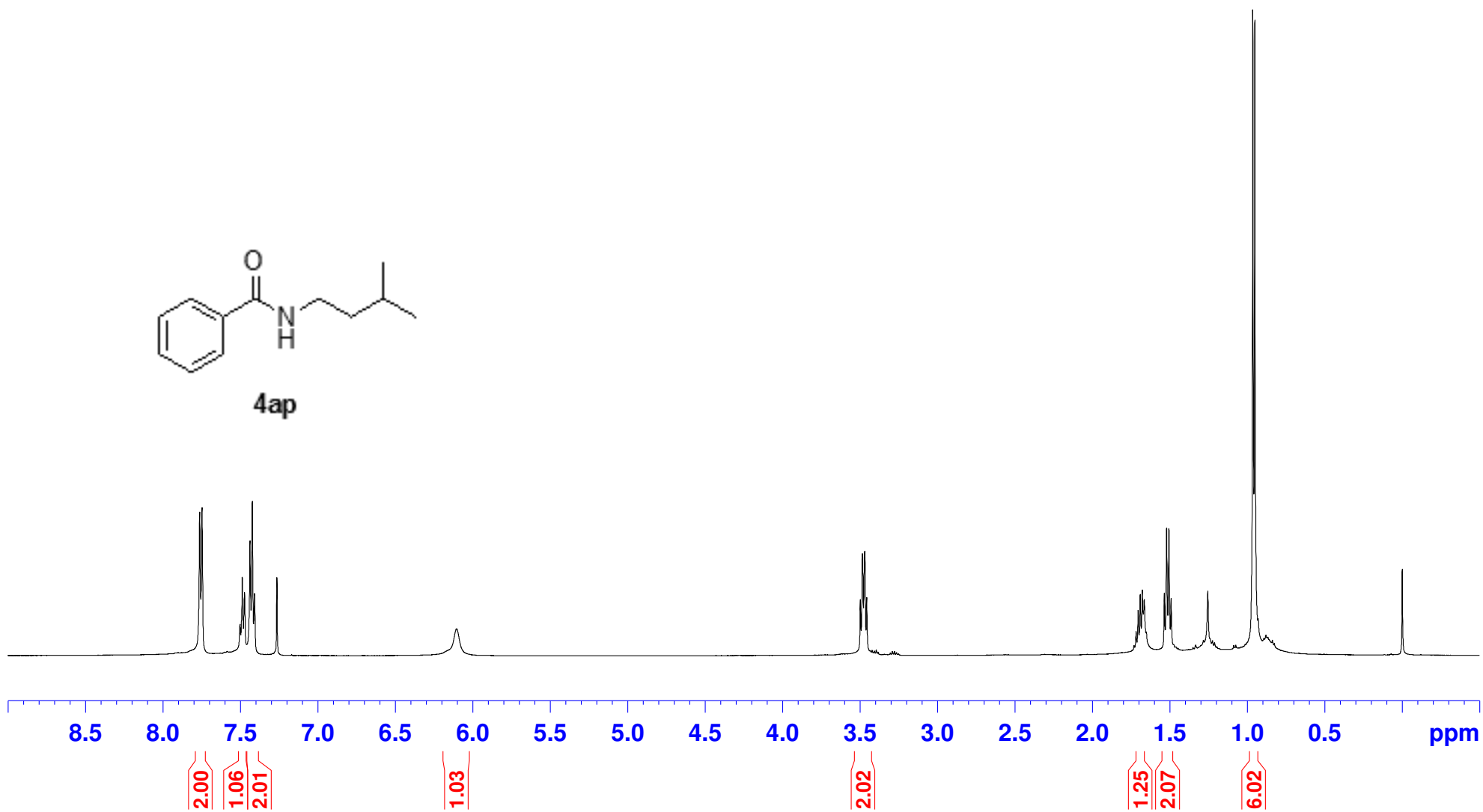
6.106

3.498
3.486
3.470
3.457

1.732
1.718
1.705
1.692
1.678
1.665
1.652
1.536
1.522
1.506
1.492
0.965
0.952



4ap



N-isopentylbenzamide
C13CPD CDC13

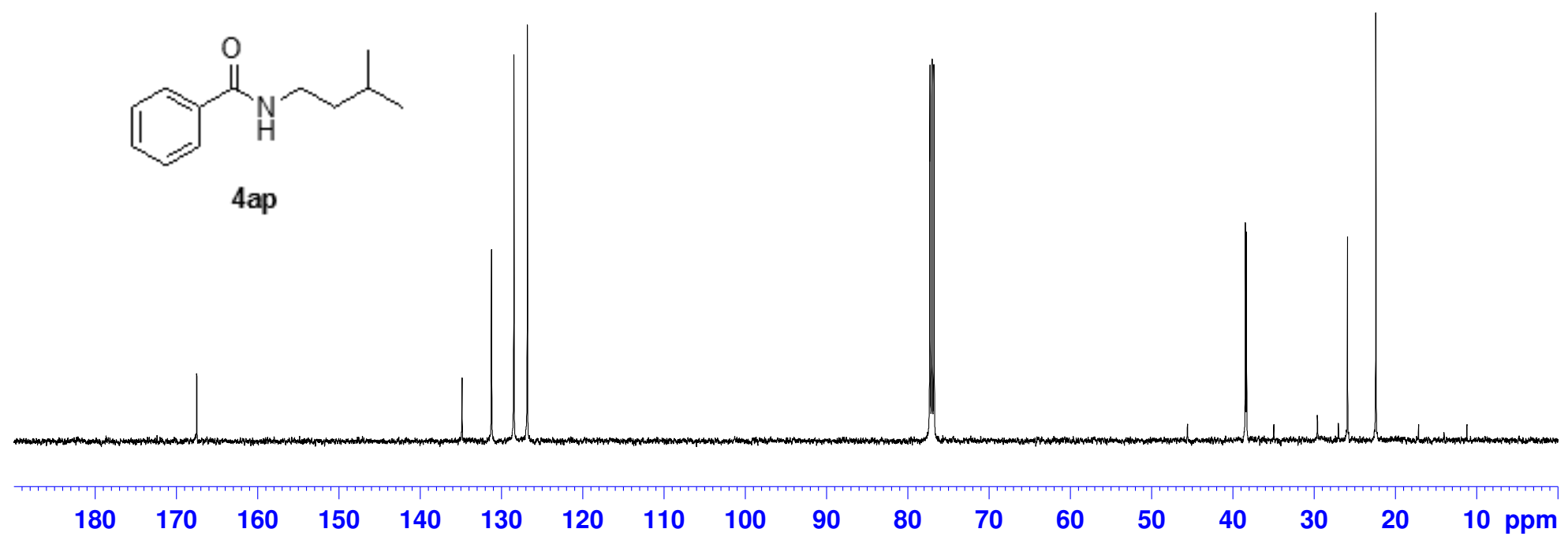
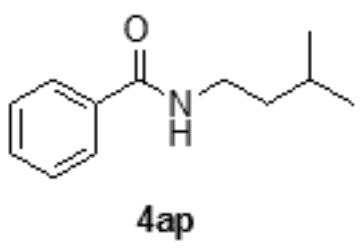
— 167.476

— 134.830
— 131.202
— 128.444
— 126.794

— 77.000

< 38.489
< 38.348

— 25.919
— 22.431

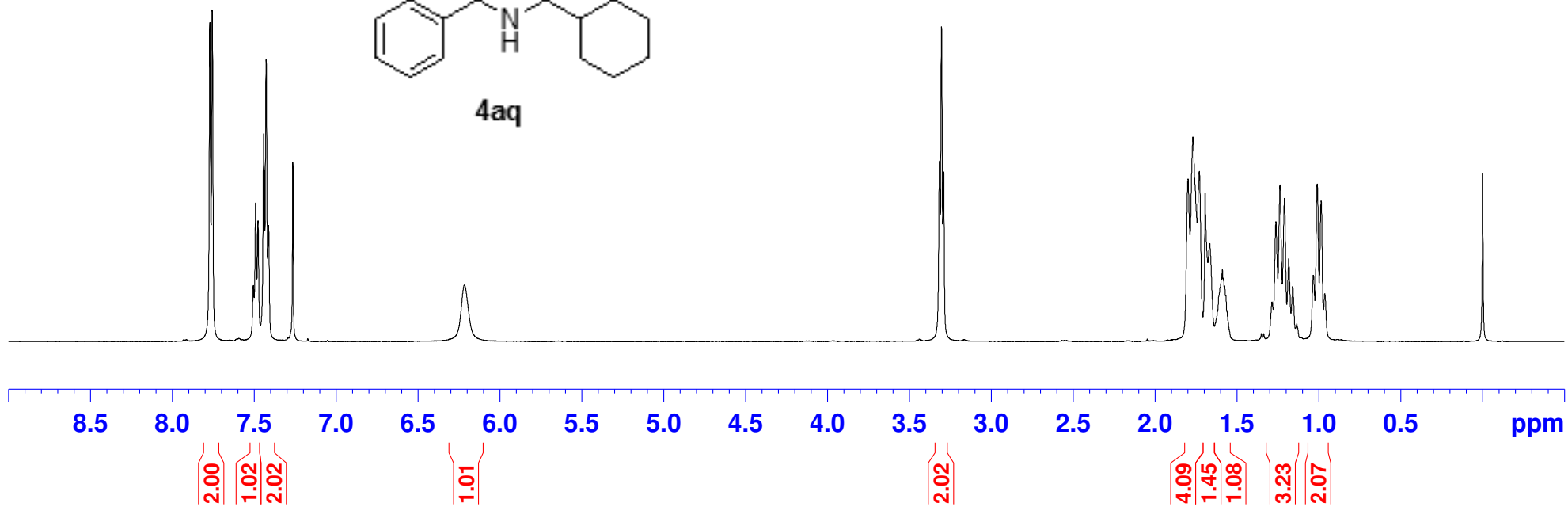
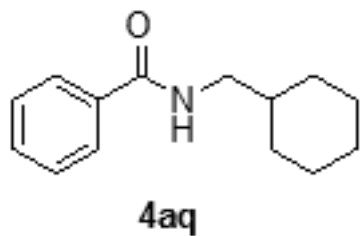


N-(cyclohexylmethyl)benzamide
Proton CDCl₃

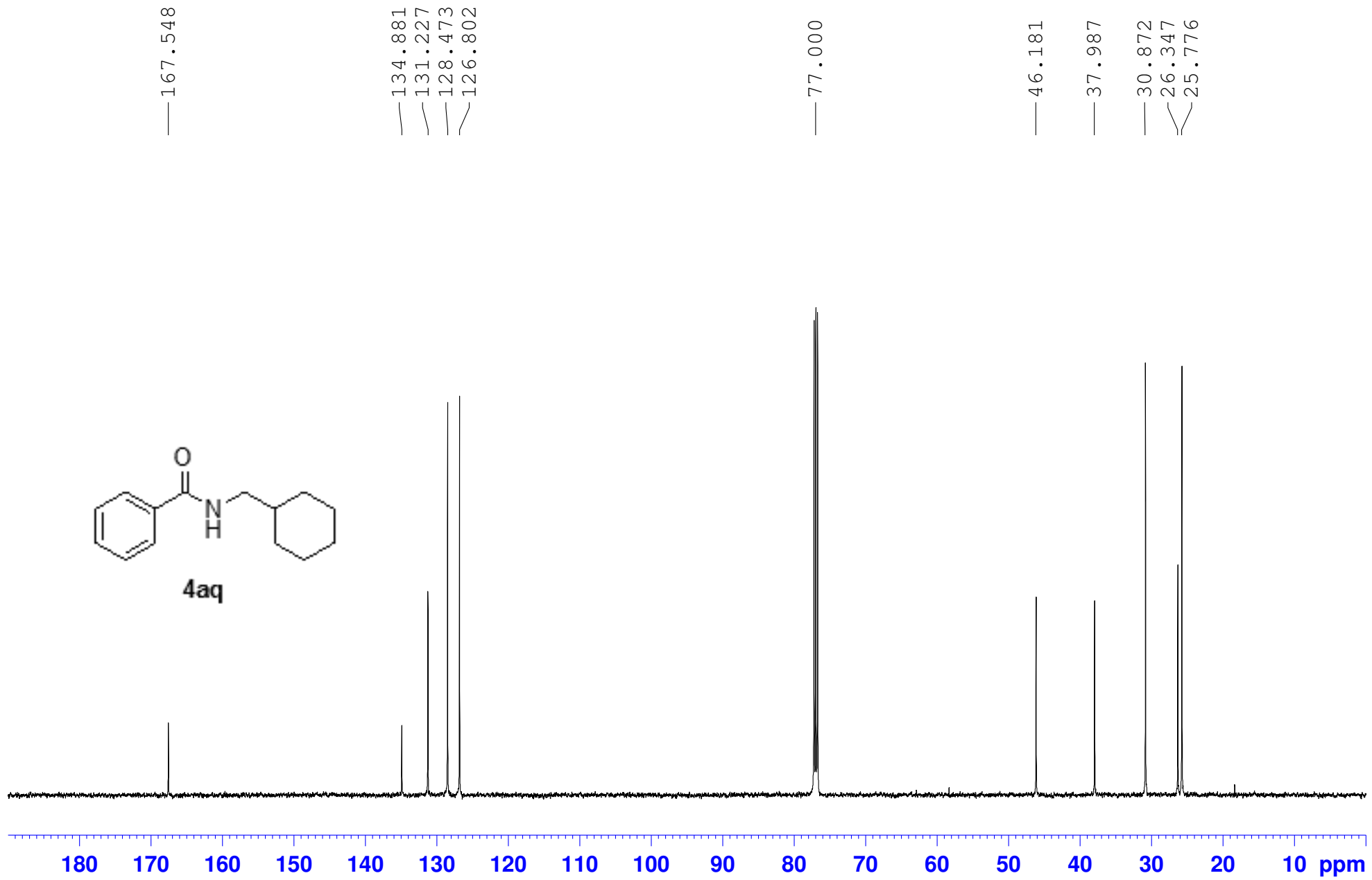
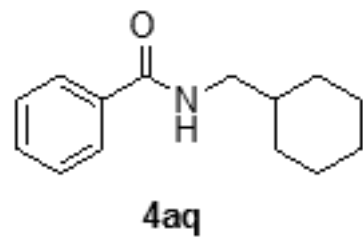
7.772
7.757
7.506
7.492
7.477
7.442
7.428
7.413
7.265

— 6.217

3.316
3.304
3.291
1.799
1.769
1.730
1.694
1.667
1.596
1.589
1.583
1.575
1.286
1.262
1.237
1.210
1.184
1.160
1.135
1.034
1.010
0.986
0.963



N-(cyclohexylmethyl)benzamide
C13CPD CDC13

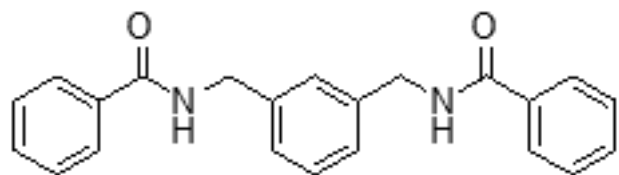


N,N'-m-xylylene-bis-benzamide
Proton DMSO-d6

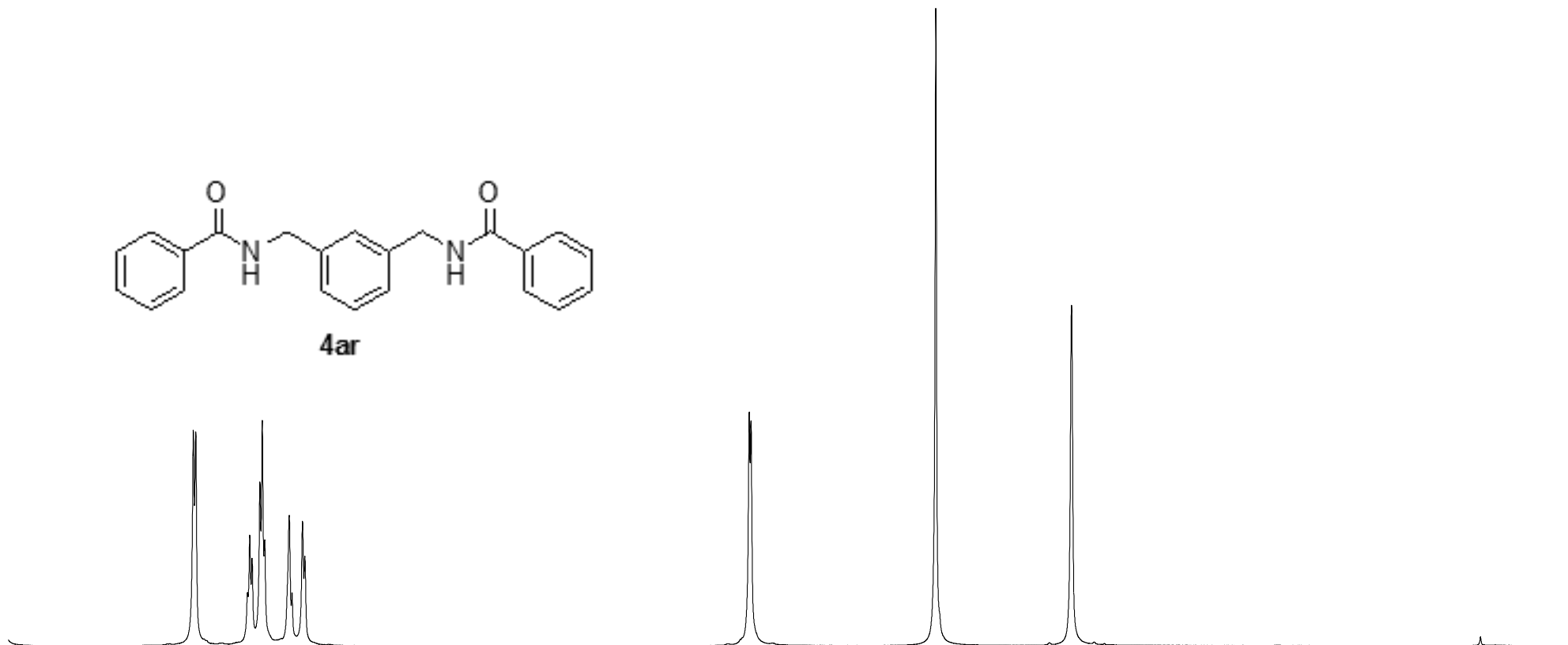
7.871
7.856
7.540
7.526
7.512
7.464
7.449
7.434
7.285
7.267
7.203
7.189

4.471
4.460

2.500



4ar

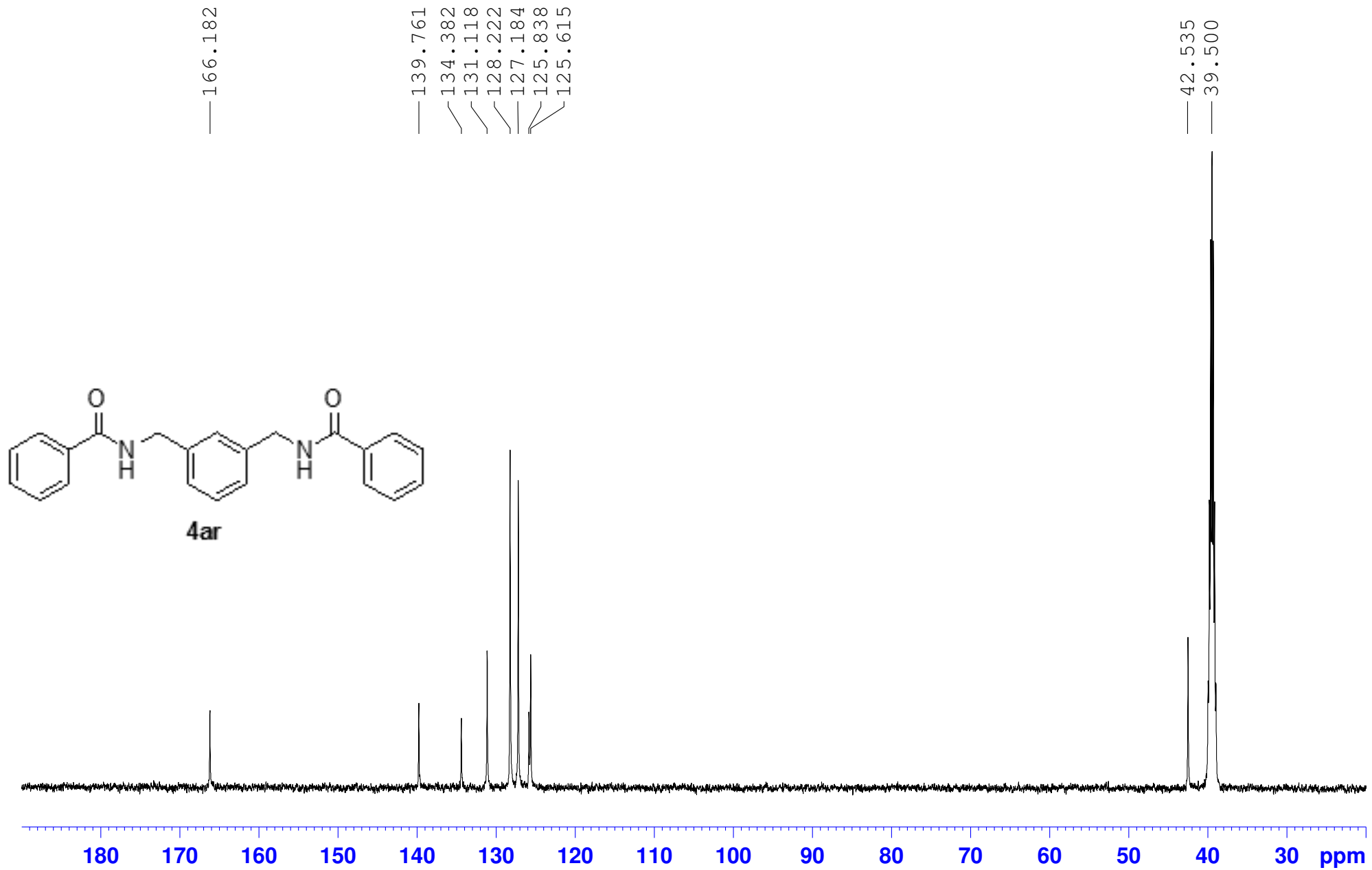


8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

4.05
2.03
4.08
2.02
2.02

4.08

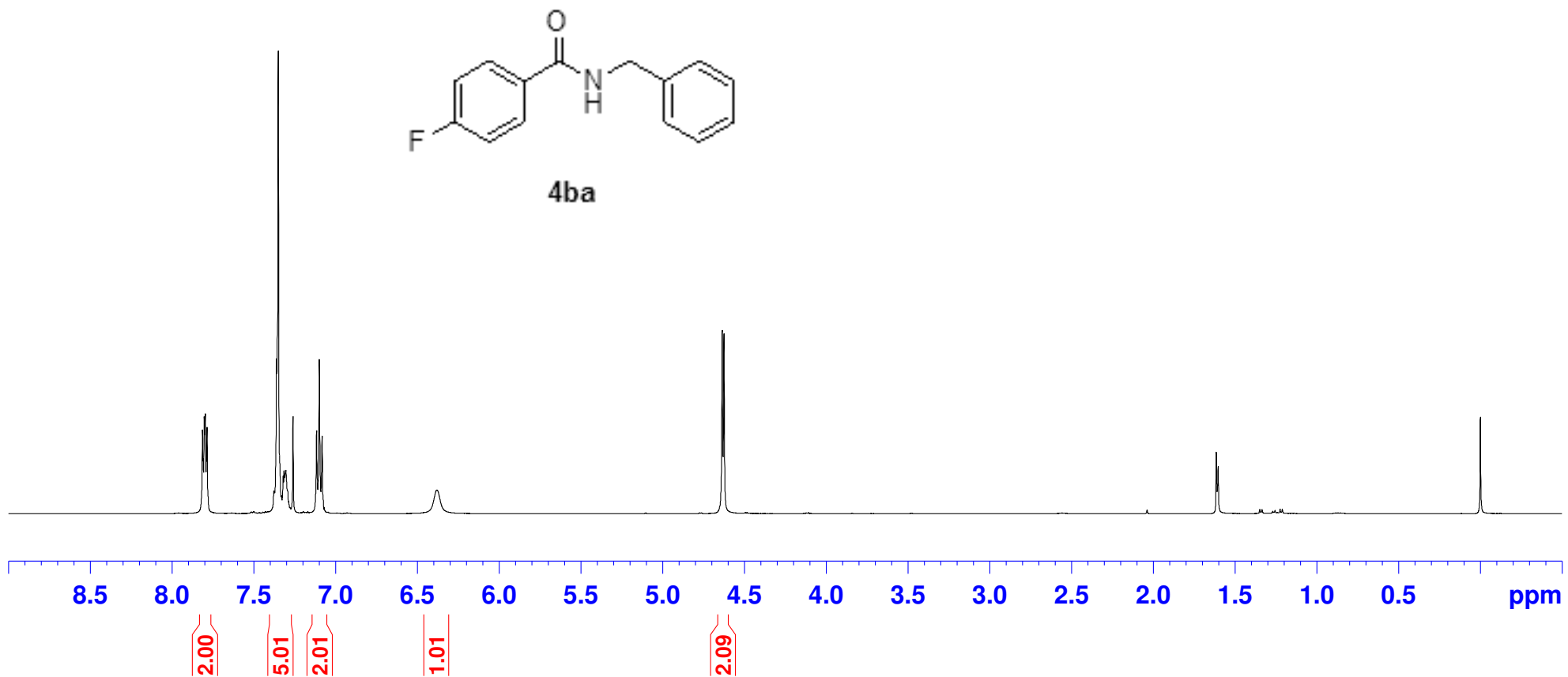
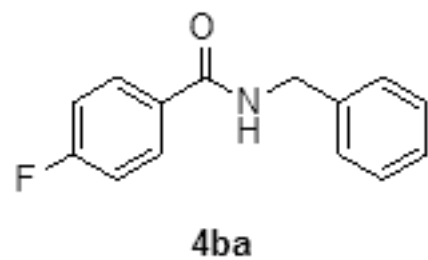
N,N'-m-xylene-bis-benzamide
C13CPD DMSO-d6



N-benzyl-4-fluorobenzamide
Proton CDCl₃

7.812
7.802
7.795
7.784
7.376
7.360
7.354
7.349
7.330
7.319
7.313
7.305
7.302
7.285
7.259
7.115
7.098
7.081
6.382

4.637
4.626



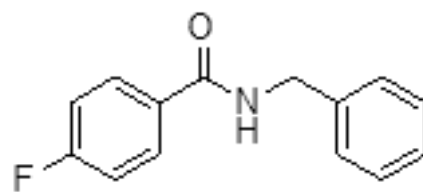
N-benzyl-4-fluorobenzamide
C13CPD CDC13

166.320
165.713
163.705

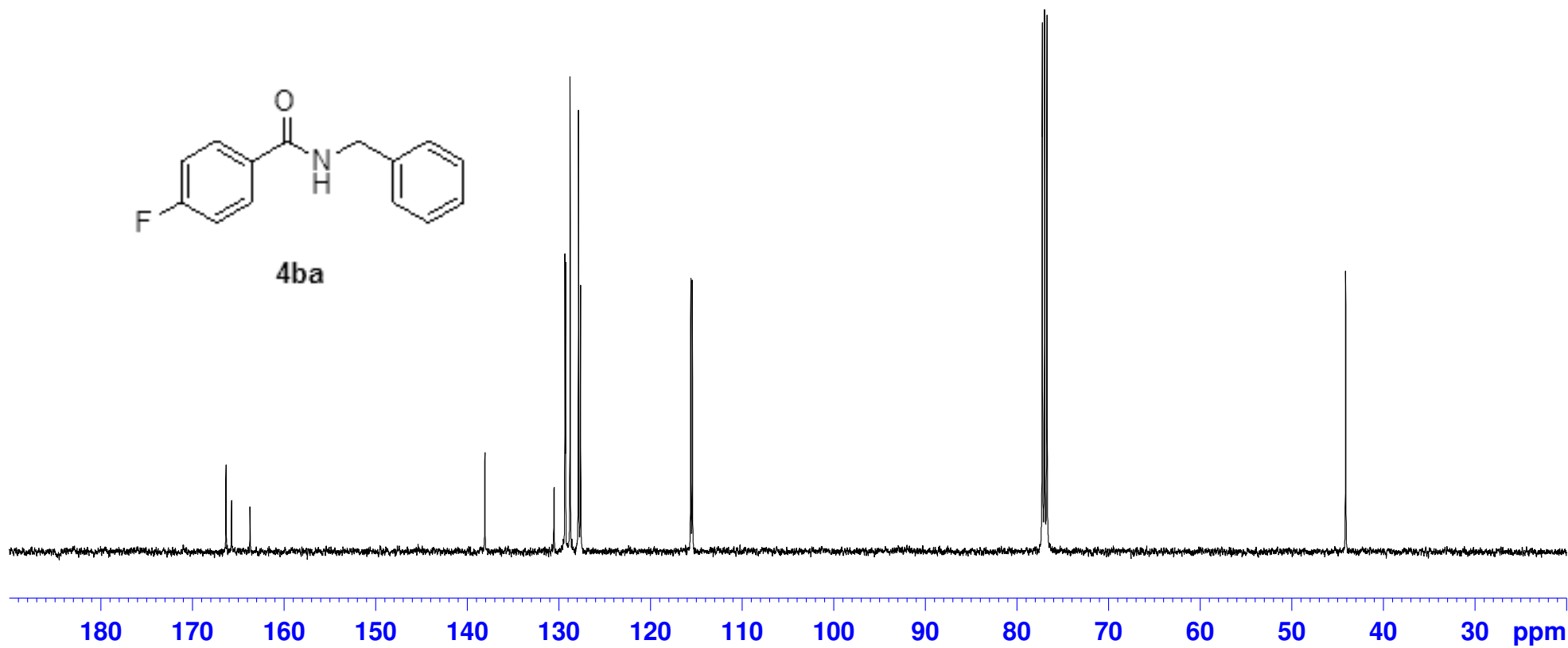
138.056
130.516
129.322
129.250
128.755
127.843
127.618
115.632
115.459

77.000

44.141



4ba

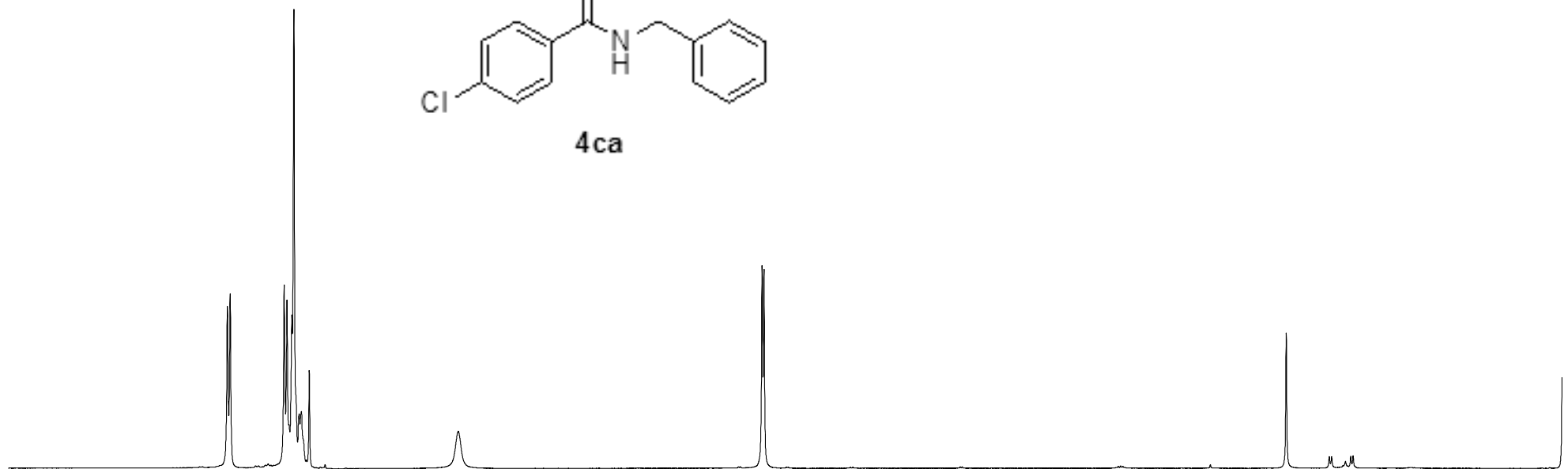
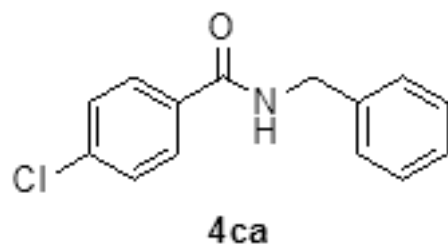


N-benzyl-4-chlorobenzamide
Proton CDCl₃

7.733
7.717
7.404
7.388
7.377
7.359
7.348
7.317
7.304
7.258

6.395

4.635
4.624



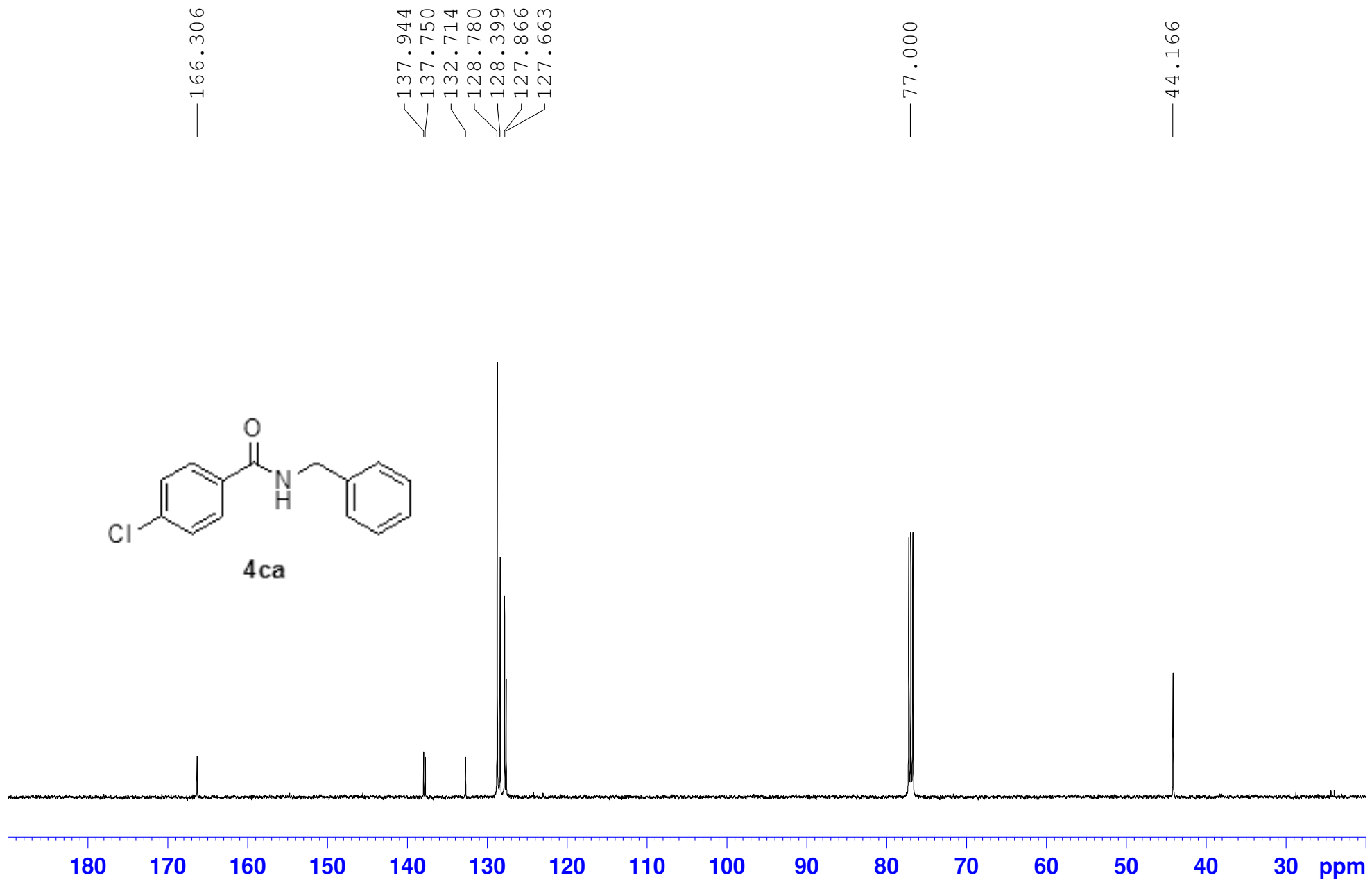
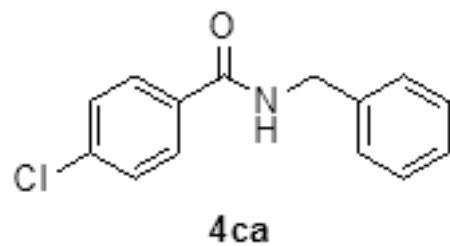
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

2.00
2.00
5.02

1.05

2.07

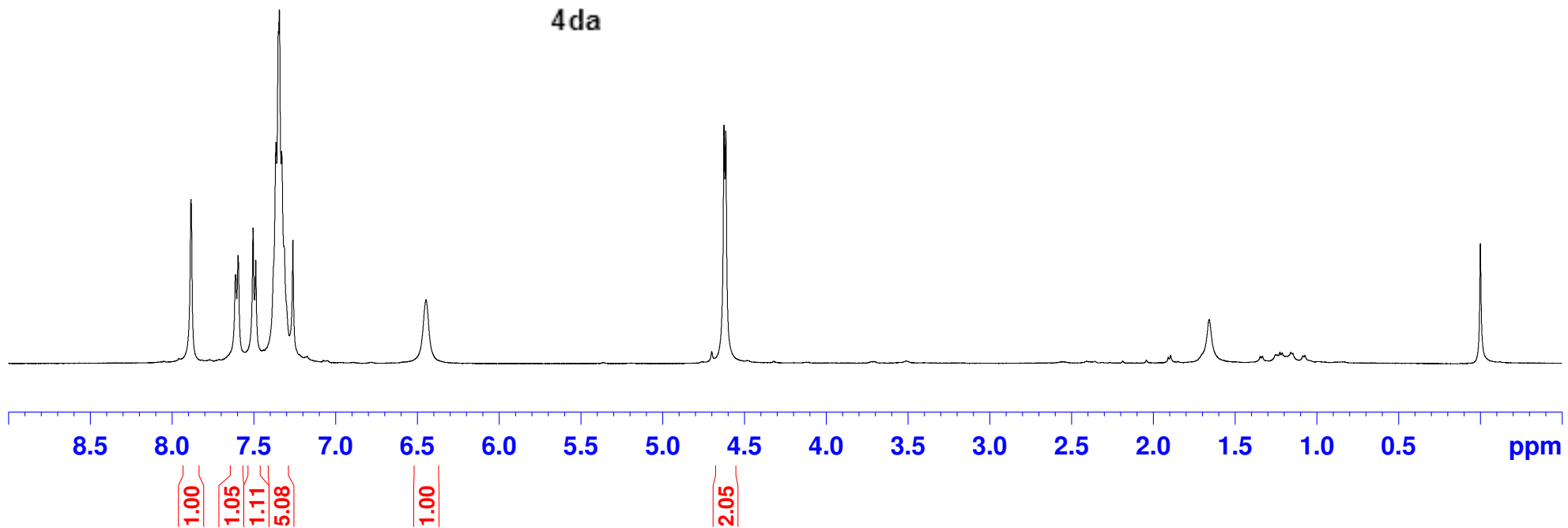
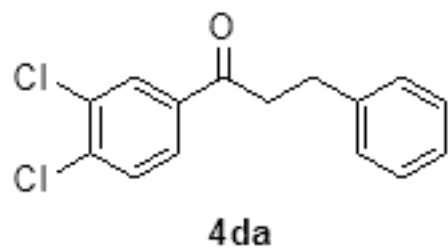
N-benzyl-4-chlorobenzamide
C13CPD CDC13



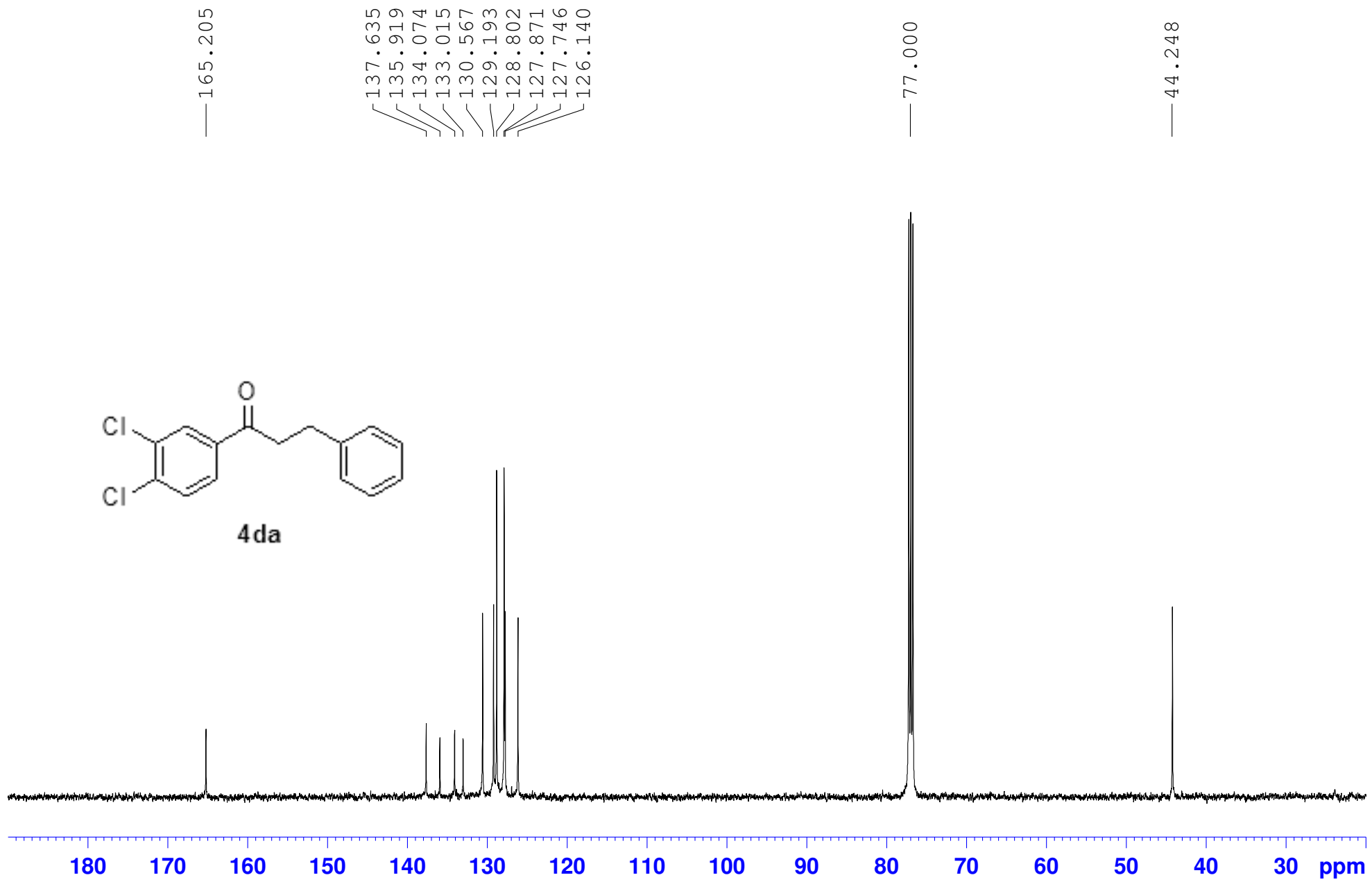
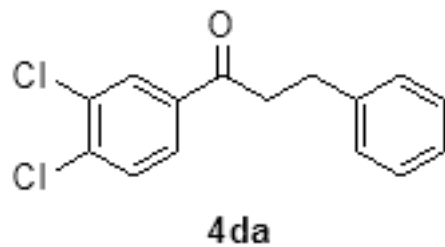
N-benzyl-3,4-dichlorobenzamide
Proton CDCl₃

7.885
7.613
7.597
7.505
7.489
7.366
7.351
7.345
7.330
7.315
7.262
— 6.448

4.625
4.614



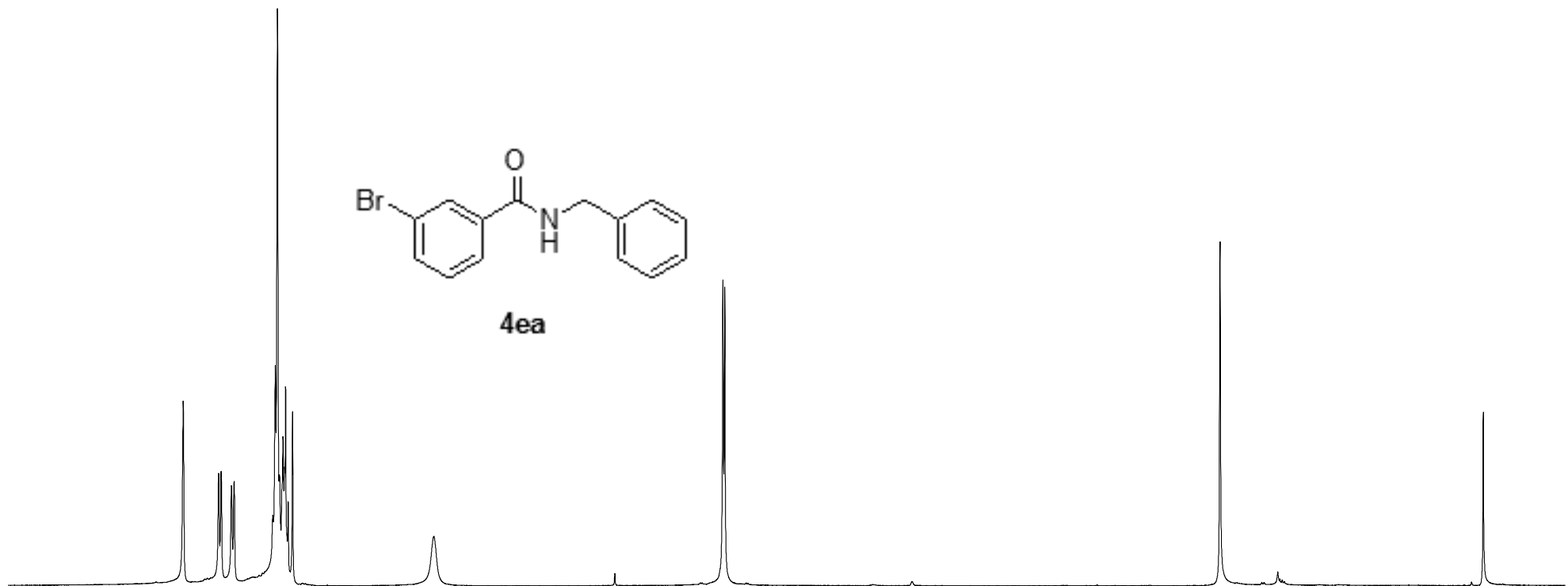
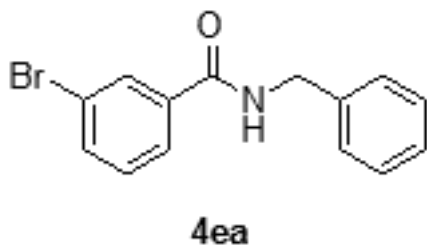
N-benzyl-3,4-dichlorobenzamide
C13CPD CDCl3



N-benzyl-3-bromobenzamide
PROTON CDC13

7.928
7.712
7.697
7.635
7.634
7.619
7.618
7.382
7.367
7.354
7.341
7.326
7.319
7.309
7.304
7.288
7.261
6.402

4.639
4.628



8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

1.00
1.00
1.00
6.00

1.00

2.00

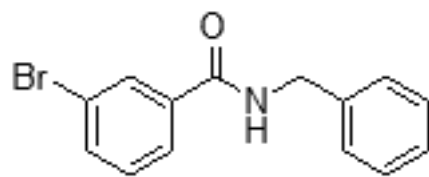
N-benzyl-3-bromobenzamide
C13CPD CDC13

— 165.921

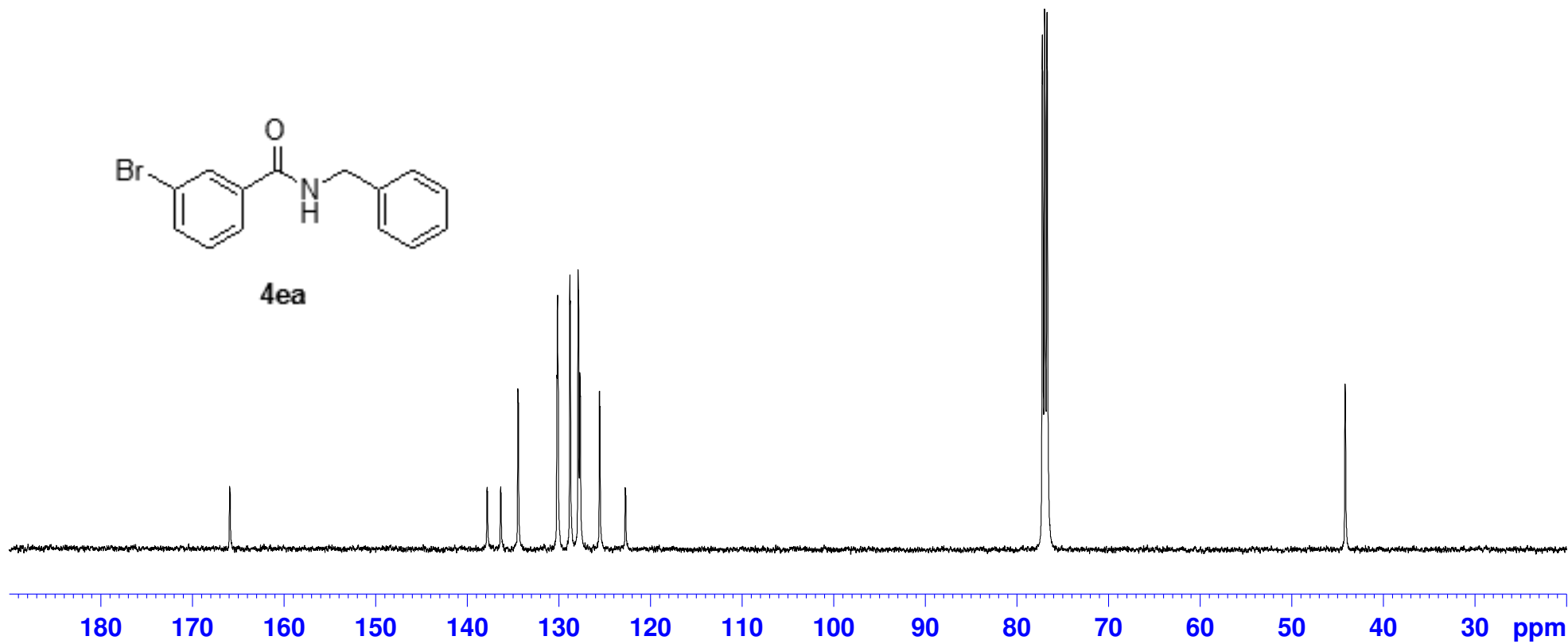
137.827
136.344
134.453
130.192
130.126
128.785
127.886
127.680
125.548
122.731

— 77.003

— 44.211



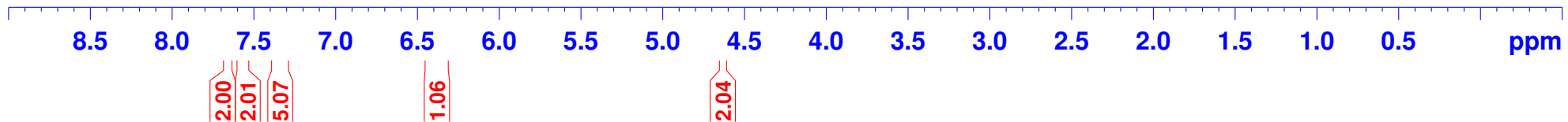
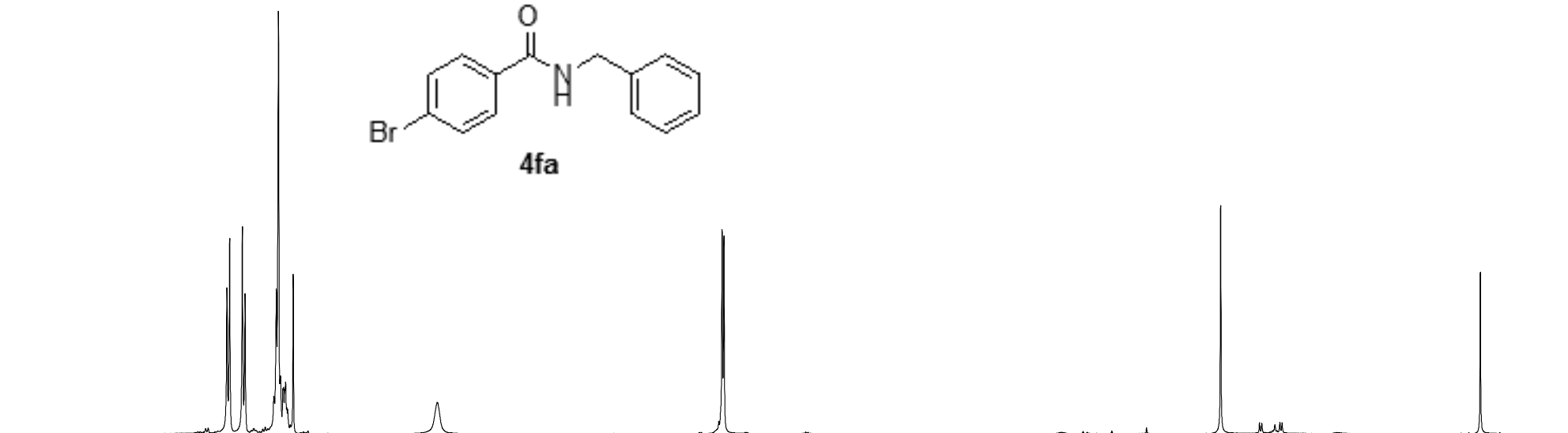
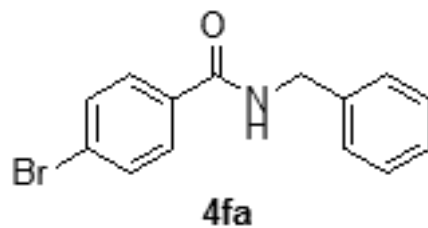
4ea



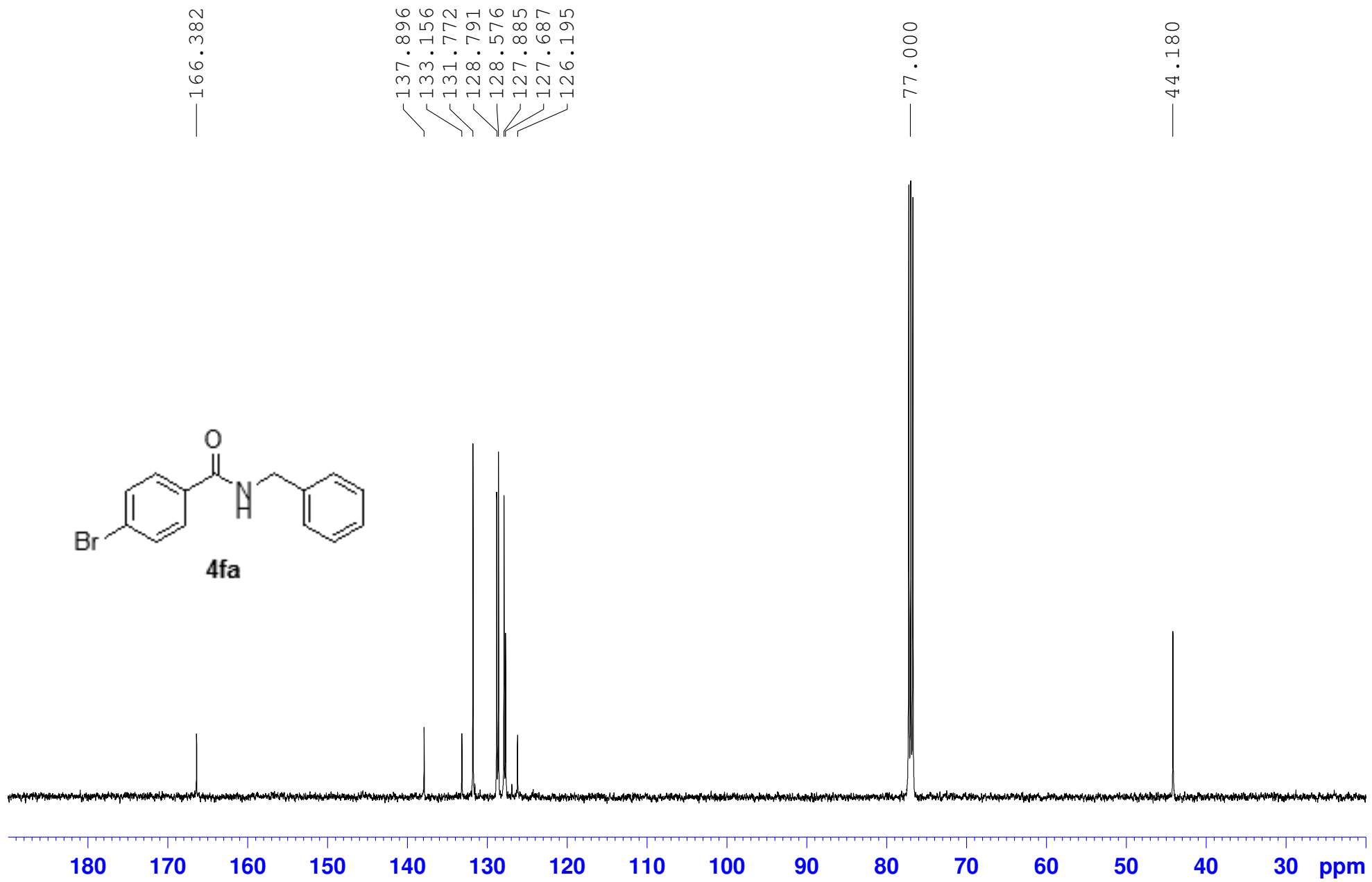
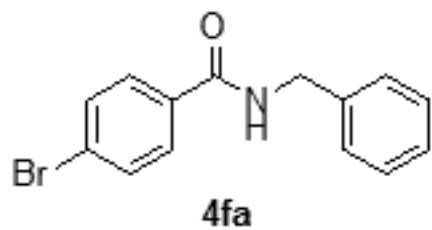
N-benzyl-4-bromobenzamide
Proton CDCl₃

7.665
7.649
7.571
7.554
7.378
7.363
7.350
7.338
7.323
7.320
7.312
7.307
7.300
7.294
7.260
6.379

4.637
4.626



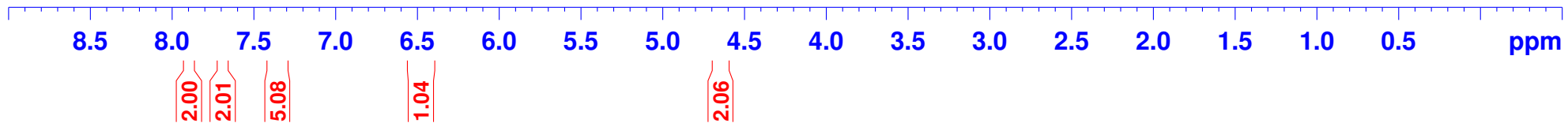
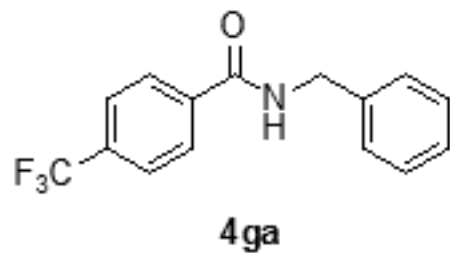
N-benzyl-4-bromobenzamide
C13CPD CDC13



N-benzyl-4-(trifluoromethyl)benzamide
Proton CDCl₃

7.908
7.892
7.702
7.686
7.374
7.362
7.335
7.332
7.324
7.319
7.262
— 6.486

4.666
4.655



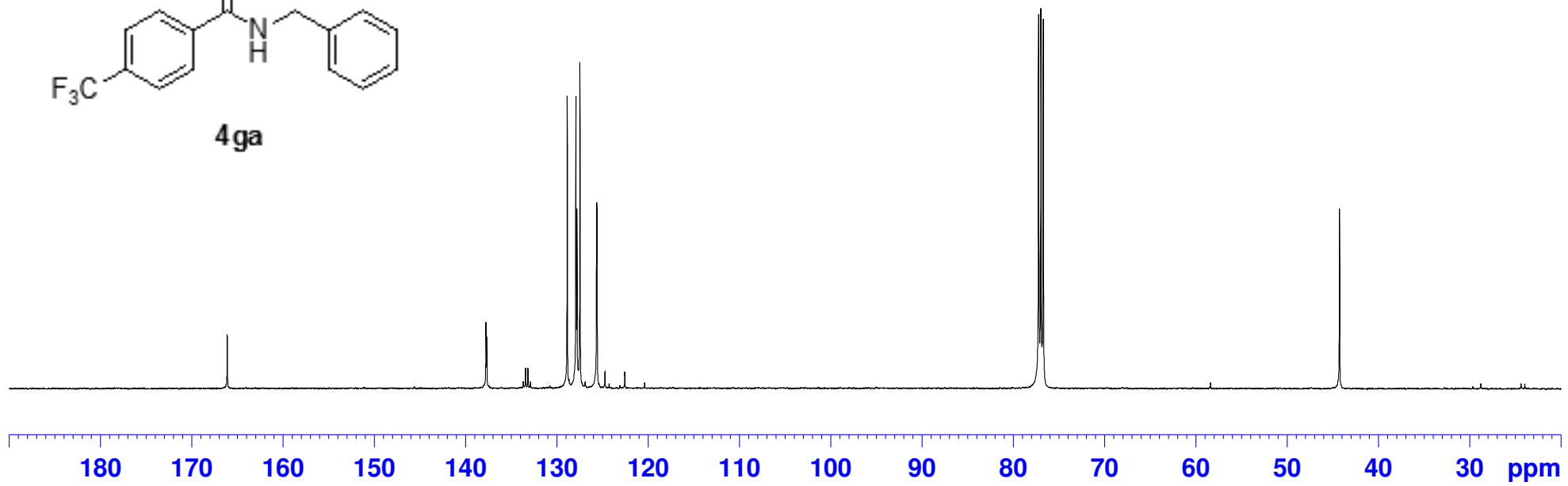
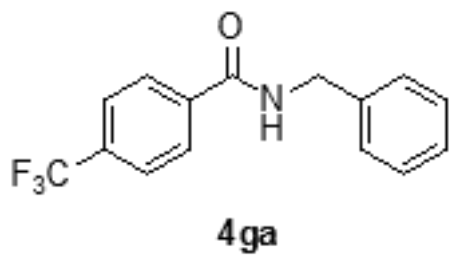
N-benzyl-4-(trifluoromethyl)benzamide
C13CPD CDCl3

— 166.098

137.753
137.664
133.672
133.413
133.150
132.892
128.846
127.895
127.784
127.454
126.882
125.601
124.714
122.544
120.376

— 77.000

— 44.284

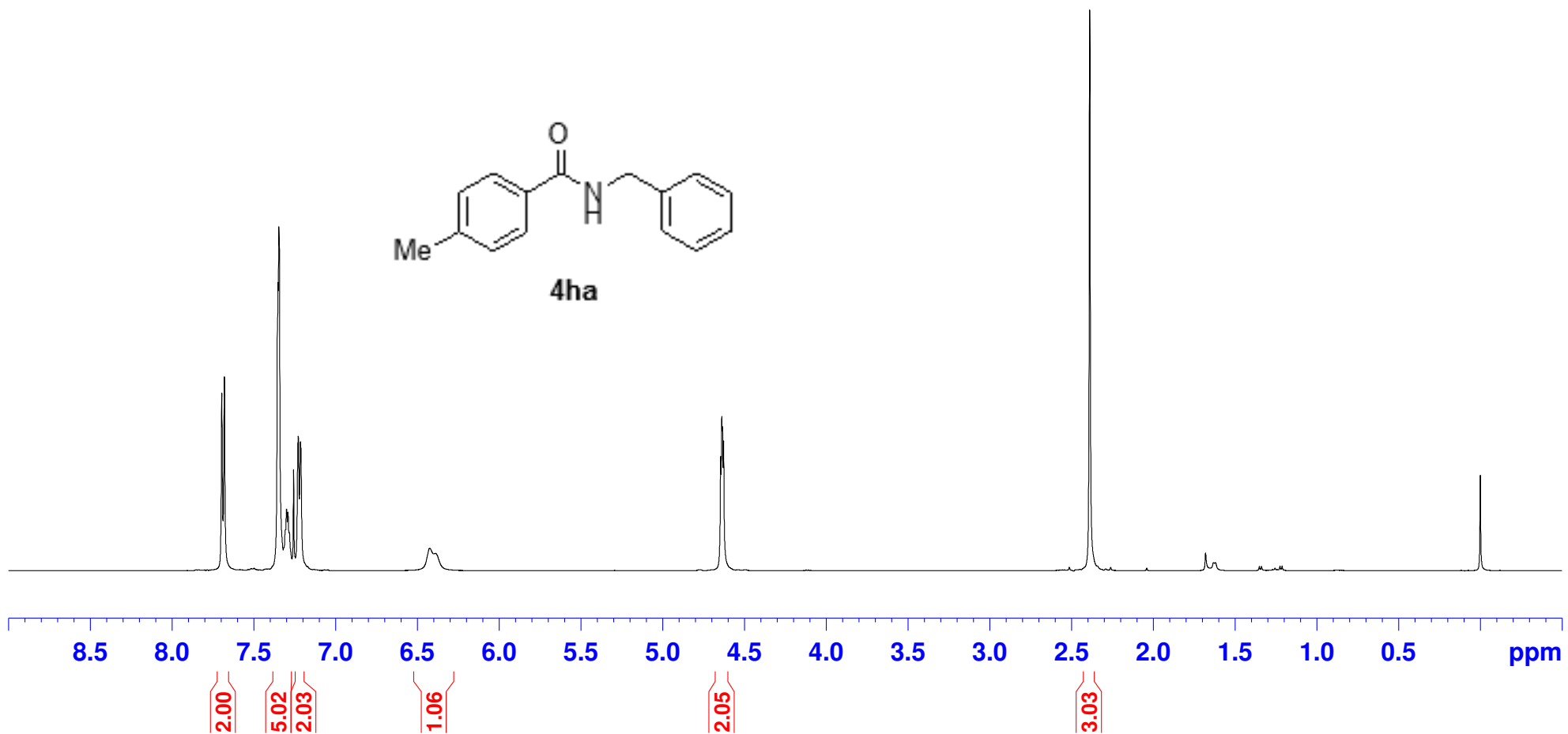
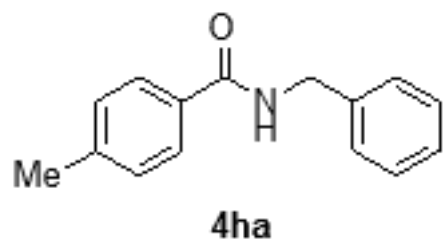


N-benzyl-4-methylbenzamide
Proton CDCl₃

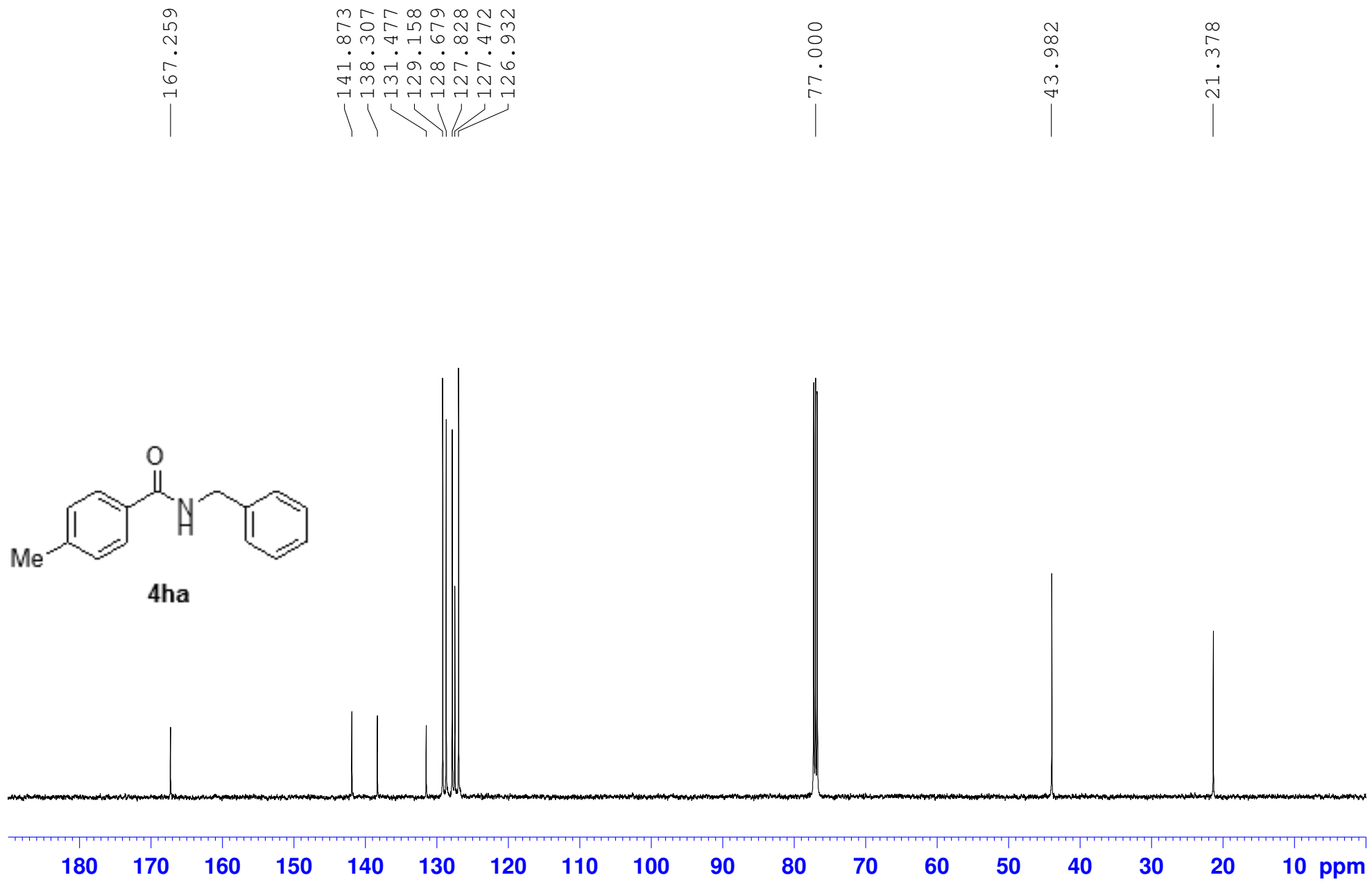
7.697
7.681
7.356
7.353
7.348
7.345
7.300
7.293
7.284
7.258
7.229
7.215
6.425
6.392

4.646
4.639
4.635
4.628

— 2.389



N-benzyl-4-methylbenzamide
C13CPD CDC13

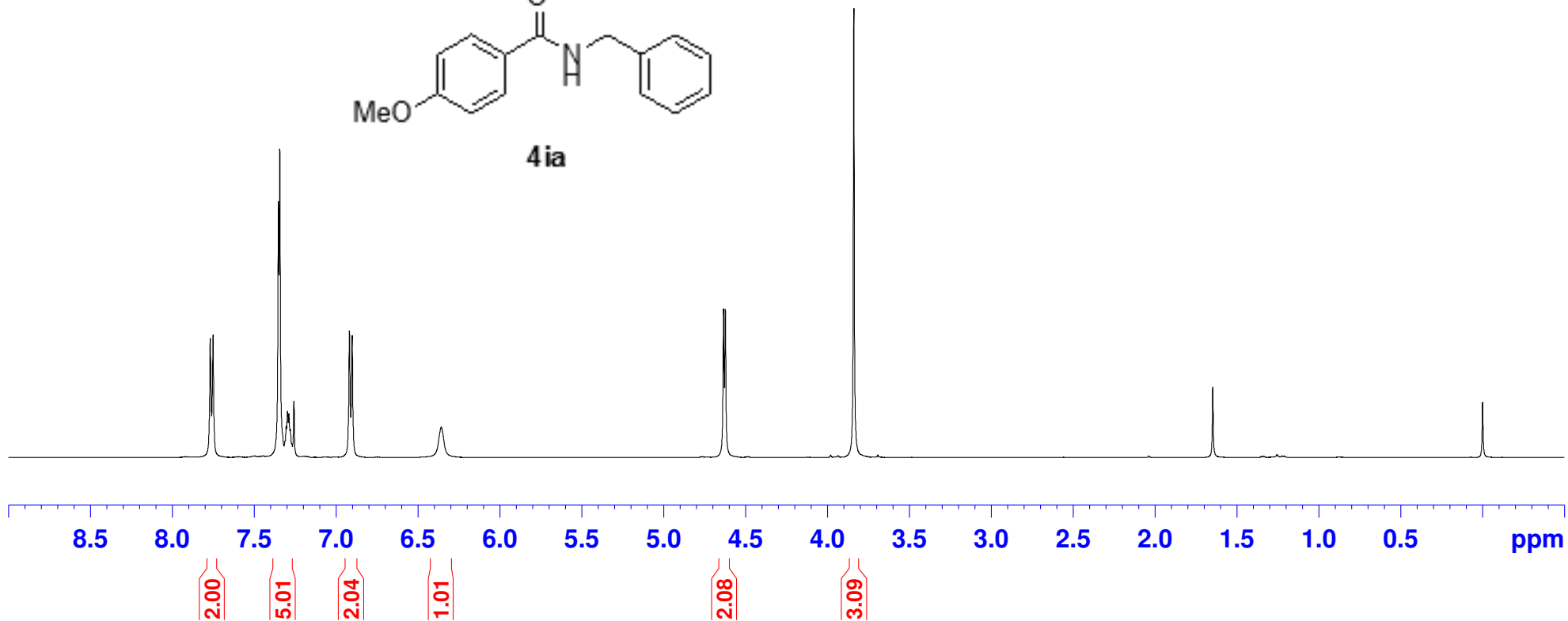
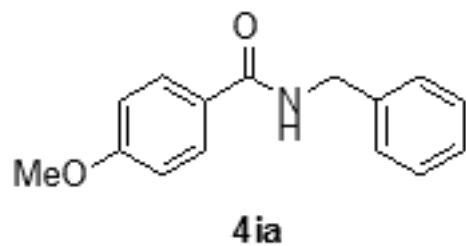


N-benzyl-4-methoxybenzamide
Proton CDCl₃

7.767
7.750
7.353
7.345
7.306
7.298
7.289
7.281
7.258
6.920
6.903
6.359

4.635
4.624

3.840



N-benzyl-4-methoxybenzamide
C13CPD CDC13

— 166.861
— 162.156

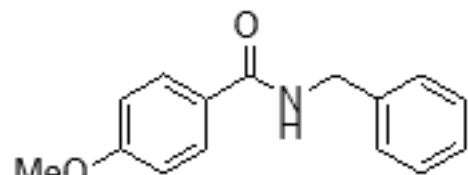
— 138.419
— 128.751
— 128.665
— 127.809
— 127.436
— 126.620

— 113.691

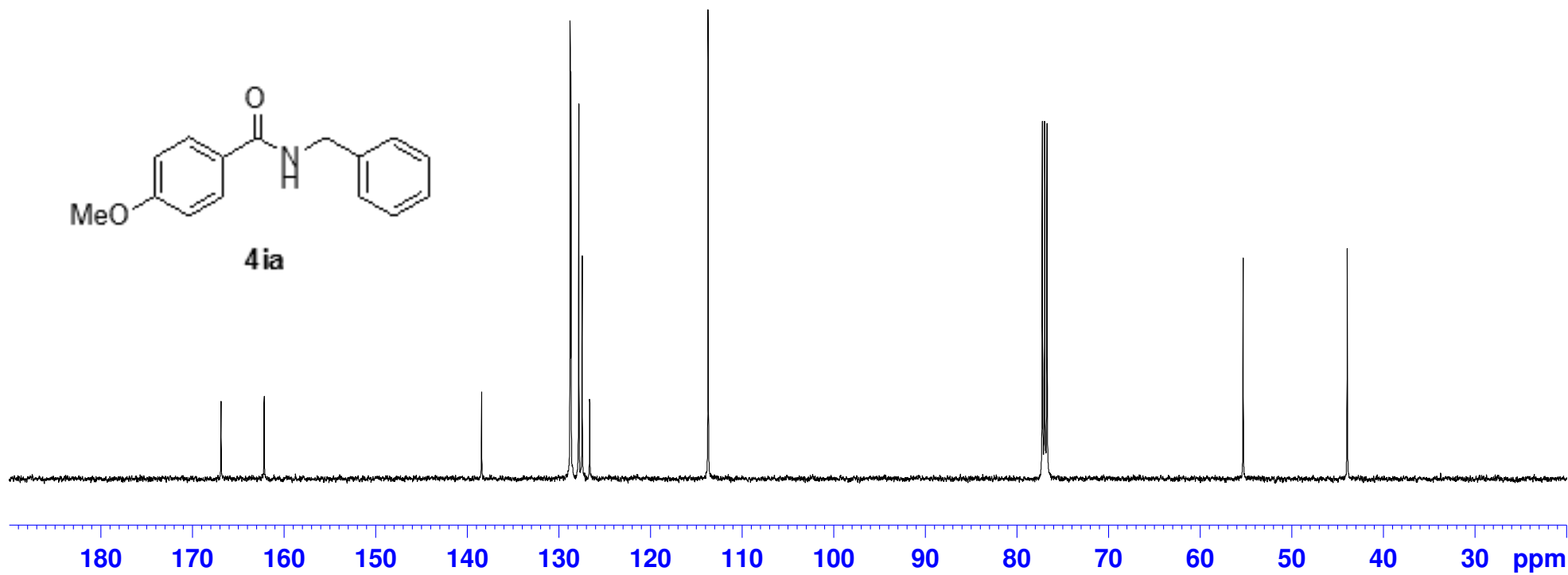
— 77.000

— 55.331

— 43.974



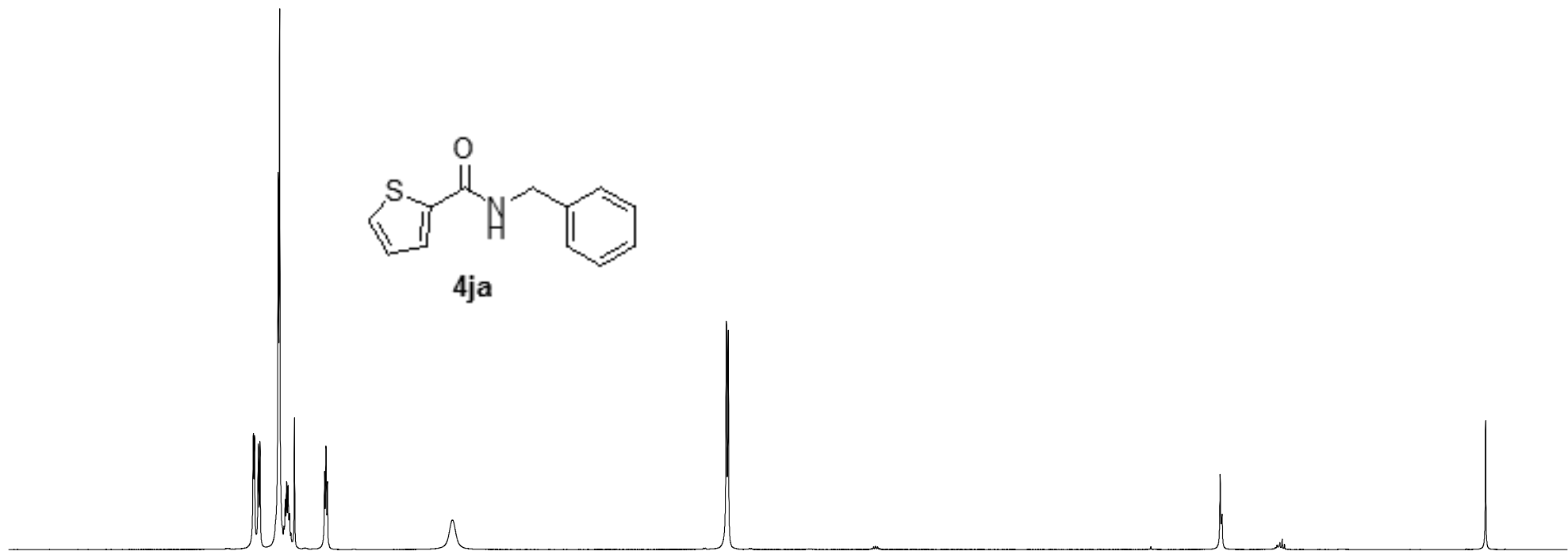
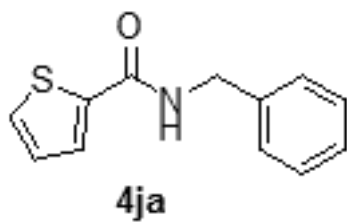
4ia



N-benzylthiophene-2-carboxamide
Proton CDCl₃

7.510
7.502
7.480
7.470
7.358
7.349
7.323
7.315
7.307
7.298
7.289
7.280
7.259
7.075
7.067
7.058
6.297

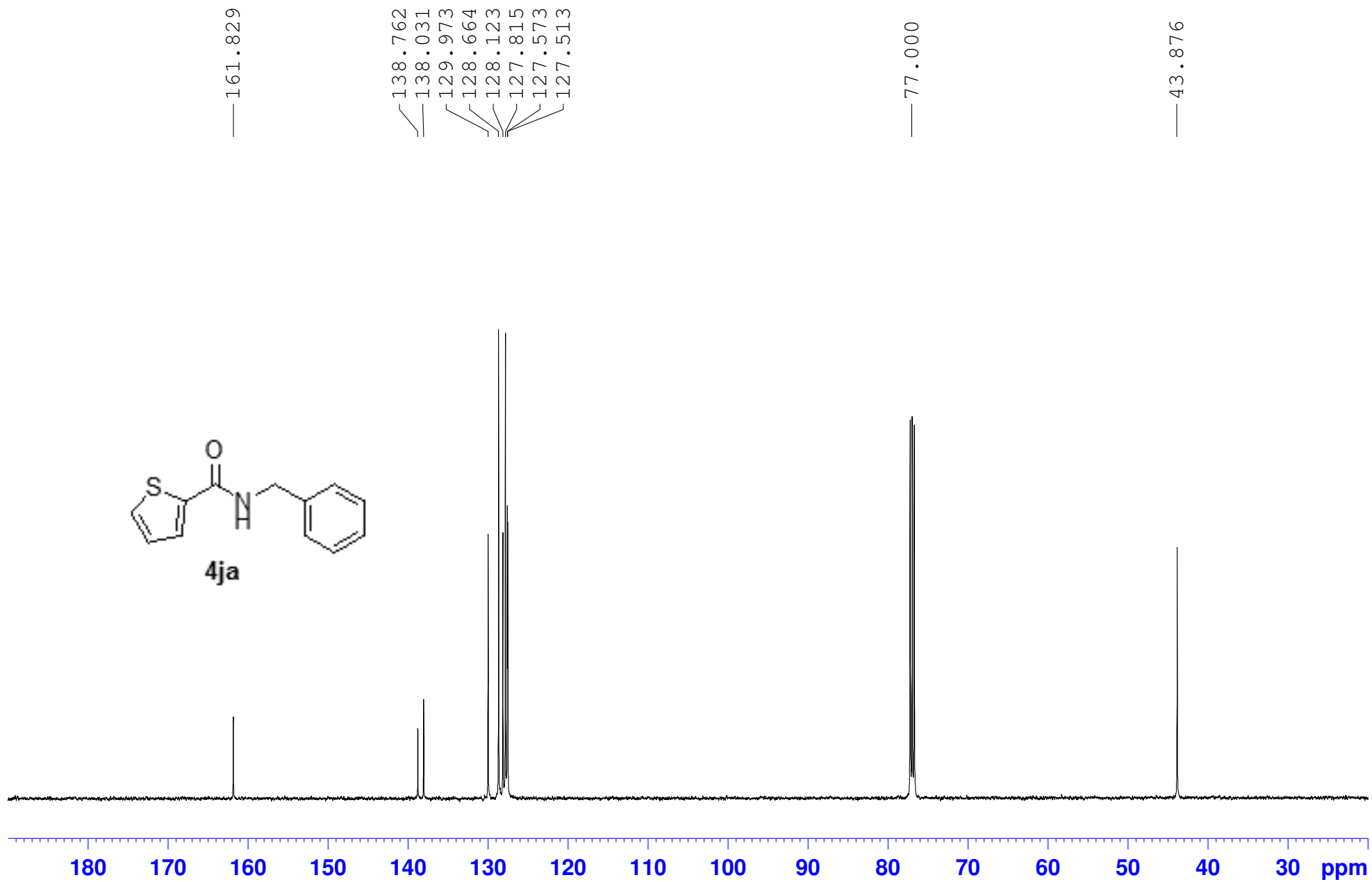
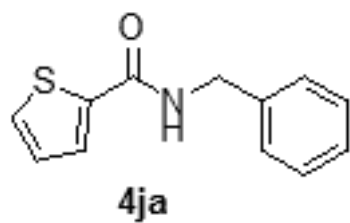
4.627
4.615



8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

1.04
0.99
4.05
1.06
1.02
1.03
2.00

N-benzylthiophene-2-carboxamide
C13CPD CDC13

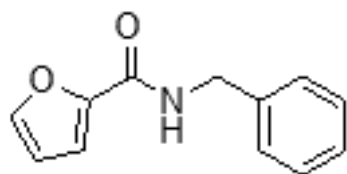


N-benzylfuran-2-carboxamide

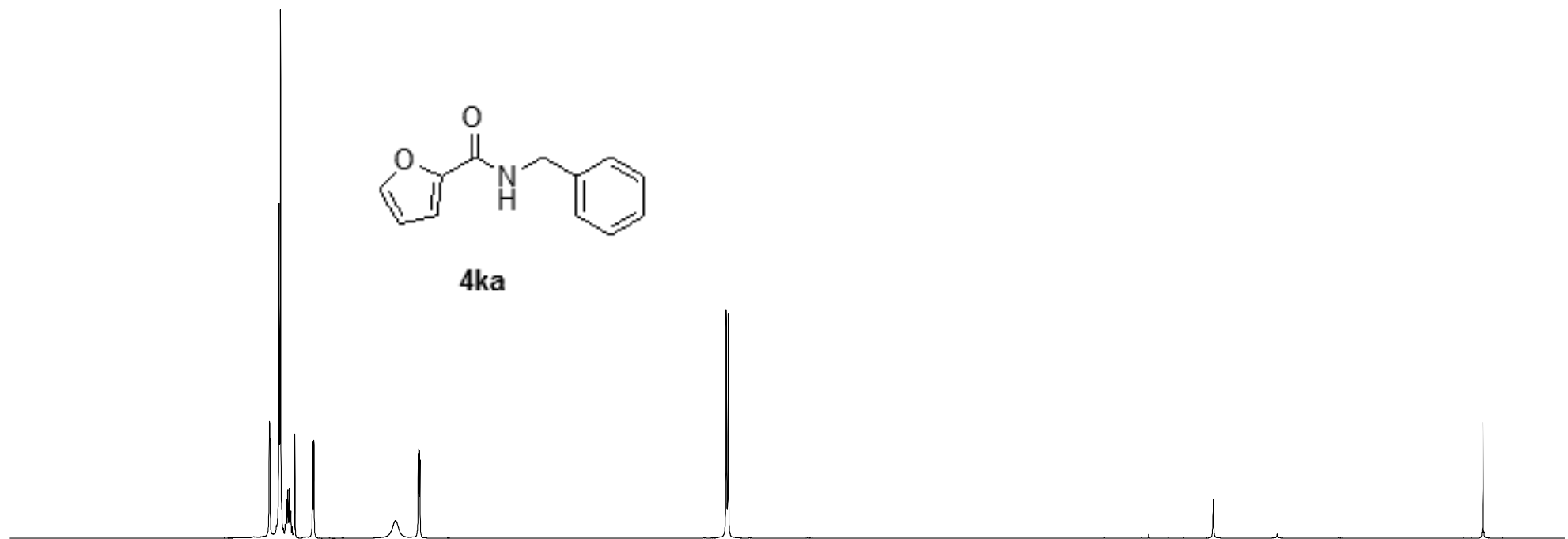
PROTON CDC13

7.415
7.413
7.412
7.356
7.348
7.319
7.311
7.302
7.294
7.287
7.284
7.277
7.260
7.151
7.150
7.144
7.143
6.645
6.506
6.502
6.499
6.495

4.624
4.612



4ka

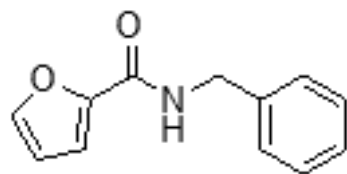


8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

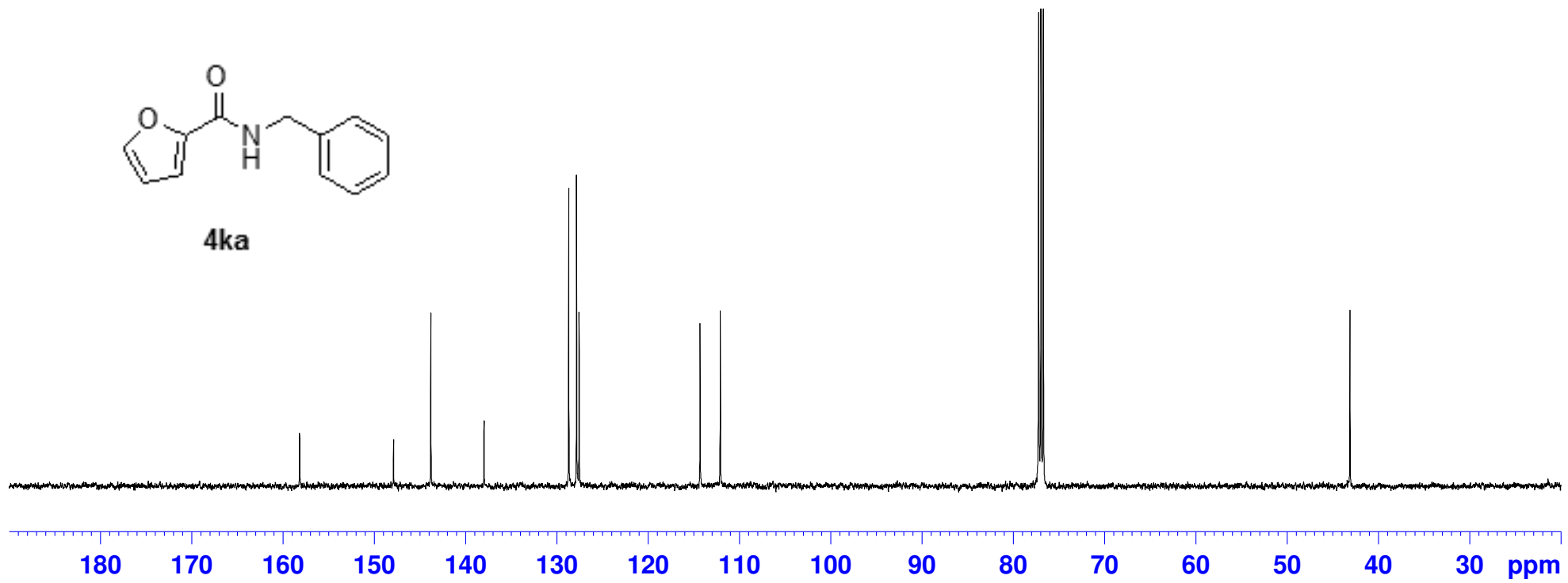
1.00
4.00
0.99
1.00
1.00
1.00
2.00

N-benzylfuran-2-carboxamide
C13CPD CDC13

— 158.218
— 147.919
— 143.835
— 138.008
— 128.728
— 127.873
— 127.591
— 114.341
— 112.130
— 76.998
— 43.141



4ka



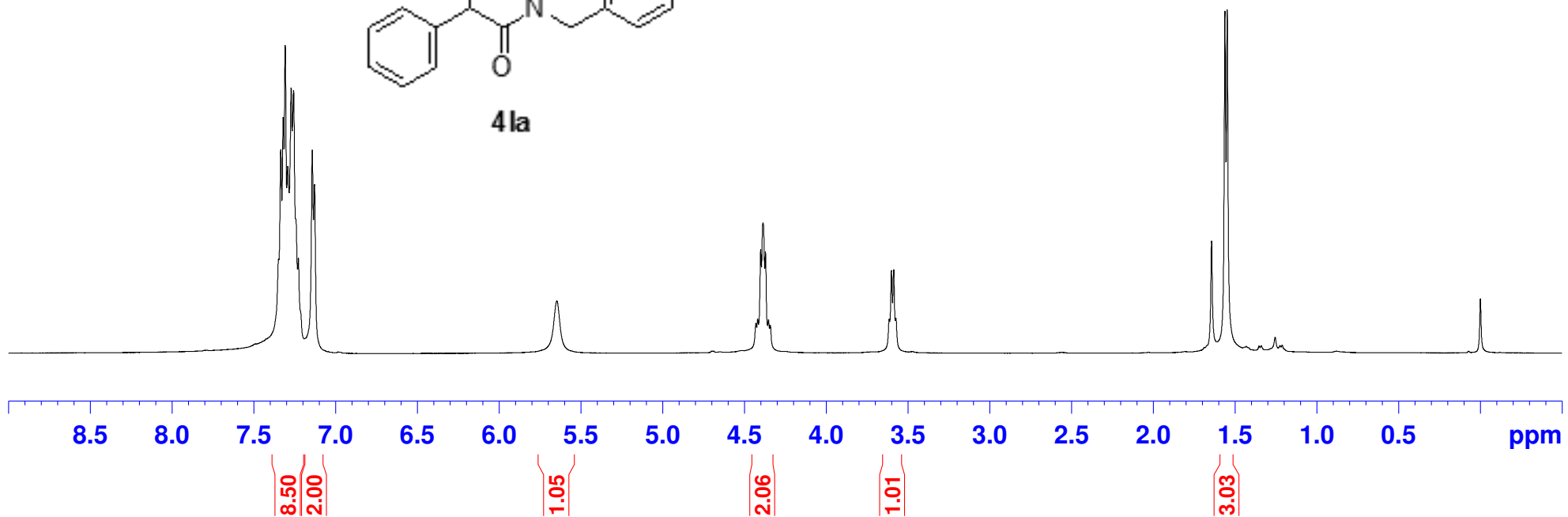
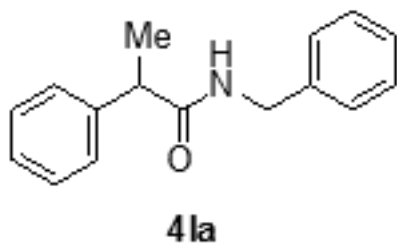
N-benzyl-2-phenylpropanamide
Proton CDCl₃

7.350
7.336
7.321
7.309
7.293
7.273
7.258
7.244
7.229
7.144
7.130

— 5.648

4.431
4.420
4.401
4.388
4.372
4.354
4.342
3.615
3.602
3.588
3.574

1.562
1.548



N-benzyl-2-phenylpropanamide
C13CPD CDCl3

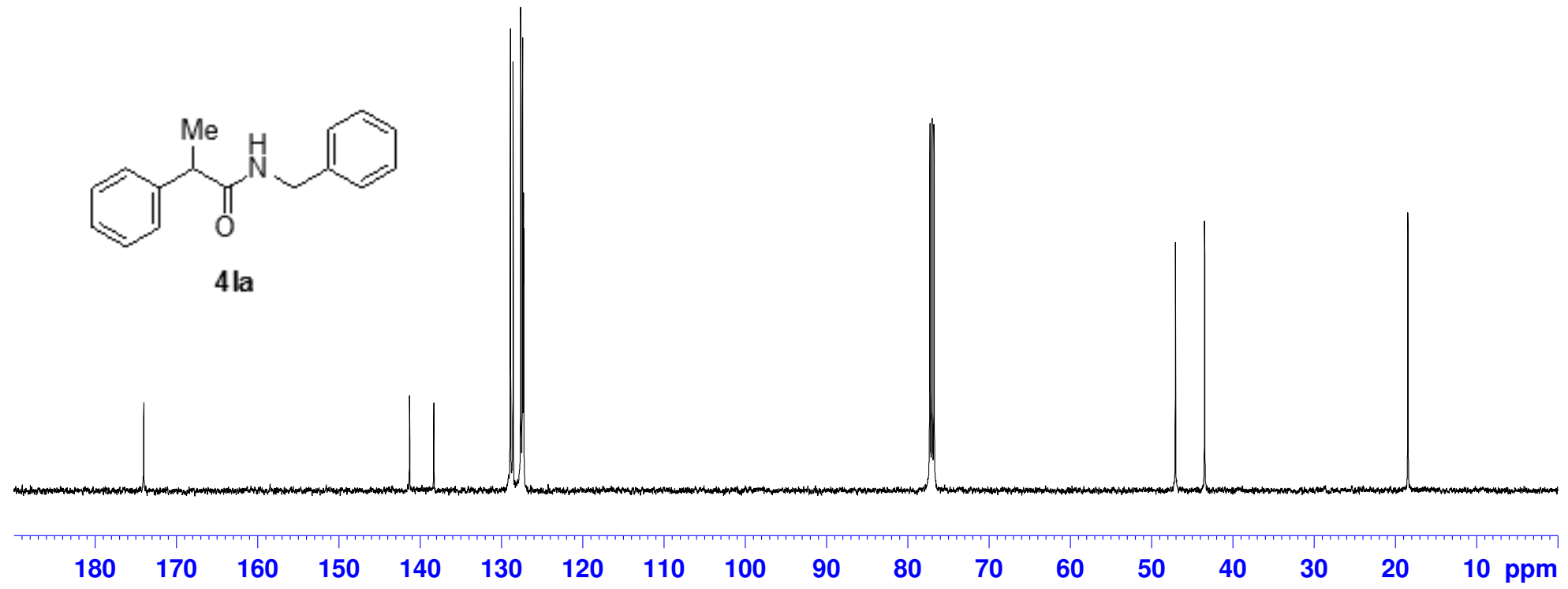
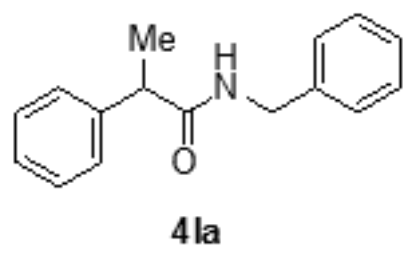
— 173.999

— 141.284
— 138.304
— 128.871
— 128.548
— 127.606
— 127.390
— 127.278
— 127.238

— 77.000

— 47.100
— 43.502

— 18.487



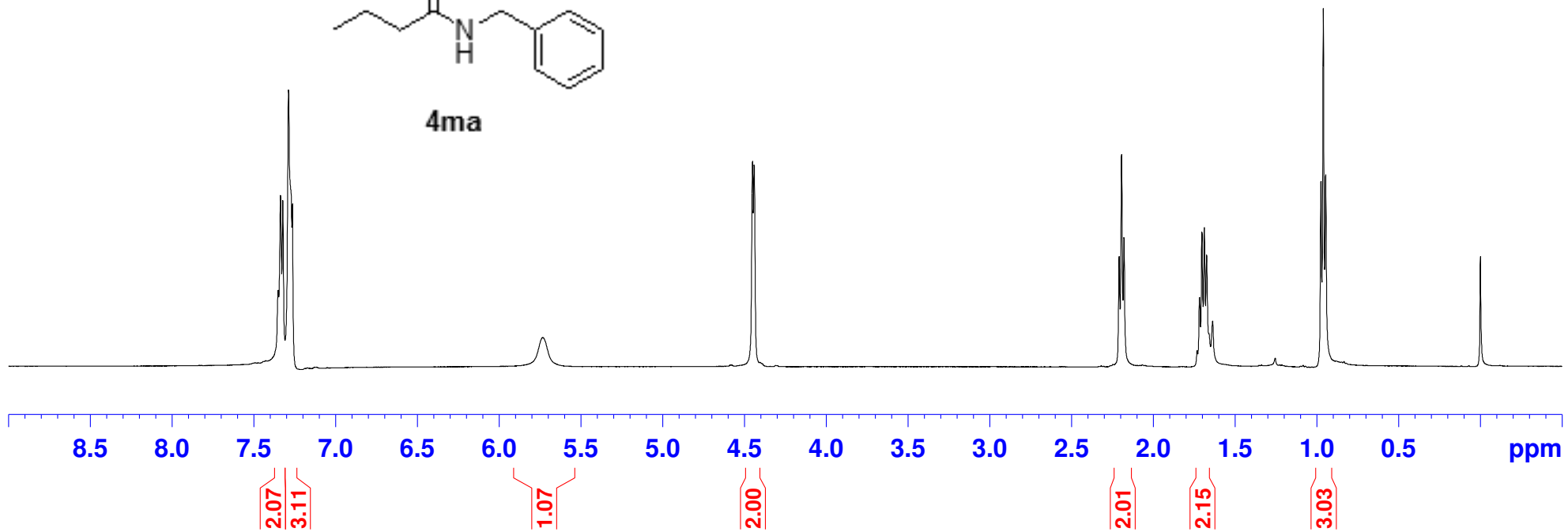
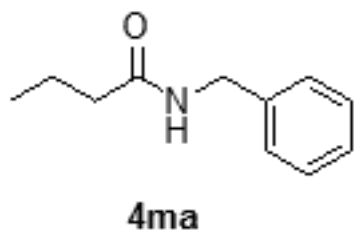
N-benzylbutyramide
Proton CDCl₃

7.350
7.335
7.321
7.286
7.262

— 5.736

4.451
4.442

2.209
2.194
2.180
1.732
1.718
1.703
1.688
1.675
1.660
0.975
0.961
0.946



N-benzylbutyramide
C13CPD CDCl3

—172.791

—138.439

128.632

127.742

127.404

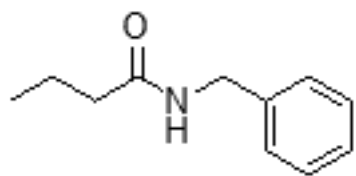
—77.000

—43.493

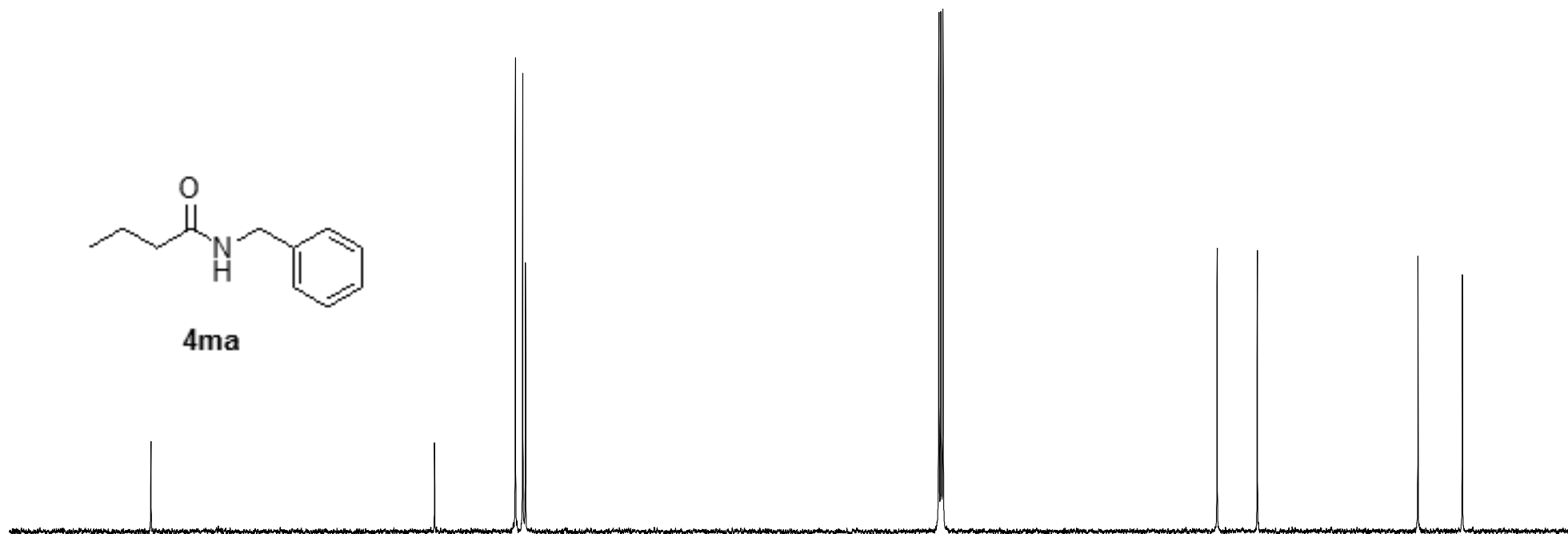
—38.616

—19.126

—13.737



4ma



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