

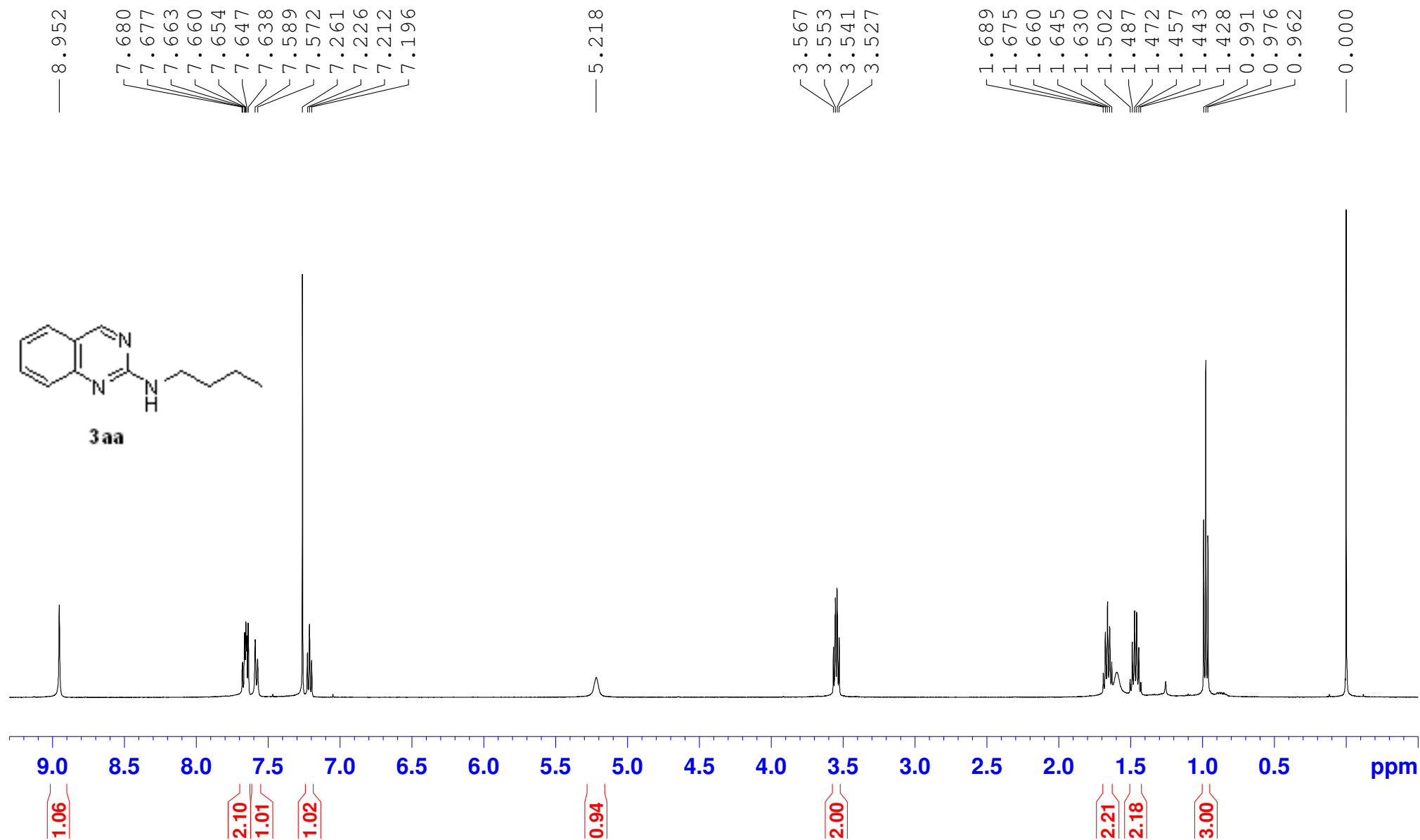
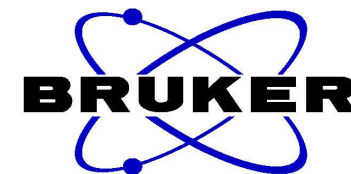
Electronic Supplementary Information (ESI)

Regioselective *N*-alkylation with alcohols for the preparation of 2-(*N*-alkylamino)quinazolines and 2-(*N*-alkylamino)pyrimidines†

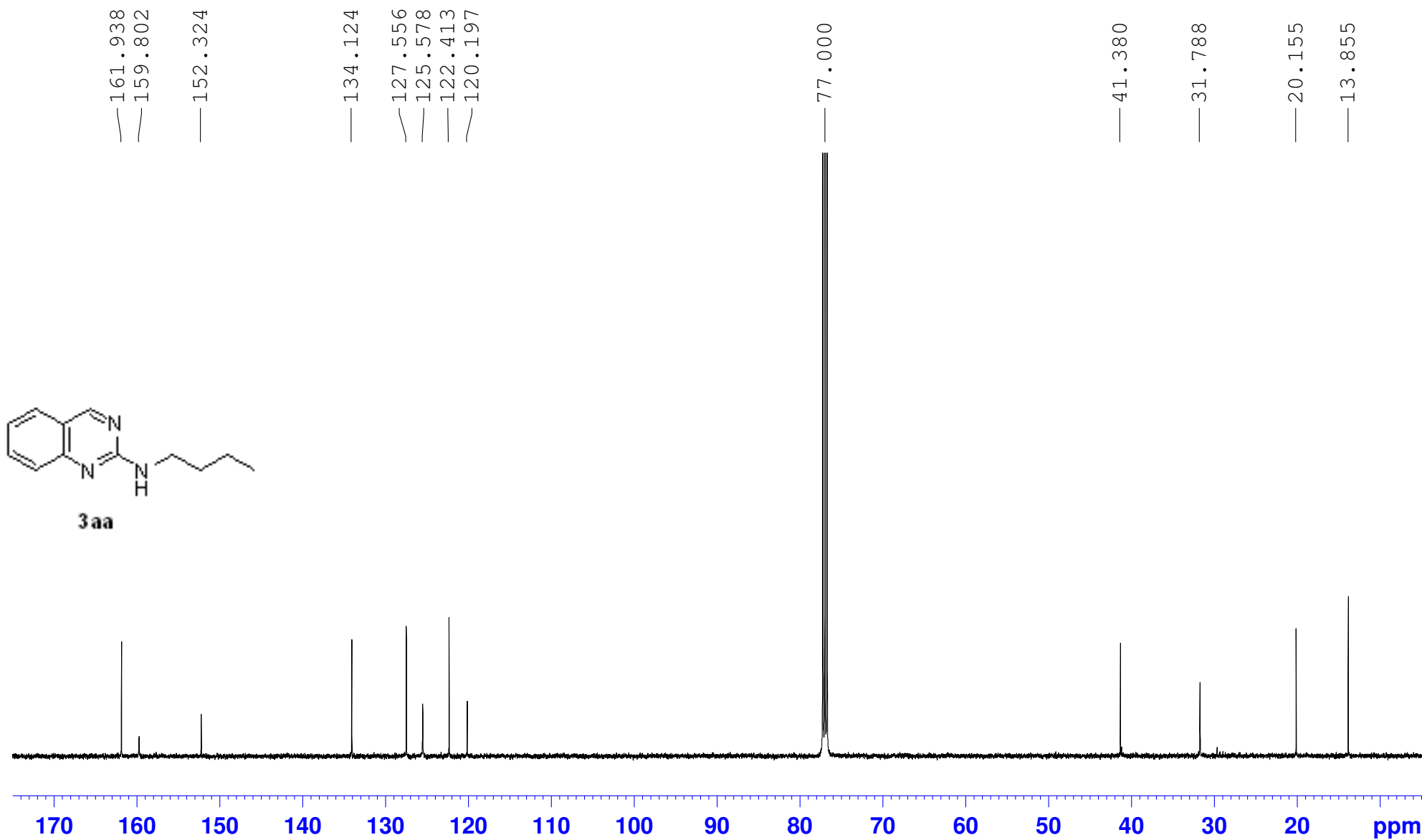
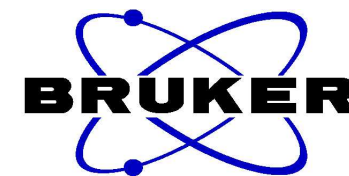
Feng Li,* Lin Chen, Qikai Kang, Jianguang Cai and Guangjun Zhu

School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, P. R. China

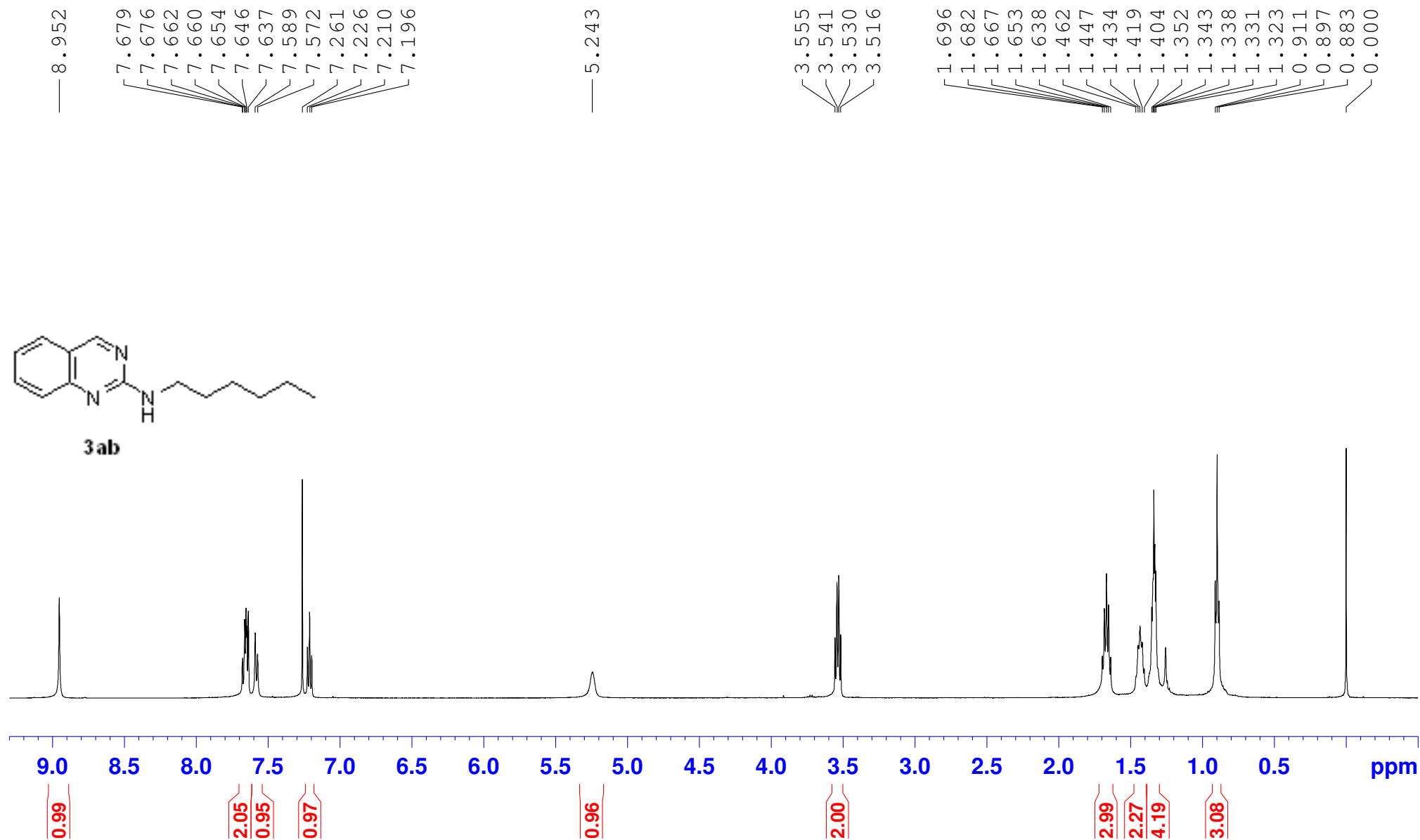
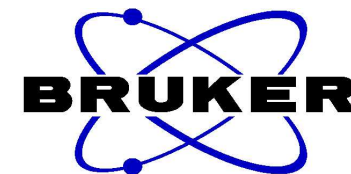
N-butylquinazolin-2-amine
Proton CDCl₃



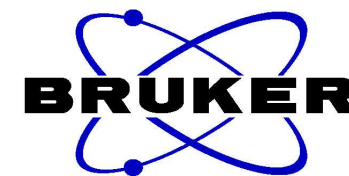
N-butylquinazolin-2-amine
C13CPD CDC13



N-hexylquinazolin-2-amine
Proton CDCl₃



N-hexylquinazolin-2-amine
C13CPD CDC13



161.860
159.719

152.258

134.158

127.526

125.523

122.345

120.134

77.000

41.626

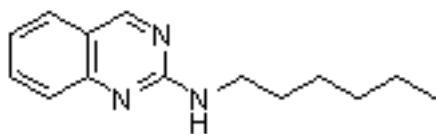
31.573

29.587

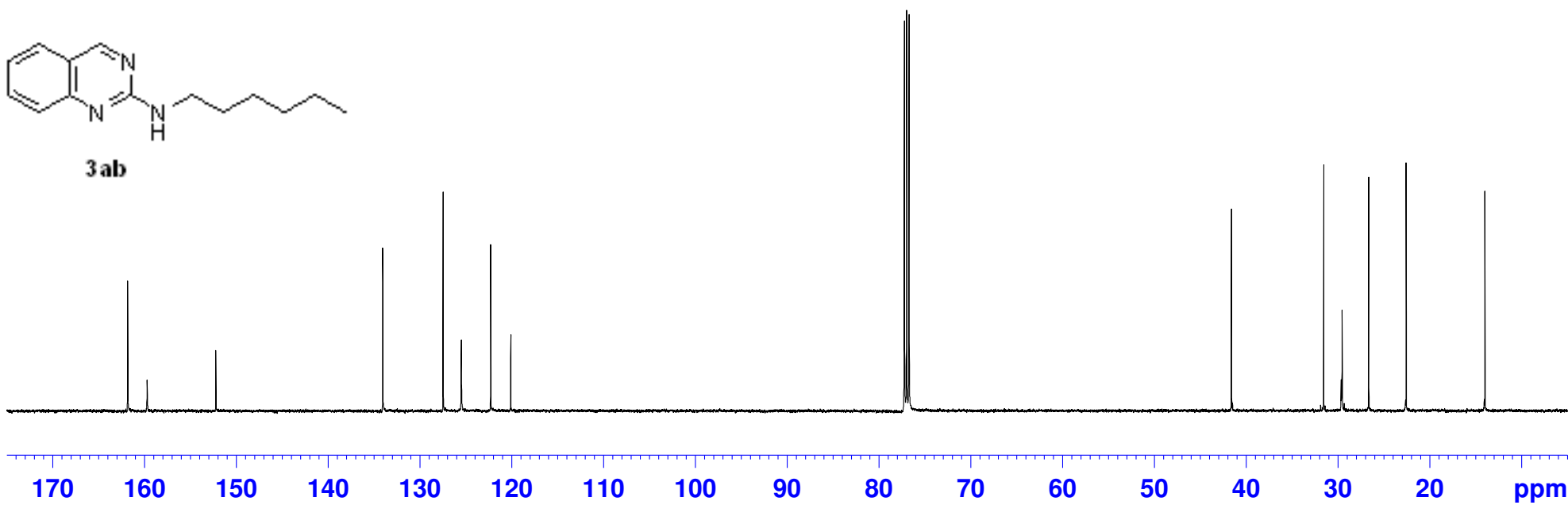
26.667

22.574

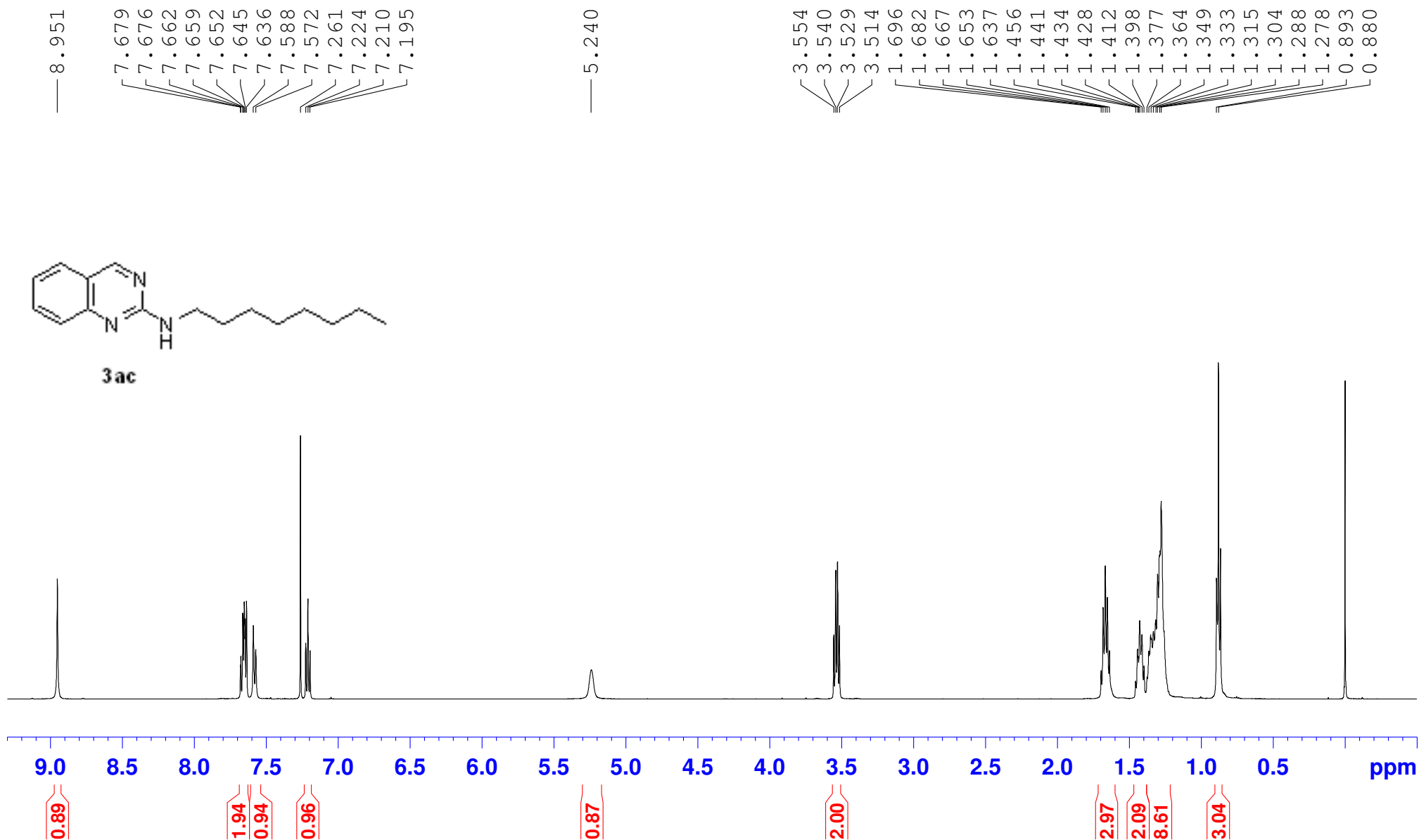
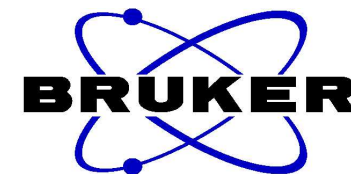
13.996



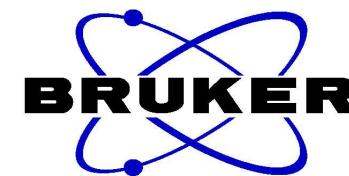
3ab



N-octylquinazolin-2-amine
Proton CDCl₃



N-octylquinazolin-2-amine
C13CPD CDC13



161.867
159.772

152.277

134.074

127.510

125.508

122.343

120.155

77.000

41.627

31.807

29.615

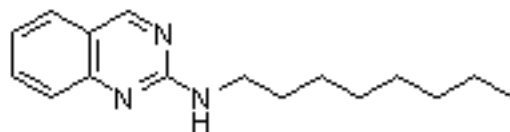
29.339

29.235

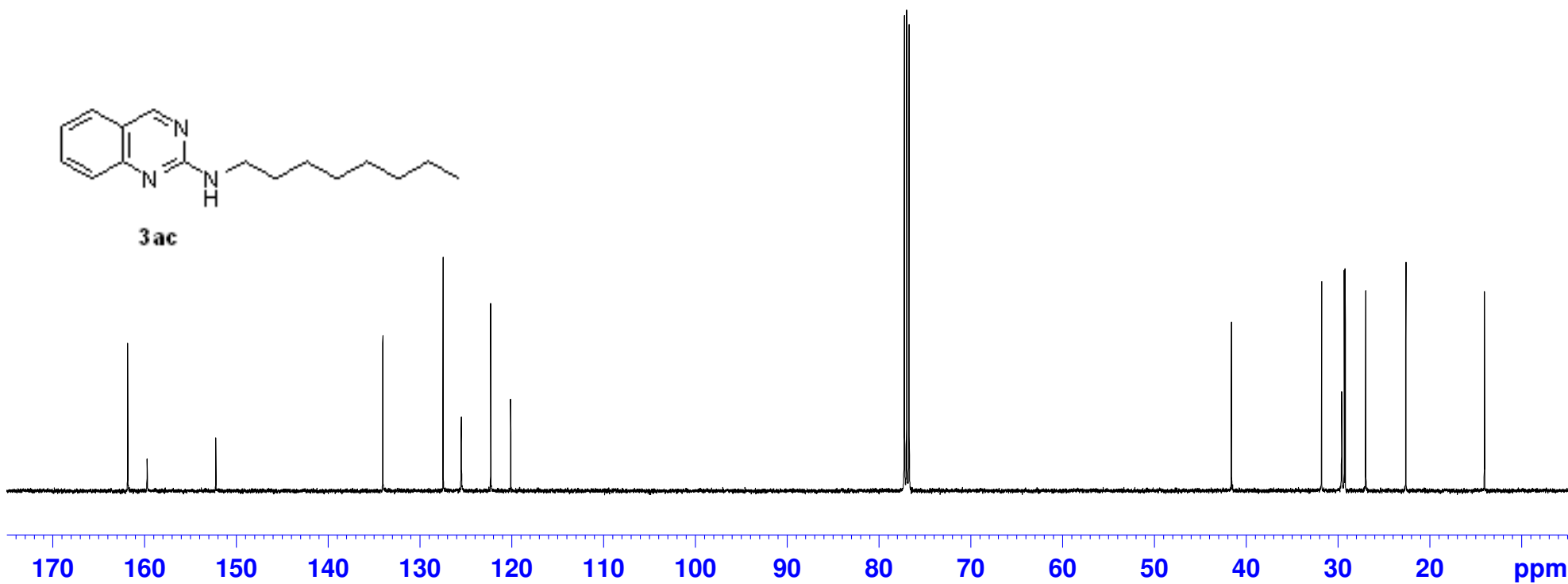
27.009

22.625

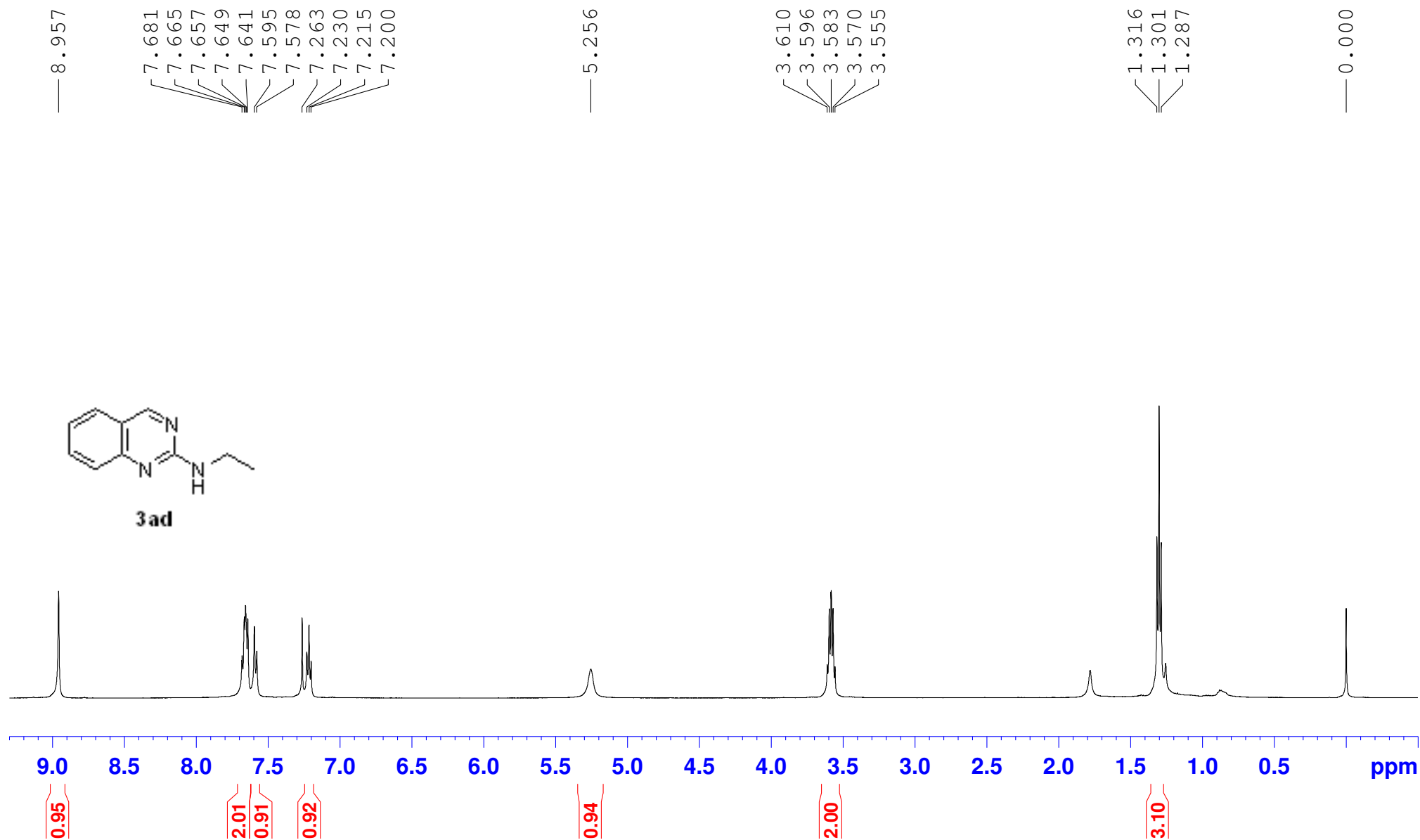
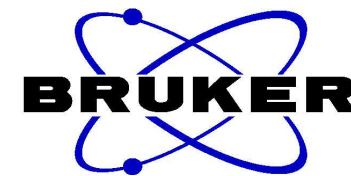
14.083



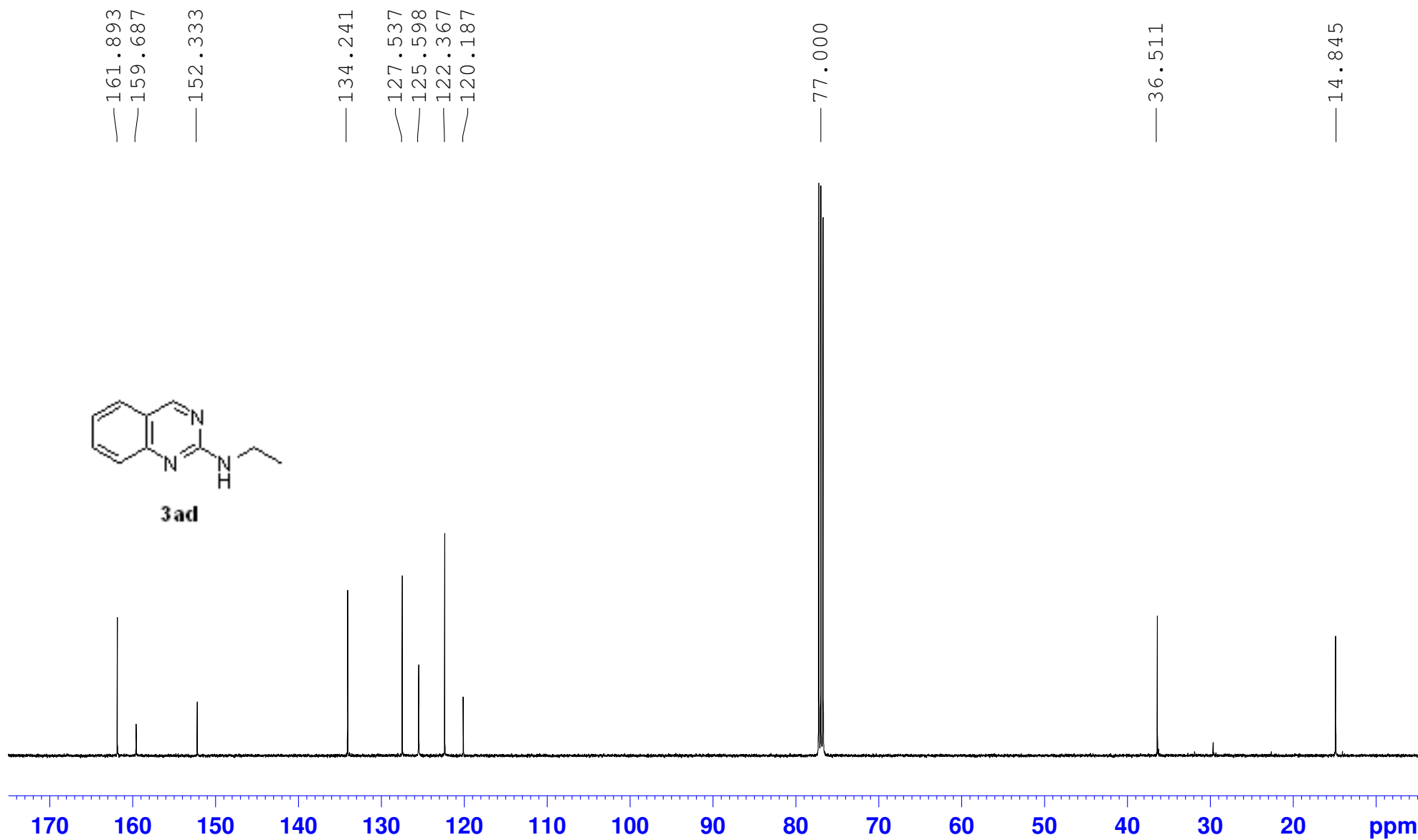
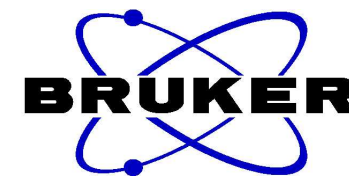
3ac



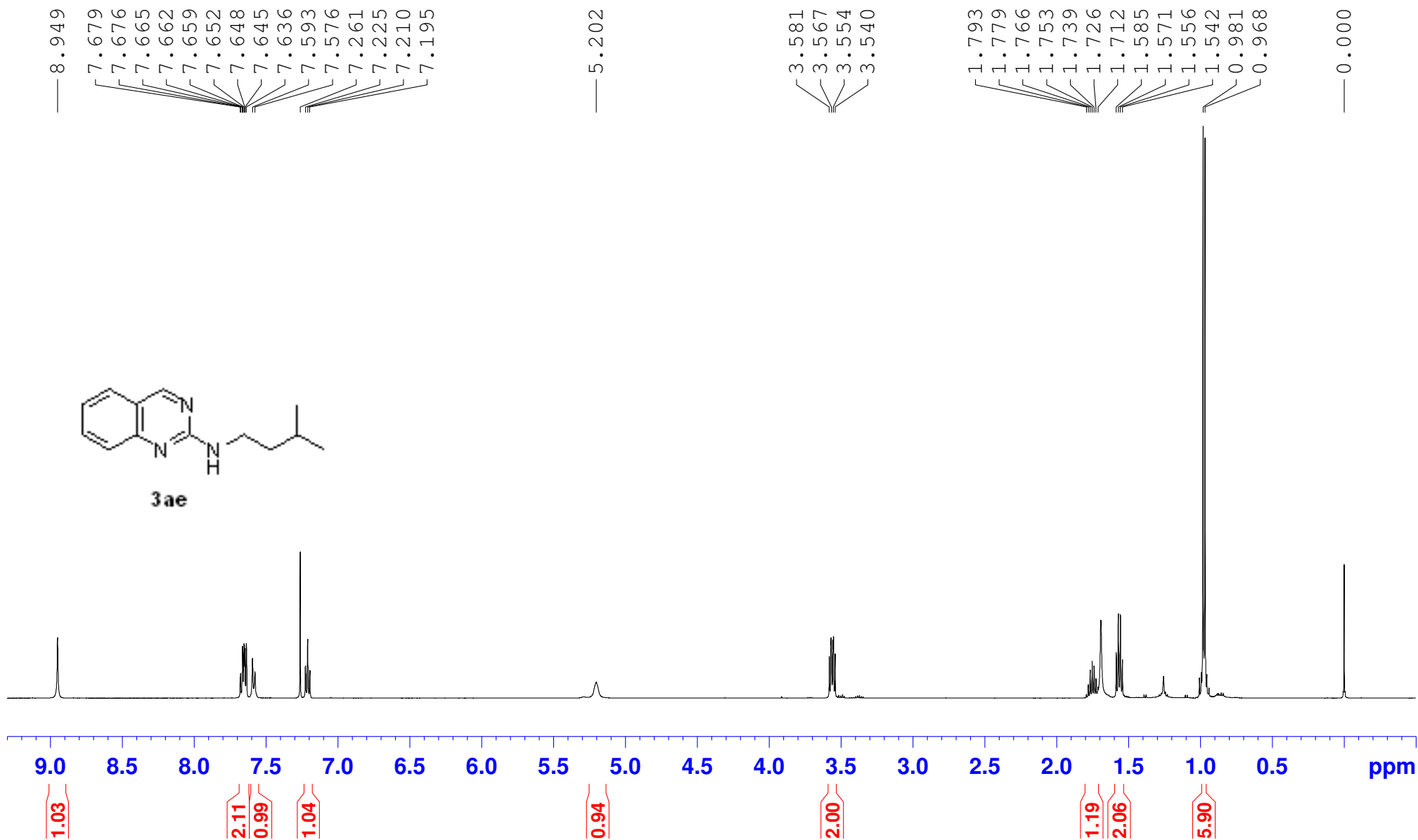
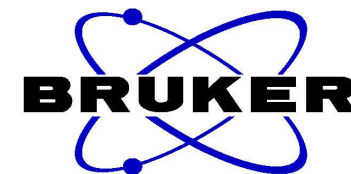
N-ethylquinazolin-2-amine
Proton CDCl₃



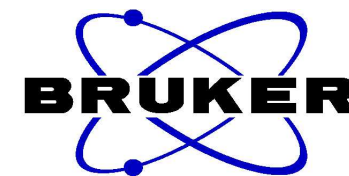
N-ethylquinazolin-2-amine
C13CPD CDC13



N-isopentylquinazolin-2-amine
Proton CDCl₃



N-isopentylquinazolin-2-amine
C13CPD CDC13



161.868
159.755

152.276

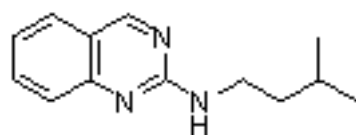
134.108

127.517
125.531
122.320
120.123

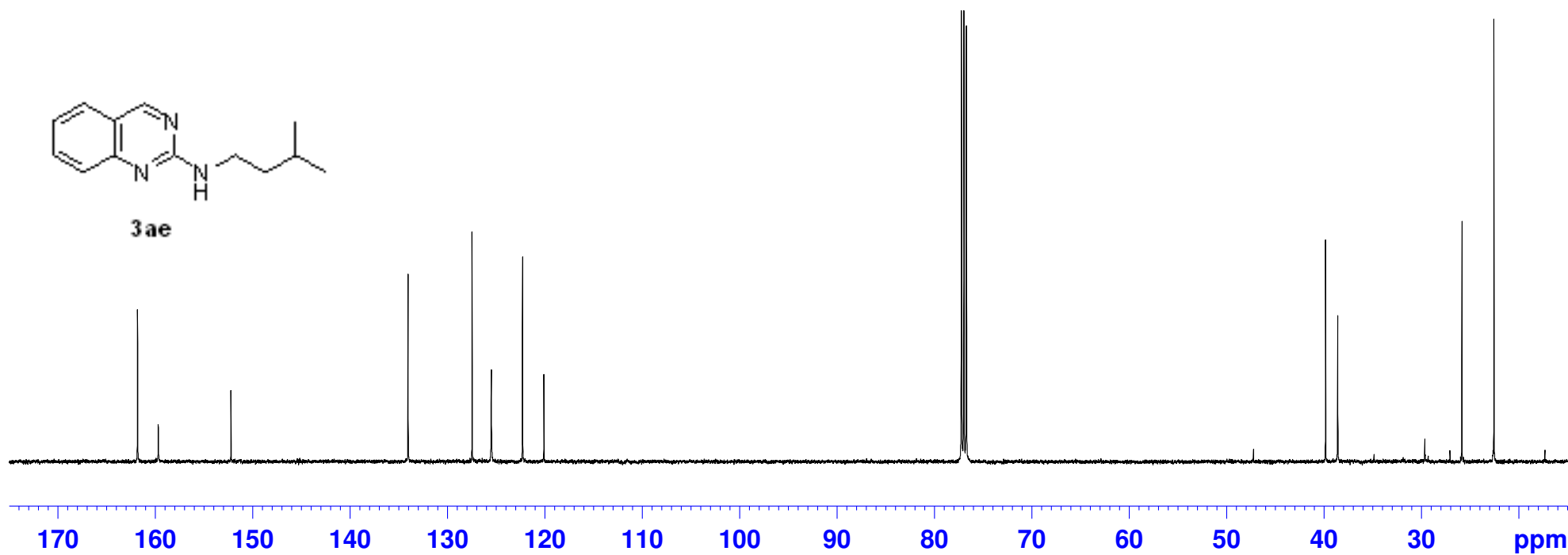
77.000

39.858
38.598

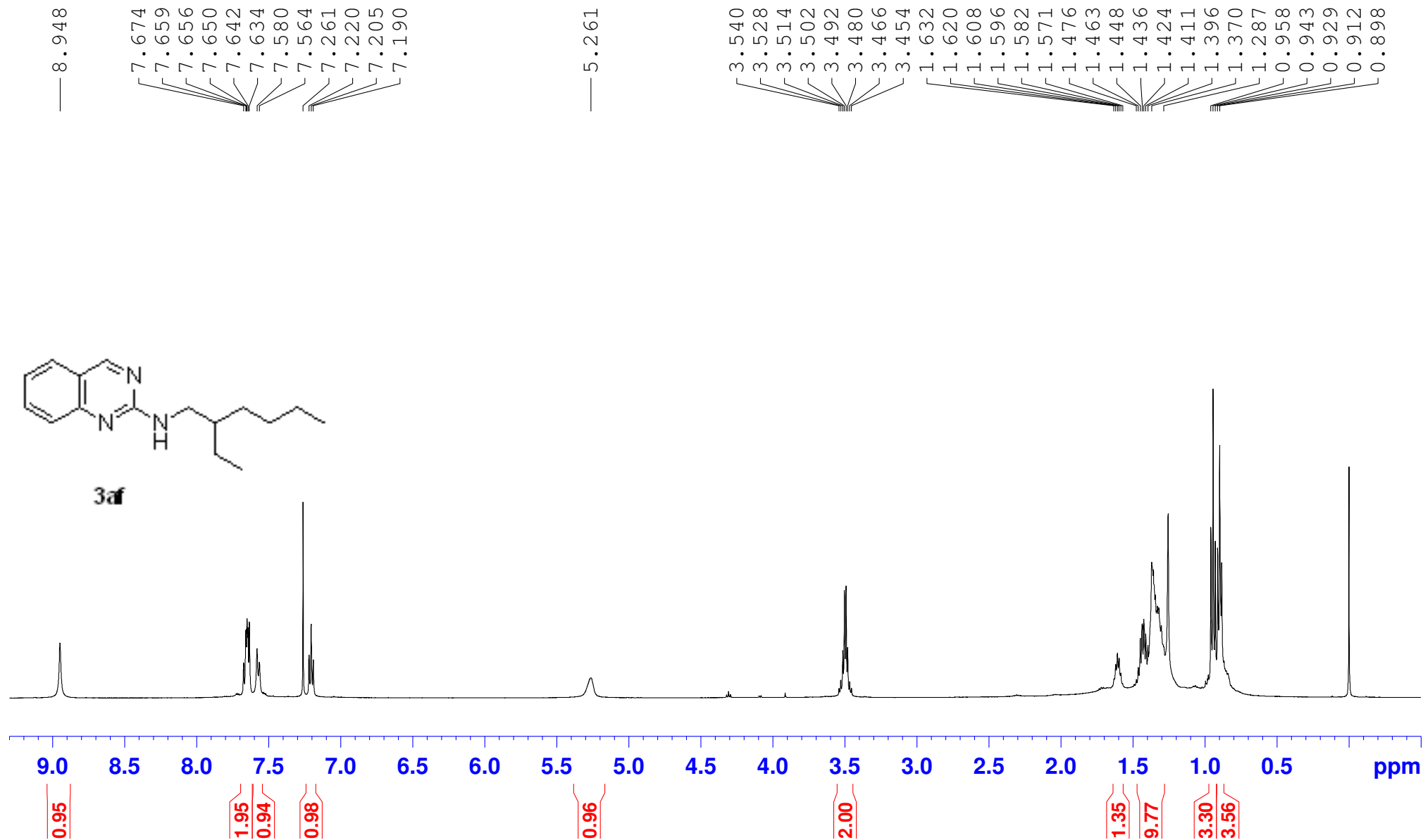
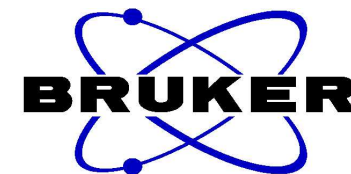
25.847
22.561



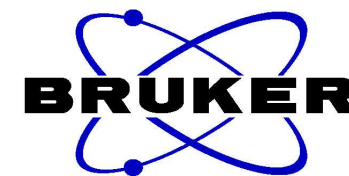
3ae



N-(2-ethylhexyl)quinazolin-2-amine
Proton CDCl₃



N-(2-ethylhexyl)quinazolin-2-amine
C13CPD CDCl₃



161.904
159.931

152.224

134.098

127.501

125.466

122.260

120.102

77.000

44.343

39.468

31.177

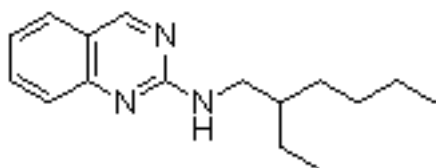
29.003

24.438

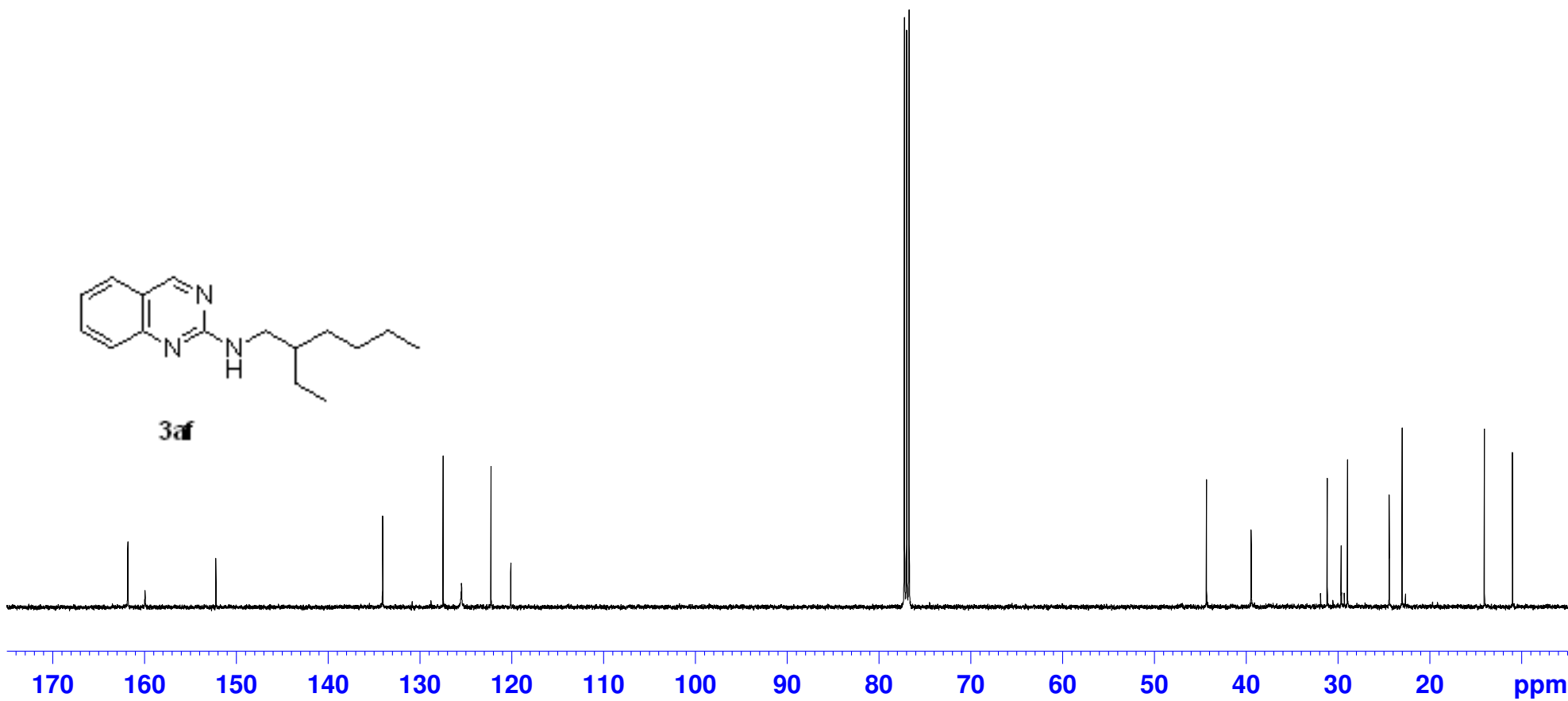
23.072

14.067

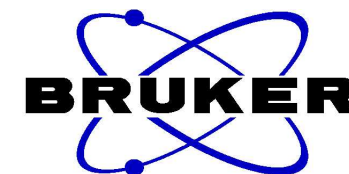
10.993



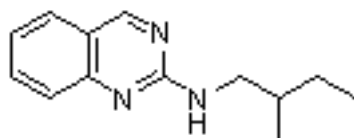
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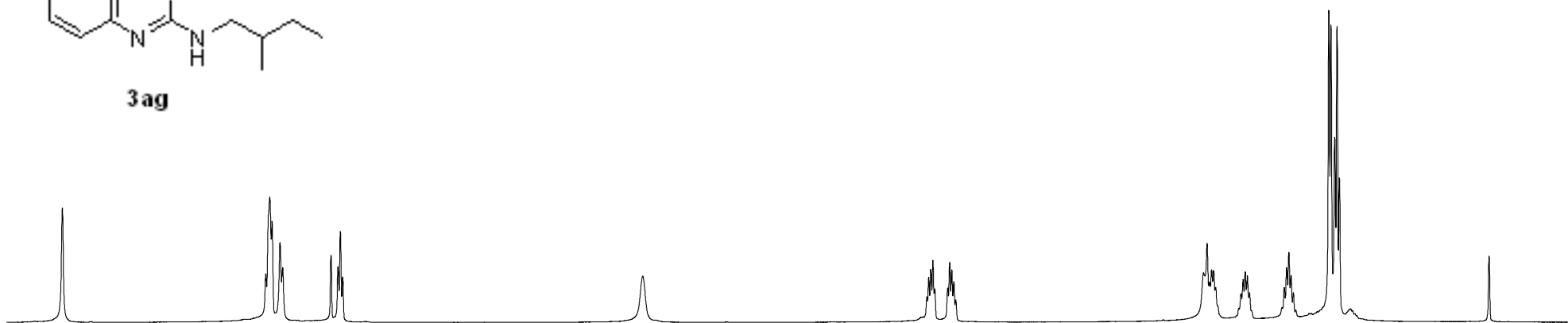
N-(2-methylbutyl)quinazolin-2-amine
Proton CDCl₃



— 8.949
7.673
7.649
7.634
7.584
7.567
7.263
7.220
7.205
7.191
— 5.312
3.528
3.516
3.503
3.490
3.478
3.396
3.385
3.371
3.358
3.346
1.795
1.771
1.756
1.742
1.730
1.716
1.701
1.571
1.558
1.543
1.531
1.516
1.503
1.488
1.301
1.286
1.271
1.256
1.243
1.229
1.214
1.006



3ag

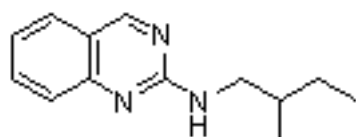


9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.86 1.92 0.95 0.92 0.97 1.00 0.97 2.11 1.12 1.29 2.82 2.88

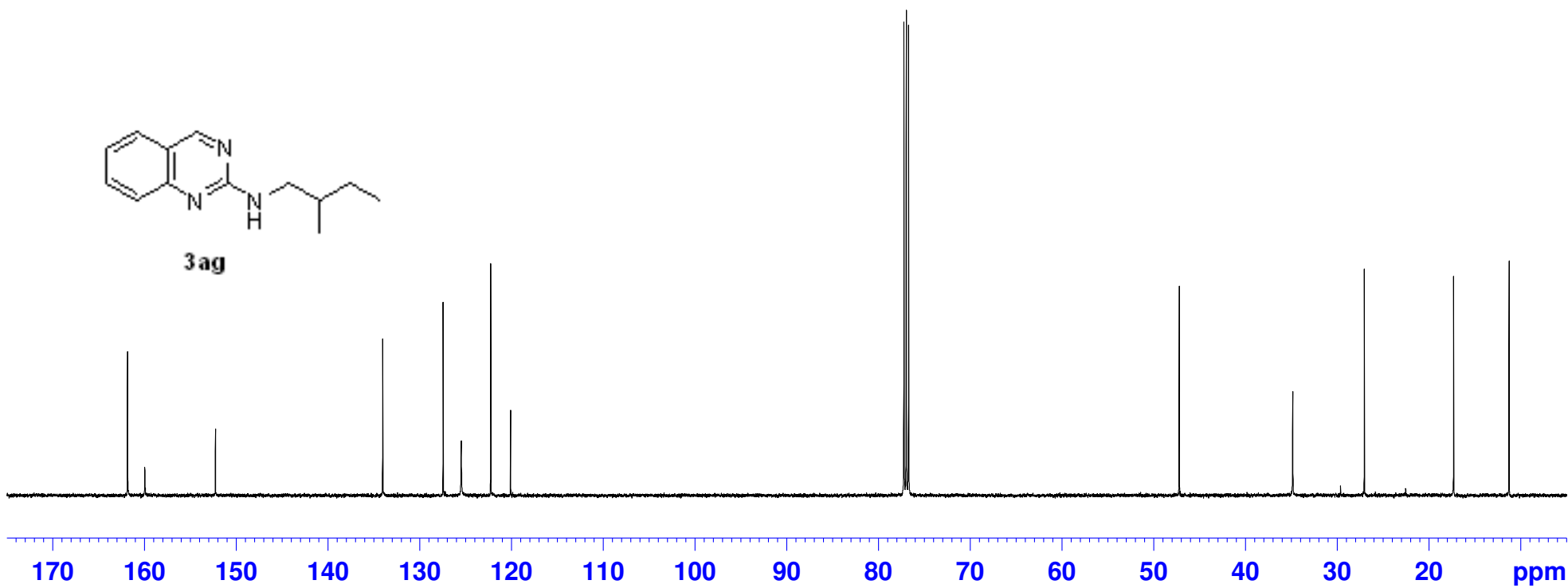
N-(2-methylbutyl)quinazolin-2-amine
C13CPD CDC13



161.925
159.941
152.223
134.068
127.526
125.468
122.381
120.103
77.000
47.342
34.928
27.353
17.464
11.572



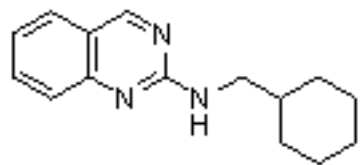
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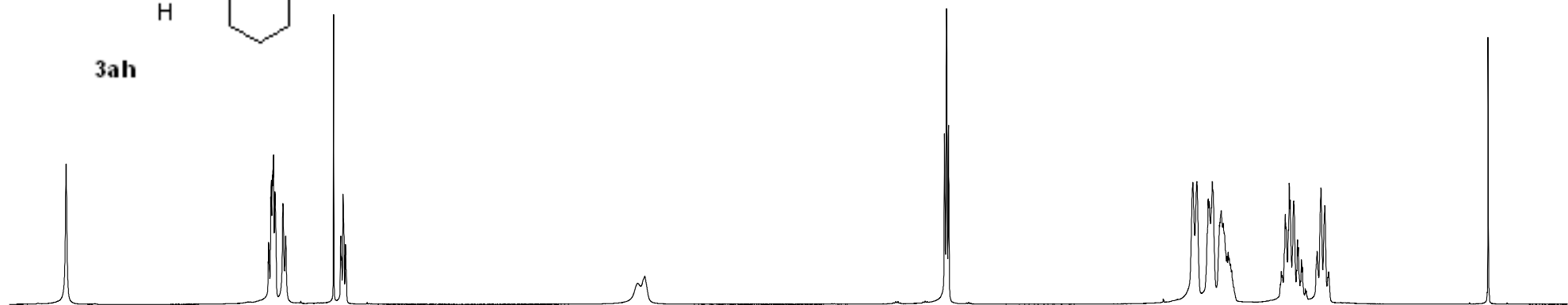
N-(cyclohexylmethyl)quinazolin-2-amine
Proton CDCl₃



8.944
7.670
7.655
7.647
7.640
7.630
7.580
7.563
7.261
7.216
7.202
7.184
5.351
5.304
3.419
3.406
3.394
1.857
1.831
1.757
1.735
1.679
1.611
1.301
1.276
1.251
1.224
1.196
1.172
1.076
1.051
1.027
1.004
0.000

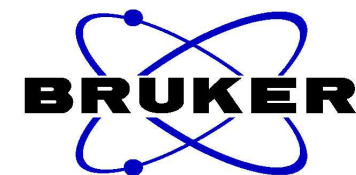


3ah



9.0 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
1.06
2.06
0.92
0.98
1.09
2.00
2.42
2.36
2.60
3.49
2.16

N-(cyclohexylmethyl)quinazolin-2-amine
C13CPD CDC13



161.807
159.958

152.272

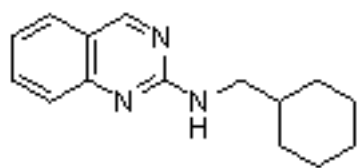
134.024

127.466
125.500
122.241
120.116

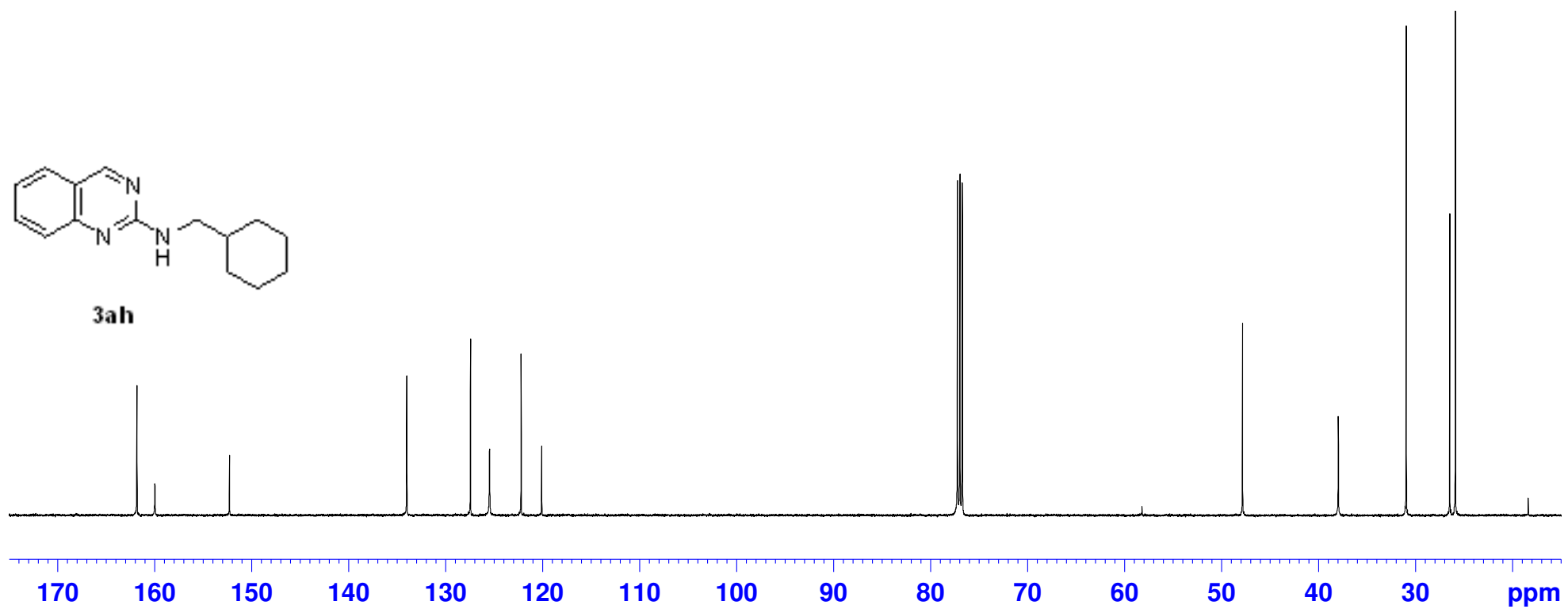
77.000

47.860

37.992
30.985
26.499
25.907



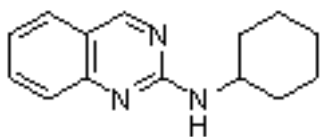
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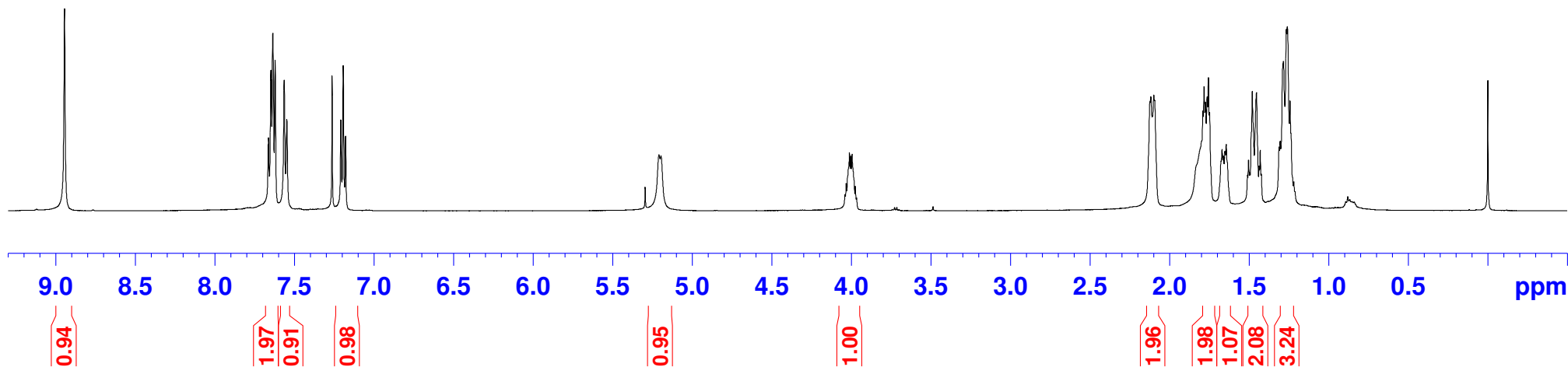
N-cyclohexylquinazolin-2-amine
Proton CDCl₃



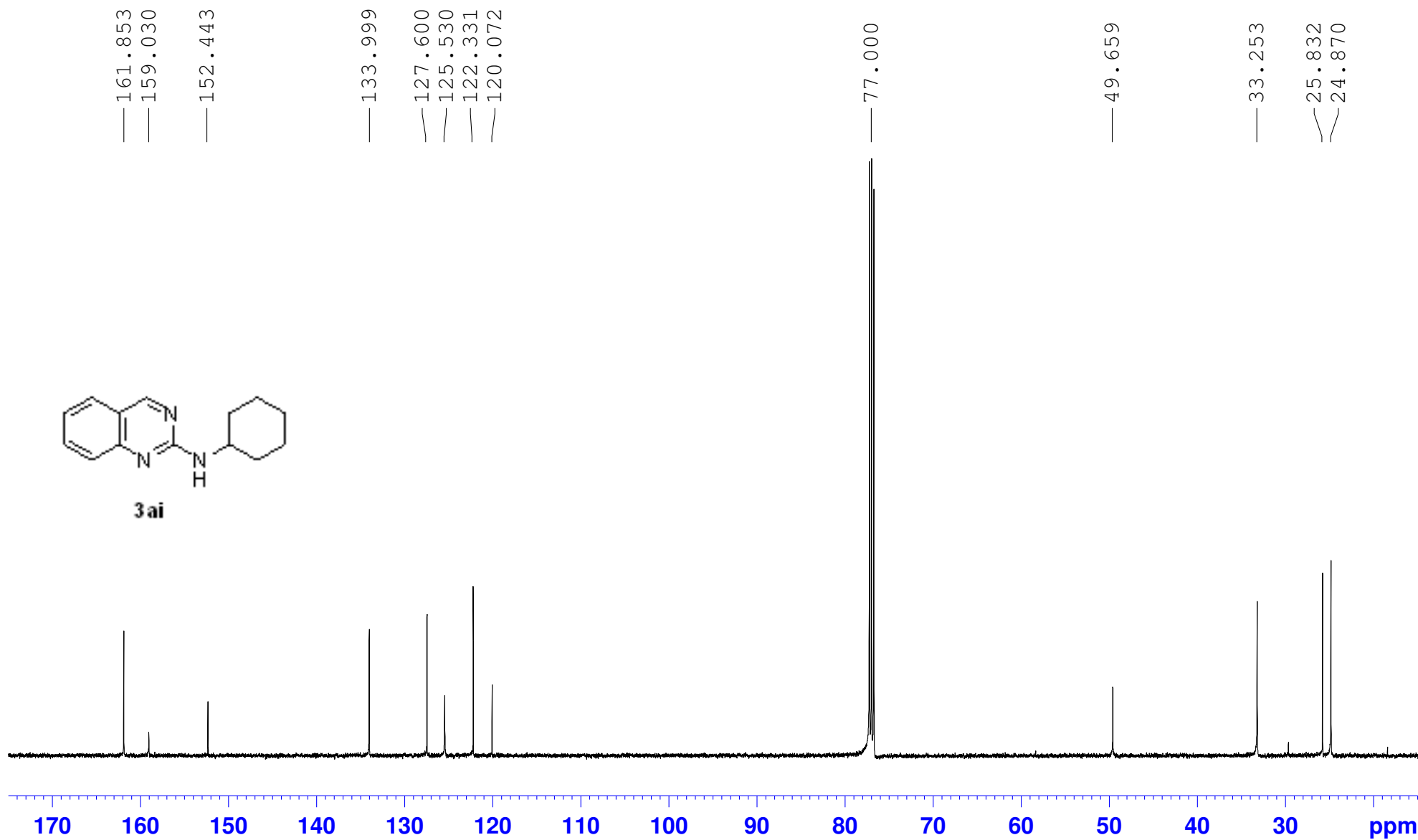
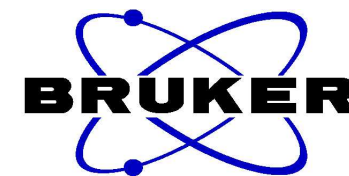
8.944
7.662
7.648
7.635
7.621
7.564
7.547
7.262
7.208
7.193
7.178
5.202
4.040
4.032
4.011
4.003
3.995
3.975
3.967
2.124
2.092
1.790
1.783
1.774
1.763
1.755
1.748
1.677
1.670
1.662
1.652
1.644
1.636
1.510
1.503
1.496
1.480
1.454
1.437
1.430
1.423
1.312
1.305
1.285



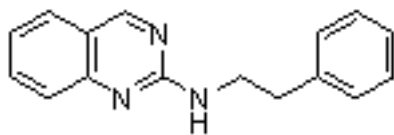
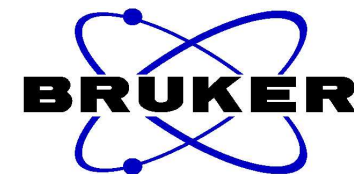
3ai



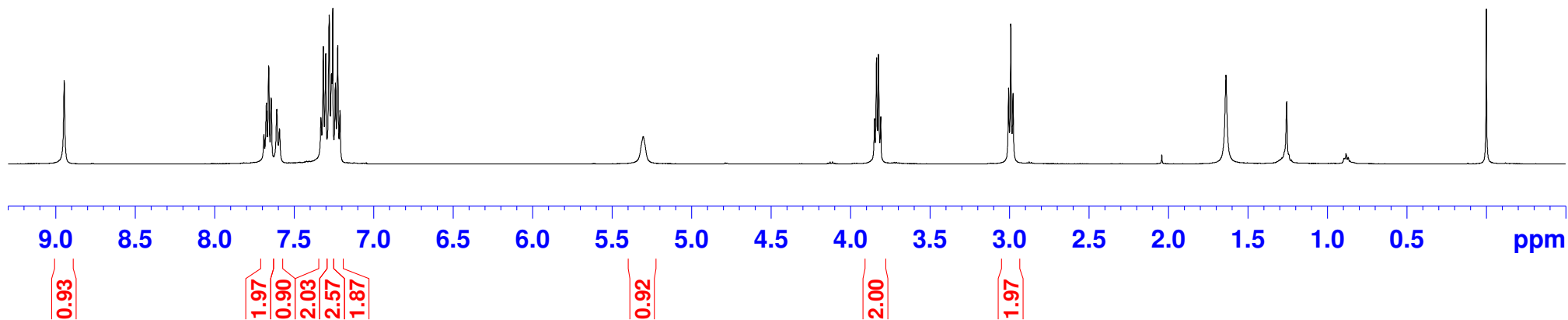
N-cyclohexylquinazolin-2-amine
C13CPD CDCl₃



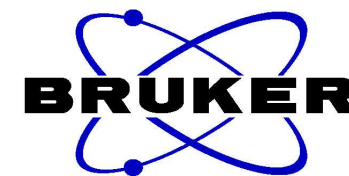
N-phenethylquinazolin-2-amine
Proton CDCl₃



3aj



N-phenethylquinazolin-2-amine
C13CPD CDC13



— 161.968
— 159.556

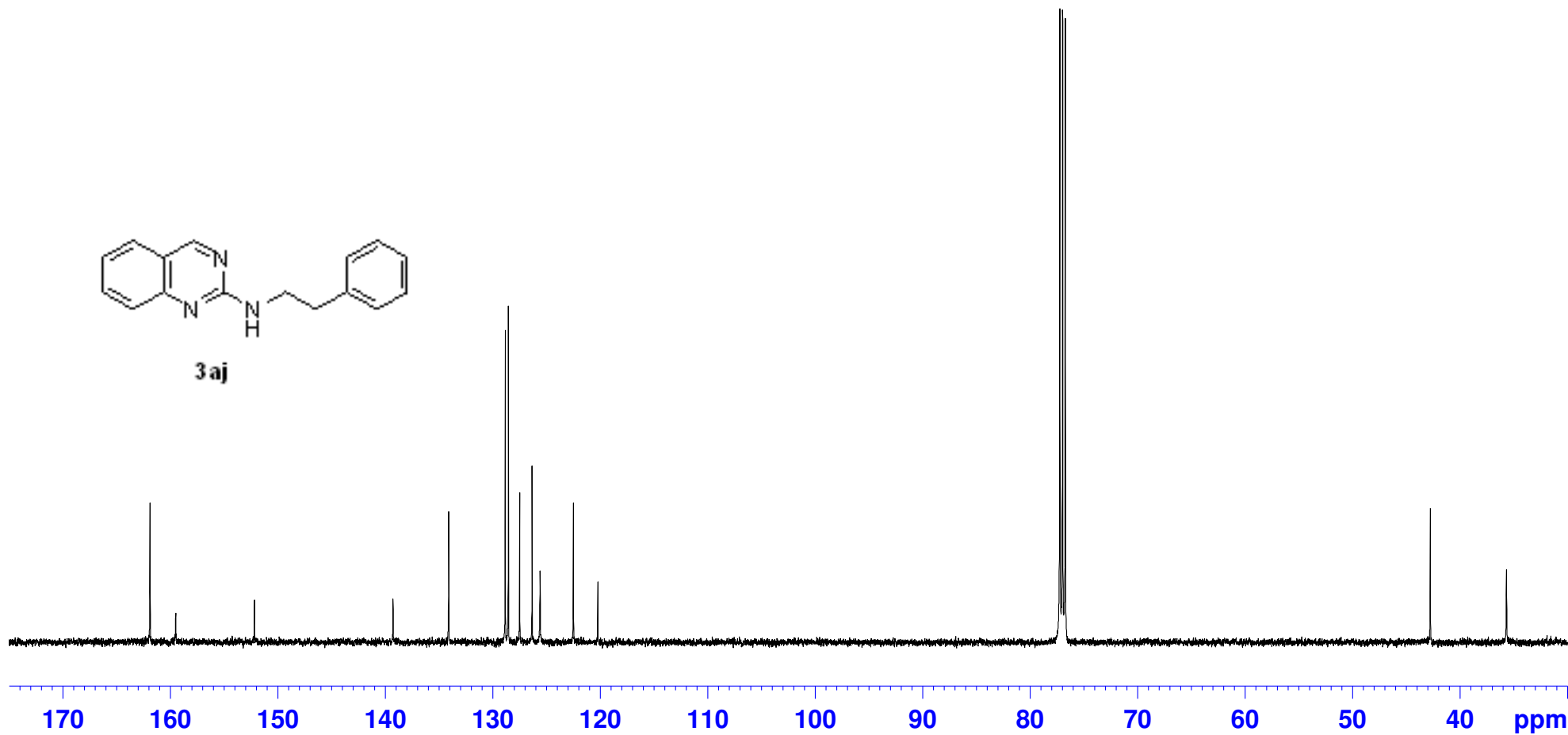
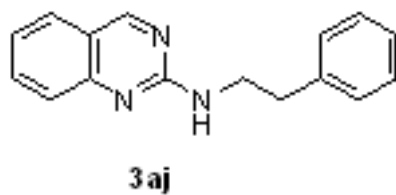
— 152.209

— 139.366
— 134.095
— 128.935
— 128.599
— 127.533
— 126.355
— 125.626
— 122.542
— 120.242

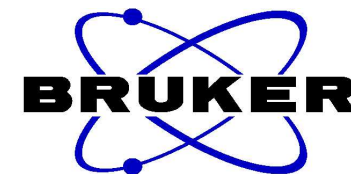
— 77.000

— 42.727

— 35.702



N-(3-phenylpropyl)quinazolin-2-amine
Proton CDCl₃



8.953
7.684
7.681
7.667
7.664
7.654
7.651
7.641
7.588
7.572
7.302
7.287
7.273
7.256
7.228
7.215
7.204
7.191
7.177

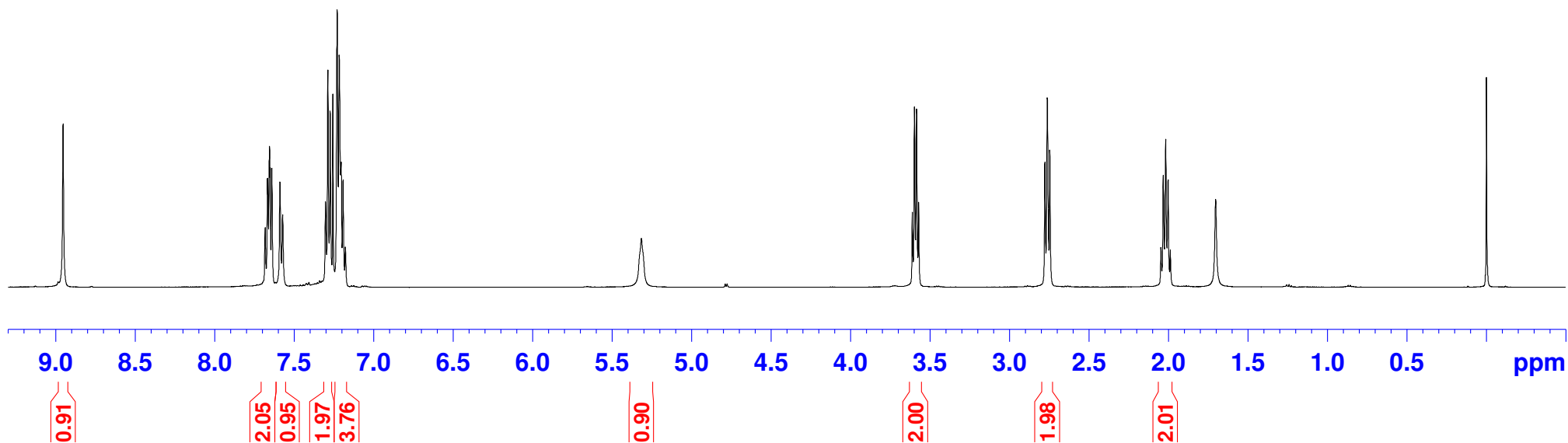
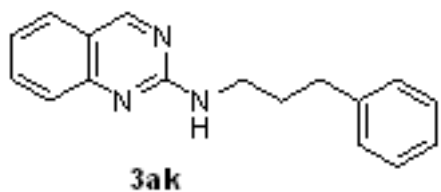
5.315

3.611
3.597
3.584
3.571

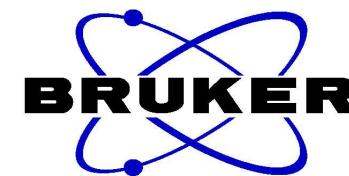
2.777
2.761
2.746

2.047
2.032
2.017
2.002
1.988

0.000



N-(3-phenylpropyl)quinazolin-2-amine
C13CPD CDCl₃

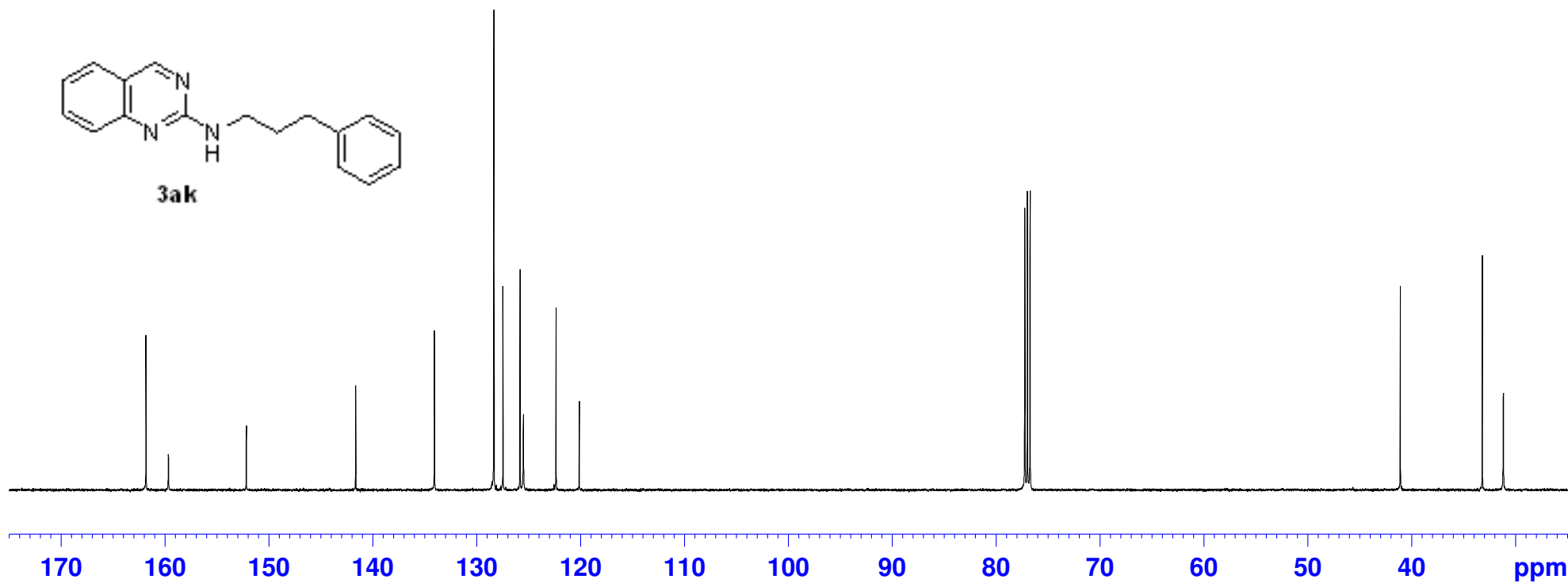
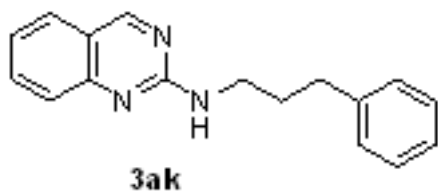


161.915
159.765
152.199
141.726
134.120
128.375
128.353
127.509
125.876
125.558
122.412
120.182

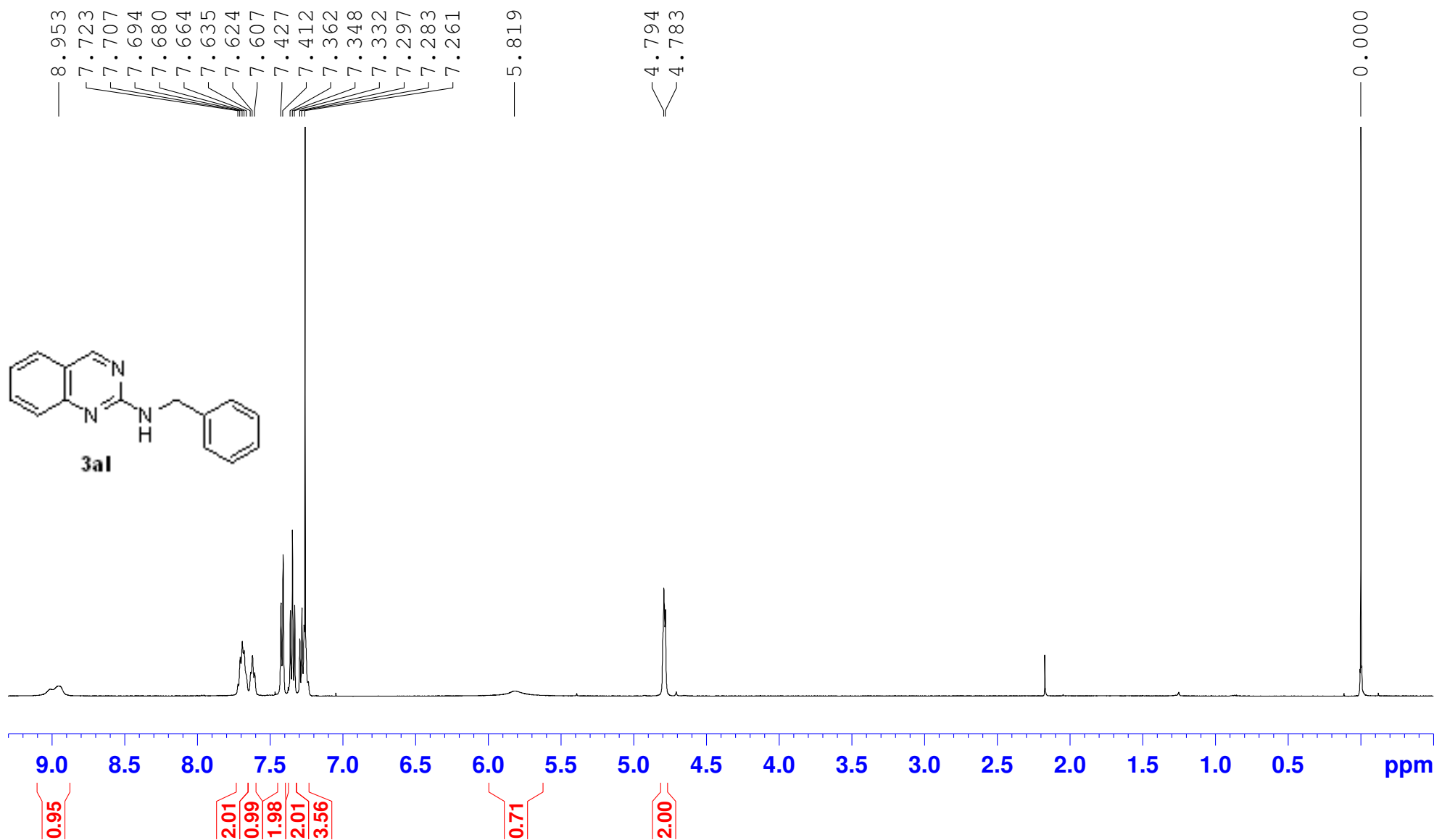
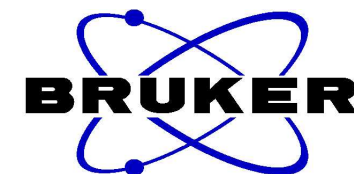
77.000

41.125

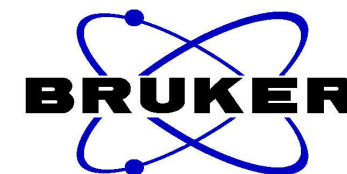
33.243
31.197



N-benzylquinazolin-2-amine
Proton CDCl₃



N-benzylquinazolin-2-amine
C13CPD CDCl3

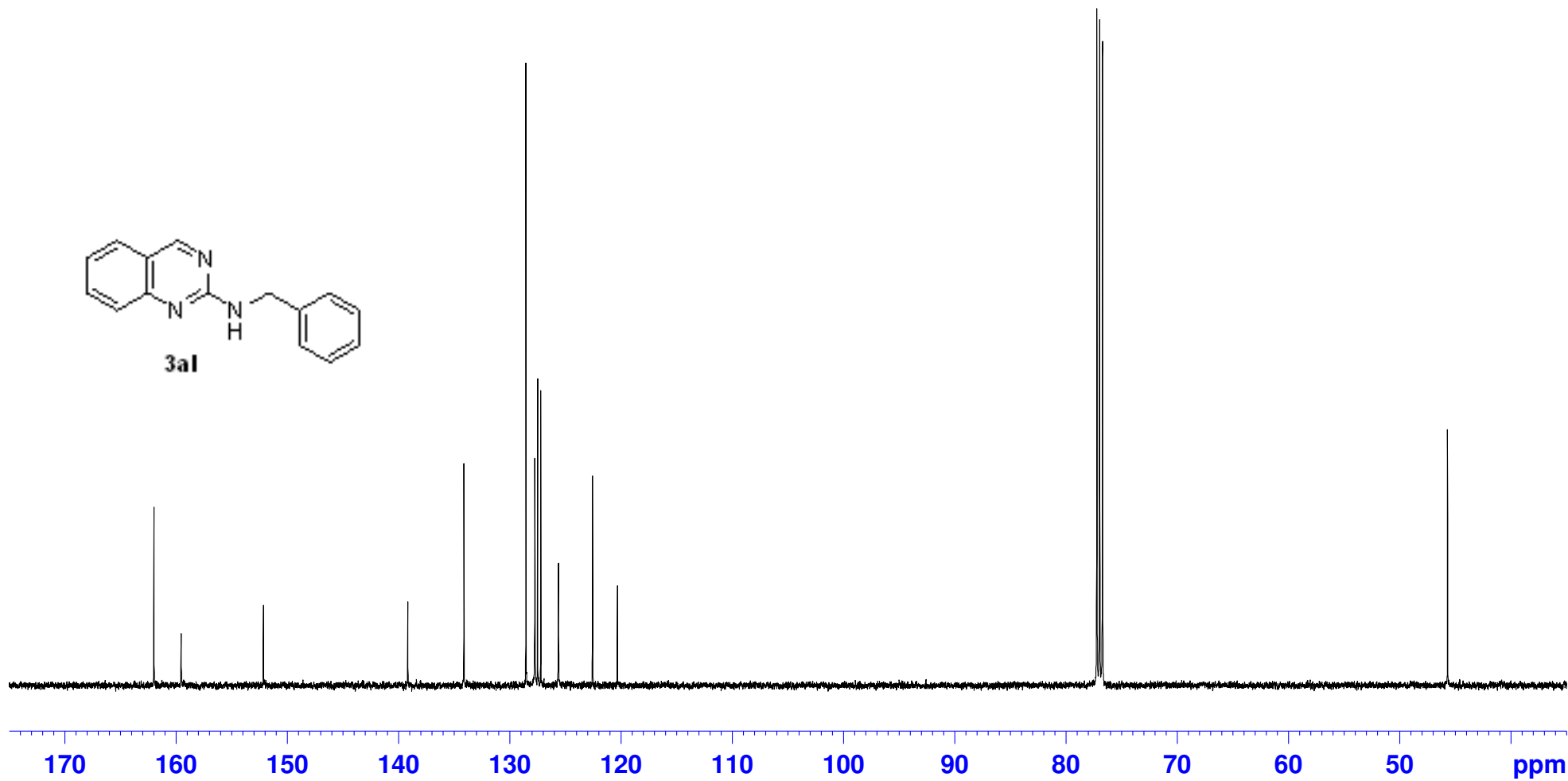
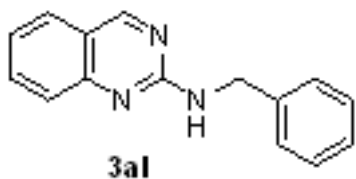


— 162.016
— 159.565

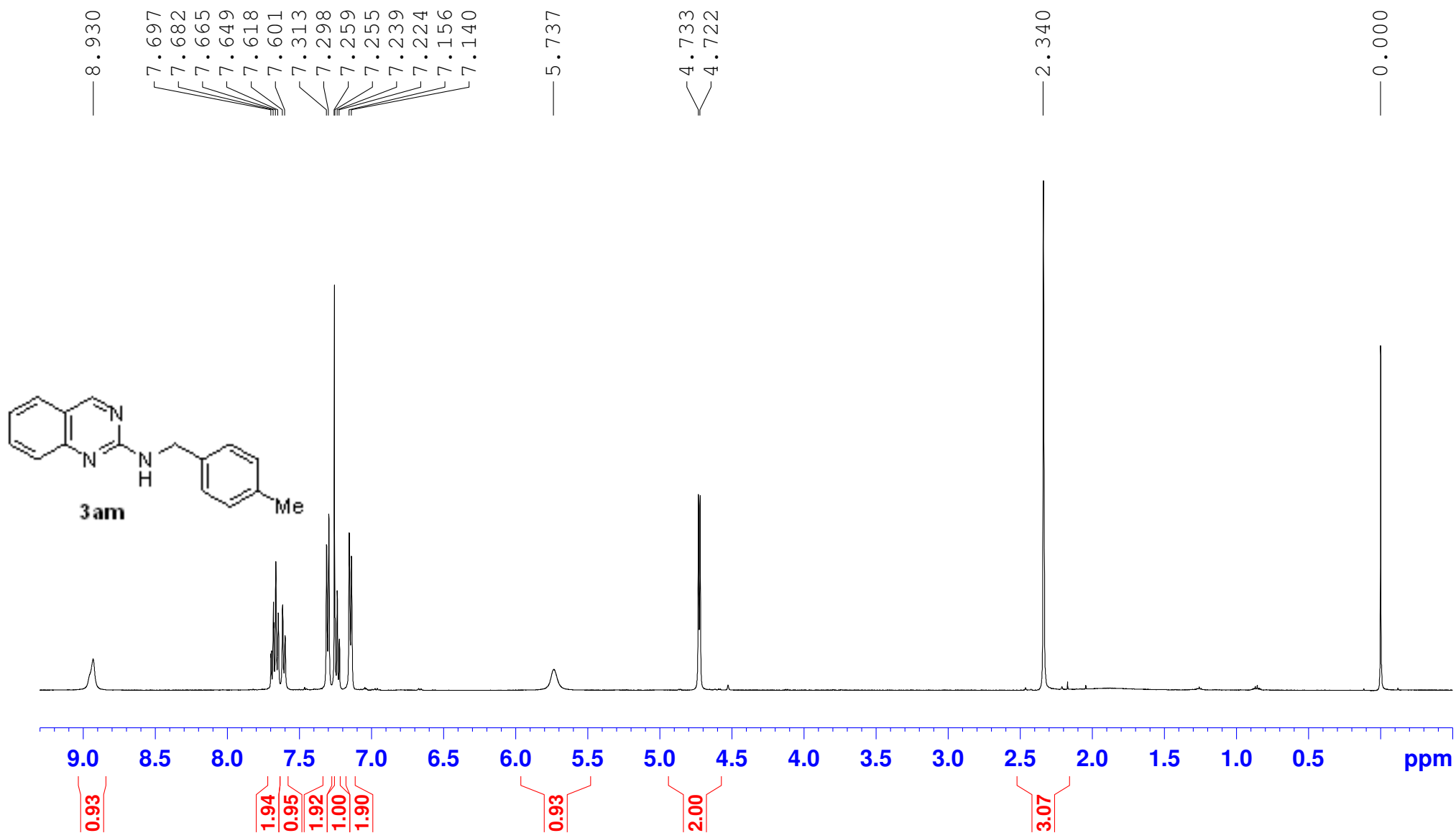
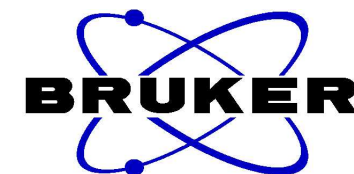
— 152.167

— 139.209
— 134.175
— 128.571
— 127.774
— 127.514
— 127.243
— 125.648
— 122.578
— 120.344

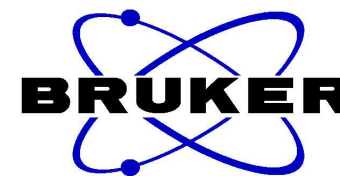
— 45.



N-(4-methylbenzyl)quinazolin-2-amine
Proton CDCl₃



N-(4-methylbenzyl)quinazolin-2-amine
C13CPD CDC13

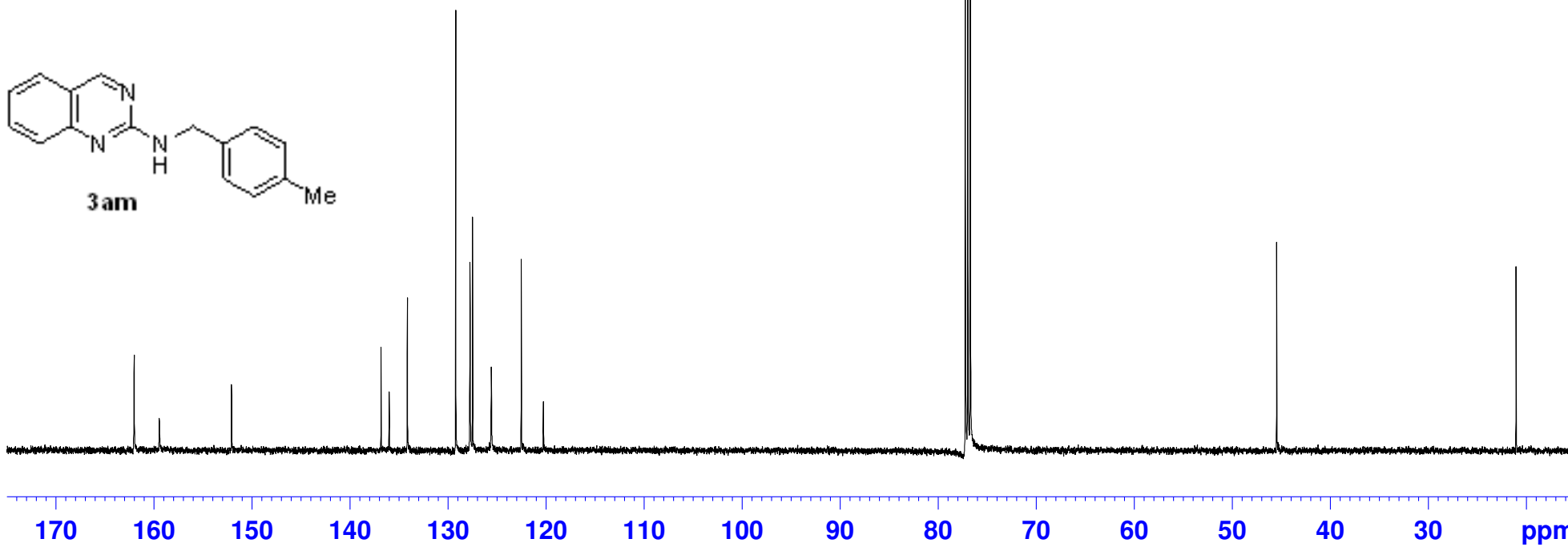
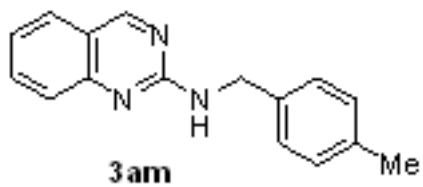


162.003
159.457
152.121
136.866
136.043
134.162
129.238
127.790
127.531
125.611
122.545
120.298

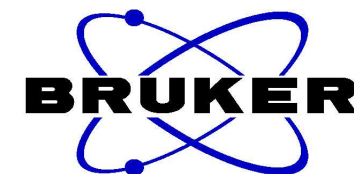
77.000

45.500

21.0



N-(4-(trifluoromethyl)benzyl)quinazolin-2-amine
Proton CDCl₃

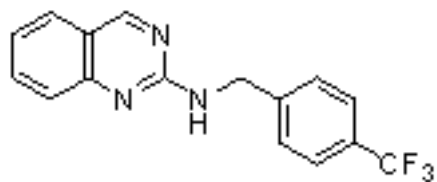


8.956
7.707
7.703
7.693
7.690
7.686
7.684
7.676
7.673
7.668
7.596
7.576
7.533
7.517
7.275
7.260
7.245

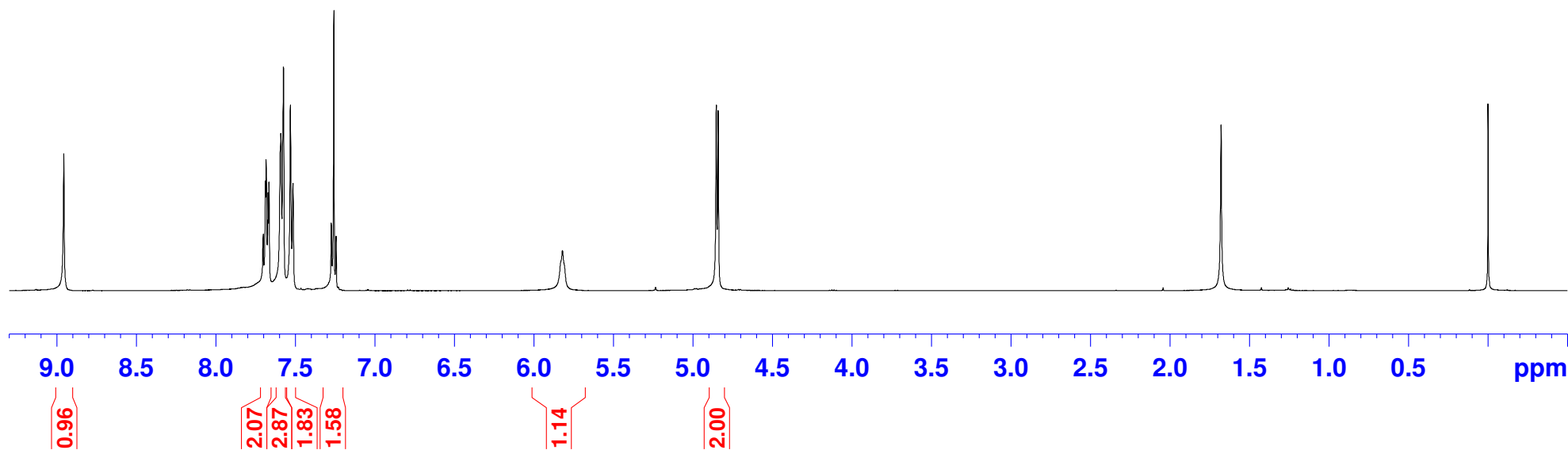
5.822

4.855
4.842

0.000



3an



N-(4-(trifluoromethyl)benzyl)quinazolin-2-amine
C13CPD CDCl₃



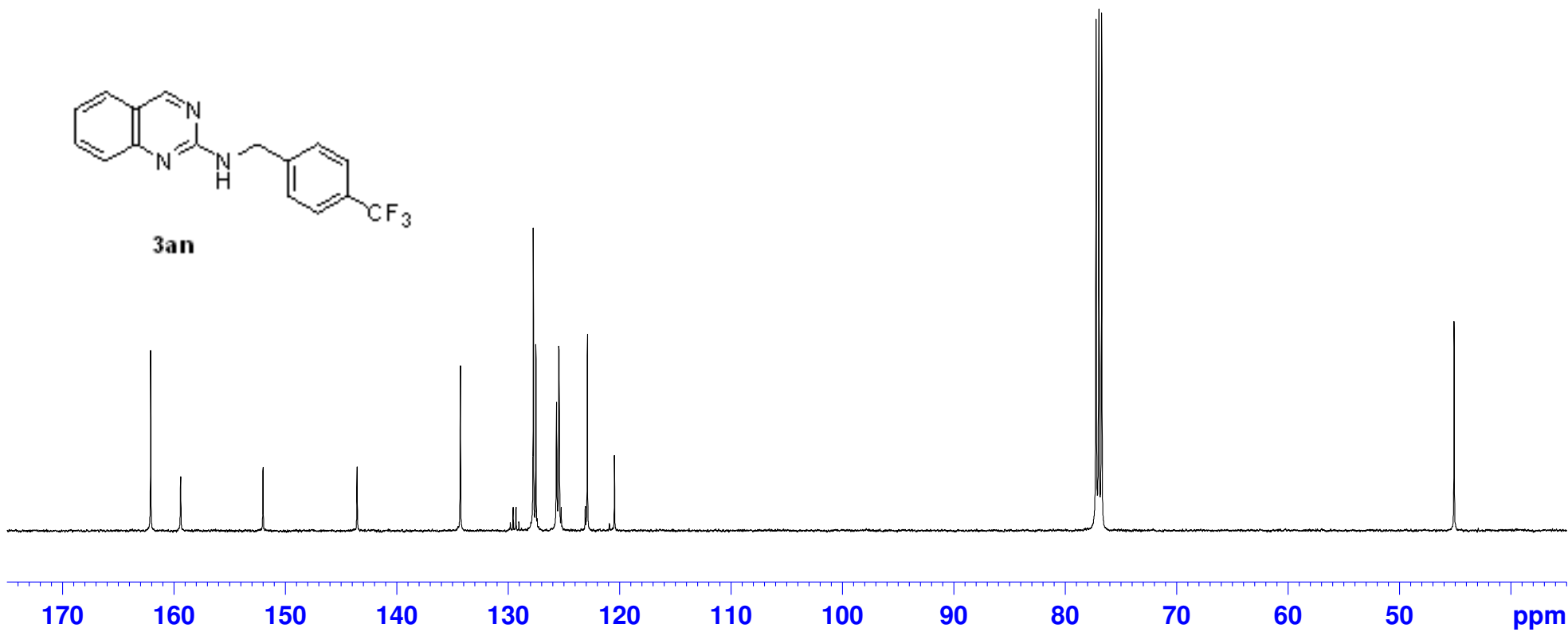
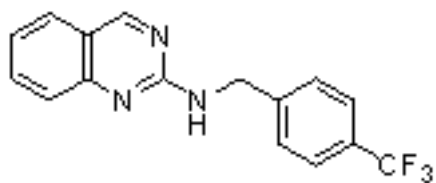
— 162.073
— 159.423

— 152.026

— 143.587
— 134.305
— 129.837
— 129.581
— 129.321
— 129.065
— 127.768
— 127.537
— 125.680
— 125.458
— 125.265
— 123.100
— 122.913
— 120.940
— 120.484

— 77.001

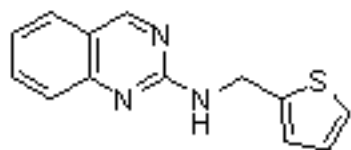
— 45.1



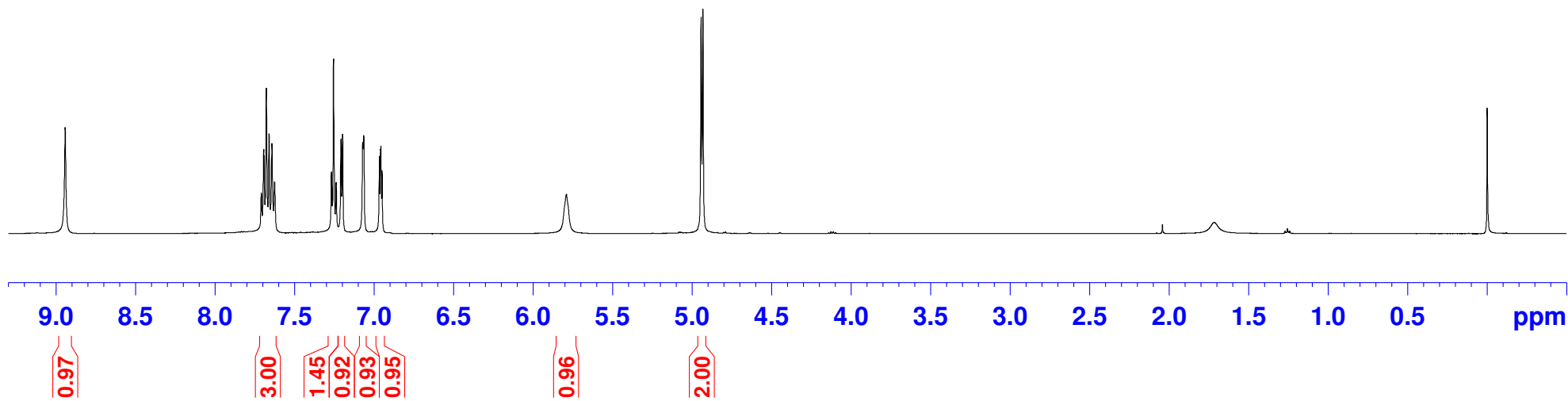
N-(thiophen-2-ylmethyl)quinazolin-2-amine
Proton CDCl₃



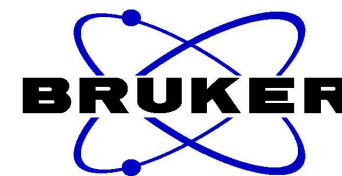
8.941
7.710
7.696
7.679
7.662
7.644
7.627
7.269
7.257
7.239
7.209
7.199
7.072
7.067
6.968
6.960
6.951
5.792
4.945
4.933
0.000



3ao



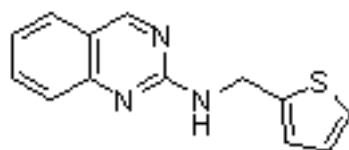
N-(thiophen-2-ylmethyl)quinazolin-2-amine
C13CPD CDCl3



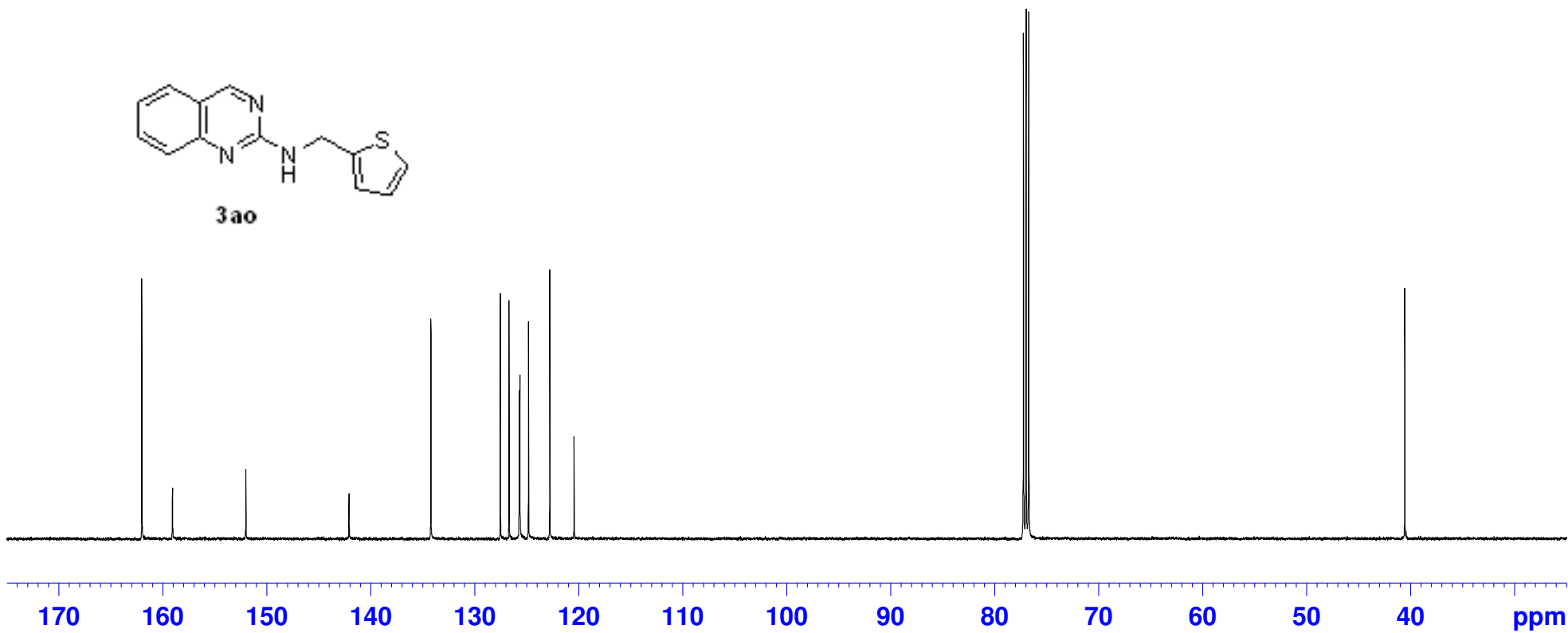
— 162.023
— 159.102
— 151.993
— 142.073
— 134.192
— 127.579
— 126.697
— 125.703
— 125.644
— 124.879
— 122.840
— 120.415

— 77.000

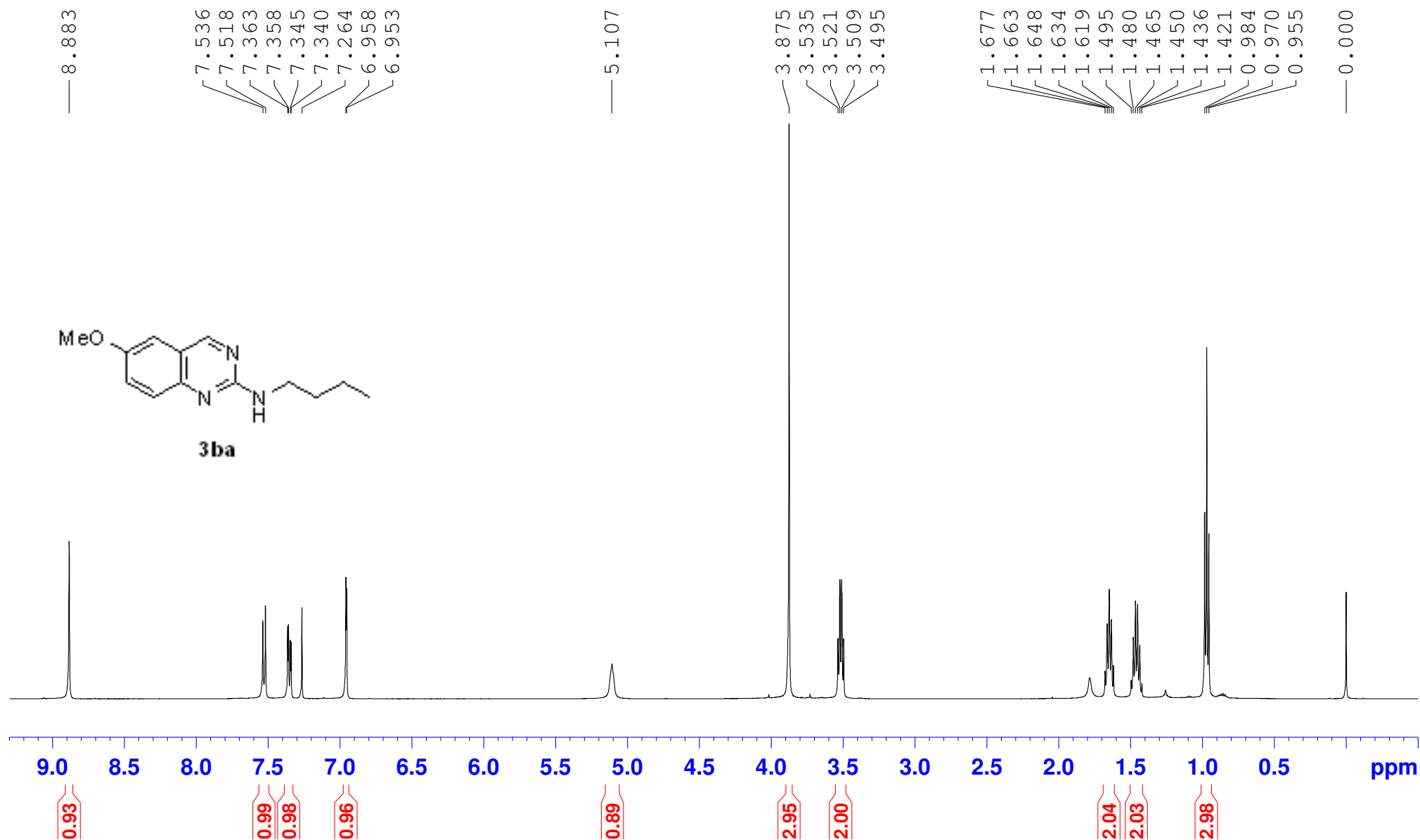
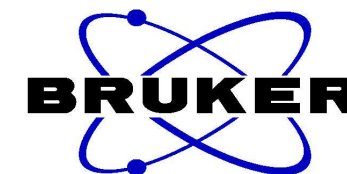
— 40.577



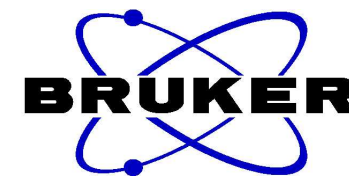
3ao



N-butyl-6-methoxyquinazolin-2-amine
Proton CDCl₃



N-butyl-6-methoxyquinazolin-2-amine
C13CPD CDC13



160.325
159.135
154.794
148.213

127.140
126.510
120.209

105.087

77.000

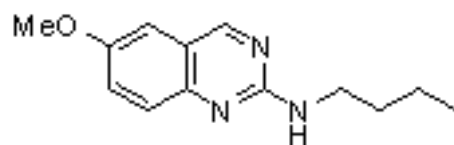
55.535

41.440

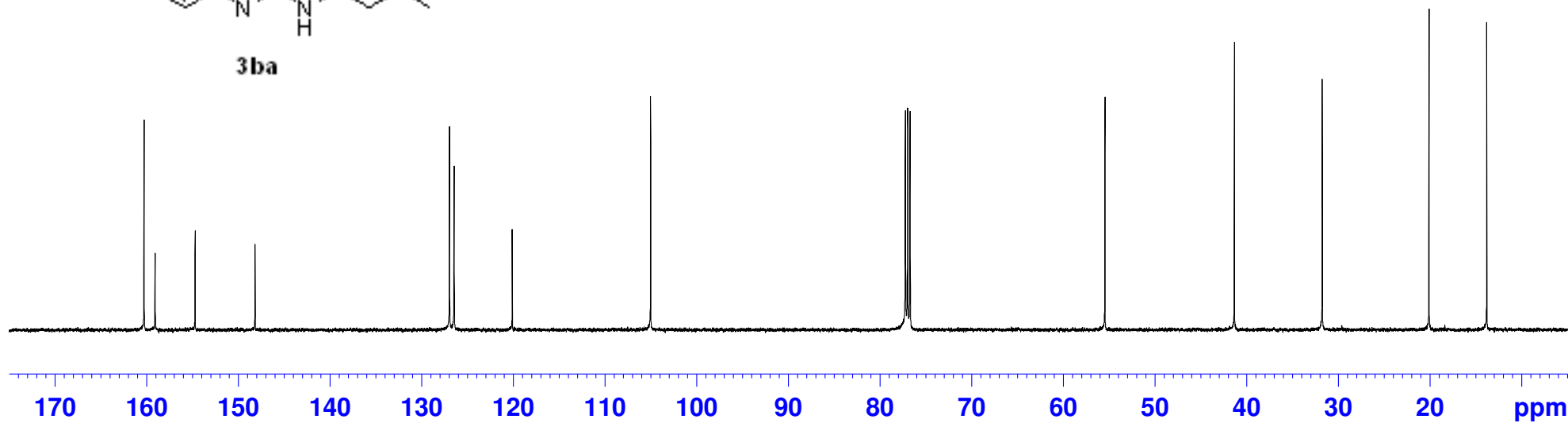
31.819

20.172

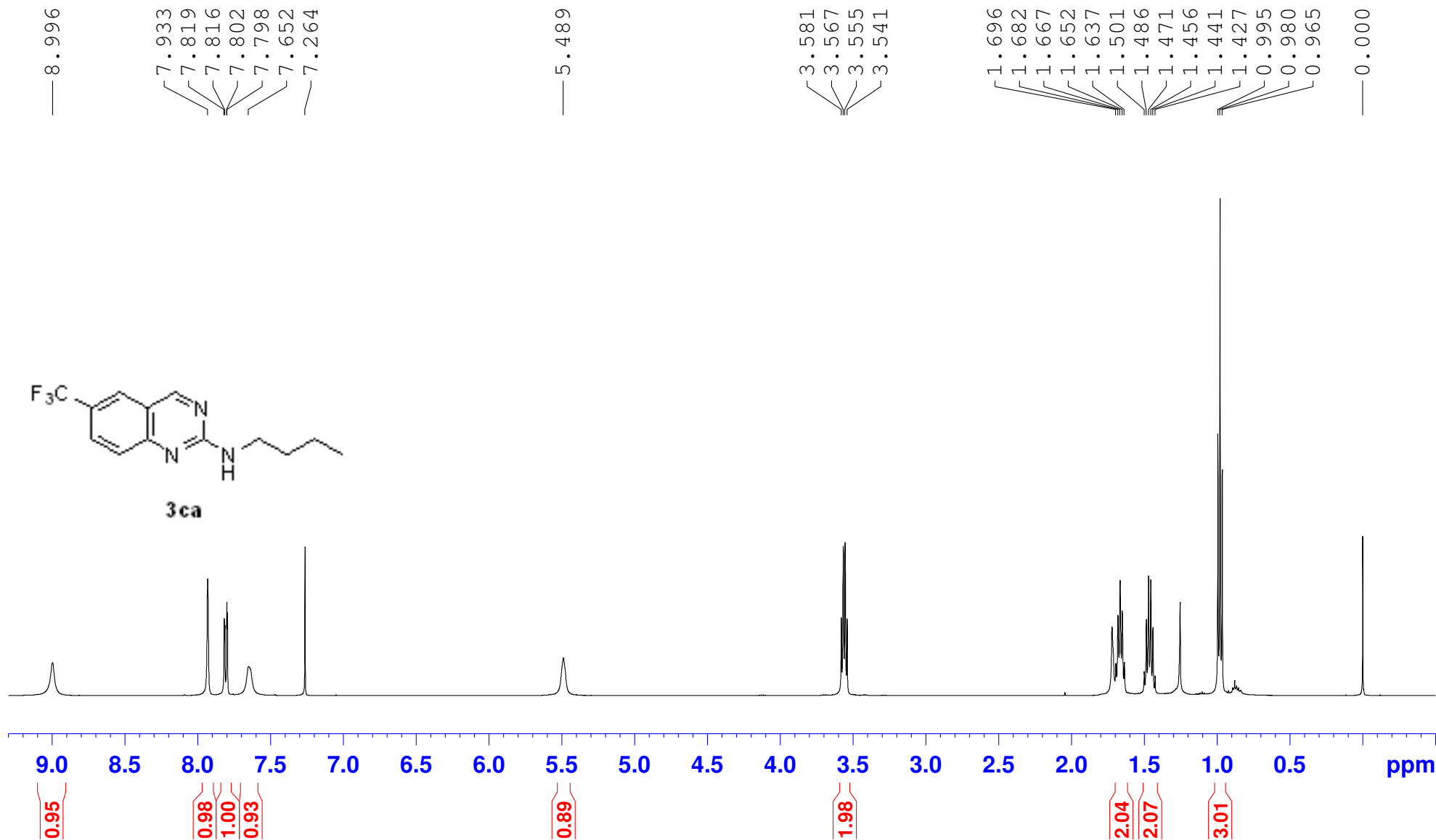
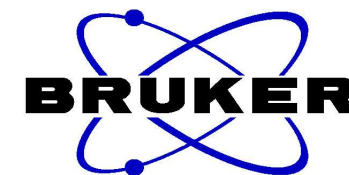
13.842



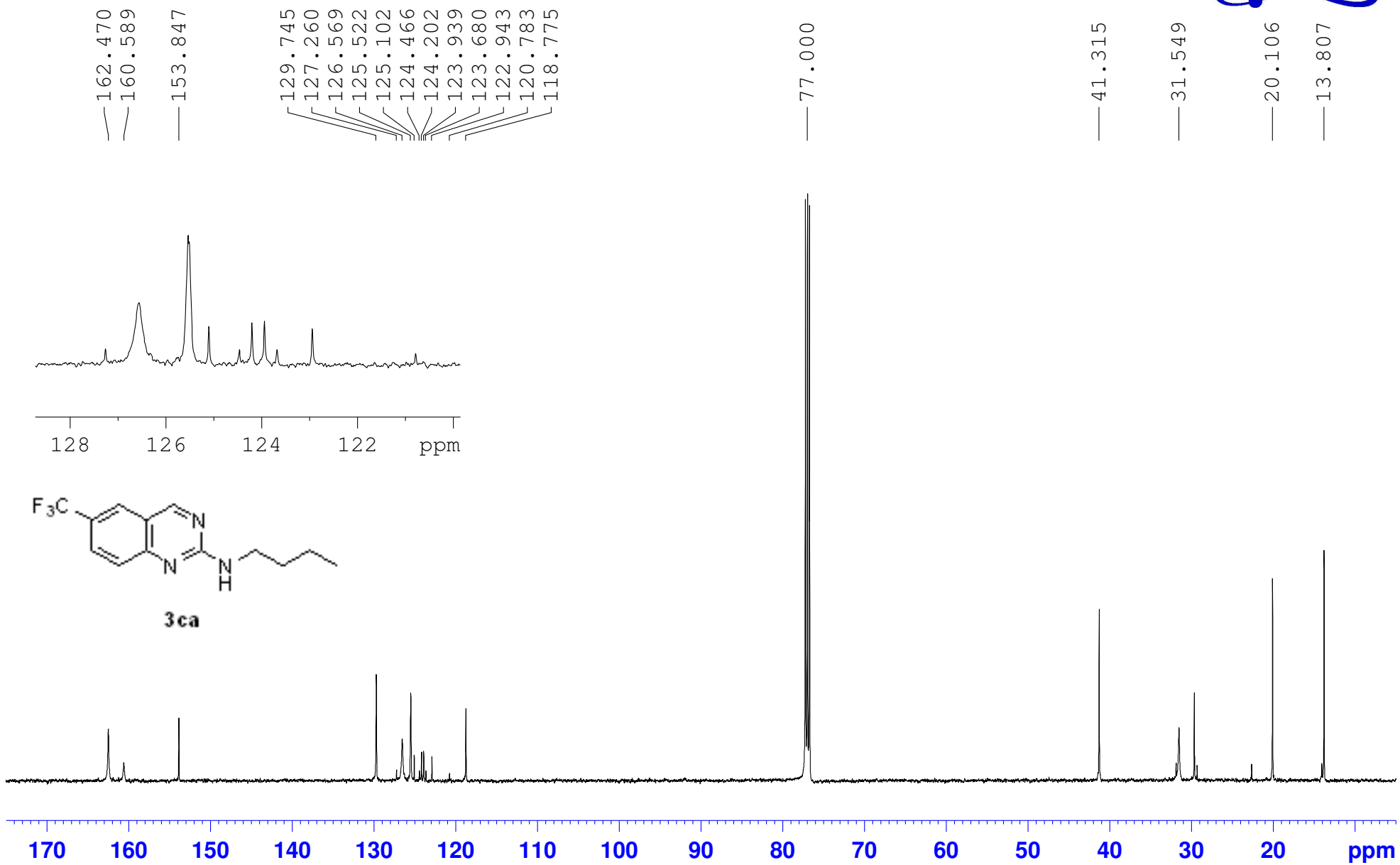
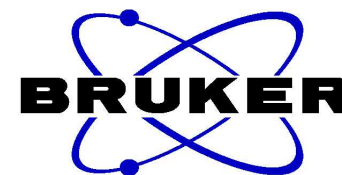
3ba



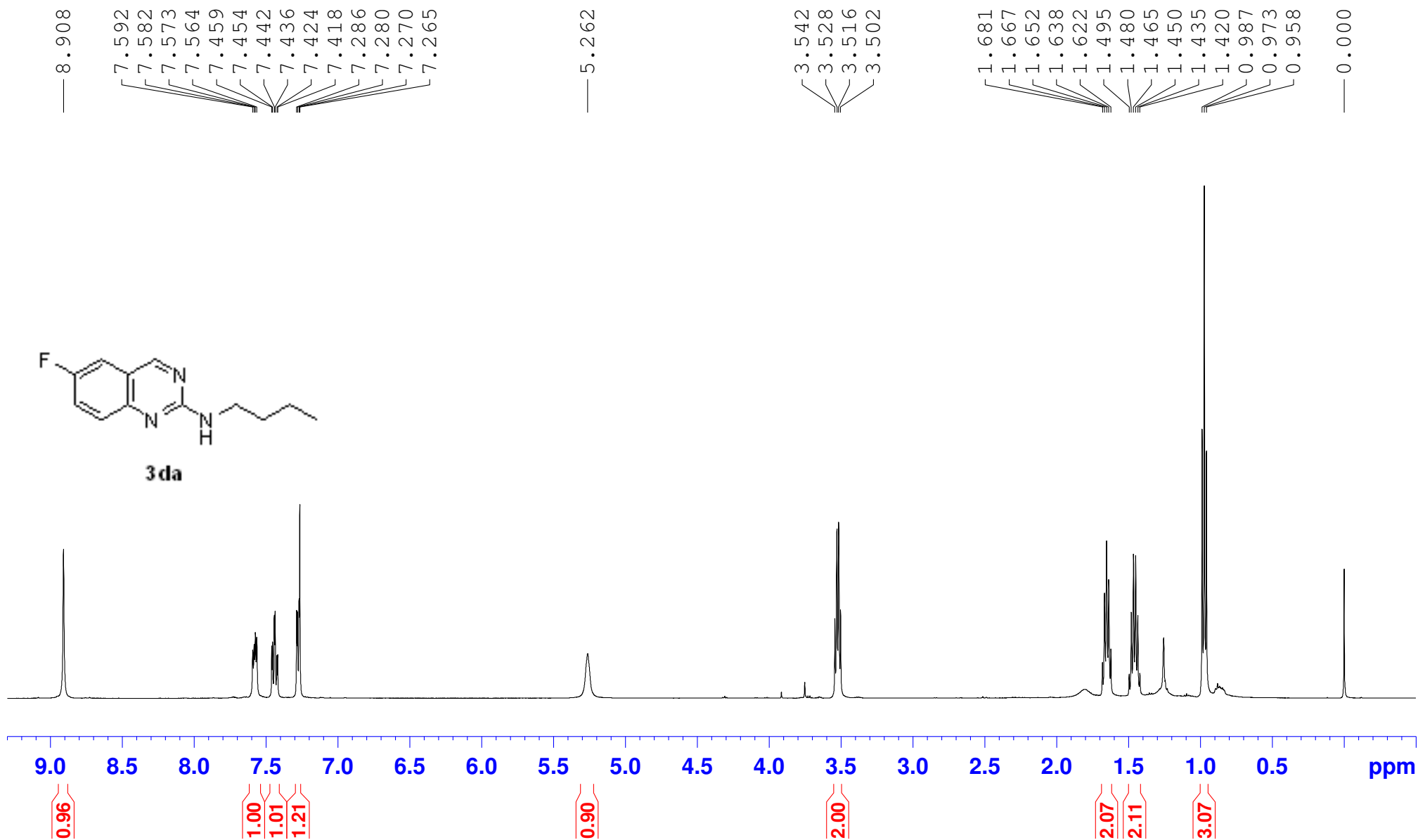
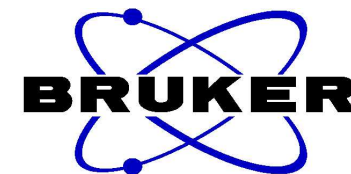
N-butyl-6-(trifluoromethyl)quinazolin-2-amine
Proton CDCl₃



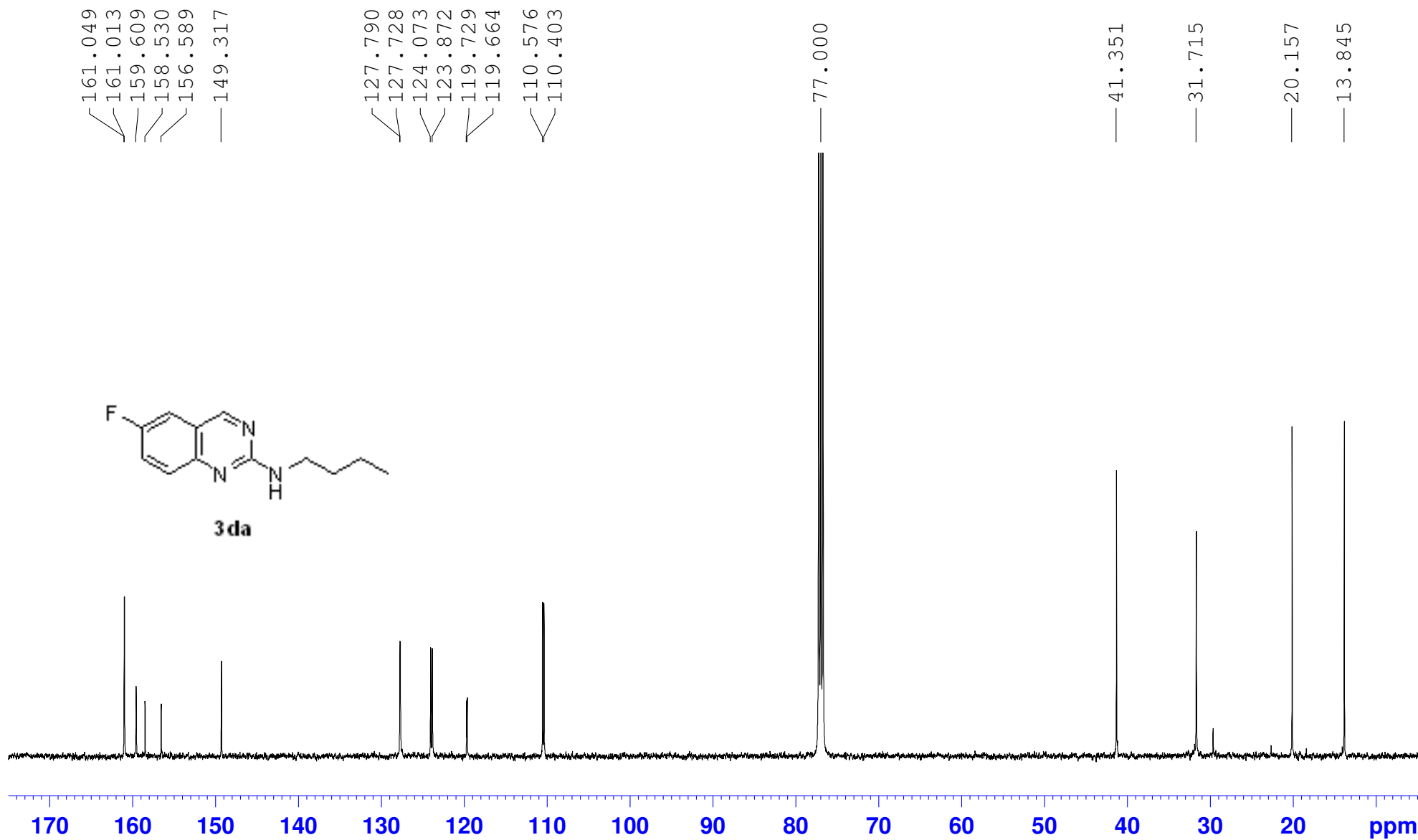
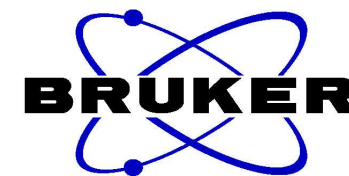
N-butyl-6-(trifluoromethyl)quinazolin-2-amine
C13CPD CDC13



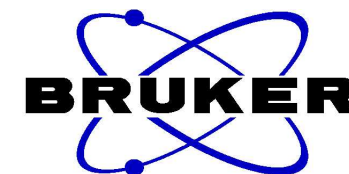
N-butyl-6-fluoroquinazolin-2-amine
Proton CDCl₃



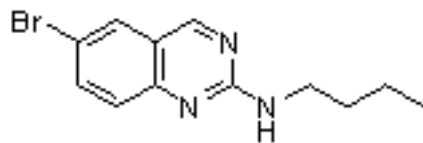
N-butyl-6-fluoroquinazolin-2-amine
C13CPD CDC13



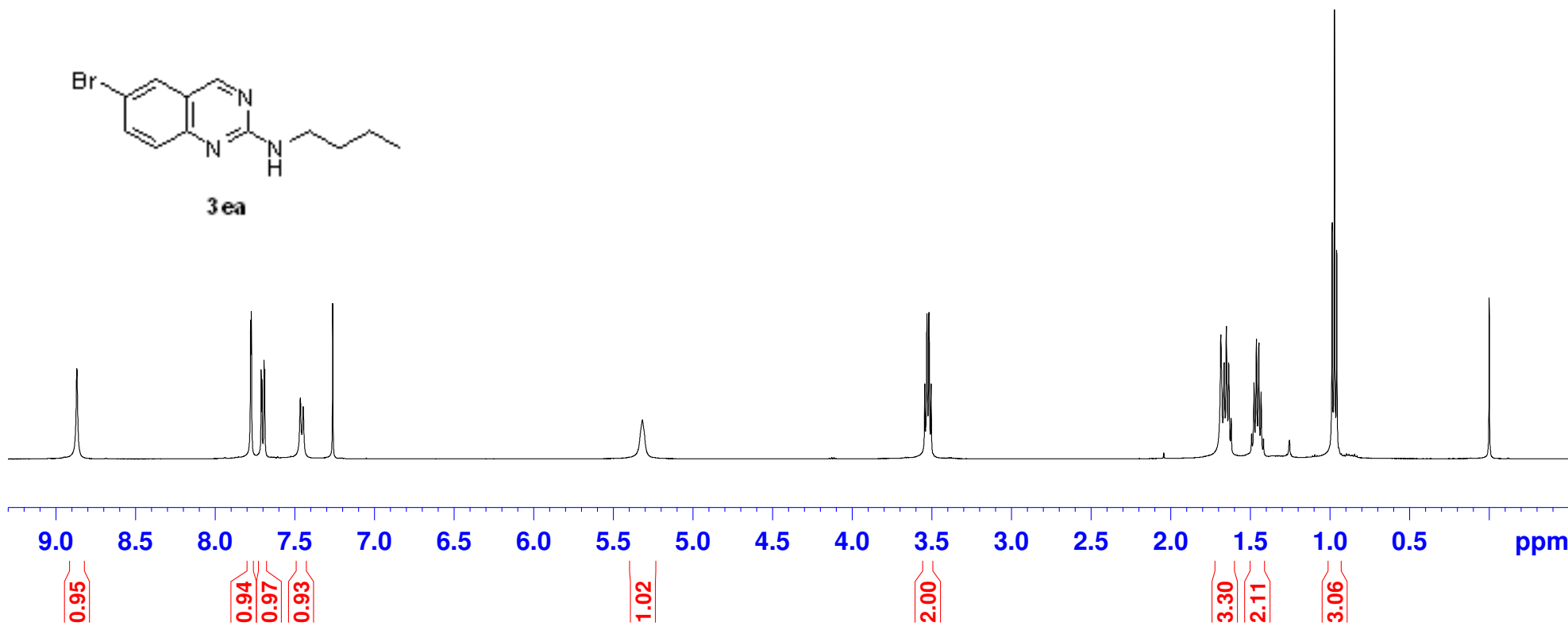
6-bromo-N-butylquinazolin-2-amine
Proton CDCl₃



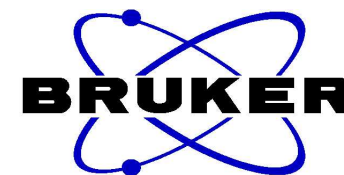
8.867
7.779
7.774
7.712
7.708
7.694
7.689
7.466
7.448
7.263
5.319
3.545
3.531
3.519
3.505
1.686
1.665
1.650
1.636
1.621
1.492
1.477
1.462
1.447
1.432
1.418
0.987
0.972
0.958
0.000



3ea



6-bromo-N-butylquinazolin-2-amine
C13CPD CDC13



160.879
159.858
151.175
137.251
129.515
127.526
121.117
114.928

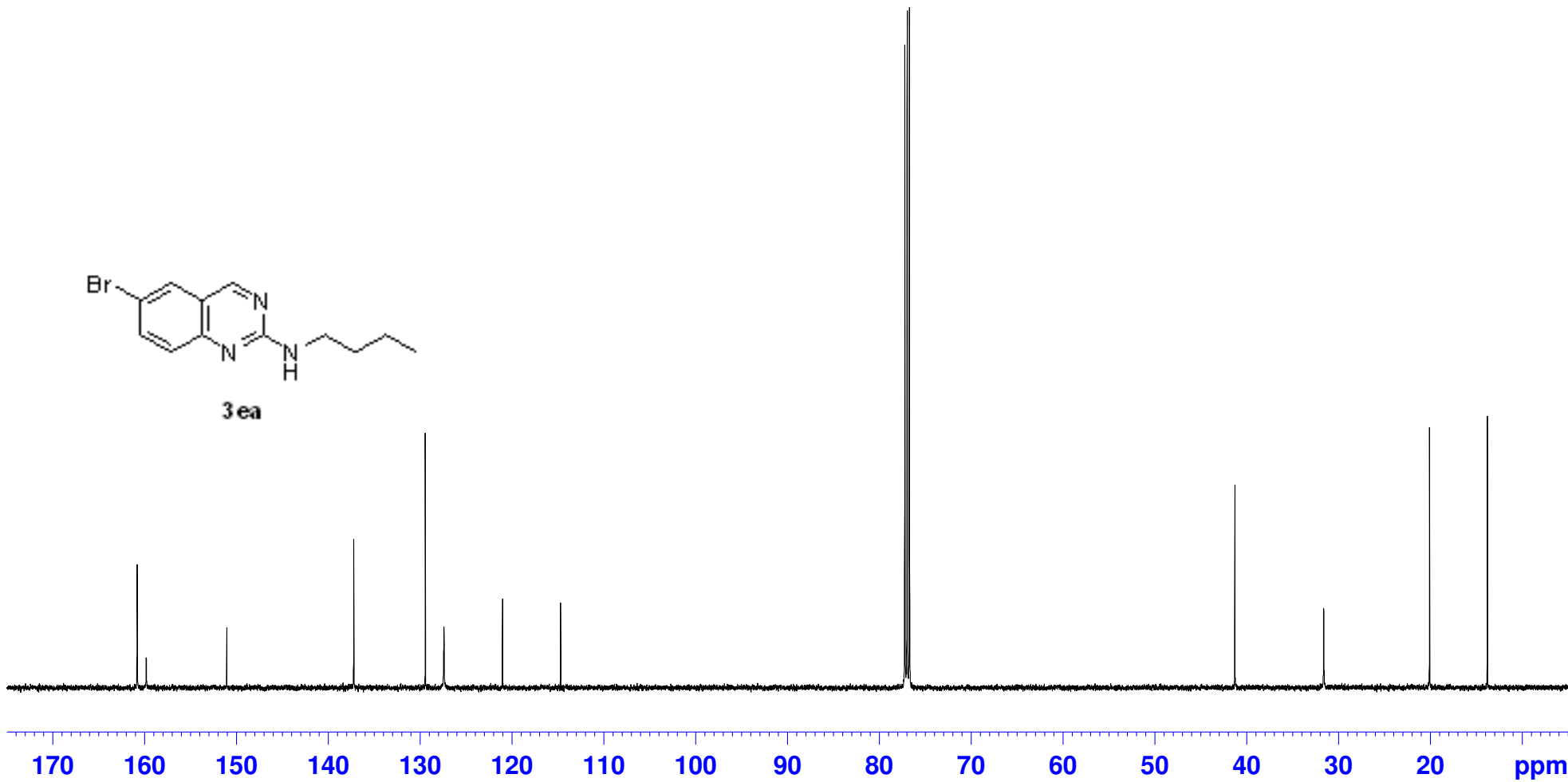
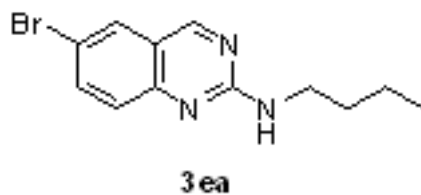
77.000

41.551

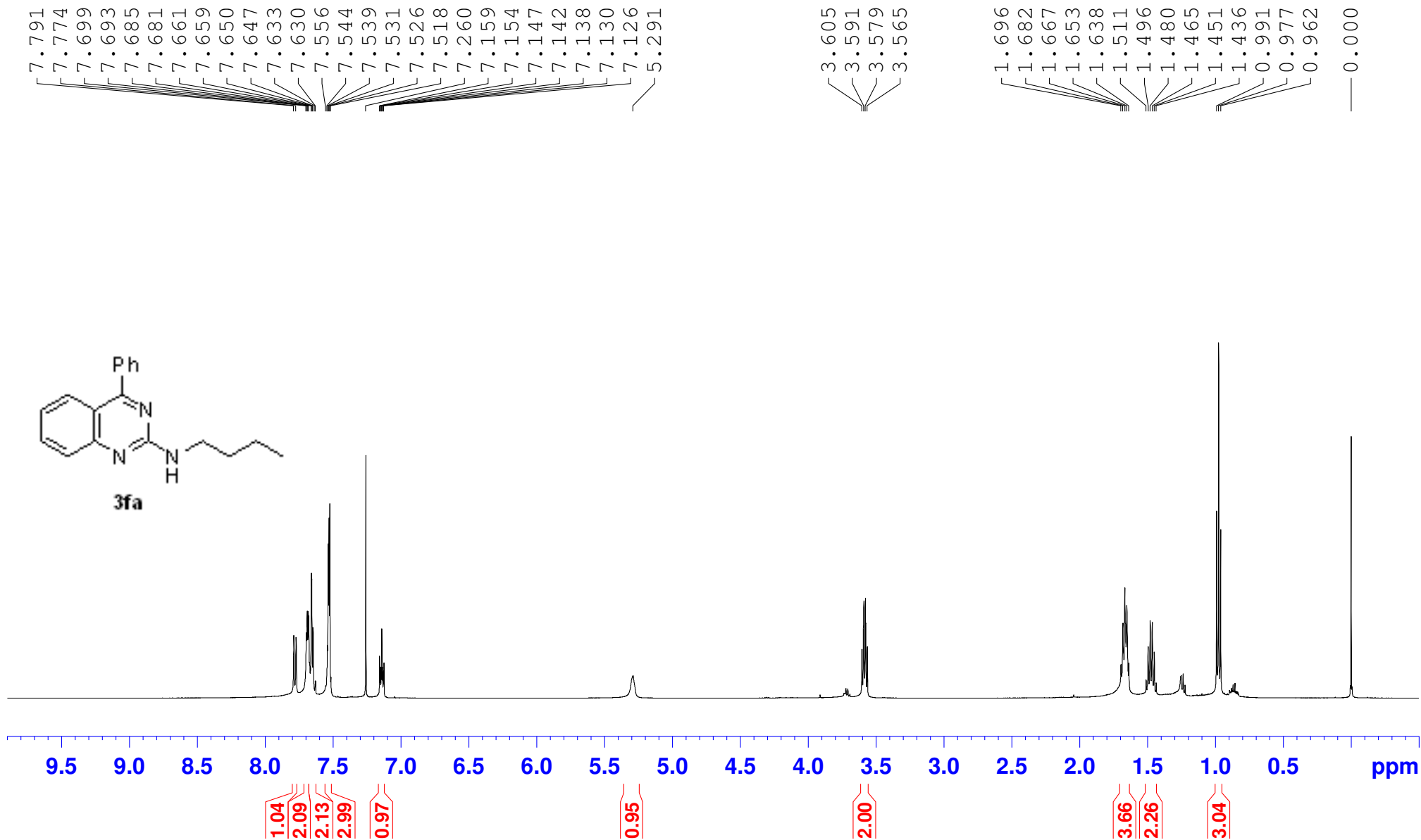
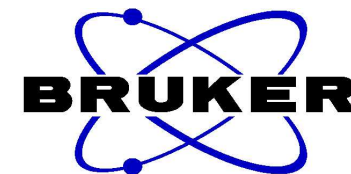
31.826

20.333

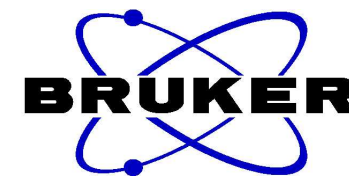
13.924



N-butyl-4-phenylnaphthalen-2-amine
Proton CDCl₃



N-butyl-4-phenylquinazolin-2-amine
C13CPD CDCl3



— 169.867
— 159.110
— 153.377
137.478
133.636
129.559
129.442
128.376
127.430
126.071
122.111
118.387

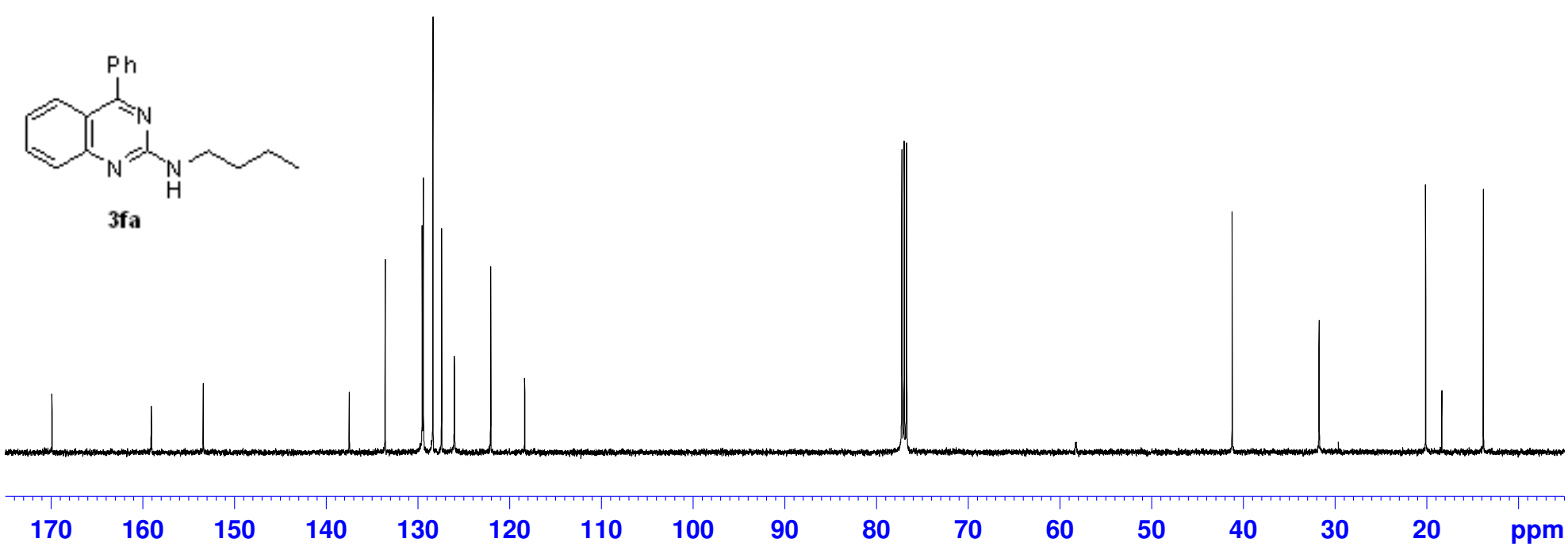
— 77.000

— 41.281

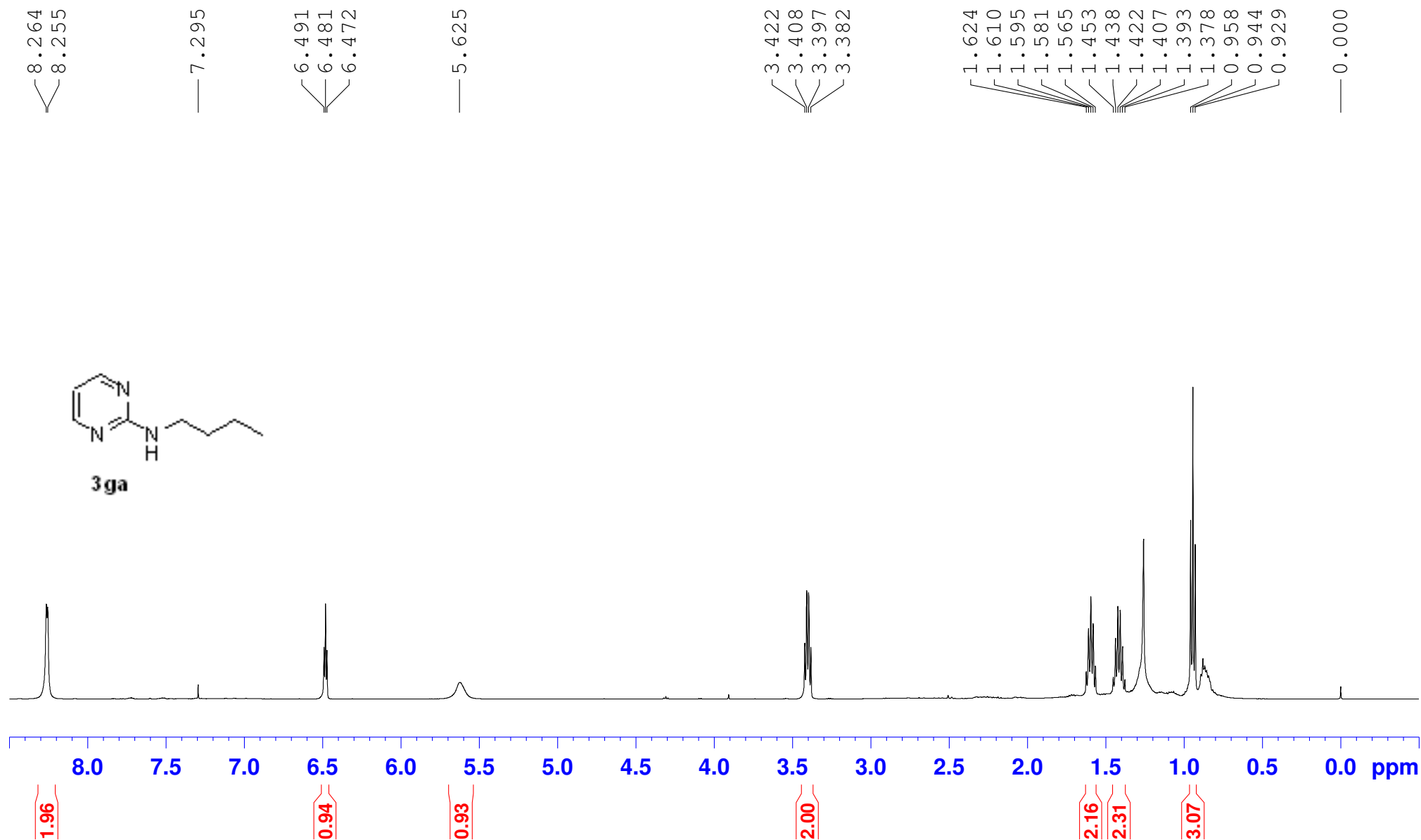
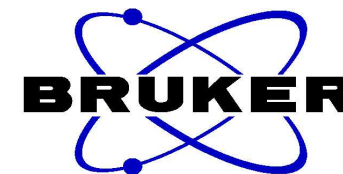
— 31.798

— 20.142

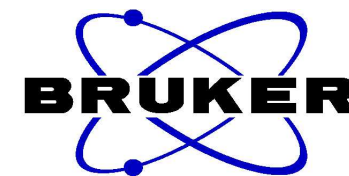
— 13.858



N-butylpyrimidin-2-amine
Proton CDCl₃



N-butylpyrimidin-2-amine
C13CPD CDCl3



— 162.460
— 158.027

— 110.153

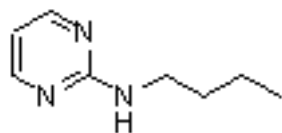
— 77.000

— 41.069

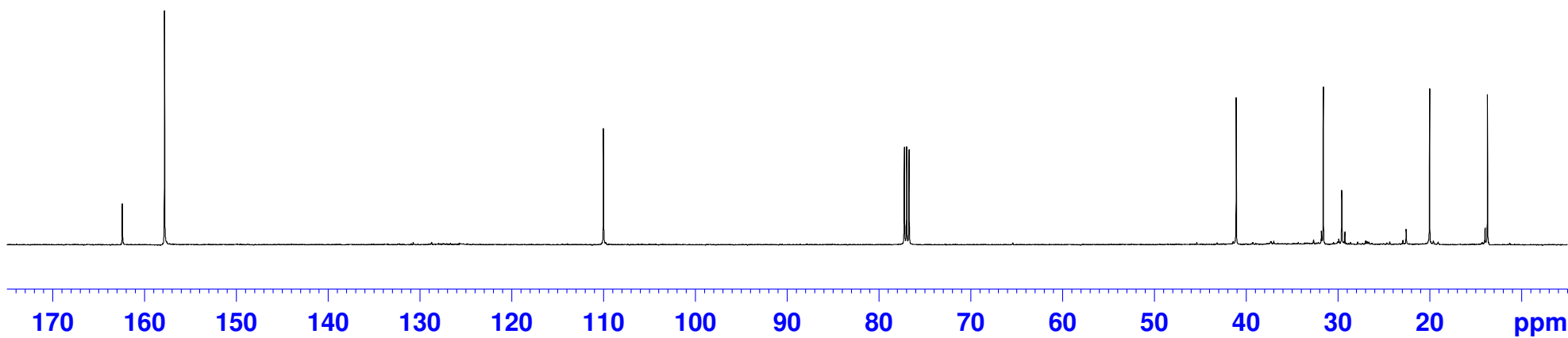
— 31.630

— 20.079

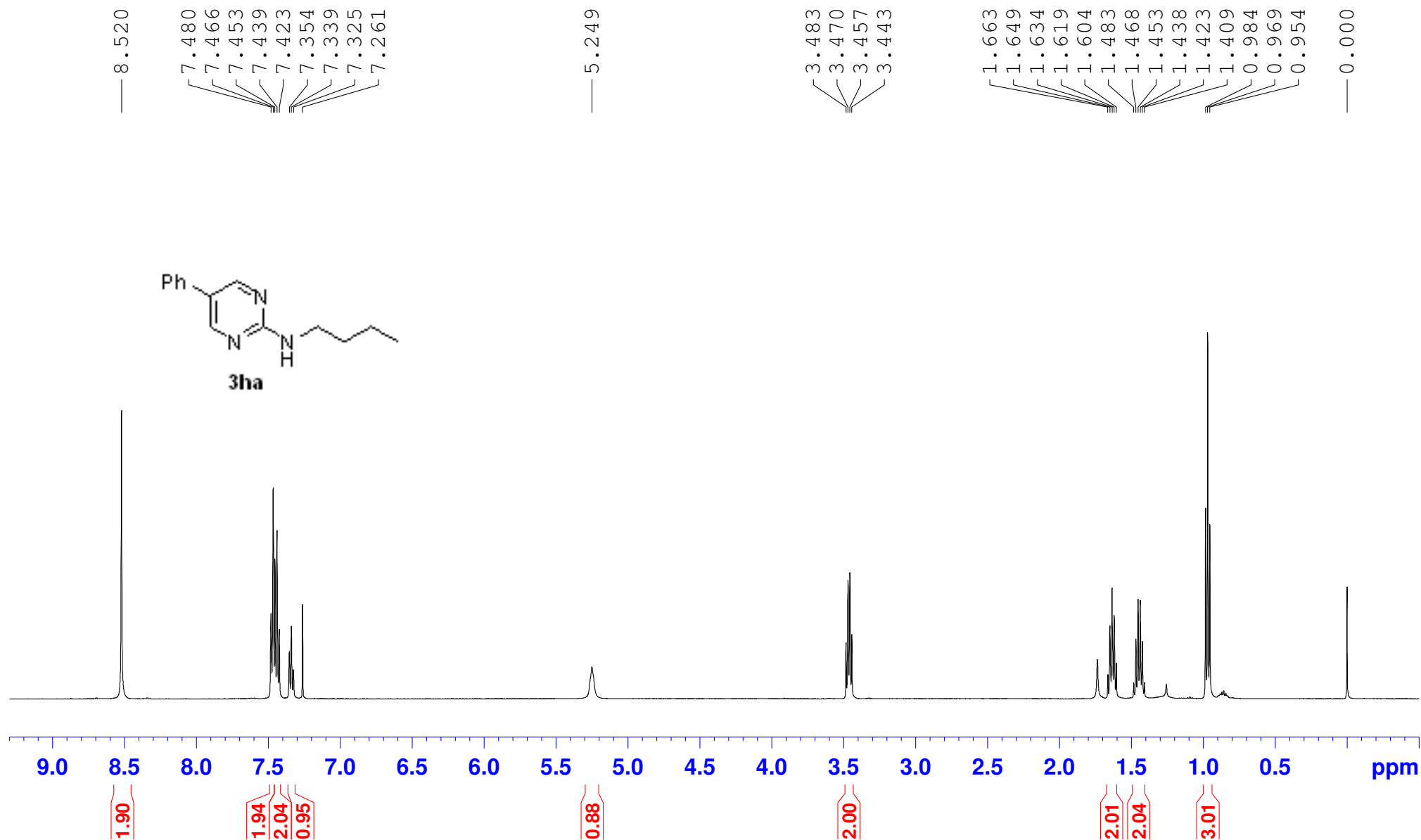
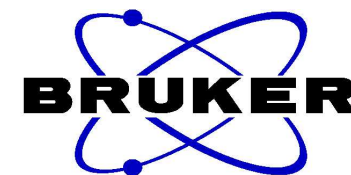
— 13.703



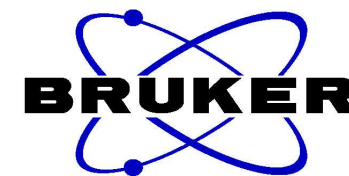
3ga



N-butyl-5-phenylpyrimidin-2-amine
Proton CDCl₃



N-butyl-5-phenylpyrimidin-2-amine
C13CPD CDCl₃



— 161.858

— 156.290

— 135.732

— 129.122

— 127.249

— 125.791

— 123.554

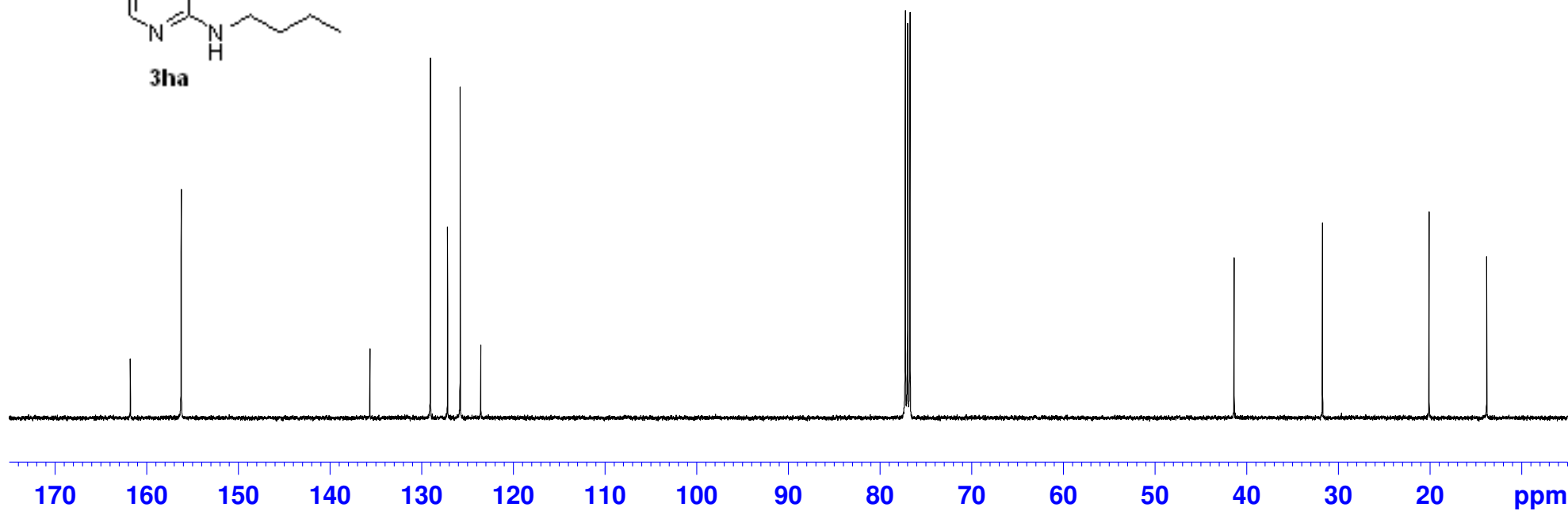
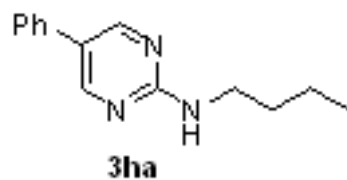
— 77.000

— 41.446

— 31.916

— 20.169

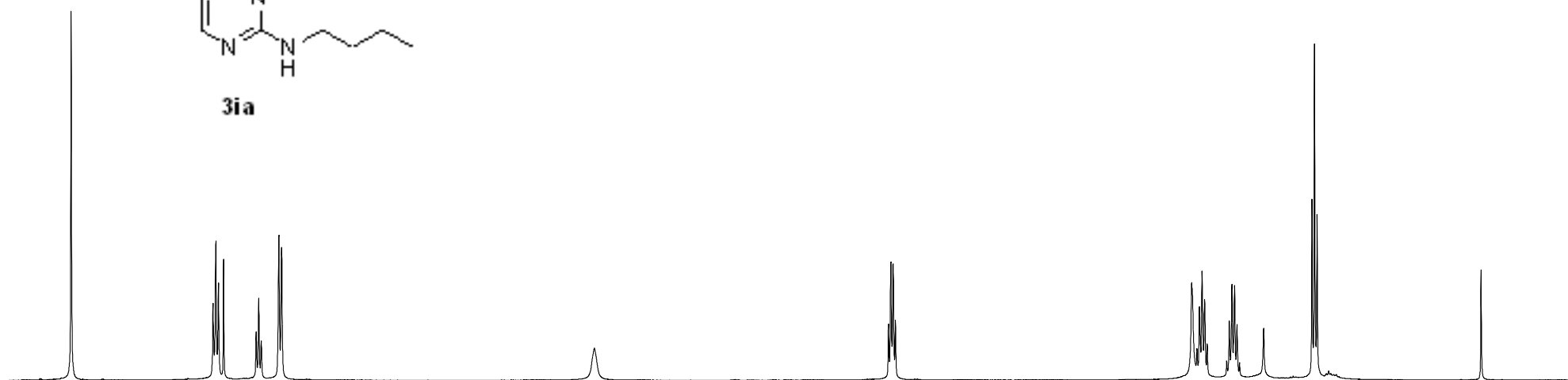
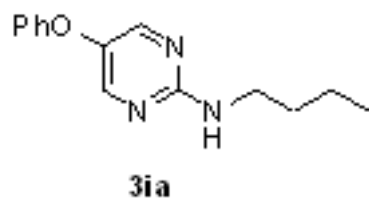
— 13.742



N-butyl-5-phenoxyimidin-2-amine
Proton CDCl₃

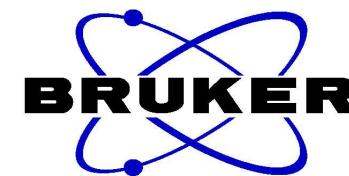


8.142
7.322
7.305
7.290
7.261
7.072
7.058
7.044
6.942
6.926
5.122
3.423
3.409
3.396
3.383
1.641
1.626
1.612
1.597
1.582
1.469
1.454
1.439
1.424
1.409
1.395
0.977
0.962
0.947
0.000



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 0.0 ppm
1.77 1.96 0.98 1.90 0.91 2.00 2.21 2.16 3.04

N-butyl-5-phoxypyrimidin-2-amine
C13CPD CDCl3



159.678
158.511
151.015
142.600
129.979
122.893
116.472

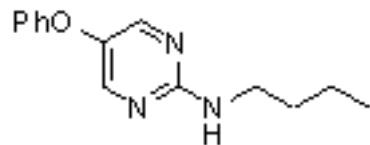
77.000

41.629

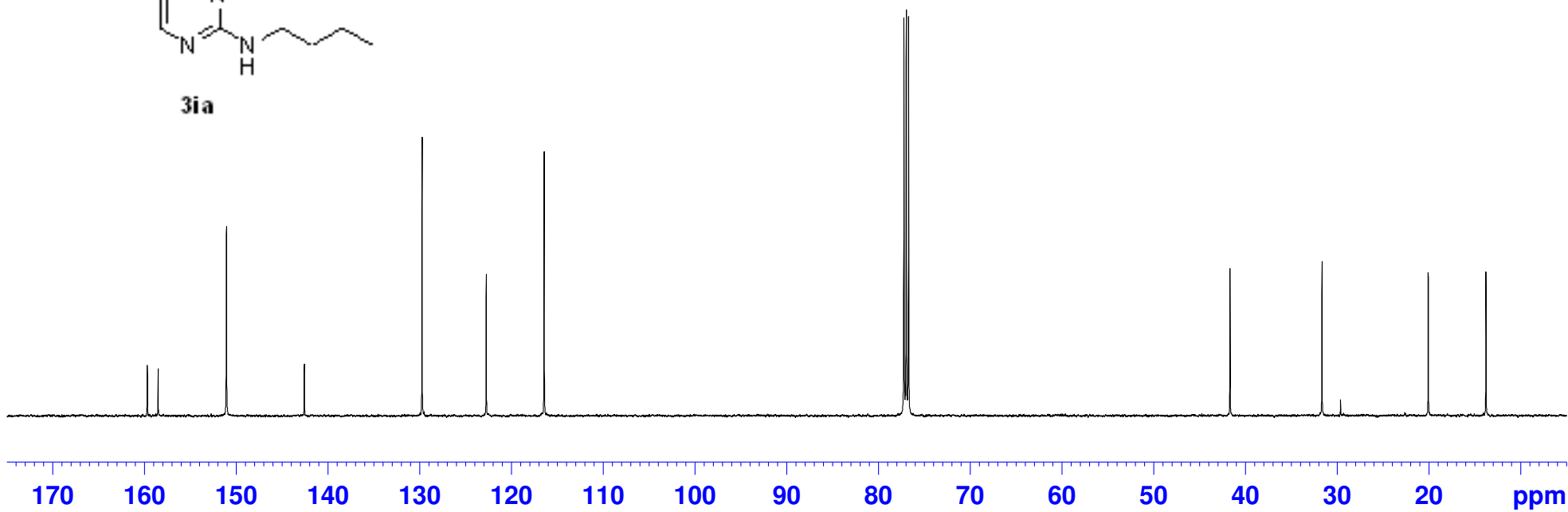
31.

20.

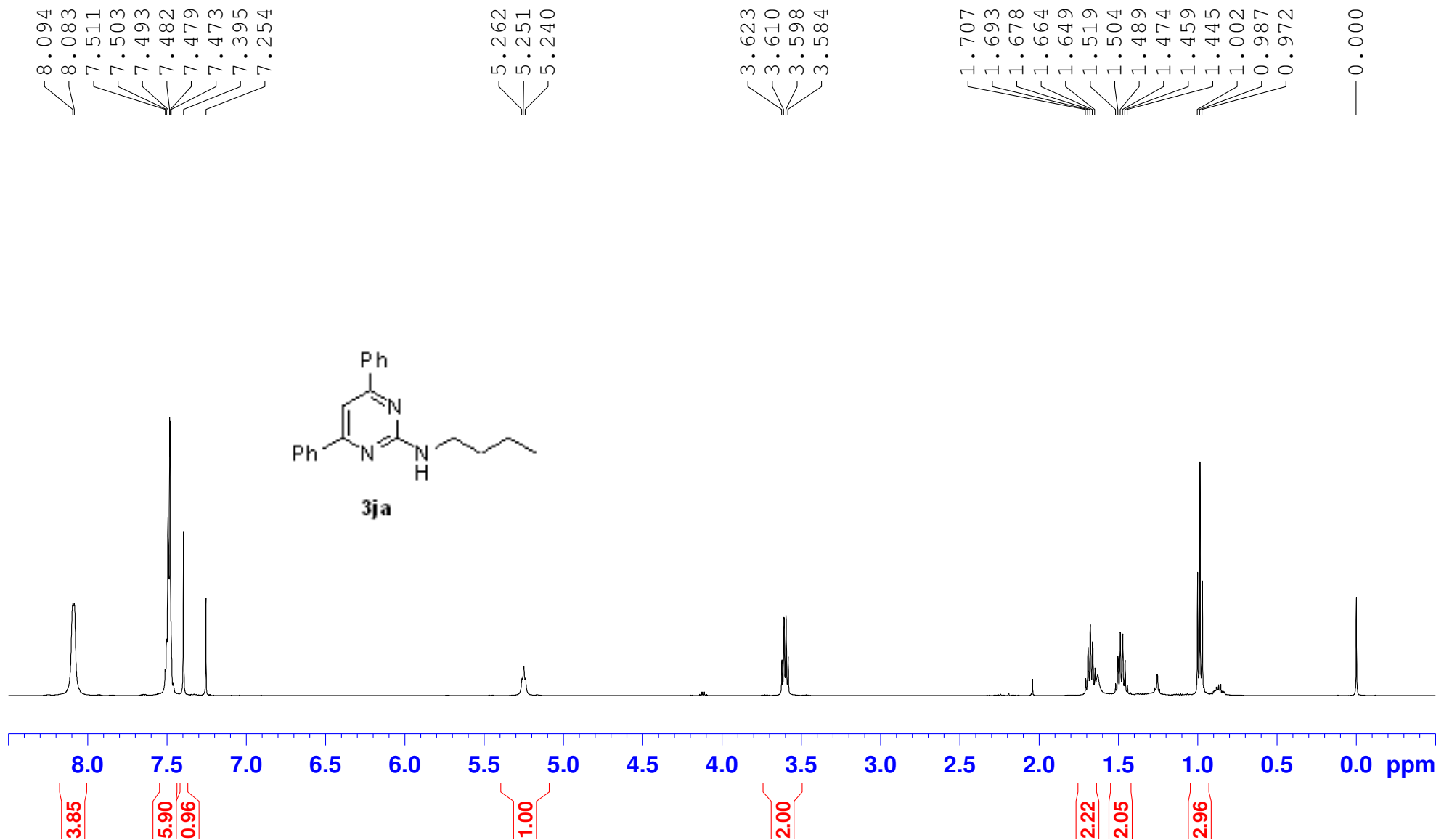
13.



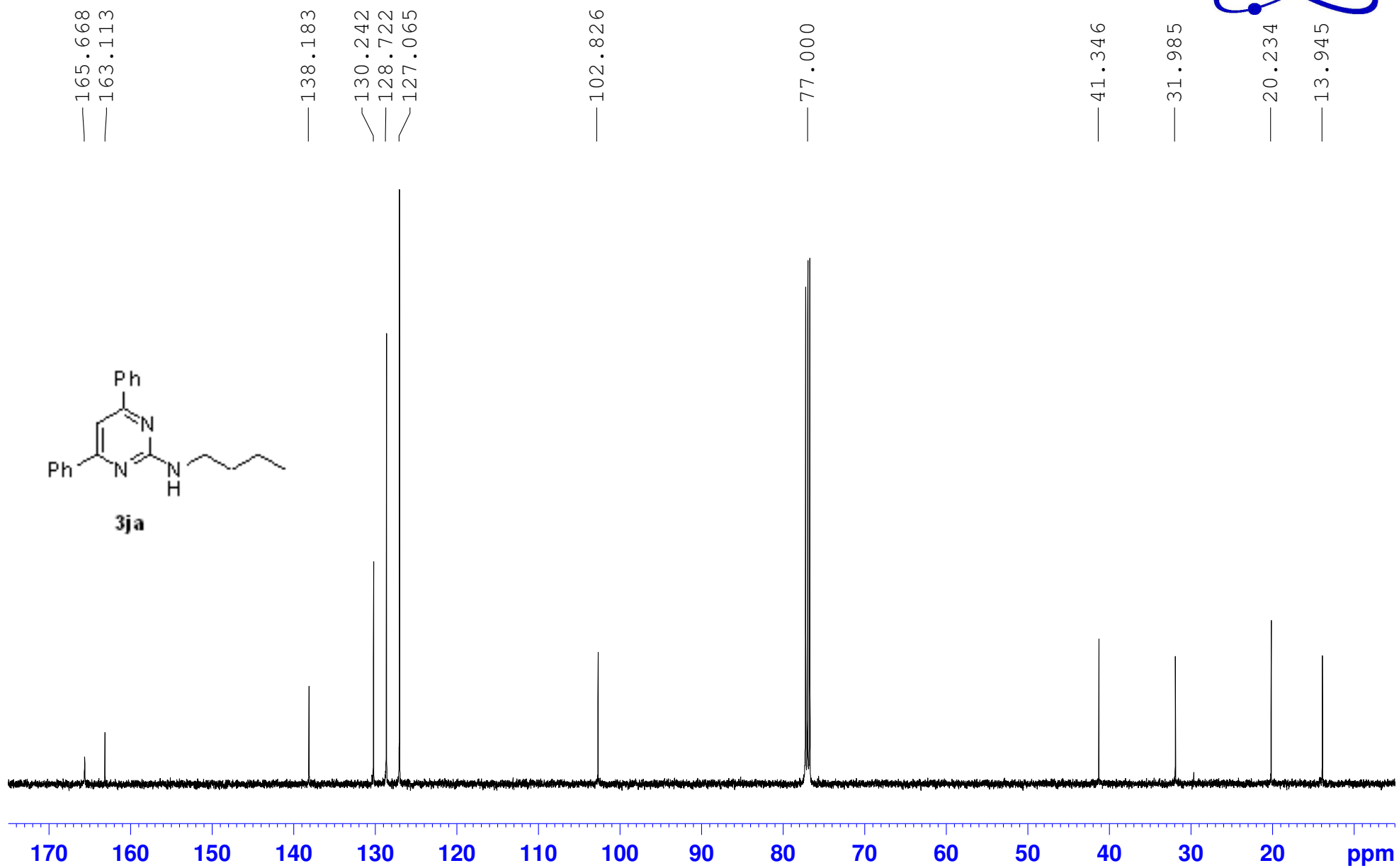
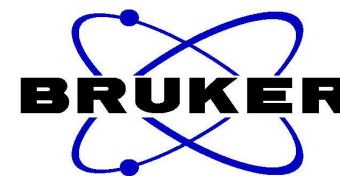
3ia



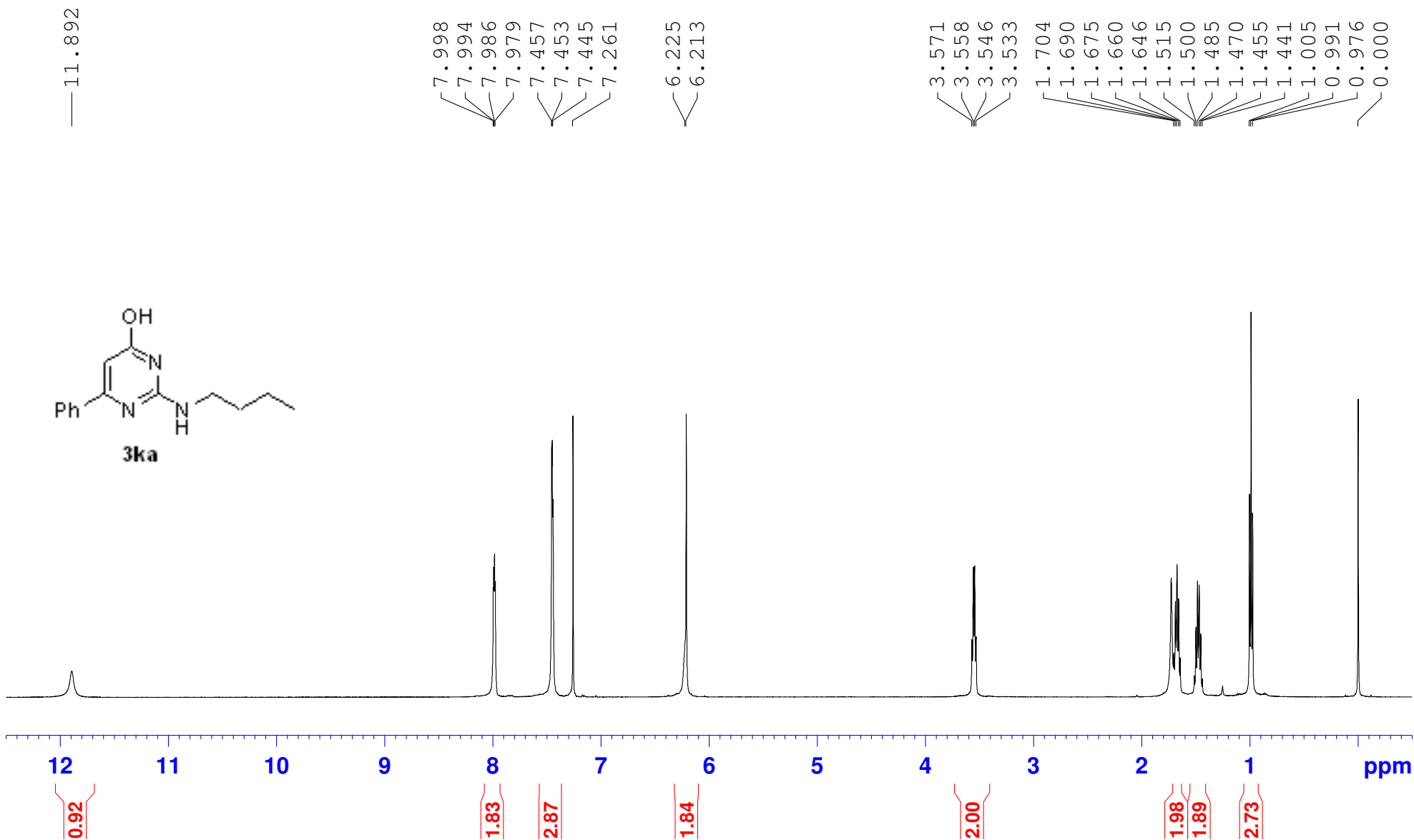
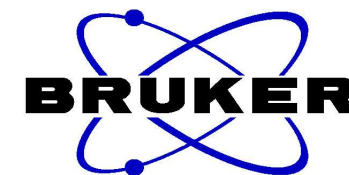
N-butyl-4,6-diphenylpyrimidin-2-amine
Proton CDCl₃



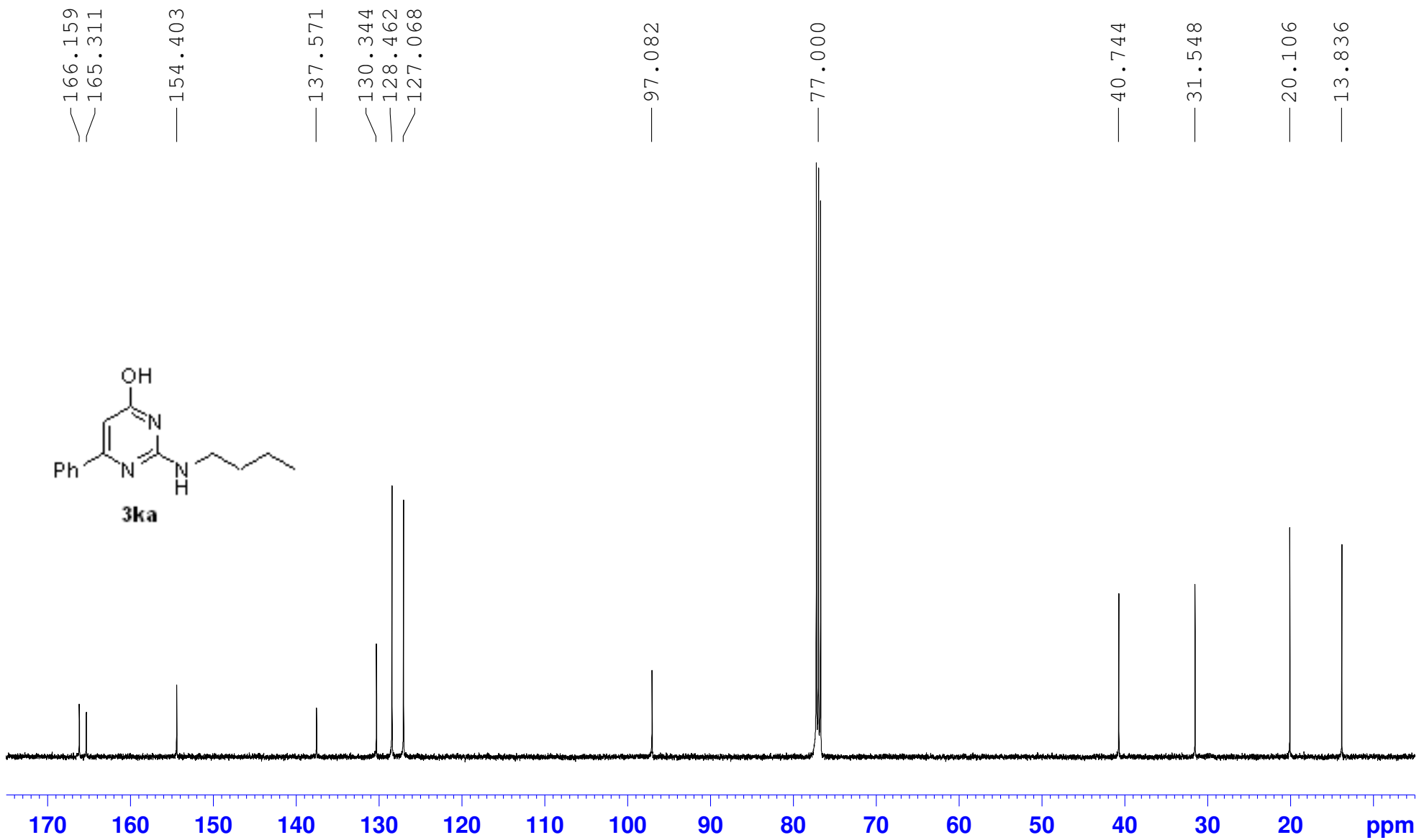
N-butyl-4,6-diphenylpyrimidin-2-amine
C13CPD CDC13



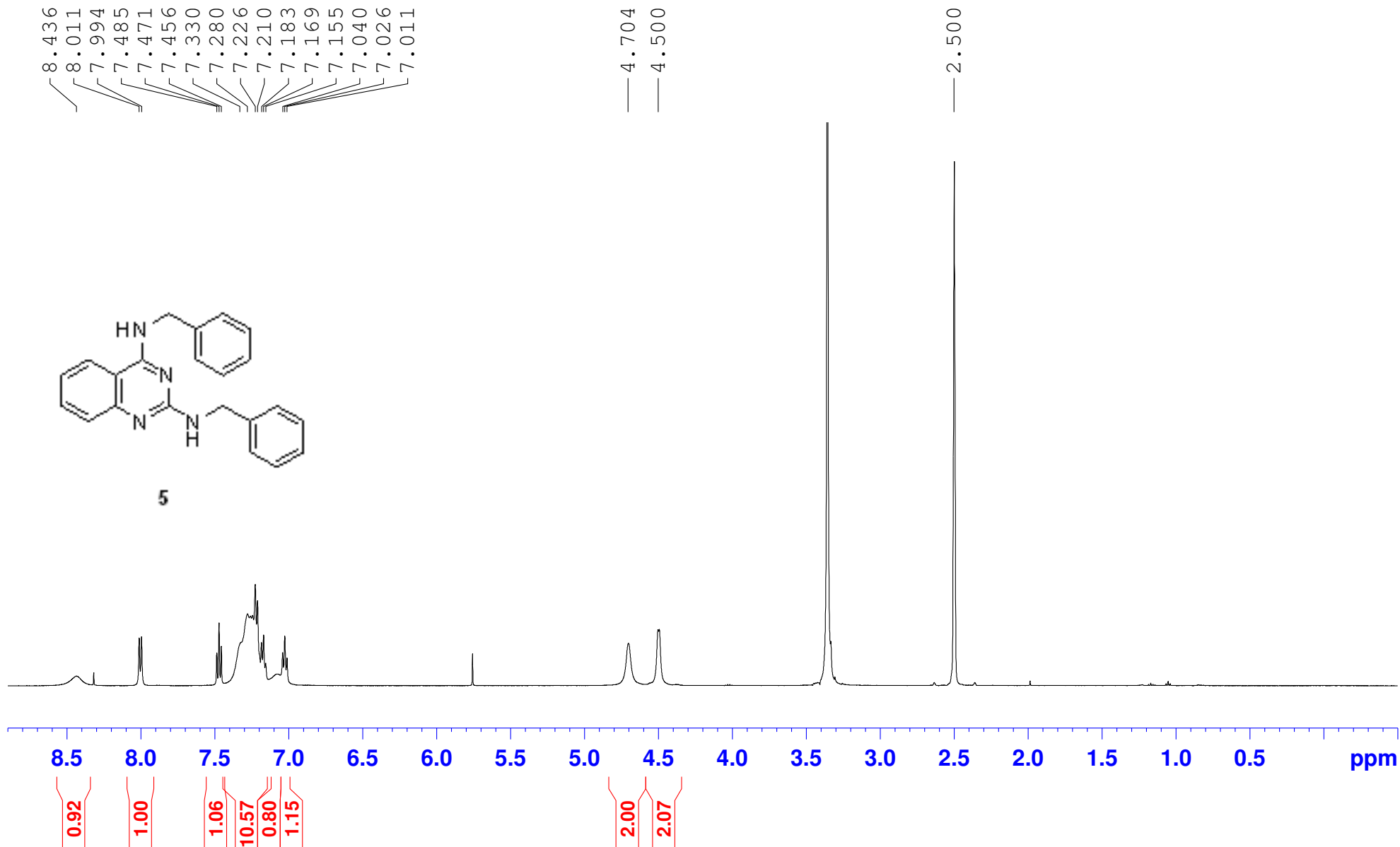
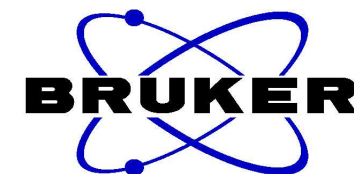
2-(butylamino)-6-phenylpyrimidin-4-ol
Proton CDCl₃



2-(butylamino)-6-phenylpyrimidin-4-ol
C13CPD CDC13



N2,N4-dibenzylquinazoline-2,4-diamine
Proton DMSO-d6



N2,N4-dibenzylquinazoline-2,4-diamine
C13CPD DMSO-d6

