

Electronic Supplementary Information for

**Acceptorless dehydrogenative condensation of *o*-aminobenzamides  
with aldehydes to quinazolinones in water catalyzed by a  
water-soluble iridium complex [Cp\*Ir(H<sub>2</sub>O)<sub>3</sub>][OTf]<sub>2</sub>**

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Nanjing 210094, P. R. China

<sup>b</sup> State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian  
116024, P. R. China

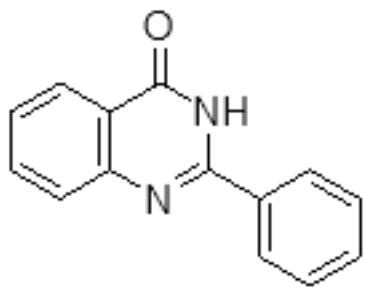
**Table of Contents:**

Copies of <sup>1</sup> H NMR and <sup>13</sup> C NMR spectra of products	S2-S57
A characteristic signal of [Ir-H] (species C in Scheme 3)	S58

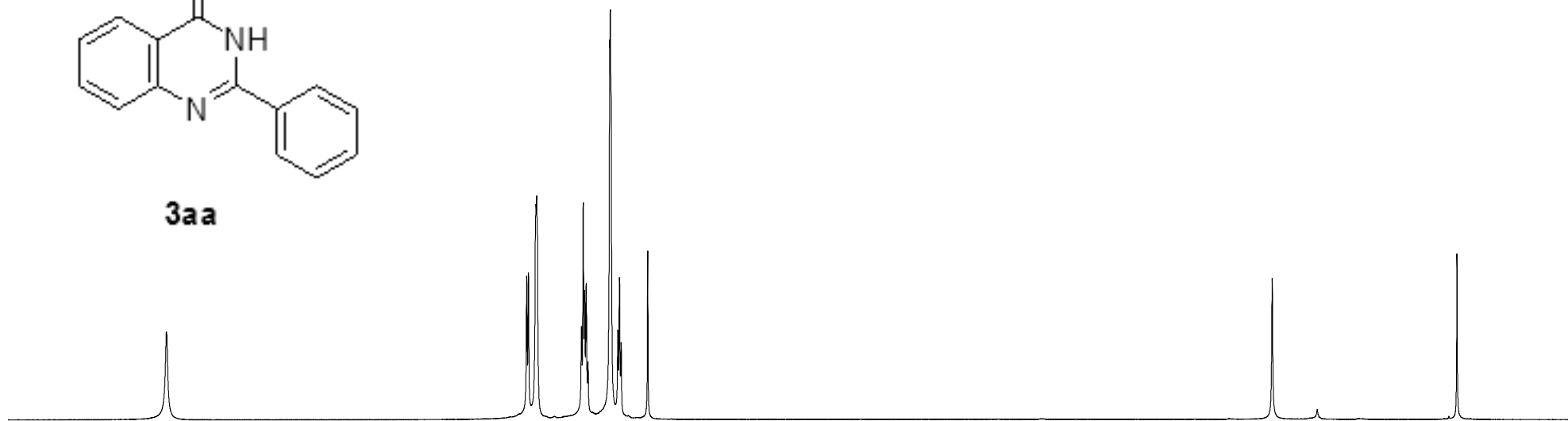
2-phenylquinazolin-4(3H)-one  
PROTON CDCl<sub>3</sub>

— 11.577

8.346  
8.330  
7.854  
7.839  
7.826  
7.812  
7.796  
7.601  
7.596  
7.590  
7.528  
7.514  
7.499  
7.260



**3aa**



12

11

10

9

8

7

6

5

4

3

2

1

0

ppm

1.01

1.00

2.00

2.00

3.00

1.00

2-phenylquinazolin-4(3H)-one  
C13CPD CDC13

— 163.920

— 151.767

— 149.540

— 134.856

— 132.834

— 131.613

— 129.006

— 128.003

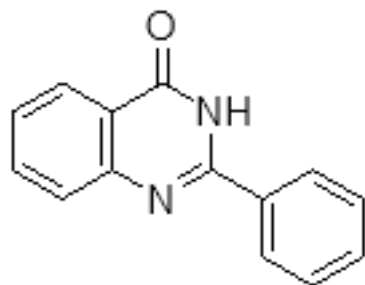
— 127.432

— 126.746

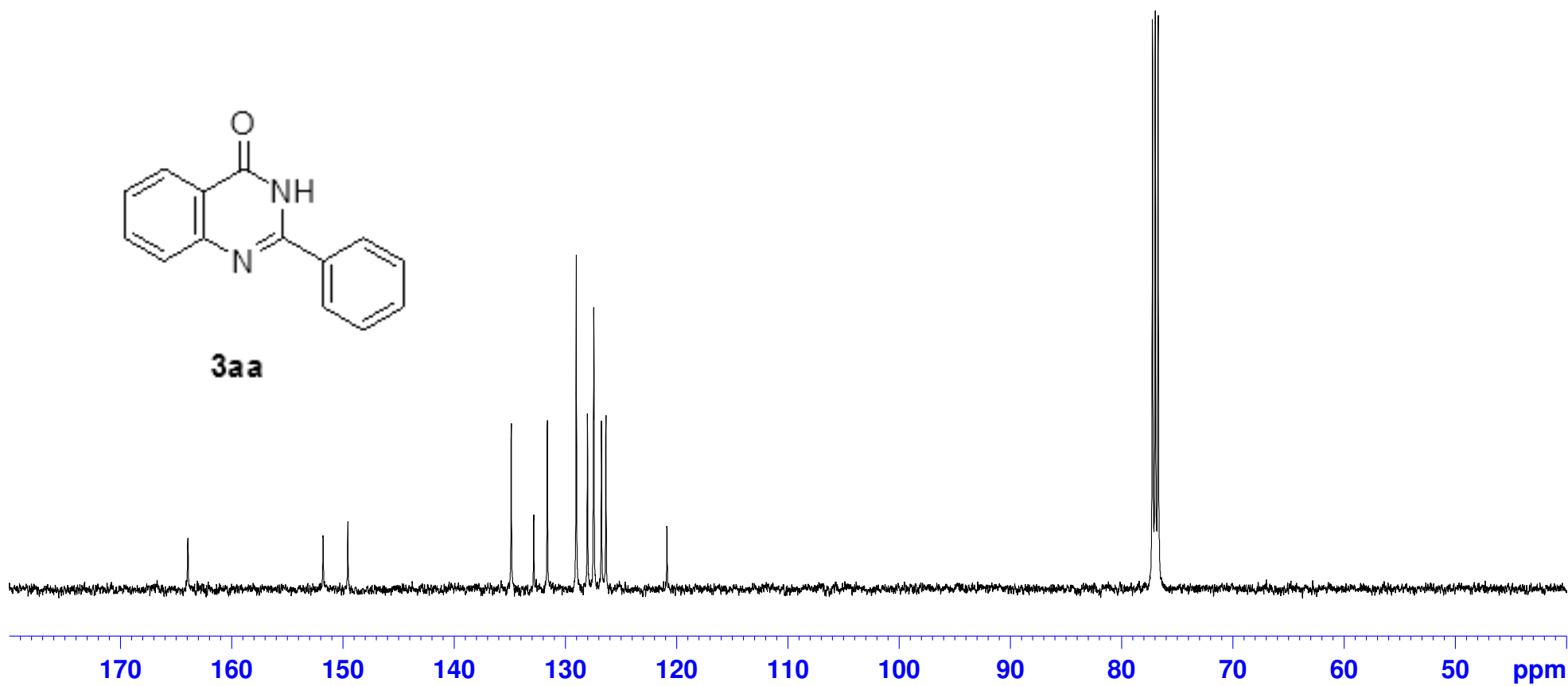
— 126.345

— 120.857

— 76.995



**3aa**

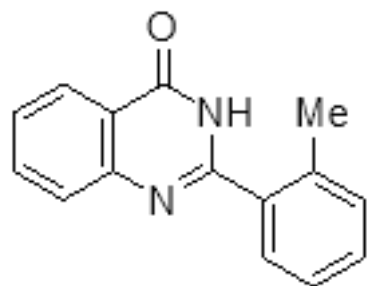


2-o-tolylquinazolin-4(3H)-one  
PROTON DMSO-d6

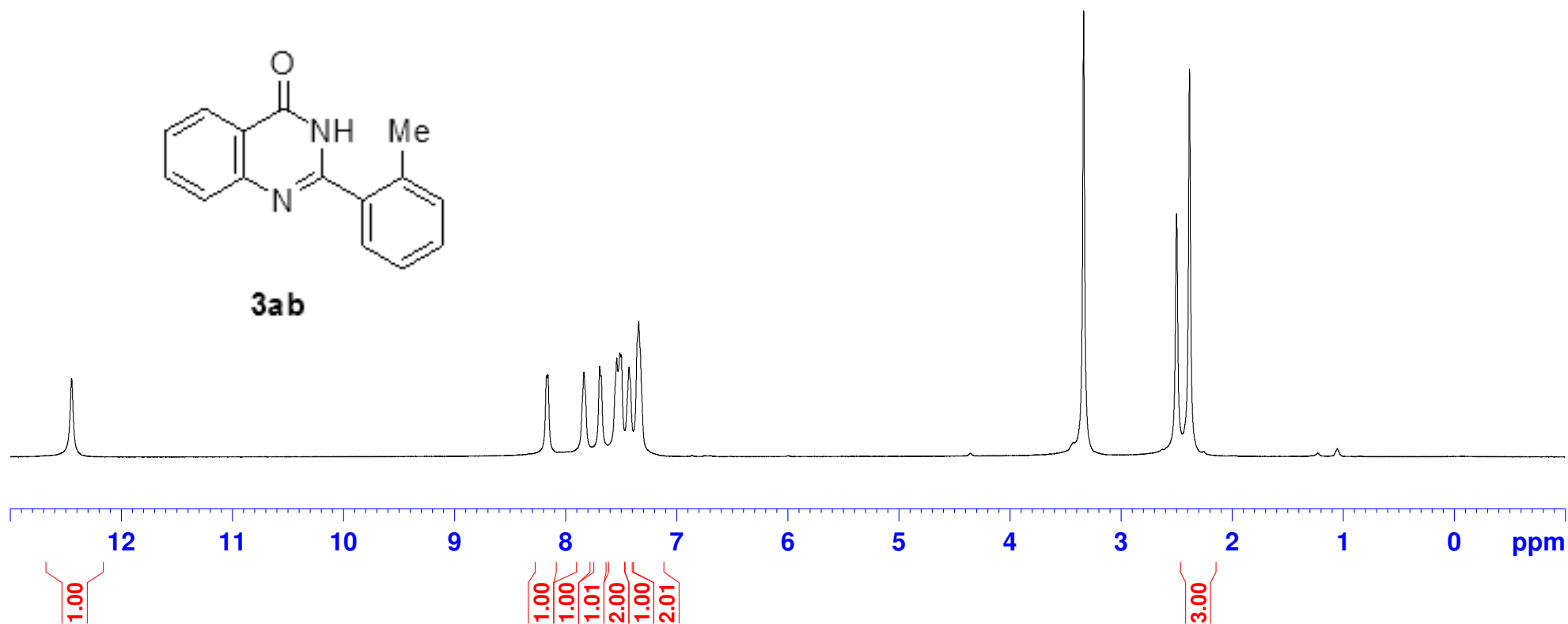
— 12.443

8.172  
8.160  
7.835  
7.694  
7.681  
7.540  
7.511  
7.500  
7.430  
7.342

2.499  
2.383

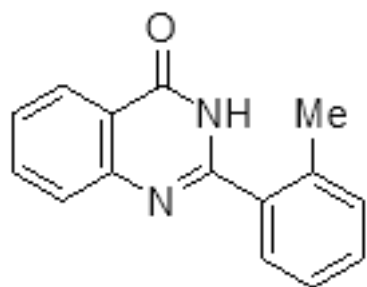


3ab

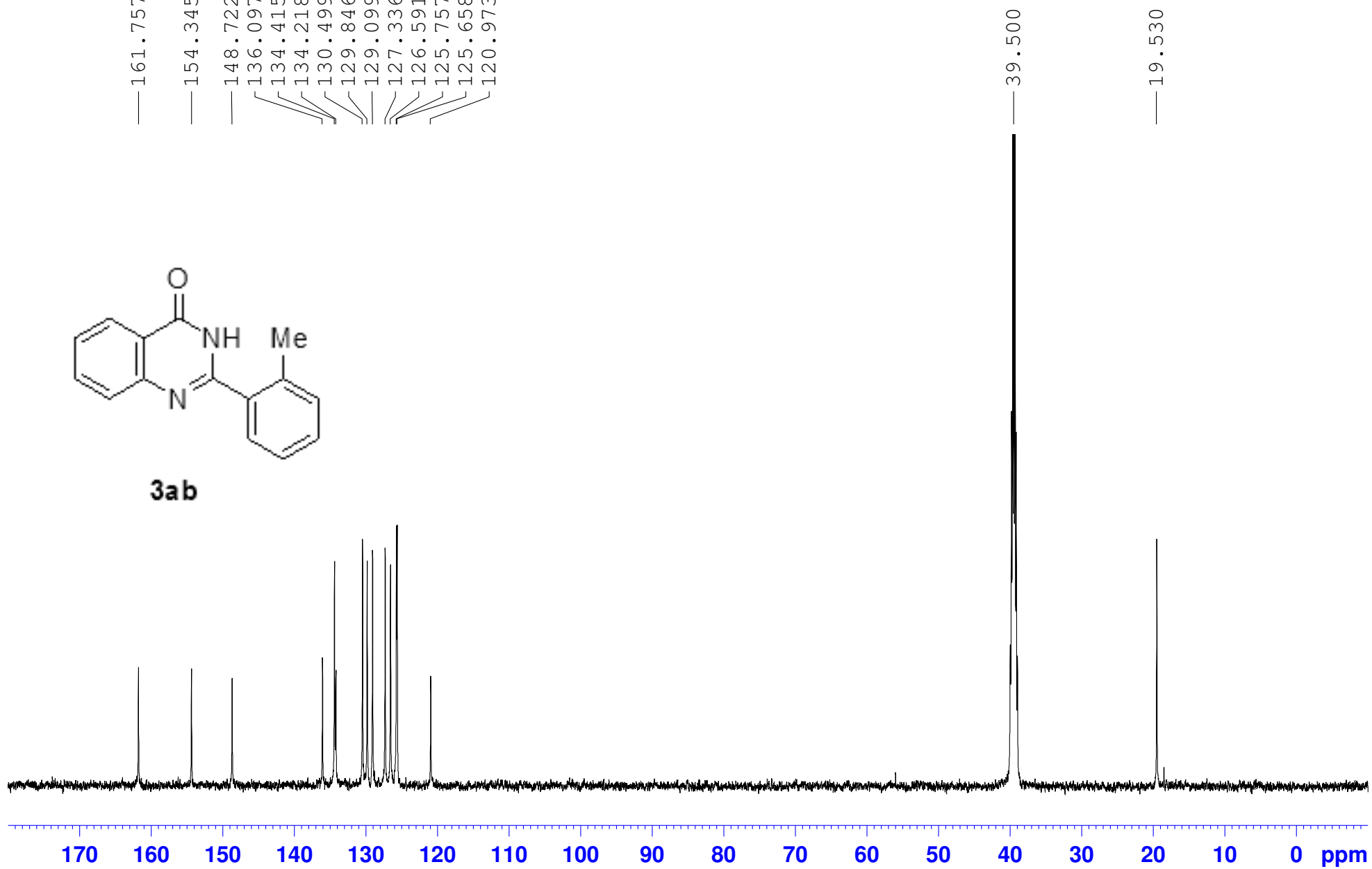


2-o-tolylquinazolin-4(3H)-one  
C13CPD DMSO-d6

— 161.757  
— 154.345  
— 148.722  
— 136.097  
— 134.415  
— 134.218  
— 130.499  
— 129.846  
— 129.099  
— 127.336  
— 126.591  
— 125.757  
— 125.658  
— 120.973



**3ab**

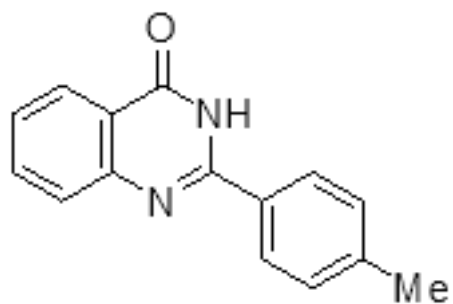


2-p-tolylquinazolin-4(3H)-one  
PROTON CDCl3

11.475

8.339  
8.323  
8.153  
8.137  
7.830  
7.814  
7.795  
7.779  
7.509  
7.495  
7.481  
7.389  
7.373  
7.260

2.463



12

11

10

9

8

7

6

5

4

3

2

1

0

ppm

1.00

1.00

2.01

2.00

1.01

2.01

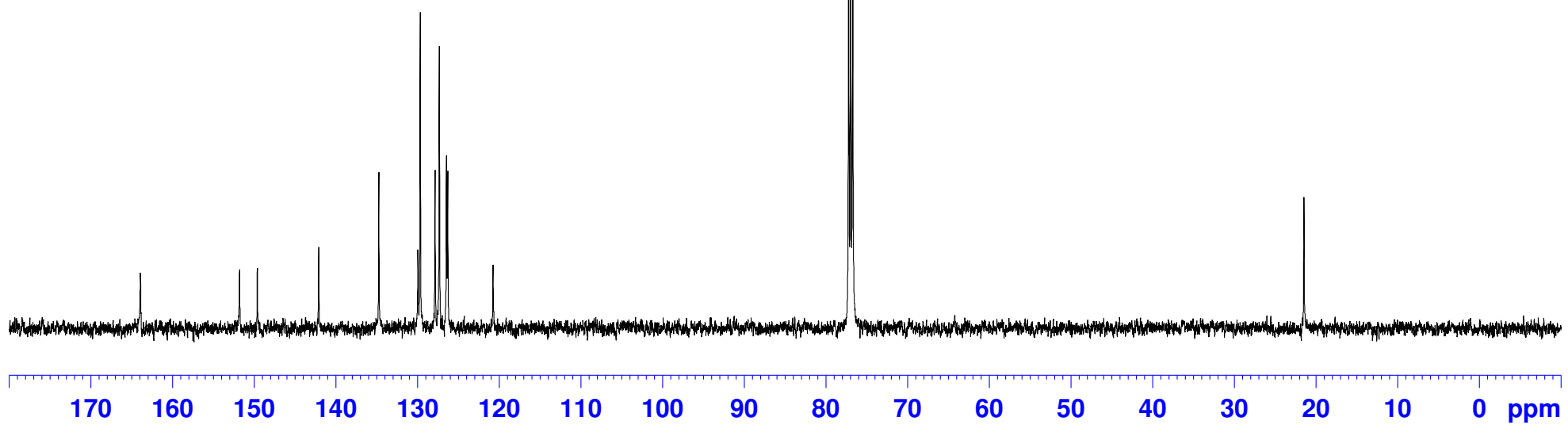
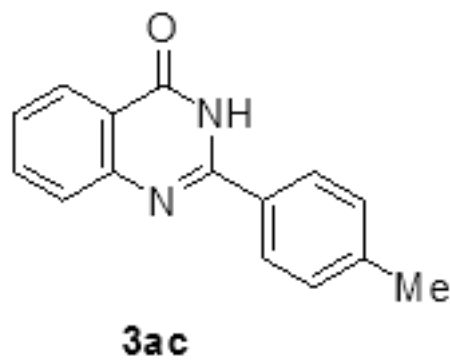
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2-p-tolylquinazolin-4(3H)-one  
C13CPD CDC13

— 163.973  
— 151.821  
— 149.649  
— 142.122  
— 134.769  
— 129.993  
— 129.701  
— 127.884  
— 127.362  
— 126.490  
— 126.331  
— 120.783

— 76.999

— 21.505

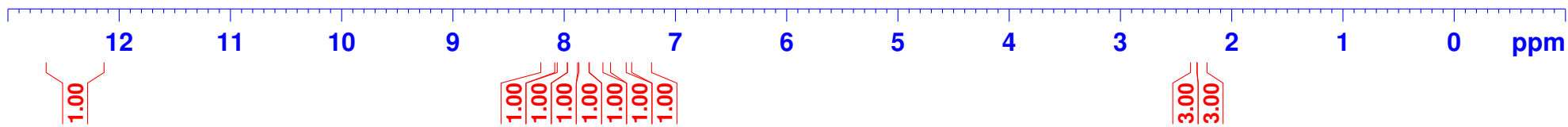
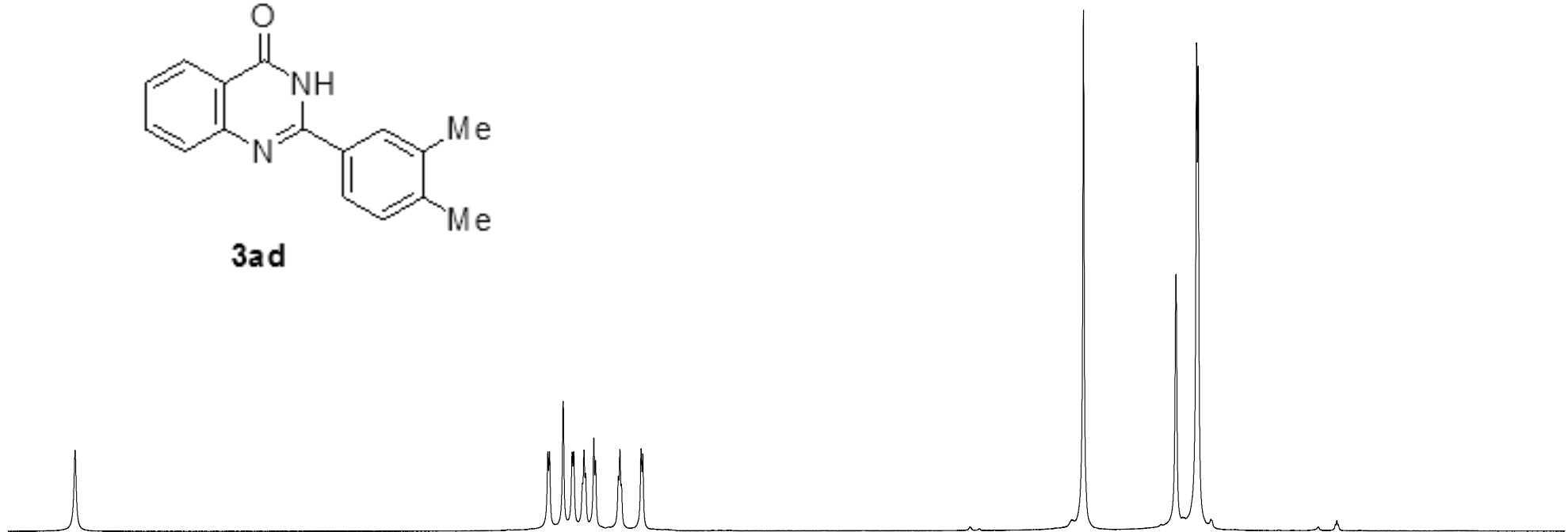
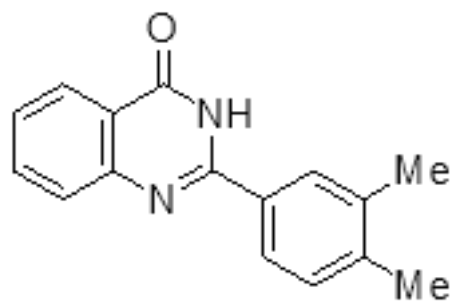


2-(3,4-dimethylphenyl)quinazolin-4(3H)-one  
PROTON DMSO-d6

12.396

8.146  
8.131  
8.008  
7.928  
7.914  
7.835  
7.821  
7.807  
7.733  
7.718  
7.513  
7.499  
7.485  
7.308  
7.293

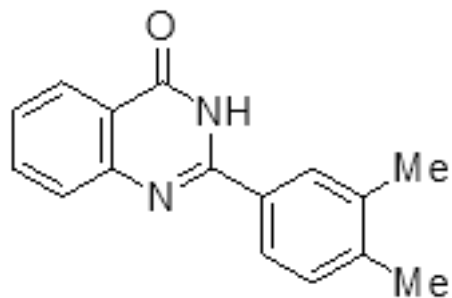
2.500  
2.315  
2.301



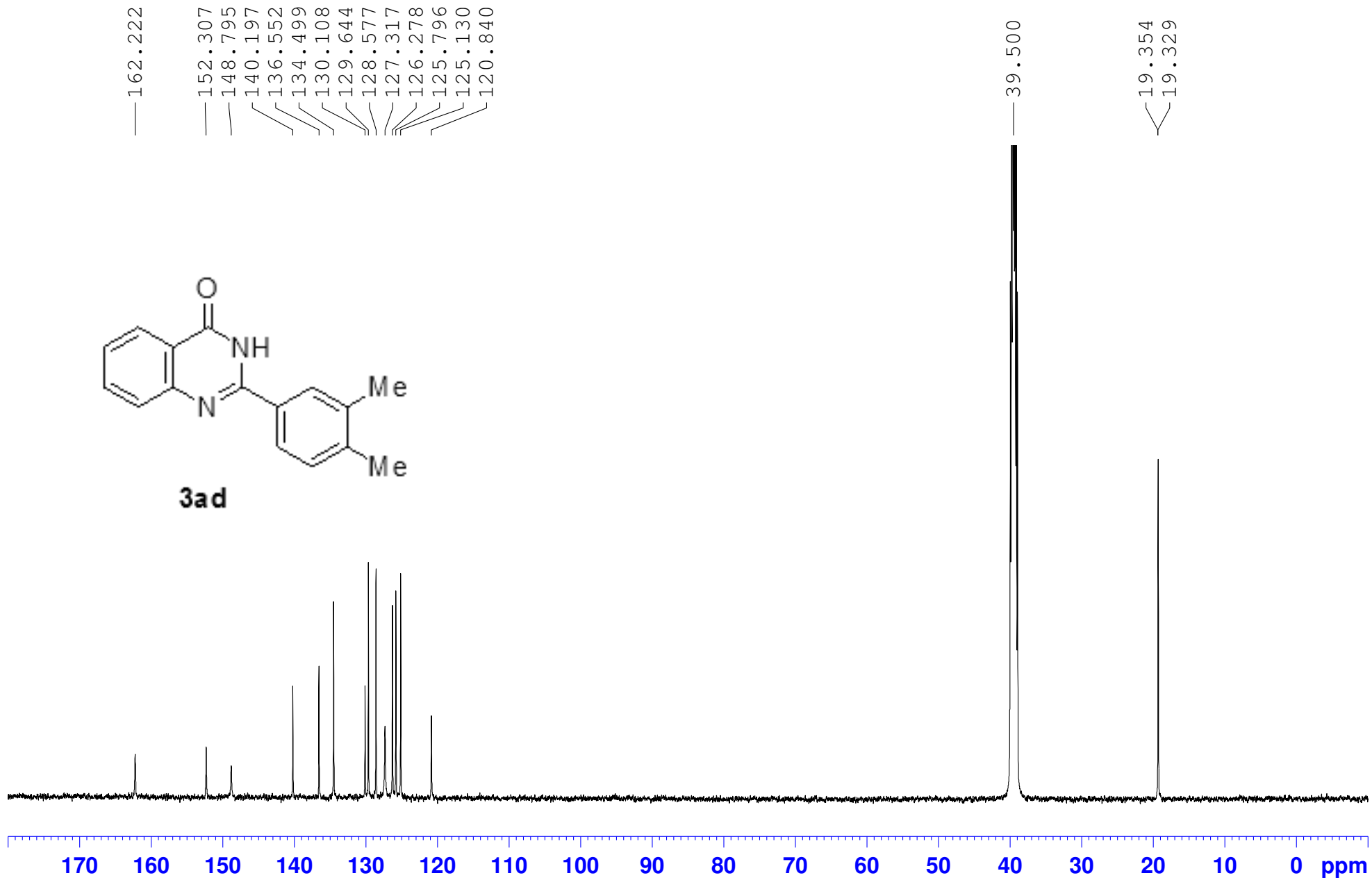


2-(3,4-dimethylphenyl)quinazolin-4(3H)-one  
C13CPD DMSO-d6

162.222  
152.307  
148.795  
140.197  
136.552  
134.499  
130.108  
129.644  
128.577  
127.317  
126.278  
125.796  
125.130  
120.840



3ad



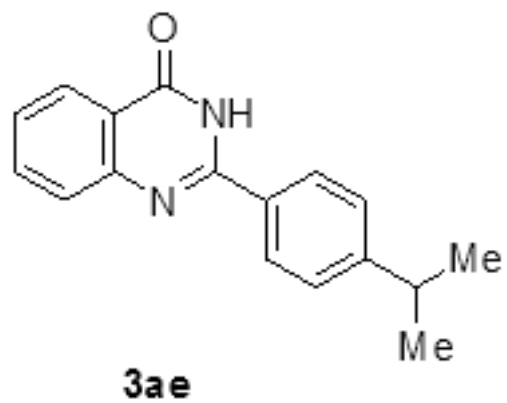
2-(4-isopropylphenyl)quinazolin-4(3H)-one  
PROTON DMSO-d6

12.478

8.155  
8.134  
8.118  
7.843  
7.829  
7.816  
7.736  
7.719  
7.523  
7.509  
7.494  
7.426  
7.412

3.008  
2.994  
2.977  
2.965  
2.952  
2.502

1.249  
1.235



1.00

3.00  
1.00  
1.00  
1.00  
2.00

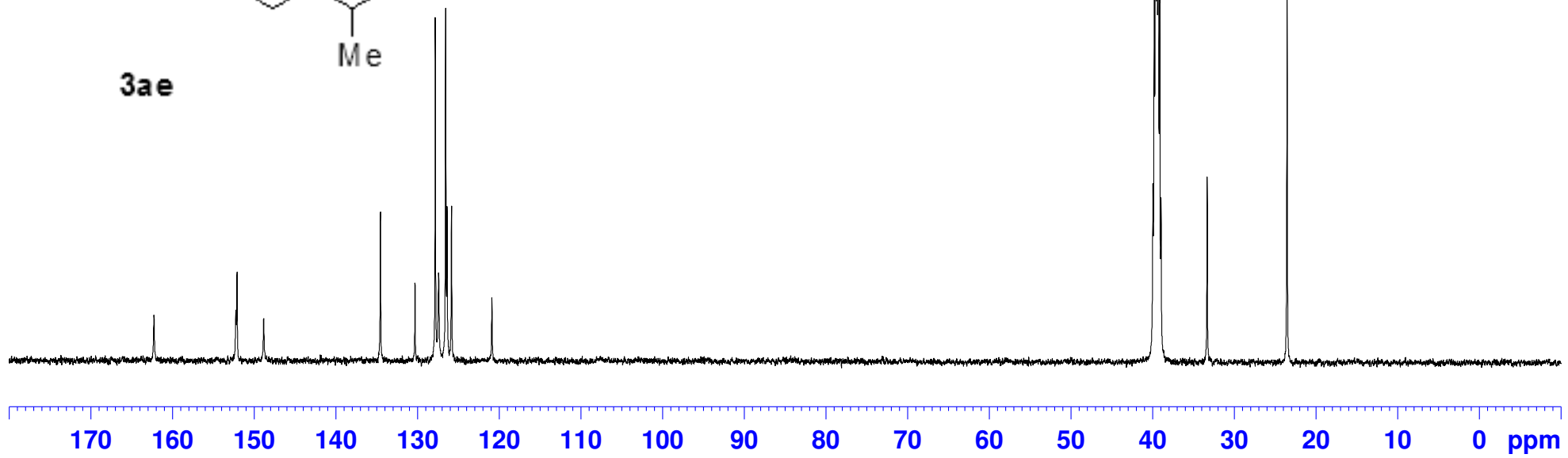
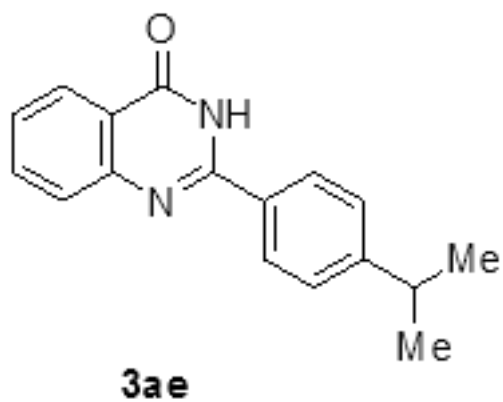
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6.00

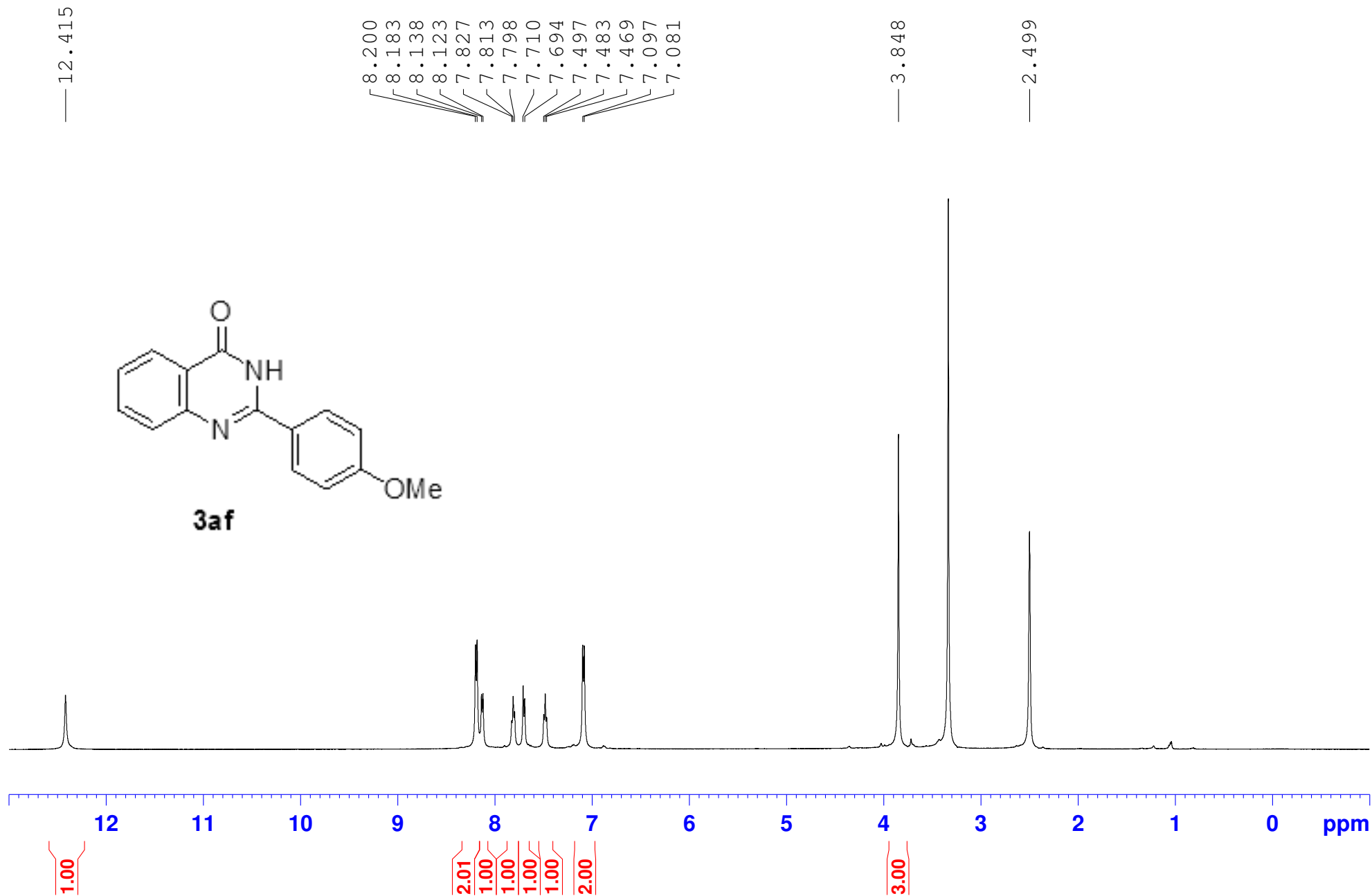
2-(4-isopropylphenyl)quinazolin-4(3H)-one  
C13CPD DMSO-d6

— 162.263  
— 152.223  
— 152.090  
— 148.821  
— 134.527  
— 130.296  
— 127.810  
— 127.407  
— 126.538  
— 126.365  
— 125.822  
— 120.883

— 39.500  
— 33.353  
— 23.571



2-(4-methoxyphenyl)quinazolin-4(3H)-one  
PROTON DMSO-d6

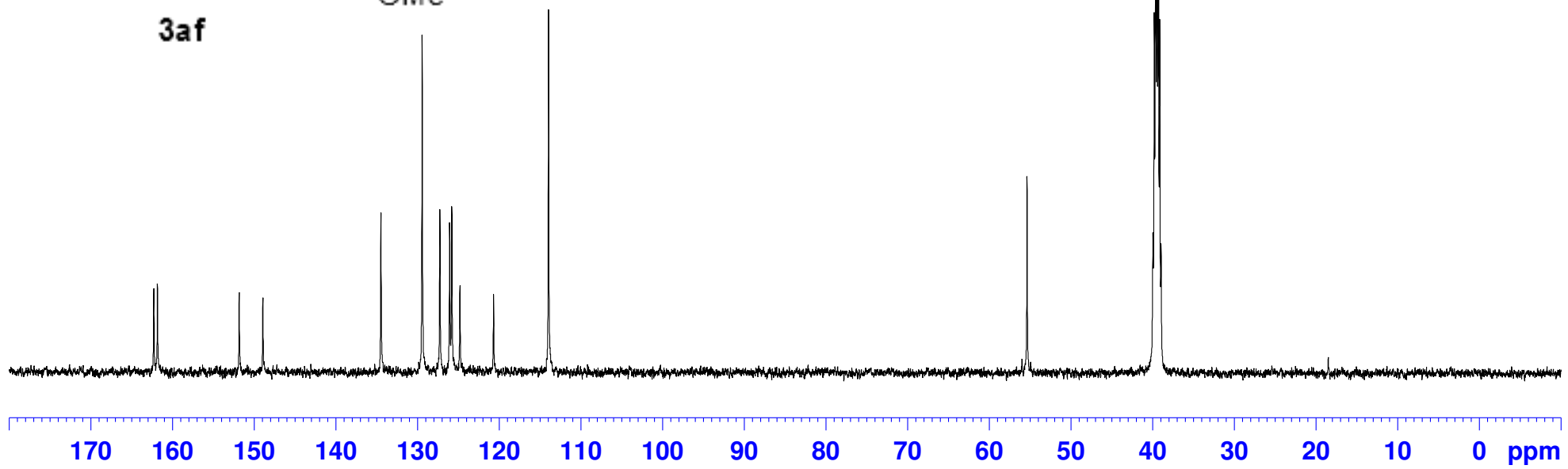
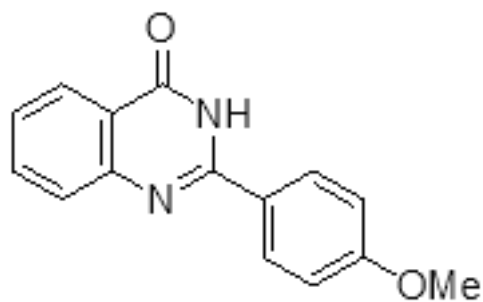


2-(4-methoxyphenyl)quinazolin-4(3H)-one  
C13CPD DMSO-d6

162.272  
161.835  
151.820  
148.925  
134.464  
129.421  
127.254  
126.056  
125.789  
124.792  
120.680  
113.946

55.408

39.501



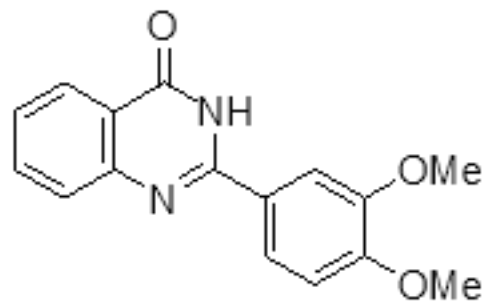
2-(3,4-dimethoxyphenyl)quinazolin-4(3H)-one  
PROTON DMSO-d6

— 12.438

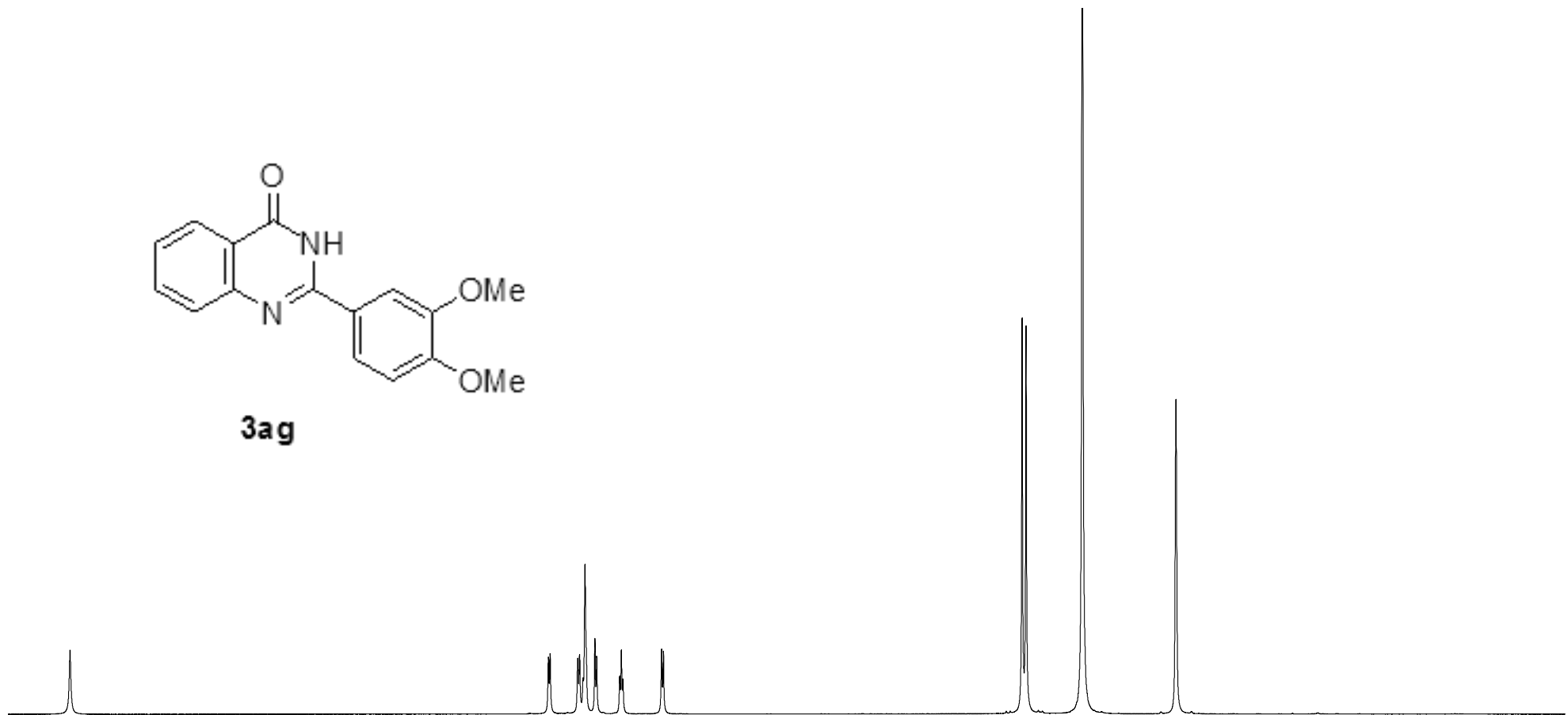
8.141  
8.126  
7.877  
7.861  
7.829  
7.812  
7.723  
7.707  
7.500  
7.485  
7.471  
7.124  
7.107

3.883  
3.847

— 2.500



**3ag**



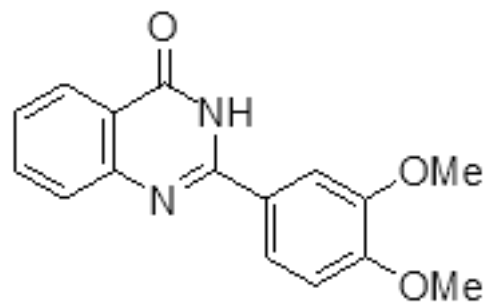
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1.00  
1.00  
2.00  
1.00  
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1.00

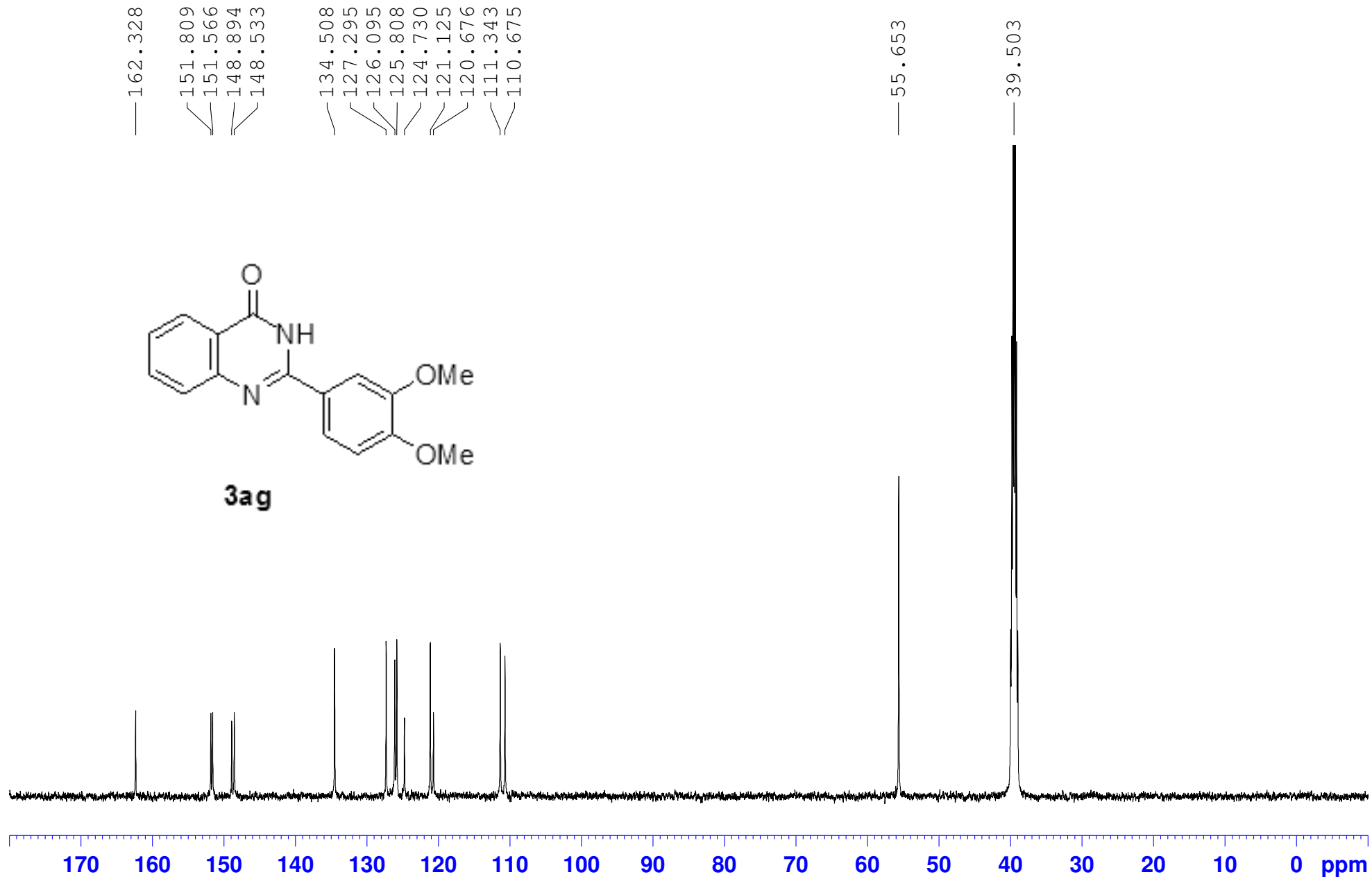
3.00  
3.00

2-(3,4-dimethoxyphenyl)quinazolin-4(3H)-one  
C13CPD DMSO-d6

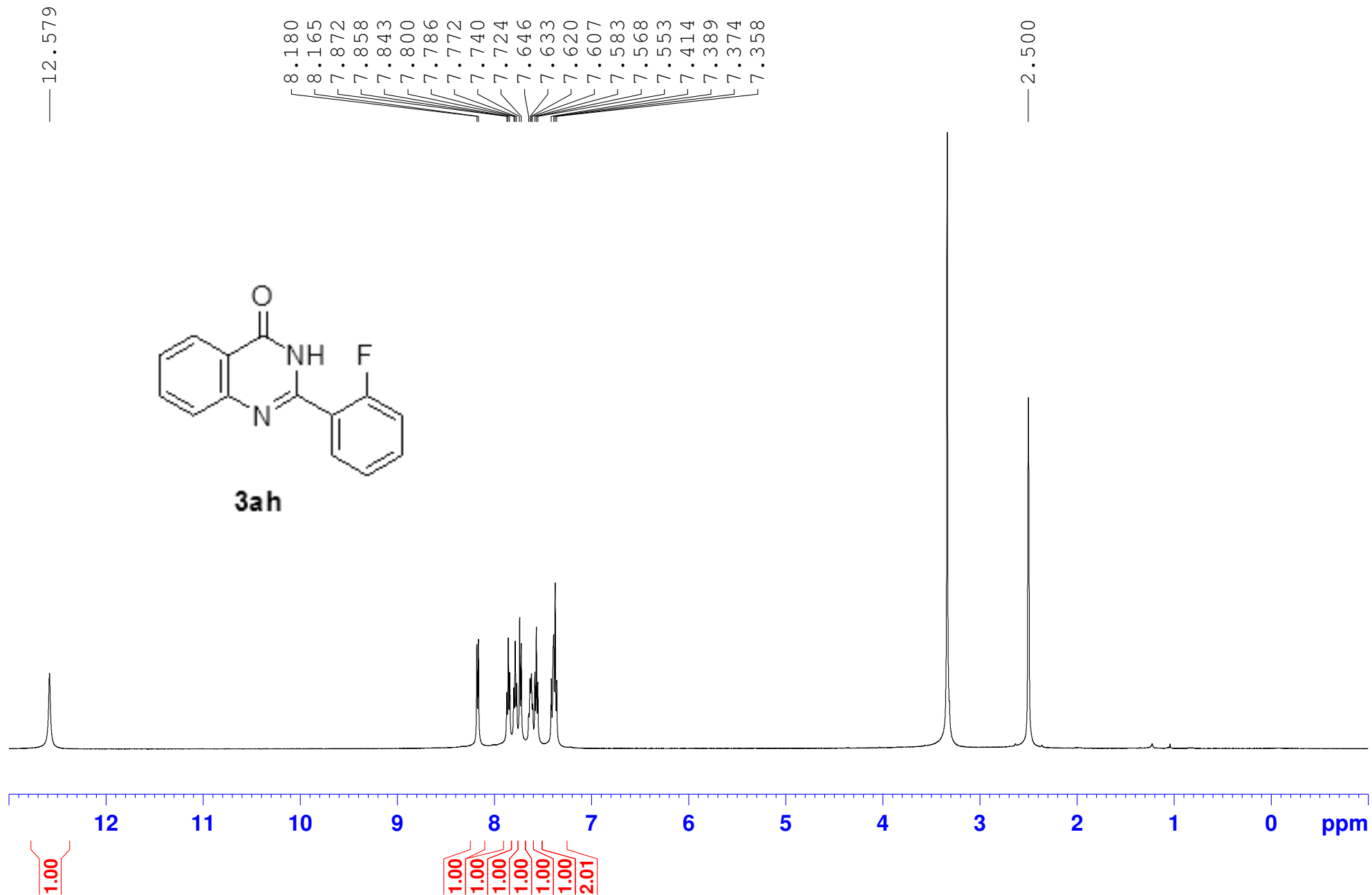
— 162.328  
151.809  
151.566  
148.894  
148.533  
134.508  
127.295  
126.095  
125.808  
124.730  
121.125  
120.676  
111.343  
110.675



3ag



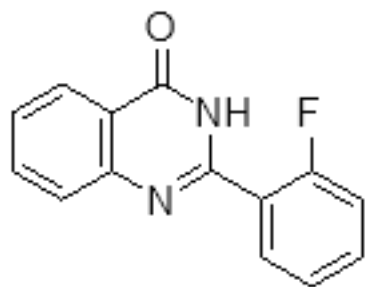
2-(2-fluorophenyl)quinazolin-4(3H)-one  
PROTON DMSO-d6



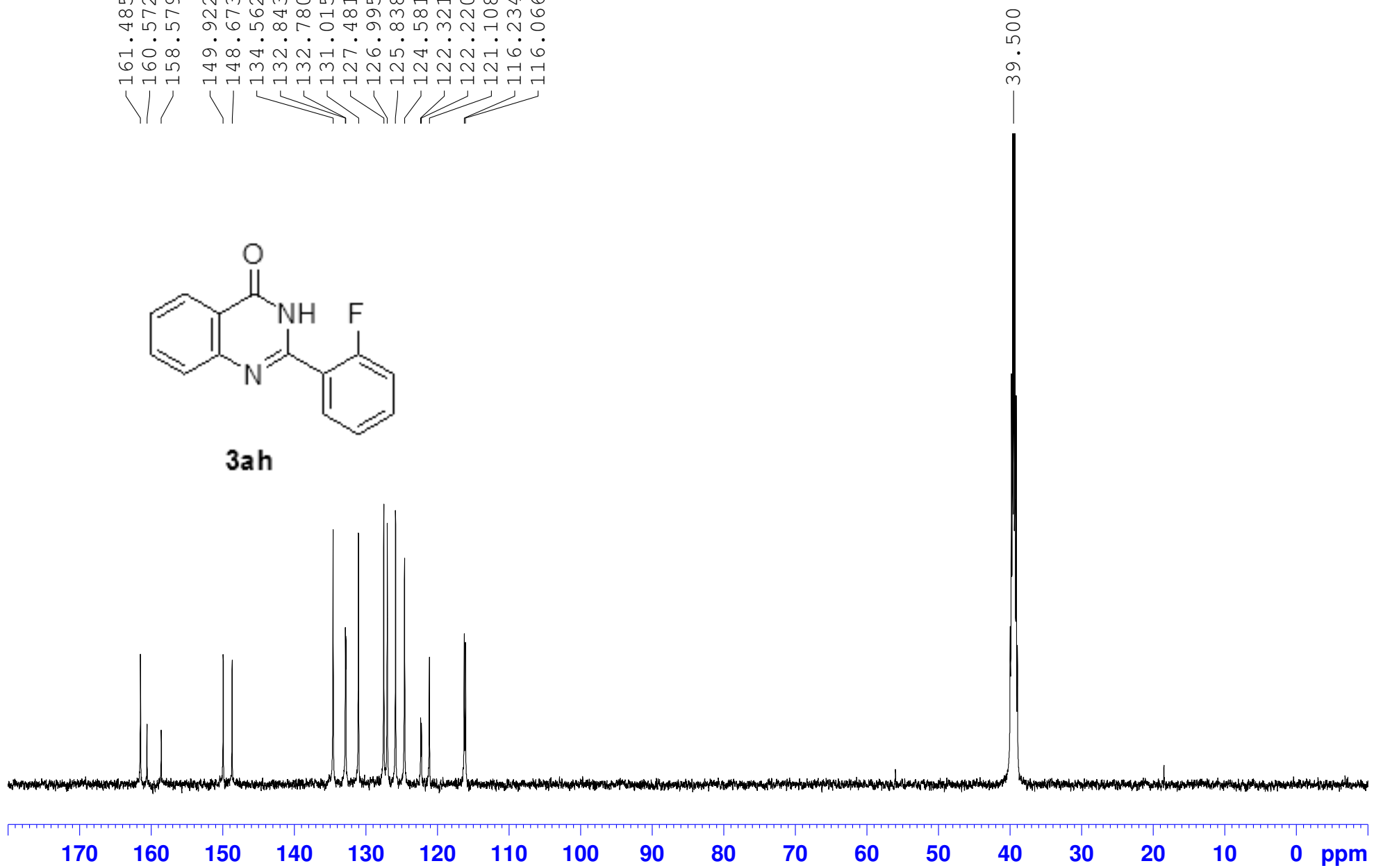


2-(2-fluorophenyl)quinazolin-4(3H)-one  
PROTON DMSO-d6

161.485  
160.572  
158.579  
149.922  
148.673  
134.562  
132.843  
132.780  
131.015  
127.481  
126.995  
125.838  
124.581  
122.321  
122.220  
121.108  
116.234  
116.066



3ah

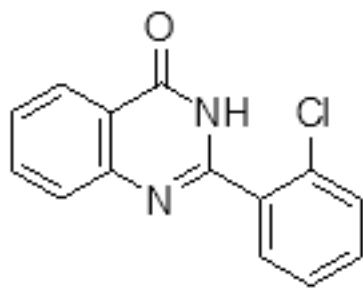


2-(2-chlorophenyl)quinazolin-4(3H)-one  
PROTON DMSO-d6

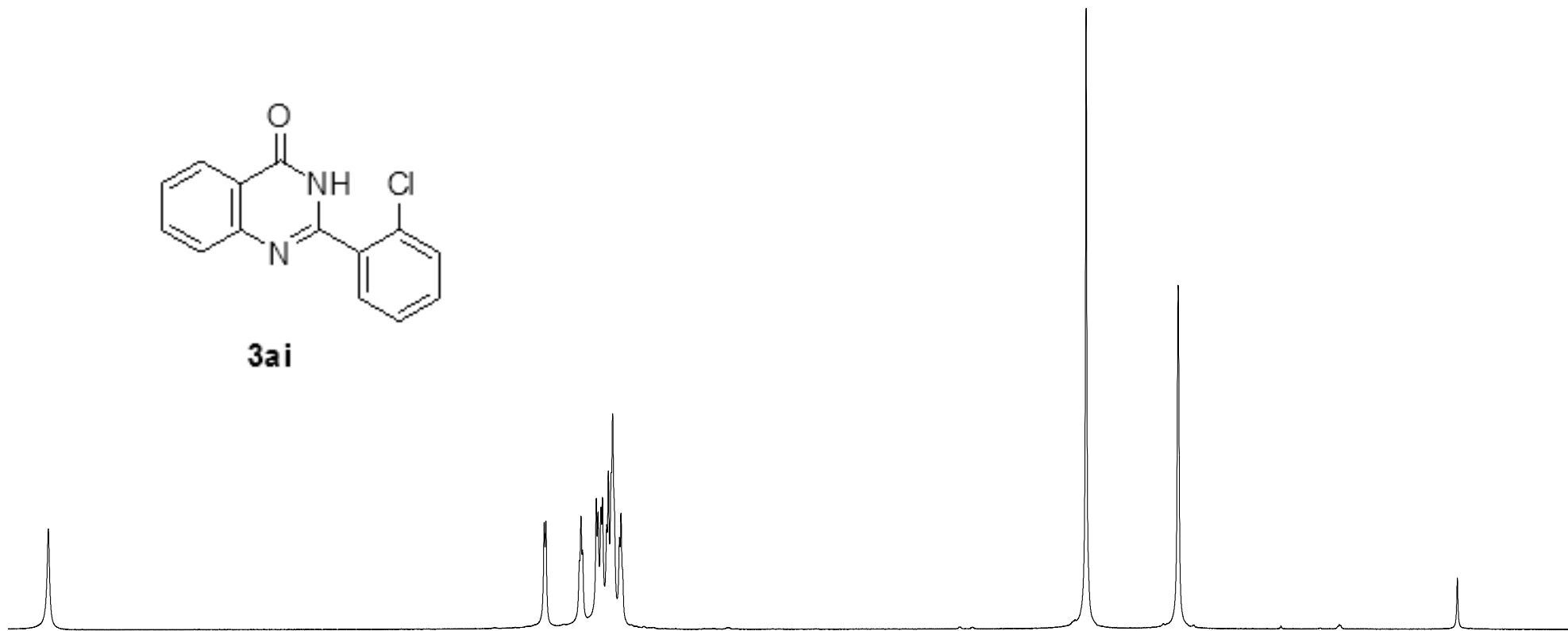
— 12.637

8.190  
8.175  
7.875  
7.860  
7.844  
7.723  
7.707  
7.682  
7.668  
7.630  
7.615  
7.590  
7.576  
7.561  
7.514  
7.500  
7.485

— 2.502



**3ai**



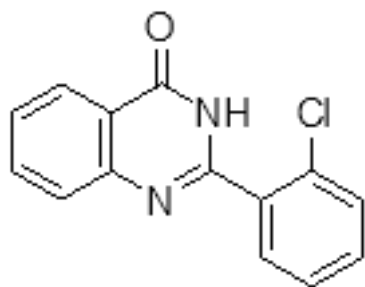
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

1.00

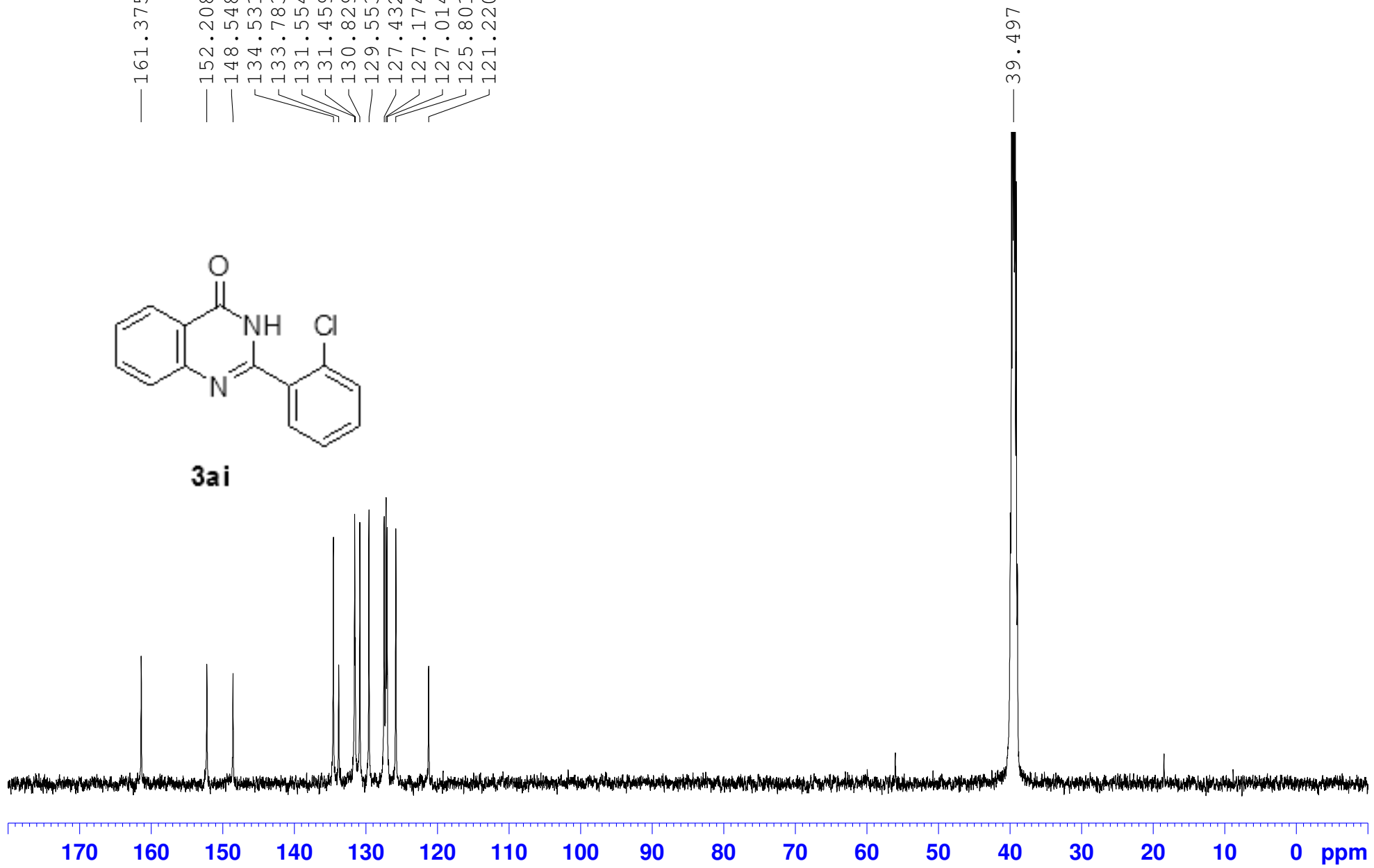
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1.00  
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C13CPD DMSO-d6

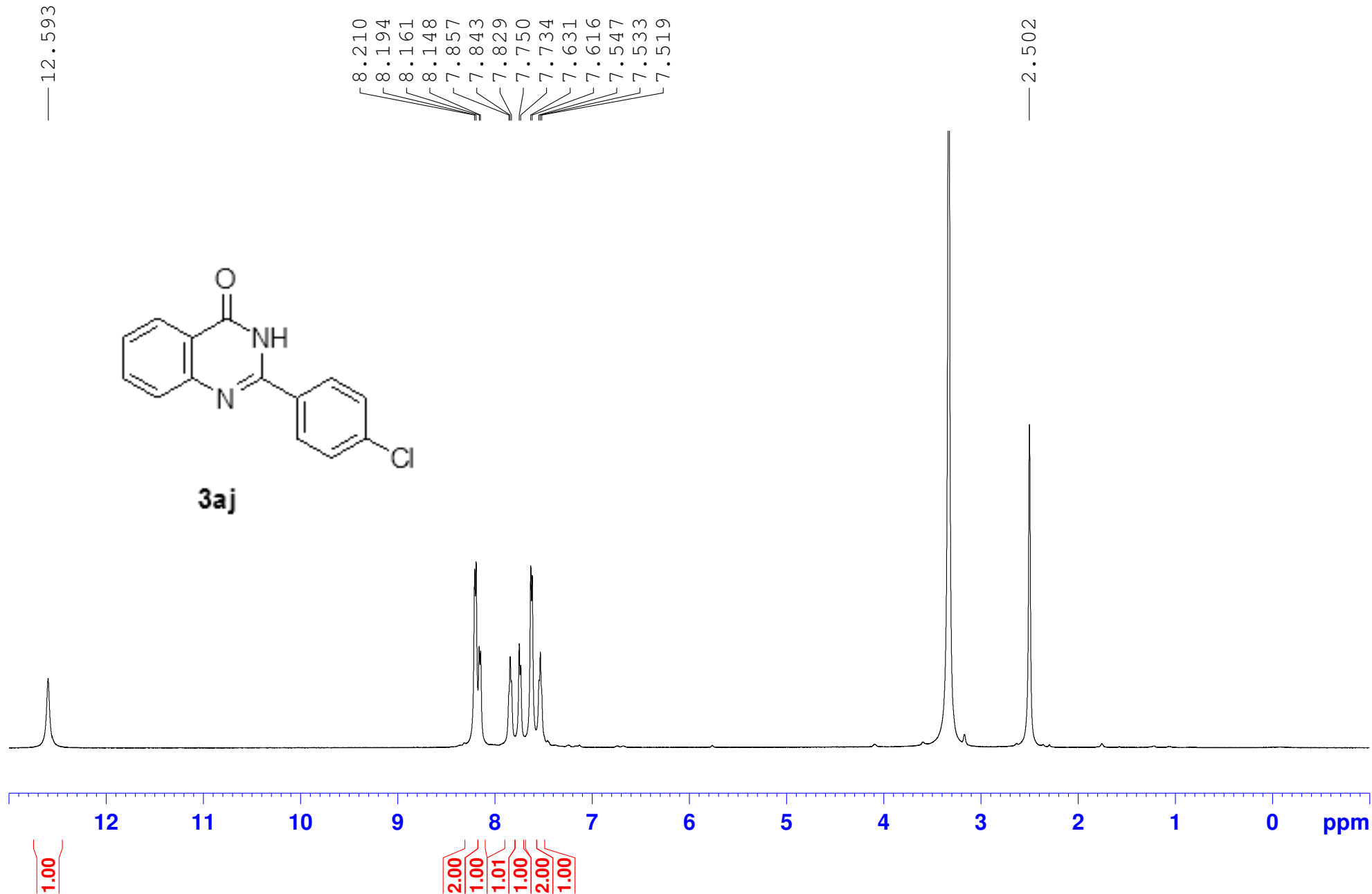
— 161.375  
— 152.208  
— 148.548  
— 134.531  
— 133.783  
— 131.554  
— 131.459  
— 130.829  
— 129.553  
— 127.432  
— 127.174  
— 127.014  
— 125.801  
— 121.220



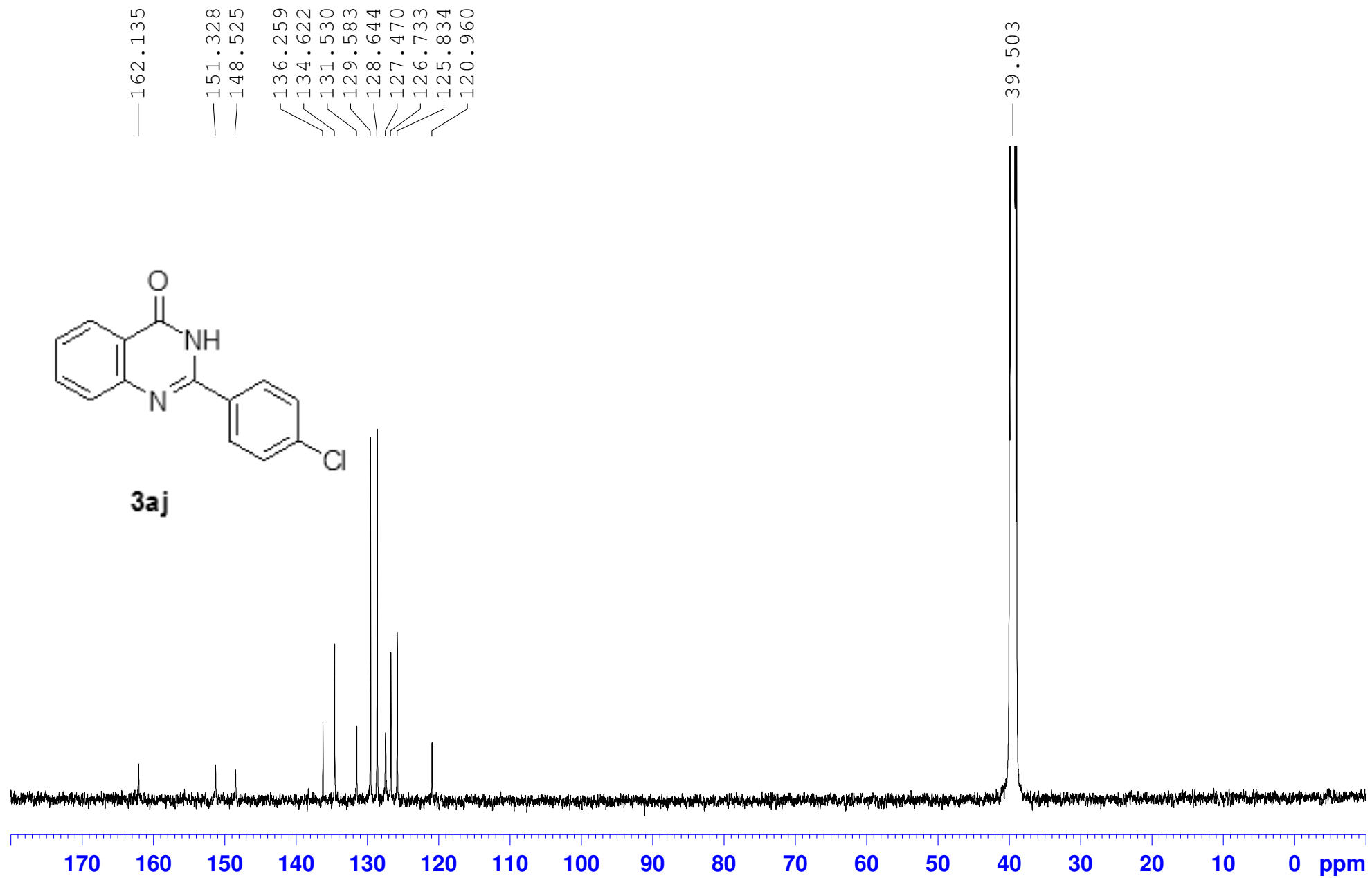
**3ai**



2-(4-chlorophenyl)quinazolin-4(3H)-one  
PROTON DMSO-d6



2-(4-chlorophenyl)quinazolin-4(3H)-one  
C13CPD DMSO-d6

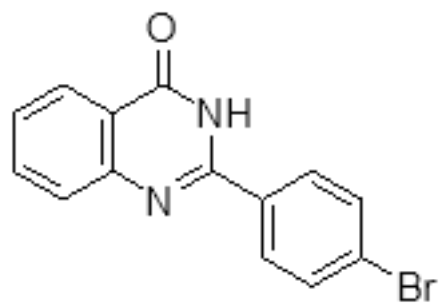


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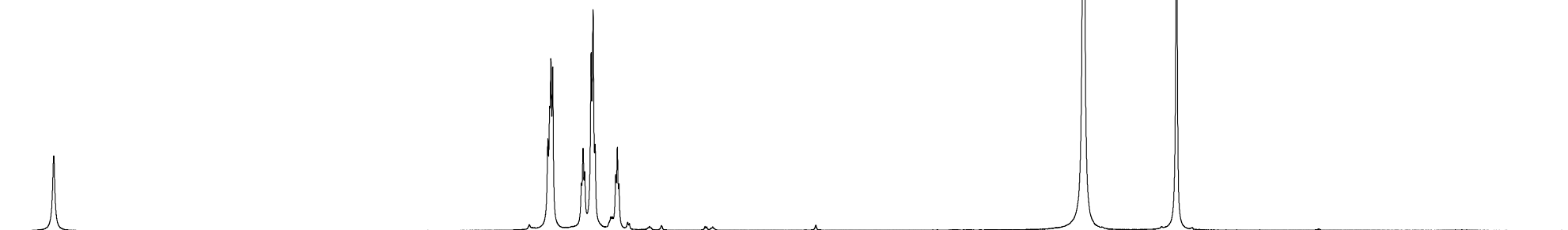
— 12.605

8.160  
8.143  
8.133  
8.117  
7.857  
7.843  
7.829  
7.771  
7.753  
7.735  
7.549  
7.535  
7.520

— 2.500



3ak



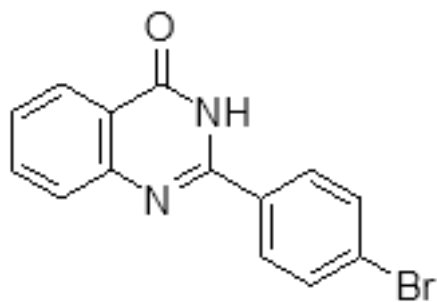
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3.00  
1.01  
3.00  
1.00

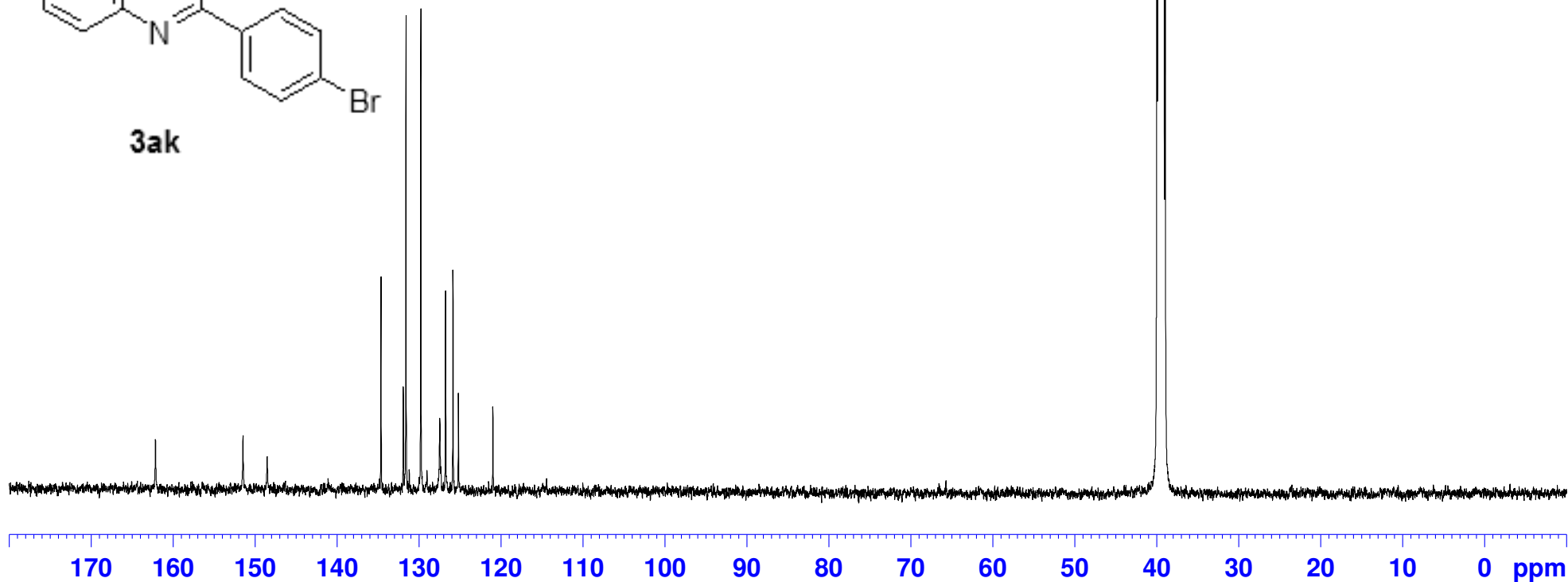
2-(4-bromophenyl)quinazolin-4(3H)-one  
C13CPD DMSO-d6

162.143  
151.461  
148.507  
134.623  
131.899  
131.577  
129.766  
127.458  
126.740  
125.838  
125.183  
120.971

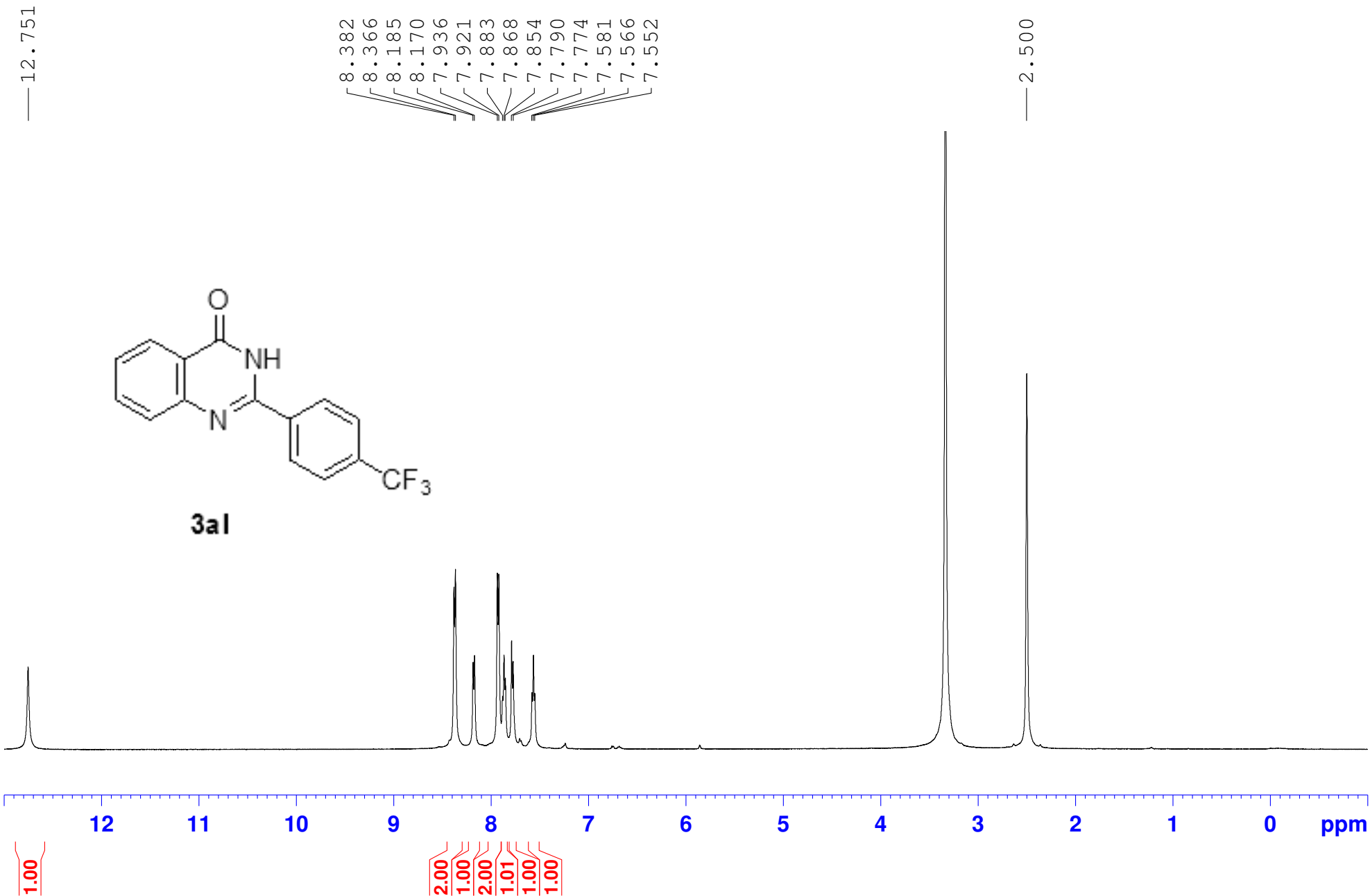
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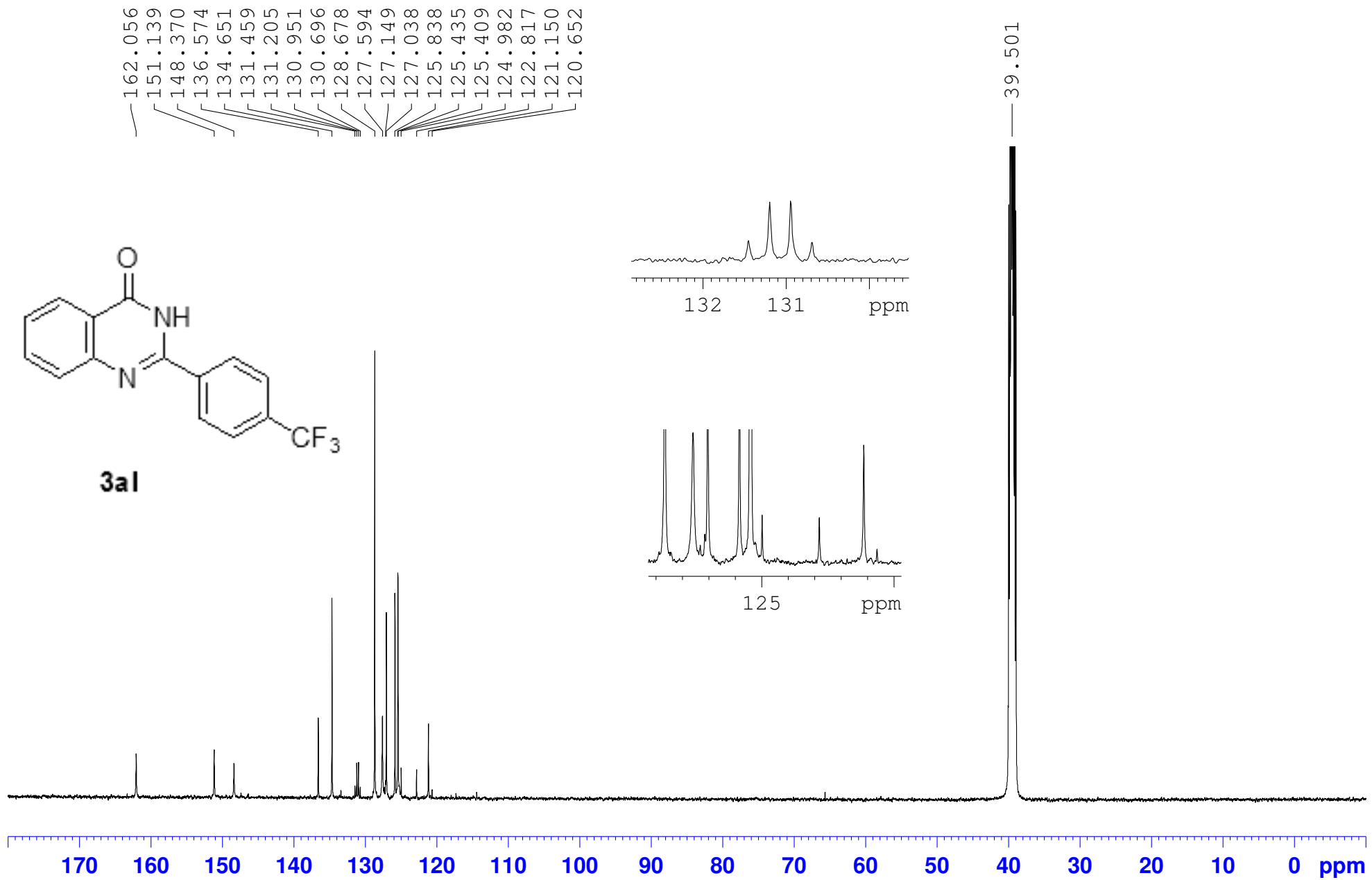


2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one  
PROTON DMSO-d6

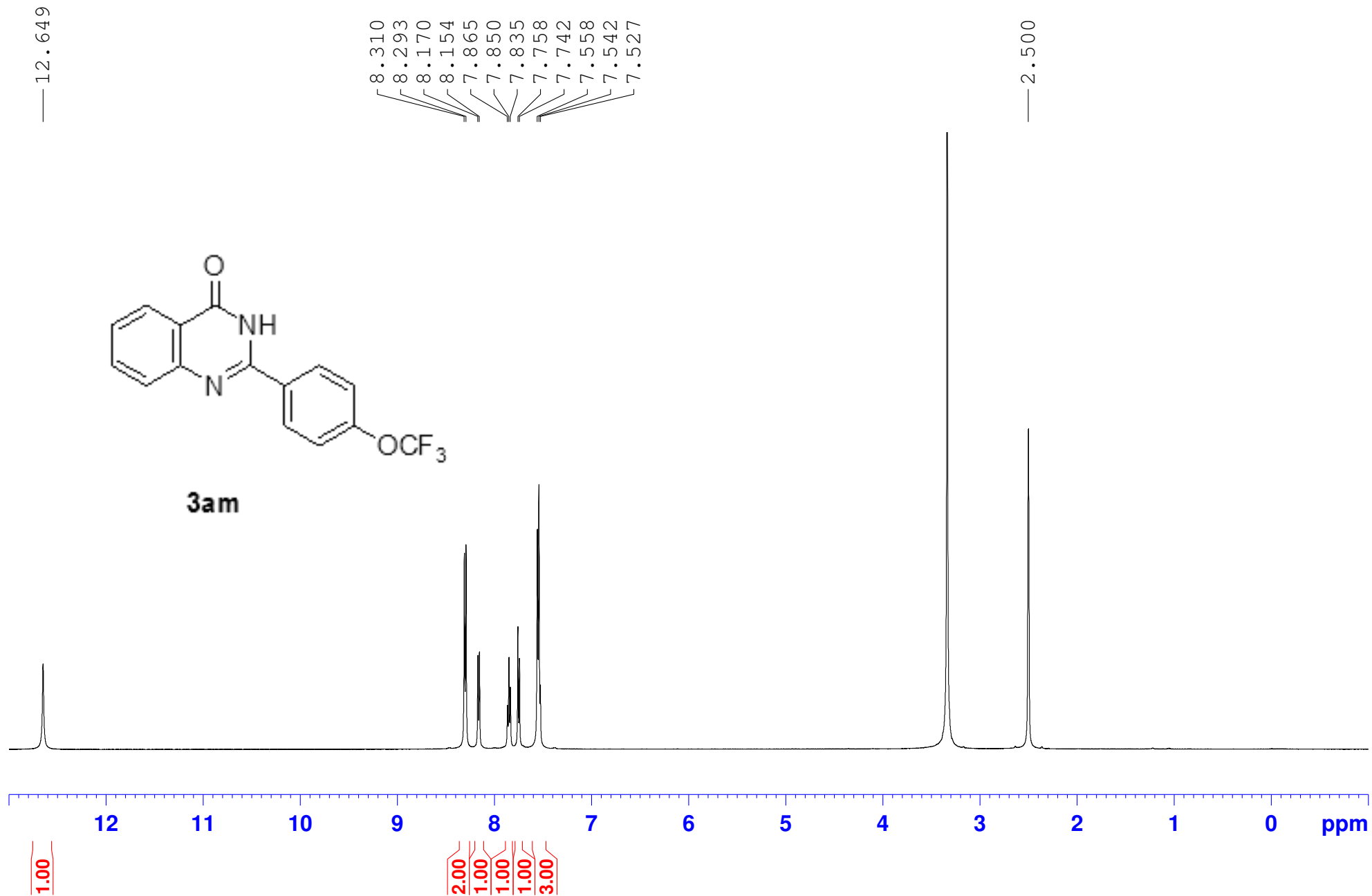




2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one  
C13CPD DMSO-d6

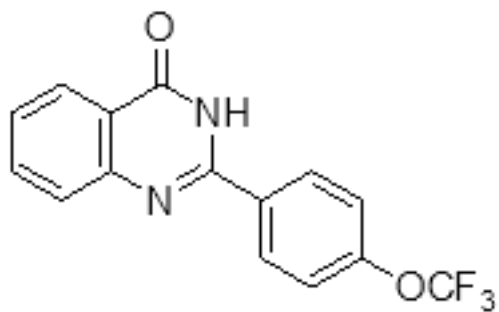


2-(4-(trifluoromethoxy)phenyl)quinazolin-4(3H)-one  
PROTON DMSO-d6

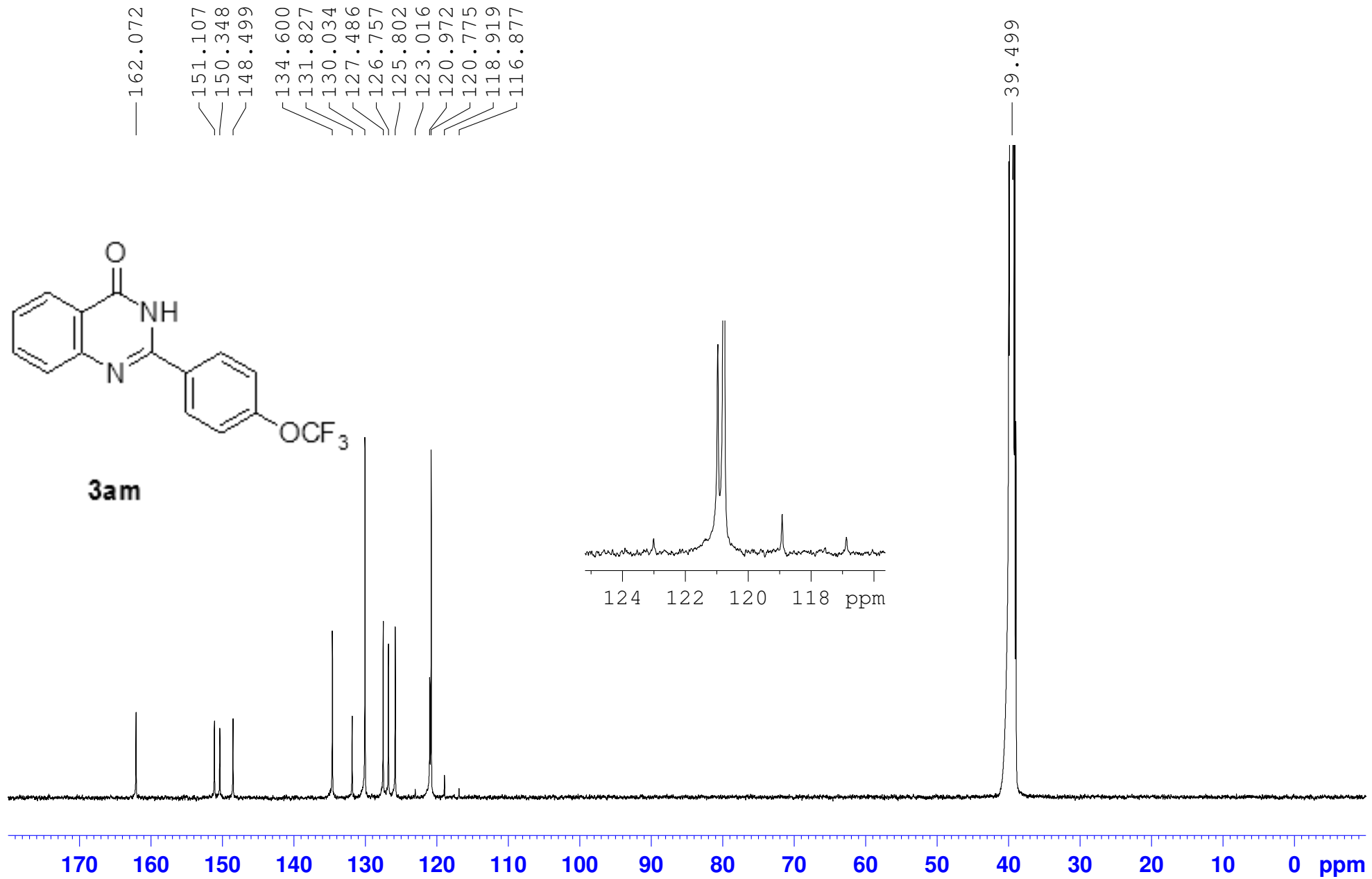


2-(4-(trifluoromethoxy)phenyl)quinazolin-4(3H)-one  
C13CPD DMSO-d6

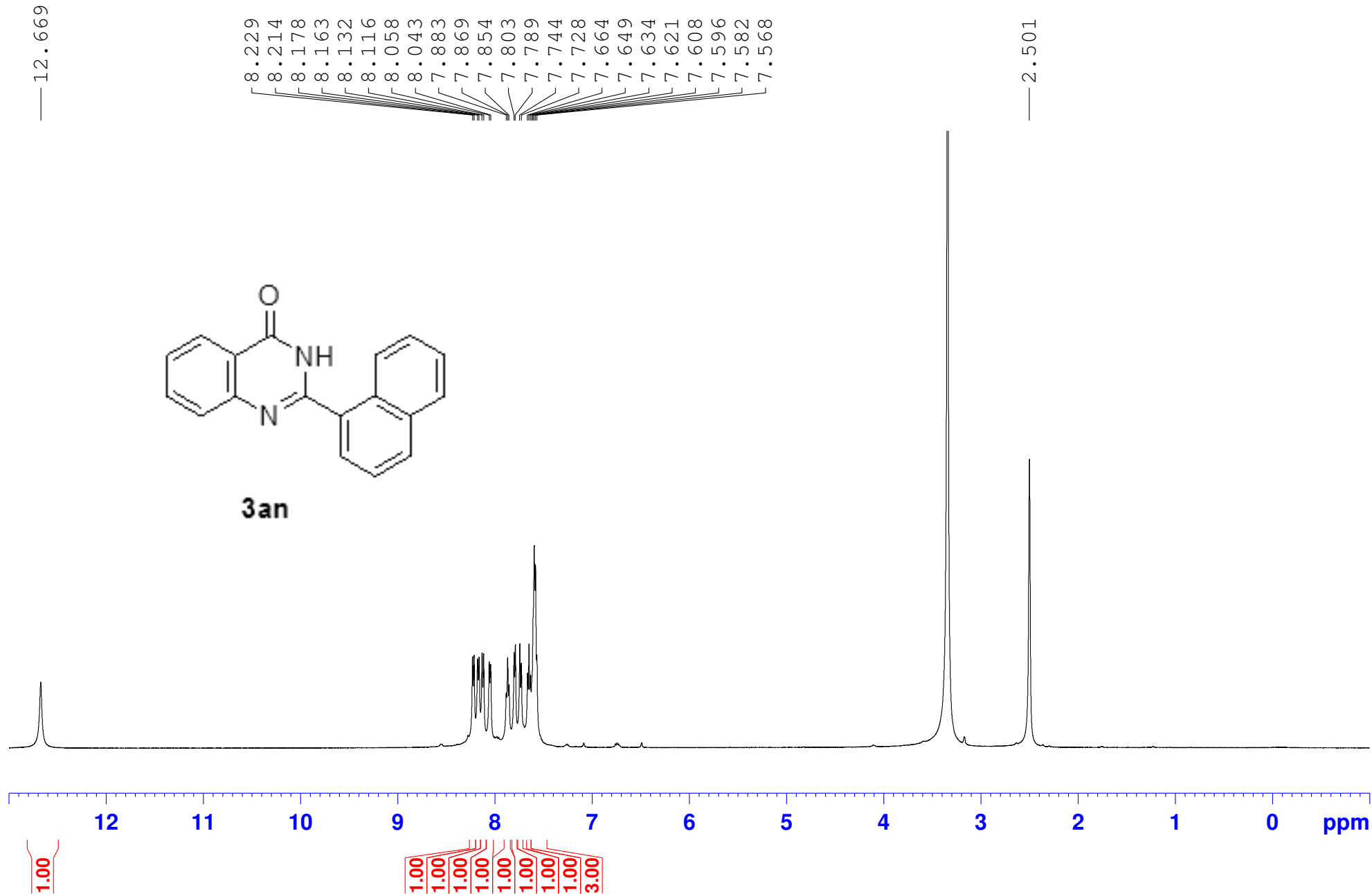
— 162.072  
— 151.107  
— 150.348  
— 148.499  
— 134.600  
— 131.827  
— 130.034  
— 127.486  
— 126.757  
— 125.802  
— 123.016  
— 120.972  
— 120.775  
— 118.919  
— 116.877



3am

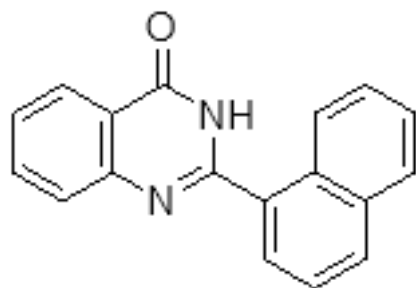


2-(naphthalen-1-yl)quinazolin-4(3H)-one  
PROTON DMSO-d6

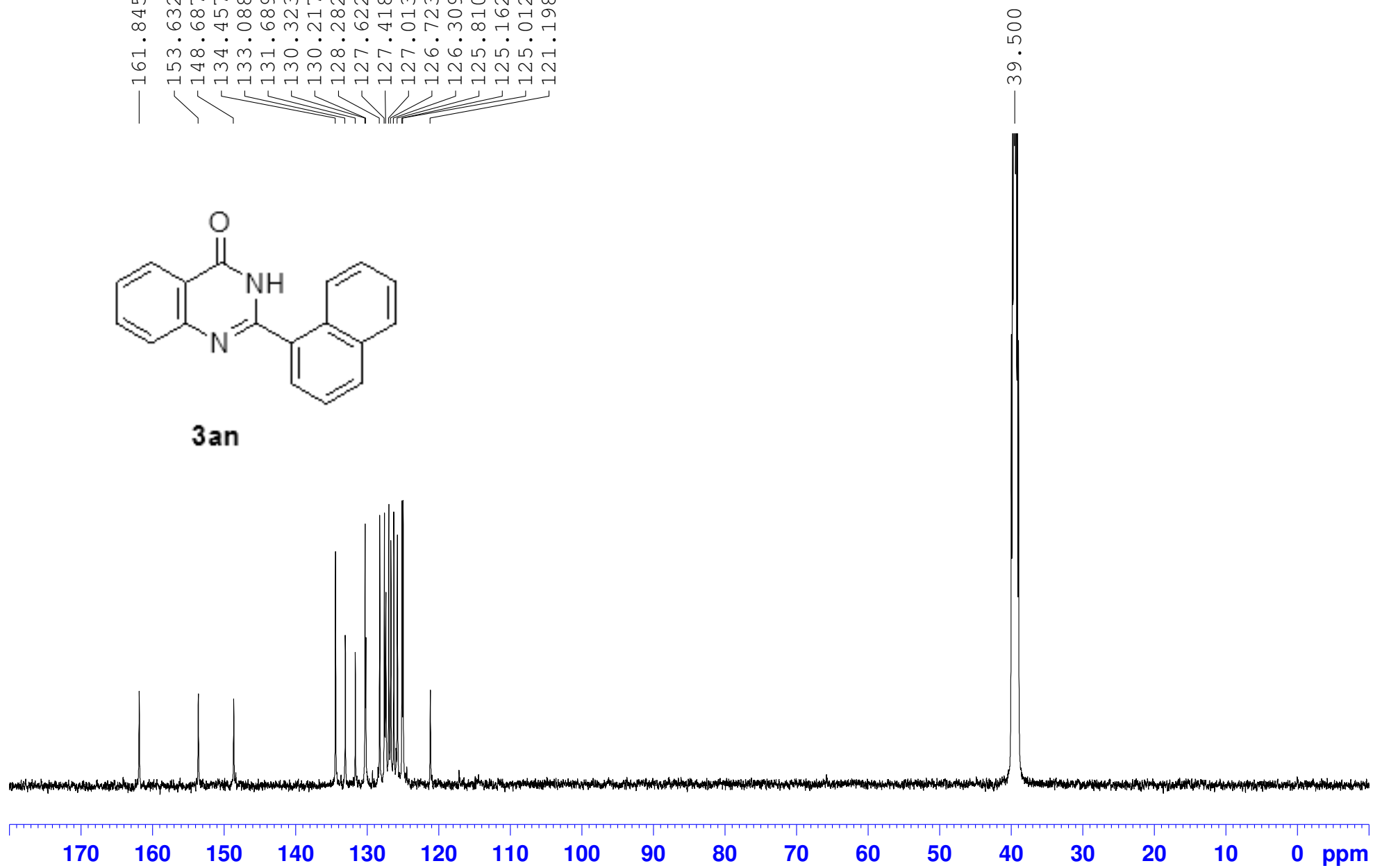


2-(naphthalen-1-yl)quinazolin-4(3H)-one  
C13CPD DMSO-d6

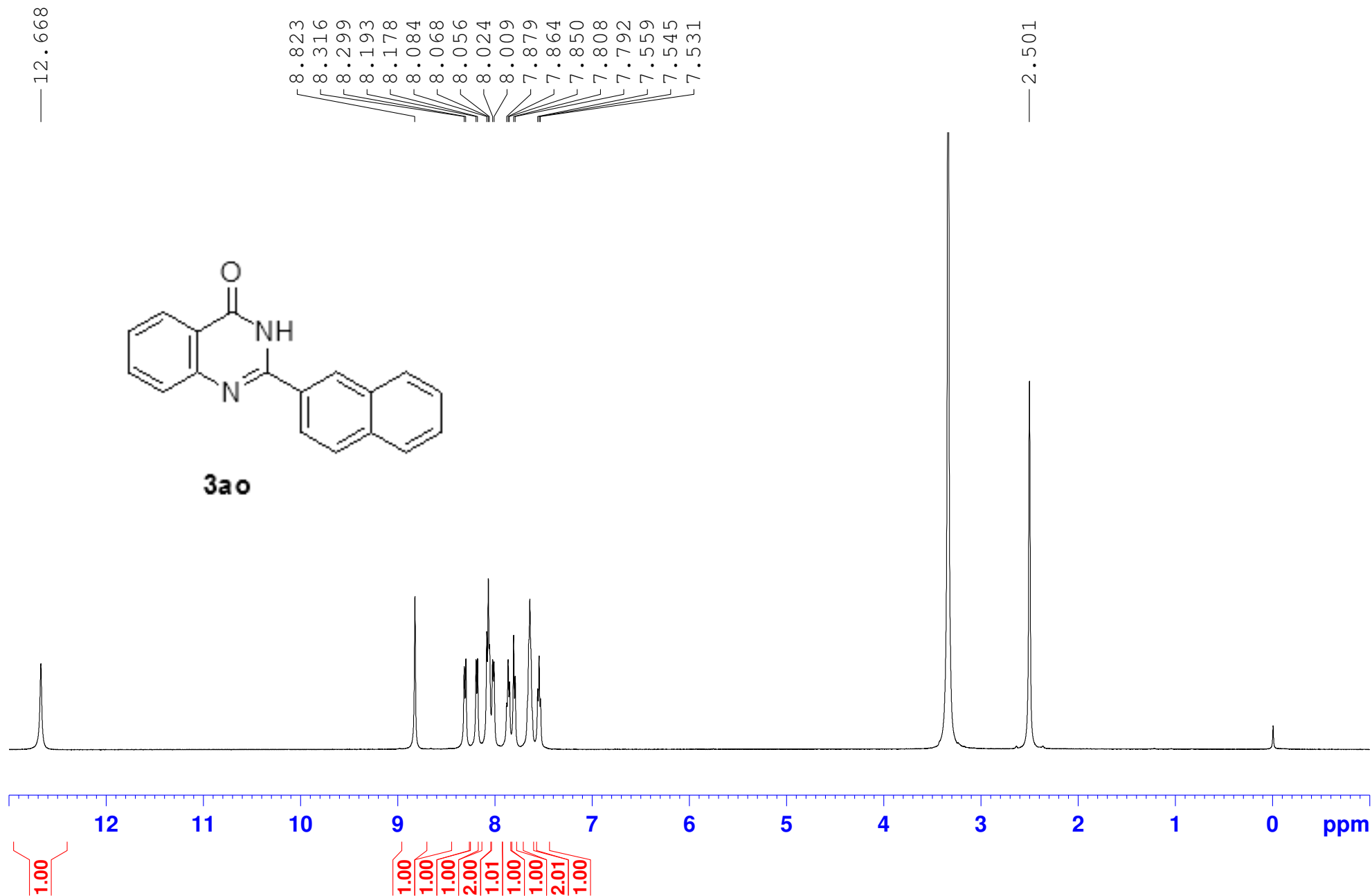
161.845  
153.632  
148.687  
134.457  
133.088  
131.689  
130.323  
130.217  
128.282  
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127.418  
127.013  
126.723  
126.309  
125.810  
125.162  
125.012  
121.198



3an

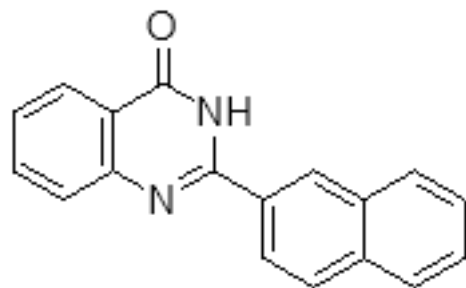


2-(naphthalen-2-yl)quinazolin-4(3H)-one  
PROTON DMSO-d6

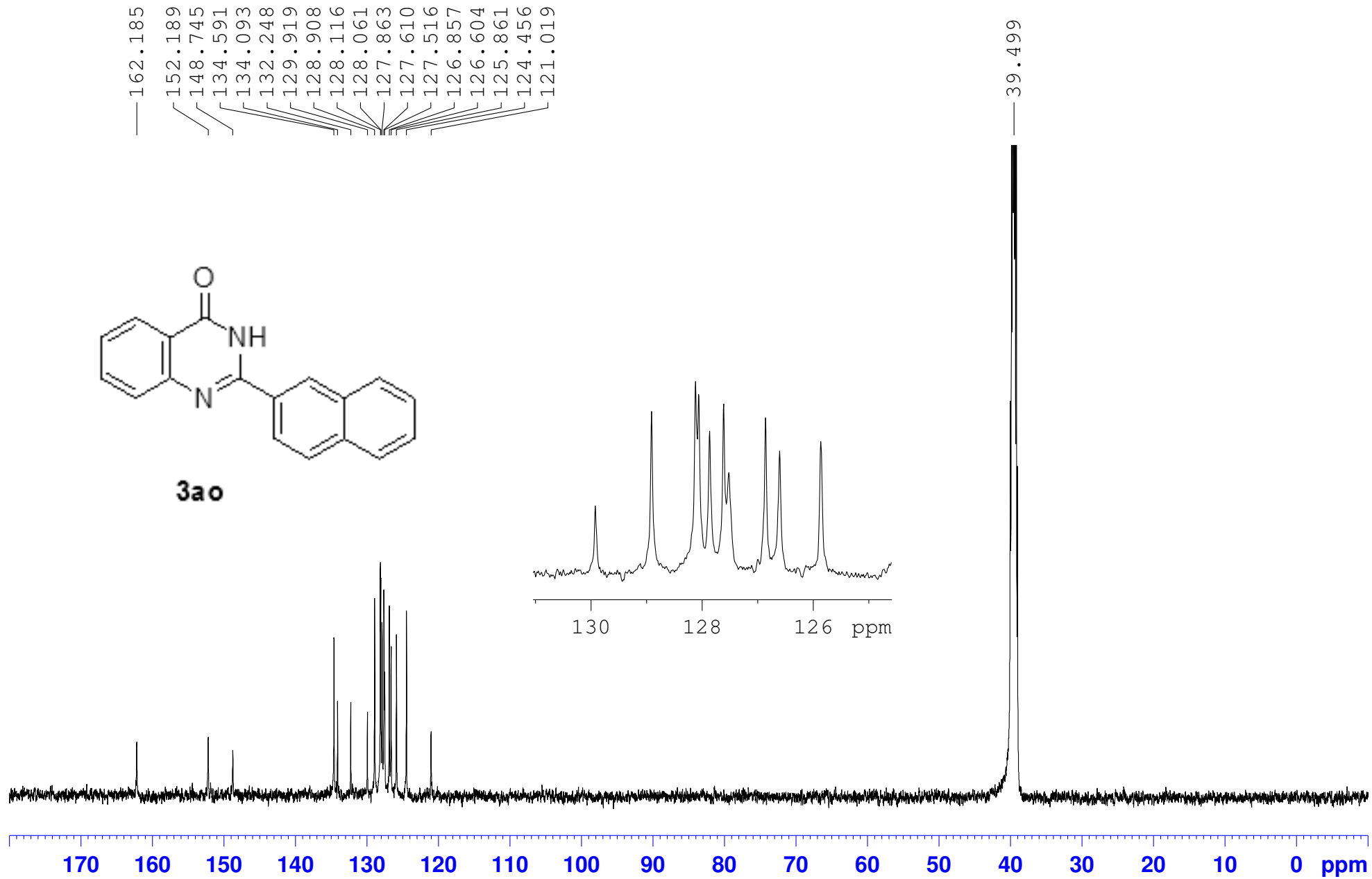


2-(naphthalen-2-yl)quinazolin-4(3H)-one  
C13CPD DMSO-d6

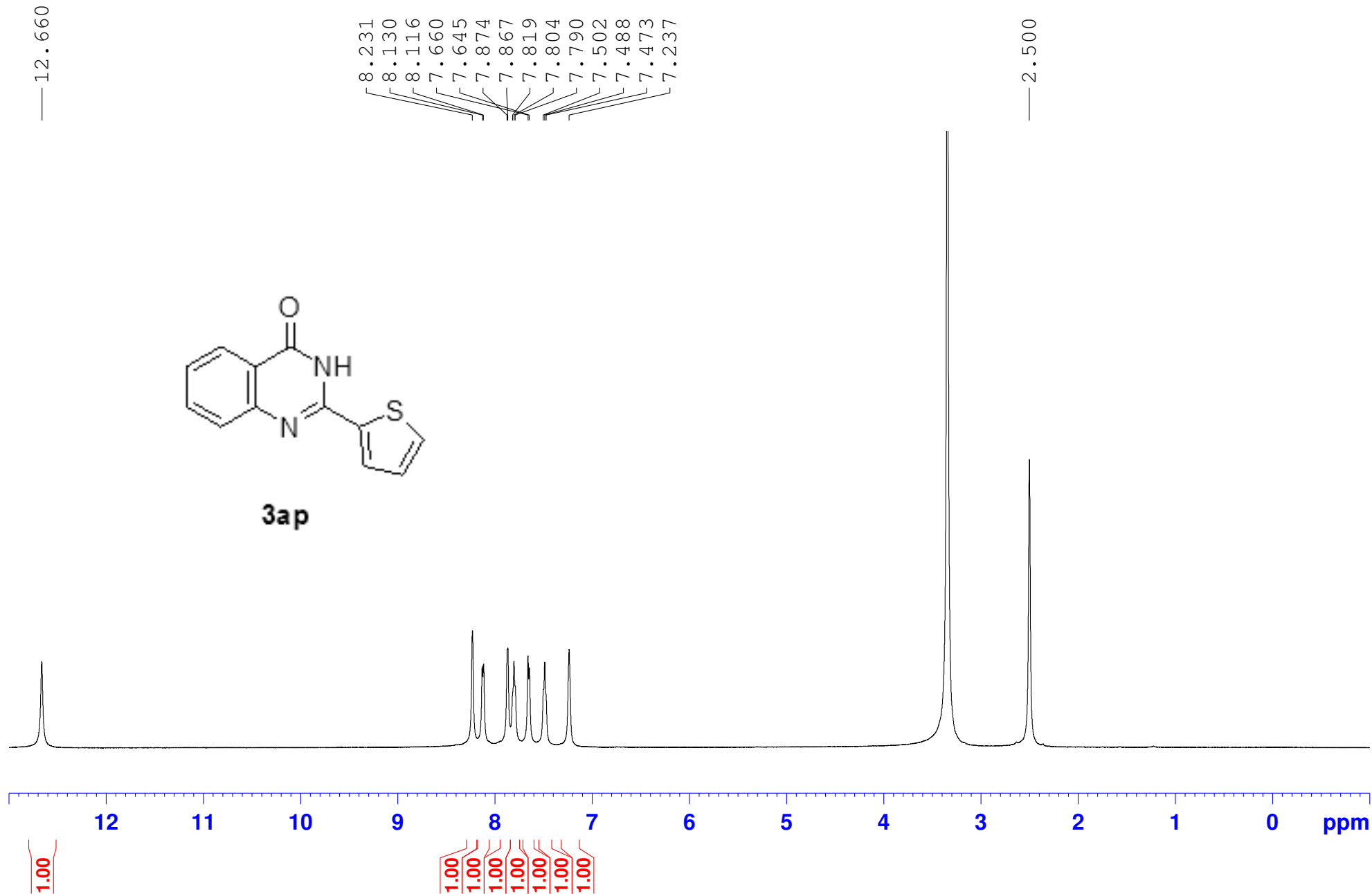
162.185  
152.189  
148.745  
134.591  
134.093  
132.248  
129.919  
128.908  
128.116  
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127.610  
127.516  
126.857  
126.604  
125.861  
124.456  
121.019



**3ao**



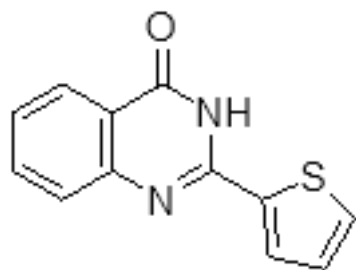
2-(thiophen-2-yl)quinazolin-4(3H)-one  
PROTON DMSO-d6



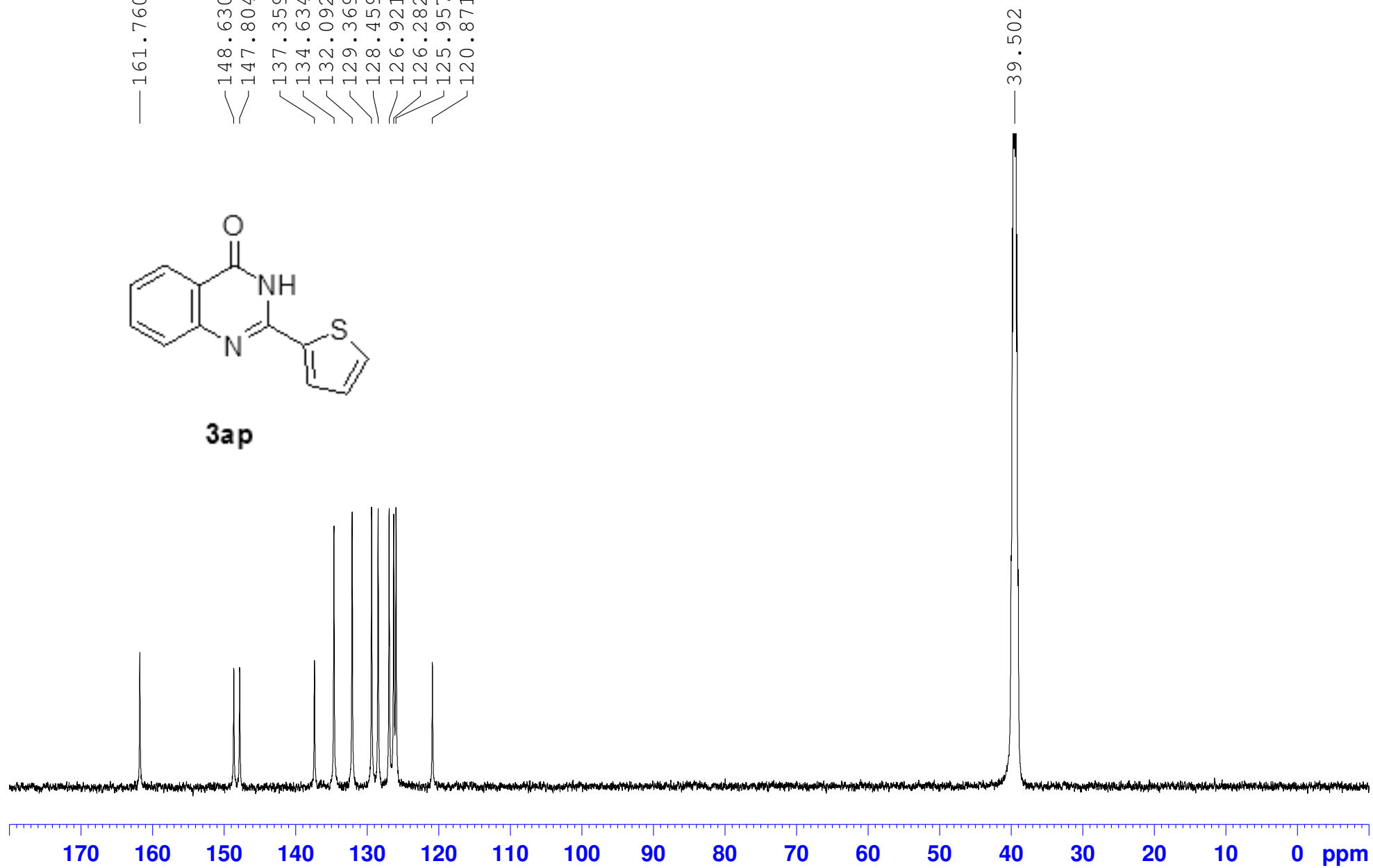


2-(thiophen-2-yl)quinazolin-4(3H)-one  
C13CPD DMSO-d6

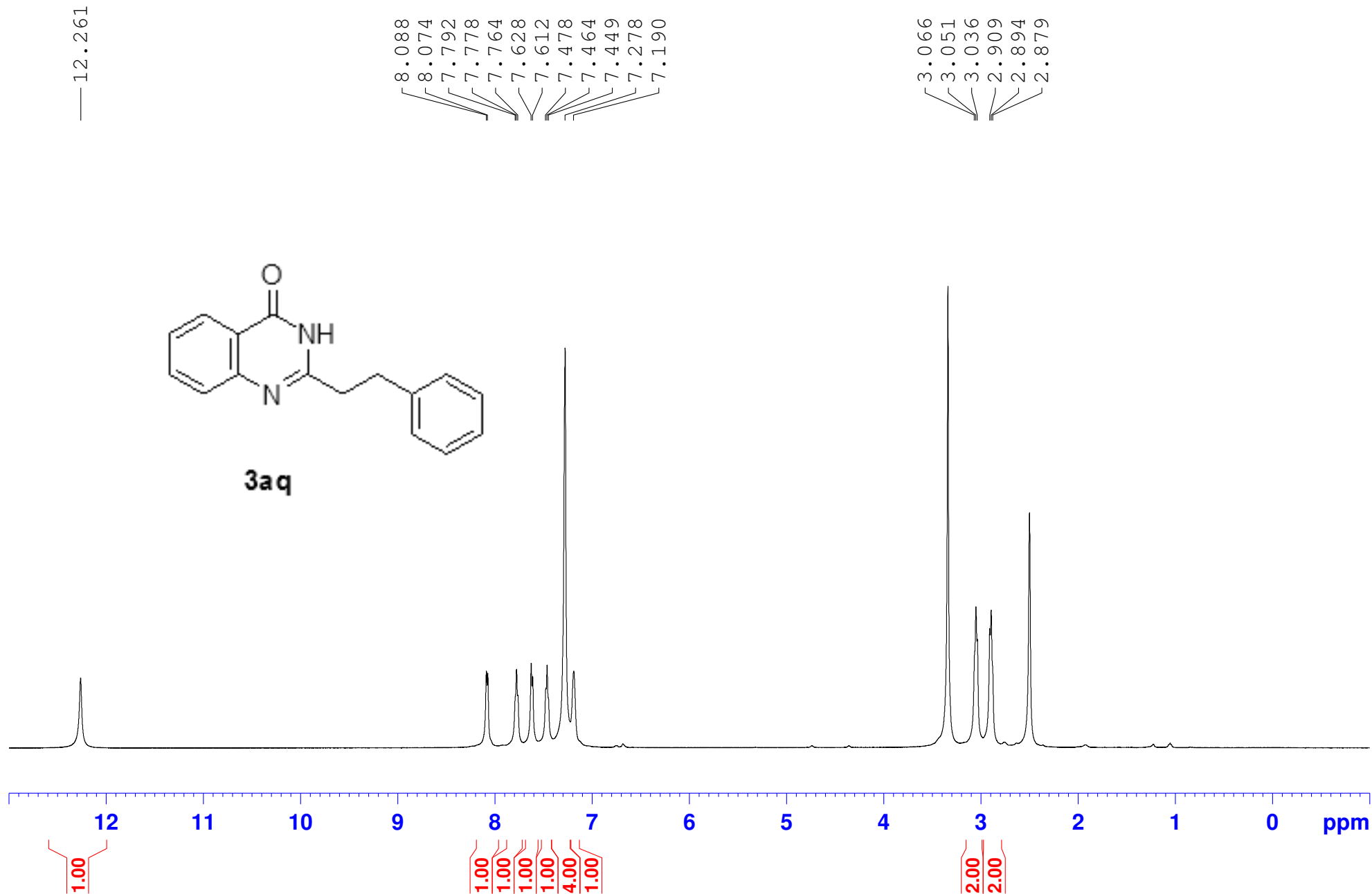
161.760  
148.630  
147.804  
137.359  
134.634  
132.092  
129.369  
128.459  
126.921  
126.282  
125.957  
120.871



3ap



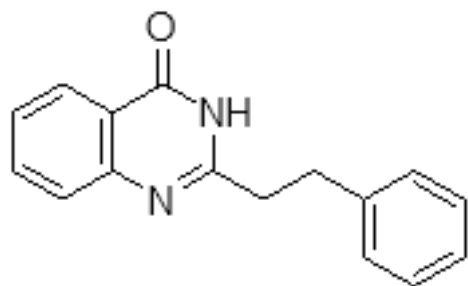
2-phenethylquinazolin-4(3H)-one  
PROTON DMSO-d6



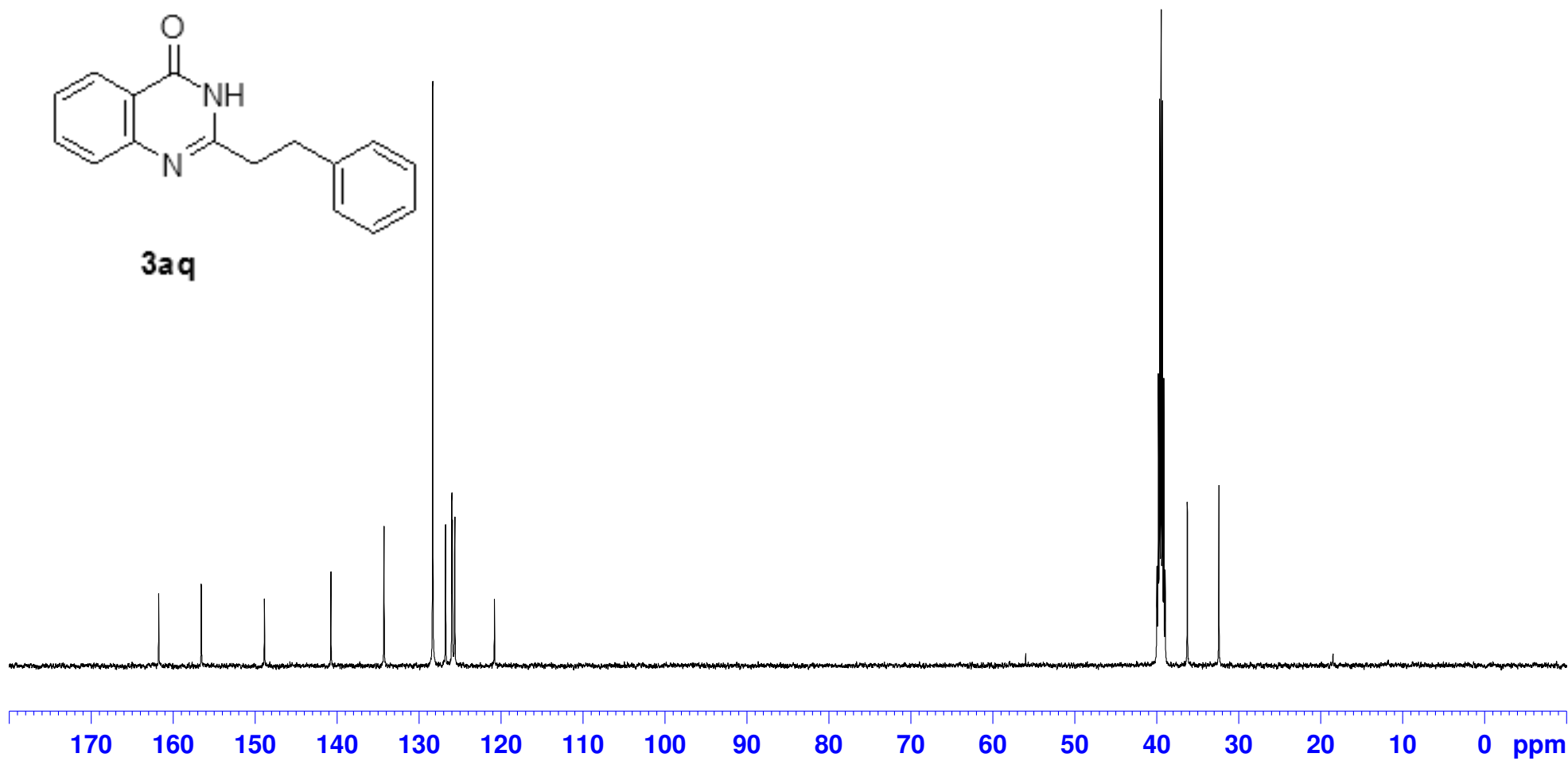
2-phenethylquinazolin-4(3H)-one  
C13CPD DMSO-d6

— 161.744  
— 156.541  
— 148.843  
— 140.730  
— 134.252  
— 128.315  
— 126.794  
— 126.039  
— 125.967  
— 125.671  
— 120.833

— 39.500  
— 36.295  
— 32.443



3aq

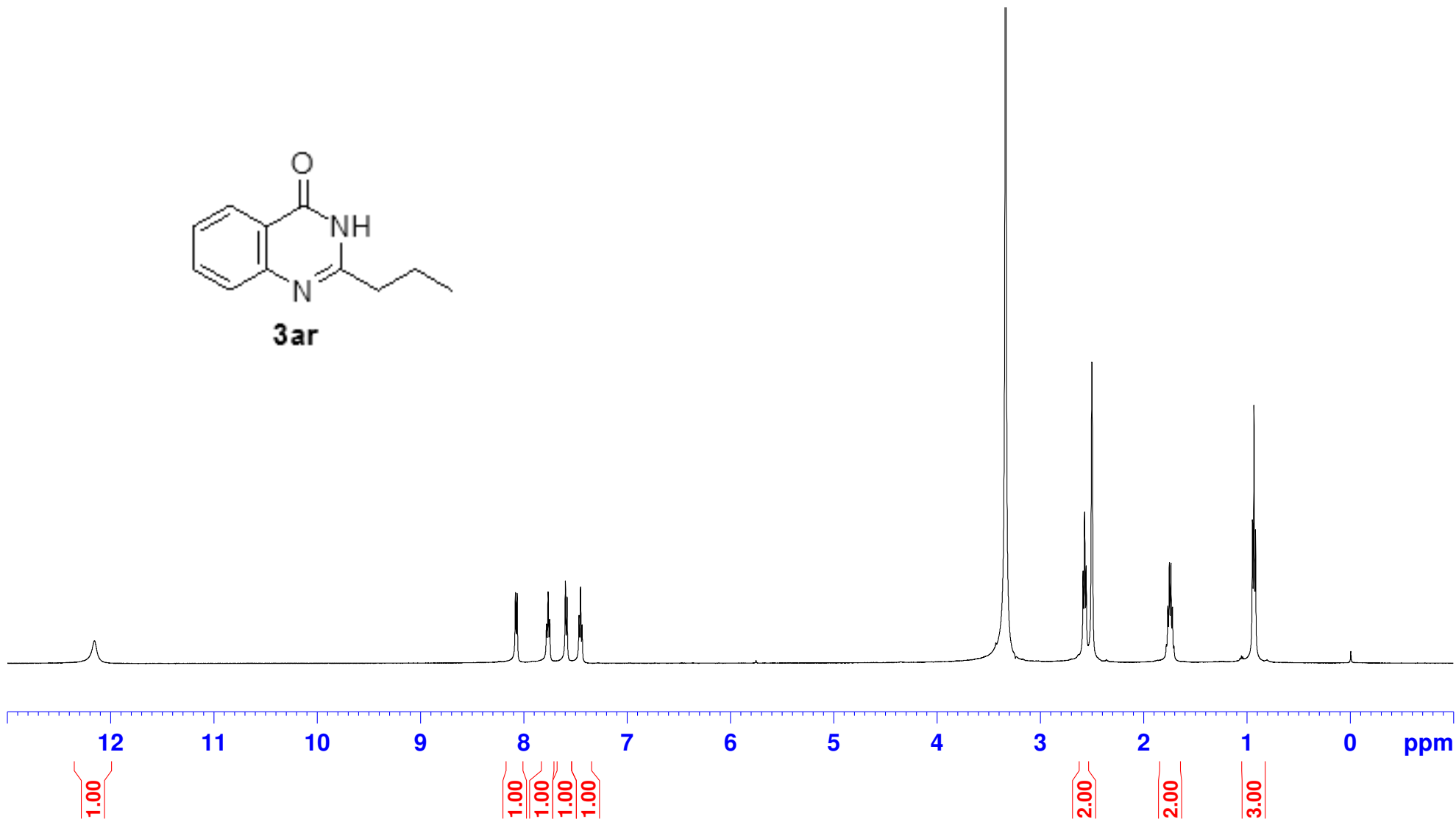
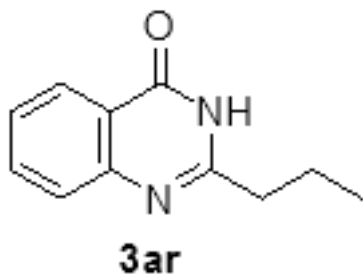


2-propylquinazolin-4(3H)-one  
PROTON DMSO-d6

— 12.157

8.080  
8.065  
7.779  
7.765  
7.750  
7.597  
7.581  
7.465  
7.451  
7.436

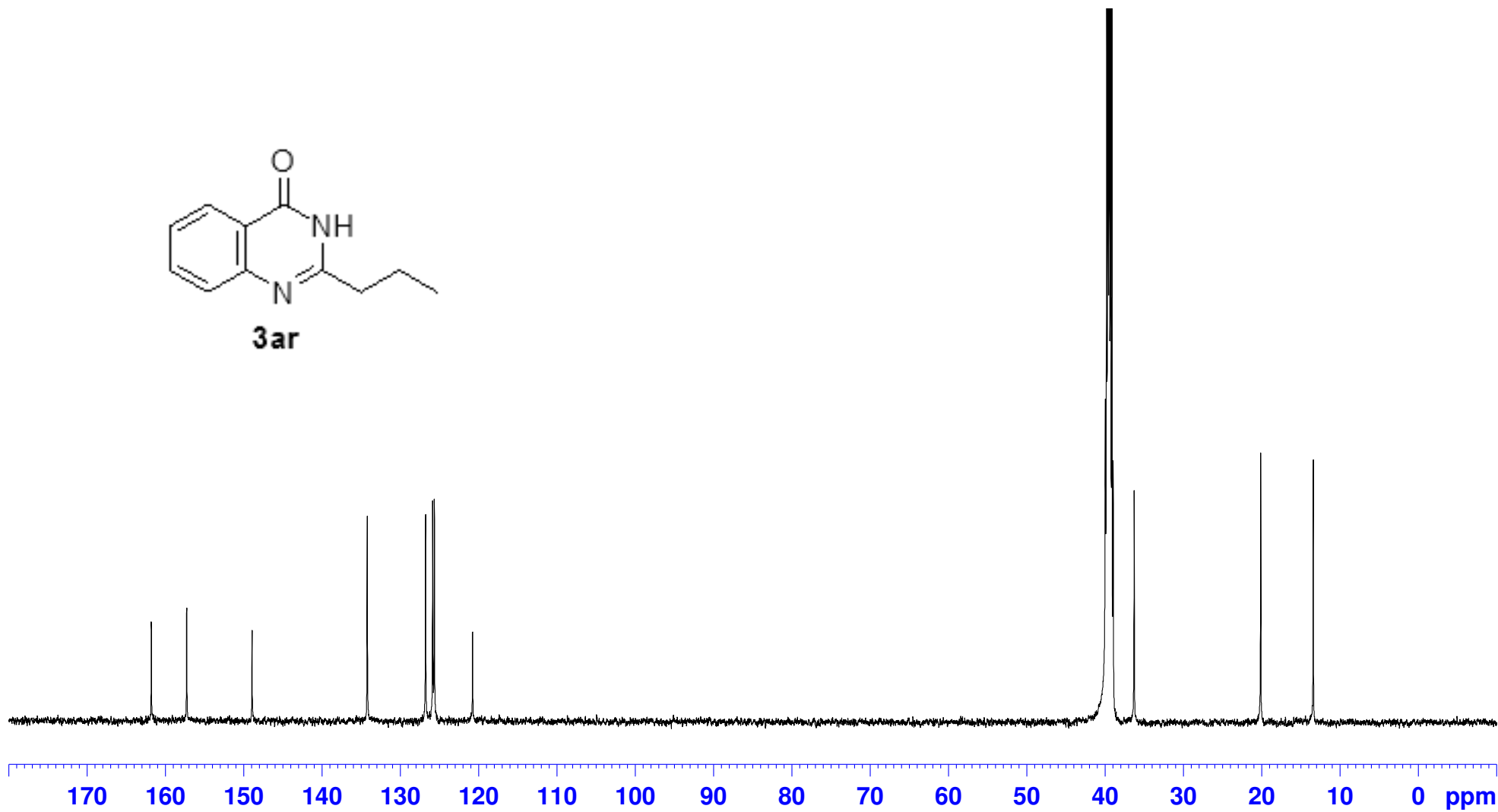
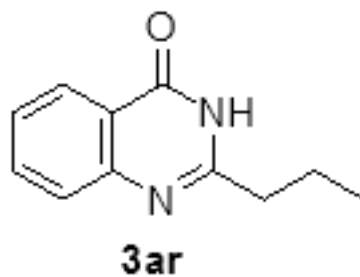
2.586  
2.571  
2.556  
2.500  
1.780  
1.765  
1.750  
1.735  
1.721  
1.706  
0.946  
0.931  
0.917



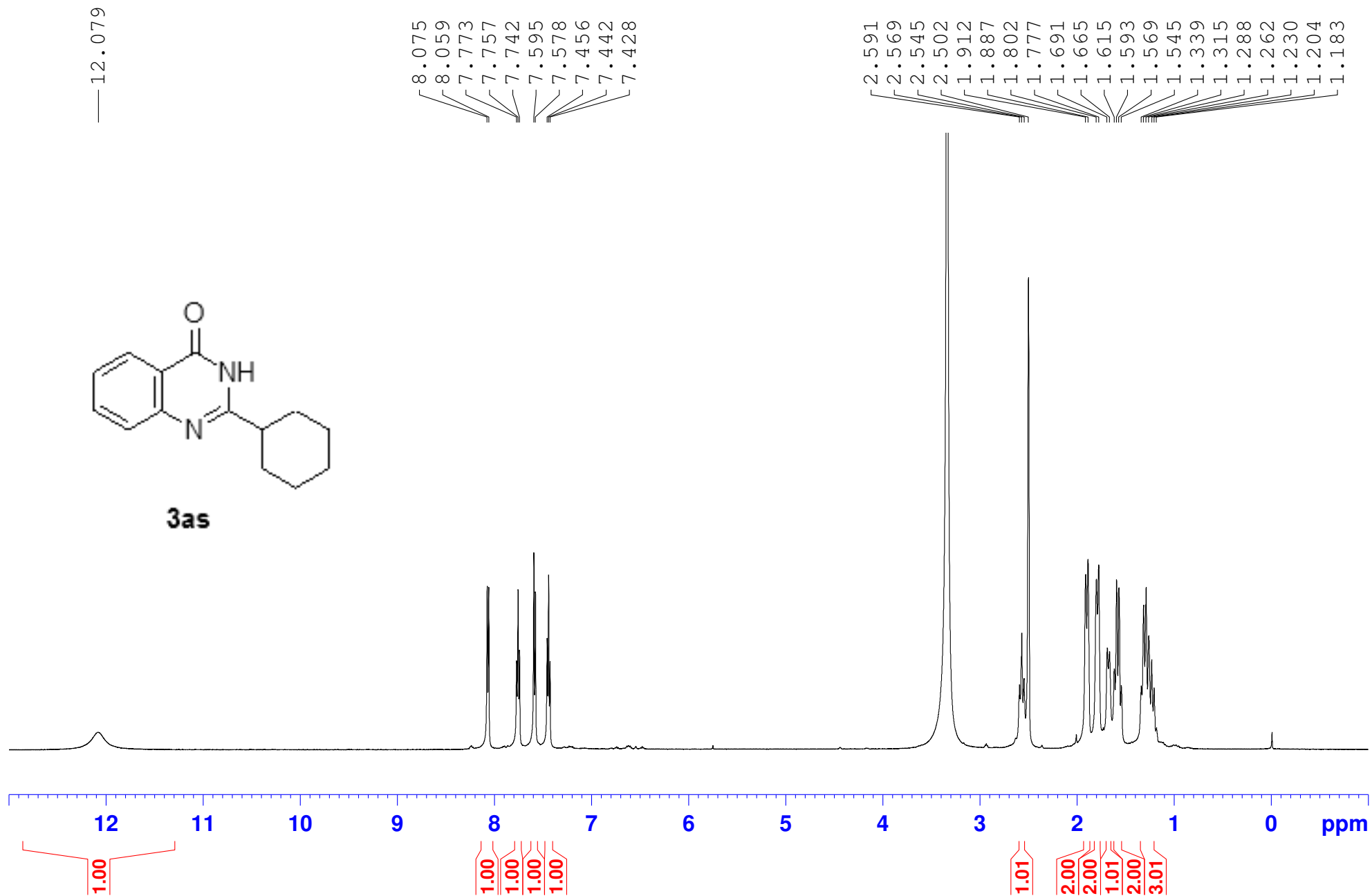
2-propylquinazolin-4(3H)-one  
C13CPD DMSO-d6

— 161.783  
— 157.270  
— 148.919  
— 134.207  
— 126.760  
— 125.858  
— 125.636  
— 120.763

— 39.501  
— 36.318  
— 20.161  
— 13.449



2-cyclohexylquinazolin-4(3H)-one  
PROTON DMSO-d6



2-cyclohexylquinazolin-4(3H)-one  
C13CPD DMSO-d6

161.895  
160.709

148.937

134.162

126.944

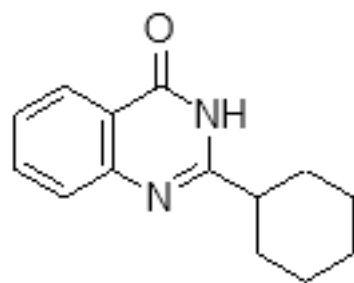
125.843

125.624

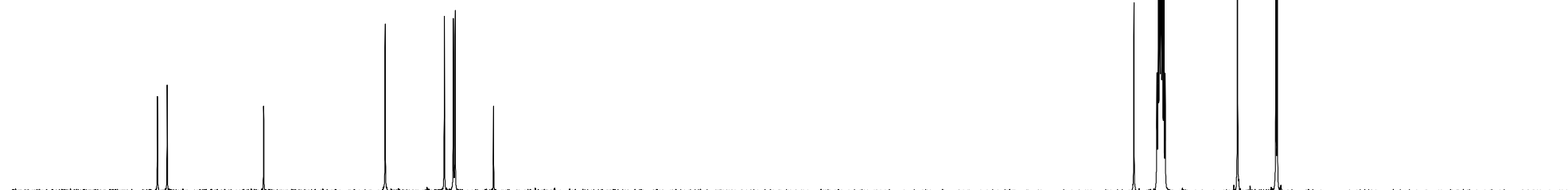
120.941

42.810  
39.500

30.168  
25.482  
25.312

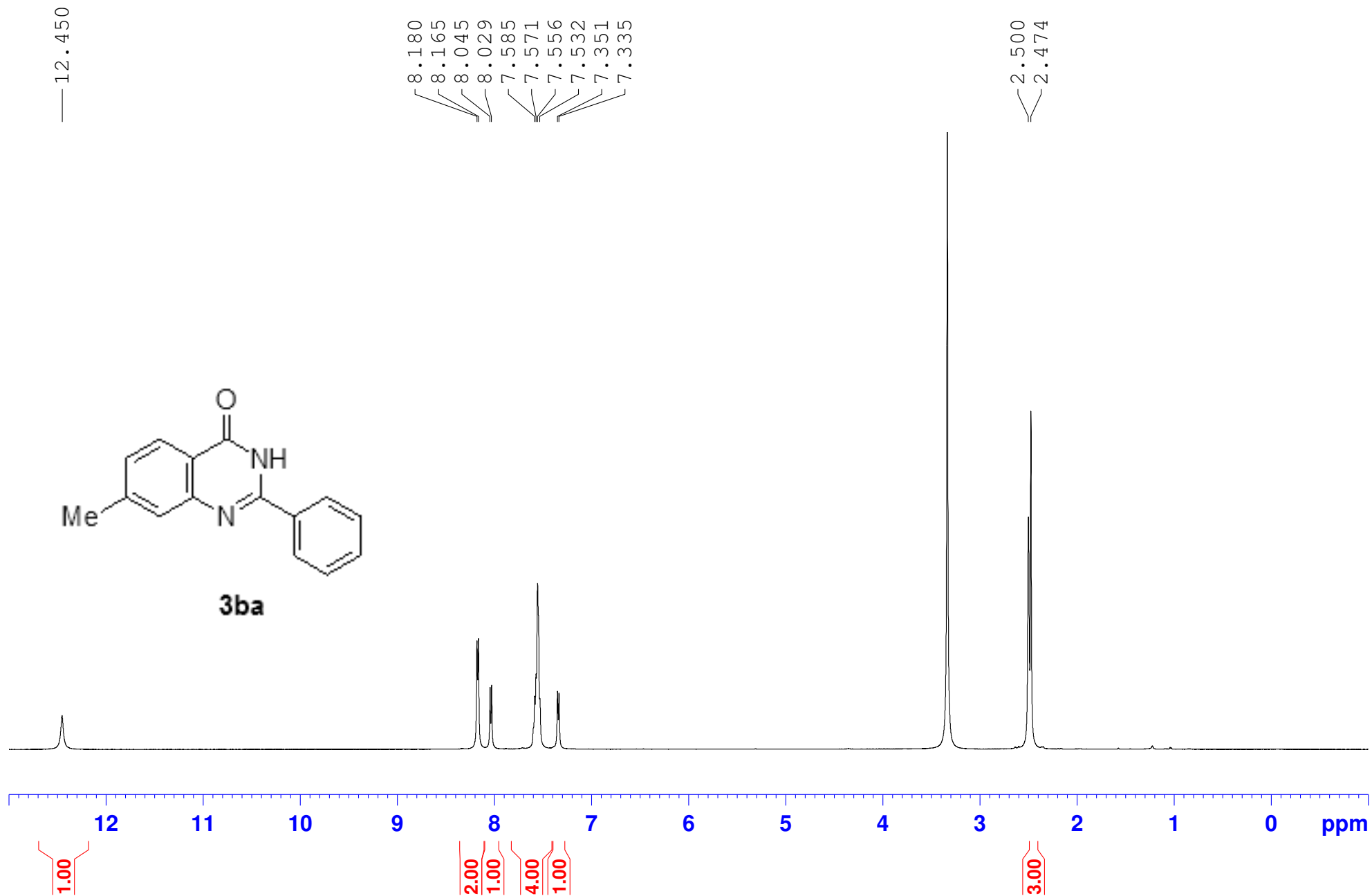


3as



170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

7-methyl-2-phenylquinazolin-4(3H)-one  
PROTON DMSO-d6



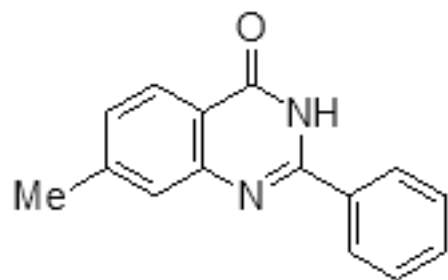


7-methyl-2-phenylquinazolin-4(3H)-one  
C13CPD DMSO-d6

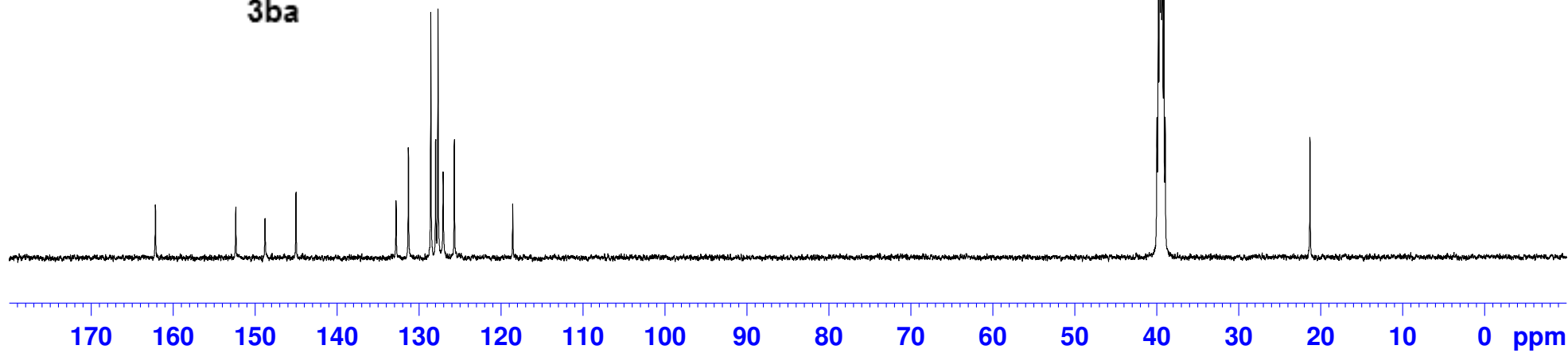
— 162.148  
— 152.340  
— 148.773  
— 144.995  
— 132.783  
— 131.279  
— 128.547  
— 127.954  
— 127.669  
— 127.038  
— 125.677  
— 118.555

— 39.499

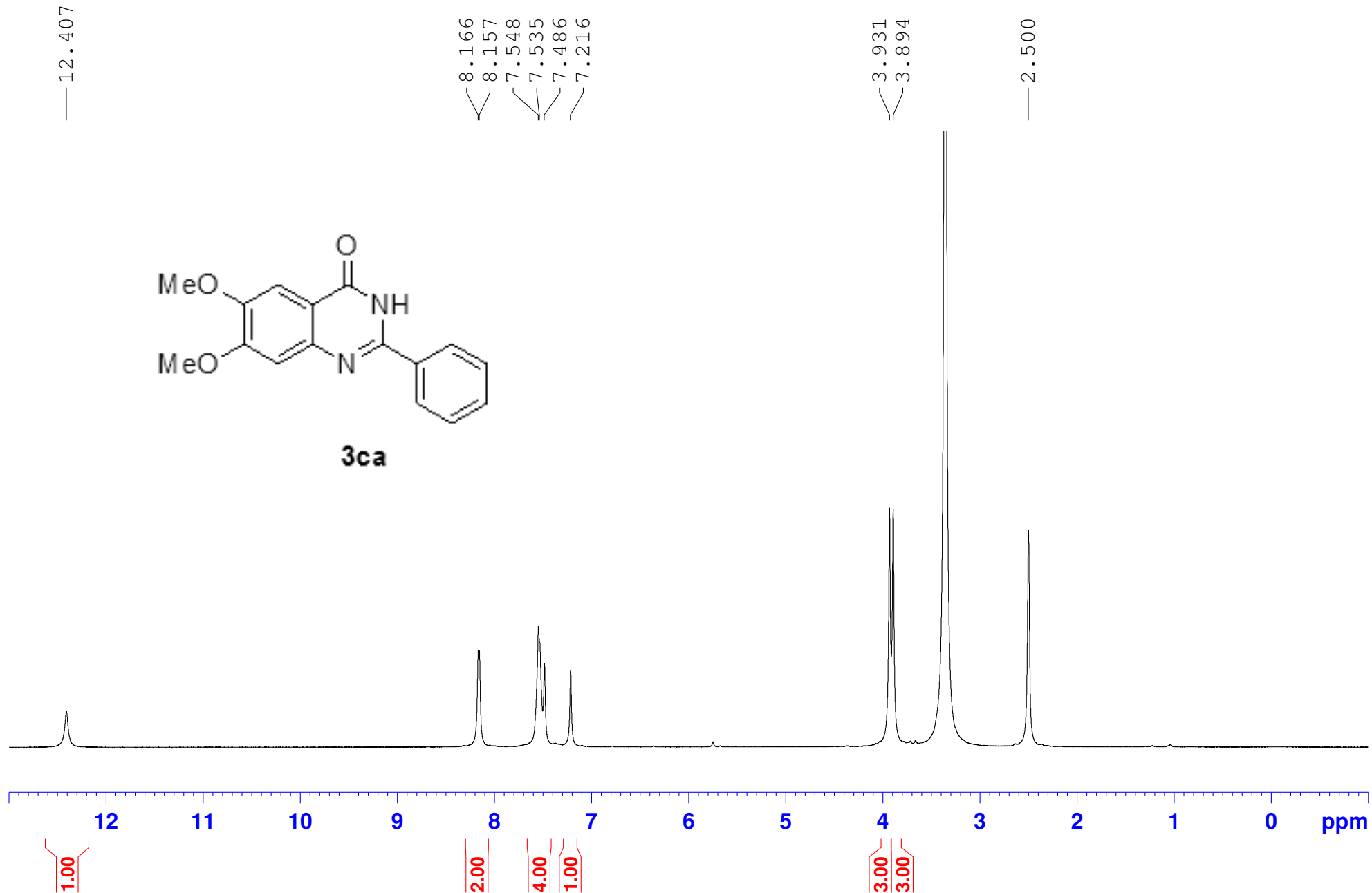
— 21.328



3ba



6,7-dimethoxy-2-phenylquinazolin-4(3H)-one  
PROTON DMSO-d6

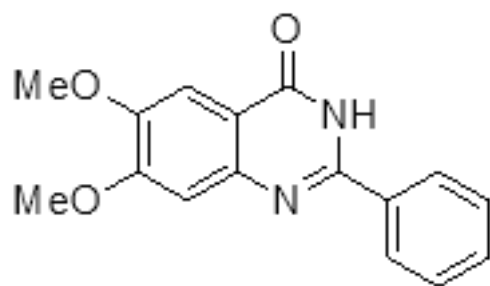


6,7-dimethoxy-2-phenylquinazolin-4(3H)-one  
C13CPD DMSO-d6

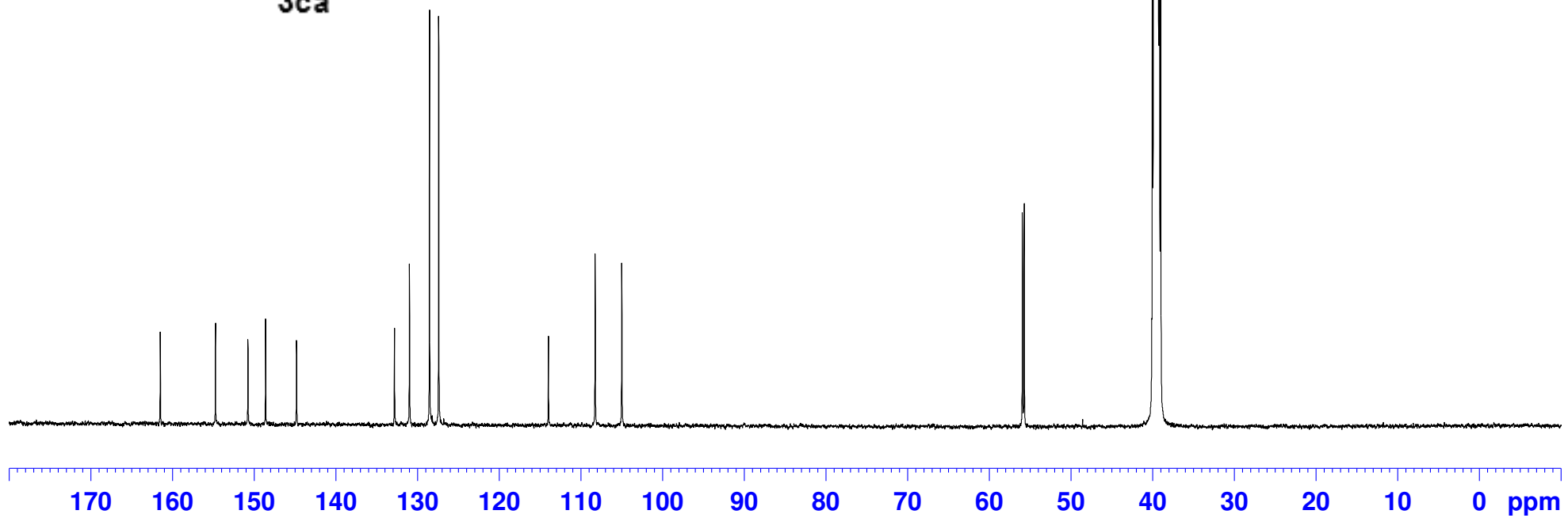
— 161.489  
— 154.731  
— 150.754  
— 148.595  
— 144.796  
  
— 132.805  
— 130.975  
— 128.518  
— 127.390  
  
— 113.957  
— 108.243  
— 104.978

— 55.932  
— 55.707

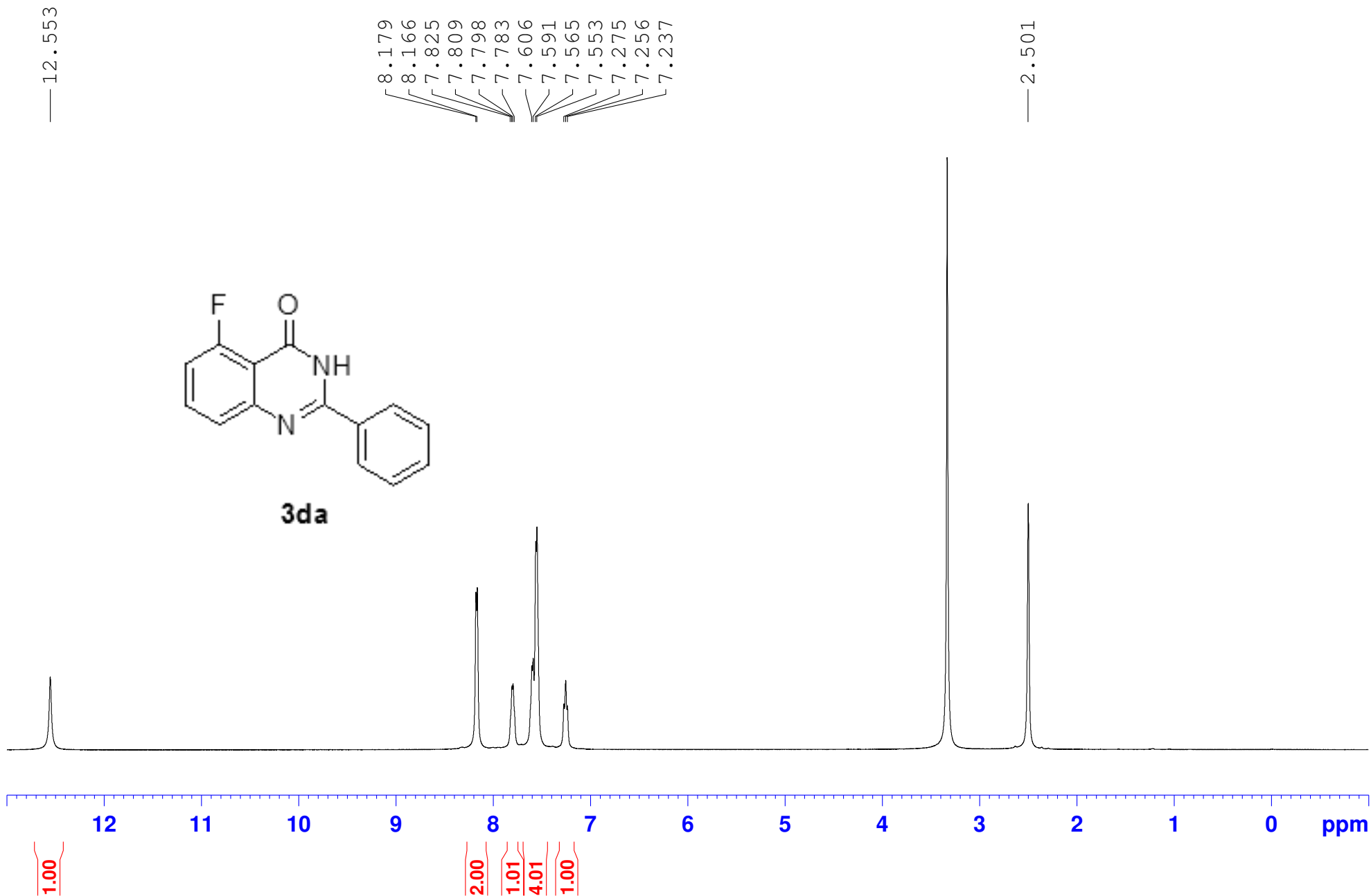
— 39.502



**3ca**

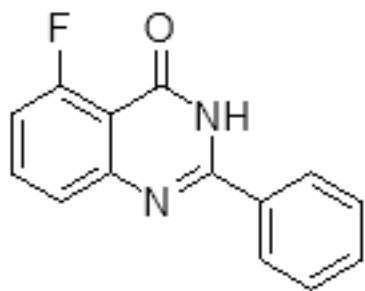


5-fluoro-2-phenylquinazolin-4(3H)-one  
PROTON DMSO-d6

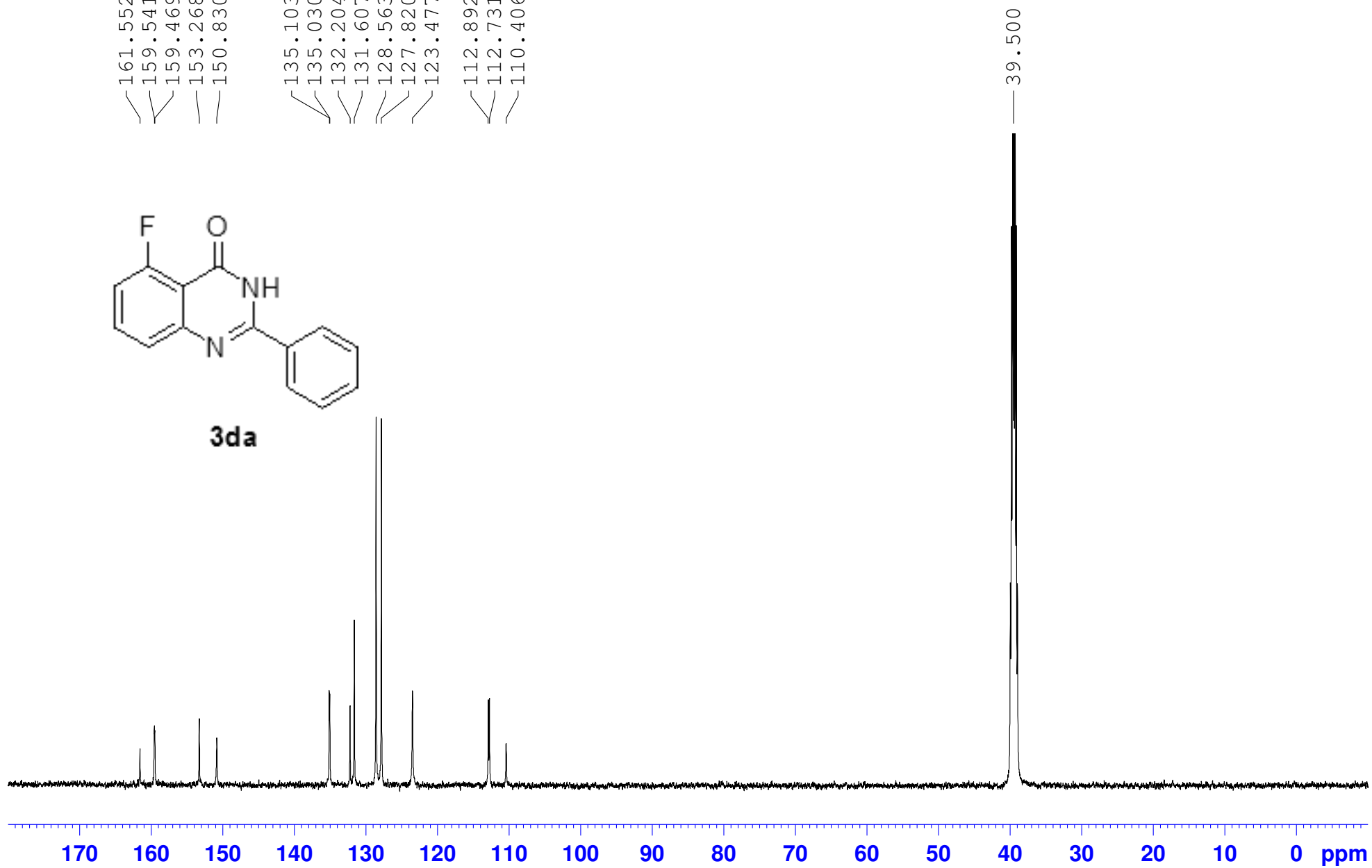


5-fluoro-2-phenylquinazolin-4(3H)-one  
C13CPD DMSO-d6

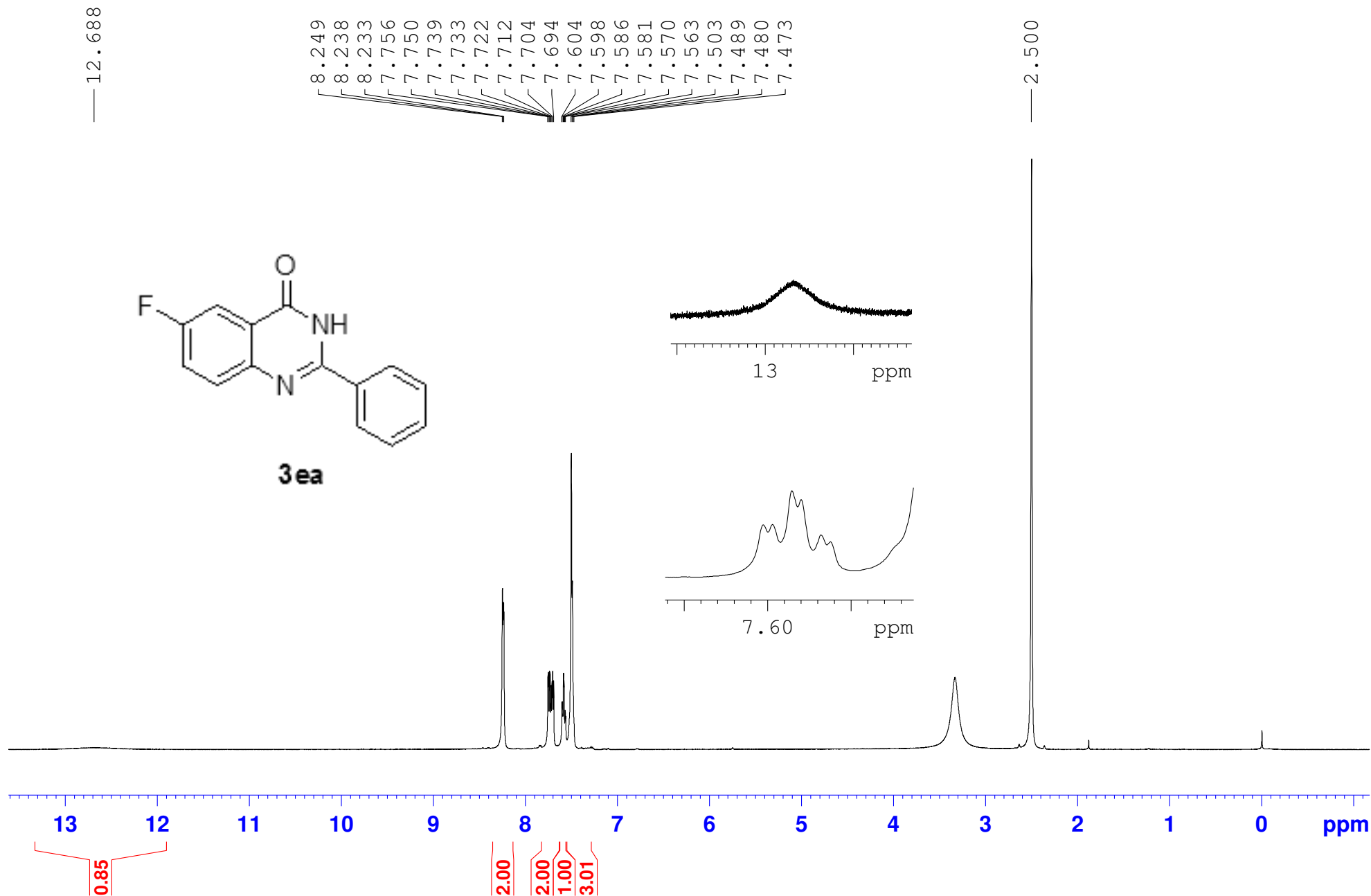
161.552  
159.541  
159.469  
153.268  
150.830  
135.103  
135.030  
132.204  
131.607  
128.563  
127.820  
123.477  
112.892  
112.731  
110.406



3da

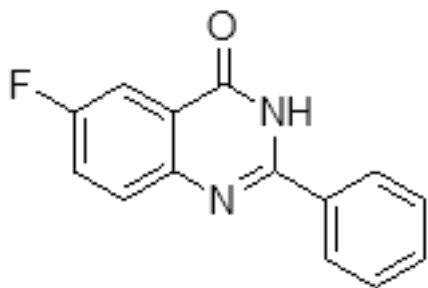


6-fluoro-2-phenylquinazolin-4(3H)-one  
PROTON DMSO-d6

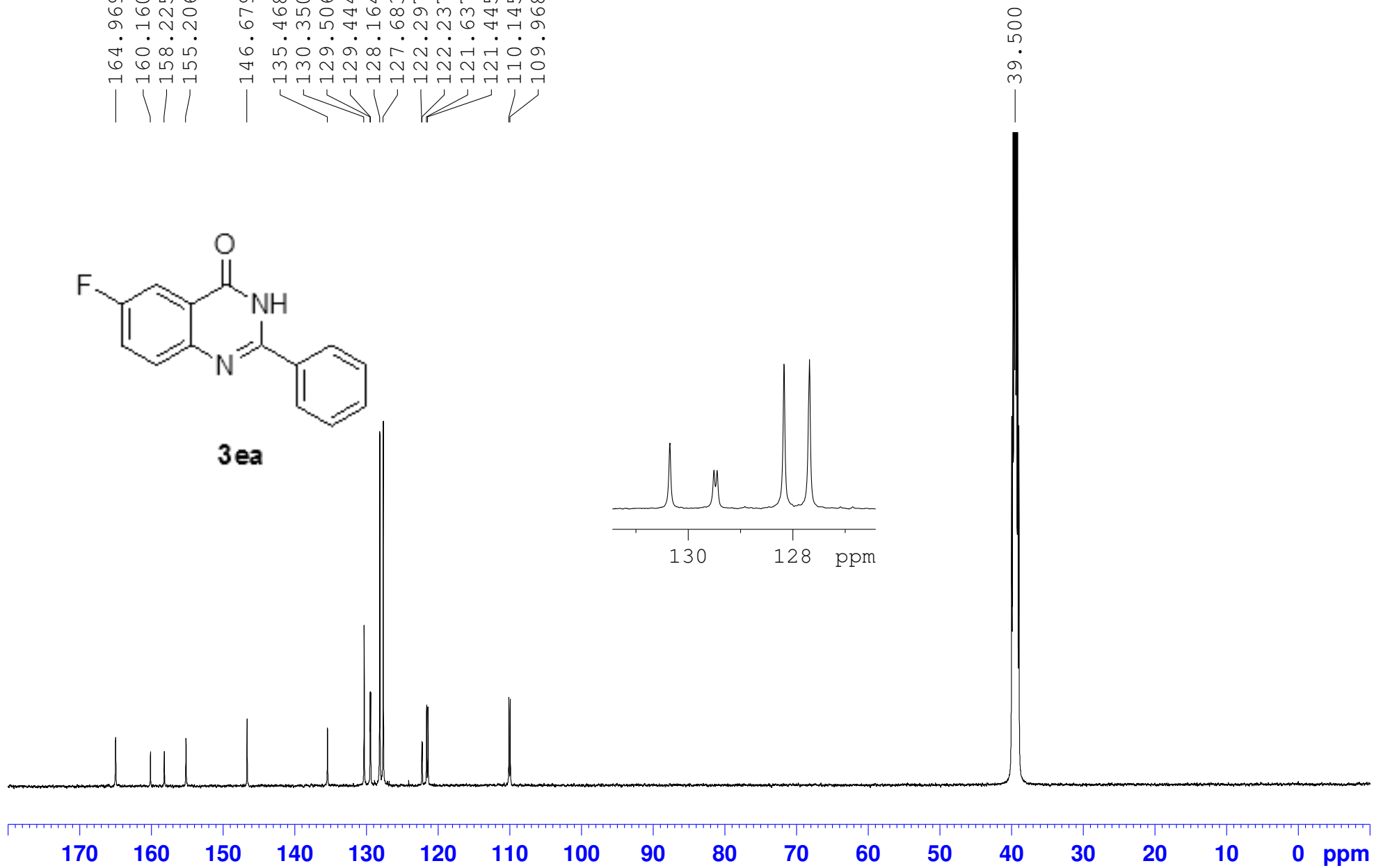


6-fluoro-2-phenylquinazolin-4(3H)-one  
C13CPD DMSO-d6

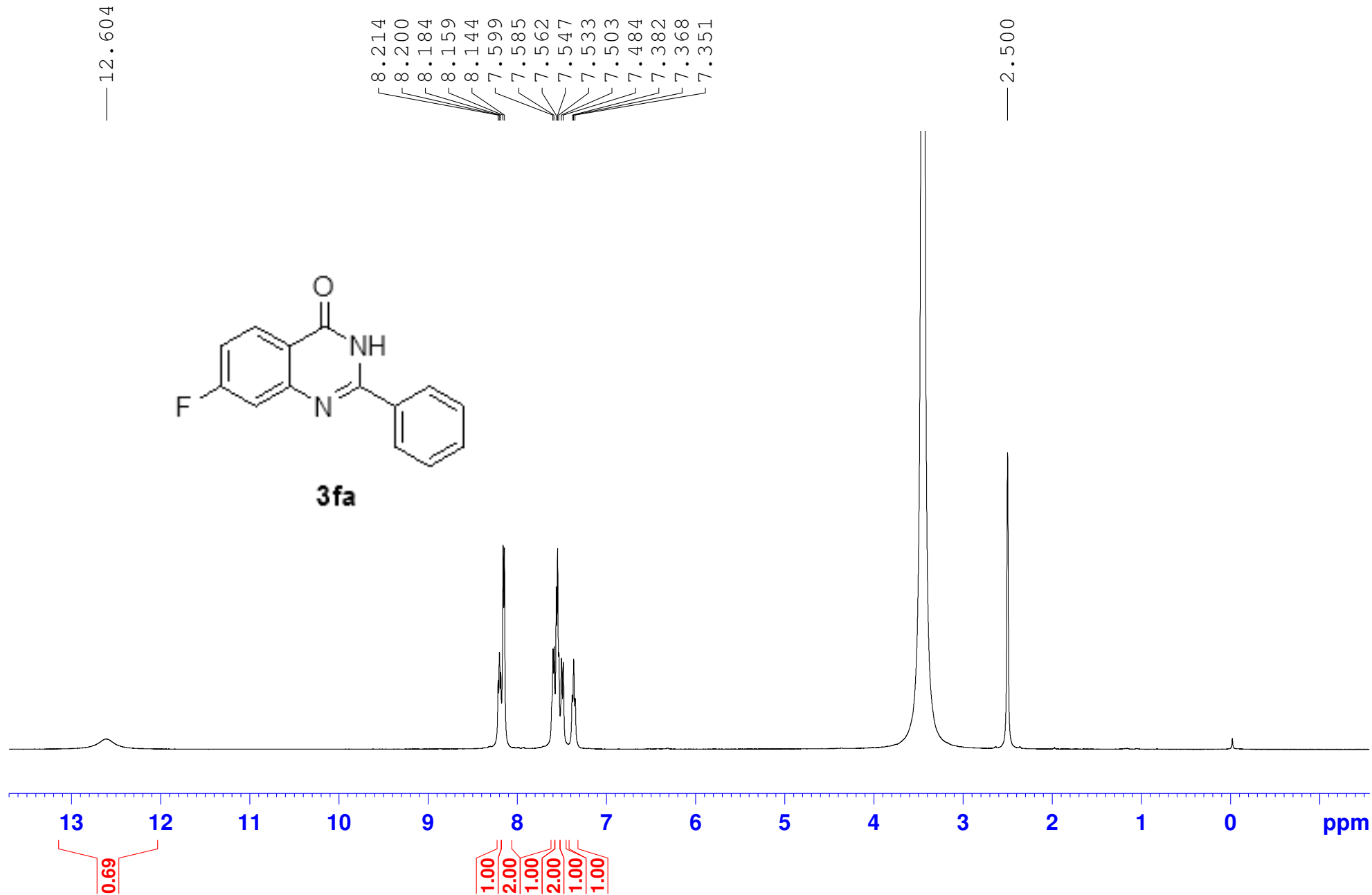
164.969  
160.160  
158.225  
155.206  
146.679  
135.468  
130.350  
129.506  
129.444  
128.164  
127.683  
122.297  
122.237  
121.637  
121.445  
110.145  
109.968



**3ea**



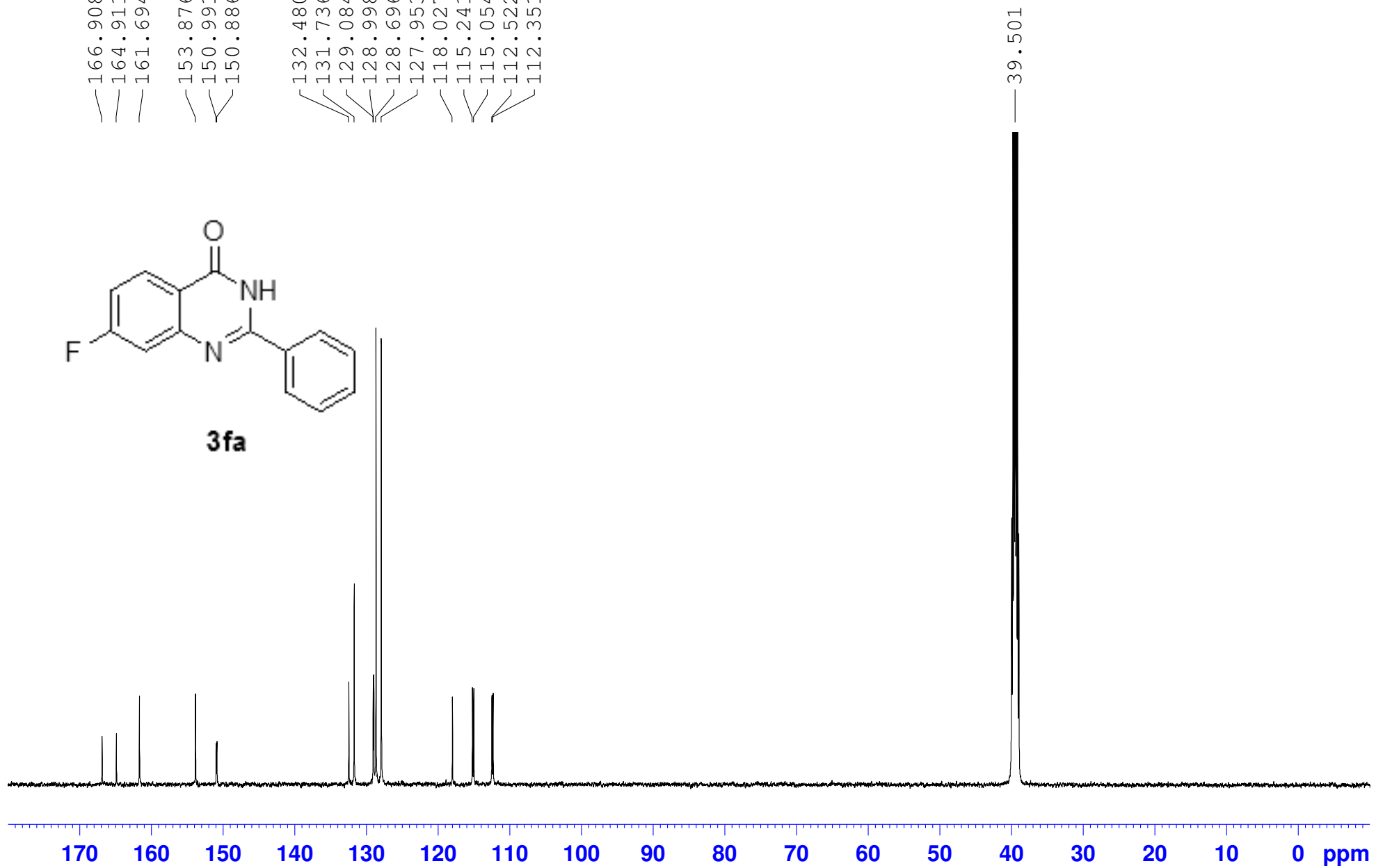
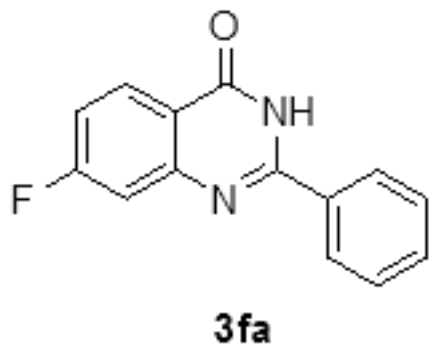
5-bromo-2-phenylquinazolin-4(3H)-one  
PROTON DMSO-d6





7-fluoro-2-phenylquinazolin-4(3H)-one  
C13CPD DMSO-d6

166.908  
164.911  
161.694  
153.876  
150.991  
150.886  
132.480  
131.736  
129.084  
128.998  
128.696  
127.953  
118.027  
115.241  
115.054  
112.522  
112.351

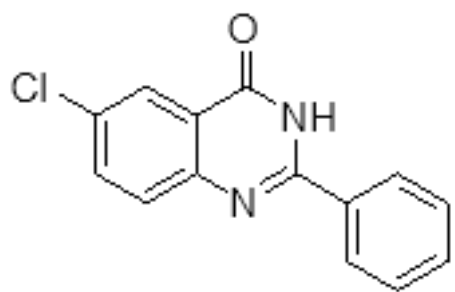


6-chloro-2-phenylquinazolin-4(3H)-one  
PROTON DMSO-d6

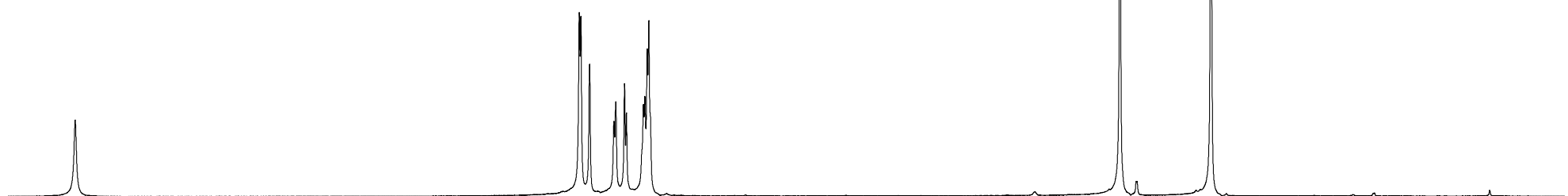
— 12.708

8.180  
8.166  
8.086  
7.868  
7.851  
7.773  
7.755  
7.619  
7.604  
7.590  
7.569  
7.555  
7.540

— 2.501



**3ga**



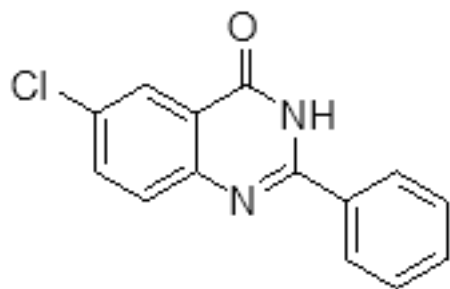
13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

1.00

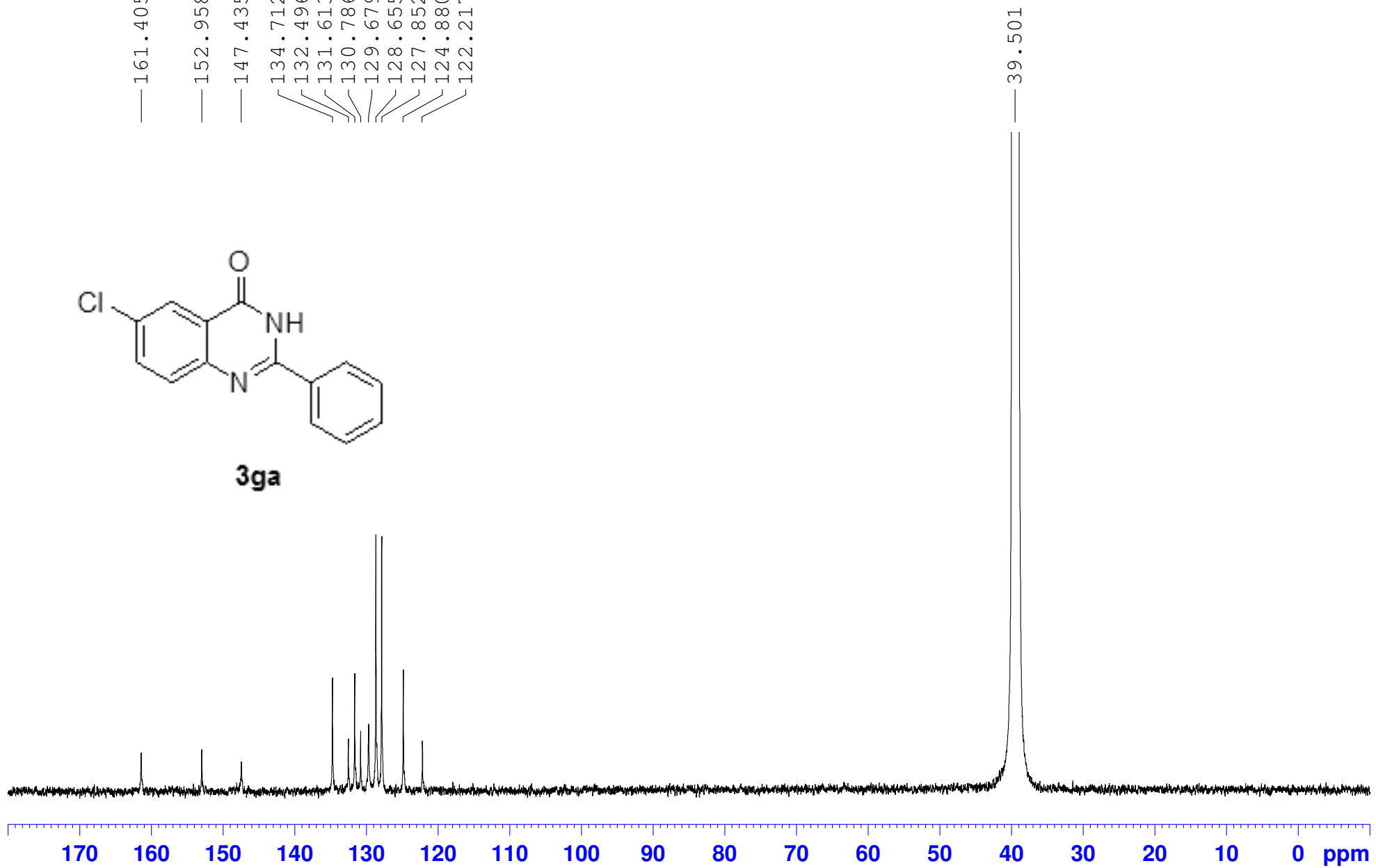
2.00  
1.00  
1.00  
1.00  
3.01

6-chloro-2-phenylquinazolin-4(3H)-one  
C13CPD DMSO-d6

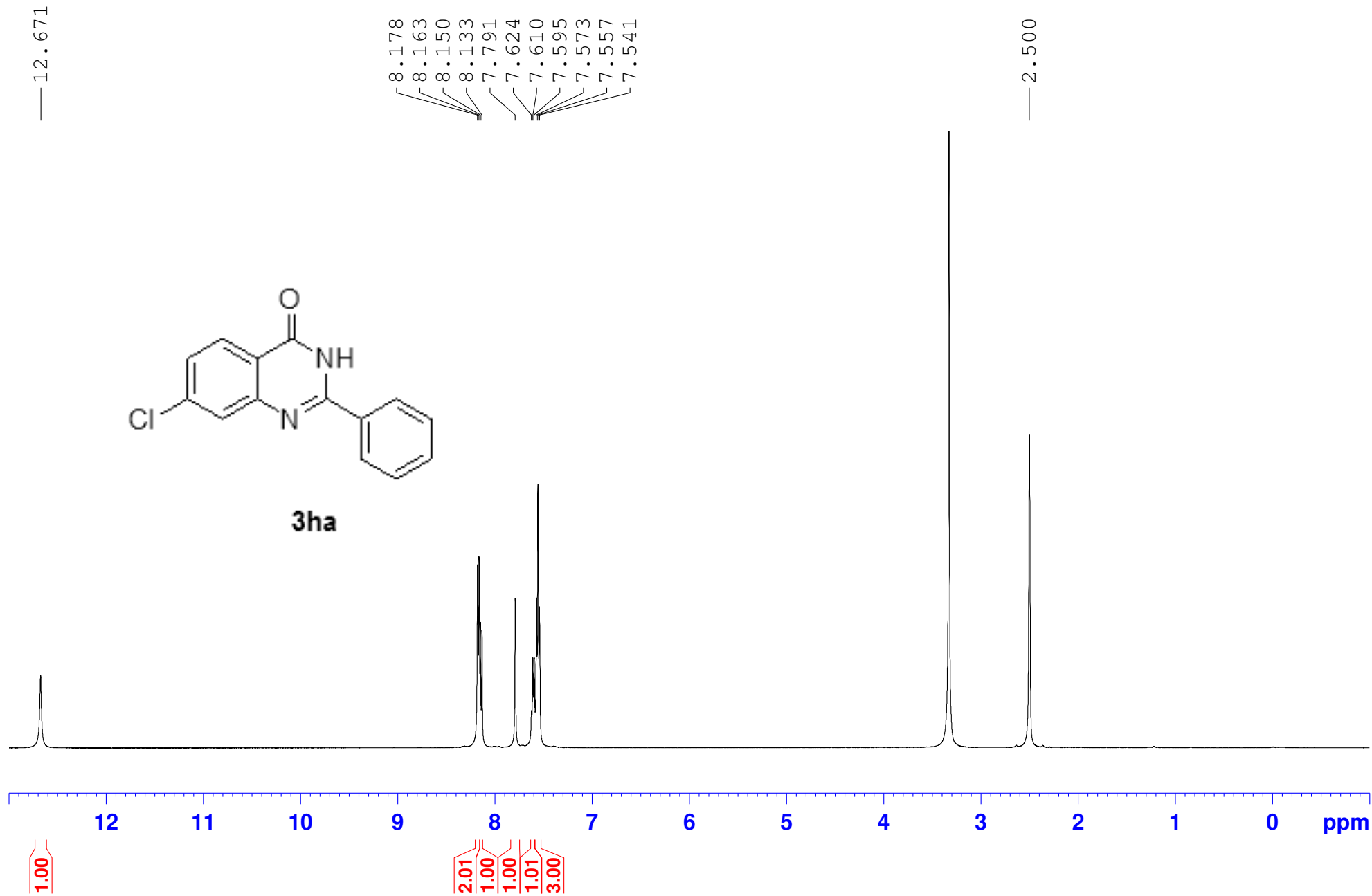
— 161.405  
— 152.958  
— 147.435  
134.712  
132.496  
131.613  
130.786  
129.679  
128.655  
127.852  
124.880  
122.217



3ga

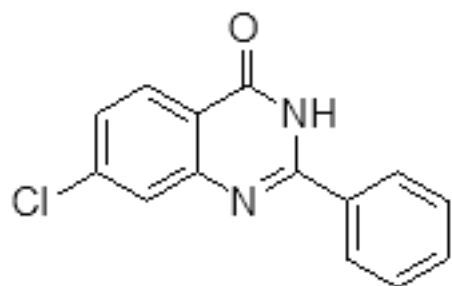


7-chloro-2-phenylquinazolin-4(3H)-one  
PROTON DMSO-d6

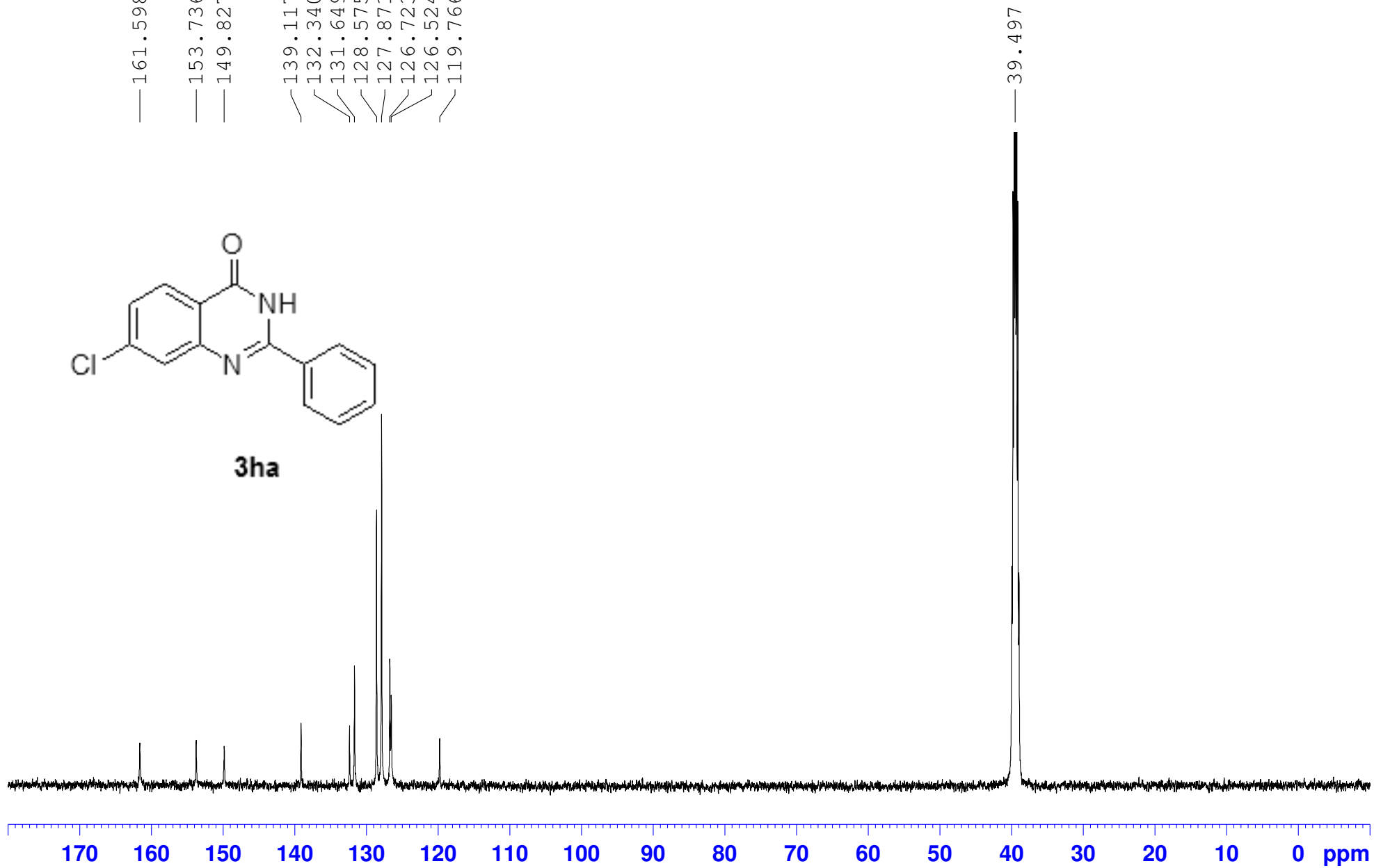


7-chloro-2-phenylquinazolin-4(3H)-one  
C13CPD DMSO-d6

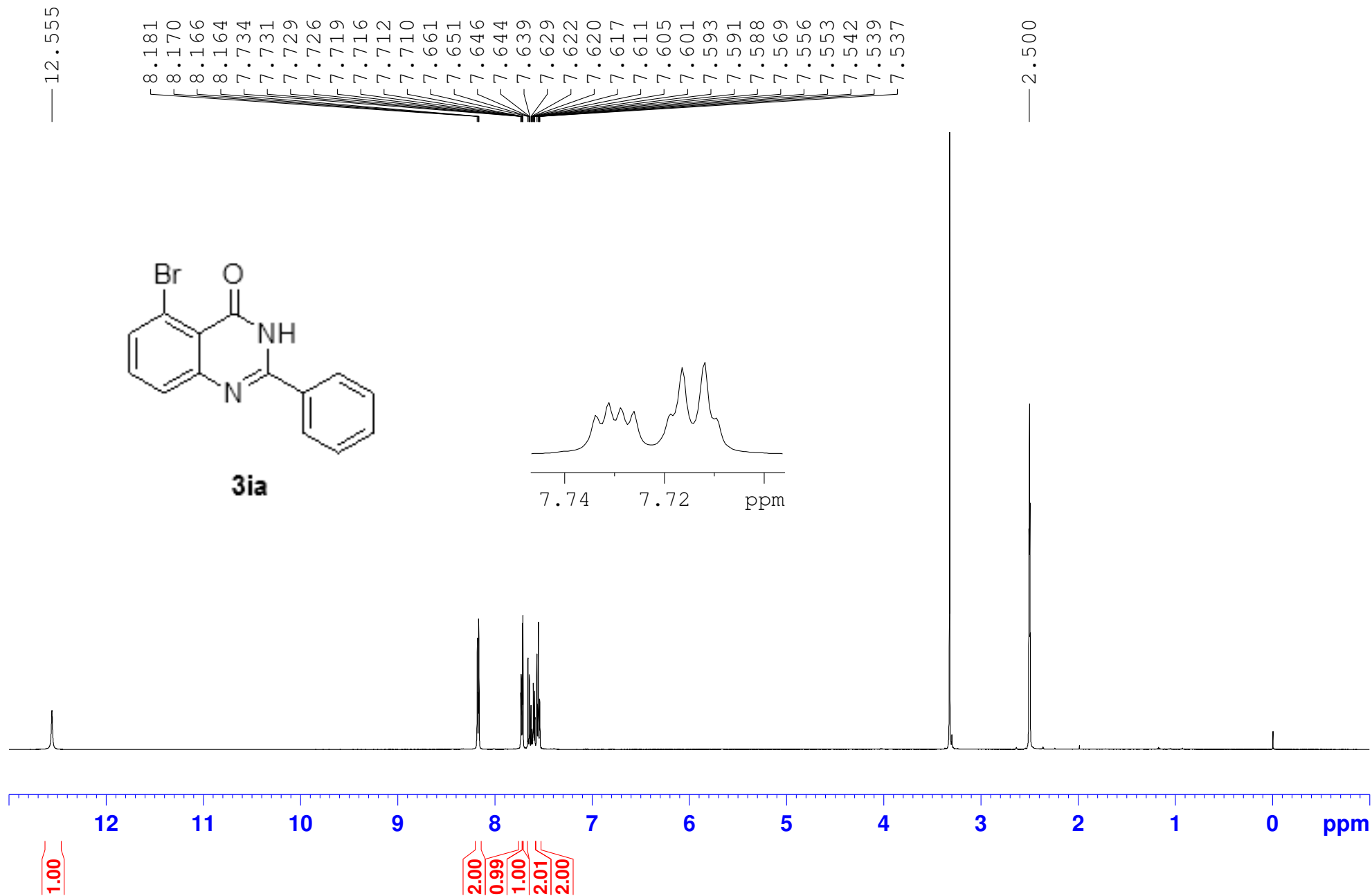
— 161.598  
— 153.736  
— 149.827  
— 139.117  
— 132.340  
— 131.649  
— 128.575  
— 127.871  
— 126.723  
— 126.524  
— 119.766



3ha

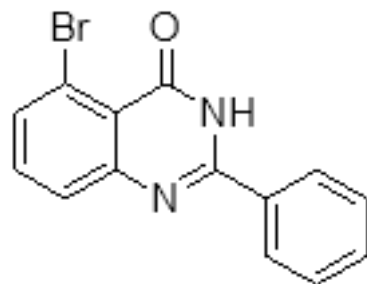


5-bromo-2-phenylquinazolin-4(3H)-one  
PROTON DMSO-d6

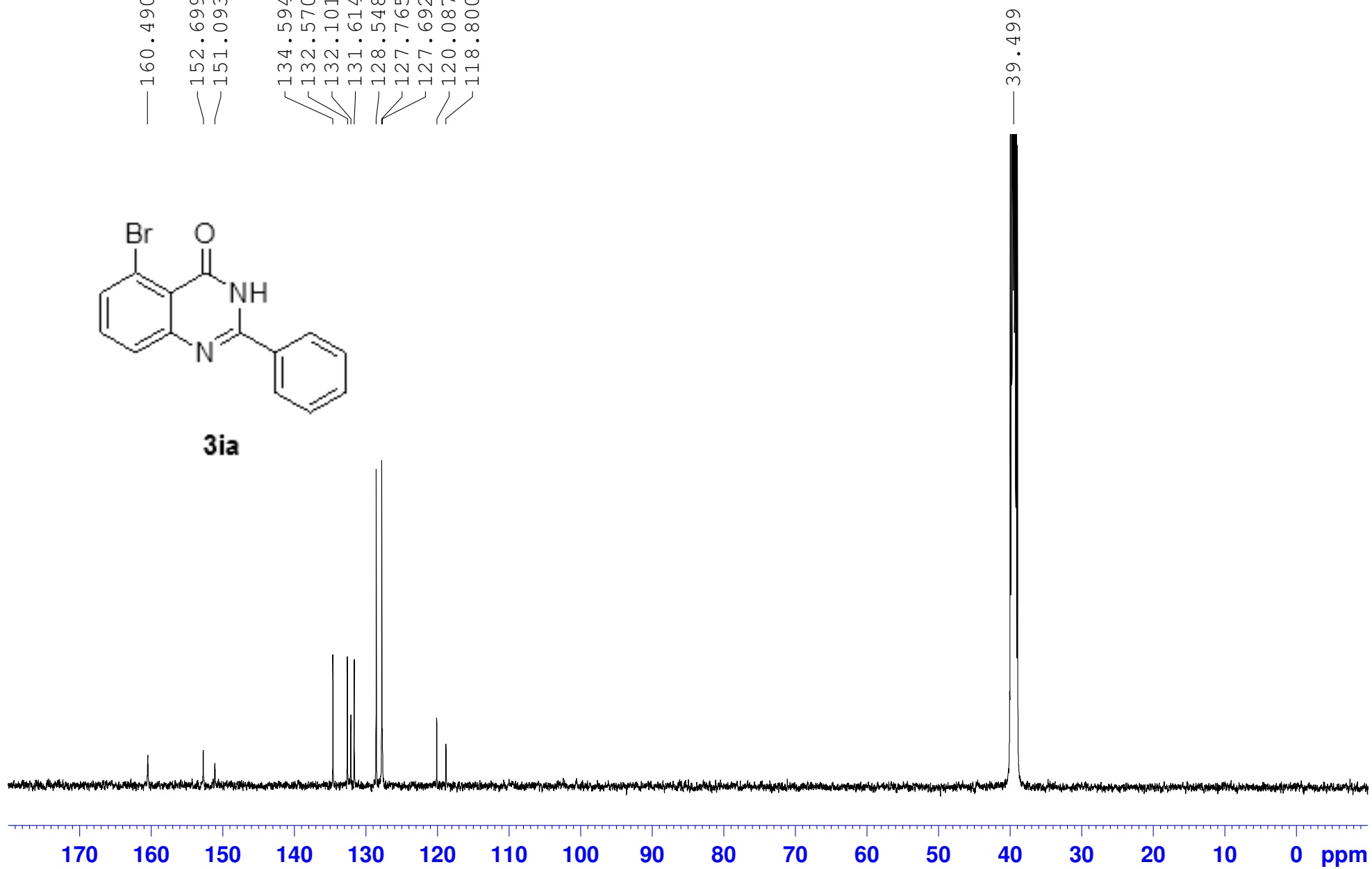


5-bromo-2-phenylquinazolin-4(3H)-one  
C13CPD DMSO-d6

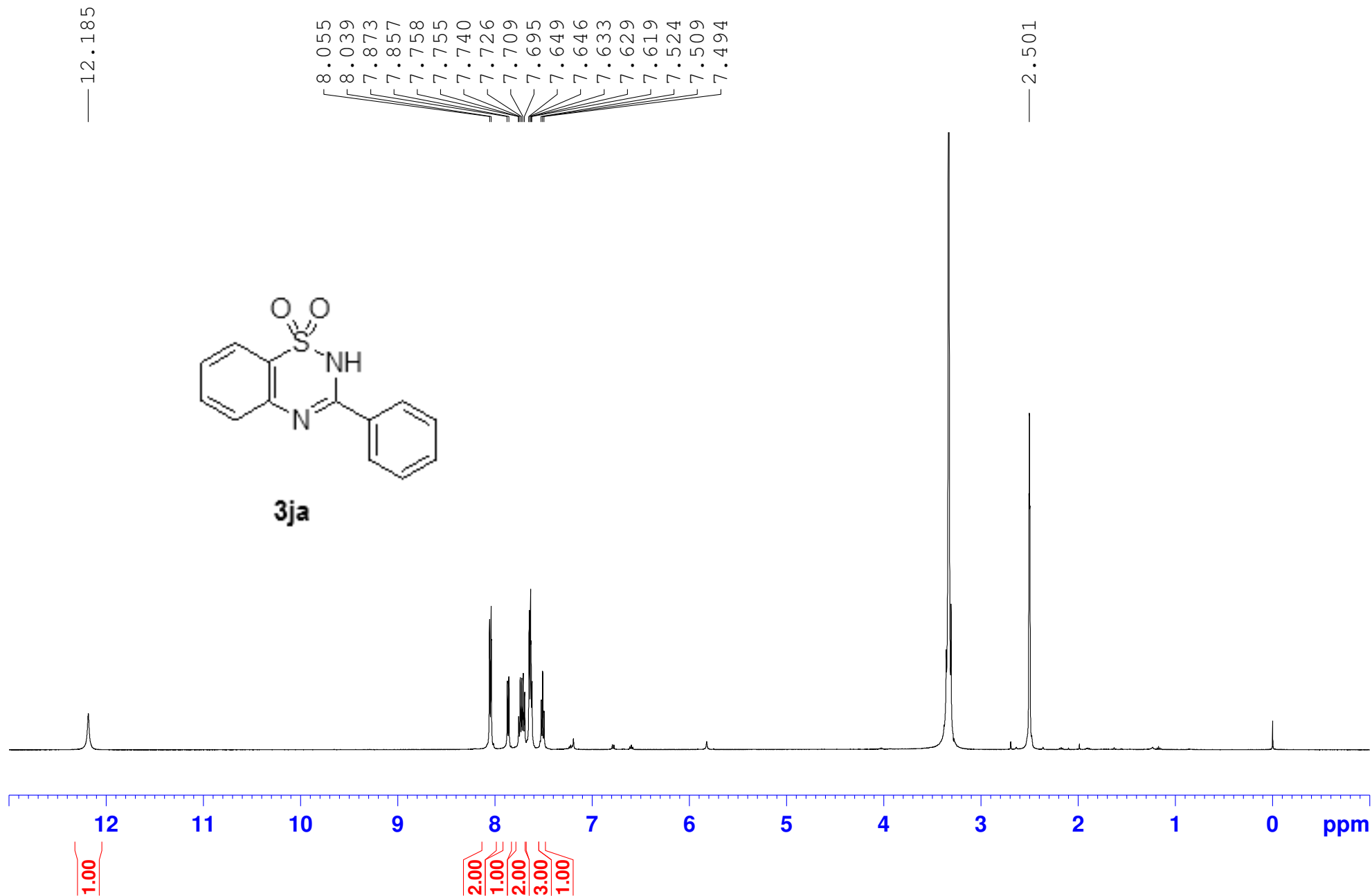
160.490  
152.699  
151.093  
134.594  
132.570  
132.101  
131.614  
128.548  
127.765  
127.692  
120.087  
118.800



3ia



3-Phenyl-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide  
PROTON DMSO-d6

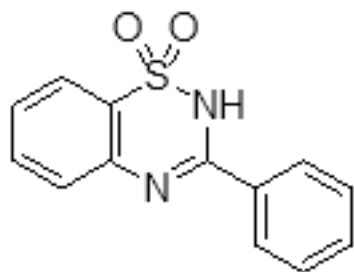




3-Phenyl-2H-benzo[e][1,2,4]thiadiazine 1,1-dioxide  
C13CPD DMSO-d6

— 154.788

135.467  
133.089  
132.797  
131.810  
128.828  
128.206  
126.687  
123.293  
121.466  
118.422



**3ja**

— 39.501

