

## A simple organic N-O $\sigma$ bond heterolysis of 3,6-dihydro-1,2-oxazines

Gilles Galvani,<sup>a</sup> Géraldine Calvet,<sup>a</sup> Nicolas Blanchard,<sup>b\*</sup> and Cyrille Kouklovsky<sup>a\*</sup>

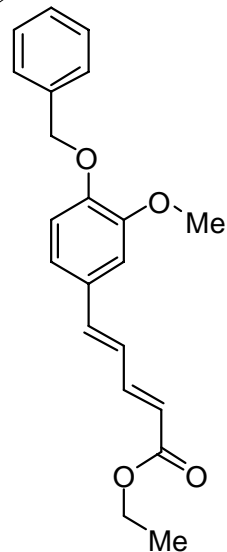
*Laboratoire de Procédés et Substances Naturelles, Institut de Chimie Moléculaire et des matériaux d'ORSAY, ICMMO - UMR 8182-Bâtiment 410 Université Paris-Sud XI  
15 rue Georges Clémenceau 91405 Orsay Cedex, France and Laboratoire de Chimie Organique, ENSCMu – UMR 7015, 3 rue A. Werner 68093 Mulhouse Cedex France*

*Nicolas.blanchard@uha.fr; cykouklo@icmo.u-psud.fr*

Copies of <sup>1</sup> H and <sup>13</sup> C NMR spectra of compound 22	2
Copies of <sup>1</sup> H and <sup>13</sup> C NMR spectra of compound 23	4
Copies of <sup>1</sup> H and <sup>13</sup> C NMR spectra of compound 24	6
Copies of <sup>1</sup> H and <sup>13</sup> C NMR spectra of compound 15	8
Copies of <sup>1</sup> H and <sup>13</sup> C NMR spectra of compound 26	10
Copies of <sup>1</sup> H and <sup>13</sup> C NMR spectra of compound 27	12
Copies of <sup>1</sup> H and <sup>13</sup> C NMR spectra of compound 28	14
Copies of <sup>1</sup> H and <sup>13</sup> C NMR spectra of compound 17	16
Copies of <sup>1</sup> H and <sup>13</sup> C NMR spectra of compound 18	18
Copy of <sup>1</sup> H spectra of compound 30	20
Copies of <sup>1</sup> H and <sup>13</sup> C NMR spectra of compound 31	21
Copies of <sup>1</sup> H and <sup>13</sup> C NMR spectra of compound 32	23
Copies of <sup>1</sup> H and <sup>13</sup> C NMR spectra of compound 19	25
Copies of <sup>1</sup> H and <sup>13</sup> C NMR spectra of compound 20	27

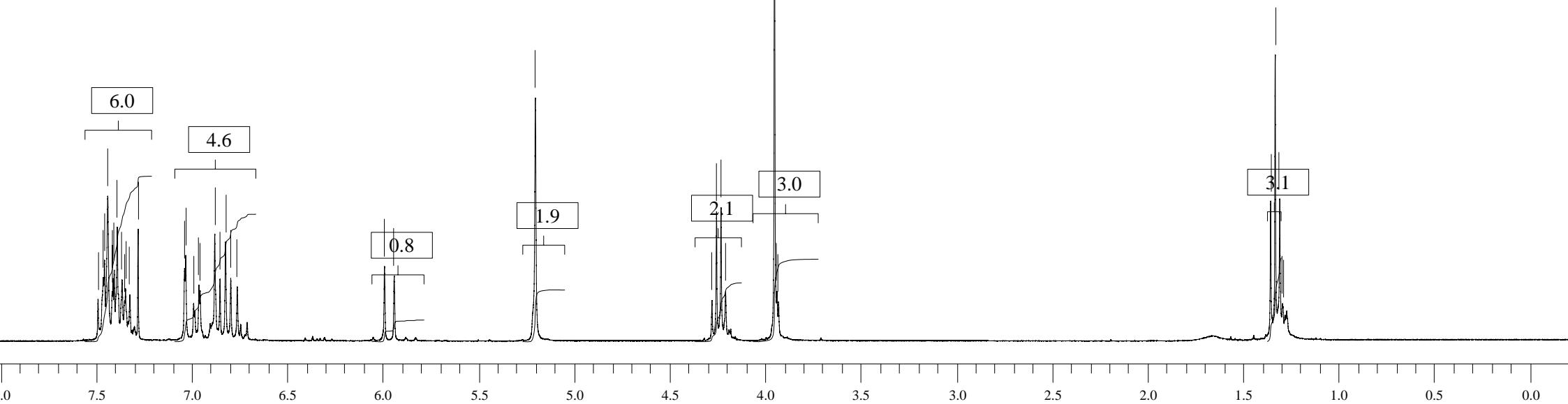
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7.461  
7.455  
7.438  
7.415  
7.410  
7.404  
7.388  
7.363  
7.350  
7.345  
7.322  
7.278  
7.036  
7.030  
6.988  
6.961  
6.954  
6.878  
6.851  
6.822  
6.795  
6.761  
5.990  
5.939  
5.201  
4.277  
4.253  
4.230  
4.206  
3.950  
3.937  
3.929

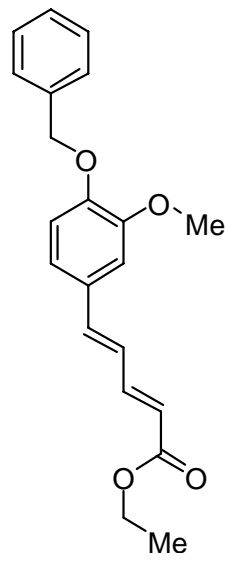
1.355  
1.331  
1.308  
1.294  
1.291



300 MHz, CDCl<sub>3</sub>

Chemical Formula: C<sub>21</sub>H<sub>22</sub>O<sub>4</sub>  
Molecular Weight: 338,40





167.196

149.682

149.146

144.810

140.259

136.666

129.467

128.581

127.928

127.161

124.428

120.976

120.202

113.543

109.540

77.420

76.987

76.576

70.820

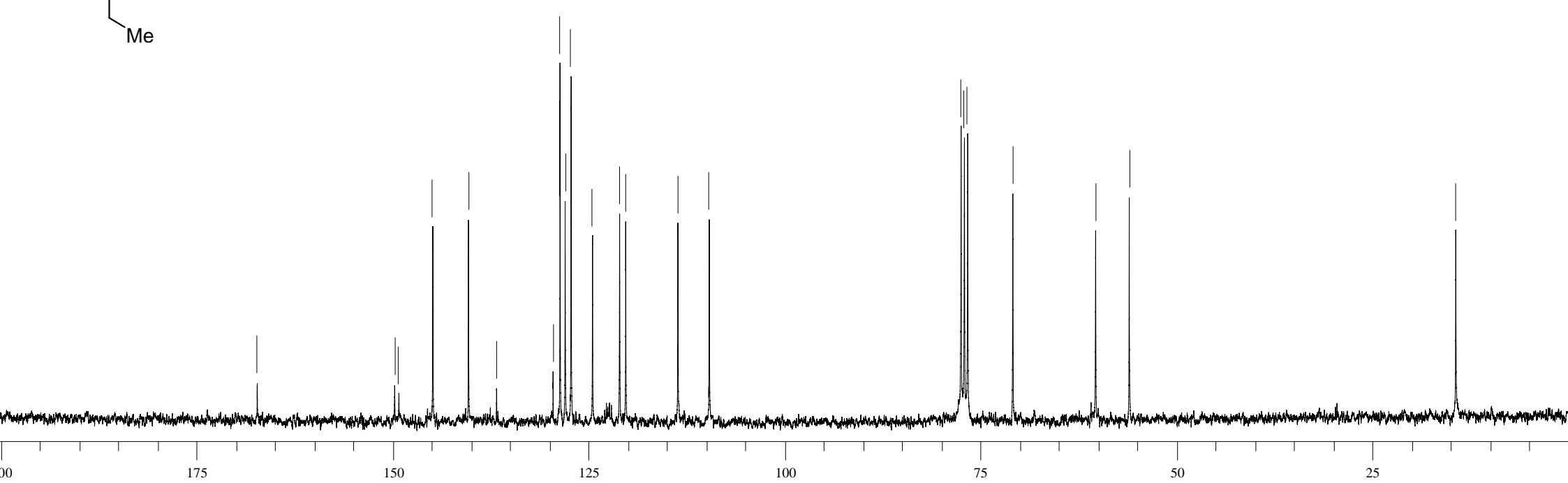
60.253

55.970

14.313

75 MHz, CDCl<sub>3</sub>

Chemical Formula: C<sub>21</sub>H<sub>22</sub>O<sub>4</sub>  
Molecular Weight: 338,40



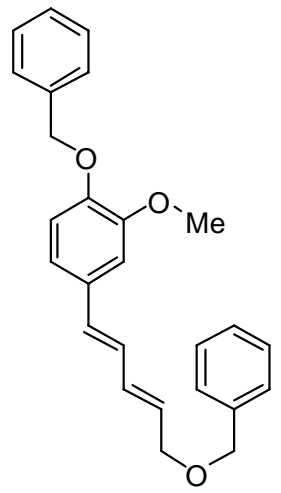
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7.384  
7.000  
6.995  
6.861  
6.536  
6.484

5.944  
5.893

5.189

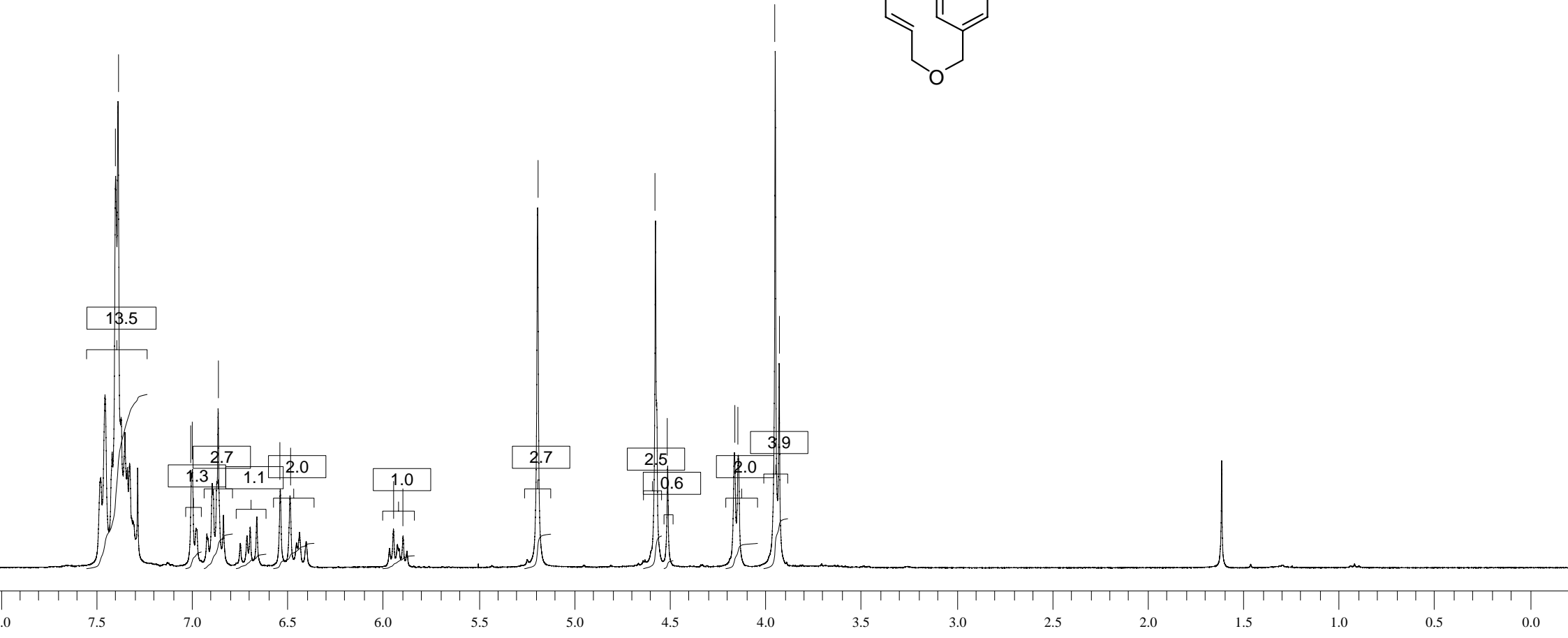
4.573  
4.509

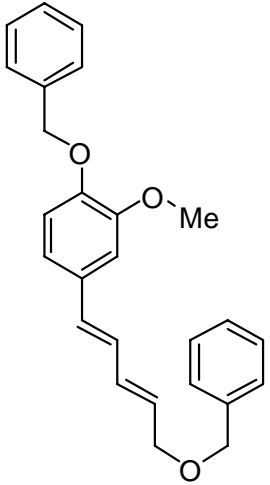
4.160  
4.140  
3.947  
3.926



300 MHz, CDCl<sub>3</sub>

Chemical Formula: C<sub>26</sub>H<sub>26</sub>O<sub>3</sub>  
Molecular Weight: 386,48

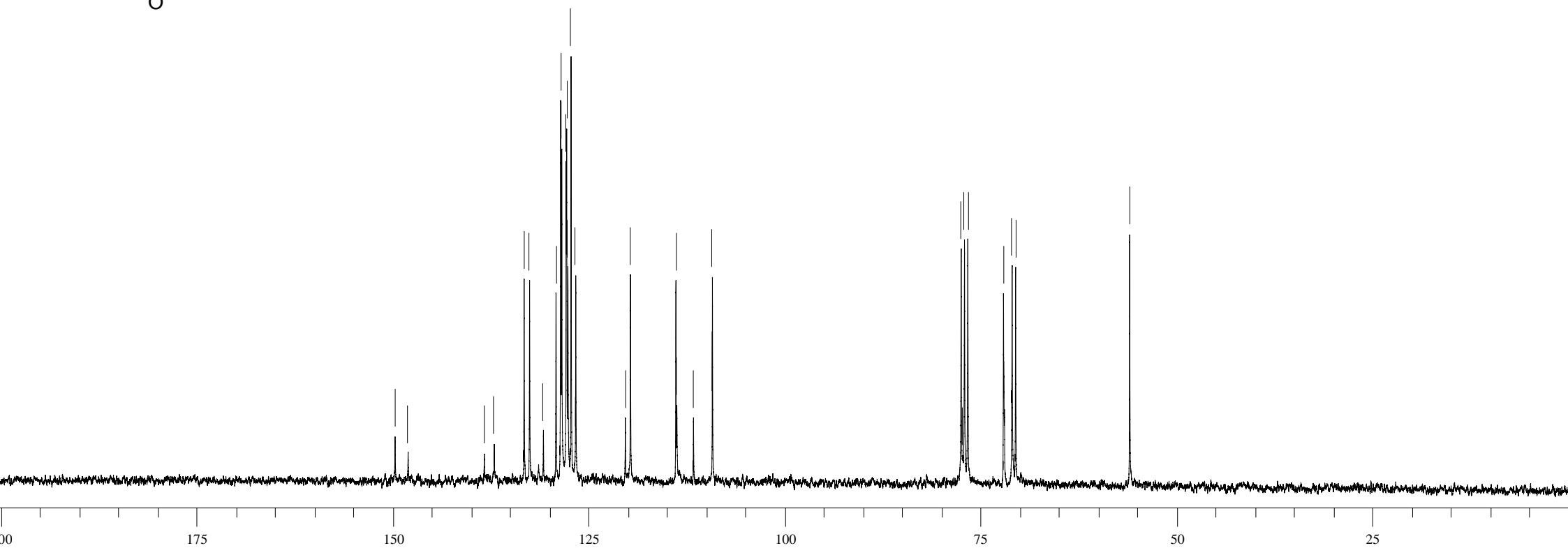




75 MHz, CDCl<sub>3</sub>

Chemical Formula: C<sub>26</sub>H<sub>26</sub>O<sub>3</sub>  
Molecular Weight: 386,48

- 149.631
- 147.957
- 138.238
- 136.966
- 133.163
- 132.467
- 130.697
- 129.100
- 128.504
- 128.357
- 127.805
- 127.740
- 127.579
- 127.174
- 126.572
- 120.256
- 119.599
- 113.798
- 113.681
- 111.548
- 109.140
- 77.404
- 77.192
- 76.989
- 76.563
- 72.008
- 71.890
- 70.895
- 70.455
- 55.898



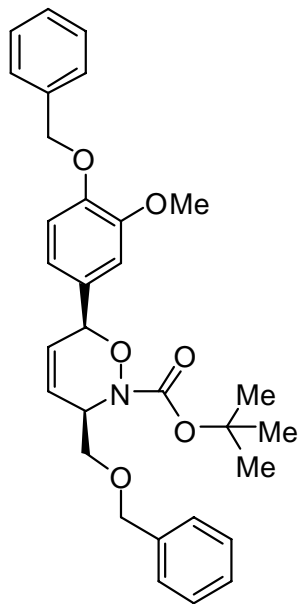
7.440  
7.387  
7.371  
7.363  
7.351  
6.871

6.096  
6.089  
6.081  
6.074  
6.022  
5.988  
5.498  
5.186

4.675  
4.635  
4.616  
4.575

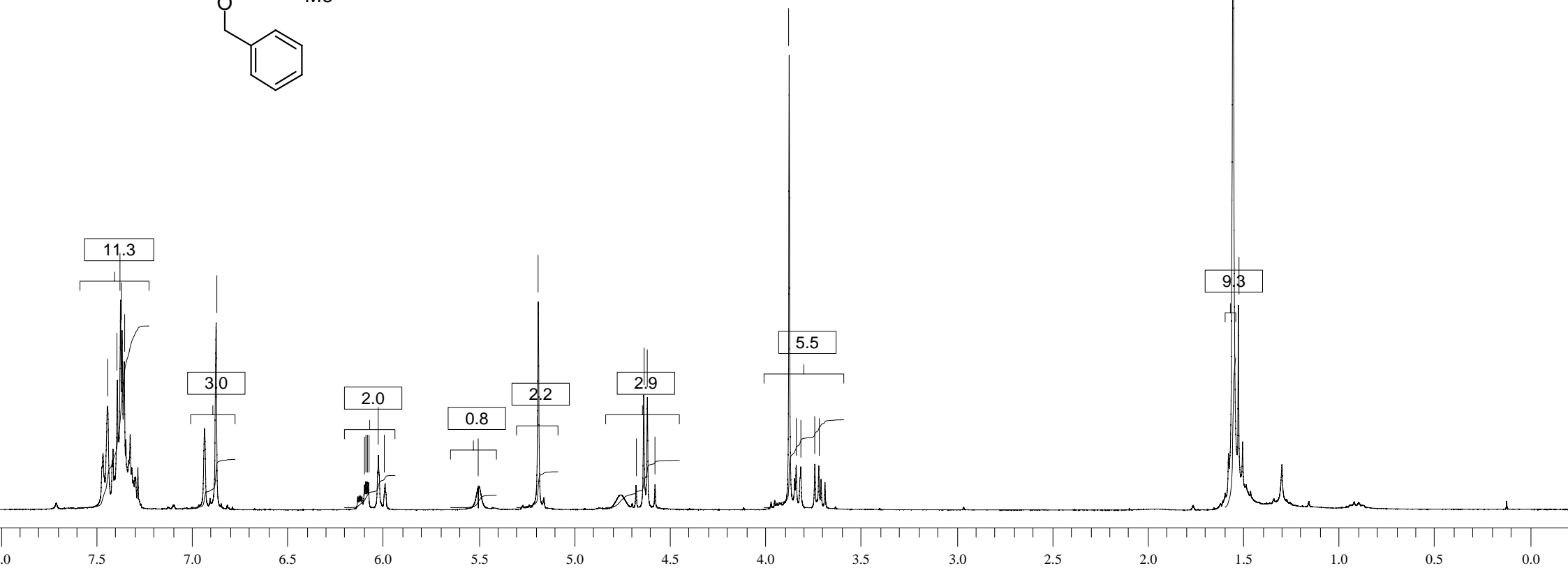
3.874  
3.837  
3.813  
3.740  
3.719

1.552  
1.524



300 MHz, CDCl<sub>3</sub>

Chemical Formula: C<sub>31</sub>H<sub>35</sub>NO<sub>6</sub>  
Molecular Weight: 517,61

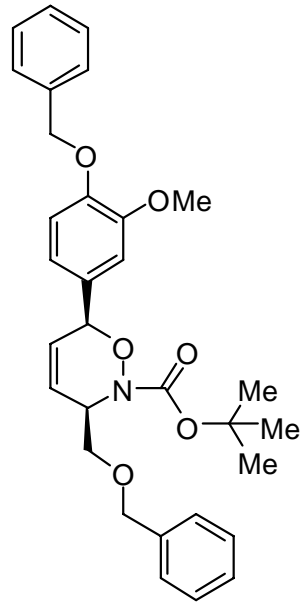


154.386  
149.453  
148.544  
138.024  
136.819  
129.868  
128.824  
128.437  
128.221  
127.725  
127.483  
127.039  
124.669  
120.751  
113.506  
111.763

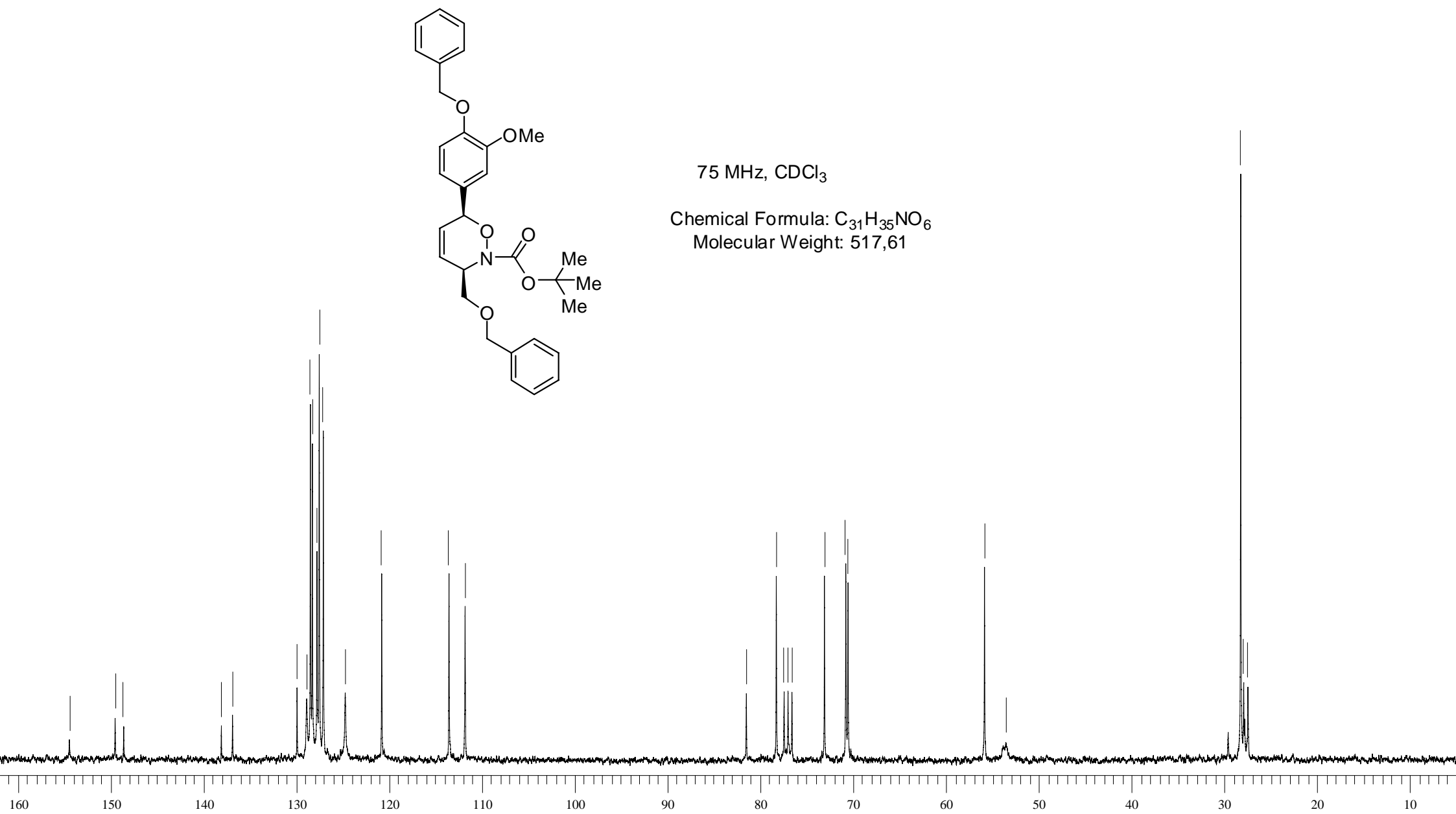
81.478  
78.251  
77.405  
76.987  
76.564  
73.068  
70.763  
70.524

55.821  
53.515

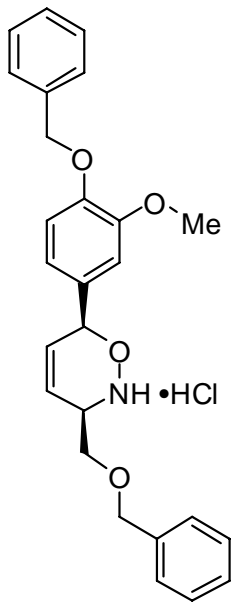
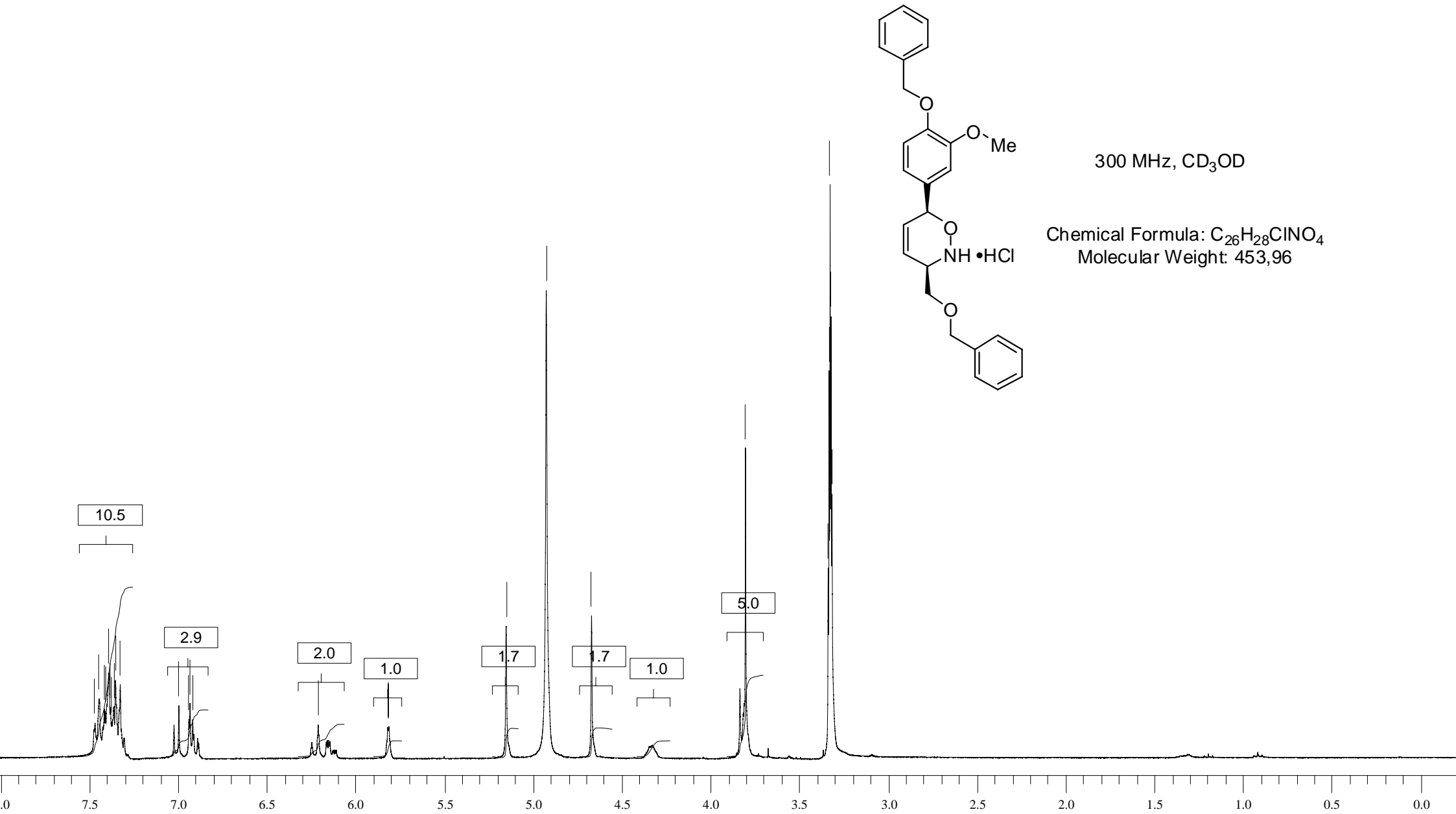
28.222  
27.902  
27.446



75 MHz, CDCl<sub>3</sub>  
Chemical Formula: C<sub>31</sub>H<sub>35</sub>NO<sub>6</sub>  
Molecular Weight: 517,61



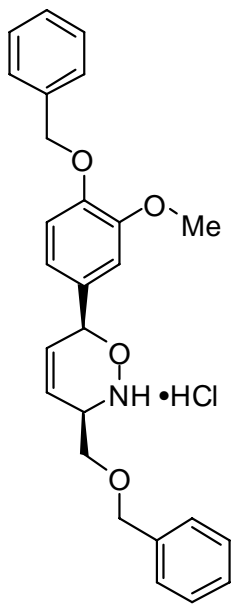
7.467  
7.443  
7.413  
7.409  
7.389  
7.379  
7.370  
7.360  
7.351  
7.324  
6.994  
6.938  
6.931  
6.916  
6.209  
5.817  
5.811  
5.150  
4.925  
4.669  
3.802  
3.337  
3.331  
3.326  
3.320  
3.314



300 MHz, CD<sub>3</sub>OD

Chemical Formula: C<sub>26</sub>H<sub>28</sub>ClNO<sub>4</sub>  
Molecular Weight: 453,96

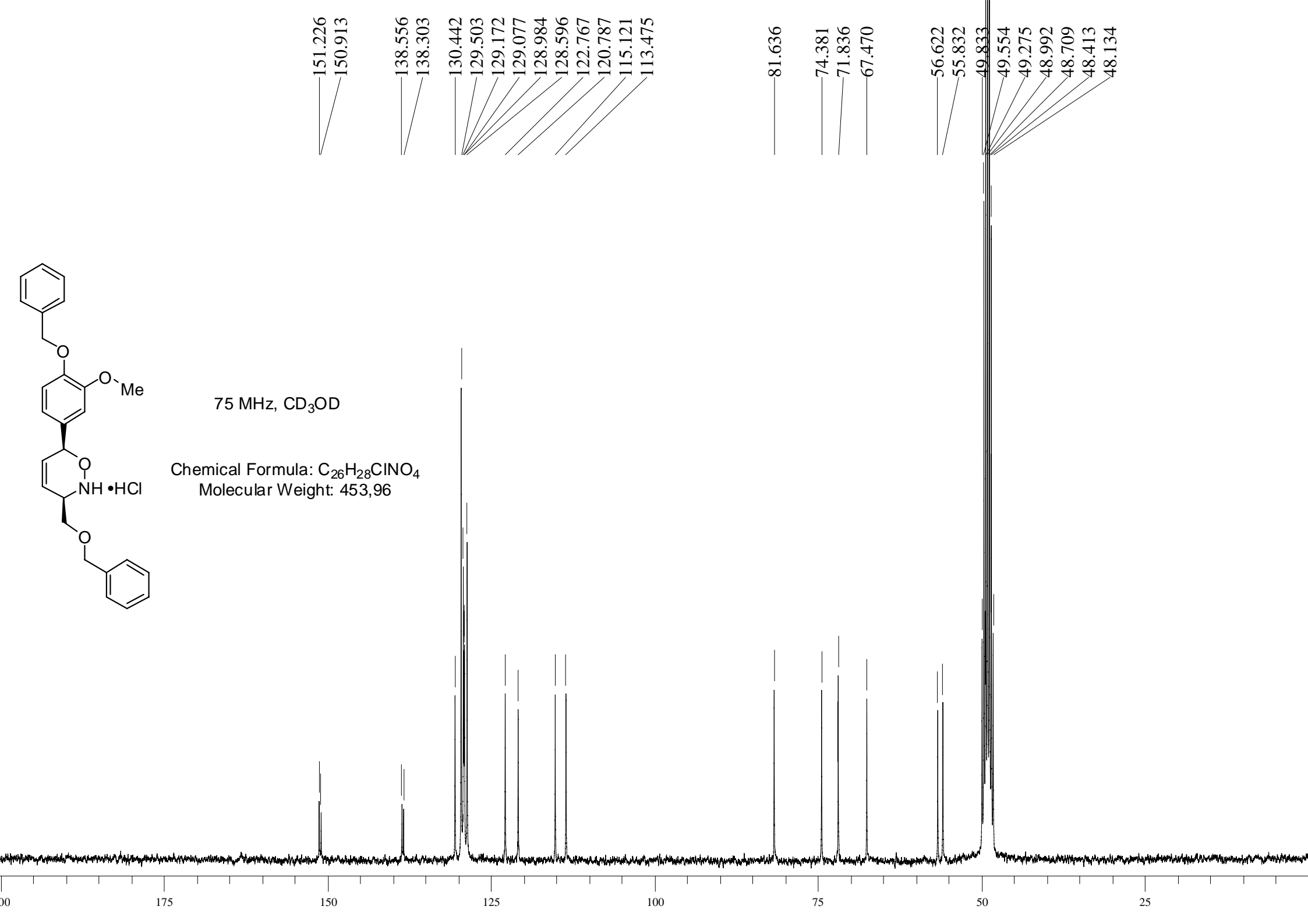




75 MHz, CD<sub>3</sub>OD

Chemical Formula: C<sub>26</sub>H<sub>28</sub>ClNO<sub>4</sub>  
Molecular Weight: 453,96

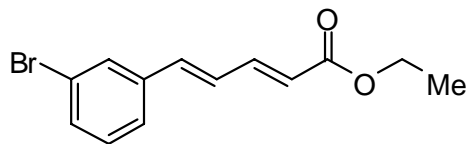
- 151.226
- 150.913
- 138.556
- 138.303
- 130.442
- 129.503
- 129.172
- 129.077
- 128.984
- 128.596
- 122.767
- 120.787
- 115.121
- 113.475
- 81.636
- 74.381
- 71.836
- 67.470
- 56.622
- 55.832
- 49.833
- 49.554
- 49.275
- 48.992
- 48.709
- 48.413
- 48.134



7.619  
7.449  
7.442  
7.419  
7.392  
7.387  
7.367  
7.269  
7.260  
7.233  
6.871  
6.840  
6.834  
6.049  
5.998

4.279  
4.255  
4.232  
4.208

1.352  
1.329  
1.305



300 MHz, CDCl<sub>3</sub>

Chemical Formula: C<sub>13</sub>H<sub>13</sub>BrO<sub>2</sub>  
Molecular Weight: 281,15

3.3

2.7

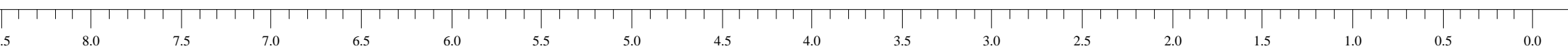
1.9

1.5

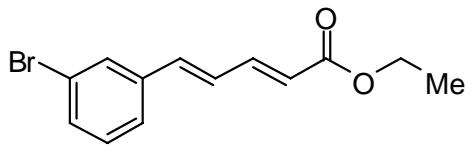
1.0

2.2

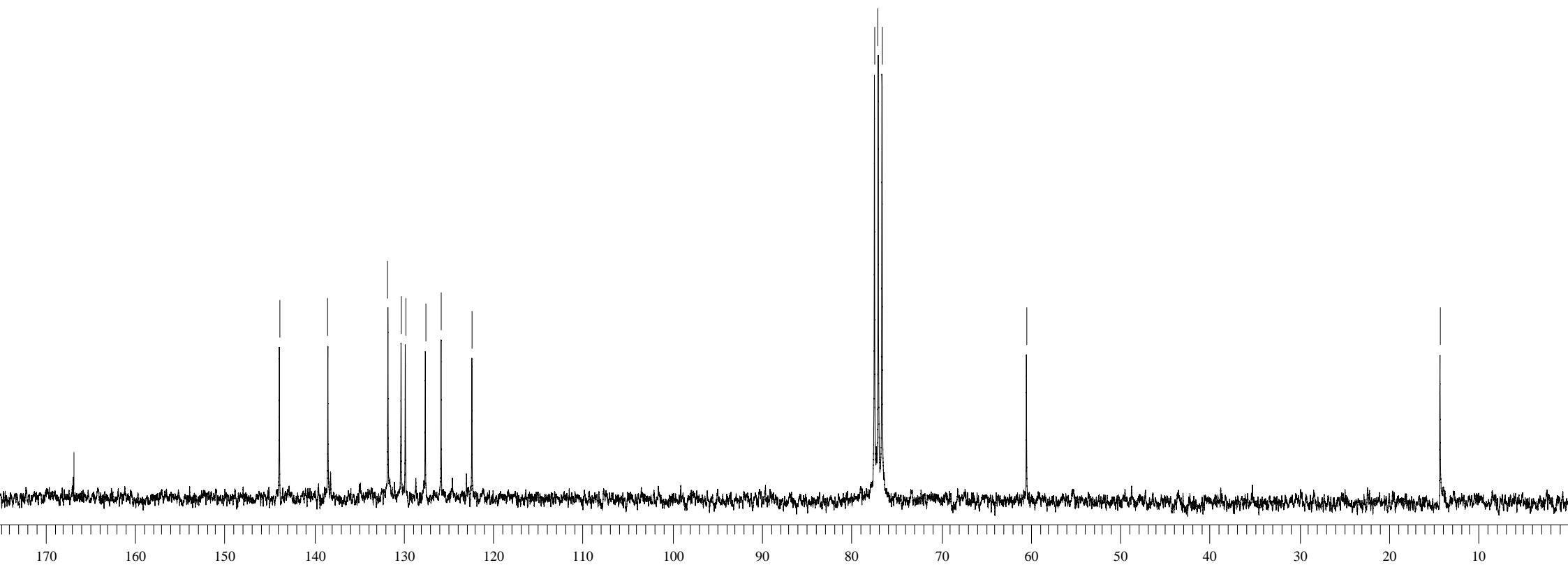
0.8

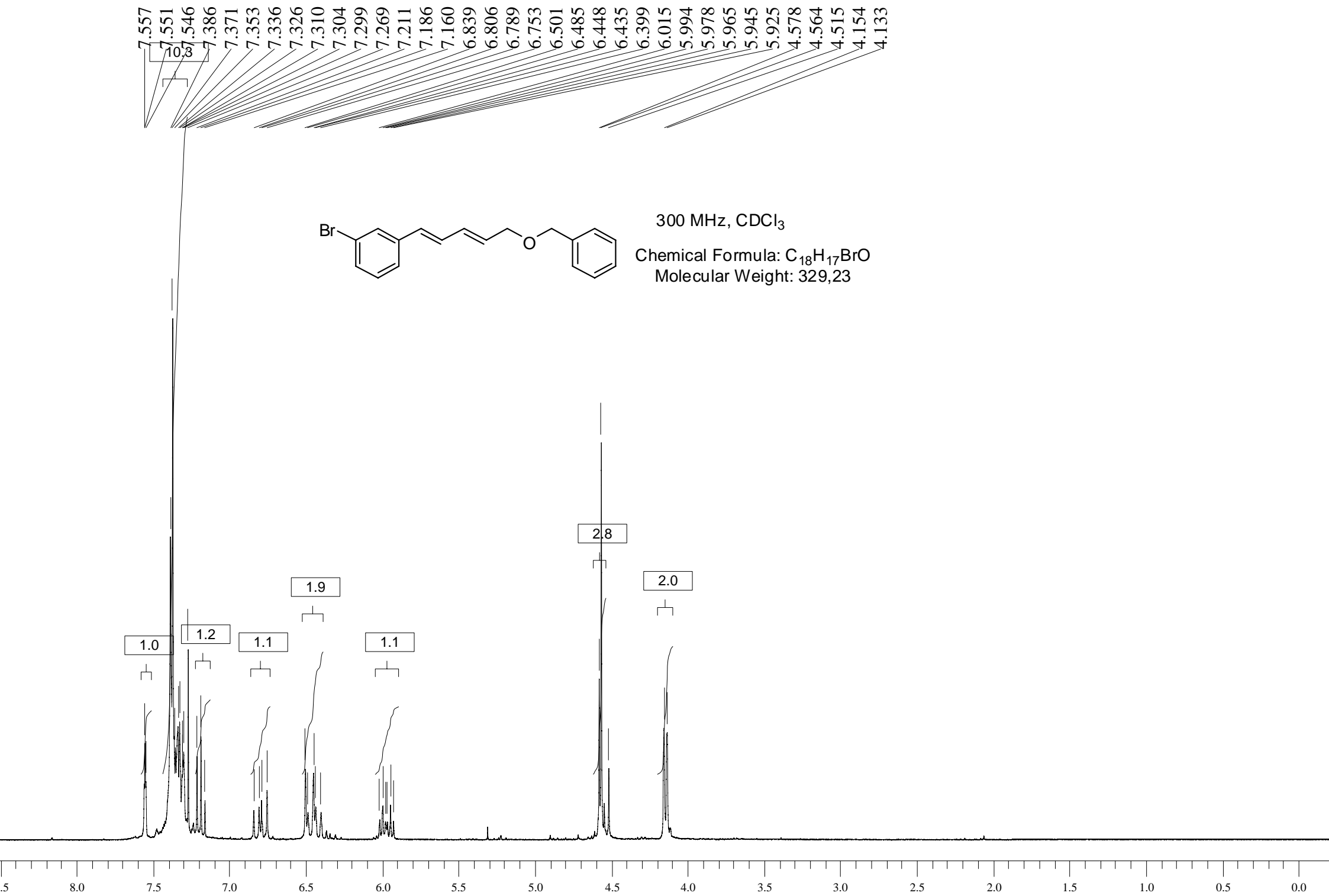


166.794  
143.845  
138.423  
131.728  
130.266  
129.787  
127.551  
125.783  
122.353  
77.419  
76.990  
76.572  
60.454  
14.286



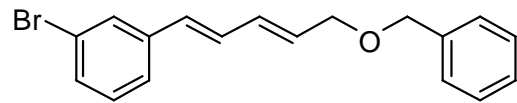
75 MHz, CDCl<sub>3</sub>  
Chemical Formula: C<sub>13</sub>H<sub>13</sub>BrO<sub>2</sub>  
Molecular Weight: 281,15





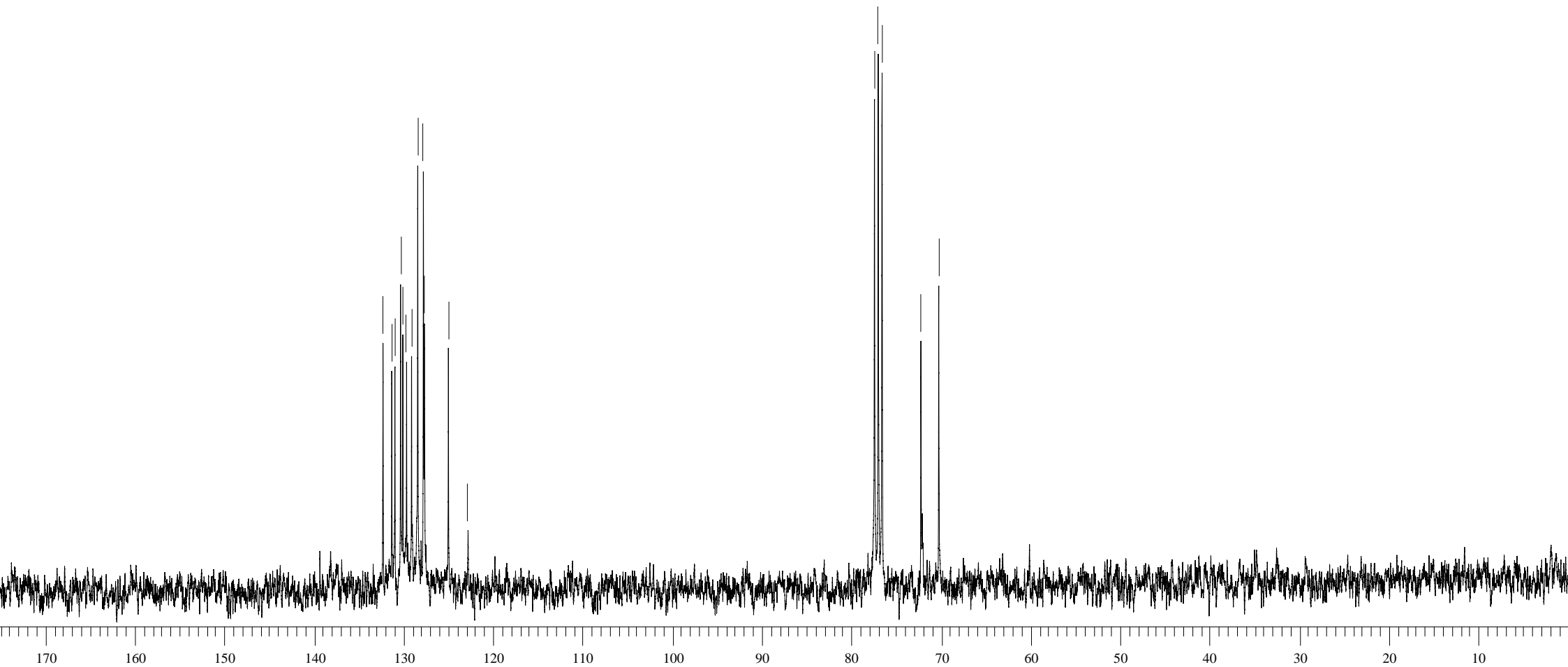
132.278  
131.298  
124.980  
122.783  
130.936  
130.312  
130.051  
129.642  
129.074  
128.394  
127.763  
127.657

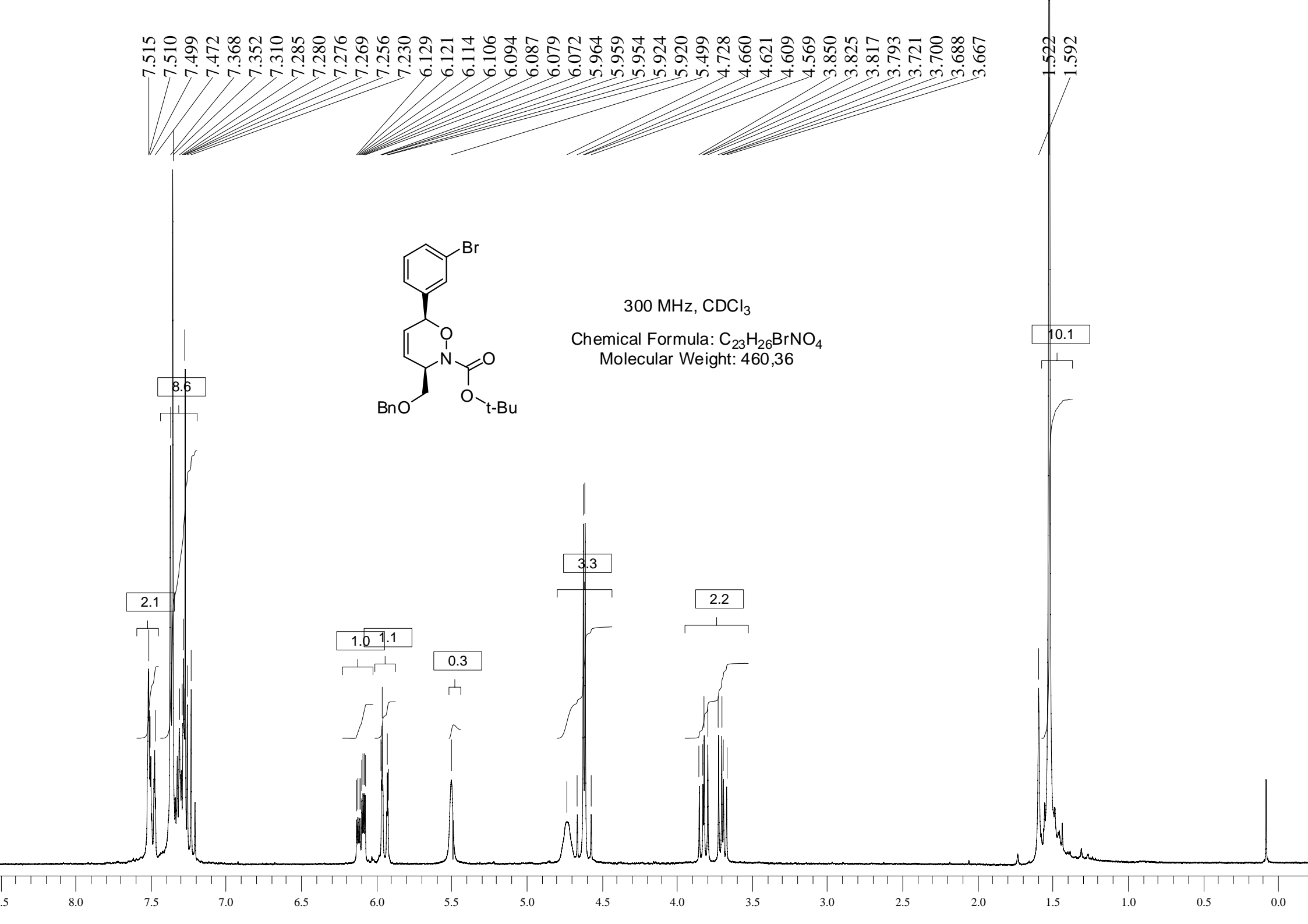
77.401  
76.991  
76.562  
72.224  
70.227



75 MHz, CDCl<sub>3</sub>

Chemical Formula: C<sub>18</sub>H<sub>17</sub>BrO  
Molecular Weight: 329,23





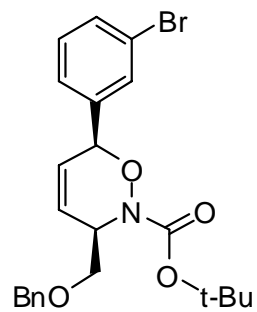
154.382

139.229  
138.019

131.999  
131.126  
130.147  
128.351  
128.248  
127.620  
126.825  
125.151  
122.553

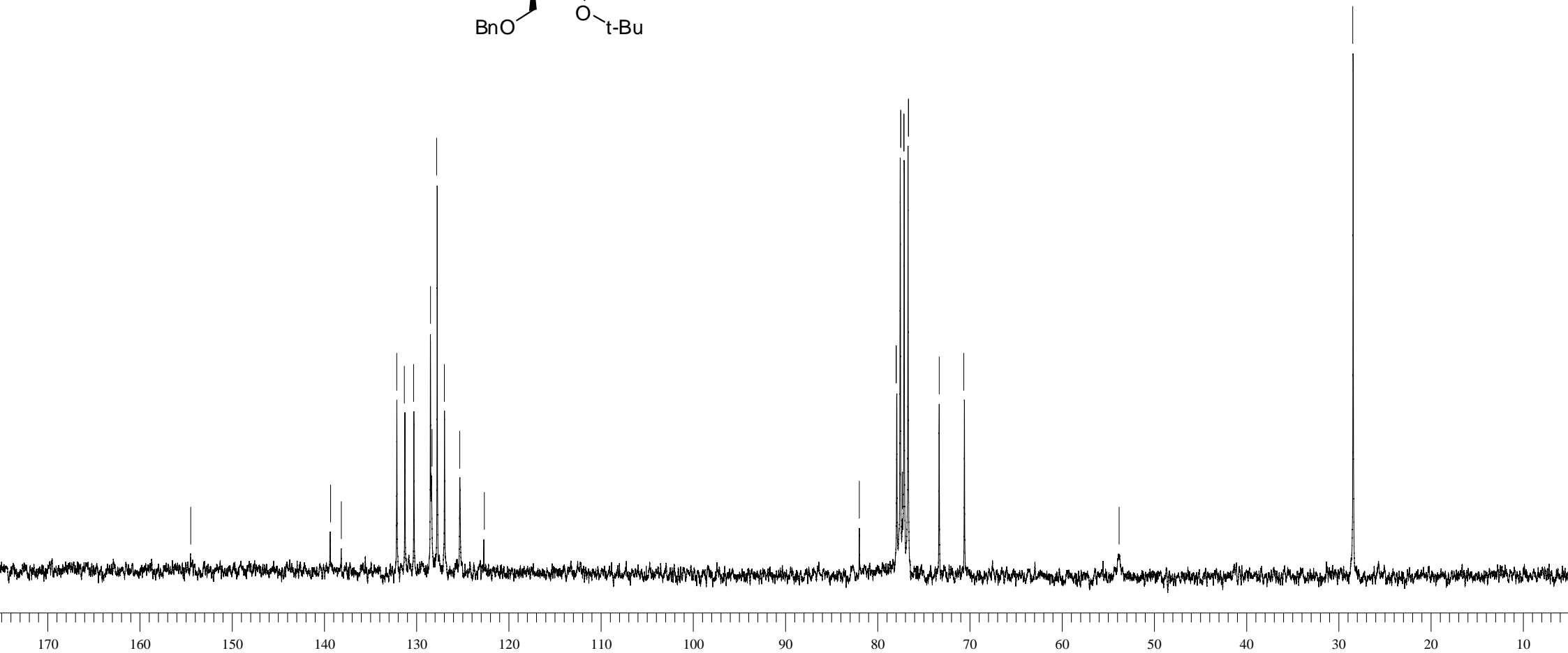
81.850  
77.777  
77.406  
76.987  
76.564  
77.777  
77.406  
77.178  
76.987  
76.564  
73.188  
70.453  
53.637

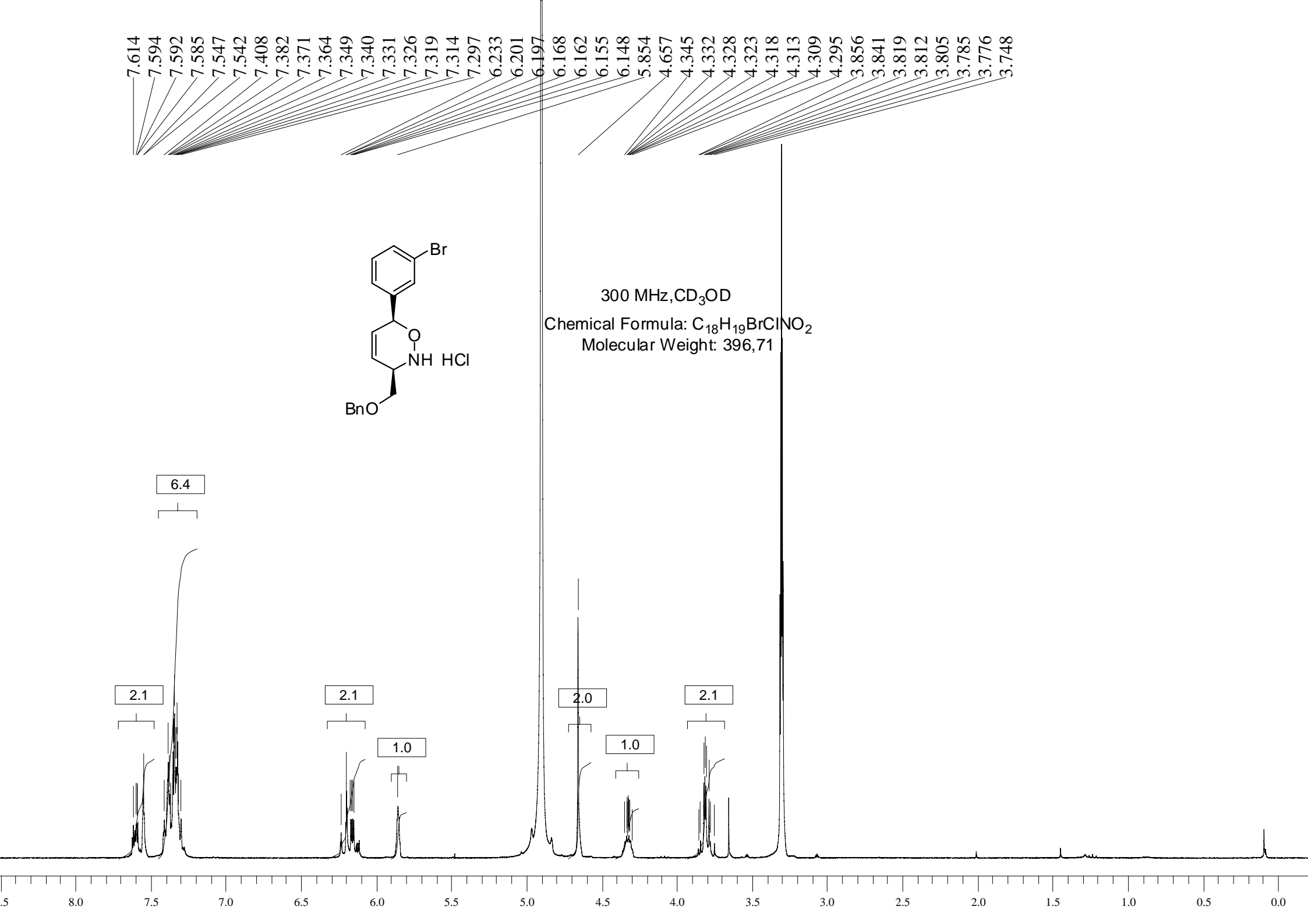
28.301



75 MHz, CDCl<sub>3</sub>

Chemical Formula: C<sub>23</sub>H<sub>26</sub>BrNO<sub>4</sub>  
Molecular Weight: 460,36







138.398  
134.152  
132.410  
131.945  
129.681  
129.560  
129.238  
129.141  
128.353  
123.722  
121.206

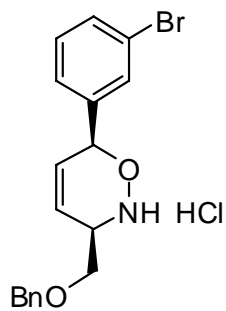
80.808

74.377

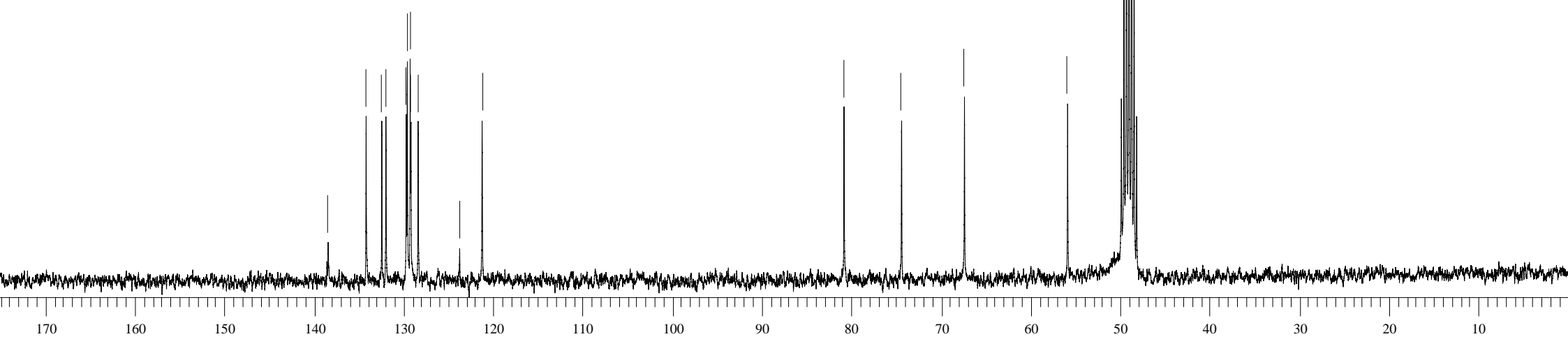
67.364

55.848

48.991



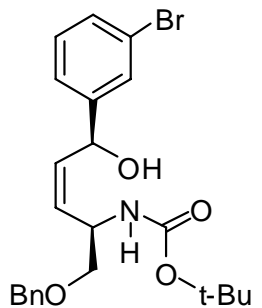
75 MHz, CD<sub>3</sub>OD  
Chemical Formula: C<sub>18</sub>H<sub>19</sub>BrClNO<sub>2</sub>  
Molecular Weight: 396,71



7.567  
7.417  
7.395  
7.389  
7.371  
7.358  
7.332  
7.308  
7.226  
7.199  
7.174

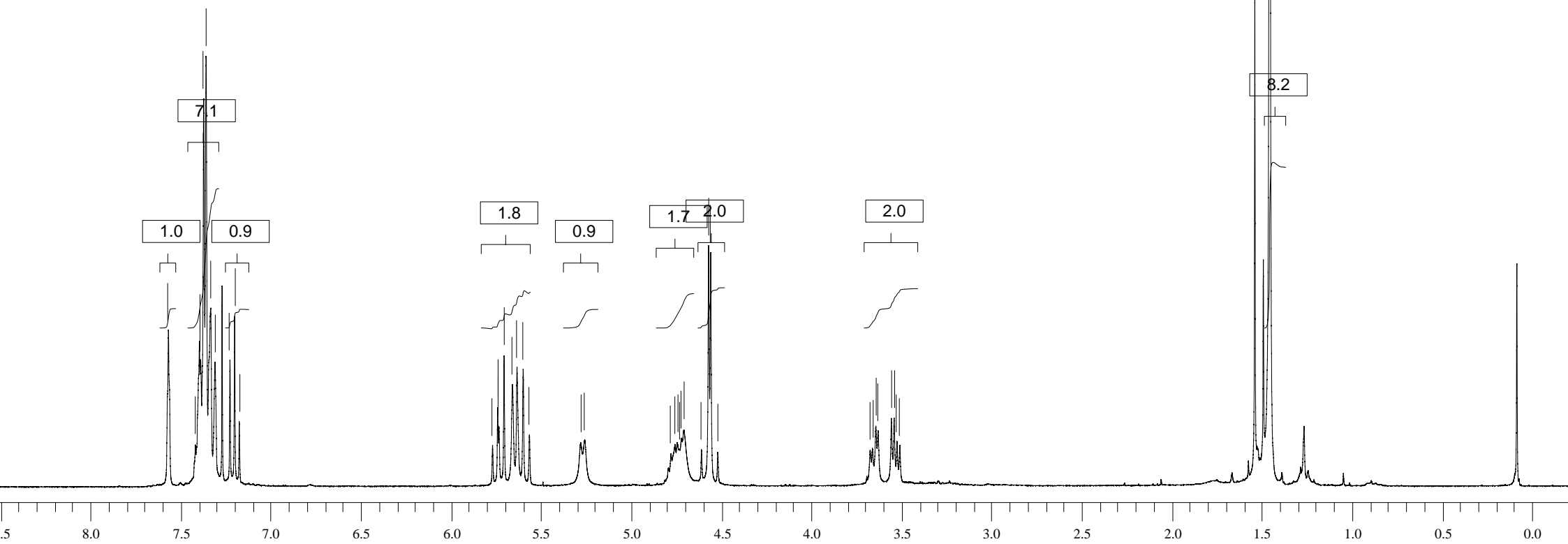
5.768  
5.740  
5.733  
5.704  
5.657  
5.633  
5.598  
5.564  
5.278  
5.257  
4.778  
4.756  
4.743  
4.731  
4.720  
4.707  
4.609  
4.569  
4.558  
4.518  
3.672  
3.659  
3.641  
3.629  
3.555  
3.540  
3.524  
3.508

1.455



300 MHz, CDCl<sub>3</sub>

Chemical Formula: C<sub>23</sub>H<sub>28</sub>BrNO<sub>4</sub>  
Molecular Weight: 462,38

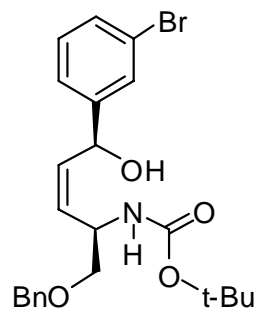


156.033  
145.345  
137.393  
134.833  
130.078  
129.839  
129.022  
128.771  
128.500  
127.966  
127.725  
124.514  
122.405

80.460  
77.407  
76.986  
76.563  
73.431  
71.246  
67.418

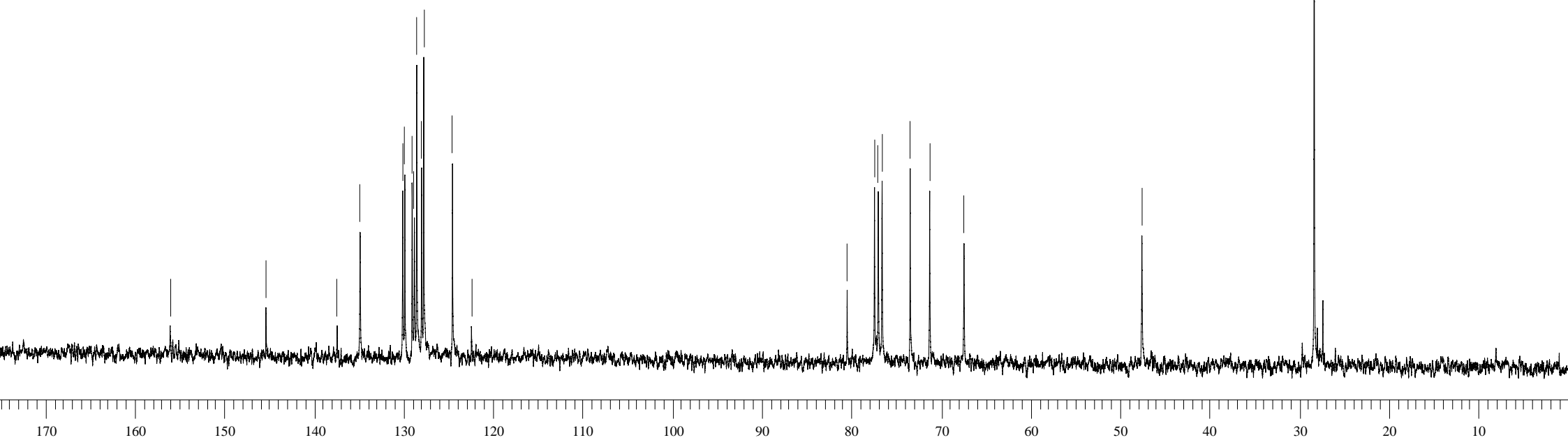
47.558

28.328



75 MHz, CDCl<sub>3</sub>

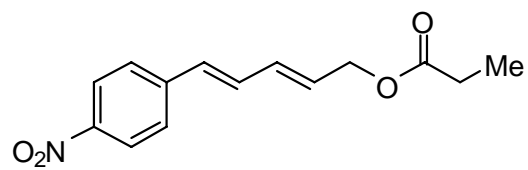
Chemical Formula: C<sub>23</sub>H<sub>28</sub>BrNO<sub>4</sub>  
Molecular Weight: 462,38



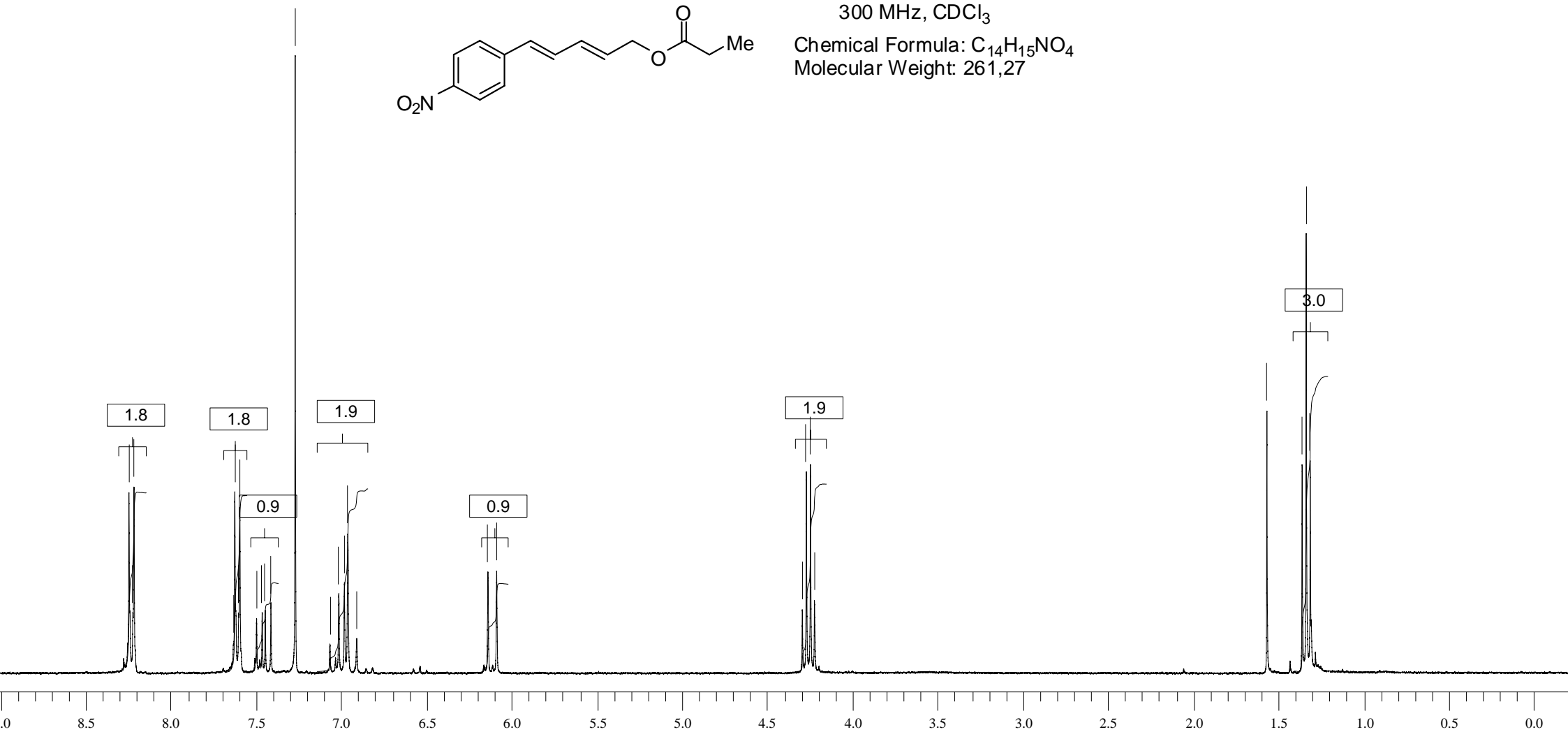
8.245  
8.222  
8.215  
7.631  
7.624  
7.600  
7.594  
7.496  
7.463  
7.445  
7.411  
7.269  
7.065  
7.013  
6.980  
6.960  
6.908  
6.138  
6.087

4.293  
4.270  
4.246  
4.222

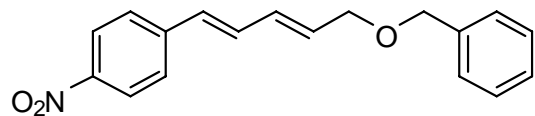
1.567  
1.360  
1.337  
1.313



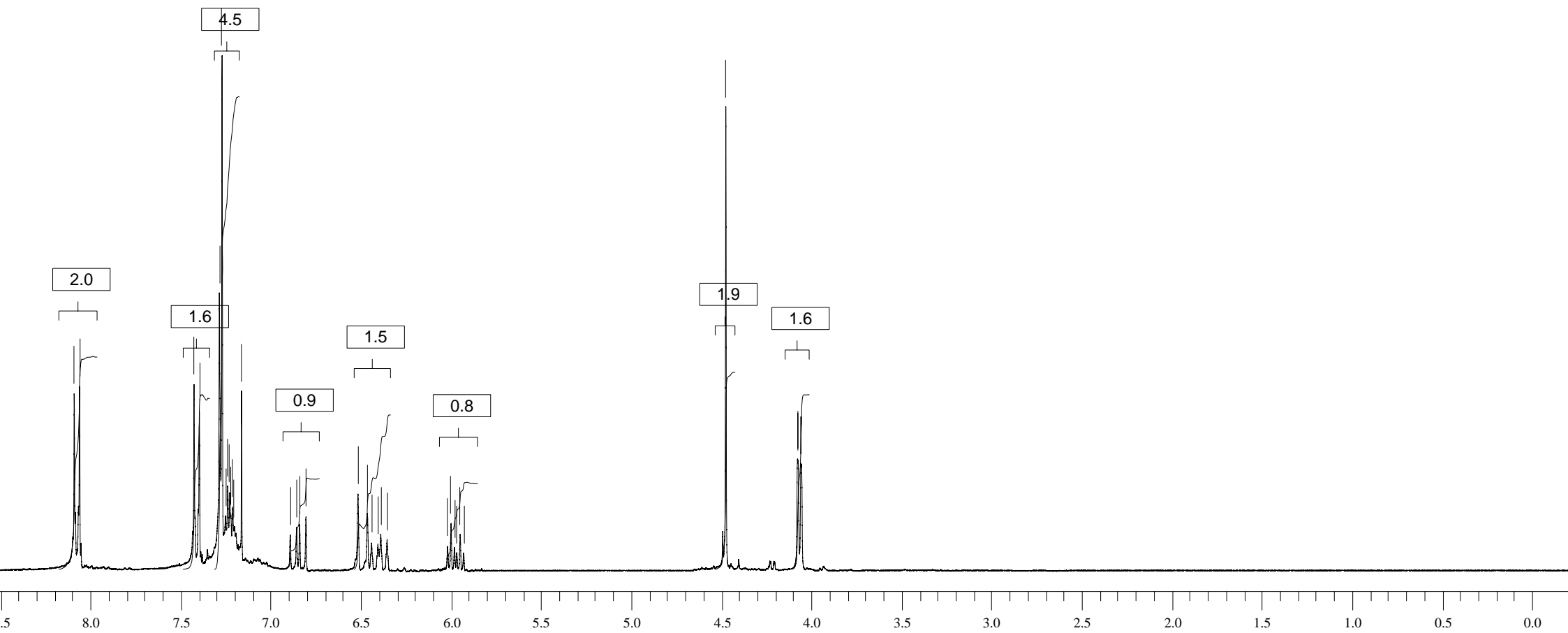
300 MHz, CDCl<sub>3</sub>  
Chemical Formula: C<sub>14</sub>H<sub>15</sub>NO<sub>4</sub>  
Molecular Weight: 261,27



8.090  
8.060  
7.425  
7.395  
7.284  
7.269  
7.250  
7.238  
7.226  
7.221  
7.210  
7.200  
7.161  
6.891  
6.856  
6.839  
6.804  
6.515  
6.463  
6.440  
6.404  
6.389  
6.353  
6.017  
5.998  
5.979  
5.966  
5.947  
5.928  
4.474  
4.076  
4.073  
4.057  
4.054



300 MHz, CDCl<sub>3</sub>  
Chemical Formula: C<sub>18</sub>H<sub>17</sub>NO<sub>3</sub>  
Molecular Weight: 295,33



143.702

133.659

132.748

131.530

130.004

128.424

127.723

126.669

124.032

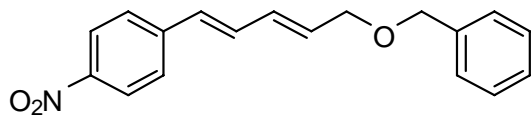
77.421

76.988

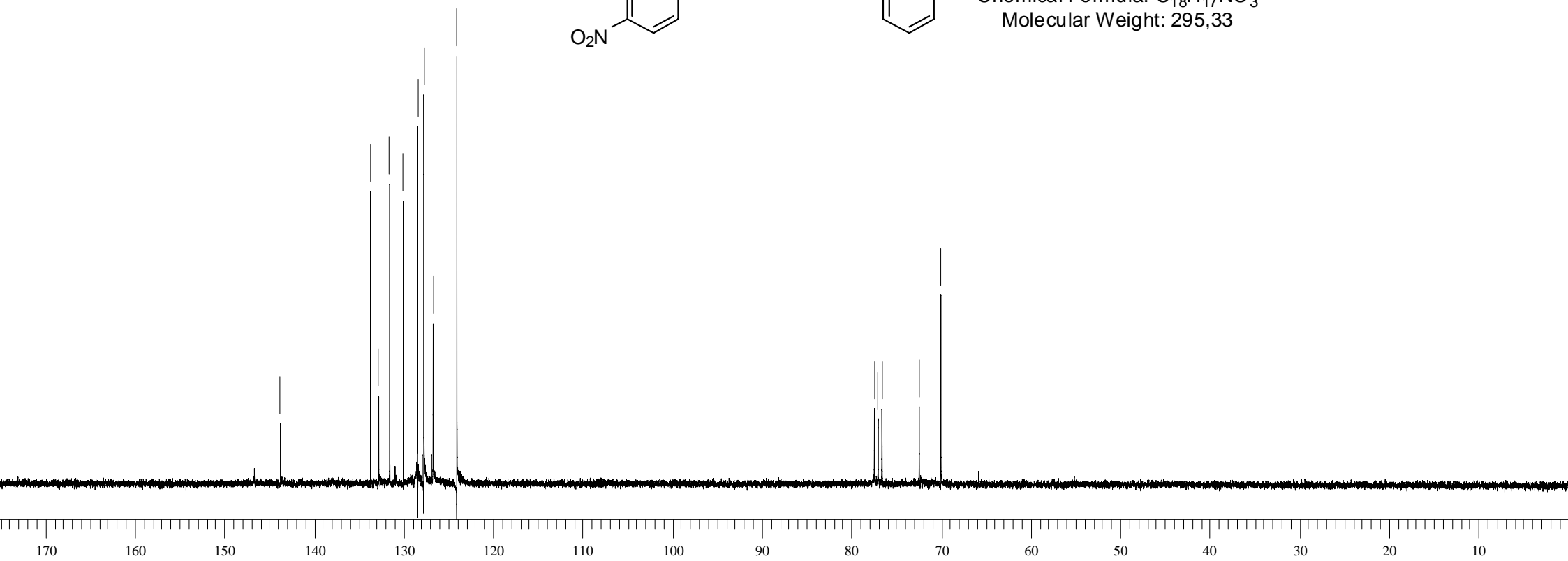
76.577

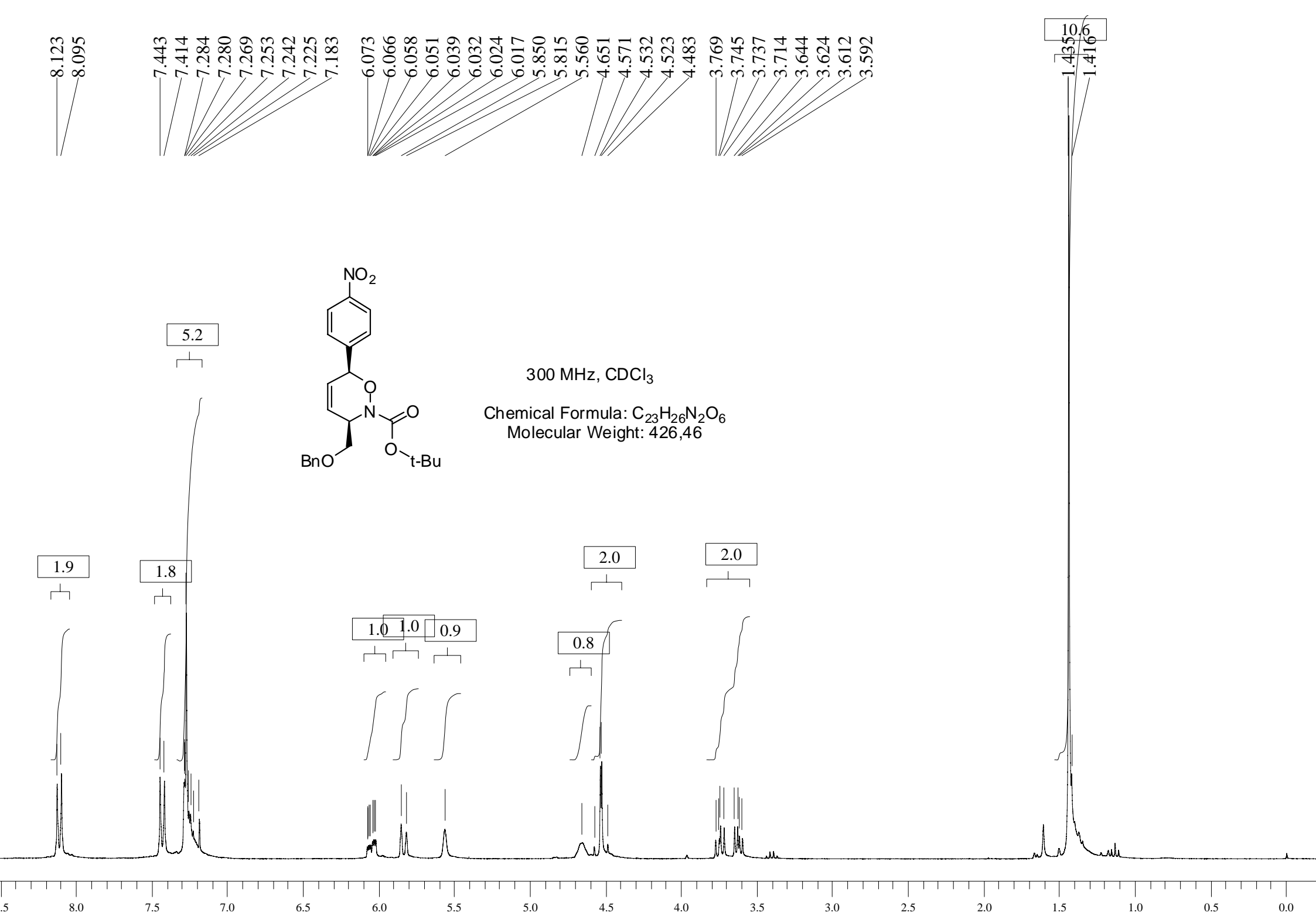
72.413

70.003



75 MHz, CDCl<sub>3</sub>  
Chemical Formula: C<sub>18</sub>H<sub>17</sub>NO<sub>3</sub>  
Molecular Weight: 295,33





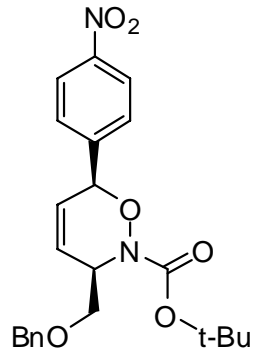
154.063  
147.743  
143.848  
137.620

128.472  
128.083  
127.417  
125.222  
123.509

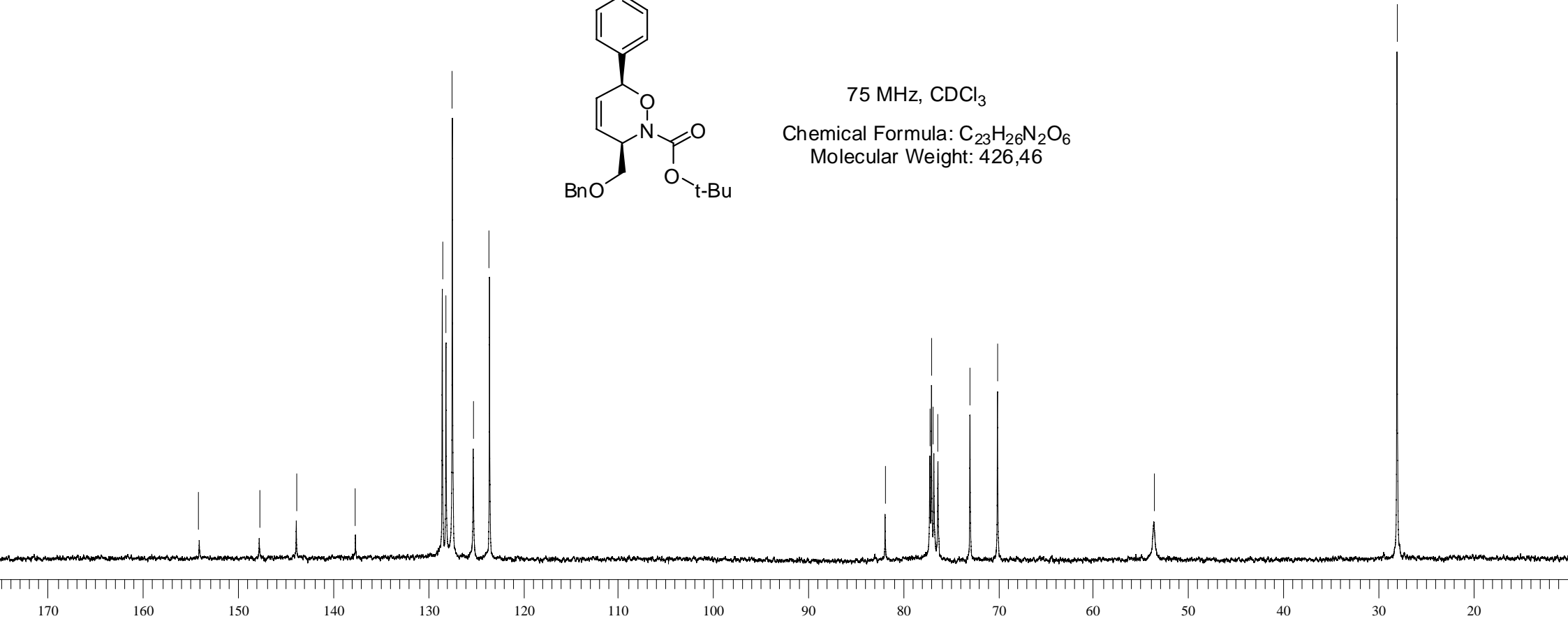
81.875  
77.164  
76.990  
76.737  
76.304  
72.929  
70.042

53.586

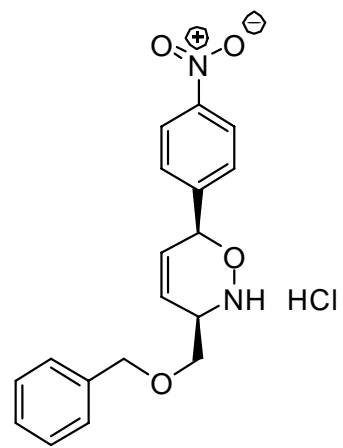
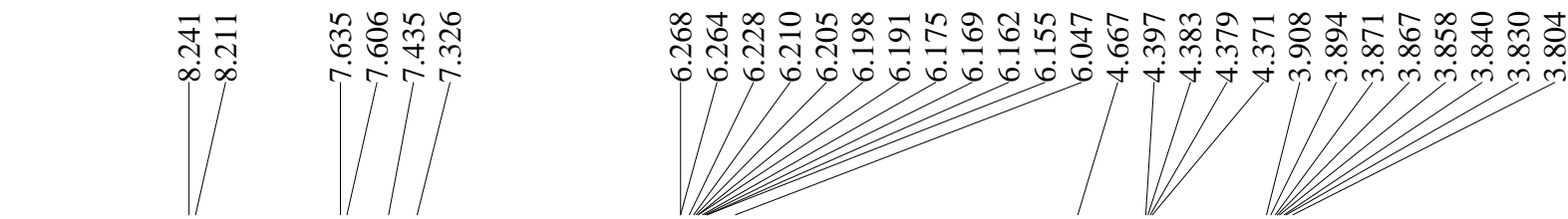
27.995



75 MHz, CDCl<sub>3</sub>  
Chemical Formula: C<sub>23</sub>H<sub>26</sub>N<sub>2</sub>O<sub>6</sub>  
Molecular Weight: 426,46

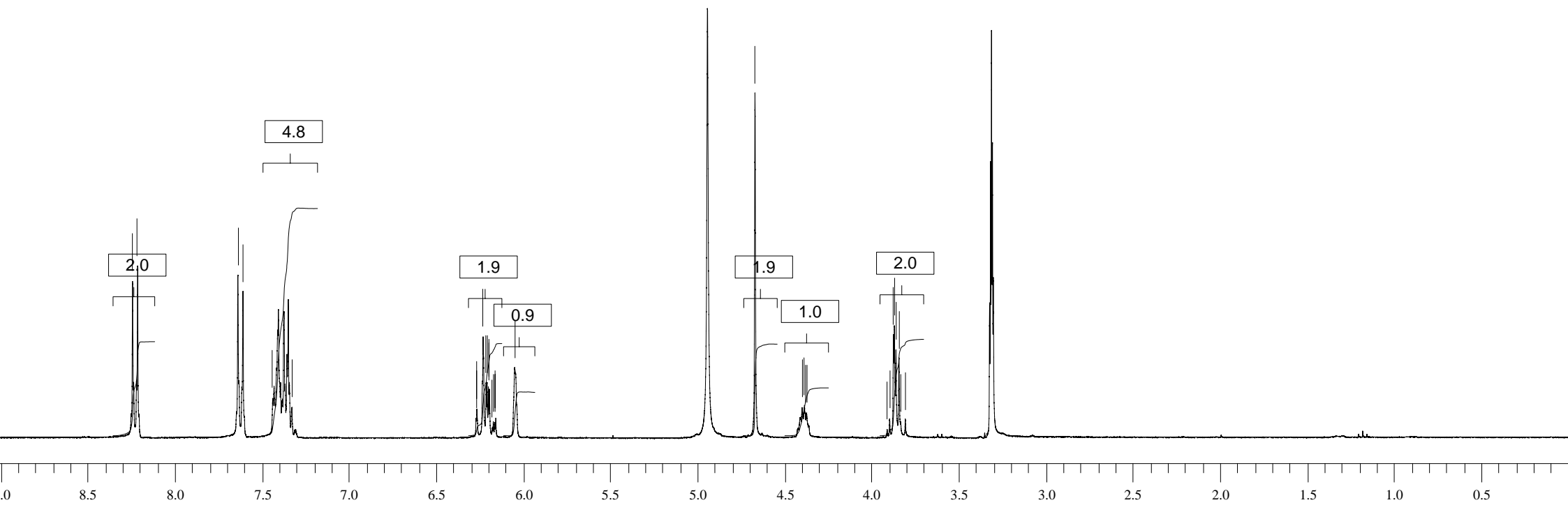






300 MHz, CD<sub>3</sub>OD

Chemical Formula: C<sub>18</sub>H<sub>19</sub>ClN<sub>2</sub>O<sub>4</sub>  
Molecular Weight: 362,81



150.087

142.925

138.583

130.526

129.573

129.401

129.306

129.173

125.007

121.431

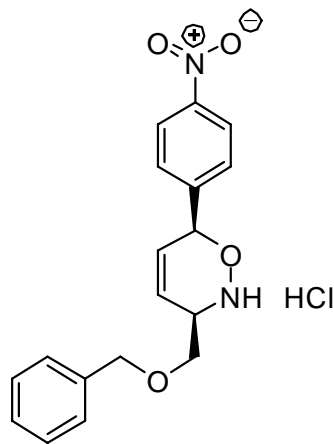
80.351

74.446

67.485

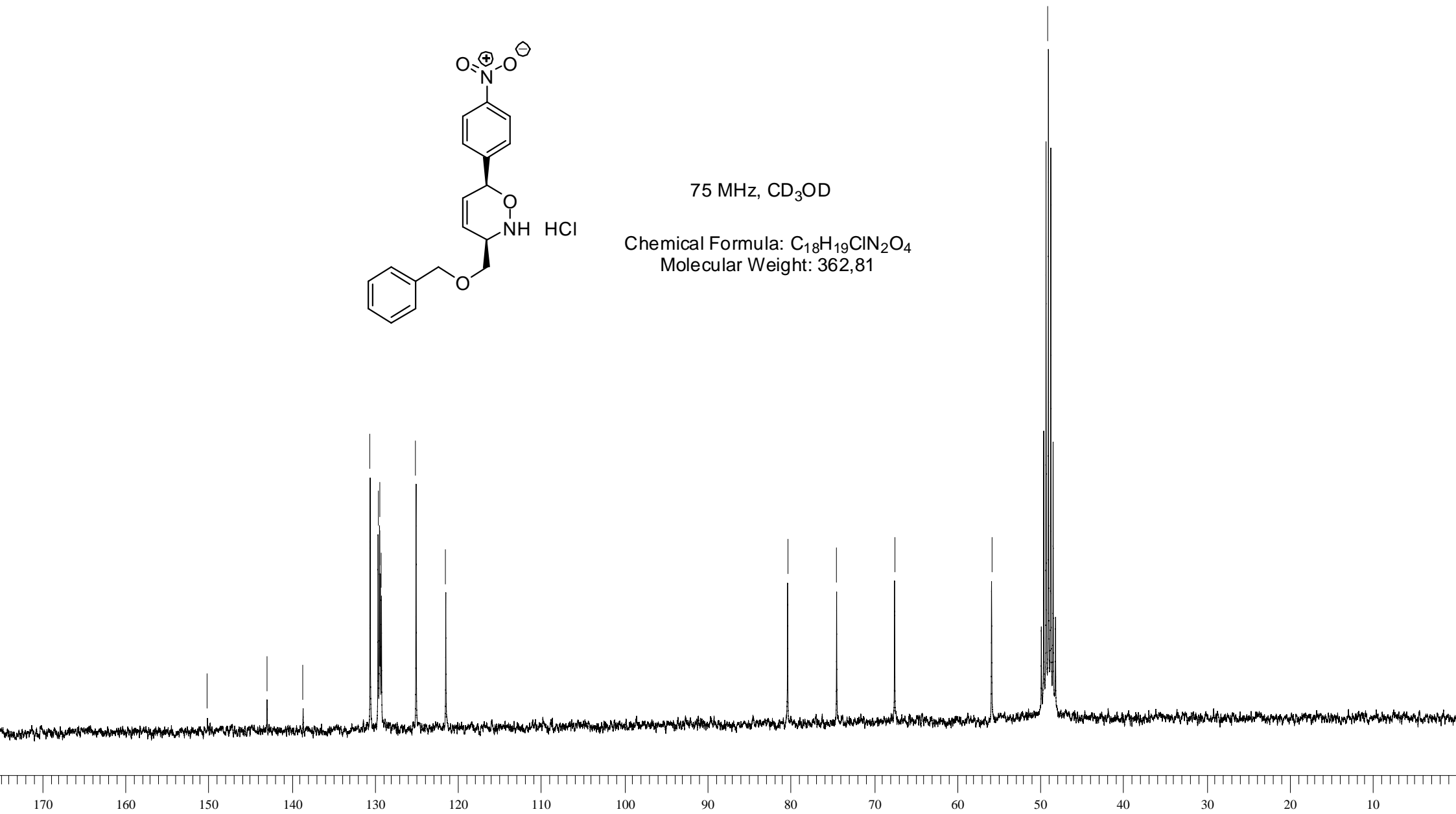
55.819

48.993



75 MHz, CD<sub>3</sub>OD

Chemical Formula: C<sub>18</sub>H<sub>19</sub>ClN<sub>2</sub>O<sub>4</sub>  
Molecular Weight: 362,81



156.113

150.460

146.953

137.300

134.058

129.614

128.543

128.043

127.775

126.628

123.492

80.658

77.401

76.991

76.561

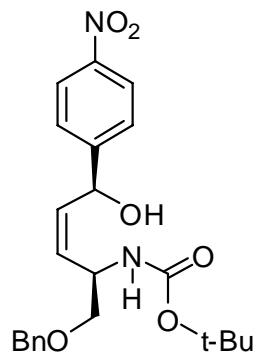
73.494

71.150

67.306

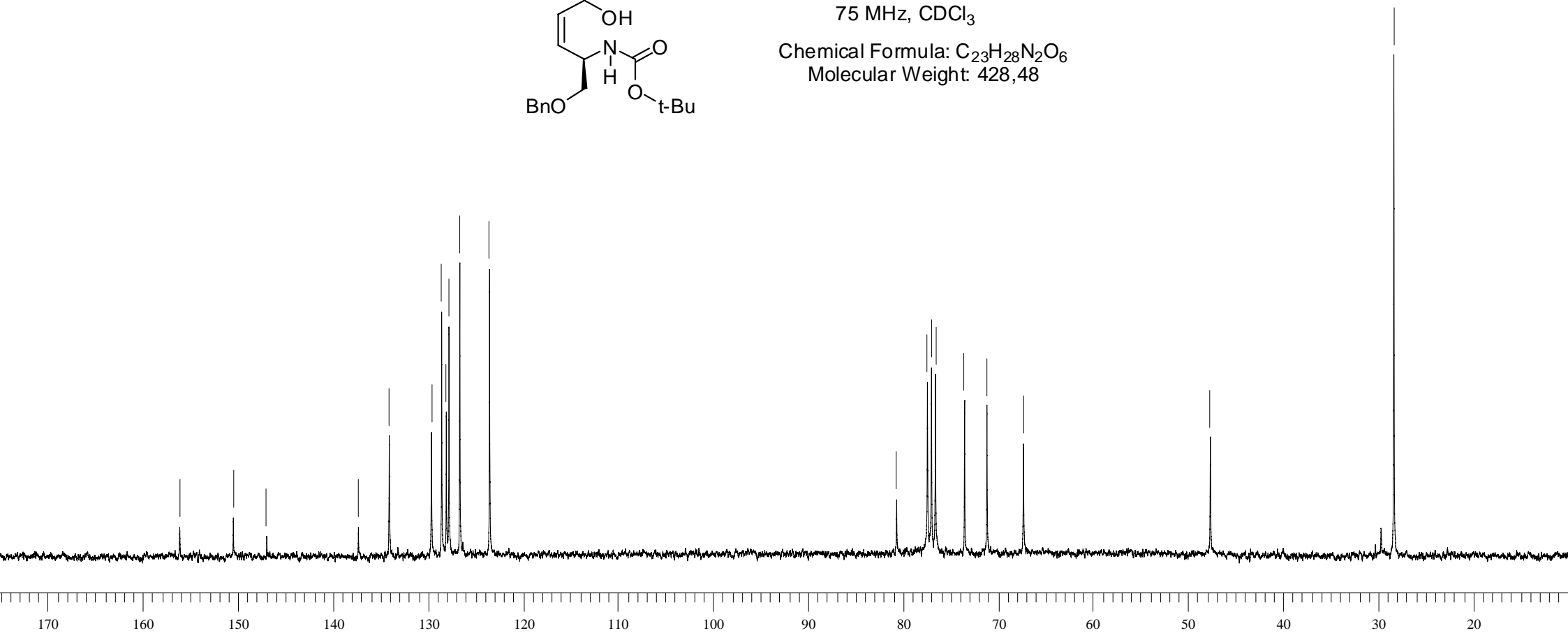
47.622

28.318



75 MHz, CDCl<sub>3</sub>

Chemical Formula: C<sub>23</sub>H<sub>28</sub>N<sub>2</sub>O<sub>6</sub>  
Molecular Weight: 428,48

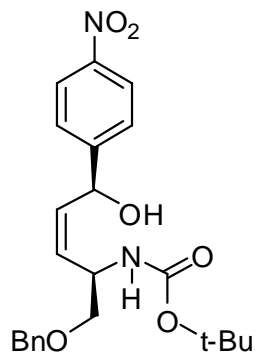


8.207  
8.178

7.574  
7.545  
7.403  
7.386  
7.372  
7.357  
7.348  
7.281

5.789  
5.763  
5.734  
5.699  
5.686  
5.680  
5.673  
5.655  
5.621  
5.308  
5.286  
4.790  
4.781  
4.774  
4.767  
4.759  
4.751  
4.745  
4.631  
4.591  
4.579  
4.540  
3.685  
3.667  
3.654  
3.591  
3.576  
3.560  
3.545

1.468



300 MHz, CDCl<sub>3</sub>  
Chemical Formula: C<sub>23</sub>H<sub>28</sub>N<sub>2</sub>O<sub>6</sub>  
Molecular Weight: 428,48

