

## Supporting Information

### Antitubercular activity of 2-mercaptobenzothiazole derivatives targeting *Mycobacterium tuberculosis* type II NADH dehydrogenase

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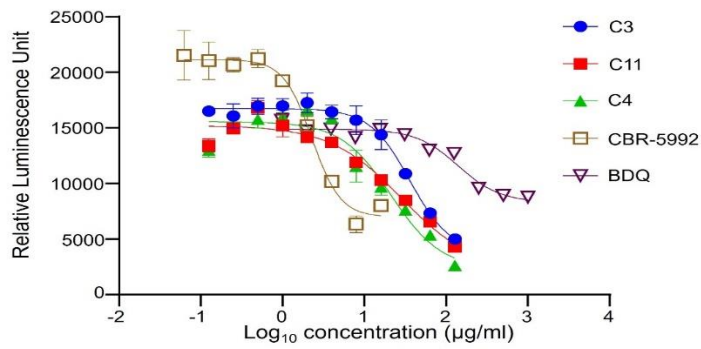
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<sup>b</sup>Department of Pharmacology and Toxicology, NIPER-Hyderabad, Hyderabad, 500037.

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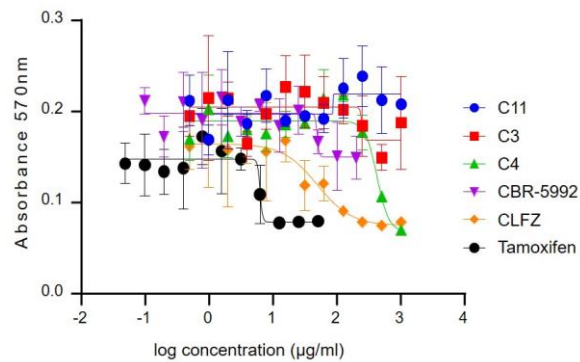
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## ATP depletion assay graph



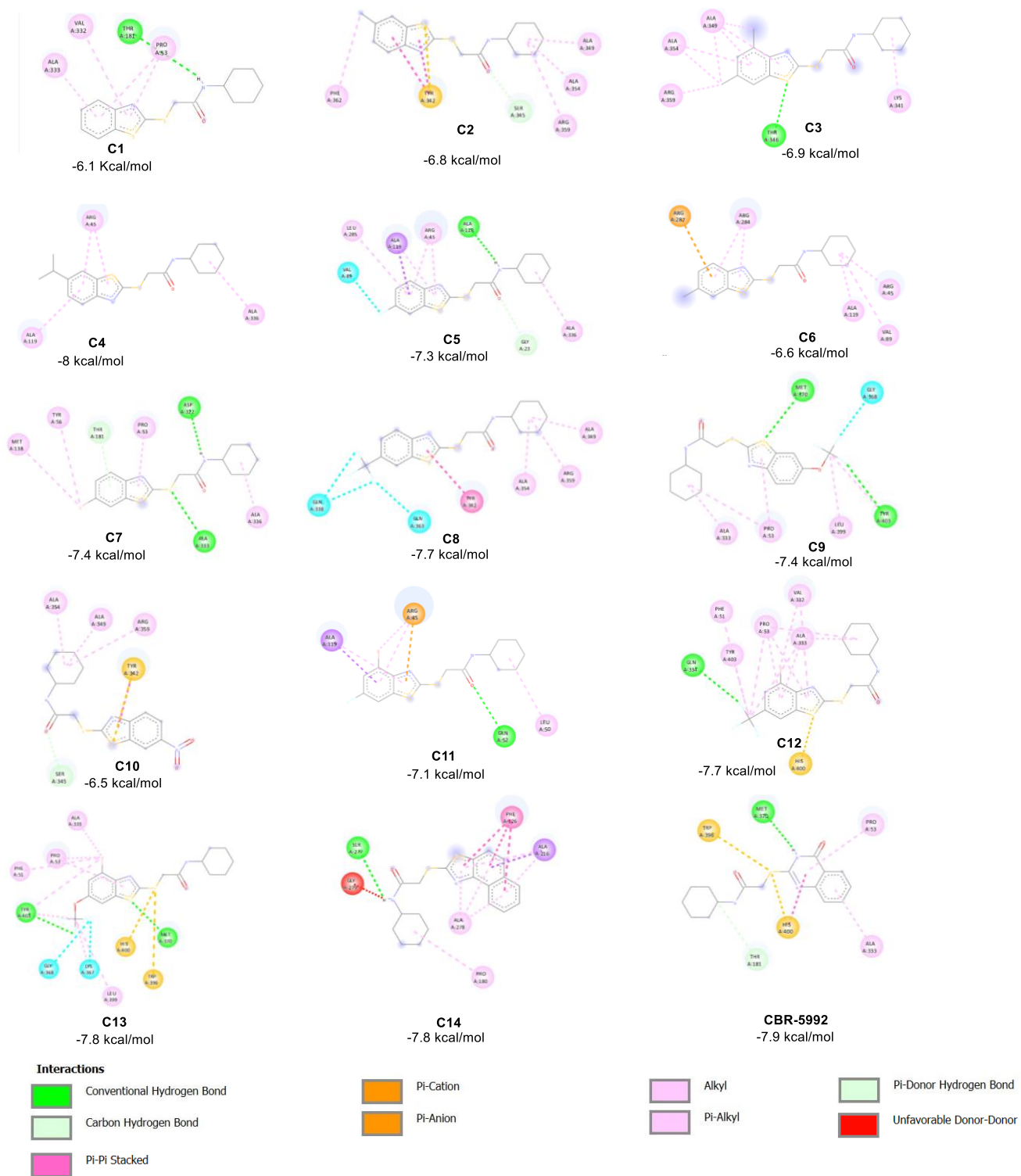
**S1.** Intracellular ATP levels were quantified using a luciferase-based assay against *Mtb* H37Rv mc<sup>2</sup> 6230.

## MTT assay graph:

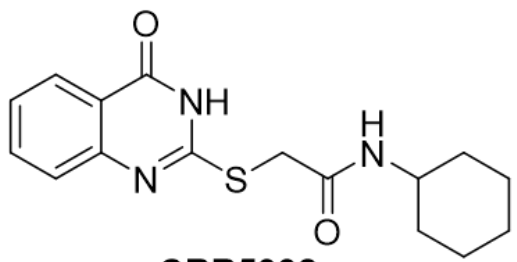


**S2.** Cytotoxicity of the test active molecules (C3, C4 and C11) and CBR-5992 against HepG2 cell lines

## In silico docking data:

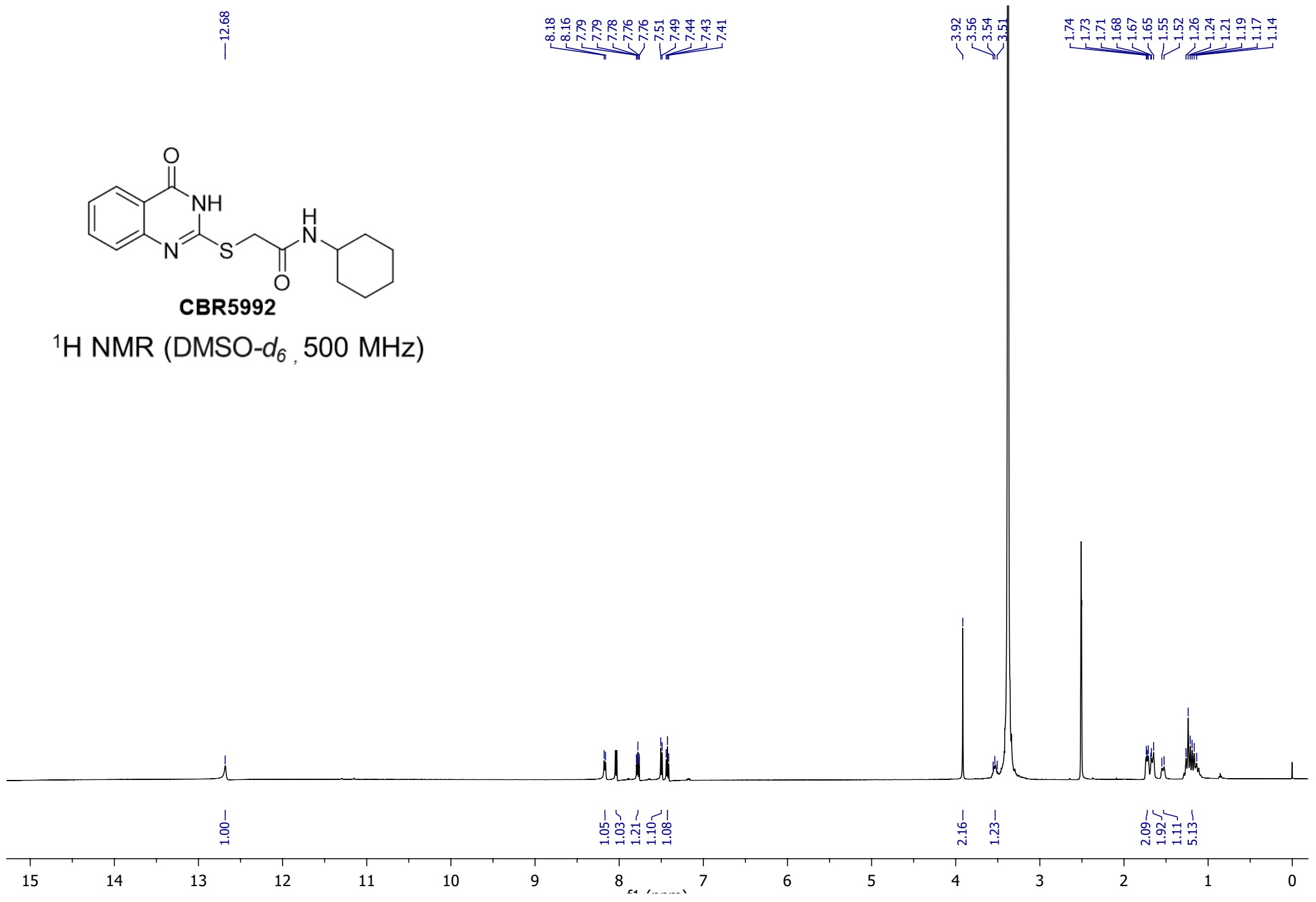


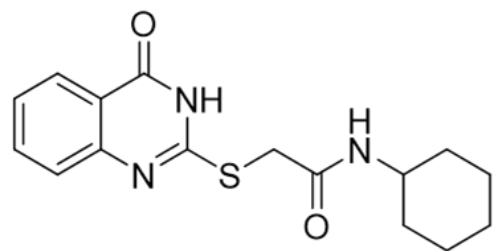
### S3. Binding interactions of C1-C14 and CBR-5992.



**CBR5992**

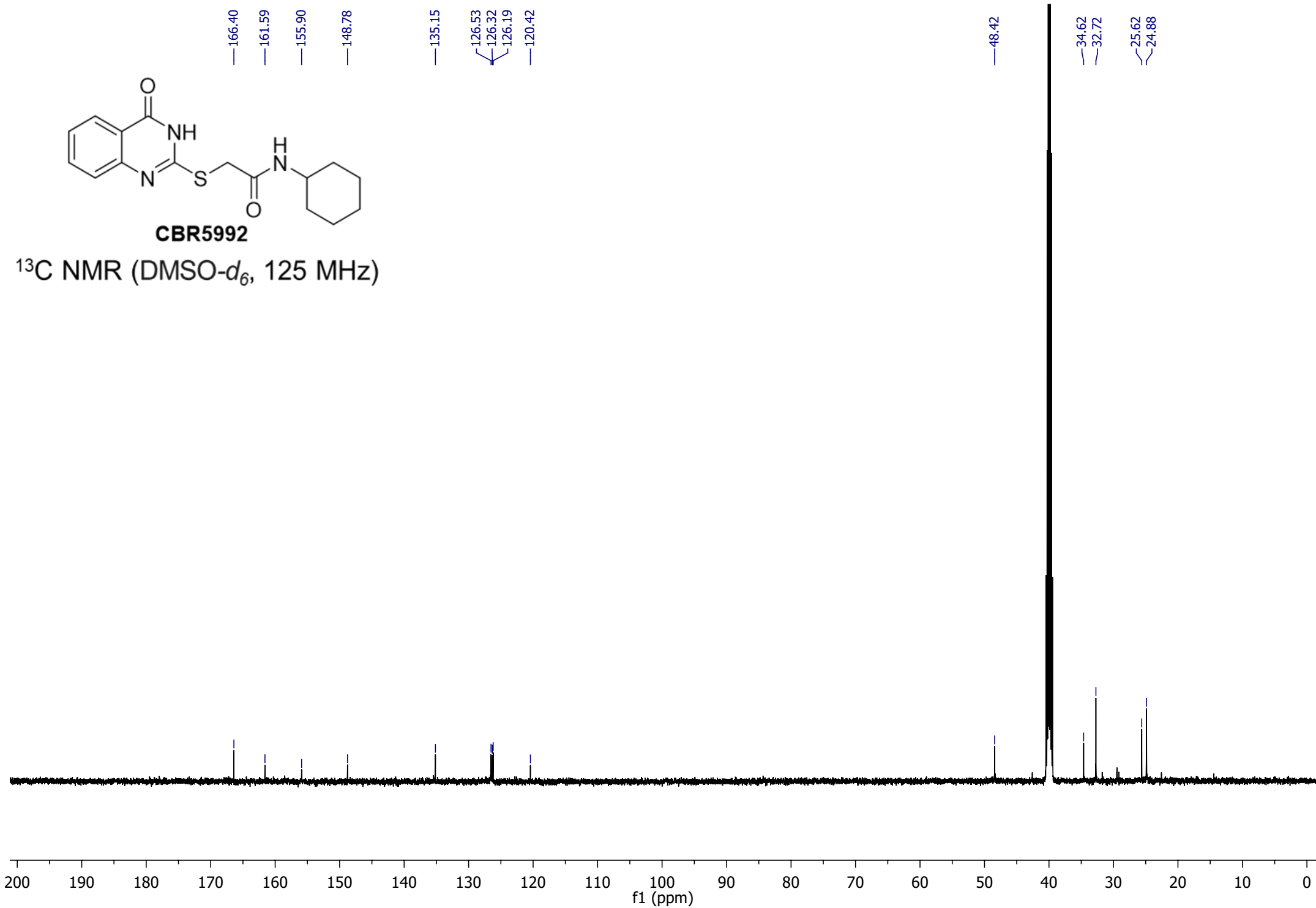
<sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 500 MHz)

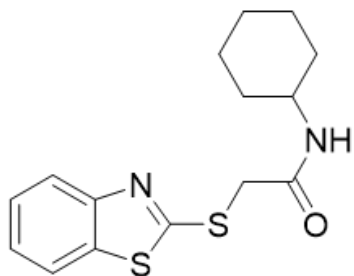




**CBR5992**

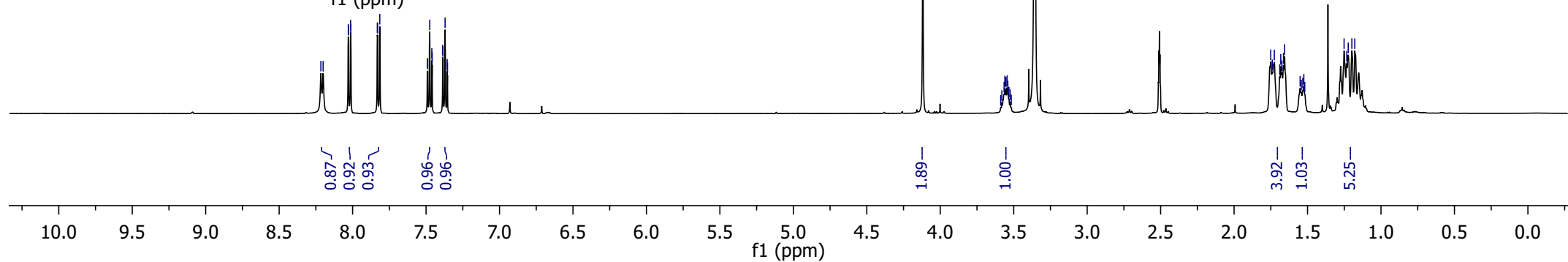
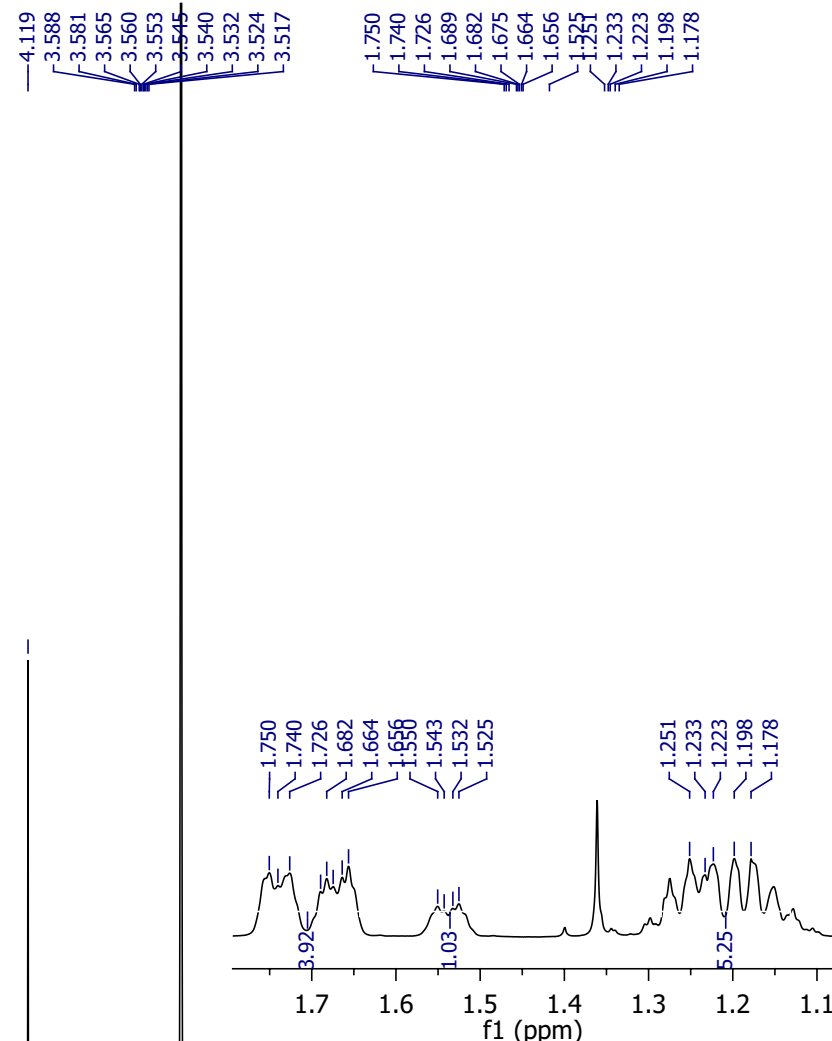
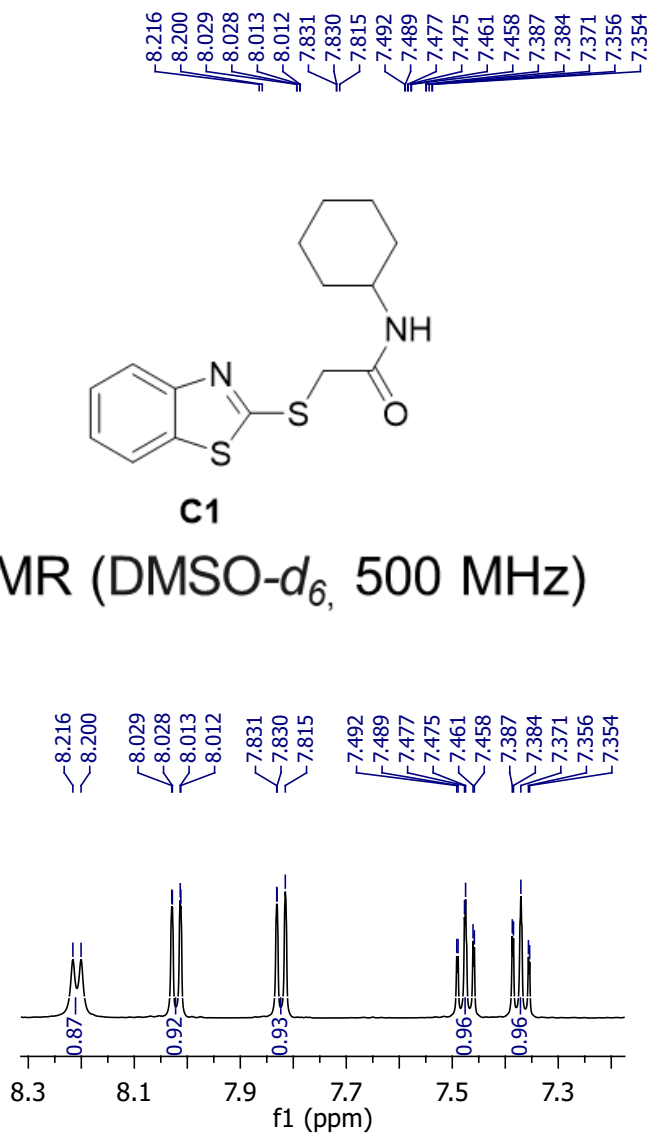
$^{13}\text{C}$  NMR (DMSO- $d_6$ , 125 MHz)

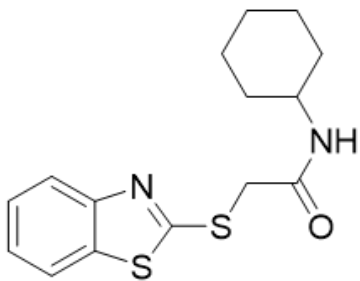




C1

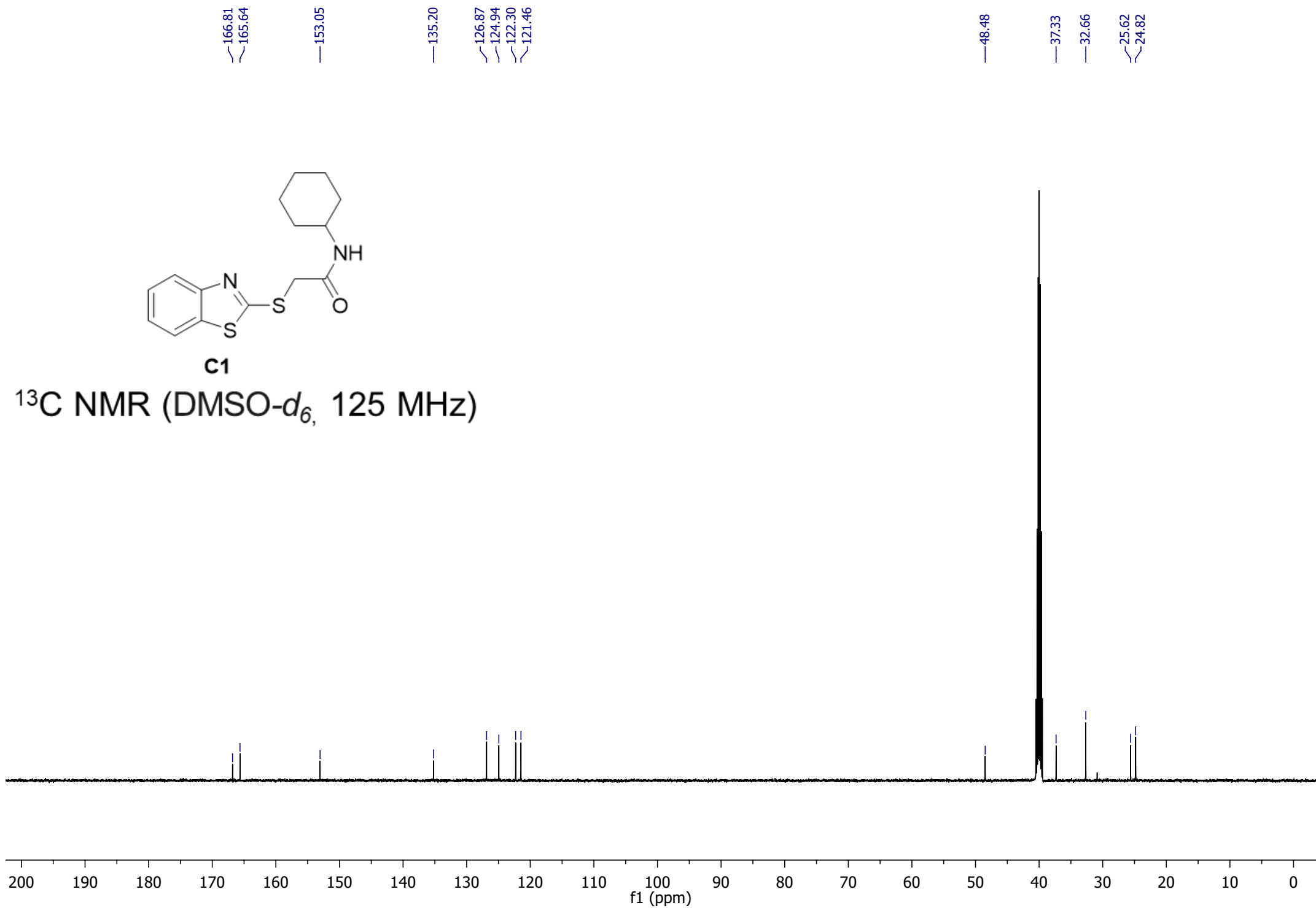
$^1\text{H}$  NMR (DMSO- $d_6$ , 500 MHz)

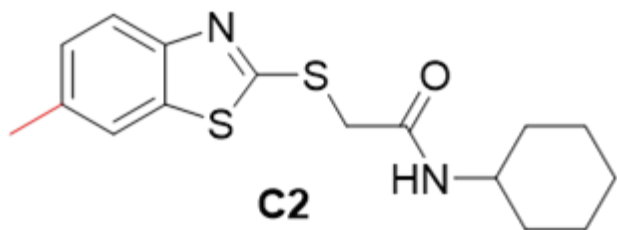




C1

$^{13}\text{C}$  NMR (DMSO- $d_6$ , 125 MHz)



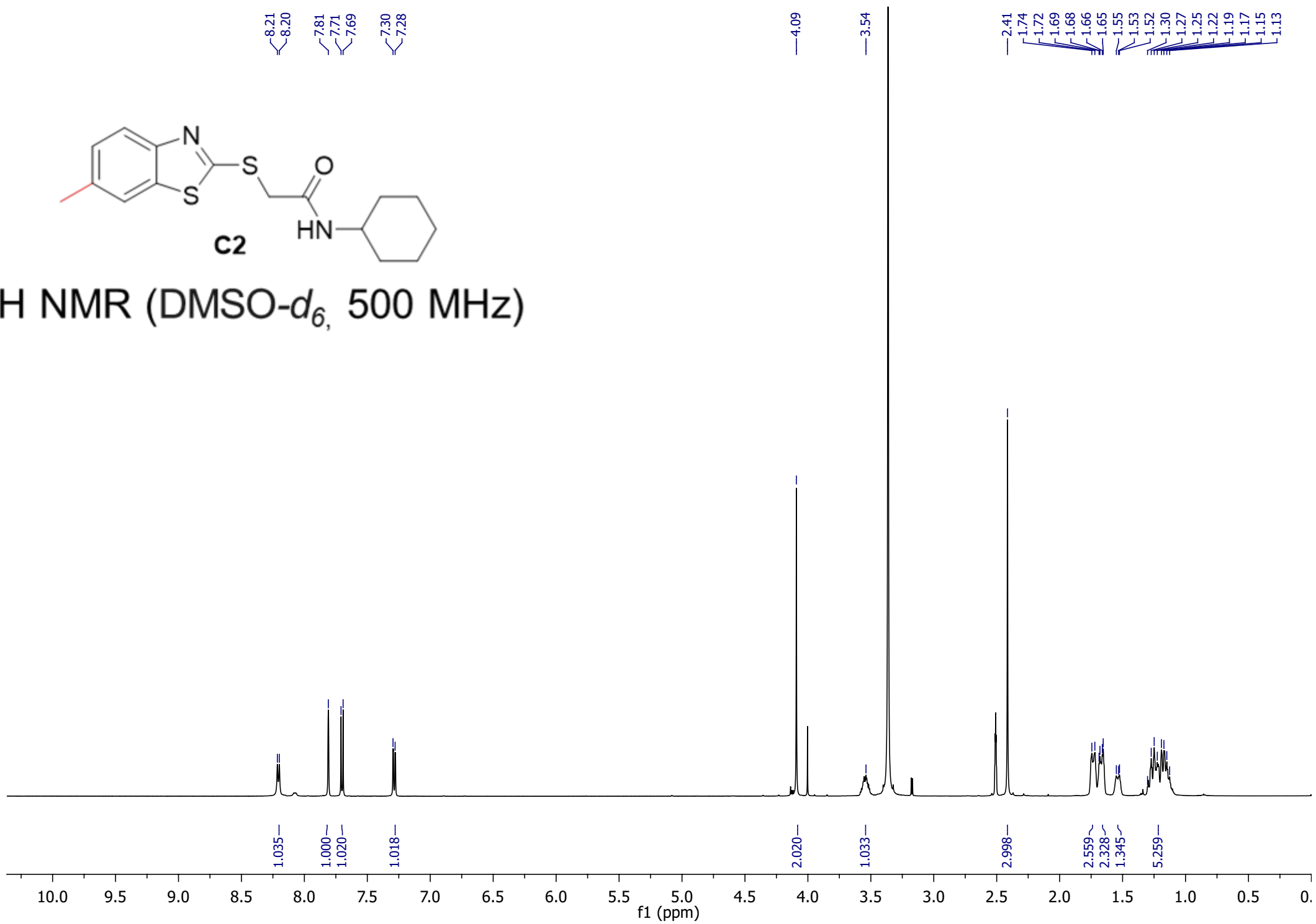


8.21  
8.20  
7.81  
7.71  
7.69  
7.30  
7.28

4.09  
3.54

2.41  
1.74  
1.72  
1.69  
1.68  
1.66  
1.65  
1.55  
1.53  
1.52  
1.30  
1.27  
1.25  
1.22  
1.19  
1.17  
1.15  
1.13

$^1\text{H}$  NMR (DMSO- $d_6$ , 500 MHz)





165.68  
165.36

151.19

135.33  
134.61

128.18

121.90  
121.05

48.45

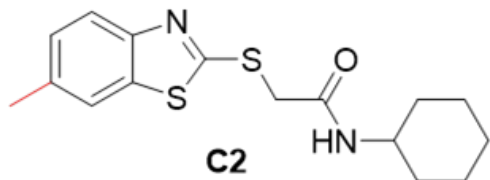
37.30

32.66

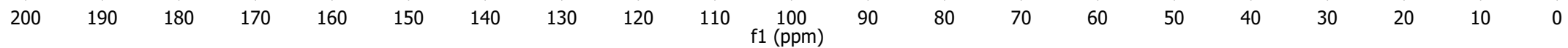
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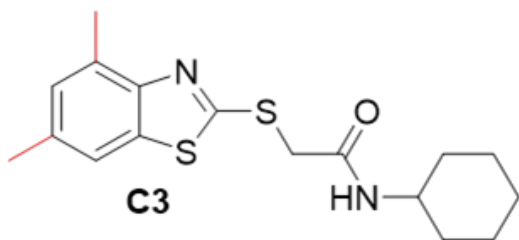
24.82

21.40

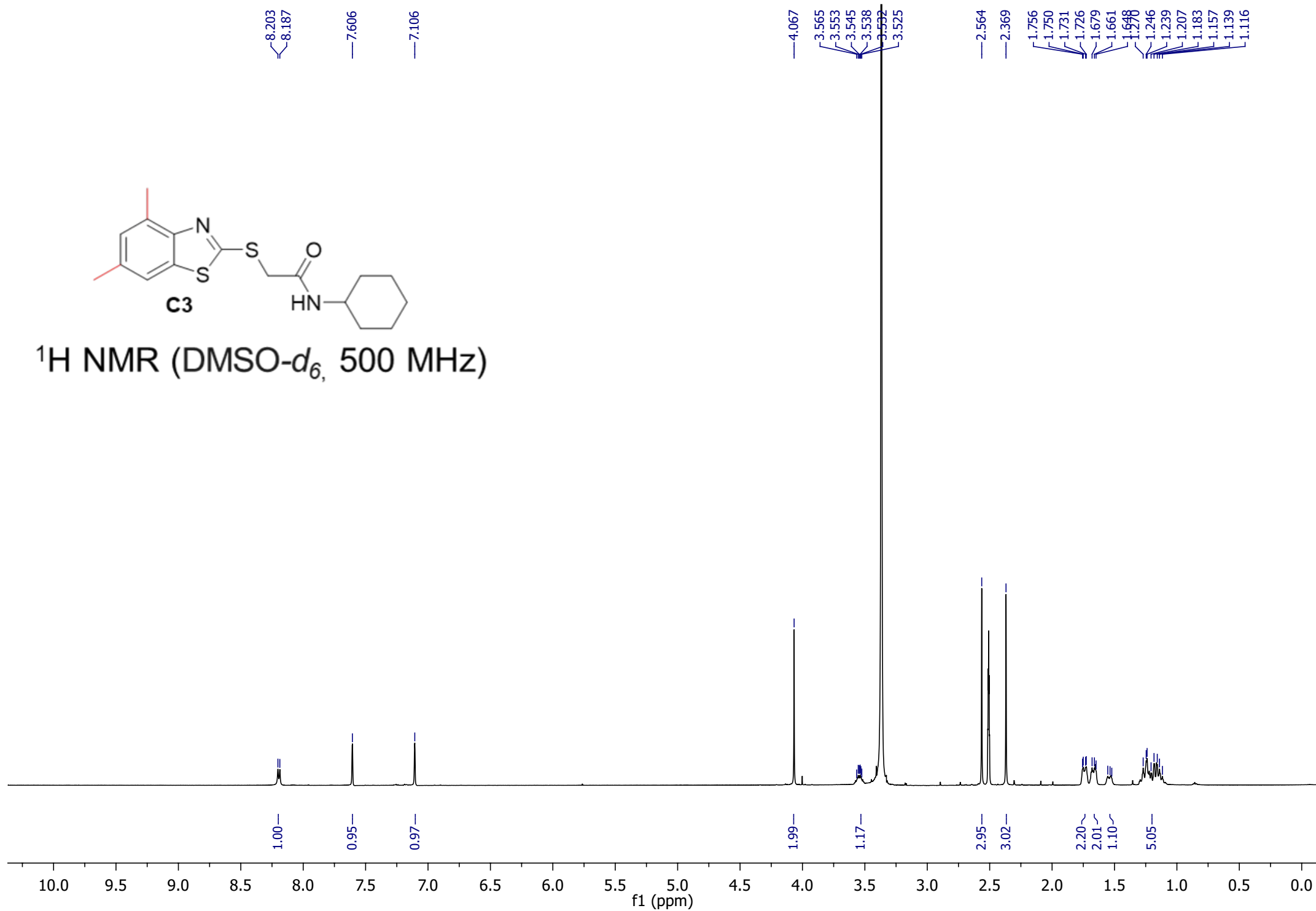


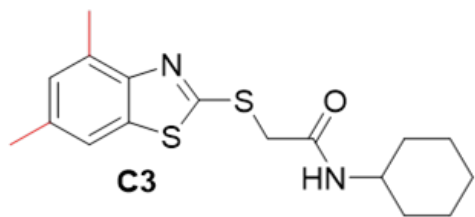
<sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 125 MHz)



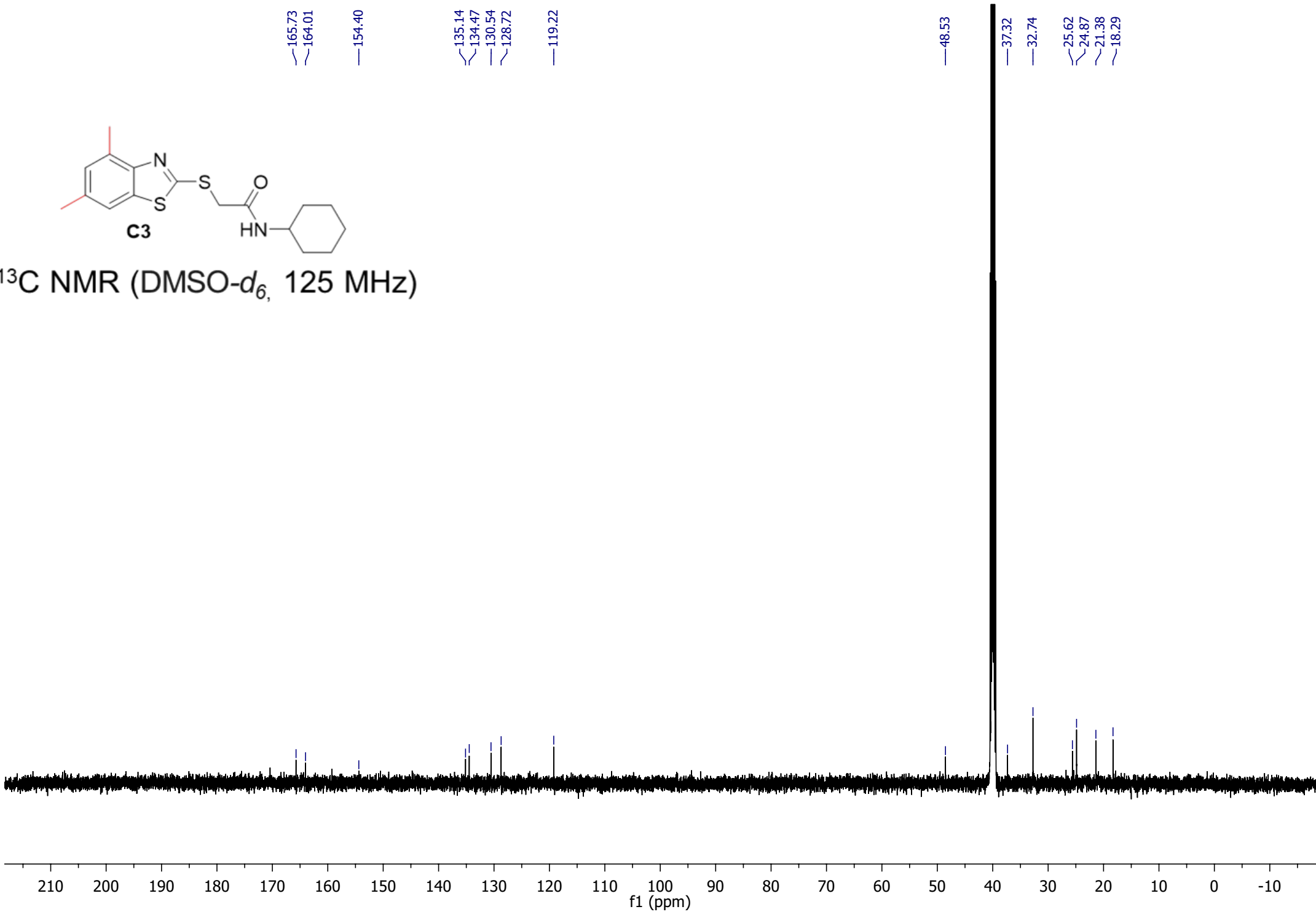


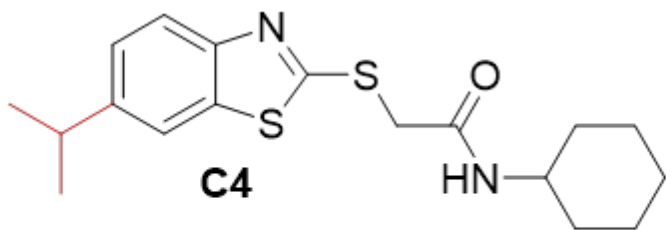
$^1\text{H NMR}$  (DMSO- $d_6$ , 500 MHz)



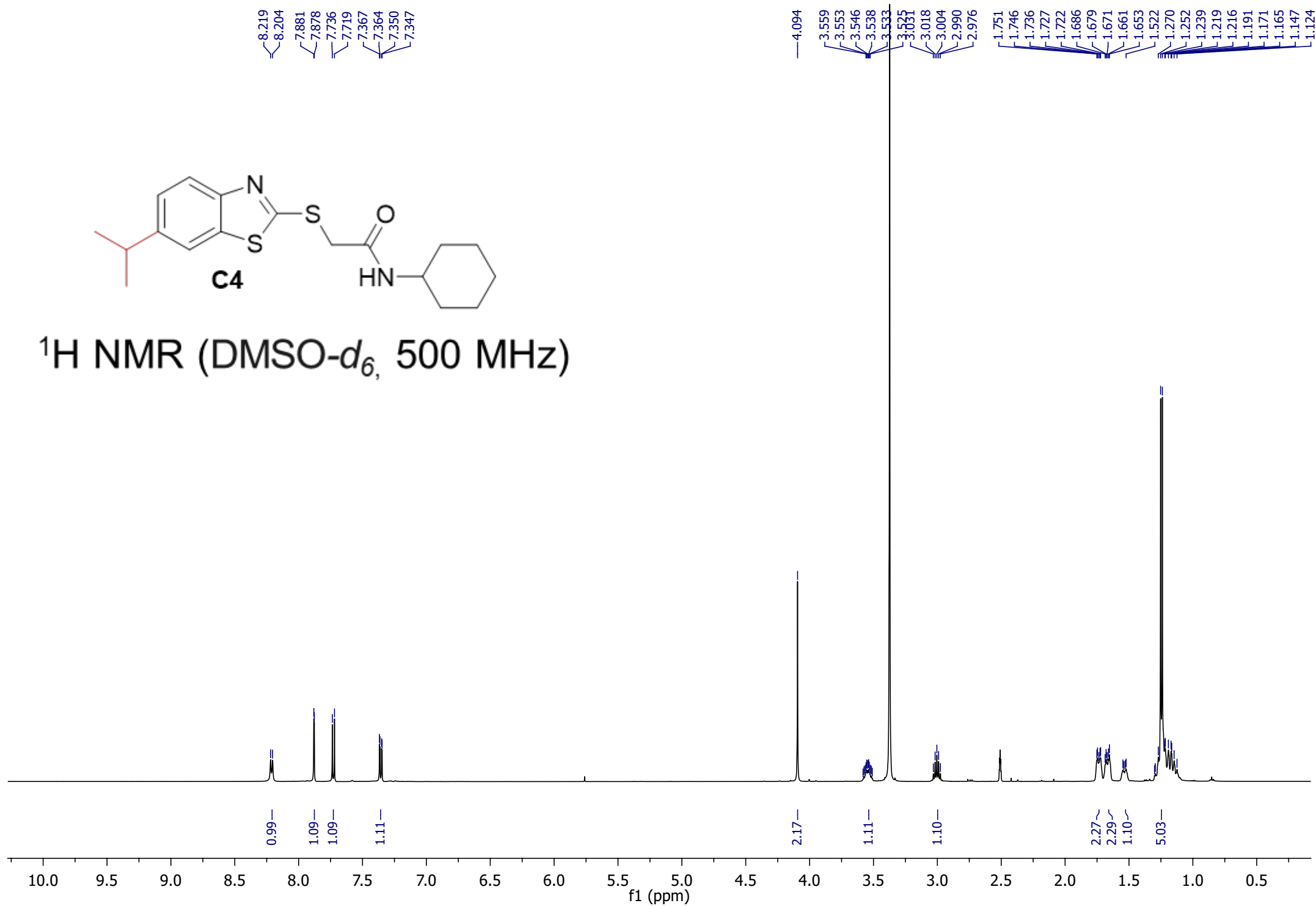


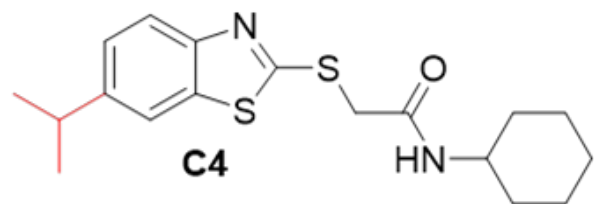
<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 125 MHz)





$^1\text{H}$  NMR (DMSO- $d_6$ , 500 MHz)

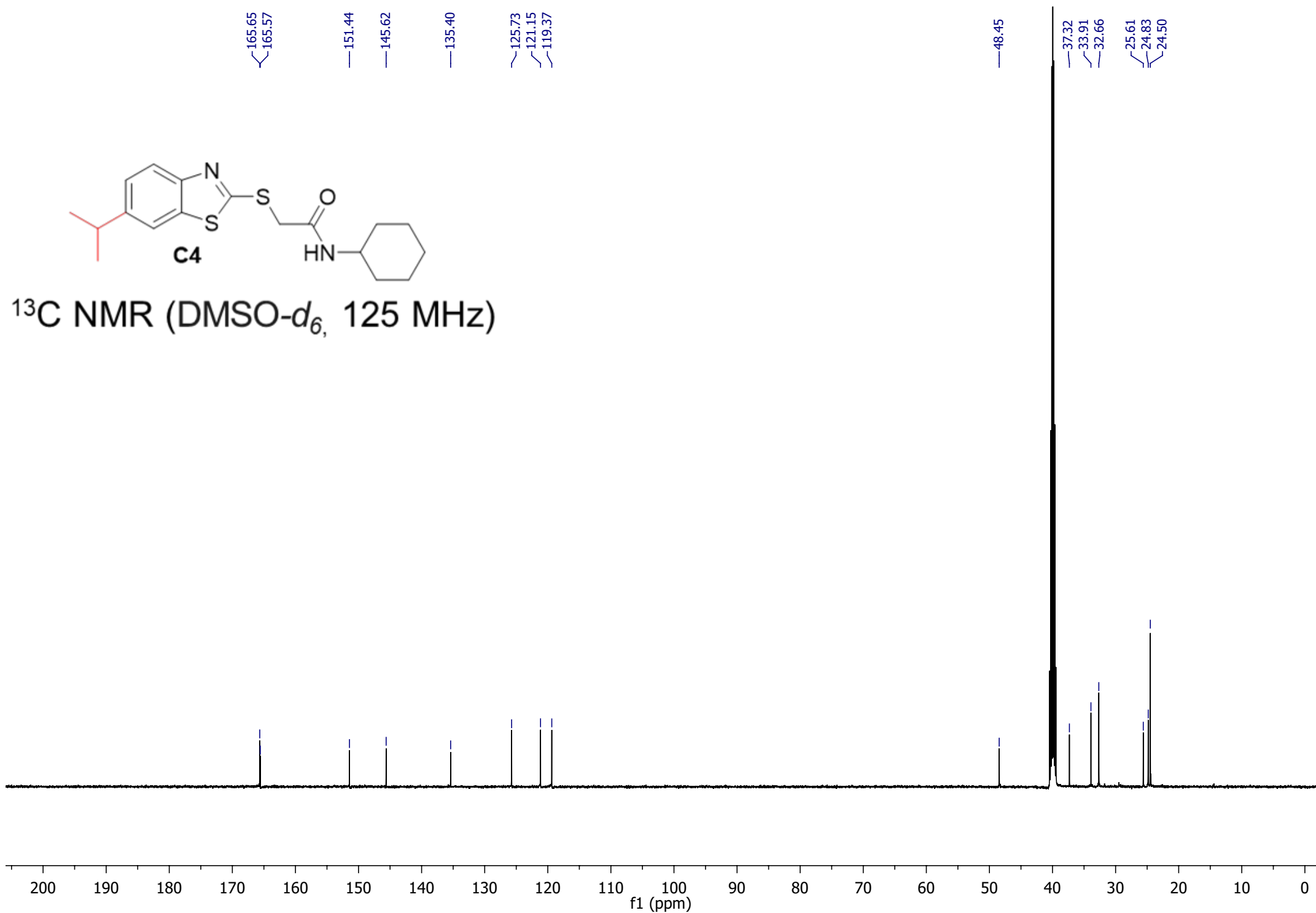




<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 125 MHz)

165.65  
165.57  
151.44  
145.62  
135.40  
125.73  
121.15  
119.37

48.45  
37.32  
33.91  
32.66  
25.61  
24.83  
24.50

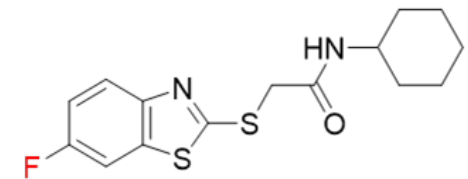


8.22  
8.21  
7.98  
7.97  
7.96  
7.95  
7.84  
7.83  
7.82  
7.81  
7.36  
7.36  
7.35  
7.34  
7.33  
7.32

4.11

3.57  
3.55  
3.53  
3.51

1.75  
1.75  
1.73  
1.72  
1.69  
1.68  
1.67  
1.66  
1.65  
1.55  
1.54  
1.54  
1.53  
1.27  
1.25  
1.24  
1.23  
1.22  
1.19  
1.17  
1.15  
1.13



C5

<sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 500 MHz)

1.00

1.10

1.12

1.24

2.08

1.26

2.39

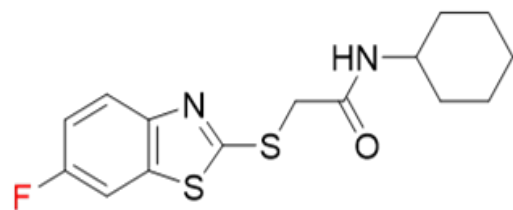
2.37

1.30

5.32

10.0 9.5 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 0.0

f1 (ppm)



C5

$^{13}\text{C}$  NMR (DMSO- $d_6$ , 125 MHz)

—165.58

—149.94

—136.53  
—136.50

—122.55  
—122.48

—115.16  
—114.97

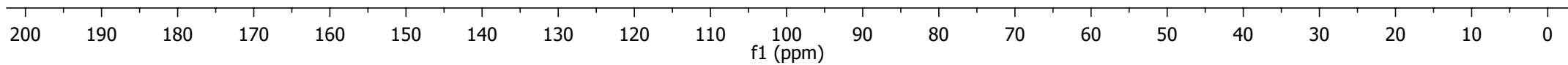
—109.08  
—108.86

—48.48

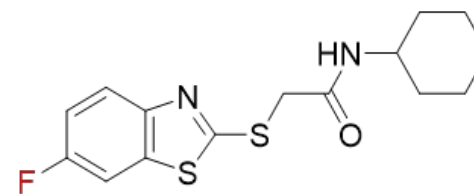
—37.37

—32.66

—25.61  
—24.83

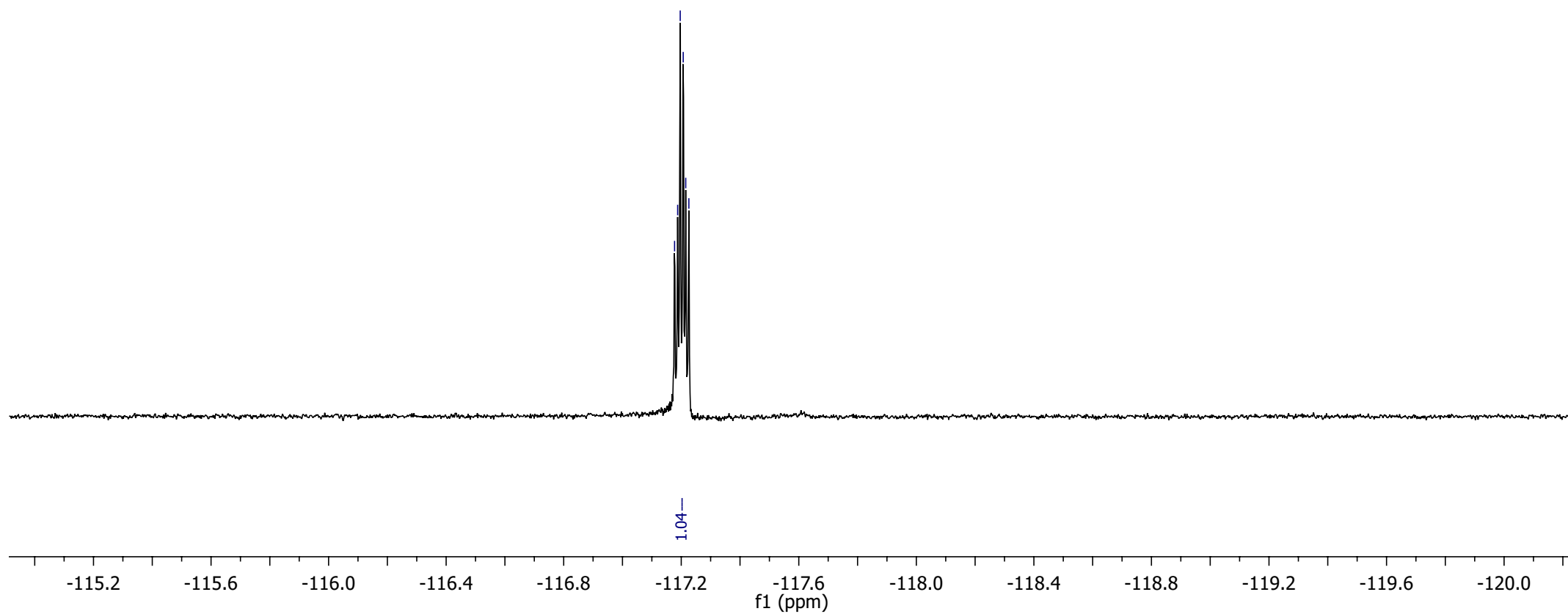


117.18  
117.19  
117.20  
117.21  
117.22  
117.23

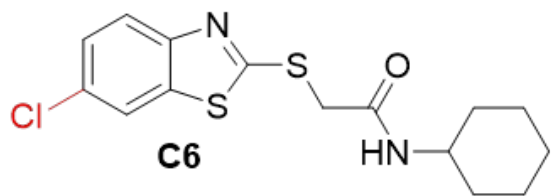


C5

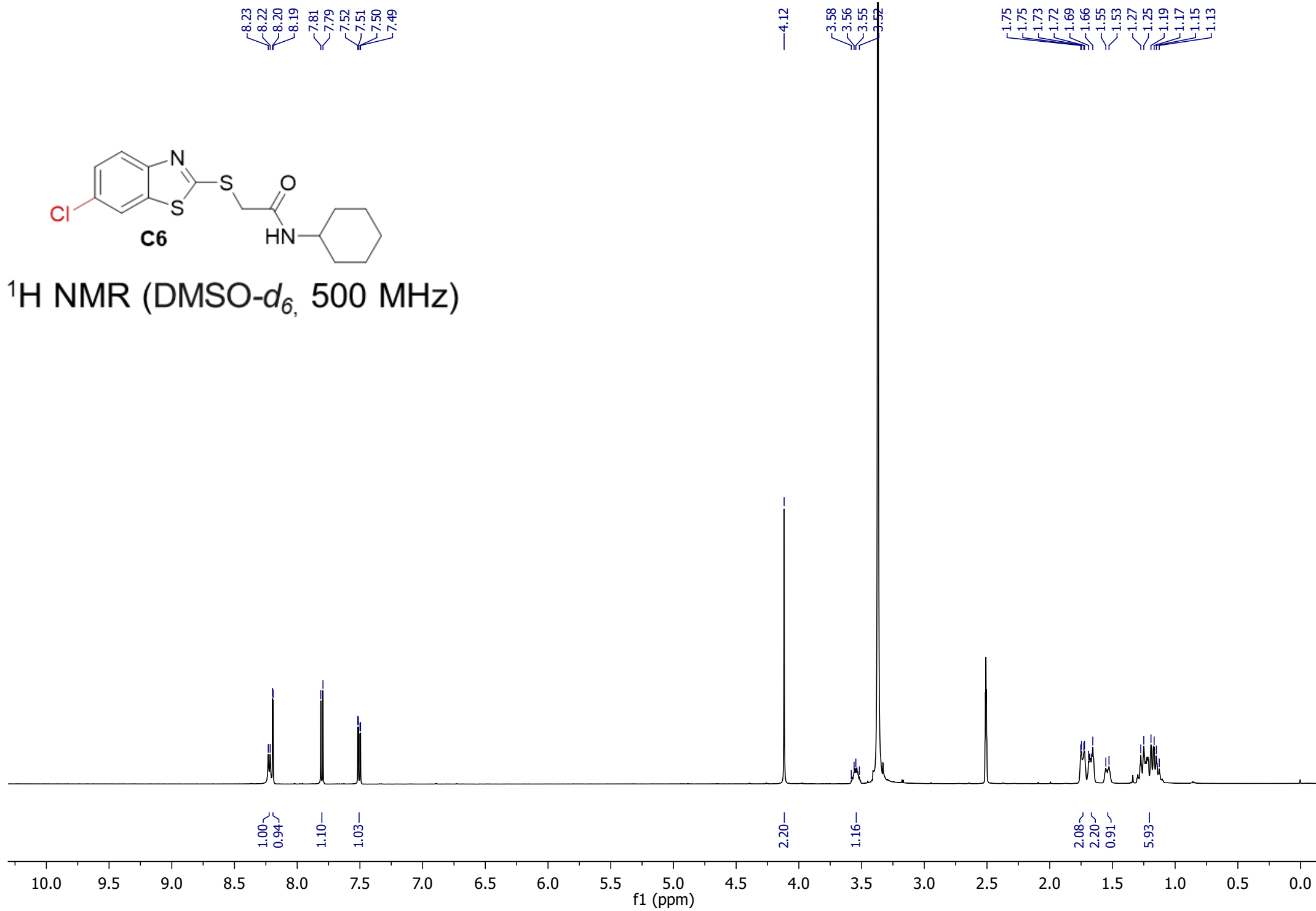
$^{19}\text{F}$  NMR (DMSO- $d_6$ , 471 MHz)

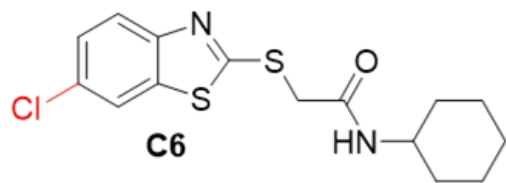






$^1\text{H}$  NMR (DMSO- $d_6$ , 500 MHz)

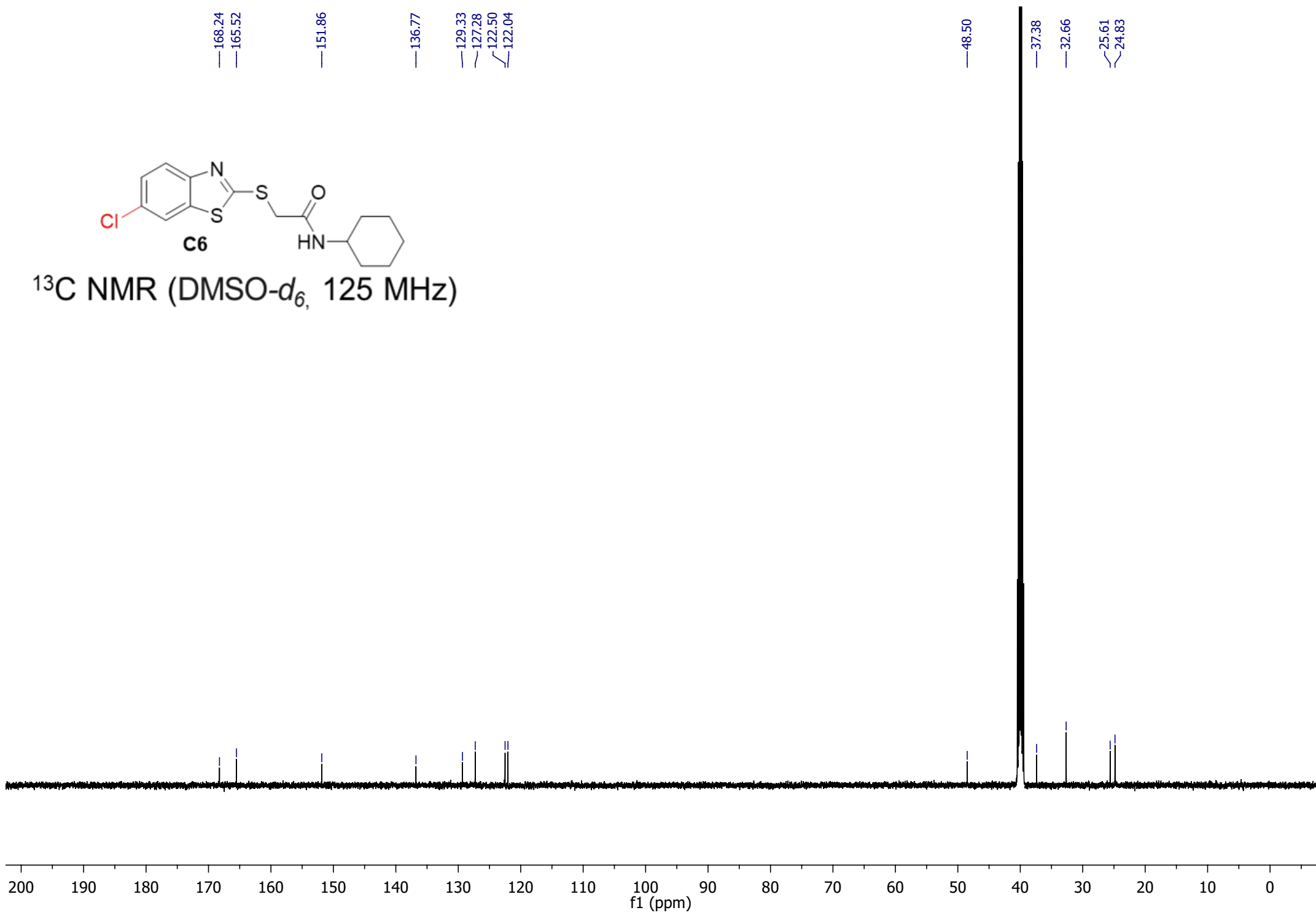


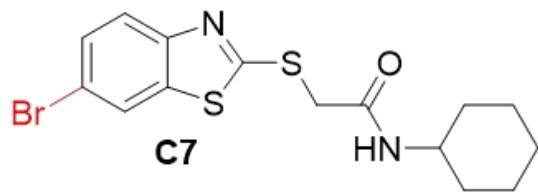


<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 125 MHz)

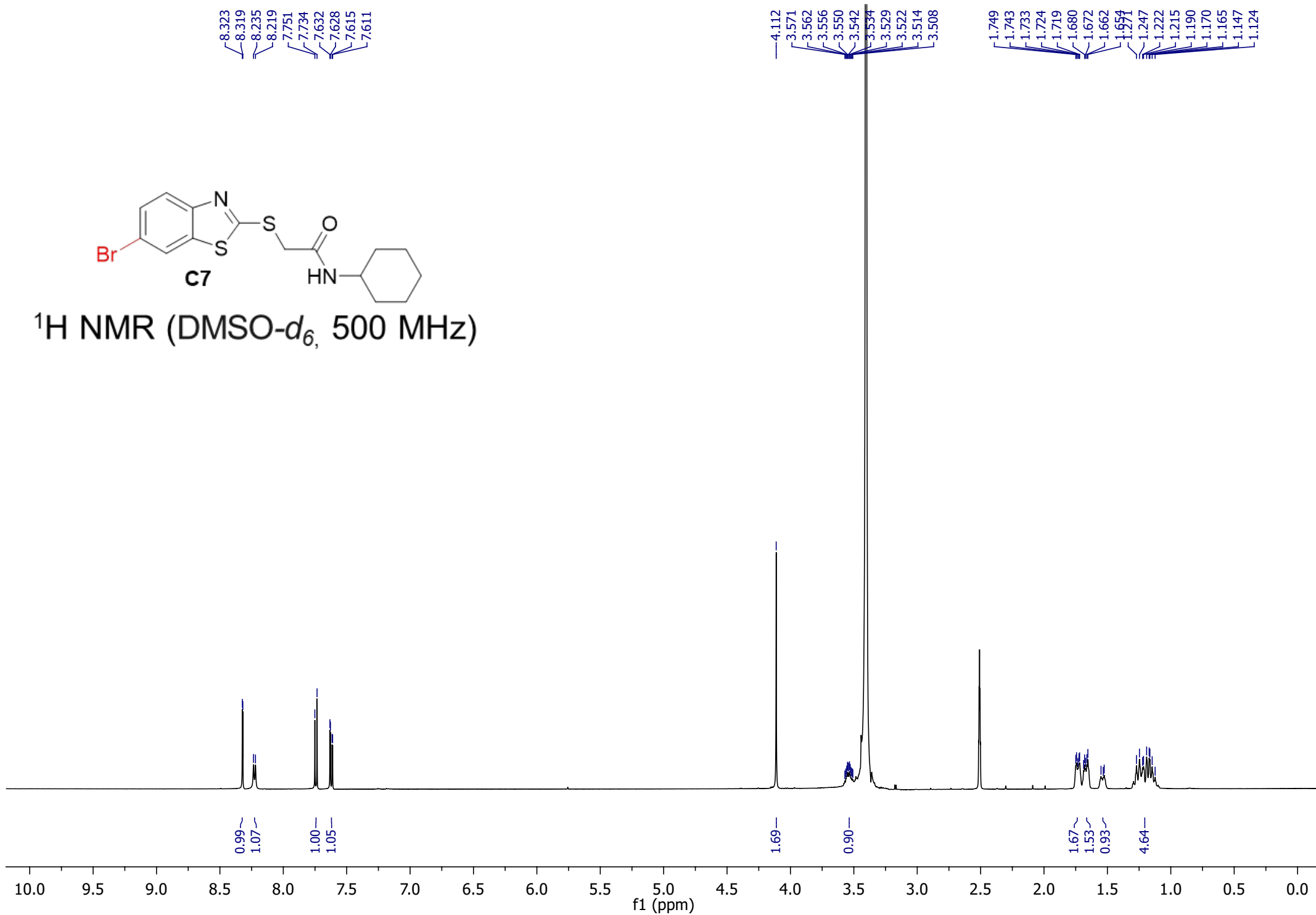
—168.24  
—165.52  
—151.86  
—136.77  
—129.33  
—127.28  
—122.50  
—122.04

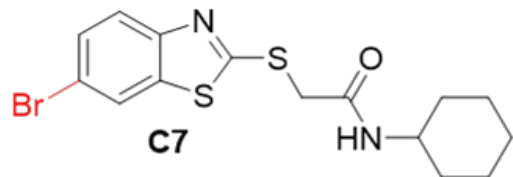
—48.50  
—37.38  
—32.66  
—25.61  
—24.83



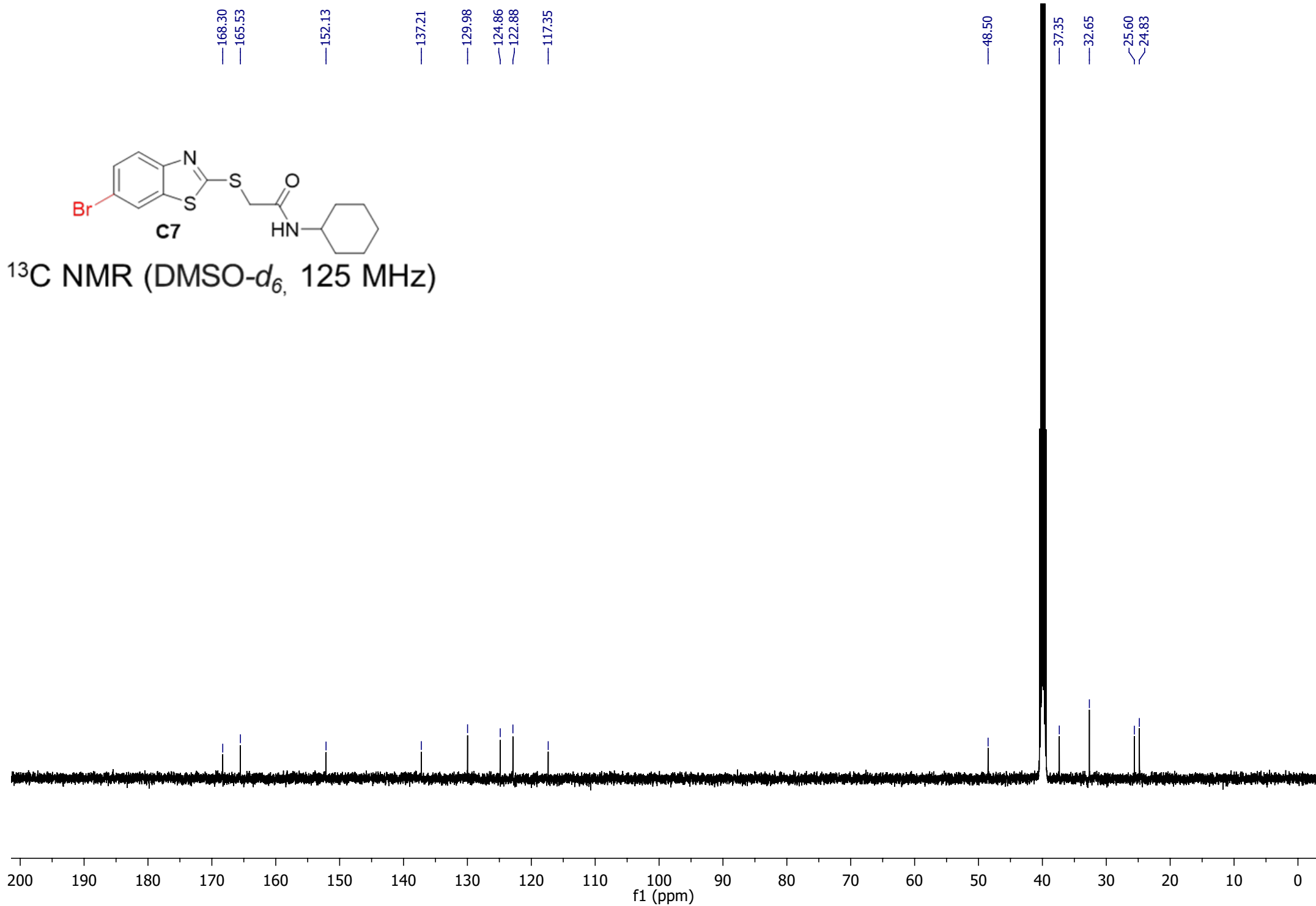


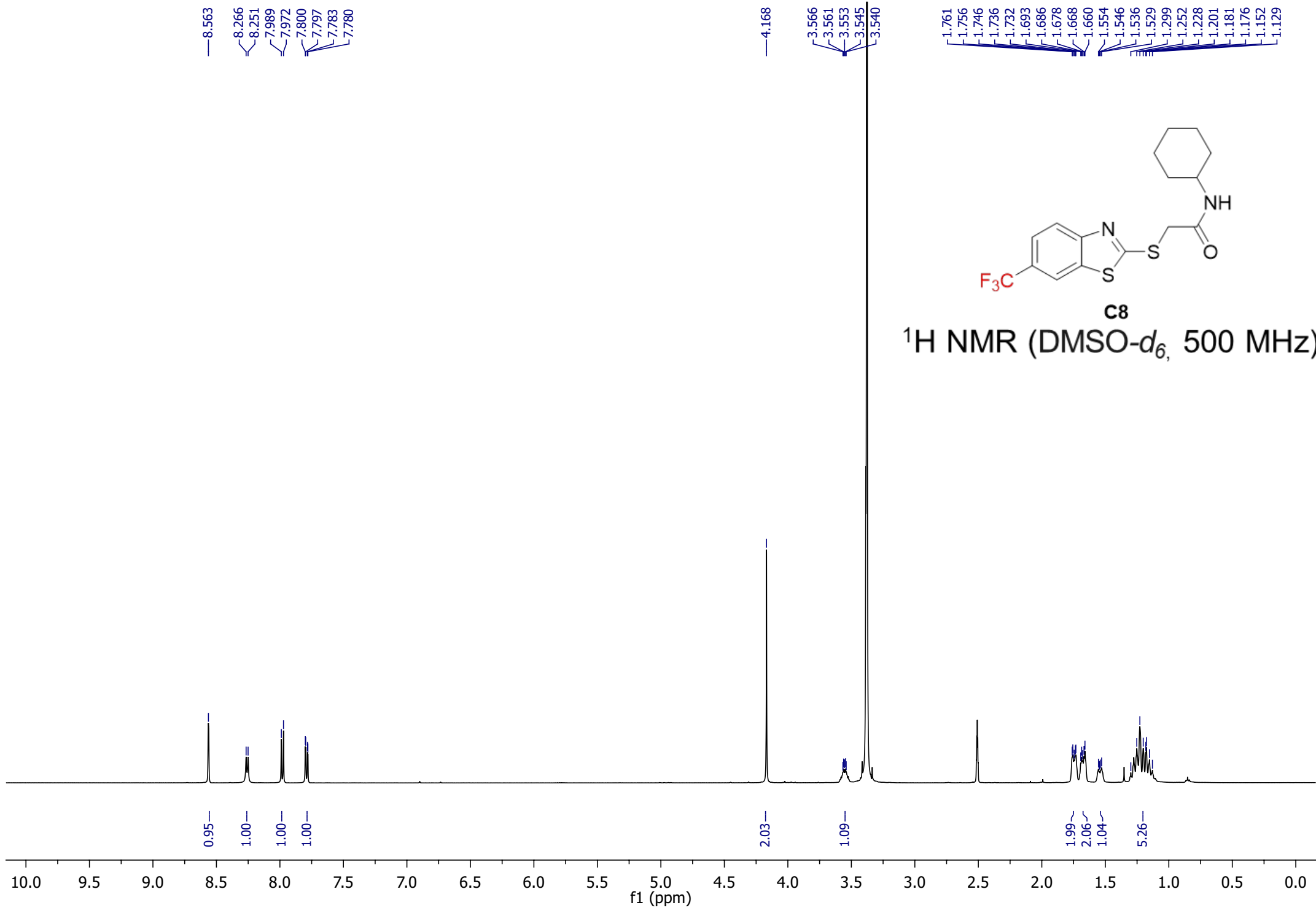
$^1\text{H}$  NMR (DMSO- $d_6$ , 500 MHz)

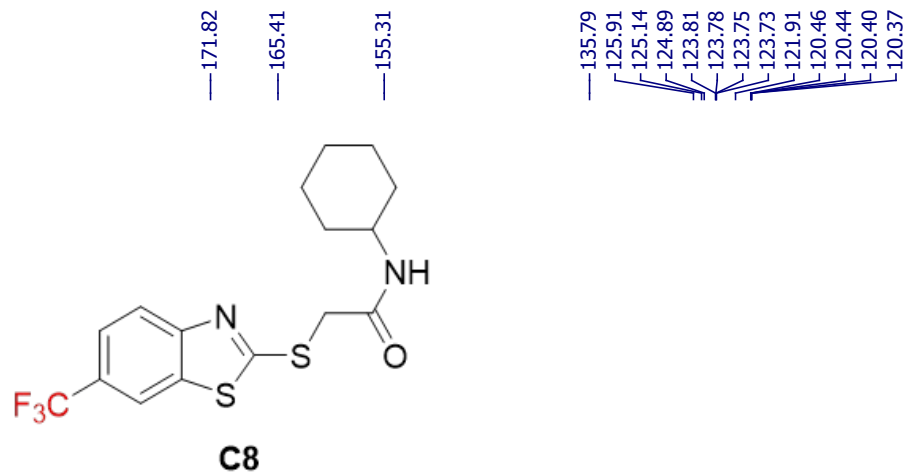




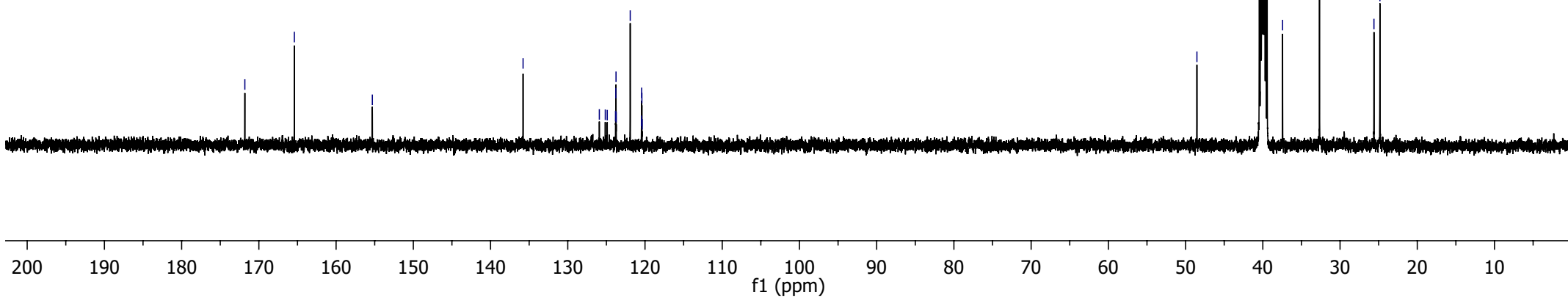
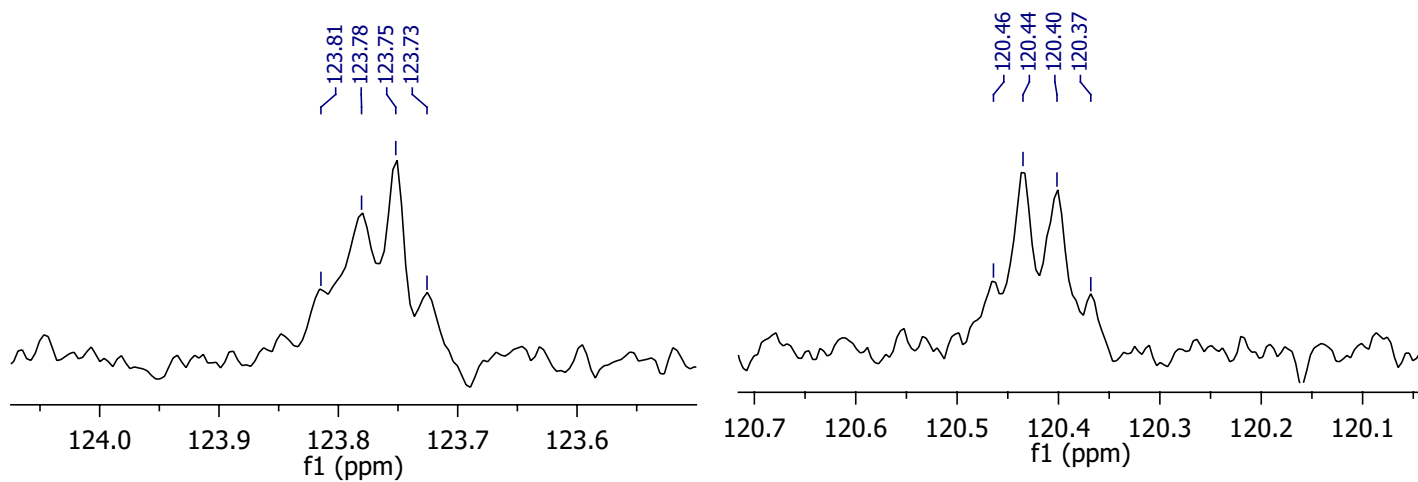
<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 125 MHz)

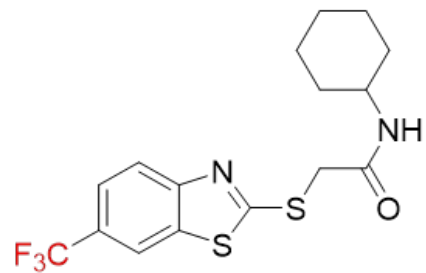






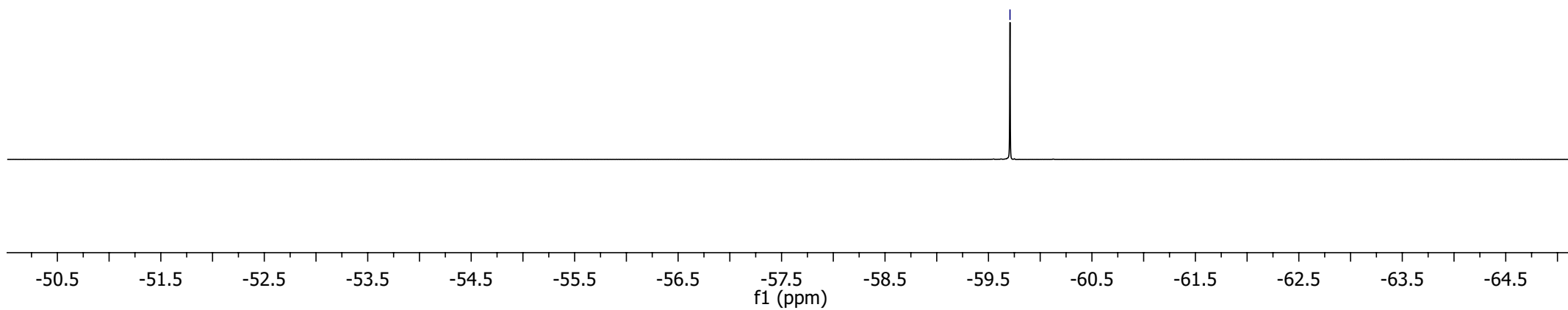
**13C NMR (DMSO-d<sub>6</sub>, 125 MHz)**





**C8**

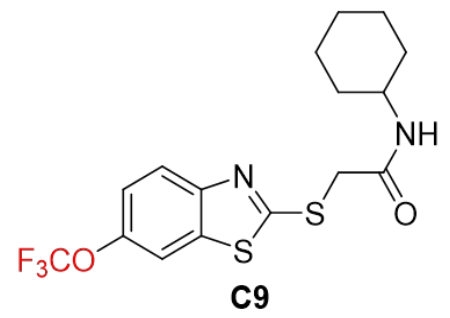
<sup>19</sup>F NMR (DMSO-*d*<sub>6</sub>, 471 MHz)



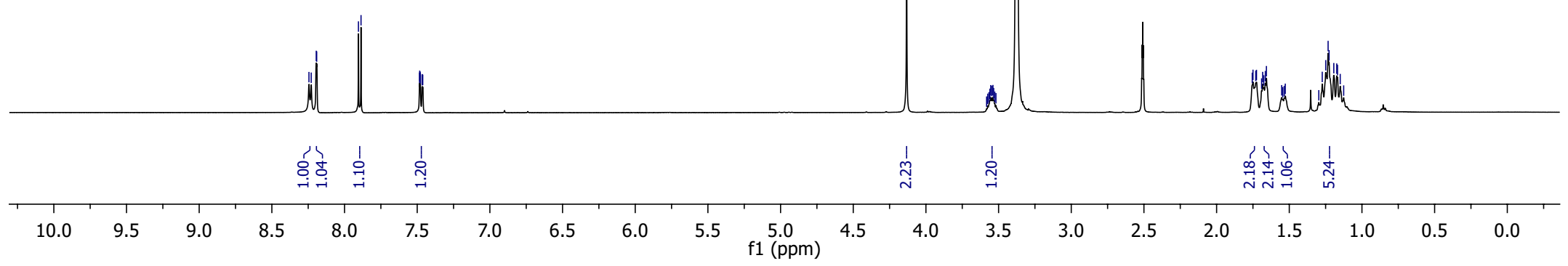
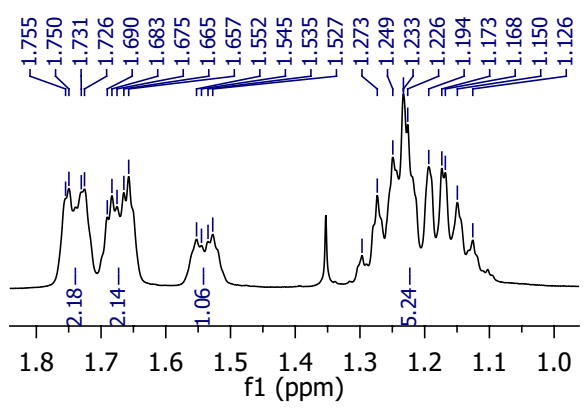
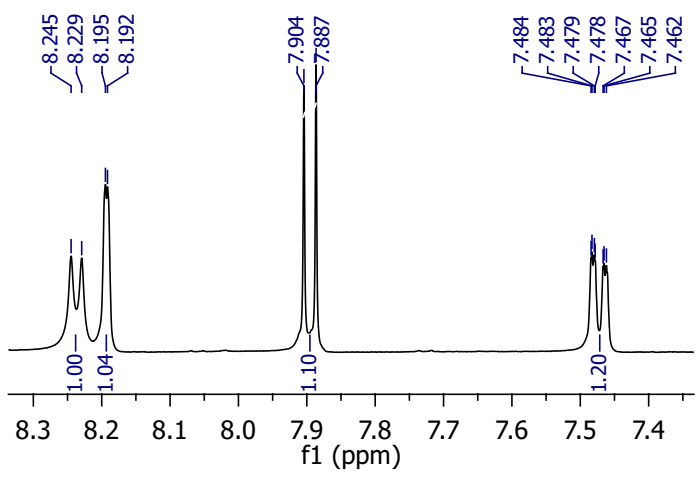
8.245  
8.229  
8.195  
8.192  
7.904  
7.887  
7.484  
7.483  
7.479  
7.478  
7.467  
7.465  
7.462

4.133  
3.582  
3.575  
3.566  
3.560  
3.554  
3.546  
3.539  
3.534  
3.526  
3.518

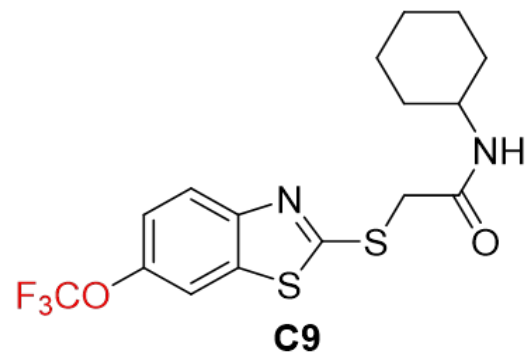
1.755  
1.750  
1.731  
1.726  
1.690  
1.683  
1.675  
1.665  
1.657  
1.552  
1.545  
1.535  
1.527  
1.297  
1.273  
1.249  
1.233  
1.226  
1.194  
1.173  
1.168  
1.150  
1.126



<sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 500 MHz)



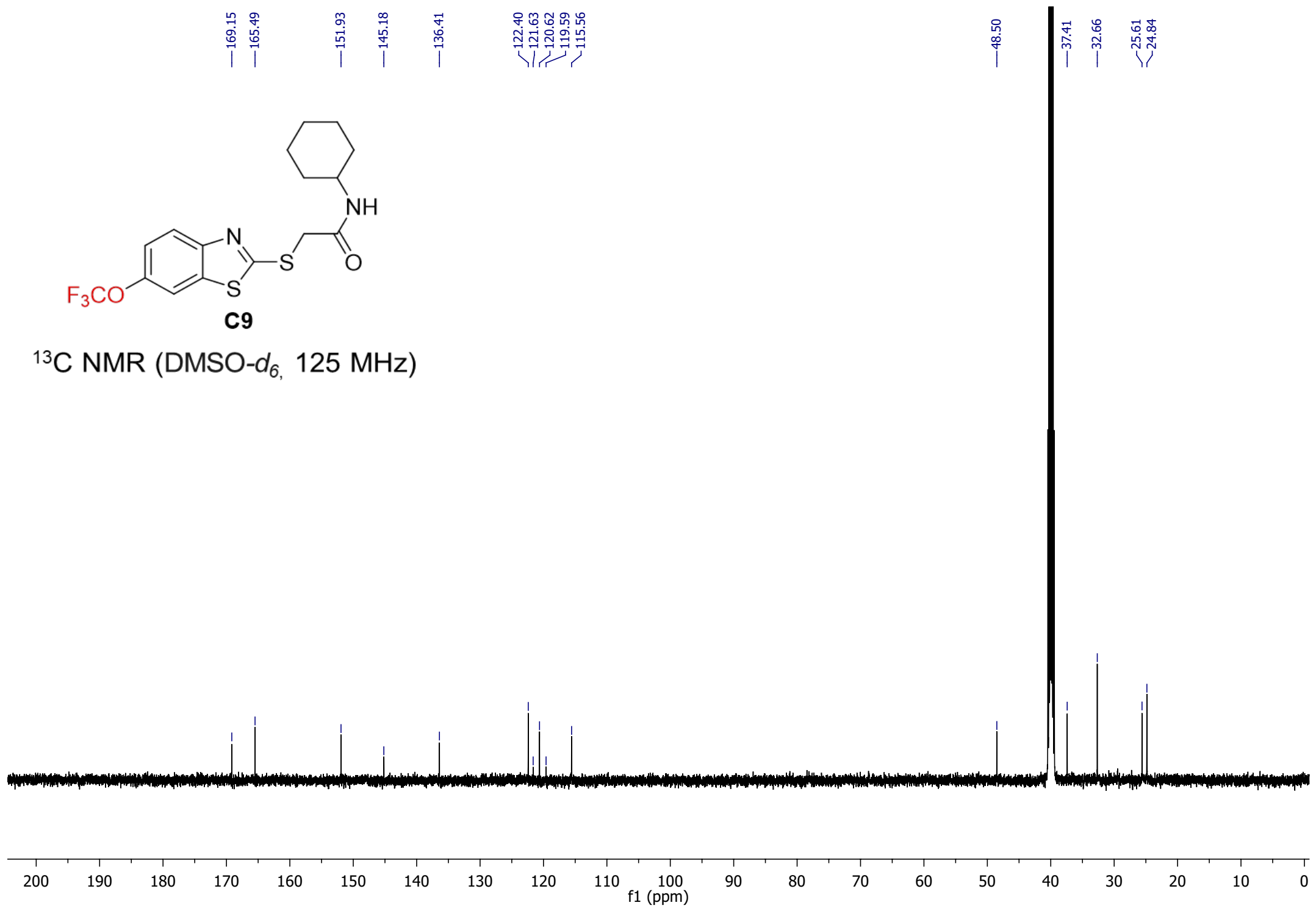


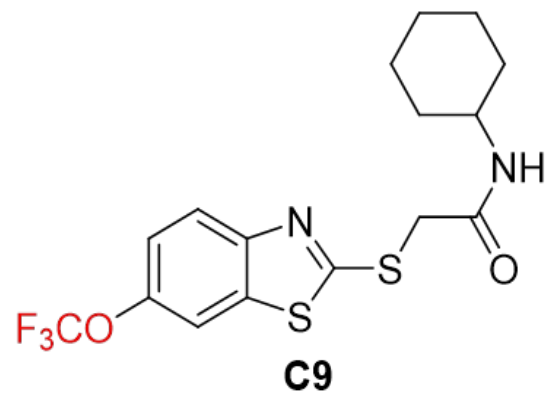


$^{13}\text{C}$  NMR (DMSO- $d_6$ , 125 MHz)

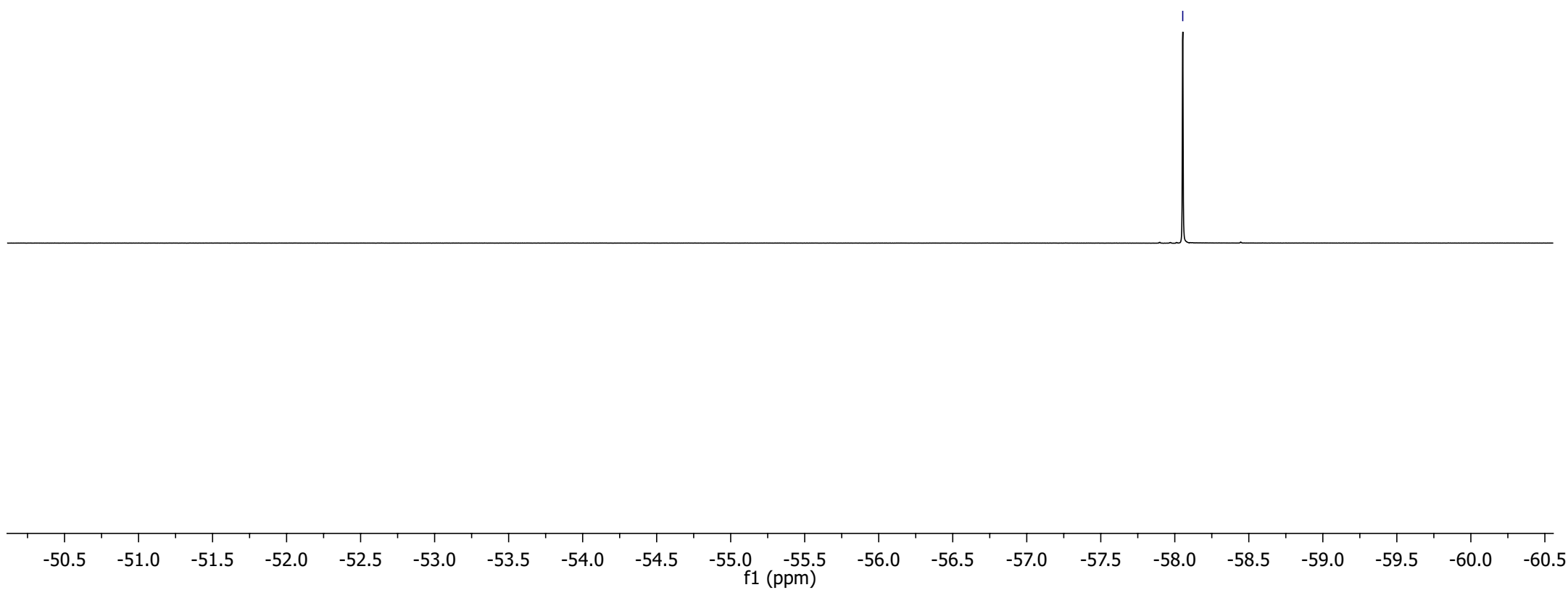
—169.15  
—165.49  
—151.93  
—145.18  
—136.41  
—122.40  
—121.63  
—120.62  
—119.59  
—115.56

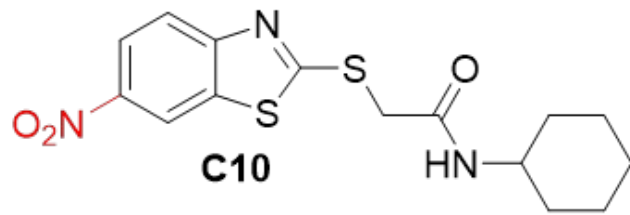
—48.50  
—37.41  
—32.66  
—25.61  
—24.84





$^{19}\text{F}$  NMR (DMSO- $d_6$ , 471 MHz)



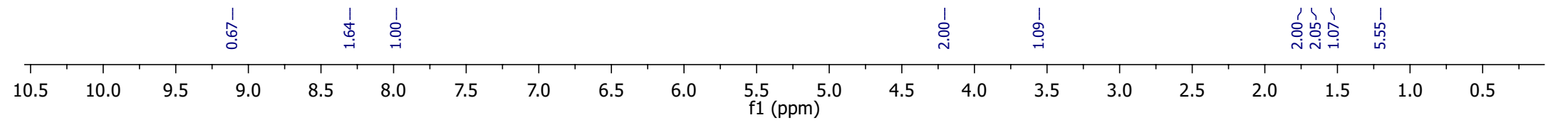


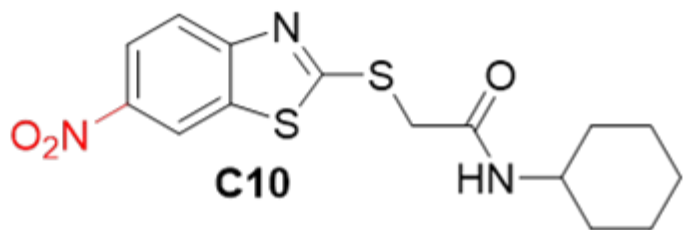
<sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 500 MHz)

9.110  
9.106  
8.321  
8.316  
8.303  
8.298  
8.289  
8.274  
7.976  
7.959

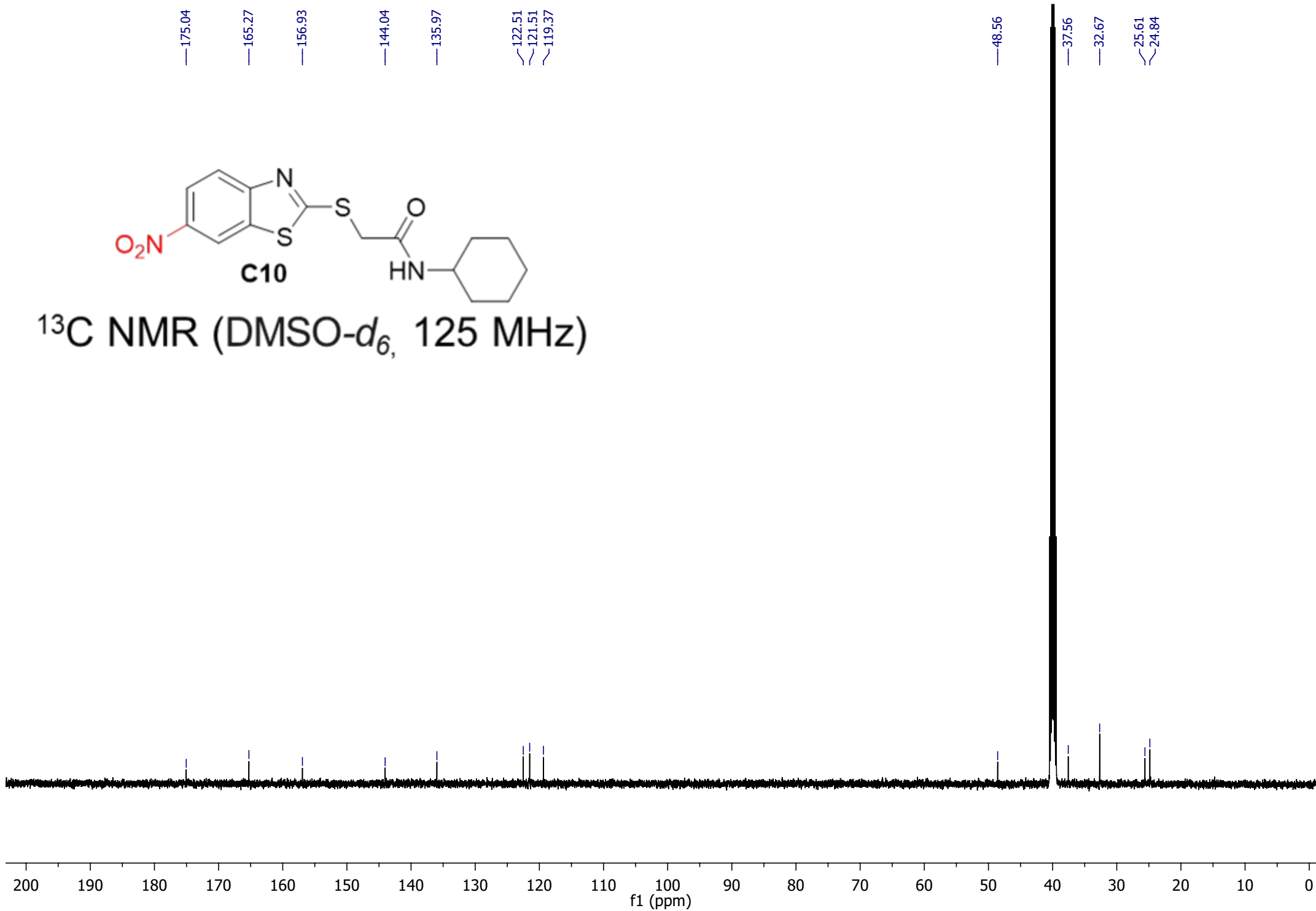
4.196  
3.584  
3.569  
3.563  
3.556  
3.548  
3.543  
3.536  
3.527

1.761  
1.751  
1.737  
1.698  
1.691  
1.684  
1.673  
1.665  
1.559  
1.551  
1.534  
1.279  
1.256  
1.231  
1.206  
1.180  
1.157  
1.134





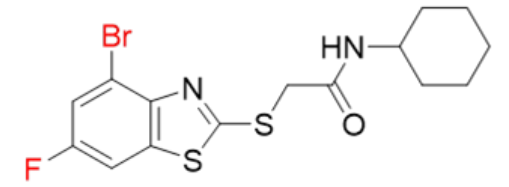
<sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 125 MHz)



8.229  
8.214  
8.035  
8.030  
8.019  
8.014  
7.744  
7.739  
7.727  
7.722

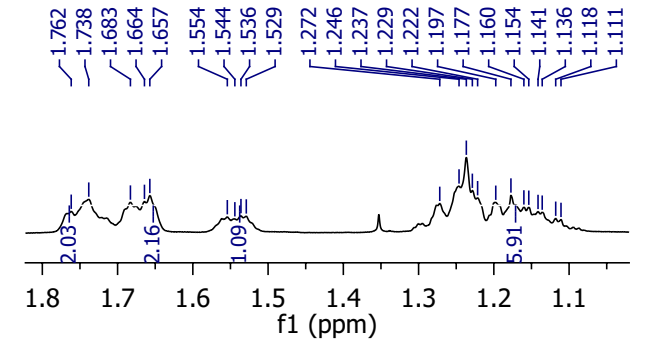
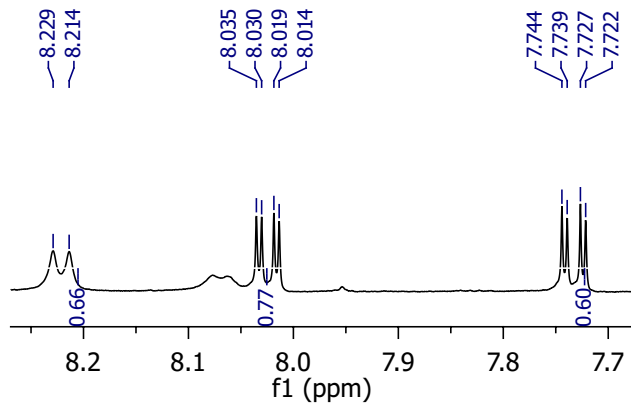
4.113  
3.998

1.762  
1.738  
1.683  
1.664  
1.657  
1.554  
1.544  
1.536  
1.529  
1.272  
1.246  
1.237  
1.229  
1.222  
1.197  
1.177  
1.160  
1.154  
1.141  
1.136  
1.118  
1.111



C11

<sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 500 MHz)



0.66  
0.77  
0.60

1.33  
0.89  
1.66

2.03  
2.16  
1.09  
5.91

10.0  
9.5  
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  
0.0  
f1 (ppm)

167.87  
167.85  
167.14

160.35  
158.36

147.53  
147.51

136.49  
136.40

118.47  
118.25

114.44  
114.36

107.25  
107.03

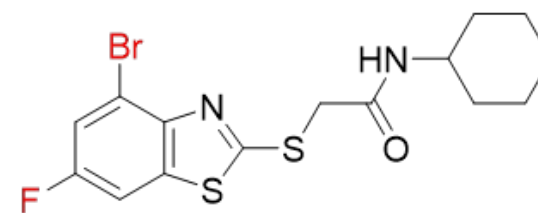
48.84

36.56

32.92

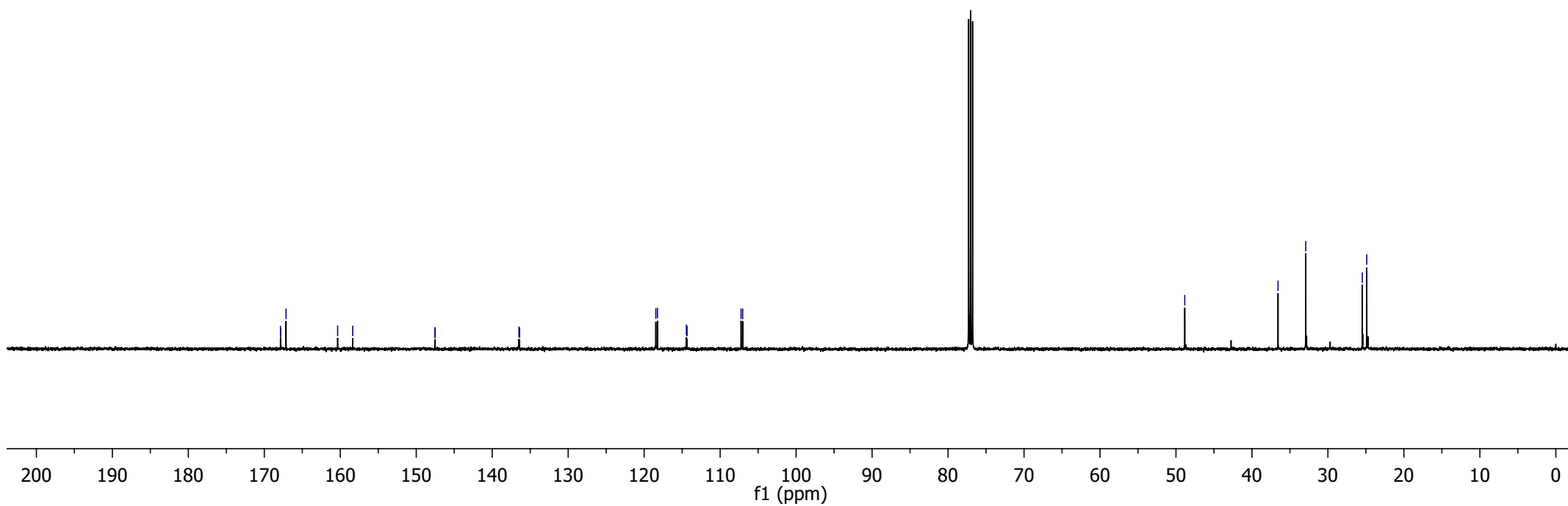
25.47

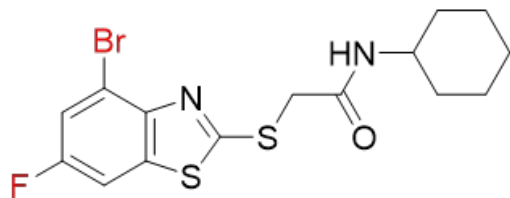
24.89



C11

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

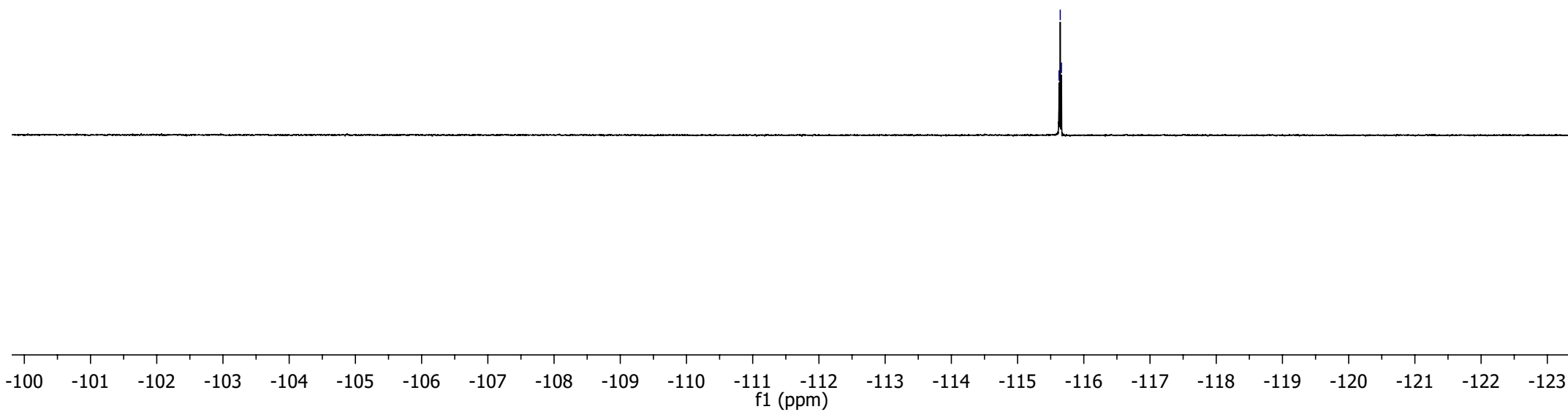


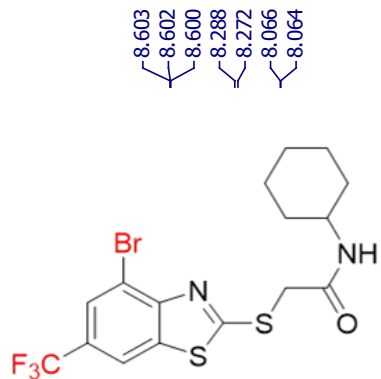


C11

$^{19}\text{F}$  NMR (DMSO- $d_6$ , 471 MHz)

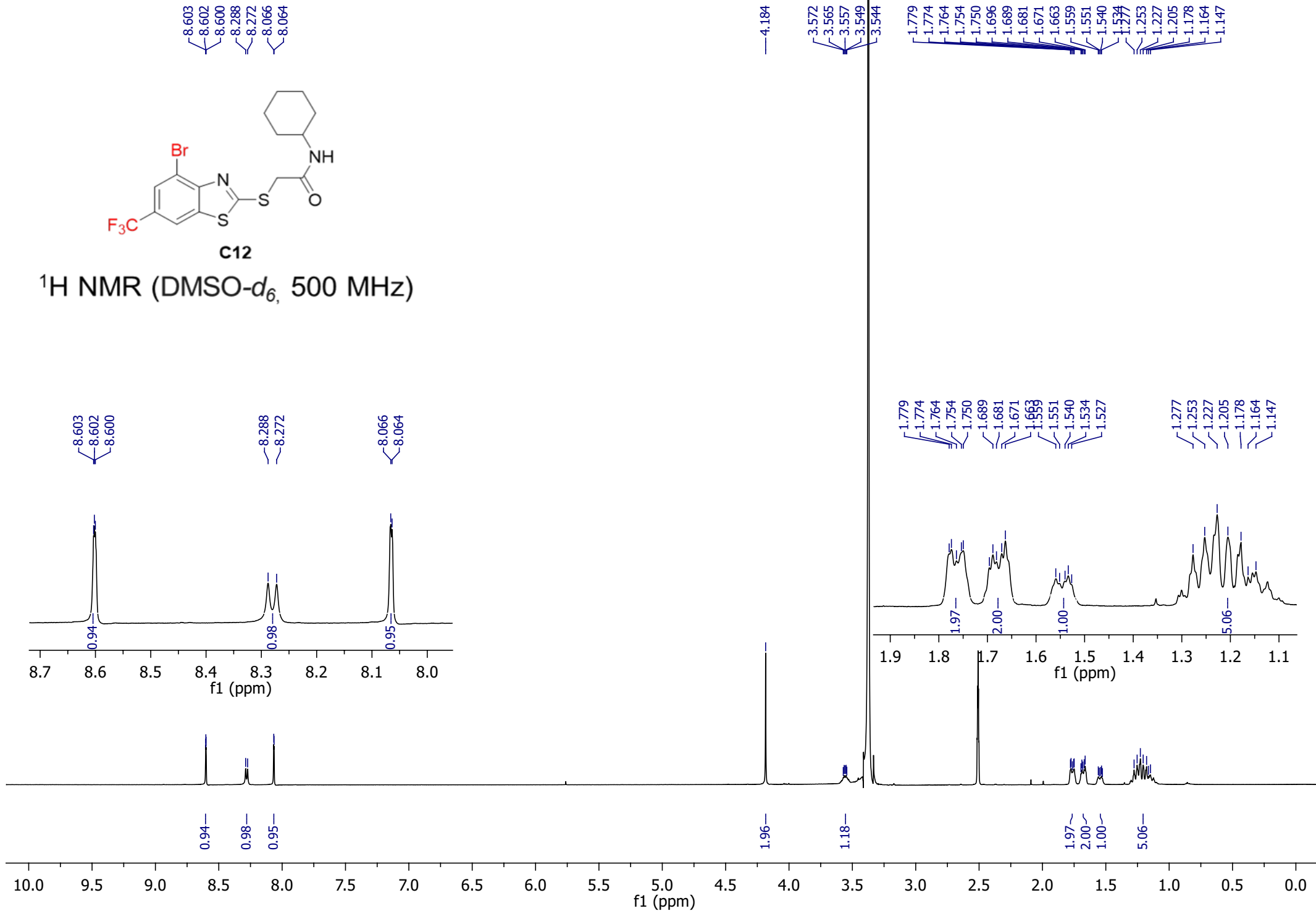
-115.626  
-115.644  
-115.663



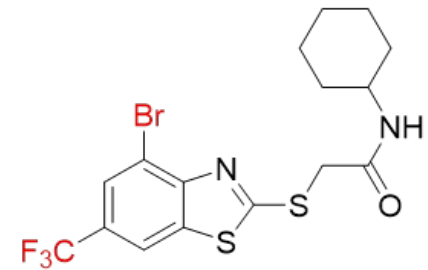
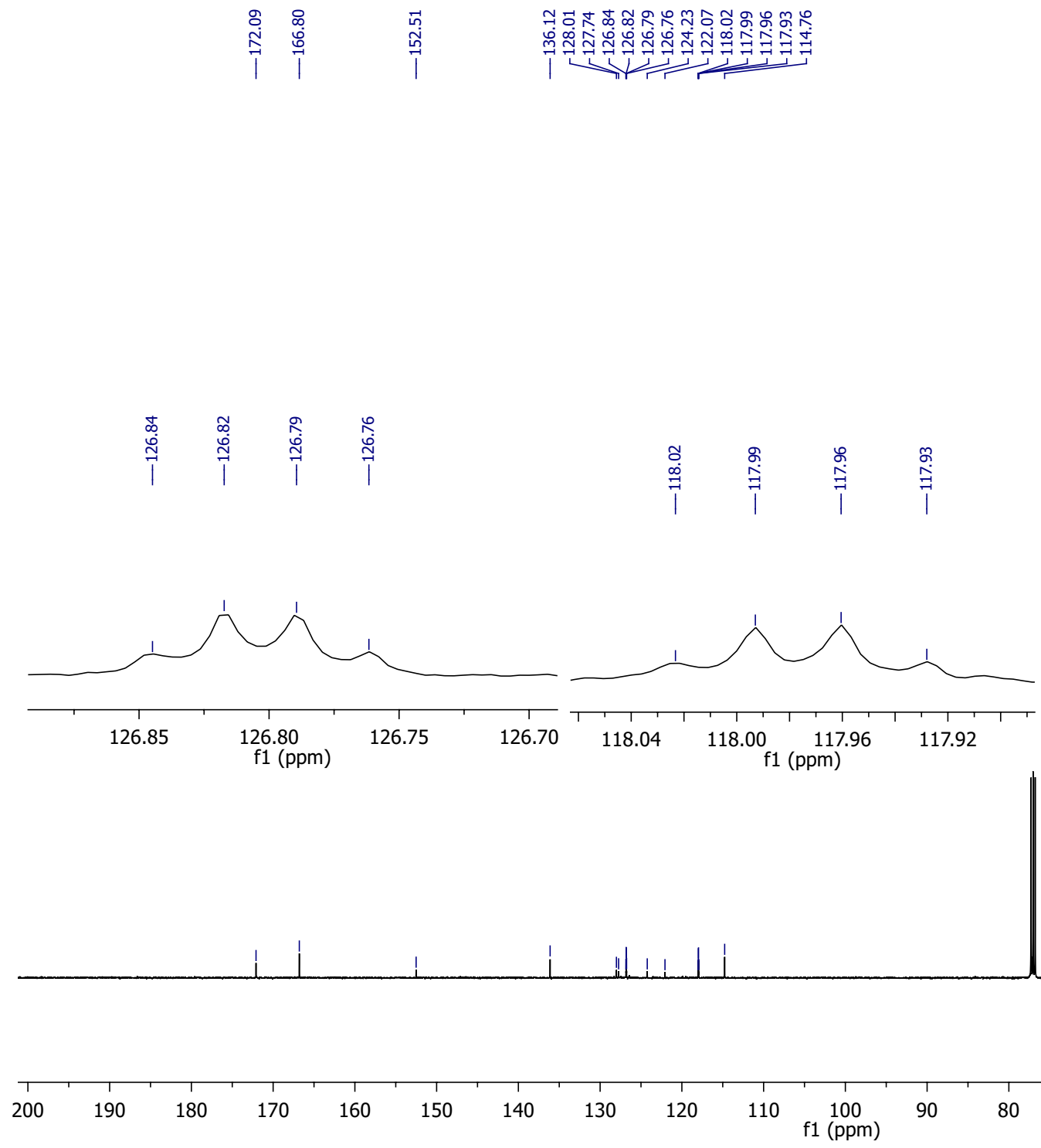


C12

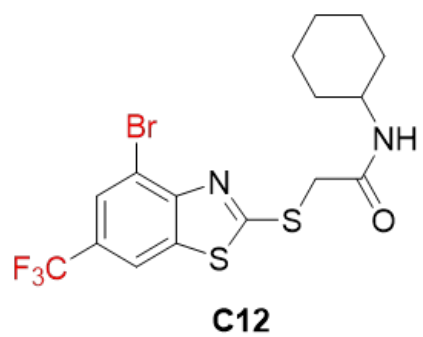
$^1\text{H}$  NMR (DMSO- $d_6$ , 500 MHz)



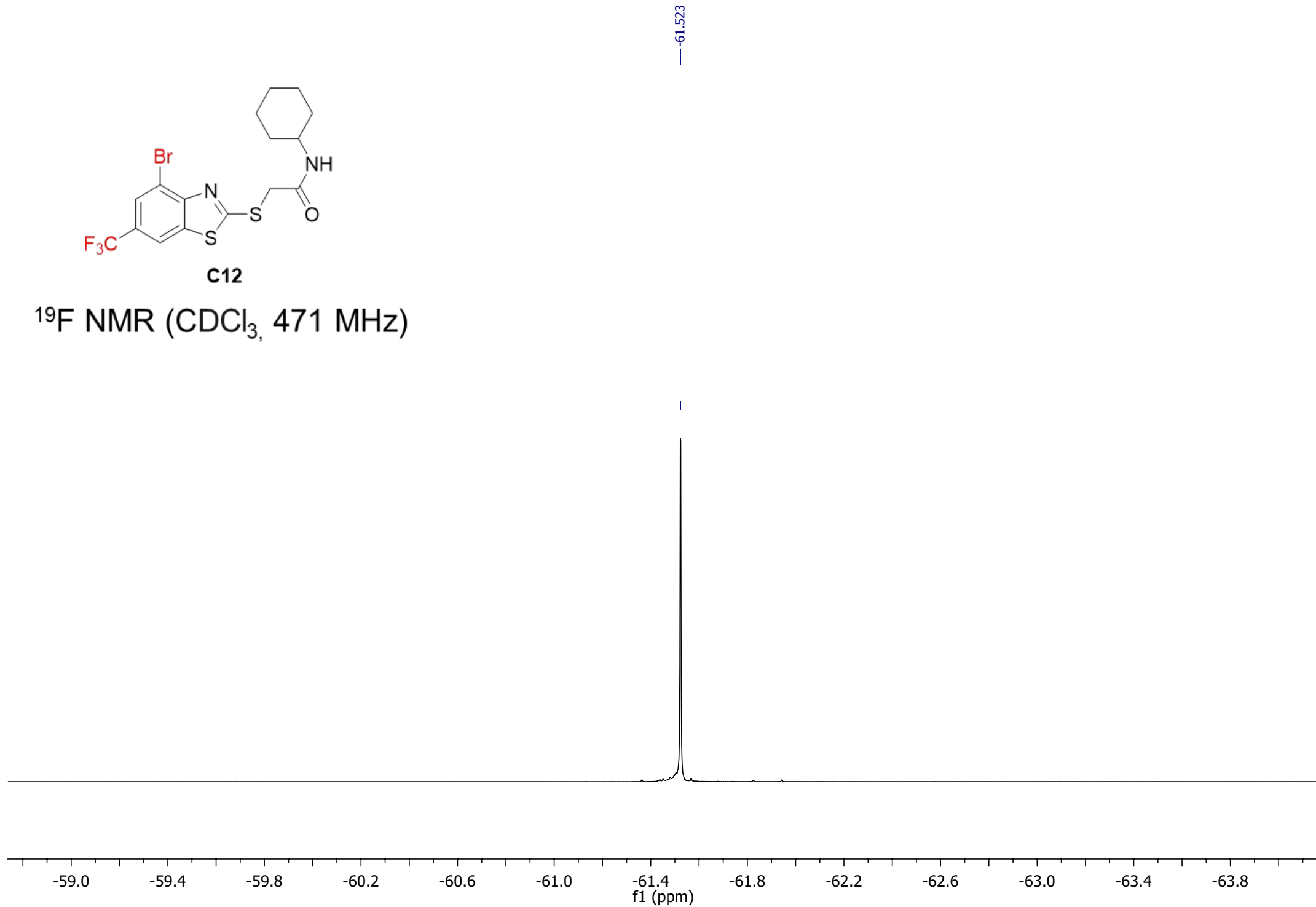


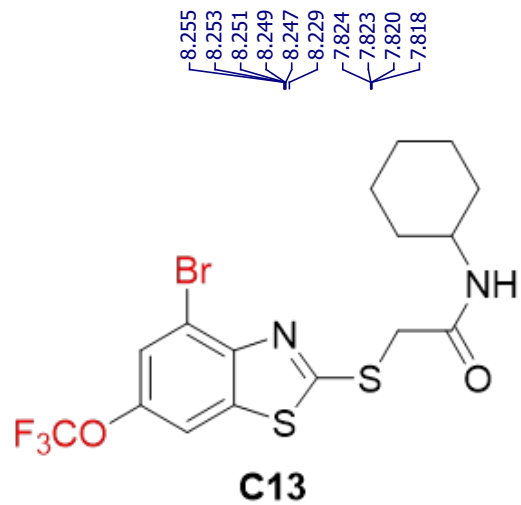


**C12**  
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)

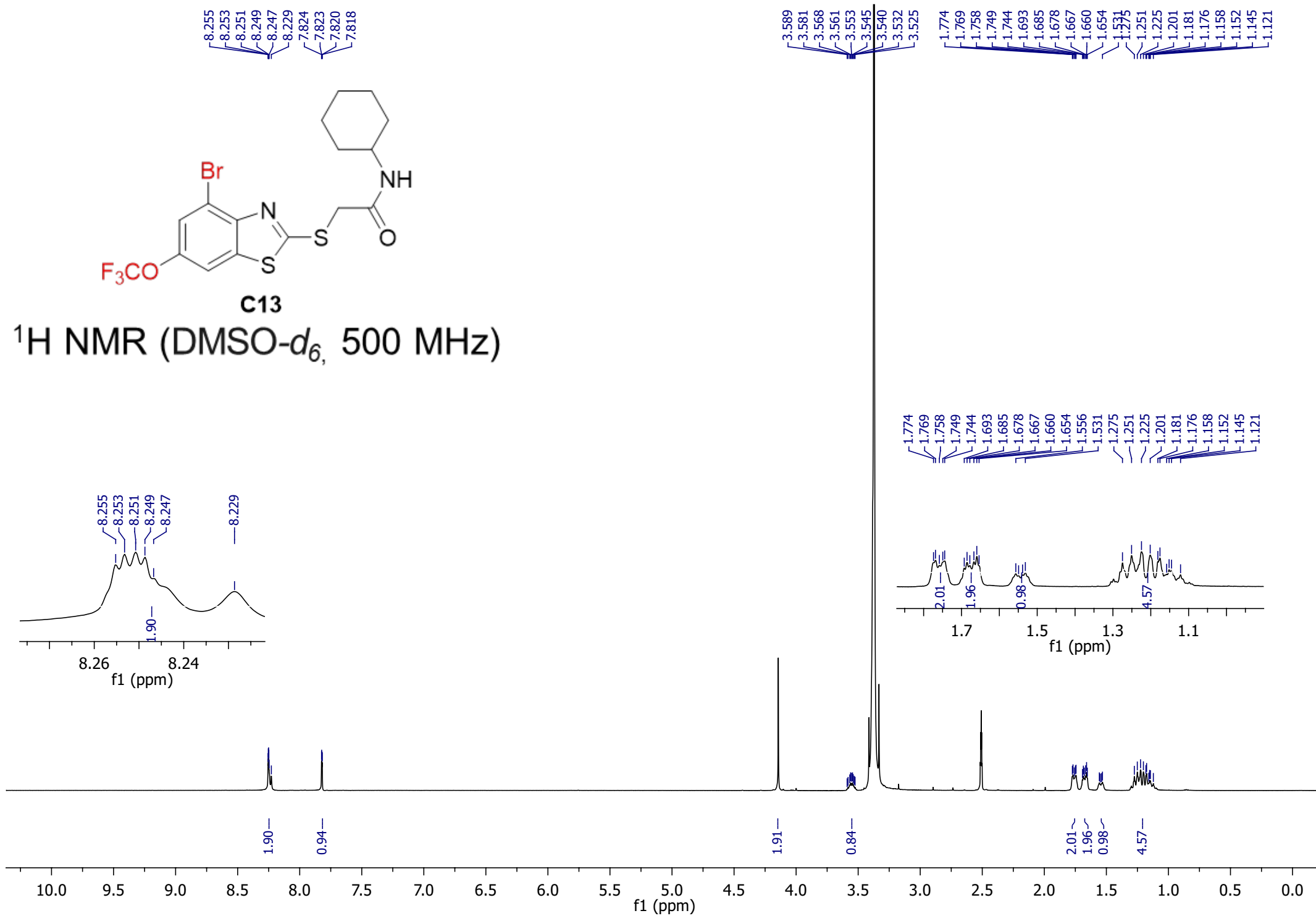


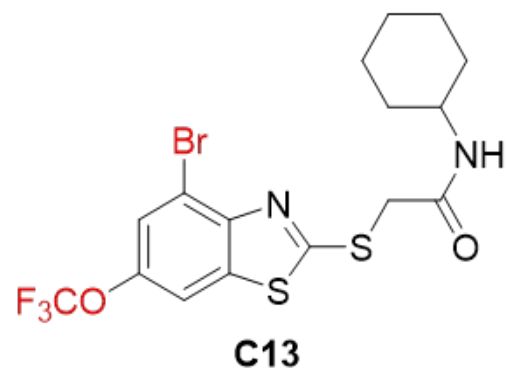
$^{19}\text{F}$  NMR ( $\text{CDCl}_3$ , 471 MHz)



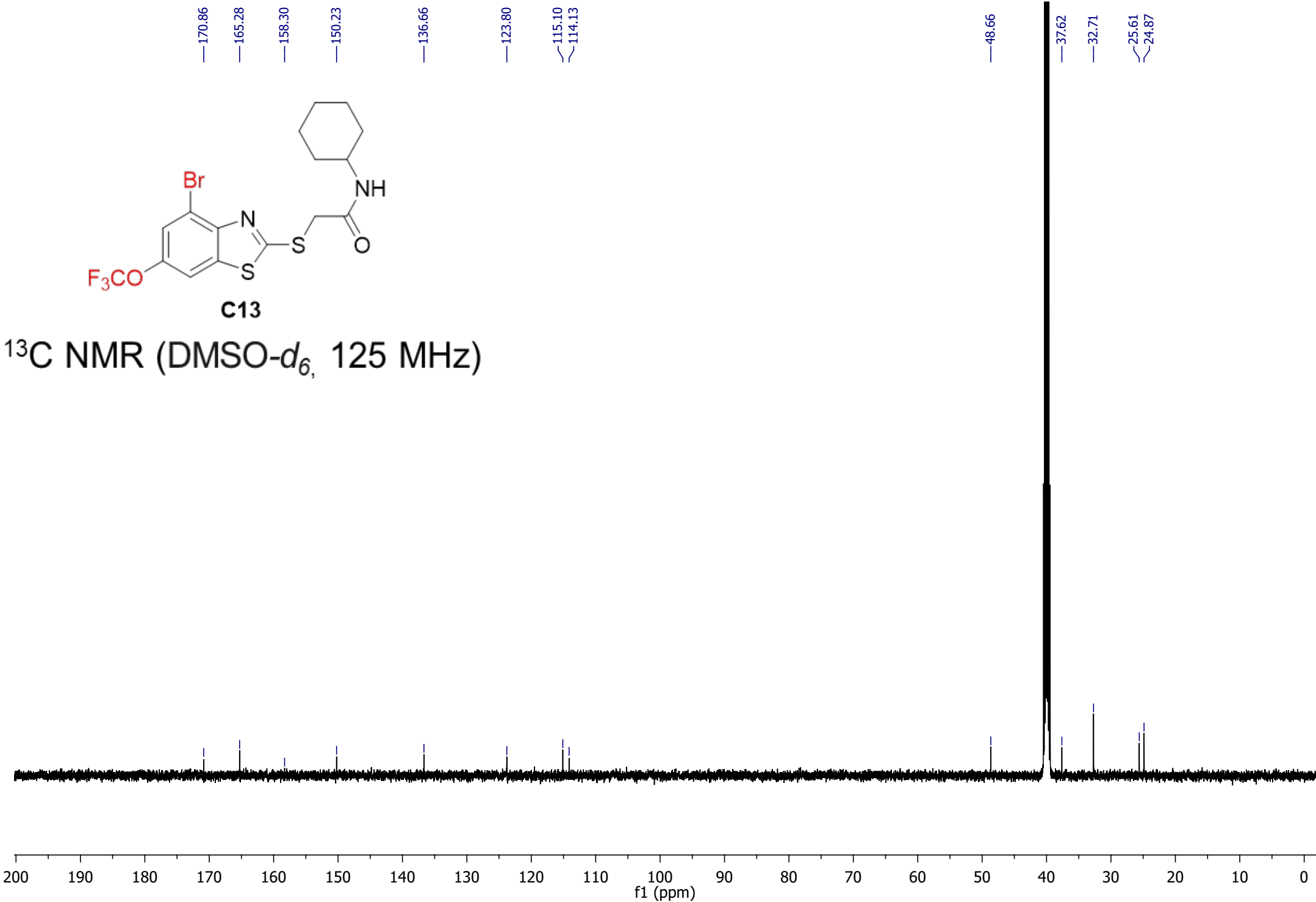


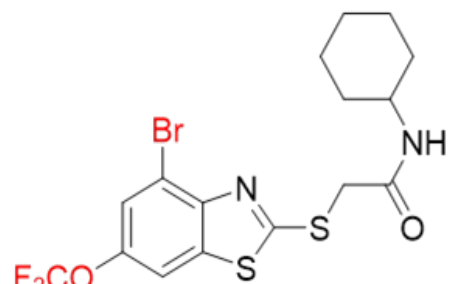
<sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 500 MHz)





<sup>13</sup>C NMR (DMSO-d<sub>6</sub>, 125 MHz)

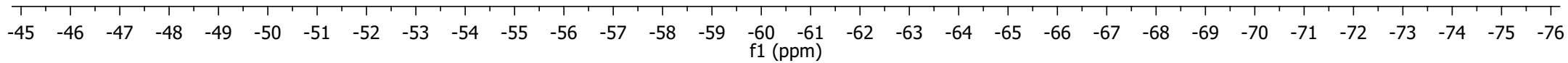




C13

<sup>19</sup>F NMR (DMSO-*d*<sub>6</sub>, 471 MHz)

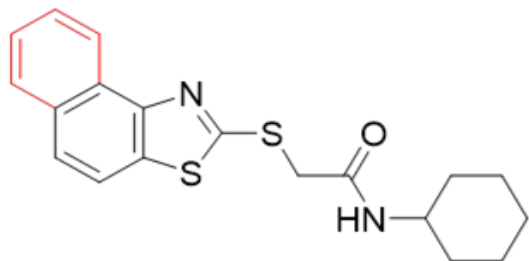
---57.179



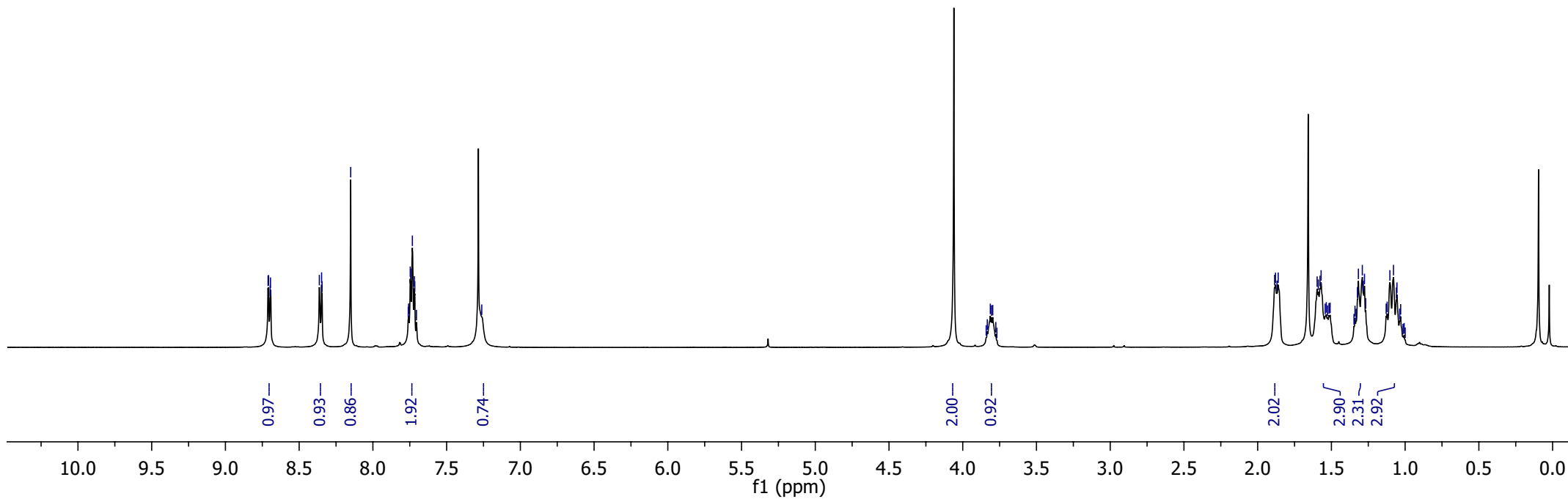
8.711  
8.708  
8.697  
8.694  
8.363  
8.348  
8.345  
8.151  
7.747  
7.744  
7.732  
7.719  
7.716  
7.262

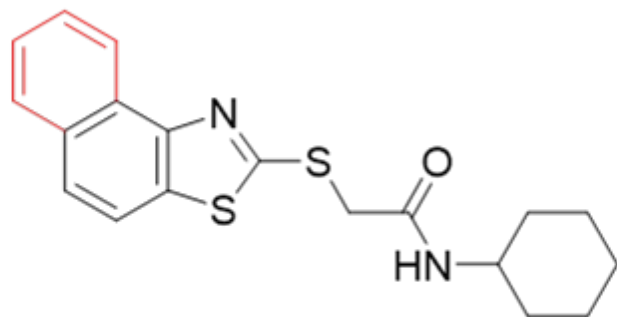
3.841  
3.833  
3.813  
3.805  
3.797  
3.776  
3.768

1.885  
1.879  
1.869  
1.861  
1.597  
1.589  
1.577  
1.570  
1.323  
1.317  
1.290  
1.284  
1.276  
1.268  
1.103  
1.079  
1.060  
1.055



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)





$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

