

## Structure-Activity Evaluation of New Uracil-Containing Non-Nucleoside Inhibitors of HIV Reverse Transcriptase

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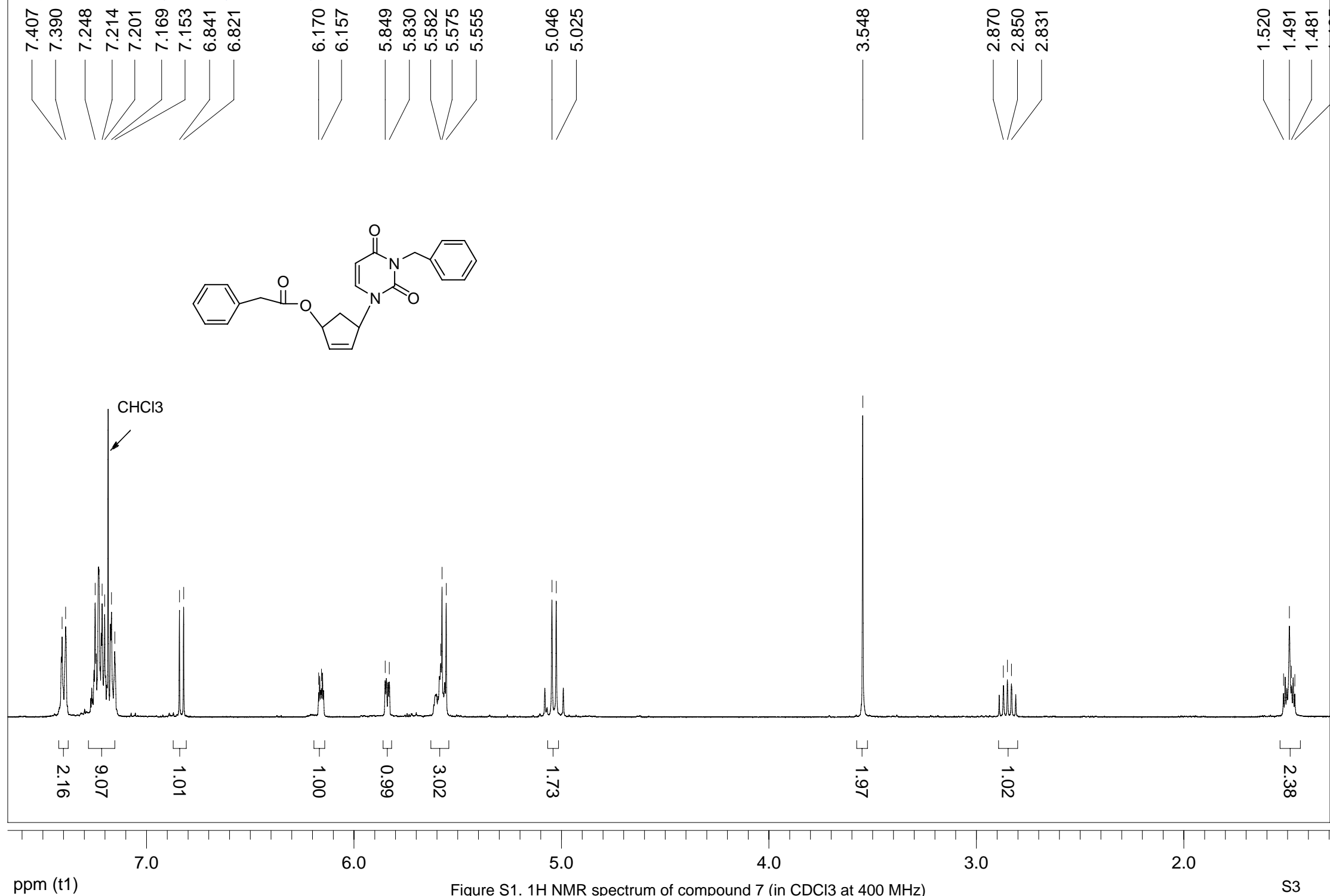


Figure S1. <sup>1</sup>H NMR spectrum of compound 7 (in CDCl<sub>3</sub> at 400 MHz)

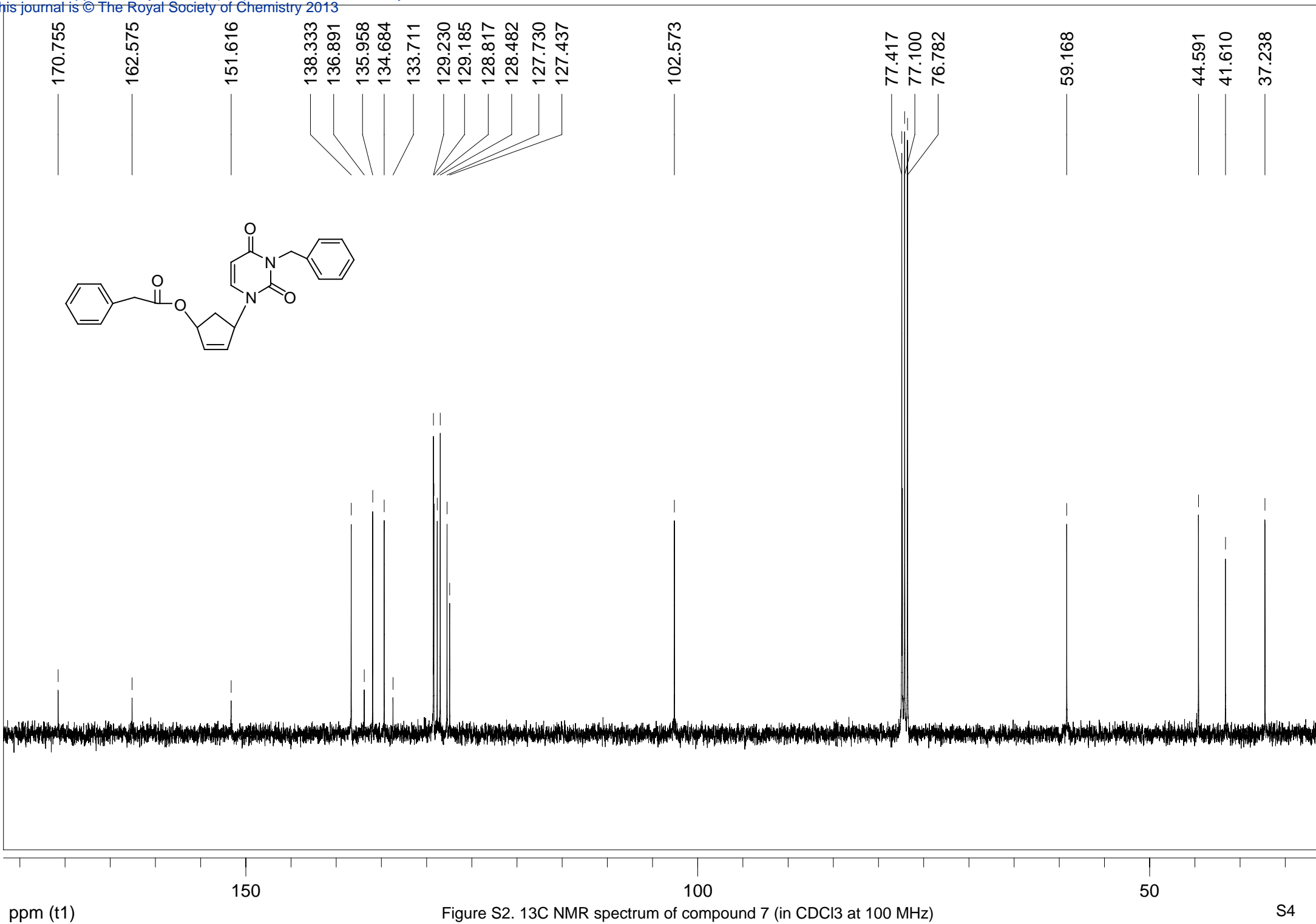
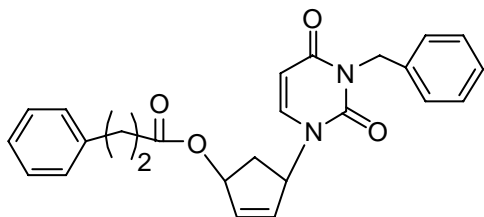


Figure S2. <sup>13</sup>C NMR spectrum of compound 7 (in CDCl<sub>3</sub> at 100 MHz)

7.492  
7.488  
7.471  
7.304  
7.286  
7.252  
7.235  
7.172  
7.158  
7.023  
7.003  
6.197  
6.192  
6.178  
6.173  
5.897  
5.892  
5.877  
5.753  
5.733  
5.655  
5.622  
5.621  
5.611  
5.602  
5.165  
5.131  
5.107  
5.073

2.955  
2.936  
2.917  
2.639  
2.620  
2.601

1.502  
1.464



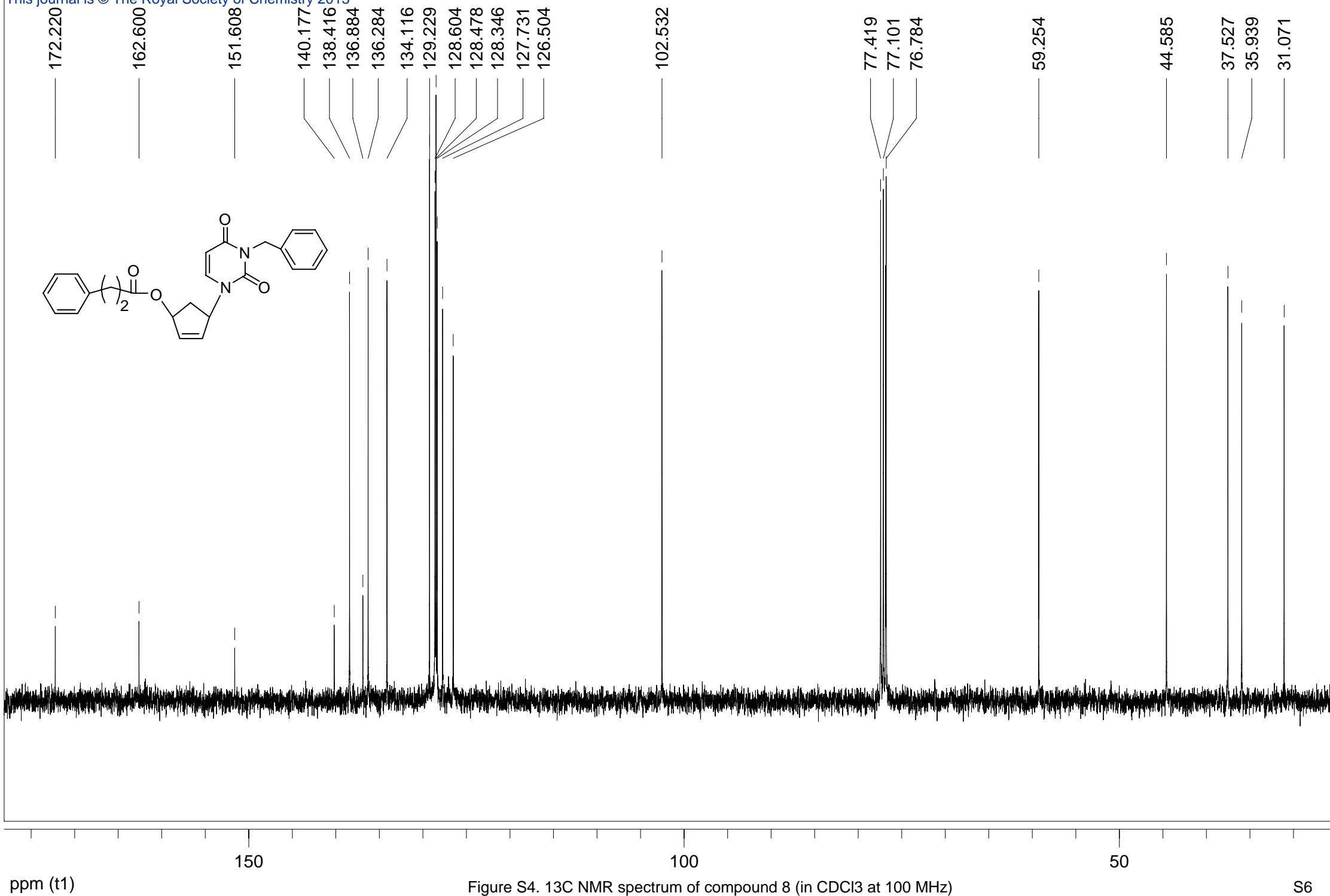
CHCl<sub>3</sub>

H<sub>2</sub>O

1.97  
5.47  
3.15  
1.02  
1.00  
0.99  
0.97  
1.94  
2.15  
3.33  
2.01  
0.77  
1.04

ppm (t1)

Figure S3. <sup>1</sup>H NMR spectrum of compound 8 (in CDCl<sub>3</sub> at 400 MHz)

Figure S4. <sup>13</sup>C NMR spectrum of compound 8 (in CDCl<sub>3</sub> at 100 MHz)

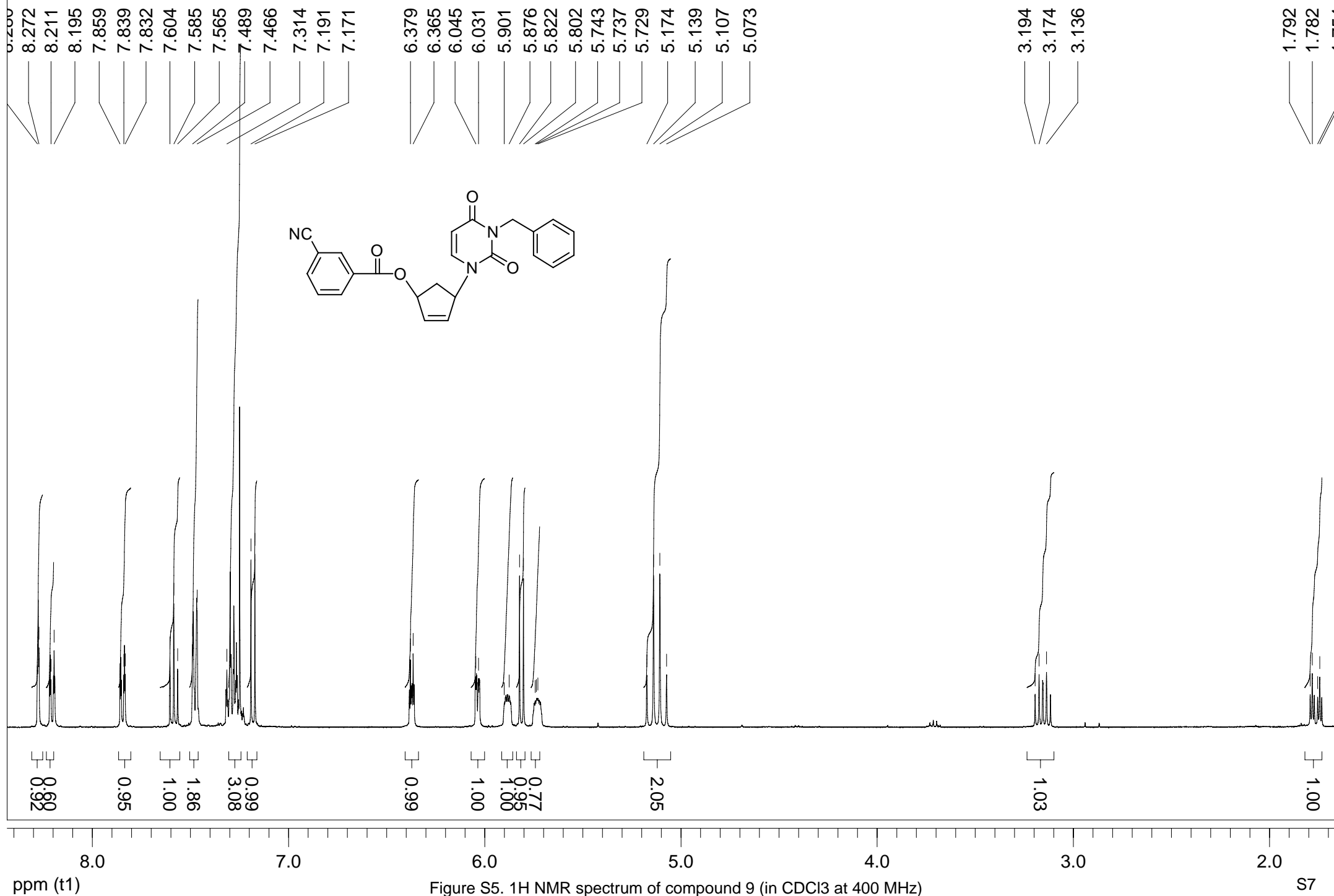


Figure S5. <sup>1</sup>H NMR spectrum of compound 9 (in CDCl<sub>3</sub> at 400 MHz)

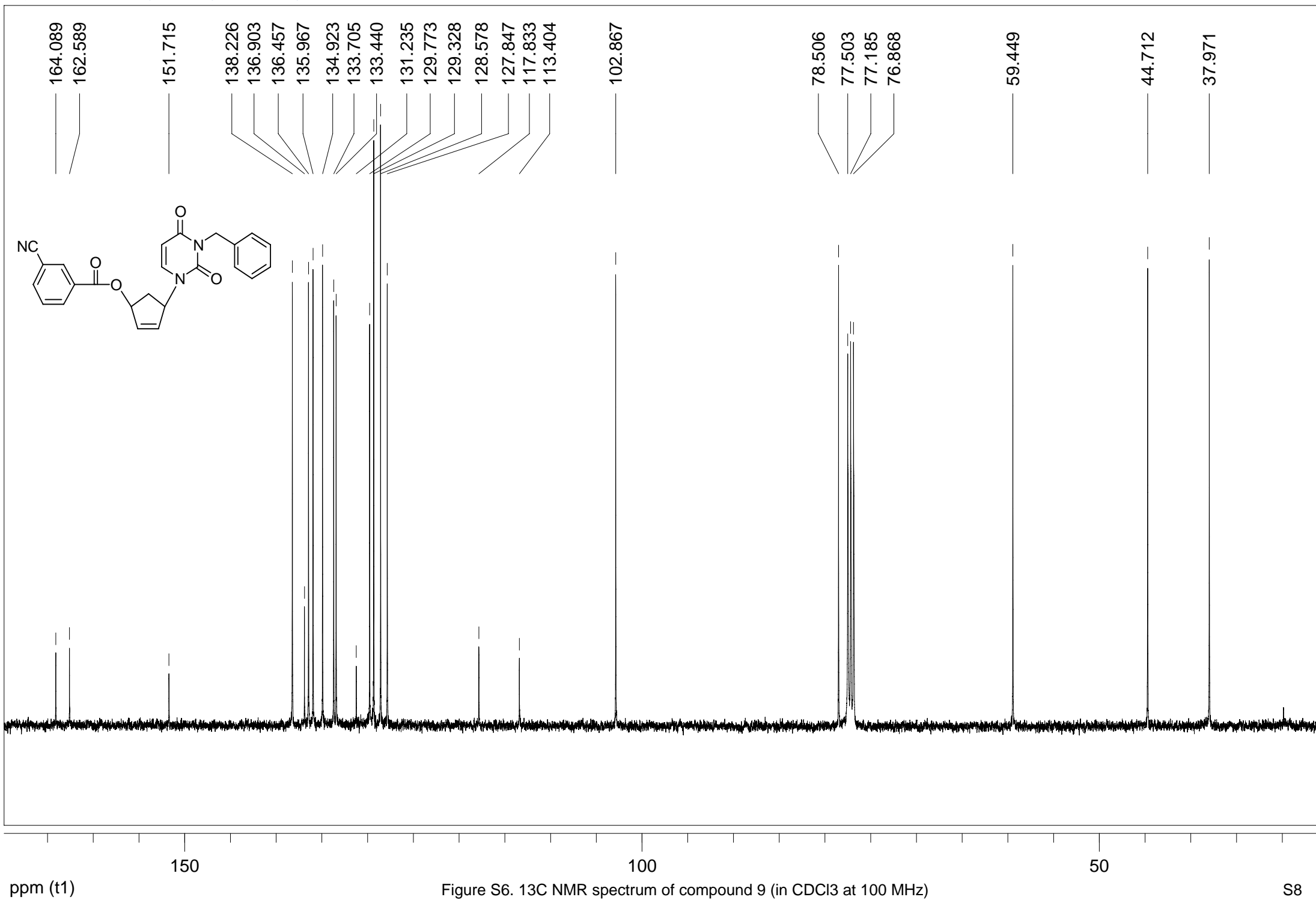


Figure S6. <sup>13</sup>C NMR spectrum of compound 9 (in CDCl<sub>3</sub> at 100 MHz)



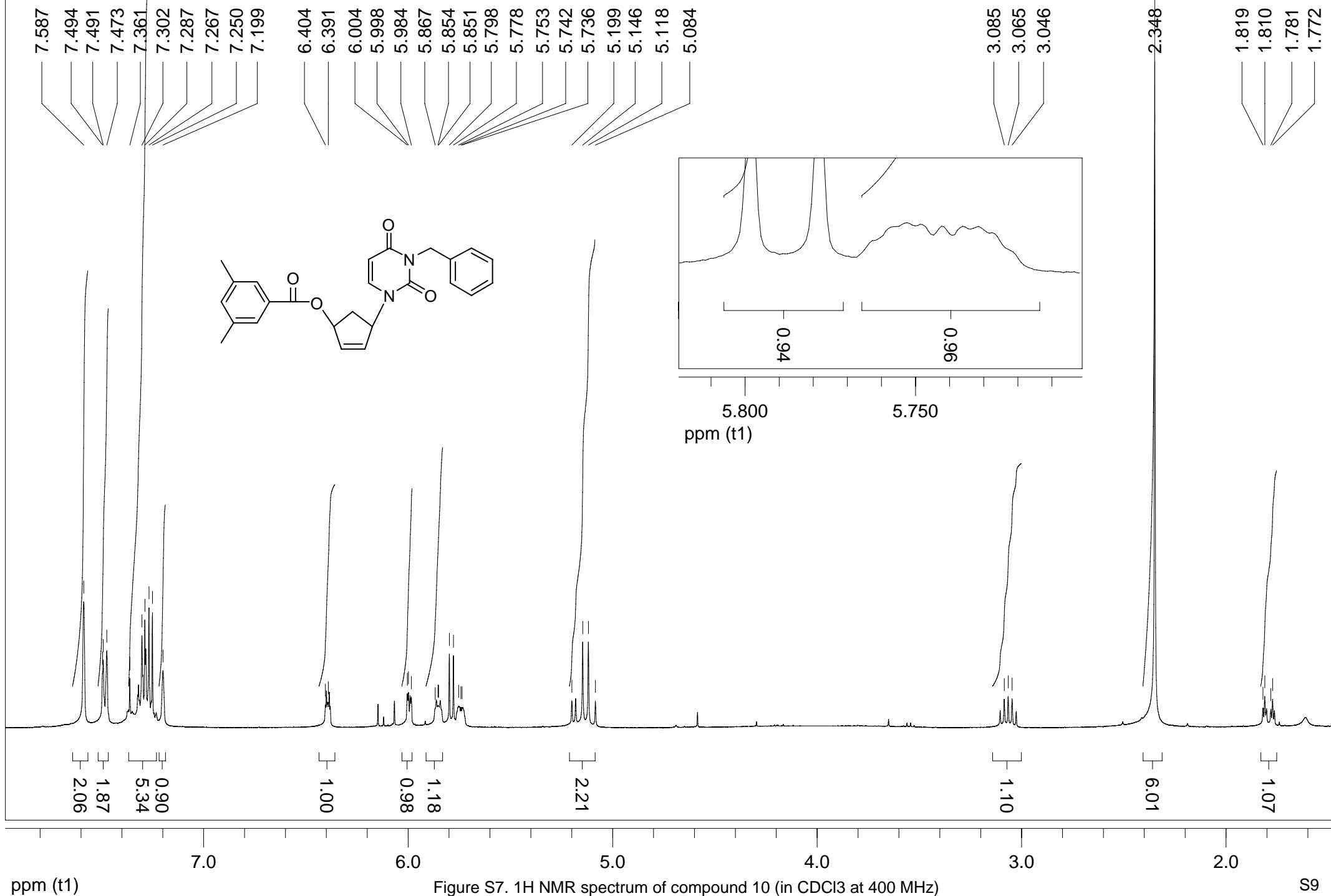


Figure S7. <sup>1</sup>H NMR spectrum of compound 10 (in CDCl<sub>3</sub> at 400 MHz)

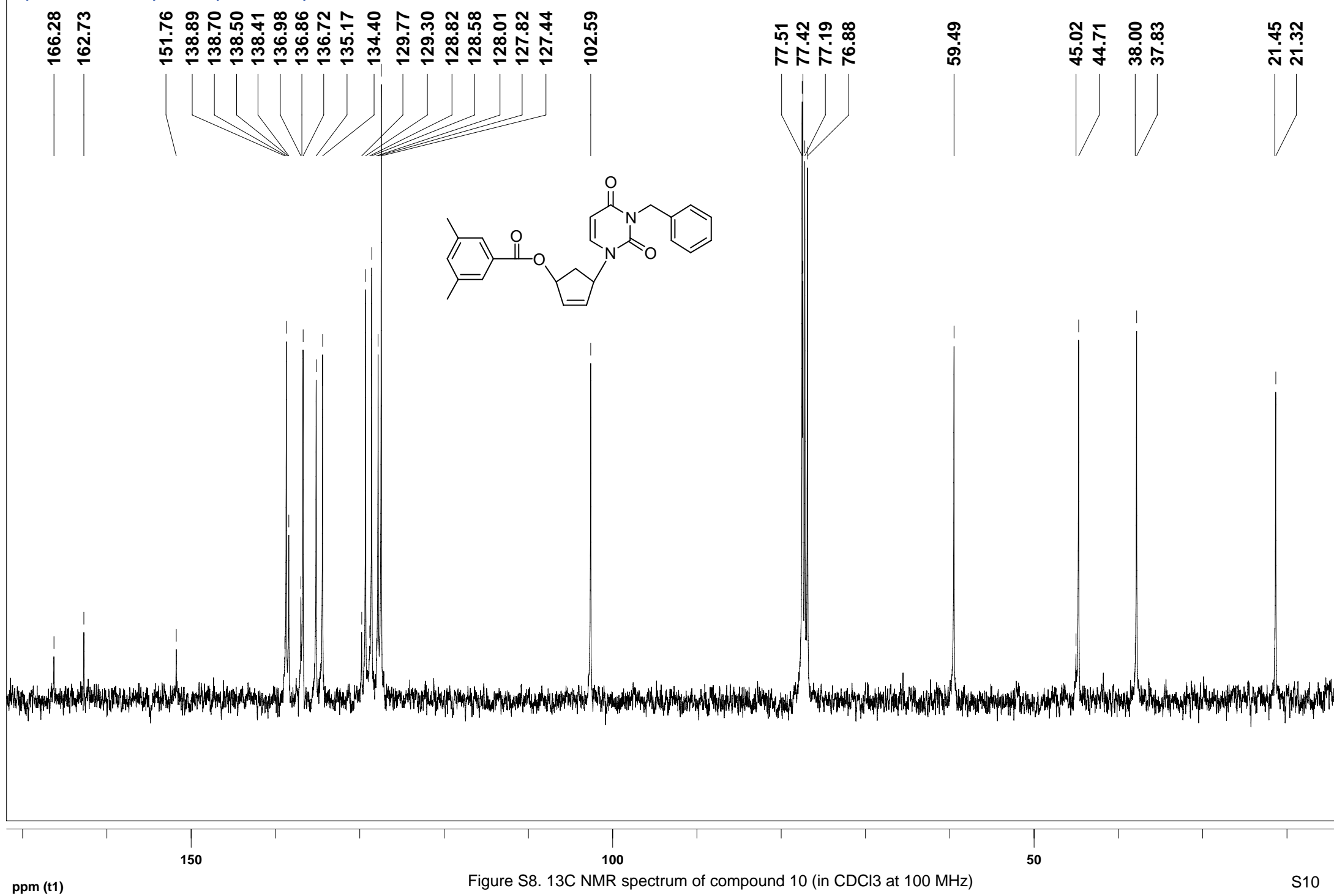


Figure S8. <sup>13</sup>C NMR spectrum of compound 10 (in CDCl<sub>3</sub> at 100 MHz)

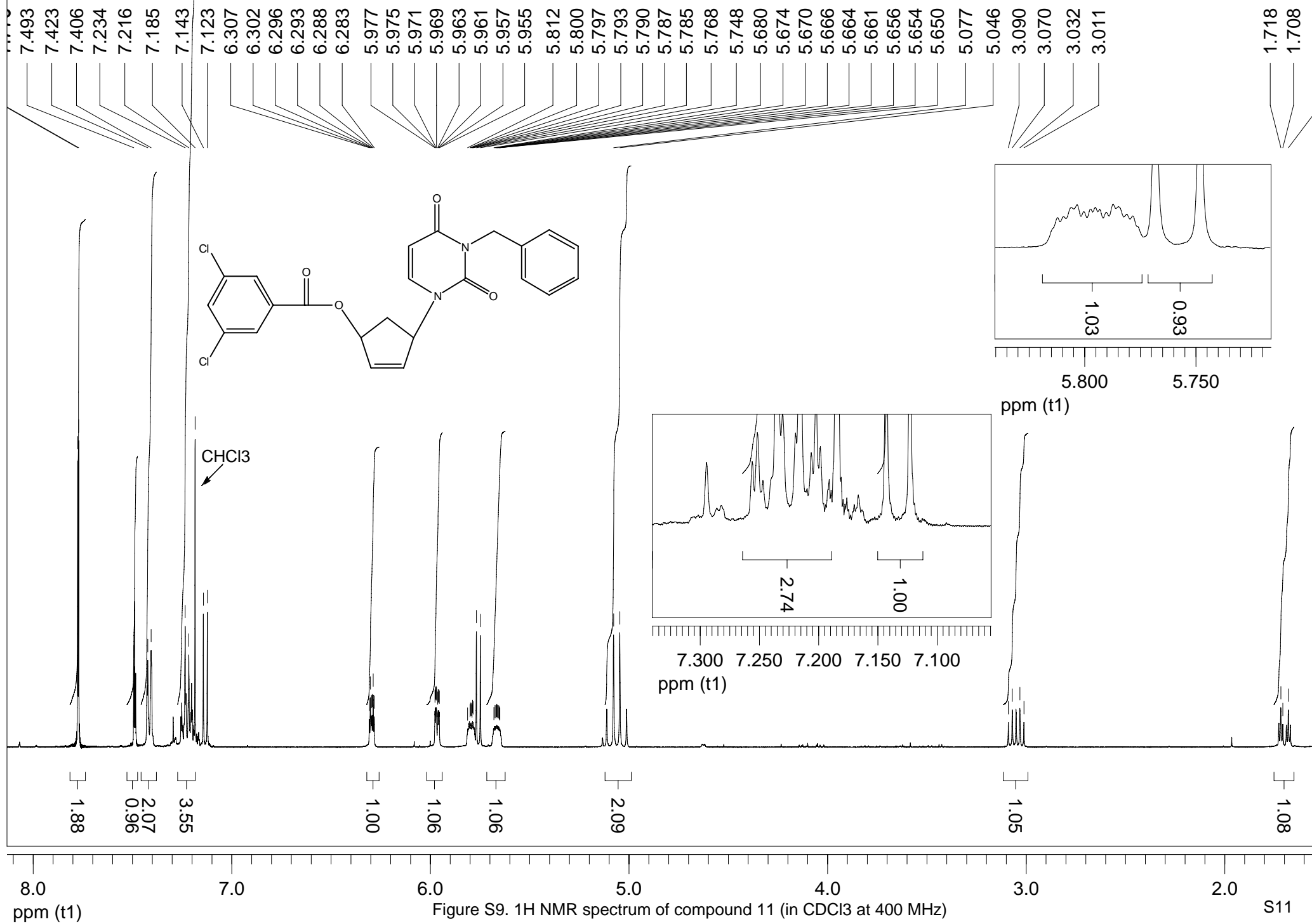


Figure S9. <sup>1</sup>H NMR spectrum of compound 11 (in CDCl<sub>3</sub> at 400 MHz)

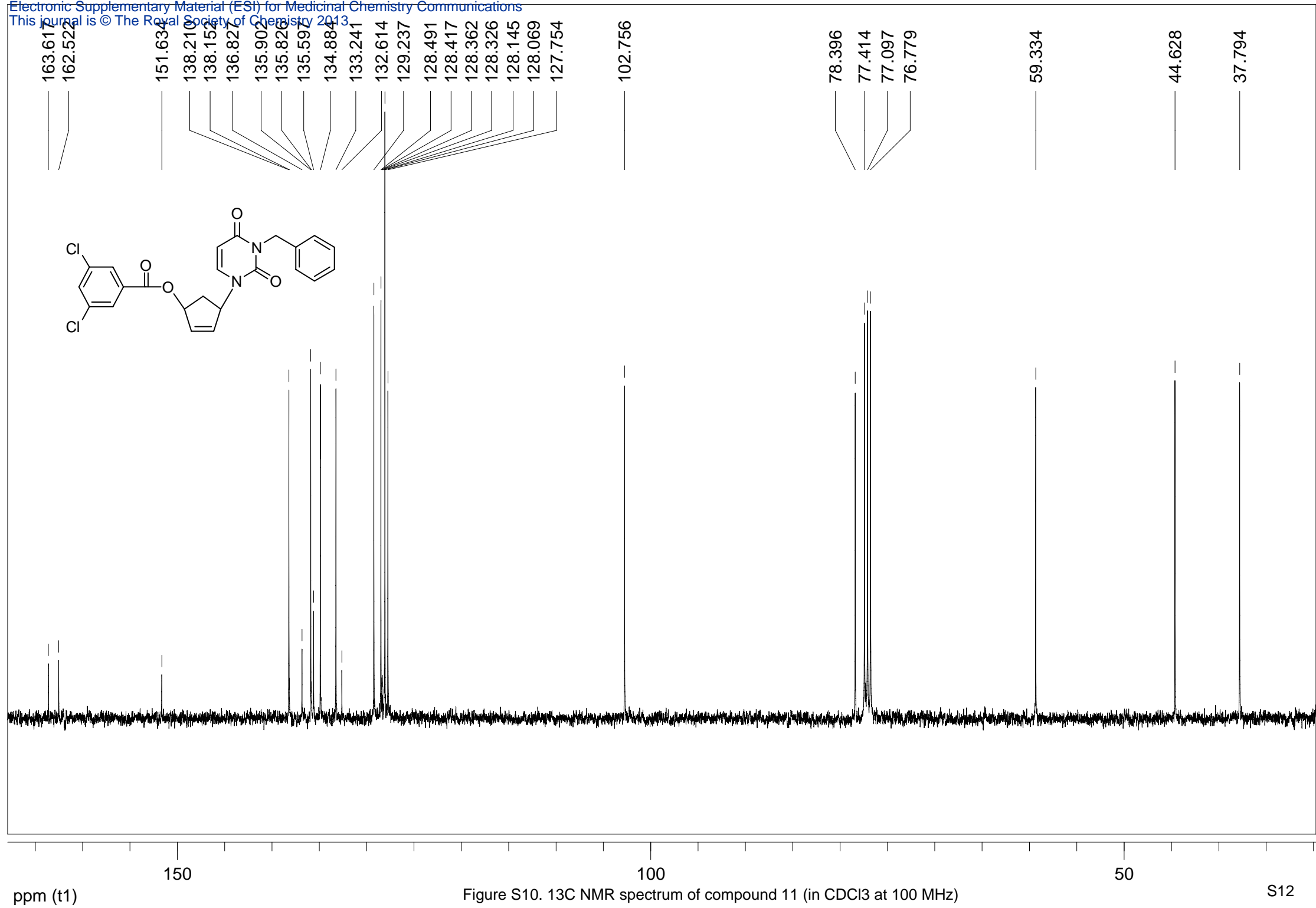


Figure S10. <sup>13</sup>C NMR spectrum of compound 11 (in CDCl<sub>3</sub> at 100 MHz)

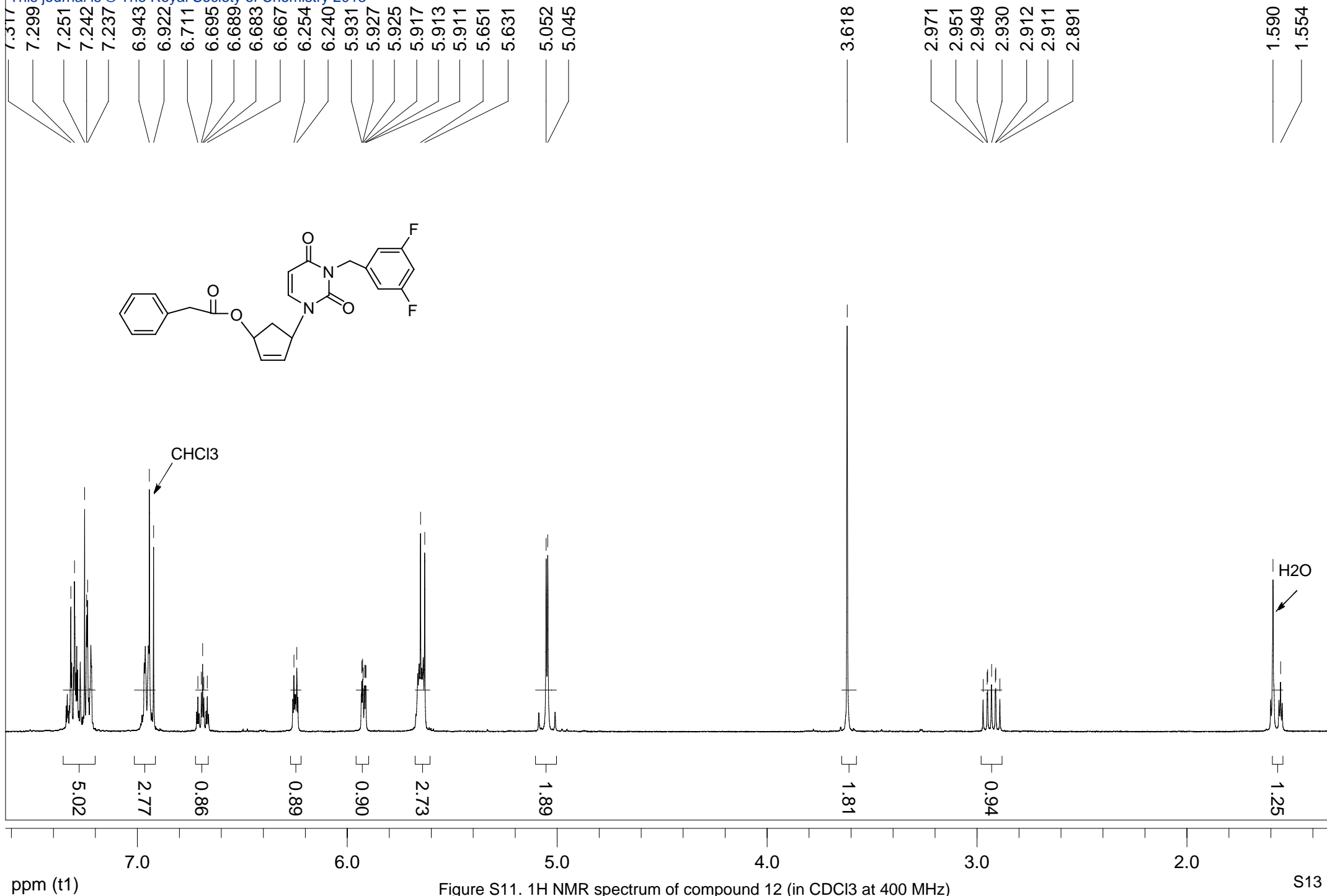


Figure S11. <sup>1</sup>H NMR spectrum of compound 12 (in CDCl<sub>3</sub> at 400 MHz)

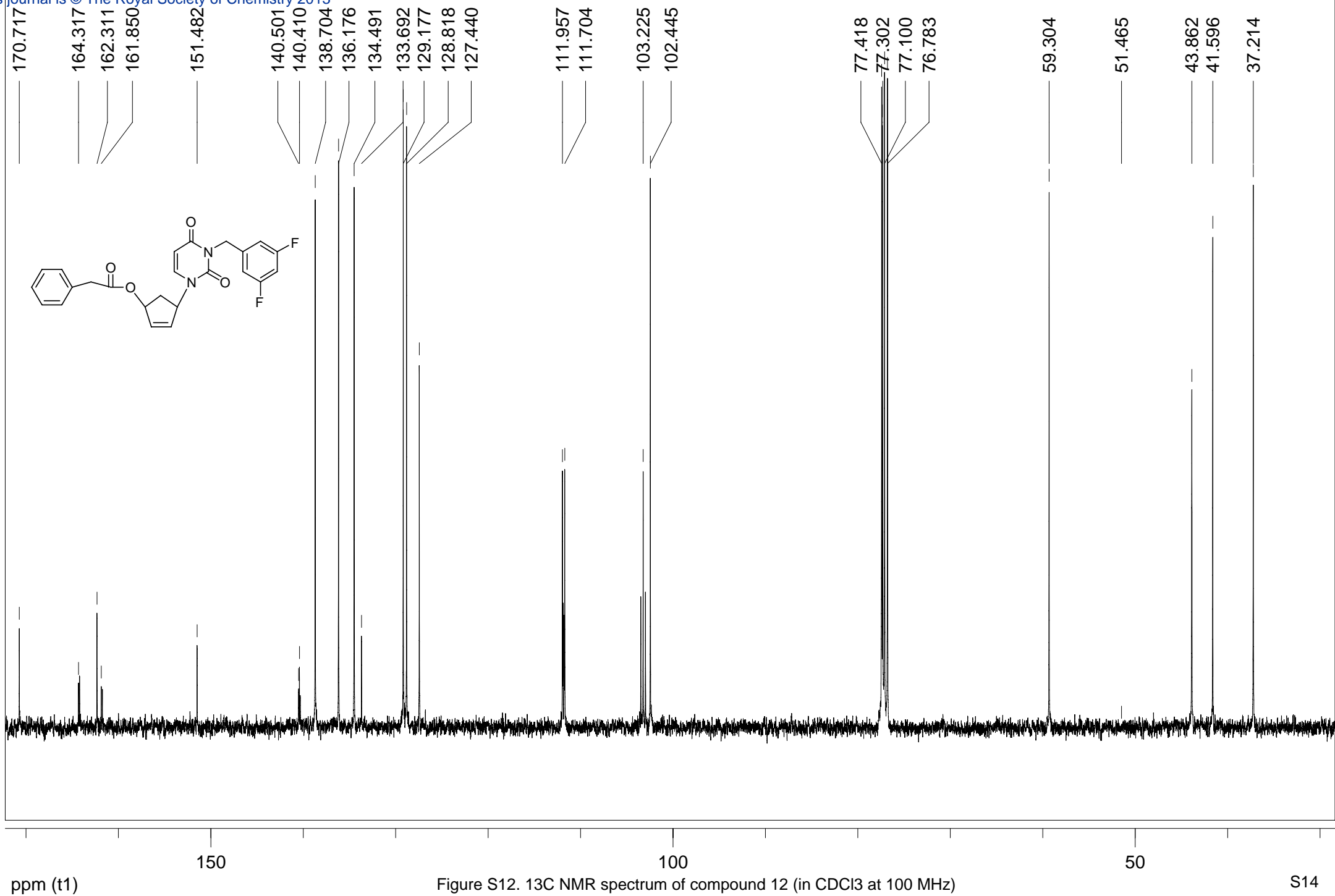


Figure S12. <sup>13</sup>C NMR spectrum of compound 12 (in CDCl<sub>3</sub> at 100 MHz)

ppm (t1)

S14

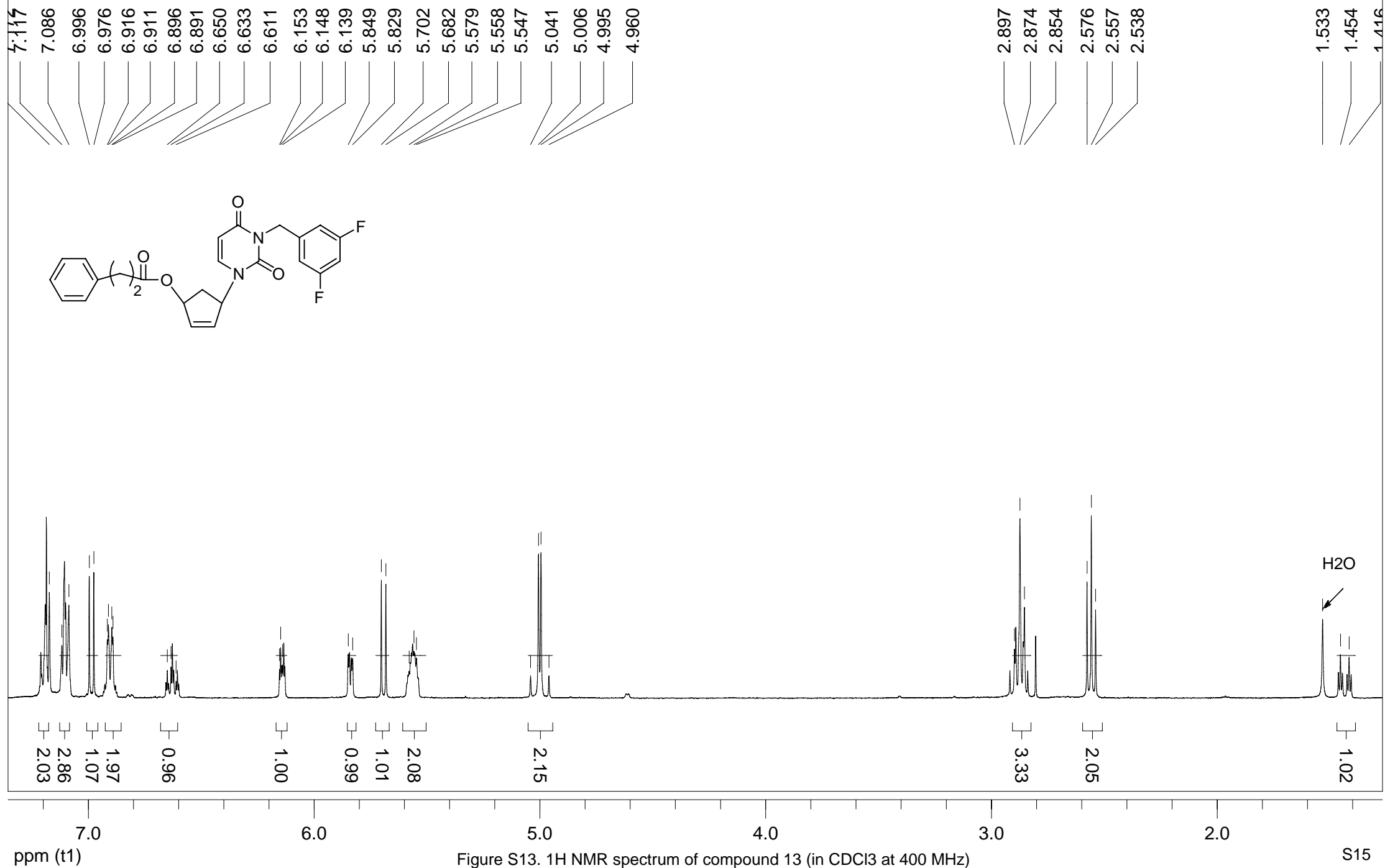
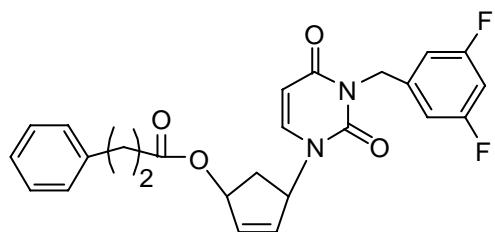


Figure S13. <sup>1</sup>H NMR spectrum of compound 13 (in CDCl<sub>3</sub> at 400 MHz)



172.205  
164.329  
164.202  
162.345  
161.857  
161.733  
151.495  
140.415  
140.180  
138.795  
136.528  
133.921  
128.612  
128.356  
126.509  
111.972  
111.719  
103.241  
102.435  
77.418  
77.100  
76.823  
76.784  
59.402  
43.871  
37.525  
35.936  
31.072

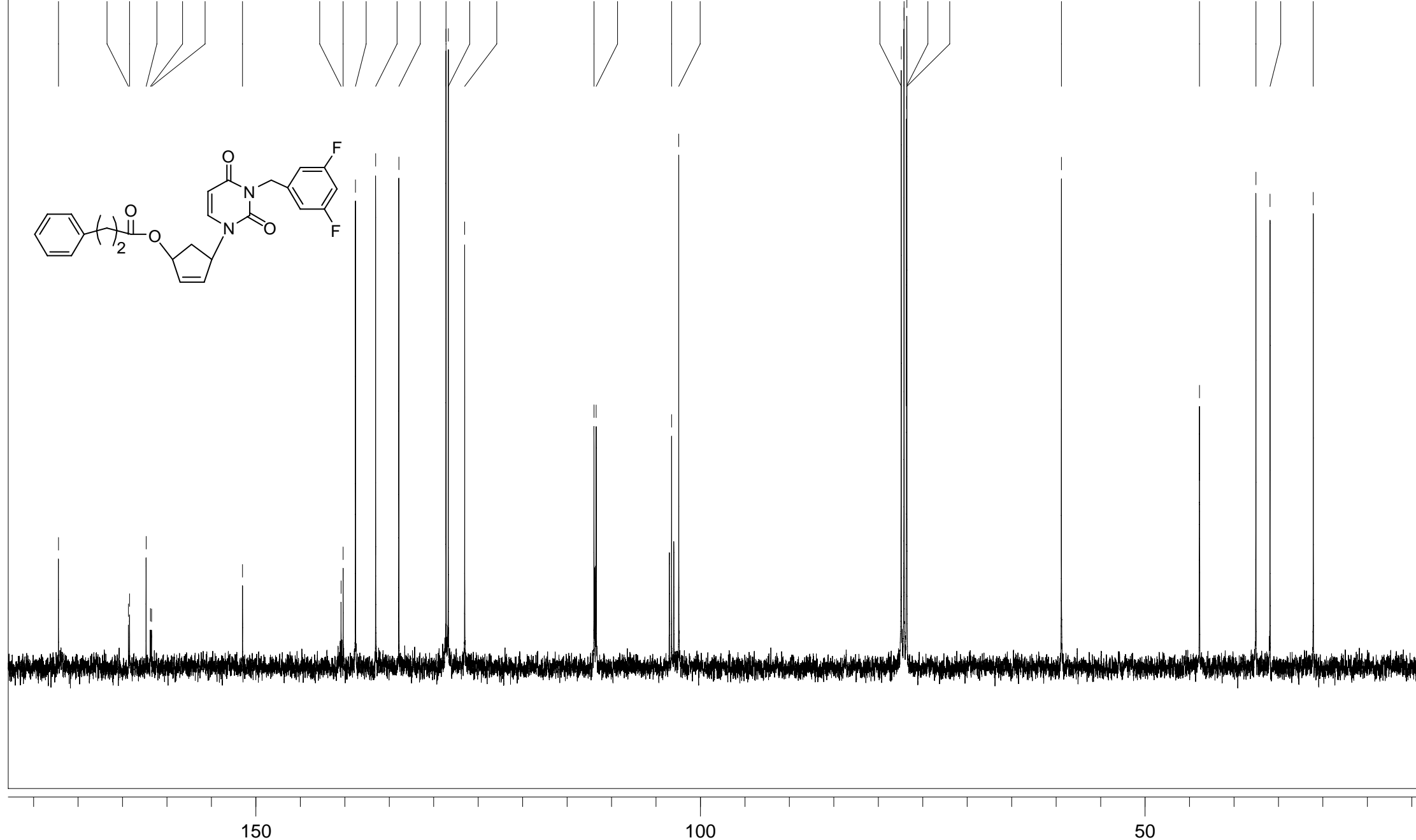


Figure S14. <sup>13</sup>C NMR spectrum of compound 13 (in CDCl<sub>3</sub> at 100 MHz)



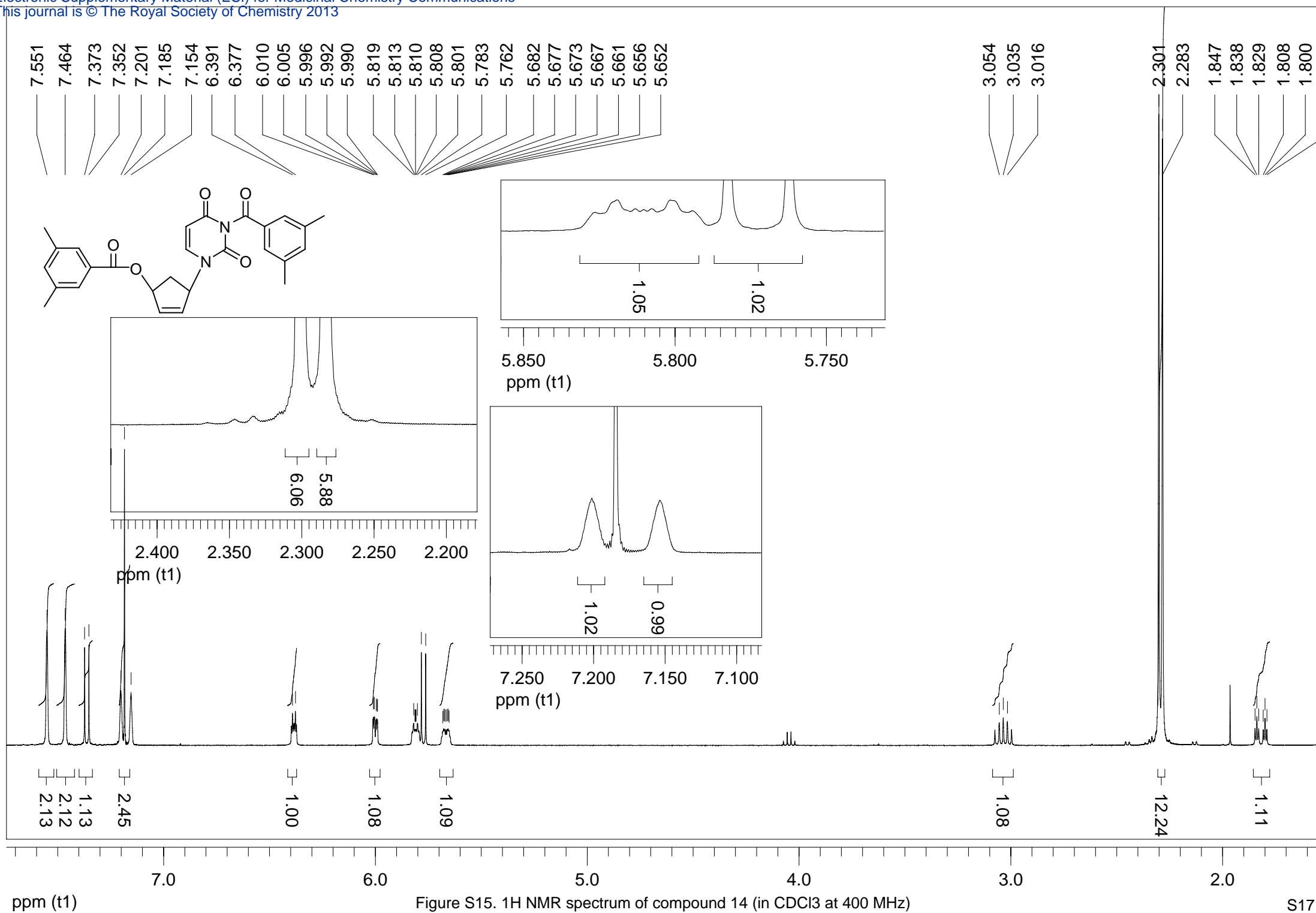


Figure S15. <sup>1</sup>H NMR spectrum of compound 14 (in CDCl<sub>3</sub> at 400 MHz)

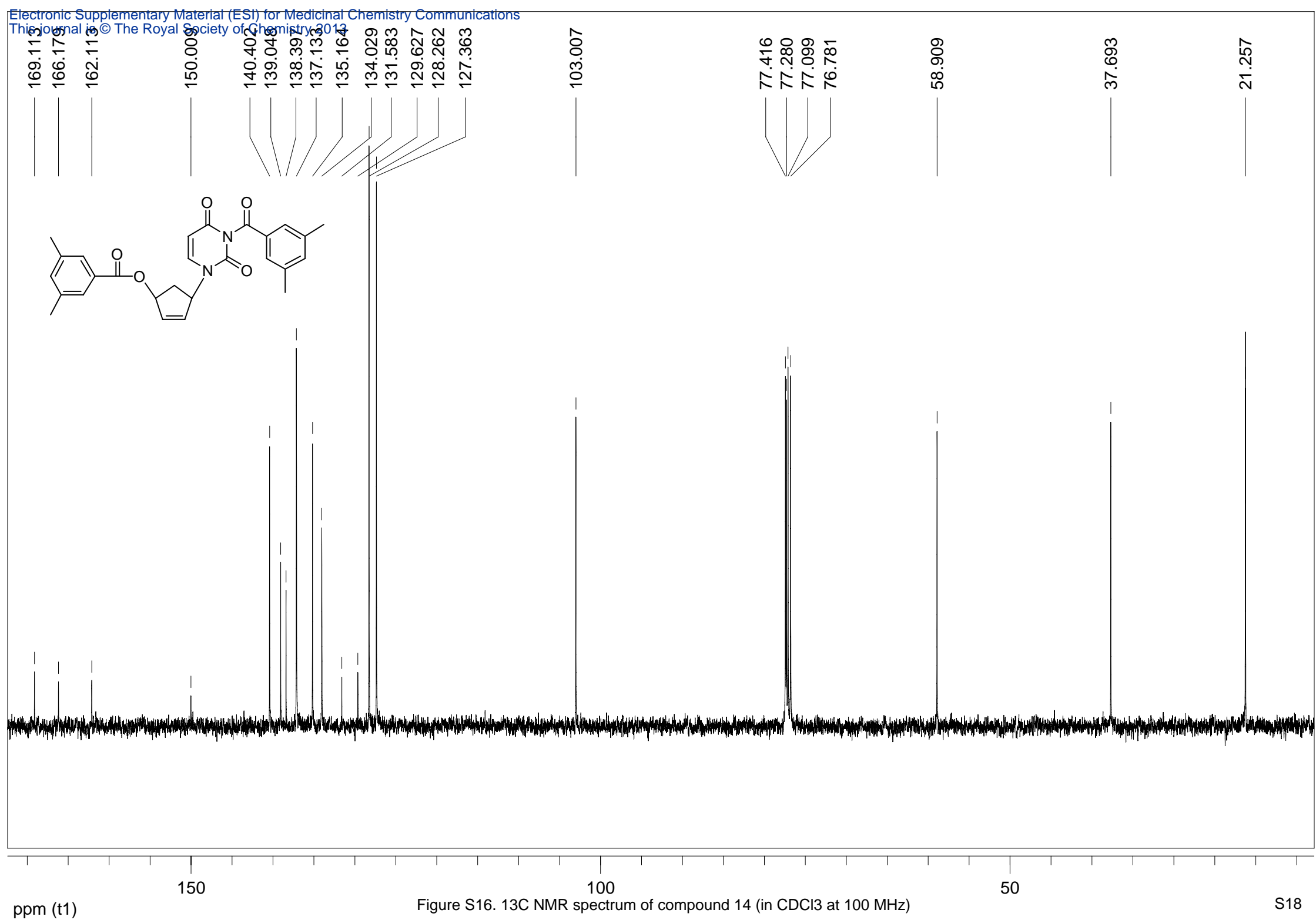


Figure S16. 13C NMR spectrum of compound 14 (in CDCl<sub>3</sub> at 100 MHz)

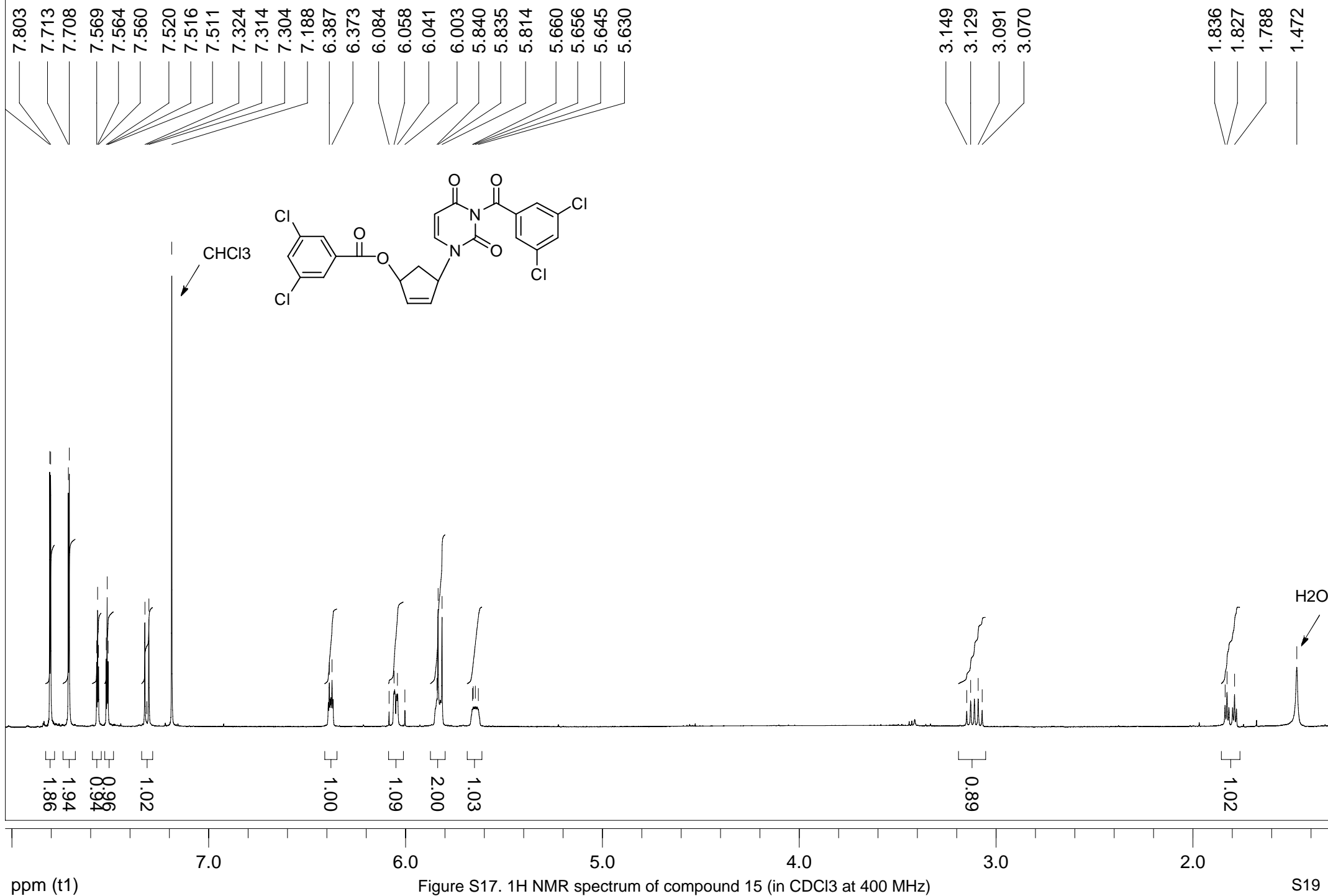


Figure S17. <sup>1</sup>H NMR spectrum of compound 15 (in CDCl<sub>3</sub> at 400 MHz)

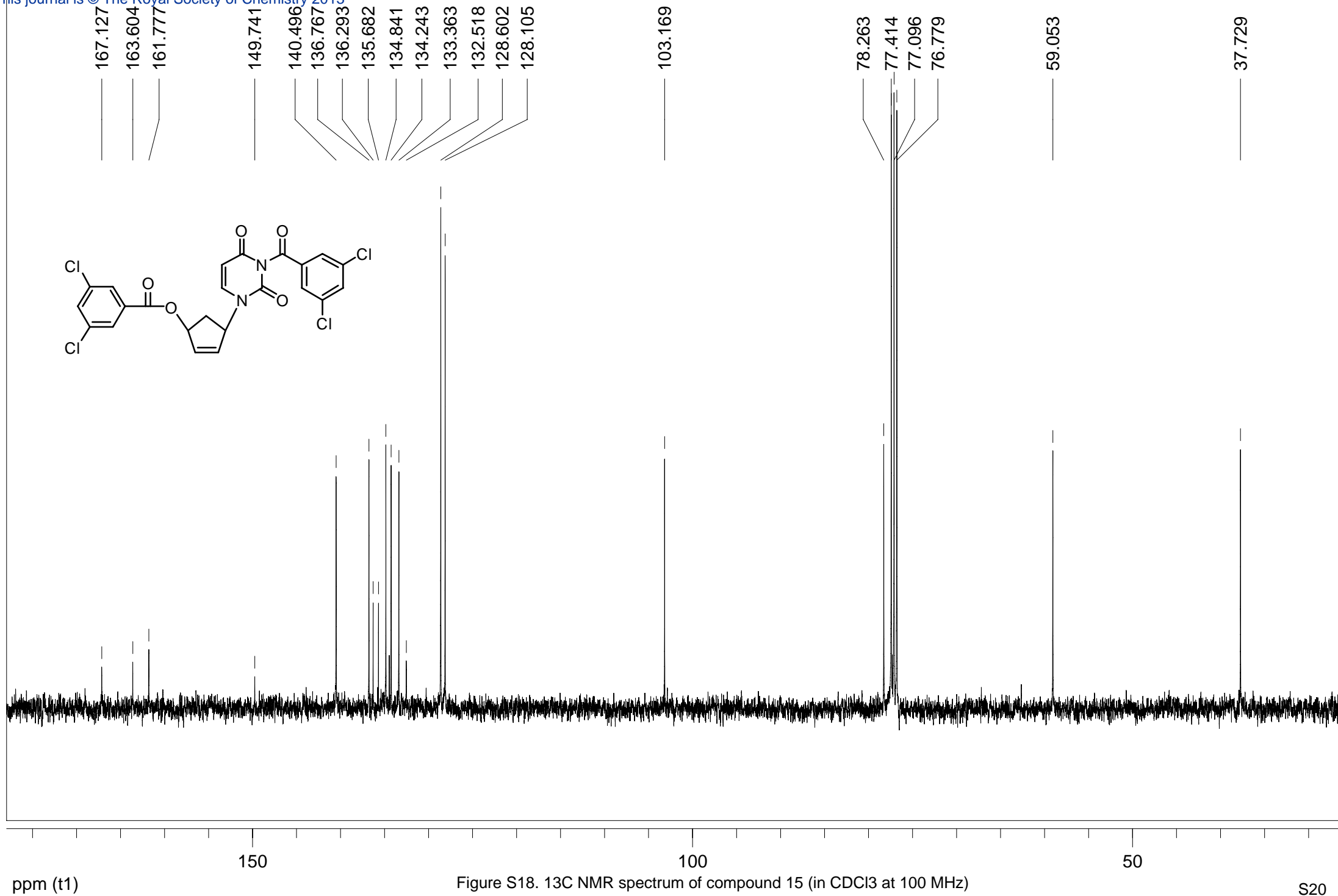


Figure S18. <sup>13</sup>C NMR spectrum of compound 15 (in CDCl<sub>3</sub> at 100 MHz)

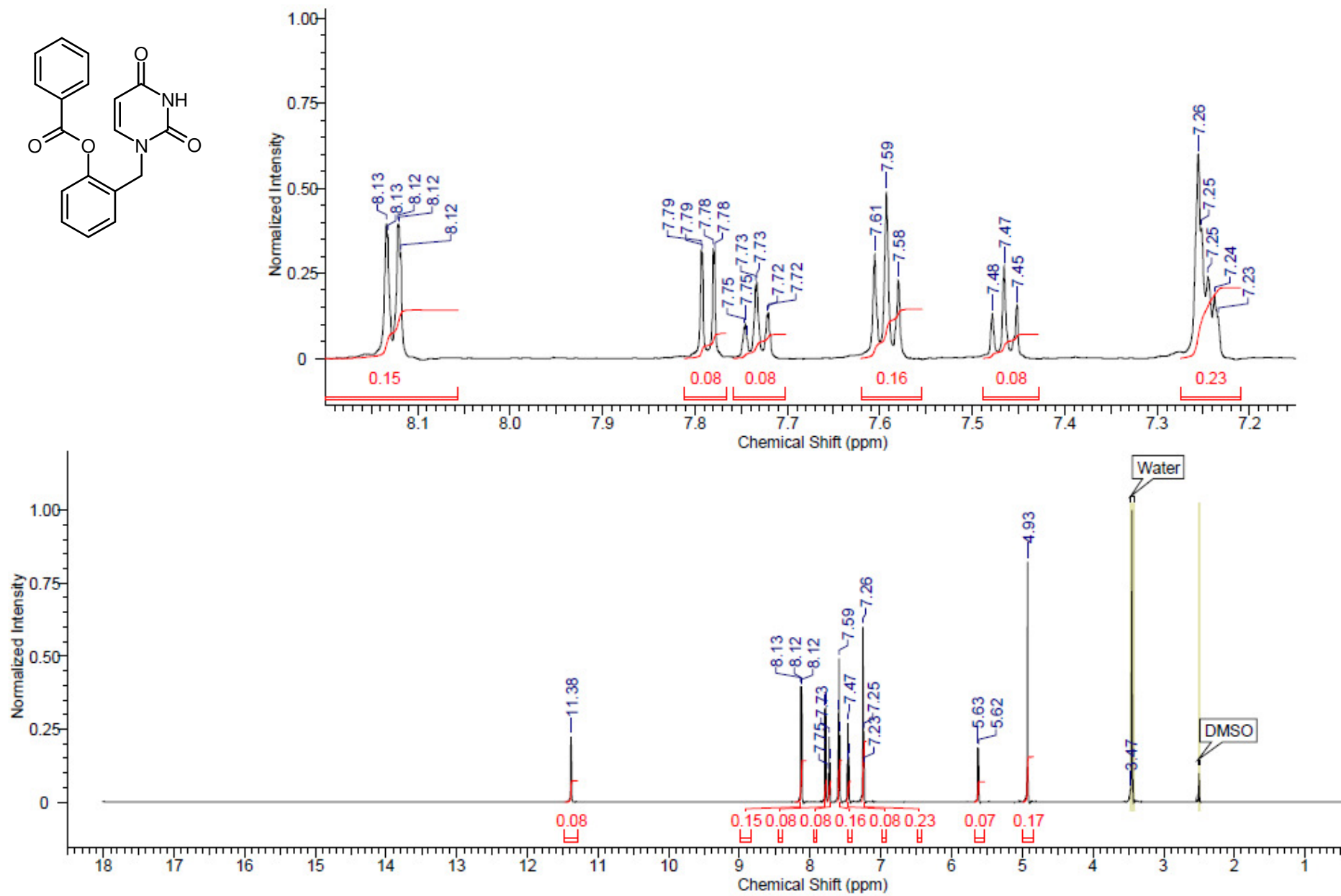
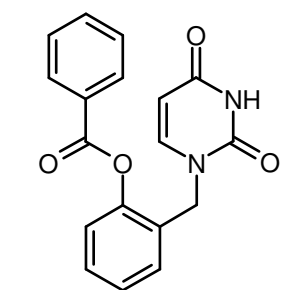


Figure S19.  $^1\text{H}$  NMR spectrum of compound 19 (in  $\text{DMSO-d}_6$  at 400 MHz)

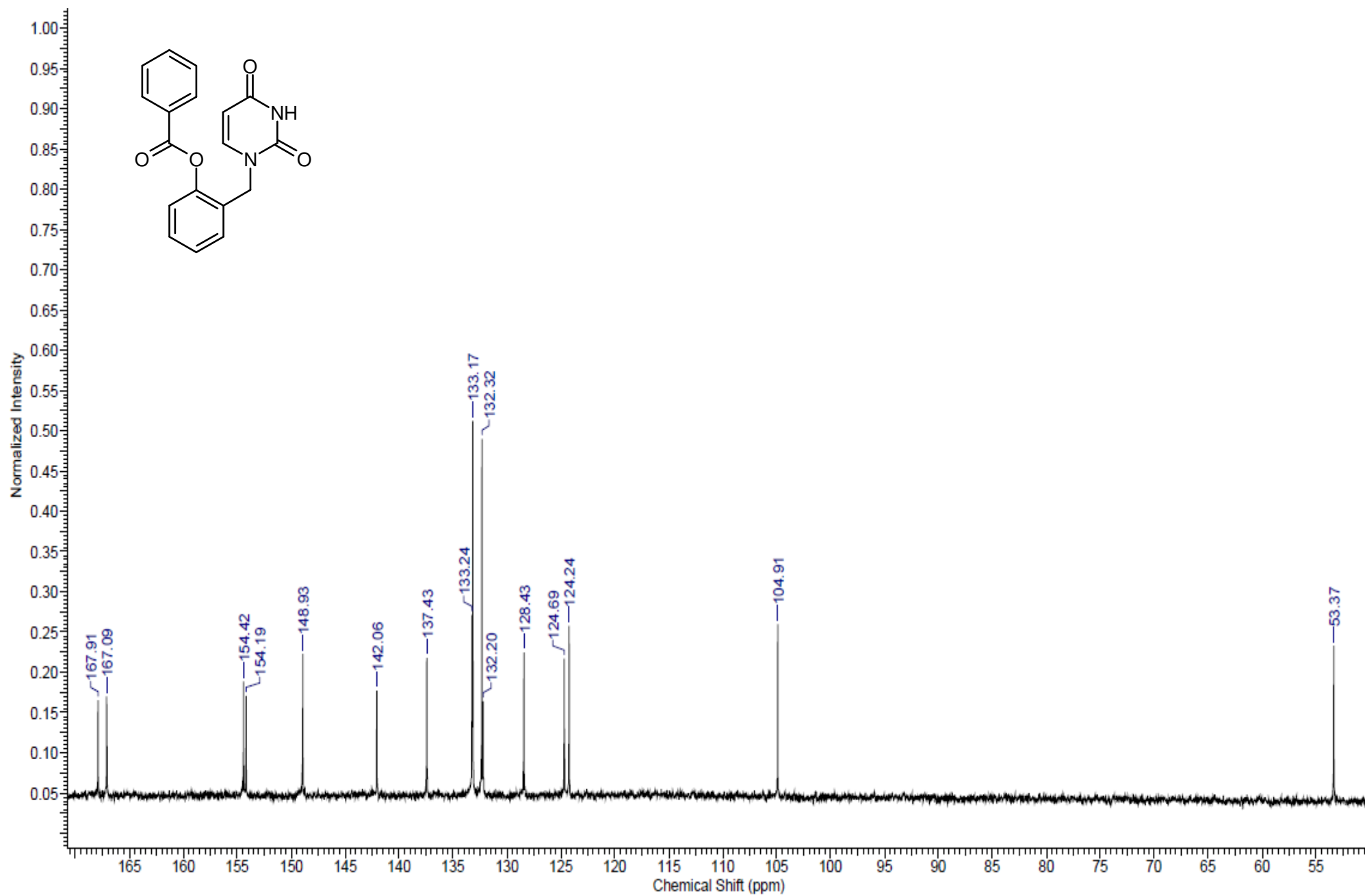


Figure S20. <sup>13</sup>C NMR spectrum of compound 19 (in DMSO-d<sub>6</sub> at 100 MHz)

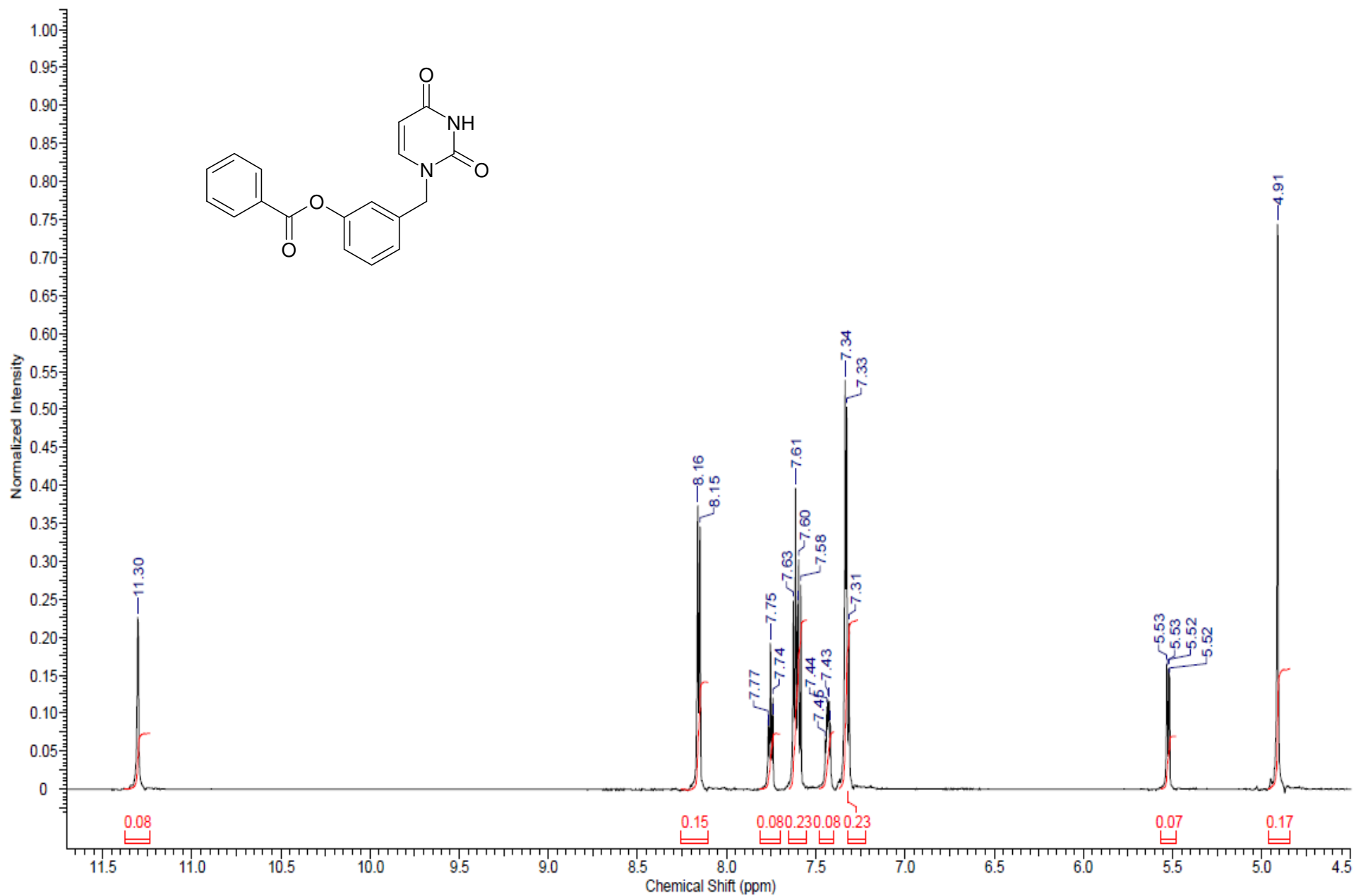


Figure S21. <sup>1</sup>H NMR spectrum of compound 20 (in DMSO-d<sub>6</sub> at 400 MHz)

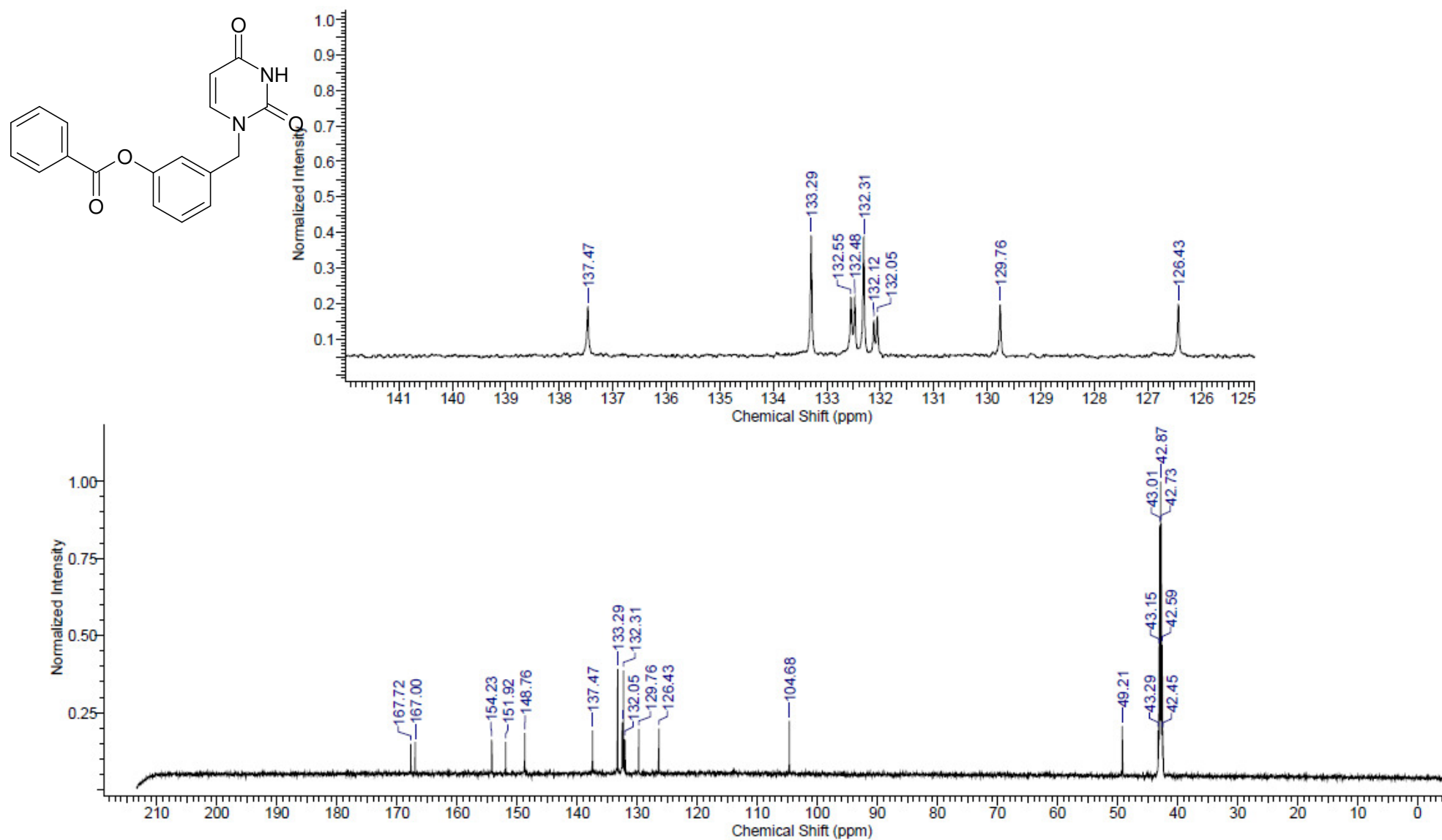


Figure S22. <sup>13</sup>C NMR spectrum of compound 20 (in DMSO-d<sub>6</sub> at 100 MHz)



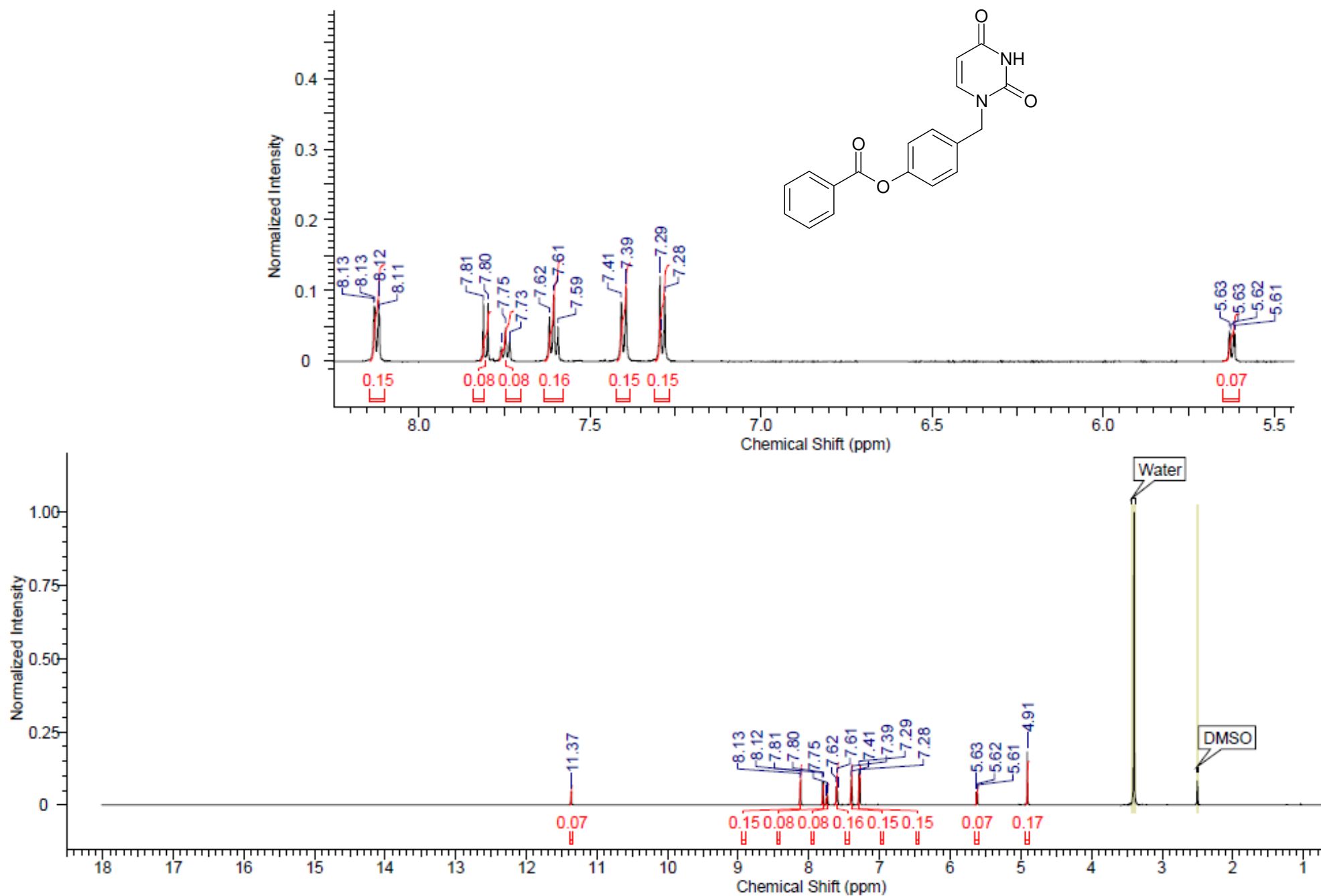


Figure S23. <sup>1</sup>H NMR spectrum of compound 21 (in DMSO-d<sub>6</sub> at 400 MHz)

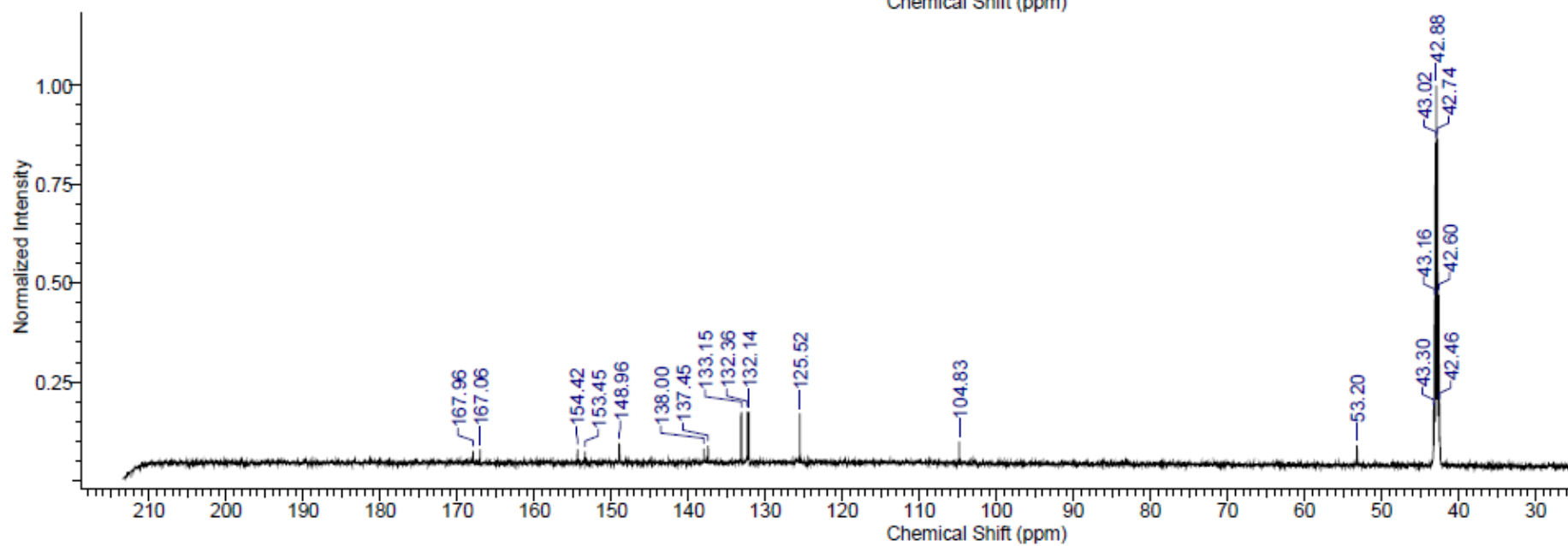
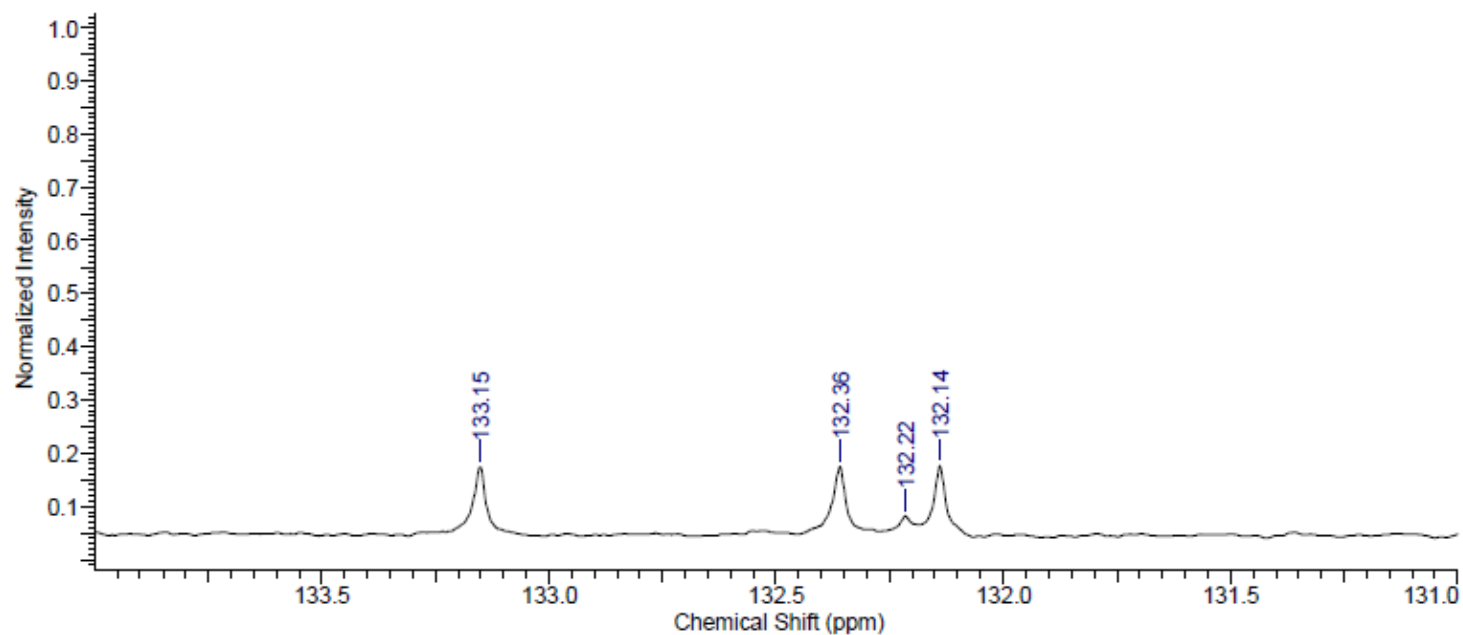
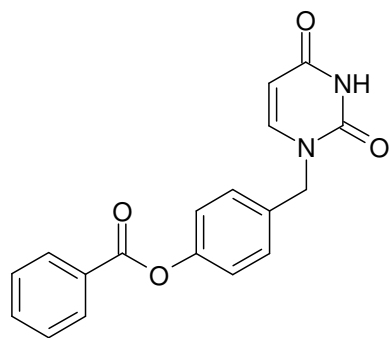


Figure S24. <sup>13</sup>C NMR spectrum of compound 21 (in DMSO-d<sub>6</sub> at 100 MHz)

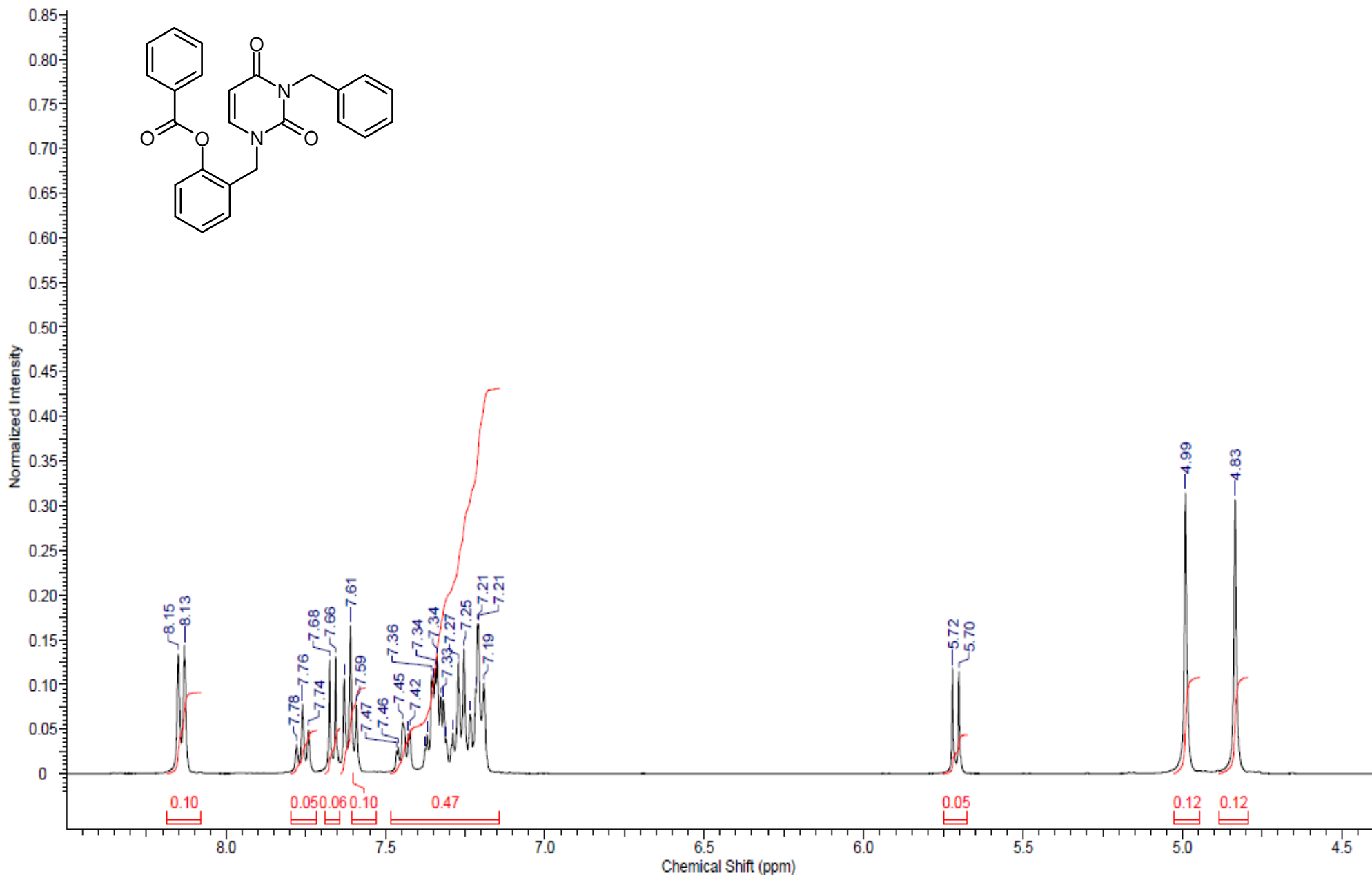


Figure S25. <sup>1</sup>H NMR spectrum of compound 22 (in DMSO-d<sub>6</sub> at 400 MHz)

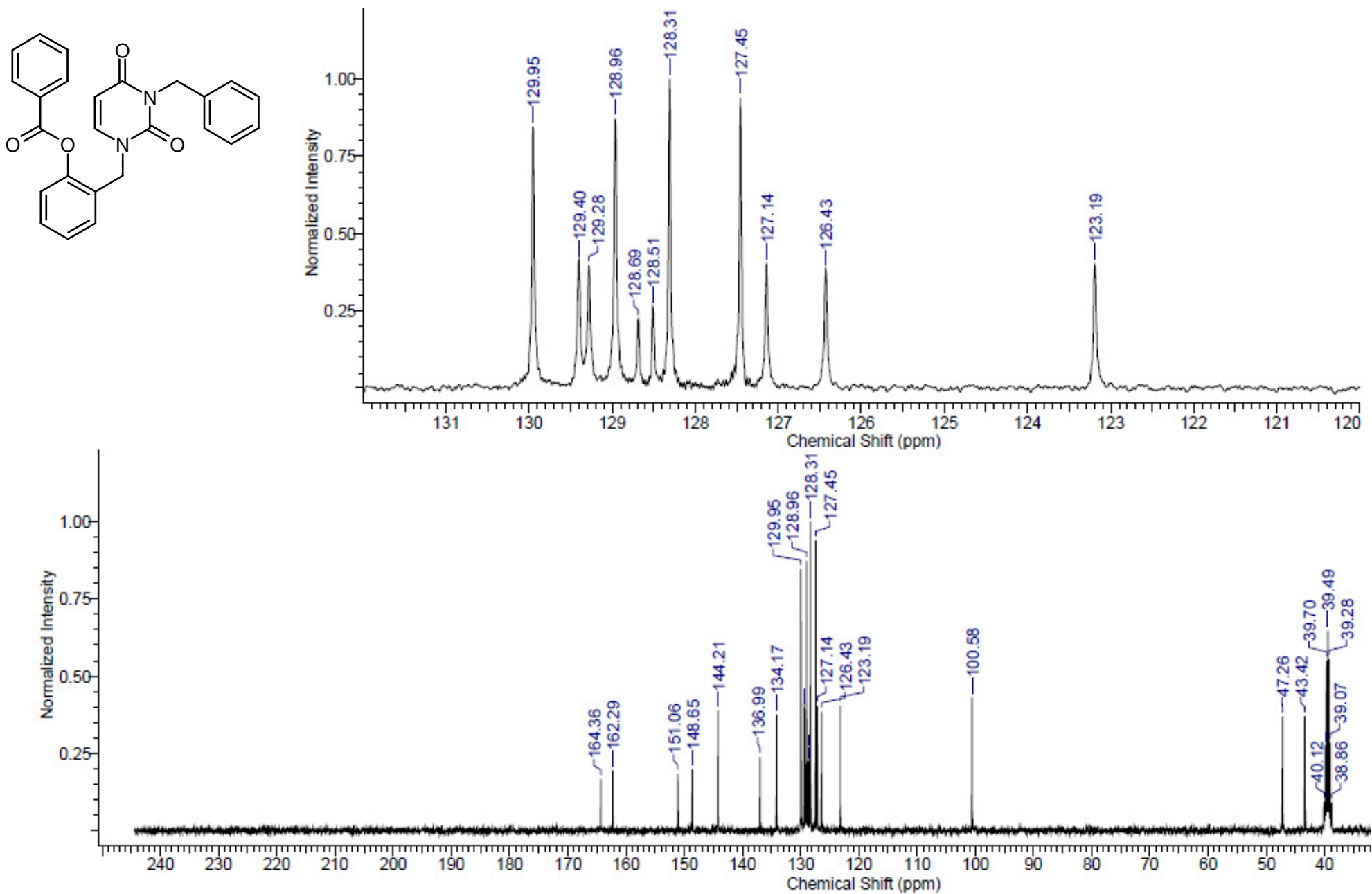


Figure S26. <sup>13</sup>C NMR spectrum of compound 22 (in CD<sub>3</sub>CN at 100 MHz)

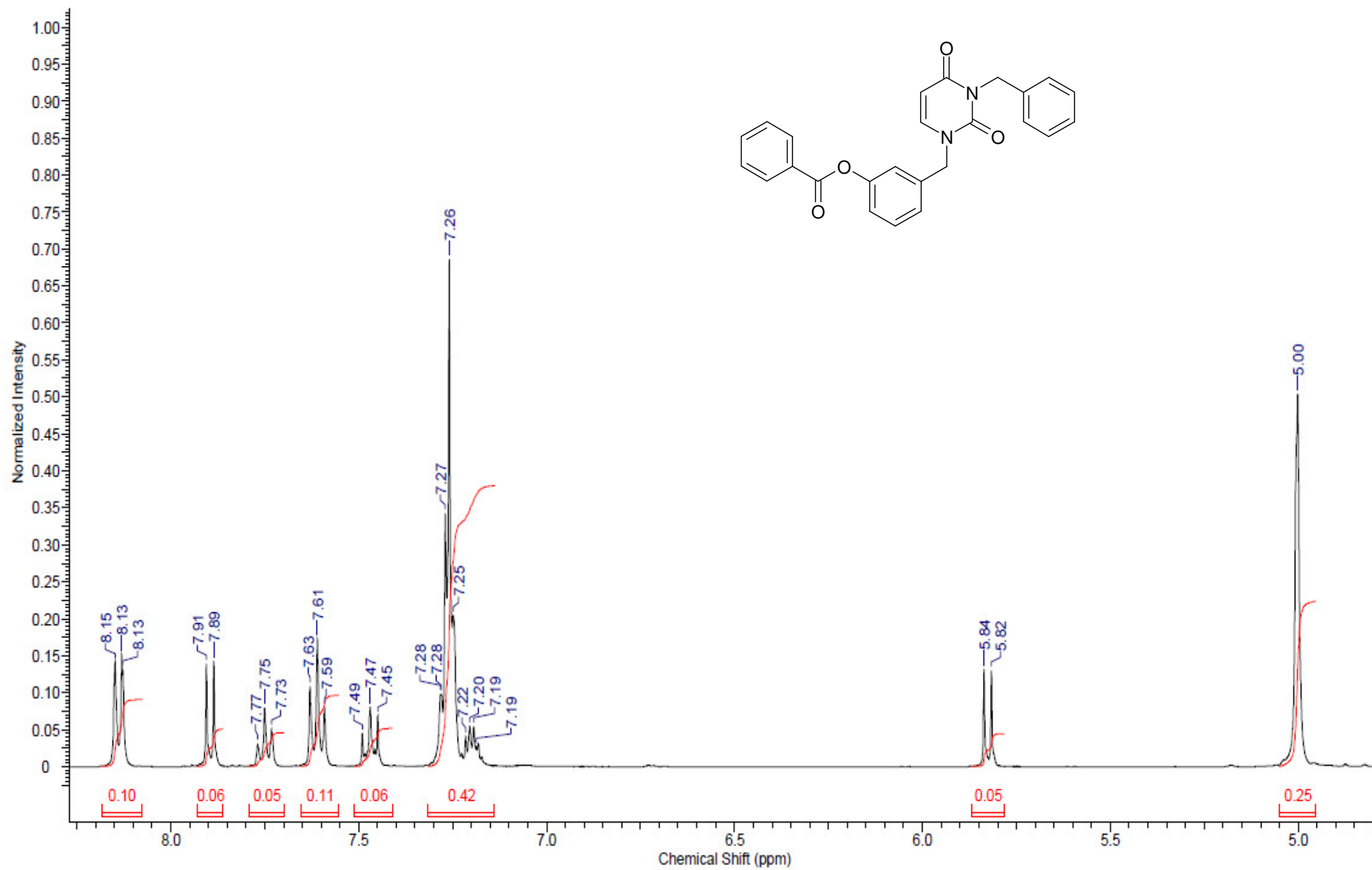


Figure S27. <sup>1</sup>H NMR spectrum of compound 23 (in DMSO-d<sub>6</sub> at 400 MHz)

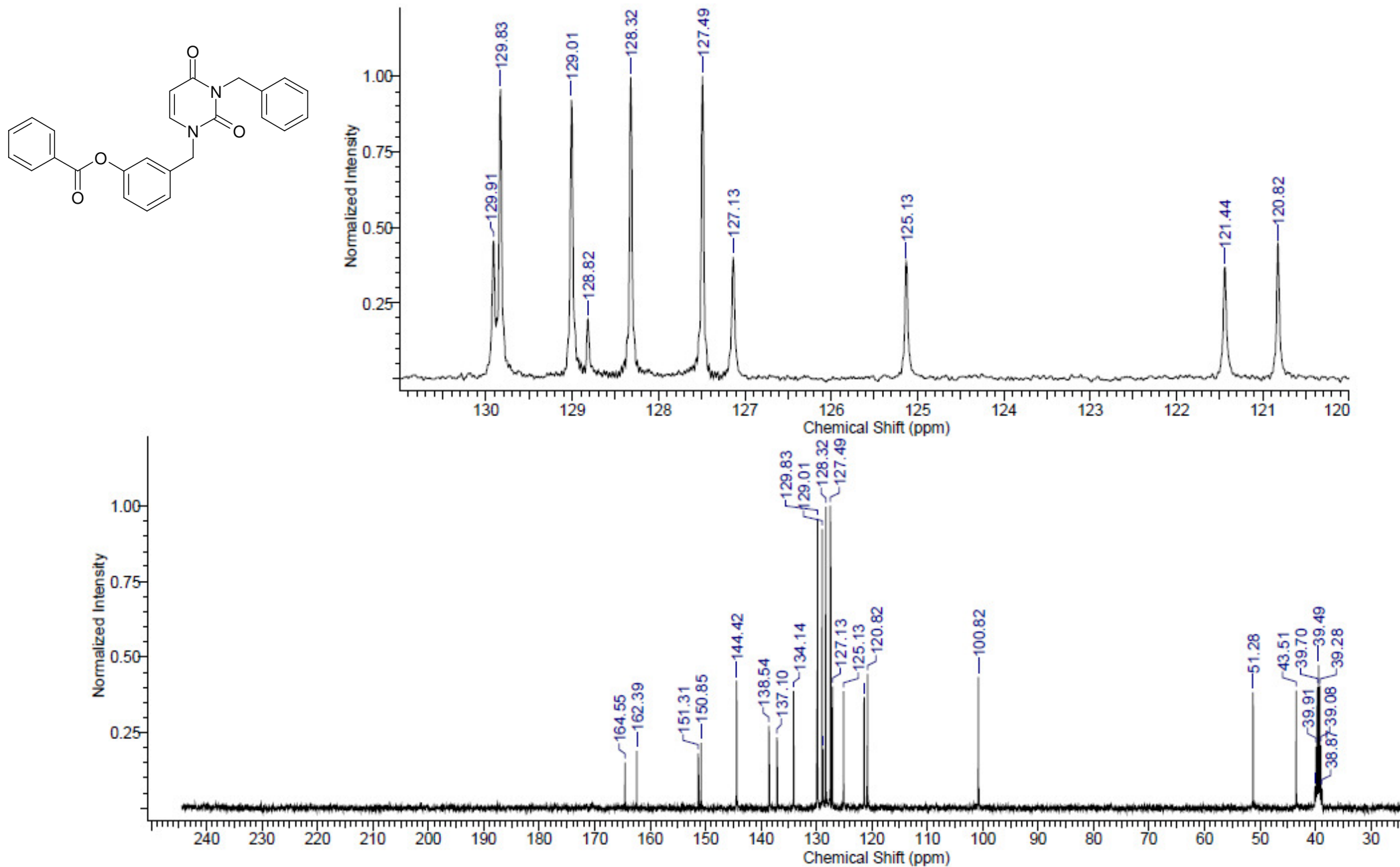


Figure S28.  $^{13}\text{C}$  NMR spectrum of compound 23 (in  $\text{CD}_3\text{CN}$  at 100 MHz)

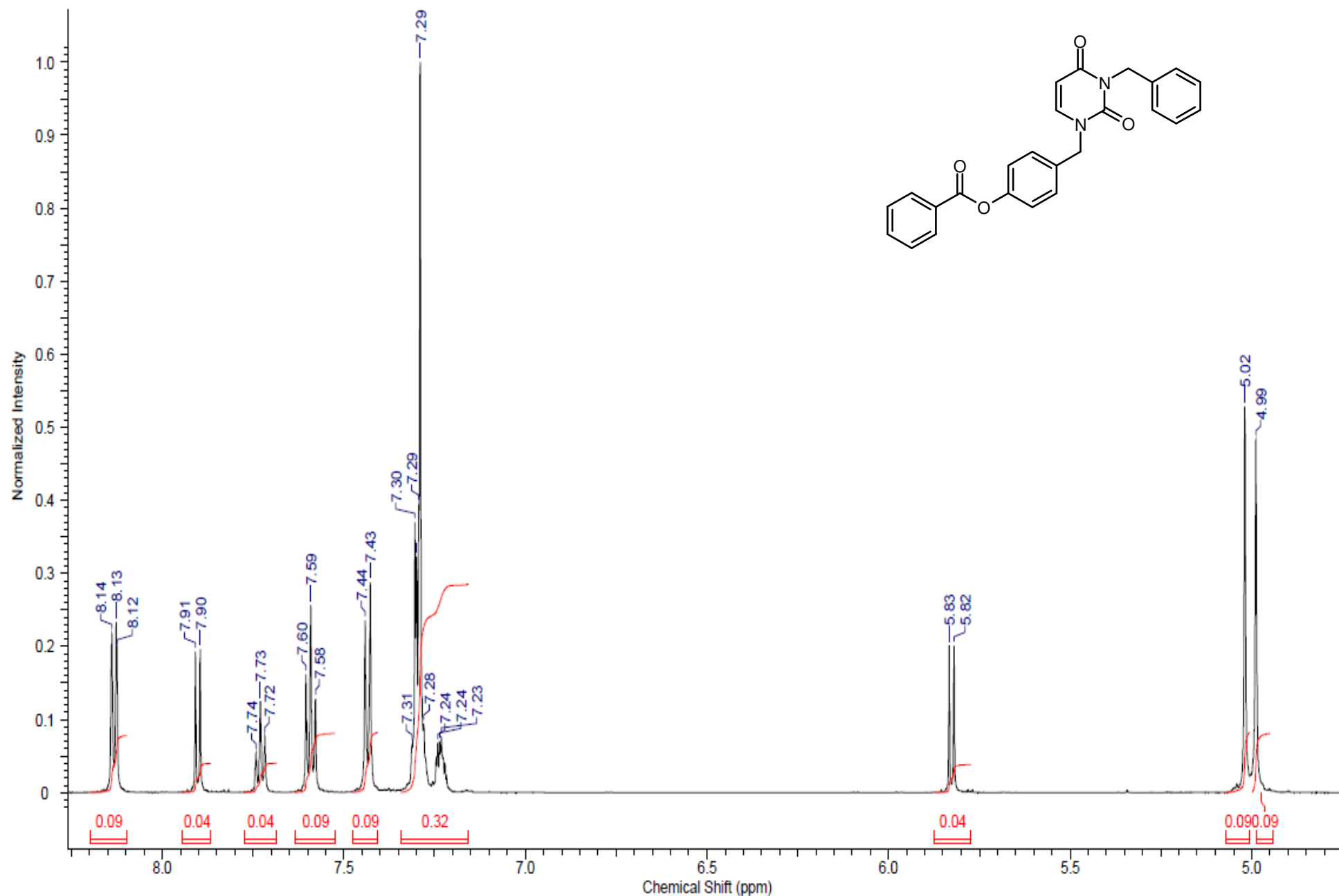


Figure S29. <sup>1</sup>H NMR spectrum of compound 24 (in DMSO-d<sub>6</sub> at 400 MHz)

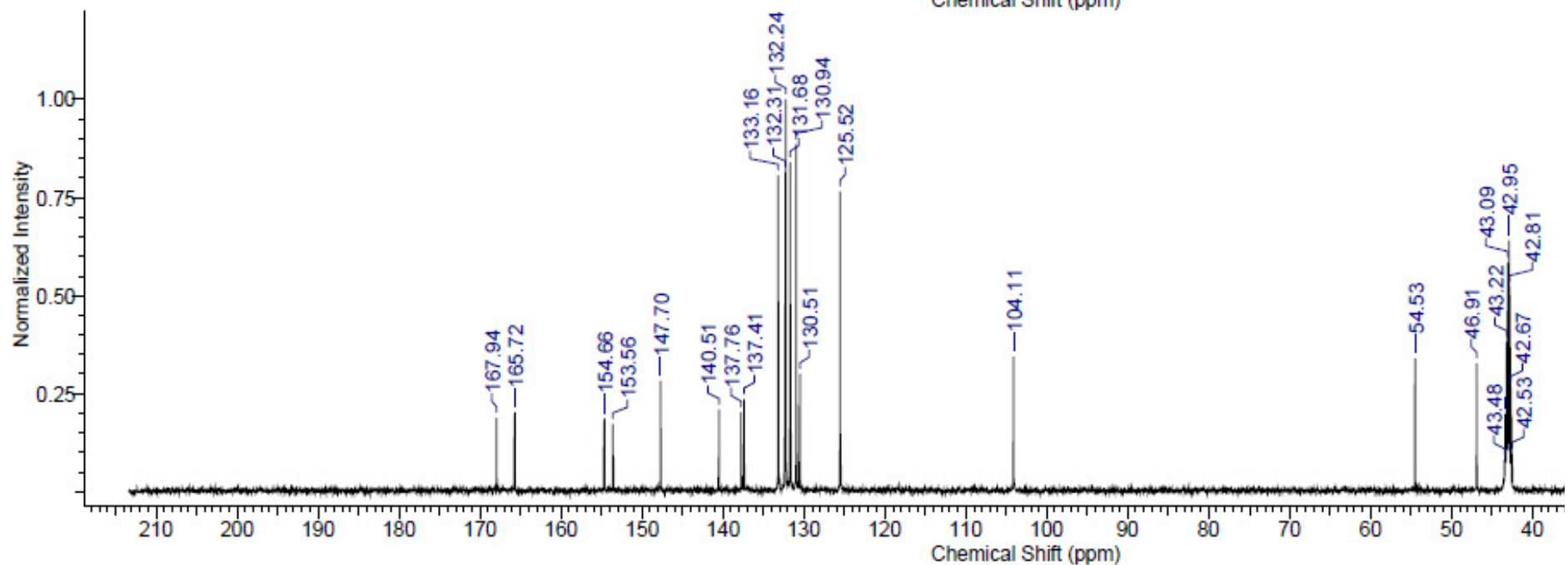
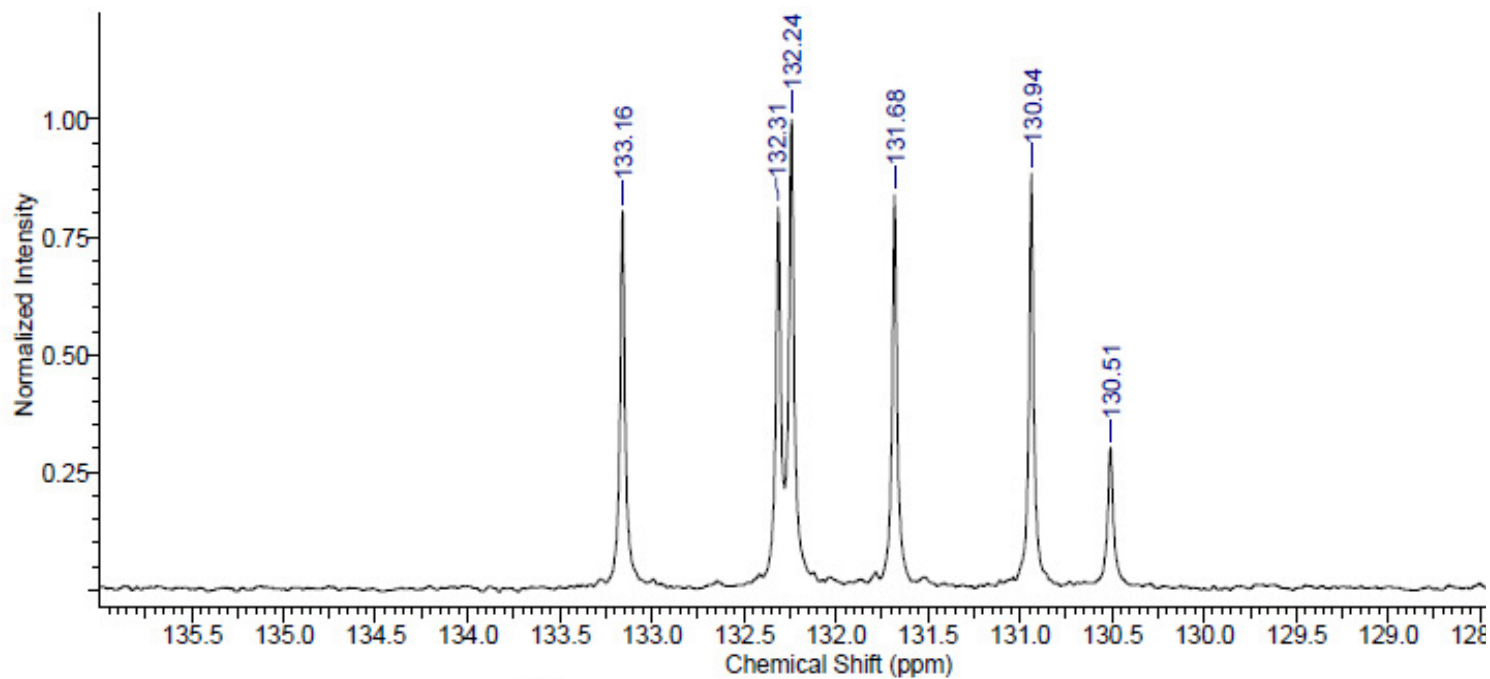
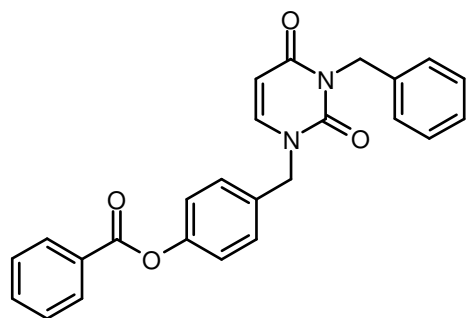


Figure S30. <sup>13</sup>C NMR spectrum of compound 24 (in DMSO-d<sub>6</sub> at 100 MHz)



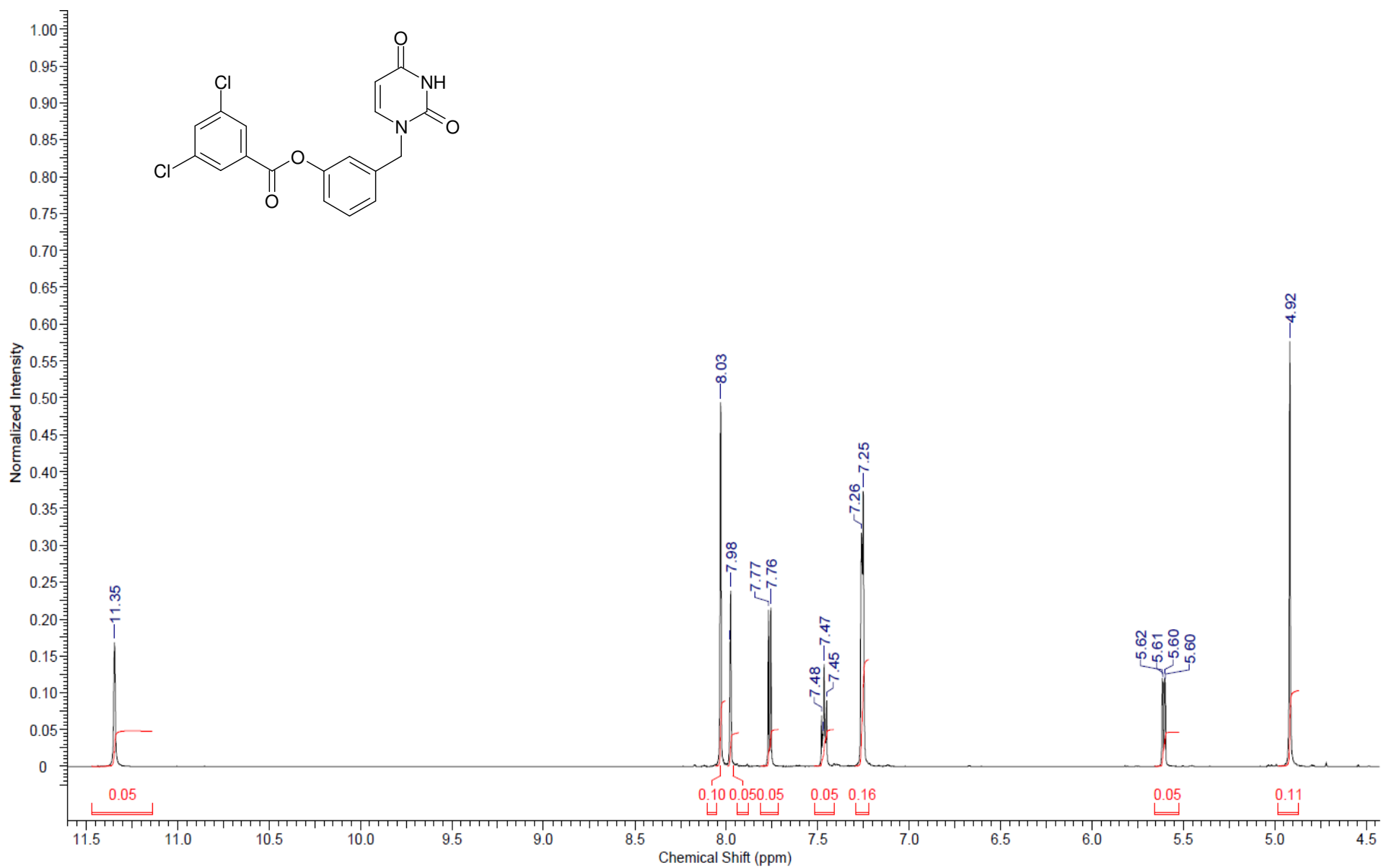


Figure S31. <sup>1</sup>H NMR spectrum of compound 25 (in DMSO-d<sub>6</sub> at 400 MHz)

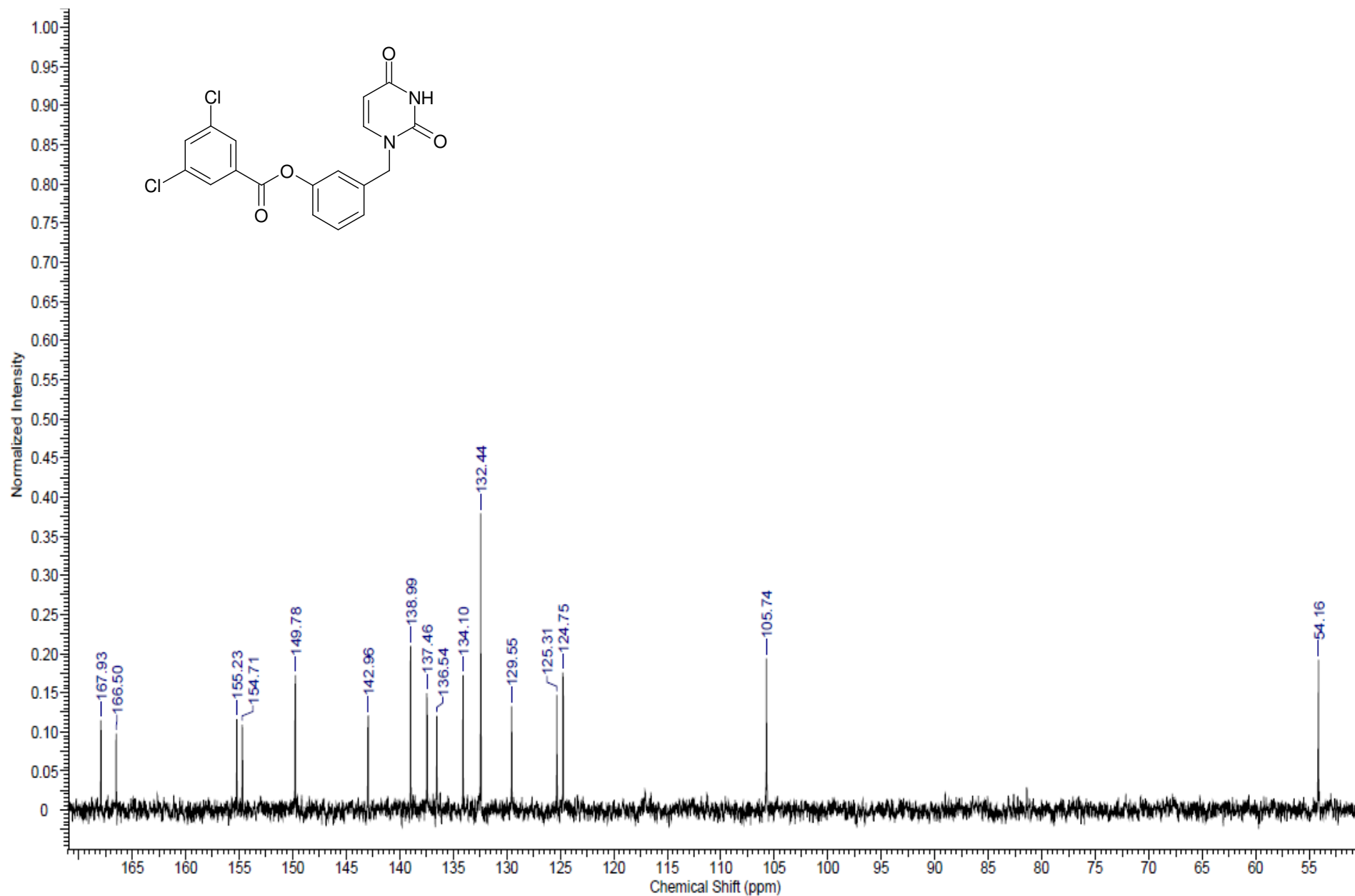


Figure S32.  $^{13}\text{C}$  NMR spectrum of compound 25 (in  $\text{DMSO-d}_6$  at 100 MHz)

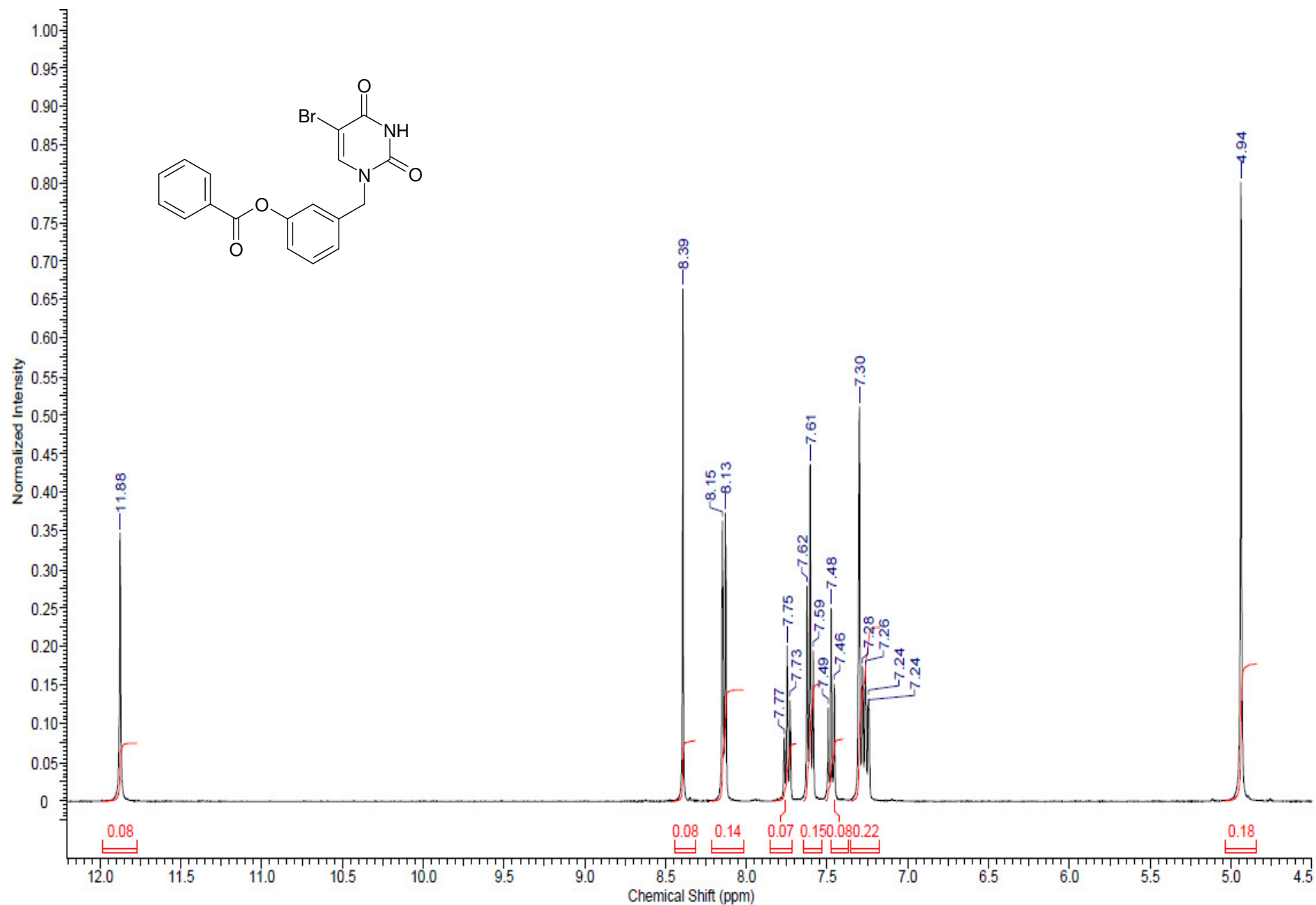


Figure S33. <sup>1</sup>H NMR spectrum of 1-[3-(benzyloxy)benzyl]-5-bromouracil (in DMSO-d<sub>6</sub> at 400 MHz)

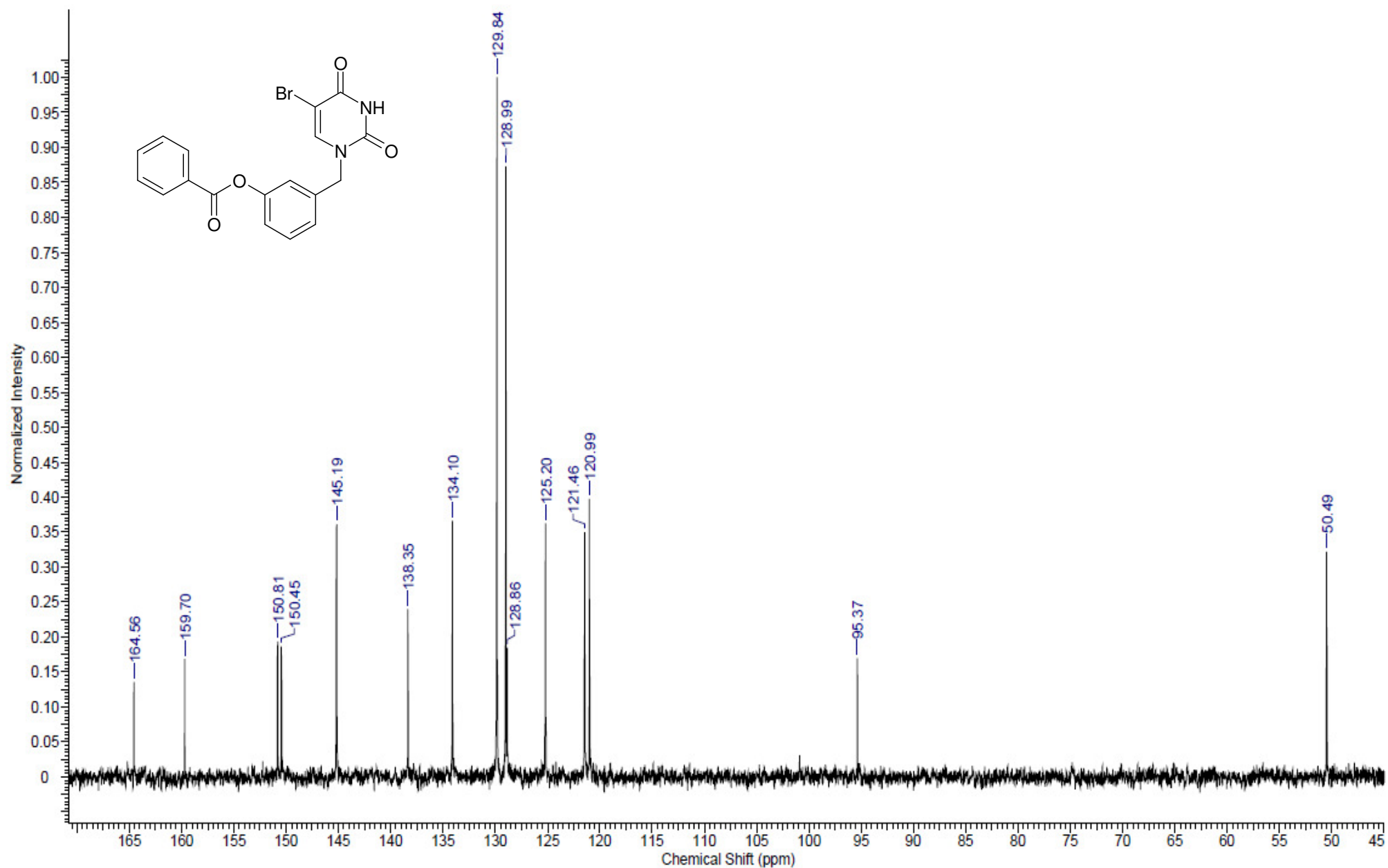


Figure S34. <sup>13</sup>C NMR spectrum of 1-[3-(benzyloxy)benzyl]-5-bromouracil (in DMSO-d<sub>6</sub> at 100 MHz)

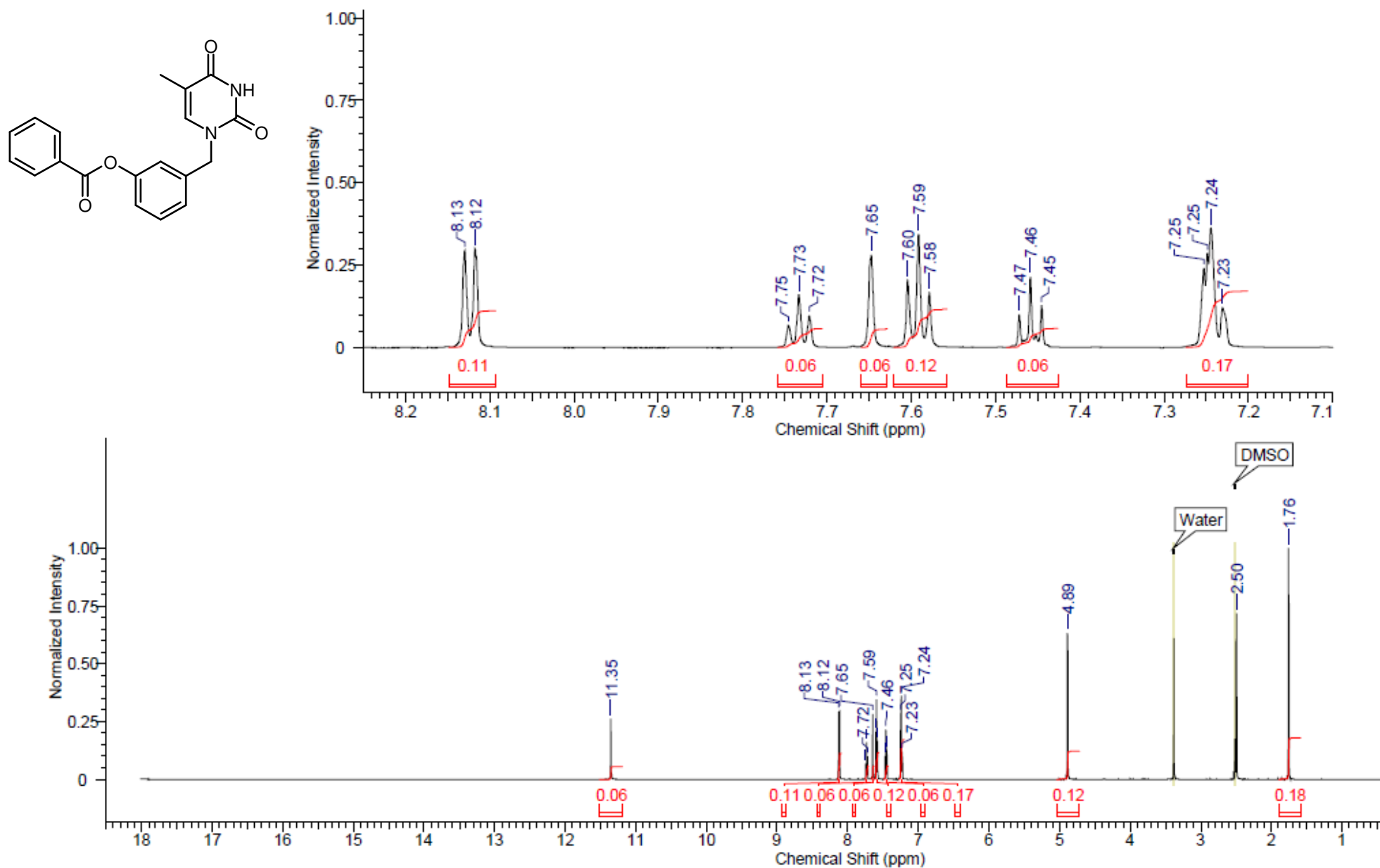


Figure S35. <sup>1</sup>H NMR spectrum of 1-[3-(benzoyloxy)benzyl]thymine (in DMSO-d<sub>6</sub> at 400 MHz)

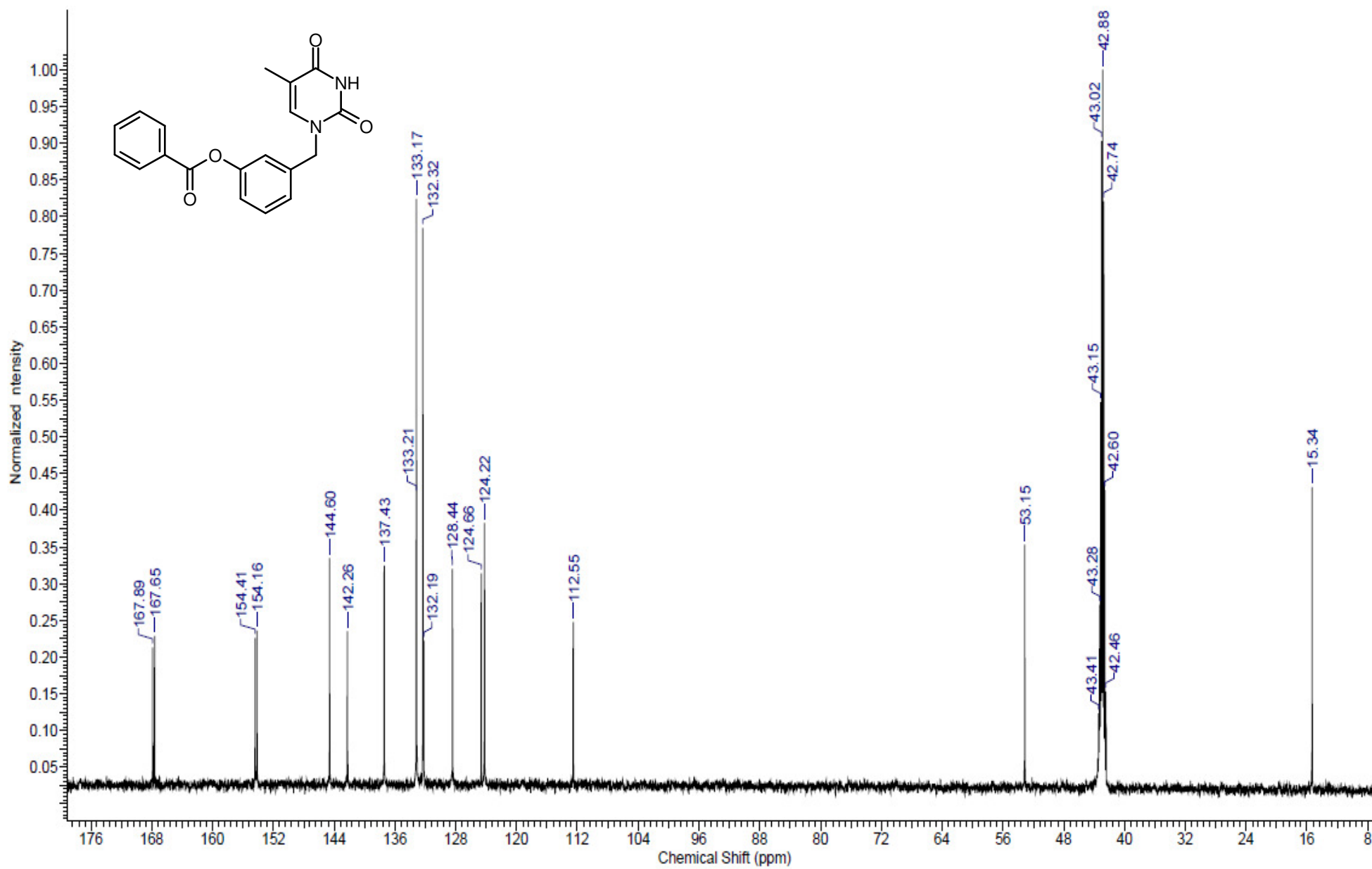


Figure S36. <sup>13</sup>C NMR spectrum of 1-[3-(benzyloxy)benzyl]thymine (in DMSO-d<sub>6</sub> at 100 MHz)

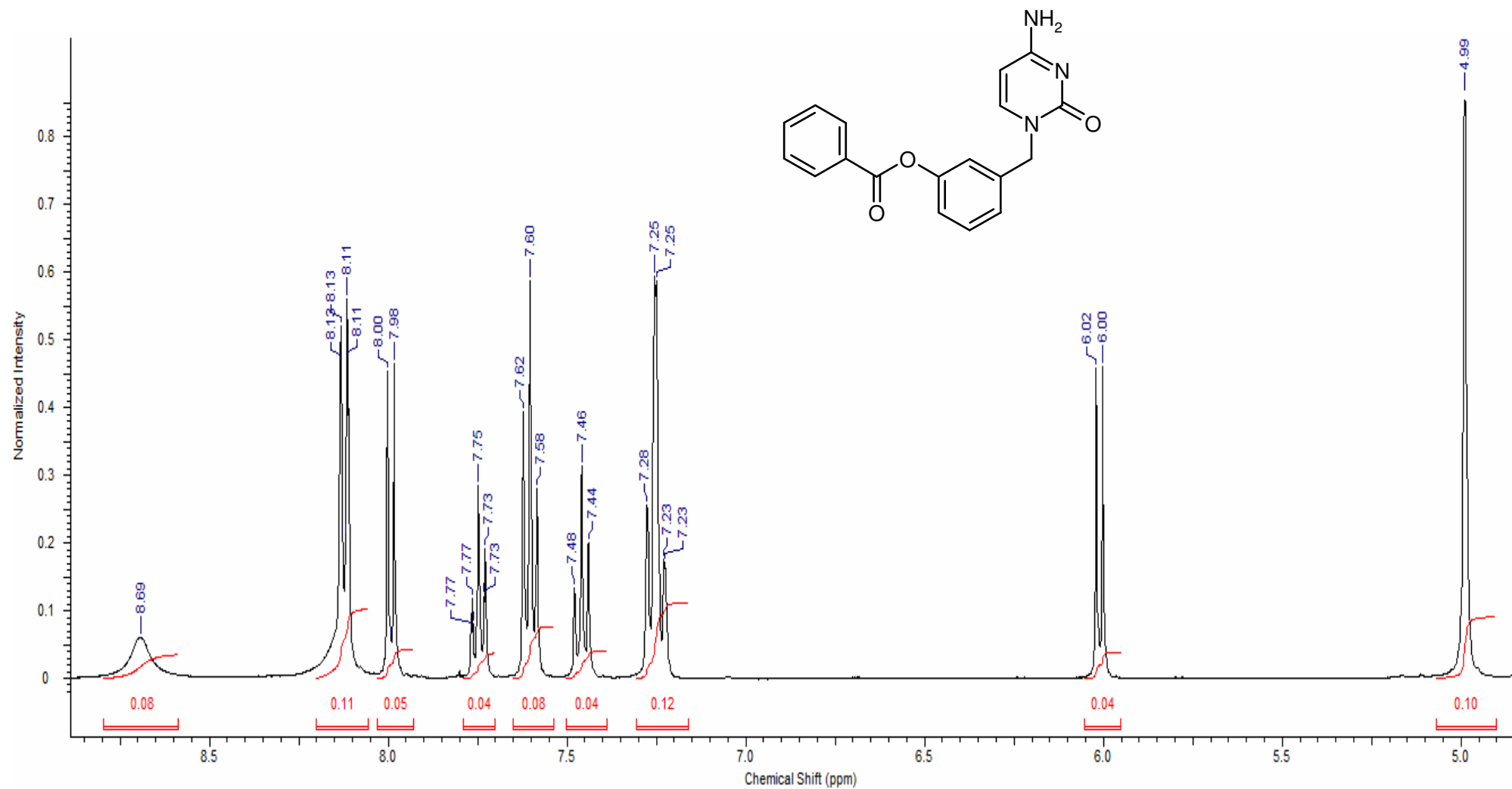


Figure S37. <sup>1</sup>H NMR spectrum of 1-[3-(benzoyloxy)benzyl]cytosine (in DMSO-d<sub>6</sub> at 400 MHz)

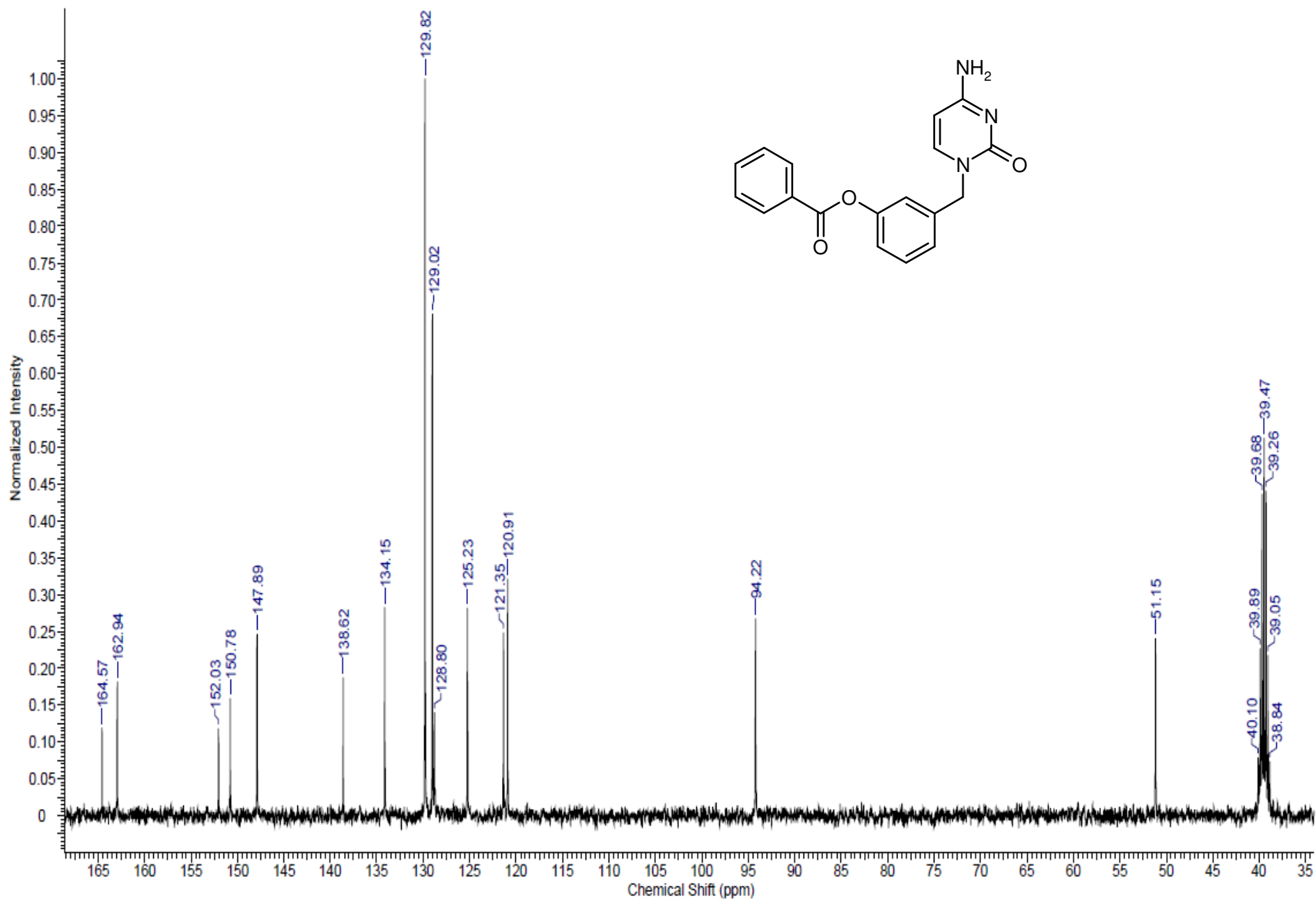


Figure S38. <sup>13</sup>C NMR spectrum of 1-[3-(benzyloxy)benzyl]cytosine (in CD<sub>3</sub>CN at 100 MHz)



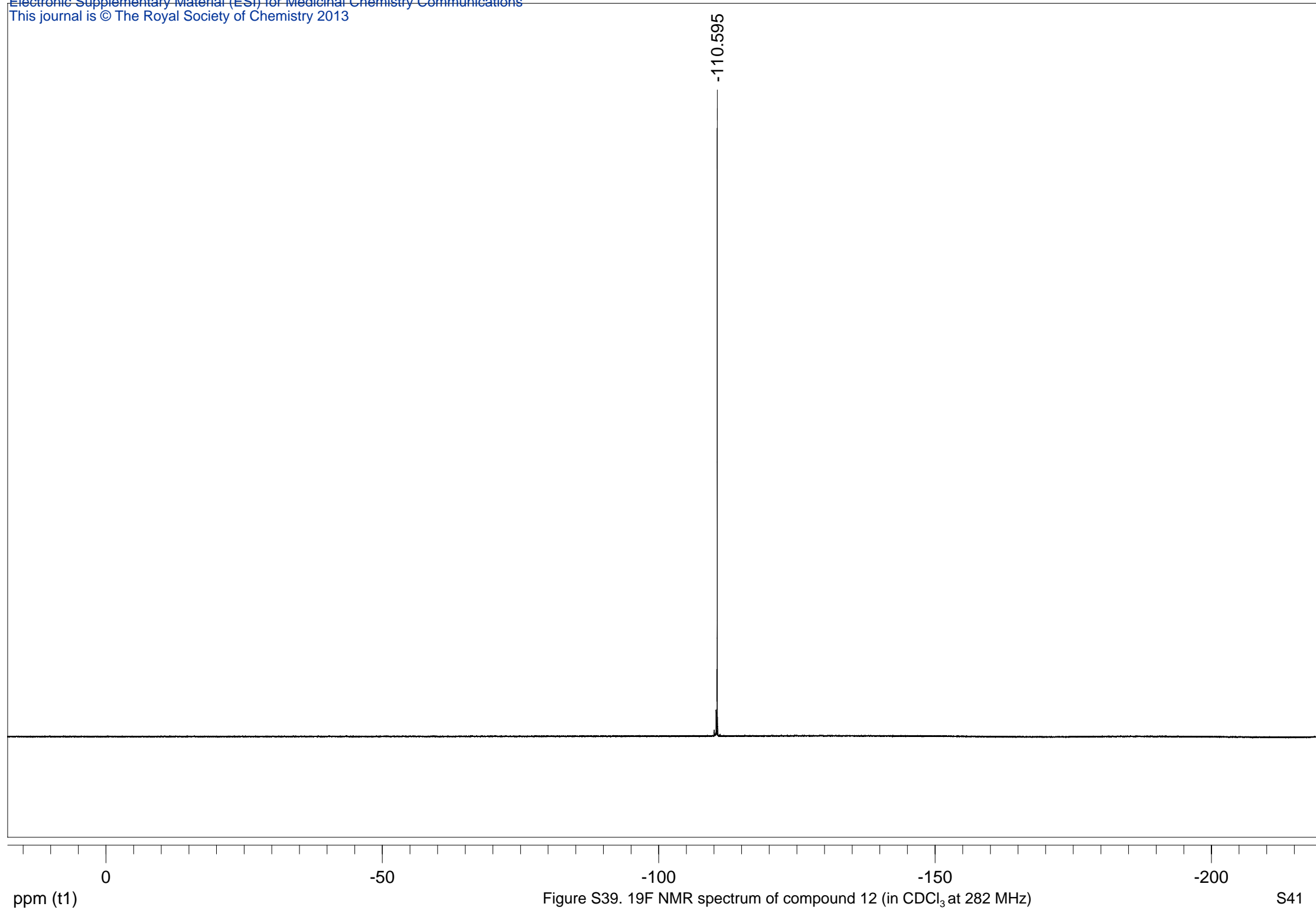


Figure S39.  $^{19}\text{F}$  NMR spectrum of compound 12 (in  $\text{CDCl}_3$  at 282 MHz)

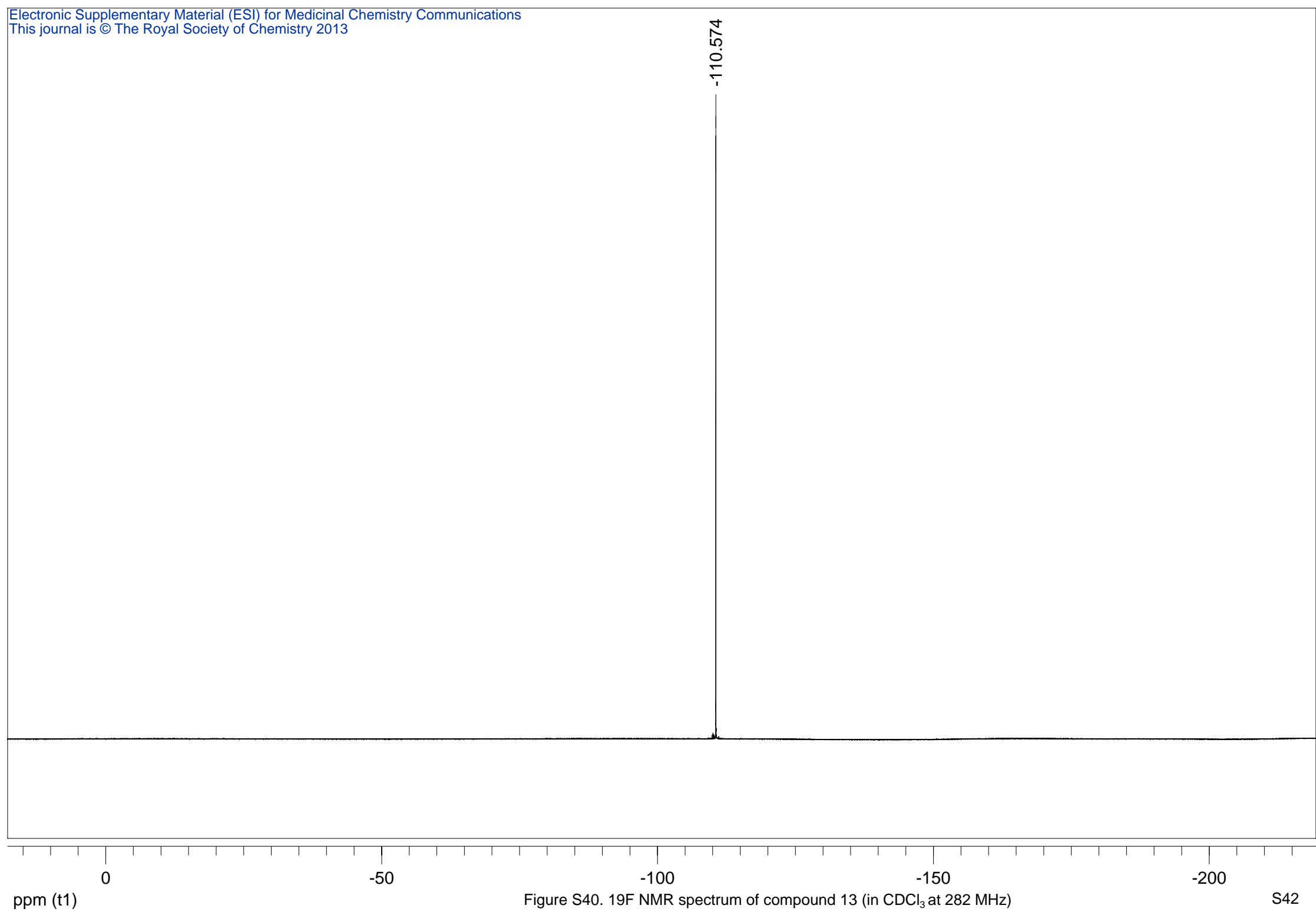


Figure S40.  $^{19}\text{F}$  NMR spectrum of compound 13 (in  $\text{CDCl}_3$  at 282 MHz)