

## **5'-Nor carbocyclic nucleosides: unusual nonnucleoside inhibitors of HIV-1 reverse transcriptase**

**Elena S. Matyugina<sup>a</sup>, Vladimir T. Valuev-Elliston<sup>a</sup>, Denis A. Babkov<sup>b</sup>, Mikhail S. Novikov<sup>b</sup>, Alexander V. Ivanov<sup>a</sup>, Sergey N. Kochetkov<sup>a</sup>, Jan Balzarini<sup>c</sup>, Katherine L. Seley-Radtke<sup>d</sup> and Anastasia L. Khandazinskaya<sup>a</sup>**

<sup>a</sup>Engelhardt Institute of Molecular Biology RAS, Vavilova 32, 119991 Moscow, Russia

<sup>b</sup>Volgograd State Medicinal University, Paversushikh Bortcov Sq., 1, 400131 Volgograd Russia

<sup>c</sup>Rega Institute for Medical Research, K.U. Leuven, Minderbroedersstraat 10, B-3000 Leuven, Belgium

<sup>d</sup>University of Maryland, Baltimore County, 1000 Hilltop Circle, Baltimore, MD USA

[kseley@umbc.edu](mailto:kseley@umbc.edu)

## Contents

$^1\text{H}$ NMR and $^{13}\text{C}$ NMR spectra	S3
Figure S1. $^1\text{H}$ NMR spectrum of compound 1 (in $\text{CDCl}_3$ at 400 MHz)	S3
Figure S2. $^{13}\text{C}$ NMR spectrum of compound 1 (in $\text{CDCl}_3$ at 100 MHz)	S4
Figure S3. $^1\text{H}$ NMR spectrum of compound 2 (in $\text{CDCl}_3$ at 400 MHz)	S5
Figure S4. $^{13}\text{C}$ NMR spectrum of compound 2 (in $\text{CDCl}_3$ at 100 MHz)	S6
Figure S5. $^1\text{H}$ NMR spectrum of compound 3 (in $\text{CDCl}_3$ at 400 MHz)	S7
Figure S6. $^{13}\text{C}$ NMR spectrum of compound 3 (in $\text{CDCl}_3$ at 100 MHz)	S8
Figure S7. $^1\text{H}$ NMR spectrum of compound 4 (in $\text{CDCl}_3$ at 400 MHz)	S9
Figure S8. $^{13}\text{C}$ NMR spectrum of compound 4 (in $\text{CDCl}_3$ at 100 MHz)	S10
Figure S9. $^1\text{H}$ NMR spectrum of compound 5 (in $\text{CDCl}_3$ at 400 MHz)	S11
Figure S10. $^{13}\text{C}$ NMR spectrum of compound 5 (in $\text{CDCl}_3$ at 100 MHz)	S12
Figure S11. $^1\text{H}$ NMR spectrum of compound 6 (in $\text{CDCl}_3$ at 400 MHz)	S13
Figure S12. $^{13}\text{C}$ NMR spectrum of compound 6 (in $\text{CDCl}_3$ at 100 MHz)	S14
Figure S13. $^1\text{H}$ NMR spectrum of compound 7 (in $\text{CDCl}_3$ at 400 MHz)	S15
Figure S14. $^{13}\text{C}$ NMR spectrum of compound 7 (in $\text{CDCl}_3$ at 100 MHz)	S16
Figure S15. $^1\text{H}$ NMR spectrum of compound 8 (in $\text{CDCl}_3$ at 400 MHz)	S17
Figure S16. $^{13}\text{C}$ NMR spectrum of compound 8 (in $\text{CDCl}_3$ at 100 MHz)	S18
Figure S17. $^1\text{H}$ NMR spectrum of compound 9 (in $\text{CDCl}_3$ at 400 MHz)	S19
Figure S18. $^{13}\text{C}$ NMR spectrum of compound 9 (in $\text{CDCl}_3$ at 100 MHz)	S20
Figure S19. $^1\text{H}$ NMR spectrum of compound 10 (in $\text{CDCl}_3$ at 400 MHz)	S21
Figure S20. $^{13}\text{C}$ NMR spectrum of compound 10 (in $\text{CDCl}_3$ at 100 MHz)	S22
Figure S21. $^1\text{H}$ NMR spectrum of compound 13 (in $\text{CDCl}_3$ at 400 MHz)	S23
Figure S22. $^{13}\text{C}$ NMR spectrum of compound 13 (in $\text{CDCl}_3$ at 100 MHz)	S24
Figure S23. $^1\text{H}$ NMR spectrum of compound 14 (in $\text{CDCl}_3$ at 400 MHz)	S25
Figure S24. $^{13}\text{C}$ NMR spectrum of compound 14 (in $\text{CDCl}_3$ at 100 MHz)	S26
Figure S25. $^1\text{H}$ NMR spectrum of compound 15 (in $\text{CDCl}_3$ at 400 MHz)	S27
Figure S26. $^{13}\text{C}$ NMR spectrum of compound 15 (in $\text{CDCl}_3$ at 100 MHz)	S28

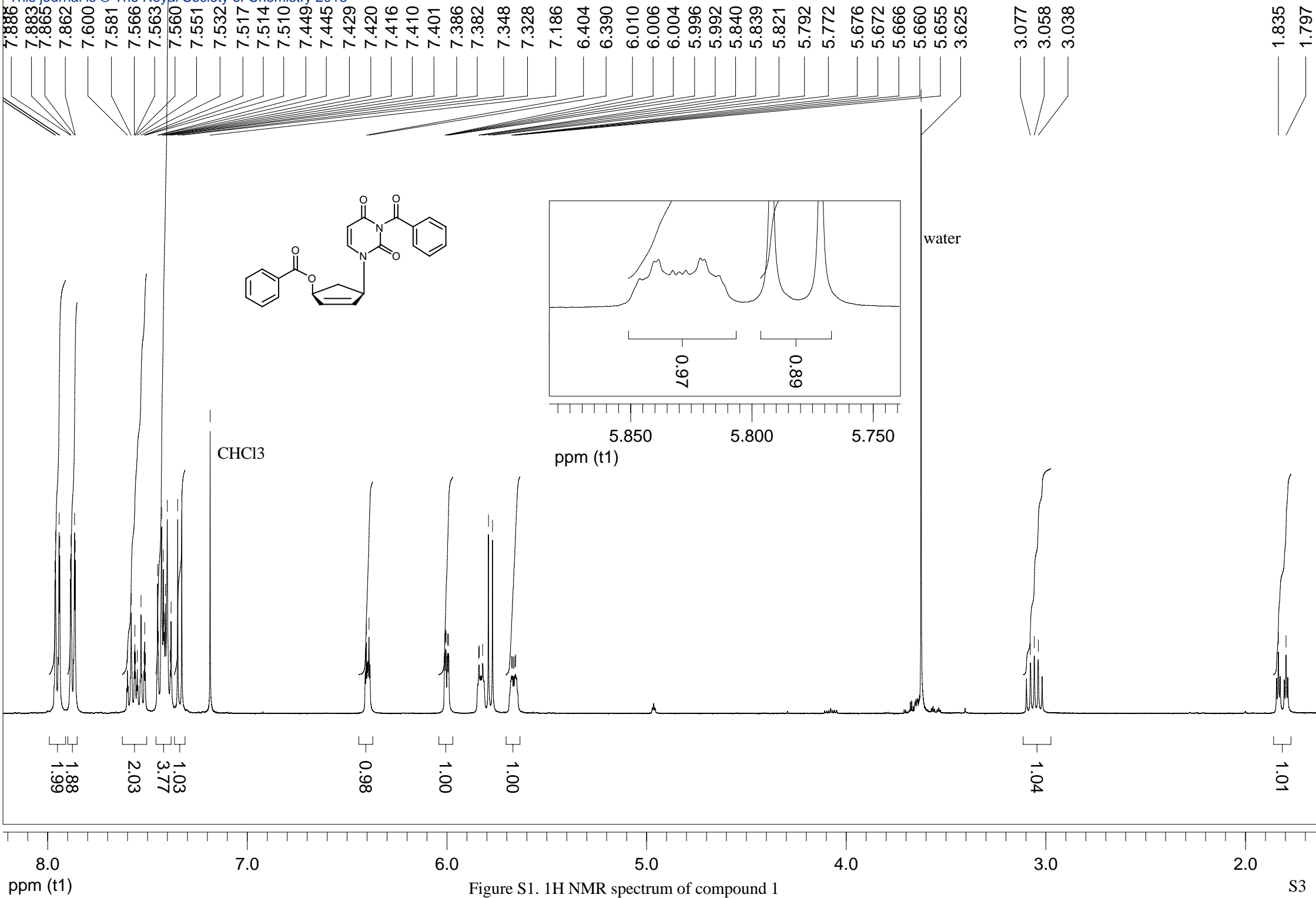


Figure S1. <sup>1</sup>H NMR spectrum of compound 1

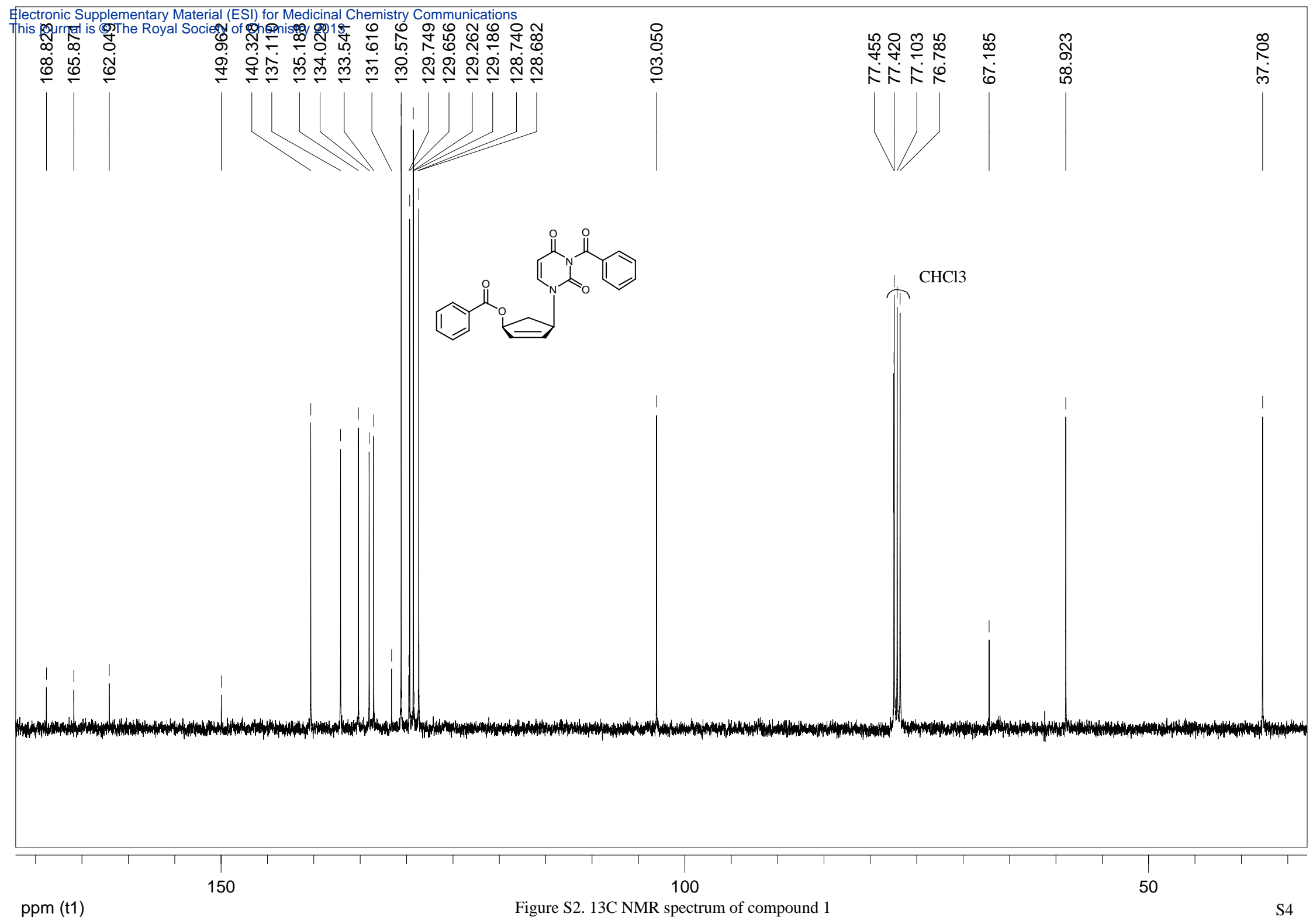
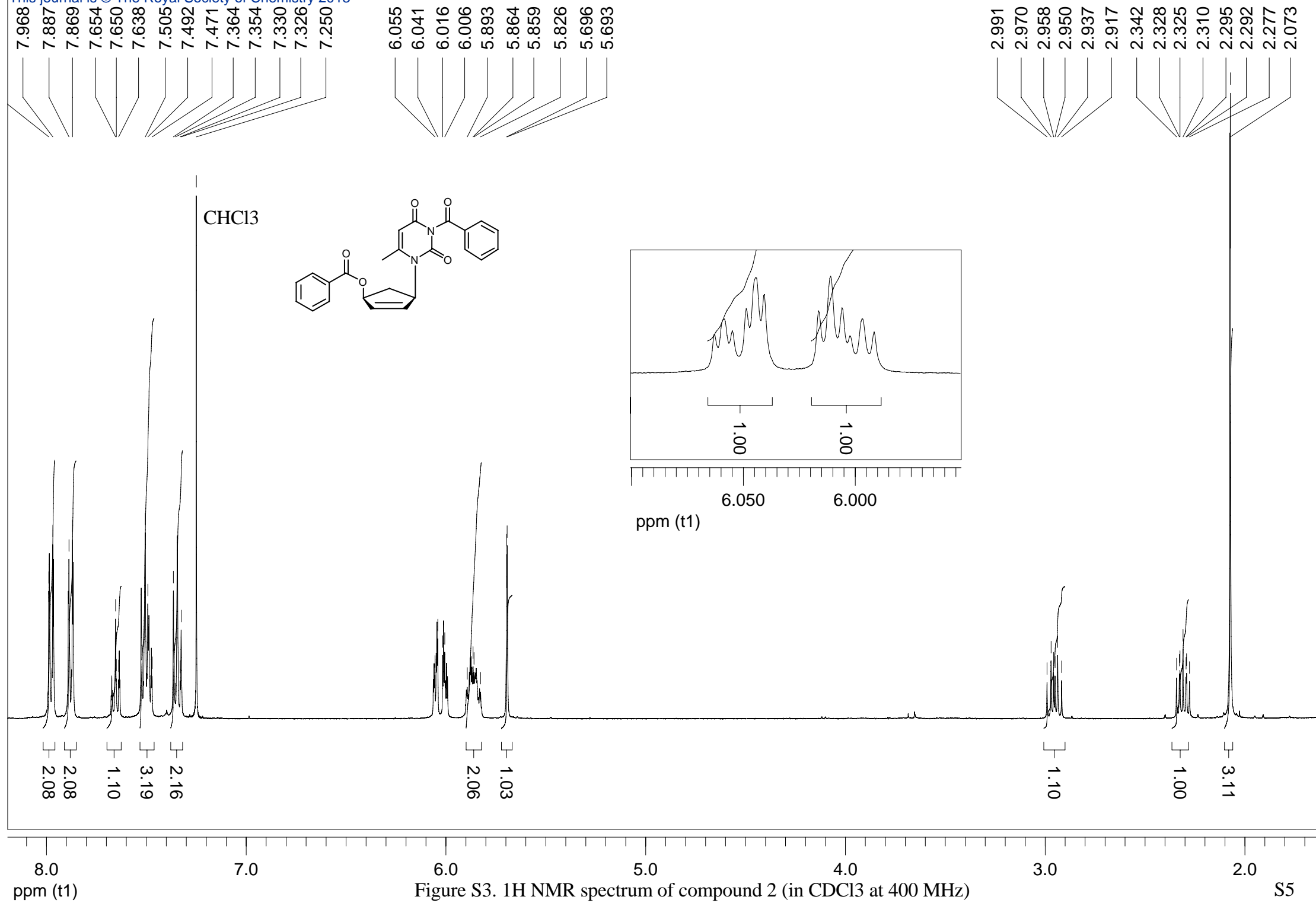


Figure S2. <sup>13</sup>C NMR spectrum of compound 1



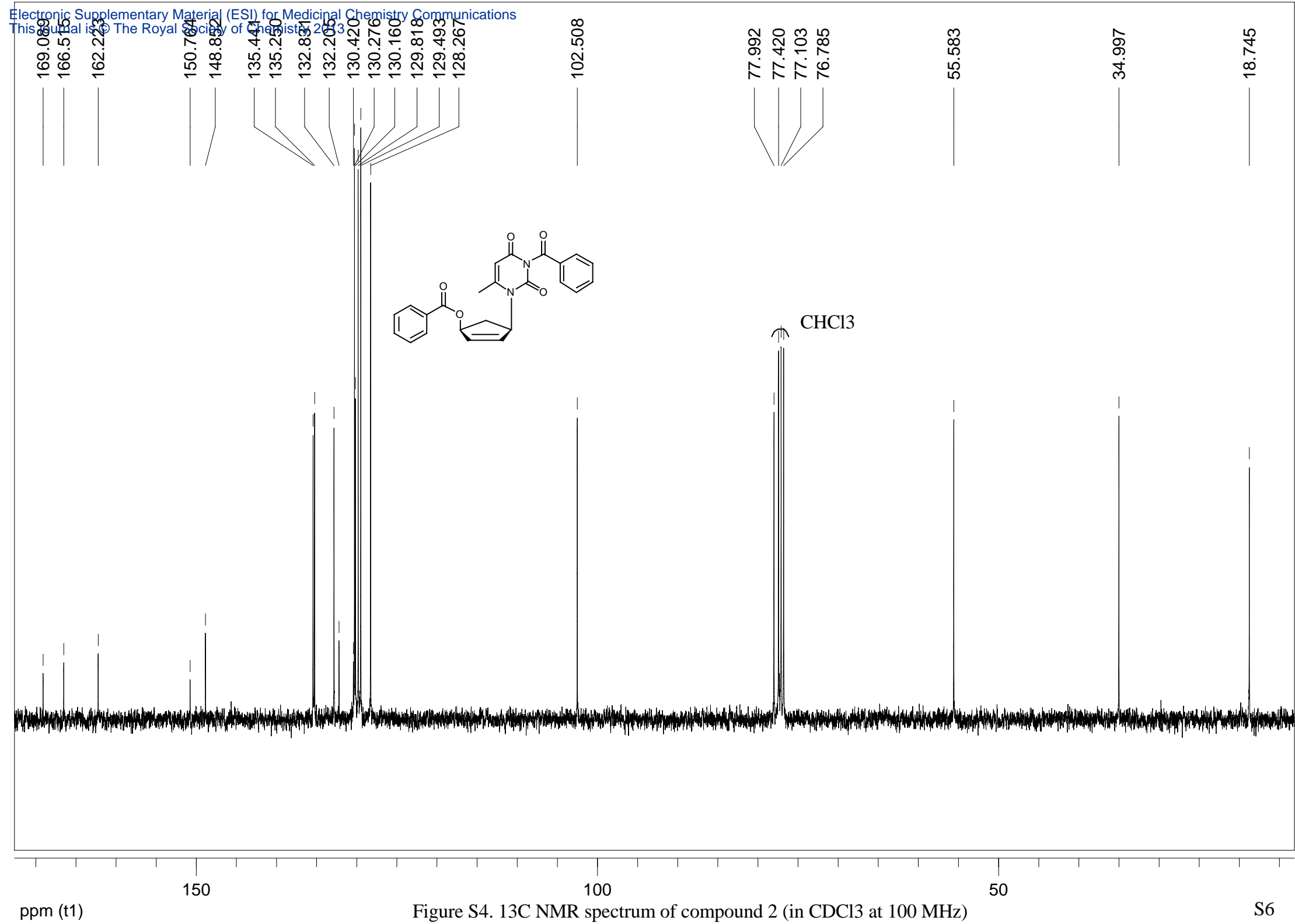
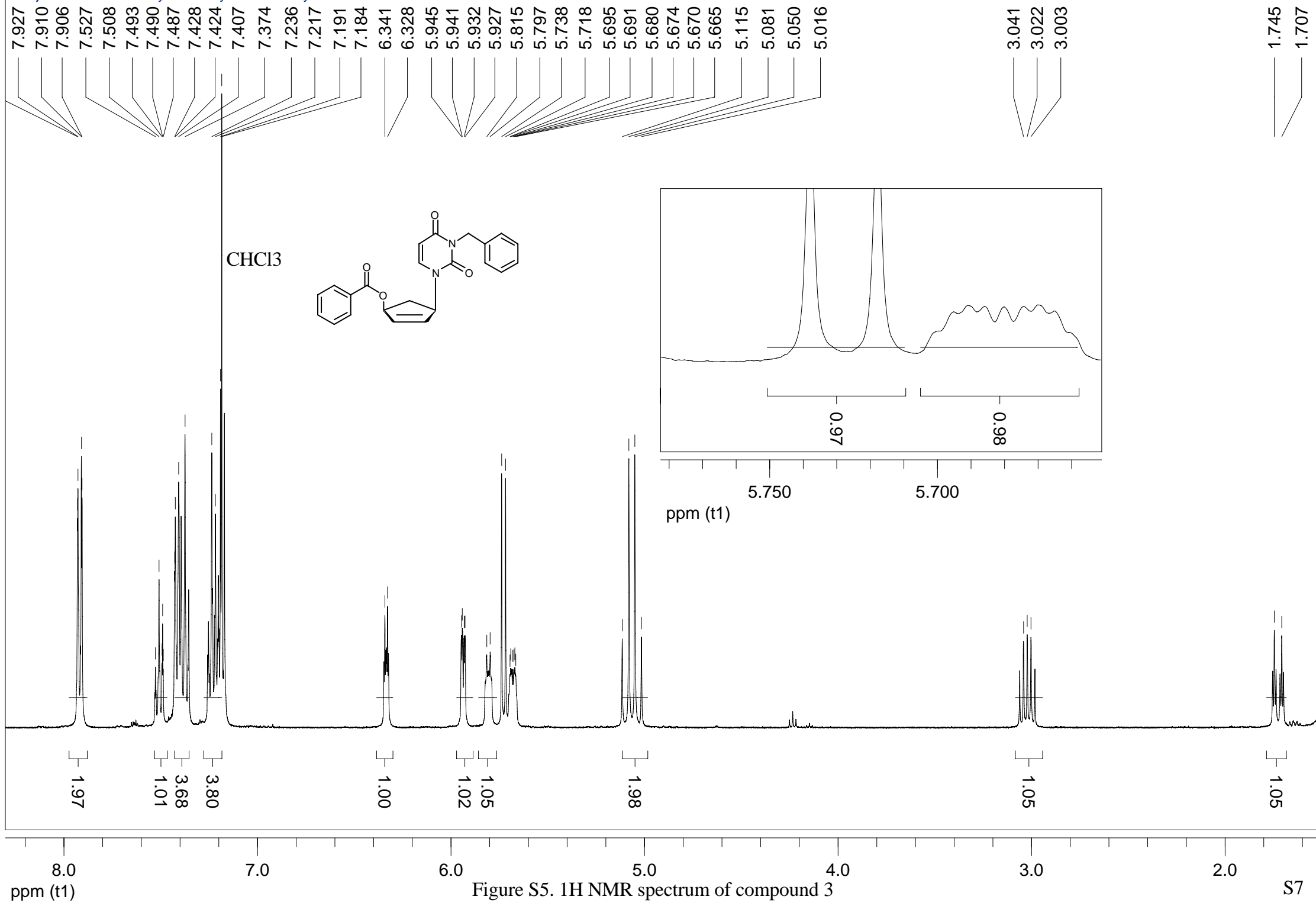


Figure S4. 13C NMR spectrum of compound 2 (in CDCl3 at 100 MHz)



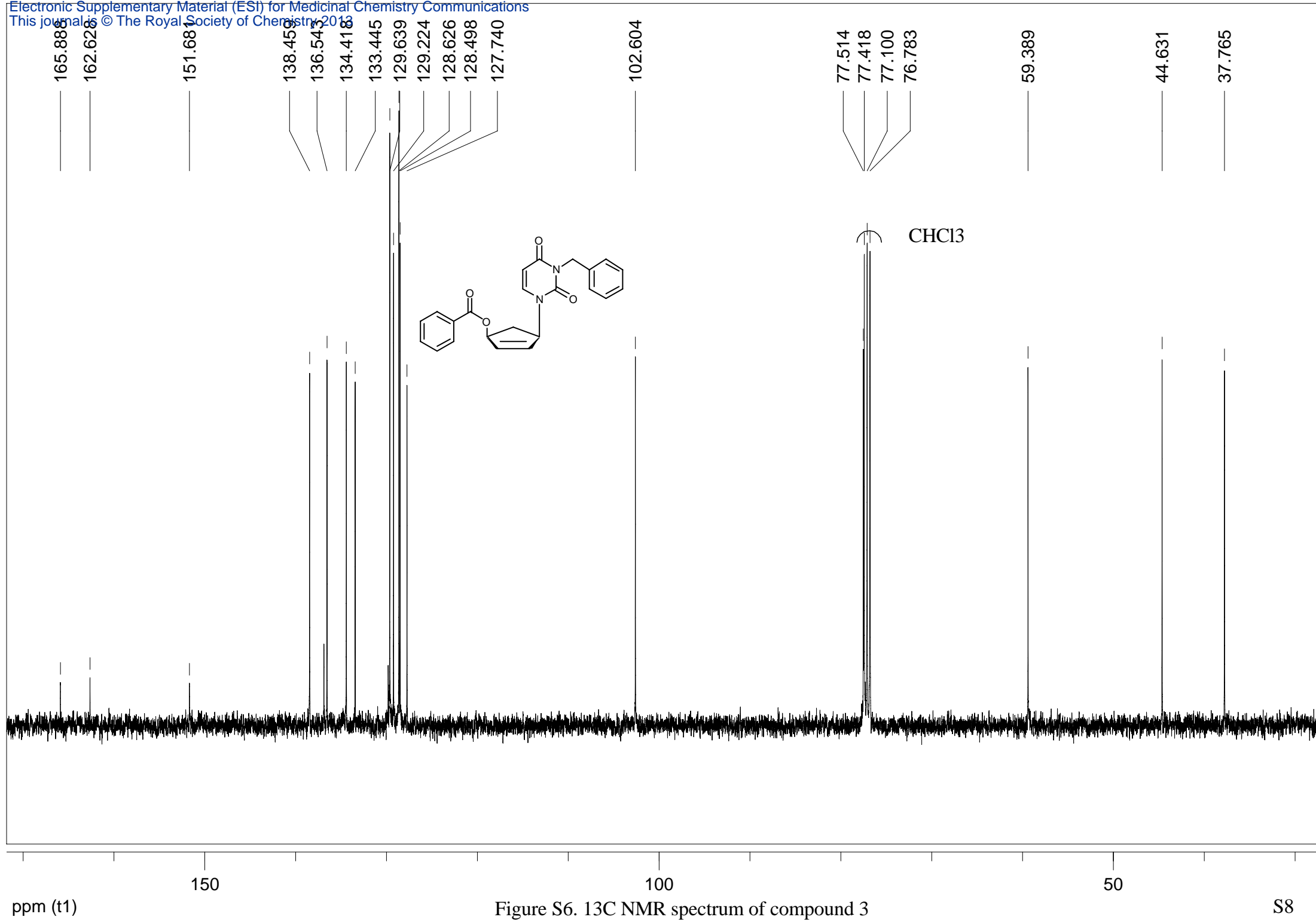


Figure S6. <sup>13</sup>C NMR spectrum of compound 3



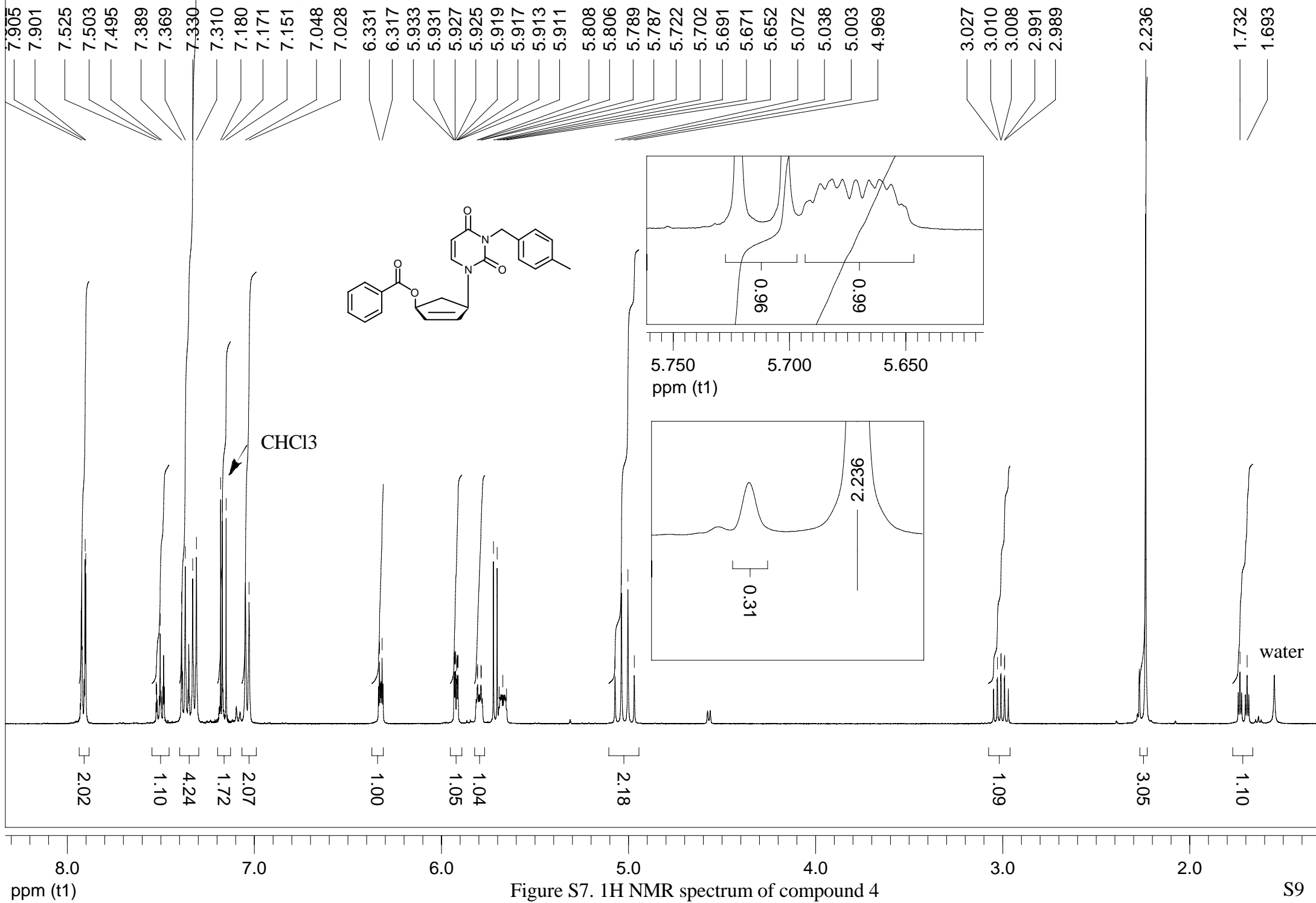
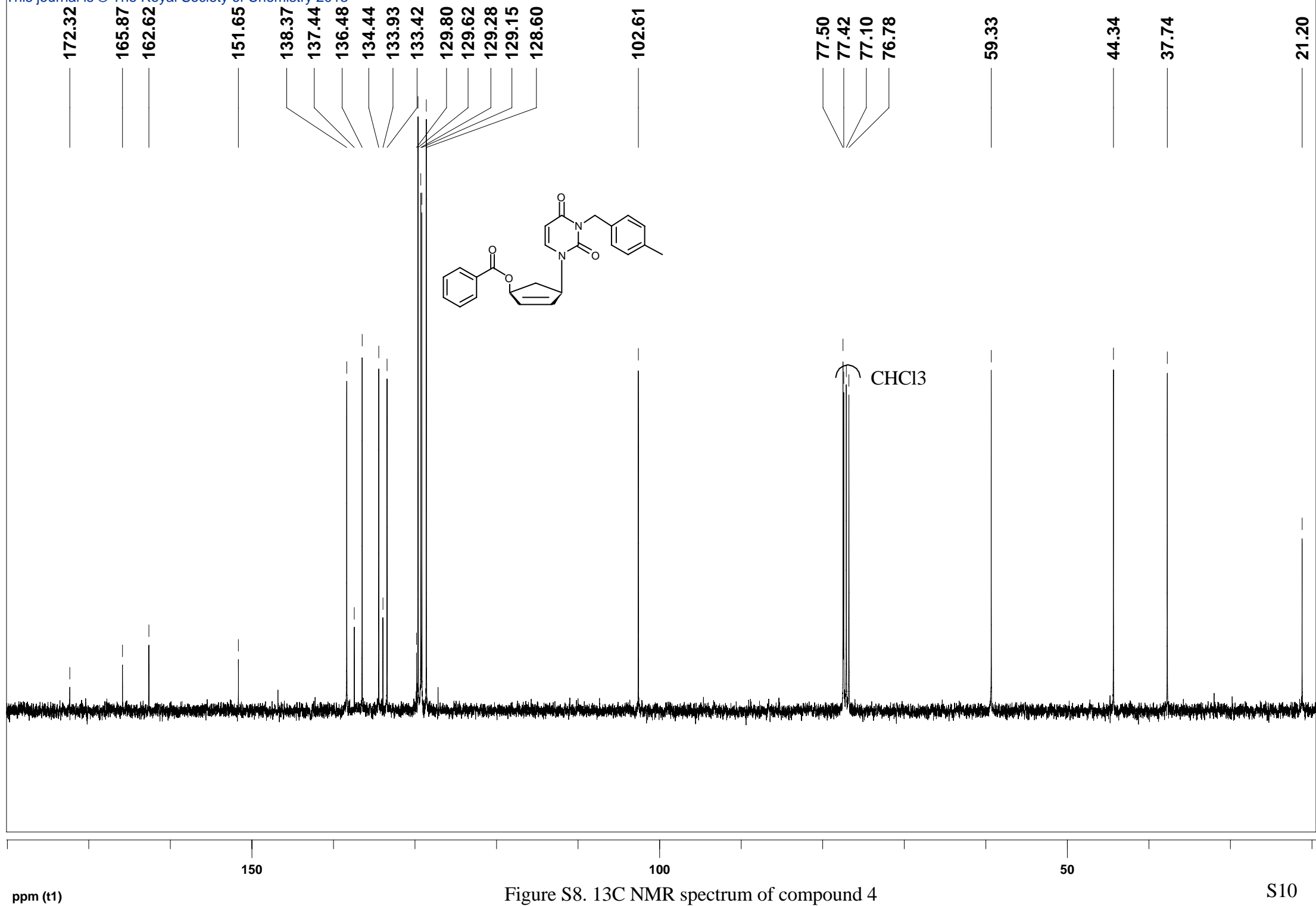


Figure S7. <sup>1</sup>H NMR spectrum of compound 4



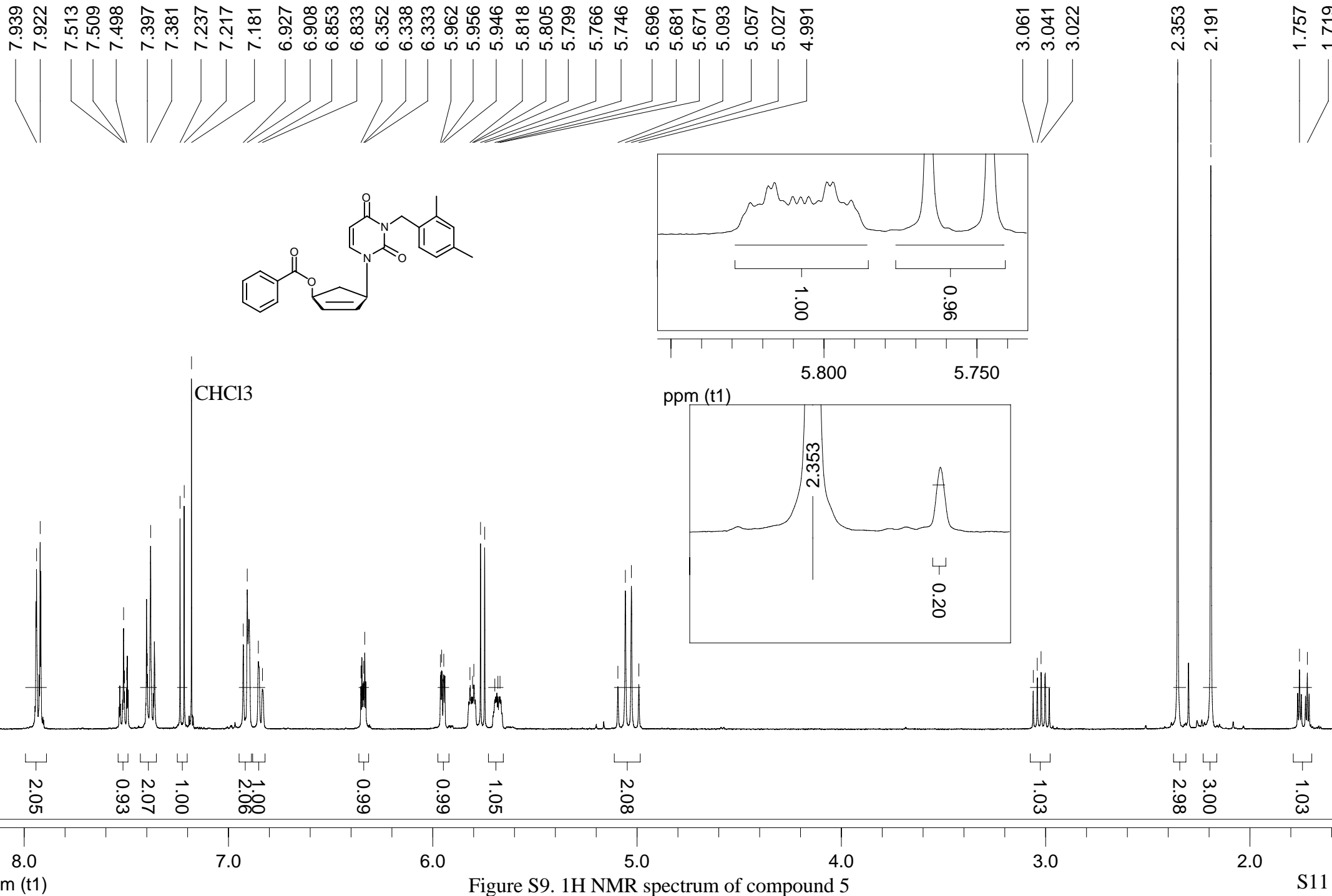


Figure S9. <sup>1</sup>H NMR spectrum of compound 5

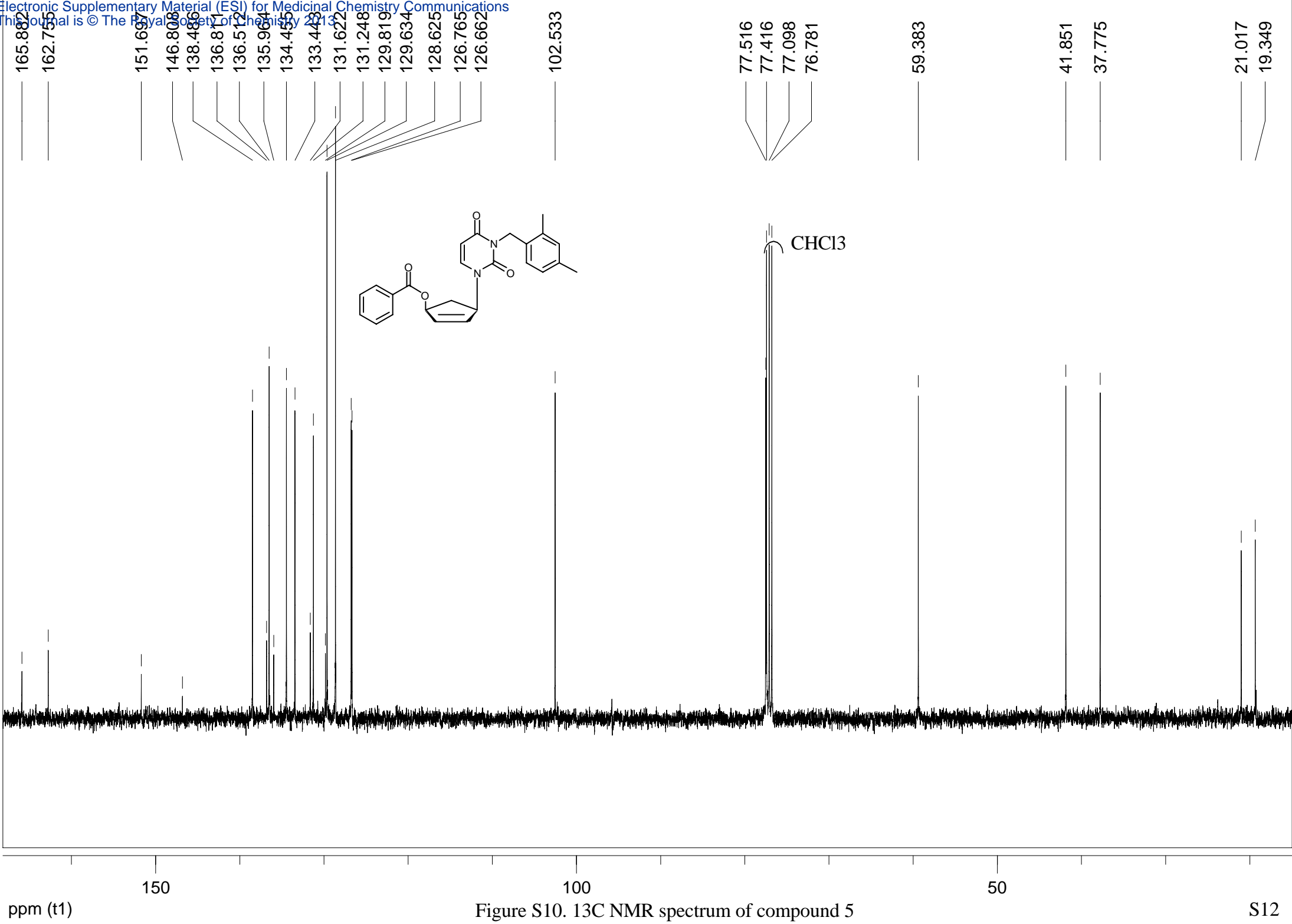


Figure S10. <sup>13</sup>C NMR spectrum of compound 5

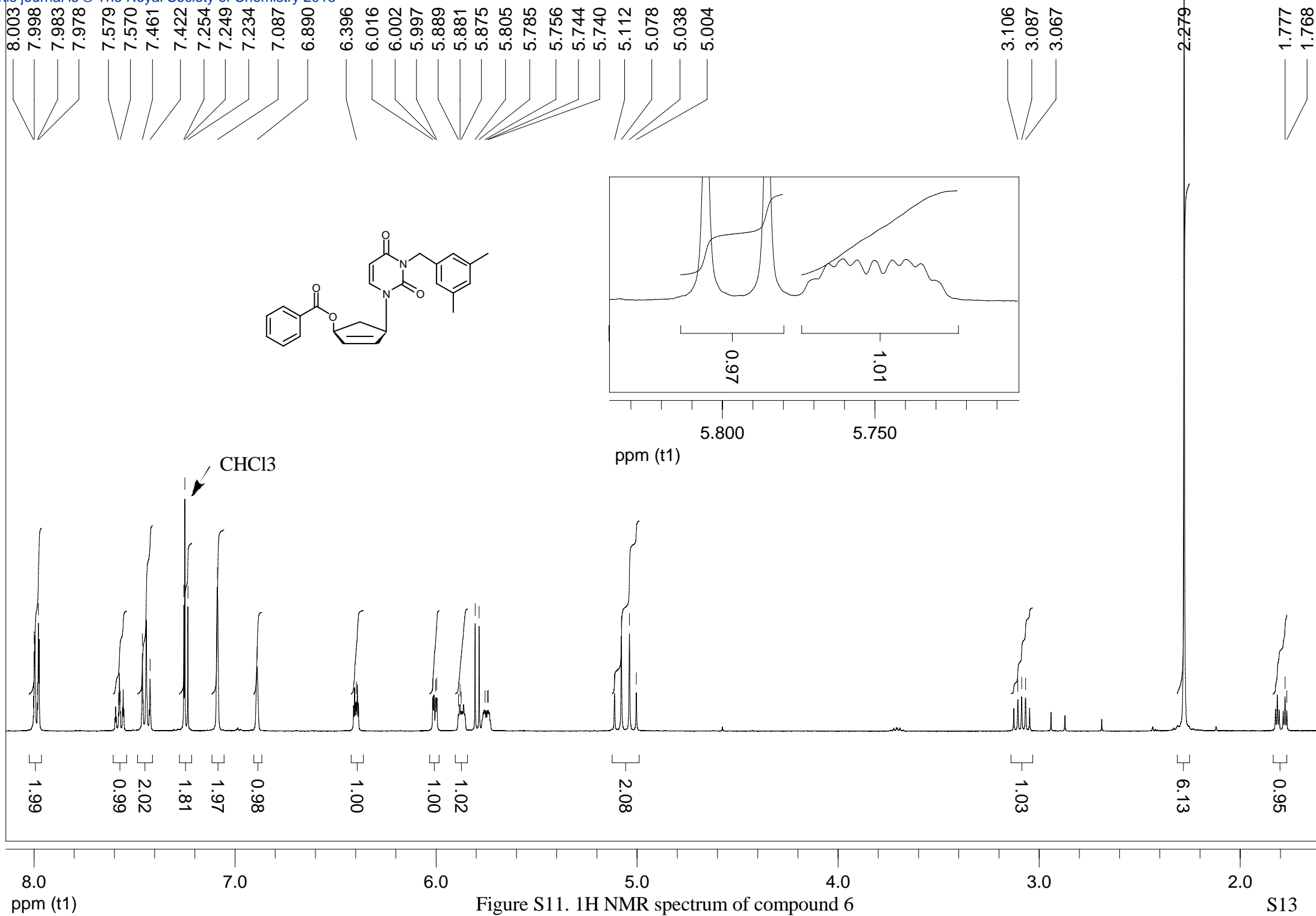


Figure S11. <sup>1</sup>H NMR spectrum of compound 6

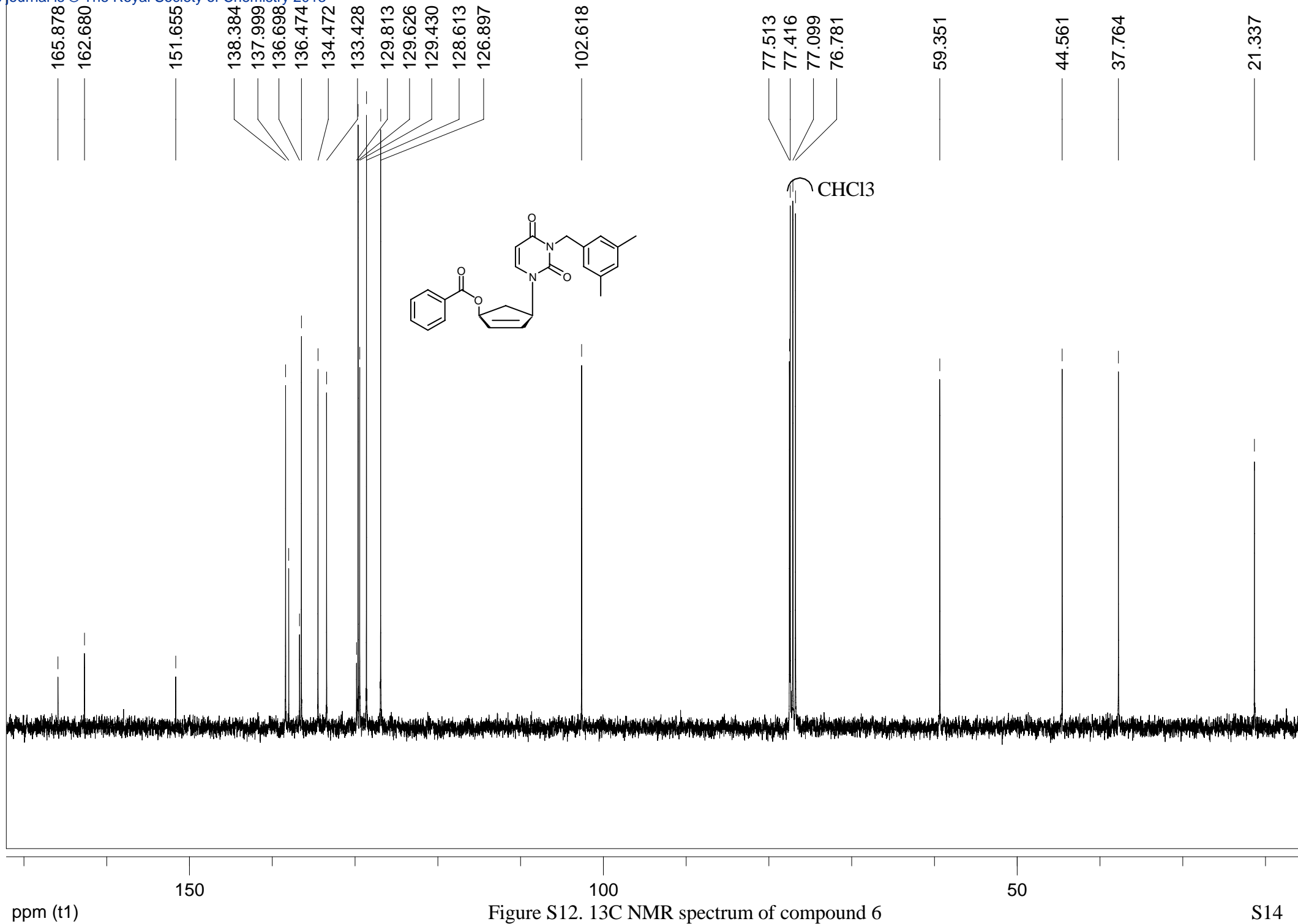


Figure S12. <sup>13</sup>C NMR spectrum of compound 6

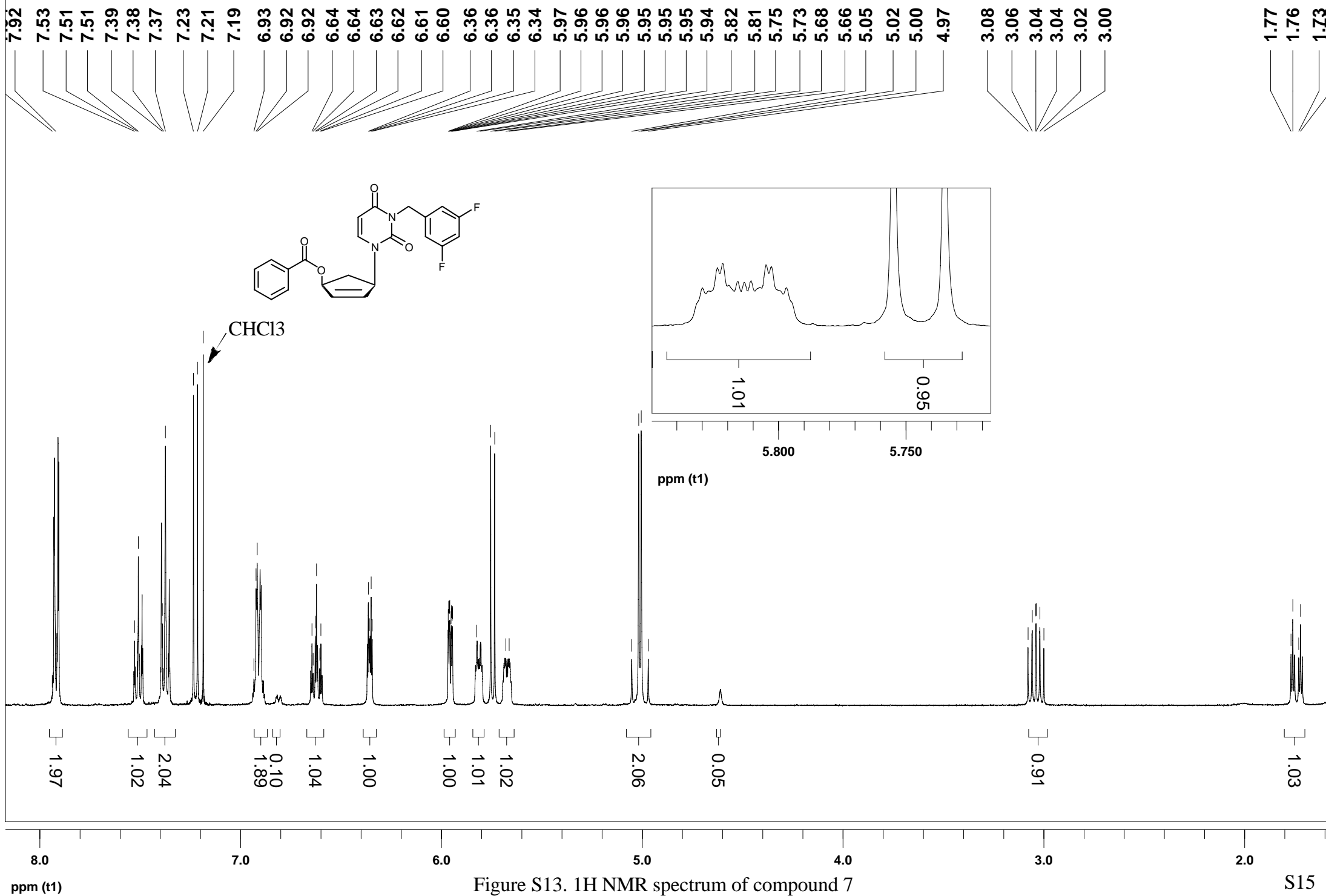


Figure S13. <sup>1</sup>H NMR spectrum of compound 7

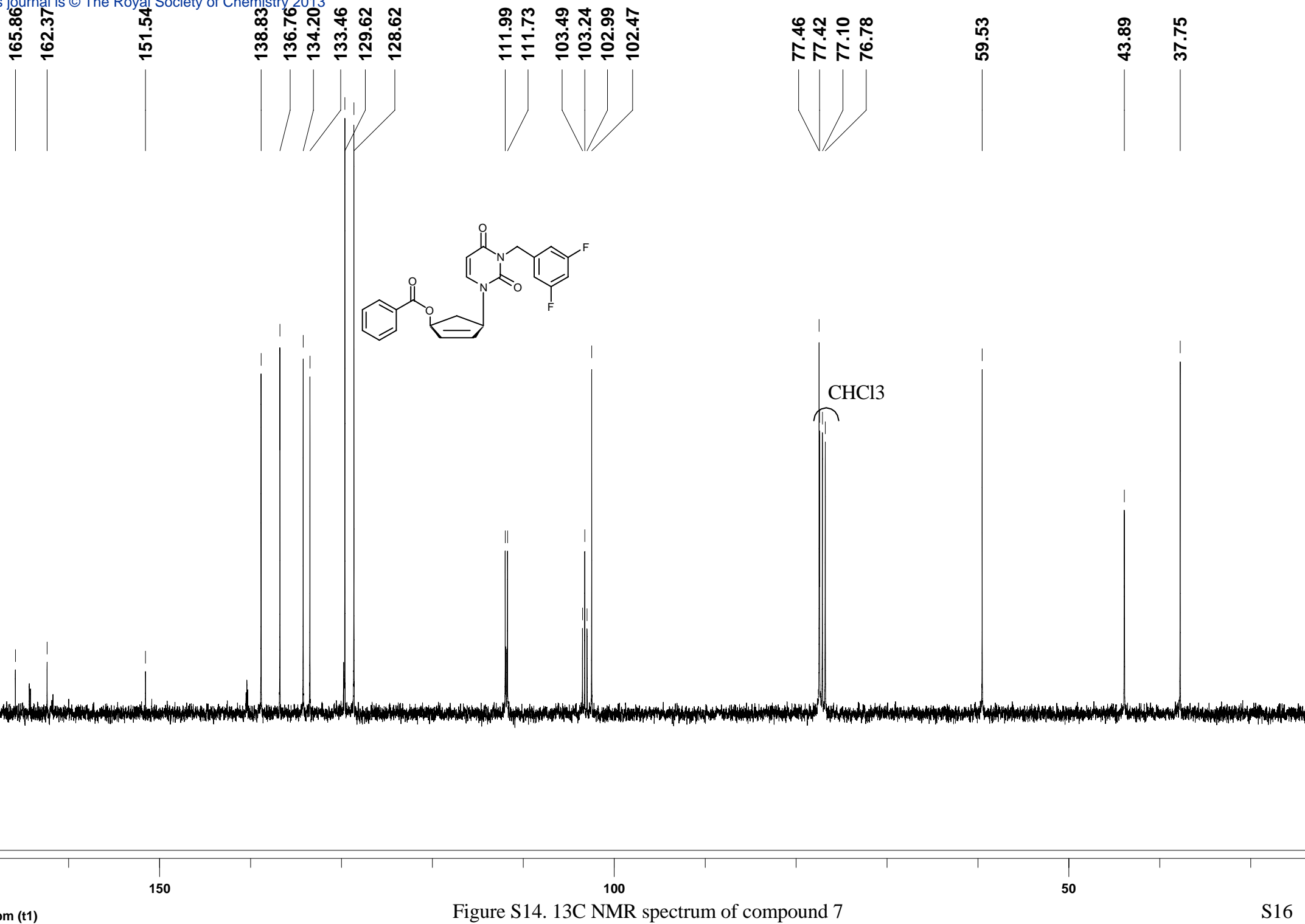


Figure S14. <sup>13</sup>C NMR spectrum of compound 7



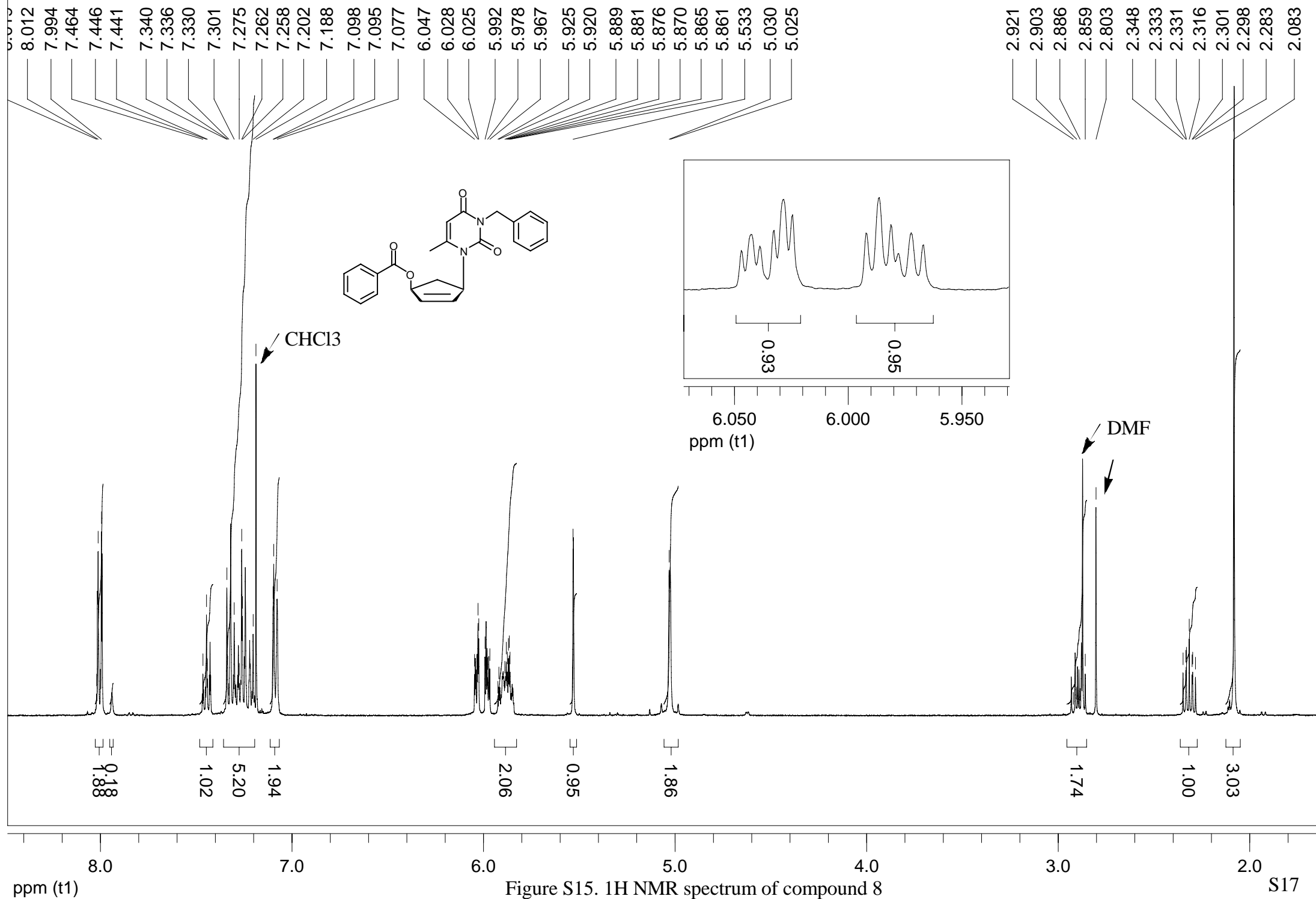


Figure S15. <sup>1</sup>H NMR spectrum of compound 8

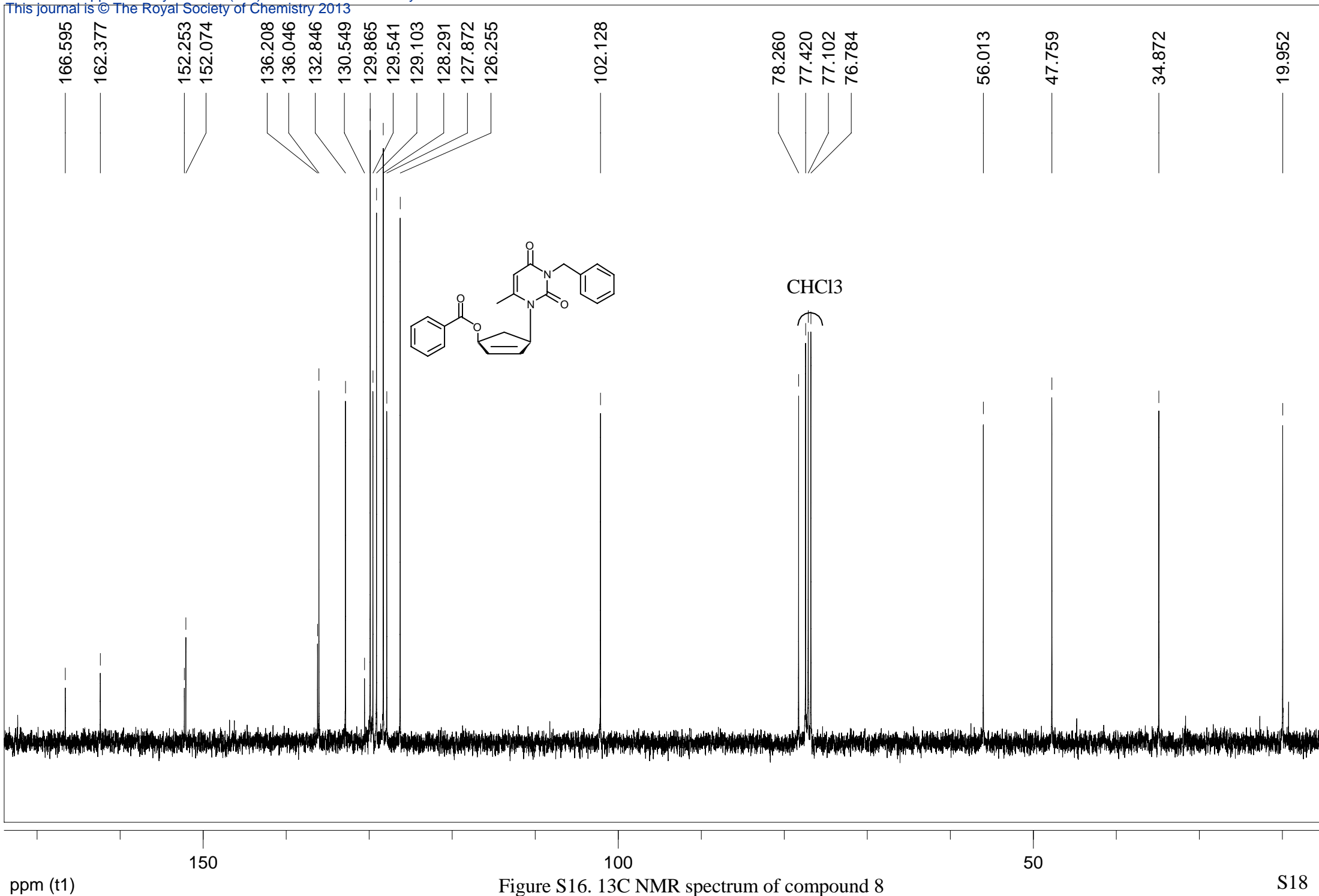


Figure S16. <sup>13</sup>C NMR spectrum of compound 8

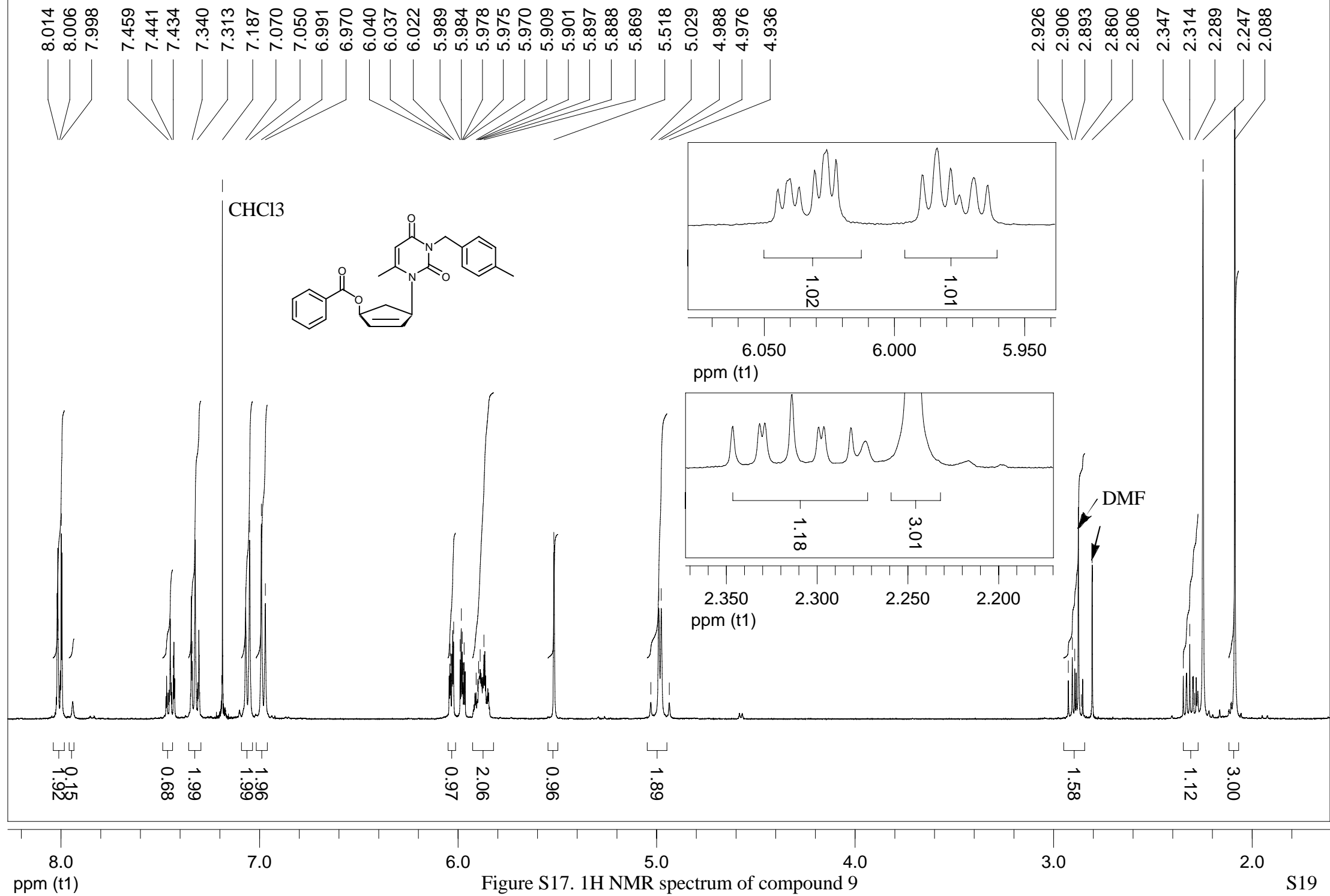


Figure S17. <sup>1</sup>H NMR spectrum of compound 9

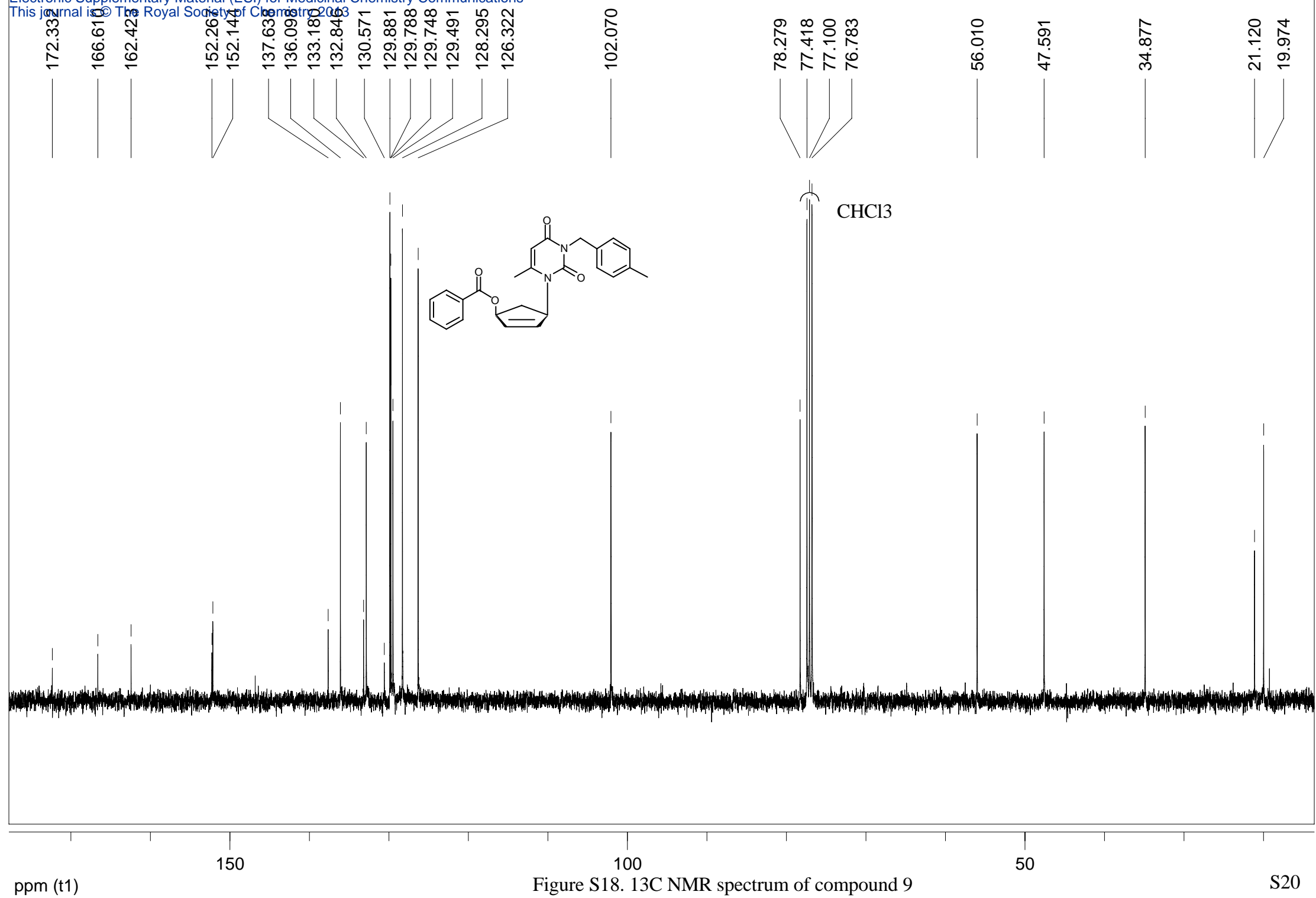


Figure S18. <sup>13</sup>C NMR spectrum of compound 9

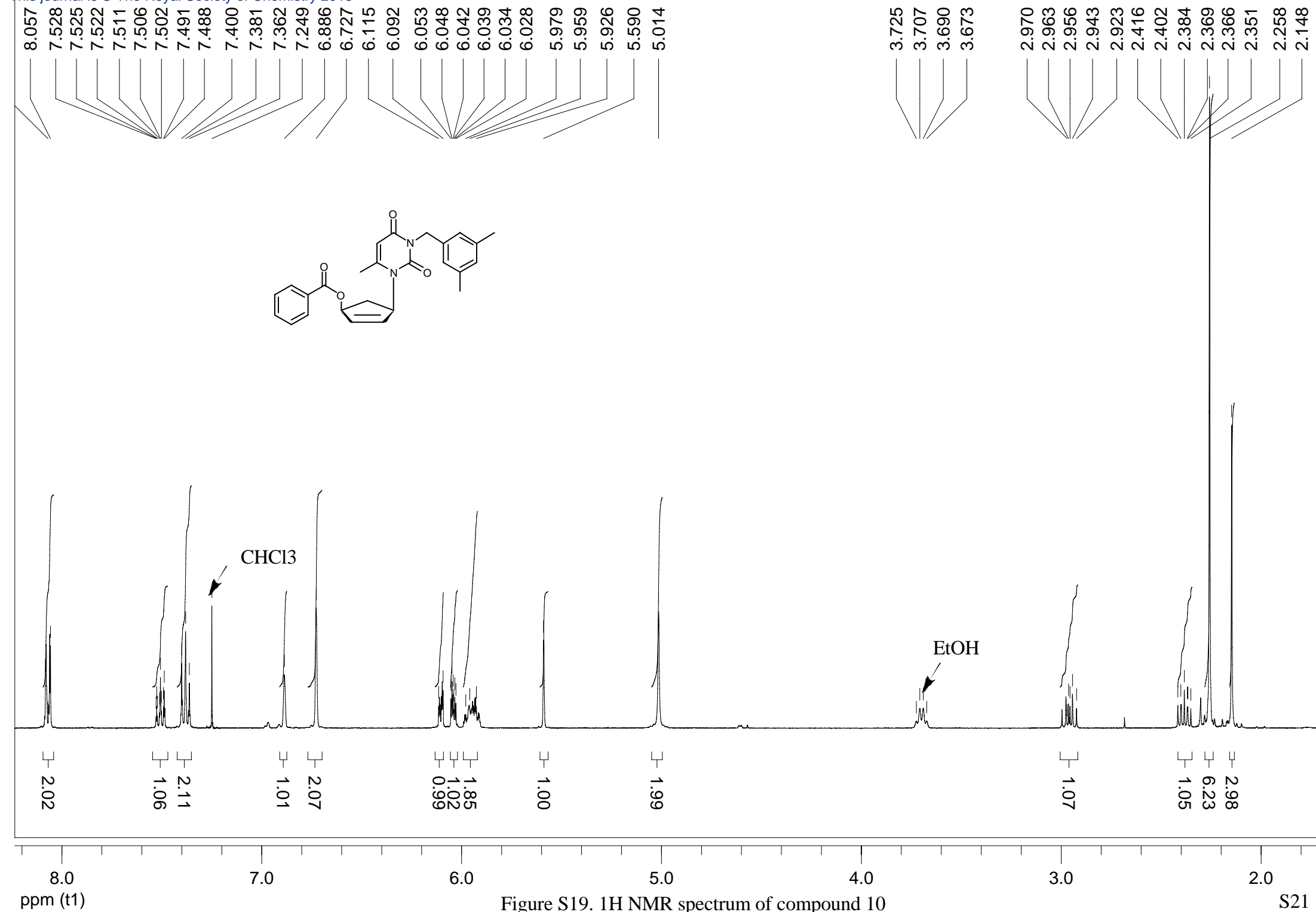
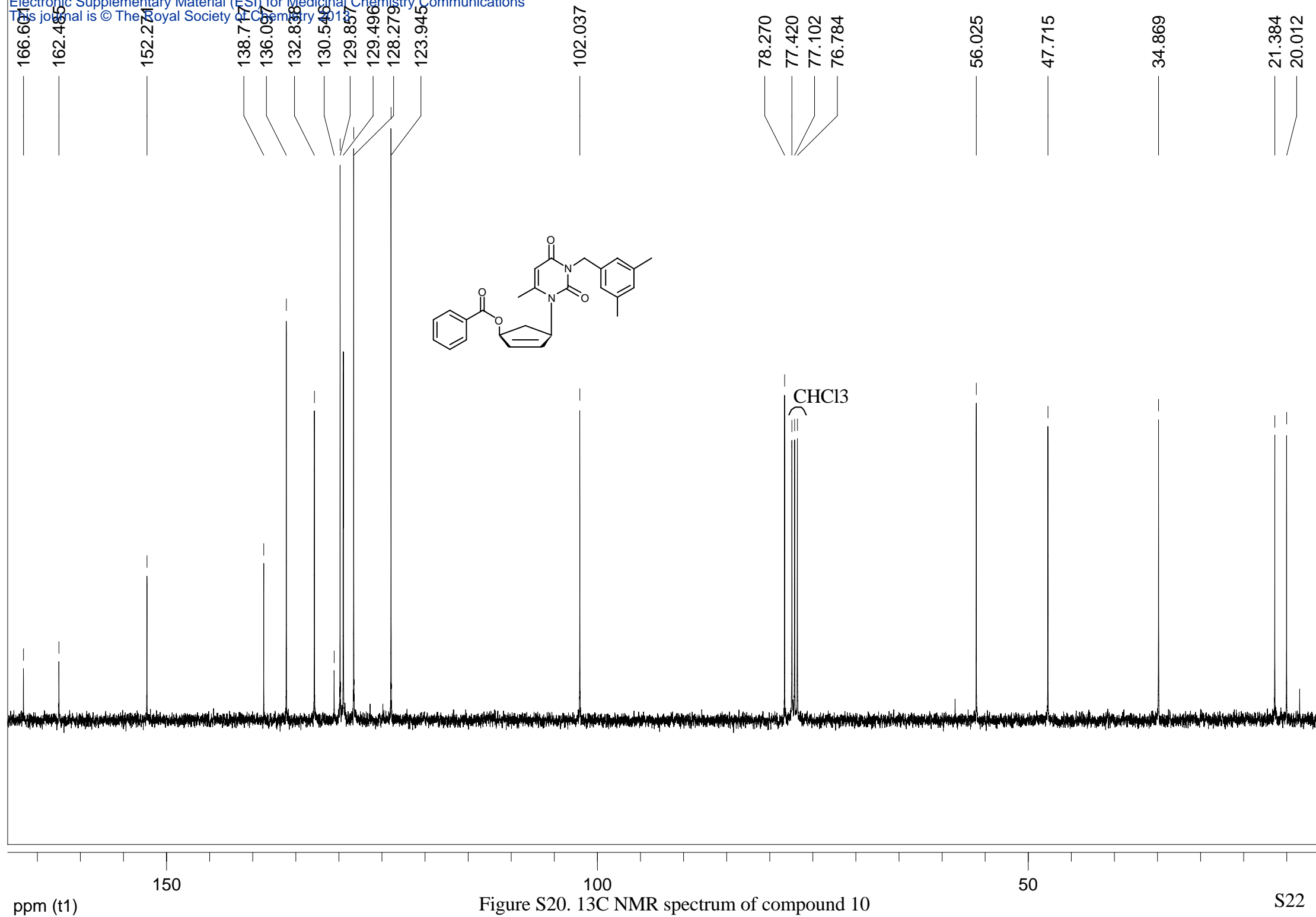


Figure S19. <sup>1</sup>H NMR spectrum of compound 10



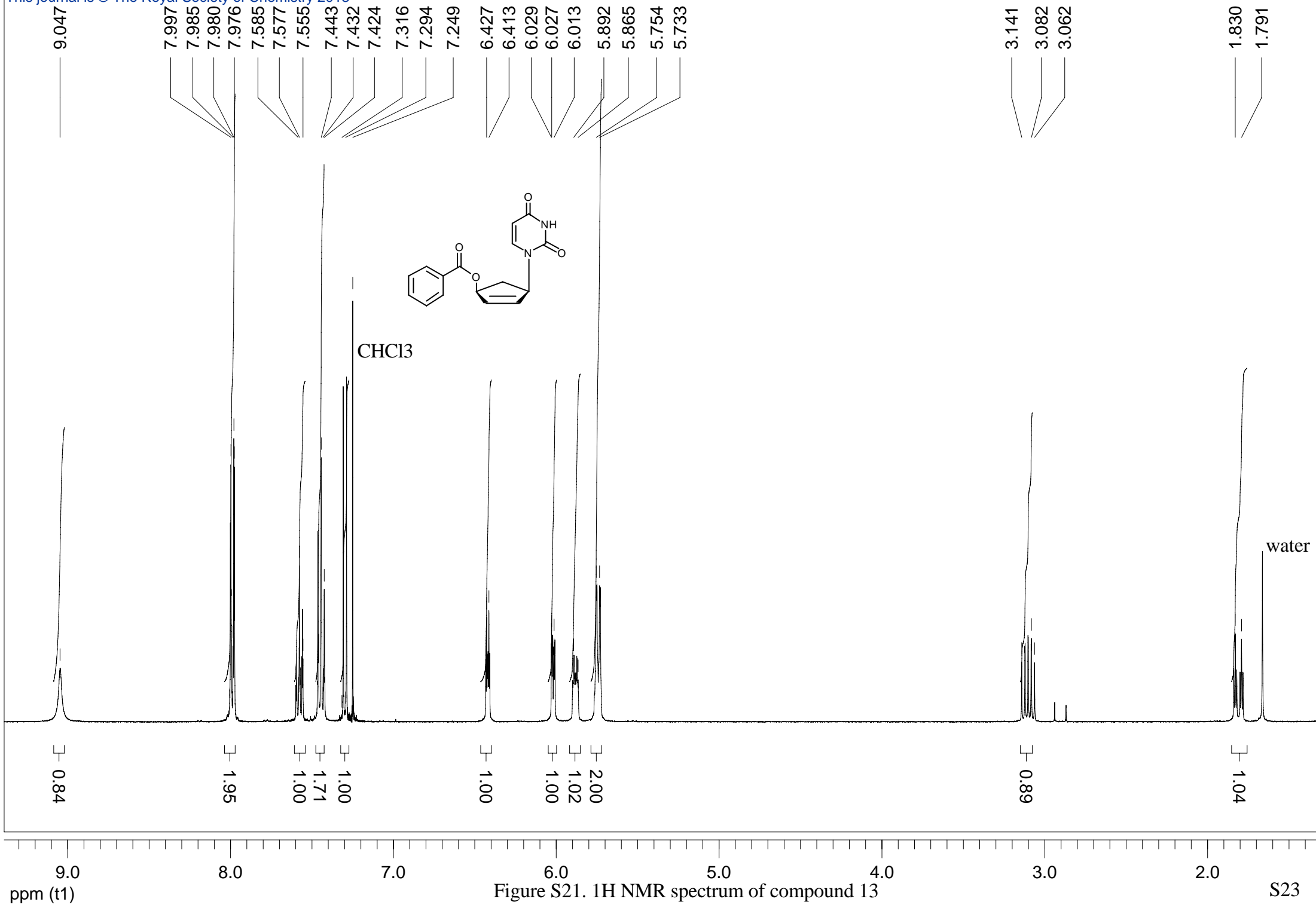


Figure S21. <sup>1</sup>H NMR spectrum of compound 13

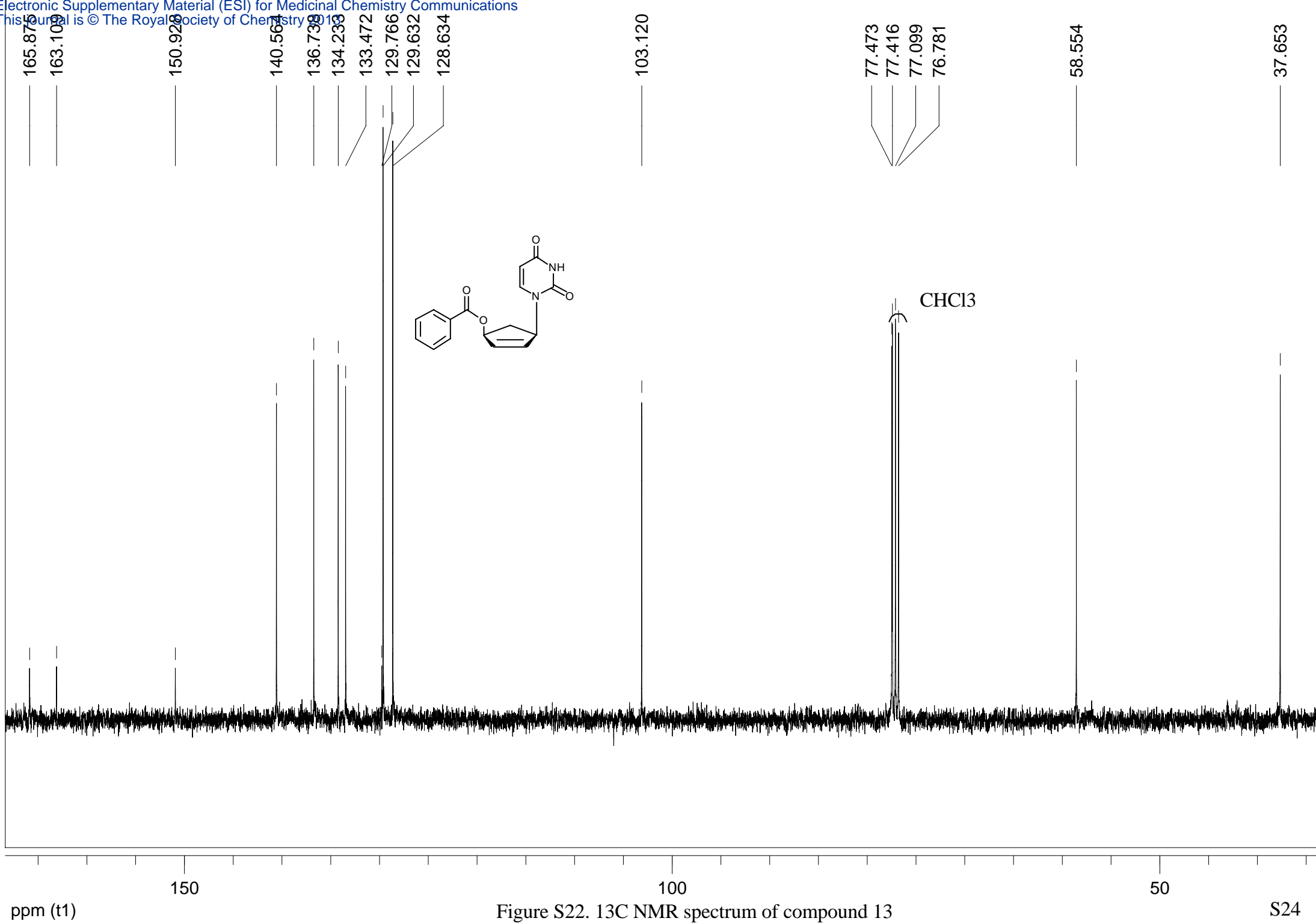
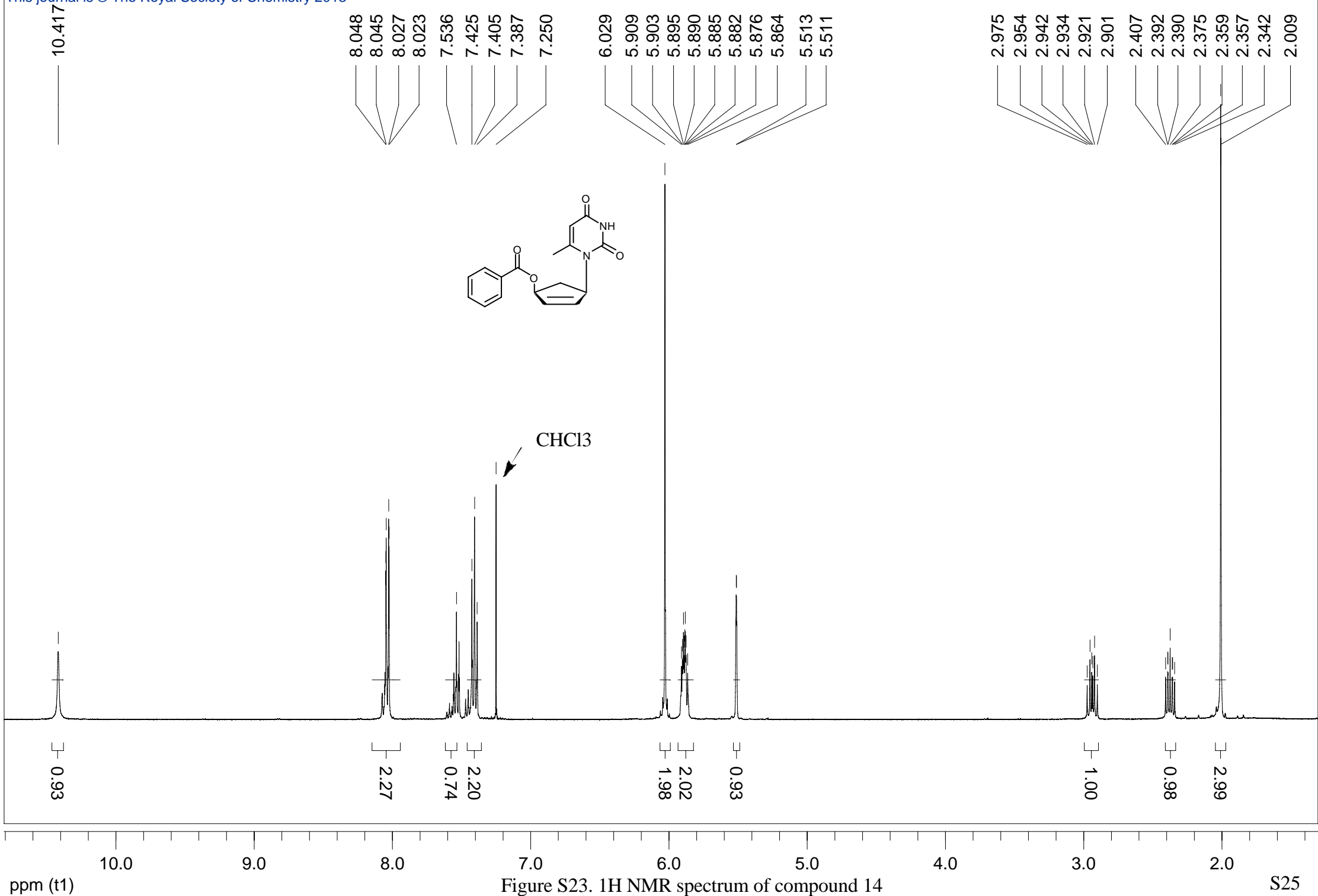


Figure S22. <sup>13</sup>C NMR spectrum of compound 13





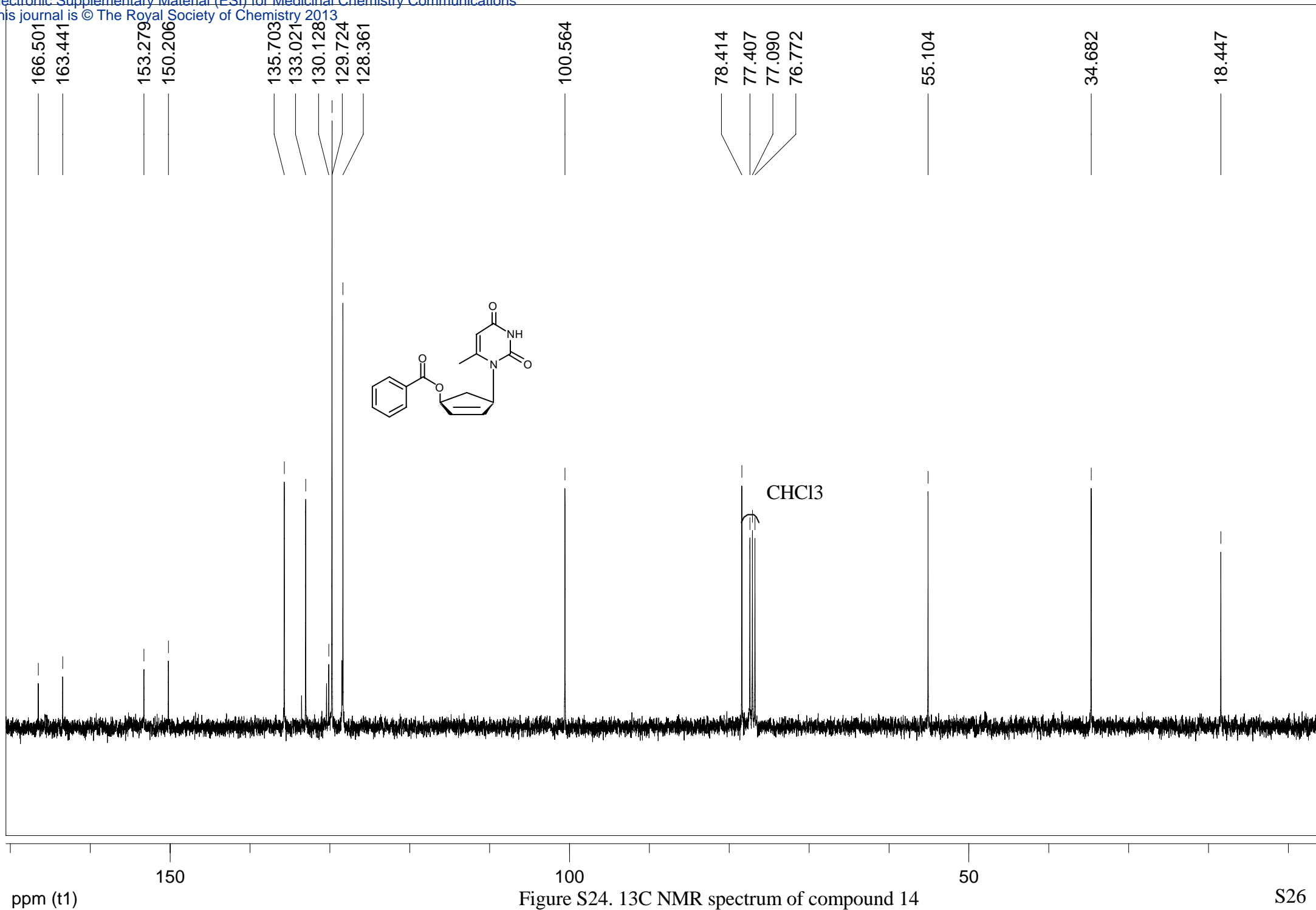


Figure S24. <sup>13</sup>C NMR spectrum of compound 14

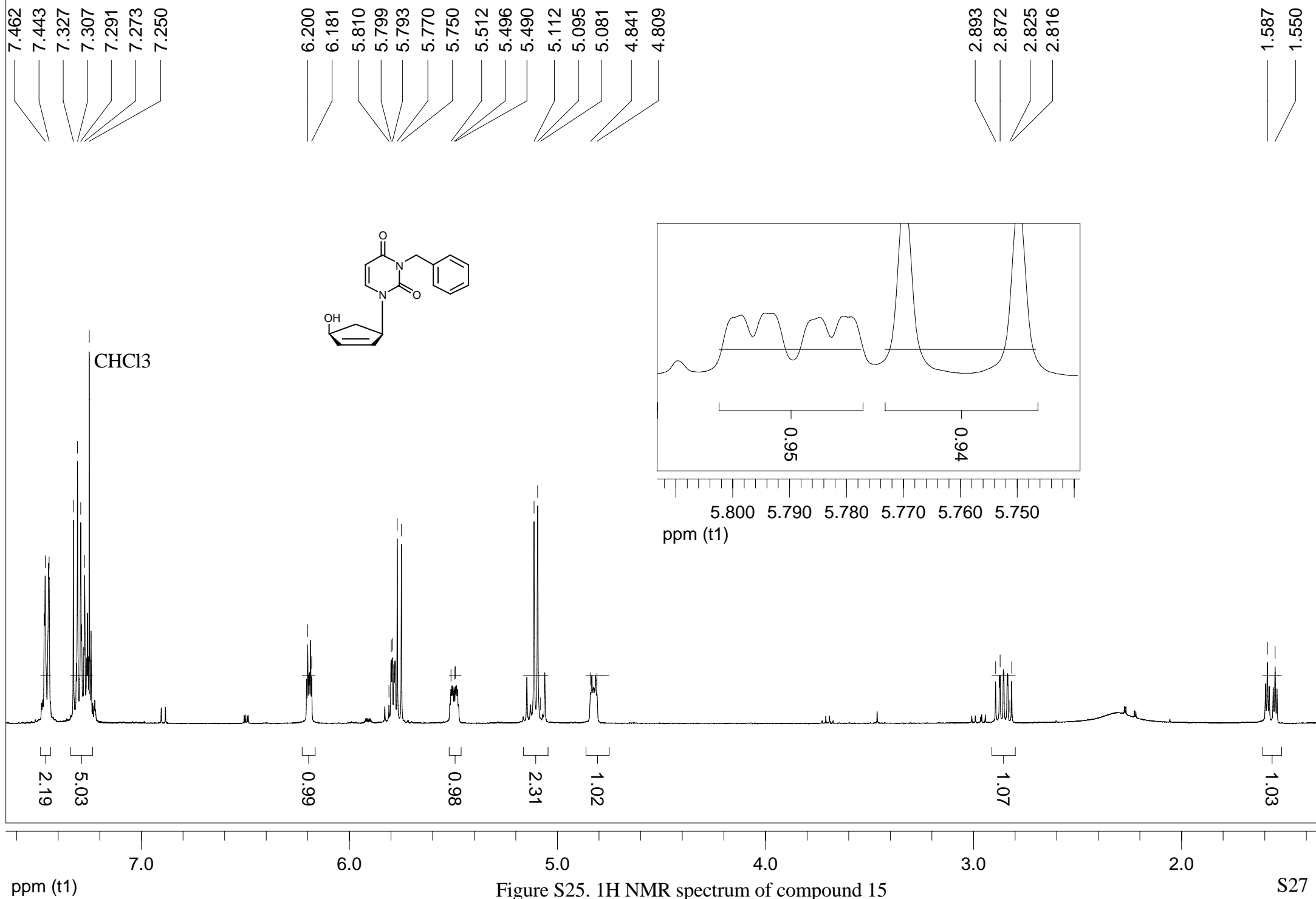


Figure S25. <sup>1</sup>H NMR spectrum of compound 15

