Supporting Online Material for

Mild and efficient synthesis of benzothiazolopyrimidine derivatives via CuAAC/ring cleavage reaction

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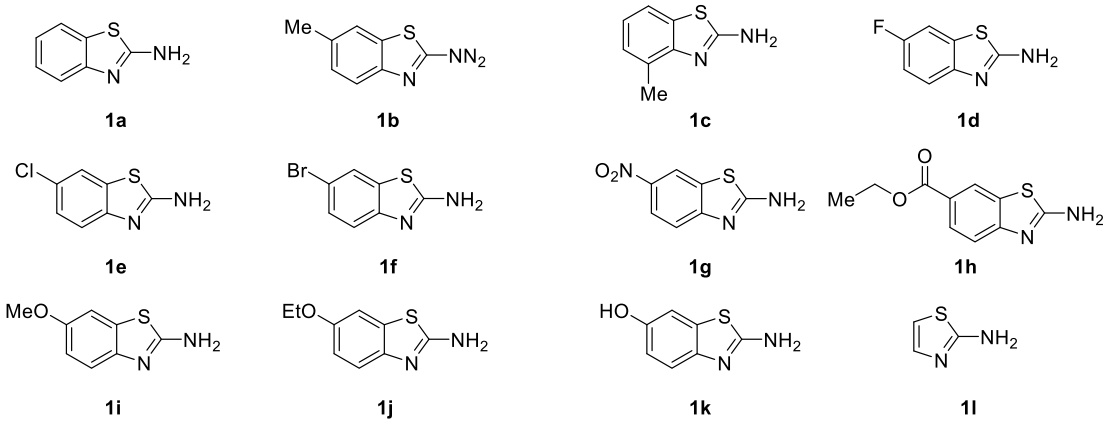
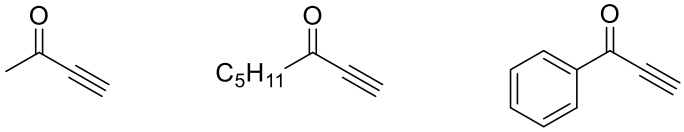
1. The structures of starting materials.

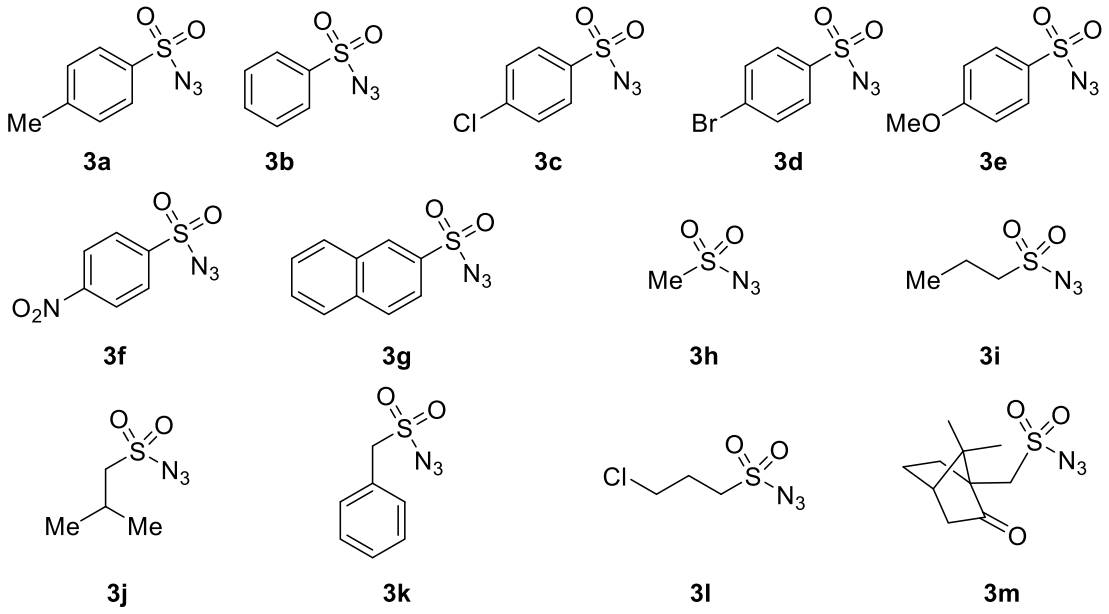
The structures of starting materials **1a-1l**.



The structures of starting materials **2a-2c**.



The structures of starting materials **3a-3m**.



2. General Information

^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were recorded at ambient temperatures on a 400 MHz Bruker spectrometer using $CDCl_3$ or DMSO-d_6 as solvent and tetramethylsilane (TMS) as the internal standard. Chemical shifts are presented as δ values relative to TMS and ^{1}H–^{1}H coupling constants (*J* values) are given in Hz. IR spectra were recorded on a BUCHI IRAffinity-1S spectrometer while HRMS measurements were carried out on a Bruker micrOTOF-Q II spectrometer. Melting points were determined on a BUCHI melting point M-565 apparatus and are uncorrected.

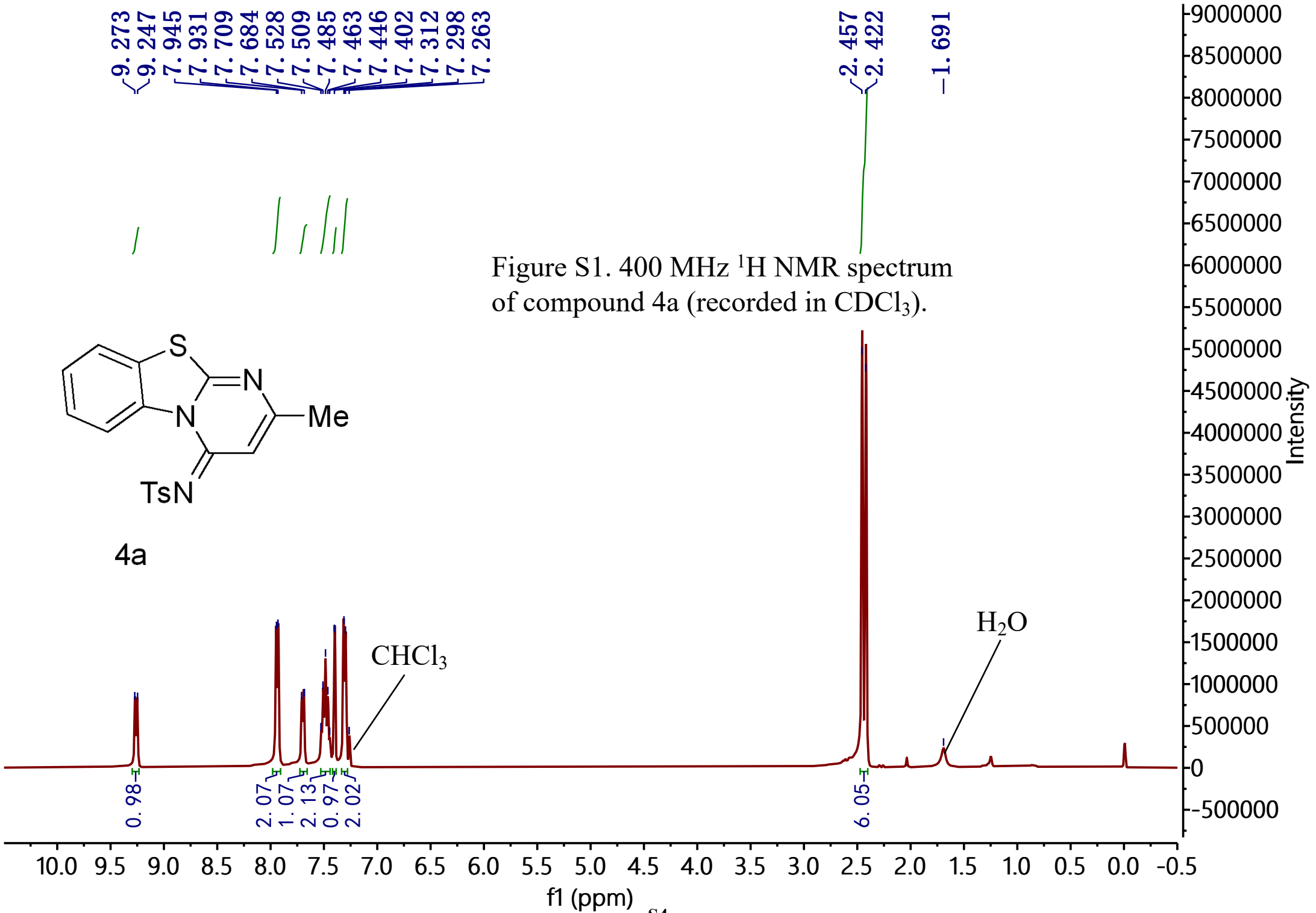


Figure S1. 400 MHz ^{1}H NMR spectrum of compound 4a (recorded in $CDCl_3$).

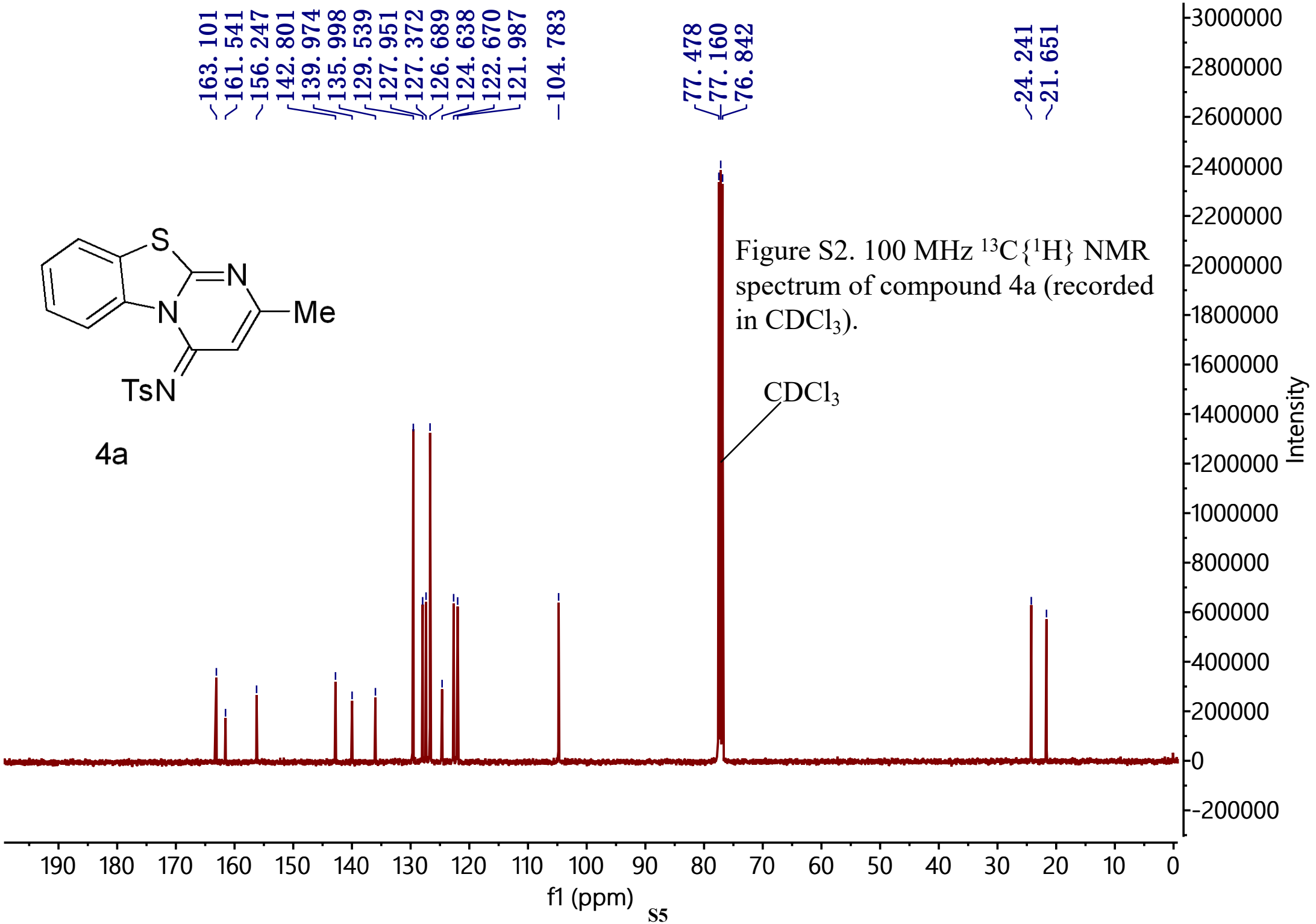


Figure S2. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4a (recorded in $CDCl_3$).

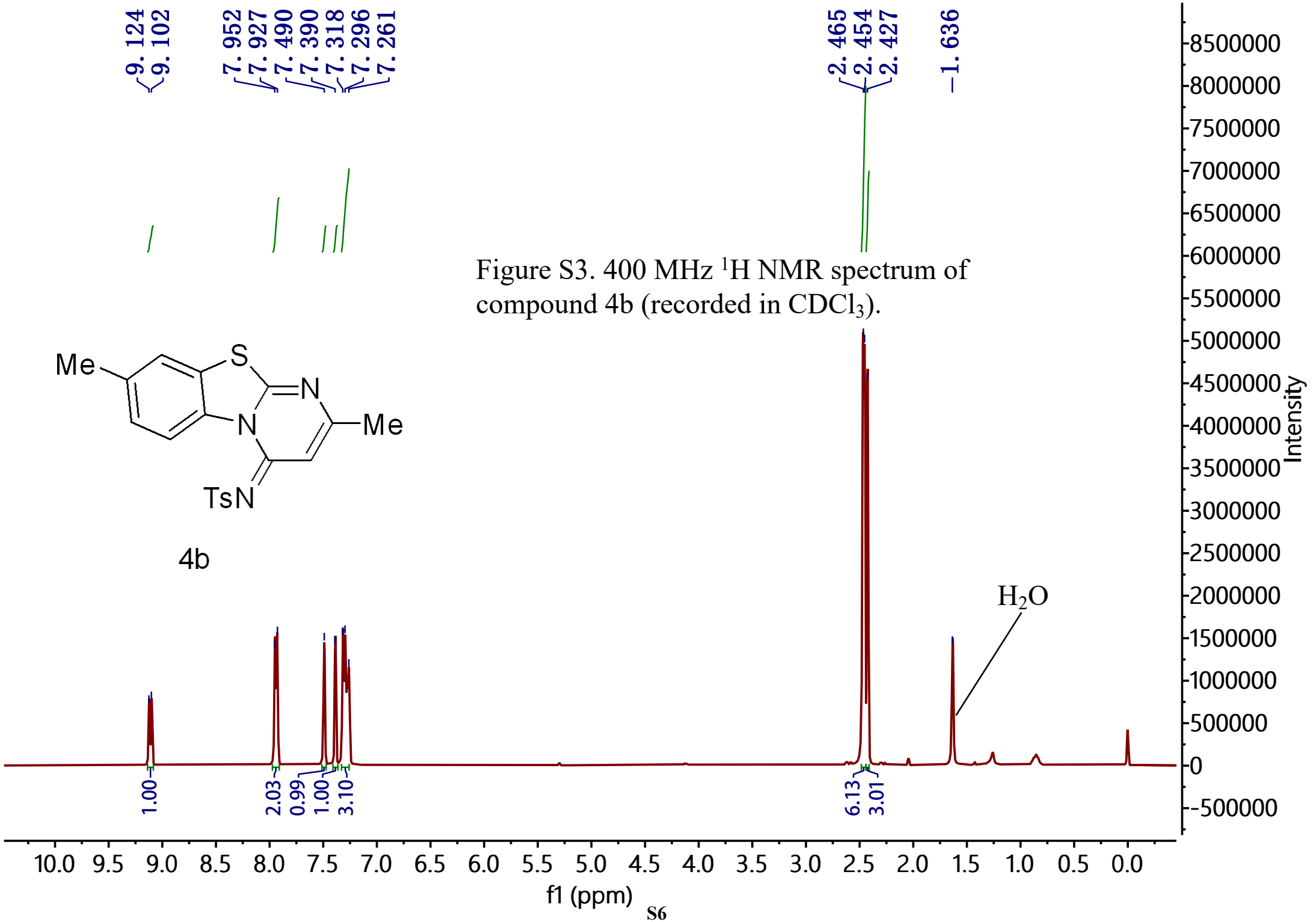


Figure S3. 400 MHz ^{1}H NMR spectrum of compound 4b (recorded in $CDCl_3$).

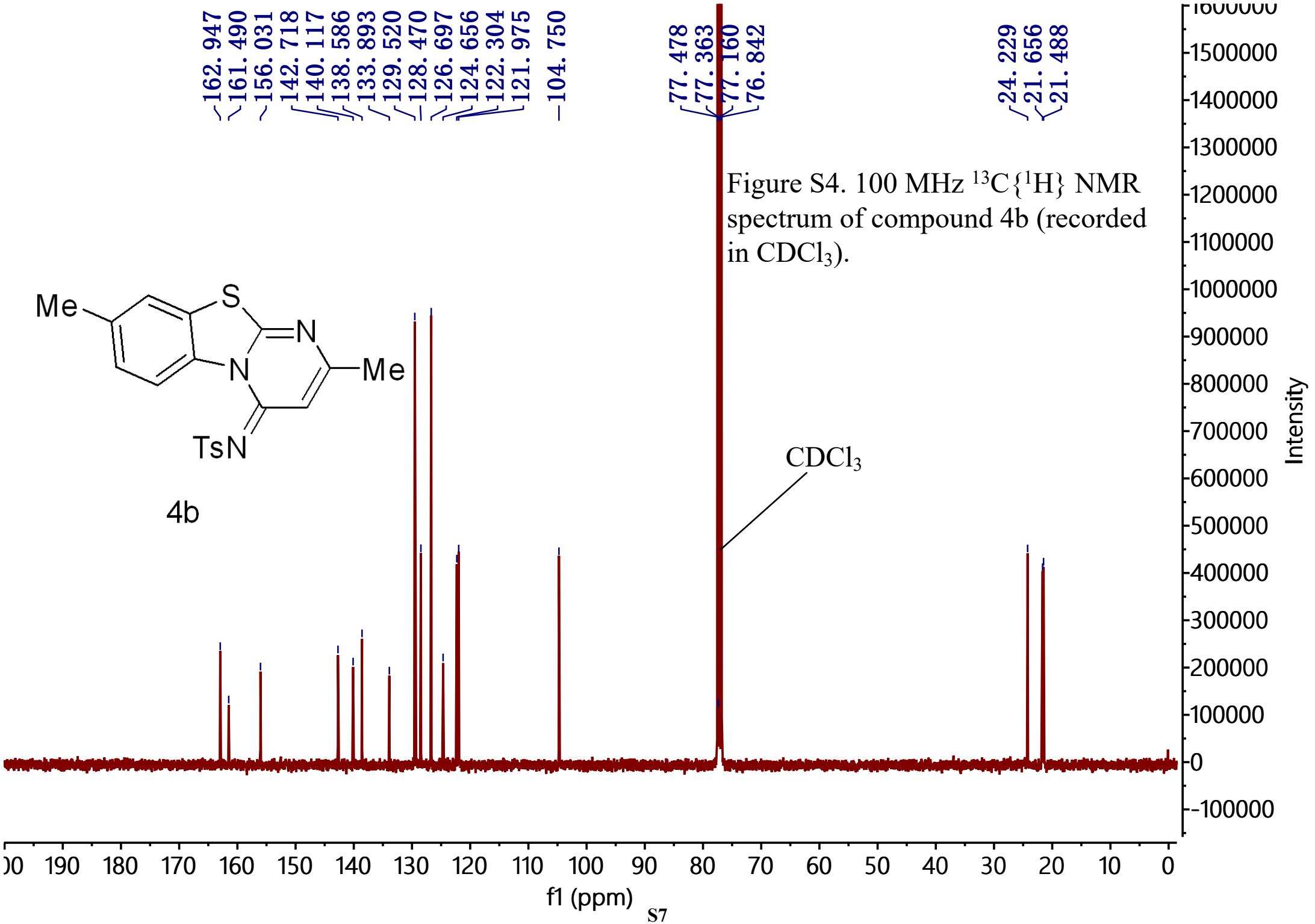


Figure S4. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4b (recorded in $CDCl_3$).

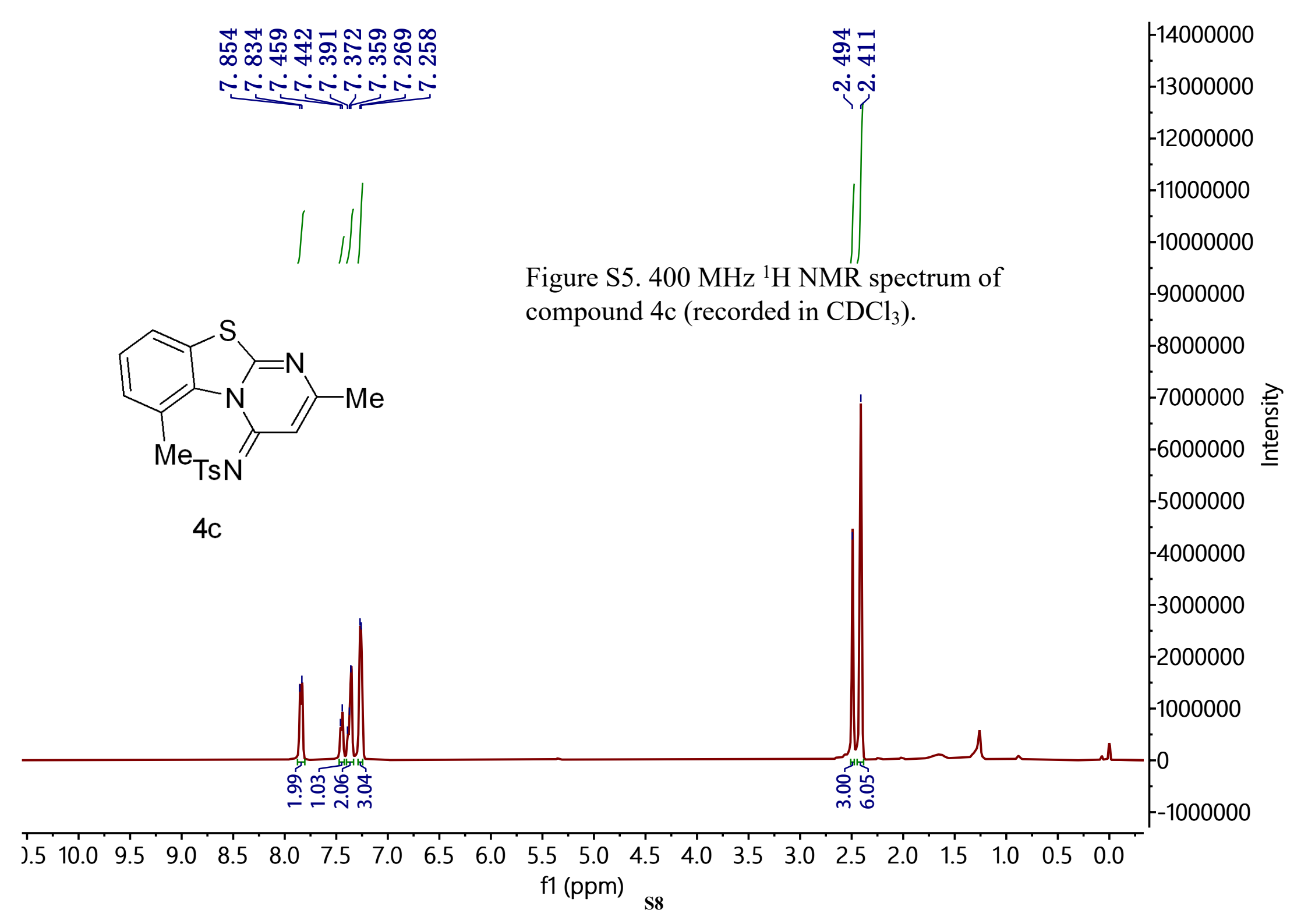


Figure S5. 400 MHz ^{1}H NMR spectrum of compound 4c (recorded in $CDCl_3$).

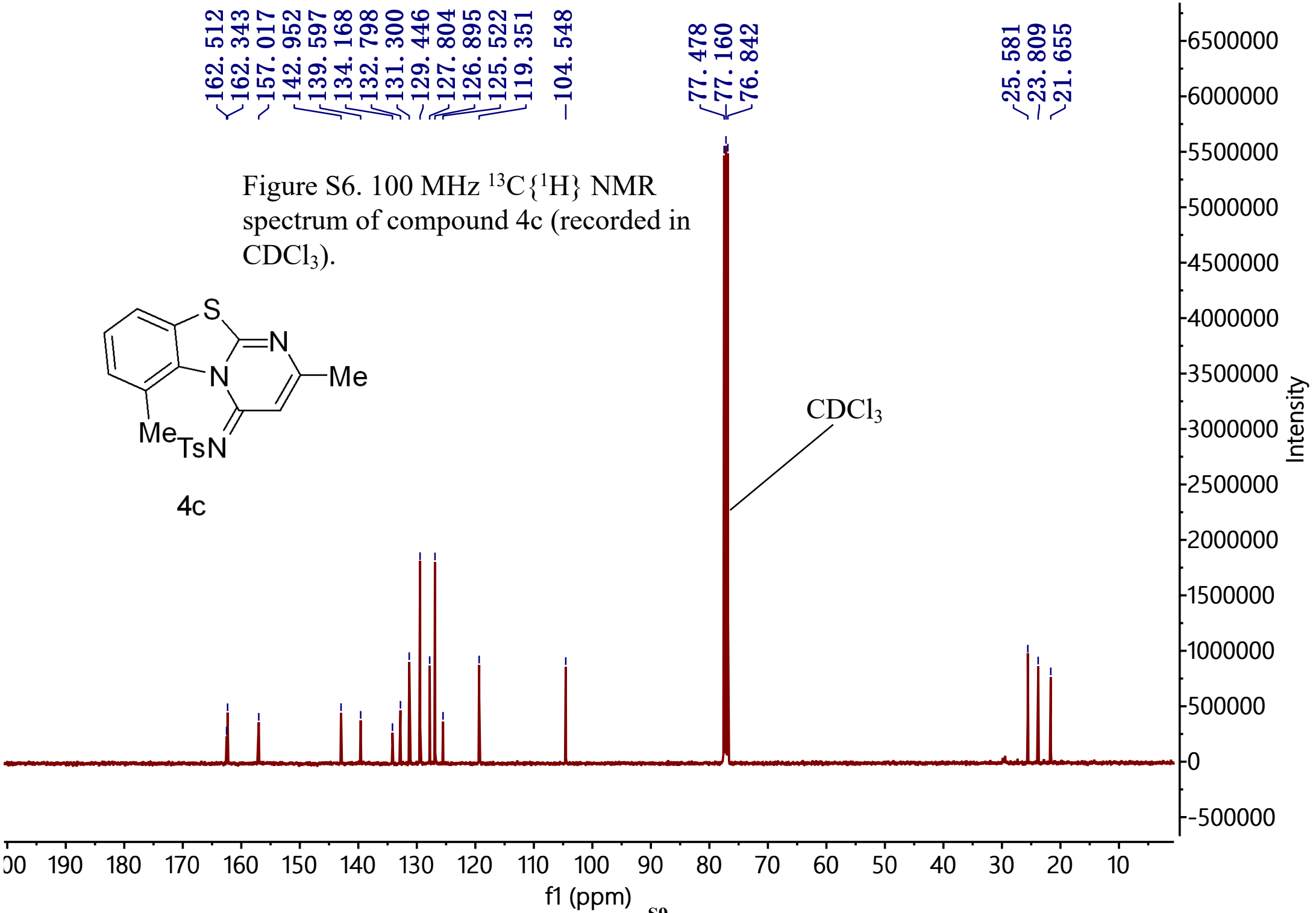


Figure S6. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4c (recorded in $CDCl_3$).

4c

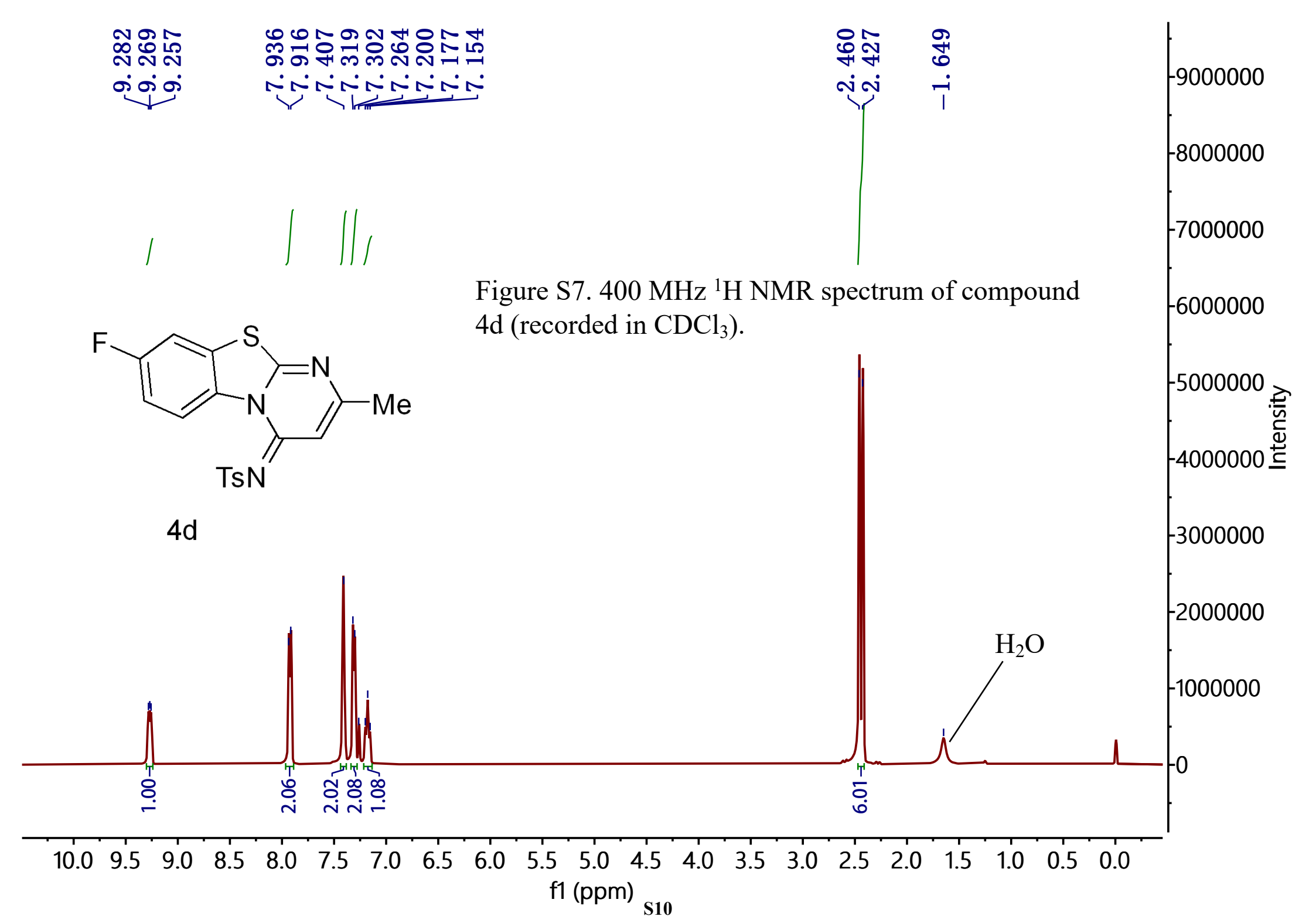


Figure S7. 400 MHz ^{1}H NMR spectrum of compound 4d (recorded in $CDCl_3$).

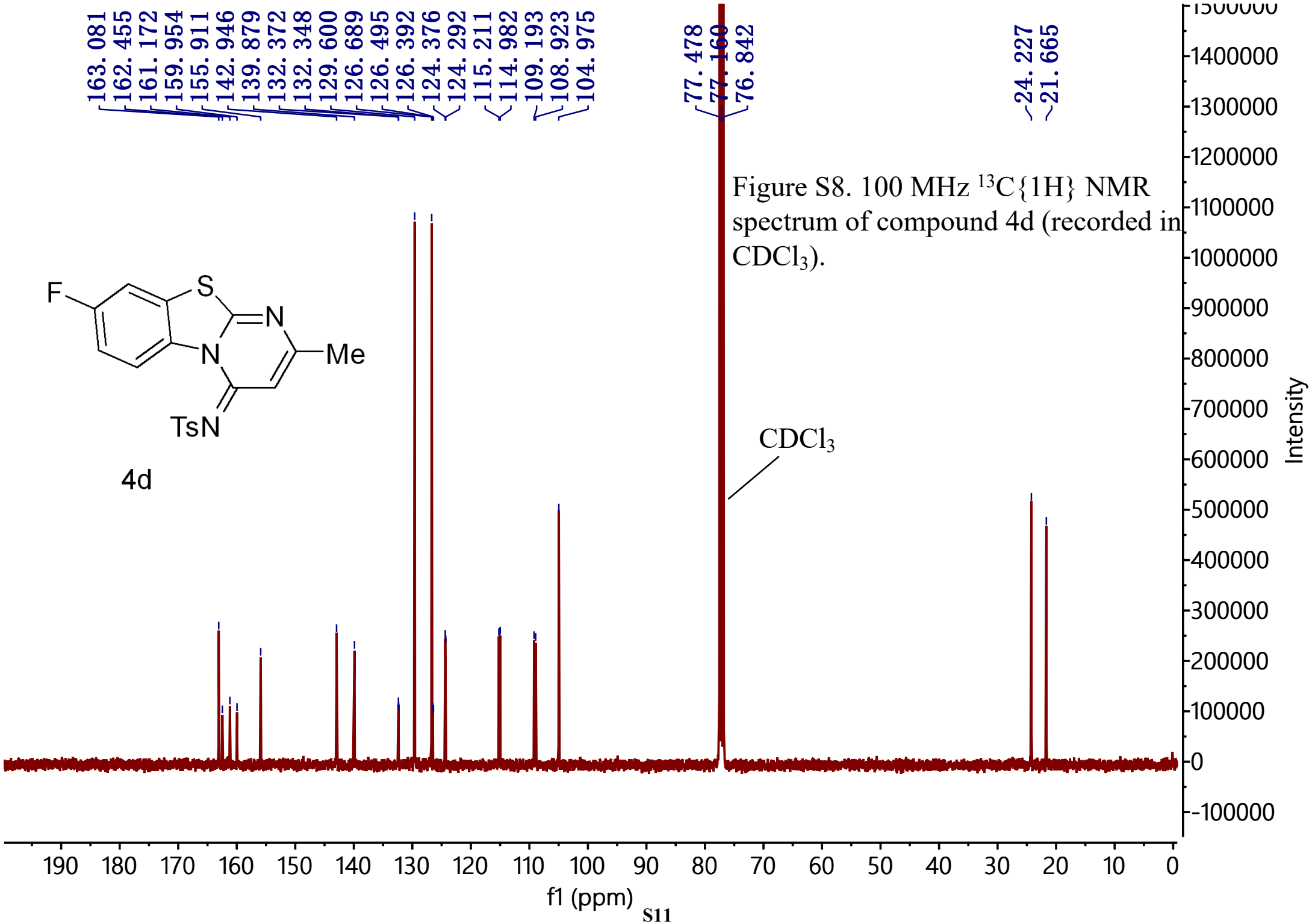


Figure S8. 100 MHz $^{13}C\{1H\}$ NMR spectrum of compound 4d (recorded in $CDCl_3$).

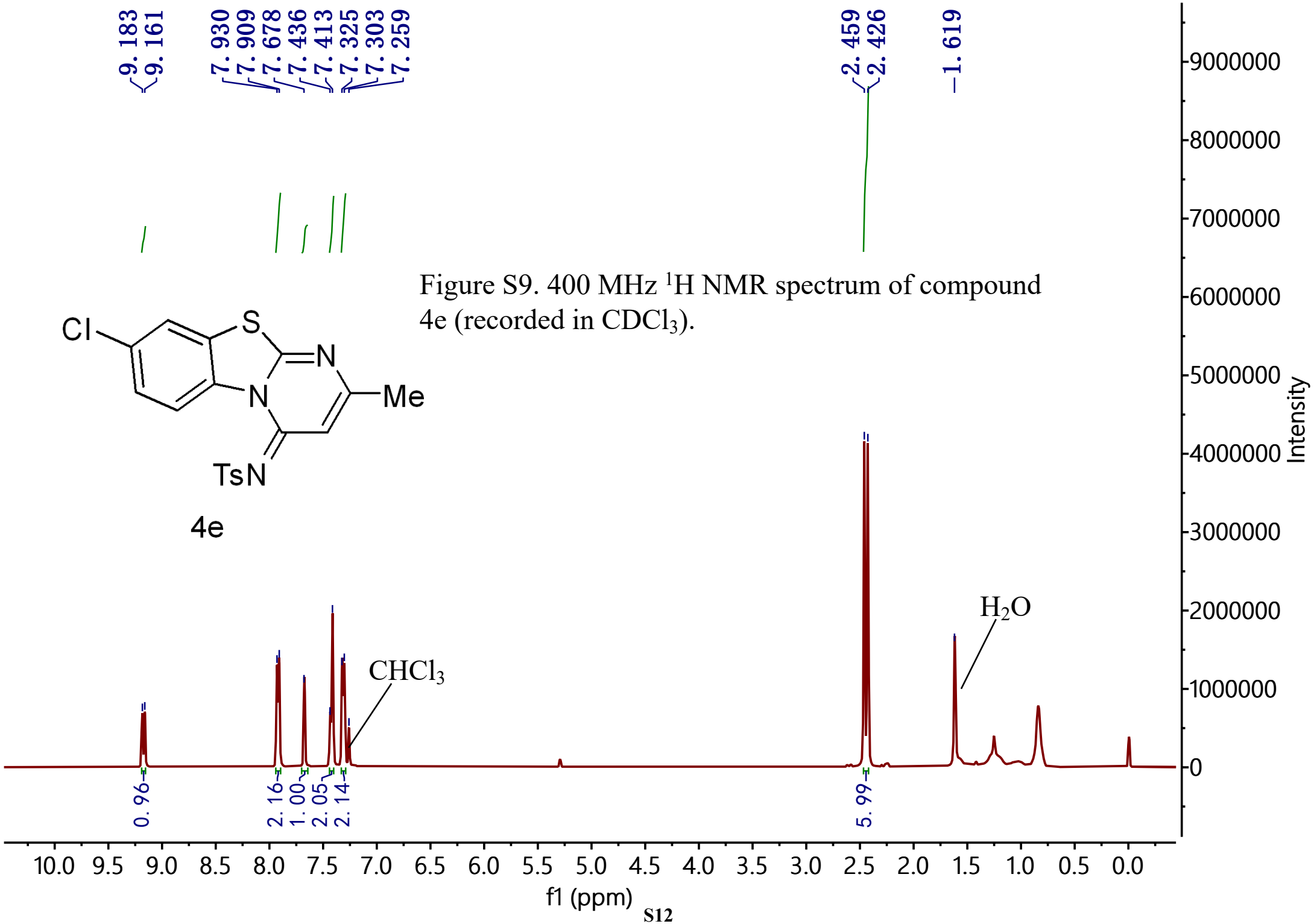


Figure S9. 400 MHz ^{1}H NMR spectrum of compound 4e (recorded in $CDCl_3$).

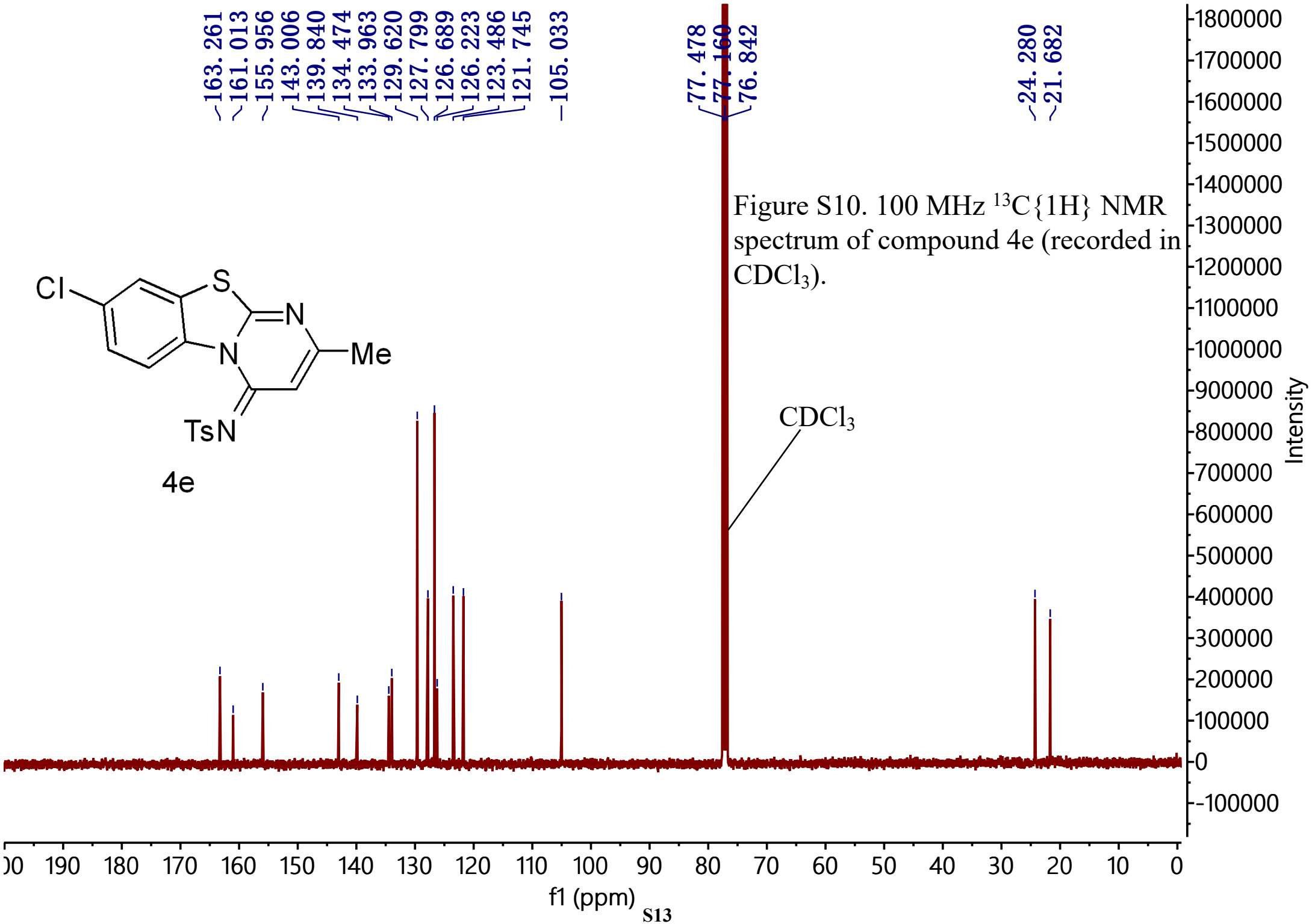


Figure S10. 100 MHz $^{13}C\{1H\}$ NMR spectrum of compound 4e (recorded in $CDCl_3$).

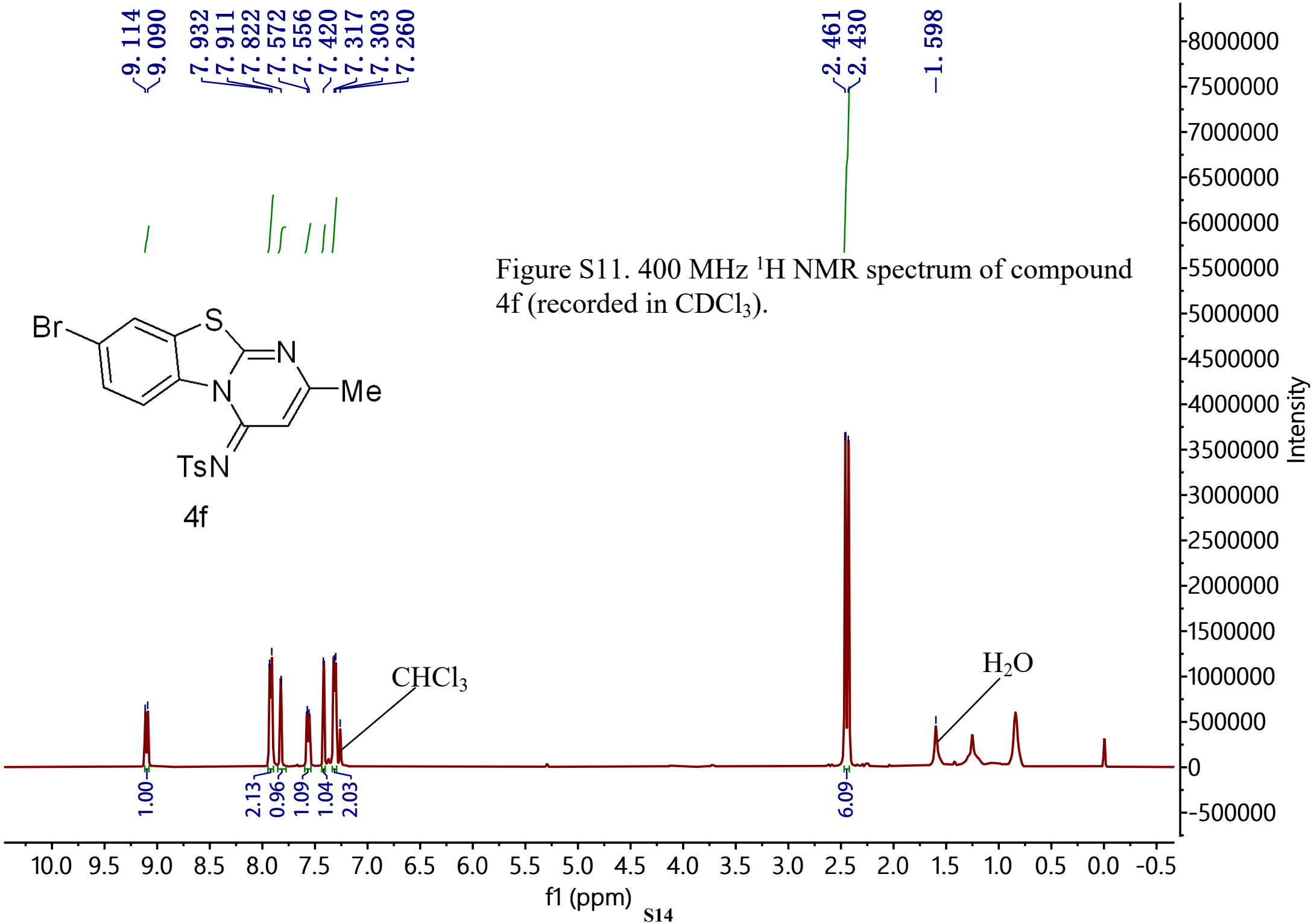


Figure S11. 400 MHz ^{1}H NMR spectrum of compound 4f (recorded in $CDCl_3$).

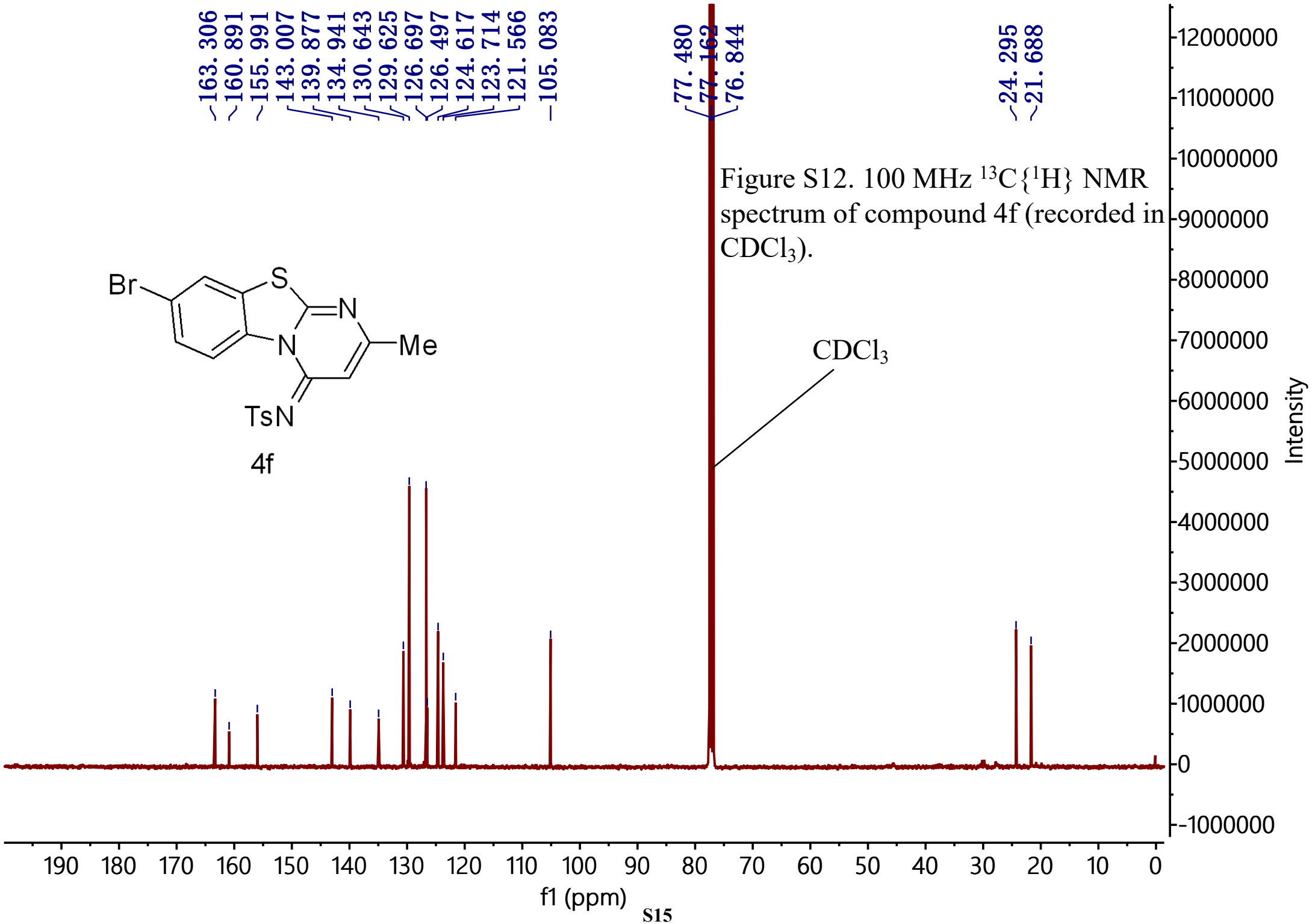


Figure S12. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4f (recorded in $CDCl_3$).

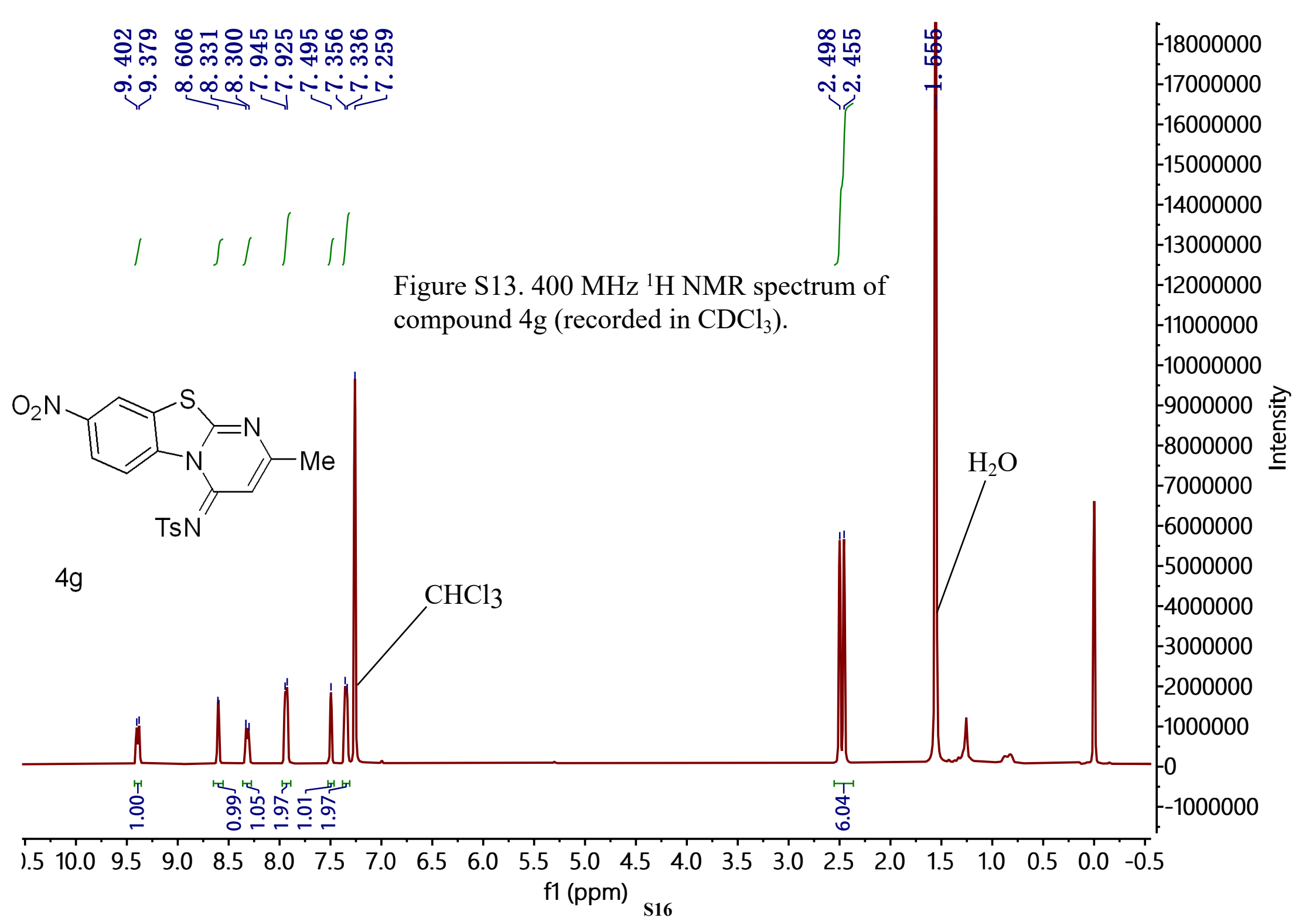


Figure S13. 400 MHz ^{1}H NMR spectrum of compound 4g (recorded in $CDCl_3$).

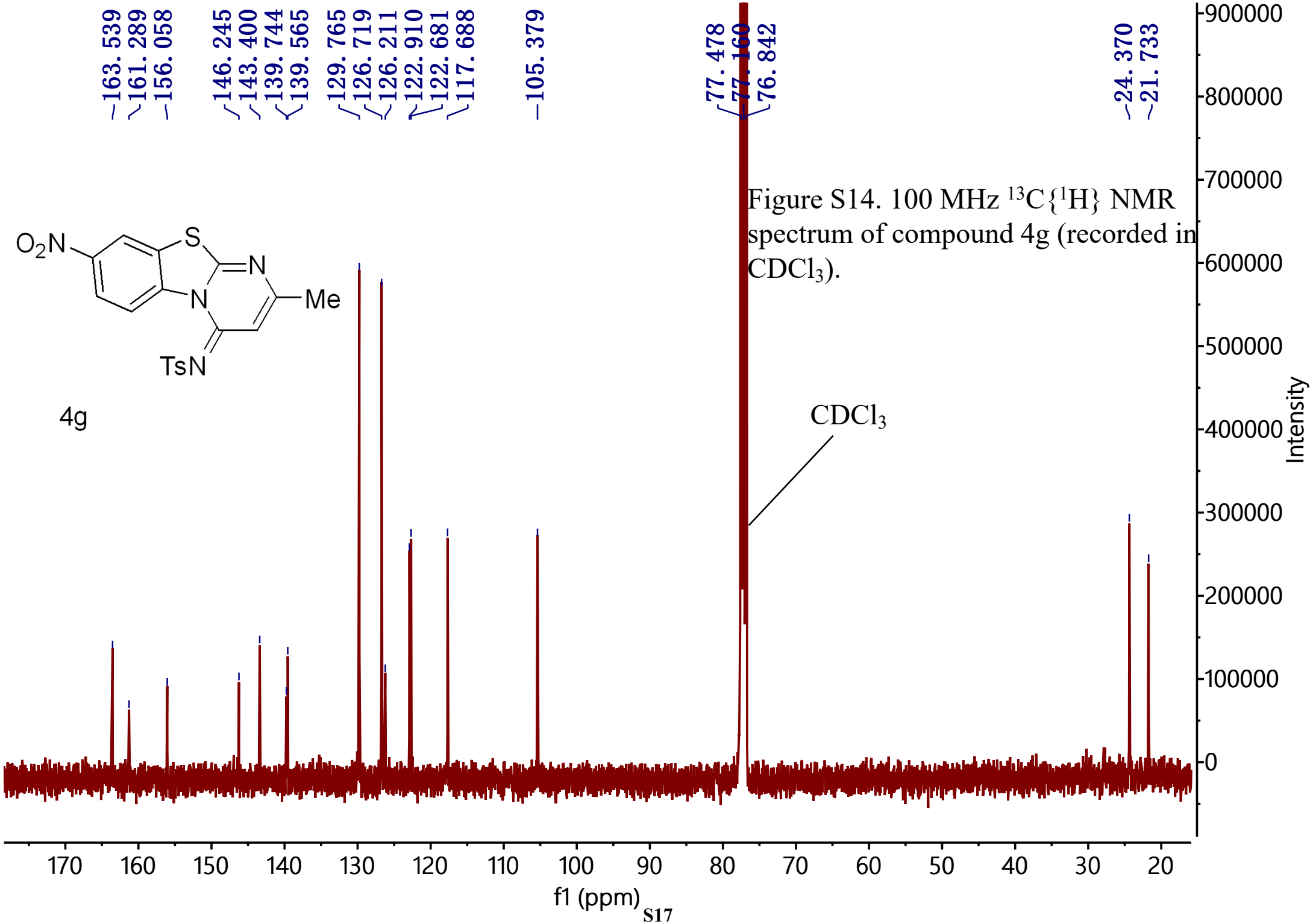


Figure S14. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4g (recorded in $CDCl_3$).

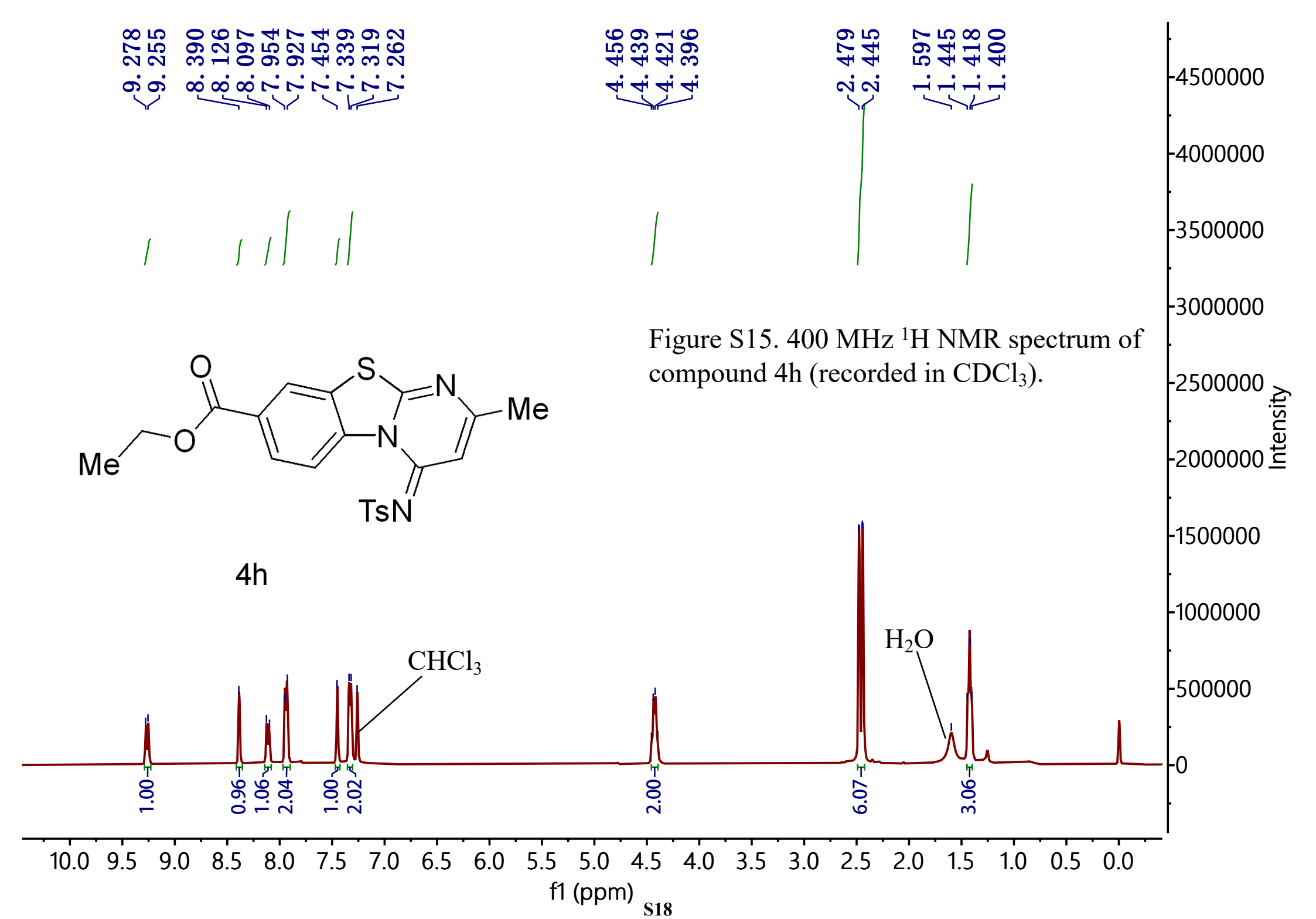


Figure S15. 400 MHz ^{1}H NMR spectrum of compound 4h (recorded in $CDCl_3$).

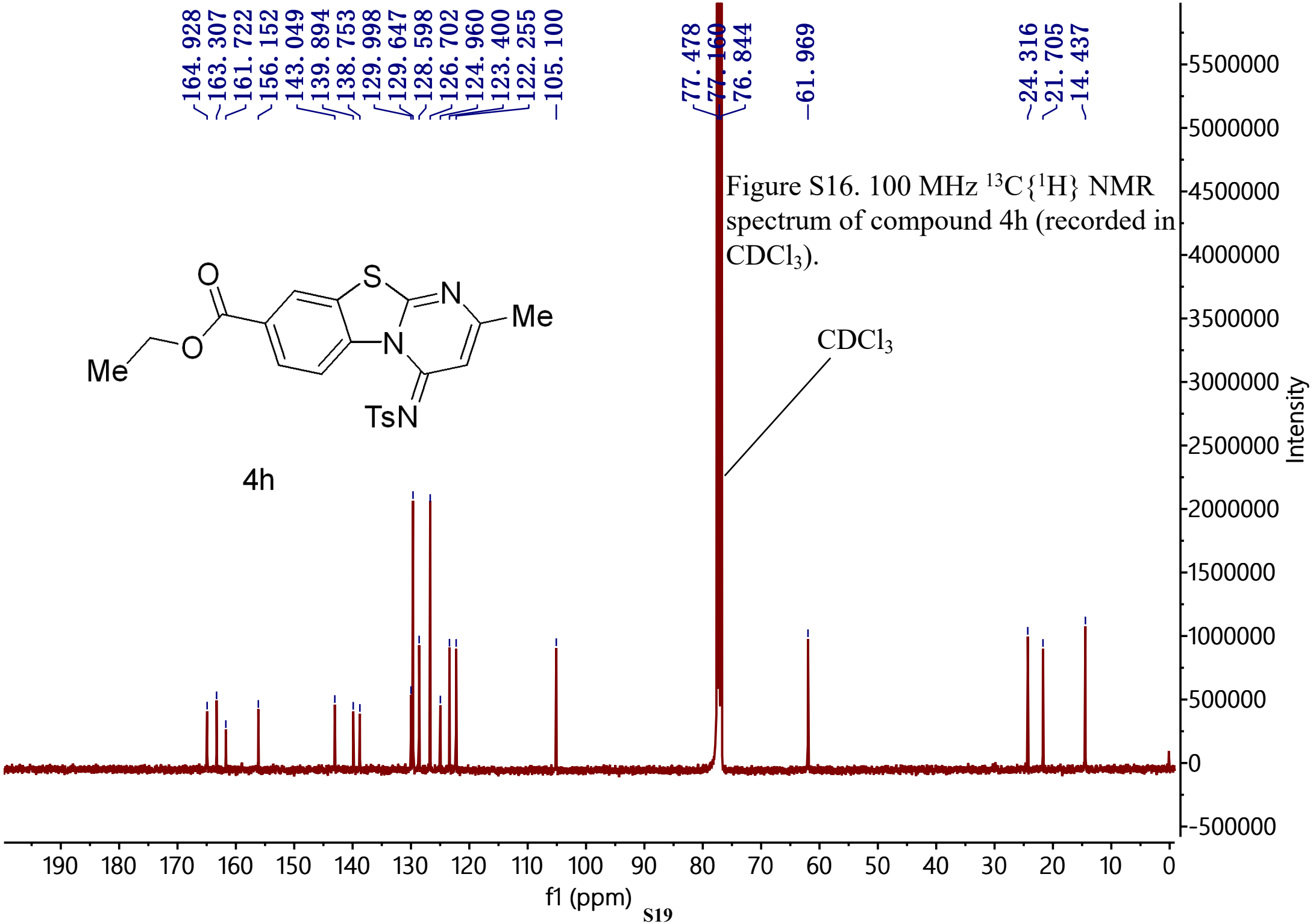


Figure S16. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4h (recorded in $CDCl_3$).

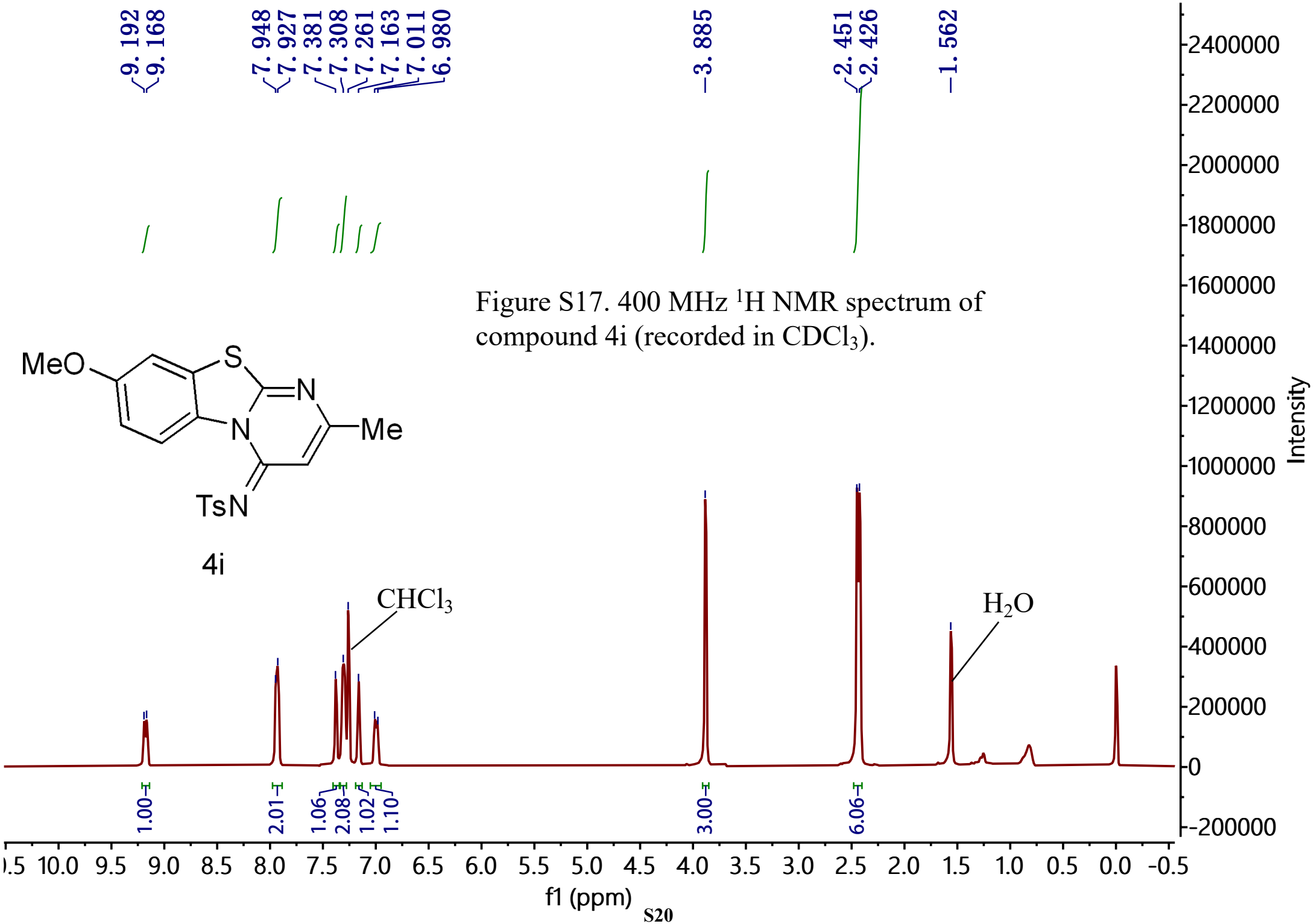


Figure S17. 400 MHz ^{1}H NMR spectrum of compound 4i (recorded in $CDCl_3$).

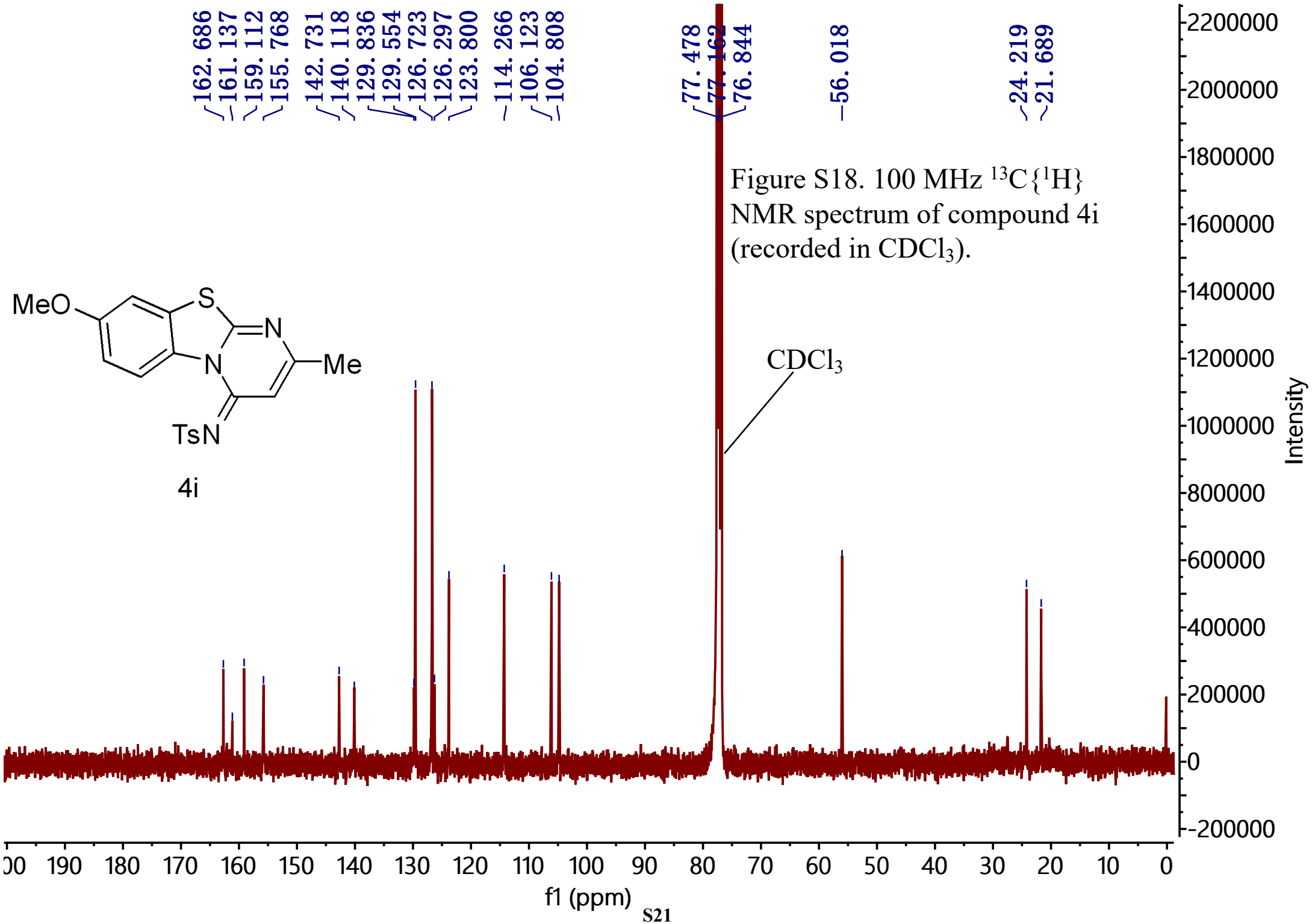


Figure S18. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4i (recorded in $CDCl_3$).

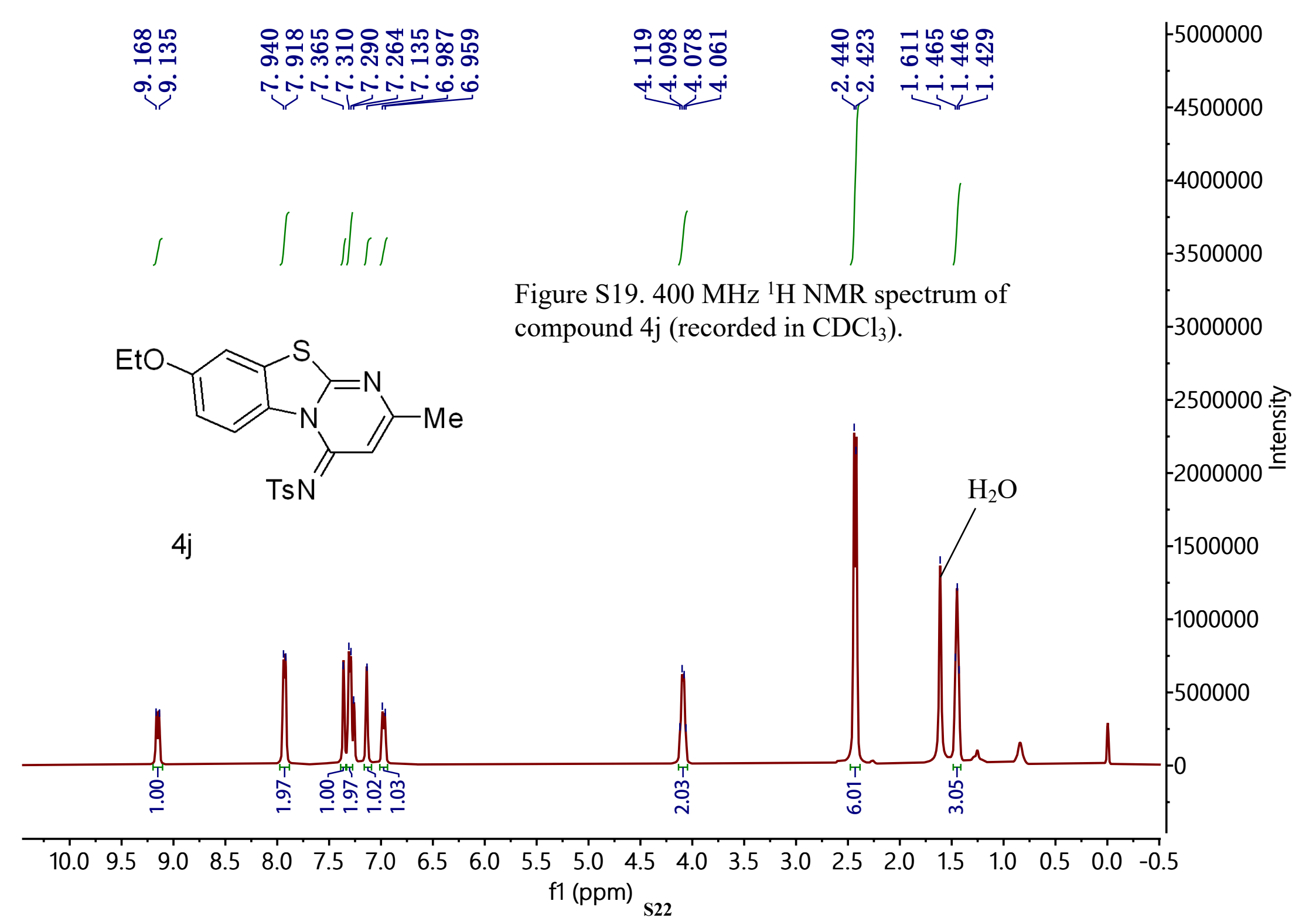


Figure S19. 400 MHz ^{1}H NMR spectrum of compound 4j (recorded in $CDCl_3$).

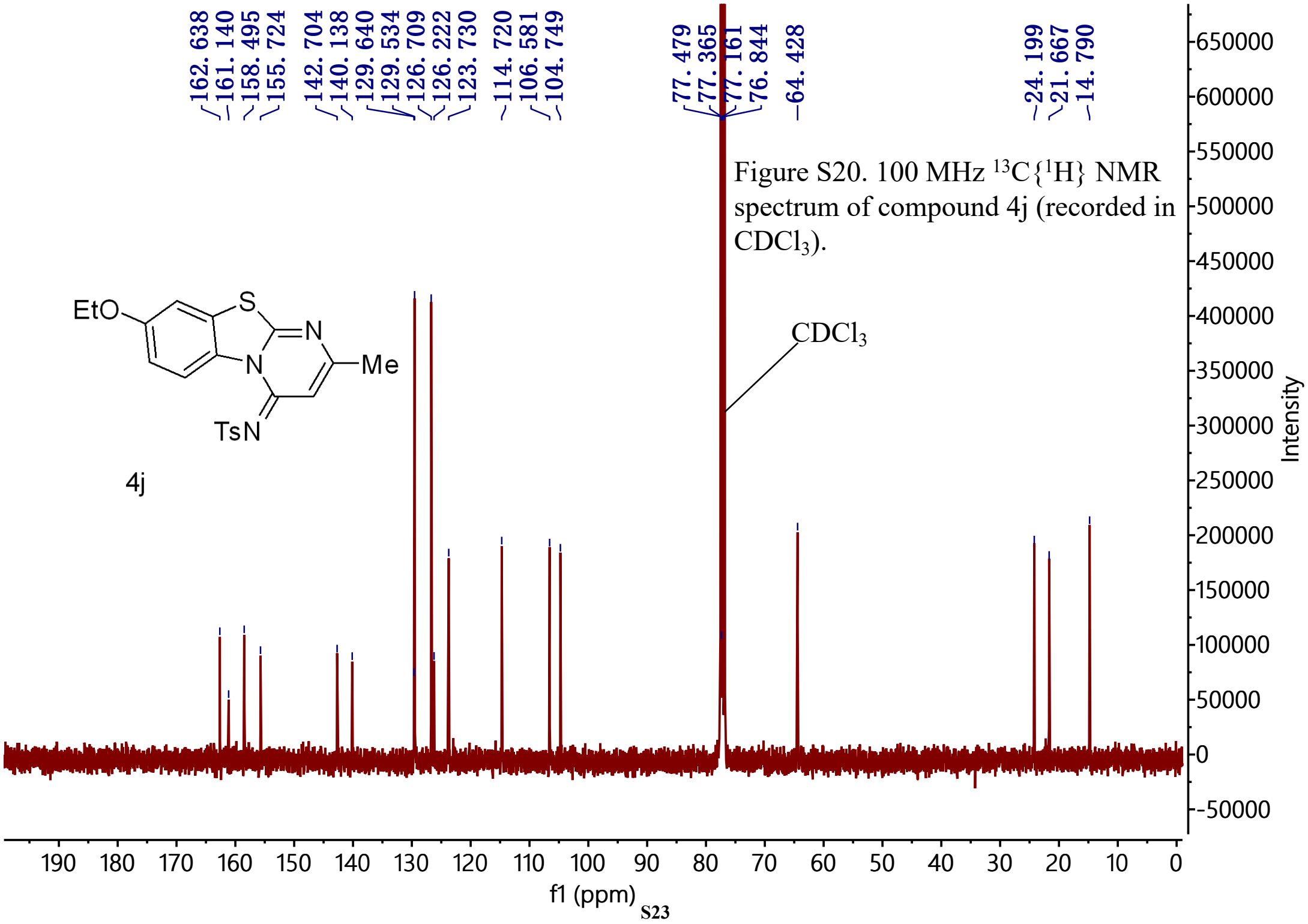


Figure S20. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4j (recorded in $CDCl_3$).

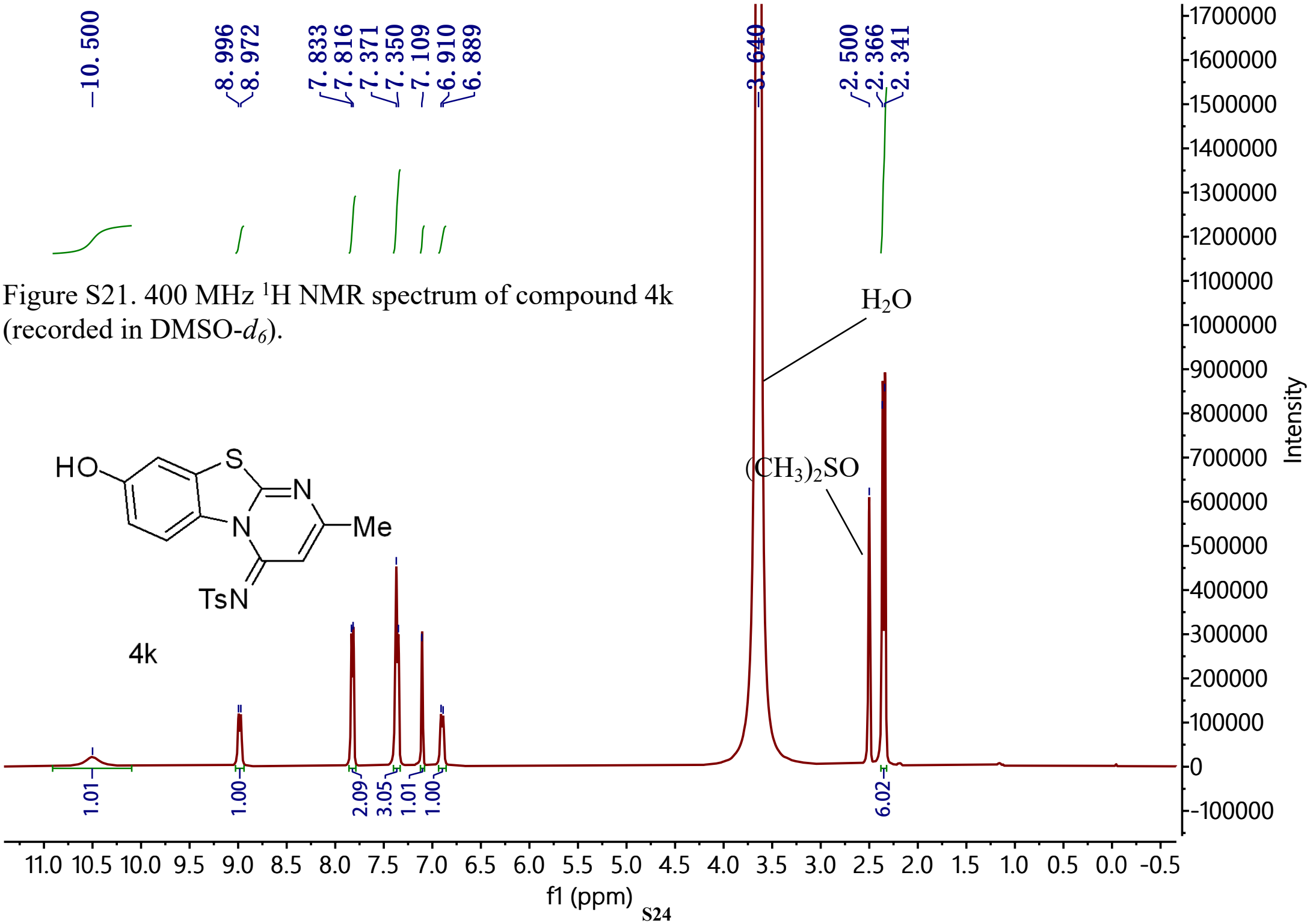


Figure S21. 400 MHz ^{1}H NMR spectrum of compound 4k (recorded in DMSO-d_6).

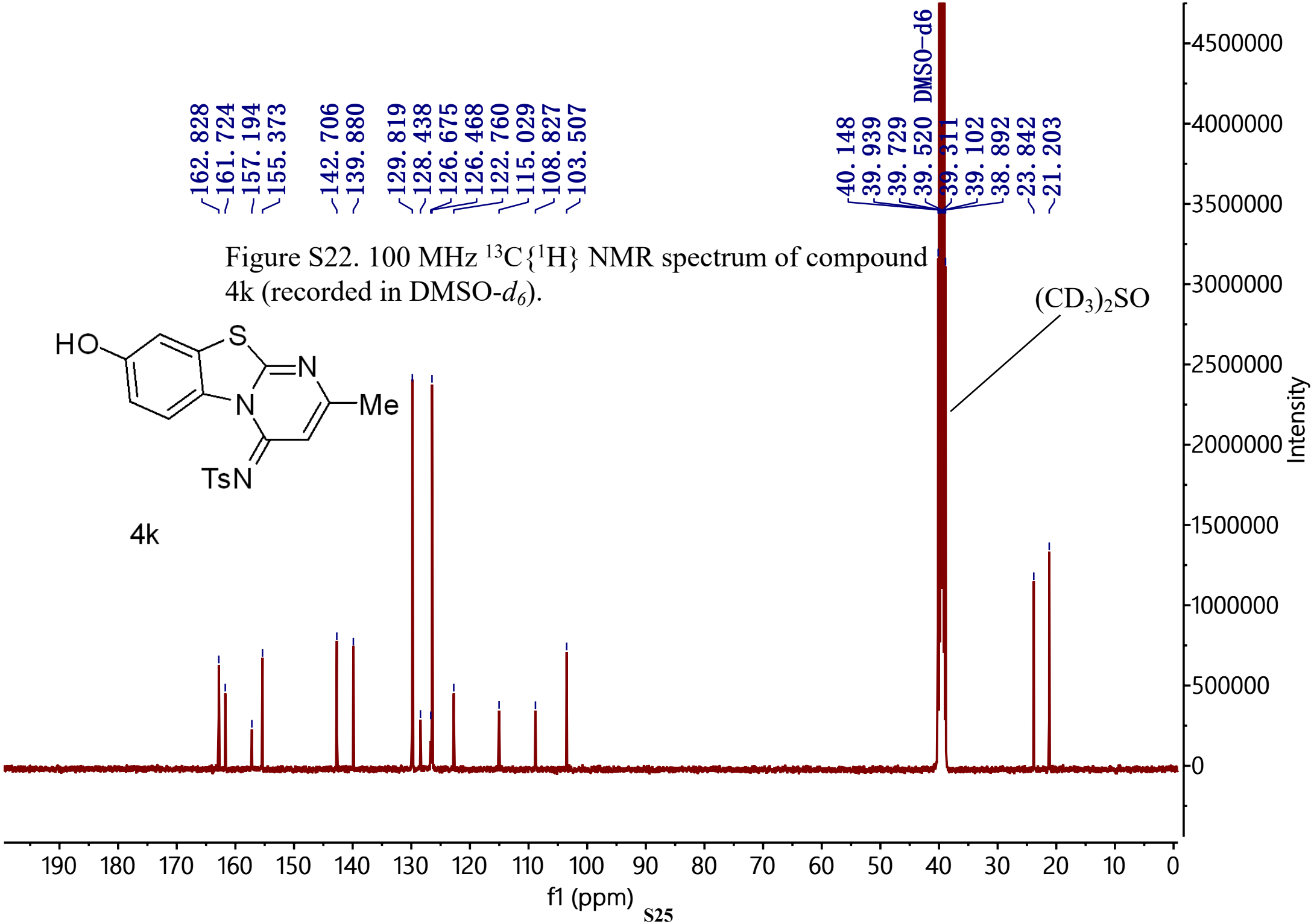


Figure S22. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4k (recorded in DMSO-d_6).

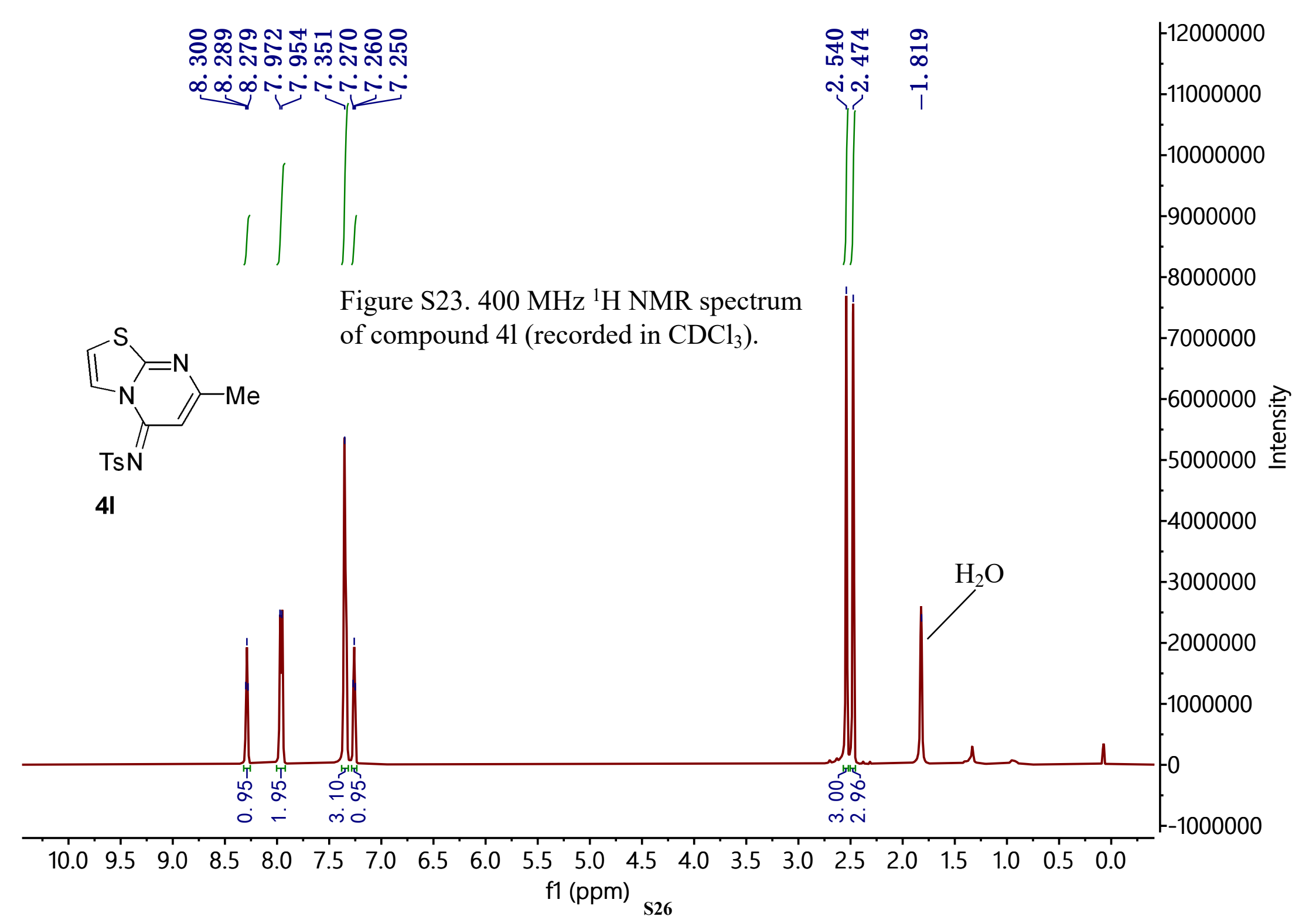


Figure S23. 400 MHz ^{1}H NMR spectrum of compound 4l (recorded in $CDCl_3$).

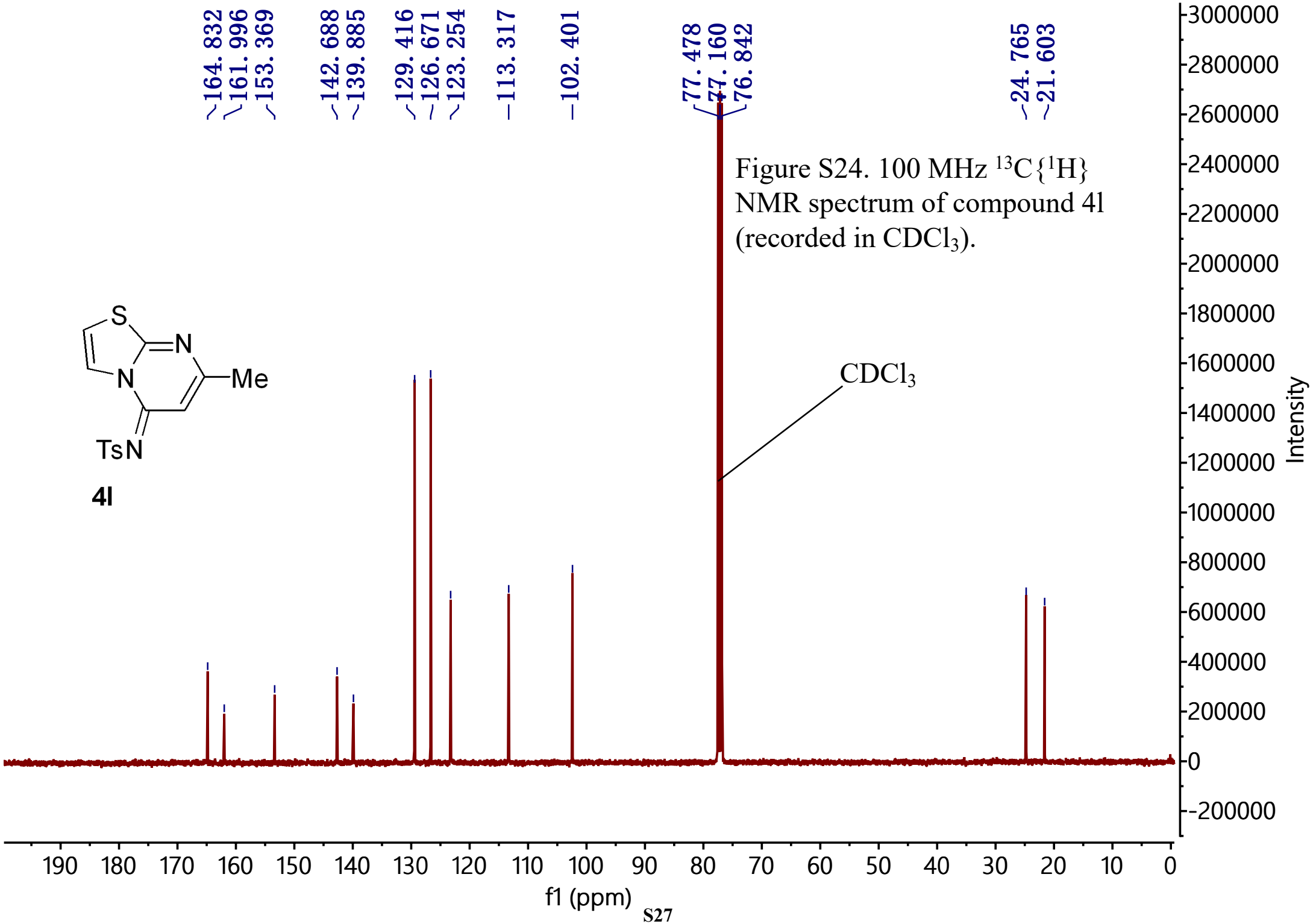


Figure S24. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4l (recorded in $CDCl_3$).

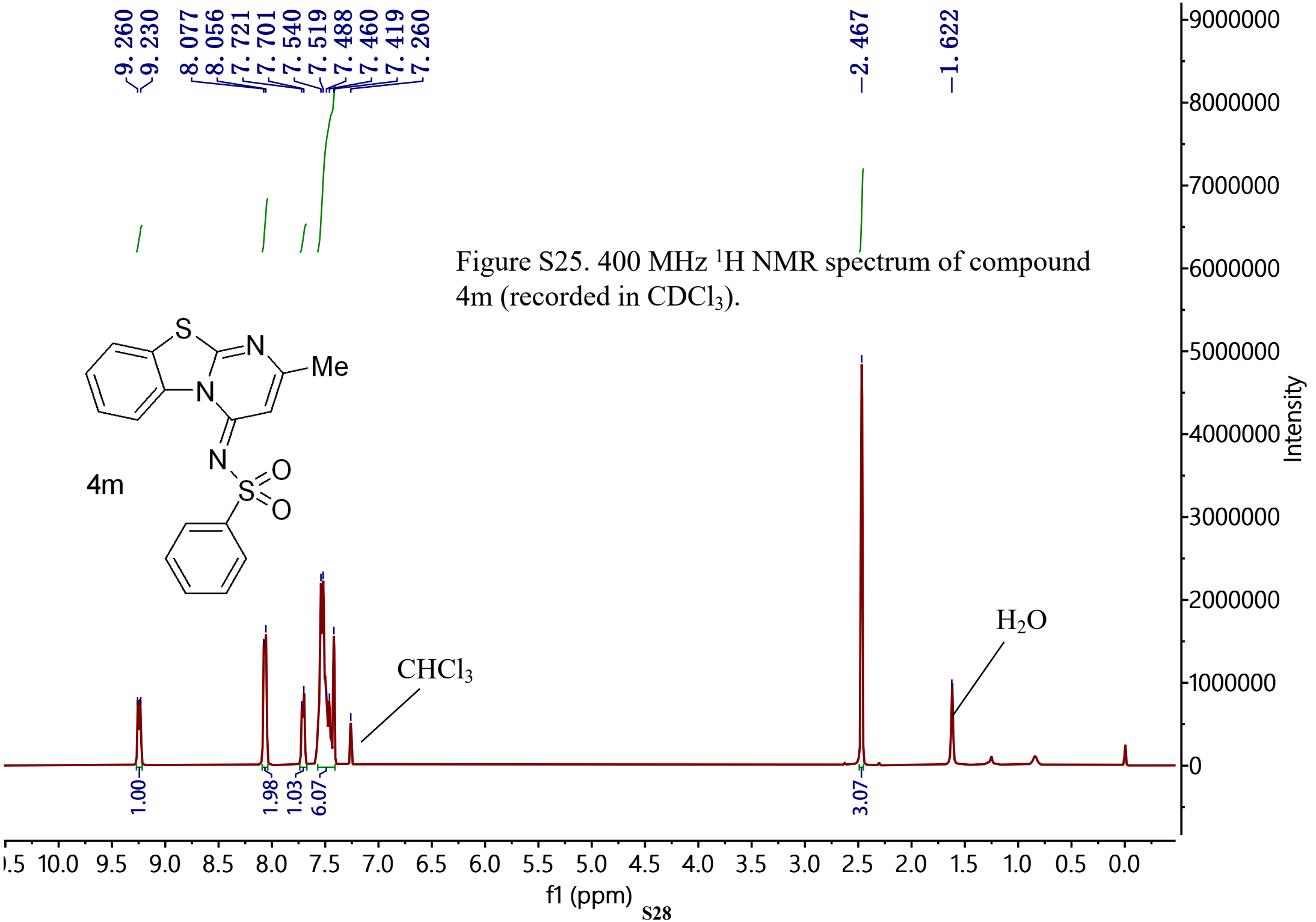


Figure S25. 400 MHz ^{1}H NMR spectrum of compound 4m (recorded in $CDCl_3$).

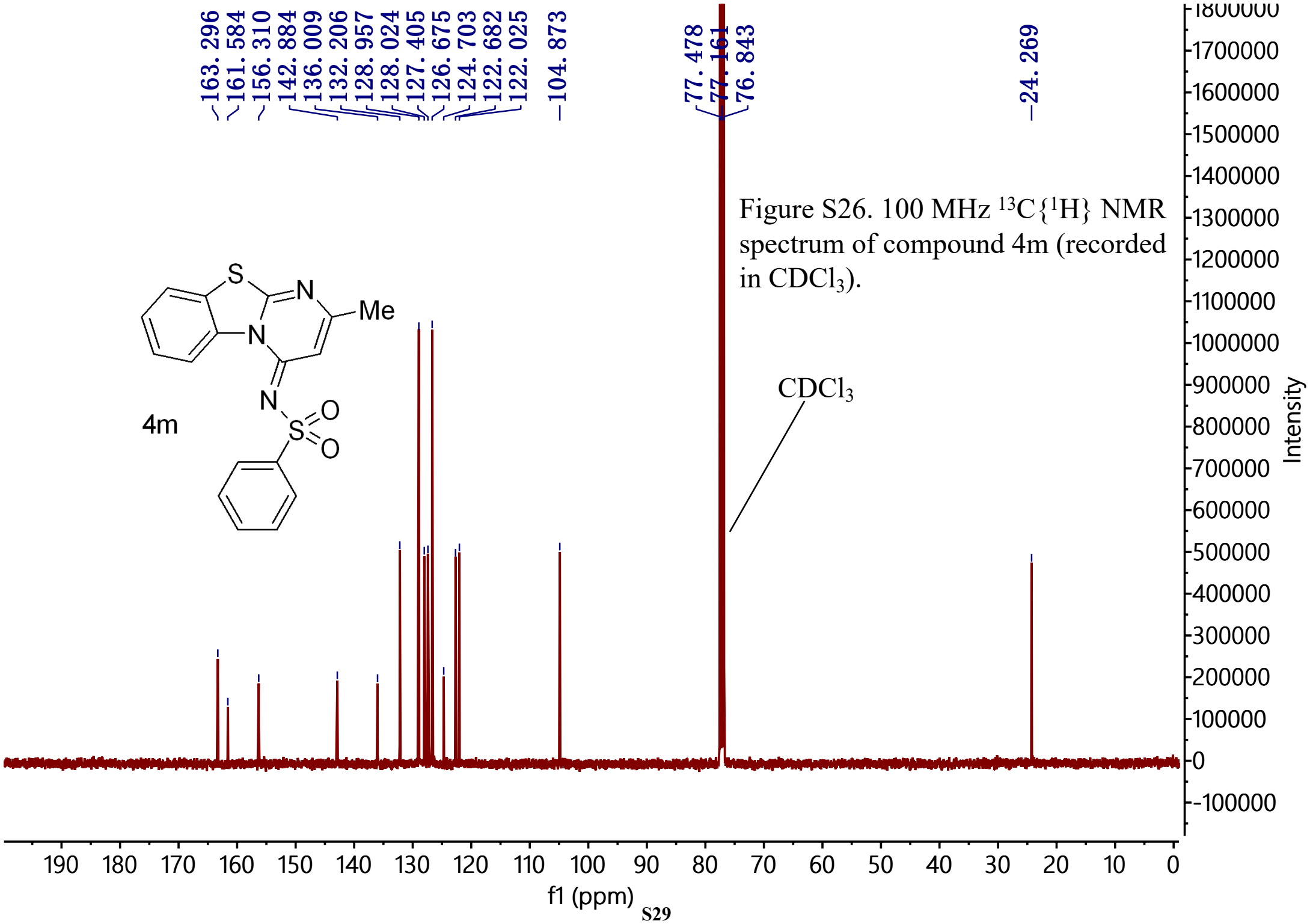


Figure S26. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4m (recorded in $CDCl_3$).

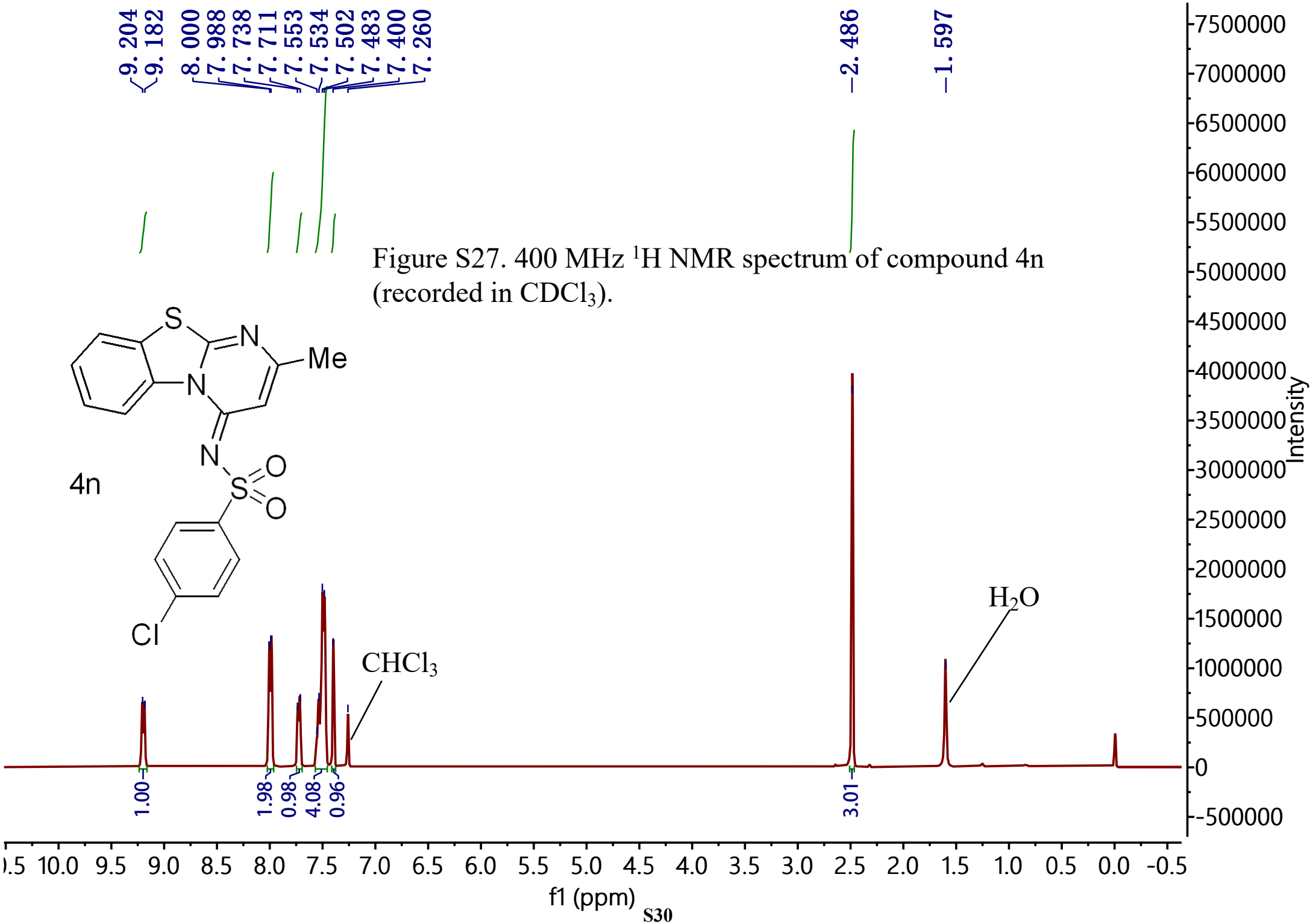


Figure S27. 400 MHz ^{1}H NMR spectrum of compound 4n (recorded in $CDCl_3$).

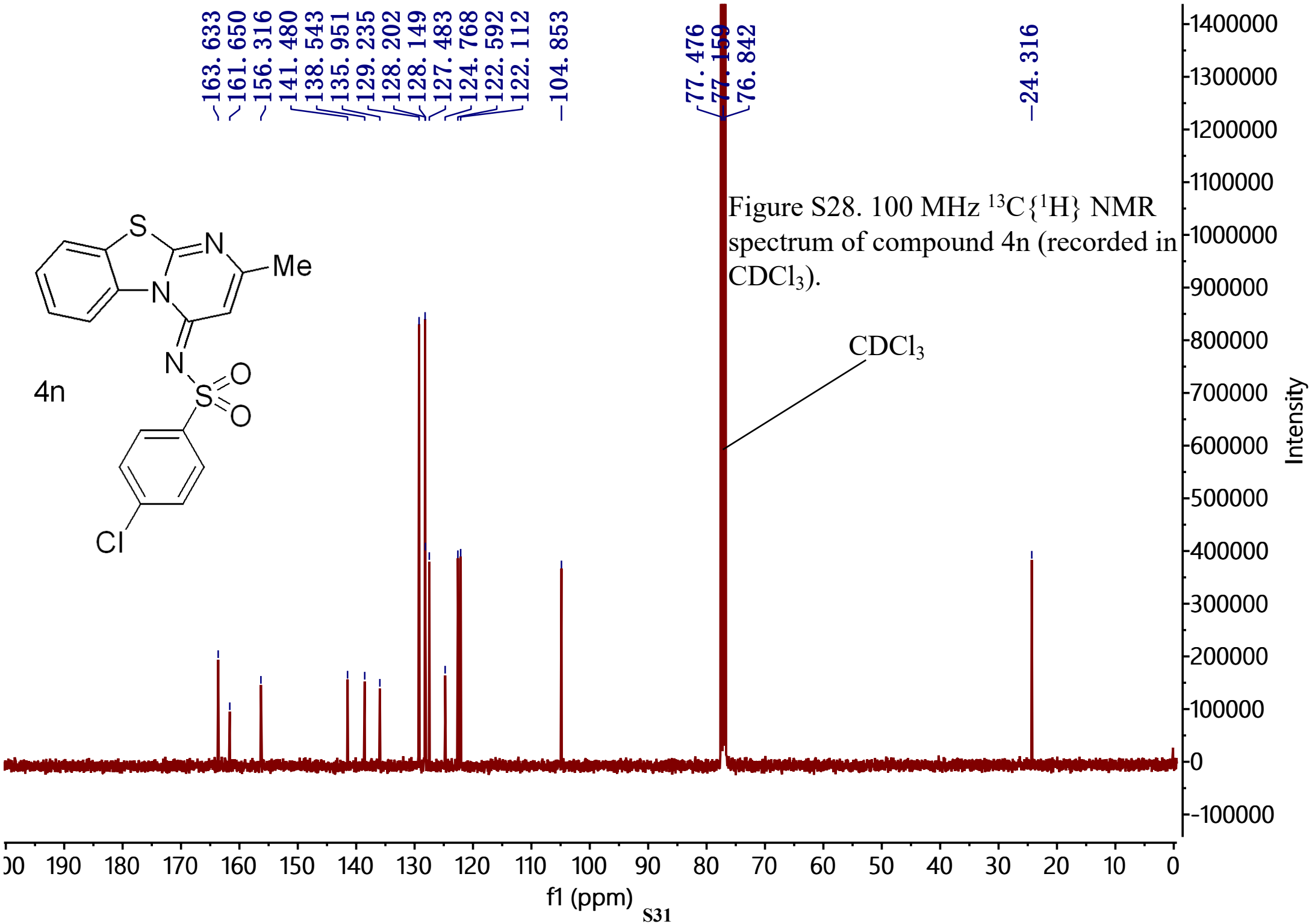


Figure S28. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4n (recorded in $CDCl_3$).

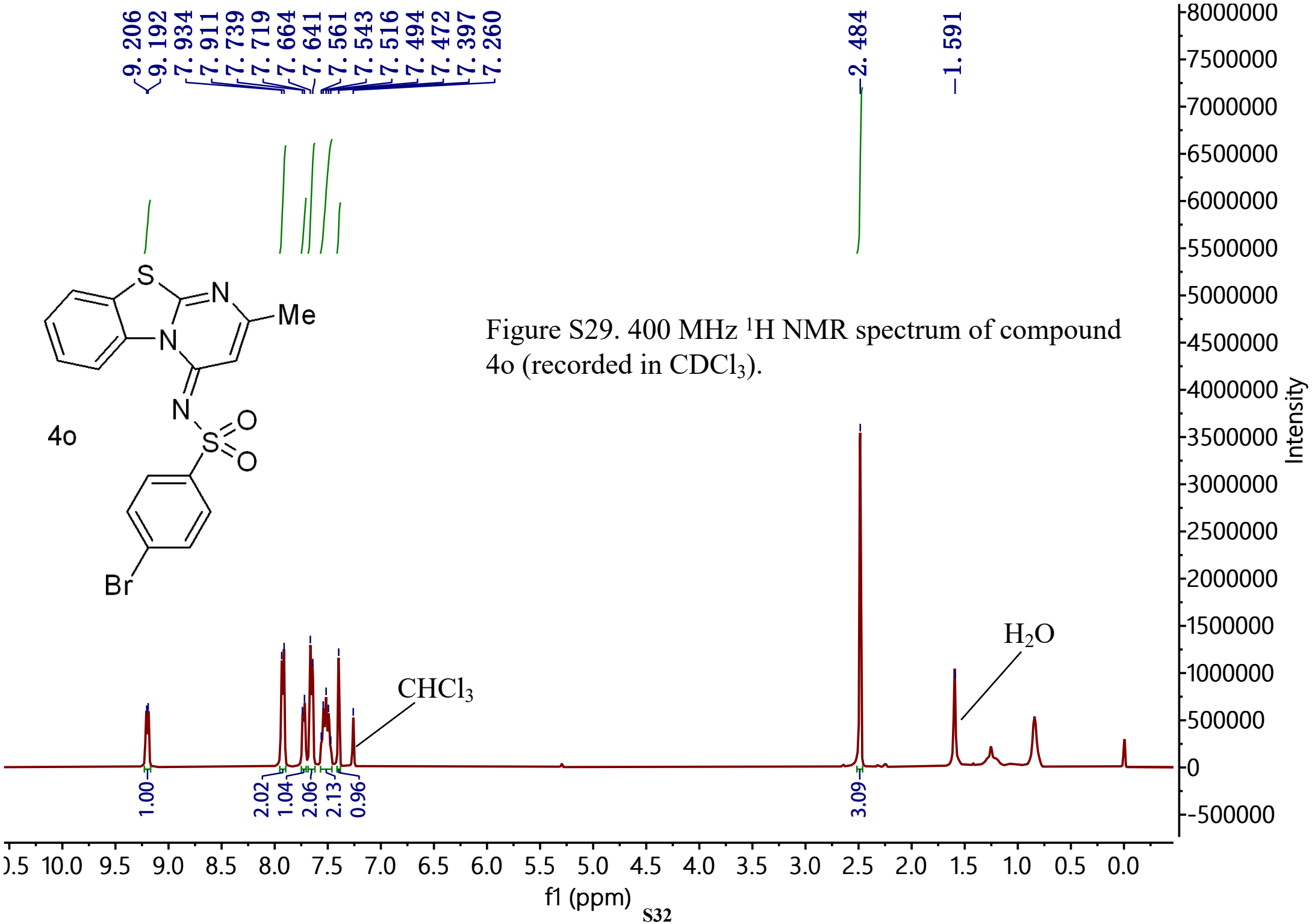


Figure S29. 400 MHz ^{1}H NMR spectrum of compound 4o (recorded in $CDCl_3$).

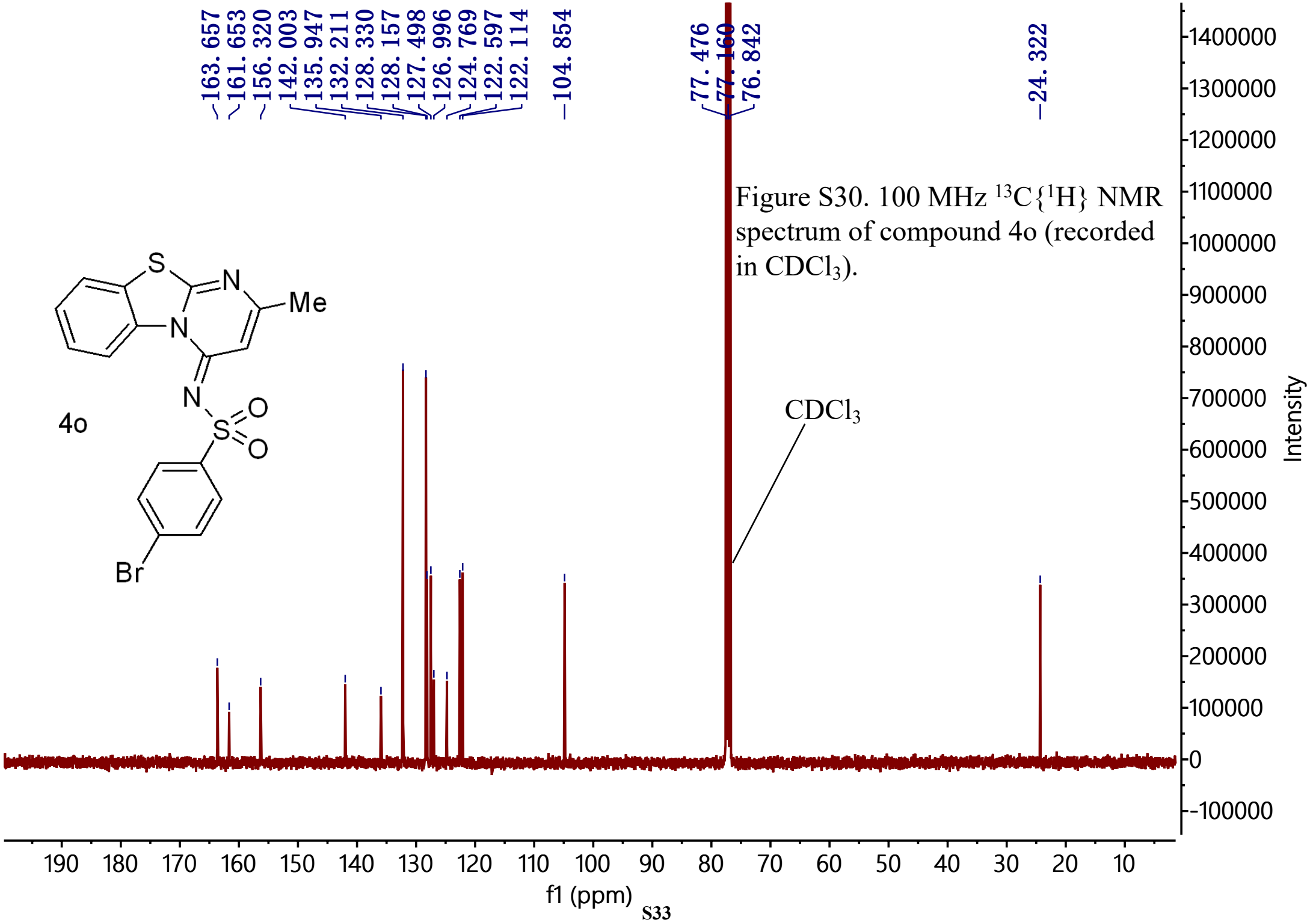


Figure S30. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4o (recorded in $CDCl_3$).

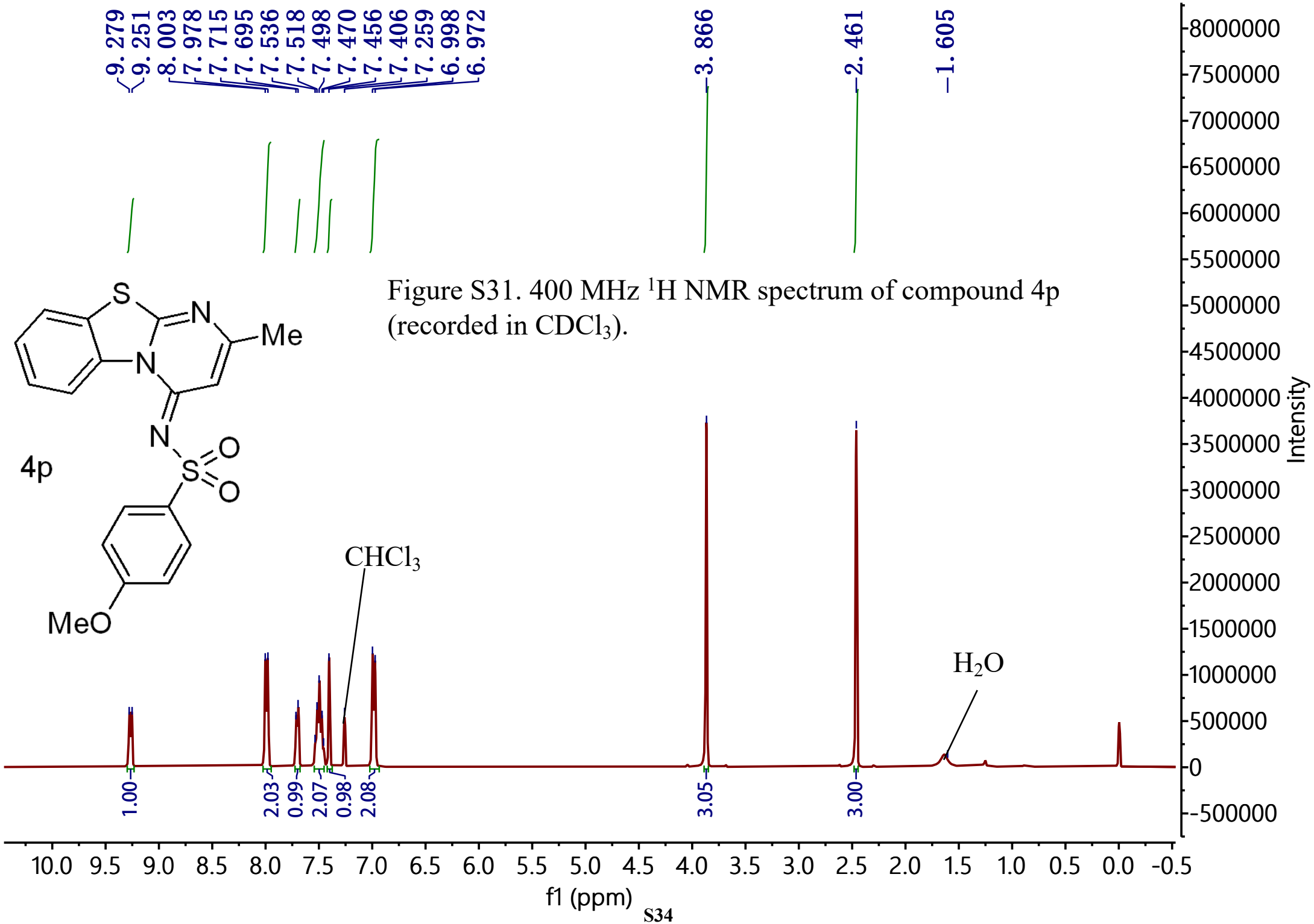


Figure S31. 400 MHz ^{1}H NMR spectrum of compound 4p (recorded in $CDCl_3$).

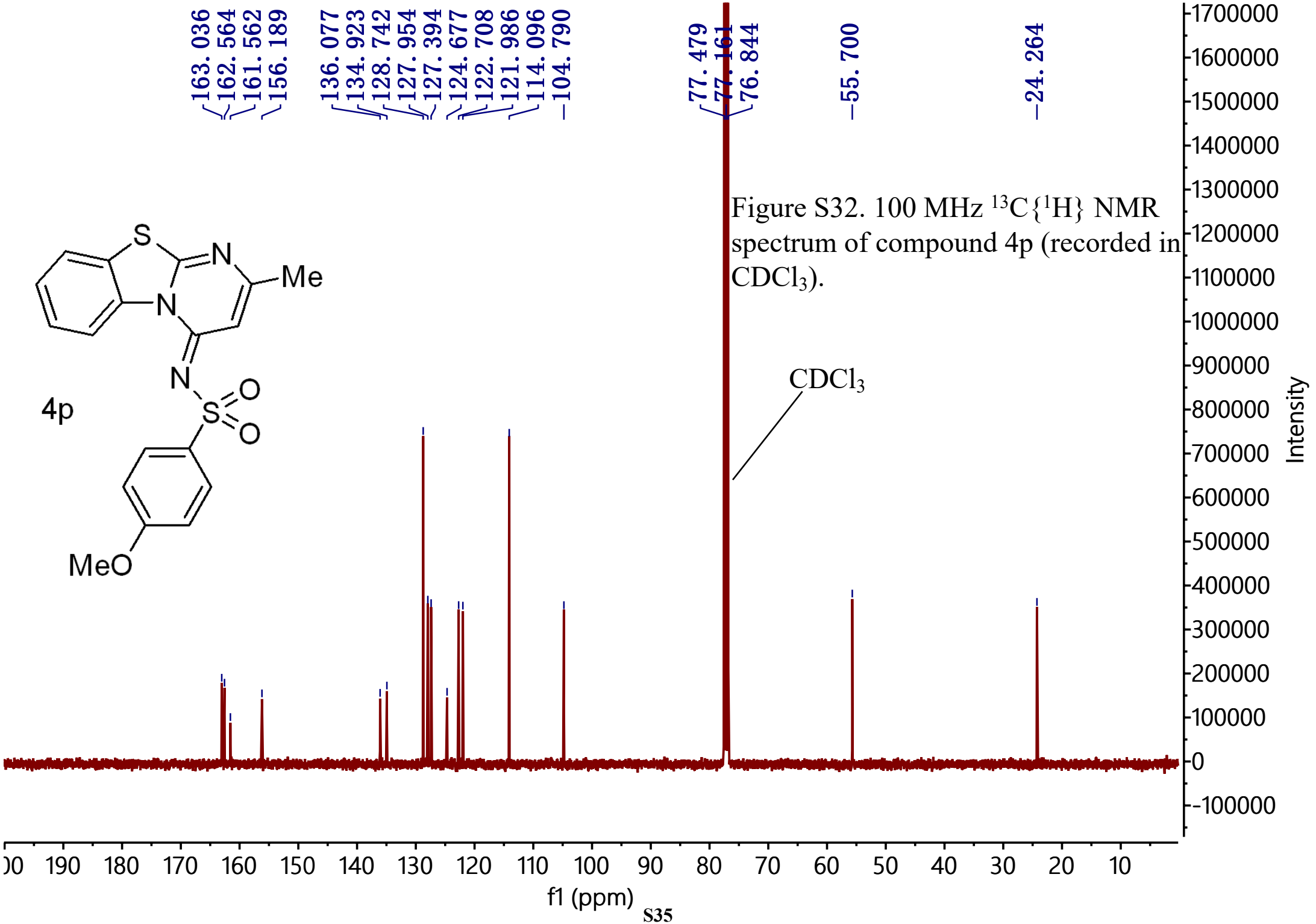


Figure S32. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4p (recorded in $CDCl_3$).

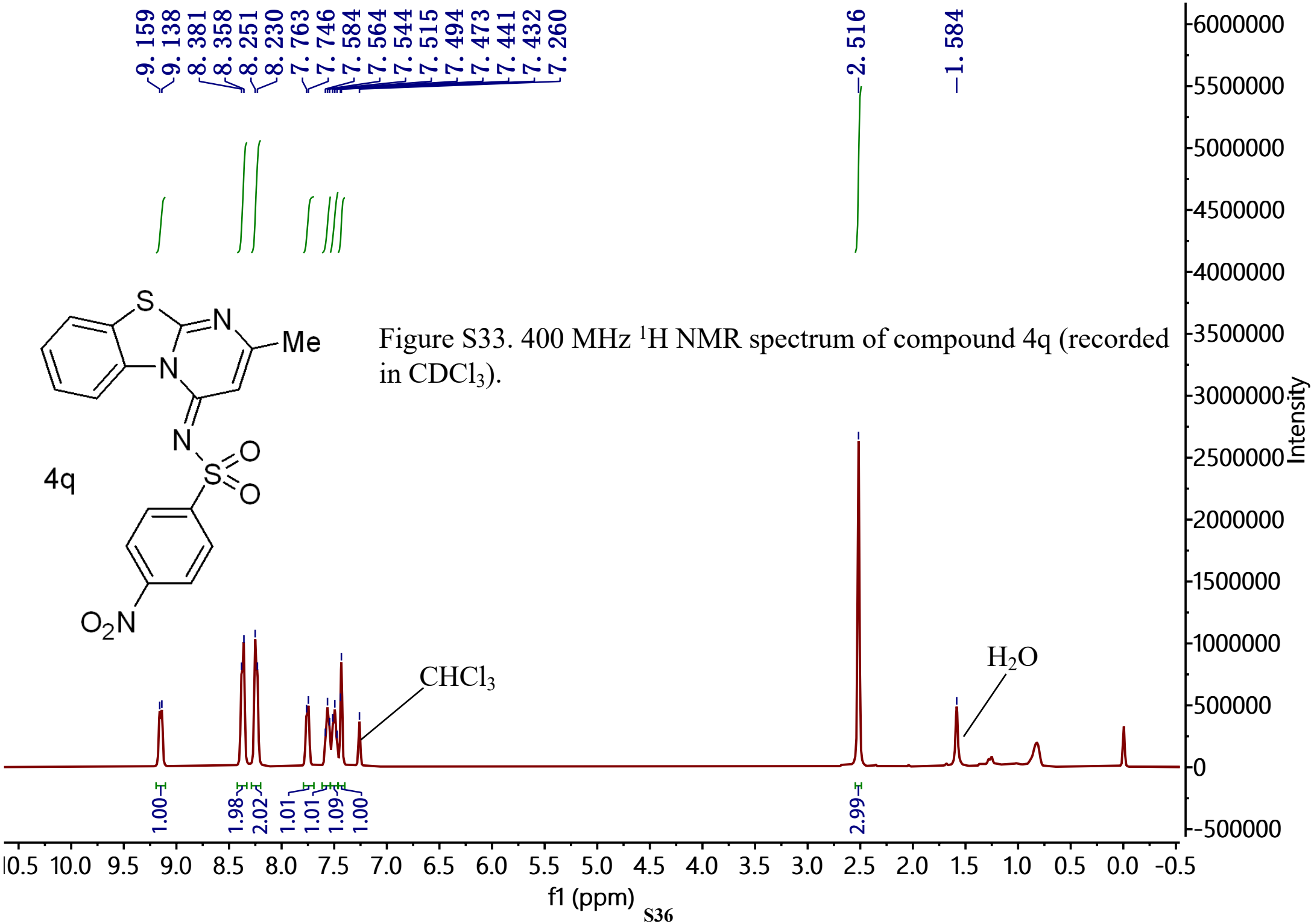


Figure S33. 400 MHz ^{1}H NMR spectrum of compound 4q (recorded in $CDCl_3$).

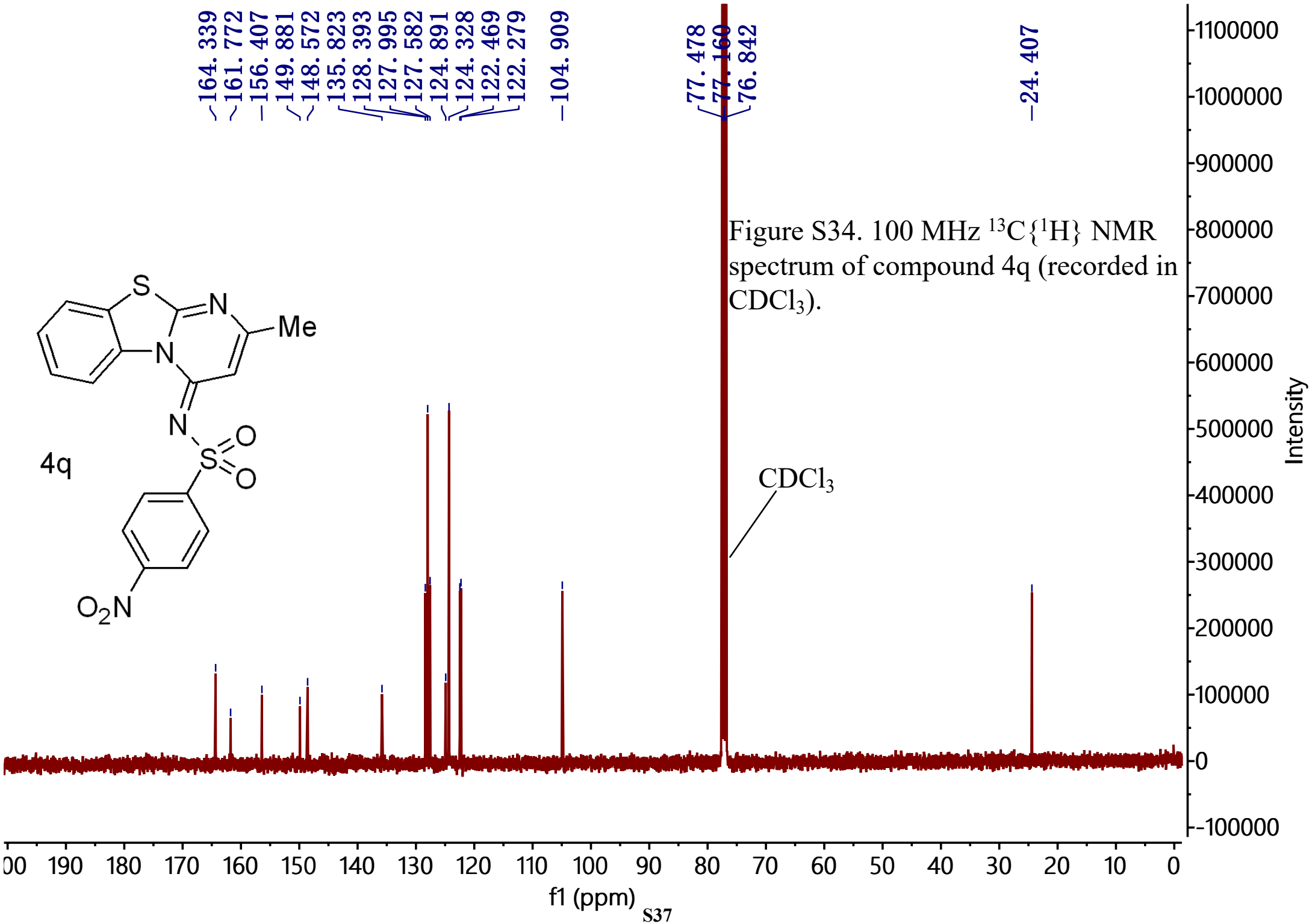


Figure S34. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4q (recorded in $CDCl_3$).

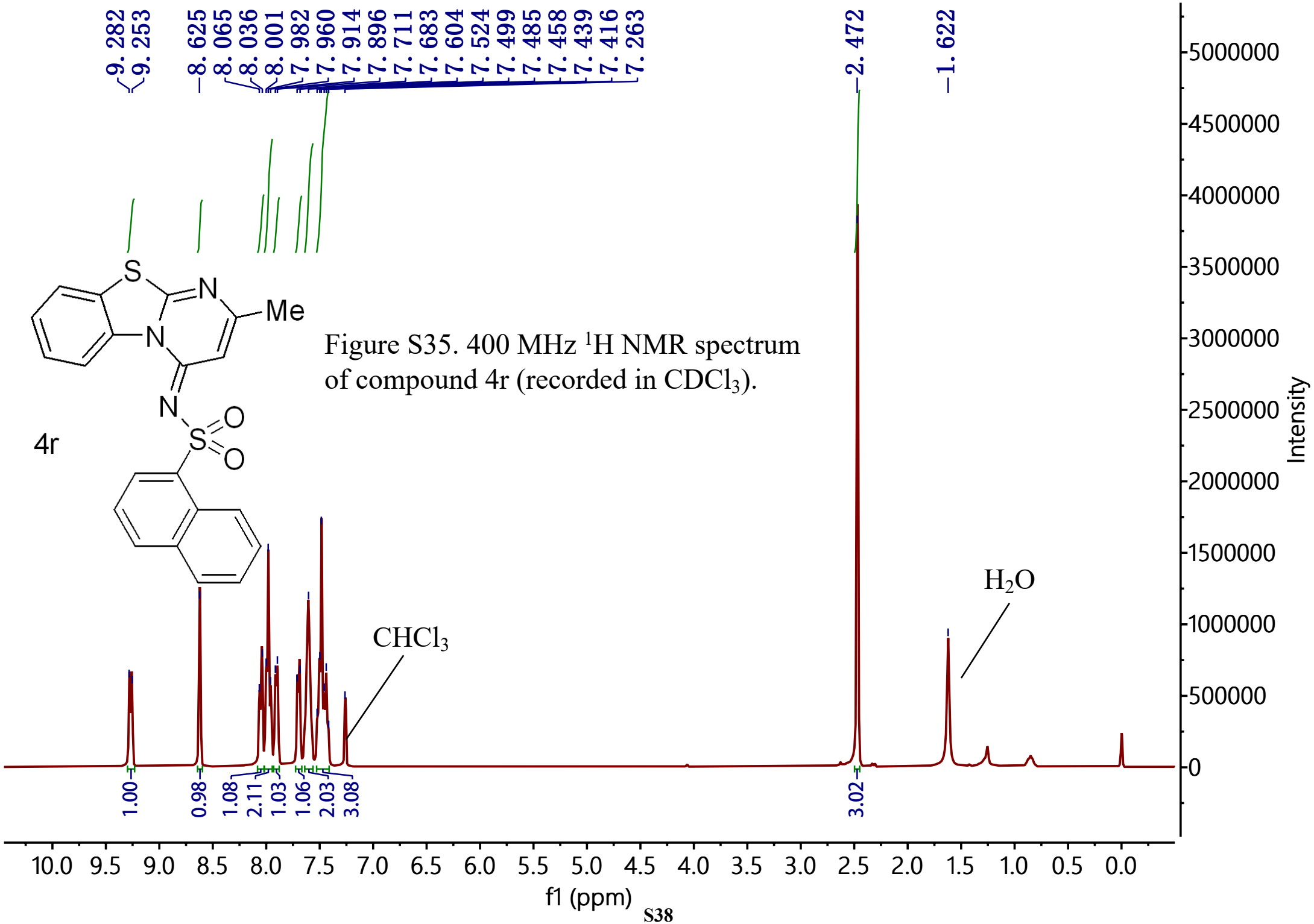


Figure S35. 400 MHz ^{1}H NMR spectrum of compound 4r (recorded in $CDCl_3$).

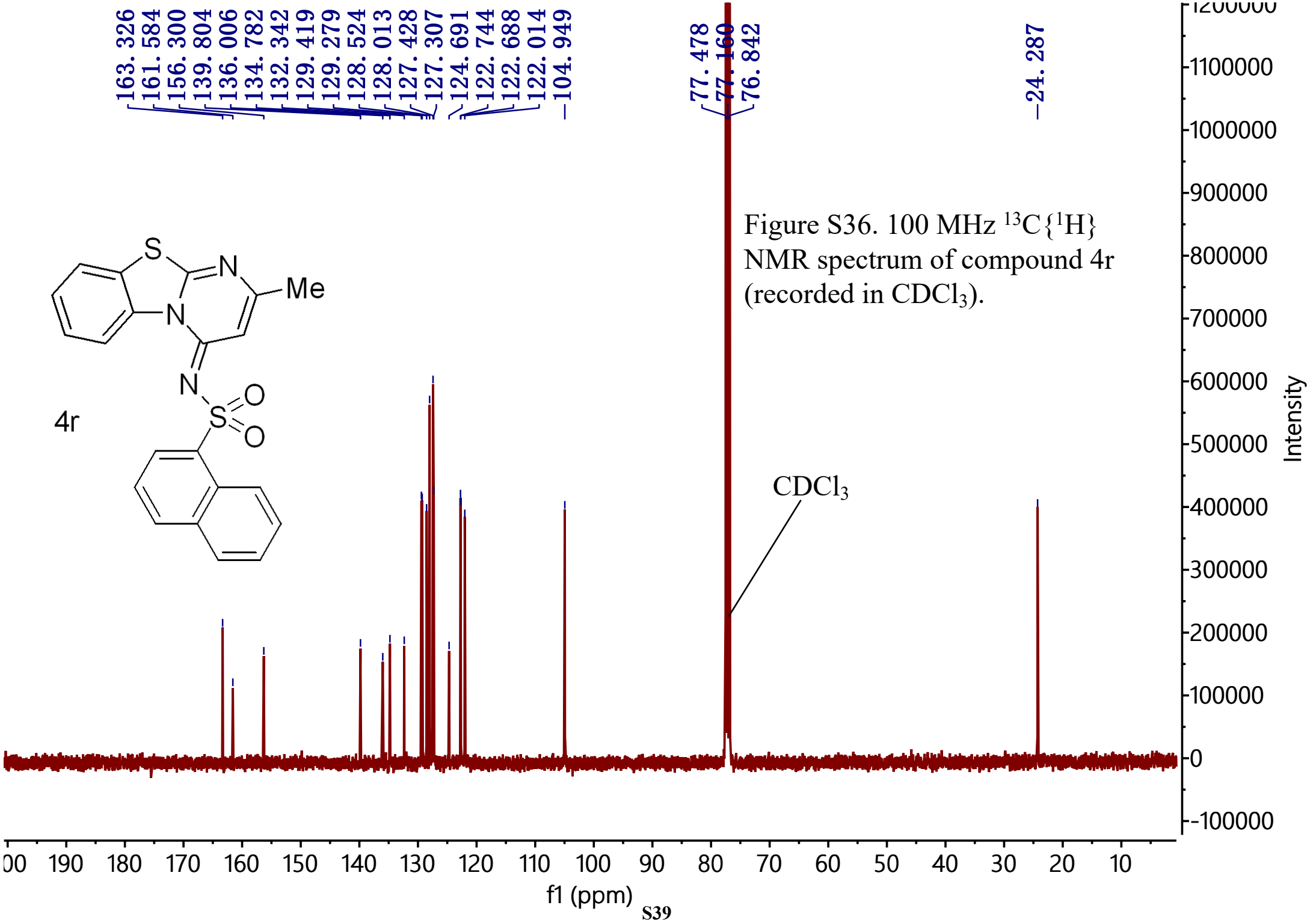


Figure S36. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4r (recorded in $CDCl_3$).

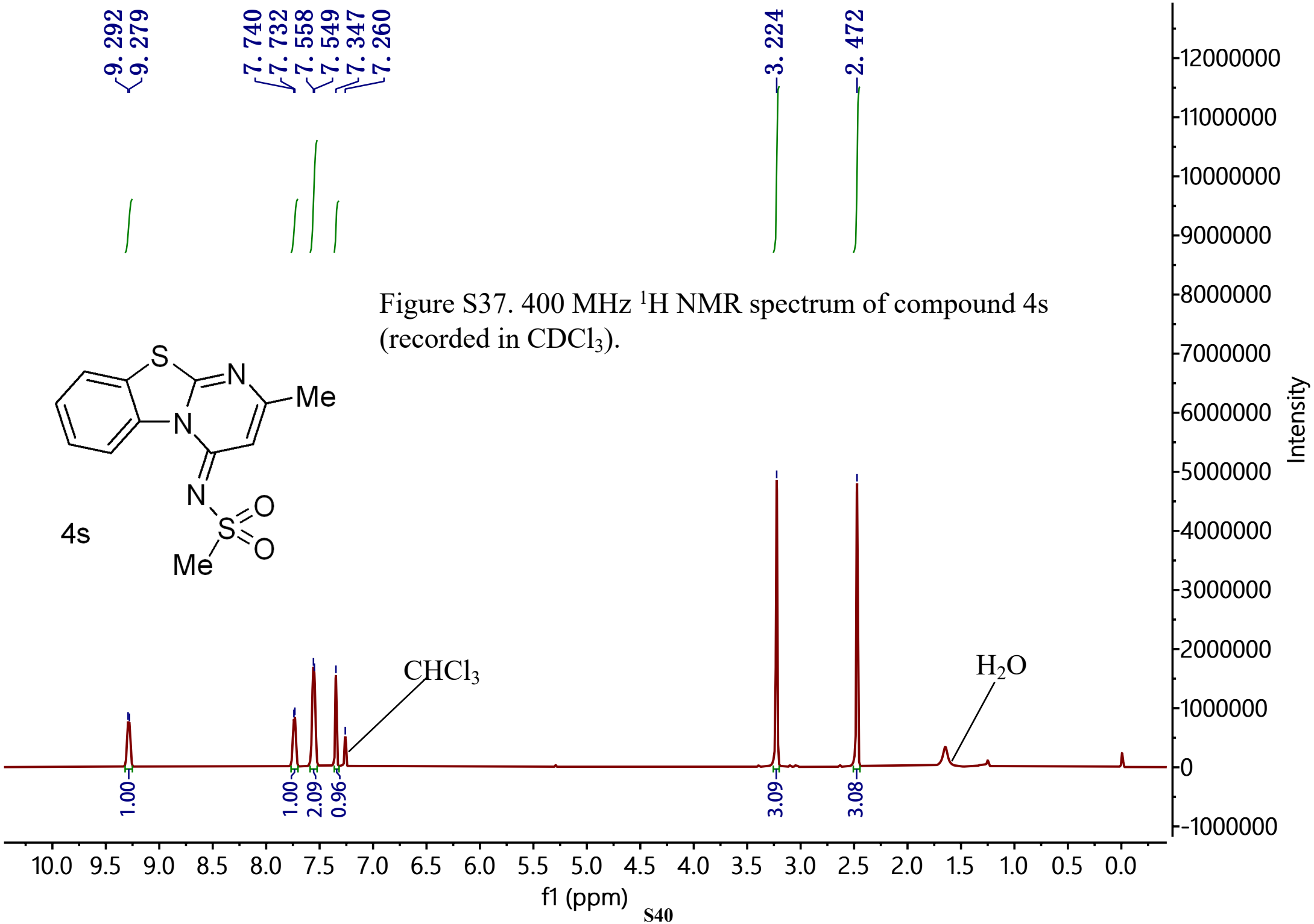


Figure S37. 400 MHz ^{1}H NMR spectrum of compound 4s (recorded in $CDCl_3$).

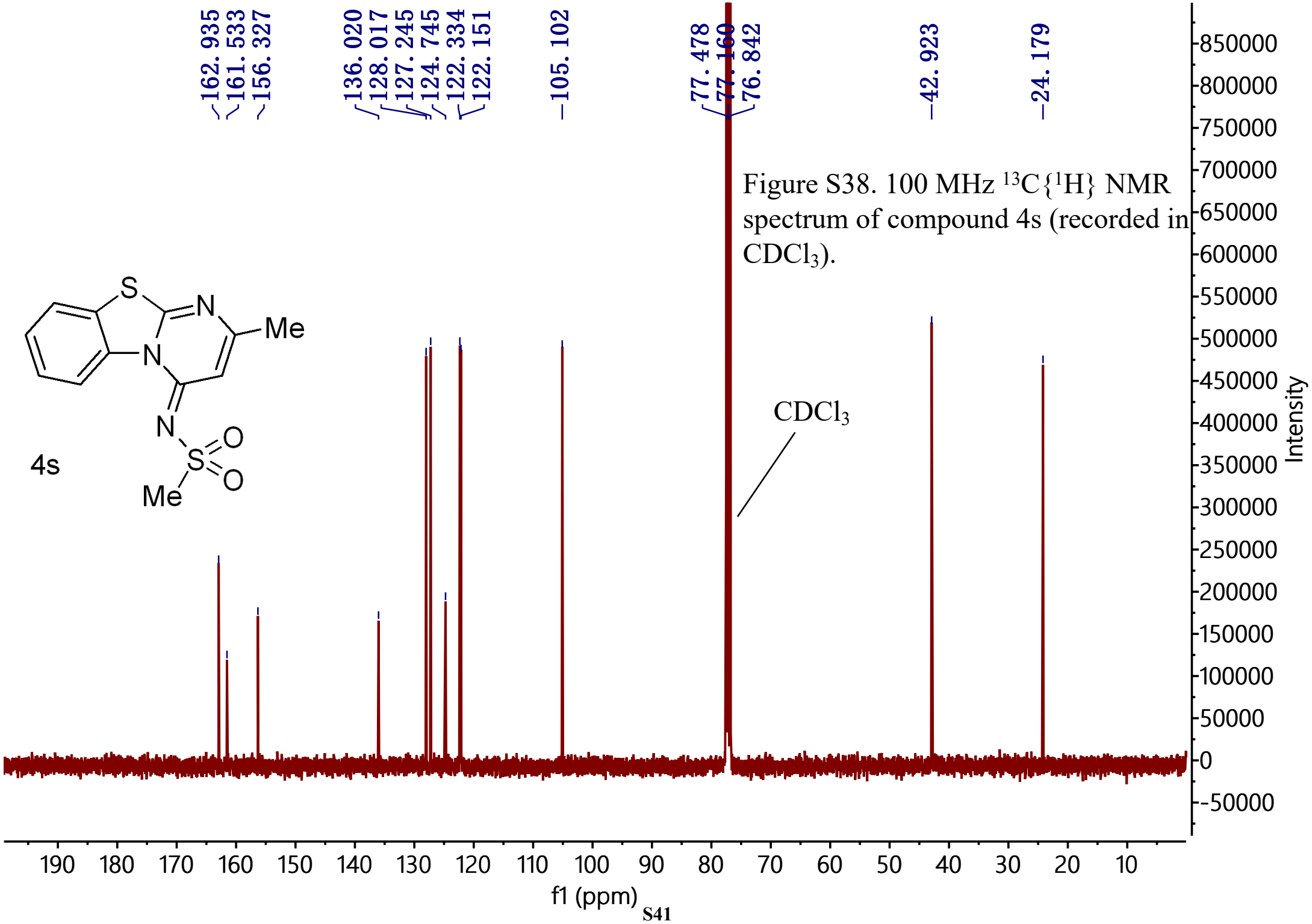


Figure S38. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4s (recorded in $CDCl_3$).

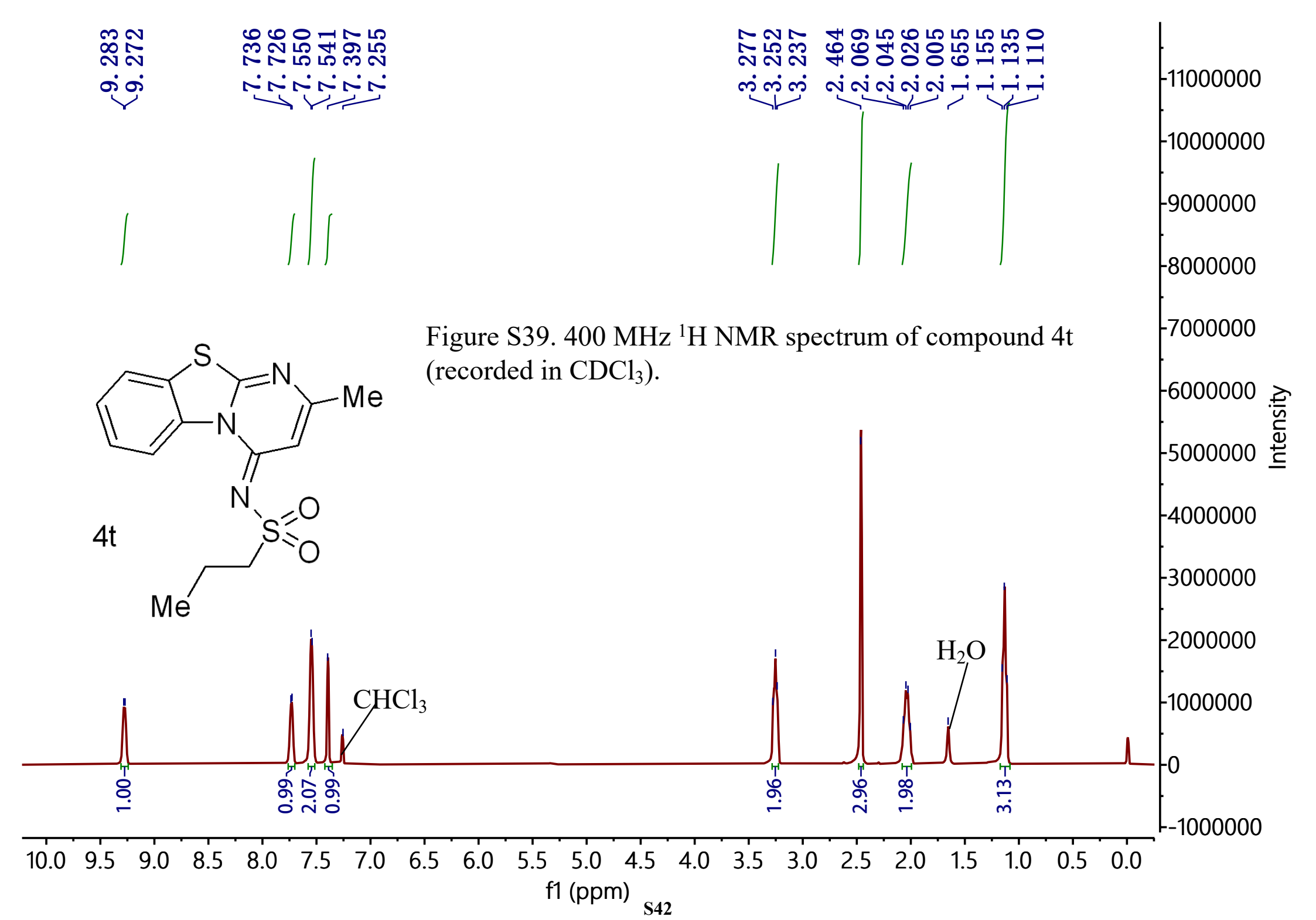


Figure S39. 400 MHz ^{1}H NMR spectrum of compound 4t (recorded in $CDCl_3$).

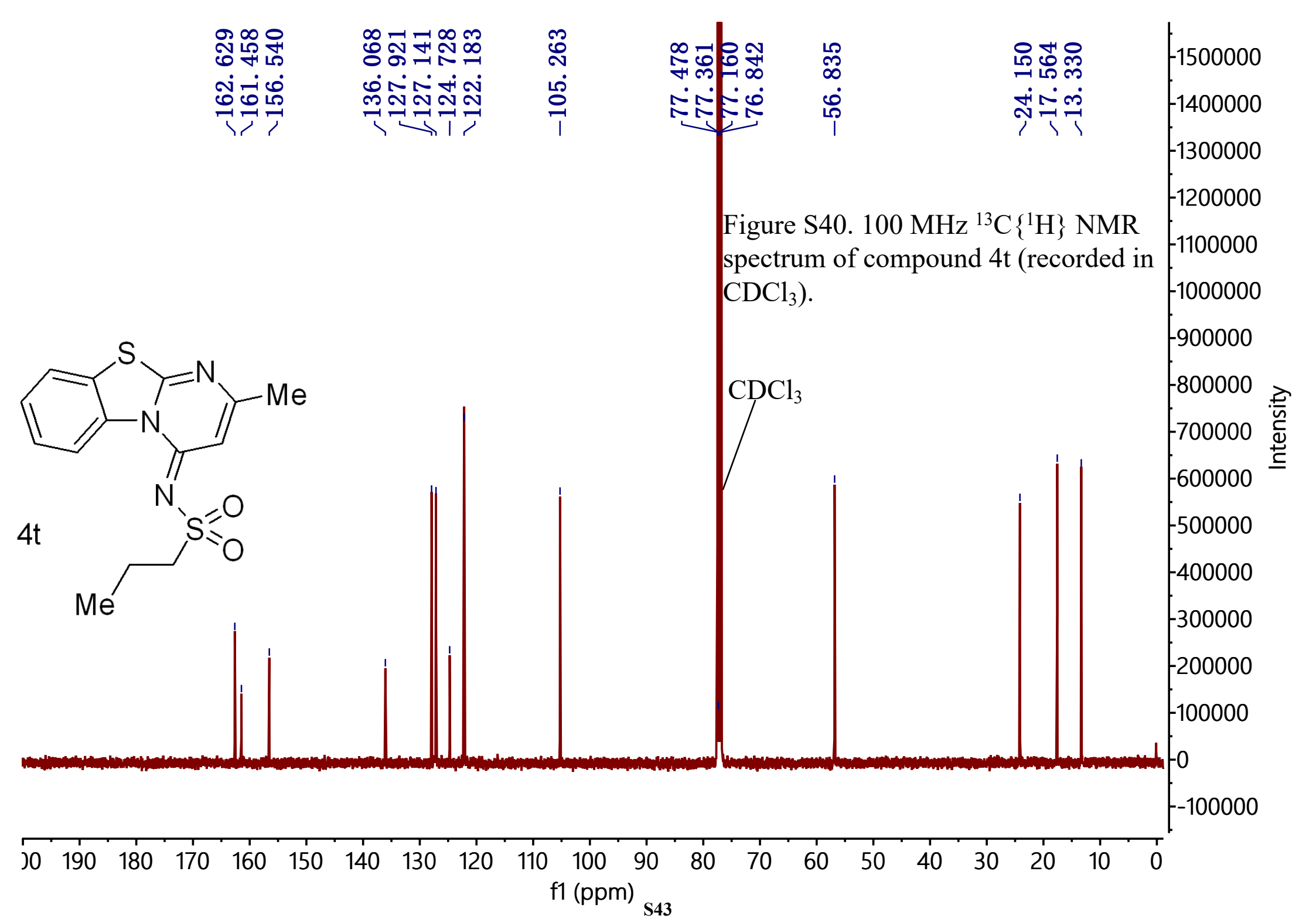


Figure S40. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4t (recorded in $CDCl_3$).

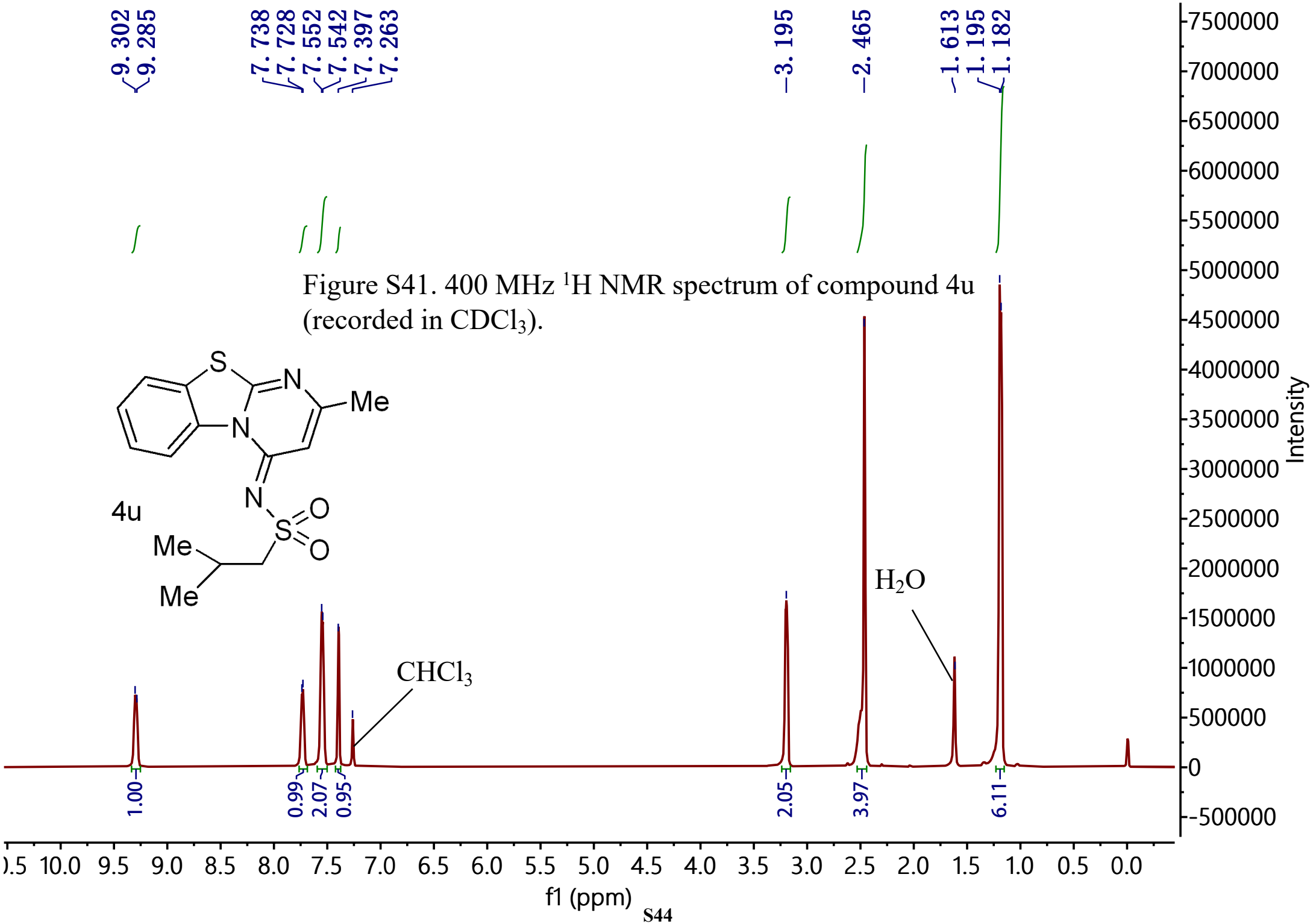


Figure S41. 400 MHz ^{1}H NMR spectrum of compound 4u (recorded in $CDCl_3$).

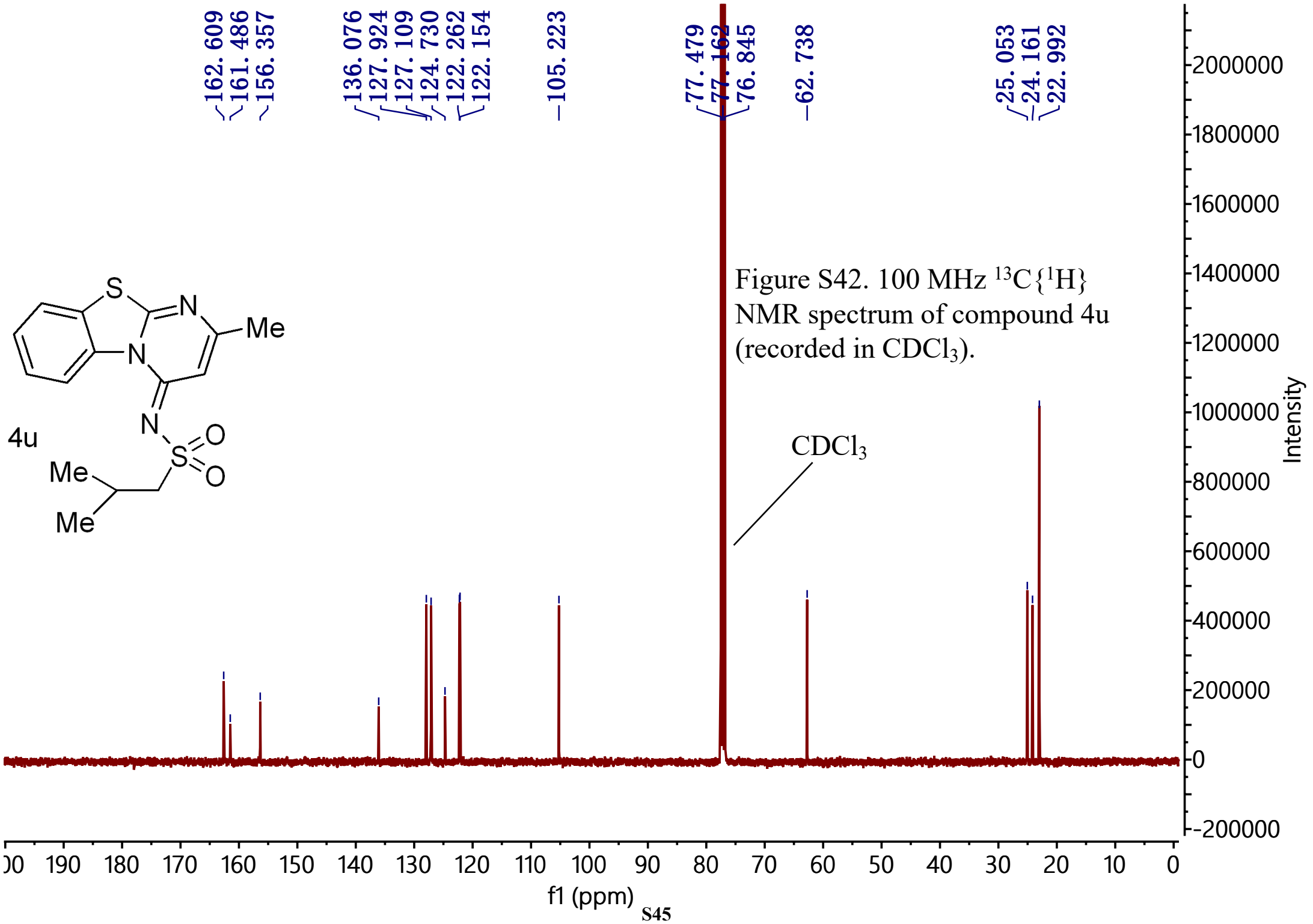


Figure S42. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4u (recorded in $CDCl_3$).

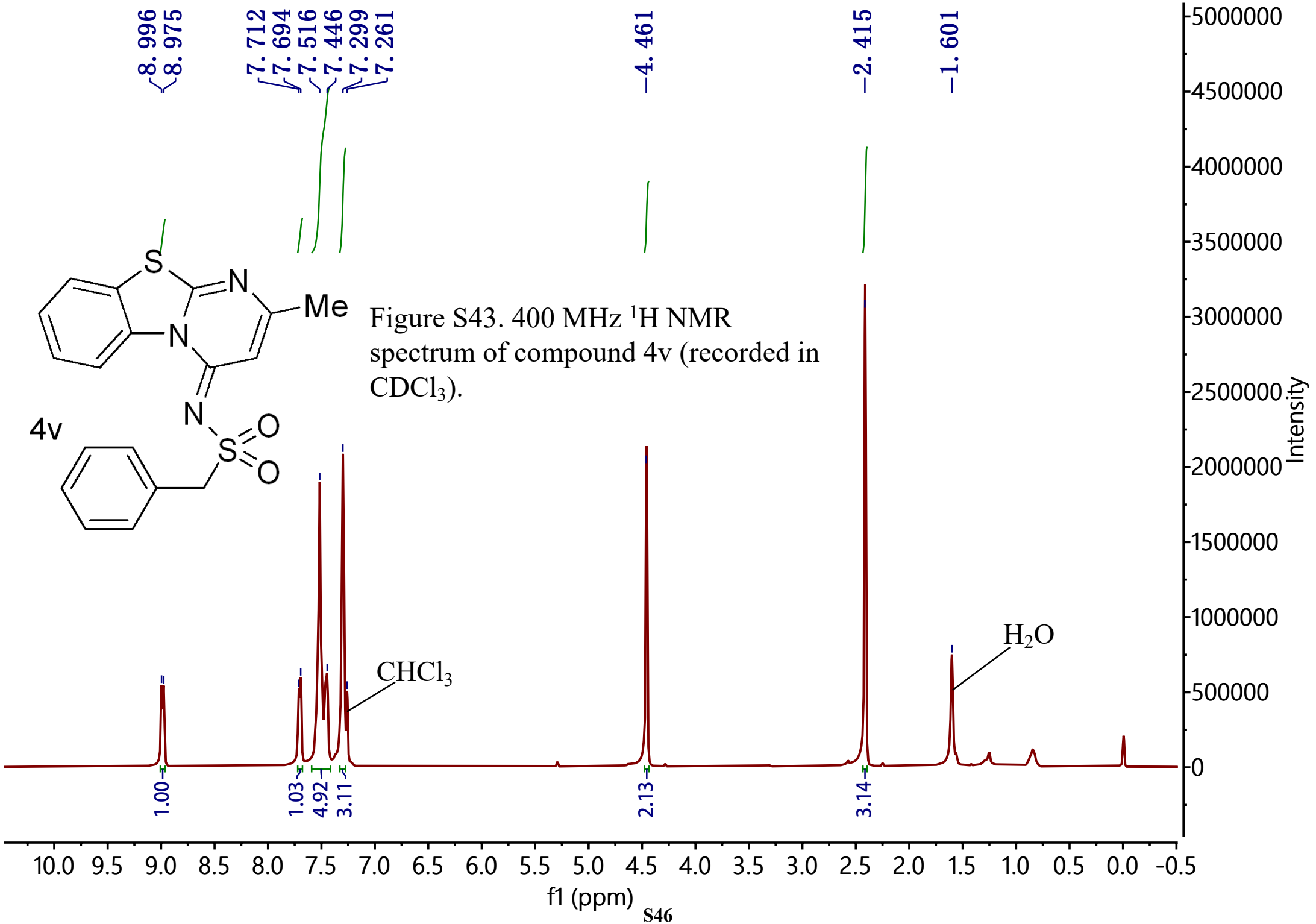


Figure S43. 400 MHz ^{1}H NMR spectrum of compound 4v (recorded in $CDCl_3$).

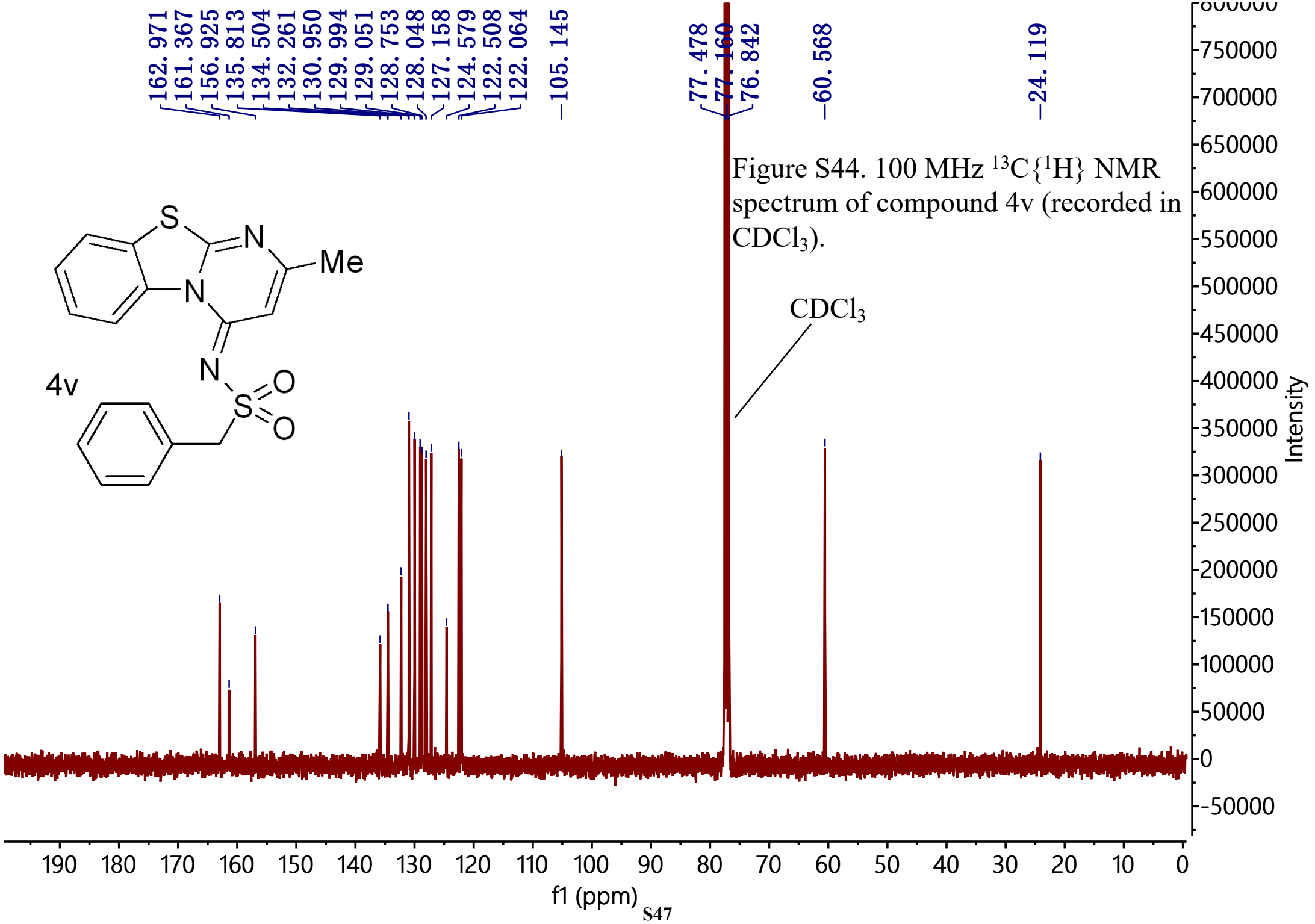


Figure S44. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4v (recorded in $CDCl_3$).

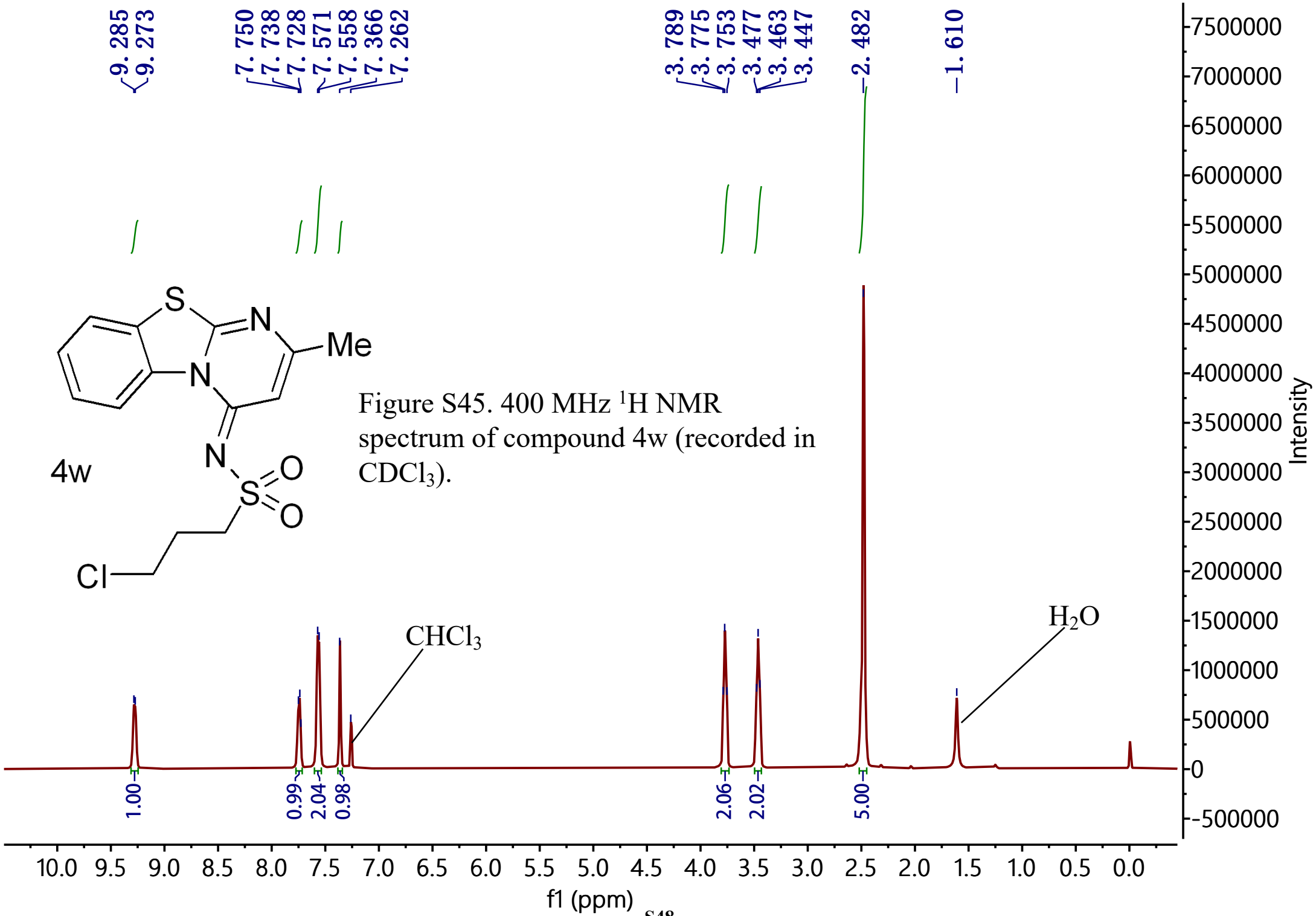


Figure S45. 400 MHz ^{1}H NMR spectrum of compound 4w (recorded in $CDCl_3$).

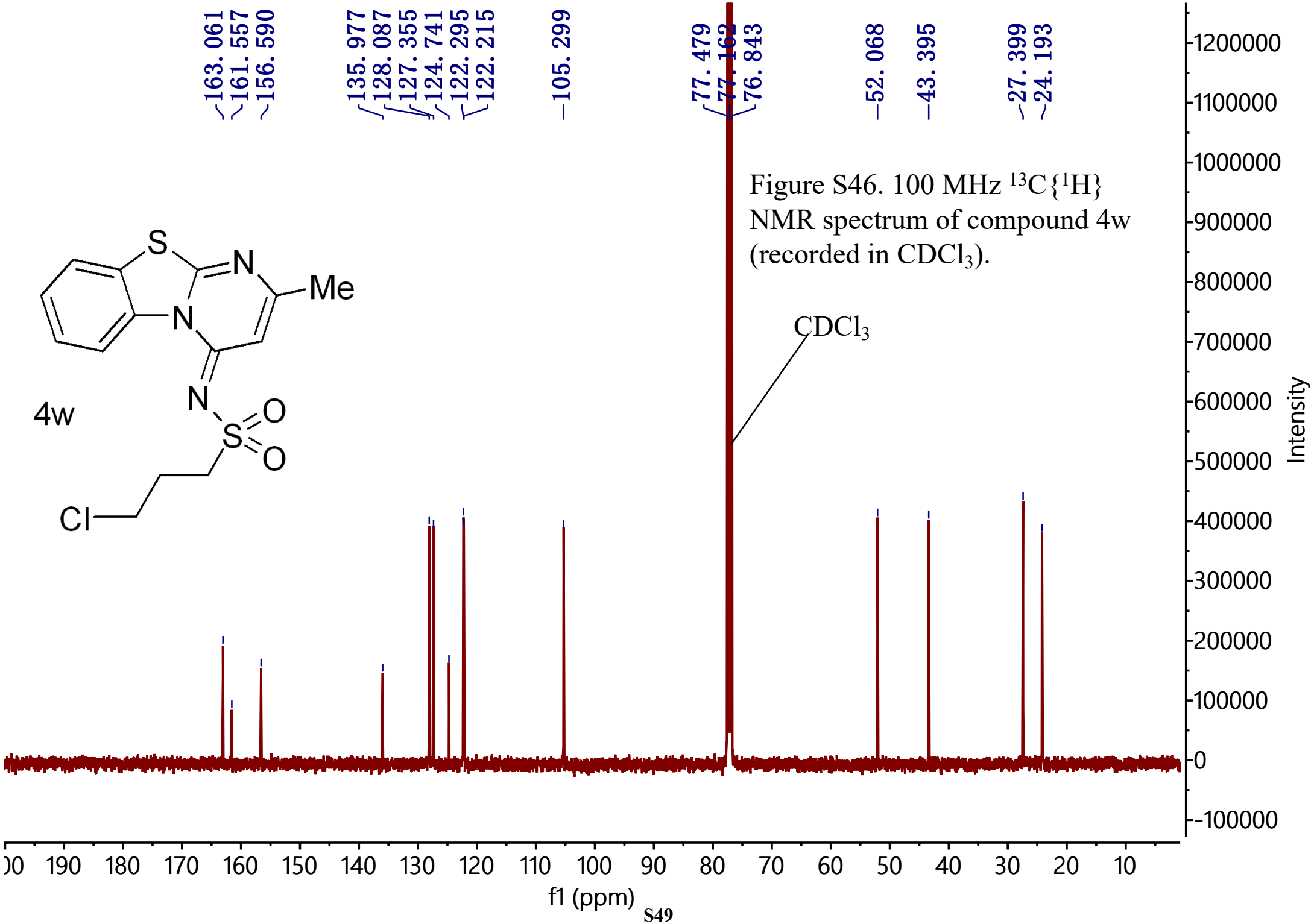


Figure S46. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4w (recorded in $CDCl_3$).

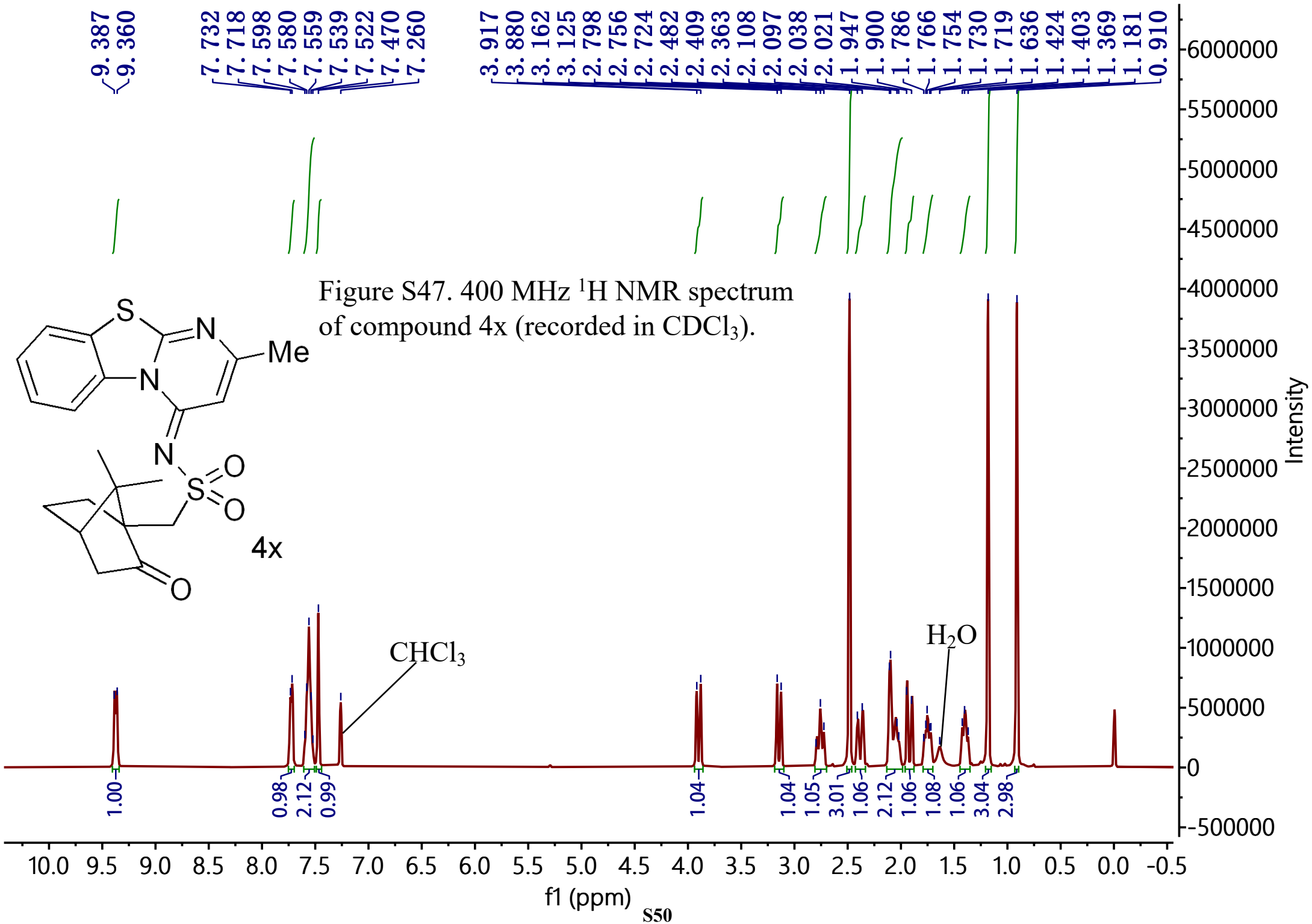


Figure S47. 400 MHz ^{1}H NMR spectrum of compound 4x (recorded in $CDCl_3$).

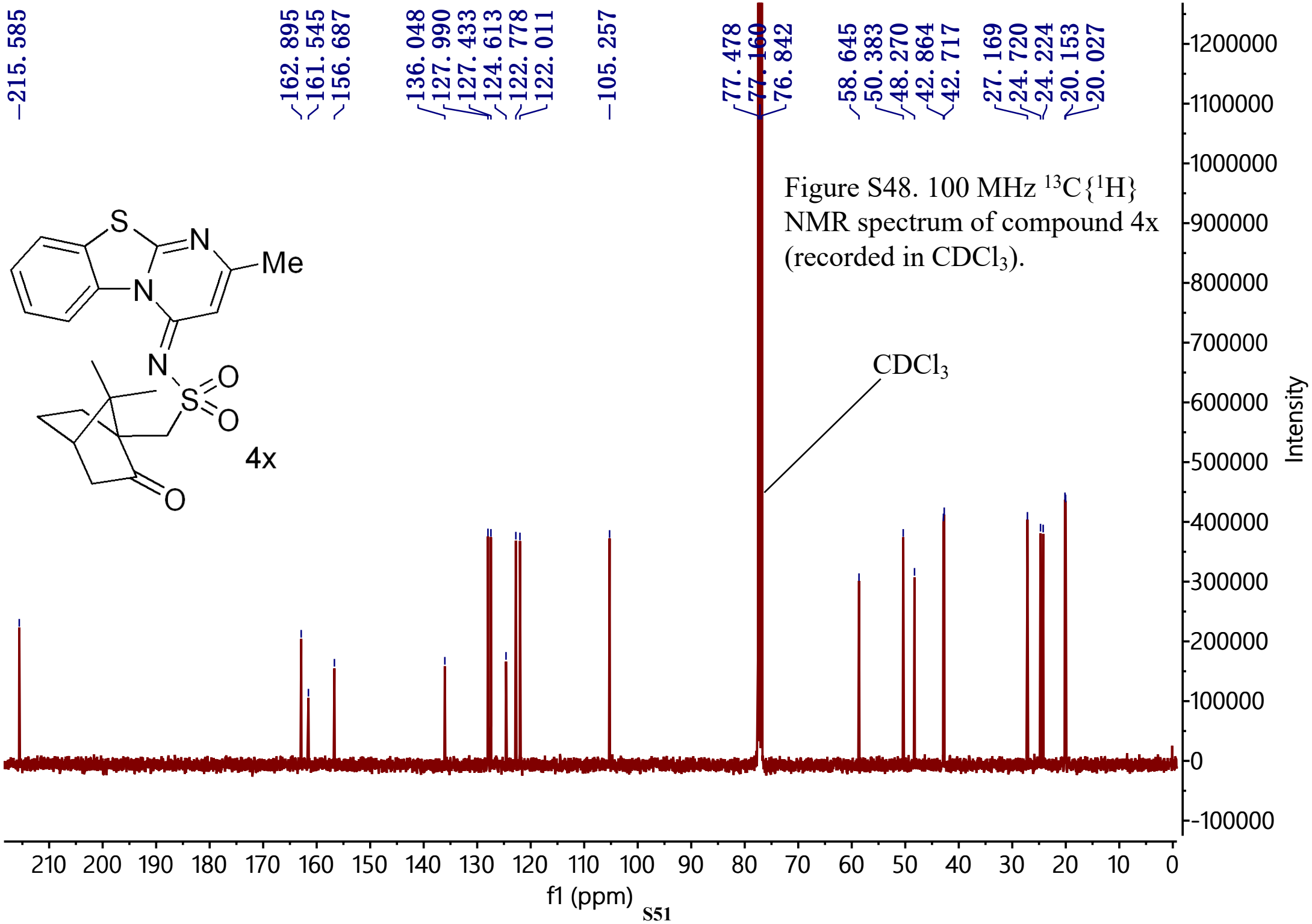


Figure S48. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4x (recorded in $CDCl_3$).

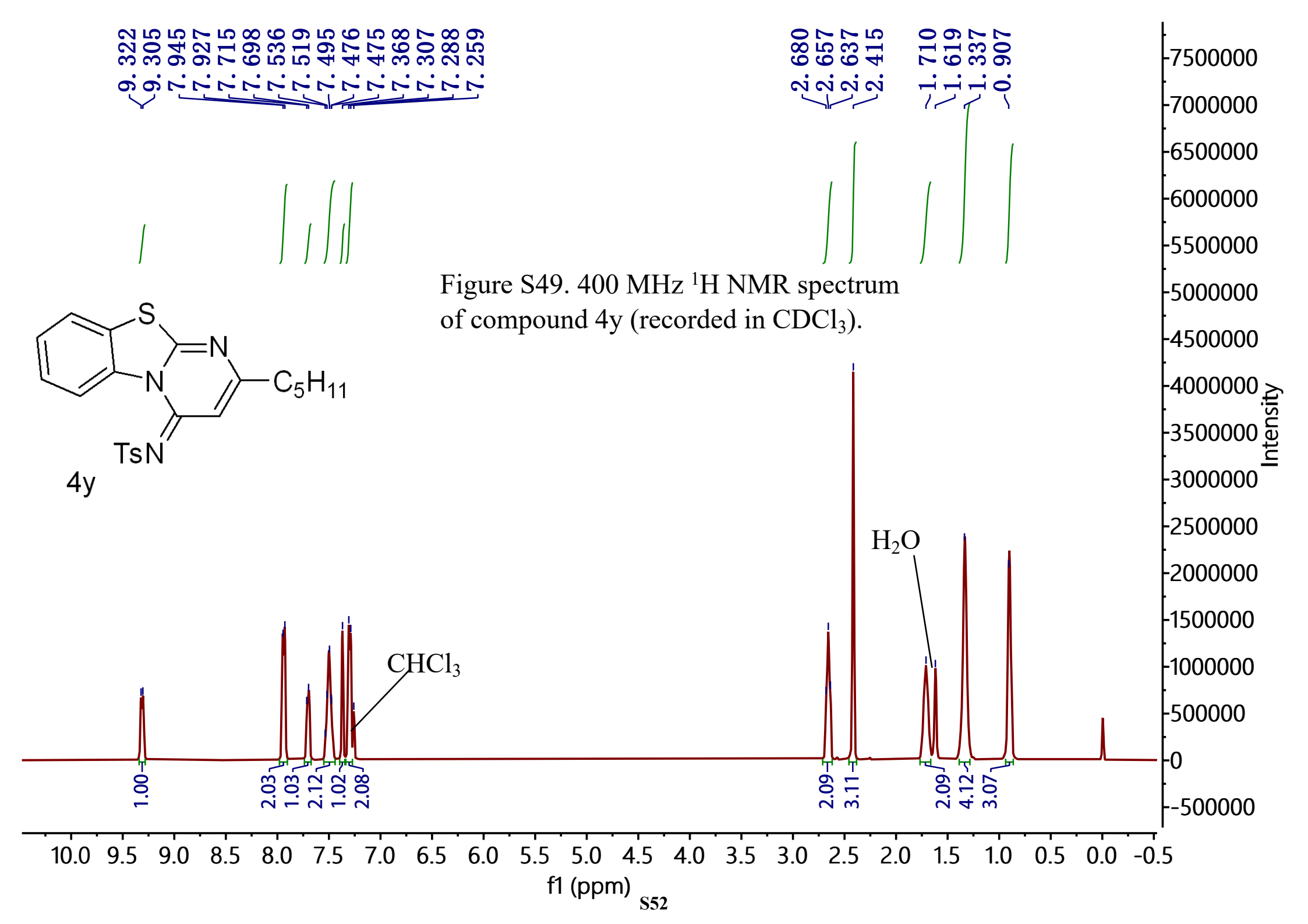


Figure S49. 400 MHz ^{1}H NMR spectrum of compound 4y (recorded in $CDCl_3$).

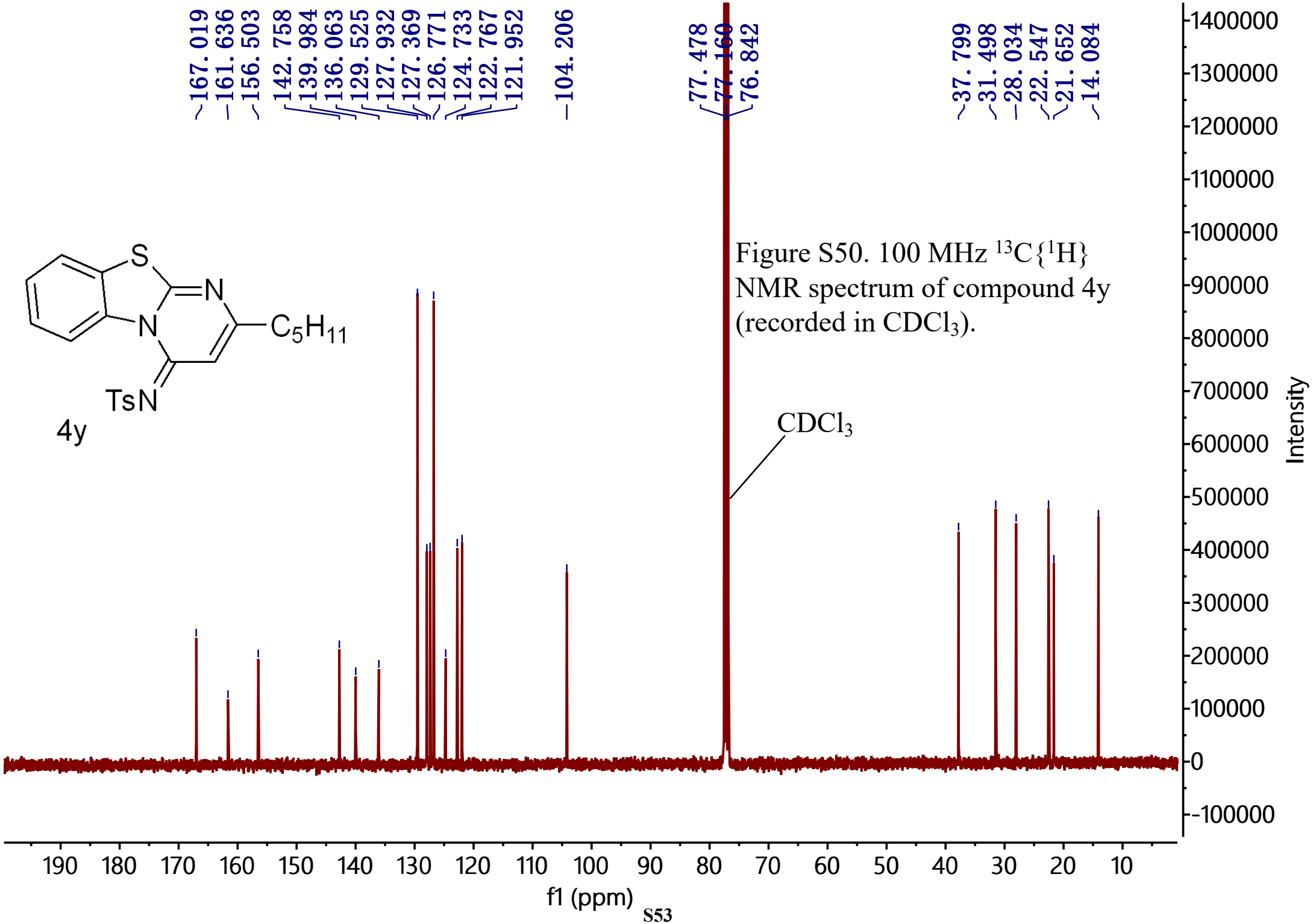


Figure S50. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4y (recorded in $CDCl_3$).

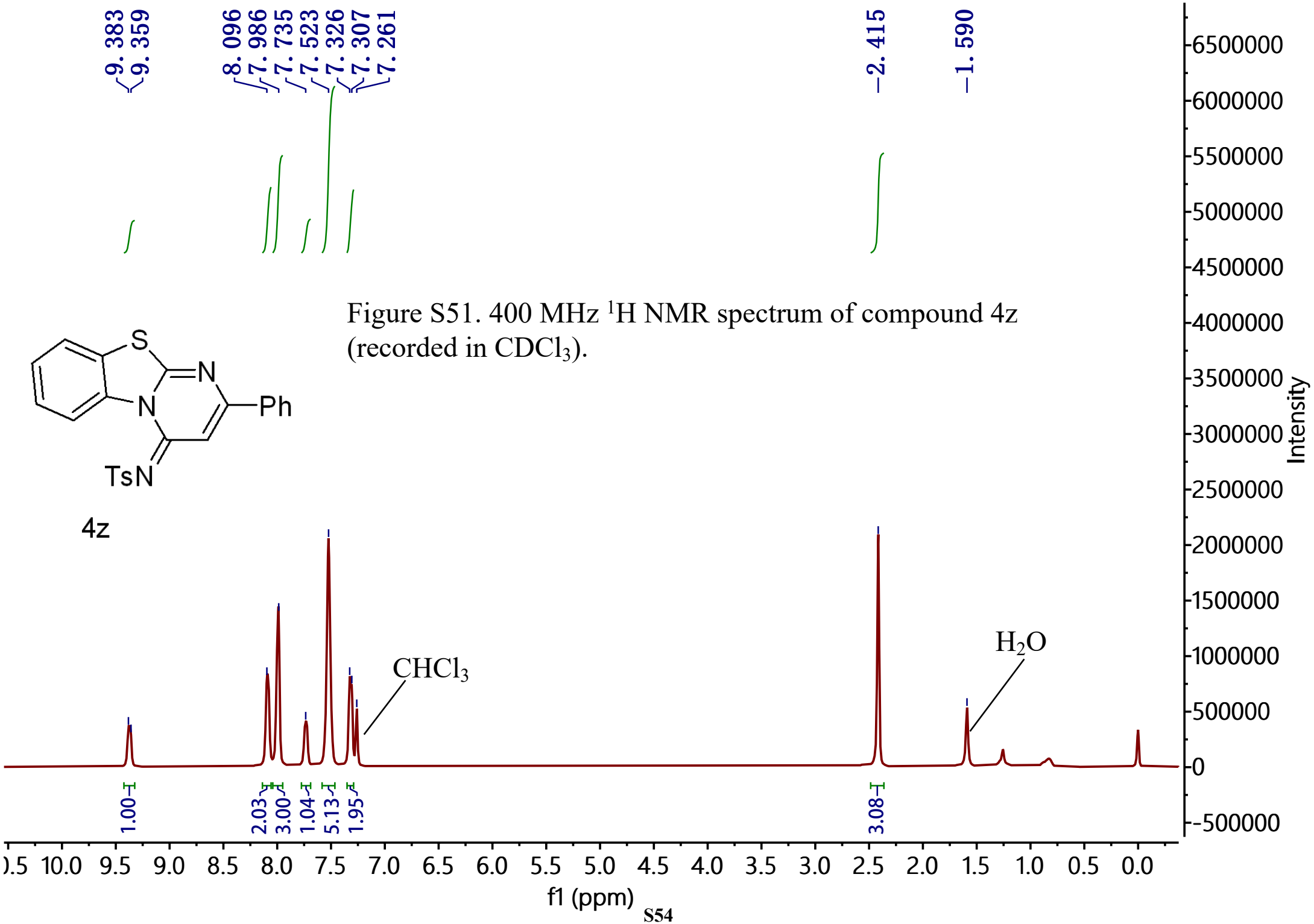


Figure S51. 400 MHz ^{1}H NMR spectrum of compound 4z (recorded in $CDCl_3$).

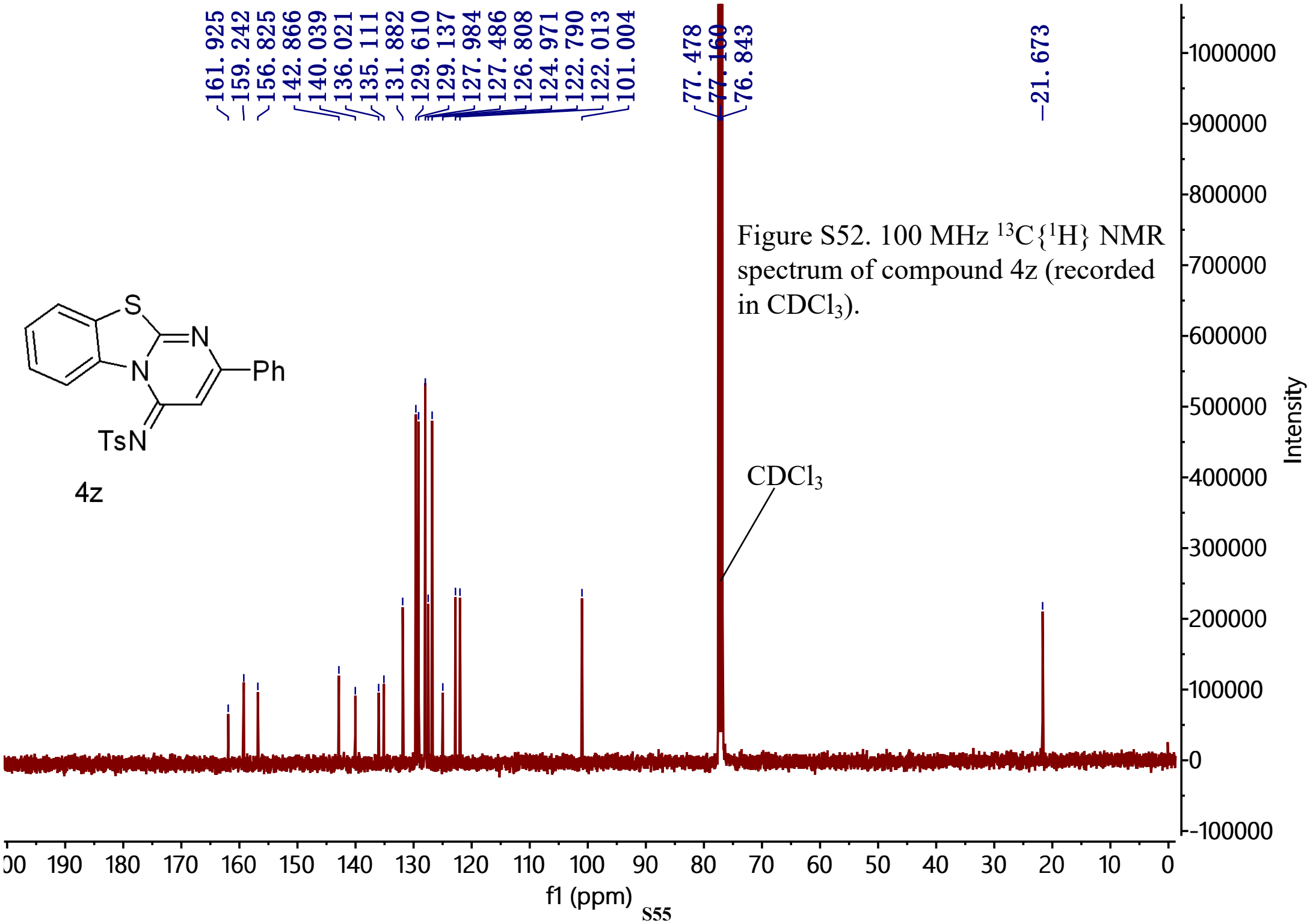


Figure S52. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 4z (recorded in $CDCl_3$).

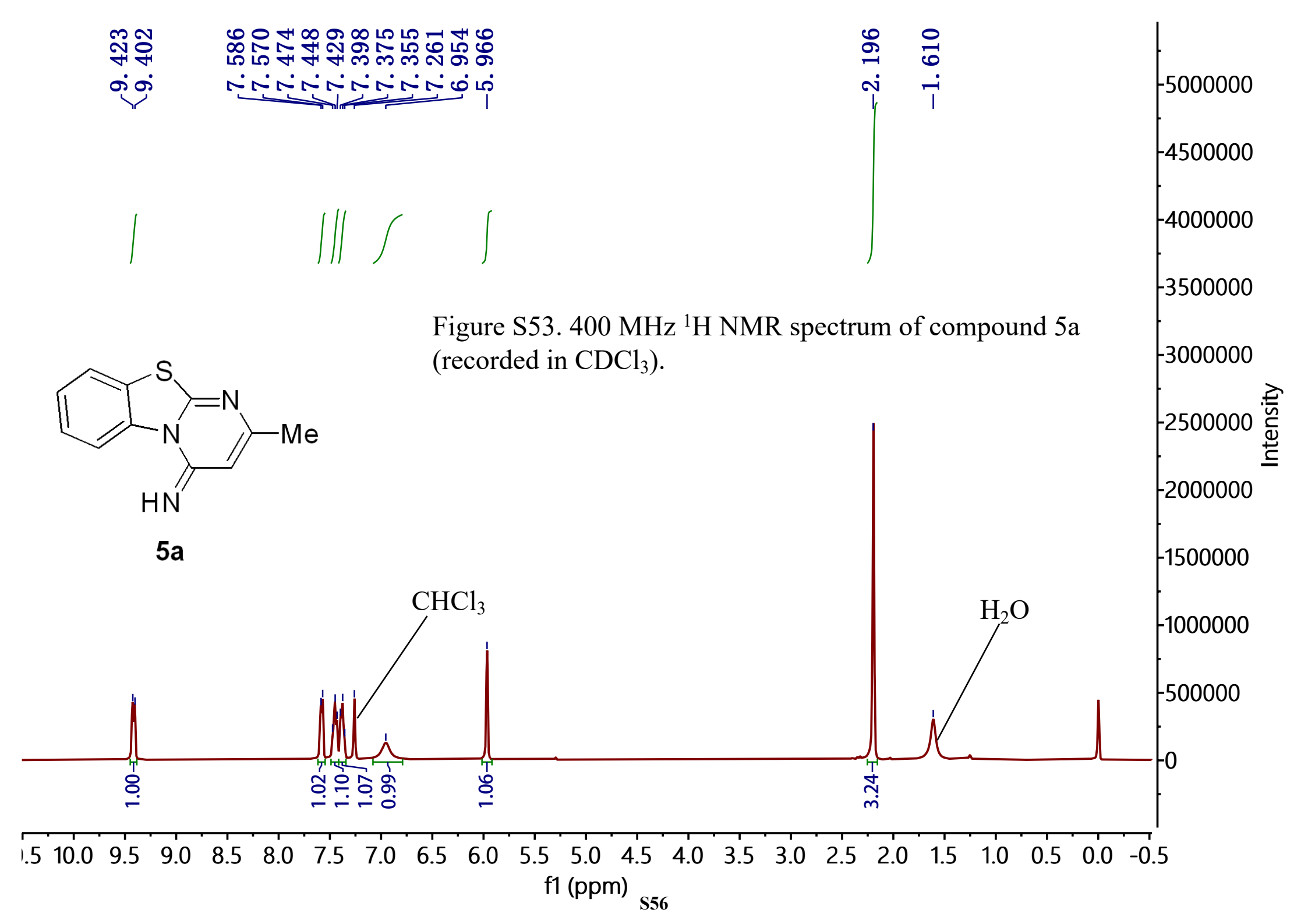


Figure S53. 400 MHz ^{1}H NMR spectrum of compound 5a (recorded in $CDCl_3$).

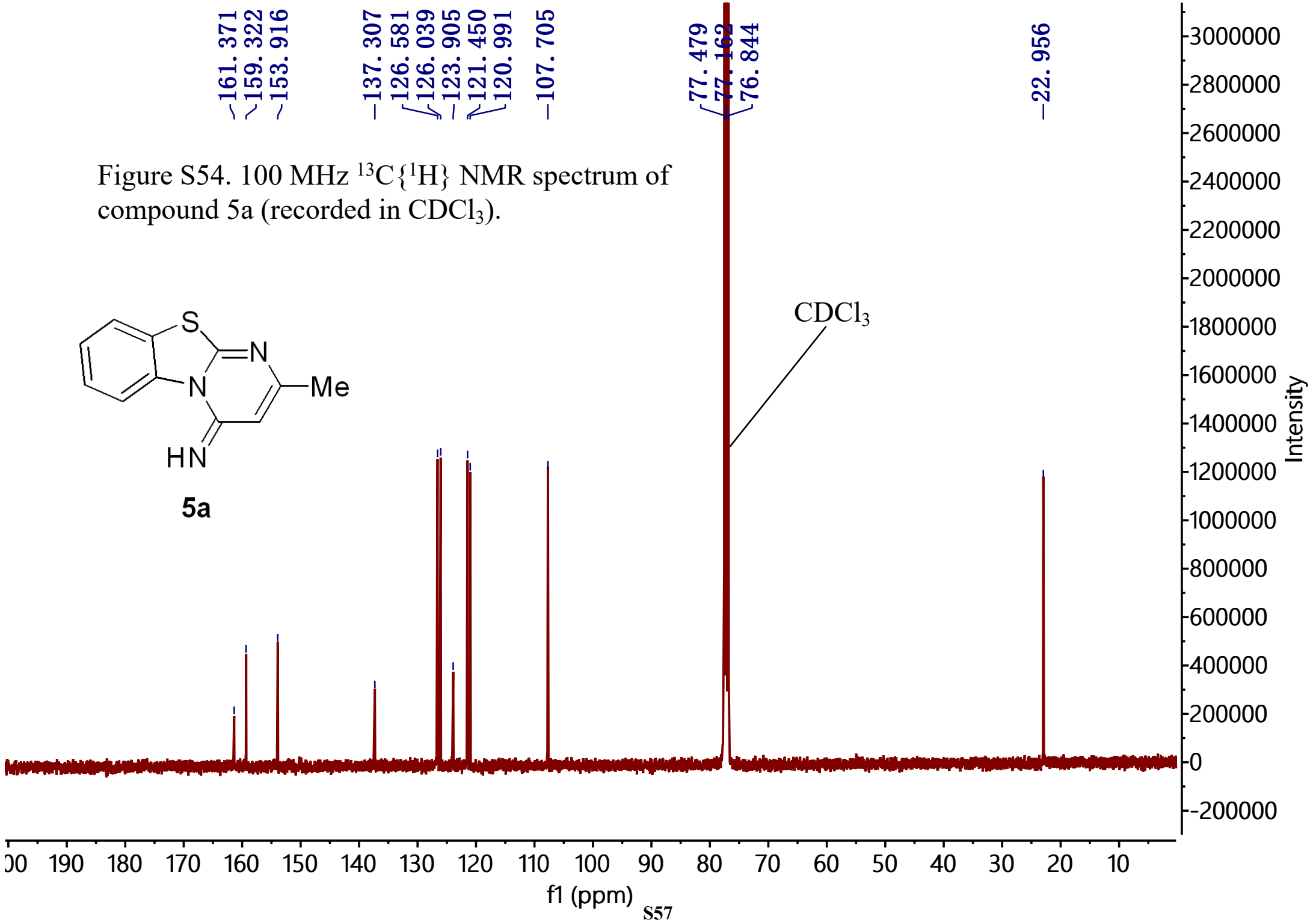


Figure S54. 100 MHz $^{13}C\{^{1}H\}$ NMR spectrum of compound 5a (recorded in $CDCl_3$).