

# **The indole motif is essential for the antitrypanosomal activity of N<sup>5</sup>-substituted paullones**

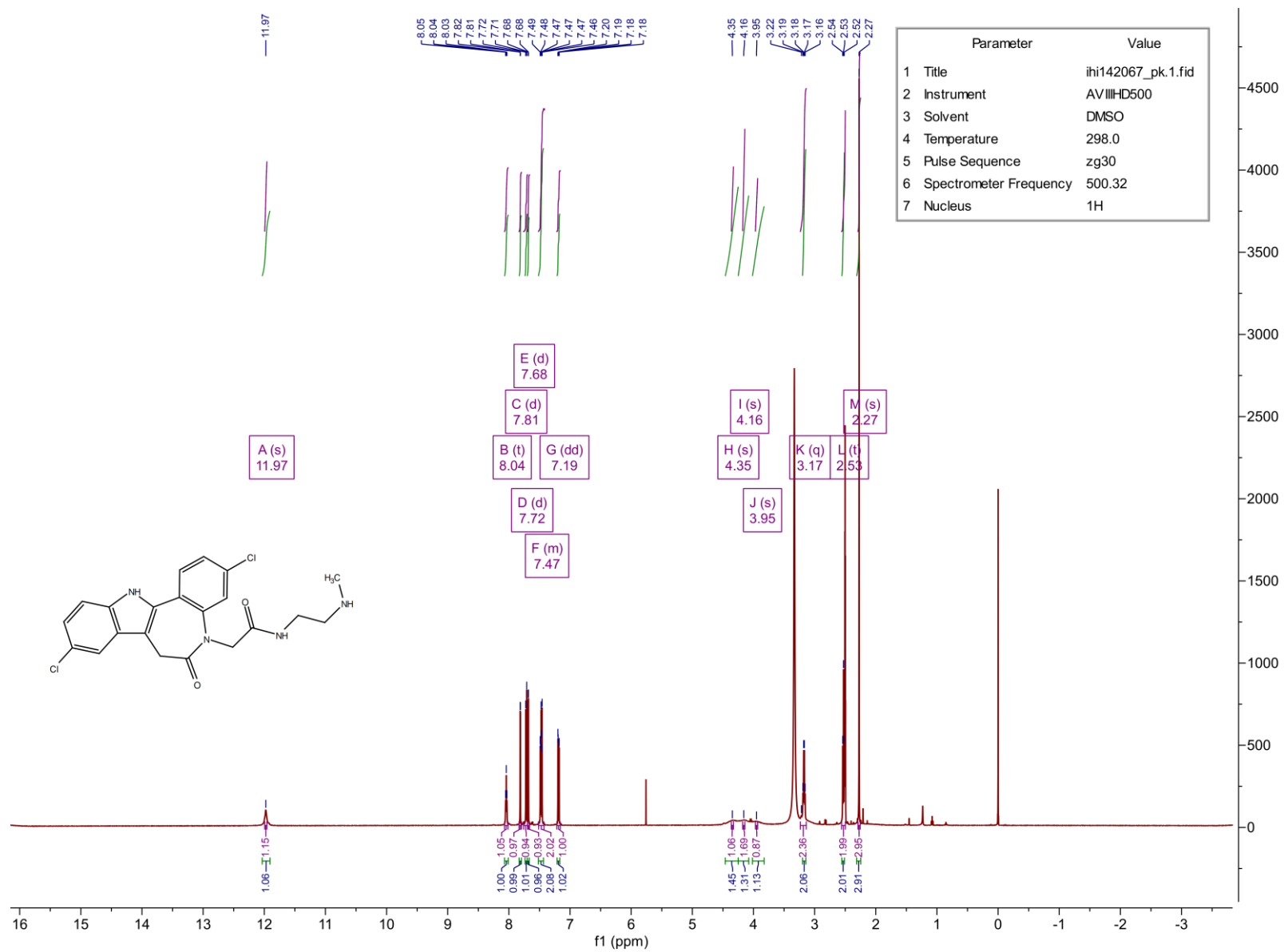
Irina Ihnatenko, Marco J. Müller, Oliver C. F. Orban, Jens C. Lindhof, Diego Benítez, Cecilia Ortíz, Estefanía Dibello, Leonardo L. Seidl, Marcelo A. Comini and Conrad Kunick\*

**S1 File. Figs 1–42. <sup>1</sup>H-NMR spectra of benzazepinones and paullones tested in biological assays.**

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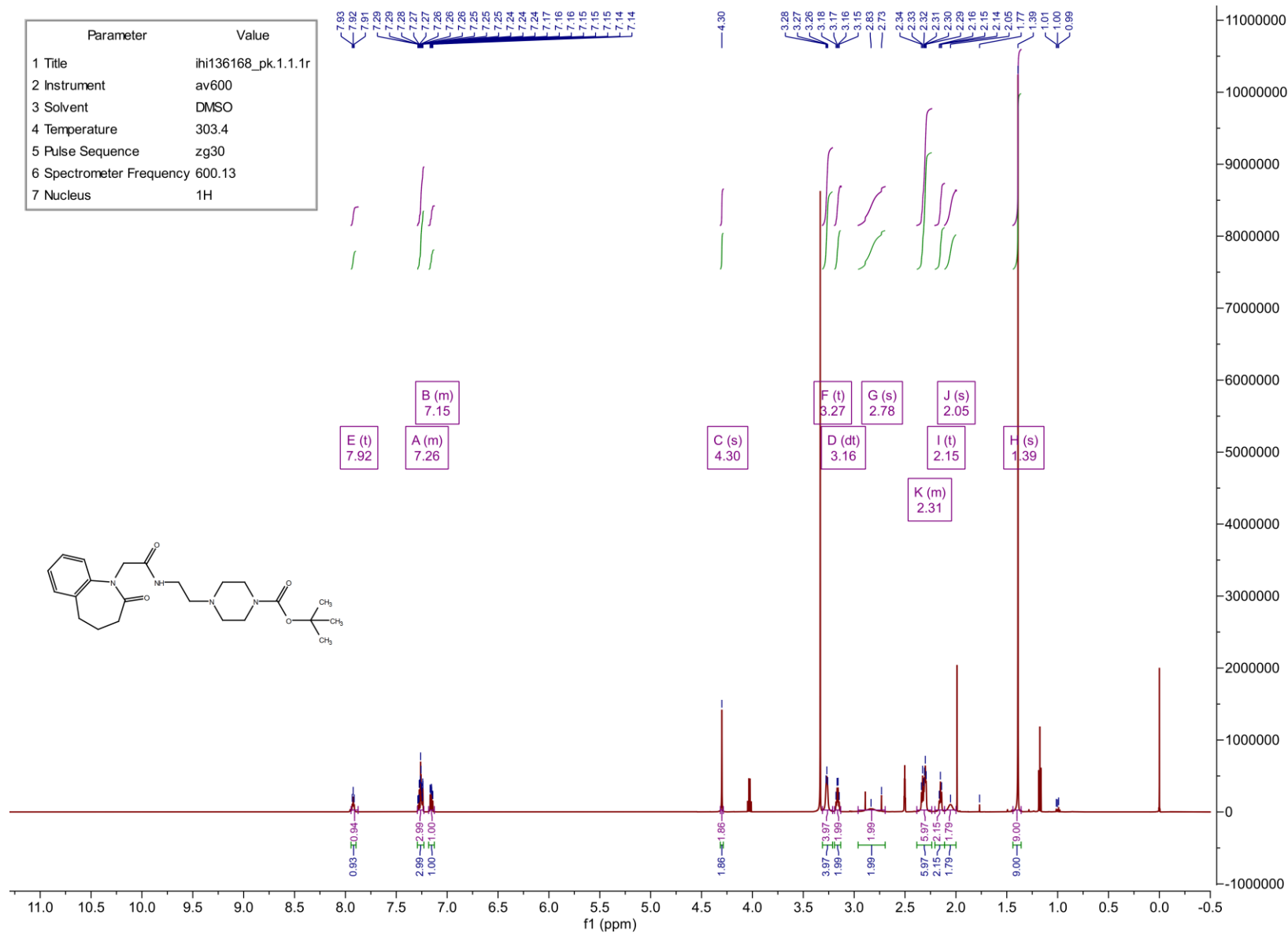
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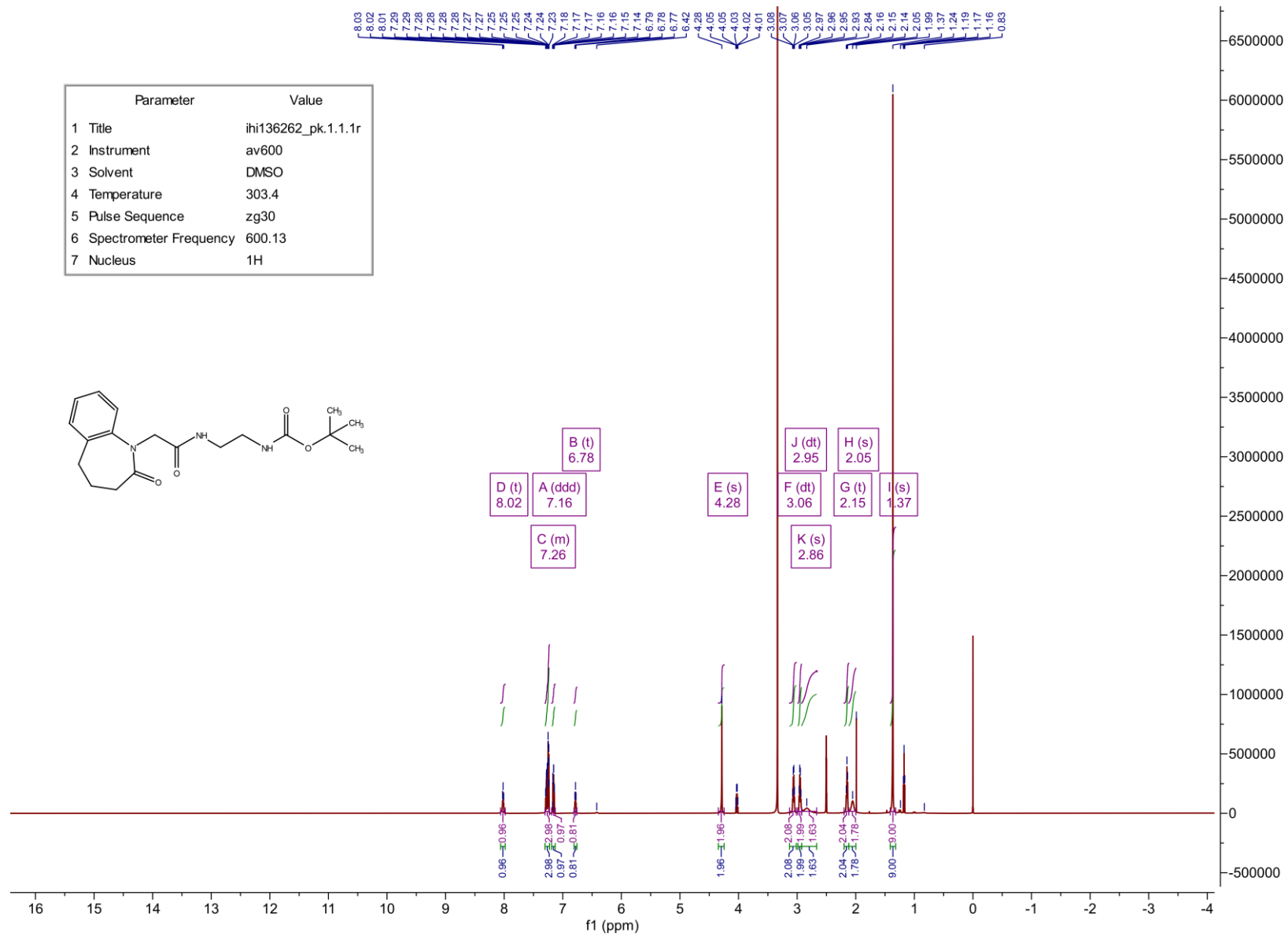


S1 File. Fig 2. <sup>1</sup>H-NMR spectrum of compound 1g.

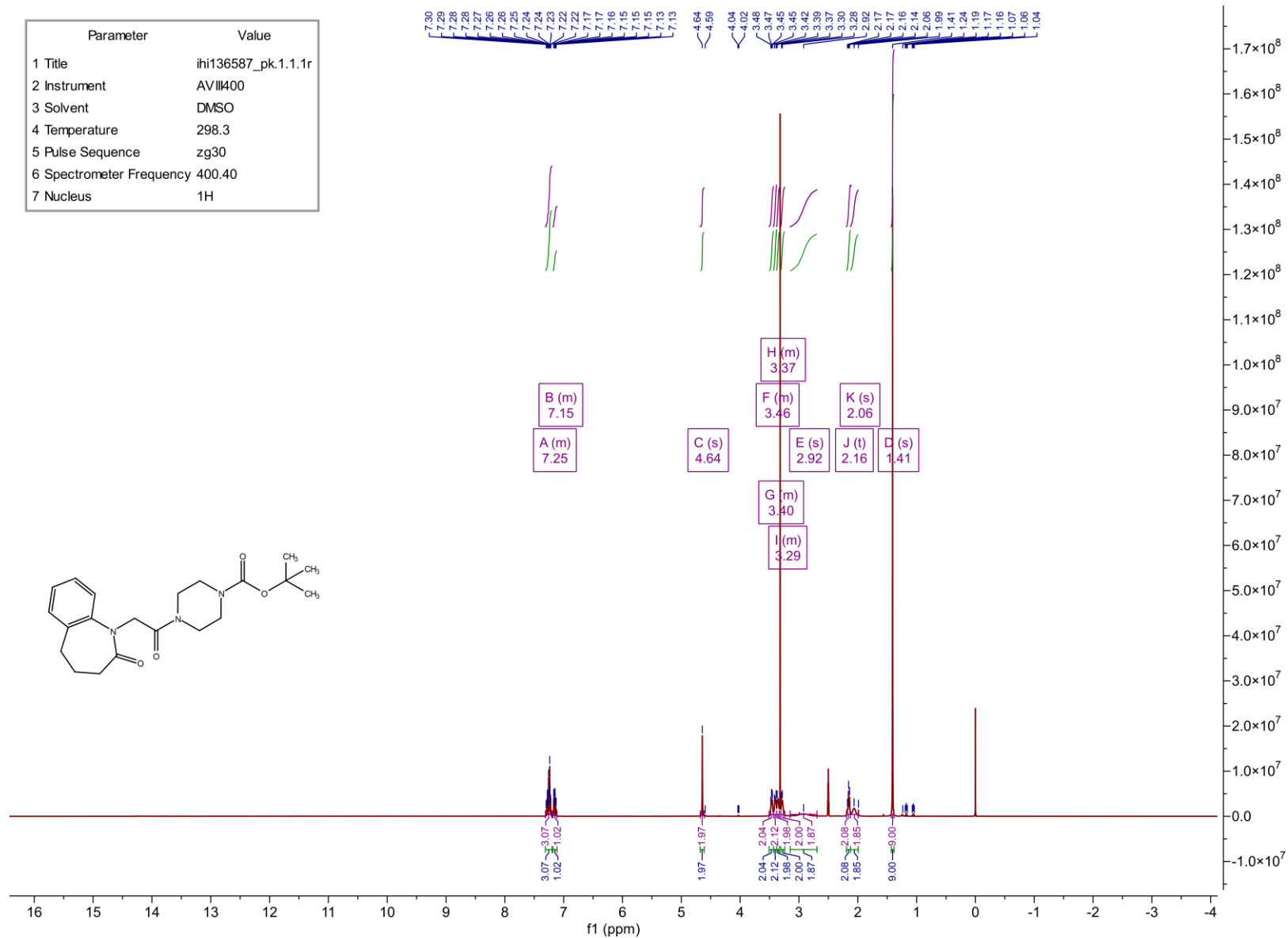




S1 File. Fig 4. <sup>1</sup>H-NMR spectrum of compound 2b.

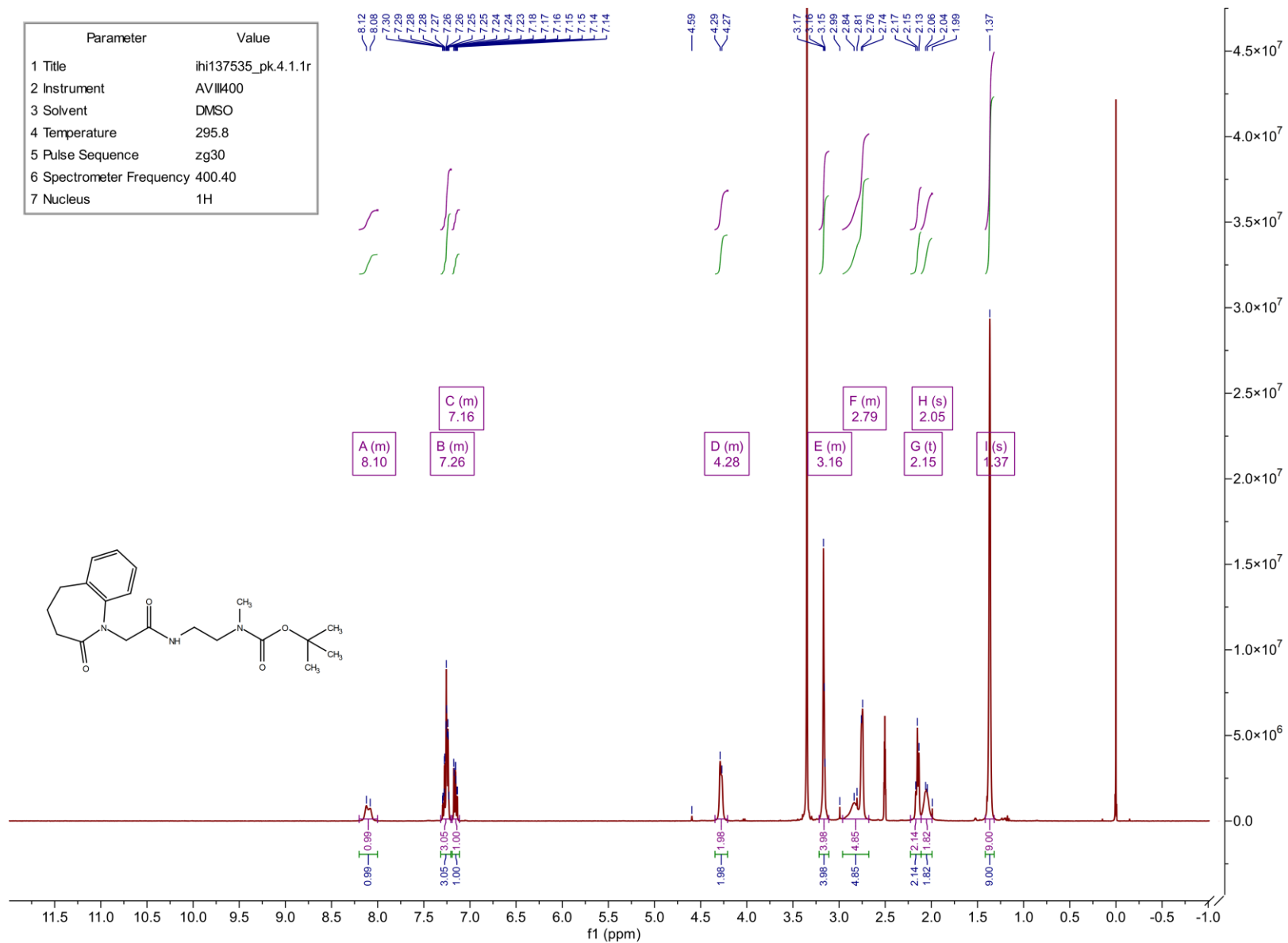


S1 File. Fig 5. <sup>1</sup>H-NMR spectrum of compound 2c.

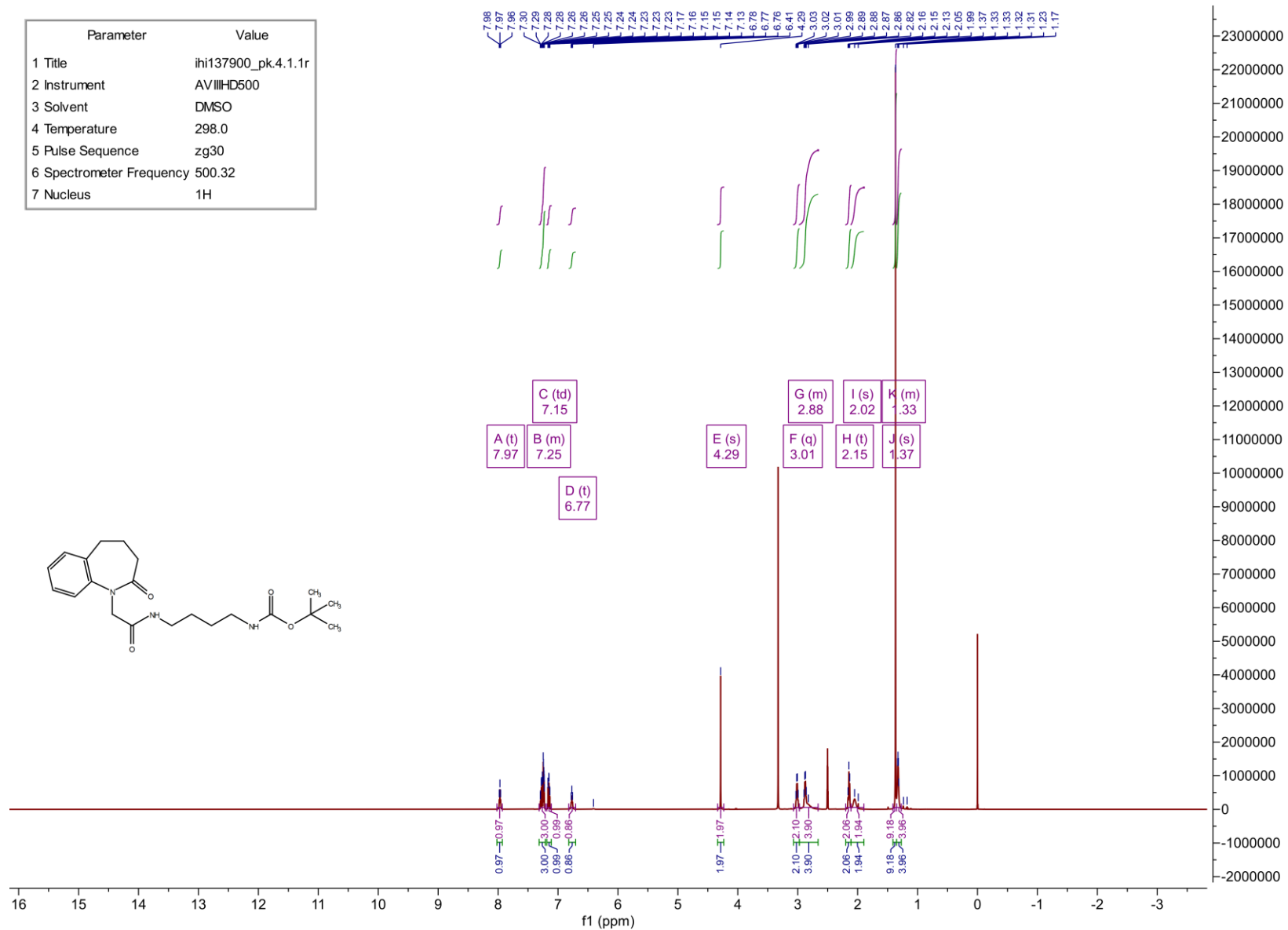


S1 File. Fig 6. <sup>1</sup>H-NMR spectrum of compound 2d.

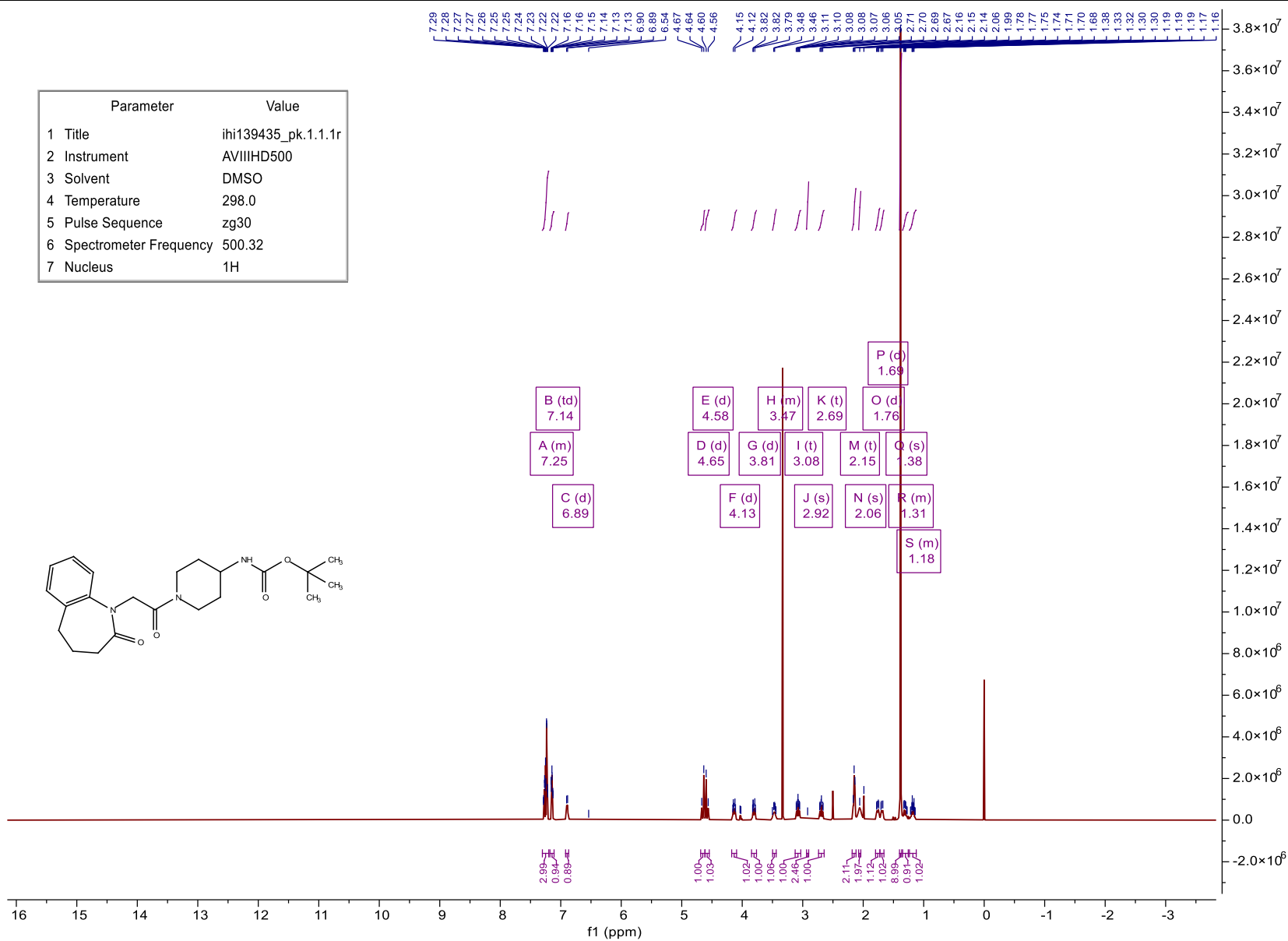




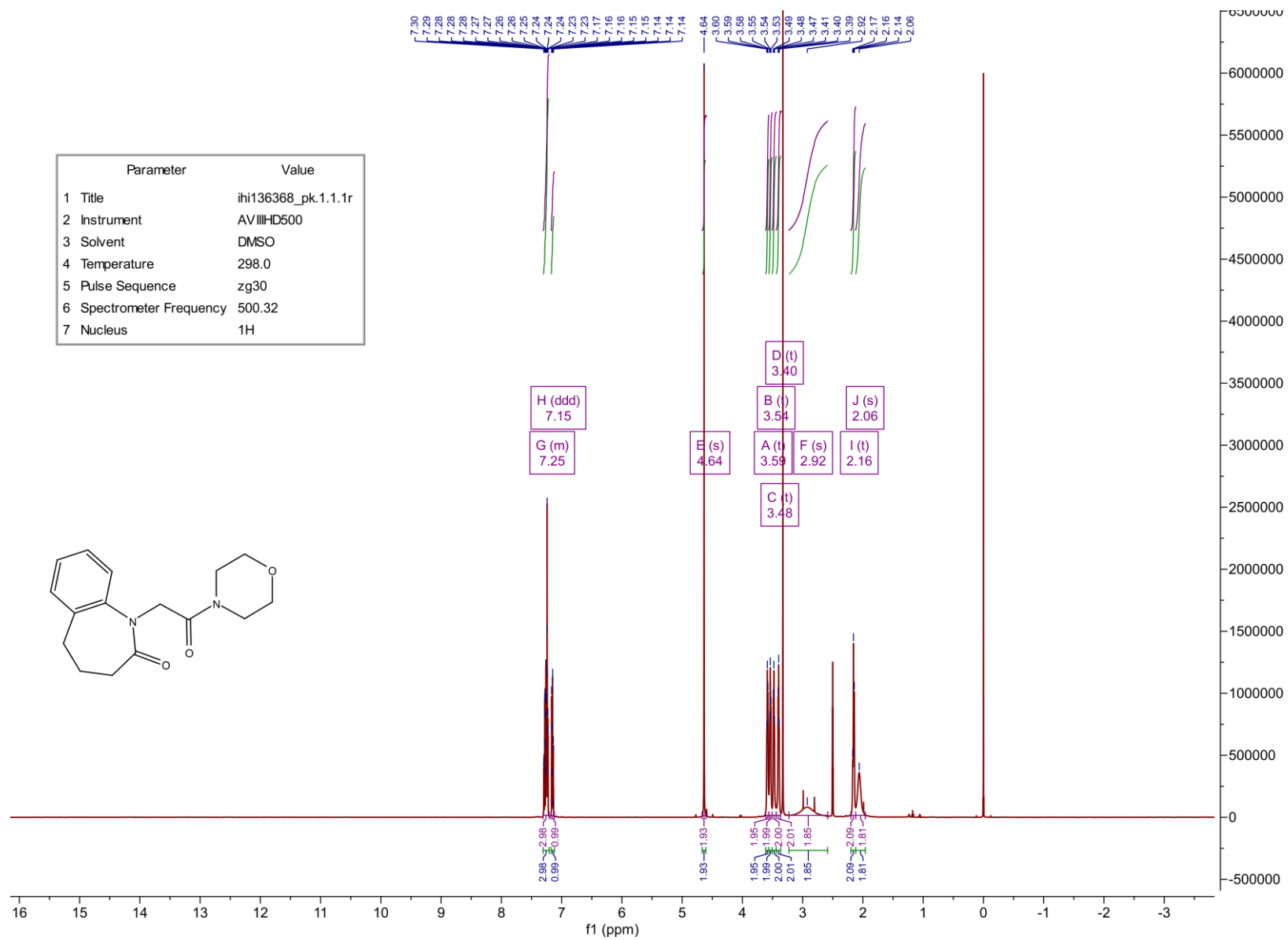
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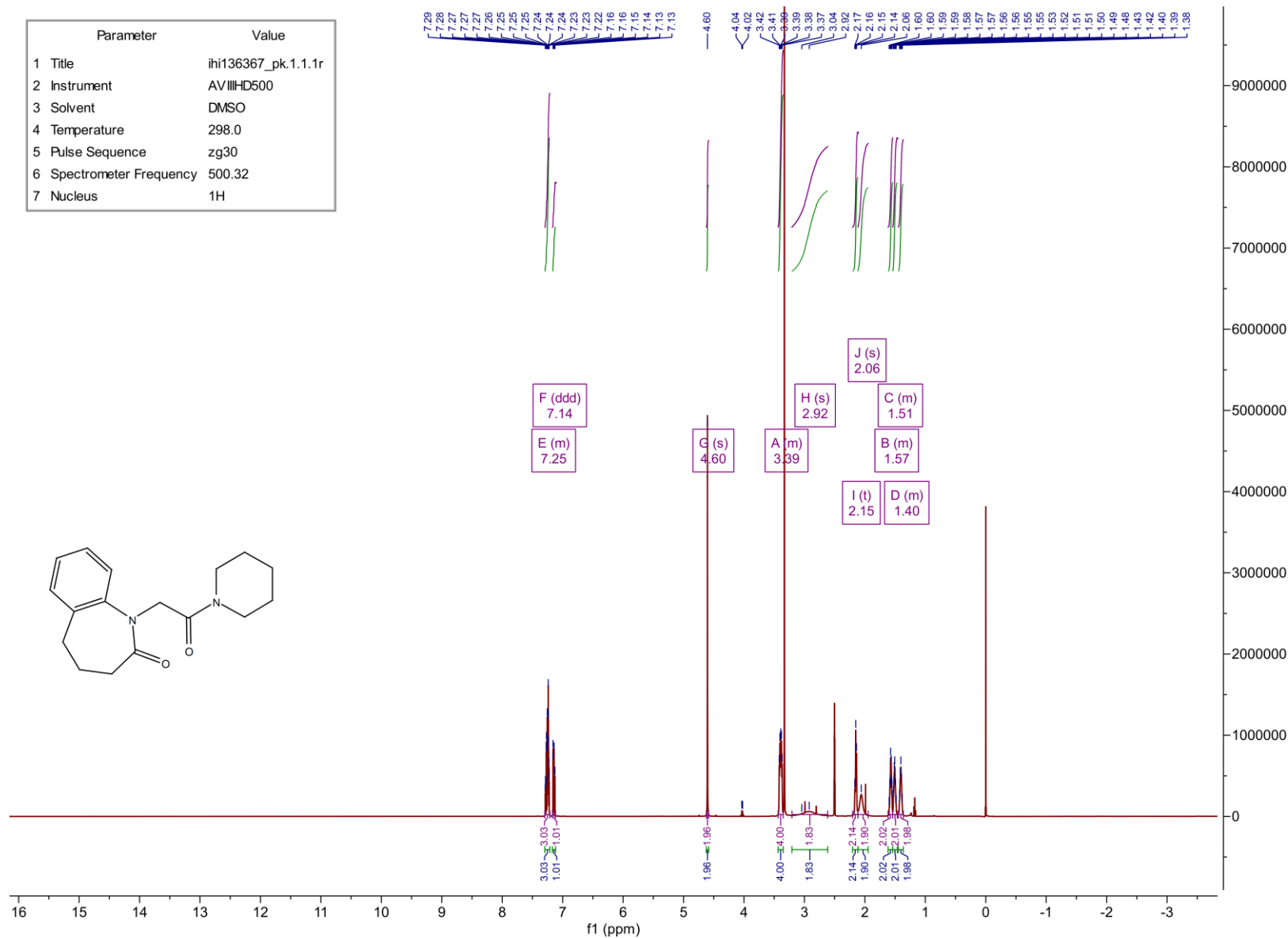
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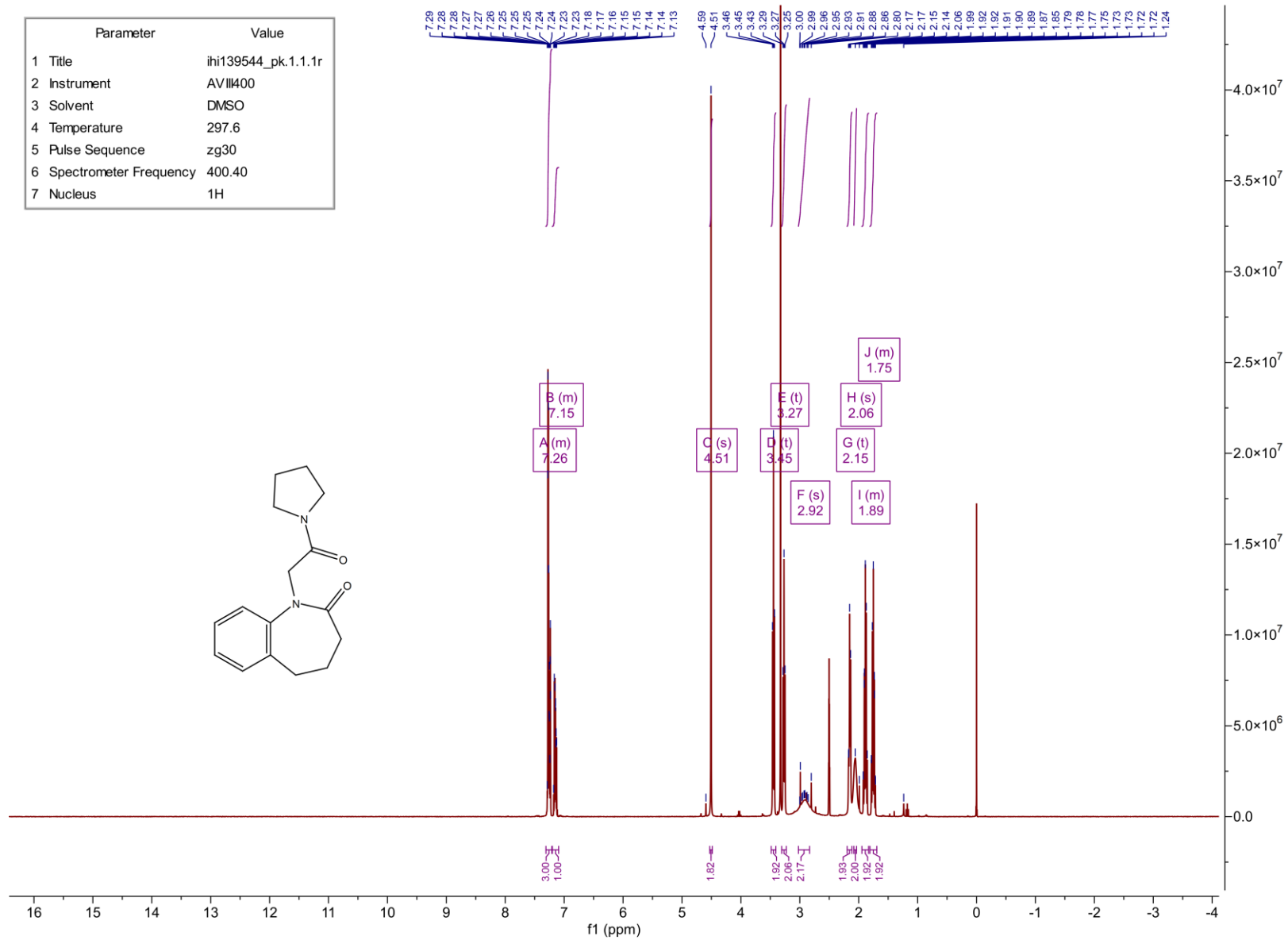
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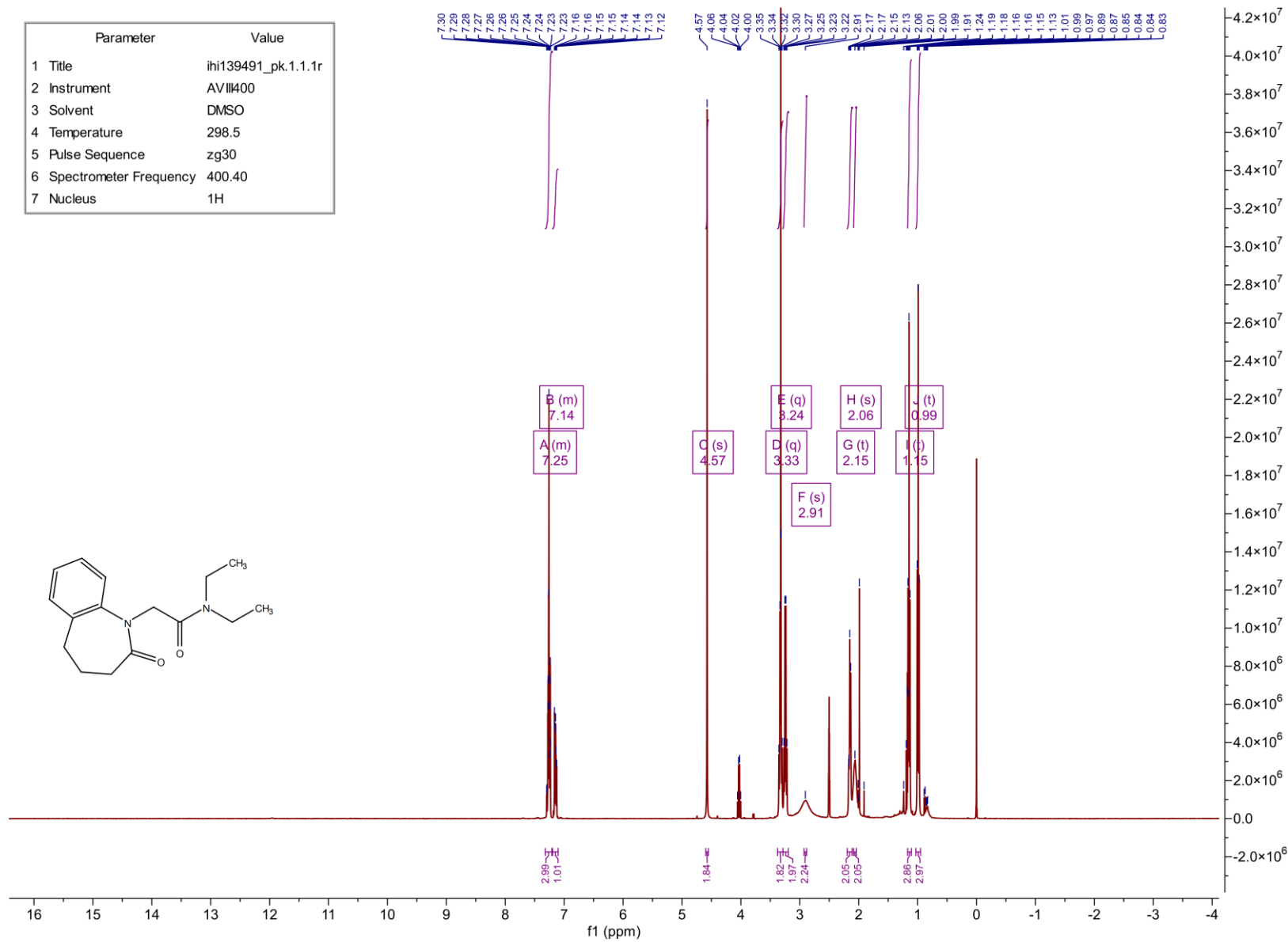


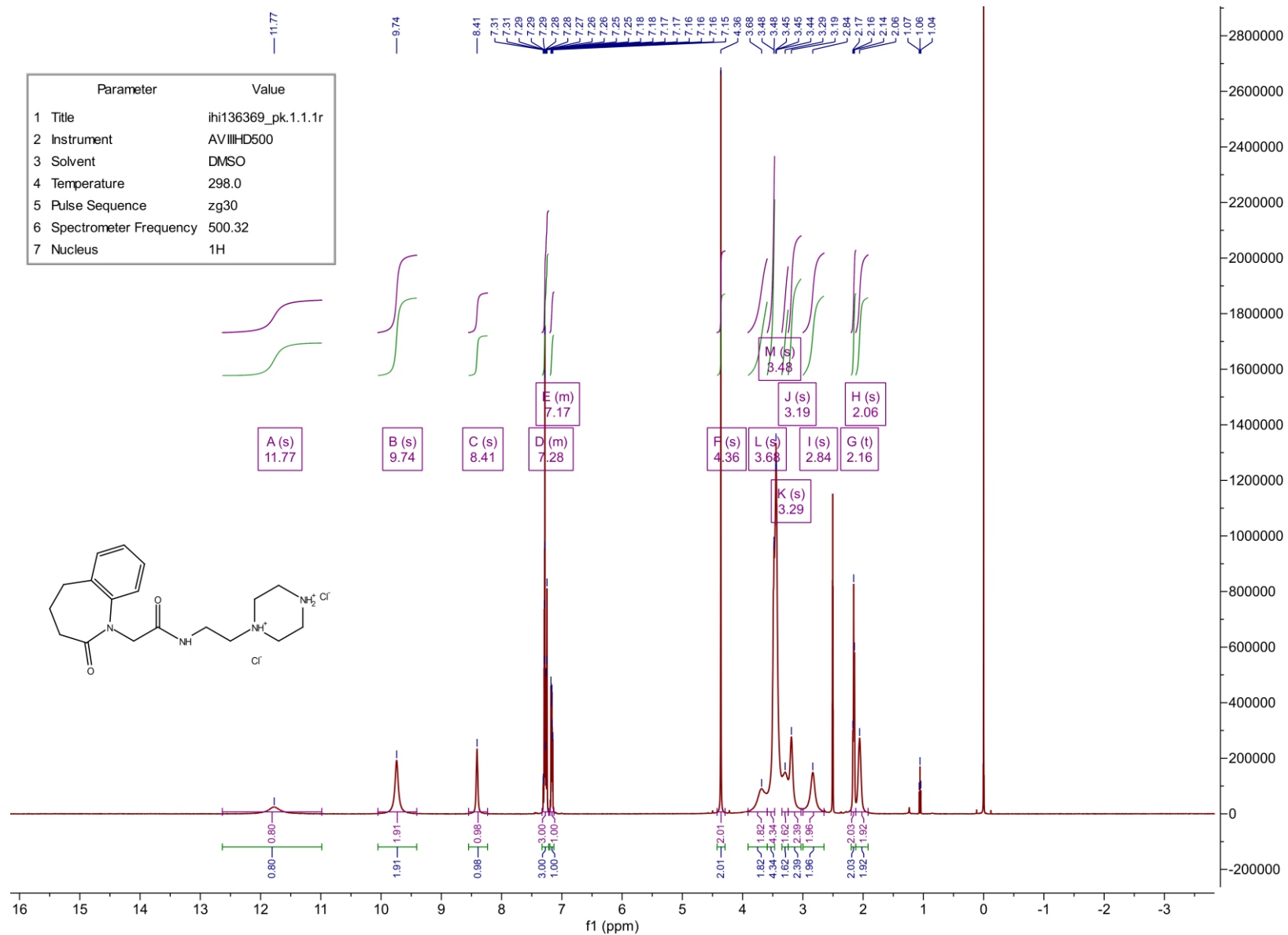
S1 File. Fig 10. <sup>1</sup>H-NMR spectrum of compound 2h.



S1 File. Fig 11. <sup>1</sup>H-NMR spectrum of compound 2i.

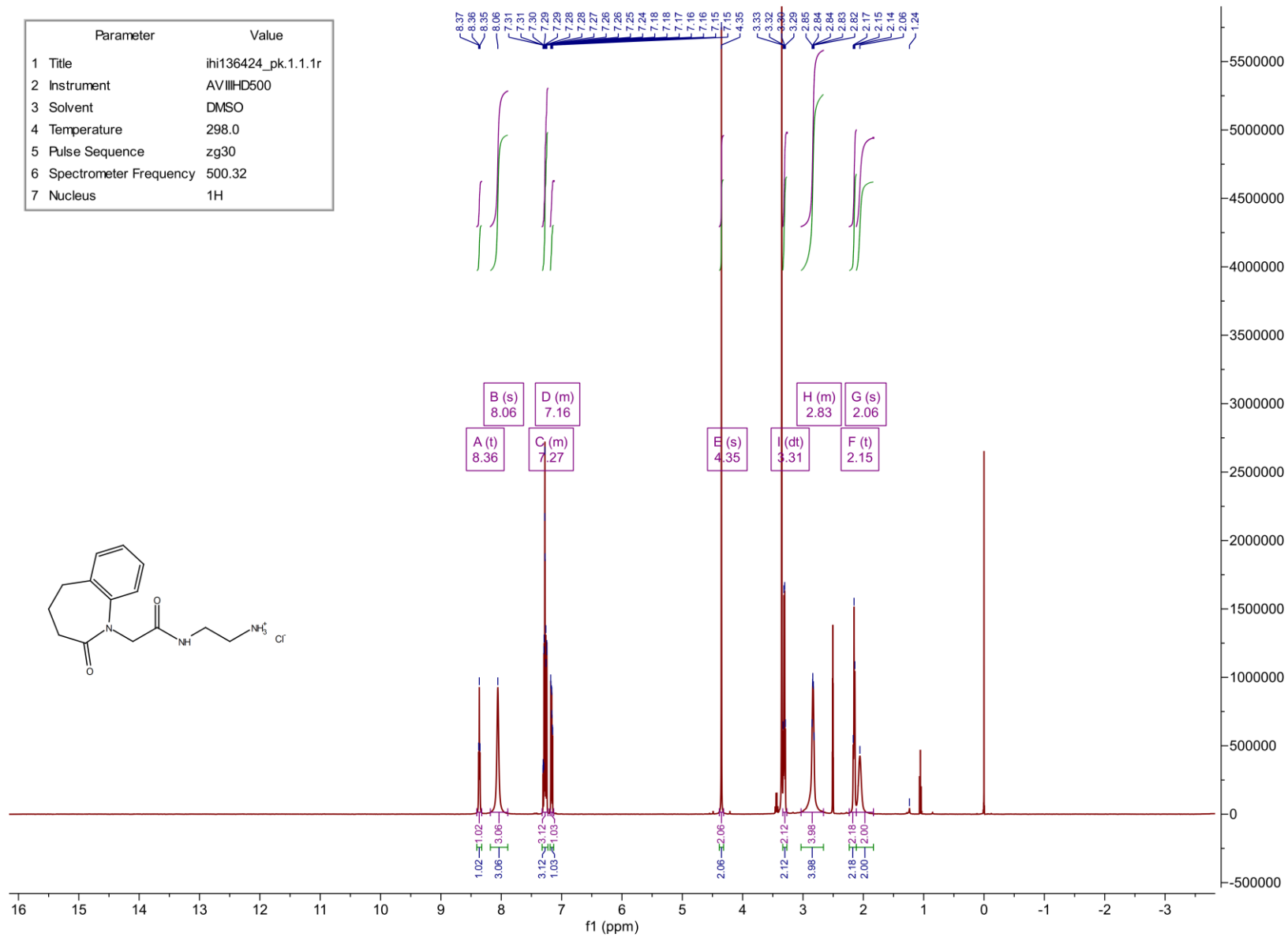
S1 File. Fig 12. <sup>1</sup>H-NMR spectrum of compound 2j.

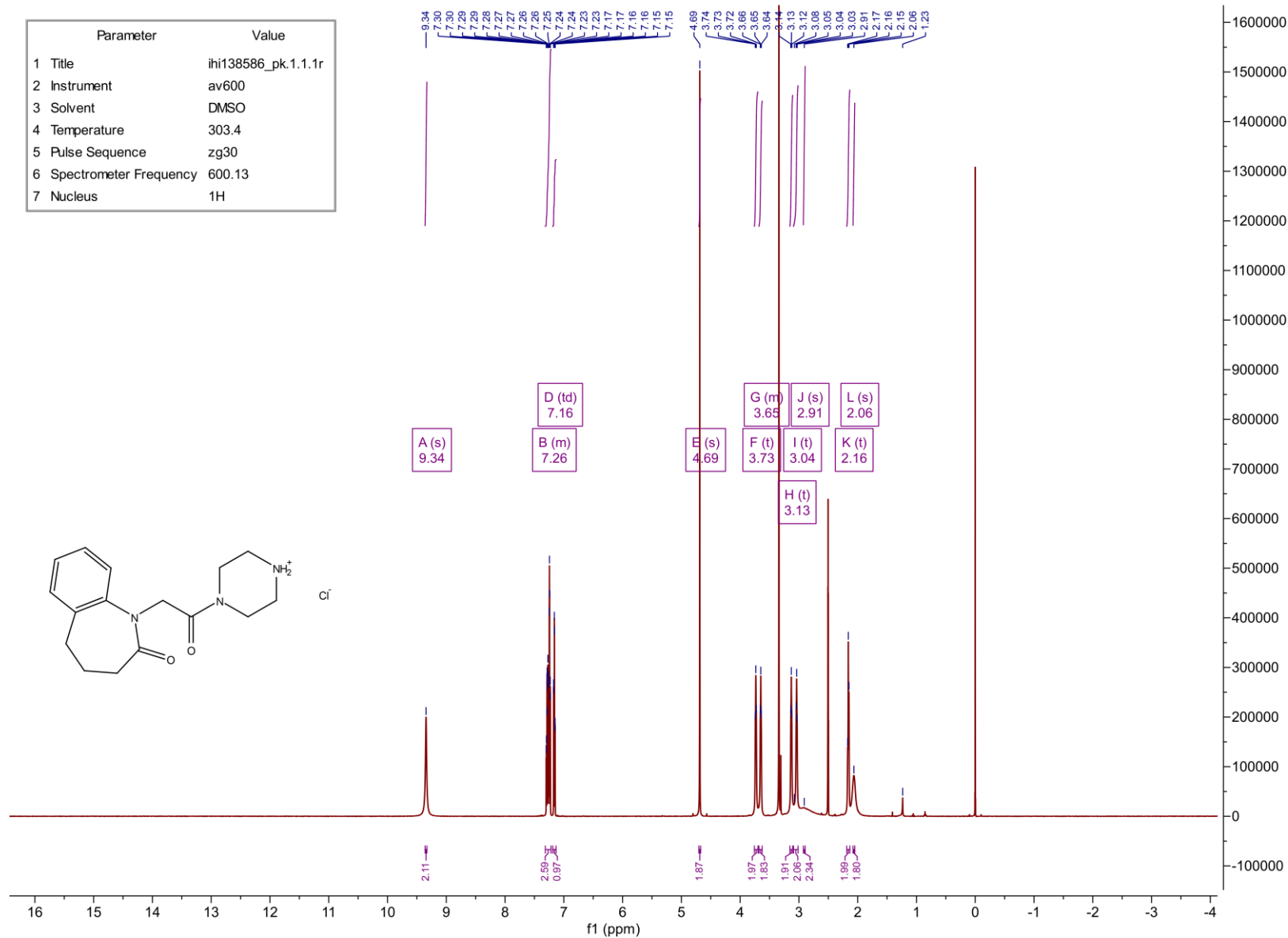
S1 File. Fig 13. <sup>1</sup>H-NMR spectrum of compound 2k.



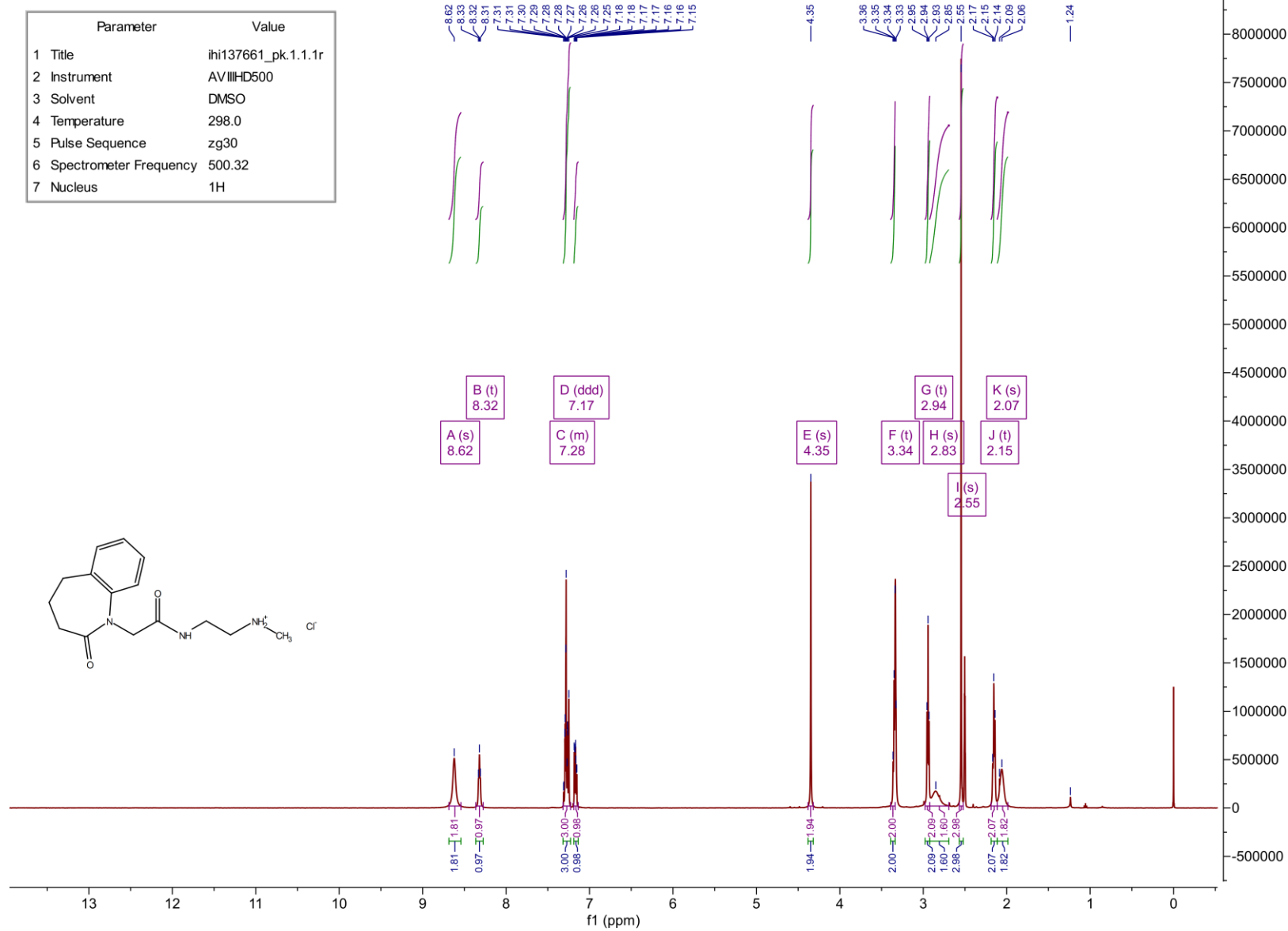
S1 File. Fig 14. <sup>1</sup>H-NMR spectrum of compound 2o.

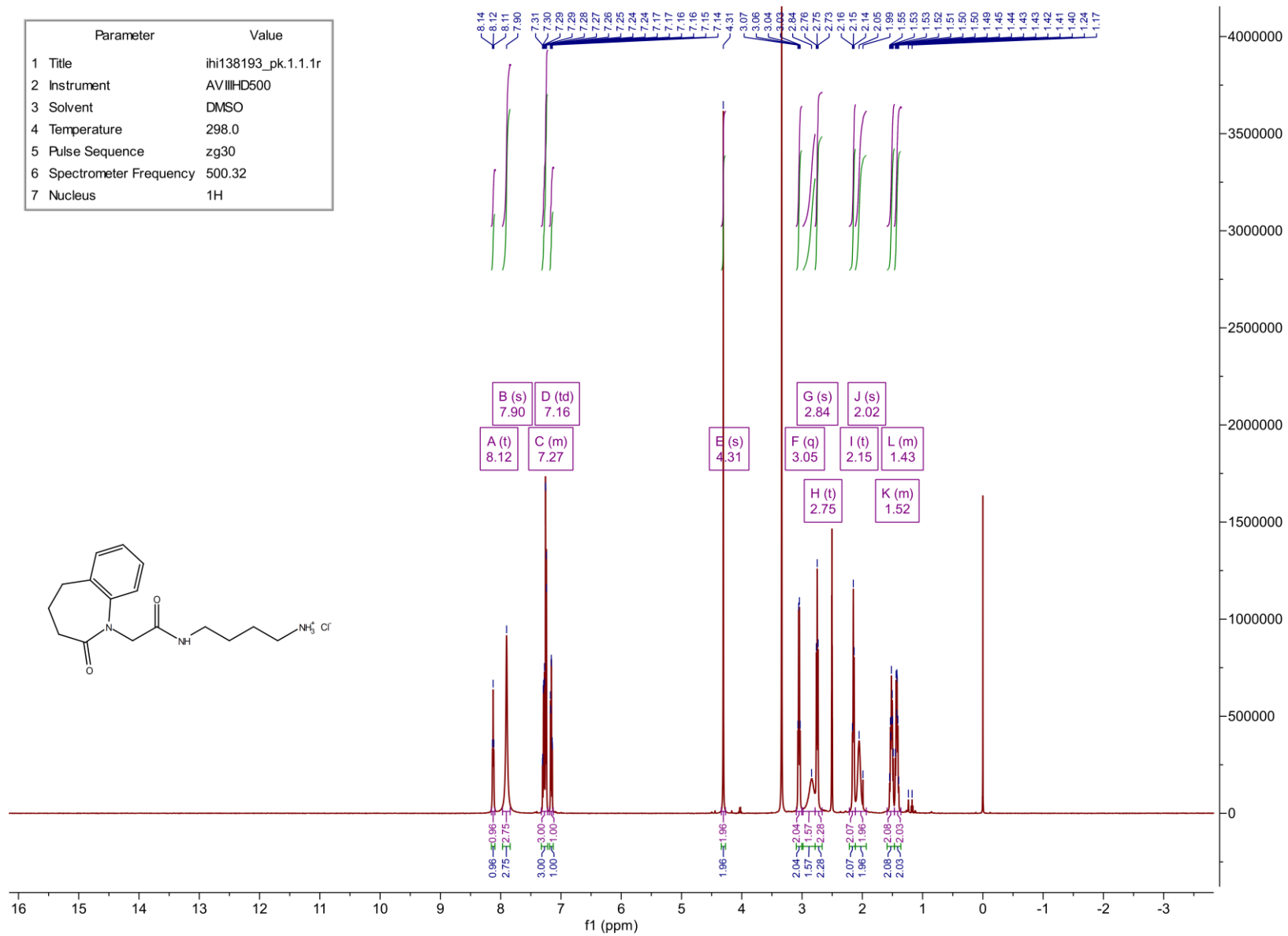


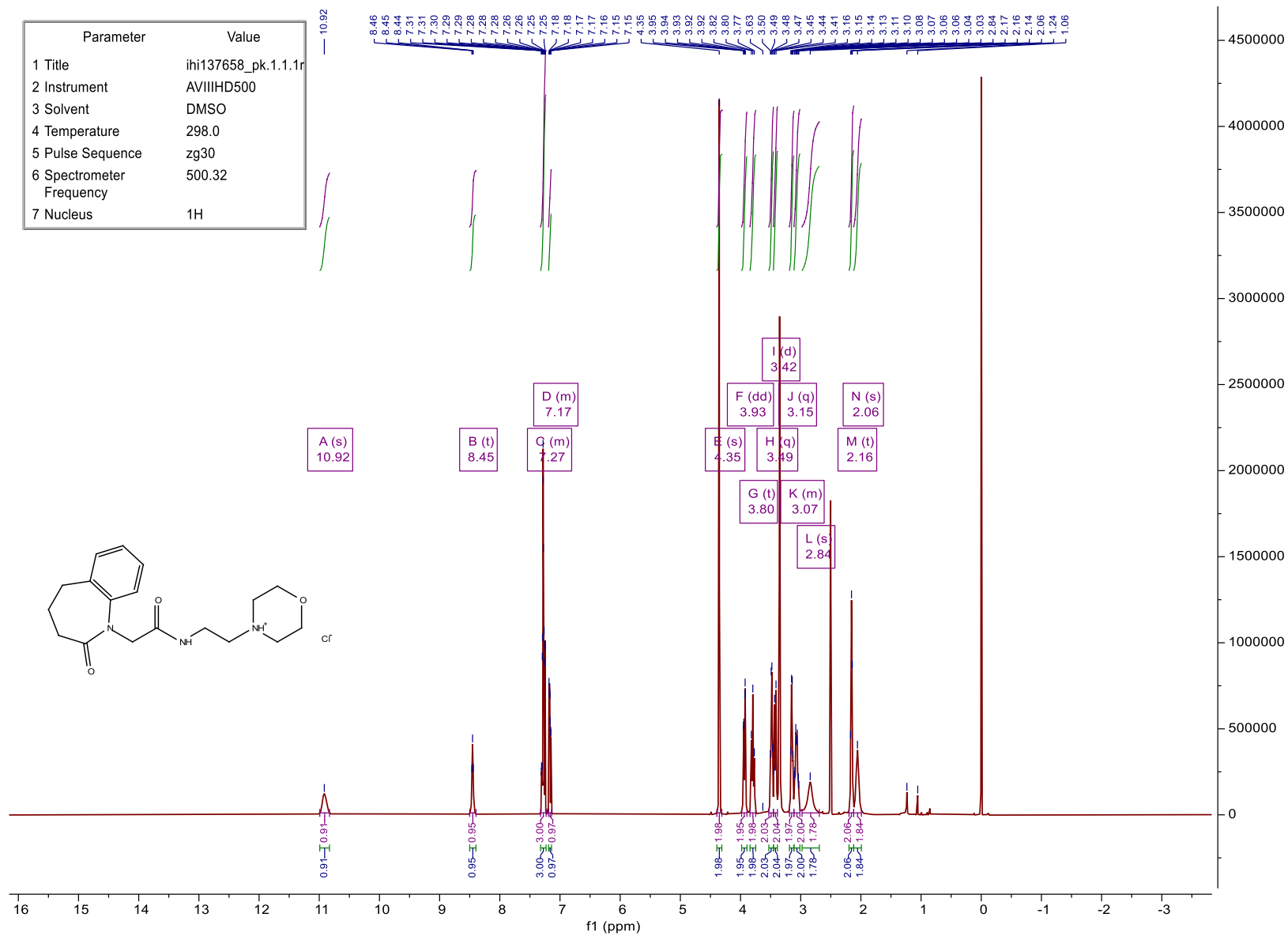
S1 File. Fig 15. <sup>1</sup>H-NMR spectrum of compound 2p.



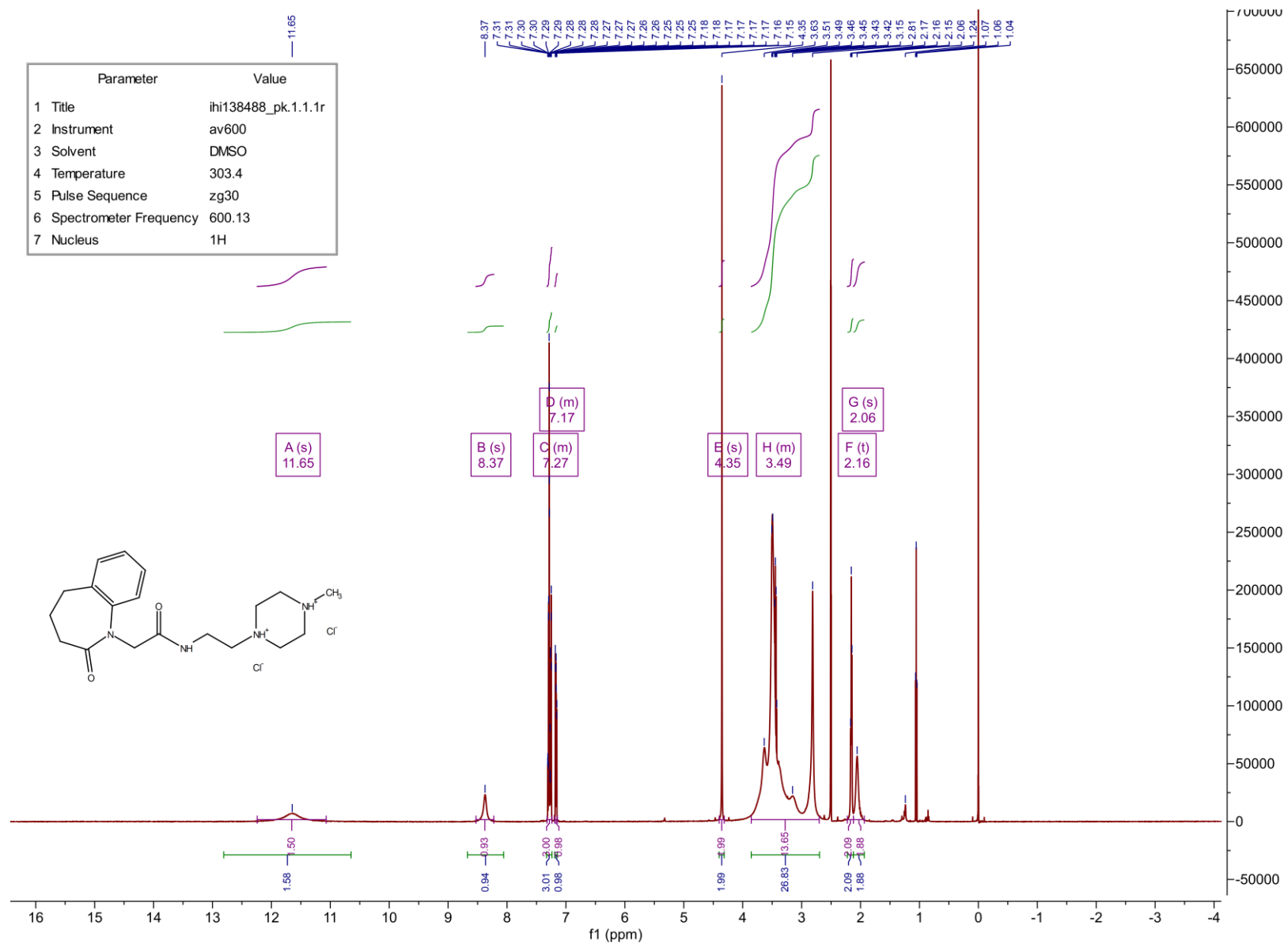
S1 File. Fig 16. <sup>1</sup>H-NMR spectrum of compound 2q.

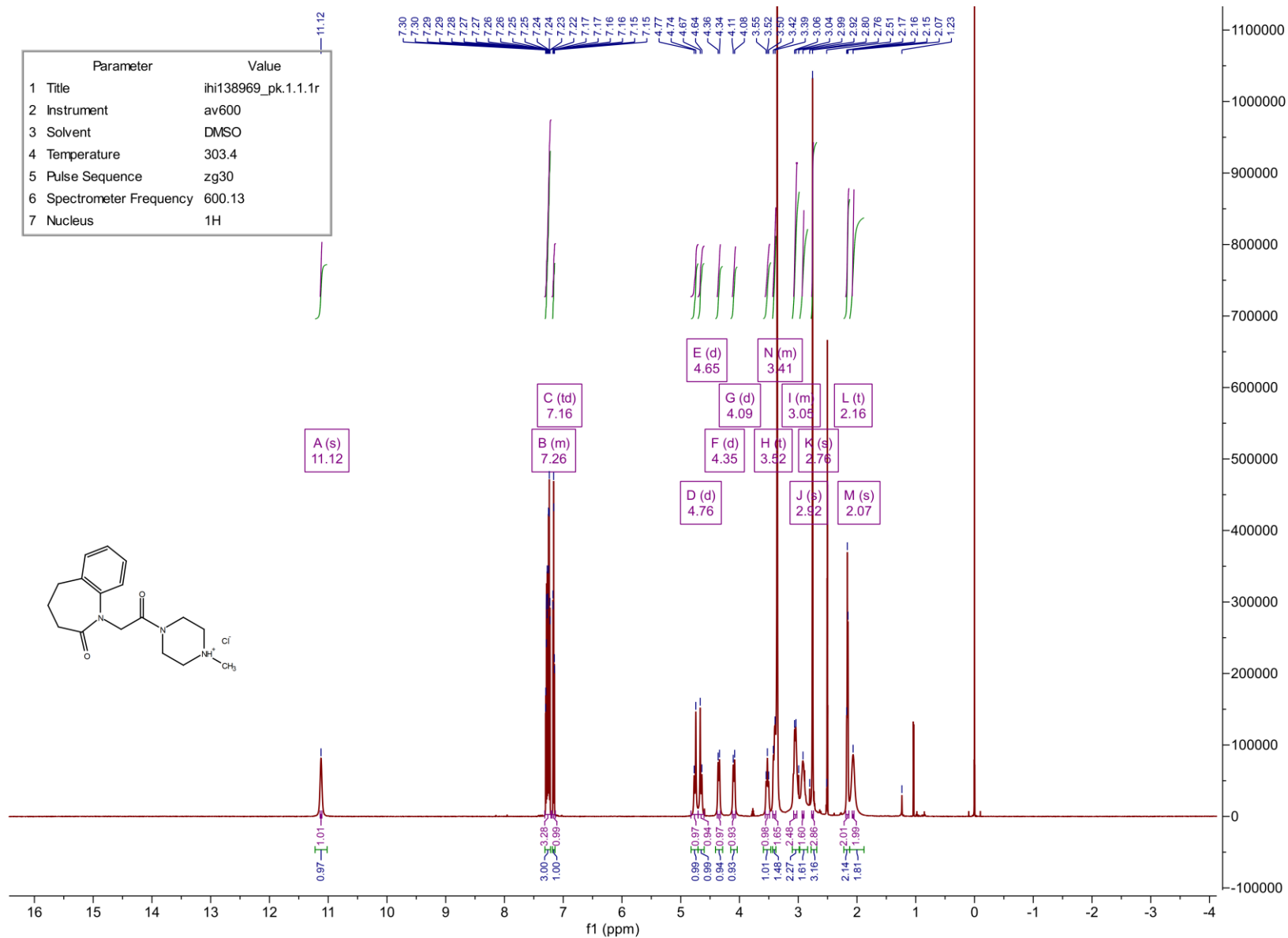
S1 File. Fig 17. <sup>1</sup>H-NMR spectrum of compound 2r.

S1 File. Fig 18. <sup>1</sup>H-NMR spectrum of compound 2s.

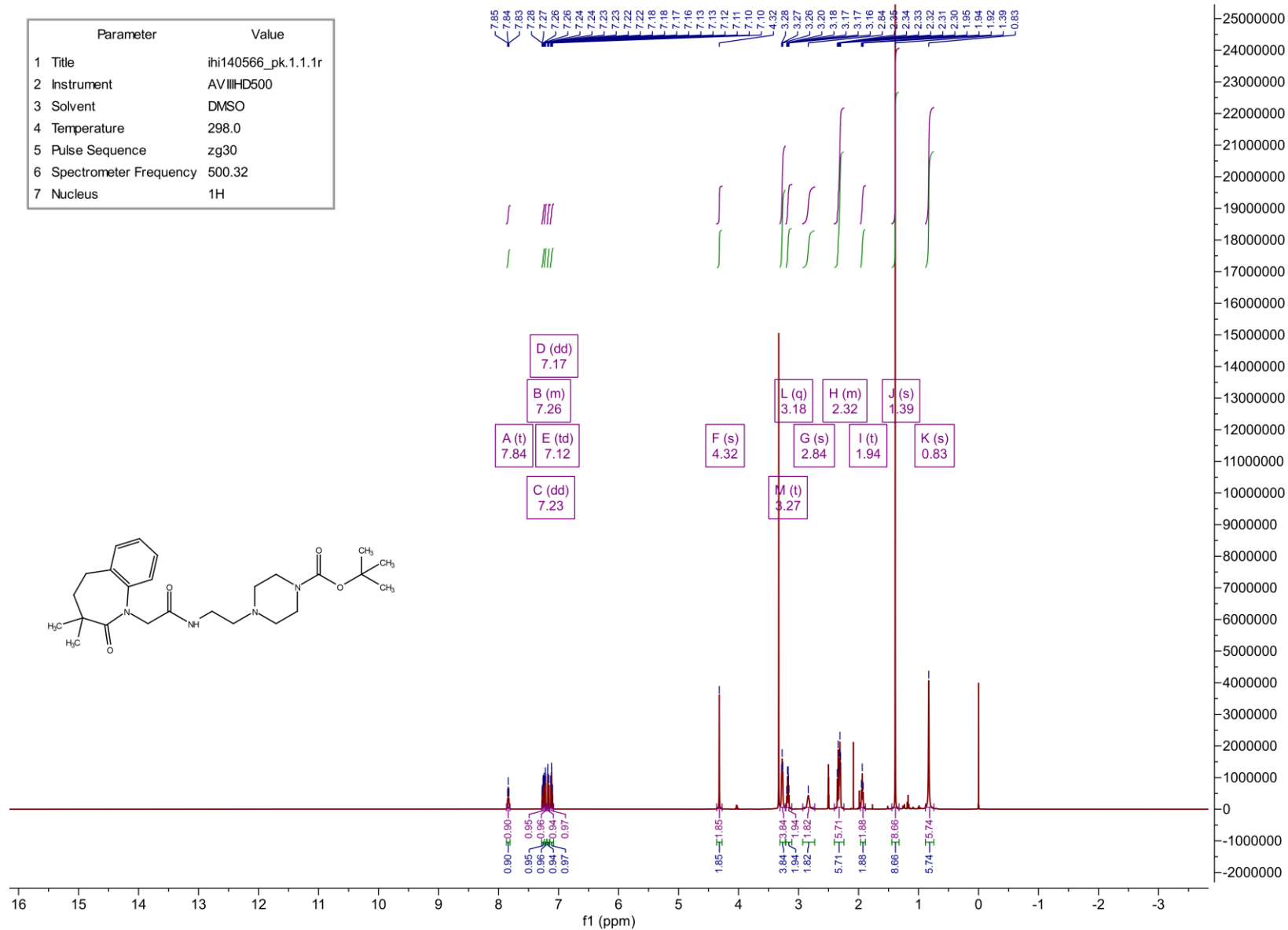


S1 File. Fig 19. <sup>1</sup>H-NMR spectrum of compound 2t.

S1 File. Fig 20. <sup>1</sup>H-NMR spectrum of compound 2u.

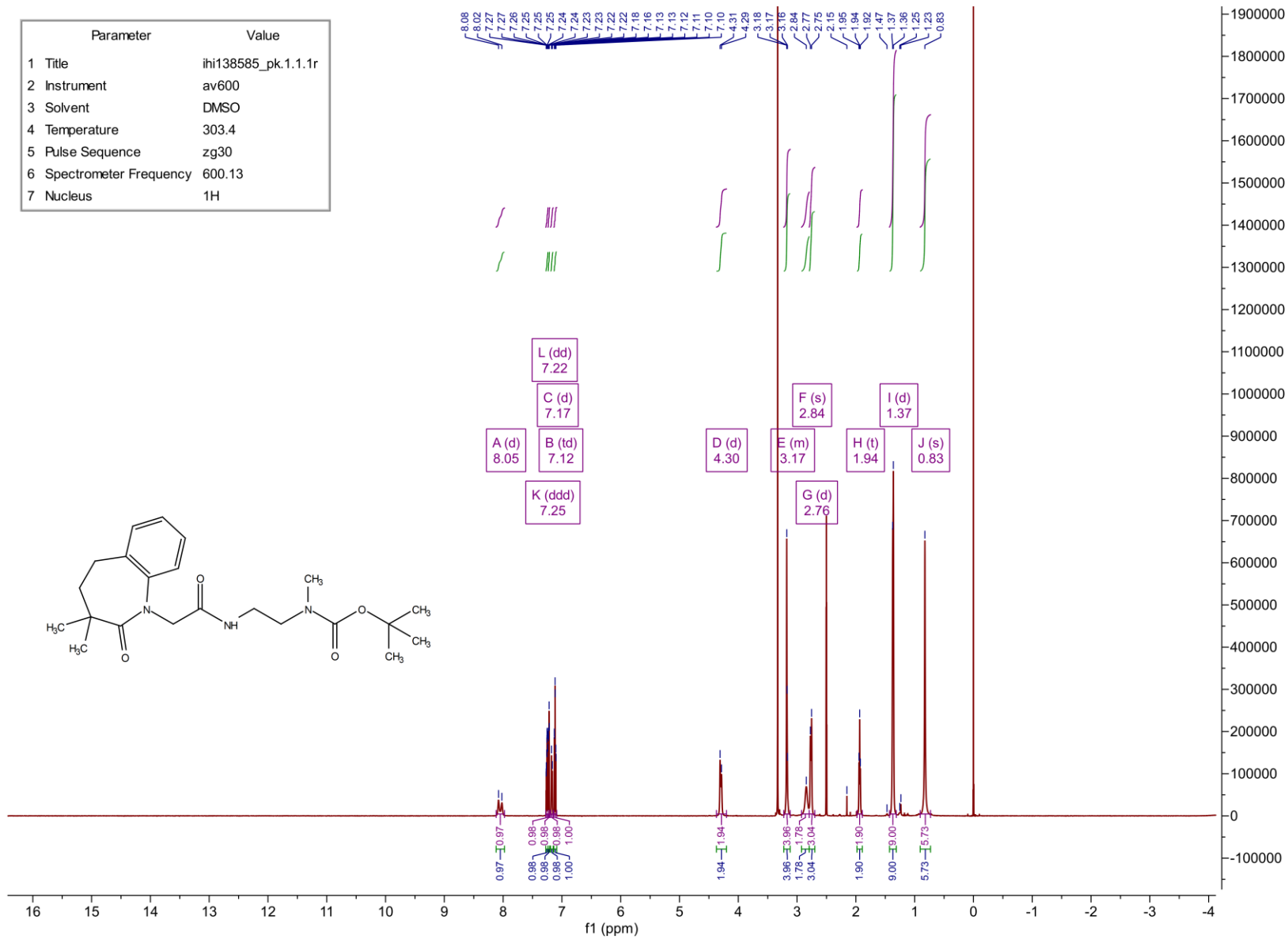


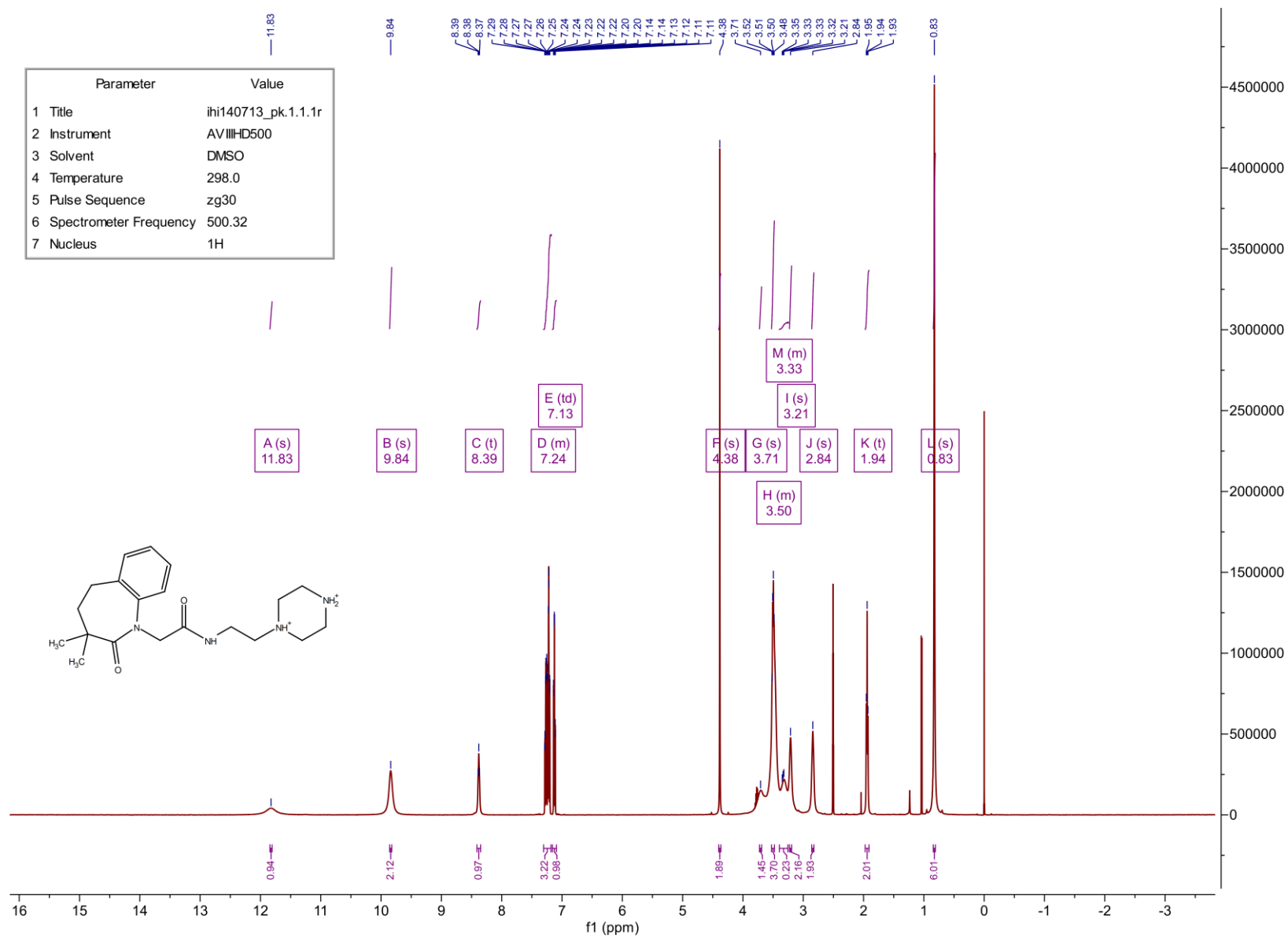
S1 File. Fig 21. <sup>1</sup>H-NMR spectrum of compound 2v.

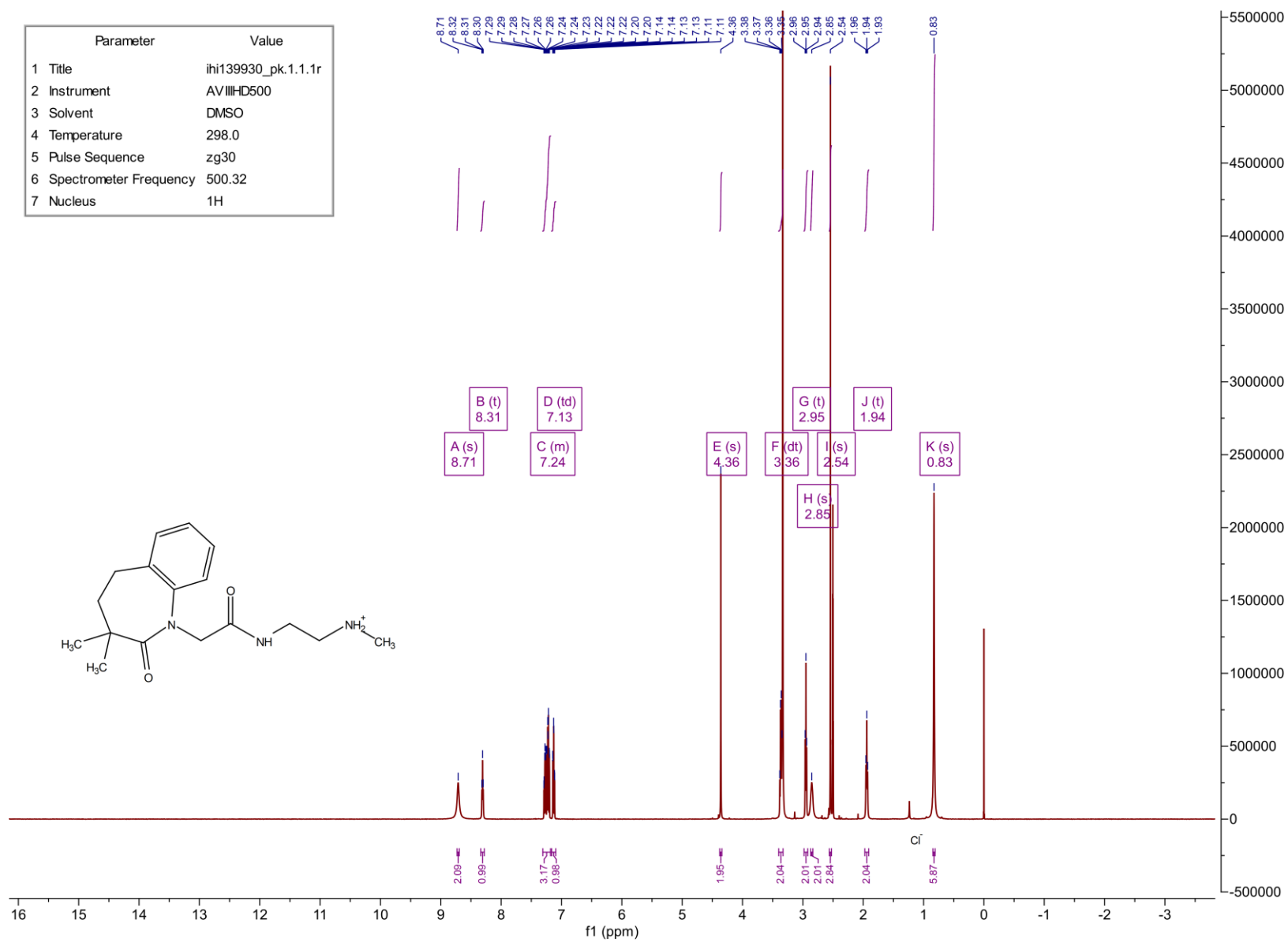


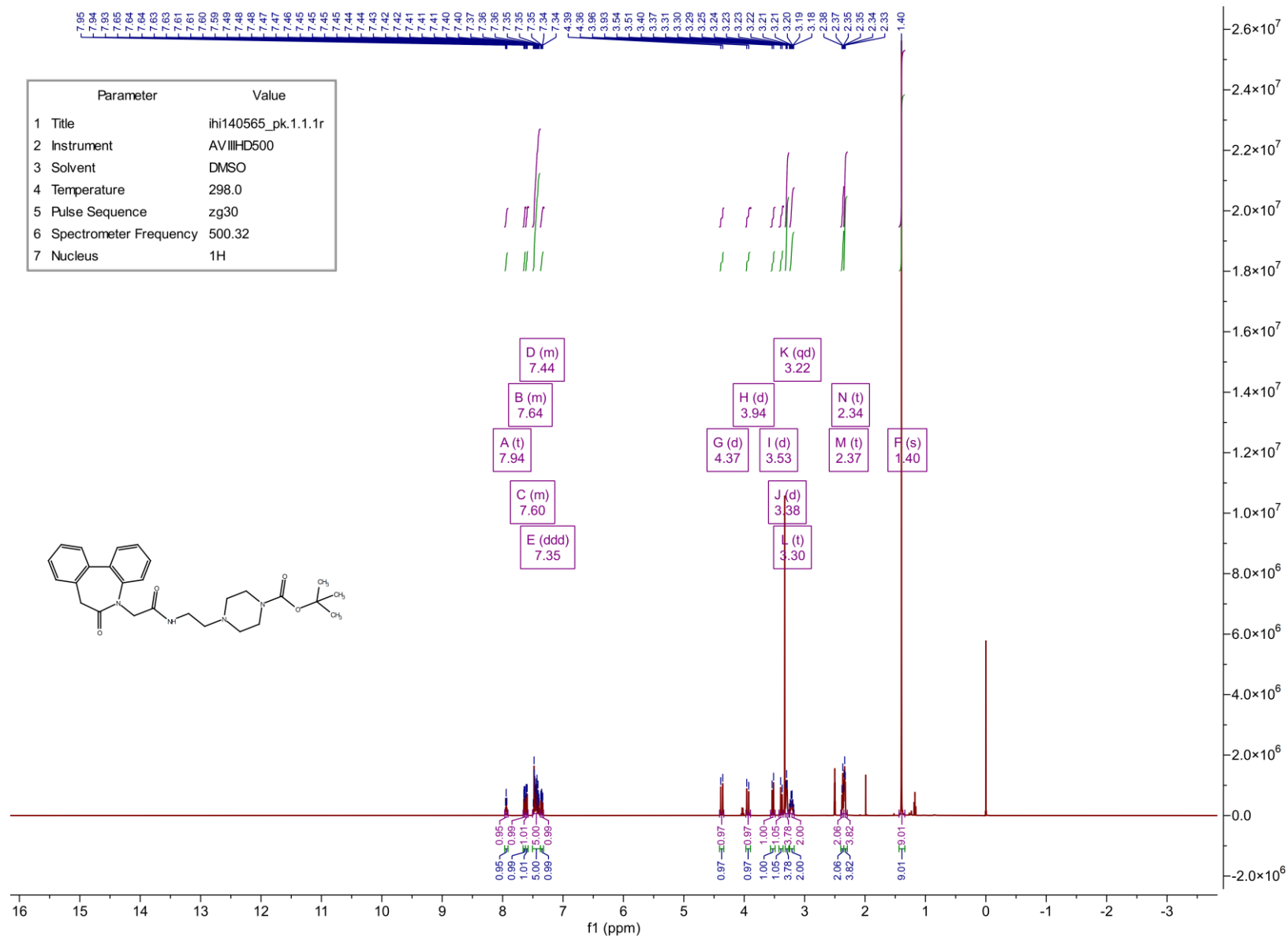
S1 File. Fig 22 <sup>1</sup>H-NMR spectrum of compound 3b.



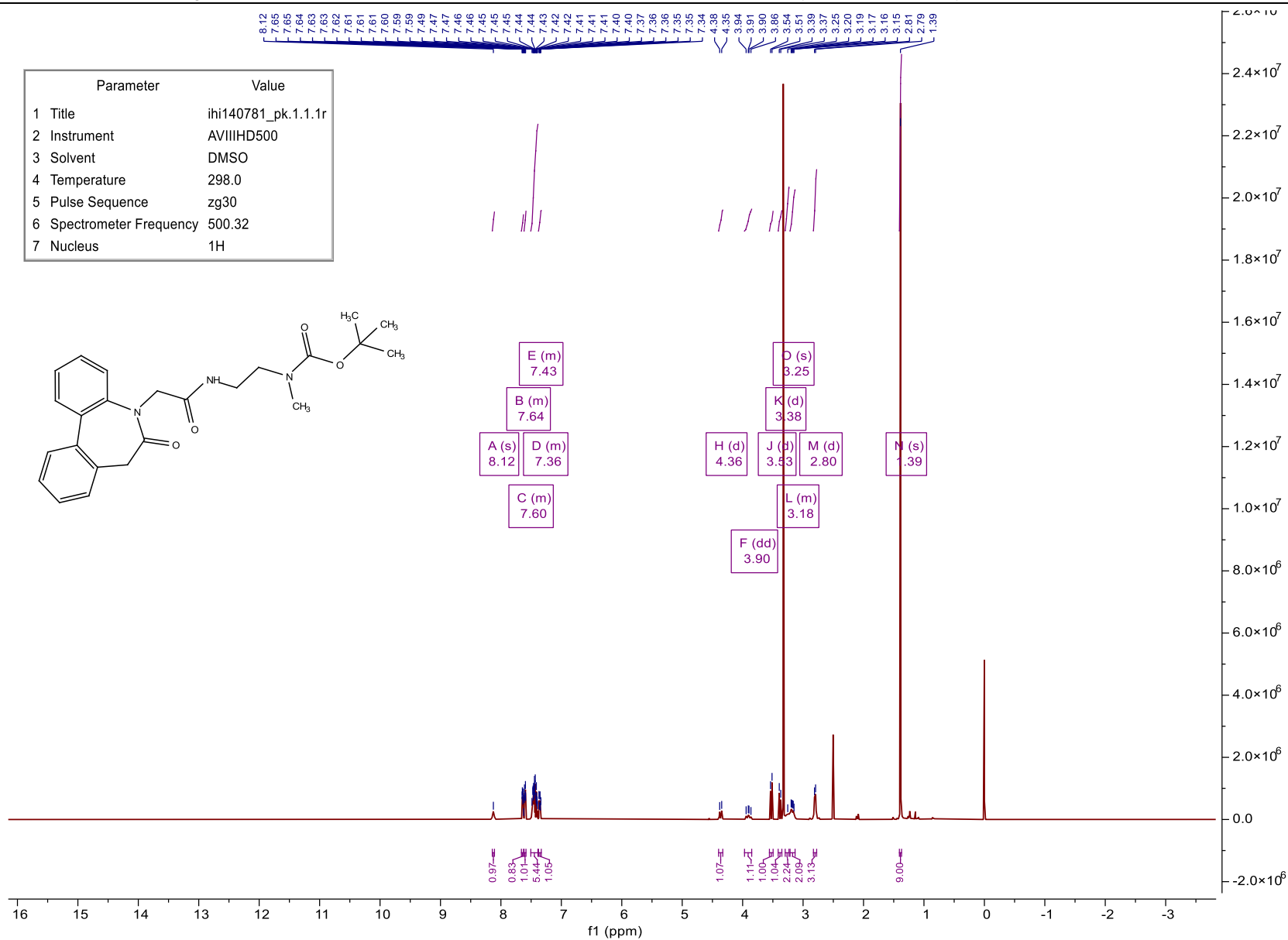
S1 File. Fig 23. <sup>1</sup>H-NMR spectrum of compound 3c.

S1 File. Fig 24. <sup>1</sup>H-NMR spectrum of compound 3d.

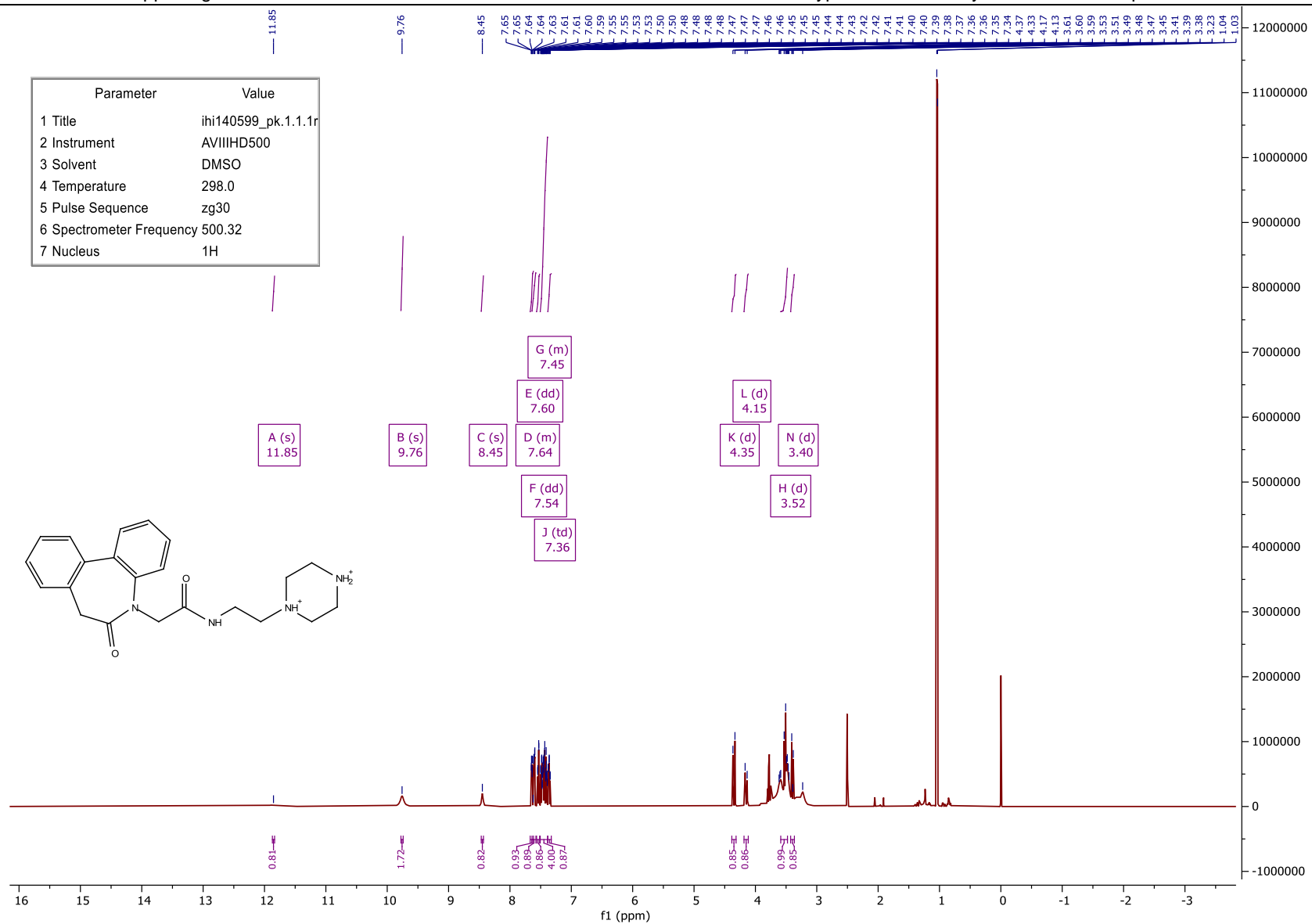
S1 File. Fig 25. <sup>1</sup>H-NMR spectrum of compound 3e.



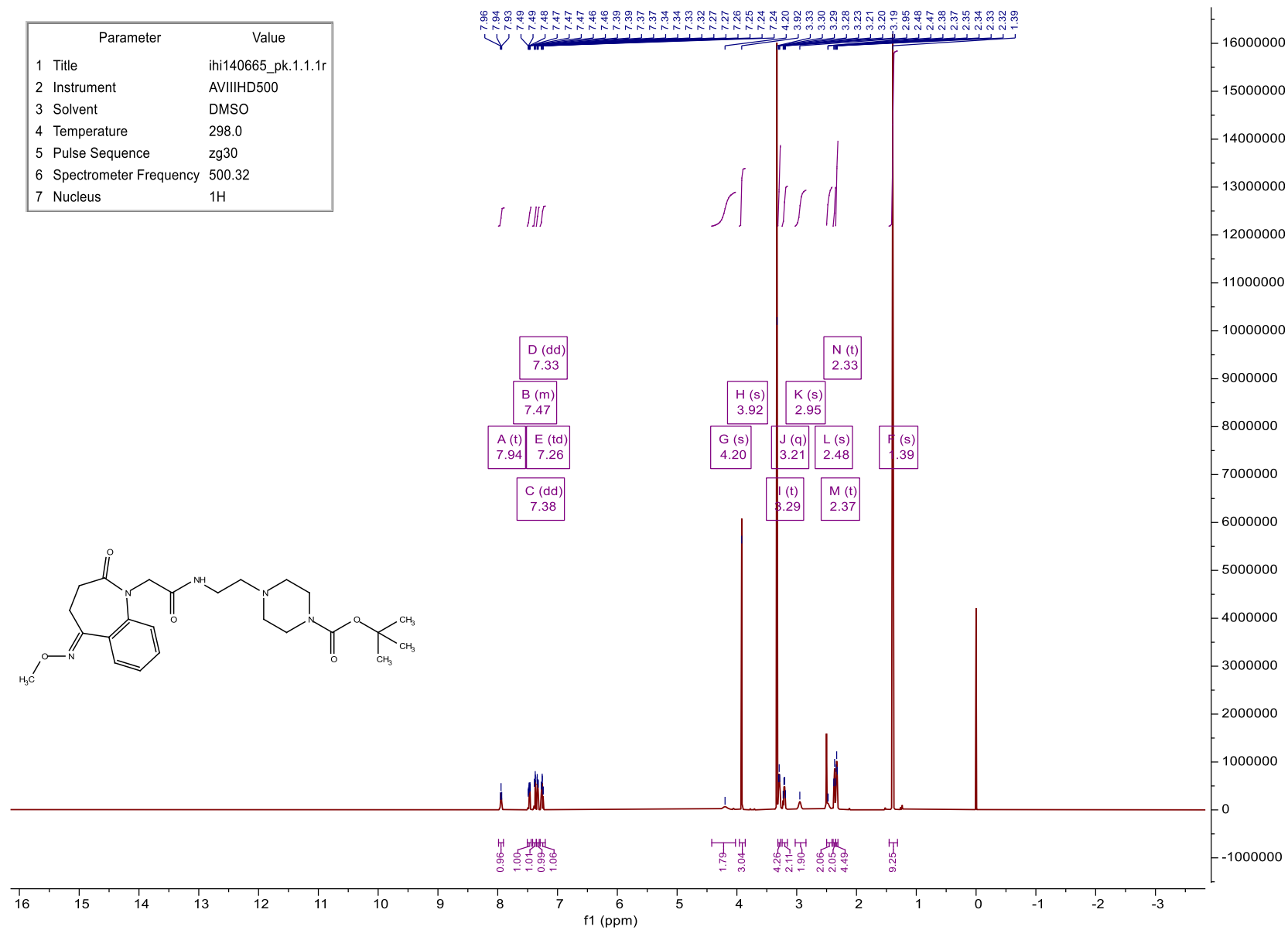
S1 File. Fig 26. <sup>1</sup>H-NMR spectrum of compound 4b.



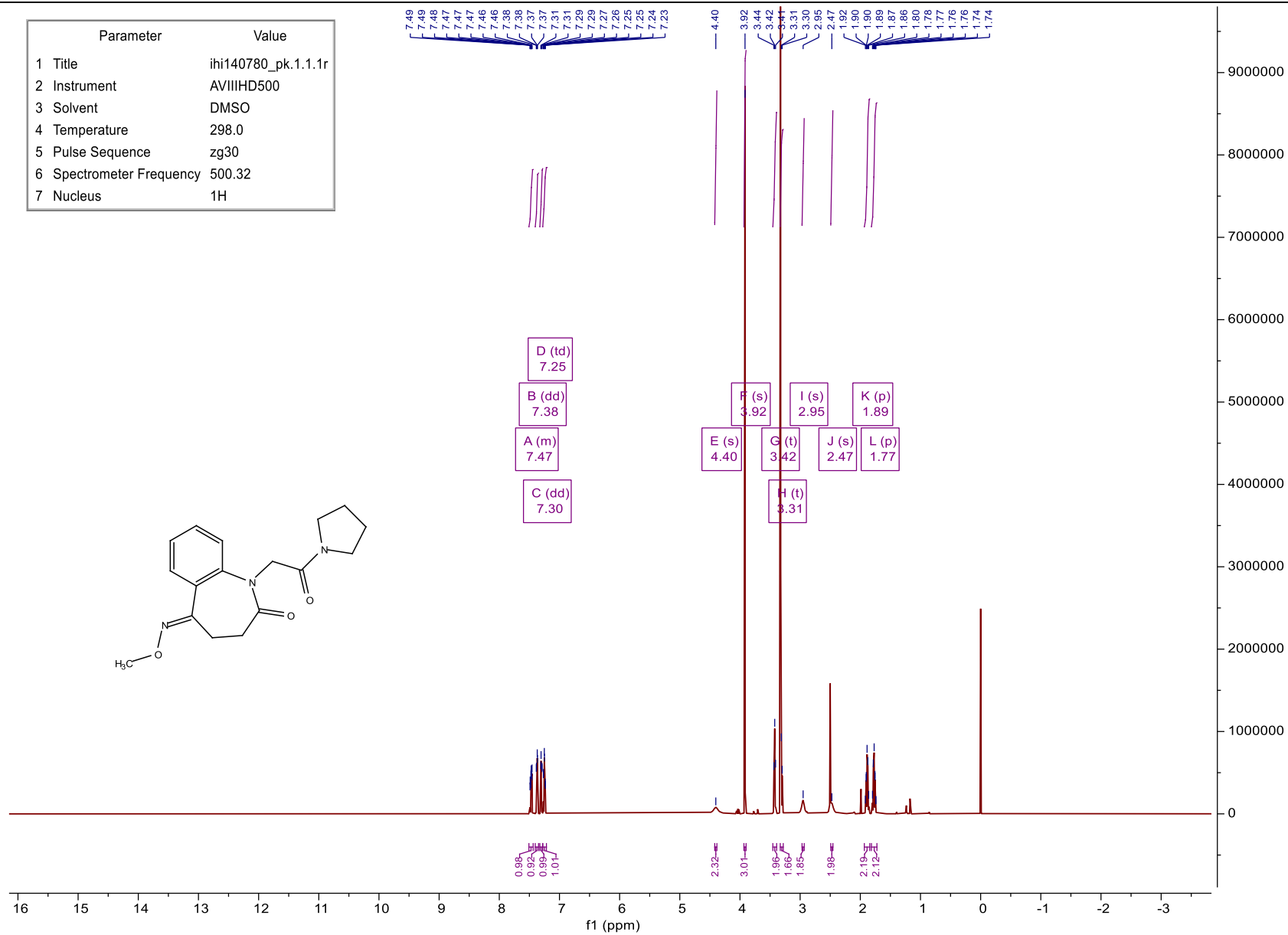
S1 File. Fig 27. <sup>1</sup>H-NMR spectrum of compound 4c.



S1 File. Fig 28. <sup>1</sup>H-NMR spectrum of compound 4d.

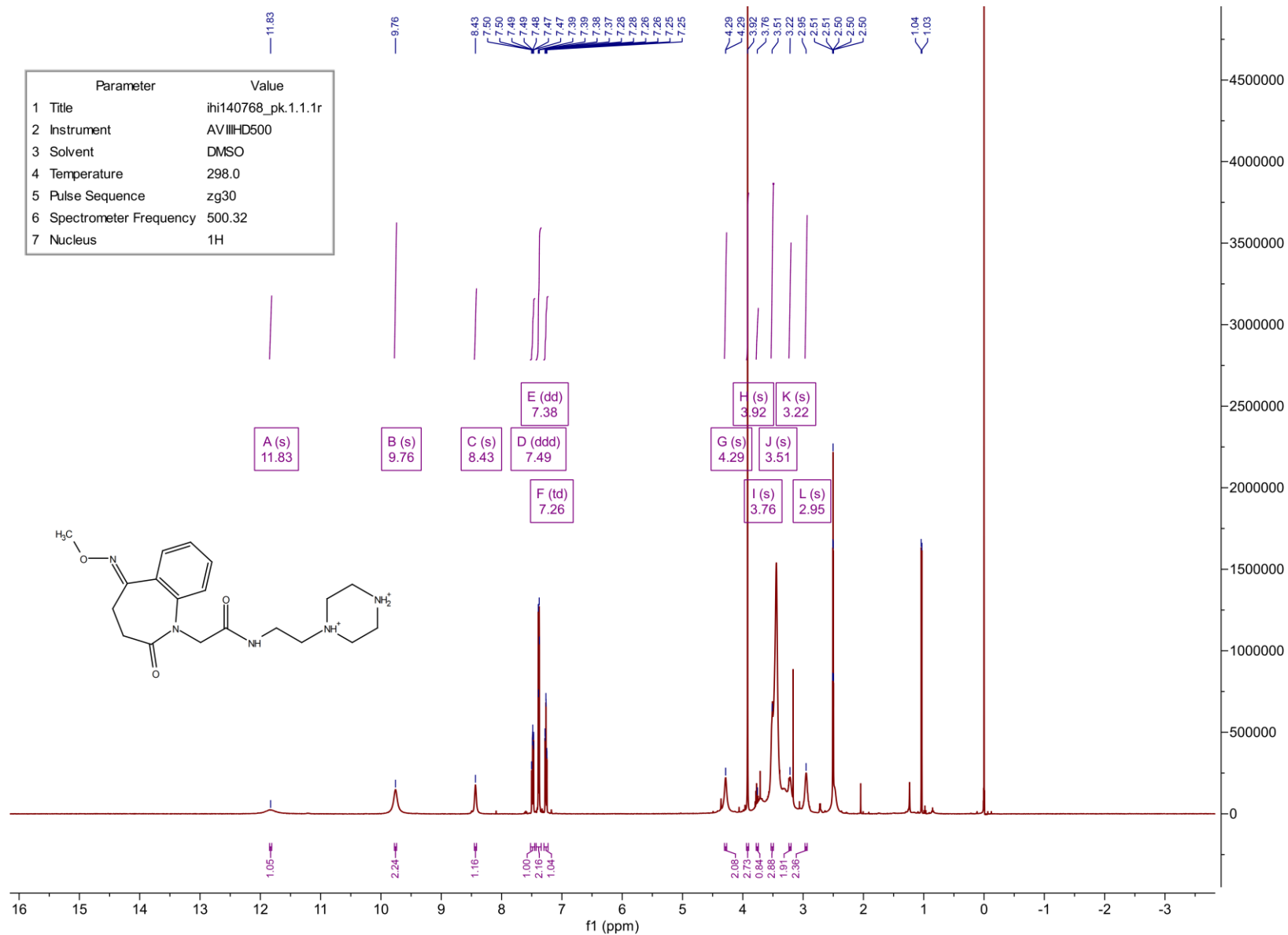


S1 File. Fig 29. <sup>1</sup>H-NMR spectrum of compound 5b.

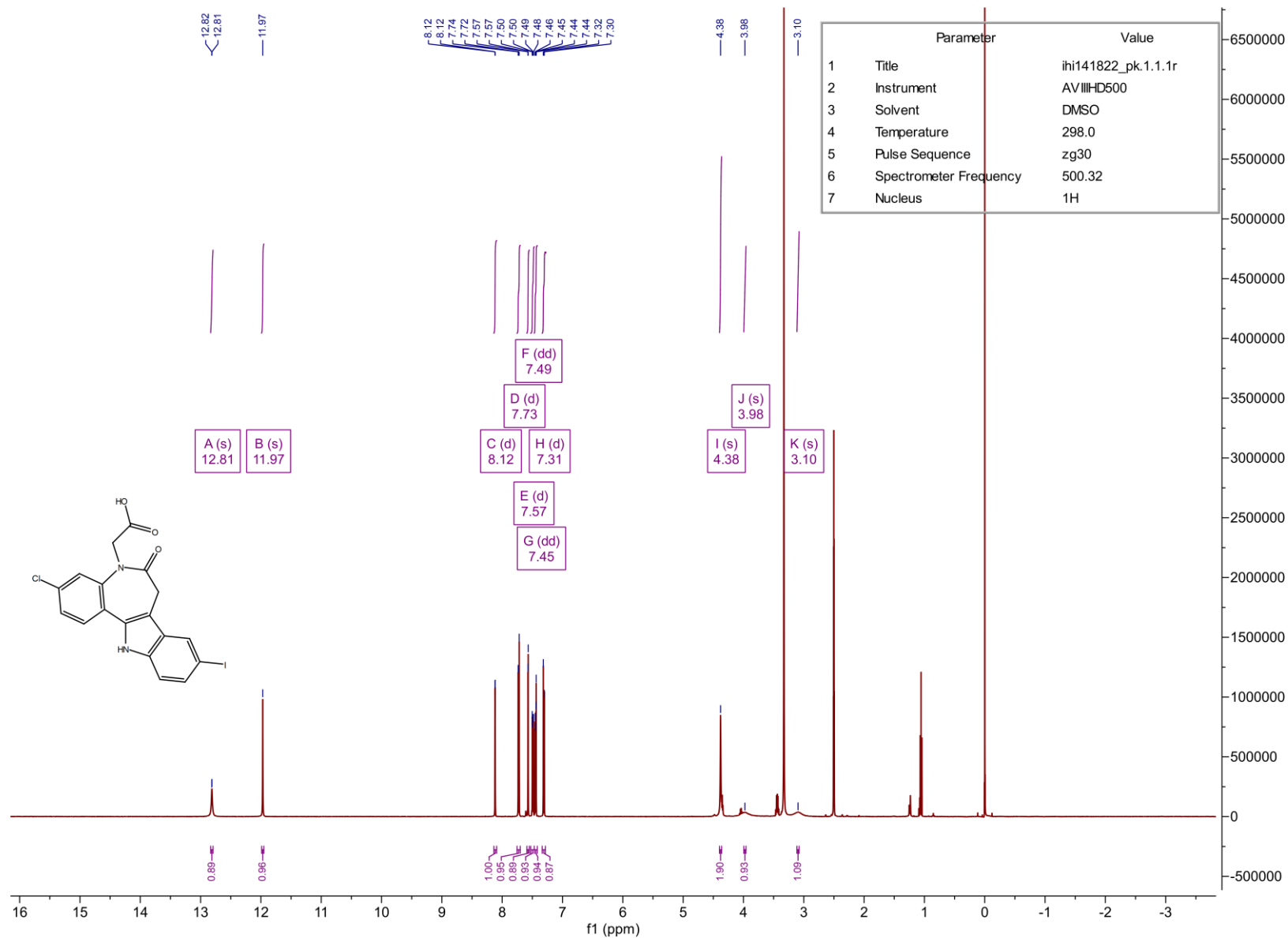


S1 File. Fig 30. <sup>1</sup>H-NMR spectrum of compound 5c.

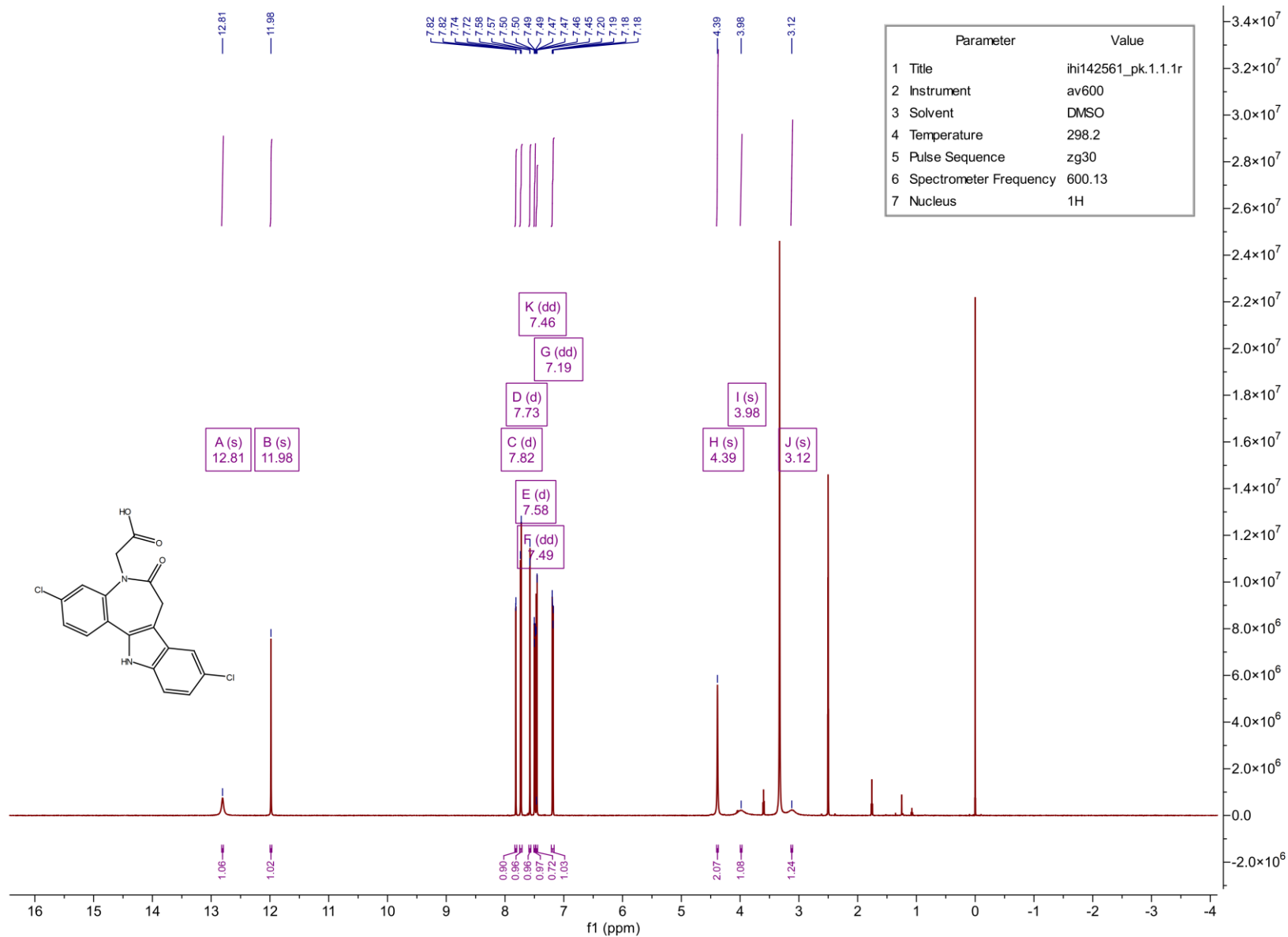




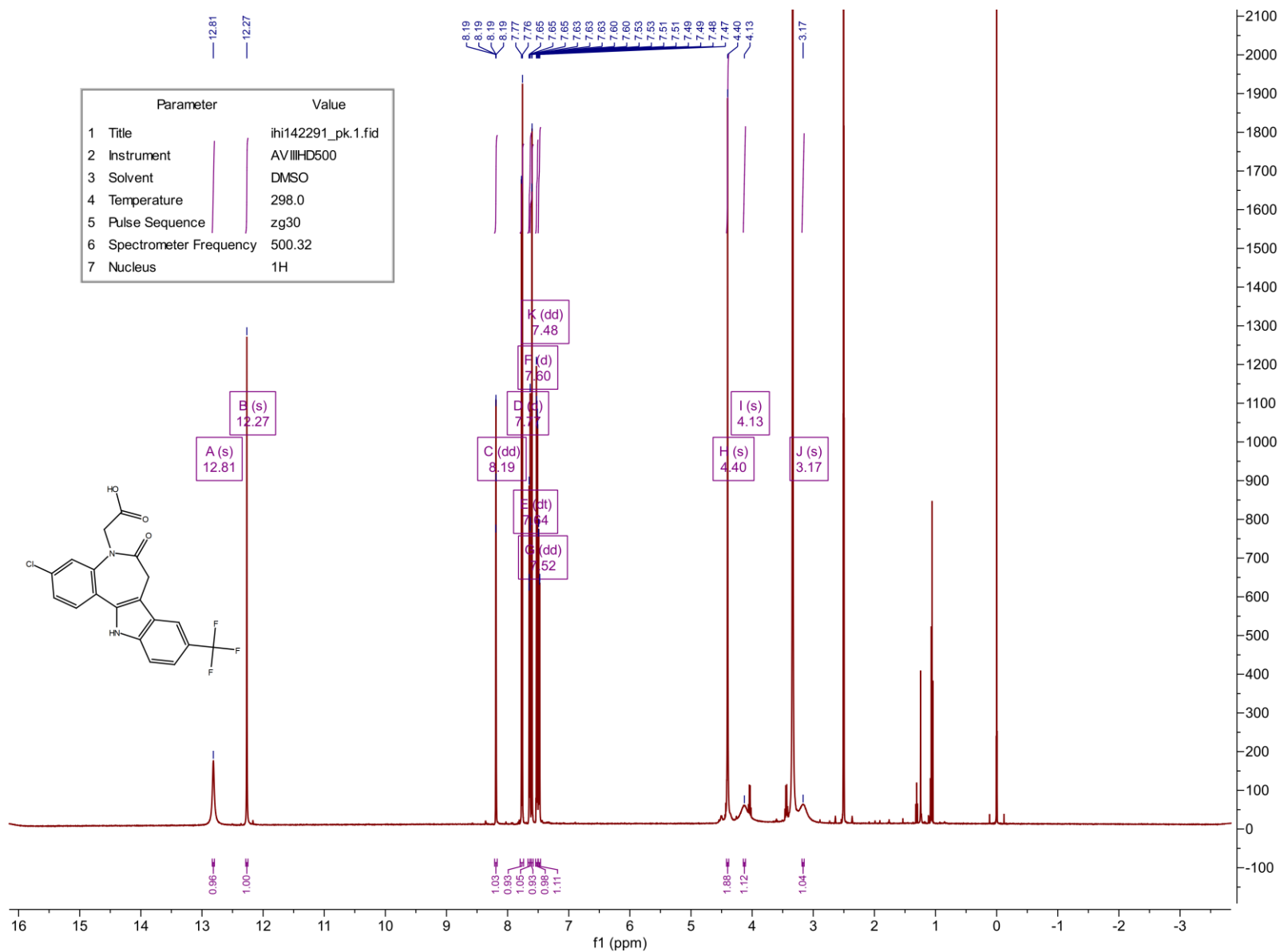
S1 File. Fig 31. <sup>1</sup>H-NMR spectrum of compound 5d.



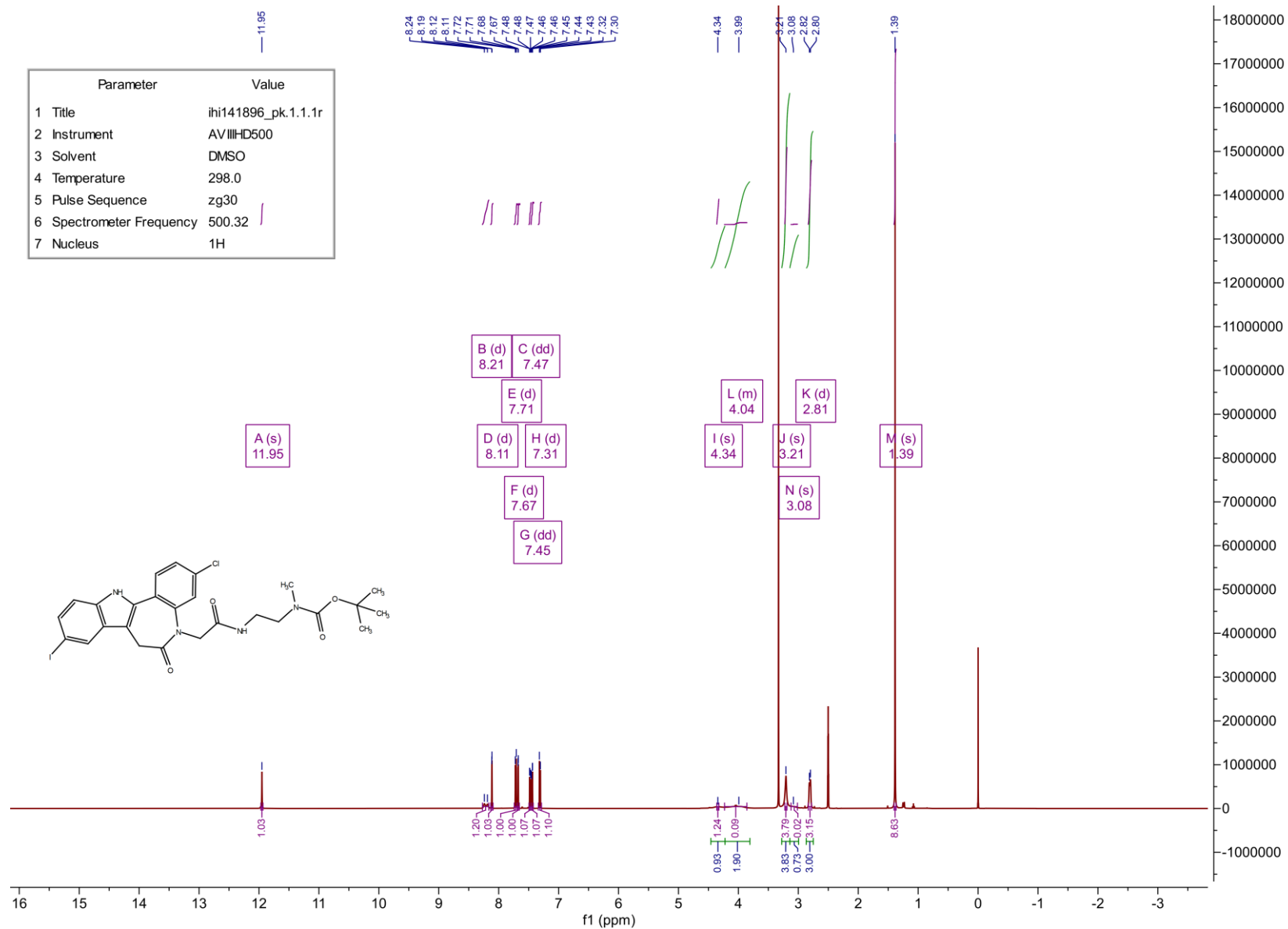
S1 File. Fig 32. <sup>1</sup>H-NMR spectrum of compound 9a.



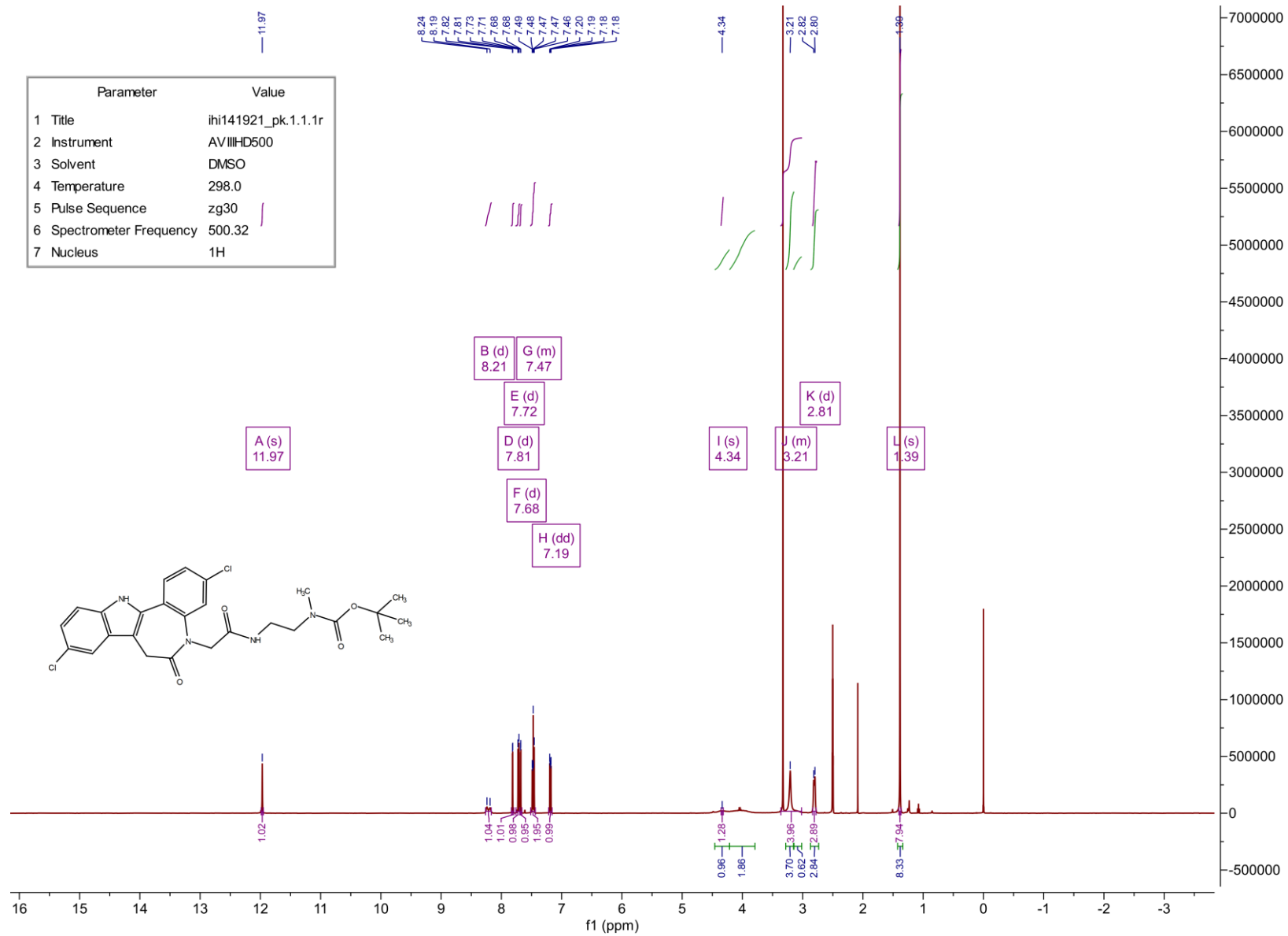
S1 File. Fig 33. <sup>1</sup>H-NMR spectrum of compound 9b.



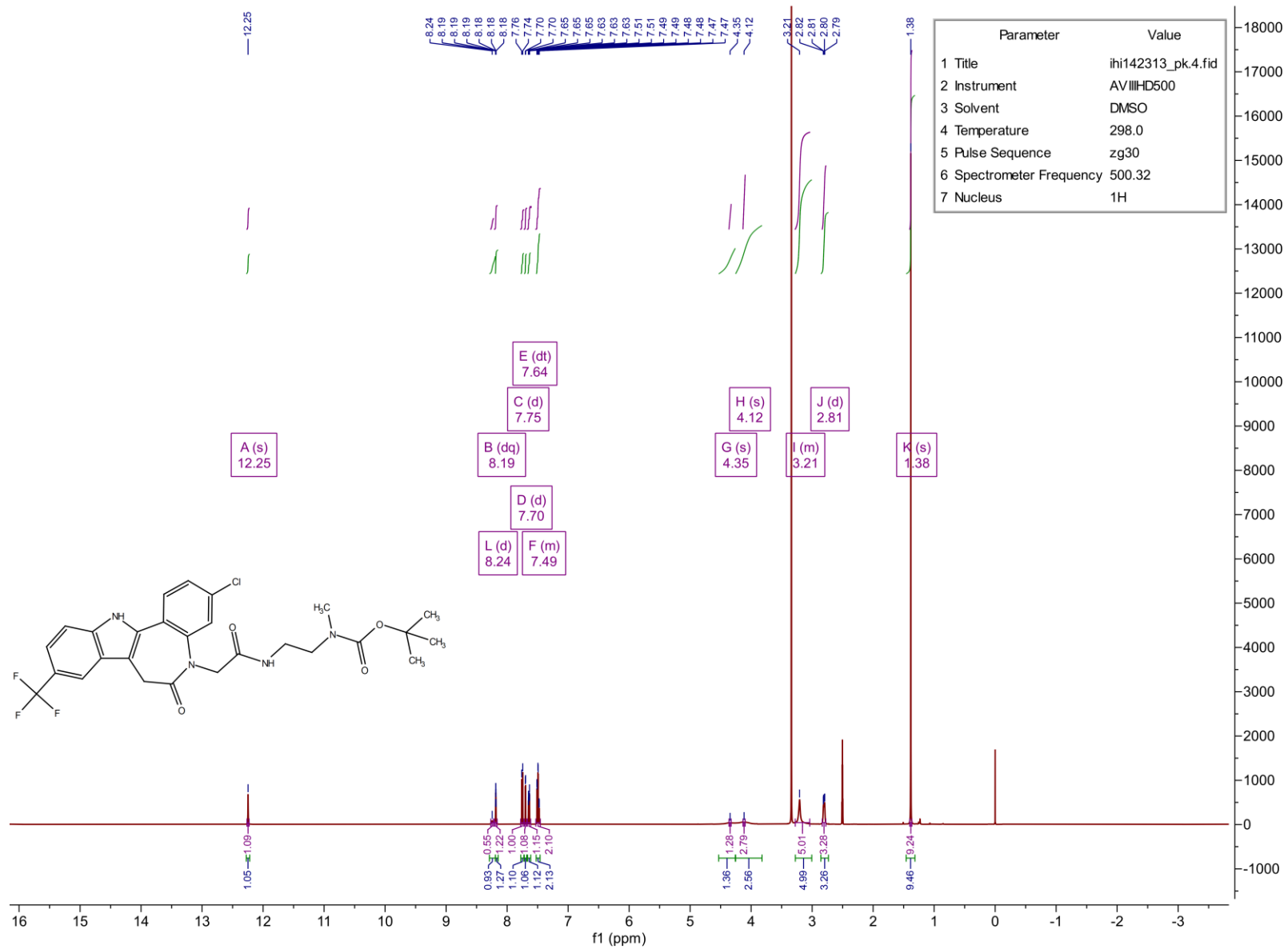
S1 File. Fig 34. <sup>1</sup>H-NMR spectrum of compound 9c.



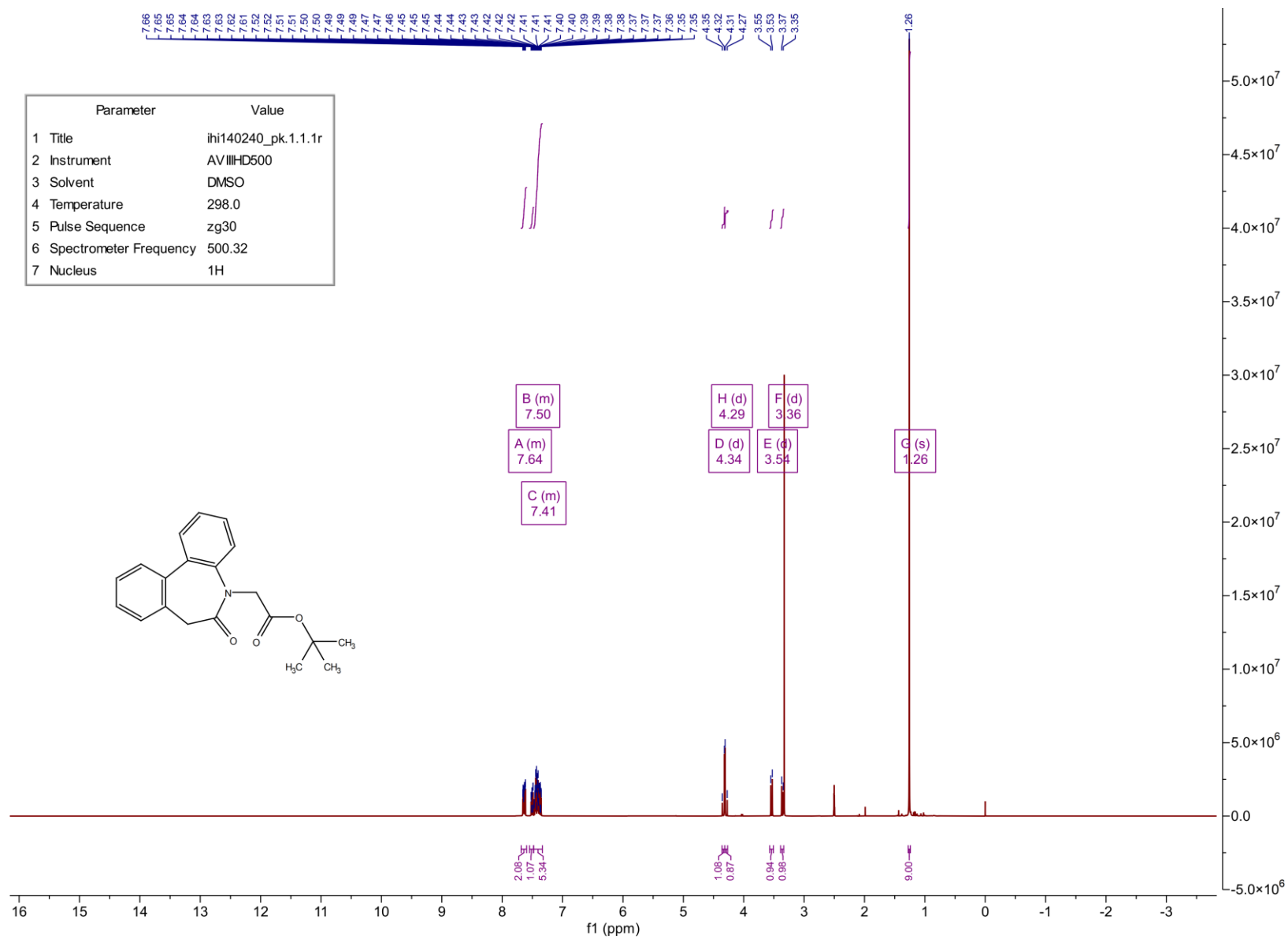
S1 File. Fig 35. <sup>1</sup>H-NMR spectrum of compound 10a.



S1 File. Fig 36. <sup>1</sup>H-NMR spectrum of compound 10b.

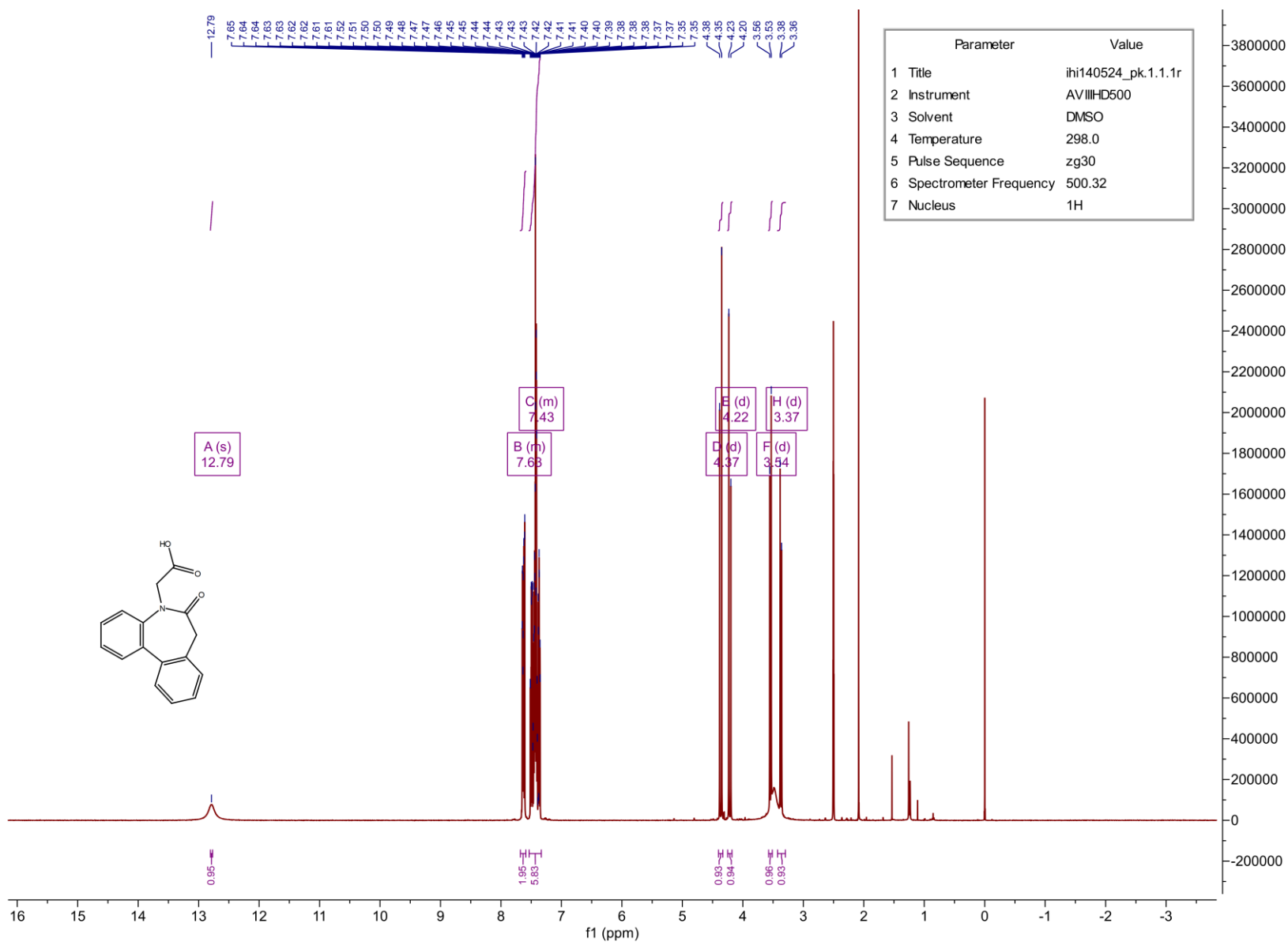


S1 File. Fig 37. <sup>1</sup>H-NMR spectrum of compound 10c.

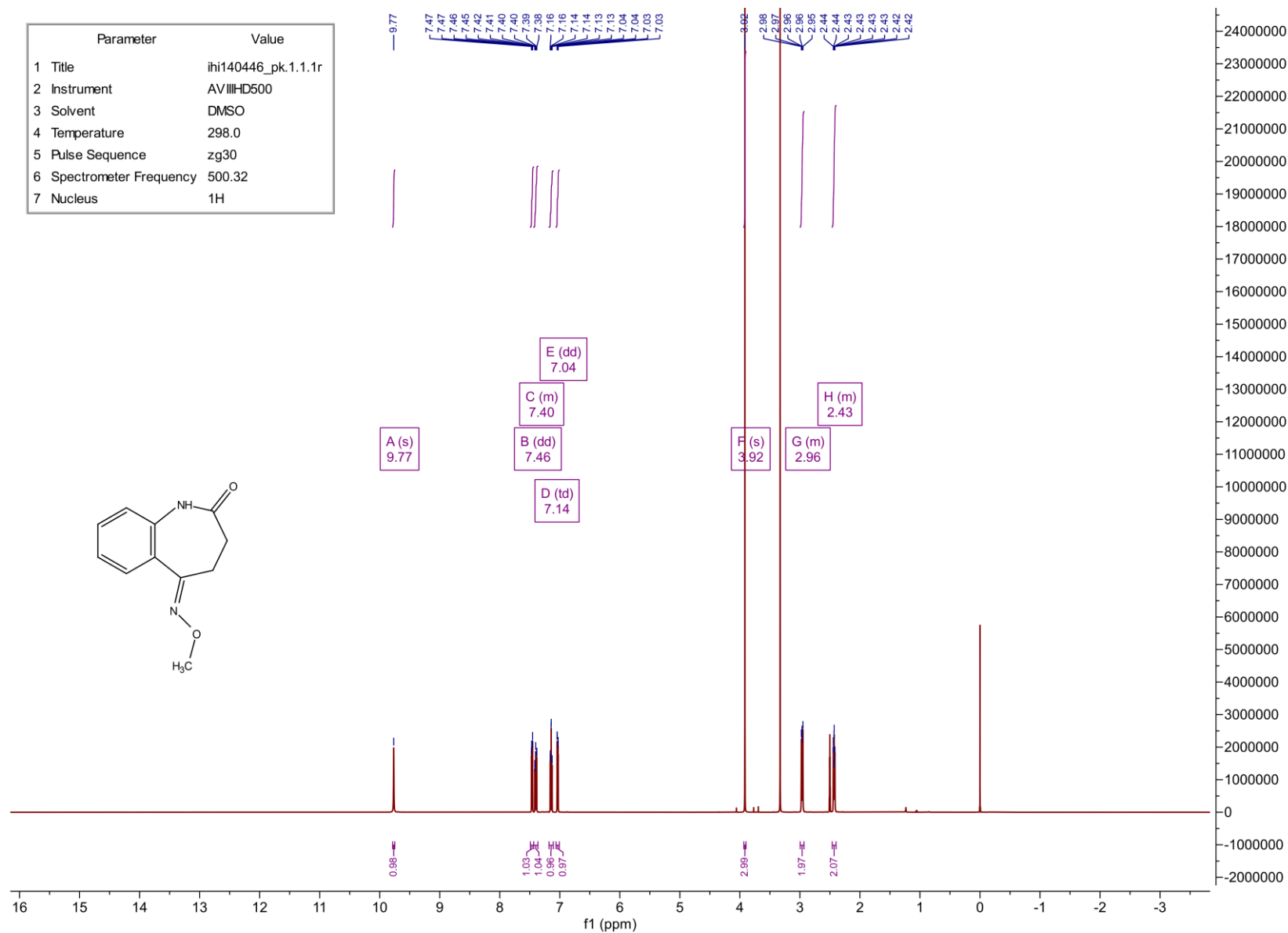


S1 File. Fig 38. <sup>1</sup>H-NMR spectrum of compound 18.

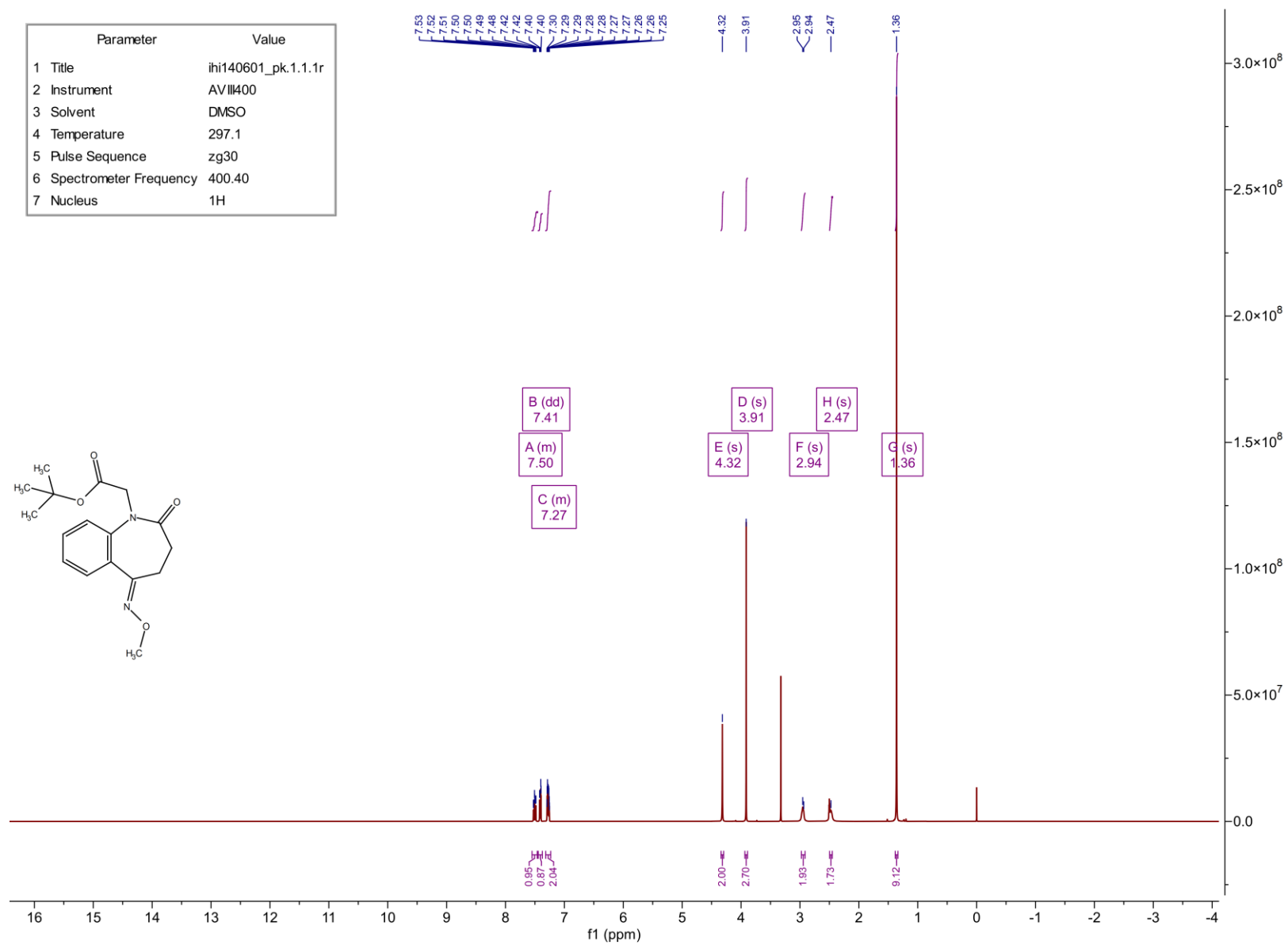




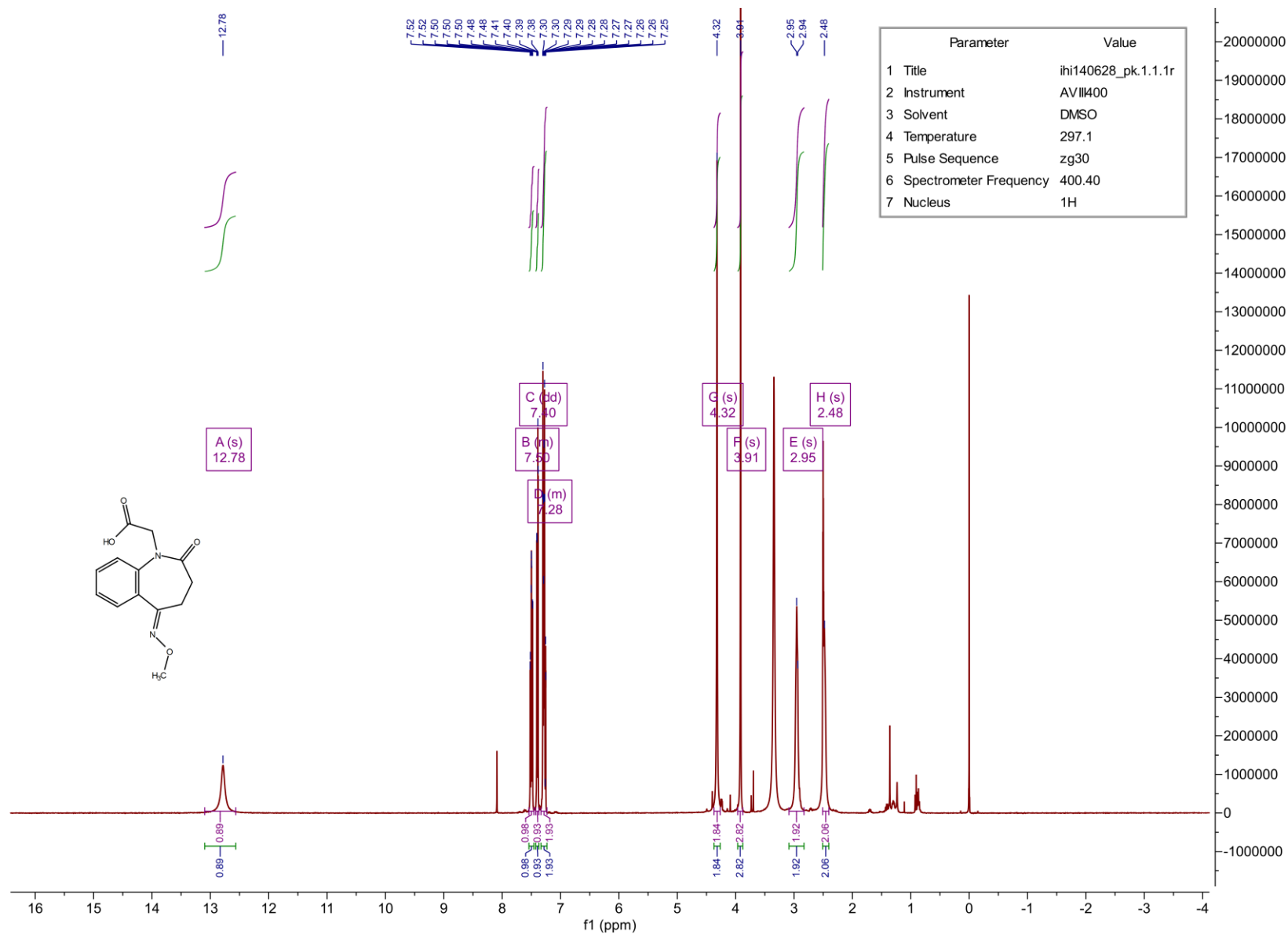
S1 File. Fig 39. <sup>1</sup>H-NMR spectrum of compound 19.



S1 File. Fig 40. <sup>1</sup>H-NMR spectrum of compound 20.



S1 File. Fig 41. <sup>1</sup>H-NMR spectrum of compound 21.



S1 File. Fig 42. <sup>1</sup>H-NMR spectrum of compound 22.