S-Containing Biginelli products based on salicylaldehydes in the reaction of aromatic nucleophilic substitution

Supporting information

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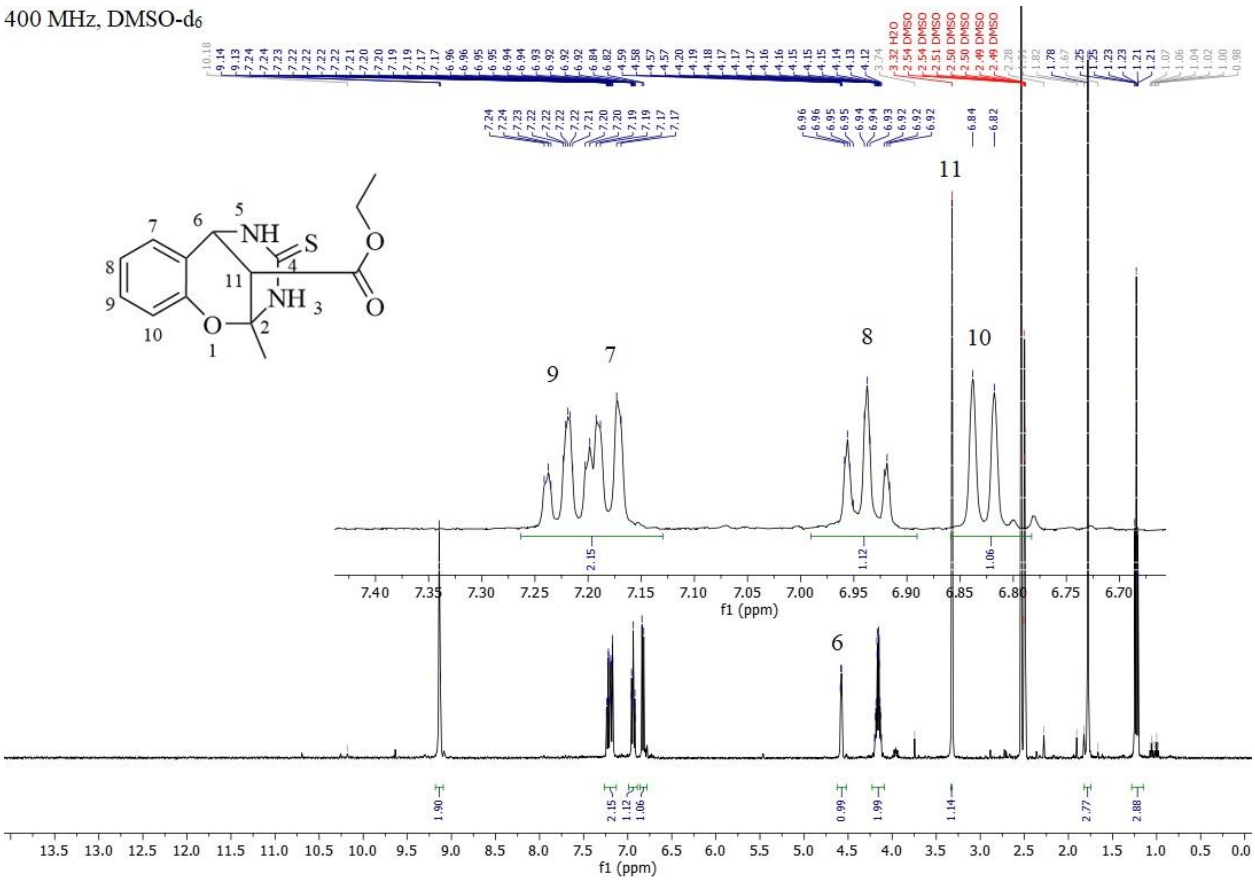

Figure SI-1. ^{1}H NMR spectrum of compound **1a**.

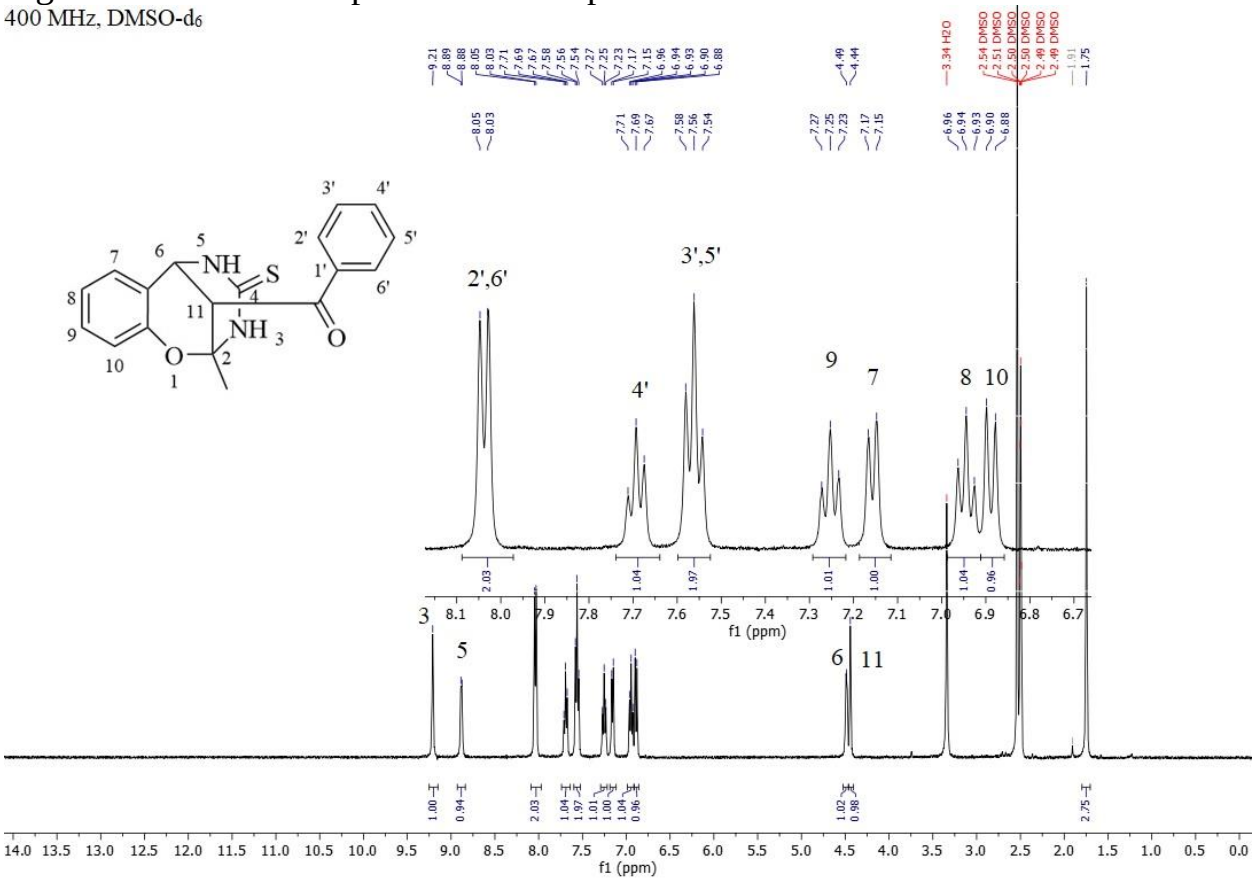

Figure SI-2. ^{1}H NMR spectrum of compound **1b**.

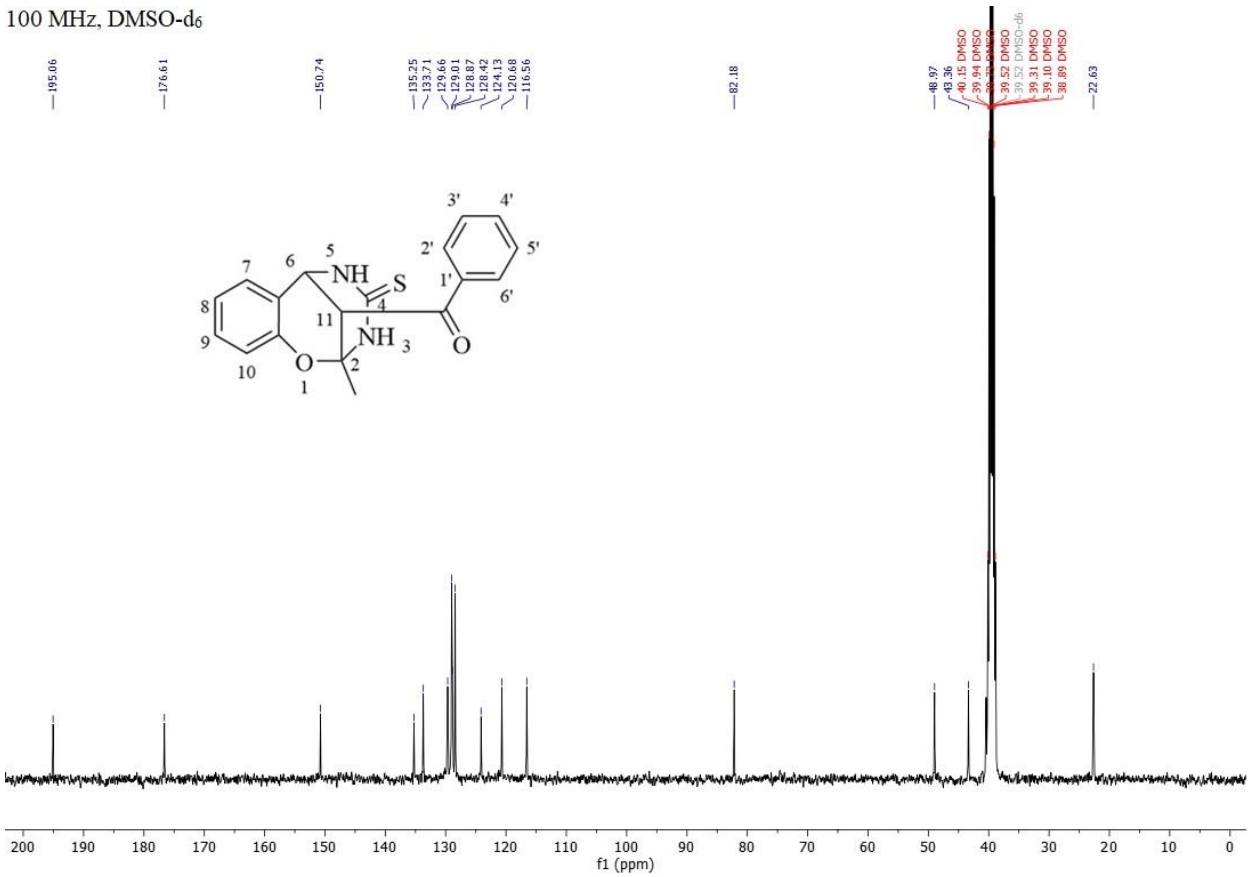

Figure SI-3. ^{13}C NMR spectrum of compound **1b**.

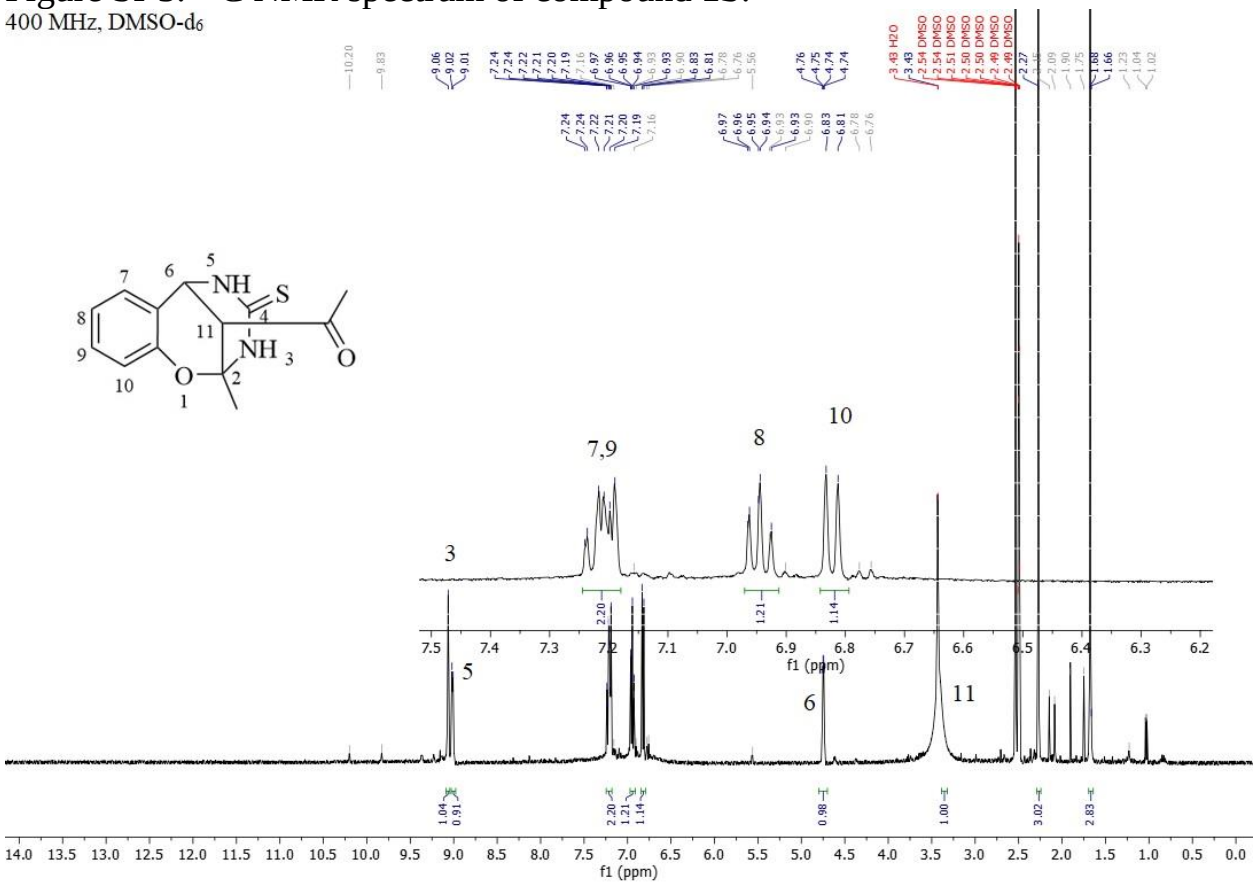

Figure SI-4. ^{1}H NMR spectrum of compound **1c**.

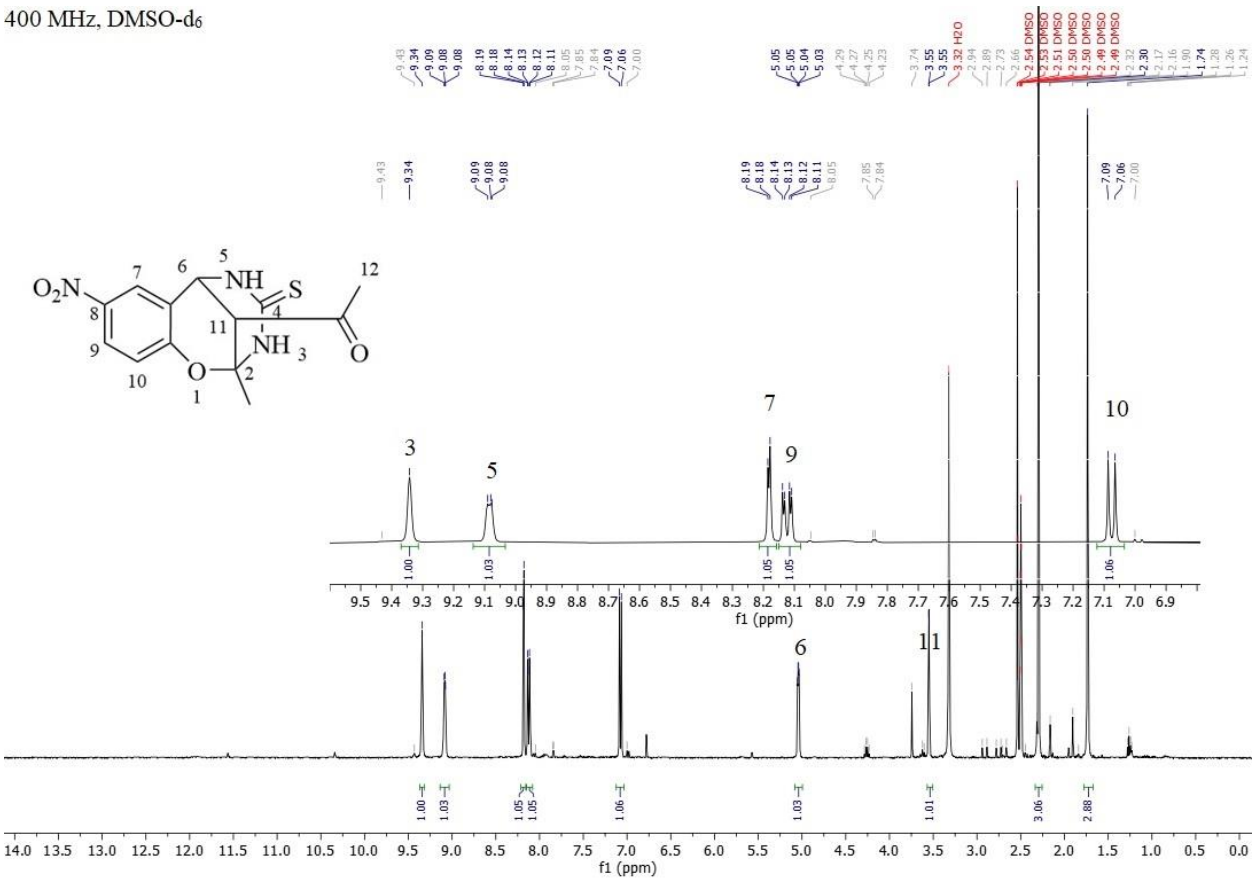

Figure SI-5. ^{1}H NMR spectrum of compound **1d**.

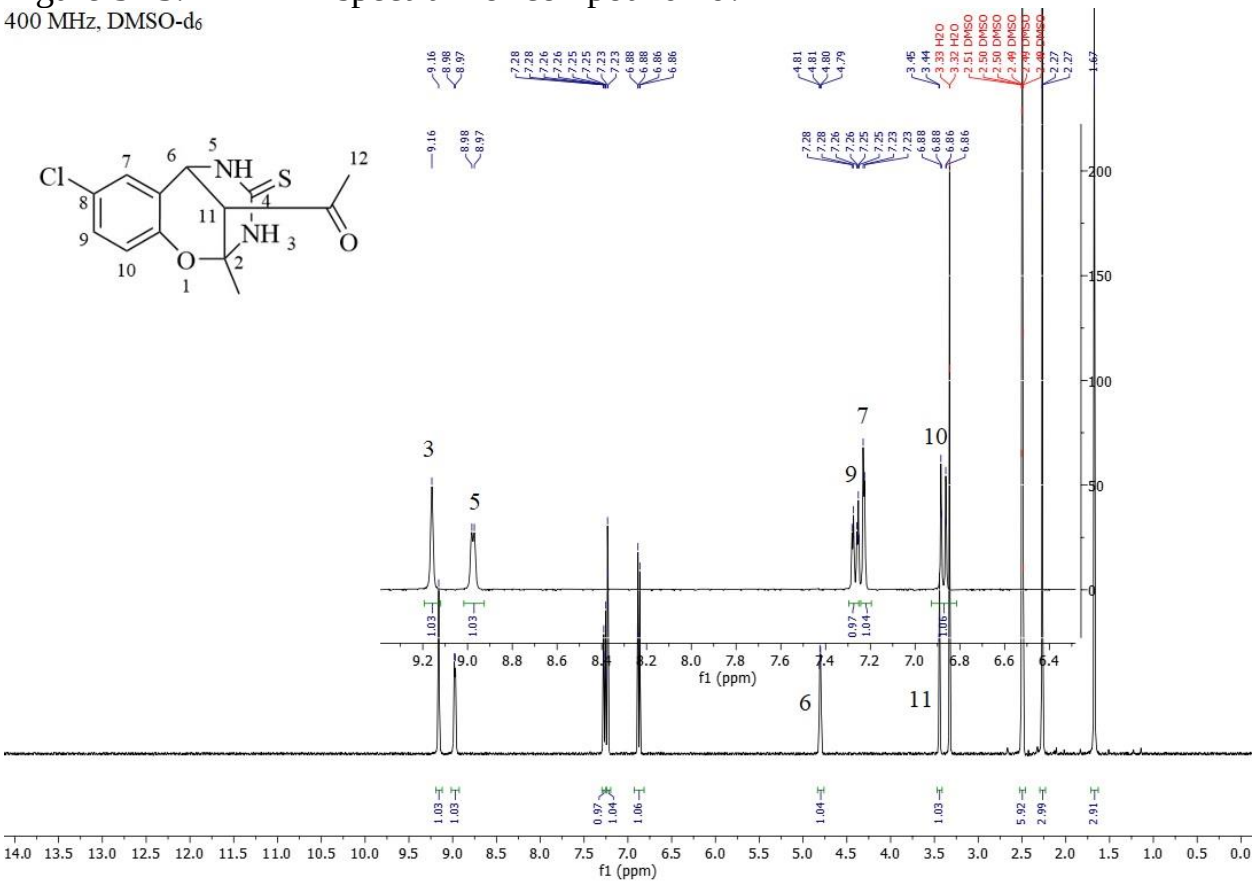

Figure SI-6. ^{1}H NMR spectrum of compound **1e**.

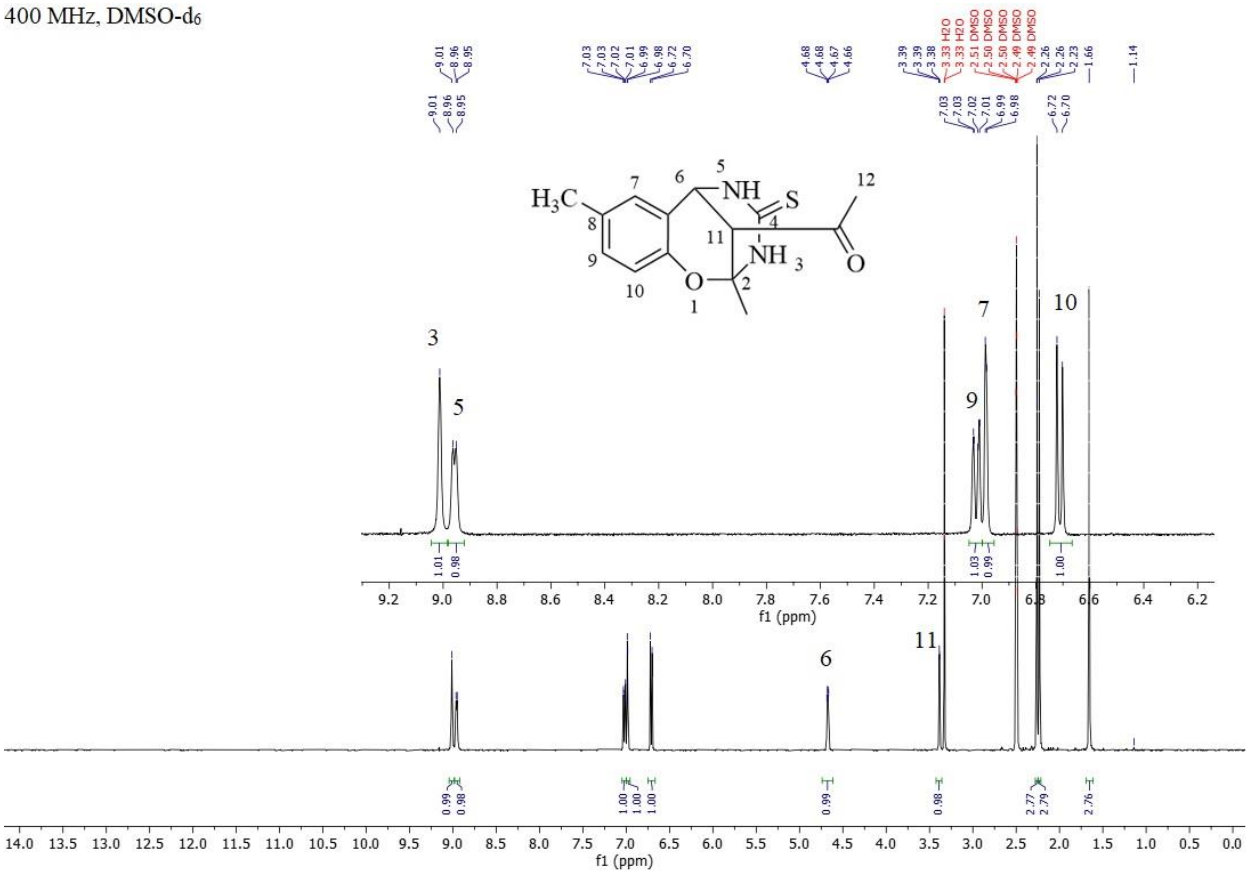

Figure SI-7. ^{1}H NMR spectrum of compound **1f**.

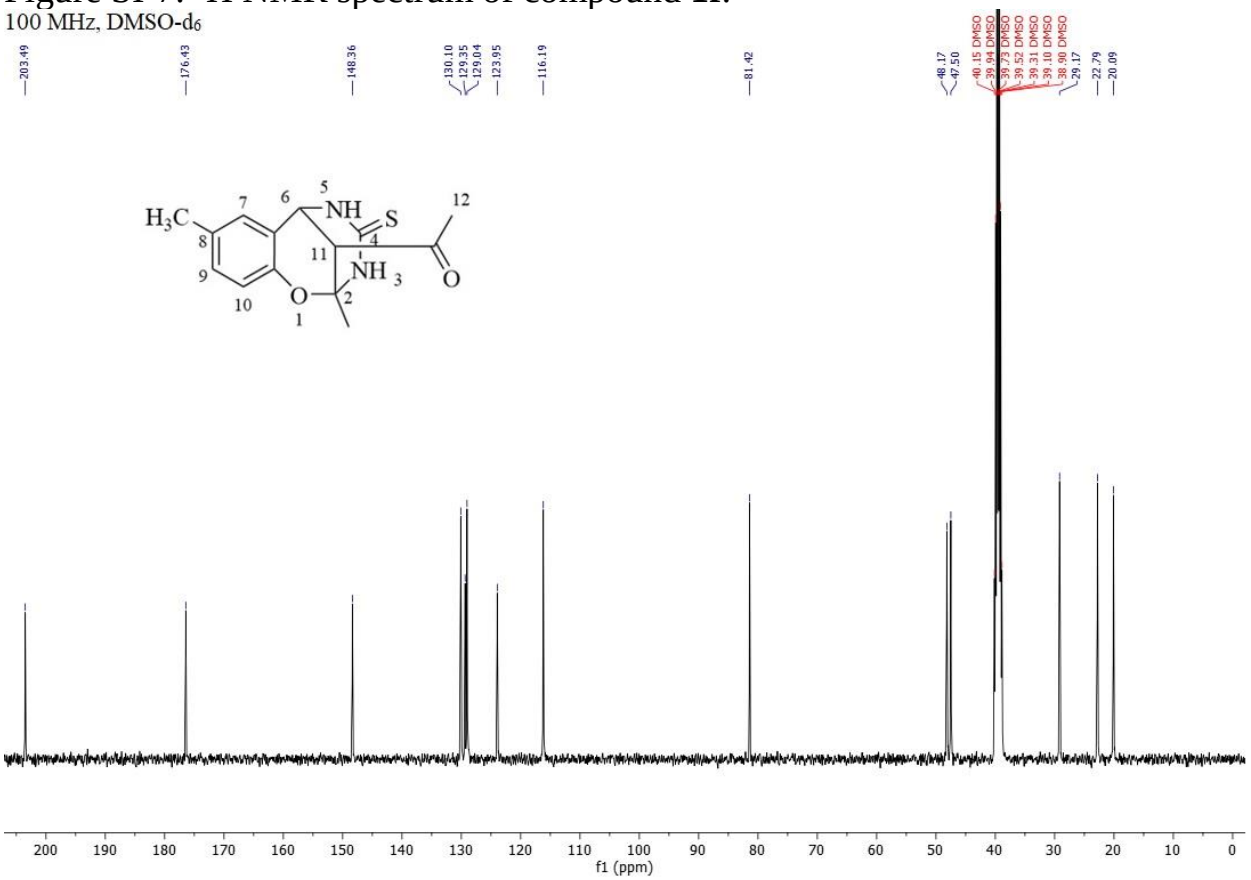

Figure SI-8. ^{13}C NMR spectrum of compound **1f**.

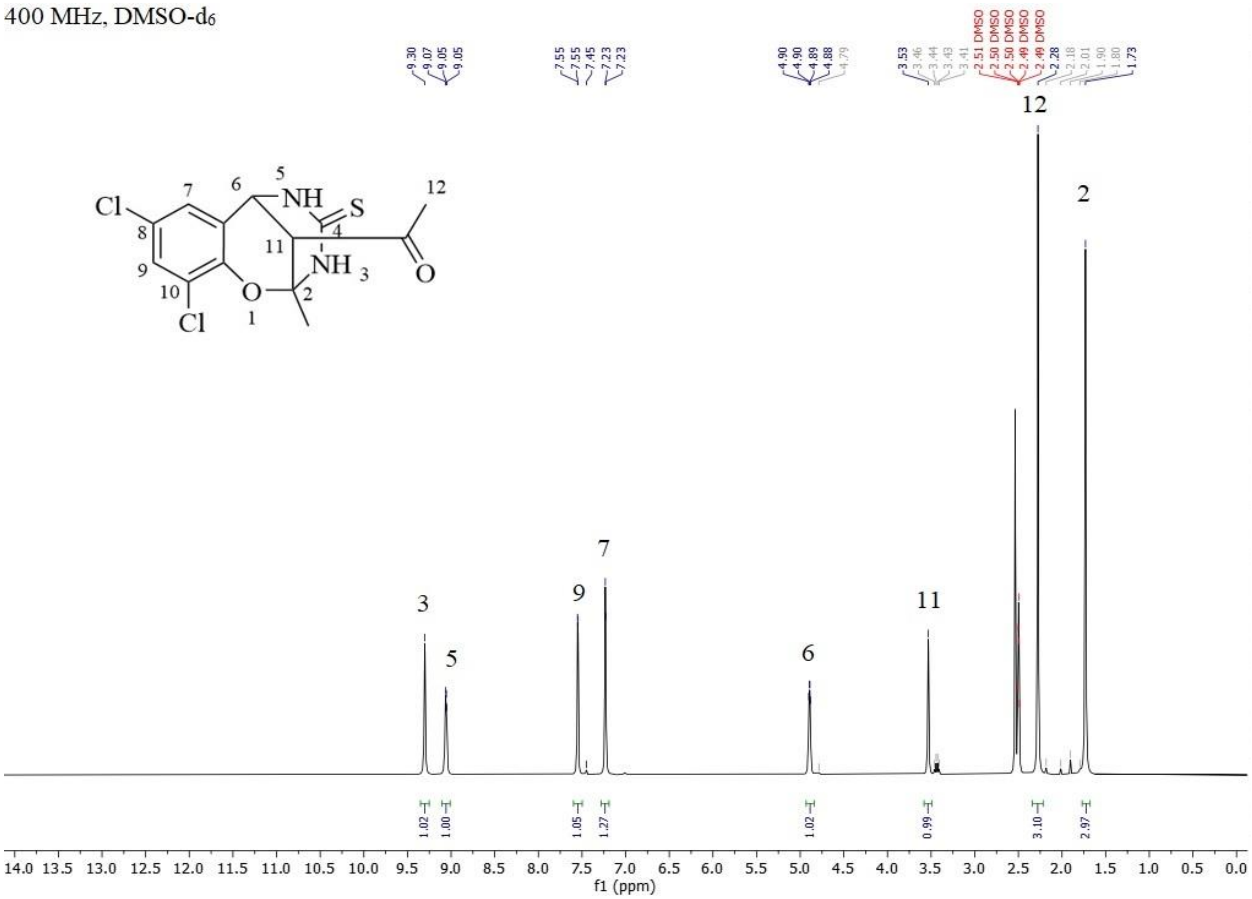

Figure SI-9. ^{1}H NMR spectrum of compound **1g**.

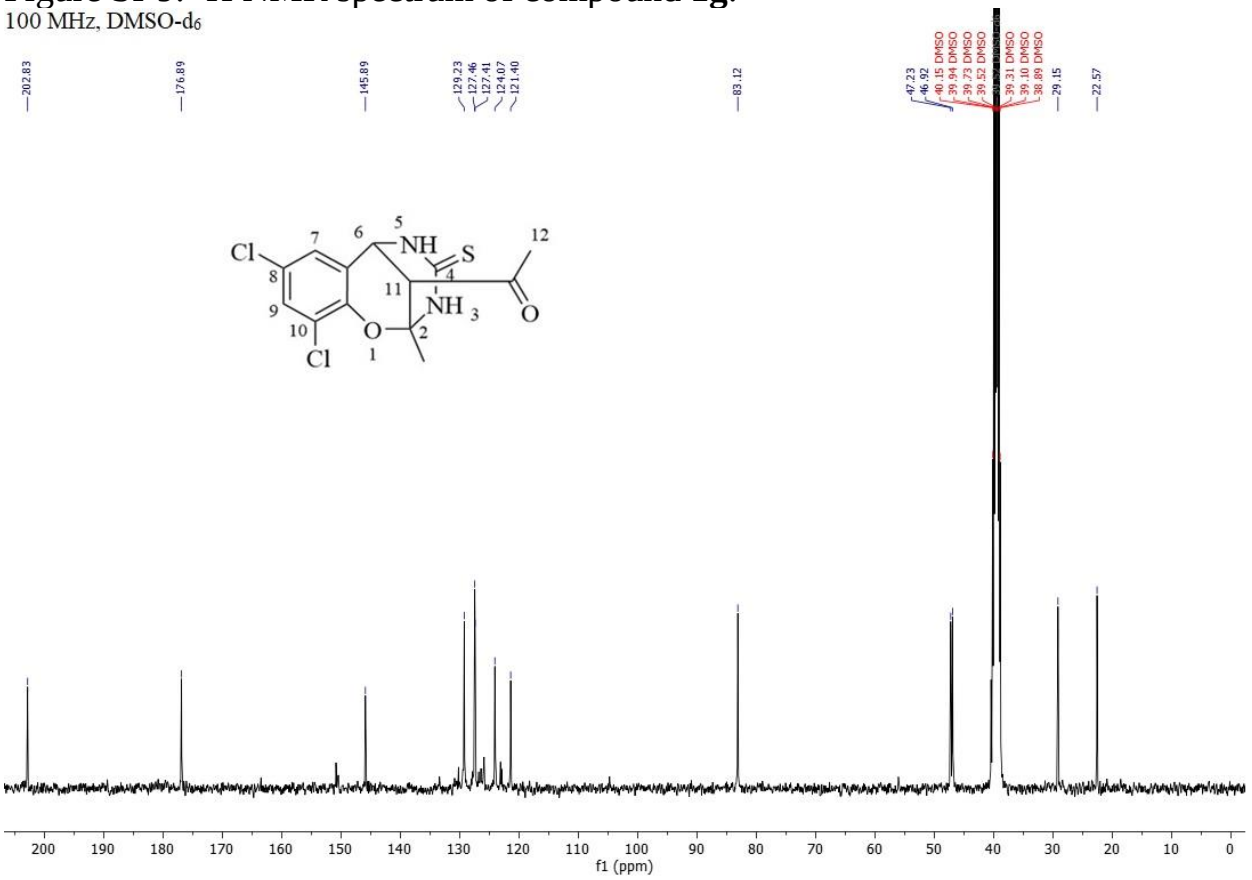

Figure SI-10. ^{13}C NMR spectrum of compound **1g**.

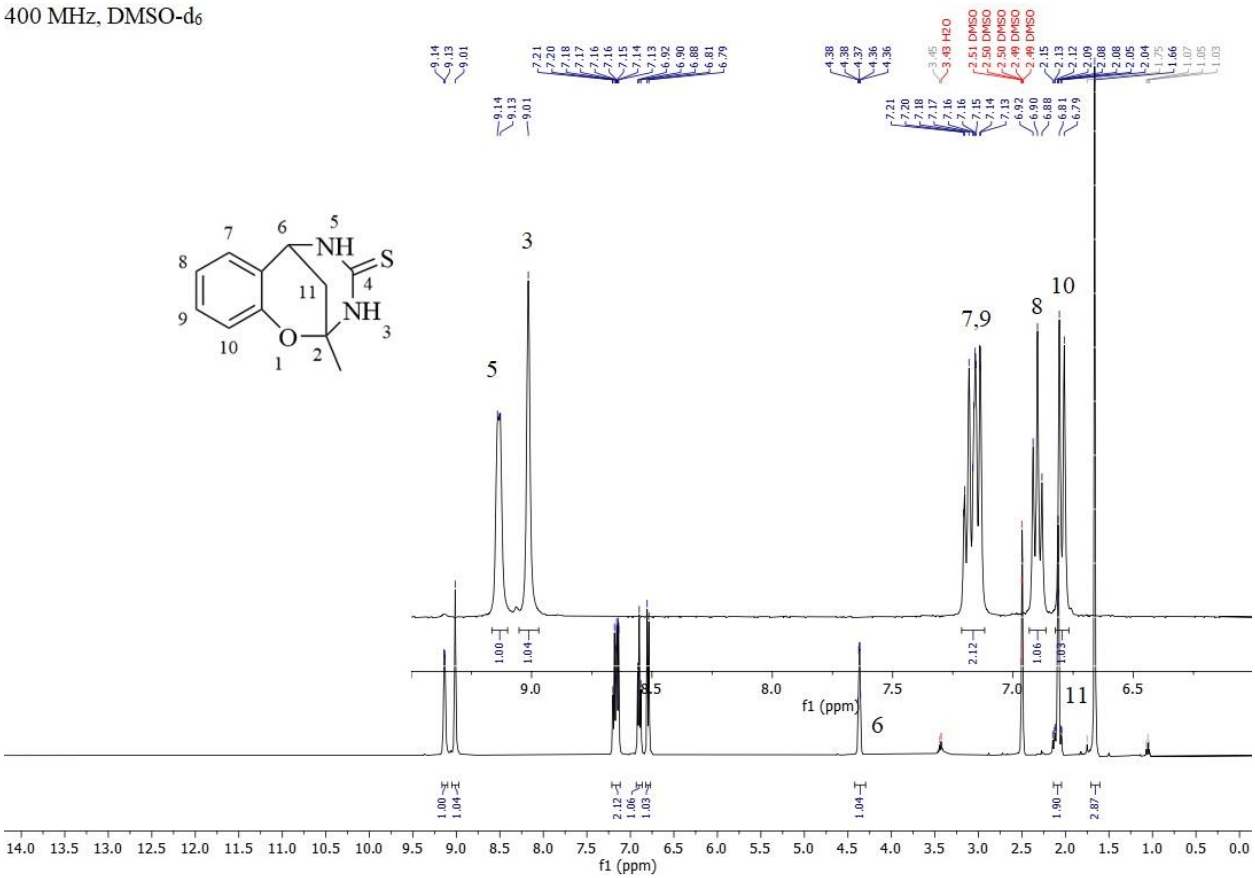

Figure SI-11. ^{13}C NMR spectrum of compound **4a**.

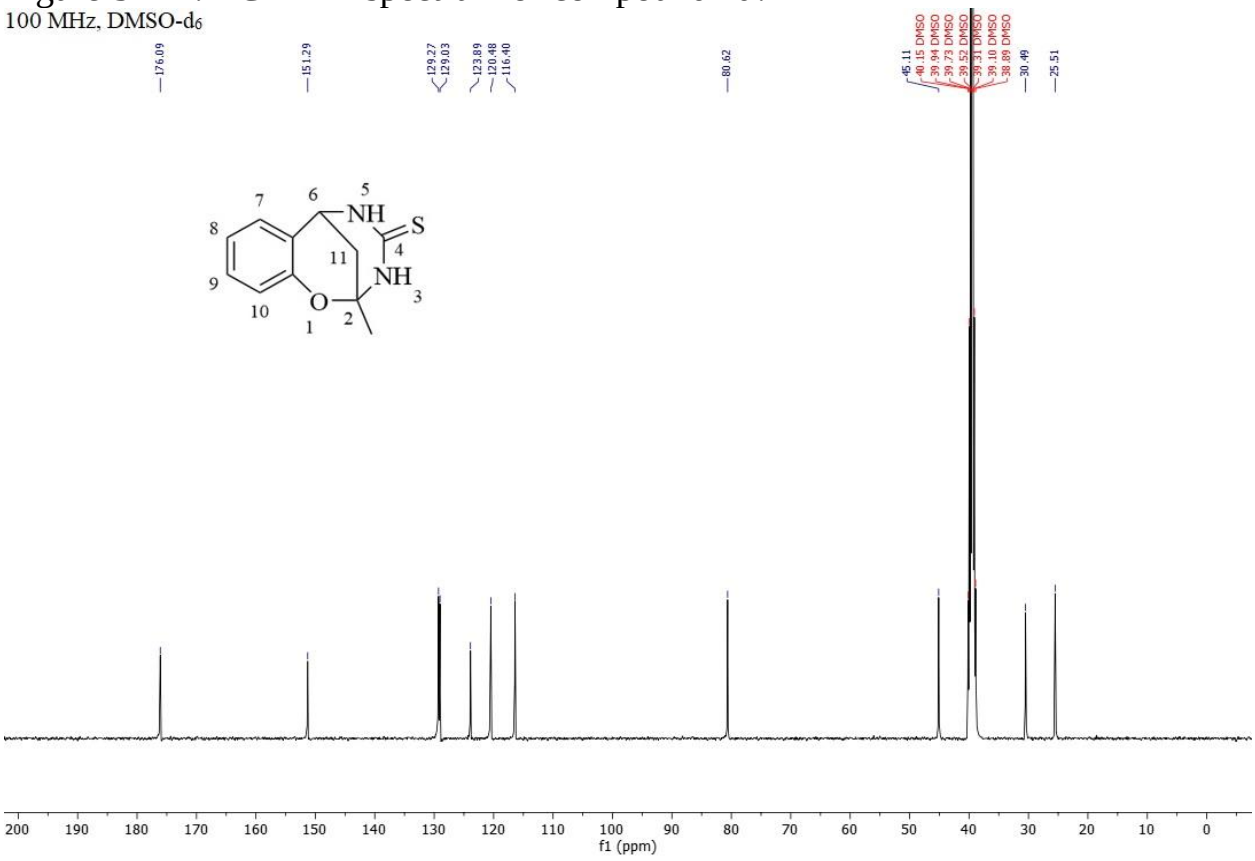

Figure SI-12. ^{13}C NMR spectrum of compound **4a**.

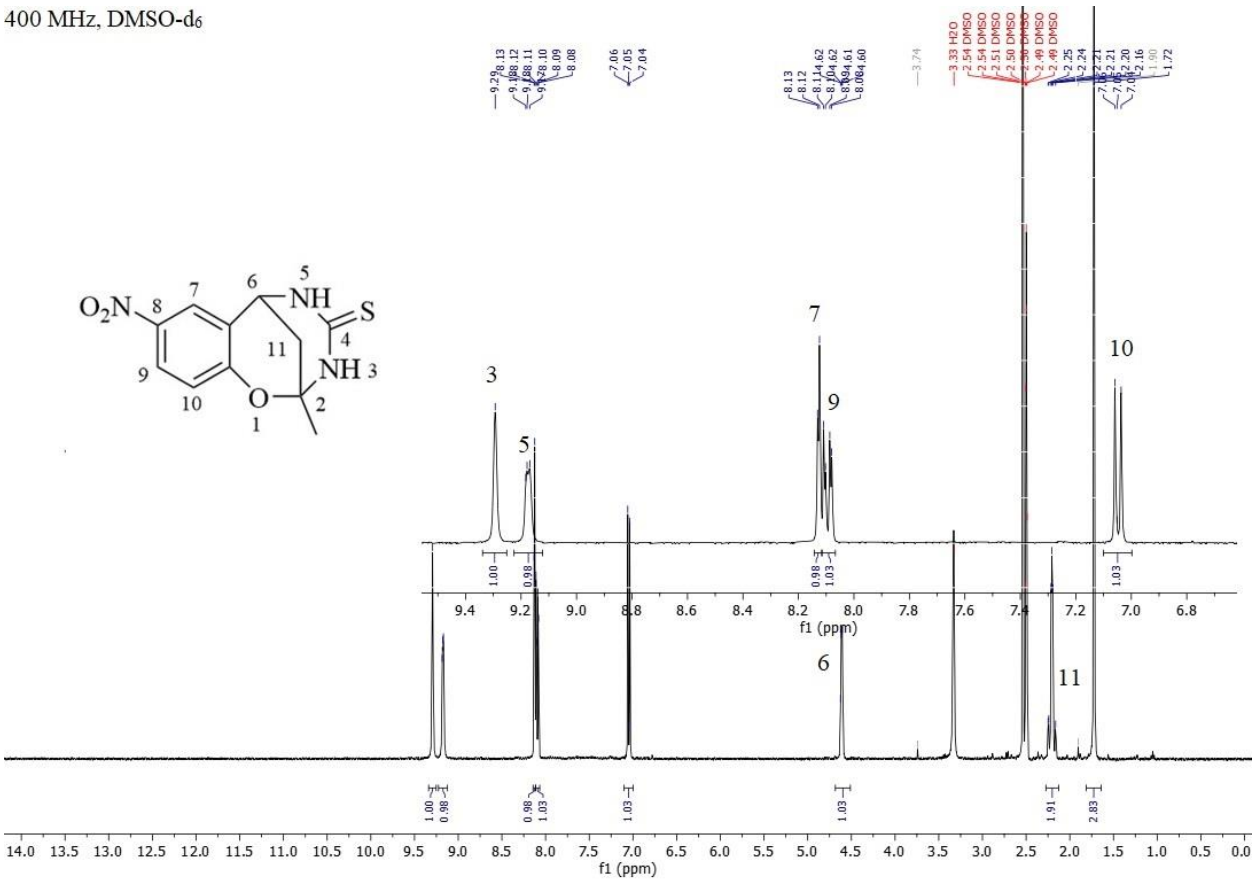

Figure SI-13. ^{1}H NMR spectrum of compound **4b**.

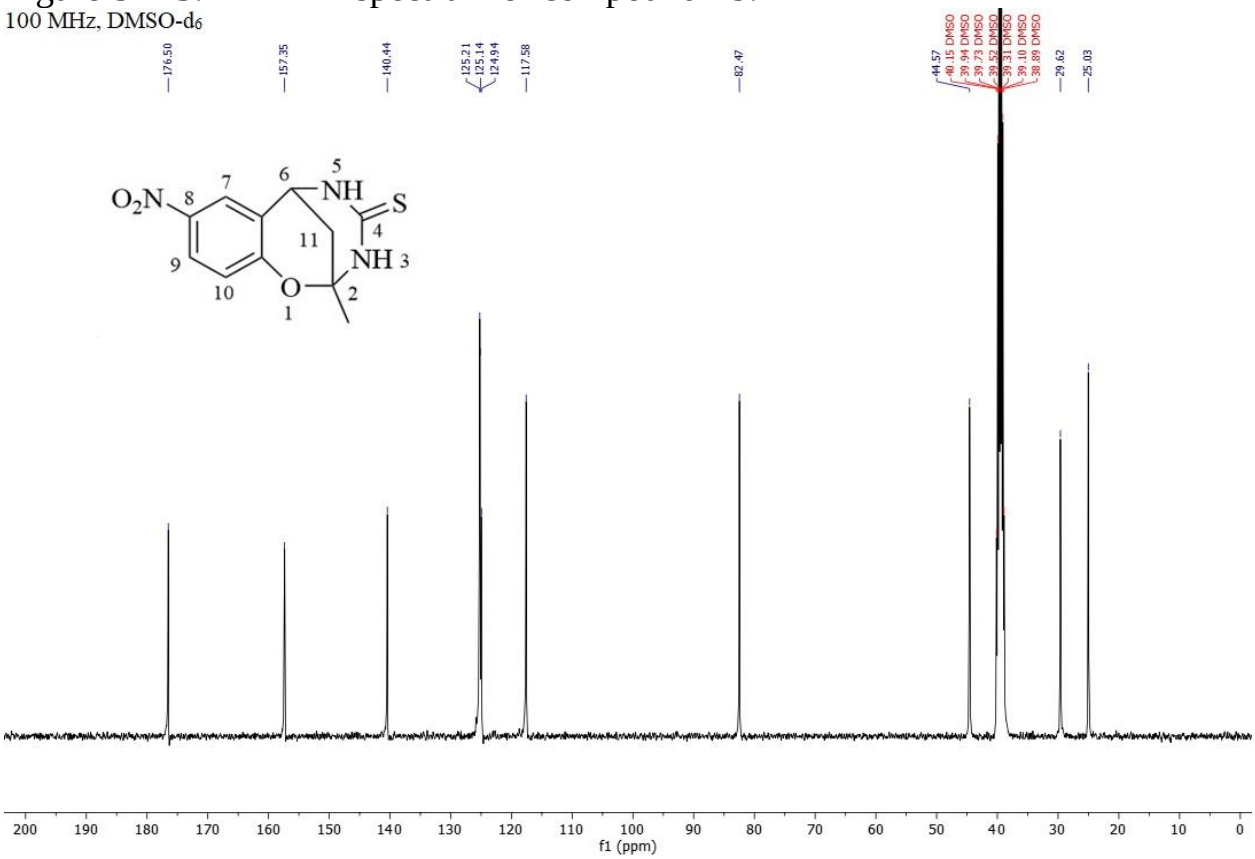

Figure SI-14. ^{13}C NMR spectrum of compound **4b**.

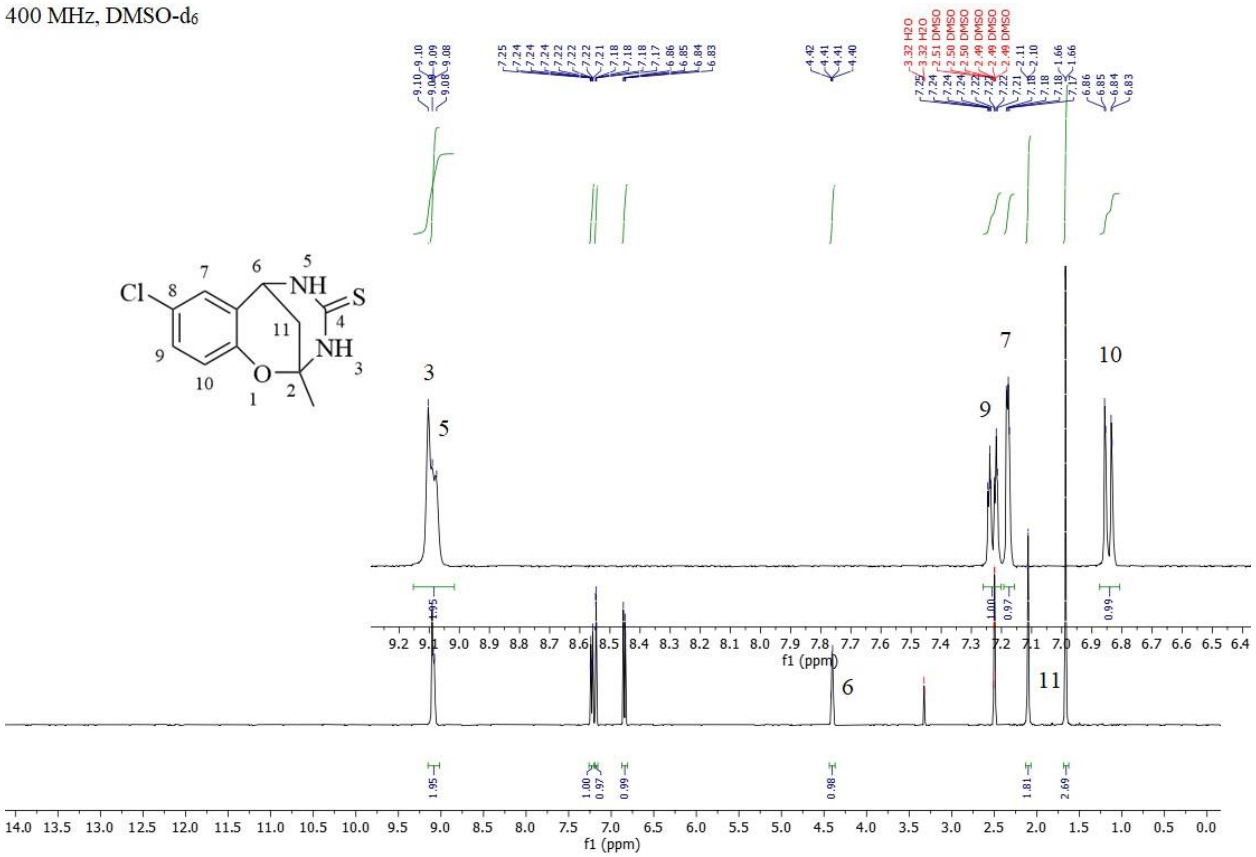

Figure SI-15. ^{1}H NMR spectrum of compound **4c**.

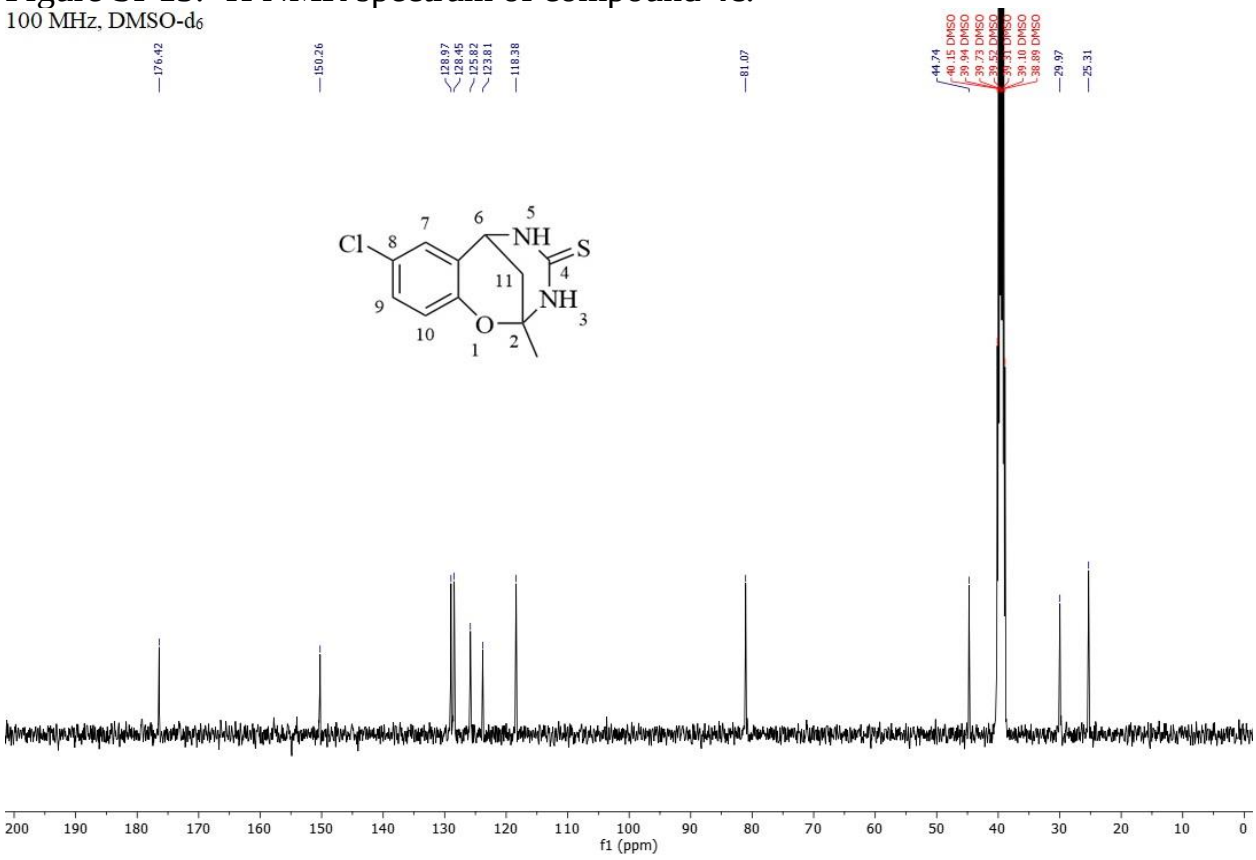

Figure SI-16. ^{13}C NMR spectrum of compound **4c**.

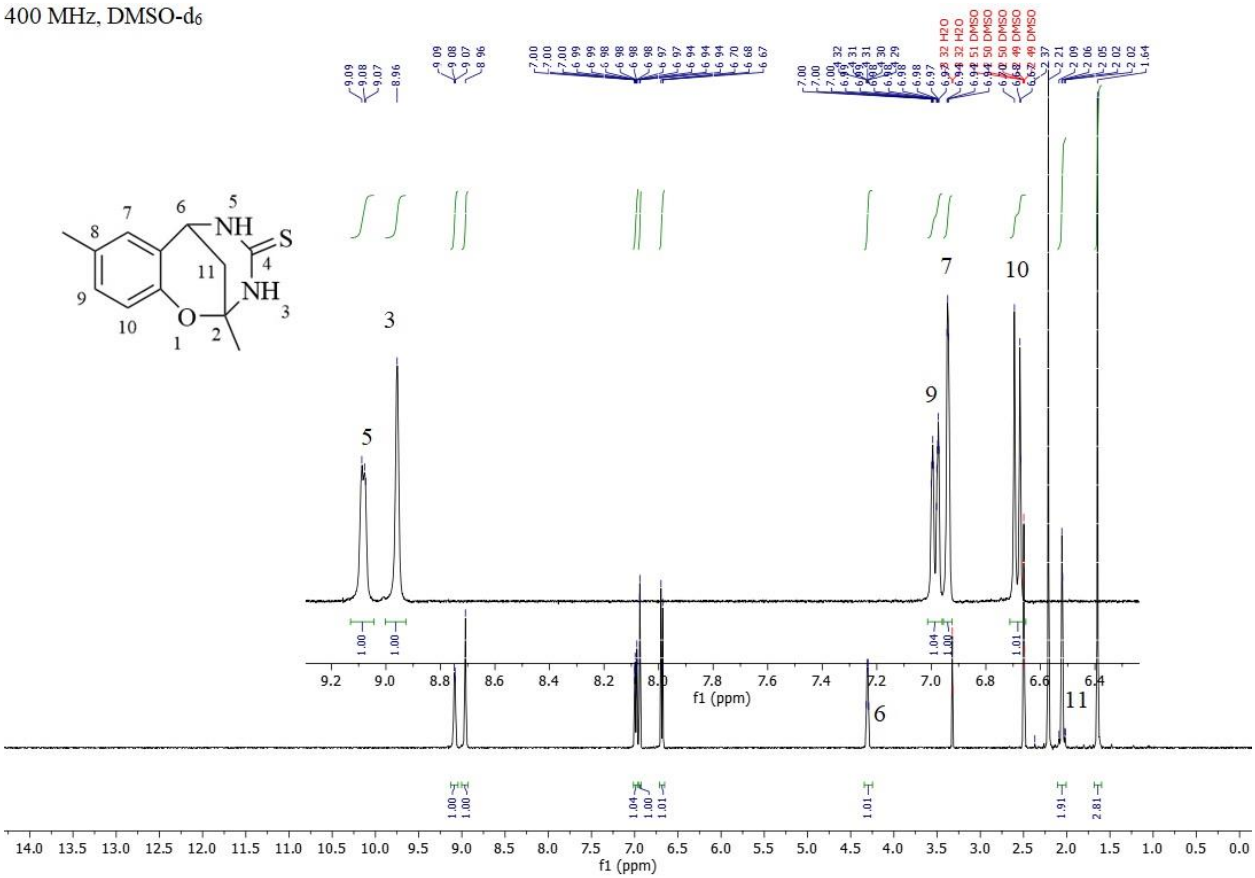

Figure SI-17. ^{1}H NMR spectrum of compound **4d**.

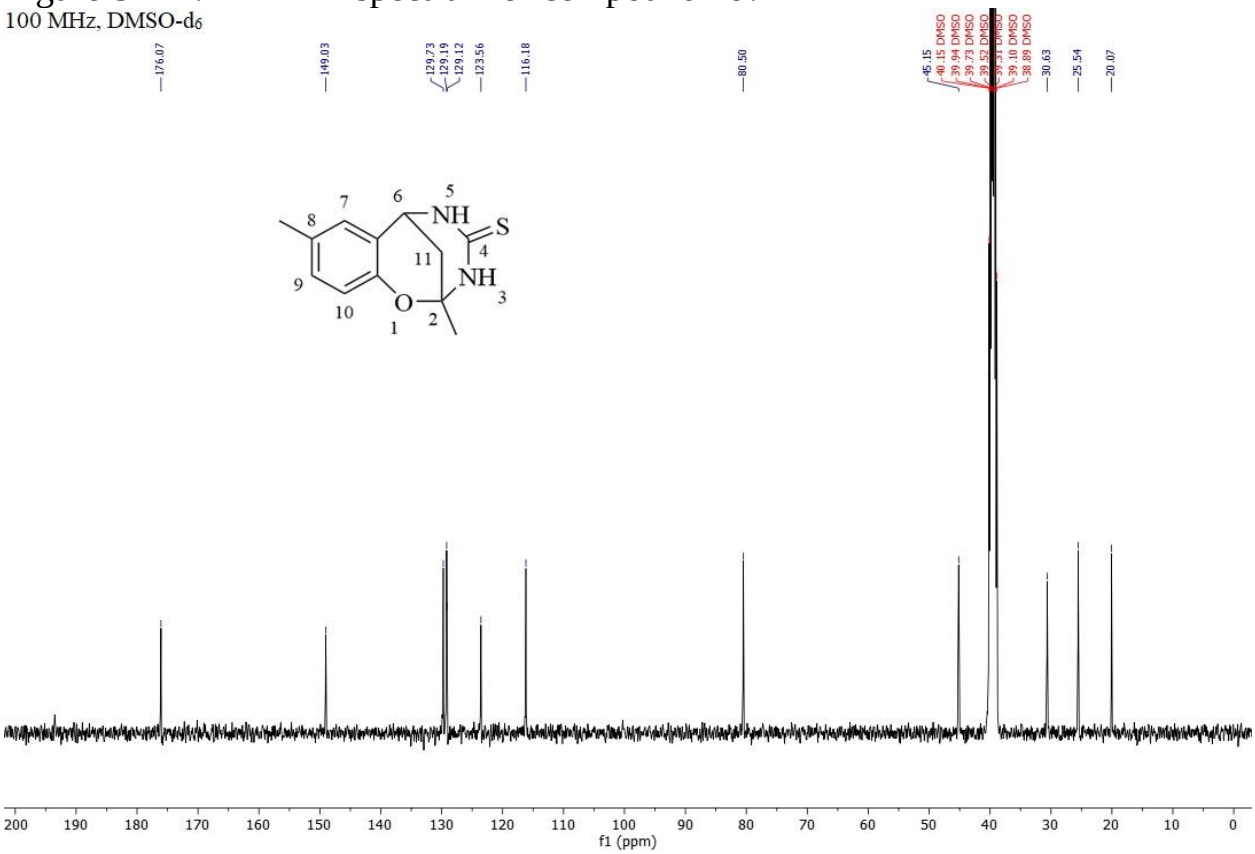

Figure SI-18. ^{13}C NMR spectrum of compound **4d**.

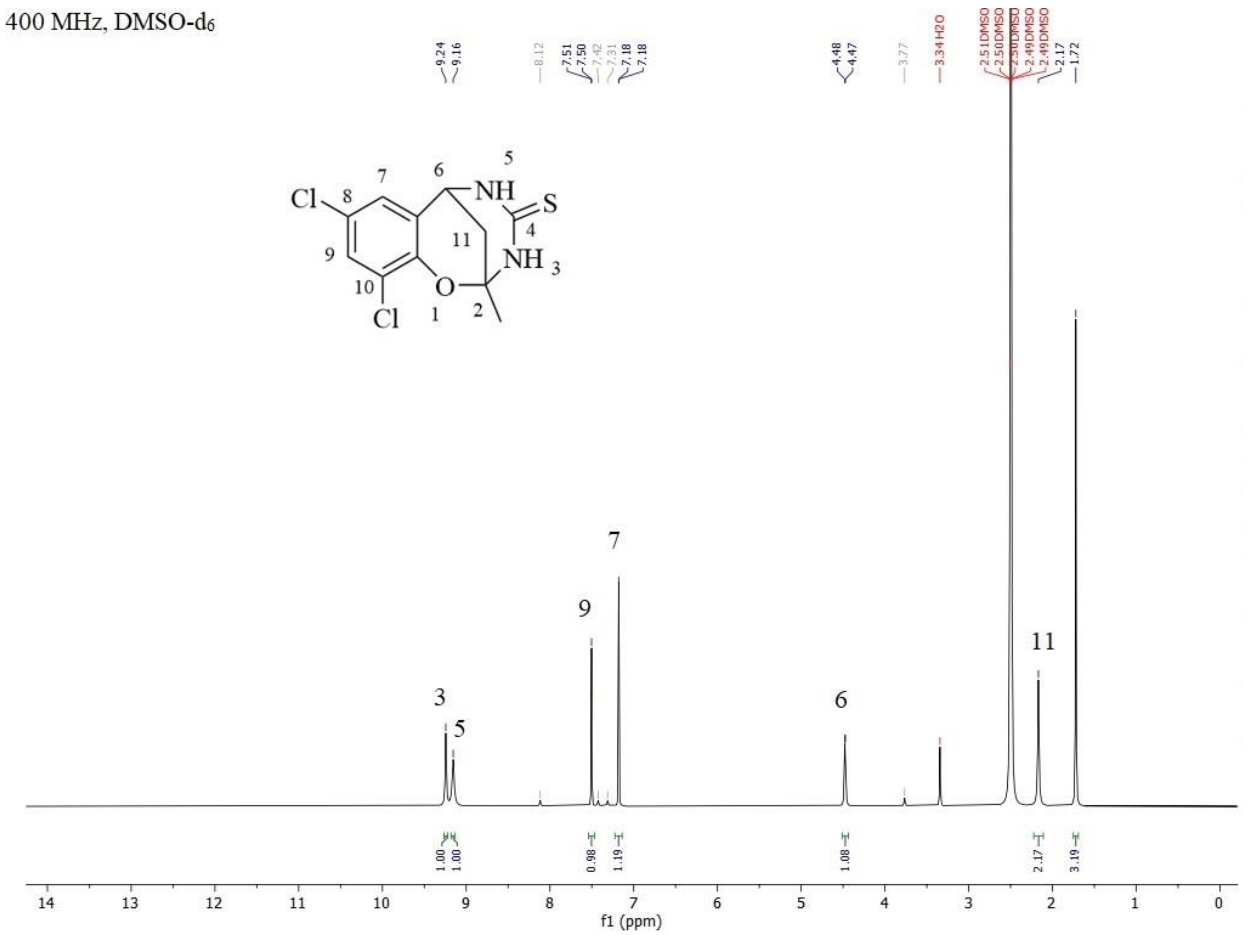

Figure SI-19. ^{1}H NMR spectrum of compound **4e**.

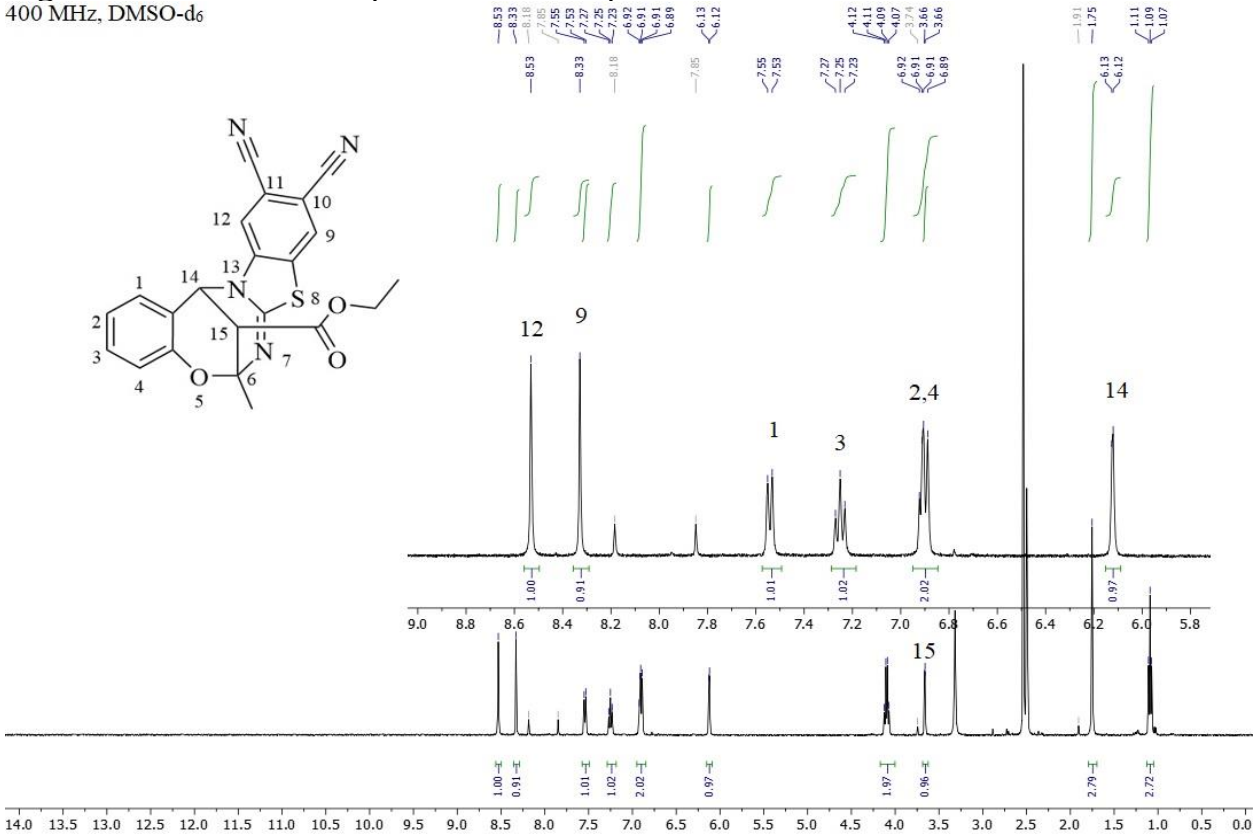

Figure SI-20. ^{1}H NMR spectrum of compound **3a**.

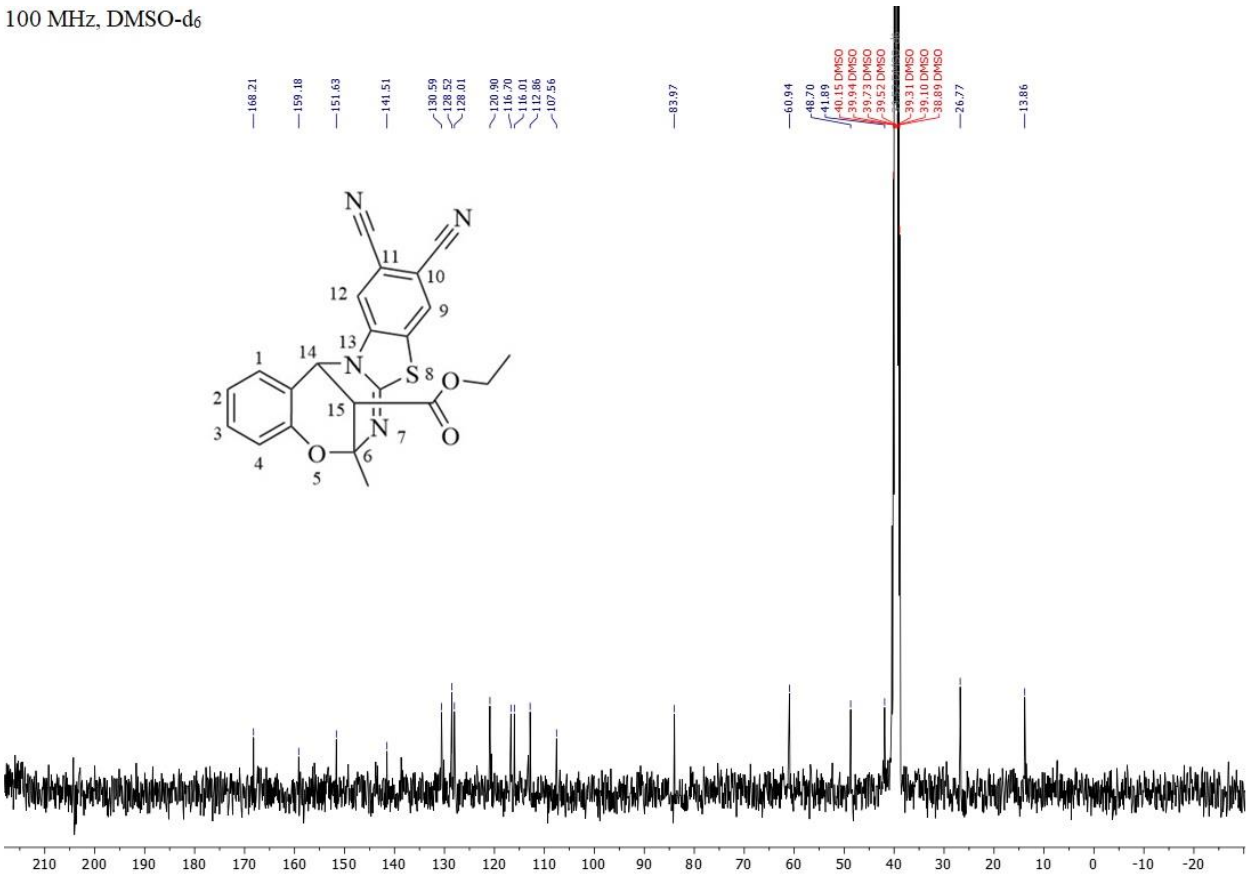

Figure SI-21. ^{13}C NMR spectrum of compound **3a**.

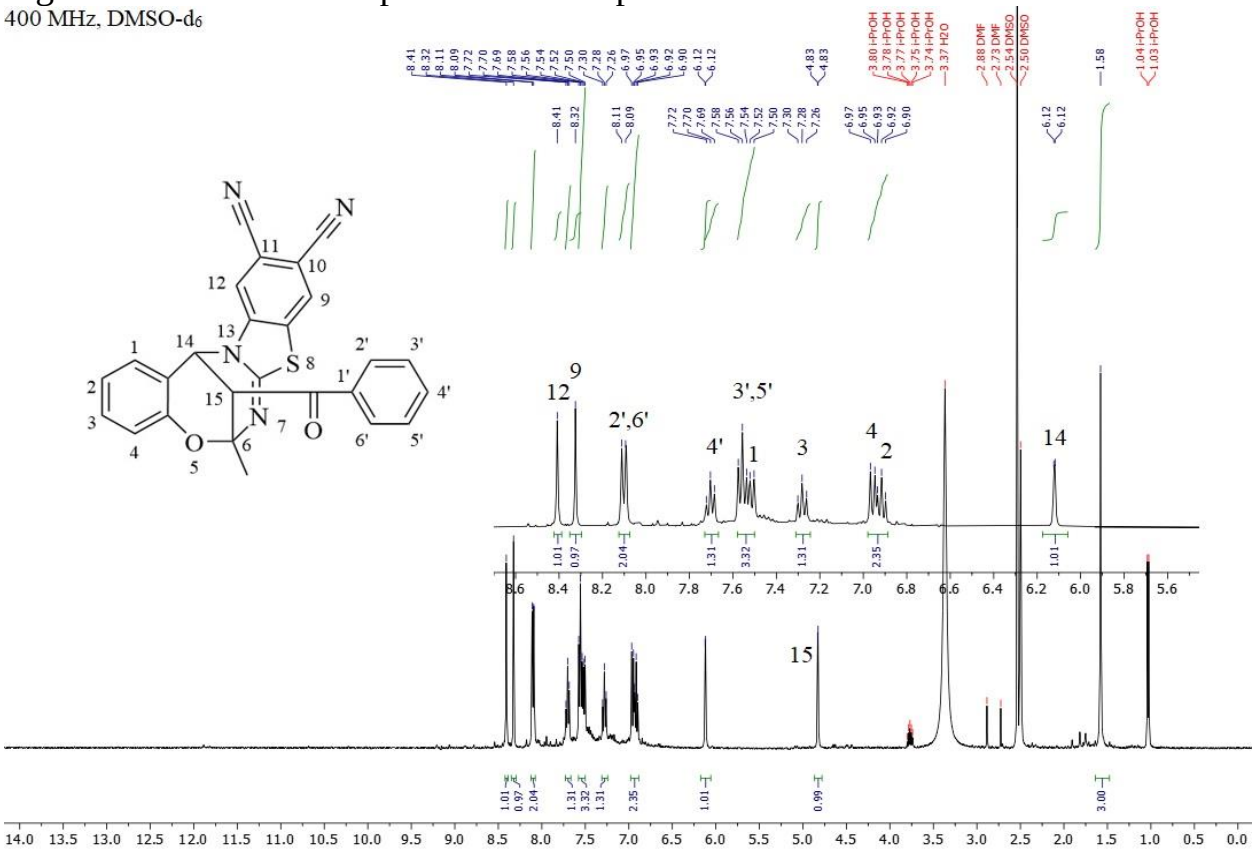

Figure SI-22. ^{1}H NMR spectrum of compound **3b**.

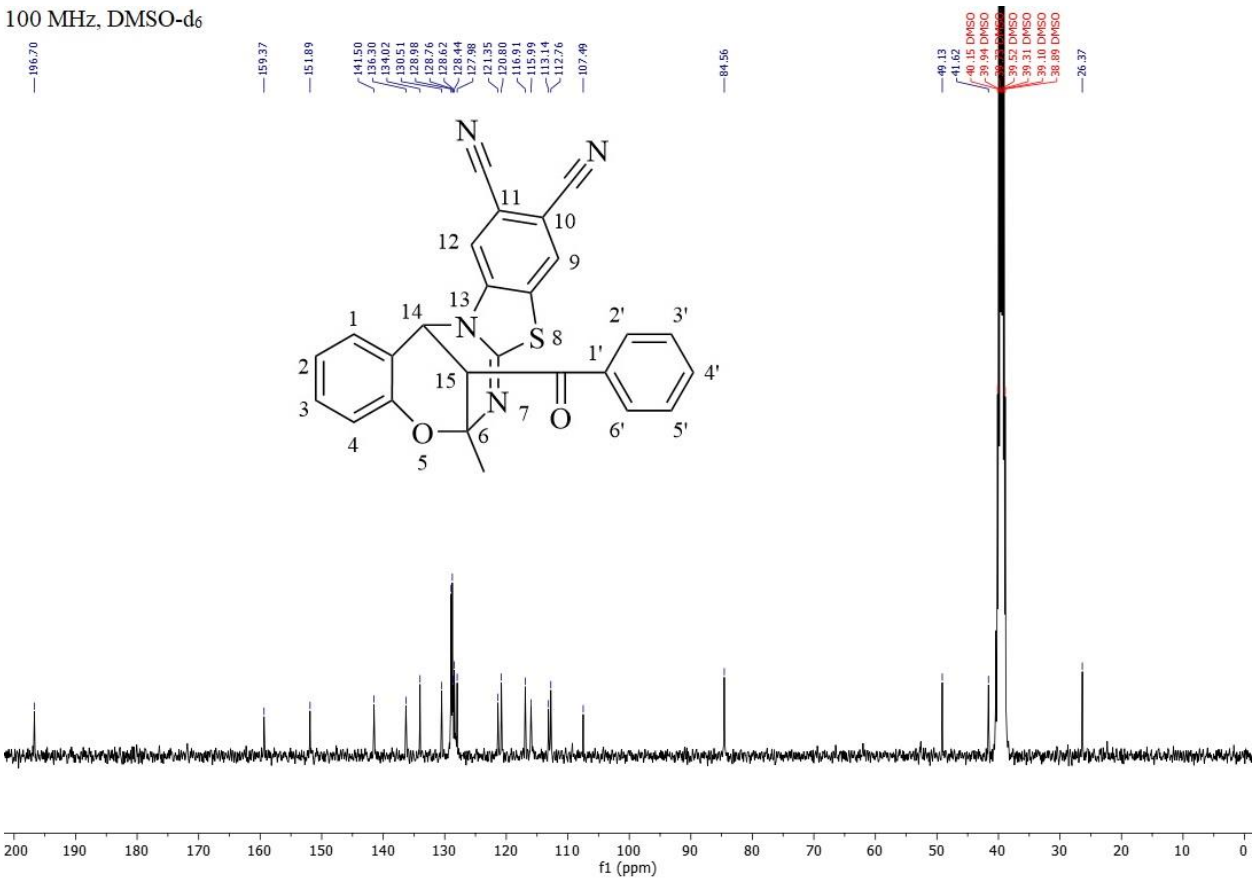

Figure SI-23. ^{13}C NMR spectrum of compound **3b**.

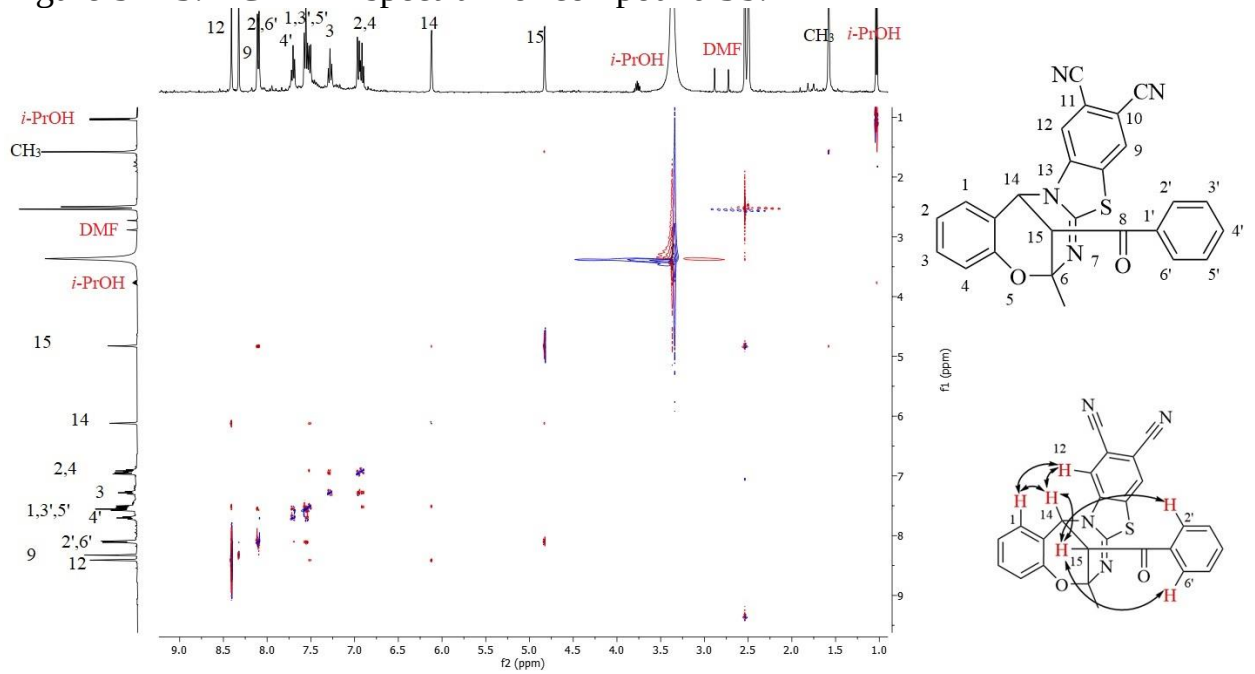

Figure SI-24. NOESY spectrum of compound **3b**.

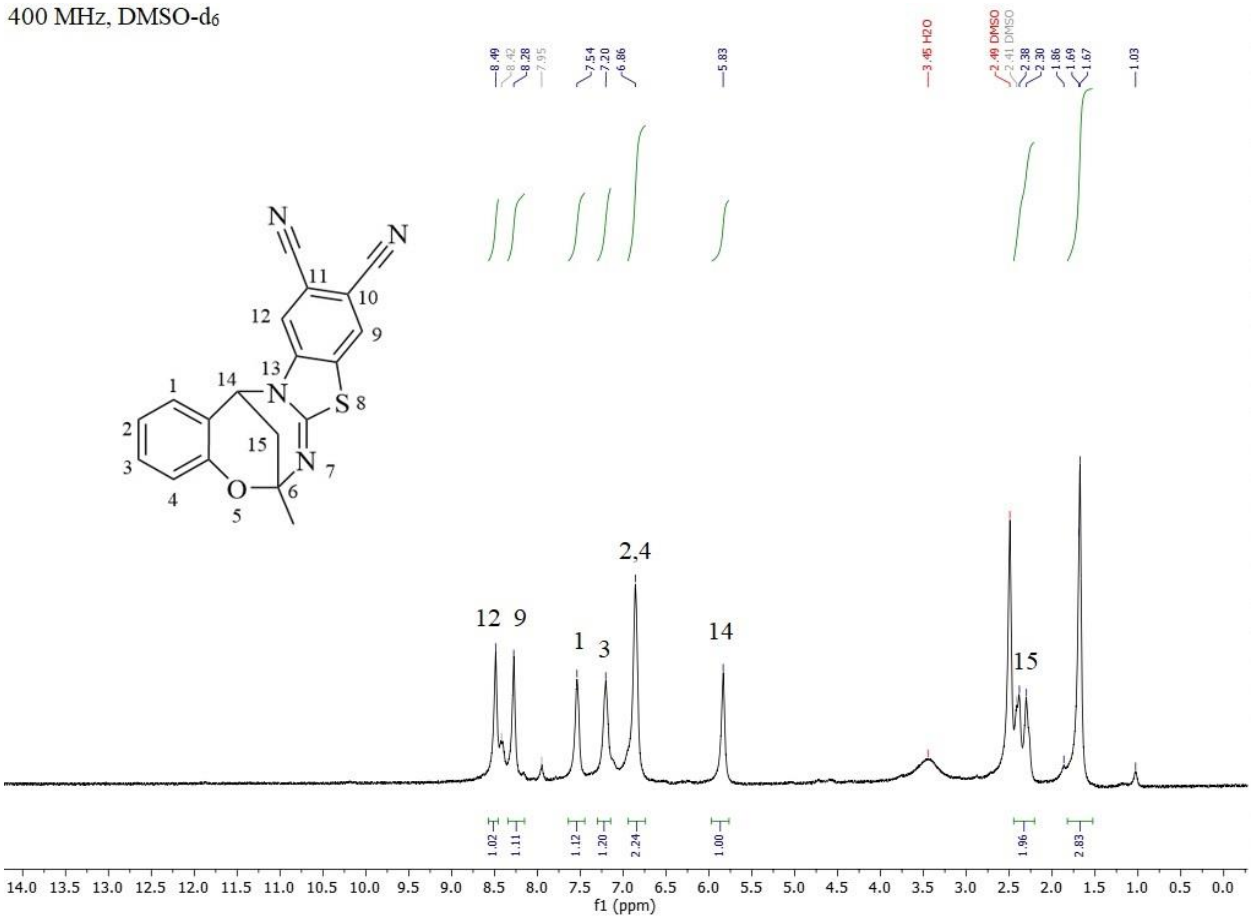

Figure SI-25. ^{1}H NMR spectrum of compound **5a**.
Compound **5a** exhibits broadened ^{1}H NMR signals due to intrinsic molecular properties, unaffected by purification.

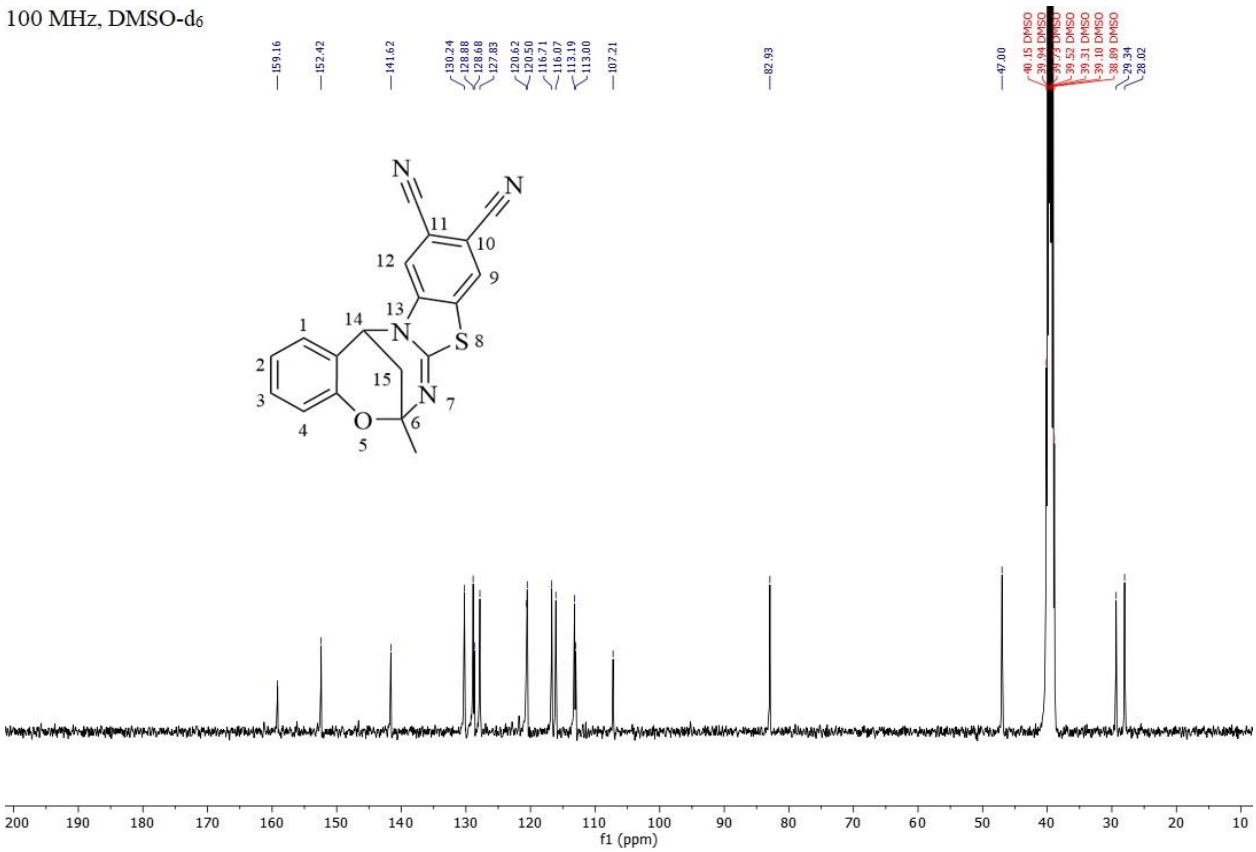

Figure SI-26. ^{13}C NMR spectrum of compound **5a**.

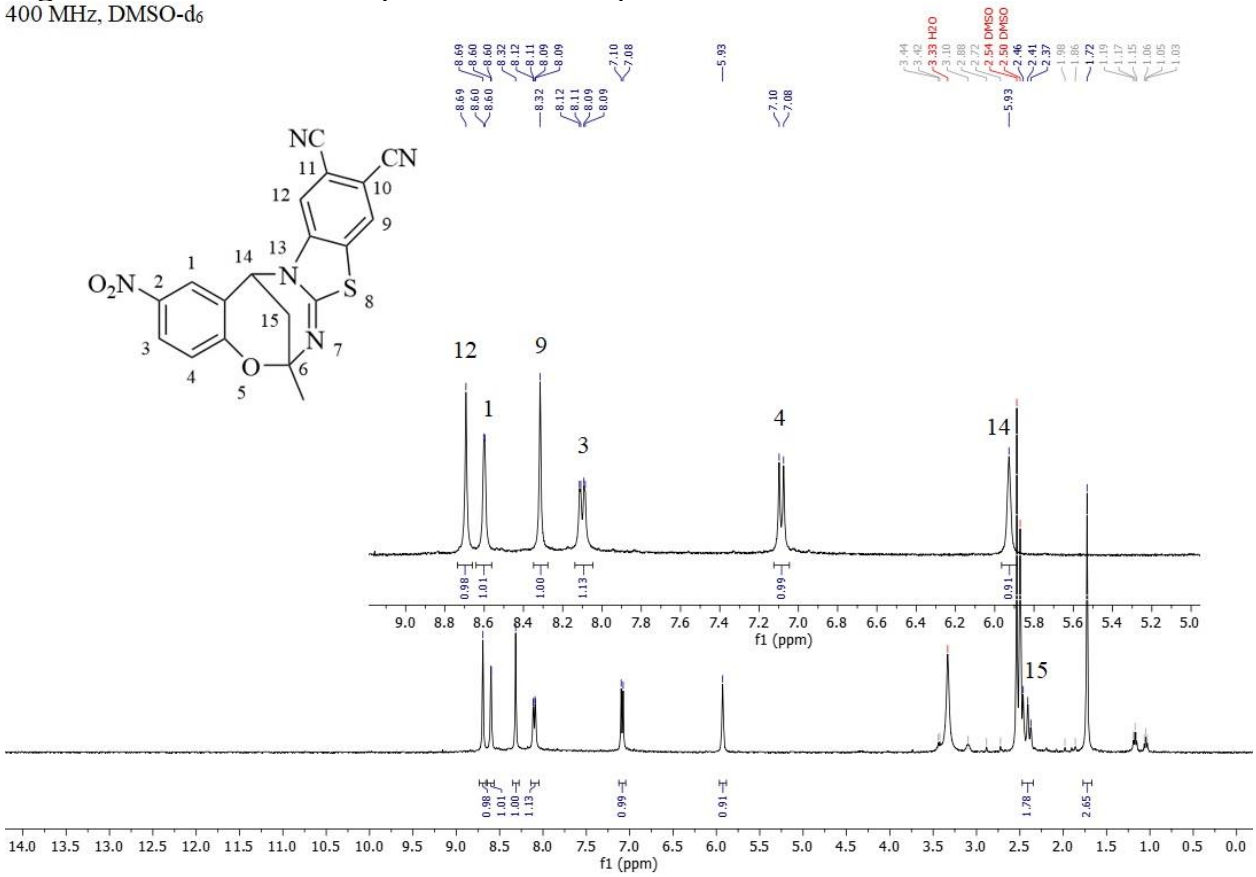

Figure SI-27. ^{1}H NMR spectrum of compound **5b**.

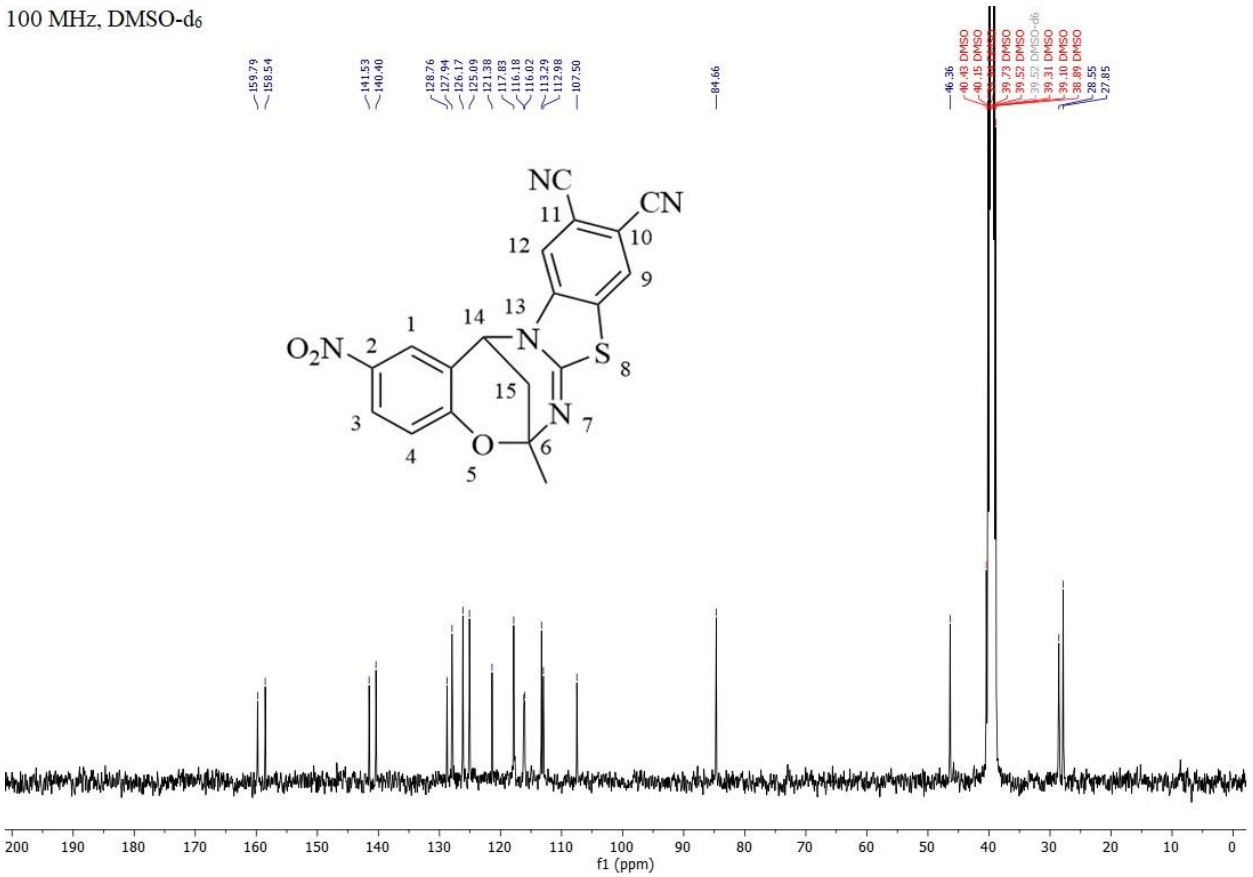

Figure SI-28. ^{13}C NMR spectrum of compound **5b**.

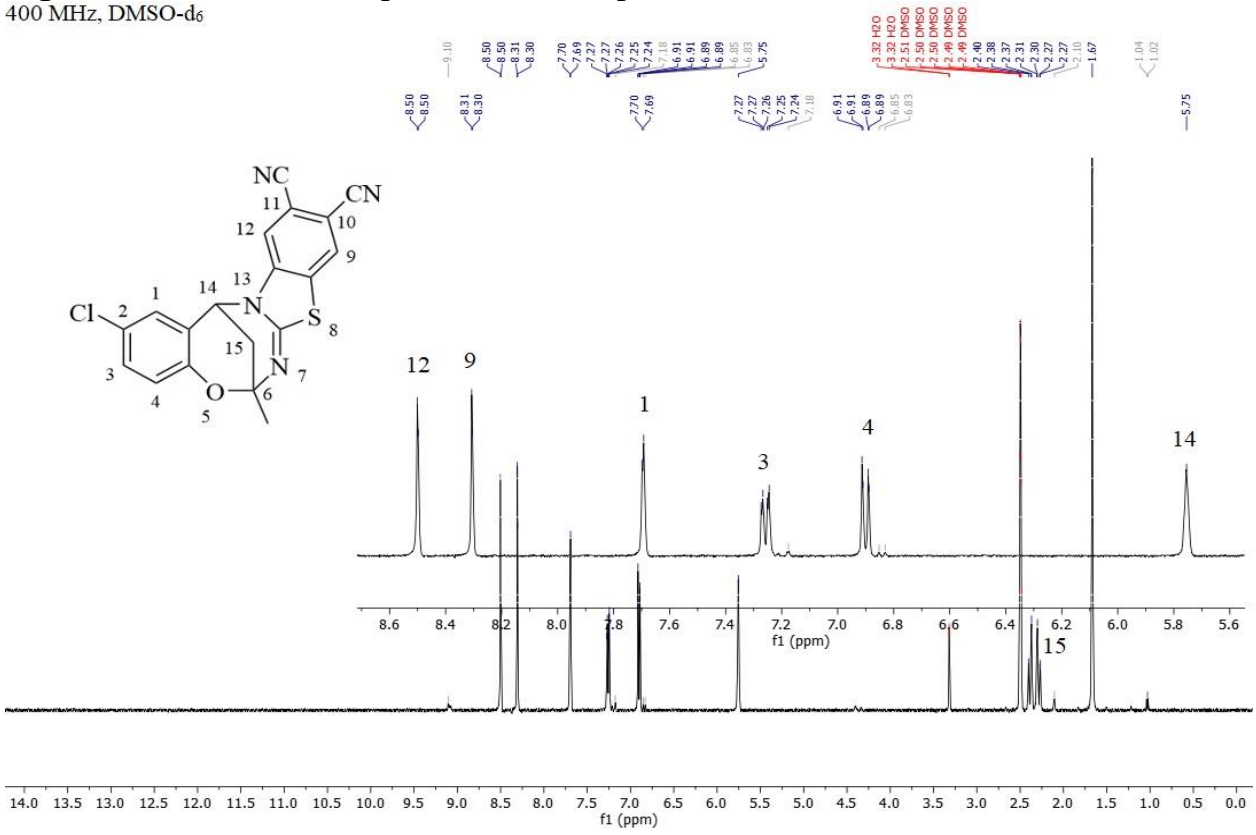

Figure SI-29. ^{1}H NMR spectrum of compound **5c**.

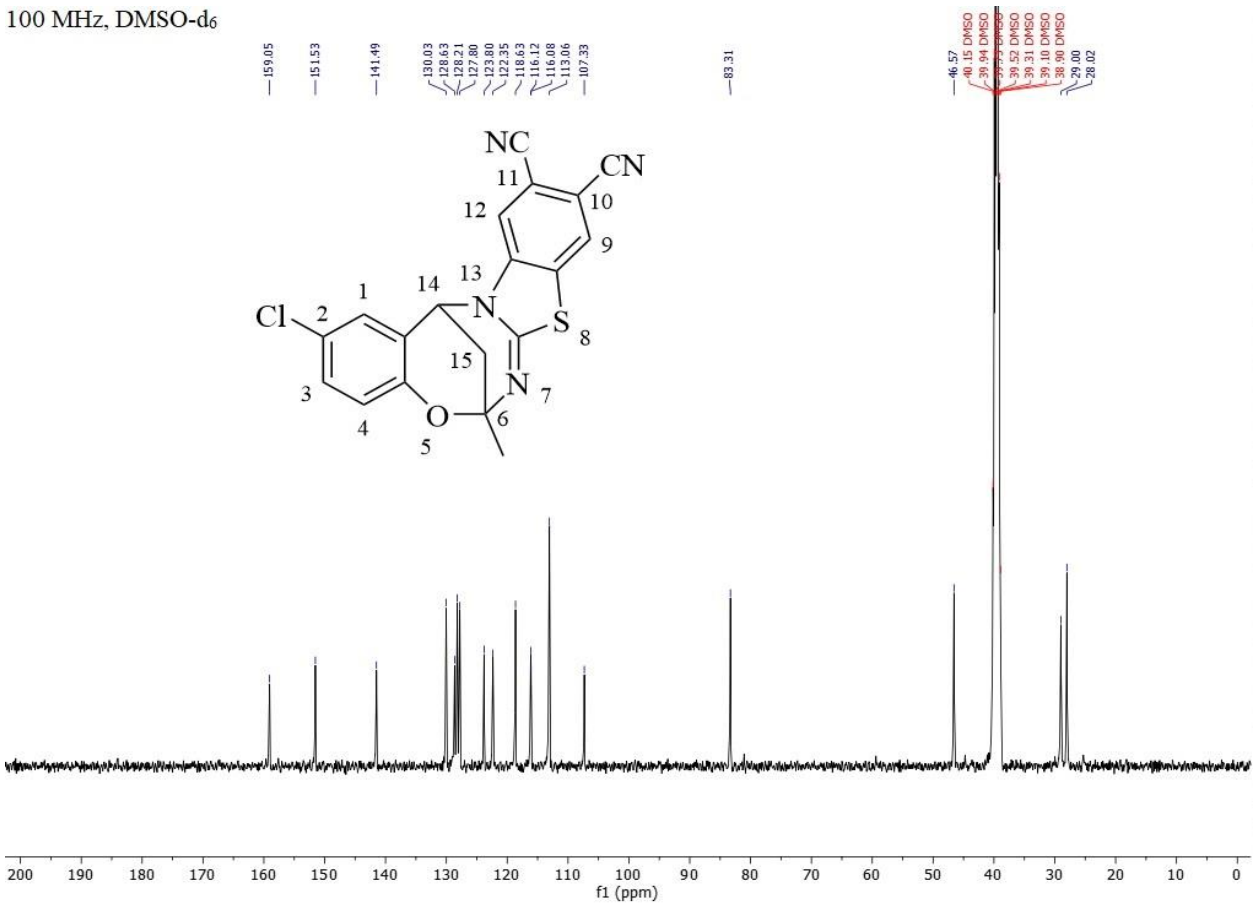

Figure SI-30. ^{13}C NMR spectrum of compound **5c**.

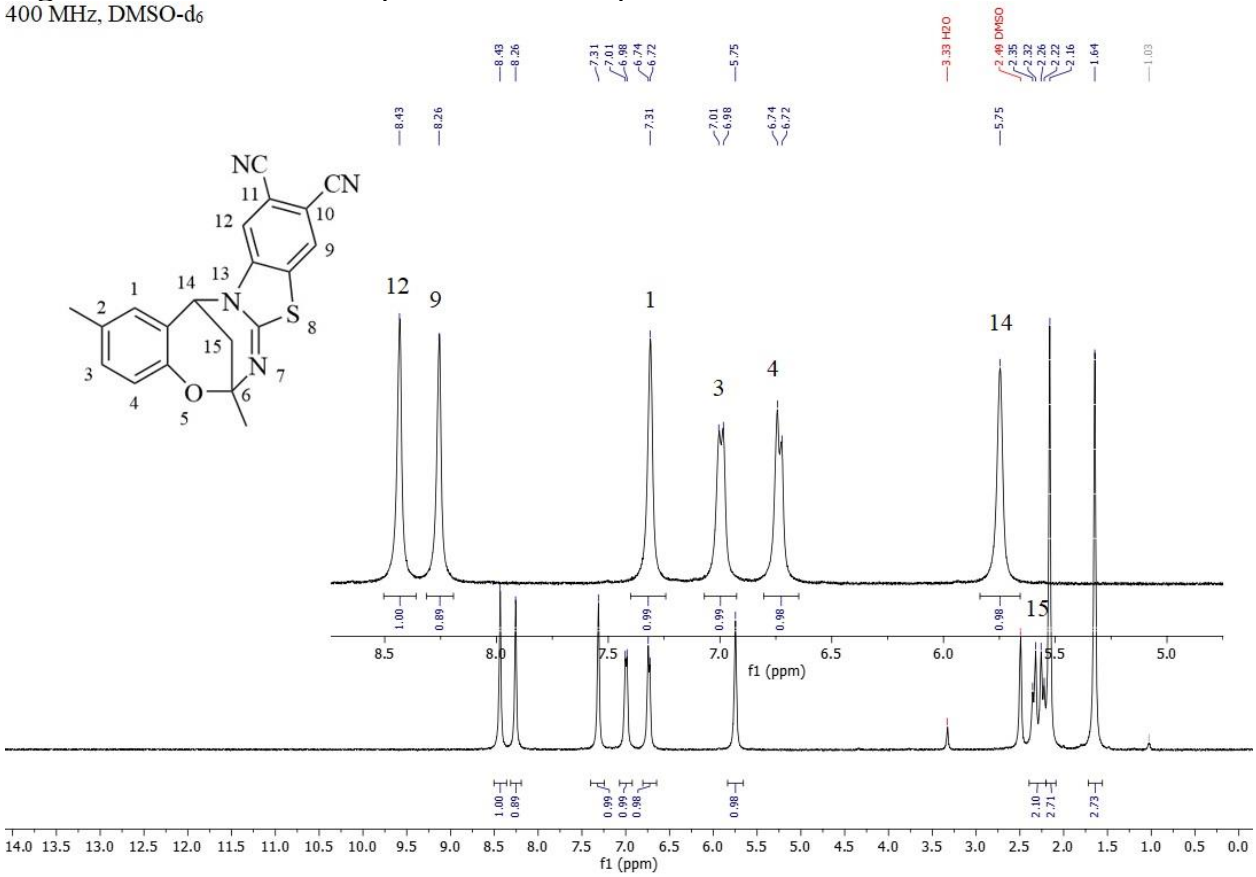

Figure SI-31. ^{1}H NMR spectrum of compound **5d**.

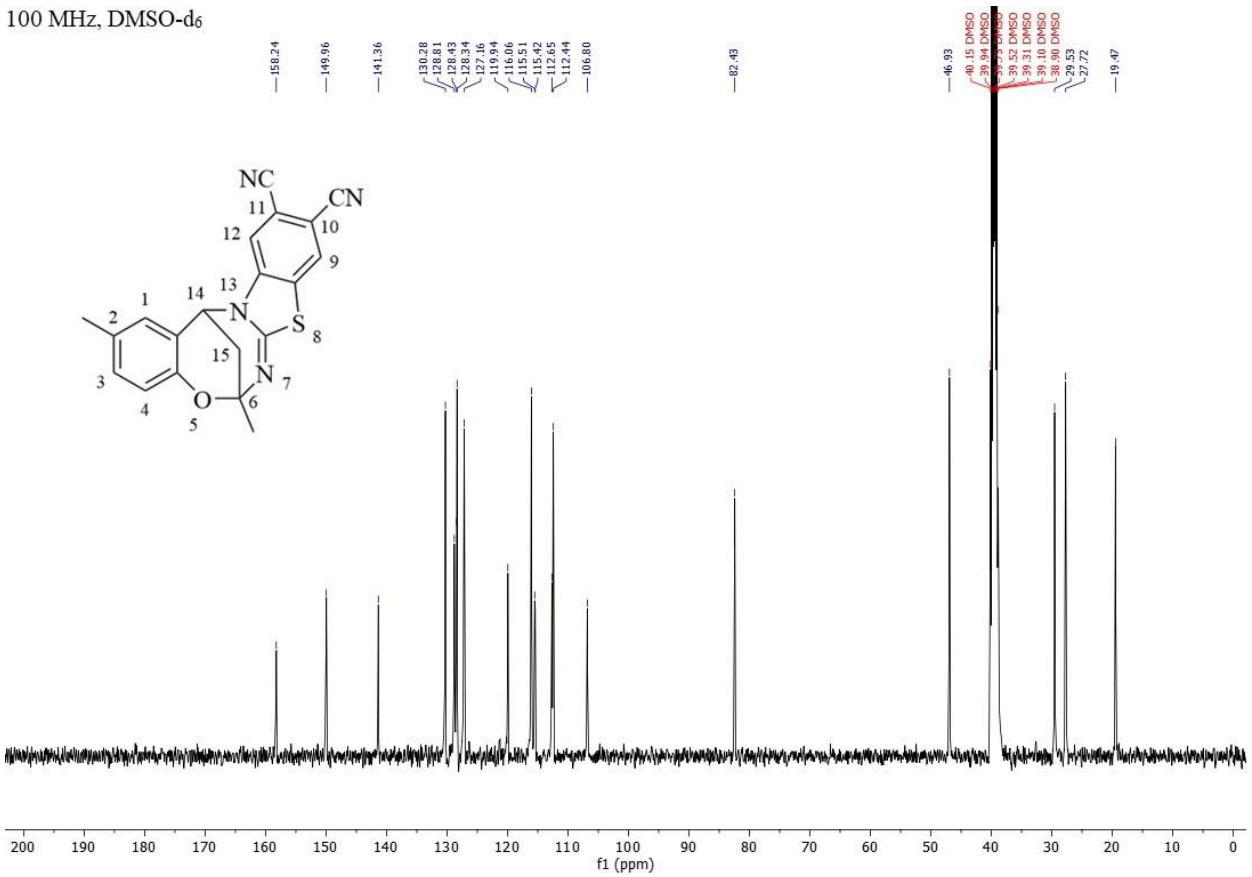

Figure SI-32. ^{13}C NMR spectrum of compound **5d**.

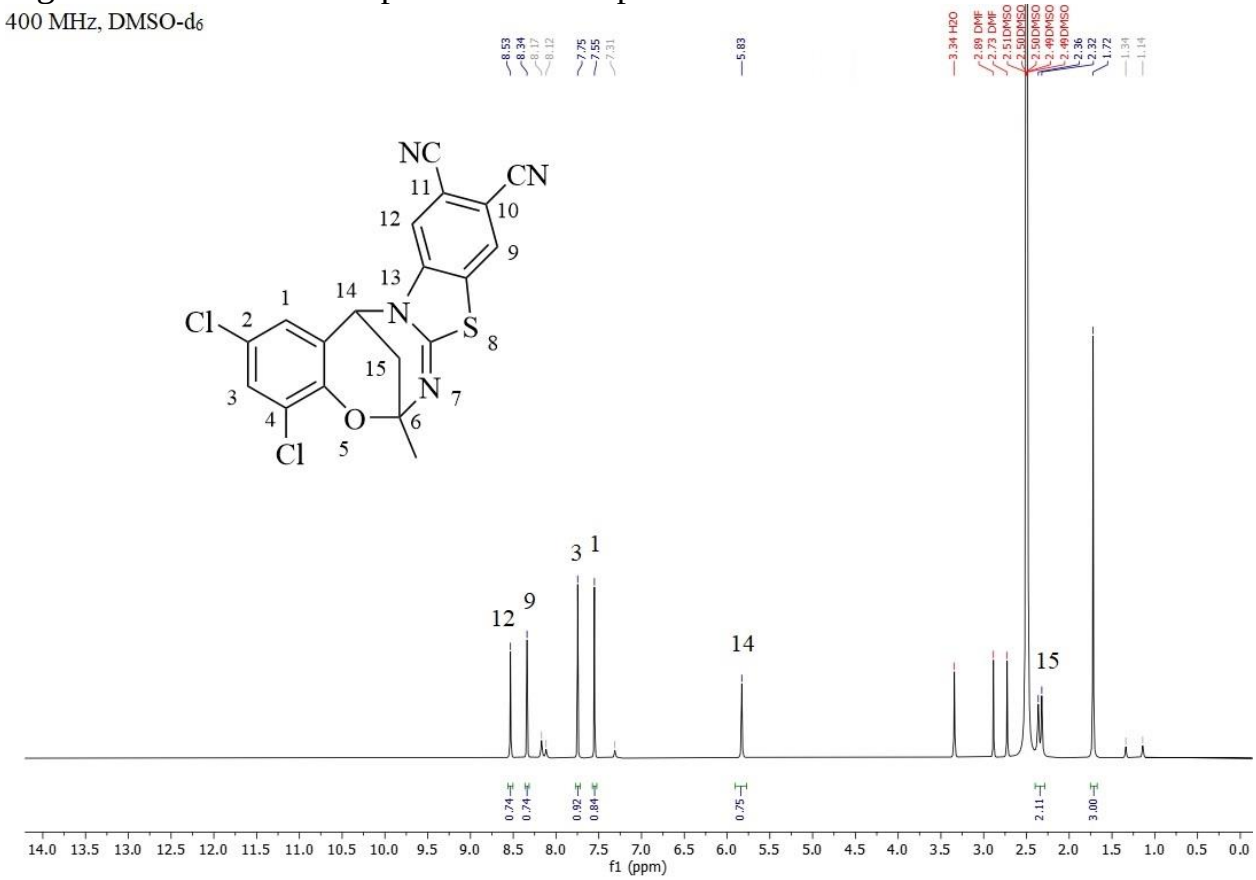

Figure SI-33. ^{1}H NMR spectrum of compound **5e**.

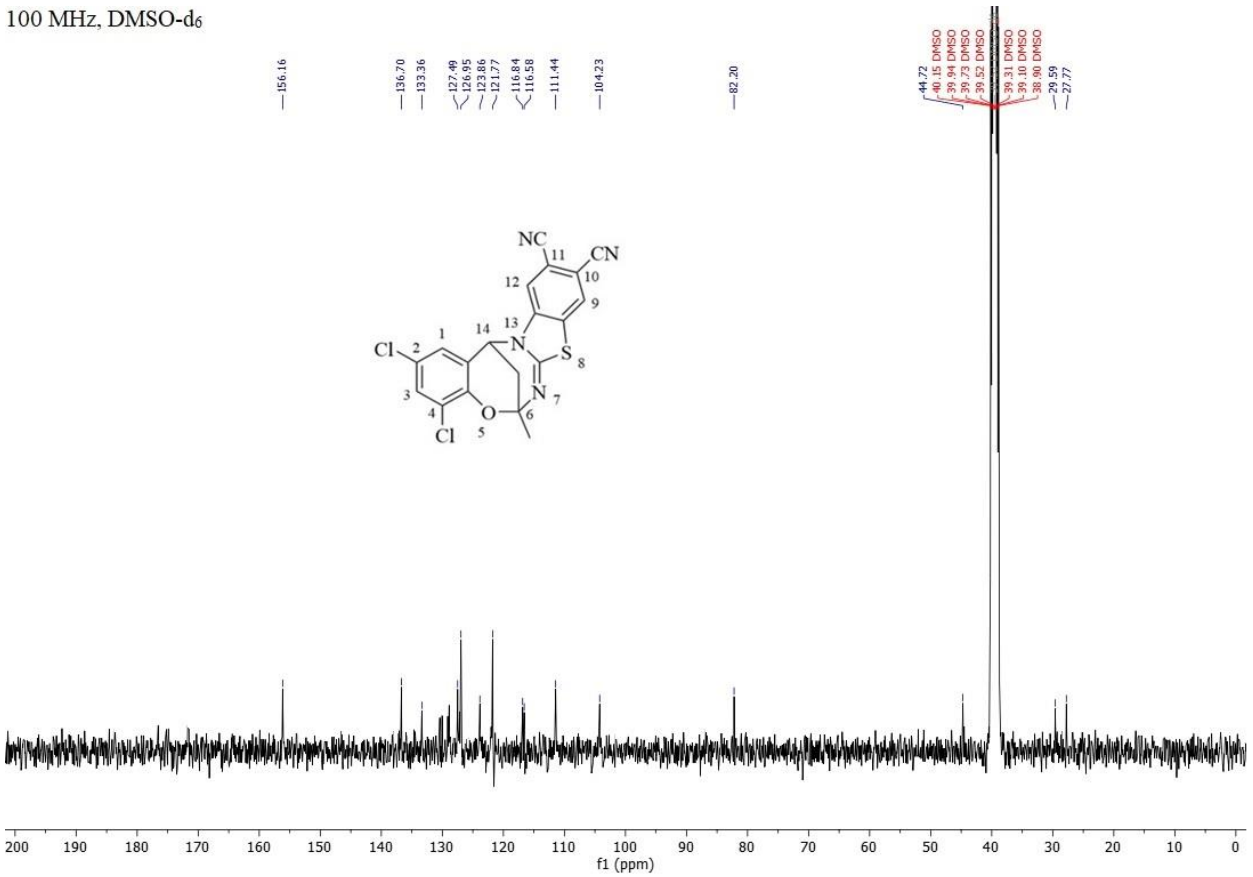

Figure SI-34. ^{13}C NMR spectrum of compound **5e**.

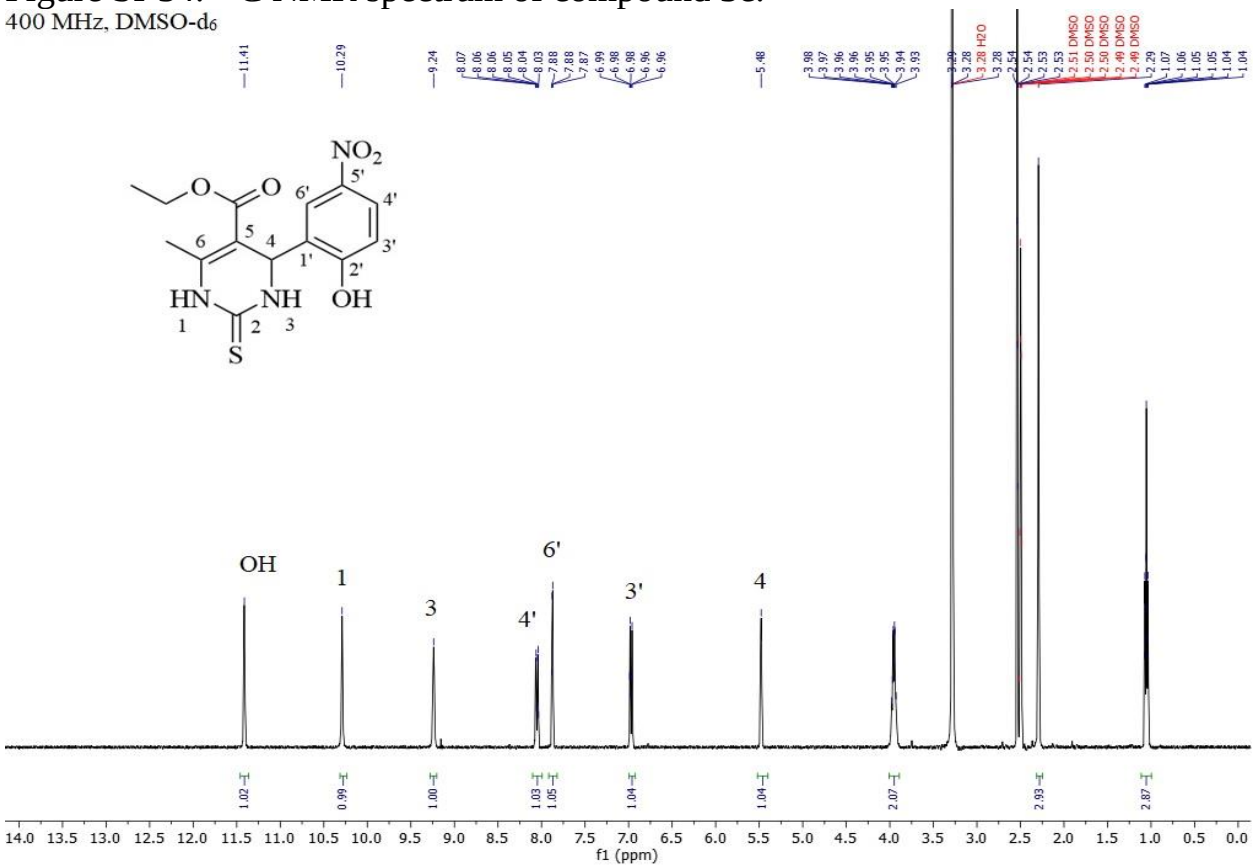

Figure SI-35. ^{1}H NMR spectrum of compound **6**.

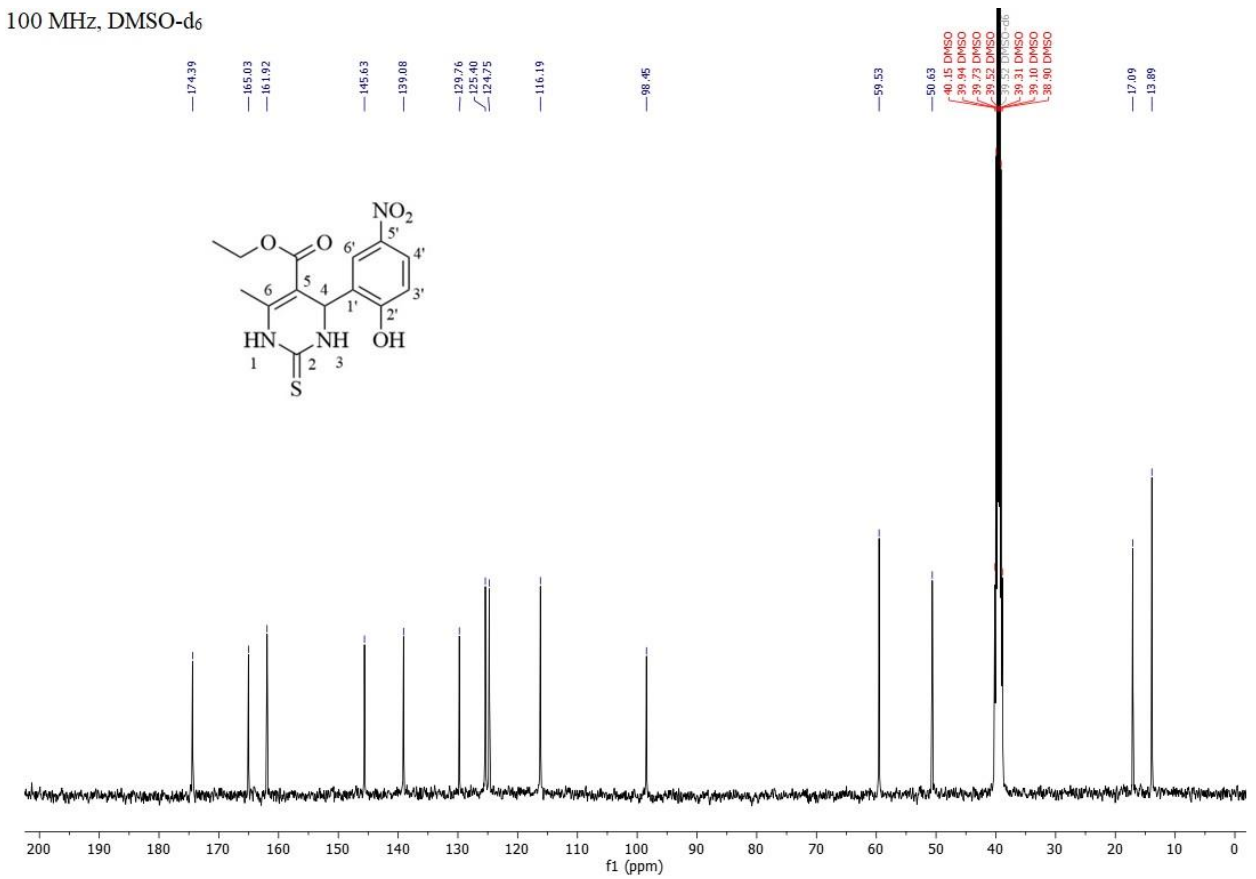

Figure SI-36. ^{13}C NMR spectrum of compound **6**.

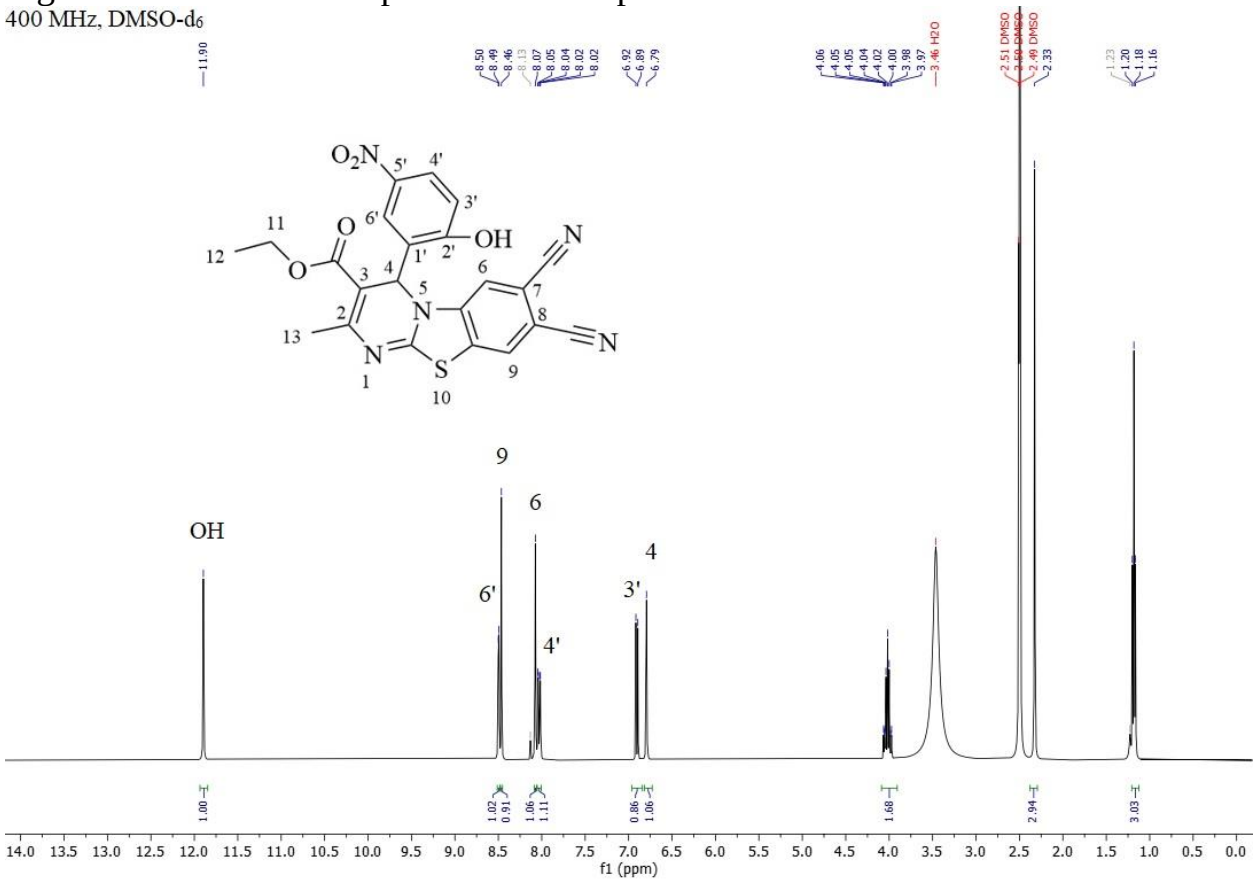

Figure SI-37. ^{1}H NMR spectrum of compound **7**.

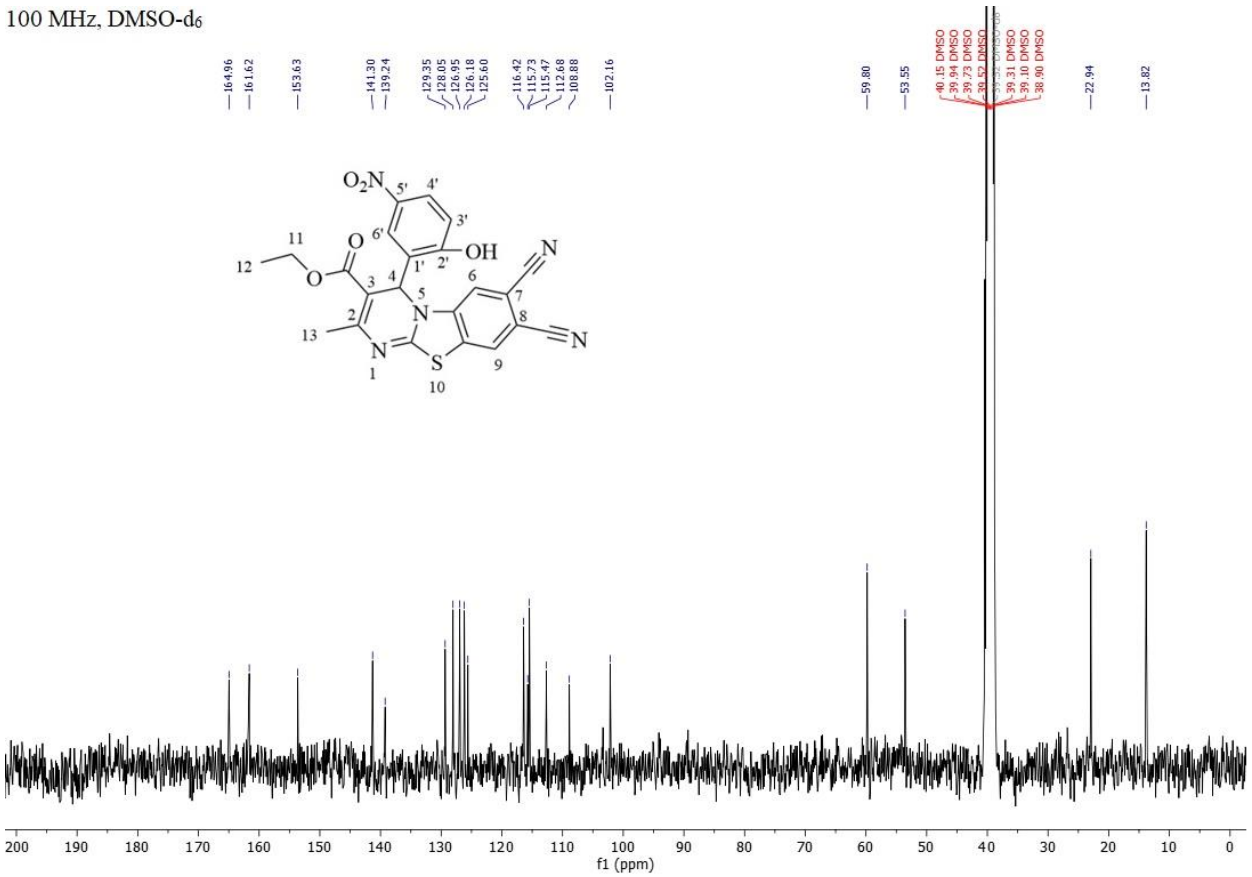

Figure SI-38. ^{13}C spectrum of compound **7**.

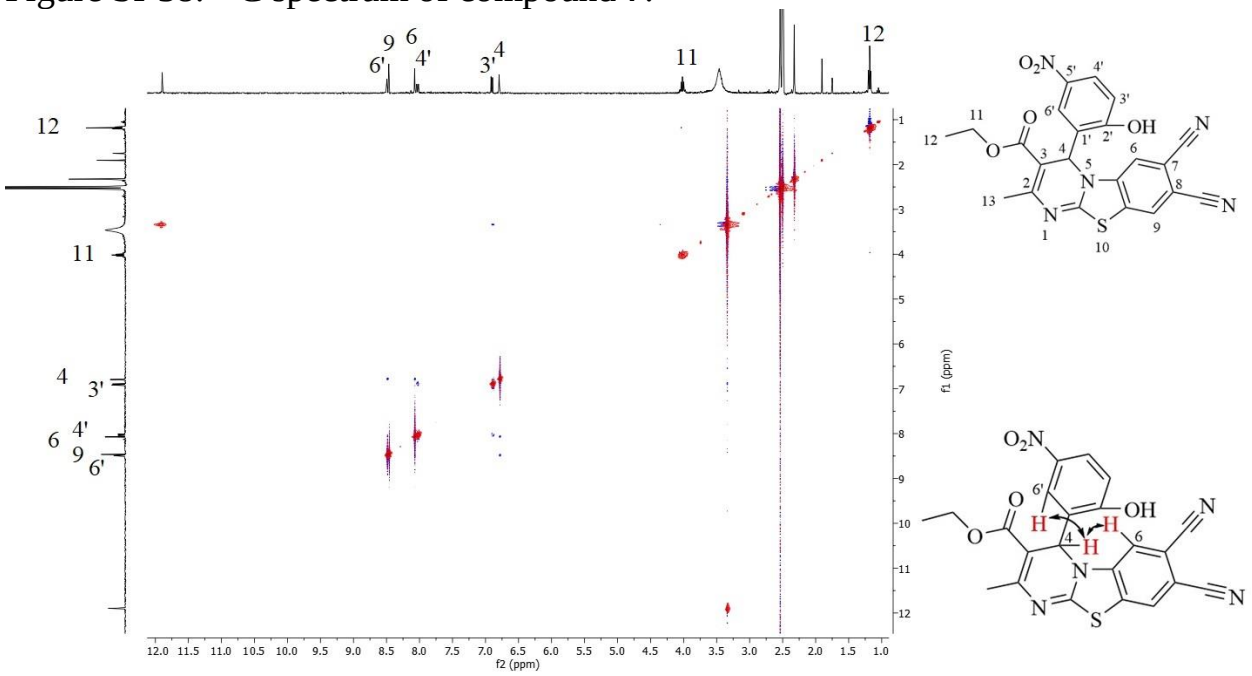

Figure SI-39. NOESY spectrum of compound **7**.

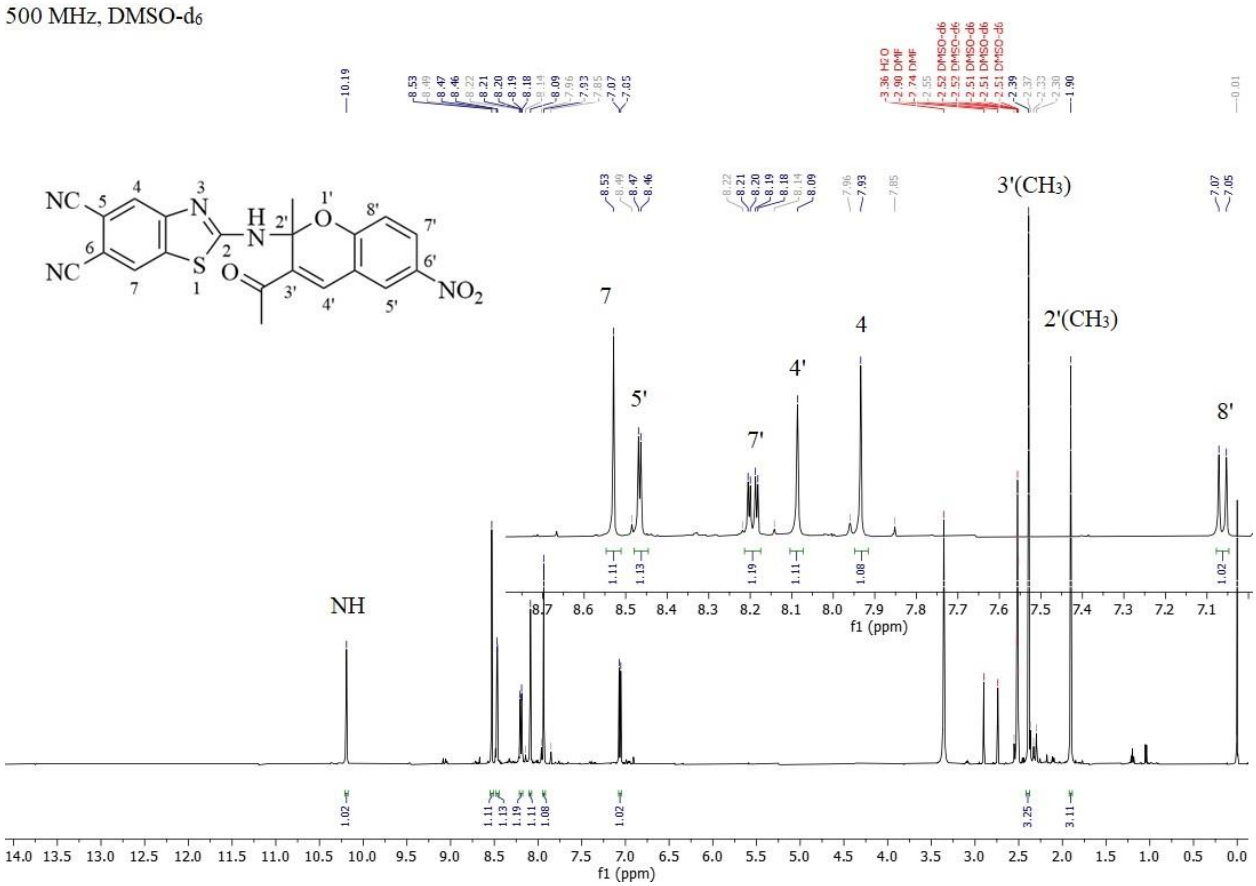

Figure SI-40. ^{1}H spectrum of compound **8**.

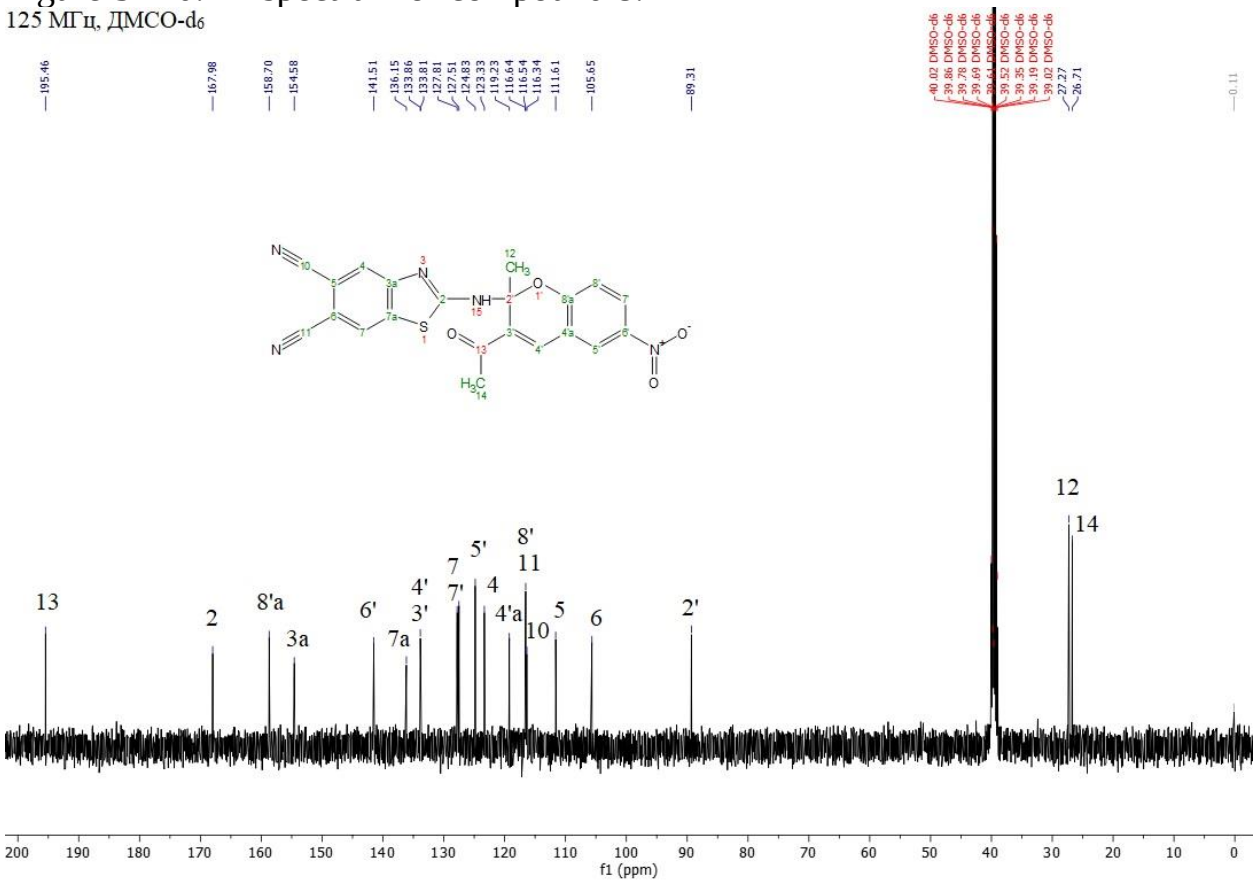

Figure SI-41. ^{13}C spectrum of compound **8**.

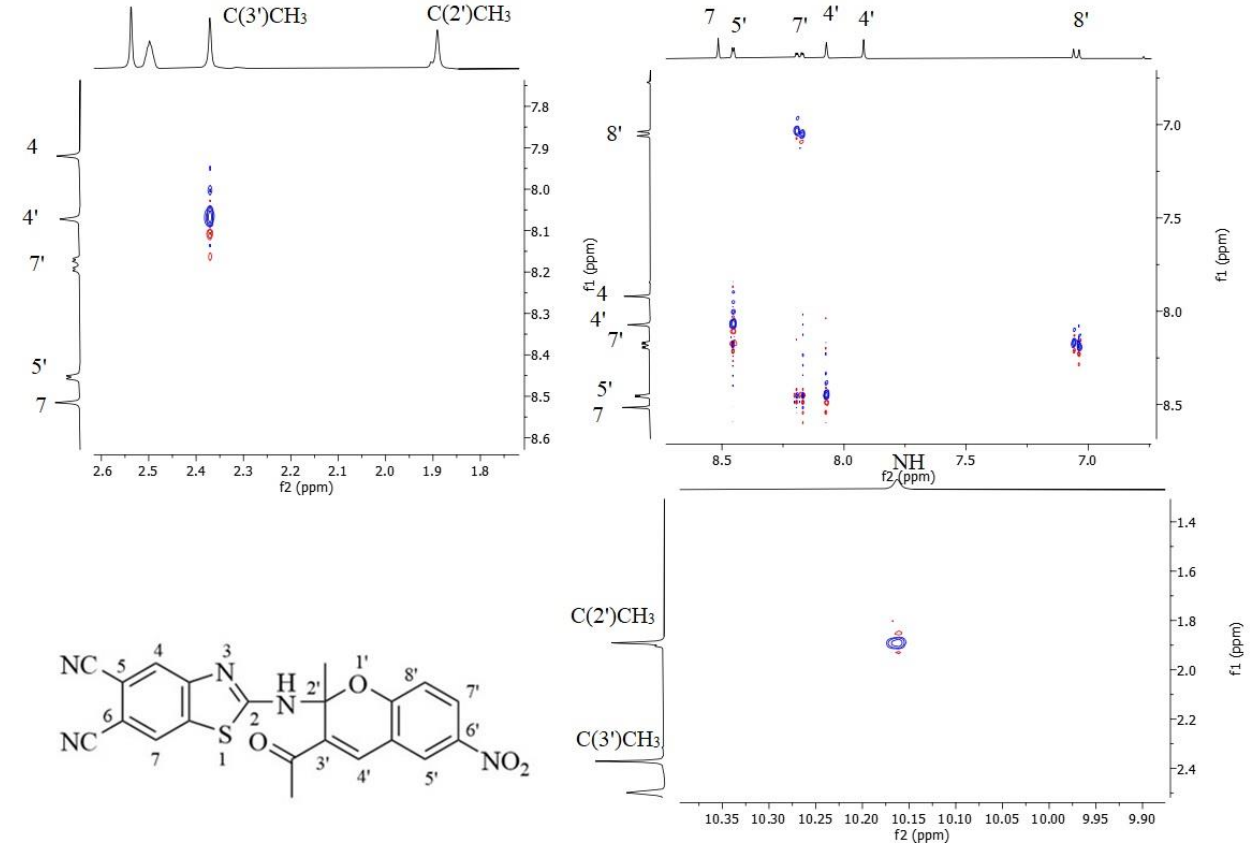

Figure SI-42. NOESY spectrum of compound **8**.

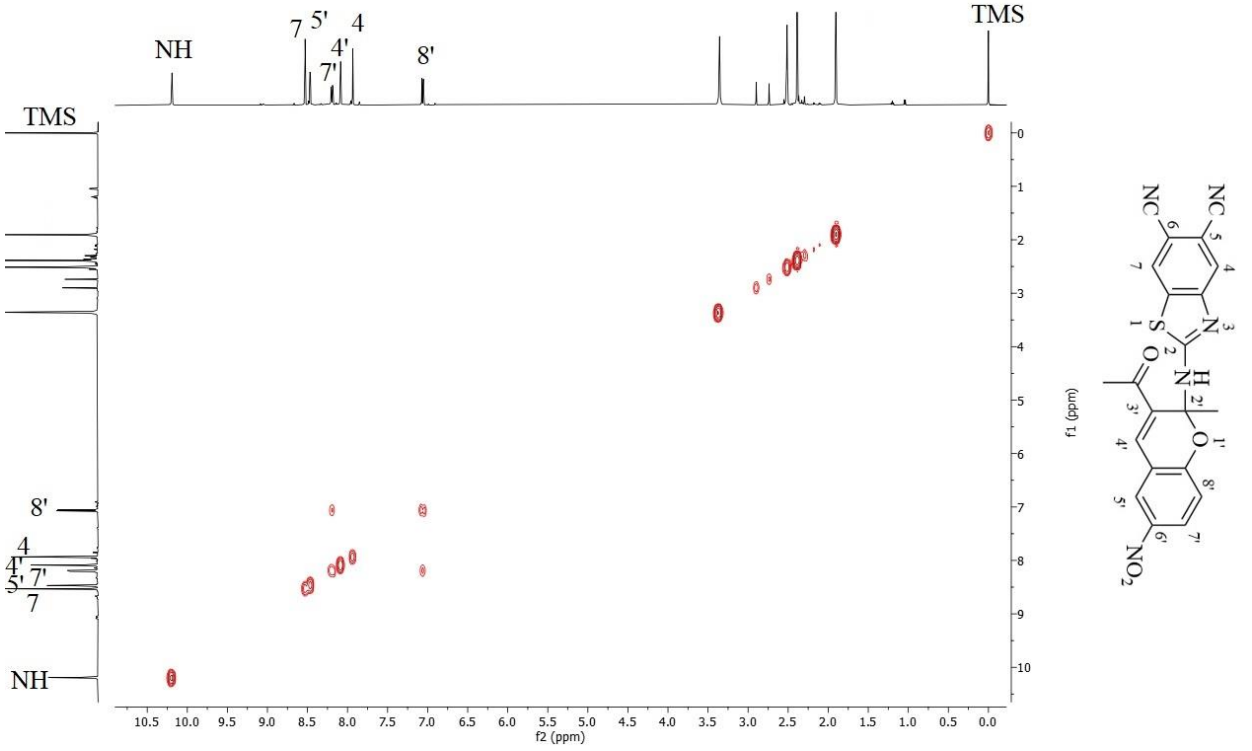

Figure SI-43. COSY spectrum of compound **8**.

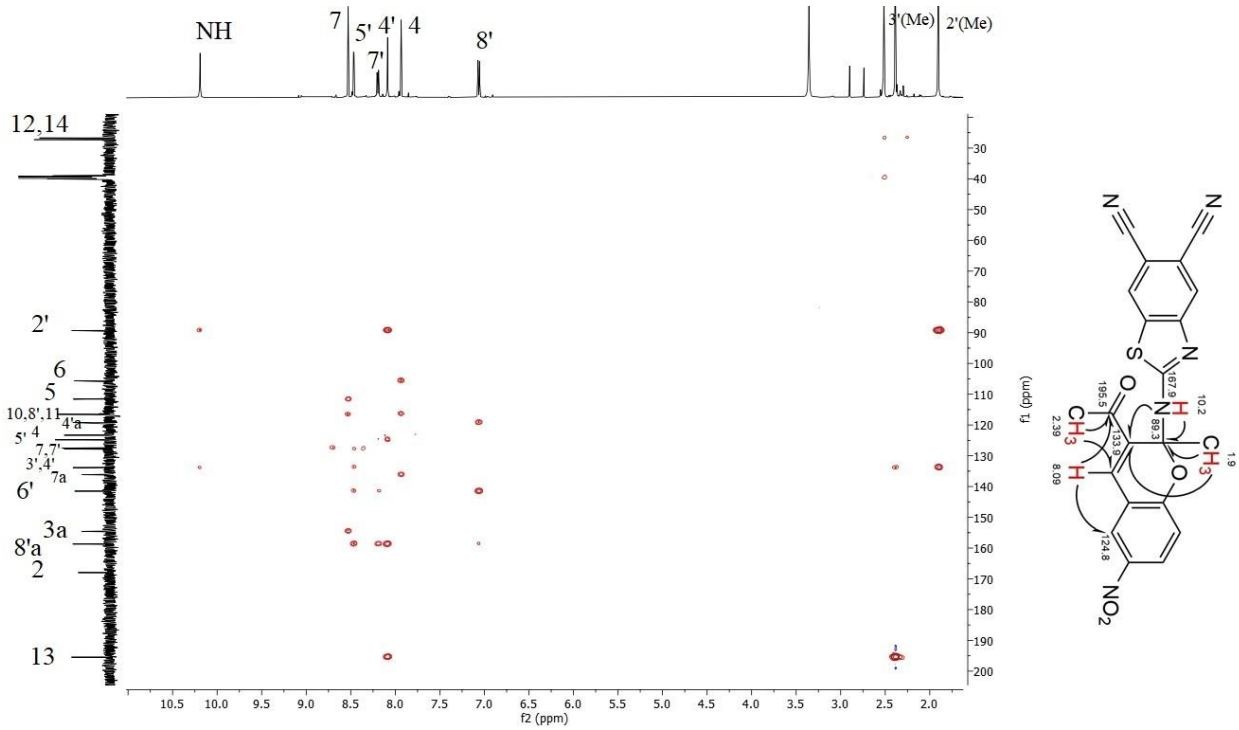

Figure SI-44. HMBC spectrum of compound **8**.

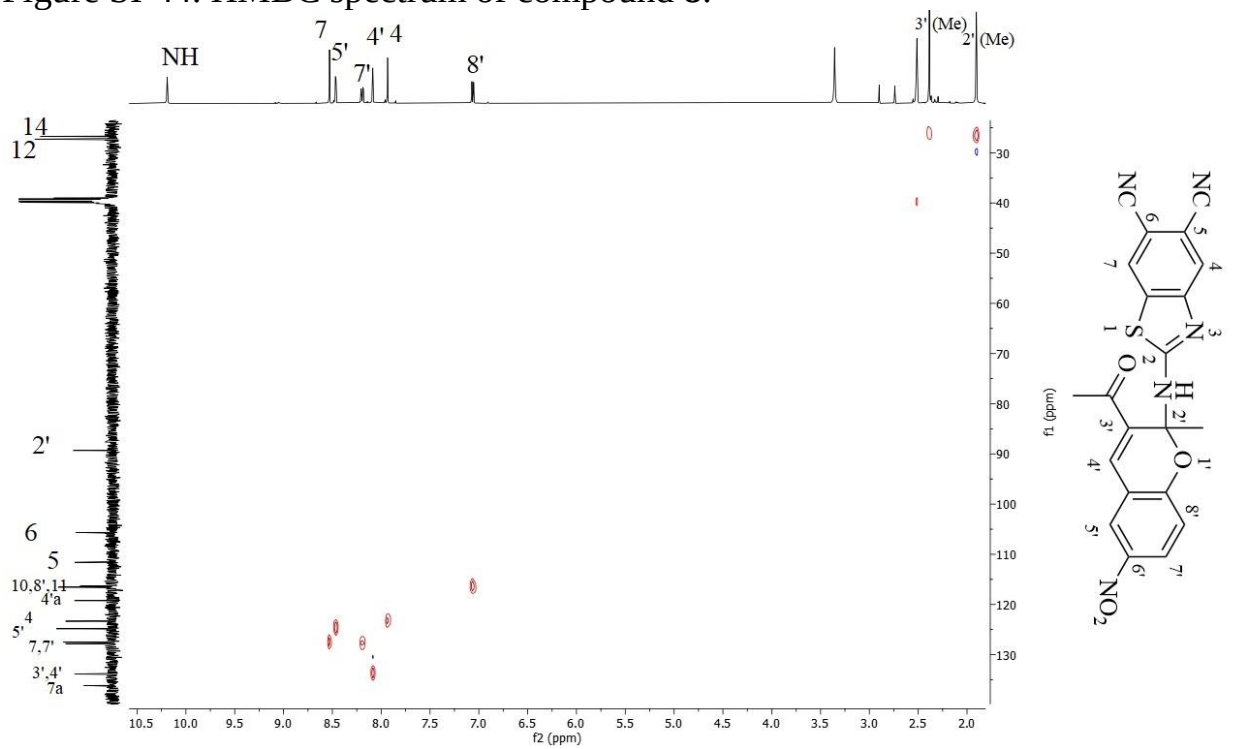

Figure SI-45. HSQC spectrum of compound **8**.

Table 1. Conditions of S_NAr reactions described in manuscript

S_NAr reaction product	Temperature of the reaction, °C	Time of the reaction, h
3a	80	2
3b	30	17
5a	80	3
5b	80	4
5c	80	5
5d	80	5
5e	80	3
7	45	3,5
8	80	1,5