

Supporting Information

Pure water induced dehalogenation of 2,4-di-*tert*-amino-6-substituted-5-halogenopyrimidines

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Contains:

Copies of ^1H NMR, ^{13}C NMR, FTIR and Mass spectra as figures

- Total number of pages: 42 (S1 - S42)
- Total number of figures: 74 (Figure S1 – Figure S74)

Figure S1. ^1H NMR spectrum for compound 2a.

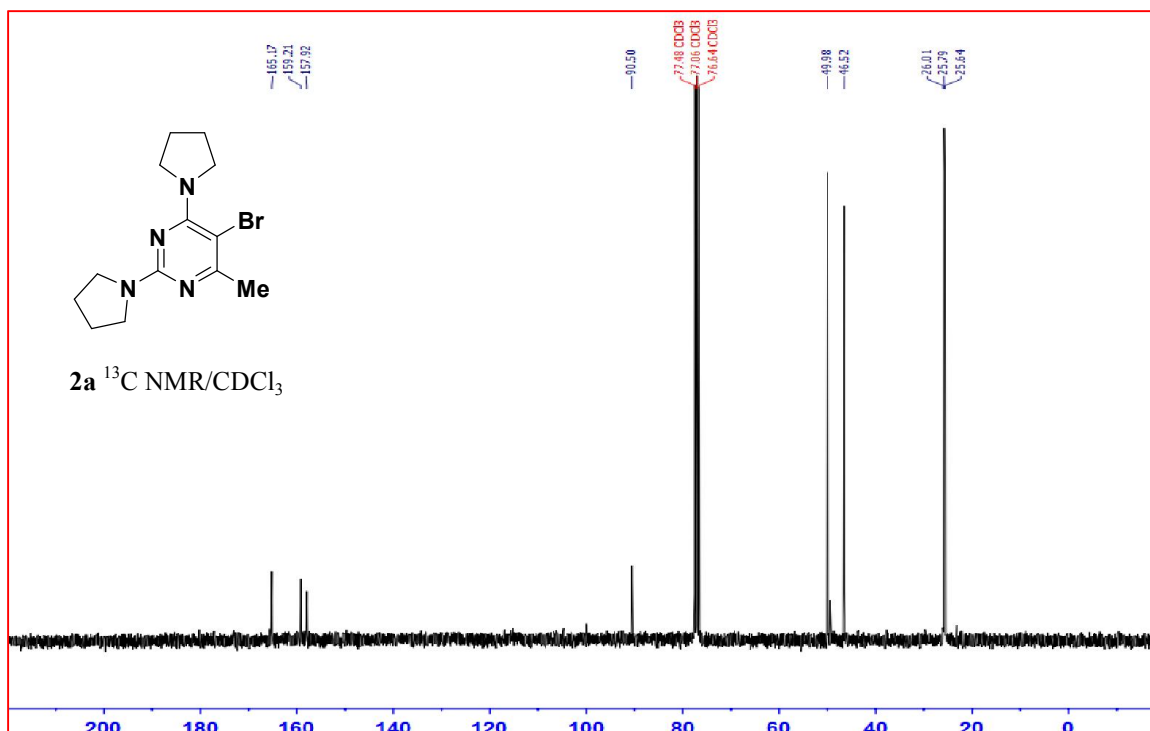
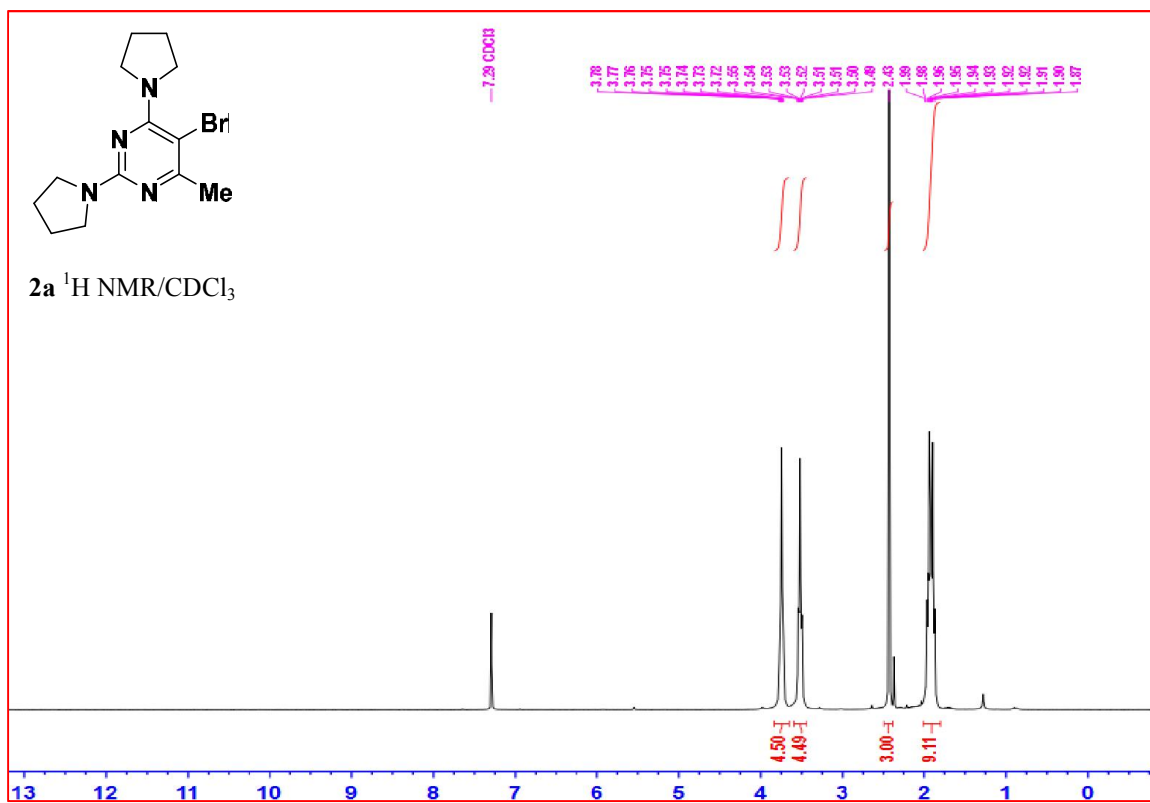


Figure S2. ^{13}C NMR spectrum for compound 2a.

Figure S3. Mass spectrum for compound 2a.

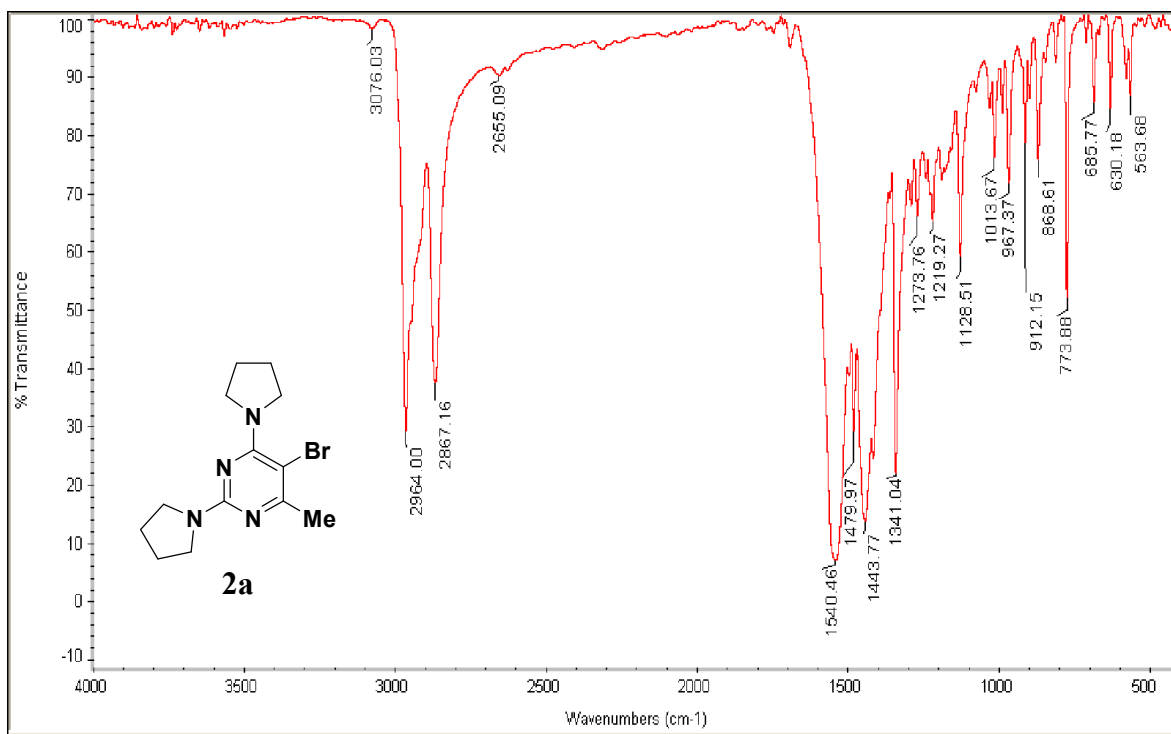
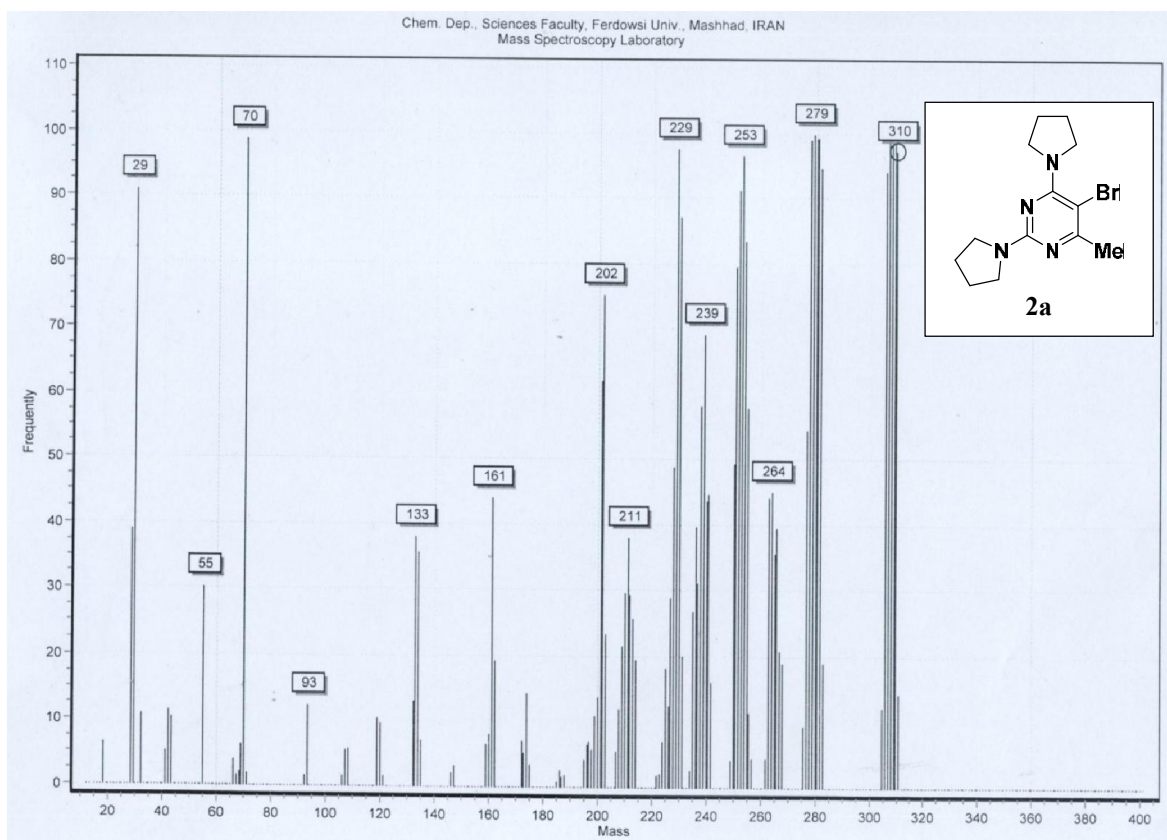


Figure S4. FTIR spectrum for compound 2a.

Figure S5. ^1H NMR spectrum for compound 2b.

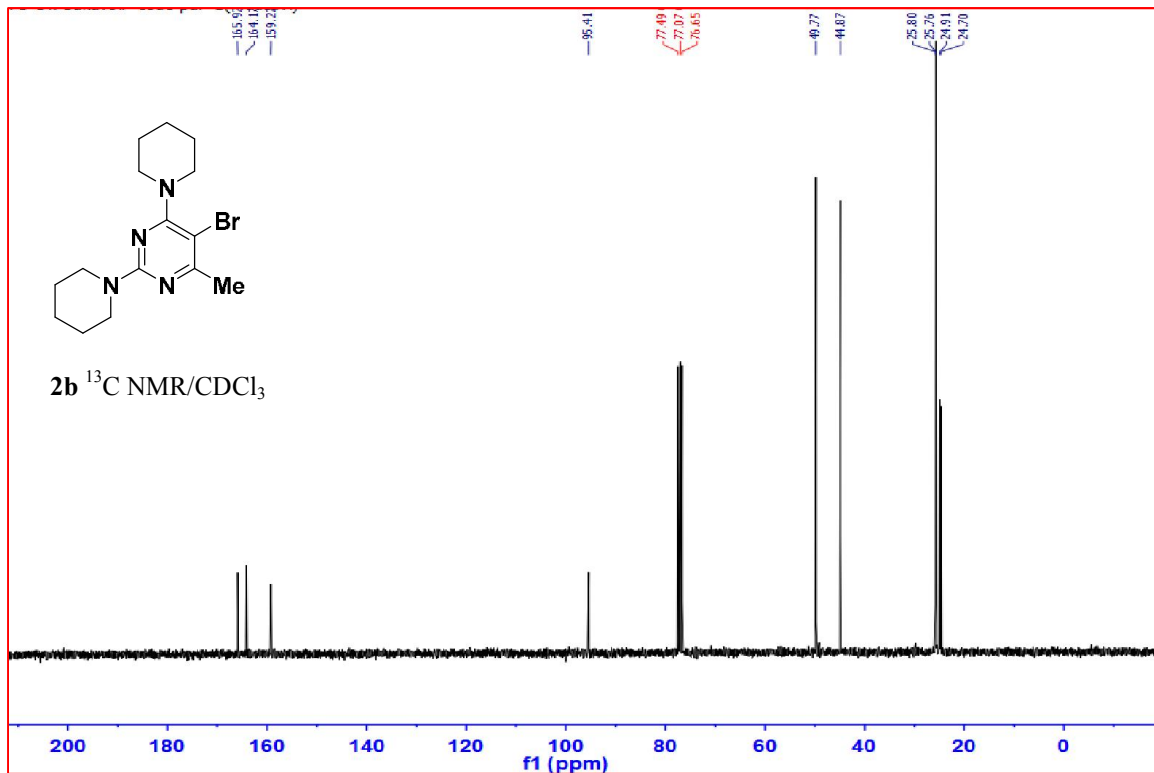
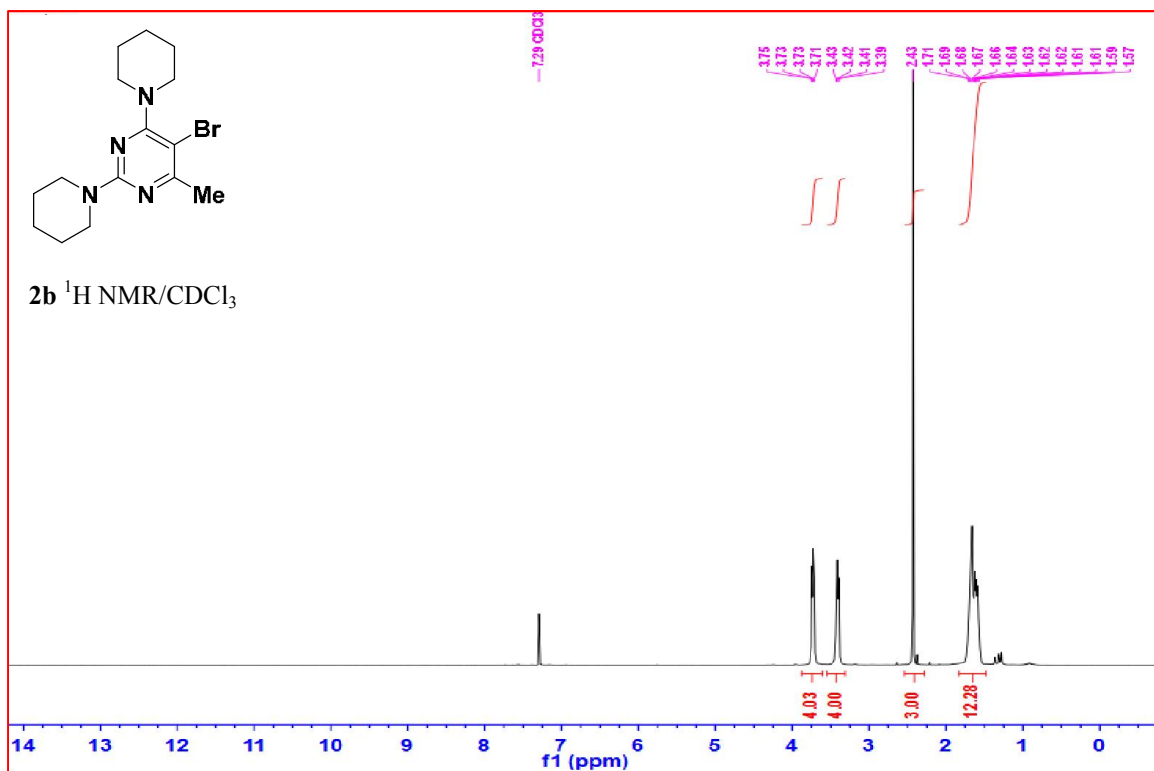


Figure S6. ^{13}C NMR spectrum for compound 2b.

Figure S7. Mass spectrum for compound 2b.

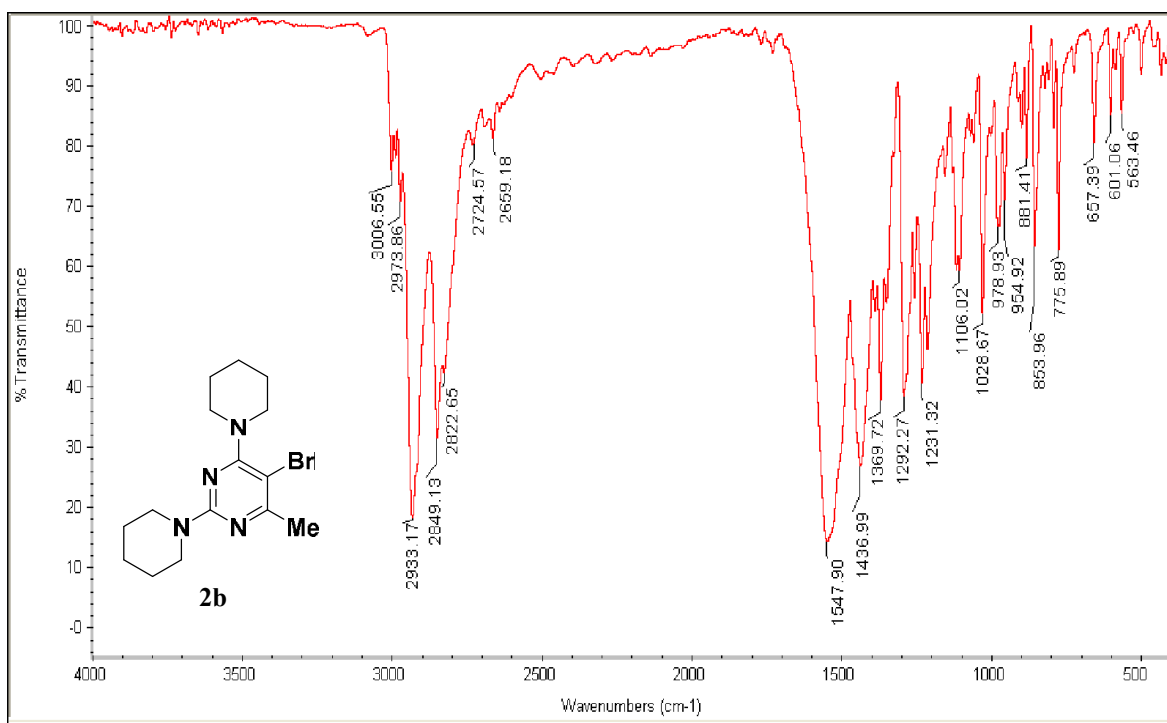
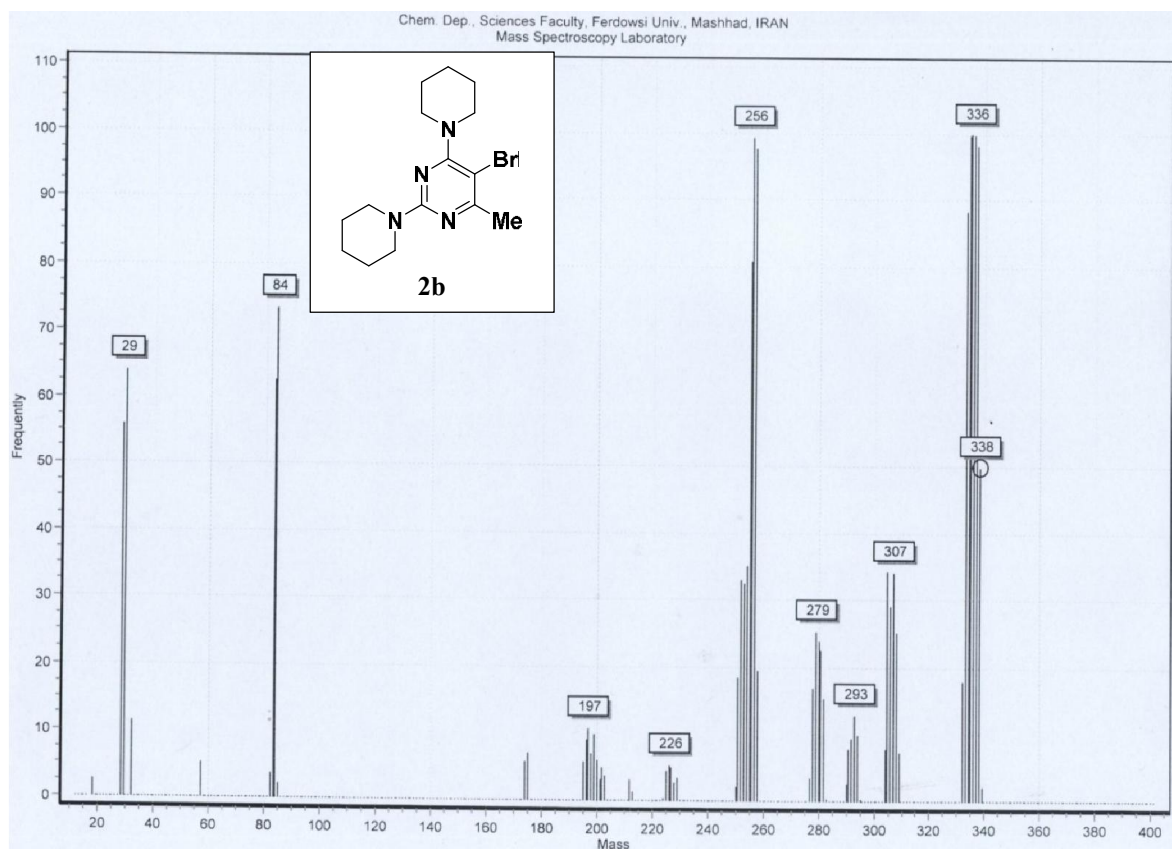


Figure S8. FTIR spectrum for compound 2b.

Figure S9. ^1H NMR spectrum for compound 2c

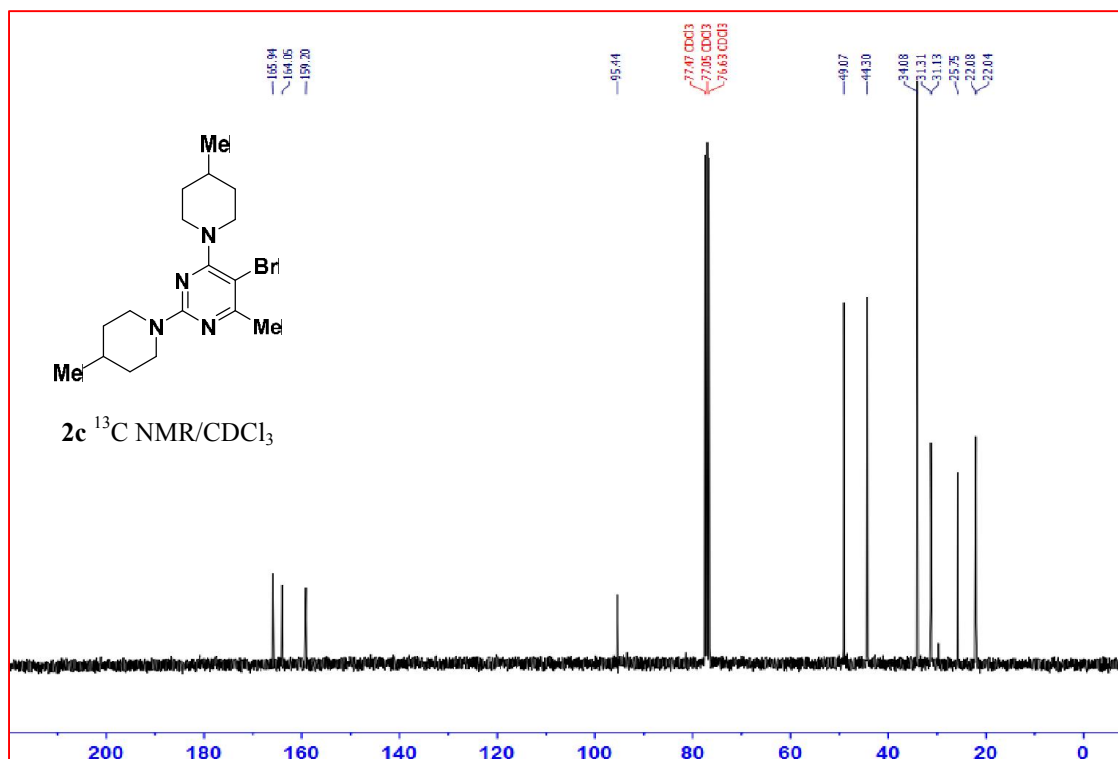
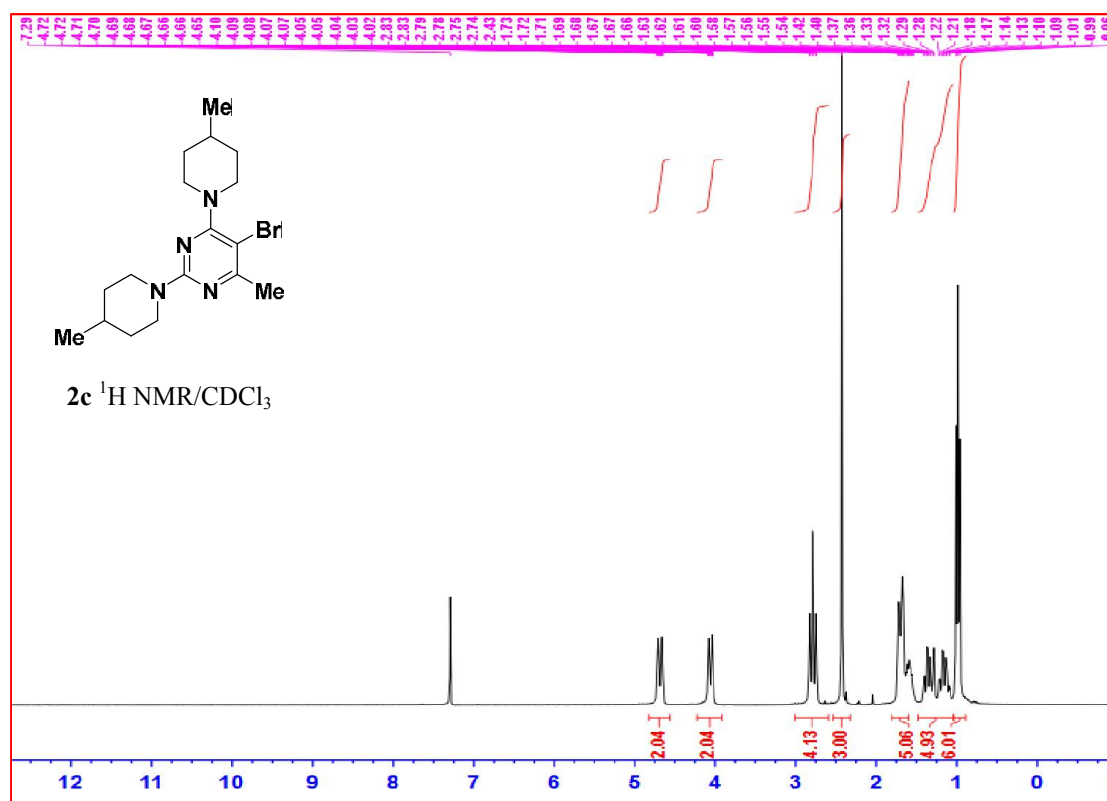


Figure S10. ^{13}C NMR spectrum for compound 2c

Figure S11. Mass spectrum for compound **2c**.

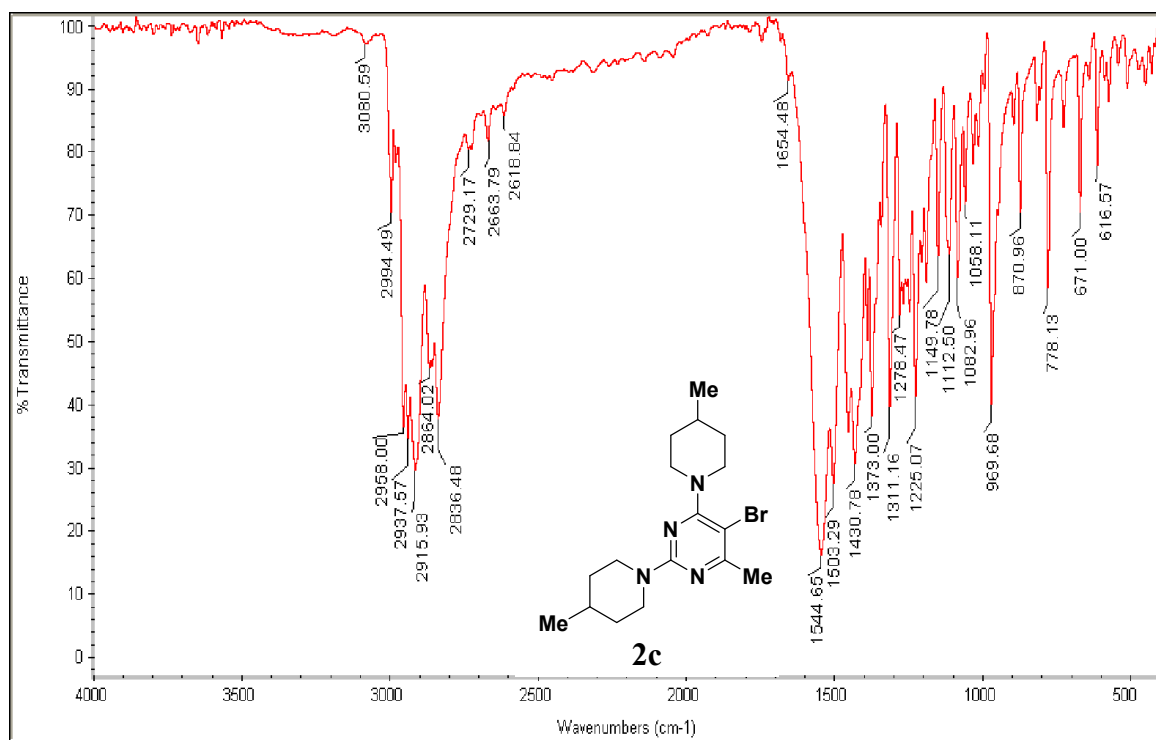
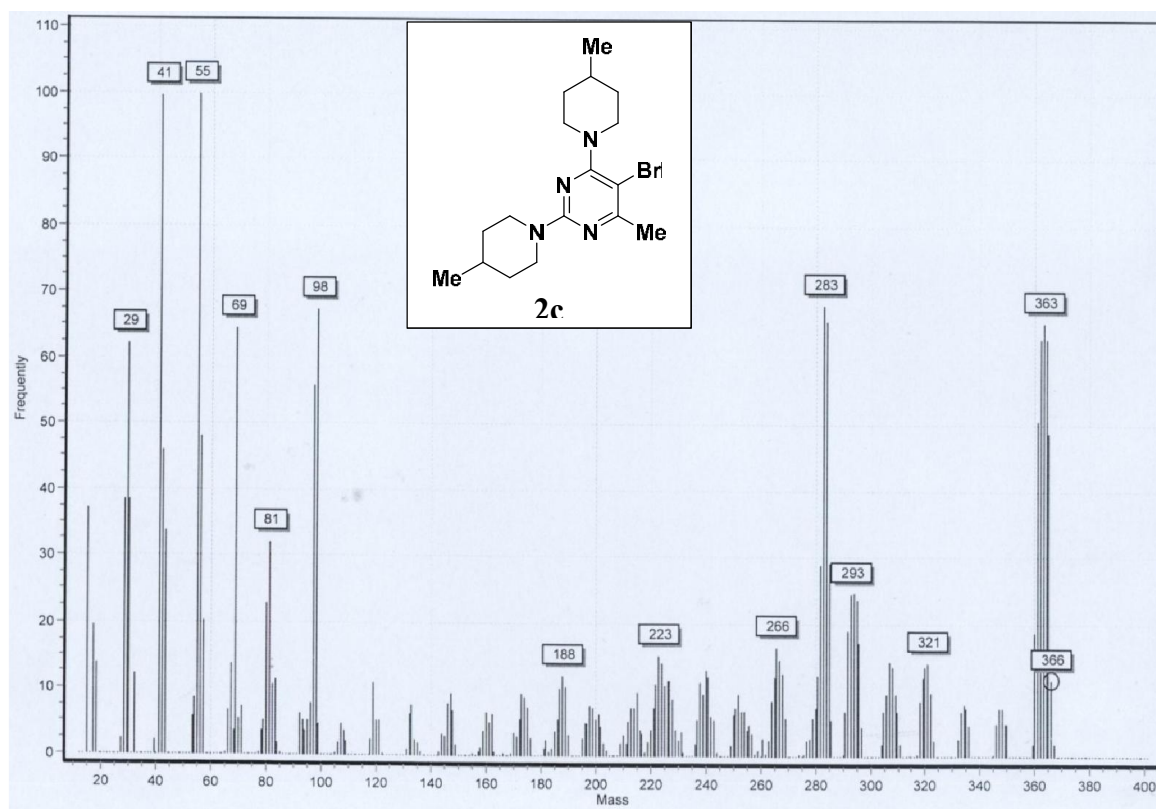


Figure S12. FTIR spectrum for compound **2c**

Figure S13. ^1H NMR spectrum for compound 2d

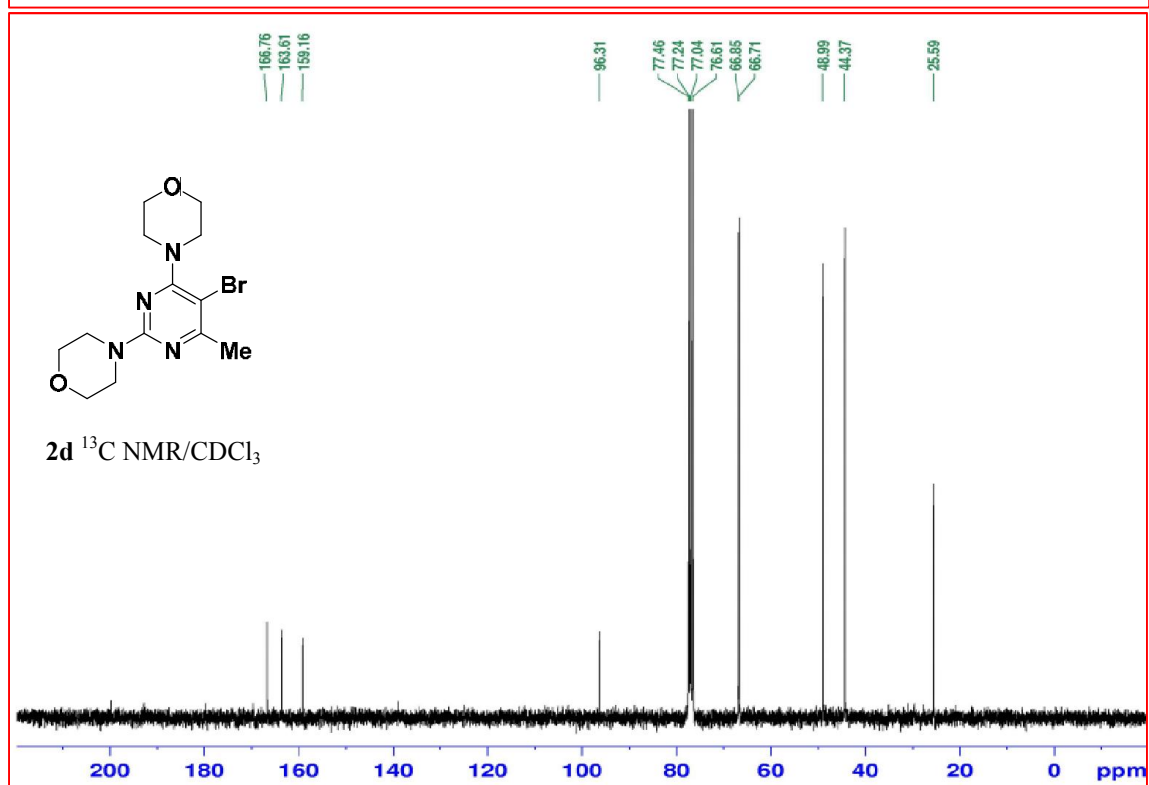
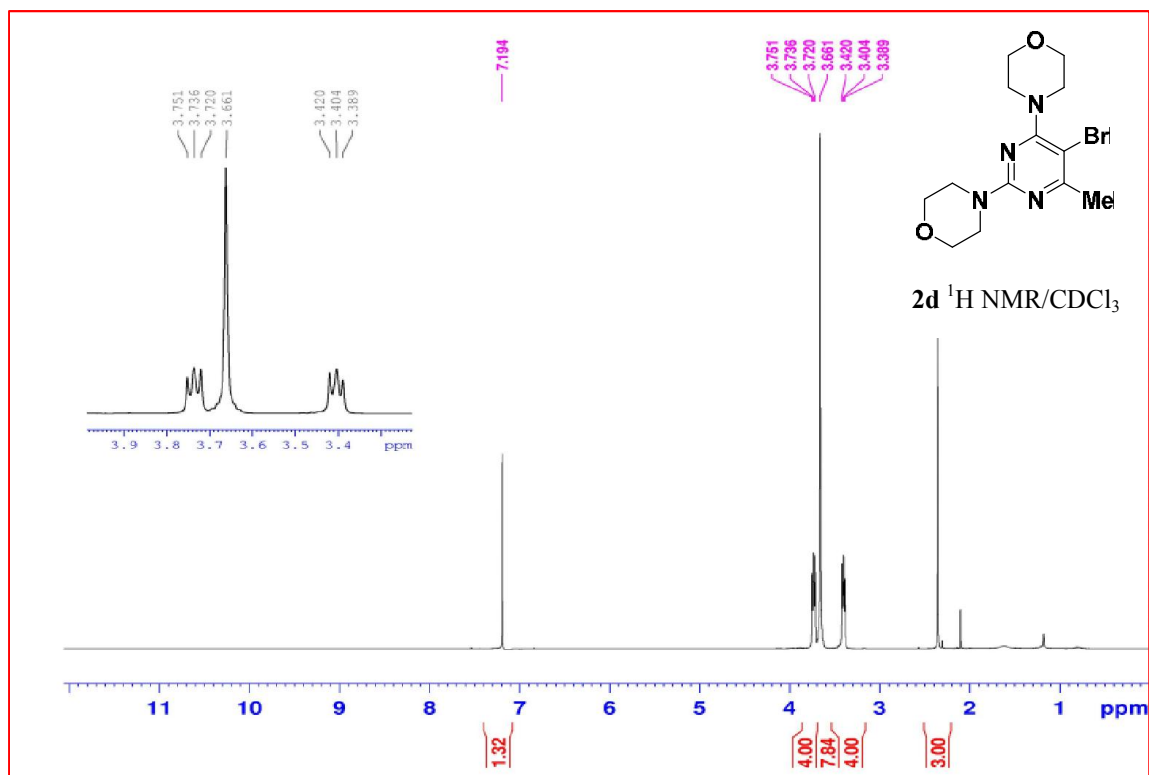


Figure S14. ^{13}C NMR spectrum for compound 2d

Figure S15. Mass spectrum for compound 2d

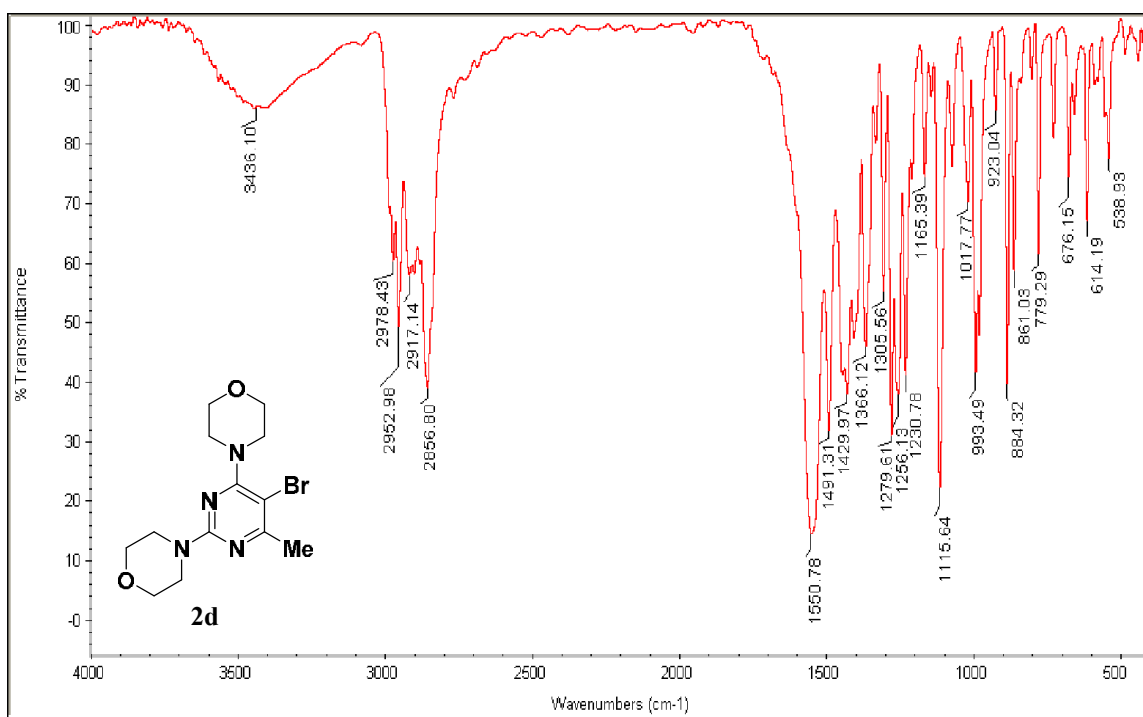
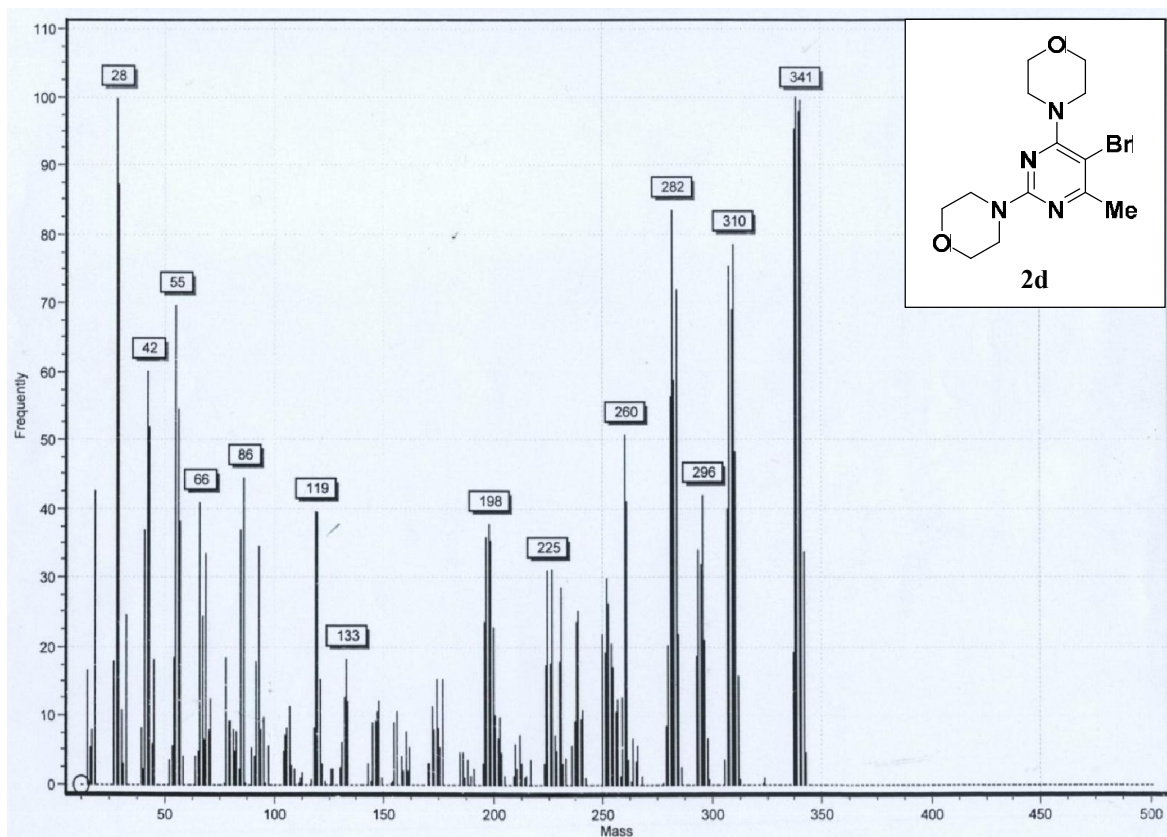


Figure S16. FTIR spectrum for compound 2d

Figure S17. ^1H NMR spectrum for compound 3a

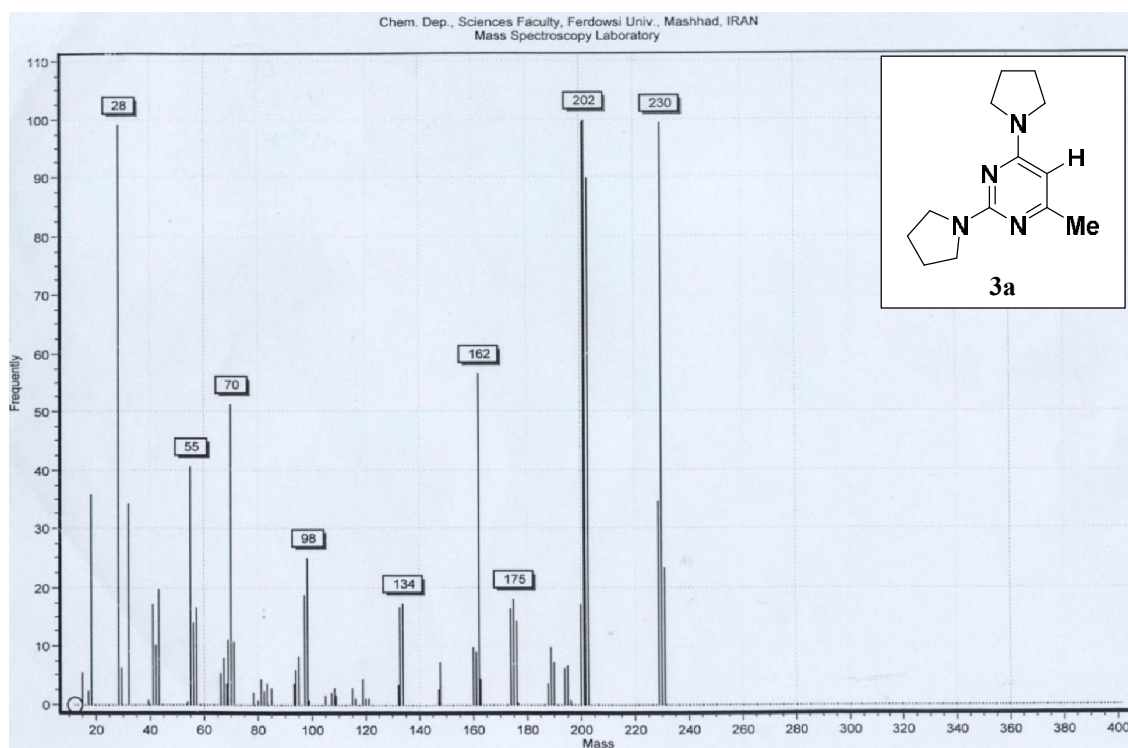
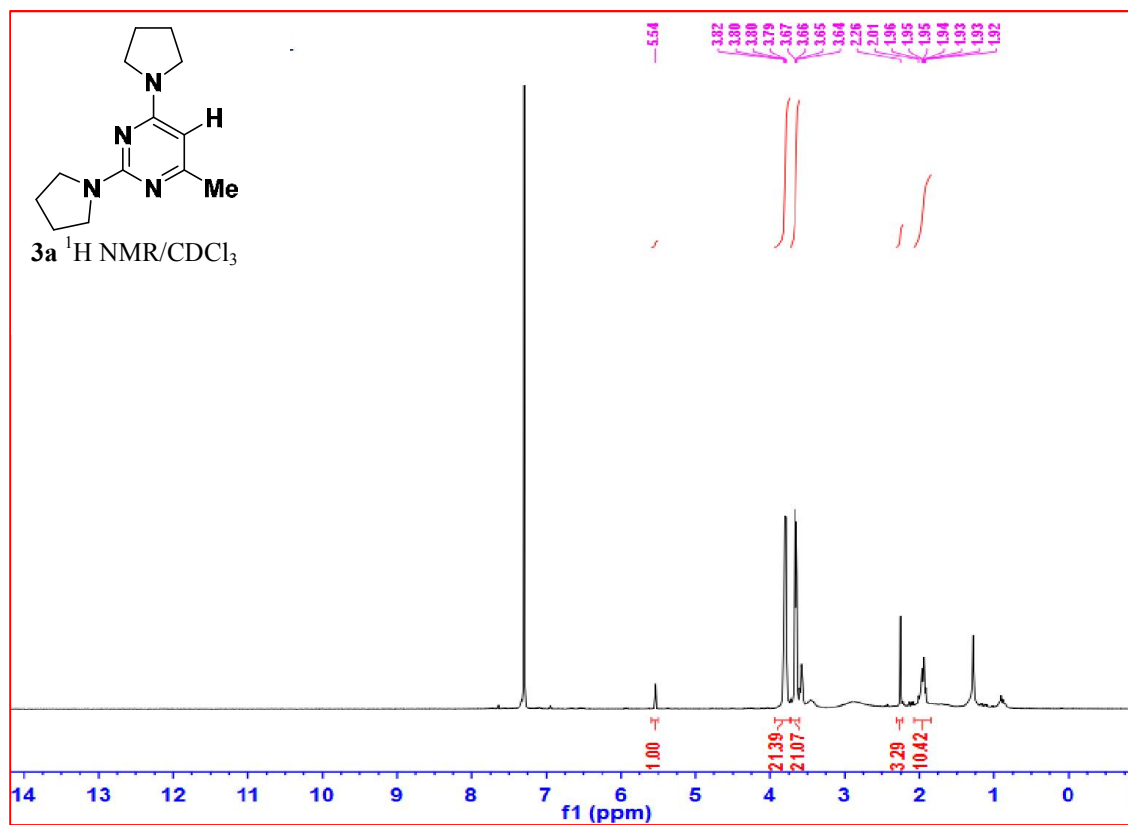


Figure S18. Mass spectrum for compound 3a

Figure S19. ^1H NMR spectrum for compound 3b

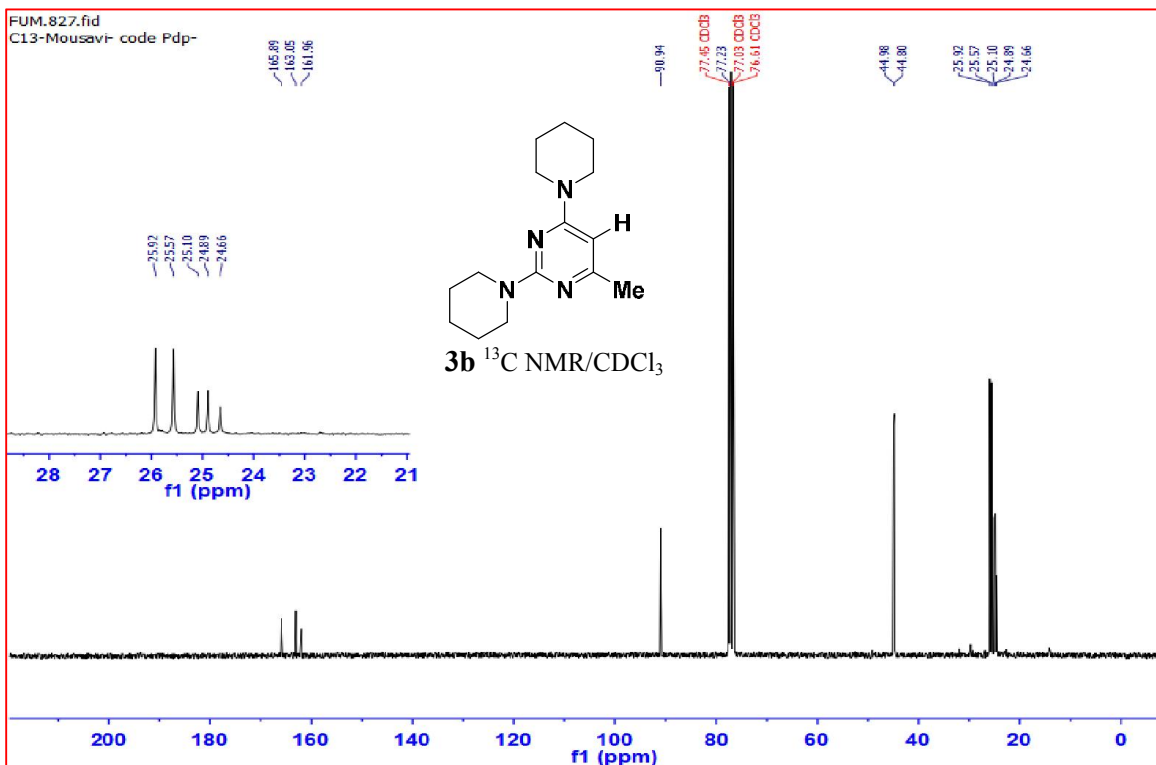
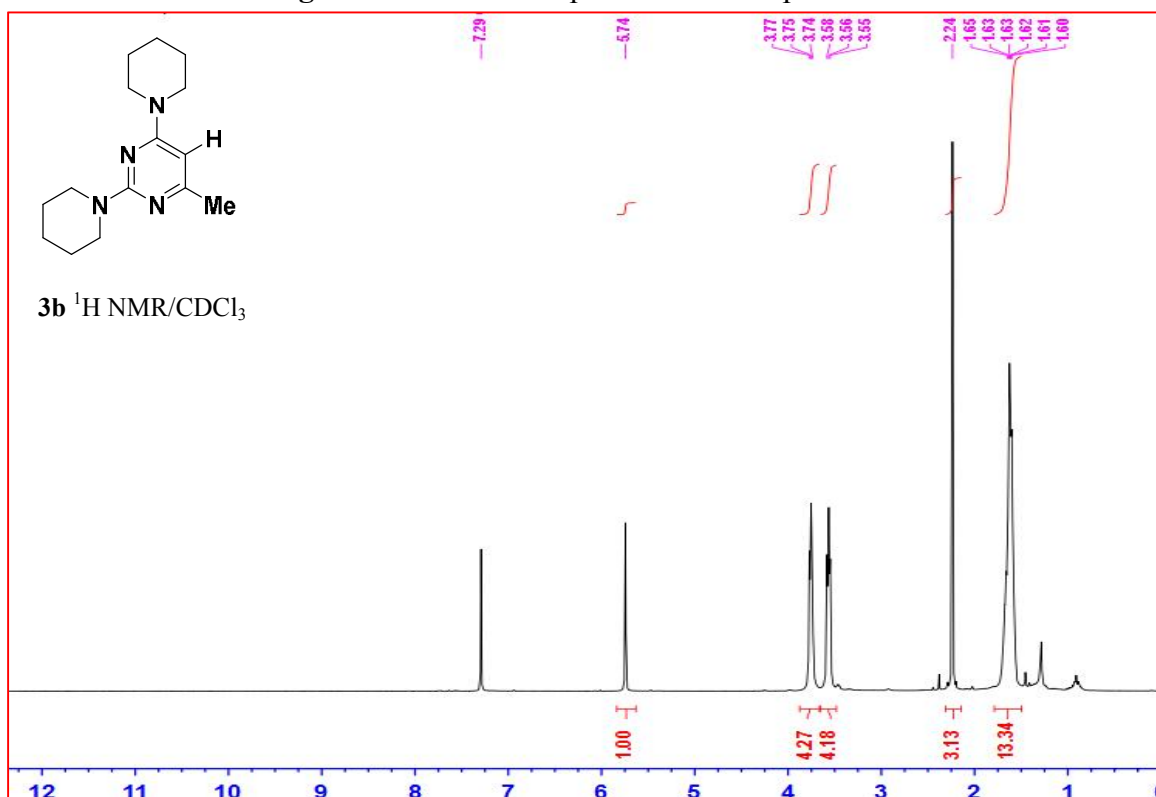


Figure S20. ^{13}C NMR spectrum for compound 3b

Figure S21. Mass spectrum for compound **3b**

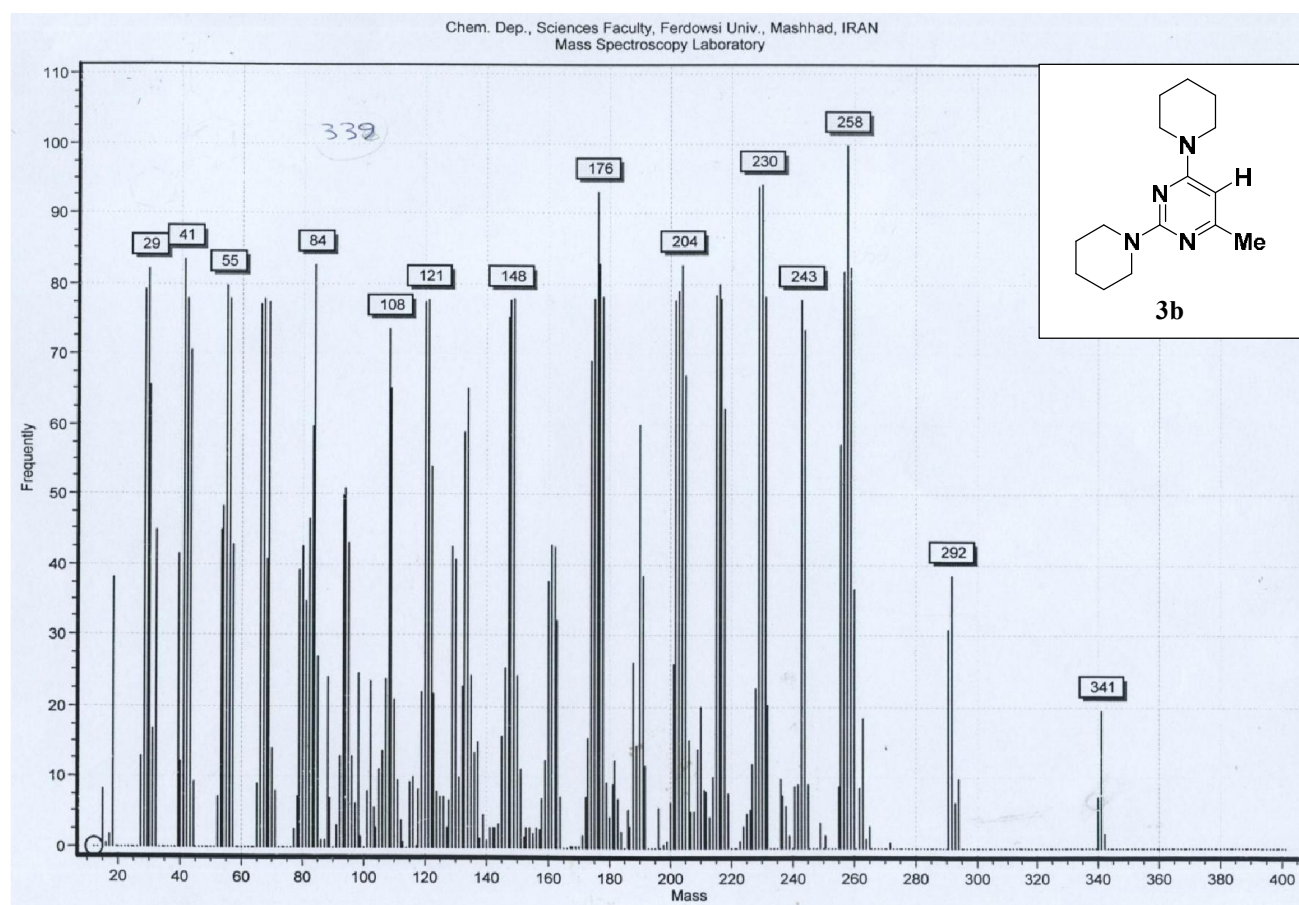


Figure S22. ^1H NMR spectrum for compound 3c

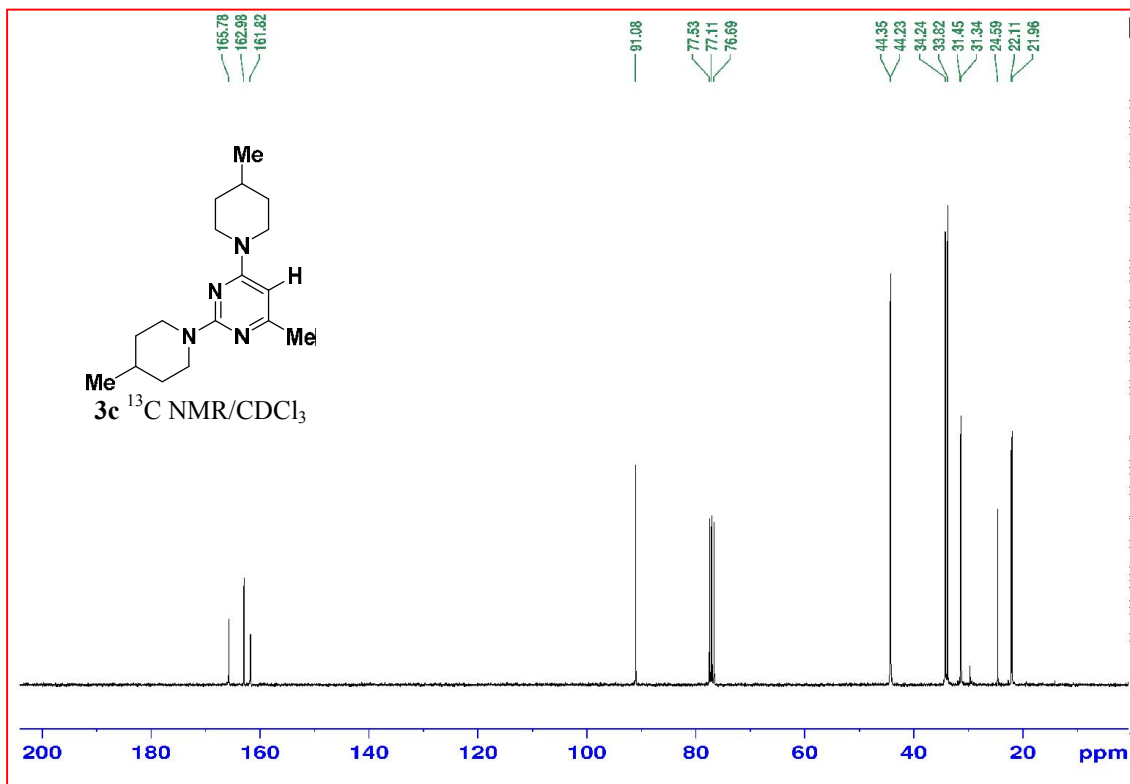
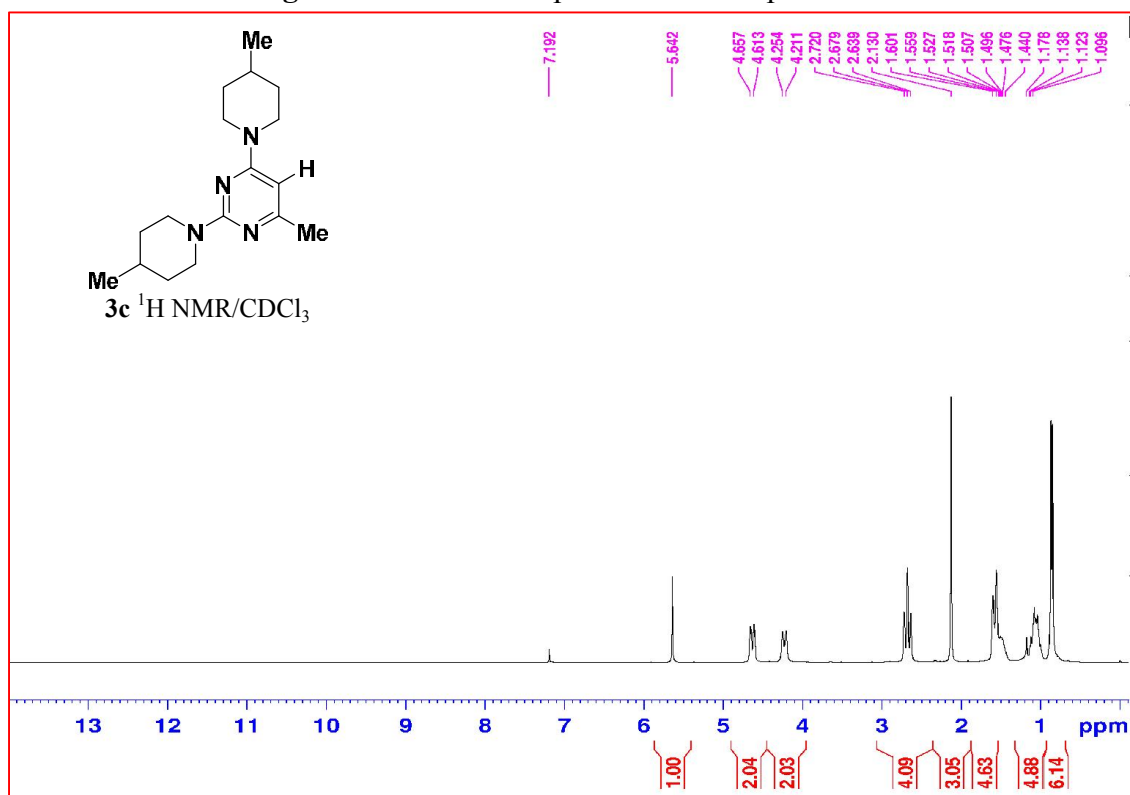


Figure S23. ^{13}C NMR spectrum for compound 3c

Figure S24. Mass spectrum for compound **3c**

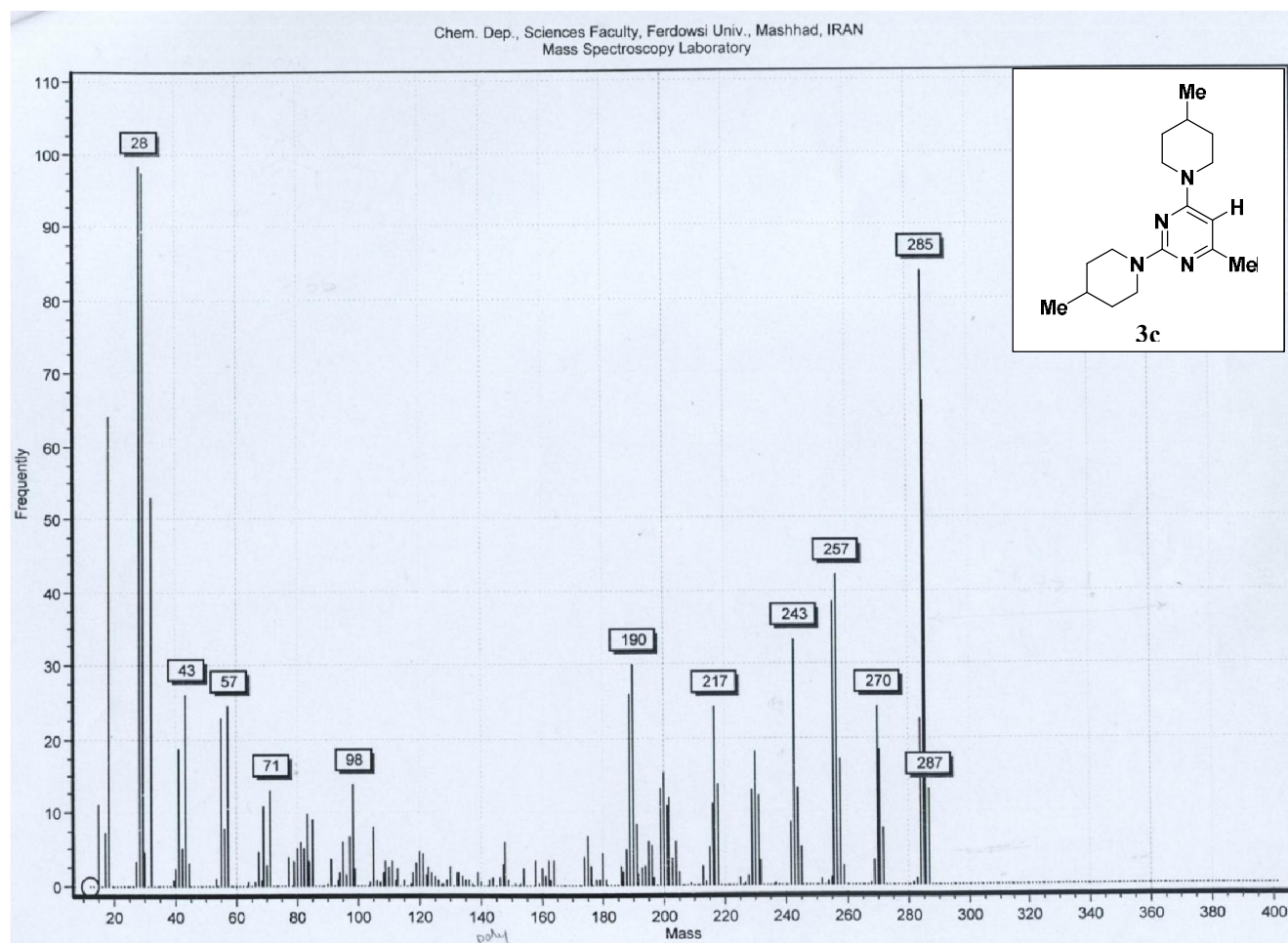


Figure S25. ^1H NMR spectrum for compound 3d.

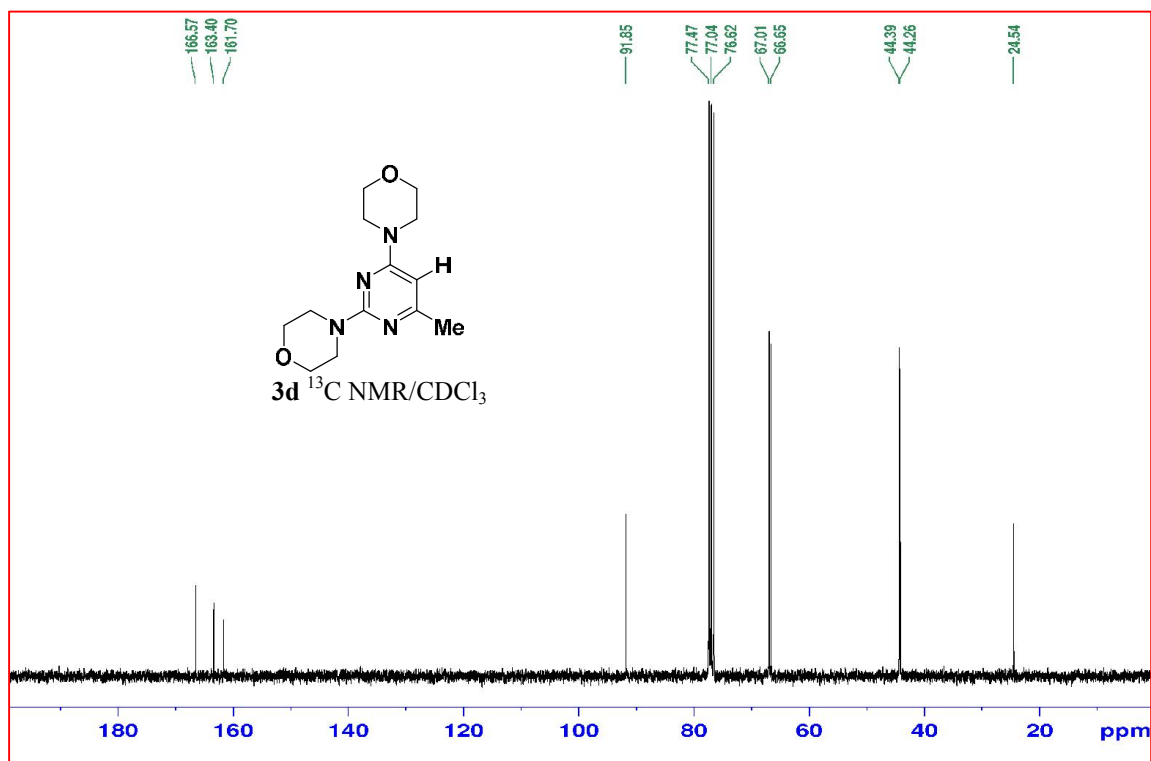
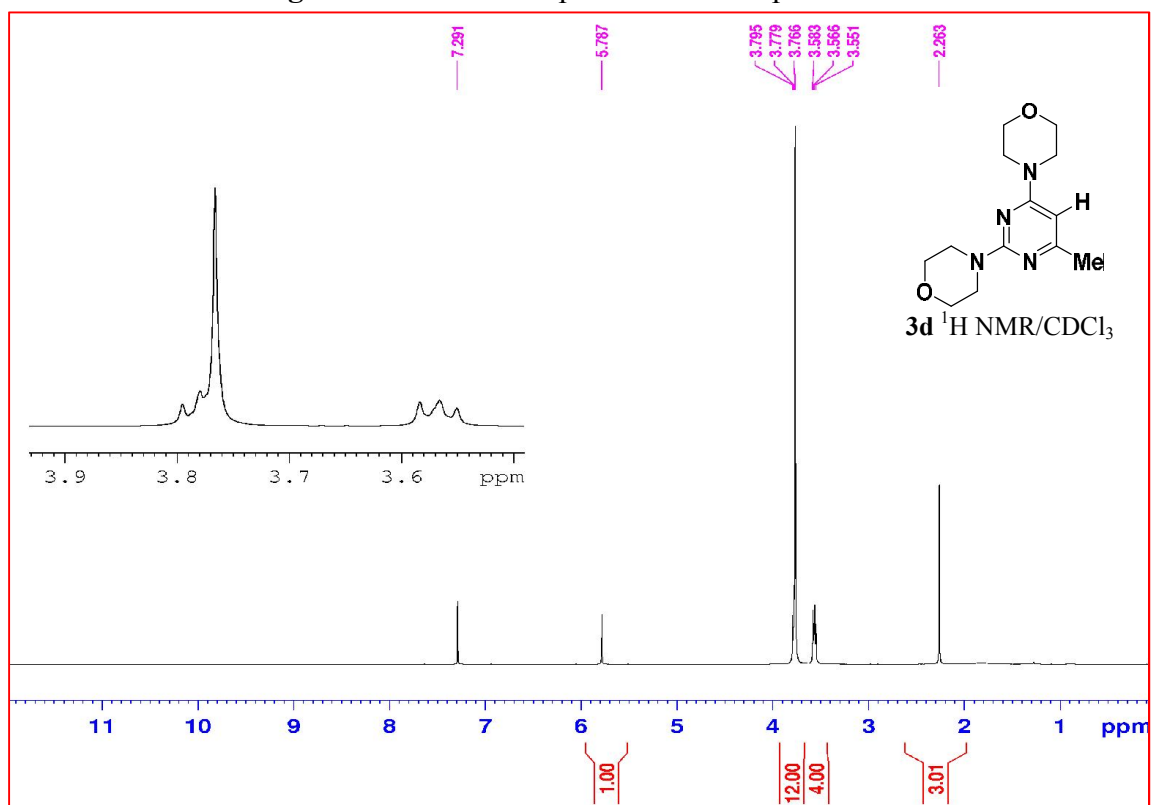


Figure S26. ^{13}C NMR spectrum for compound 3d.

Figure S27. Mass spectrum for compound 3d.

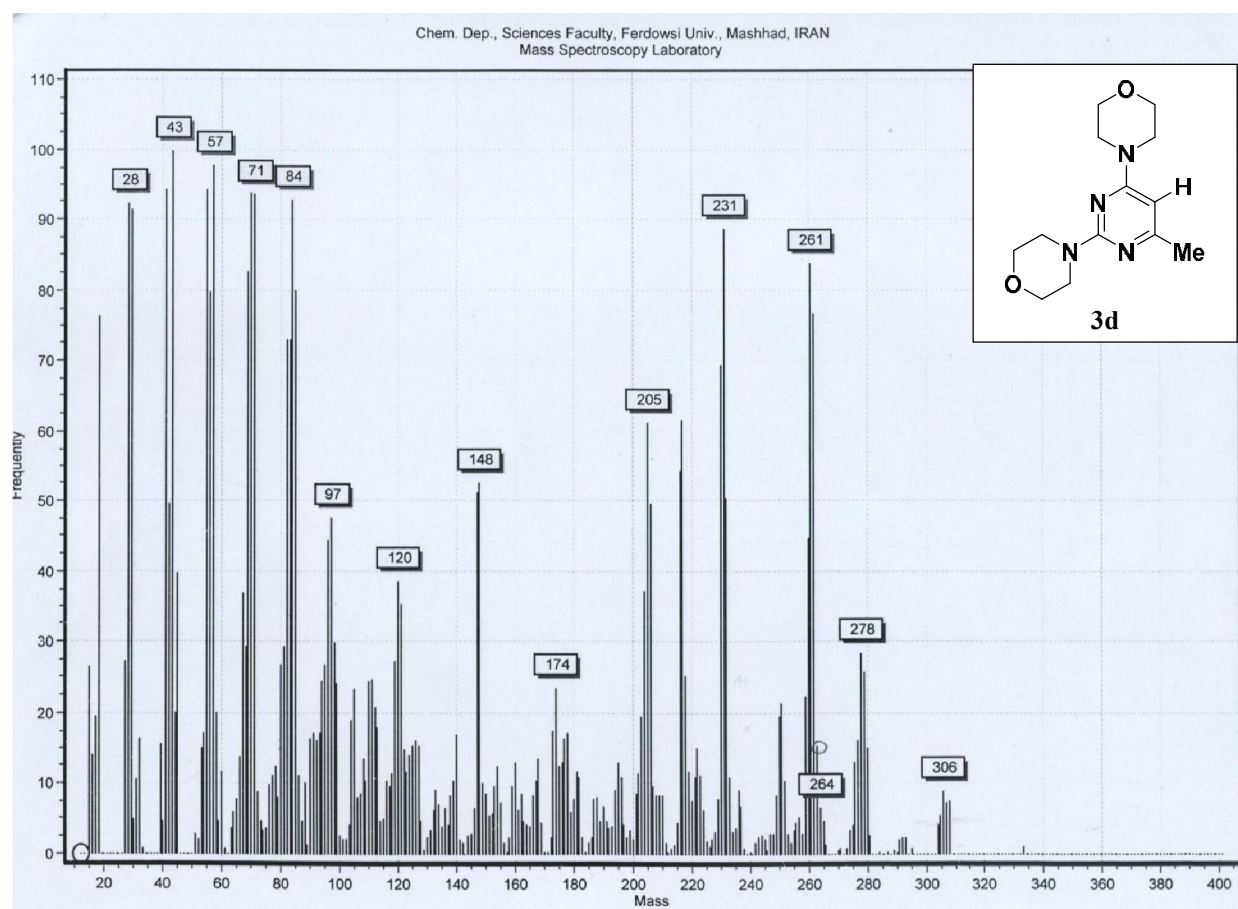


Figure S28. ^1H NMR spectrum for compound 7a.

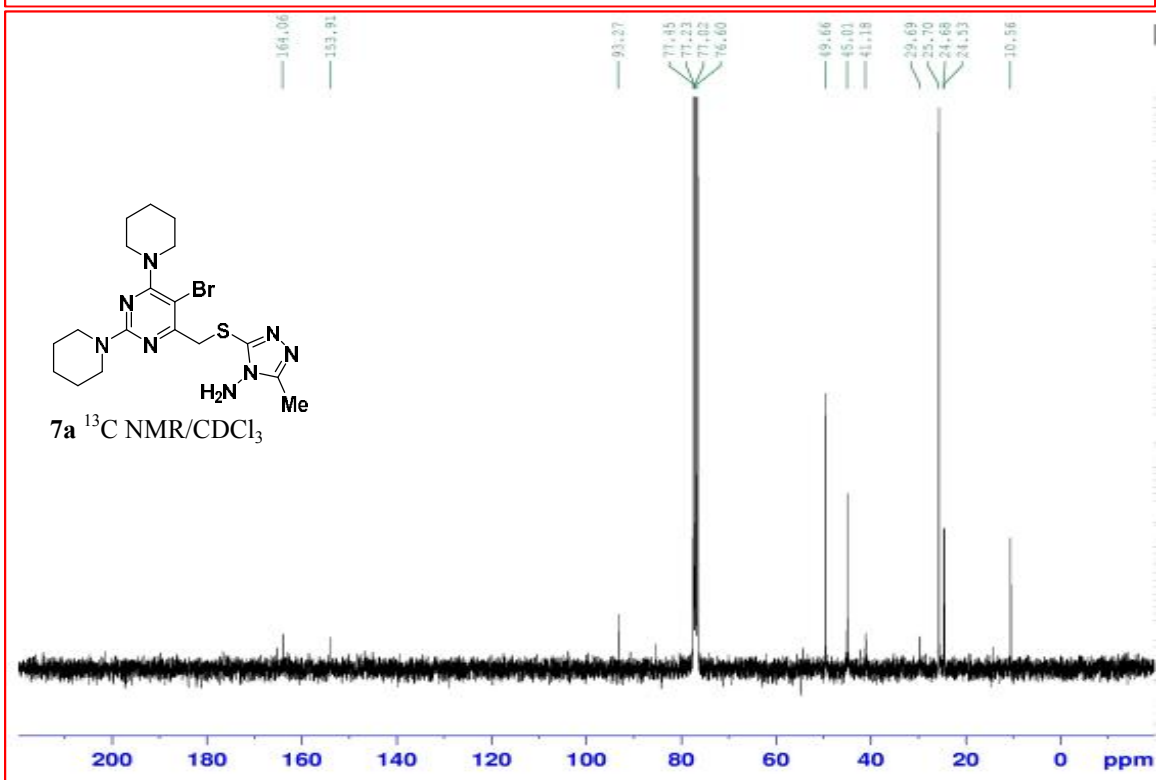
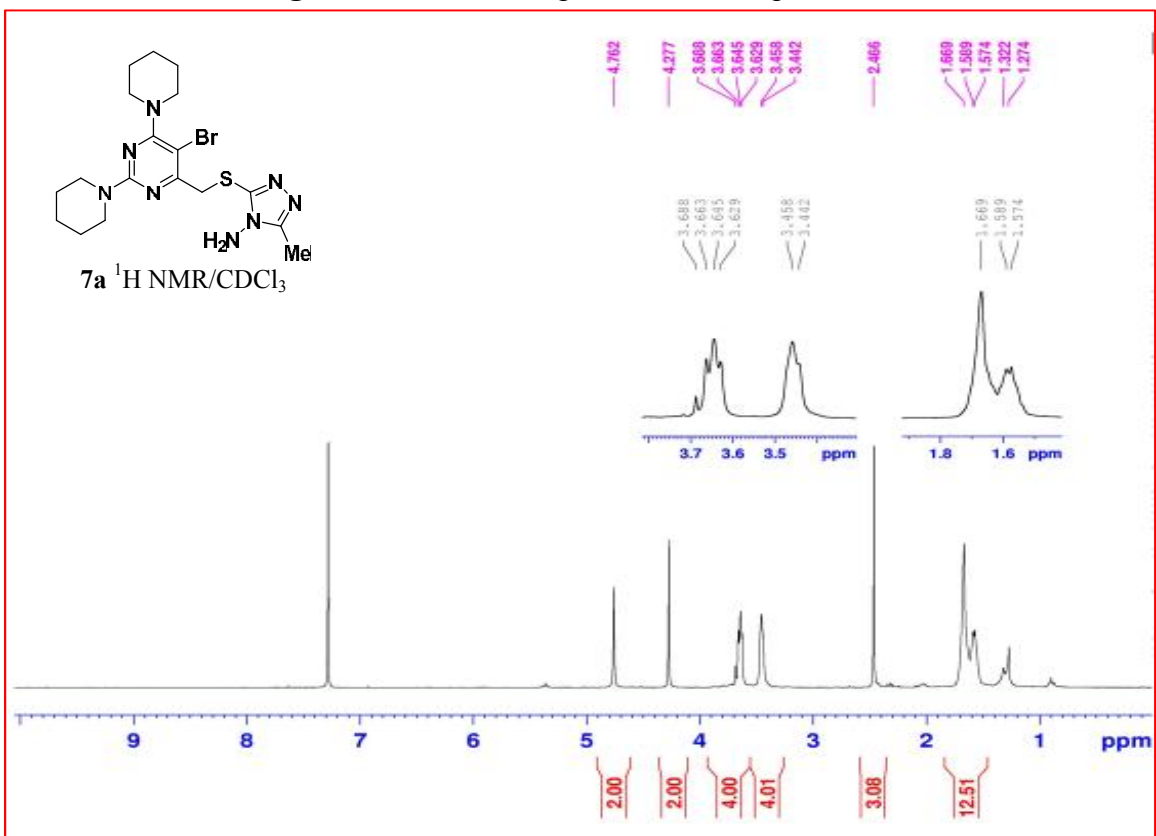


Figure S29. ^{13}C NMR spectrum for compound 7a.

Figure S30. D₂O exchange-¹H NMR spectrum for compound 7a.

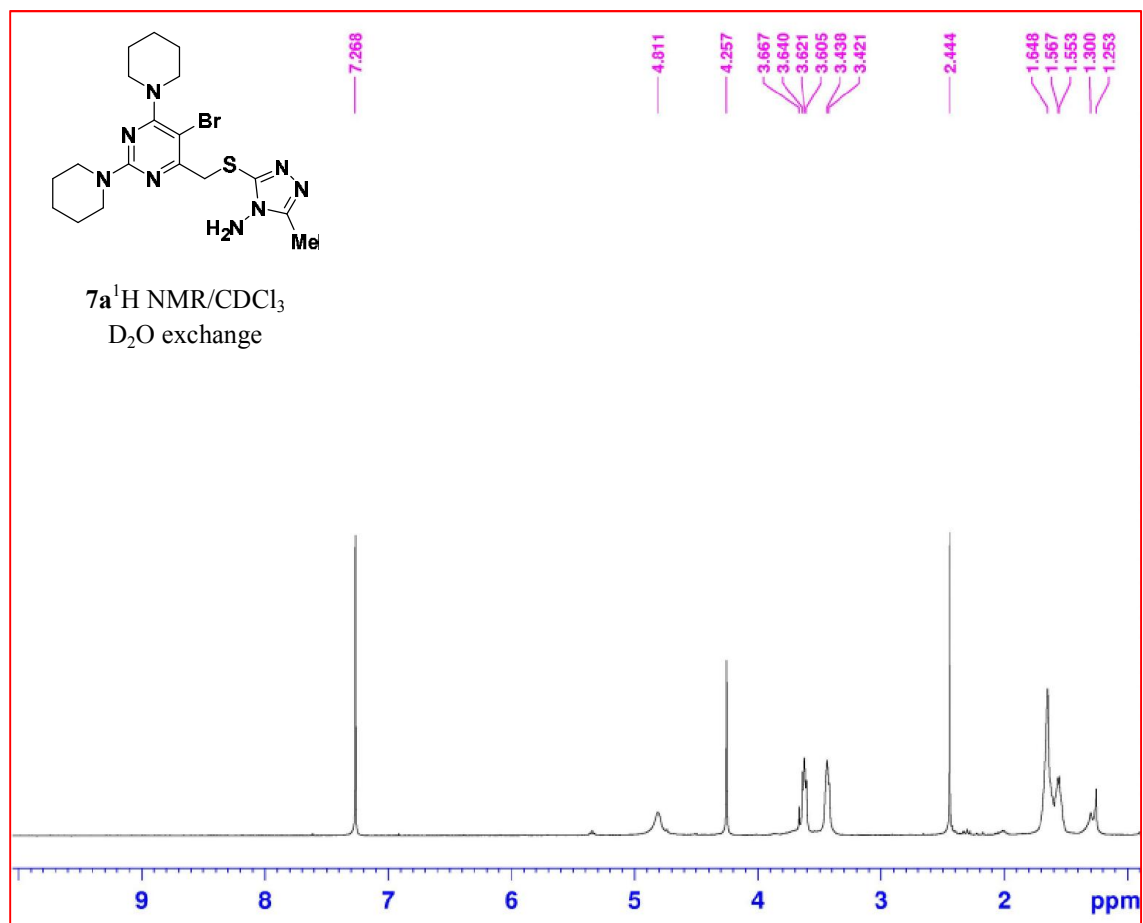


Figure S31. Mass spectrum for compound 7a.

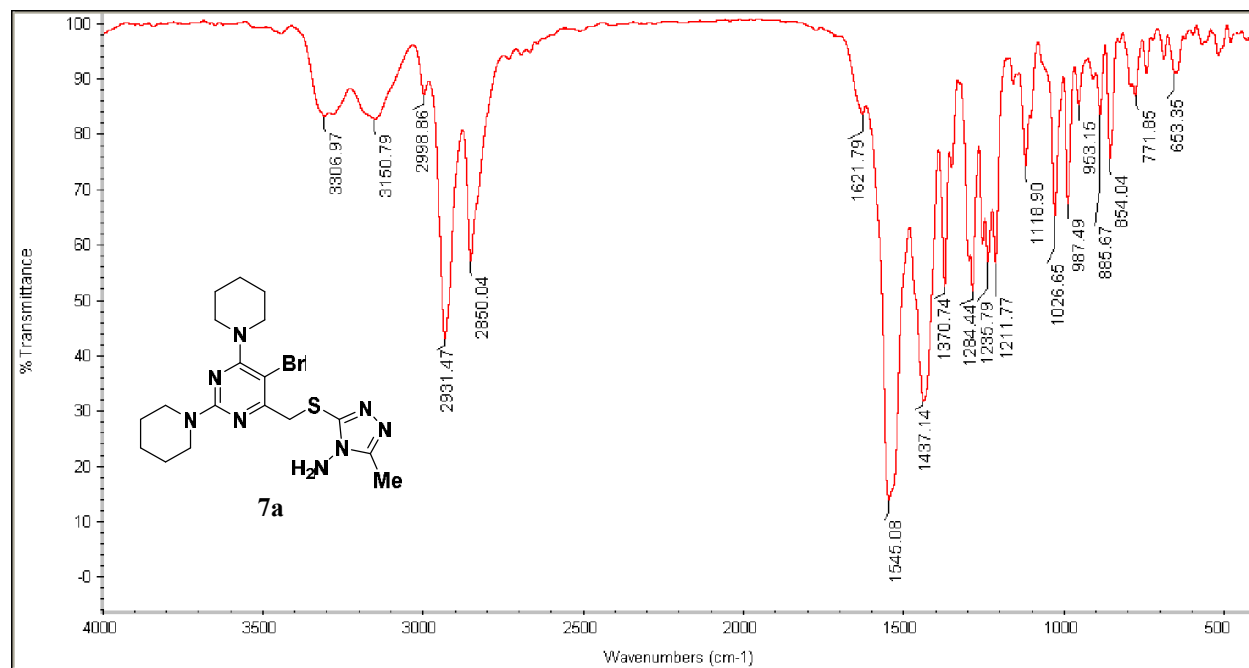
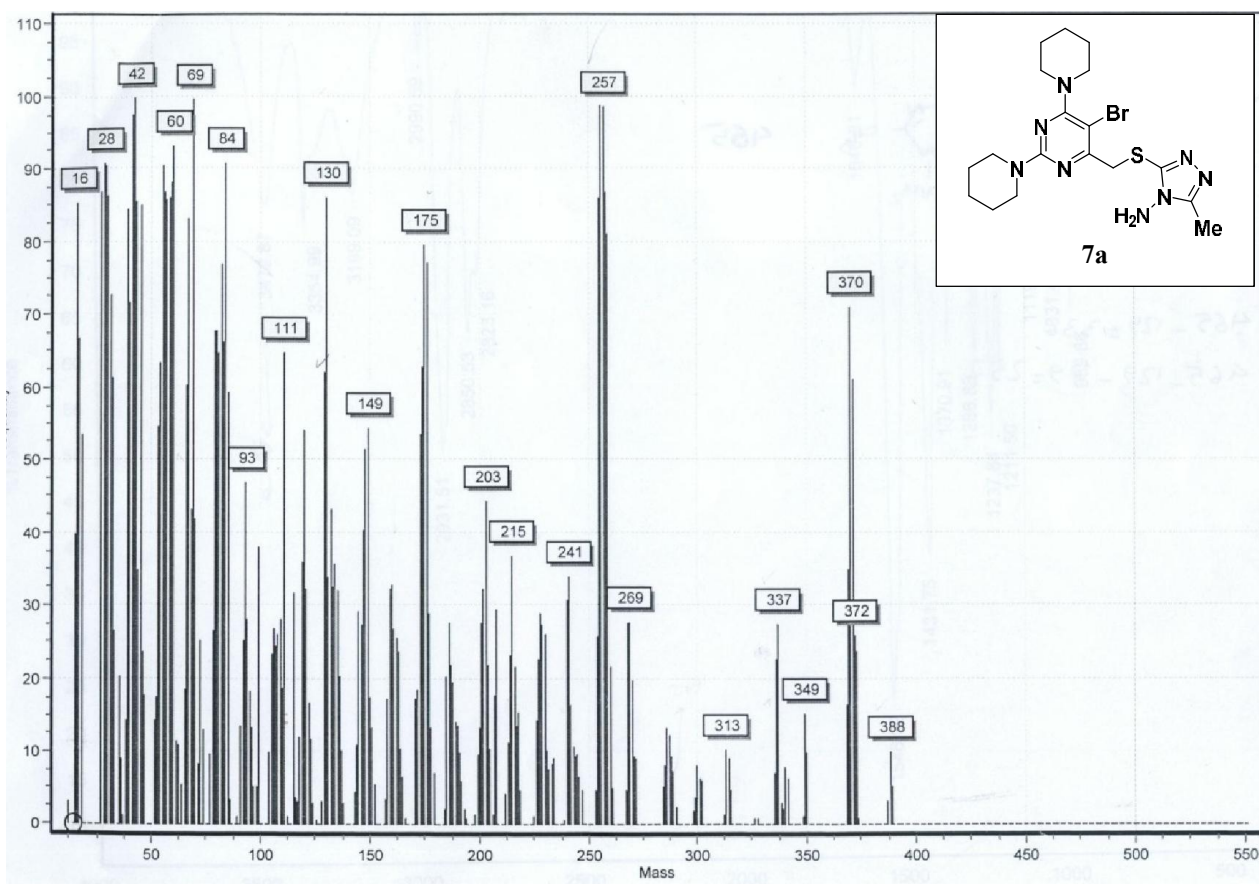


Figure S32. FTIR spectrum for compound 7a.

Figure S33. ^1H NMR spectrum for compound 7b.

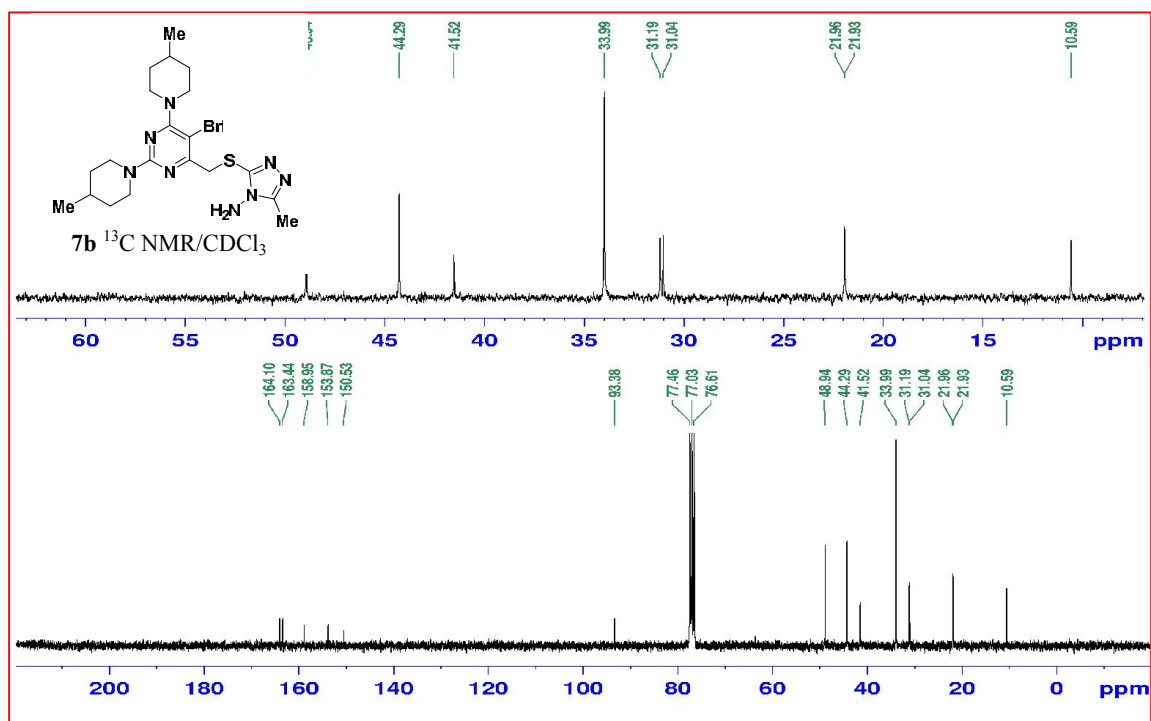
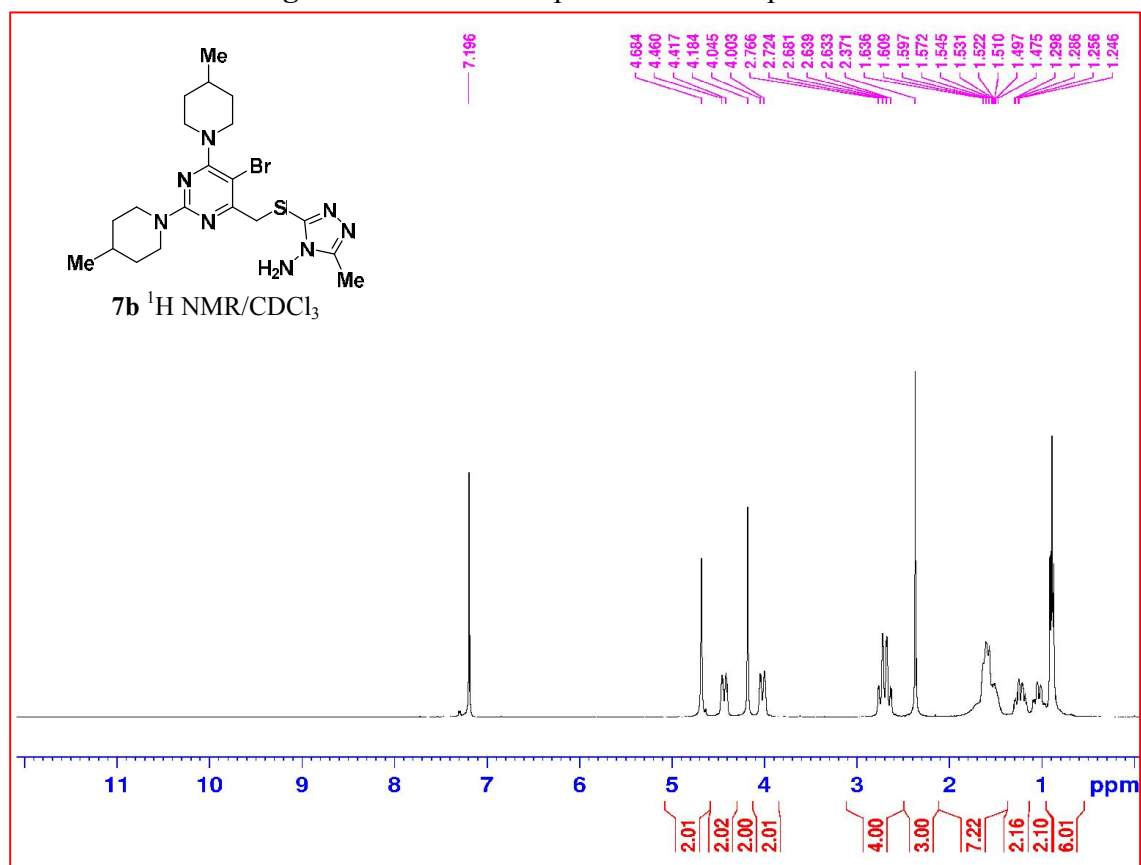


Figure S34. ^{13}C NMR spectrum for compound 7b.

Figure S35. Mass spectrum for compound 7b.

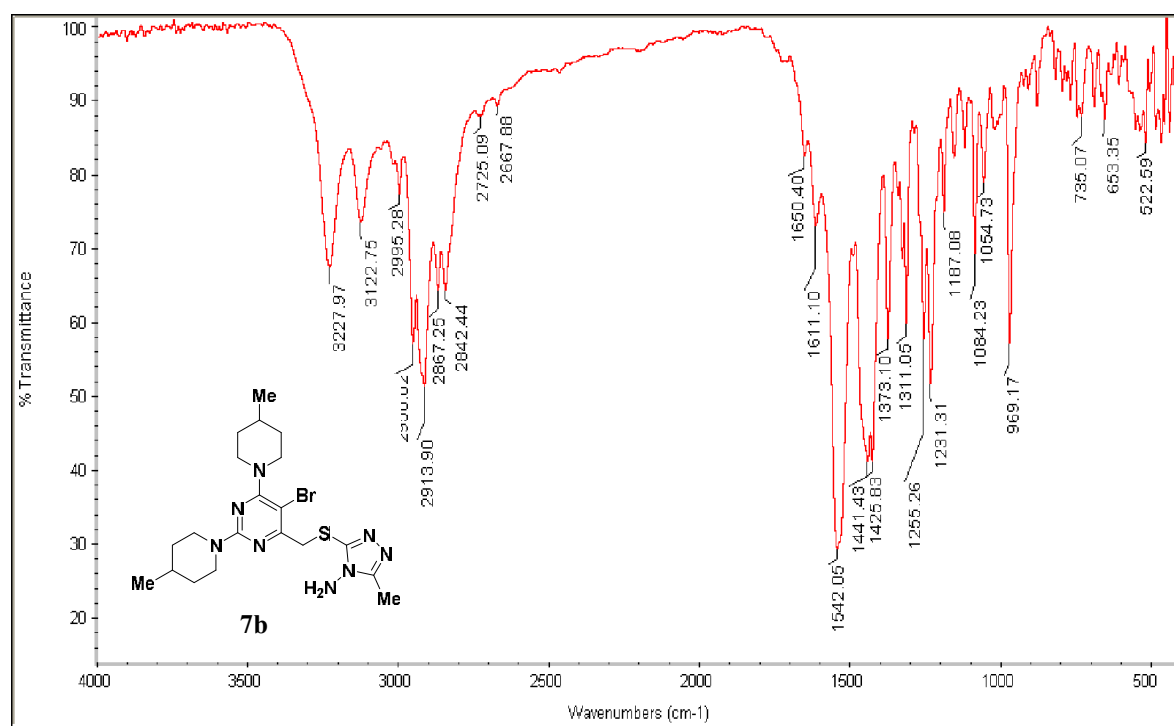
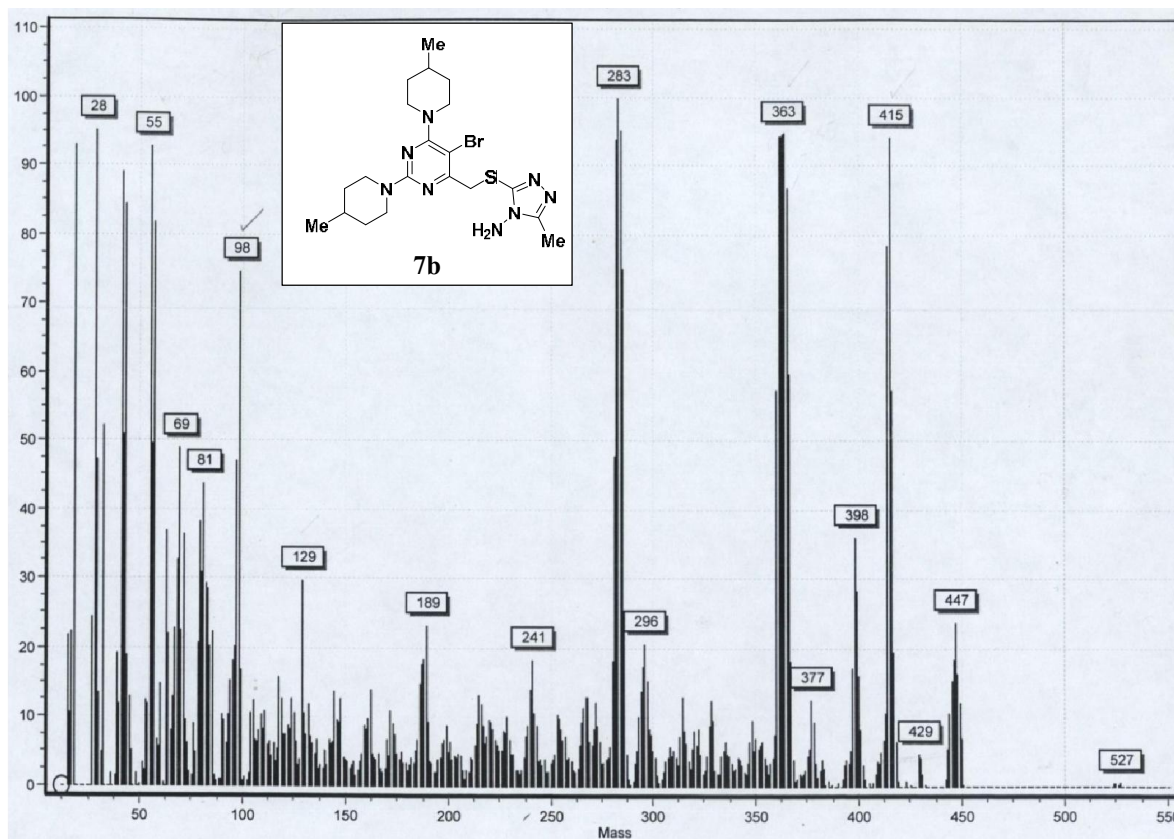


Figure S36. FTIR spectrum for compound 7b.

Figure S37. ^1H NMR spectrum for compound 7c.

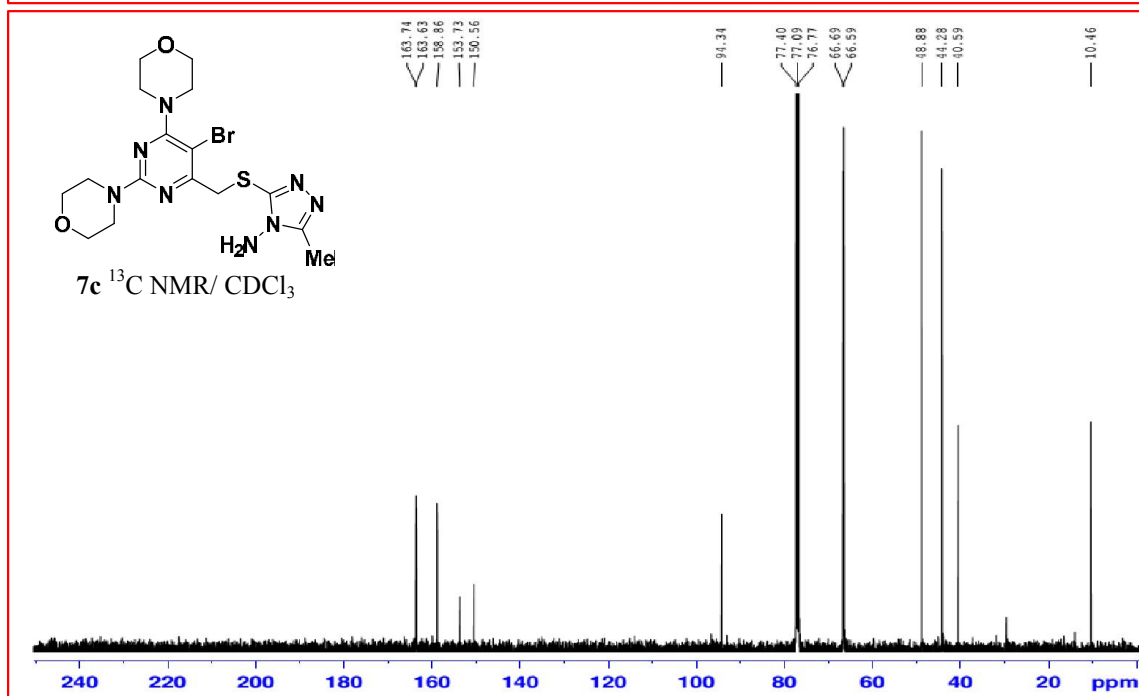
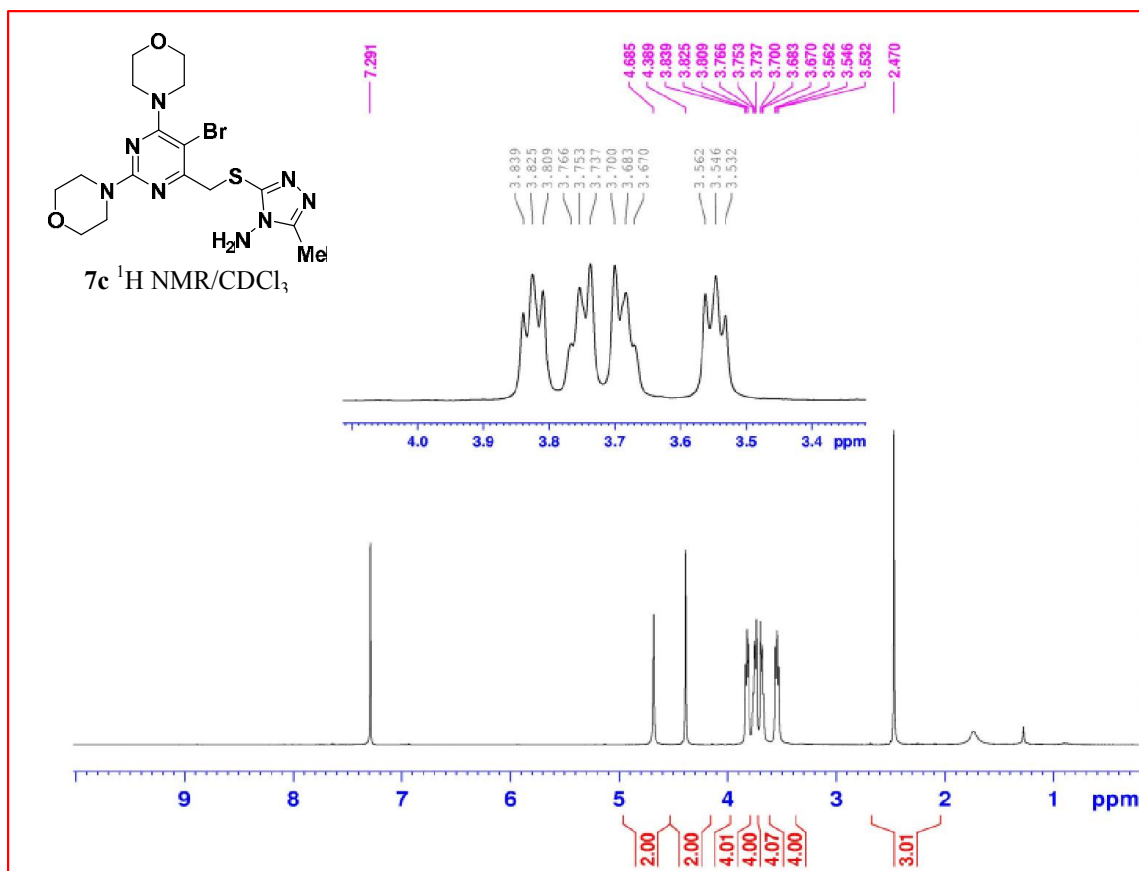


Figure S38. ^{13}C NMR spectrum for compound 7c.

Figure S39. D₂O exchange-¹H NMR spectrum for compound **7c**.

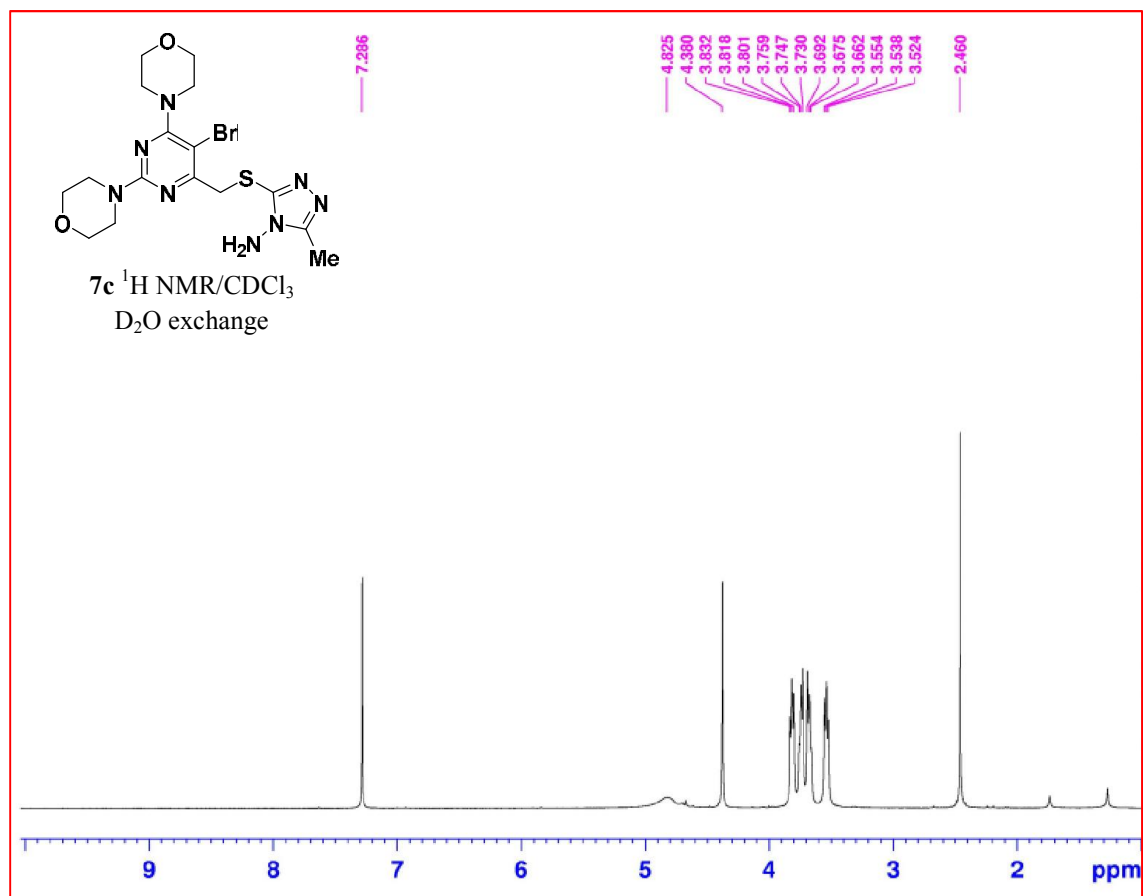


Figure S40. Mass spectrum for compound 7c.

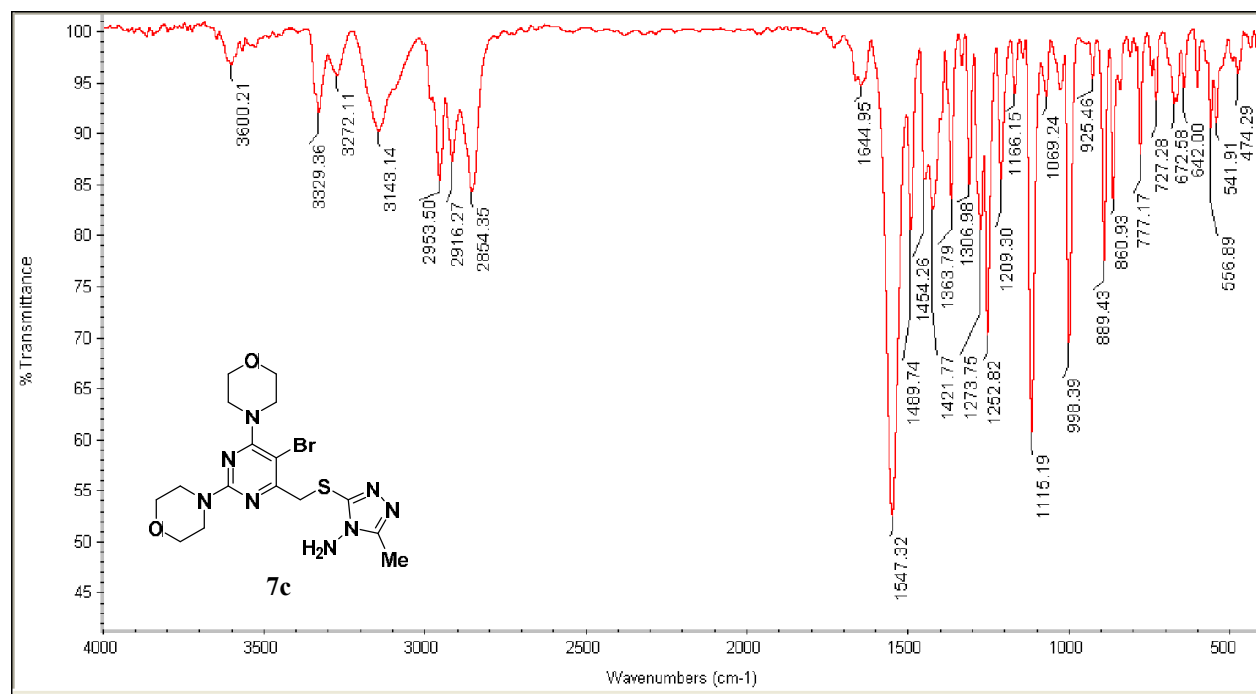
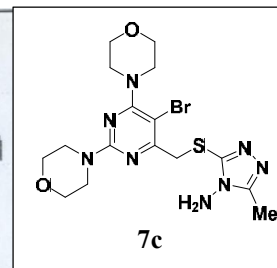
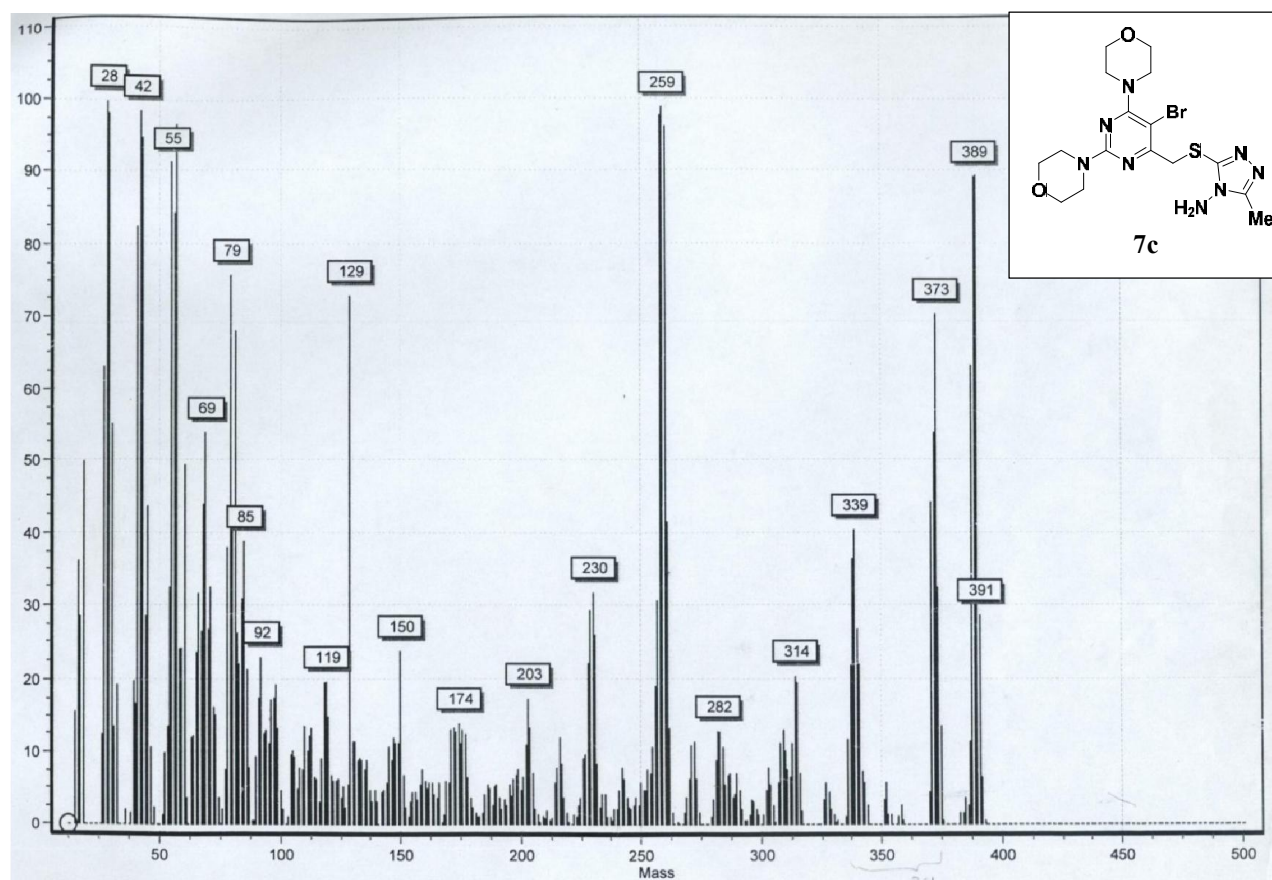


Figure S41. FTIR spectrum for compound 7c.

Figure S42. ^1H NMR spectrum for compound 7d.

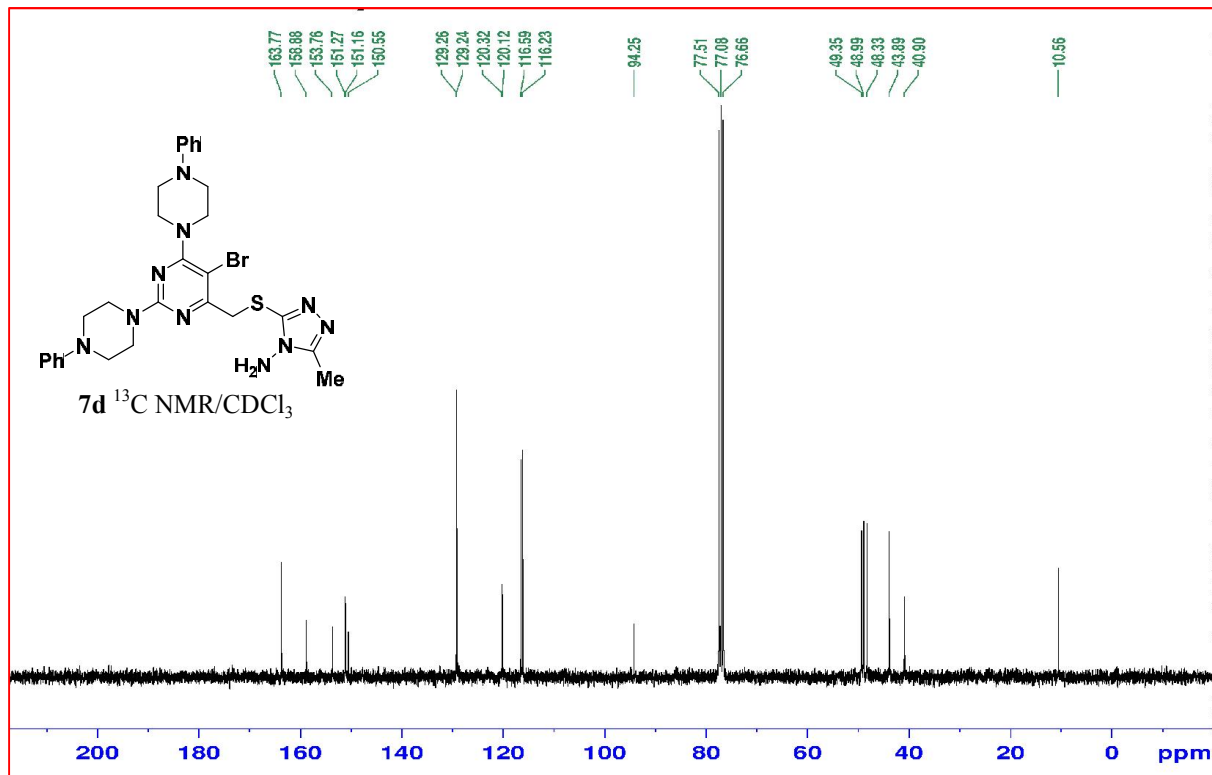
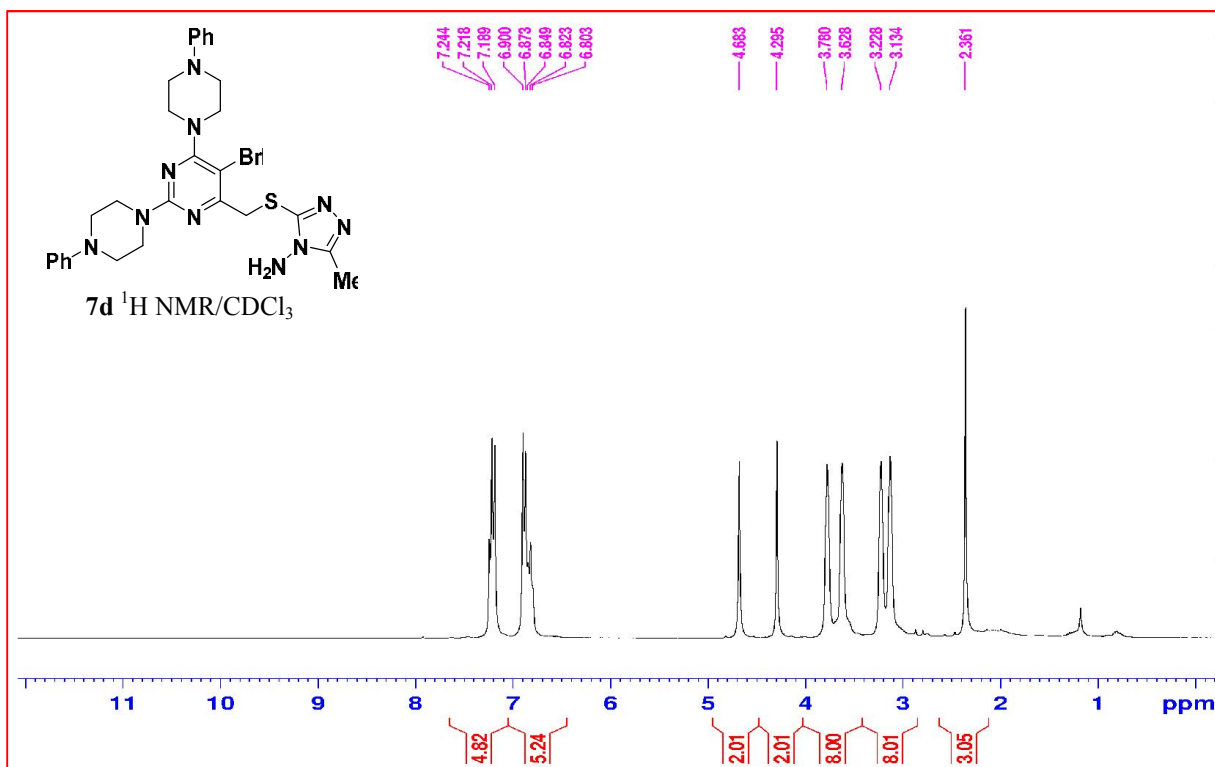


Figure S43. ^{13}C NMR spectrum for compound 7d.

Figure S44. Mass spectrum for compound 7d.

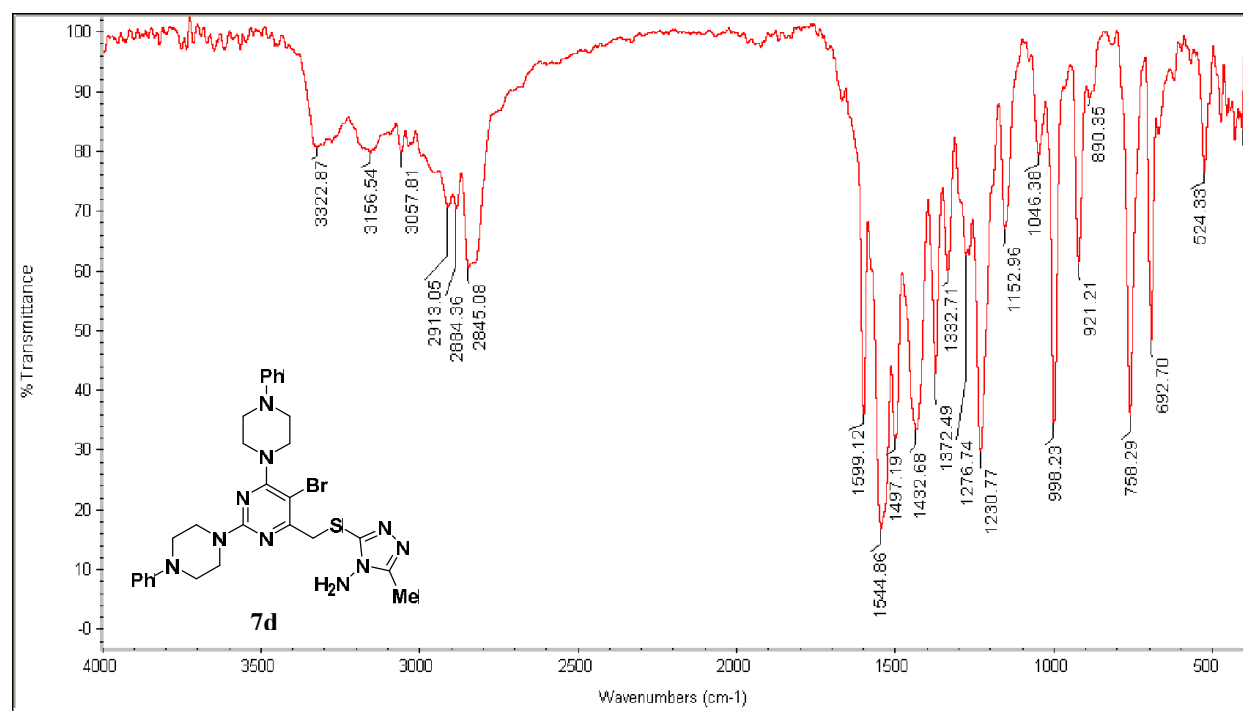
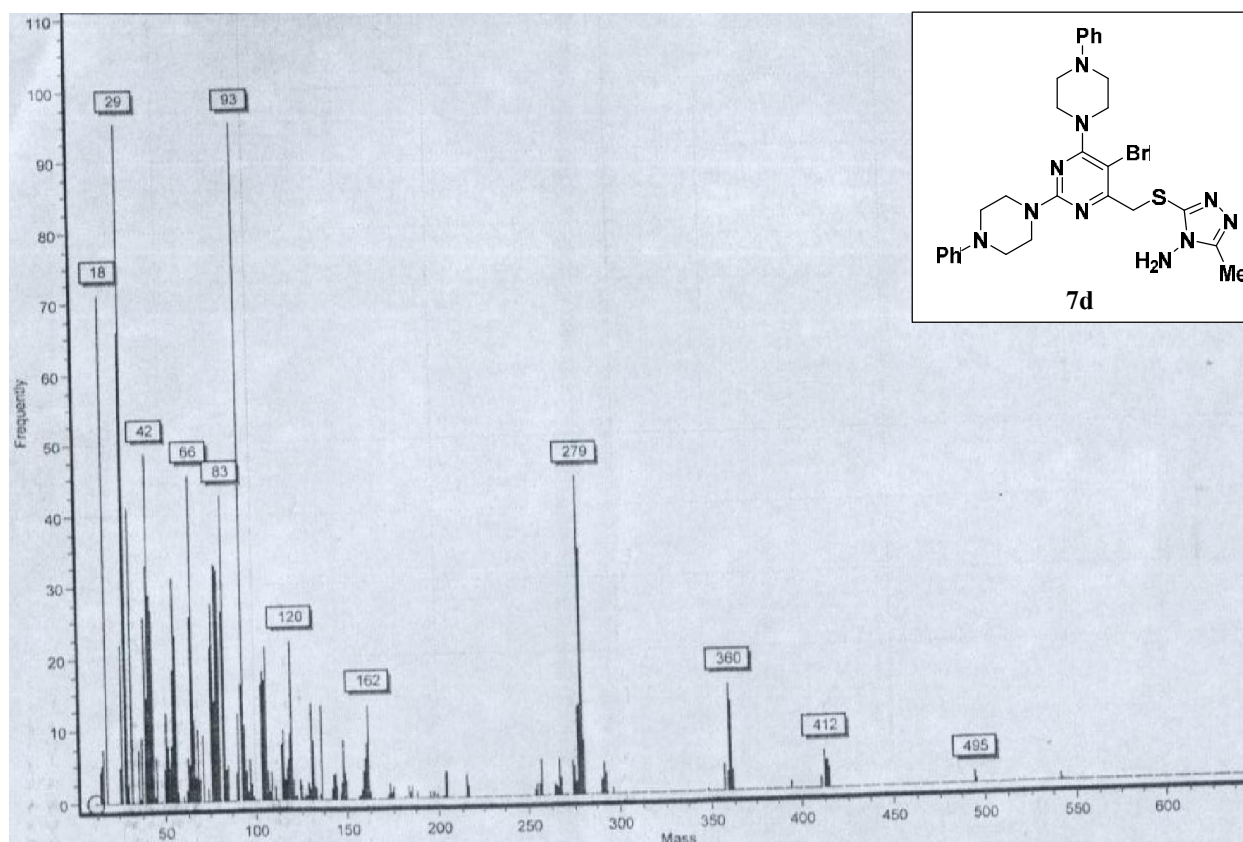


Figure S45. FTIR spectrum for compound 7d.

Figure S46. ^1H NMR spectrum for compound 7e.

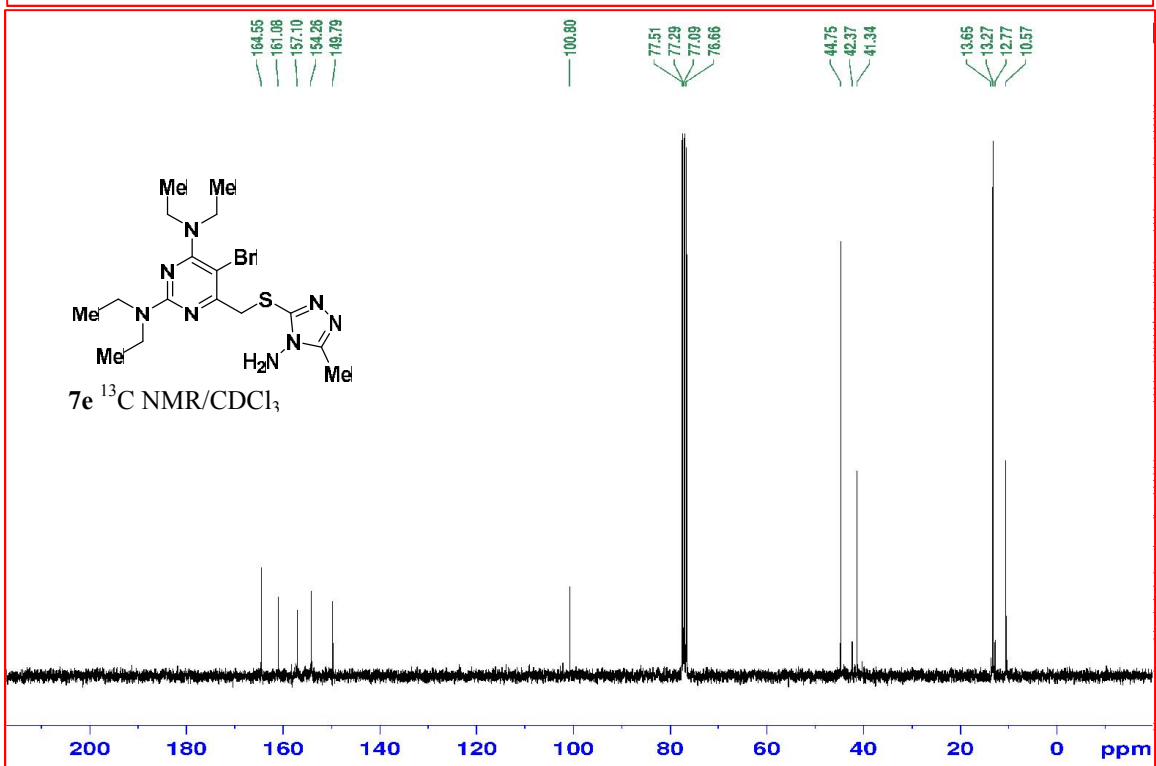
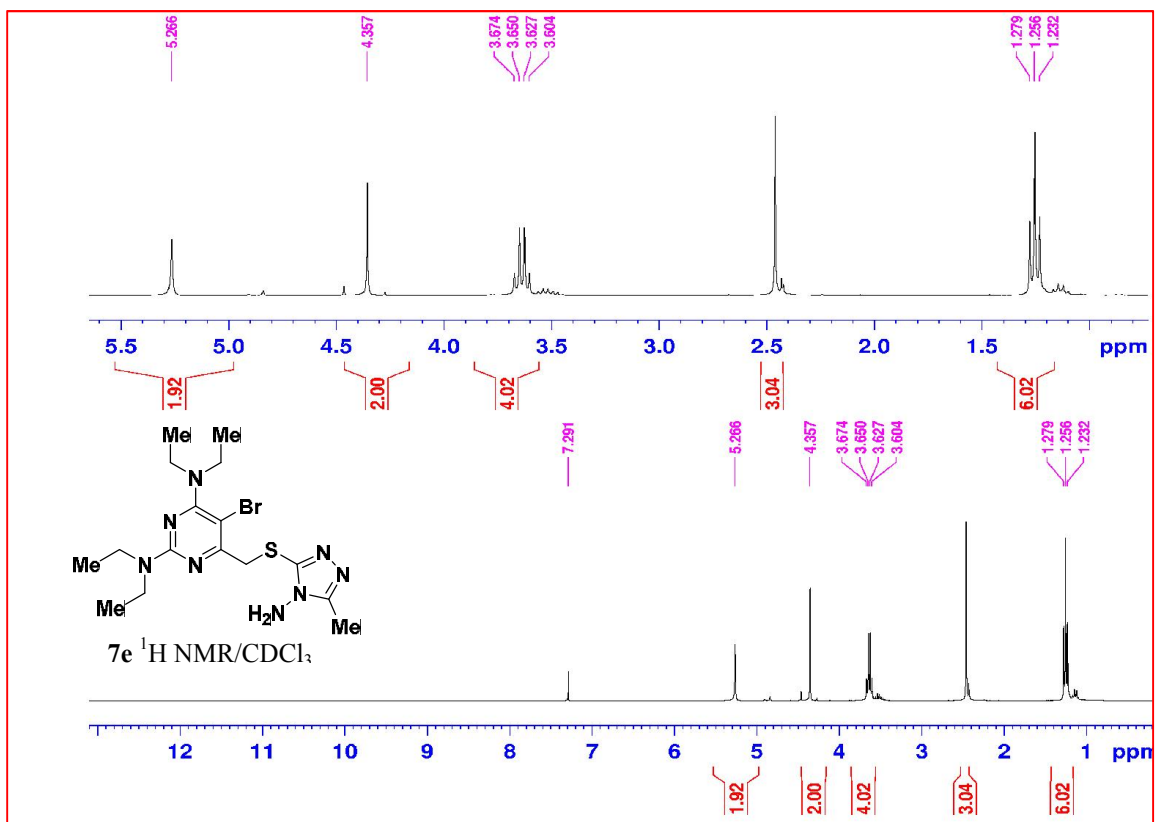


Figure S47. ^{13}C NMR spectrum for compound 7e.

Figure S48. Mass spectrum for compound 7e.

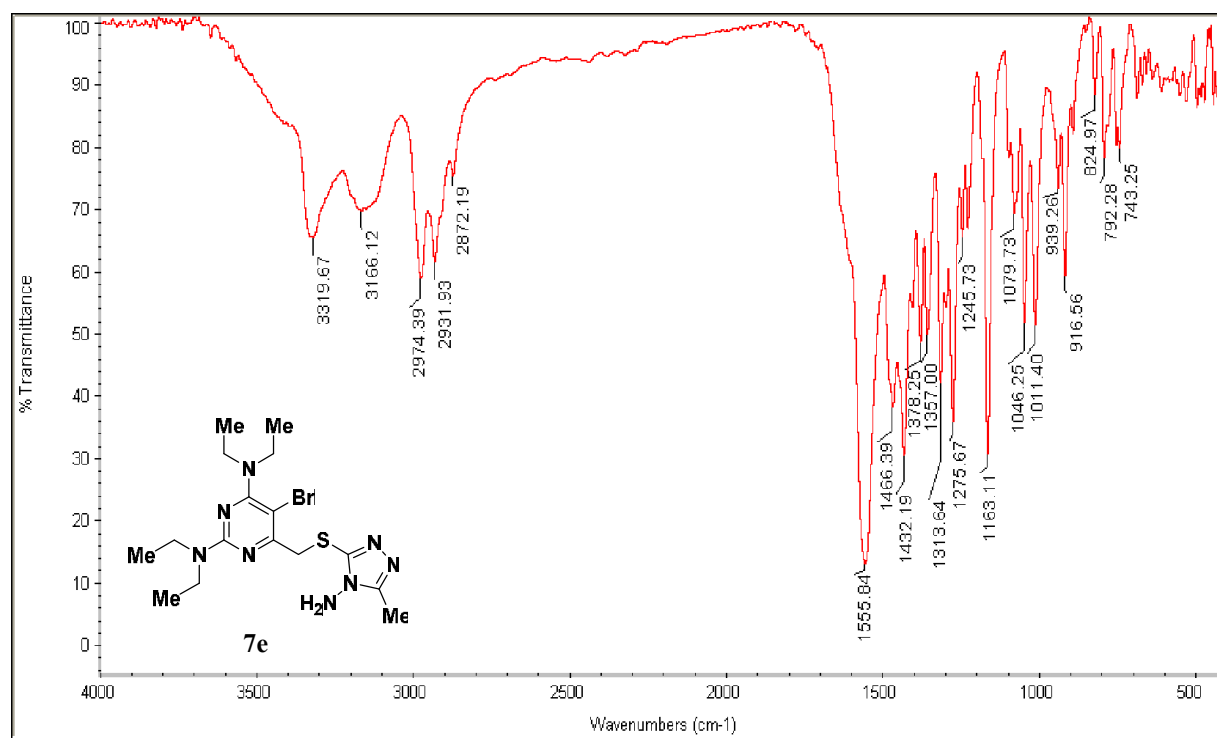
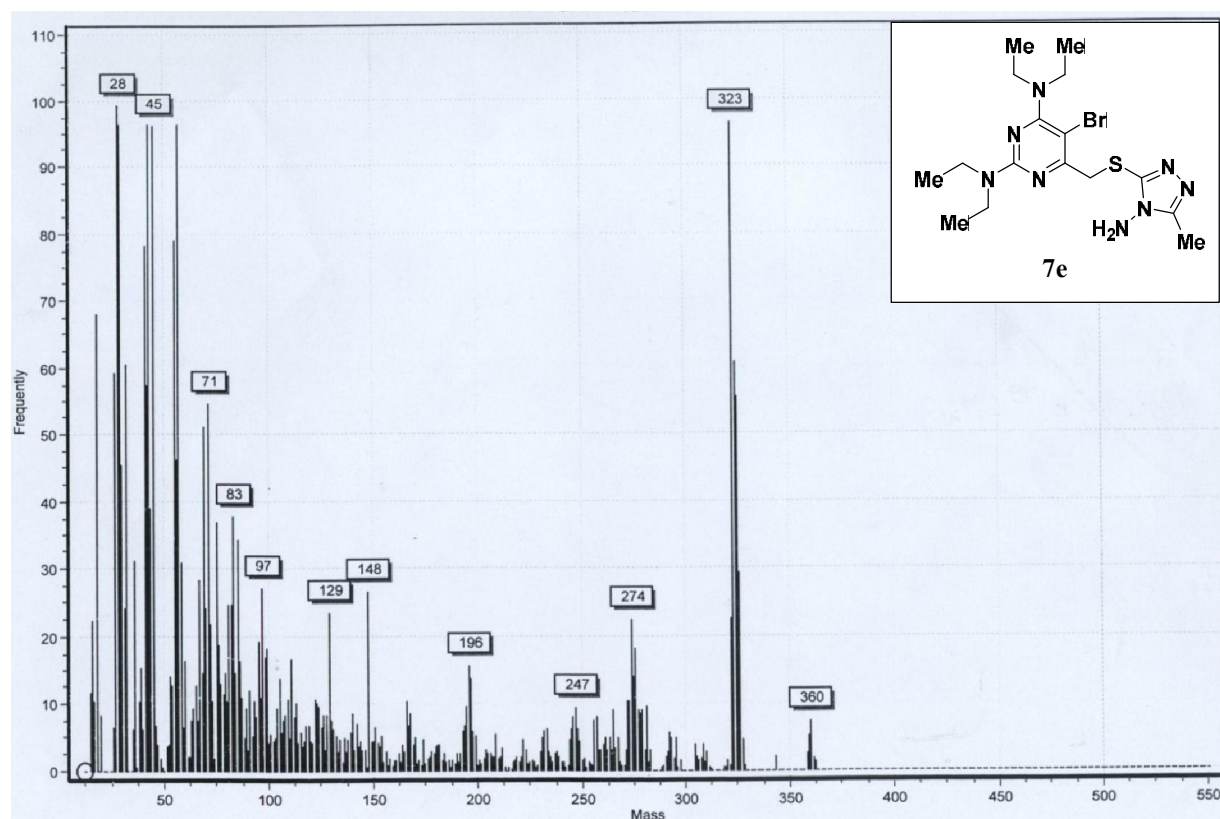


Figure S49. FTIR spectrum for compound 7e.

Figure S50. ^1H NMR spectrum for compound 8a.

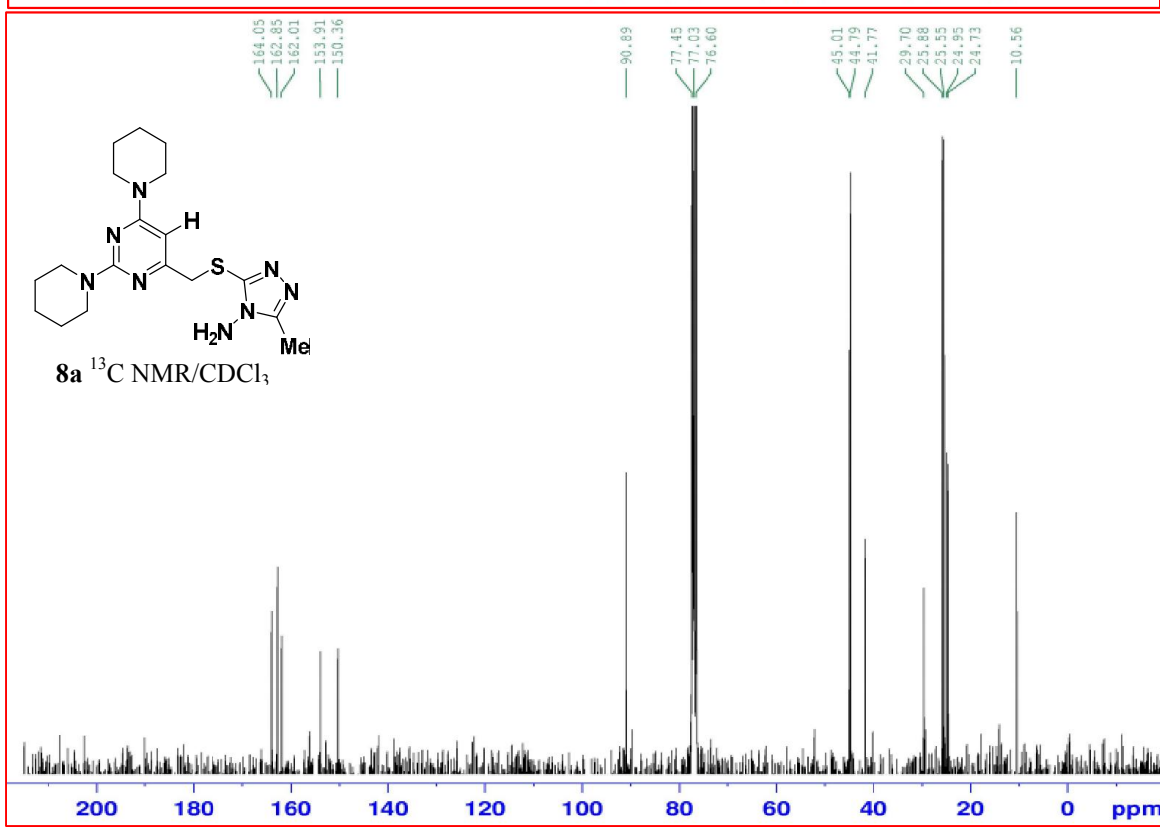
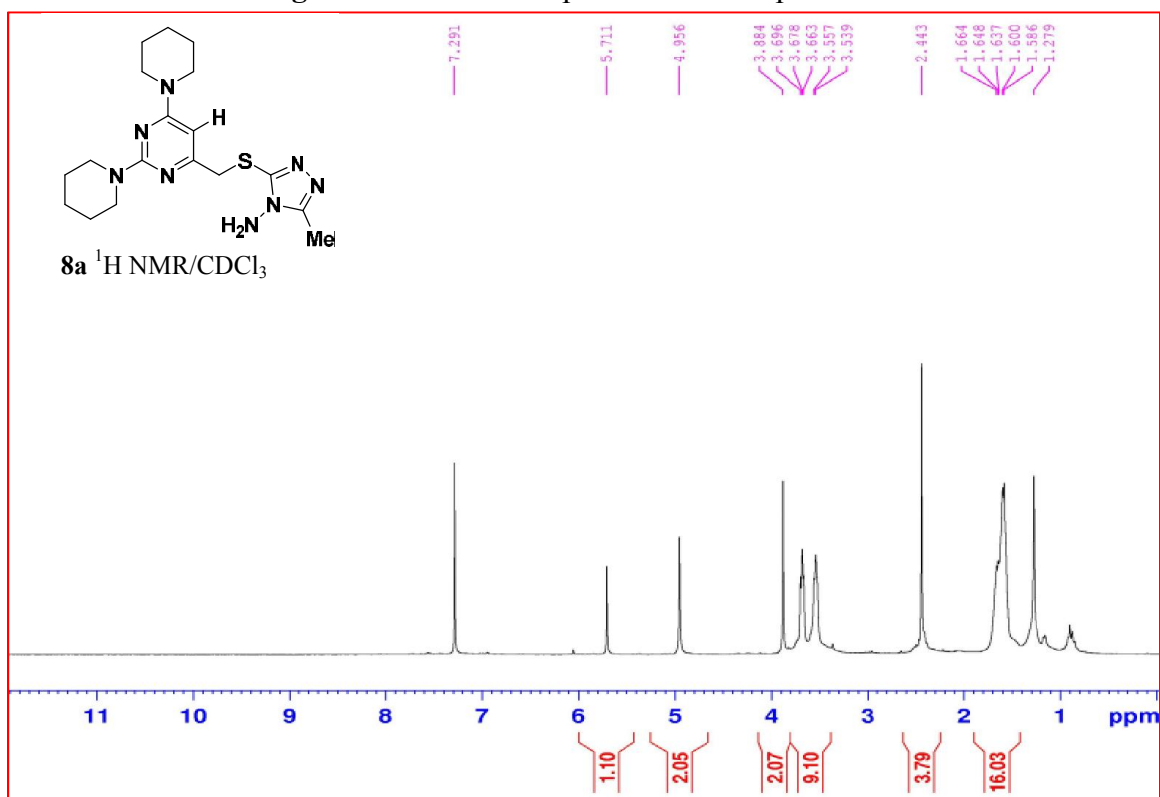


Figure S51. ^{13}C NMR spectrum for compound 8a.

Figure S52. D₂O exchange-¹H NMR spectrum for compound 8a.

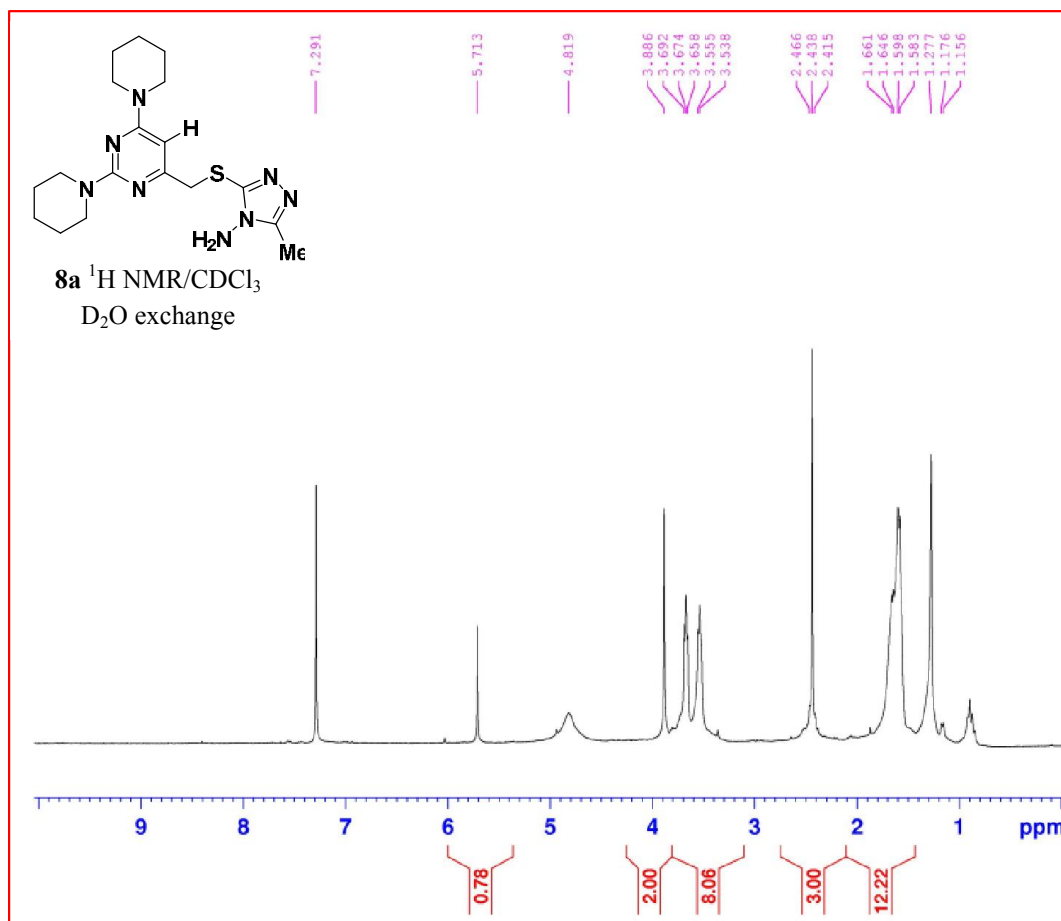


Figure S53. Mass spectrum for compound 8a.

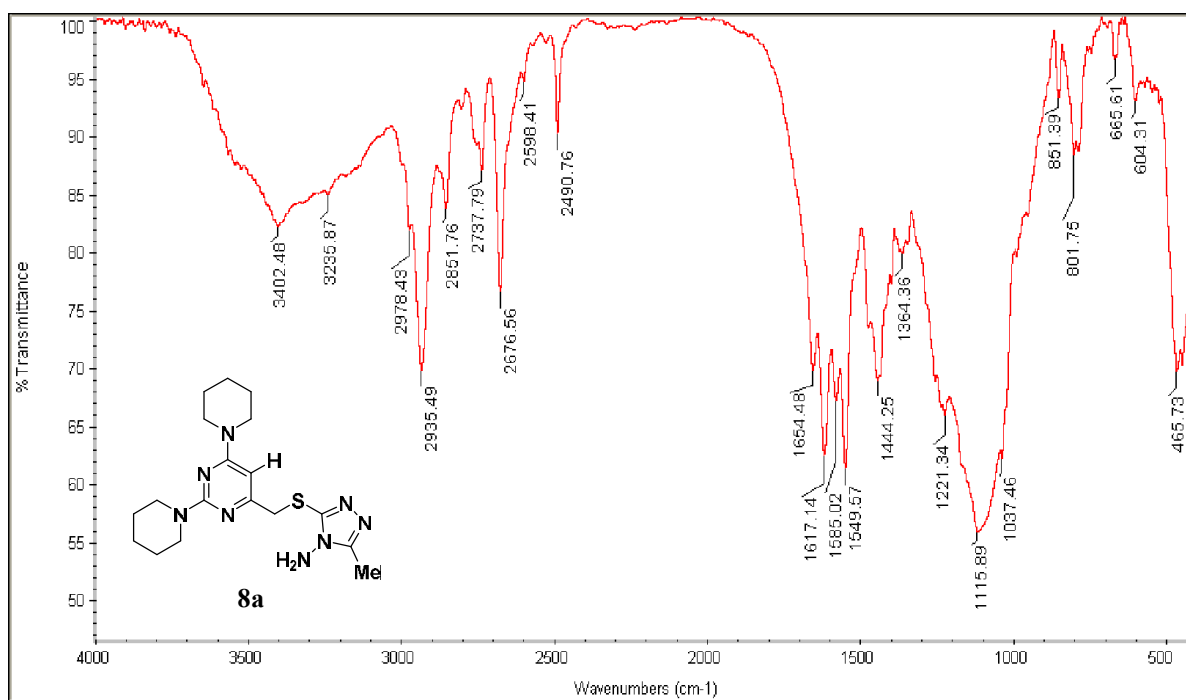
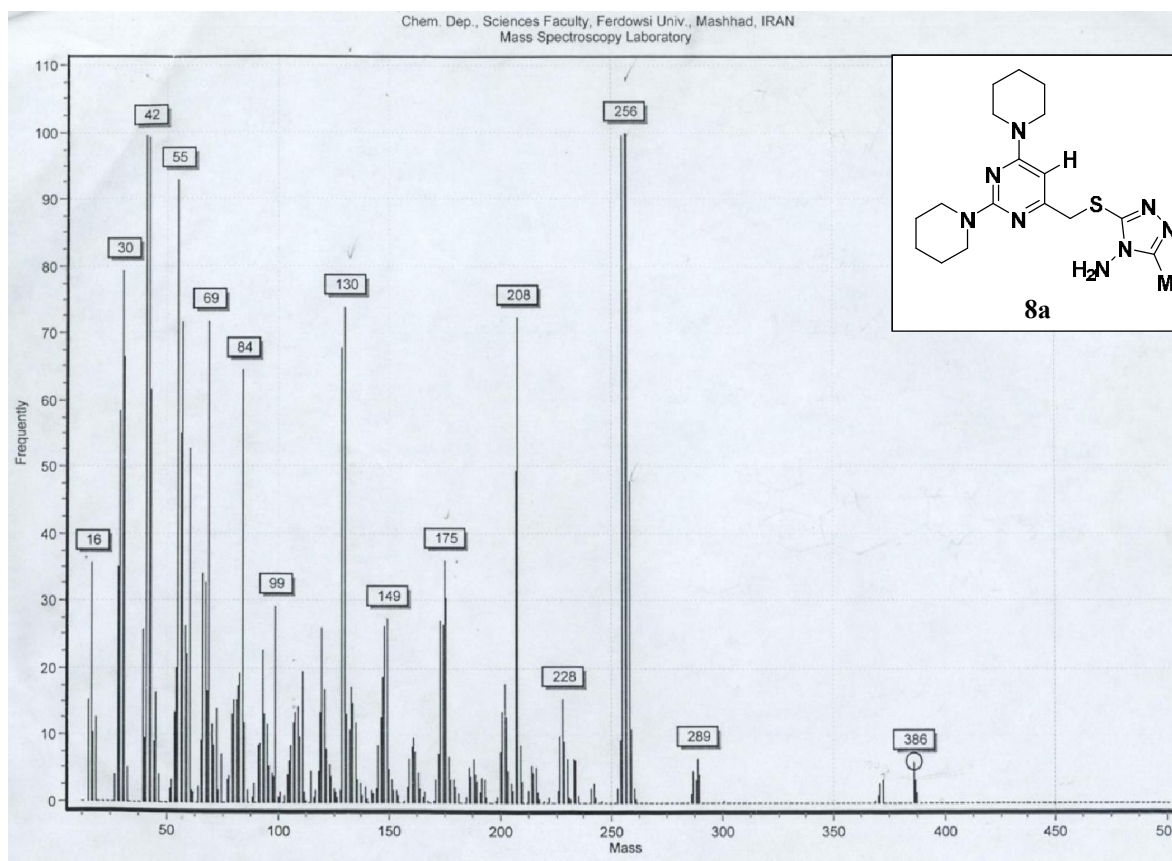


Figure S54. FTIR spectrum for compound 8a.

Figure S55. ^1H NMR spectrum for compound 8b.

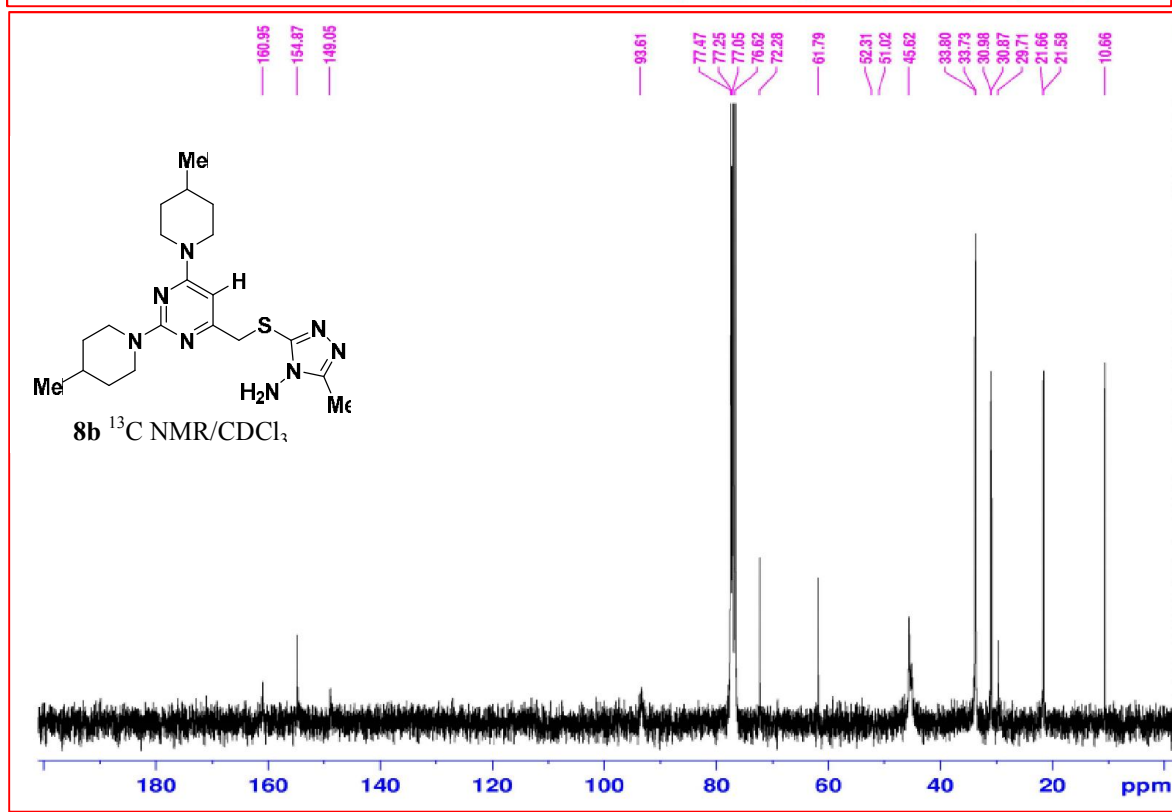
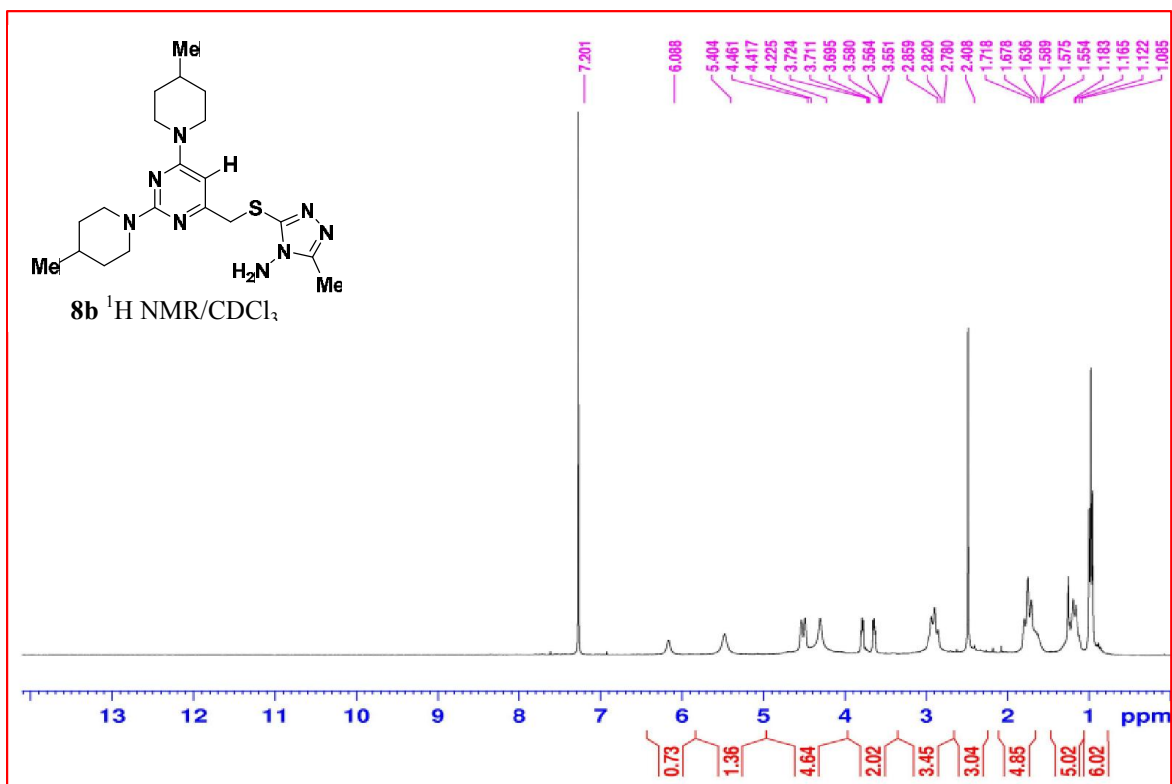


Figure S56. ^{13}C NMR spectrum for compound 8b.

Figure S57. D₂O exchange-¹H NMR spectrum for compound 8b.

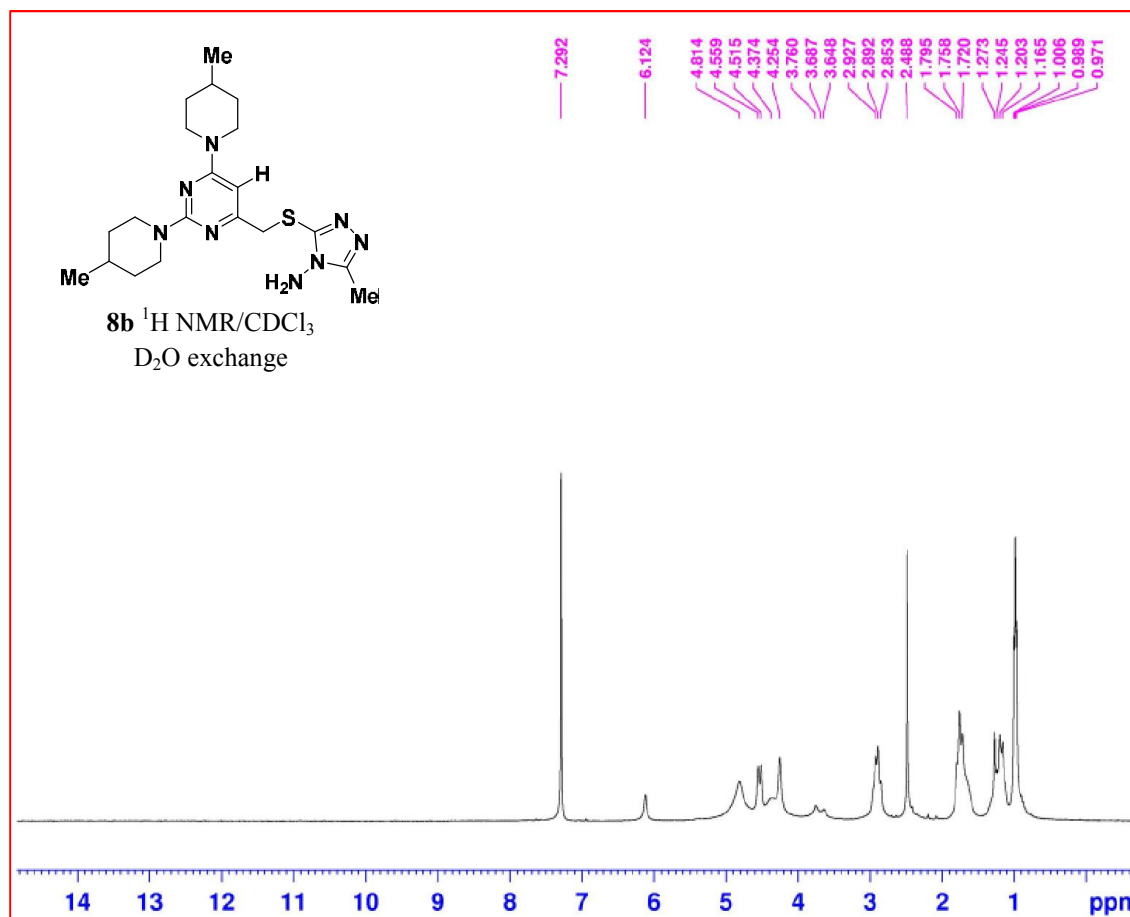


Figure S58. Mass spectrum for compound 8b

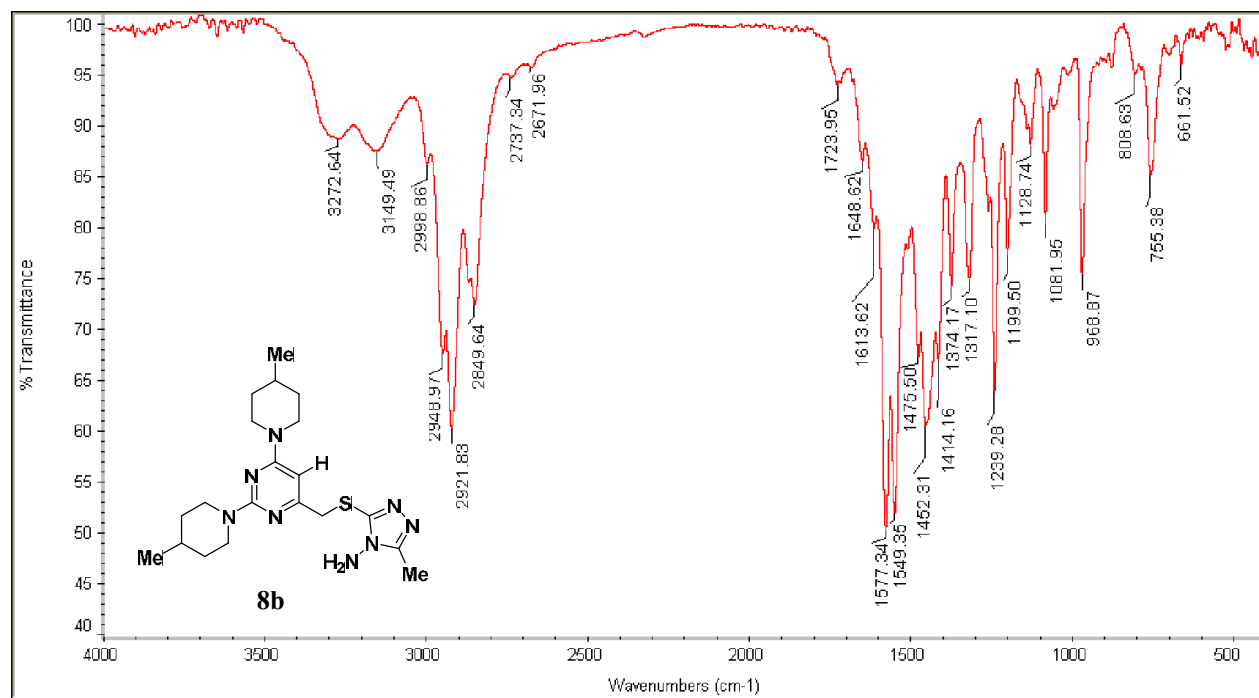
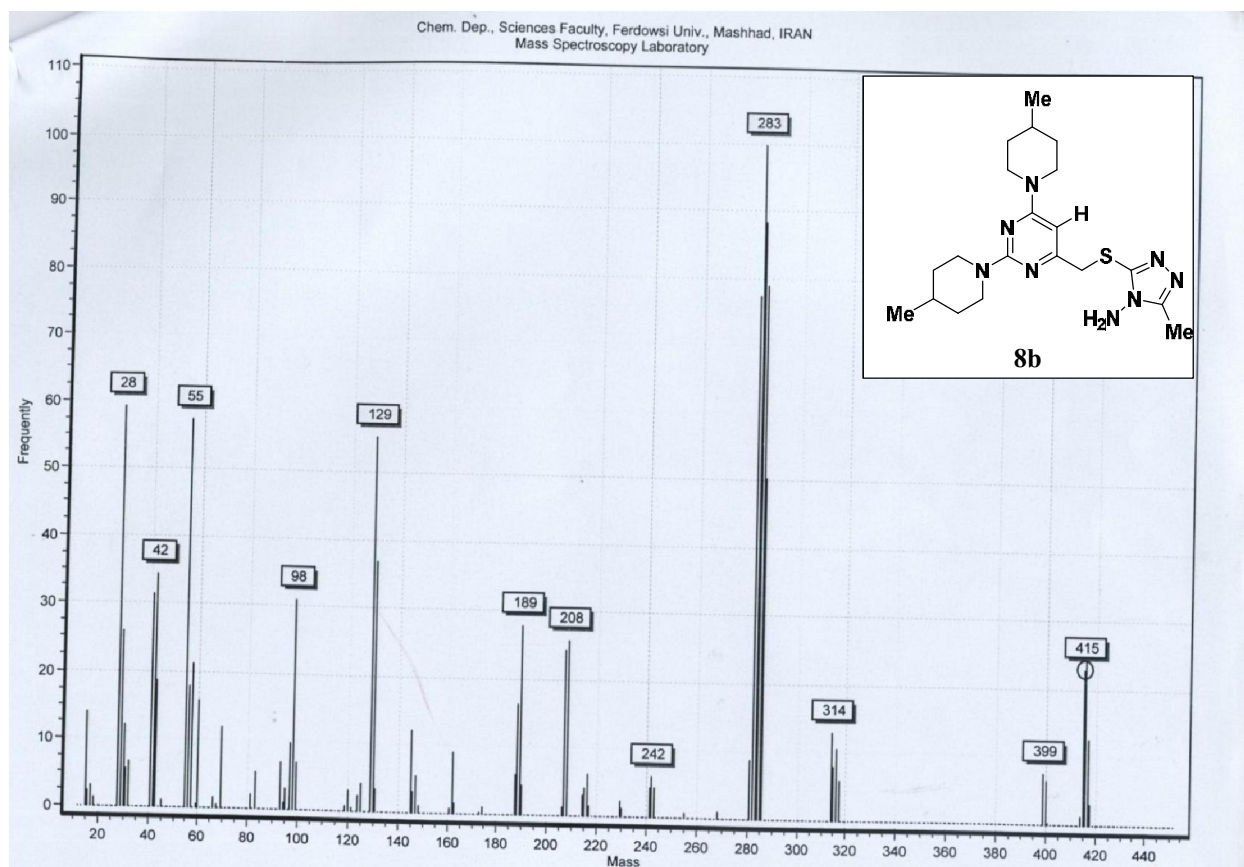


Figure S59. FTIR spectrum for compound 8b.

Figure S60. ^1H NMR spectrum for compound 8c.

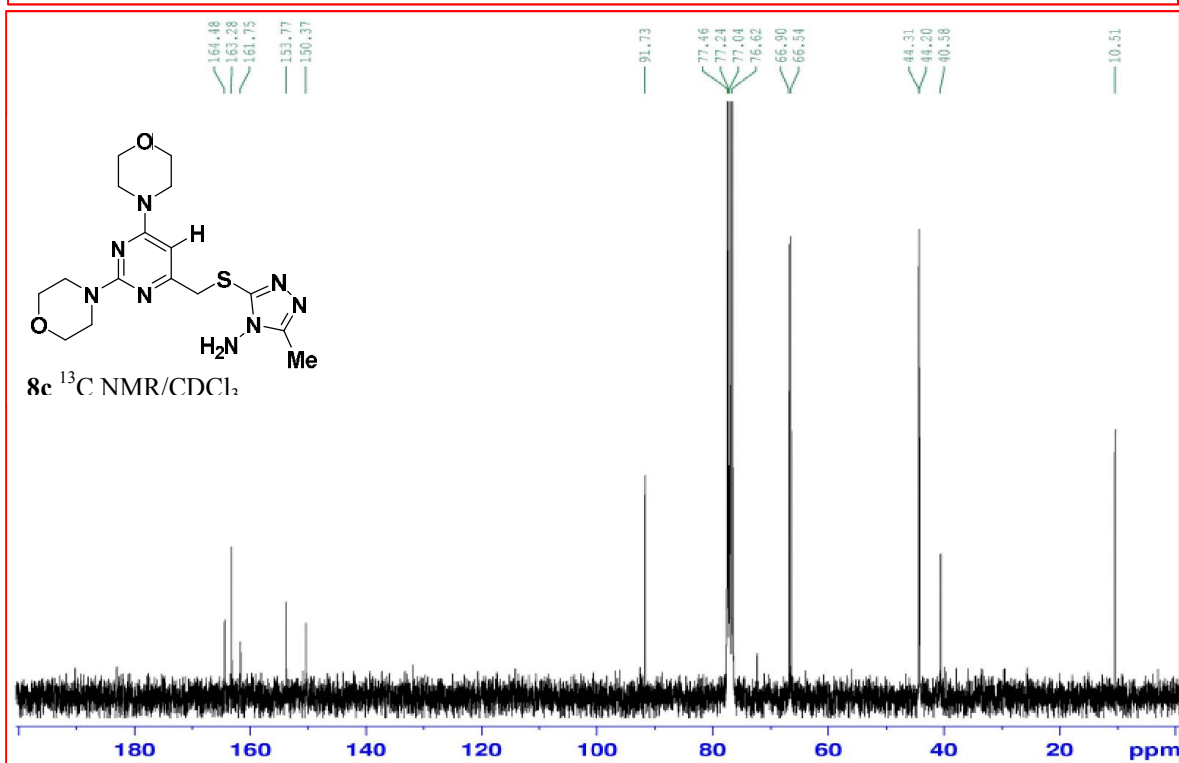
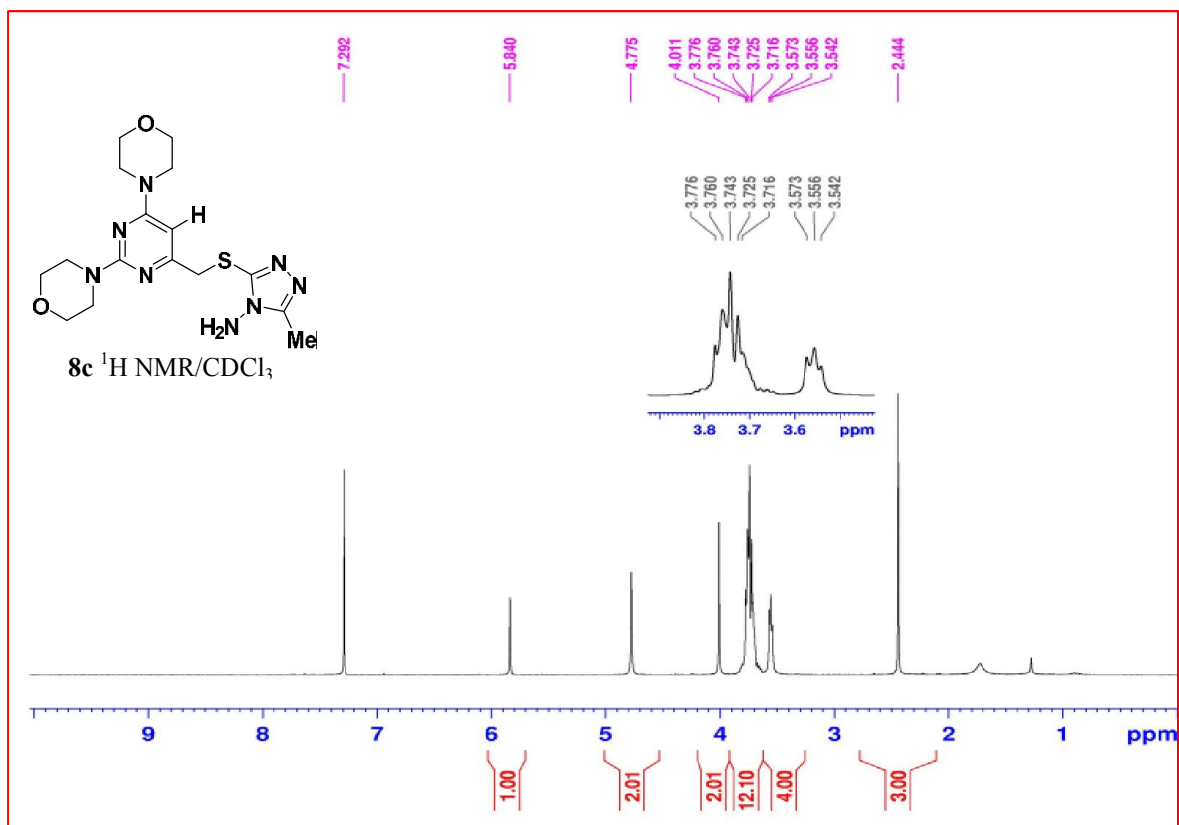


Figure S61. ^{13}C NMR spectrum for compound 8c.

Figure S62. D₂O exchange-¹H NMR spectrum for compound 8c.

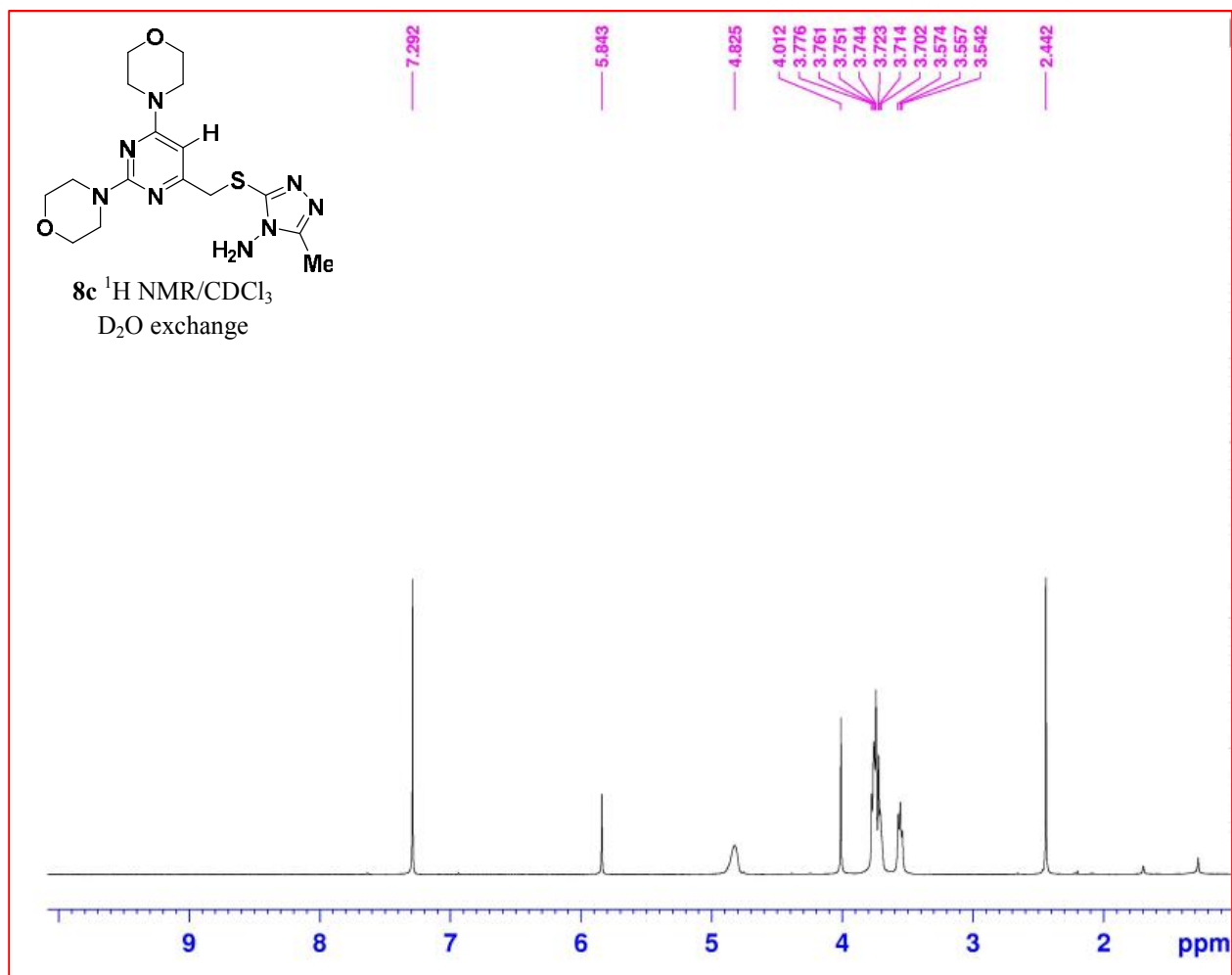


Figure S63. Mass spectrum for compound 8c.

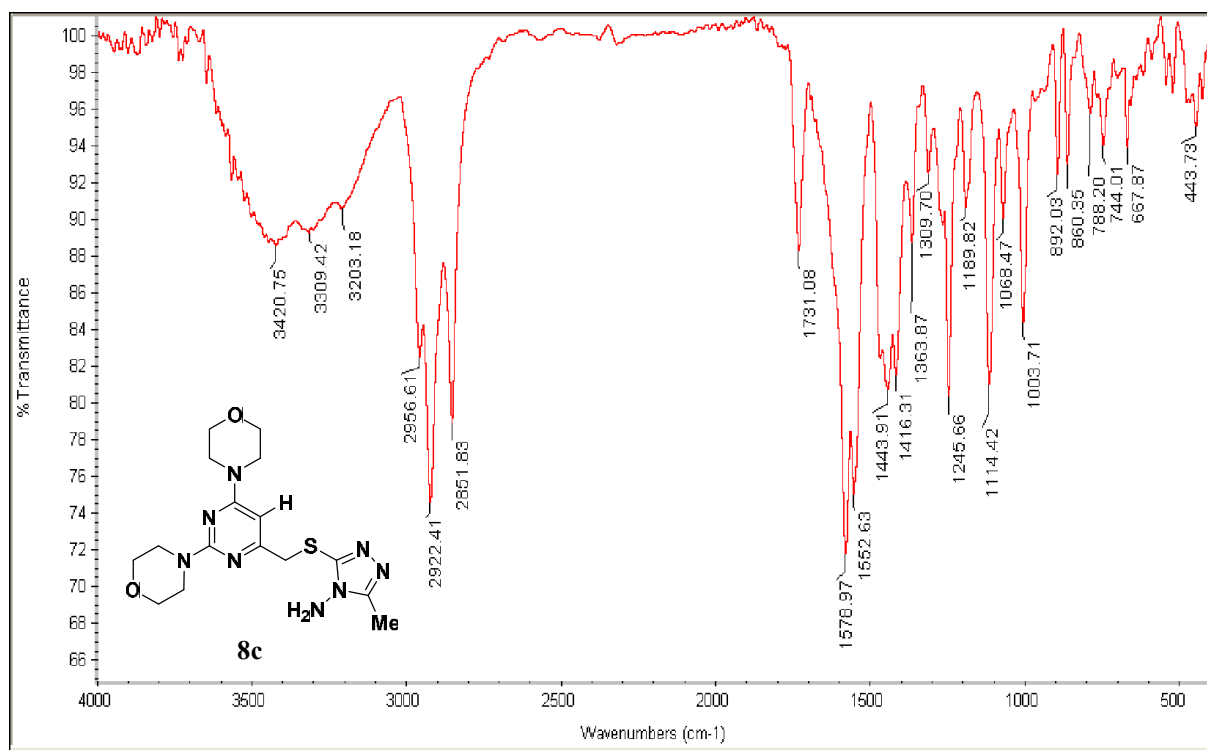
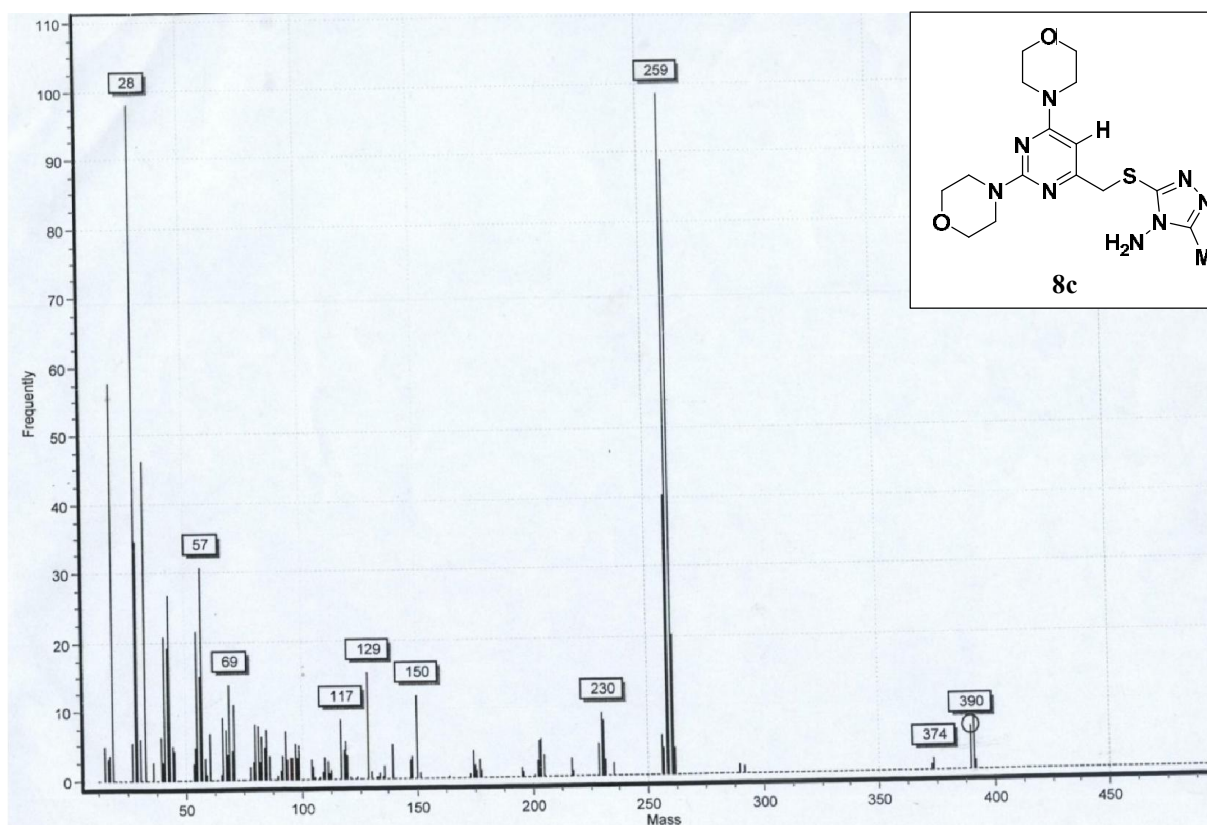


Figure S64. FTIR spectrum for compound 8c.

Figure S65. ^1H NMR spectrum for compound 8d.

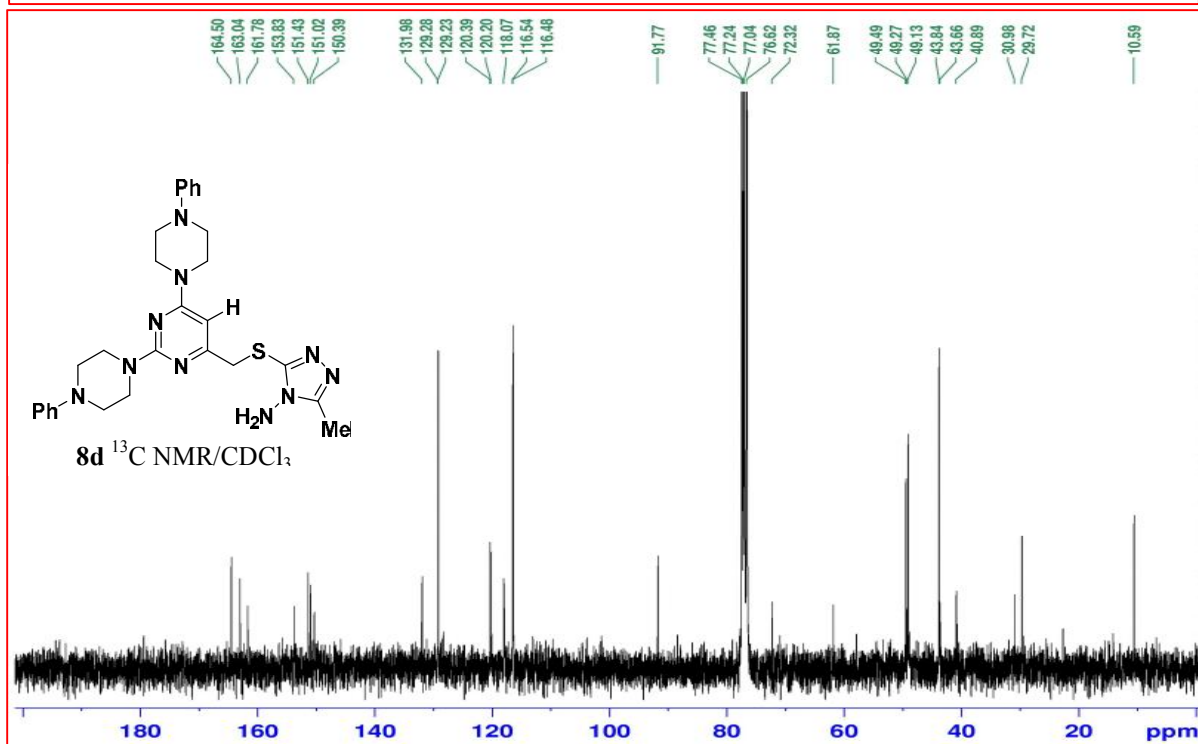
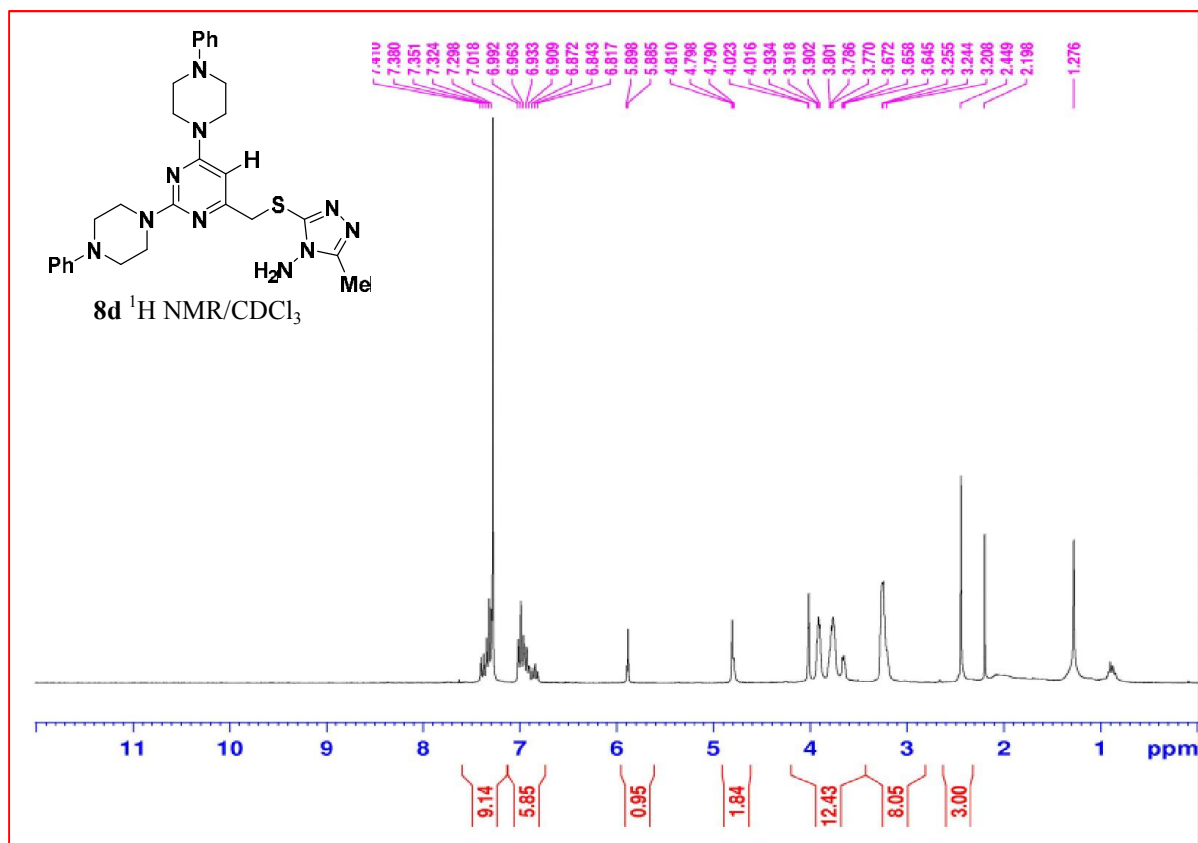


Figure S66. ^{13}C NMR spectrum for compound 8d.

Figure S67. Mass spectrum for compound 8d.

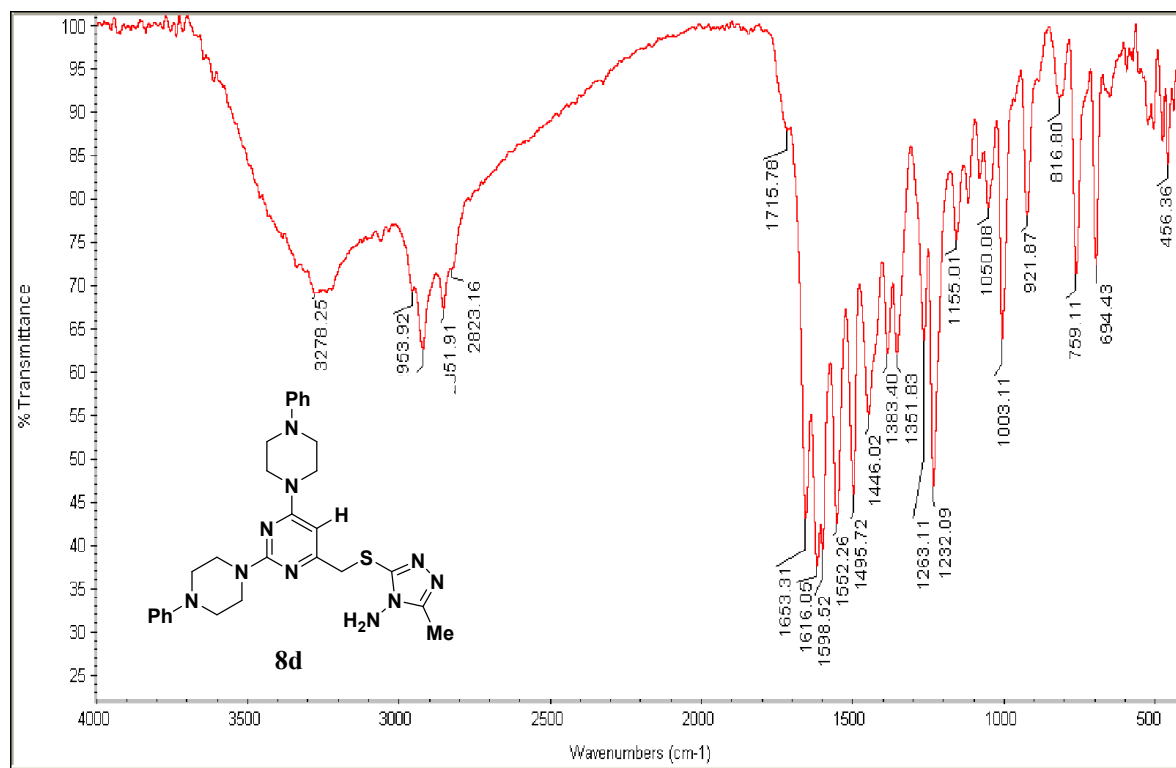
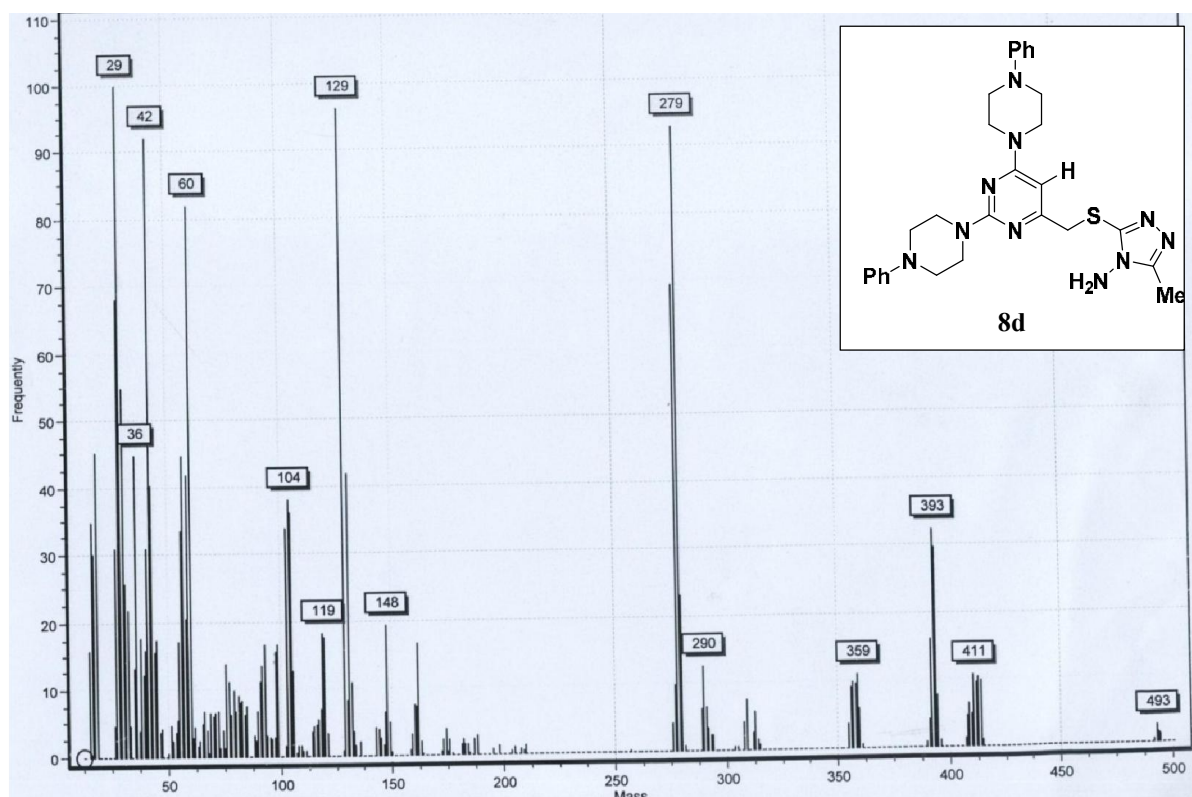


Figure S68. FTIR spectrum for compound 8d.

Figure S69. ^1H NMR spectrum for compound 8e.

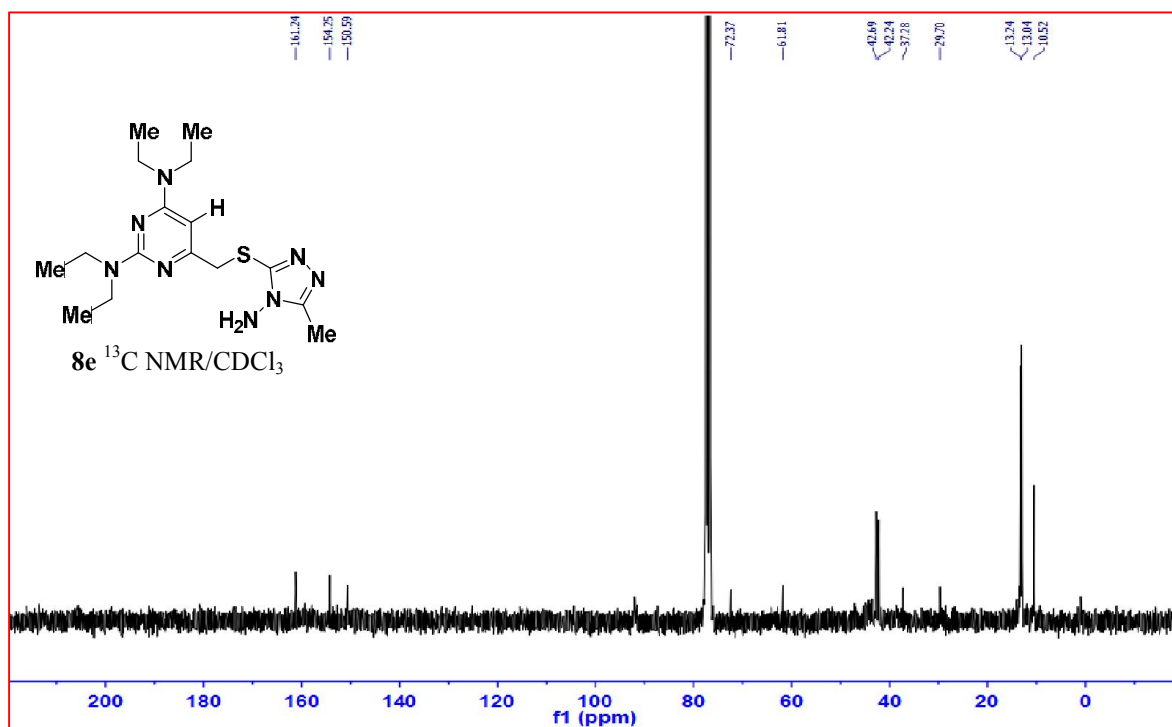
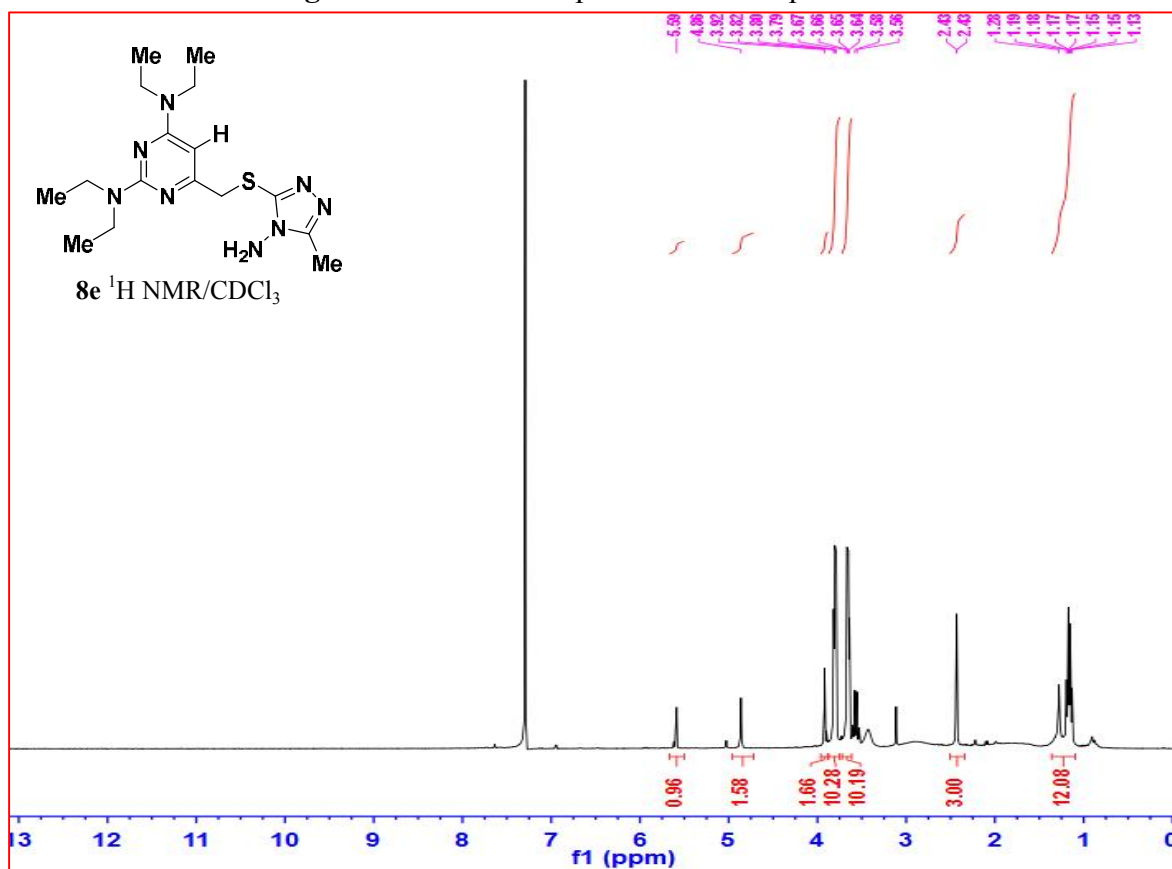


Figure S70. ^{13}C NMR spectrum for compound 8e.

Figure S71. Mass spectrum for compound **8e**.

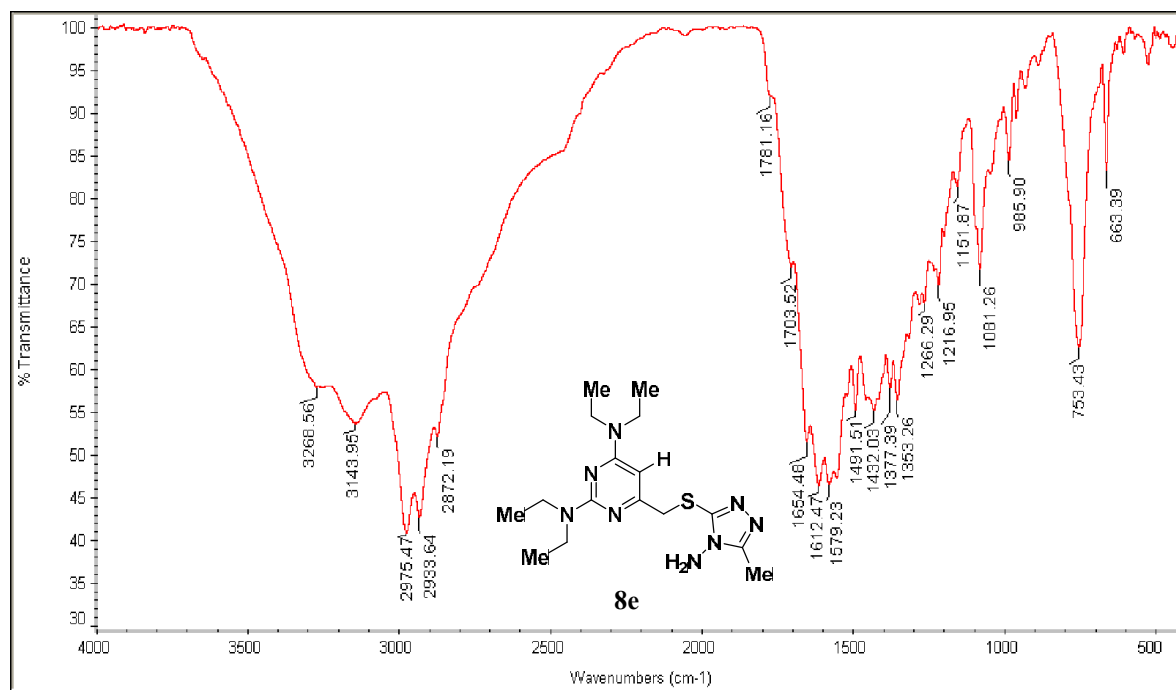
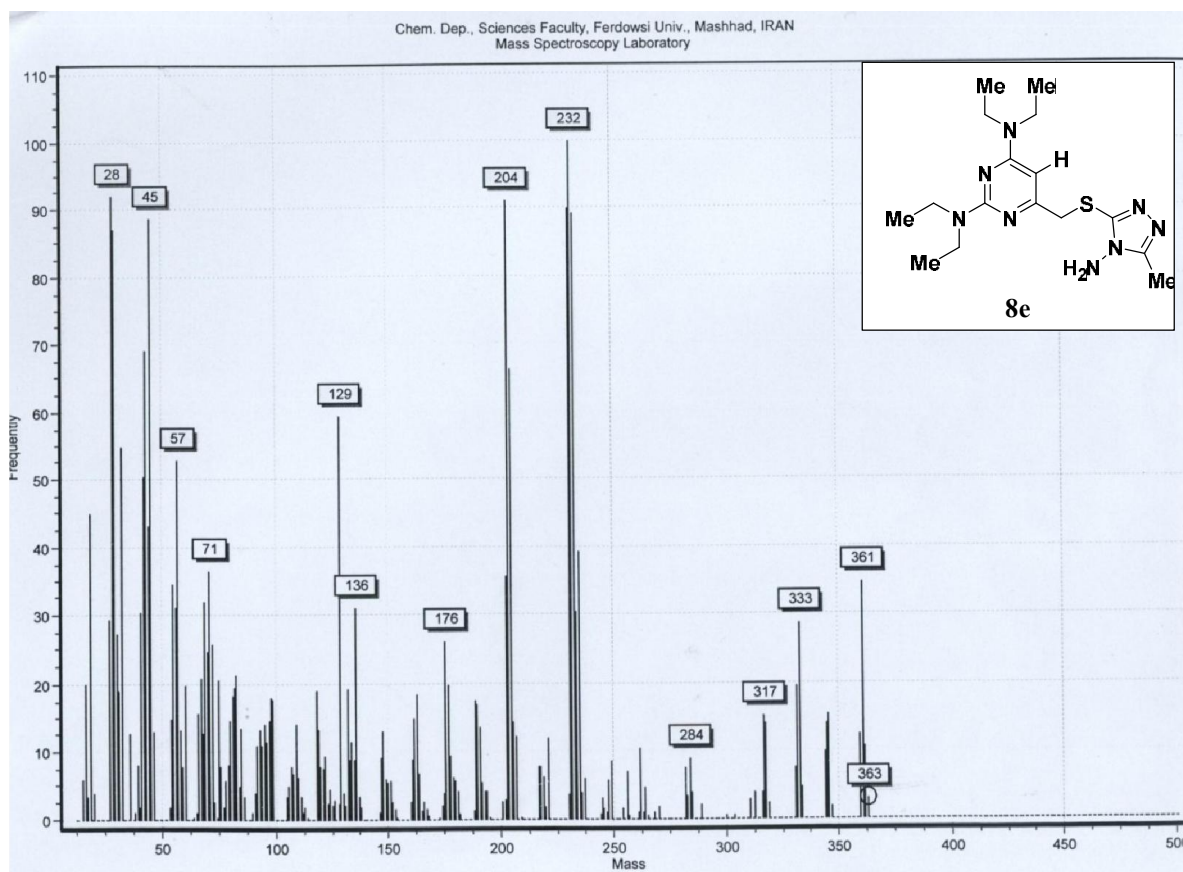


Figure S72. FTIR spectrum for compound **8e**.

Figure S73. ^1H NMR spectrum for compound 10.

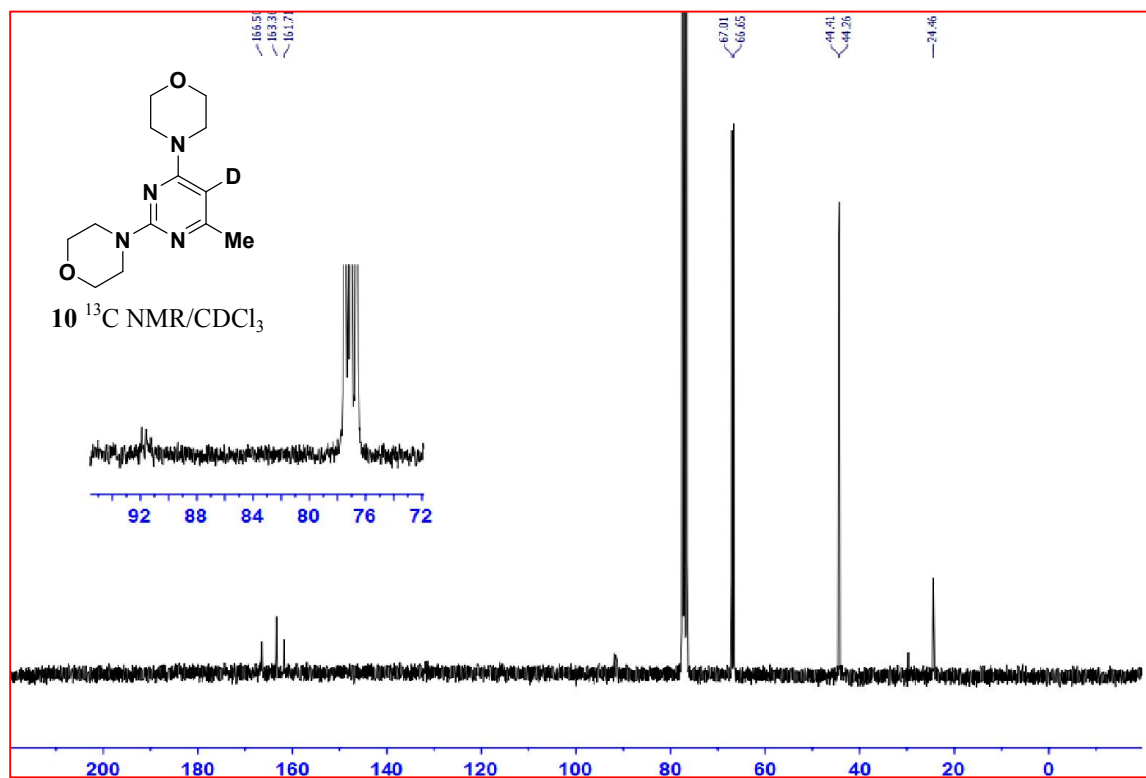
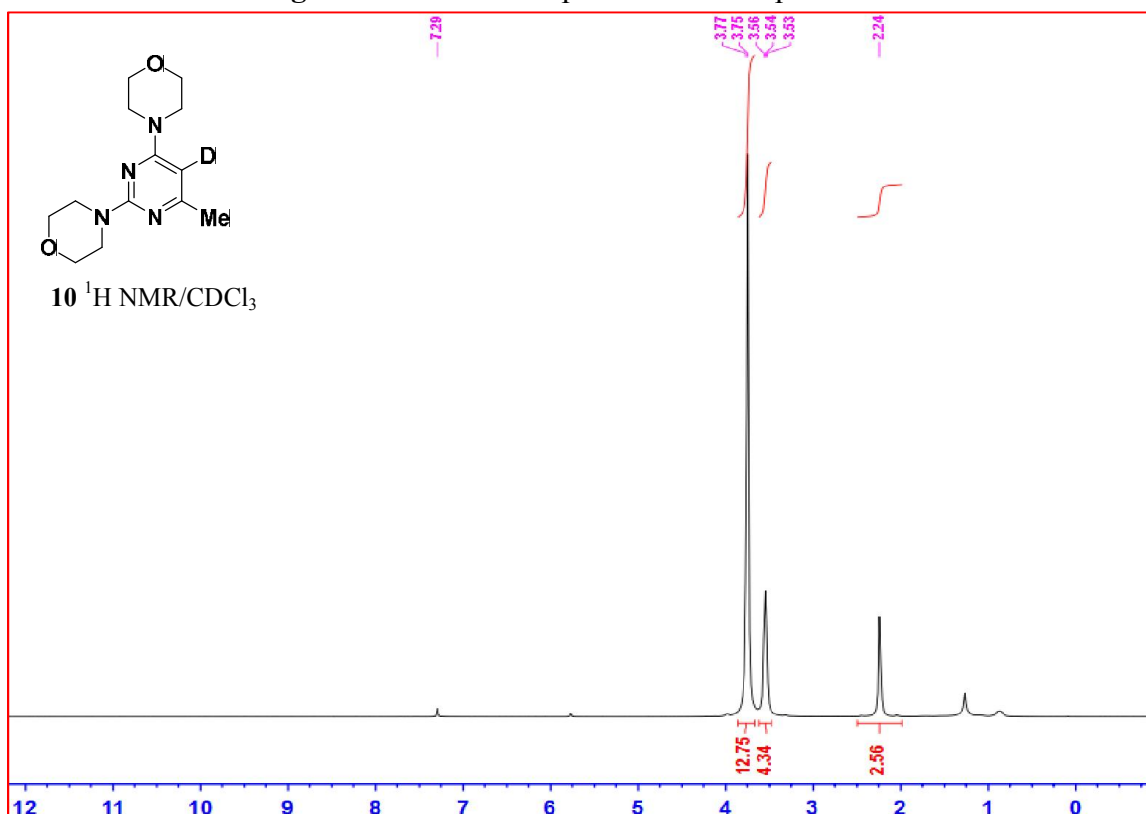


Figure S74. ^{13}C NMR spectrum for compound 10