

Mechanochemical synthesis of novel 1-[(*N*-arylthiocarbamoyl)amidino]pyrazoles and their application in thiocarbamoylguanylations

Krishnapriya K. Girija, Priya R. Maheswari, Akhila V. Radha, Sandhya V. Satheesh, and Kallikat N. Rajasekharan*

Department of Chemistry, University of Kerala, Kariavattom campus, Thiruvananthapuram 695581, Kerala, India.

E.mail: kn.rajasekharan@gmail.com

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Figure S1. ^1H NMR spectrum of 1-[(*N*-phenylthiocarbamoyl)amidino]pyrazole (**2a**) (400 MHz, CDCl_3)

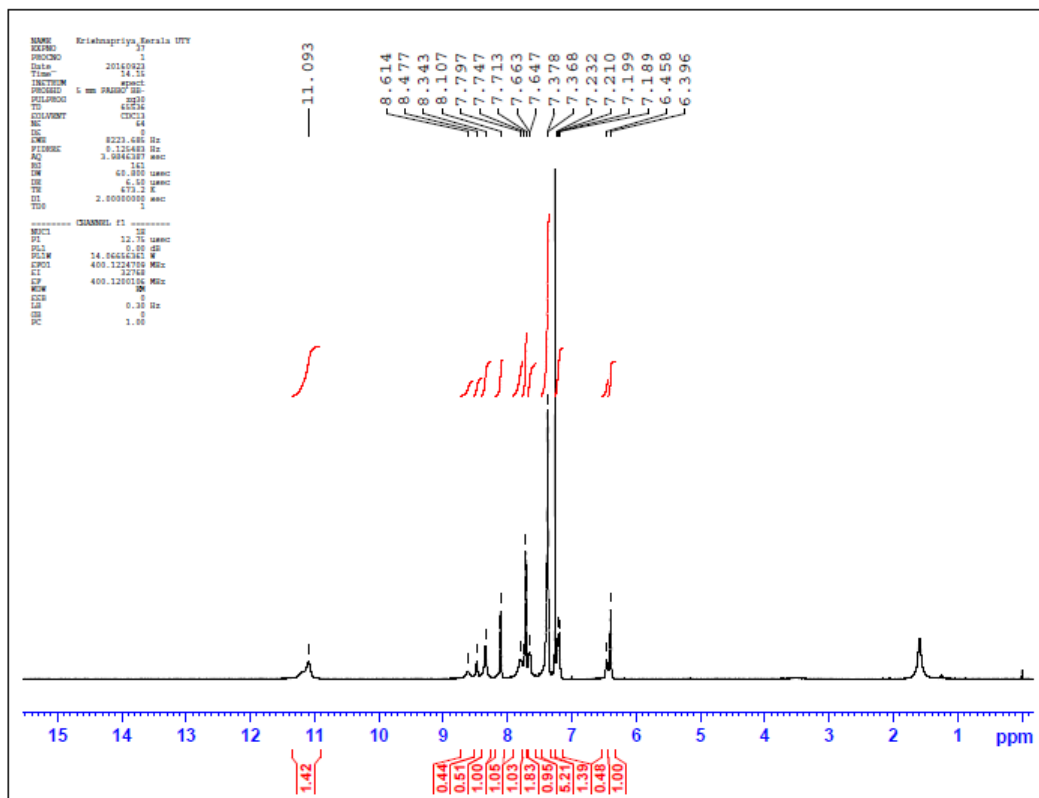


Figure S2. ^1H NMR spectrum (expanded) of 1-[(*N*-phenylthiocarbamoyl)amidino]pyrazole (**2a**) (400MHz, CDCl_3)

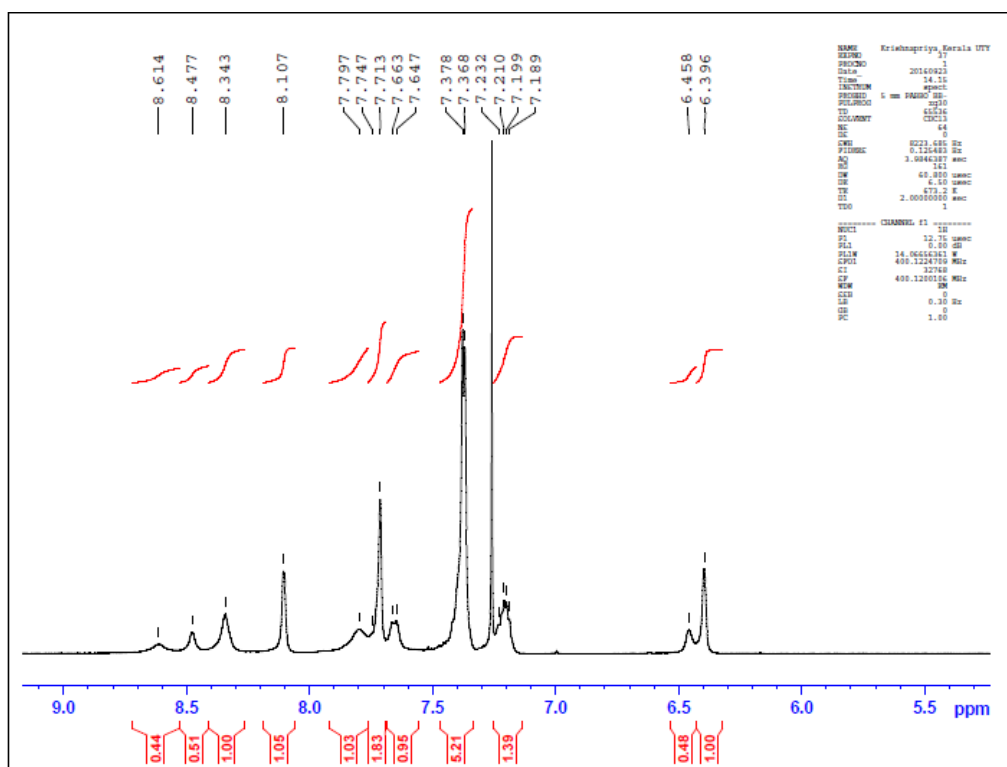


Figure S3. ^{13}C NMR spectrum of 1-[(*N*-phenylthiocarbamoyl)amidino]pyrazole (**2a**) (100 MHz, CDCl_3)

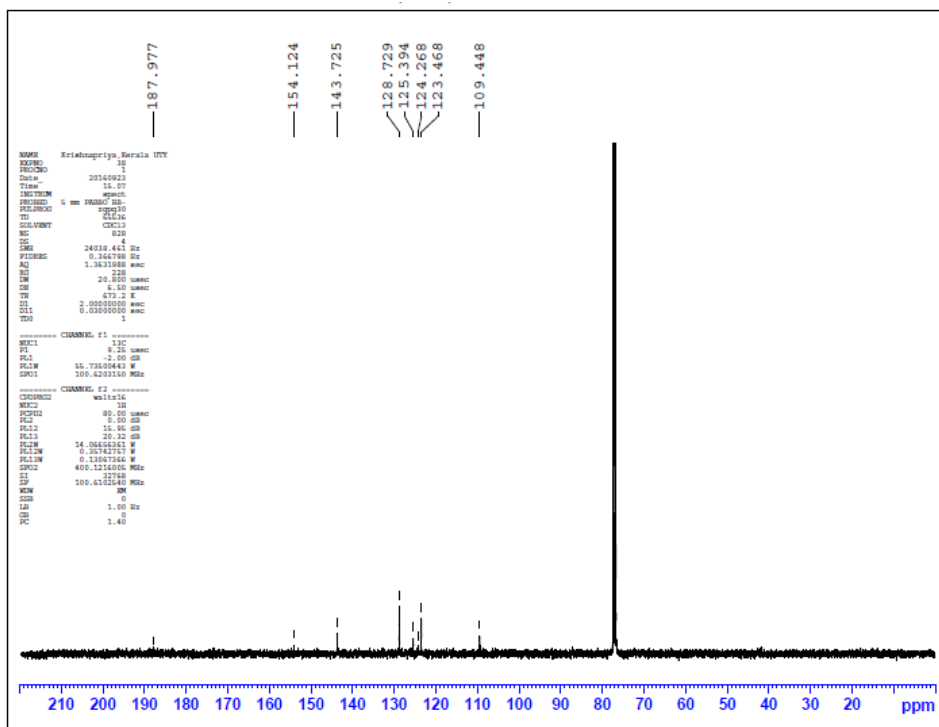


Figure S4. ESI-HRMS spectrum of 1-[(*N*-phenylthiocarbamoyl)amidino]pyrazole (**2a**)

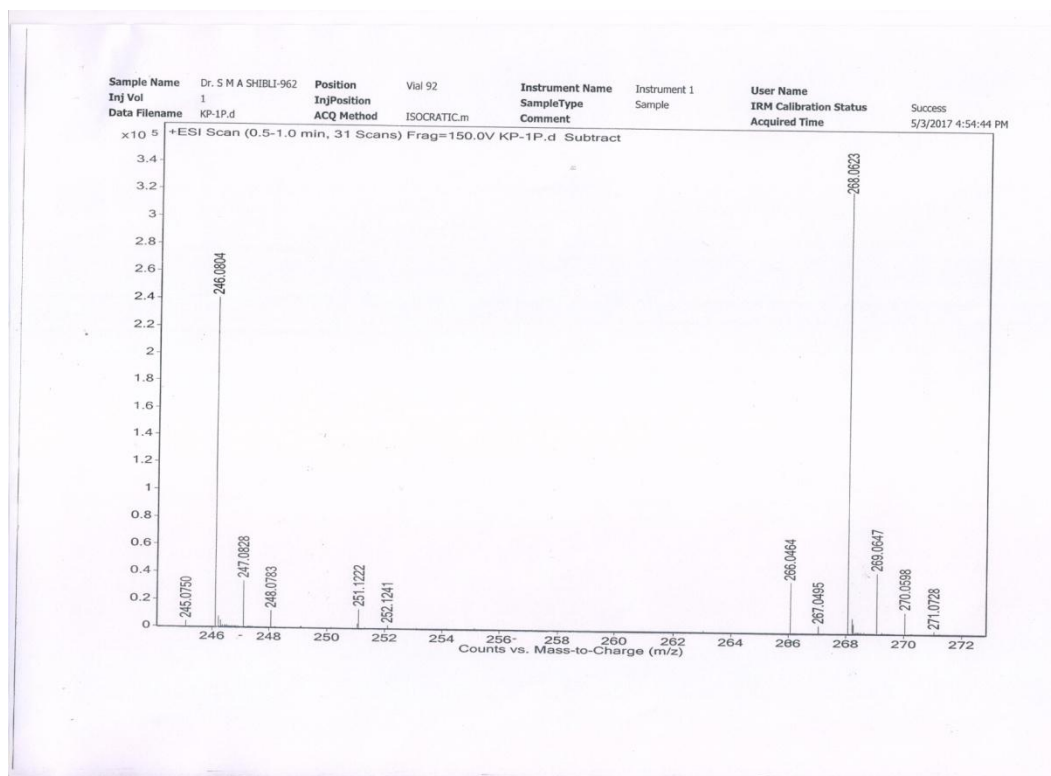


Figure S5. ^1H NMR spectrum of 1-[(*N*-4-chlorophenylthiocarbamoyl)amidino]pyrazole (**2b**) (400 MHz, CDCl_3)

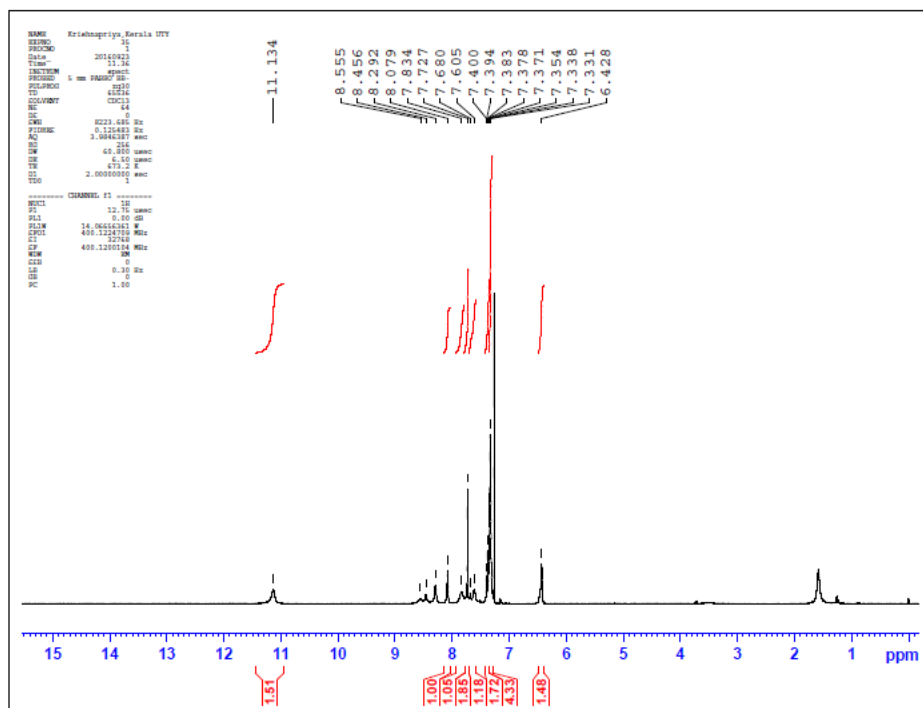


Figure S6. ^1H NMR spectrum (expanded) of 1-[(*N*-4-chlorophenylthiocarbamoyl)amidino]pyrazole (**2b**) (400 MHz, CDCl_3)

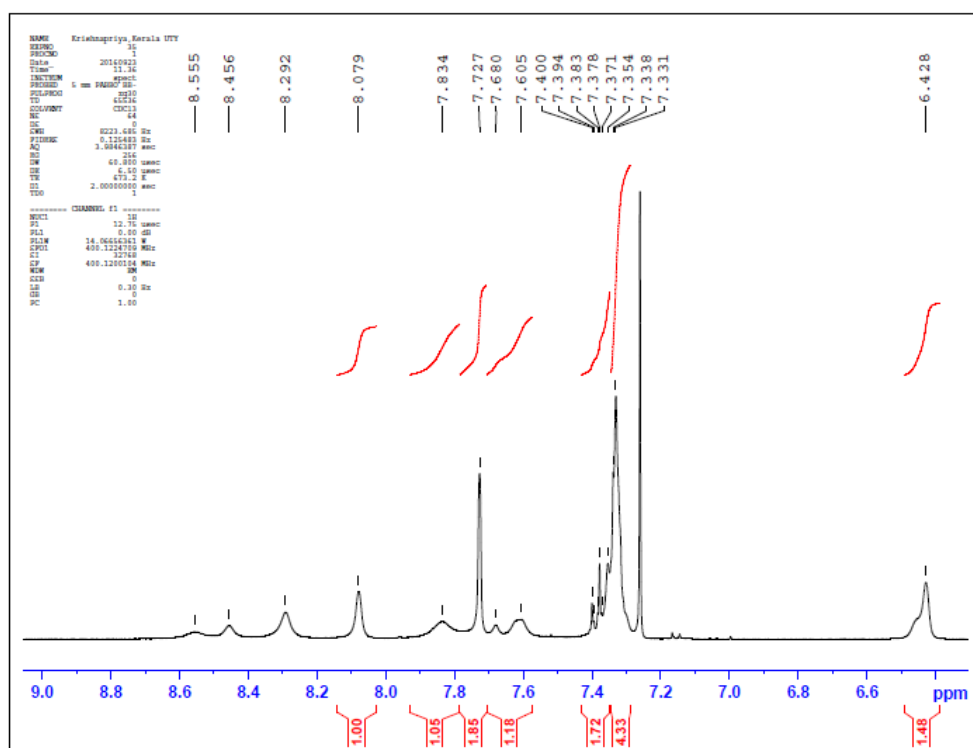


Figure S7. ^{13}C NMR spectrum of 1-[(*N*-4-chlorophenylthiocarbamoyl)amidino]pyrazole (**2b**) (100 MHz, CDCl_3)

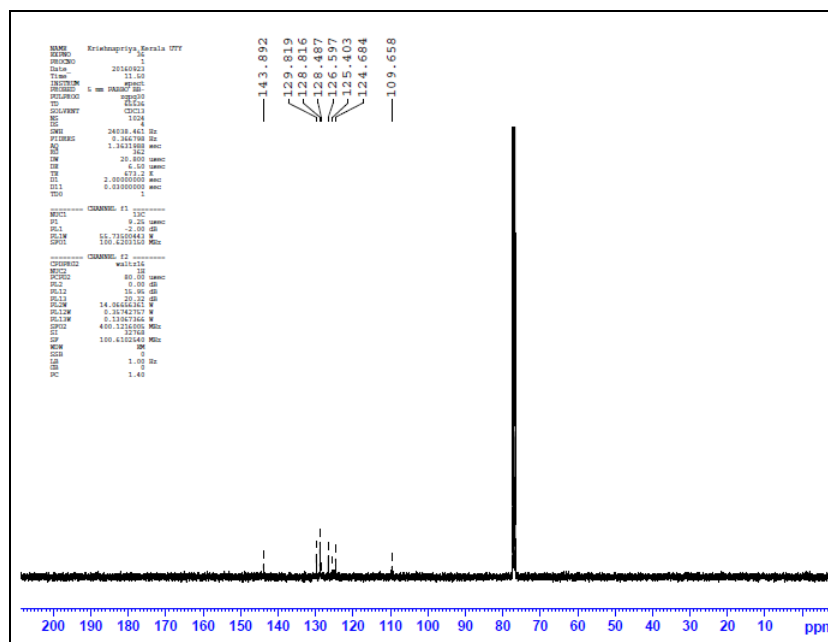


Figure S8. ESI-HRMS spectrum of 1-[(*N*-4-chlorophenylthiocarbamoyl)amidino]pyrazole (**2b**)

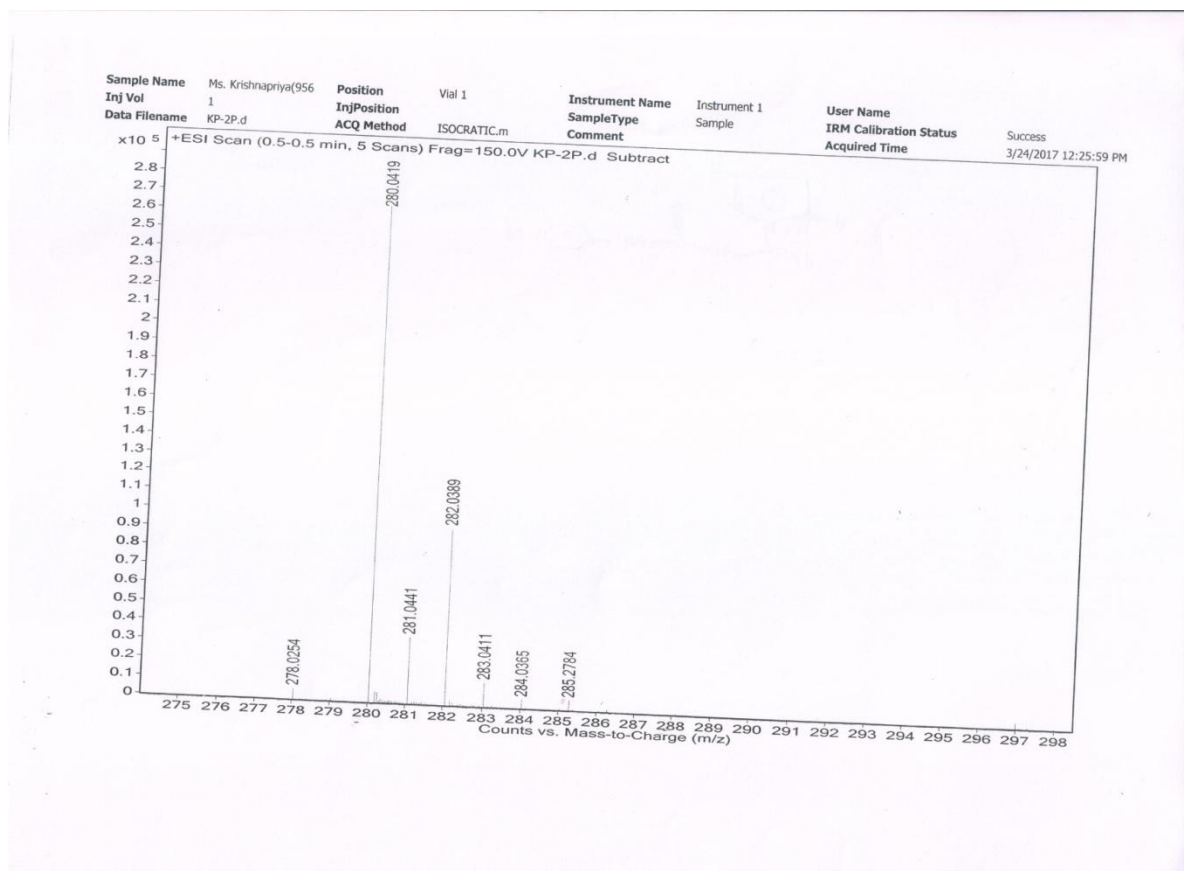


Figure S9. ^1H NMR spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrazole (**2c**) (400 MHz, CDCl_3)

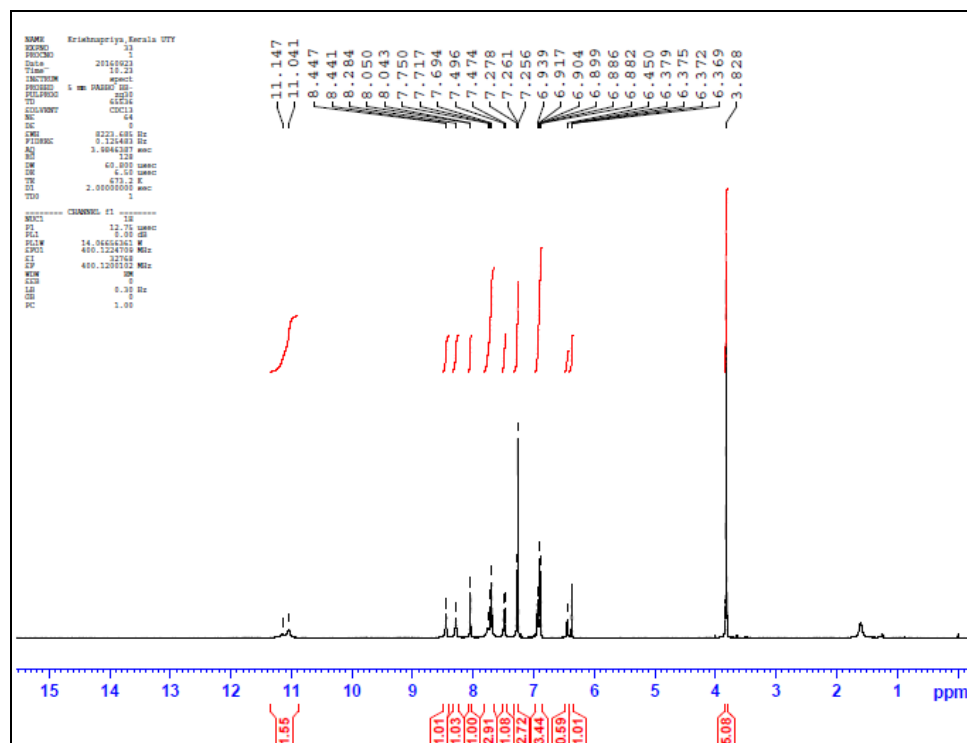


Figure S10. ^1H NMR spectrum (expanded) of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrazole (**2c**) (400 MHz, CDCl_3)

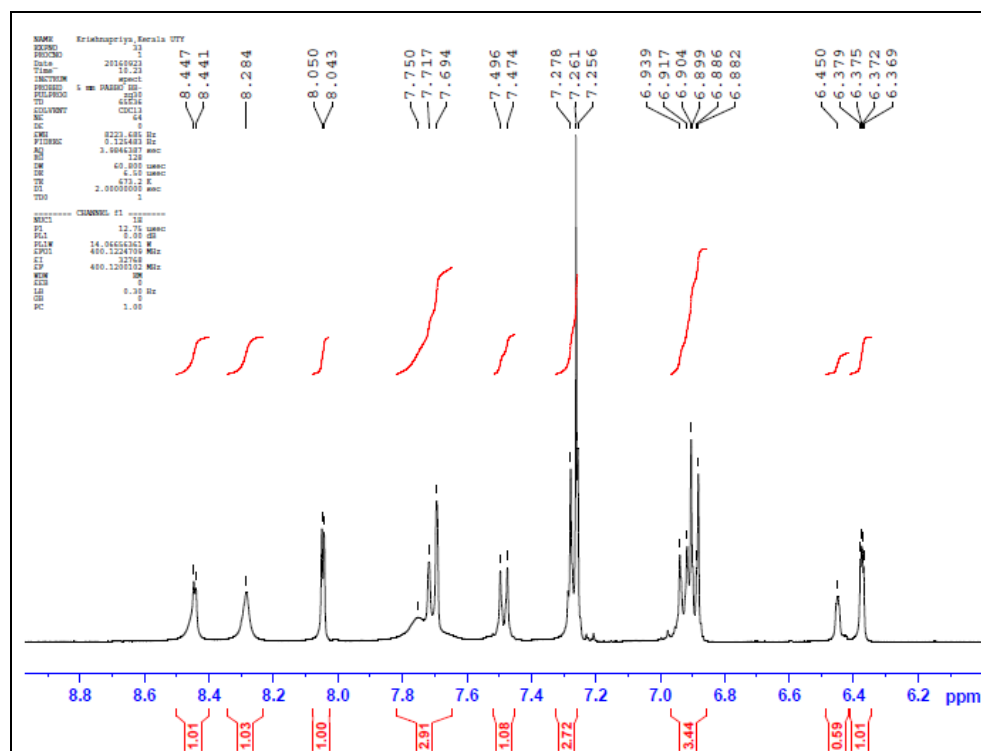


Figure S11. ^{13}C NMR spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrazole (**2c**) (100 MHz, CDCl_3)

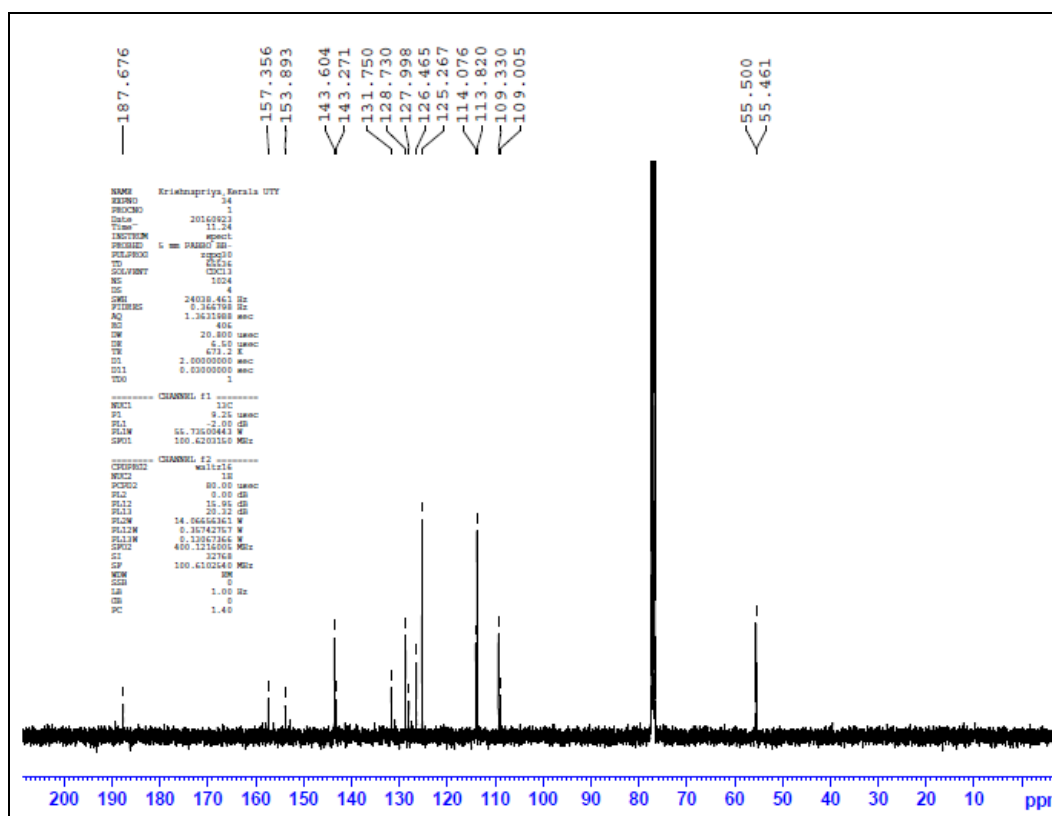


Figure S12. ^1H NMR spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrazole (**2c**) (400 MHz, CD_3OD)

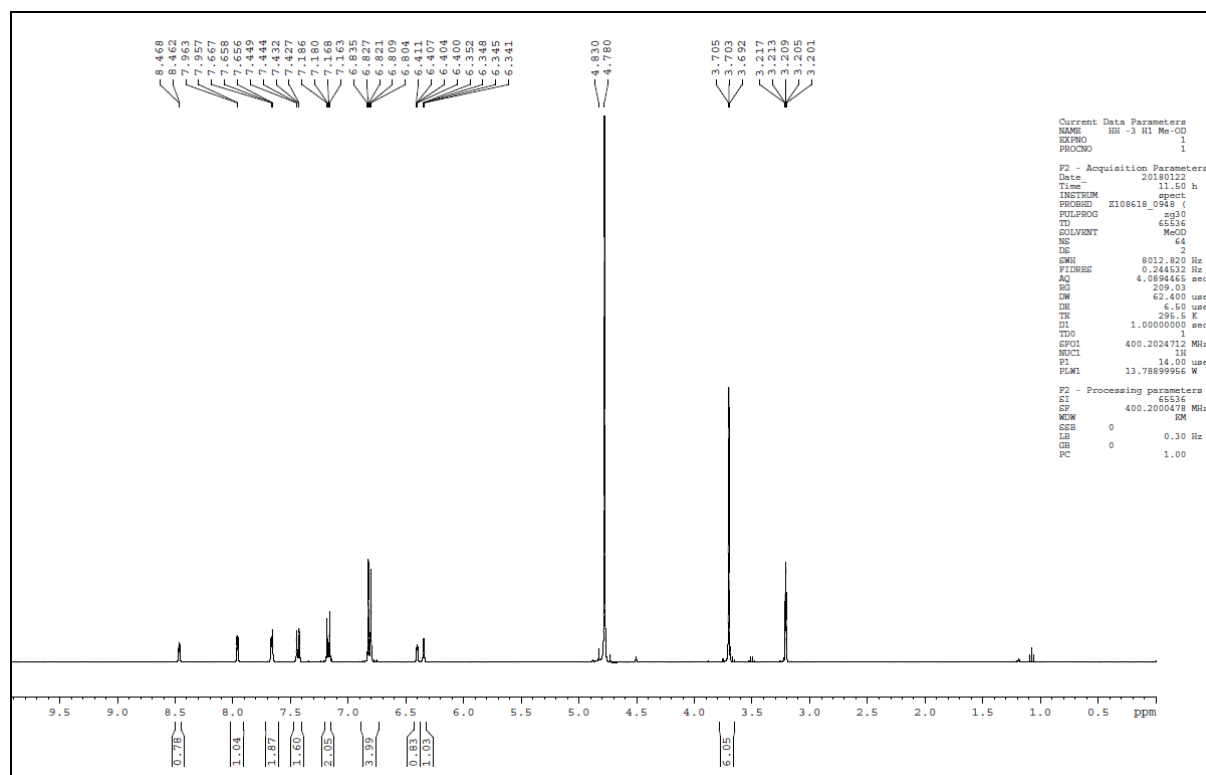


Figure S13. ^1H NMR spectrum (expanded) of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrazole (**2c**) (400 MHz, CD_3OD)

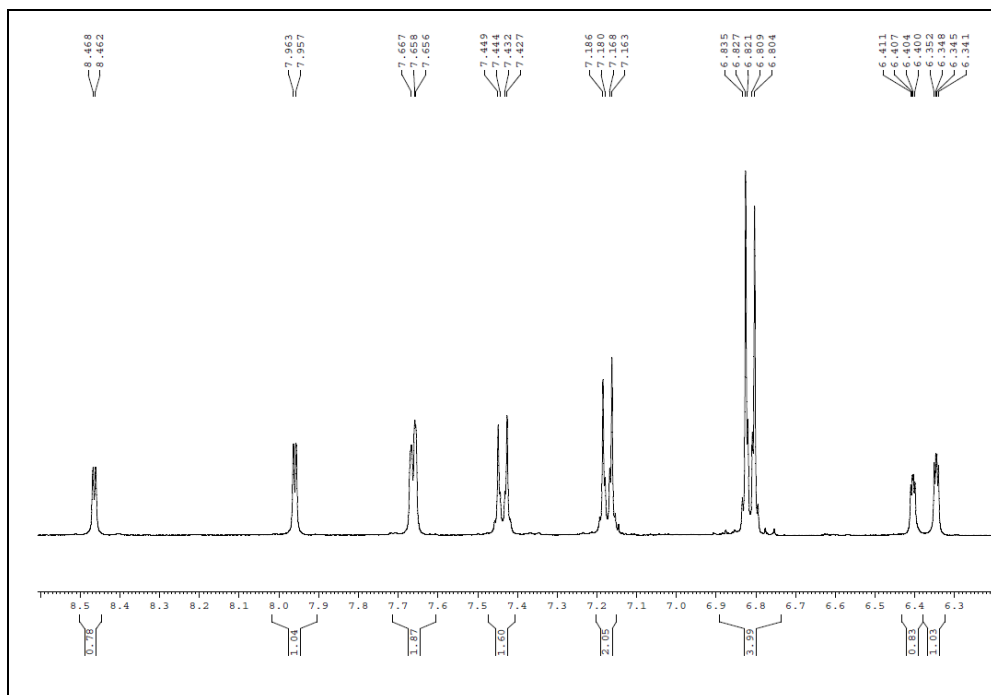


Figure S14. ^{13}C NMR spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrazole (**2c**) (100 MHz, CD_3OD)

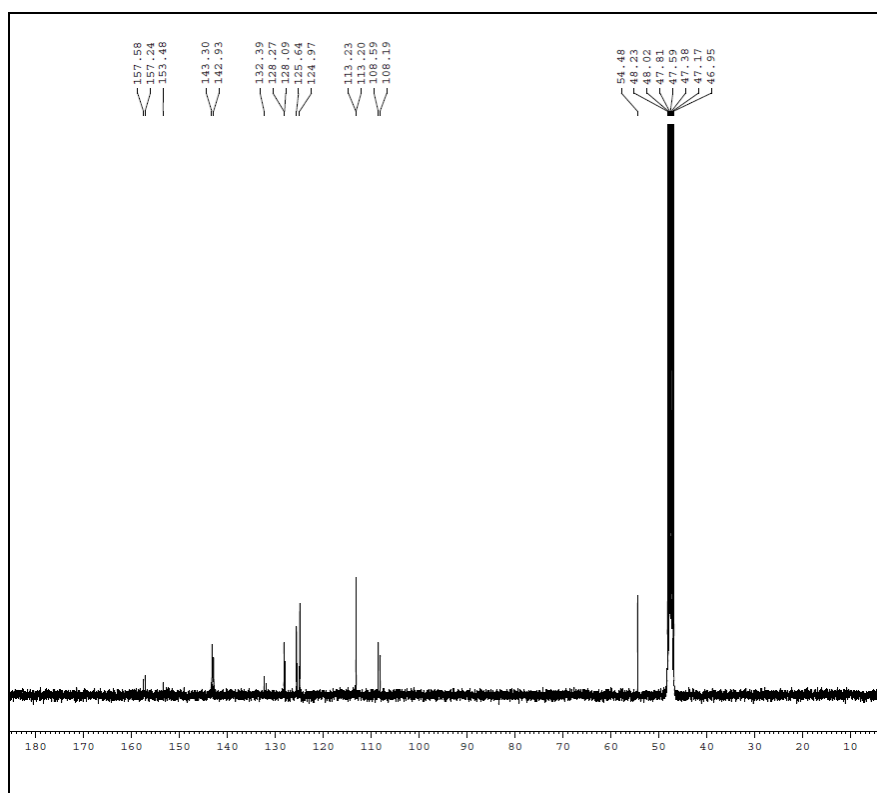


Figure S15. ESI-HRMS spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrazole (2c)

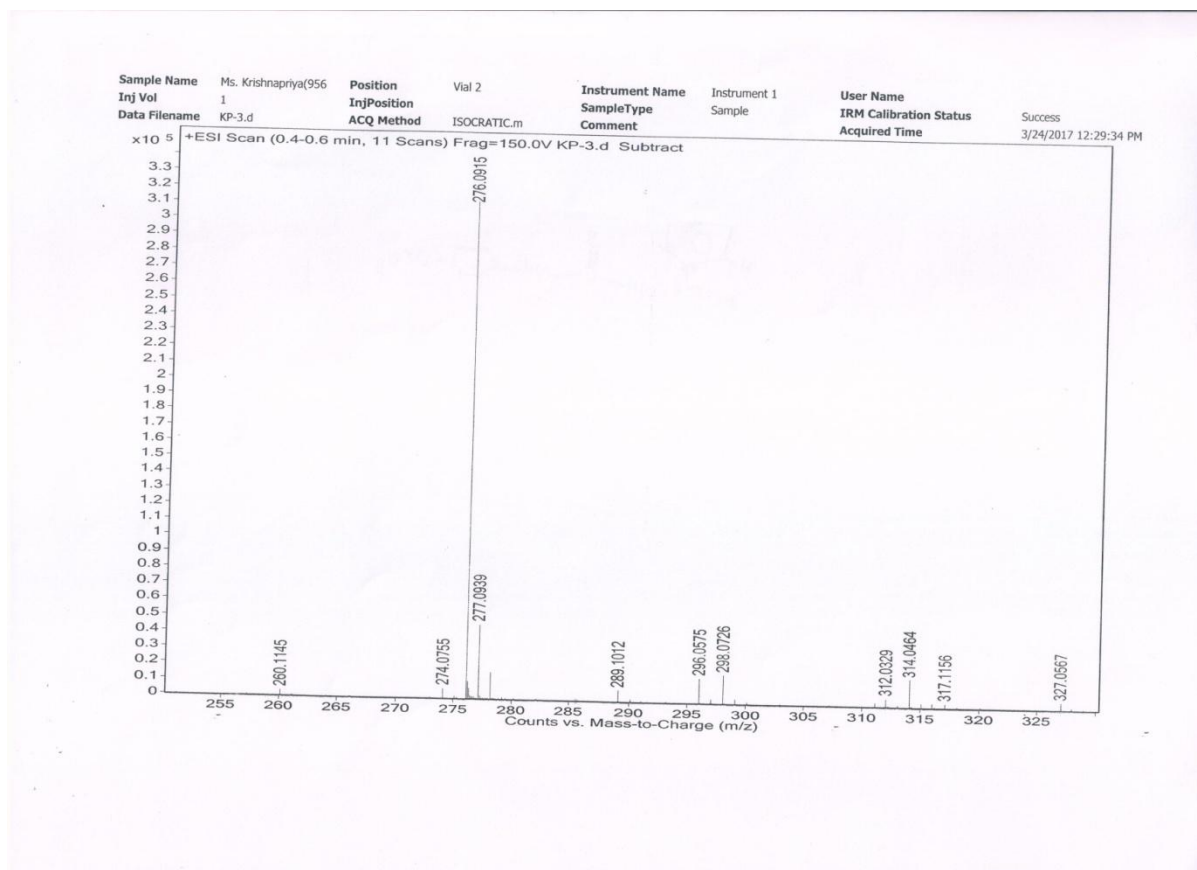


Figure S16. ^1H NMR spectrum of 1-[(*N*-4-methylphenylthiocarbamoyl)amidino]pyrazole (**2d**) (400 MHz, $\text{DMSO-}d_6$)

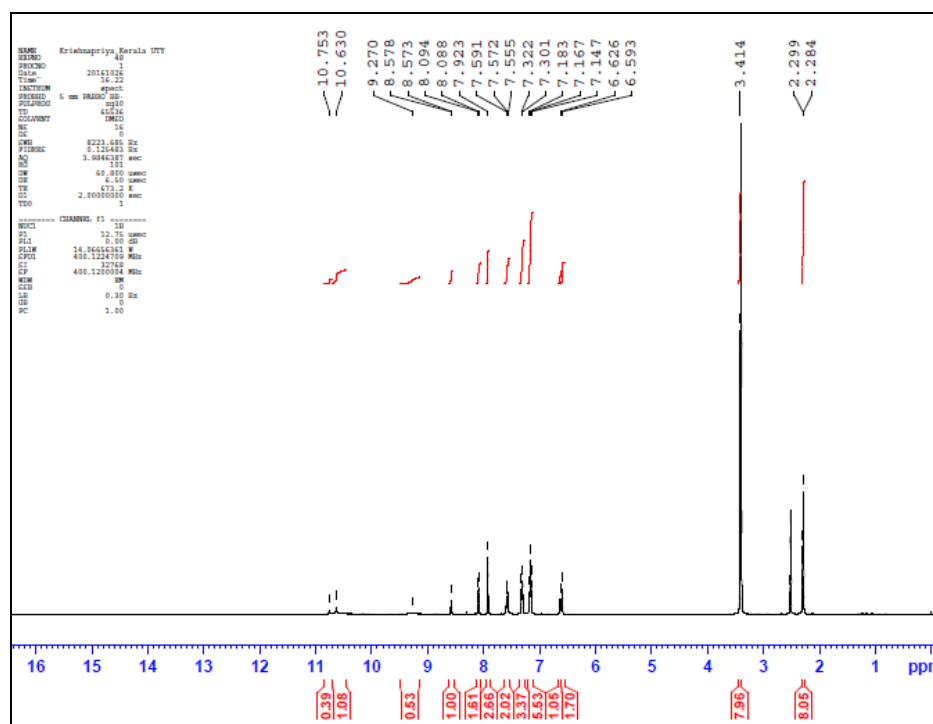


Figure S17. ^1H NMR spectrum (expanded) of 1-[(*N*-4-methylphenylthiocarbamoyl)amidino]pyrazole (**2d**) (400 MHz, $\text{DMSO-}d_6$)

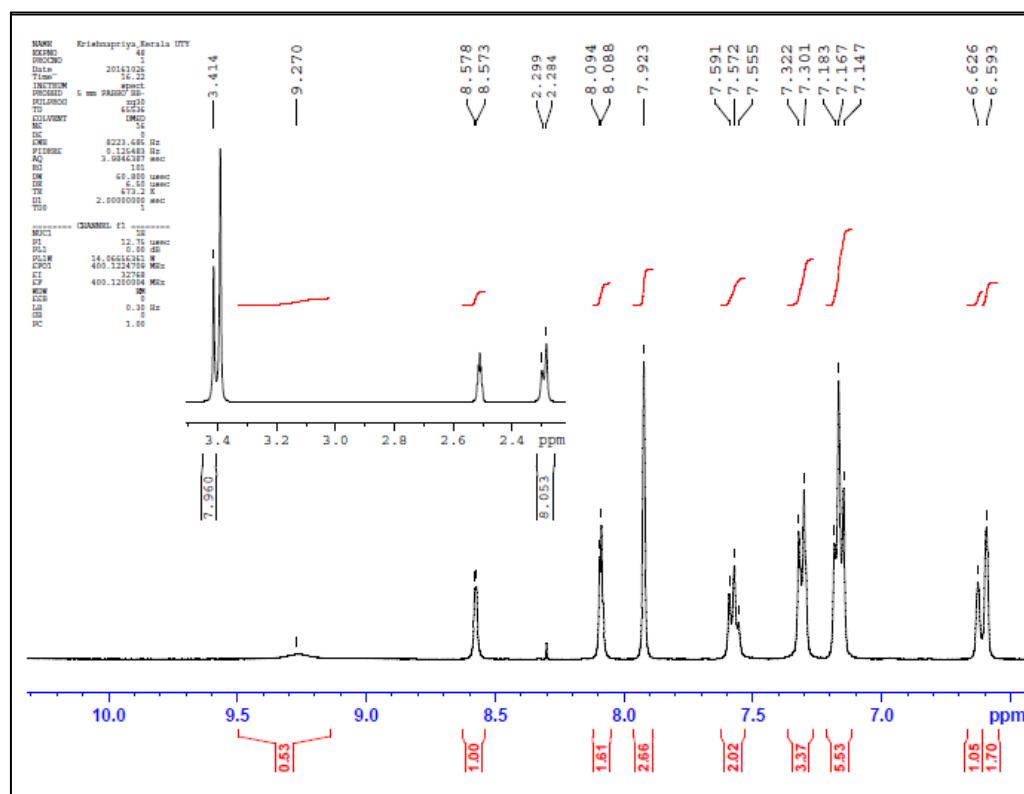


Figure S18. ^{13}C NMR spectrum of 1-[(*N*-4-methylphenylthiocarbamoyl)amidino]pyrazole (**2d**) (100 MHz, $\text{DMSO-}d_6$)

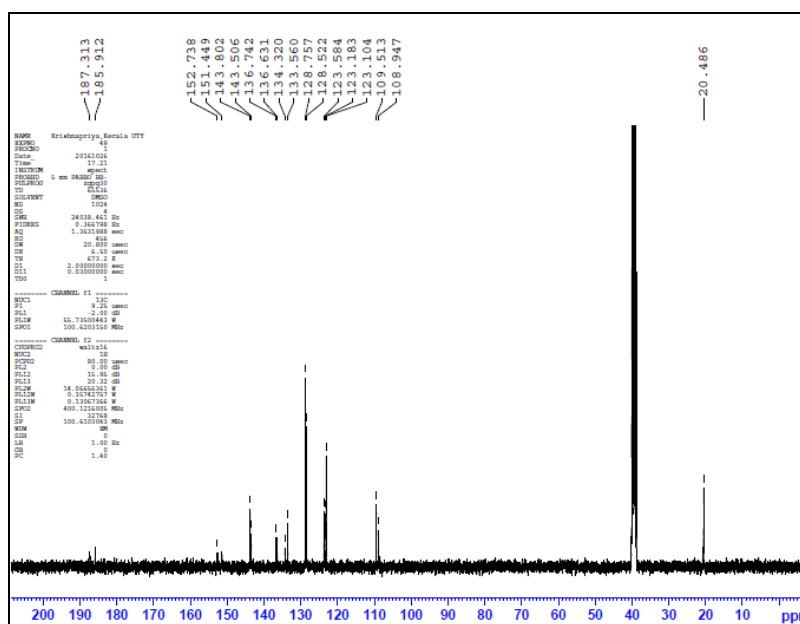


Figure S19. ESI-HRMS spectrum of 1-[(*N*-4-methylphenylthiocarbamoyl)amidino]pyrazole (**2d**)

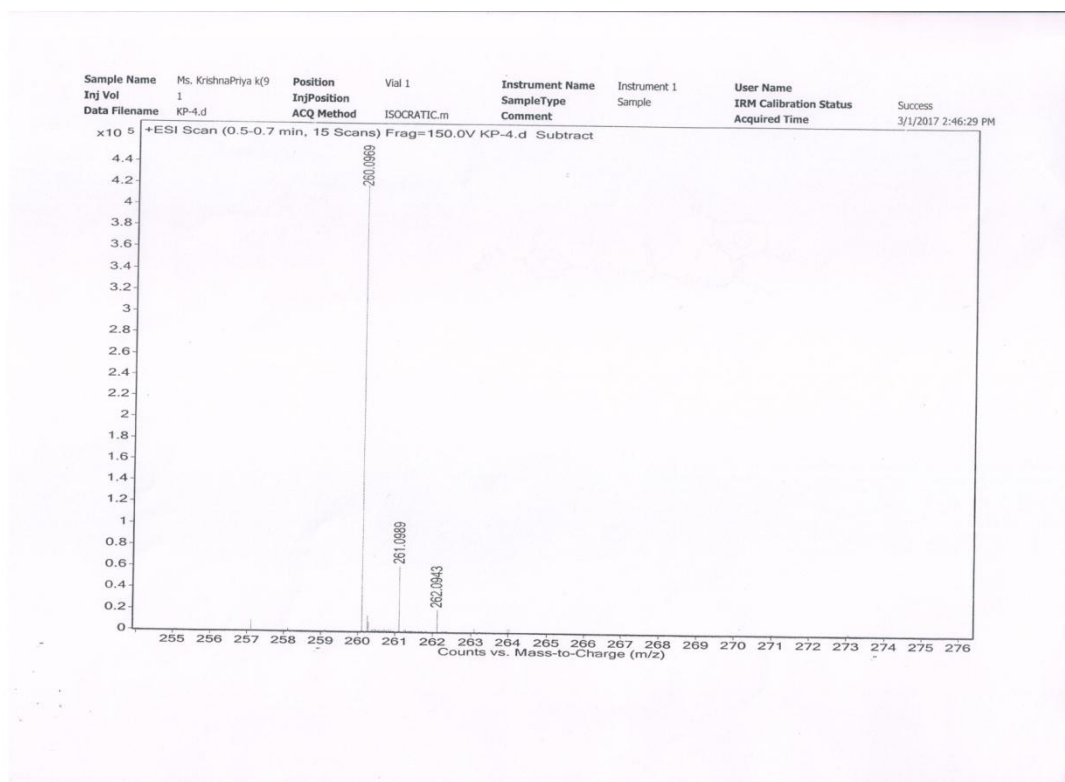


Figure S20. ^1H NMR spectrum of 1-[(*N*-3-methoxyphenylthiocarbamoyl)amidino]pyrazole (**2e**) (400 MHz, CDCl_3)

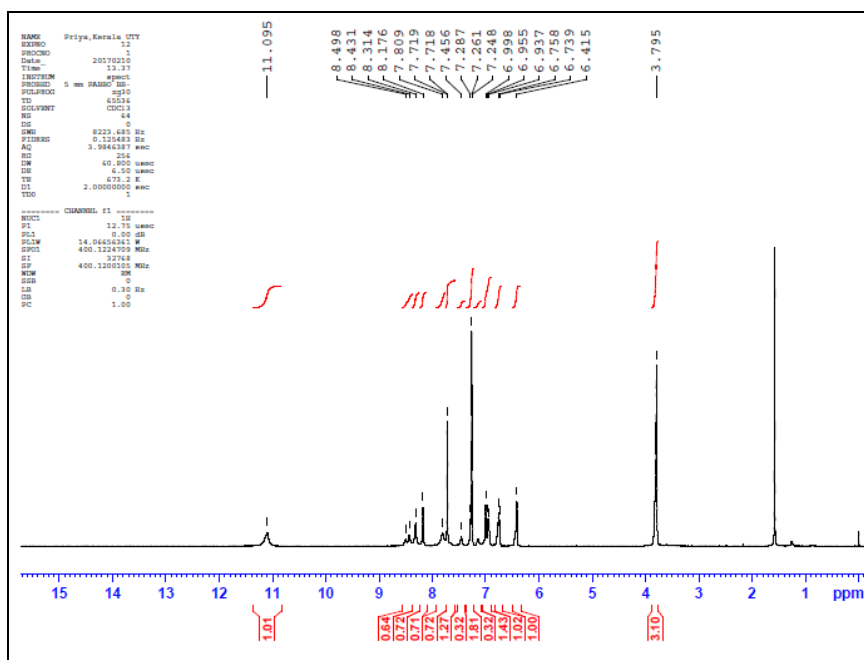


Figure S21. ^1H NMR spectrum (expanded) of 1-[(*N*-3-methoxyphenylthiocarbamoyl)amidino]pyrazole (**2e**) (400 MHz, CDCl_3)

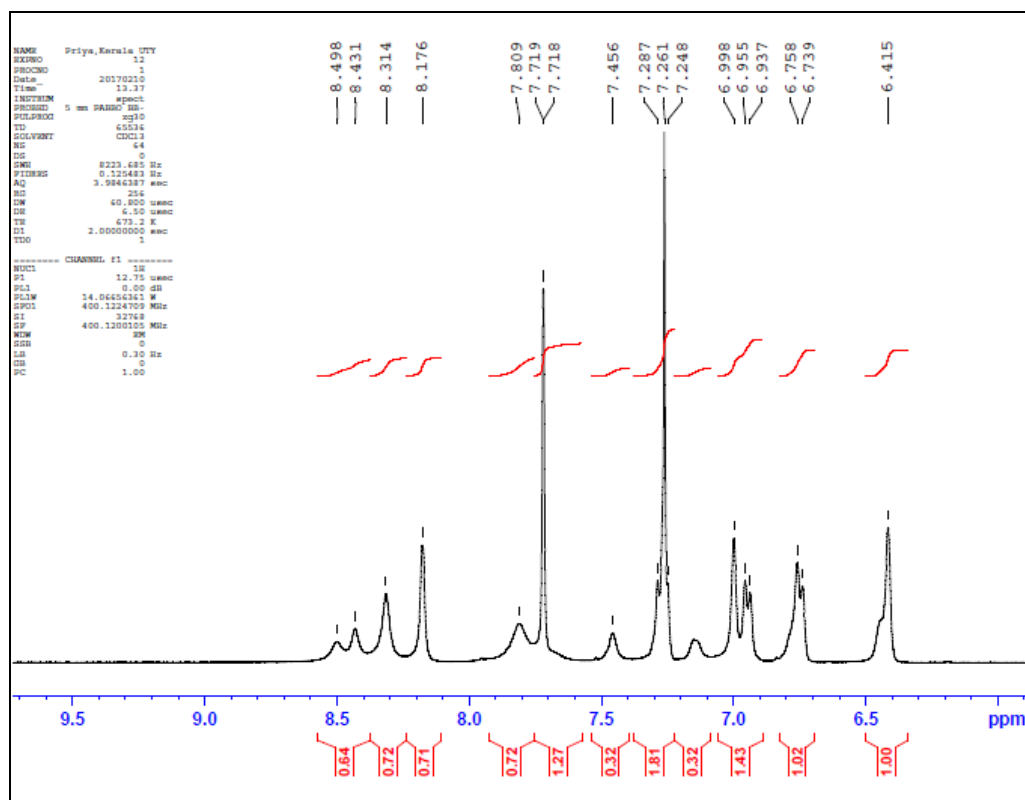


Figure S22. ^{13}C NMR spectrum of 1-[(*N*-3-methoxyphenylthiocarbamoyl)amidino]pyrazole (**2e**) (100 MHz, CDCl_3)

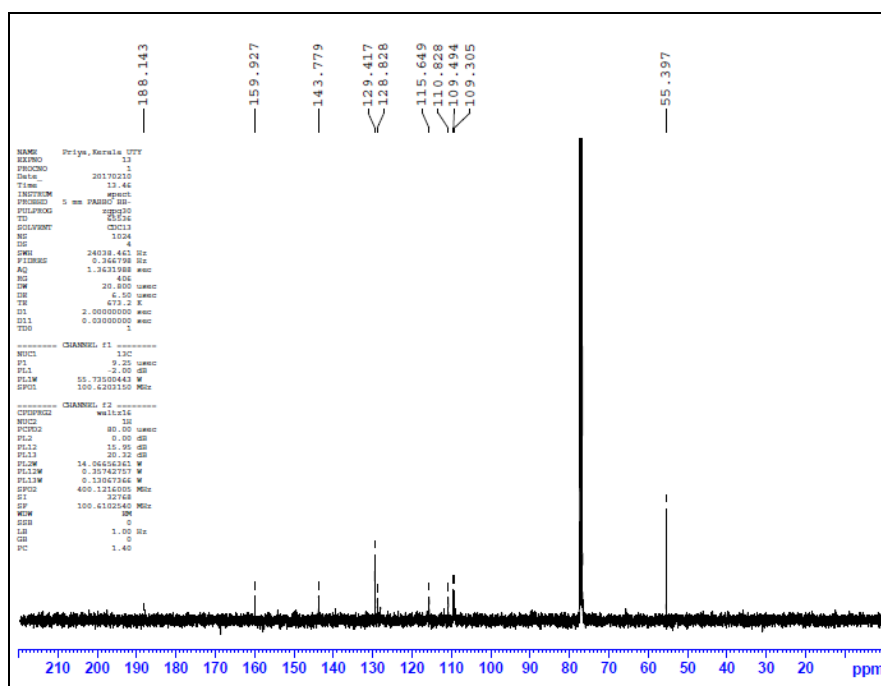


Figure S23. ESI-HRMS spectrum of 1-[(*N*-3-methoxyphenylthiocarbamoyl)amidino]pyrazole (**2e**)

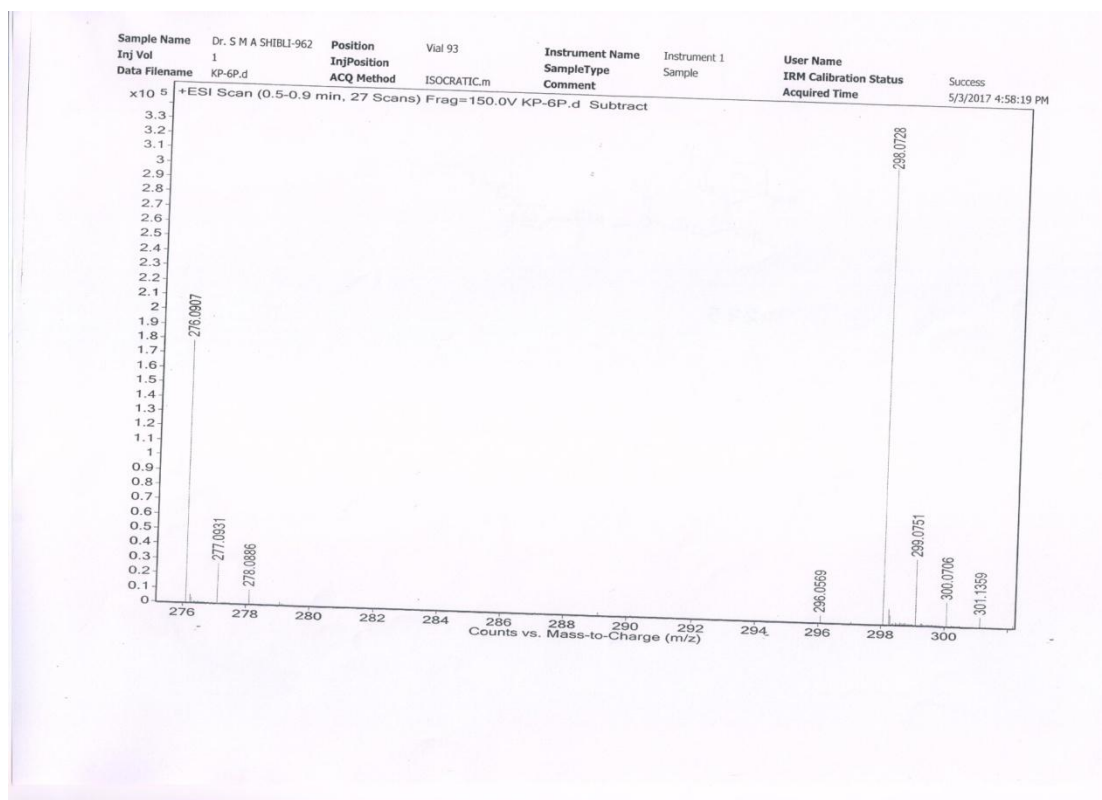


Figure S24. ¹H NMR spectrum of 1-[(N-4-bromophenylthiocarbamoyl)amidino]pyrazole (**2f**) (400 MHz, CDCl₃)

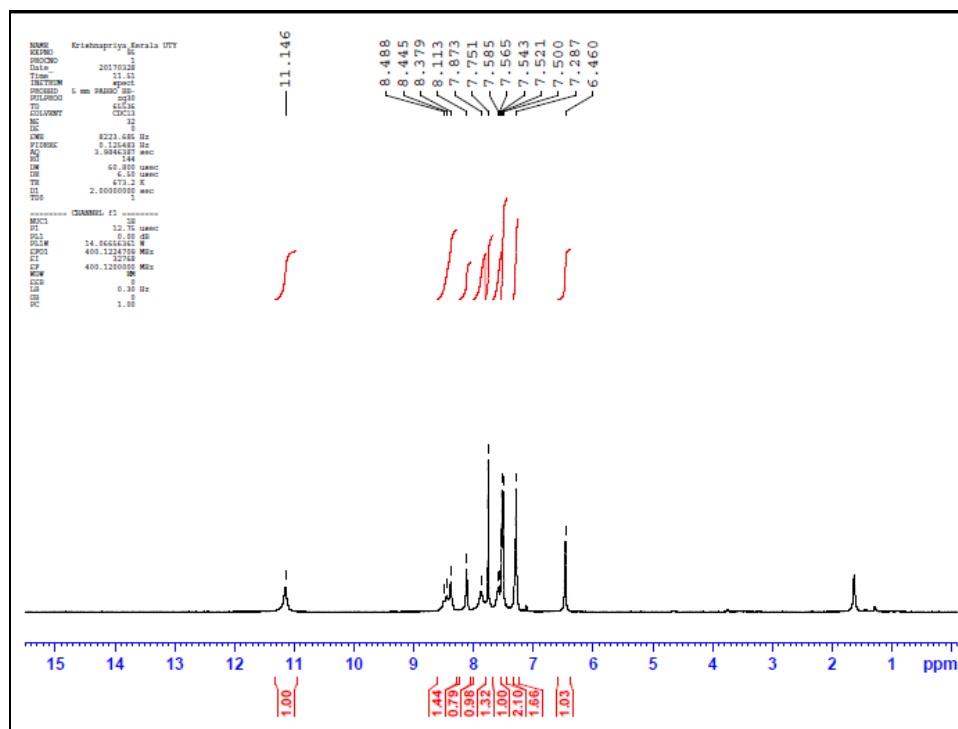


Figure S25. ¹H NMR spectrum (expanded) of 1-[(N-4-bromophenylthiocarbamoyl)amidino]pyrazole (**2f**) (400 MHz, CDCl₃)

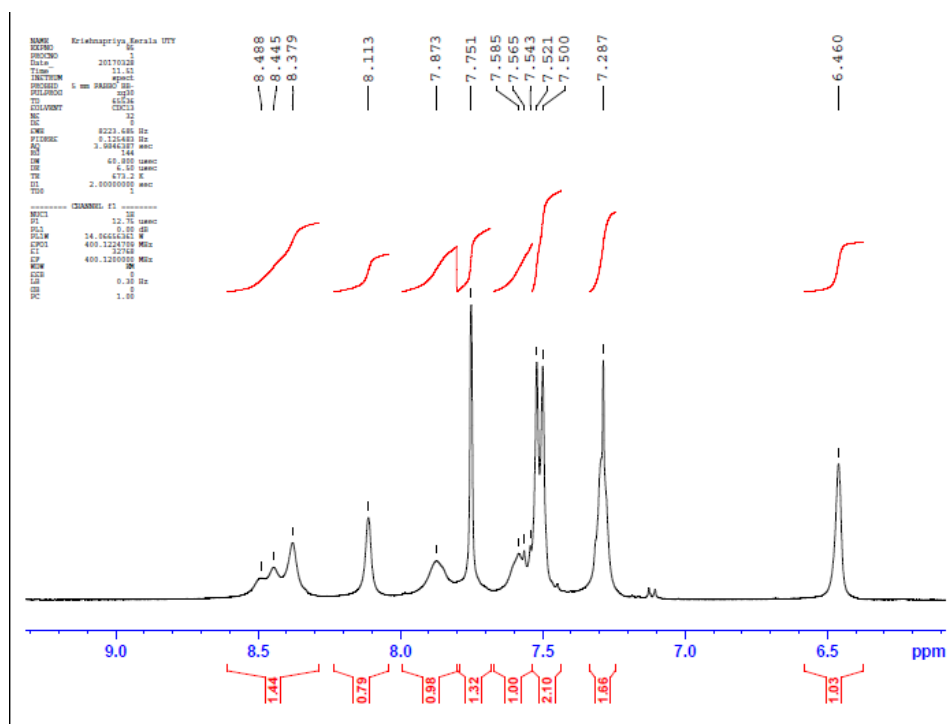


Figure S26. ^{13}C NMR spectrum (expanded) of 1-[(*N*-4-bromophenylthiocarbamoyl)amidino]pyrazole (**2f**) (100 MHz, CDCl_3)

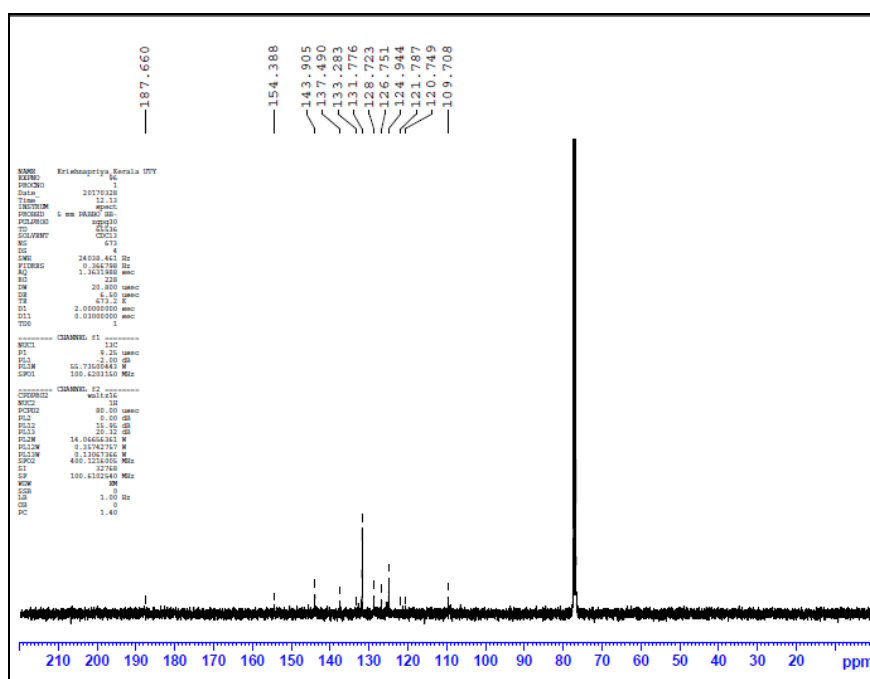


Figure S27. ESI-HRMS spectrum of 1-[(*N*-4-bromophenylthiocarbamoyl)amidino]pyrazole (**2f**)

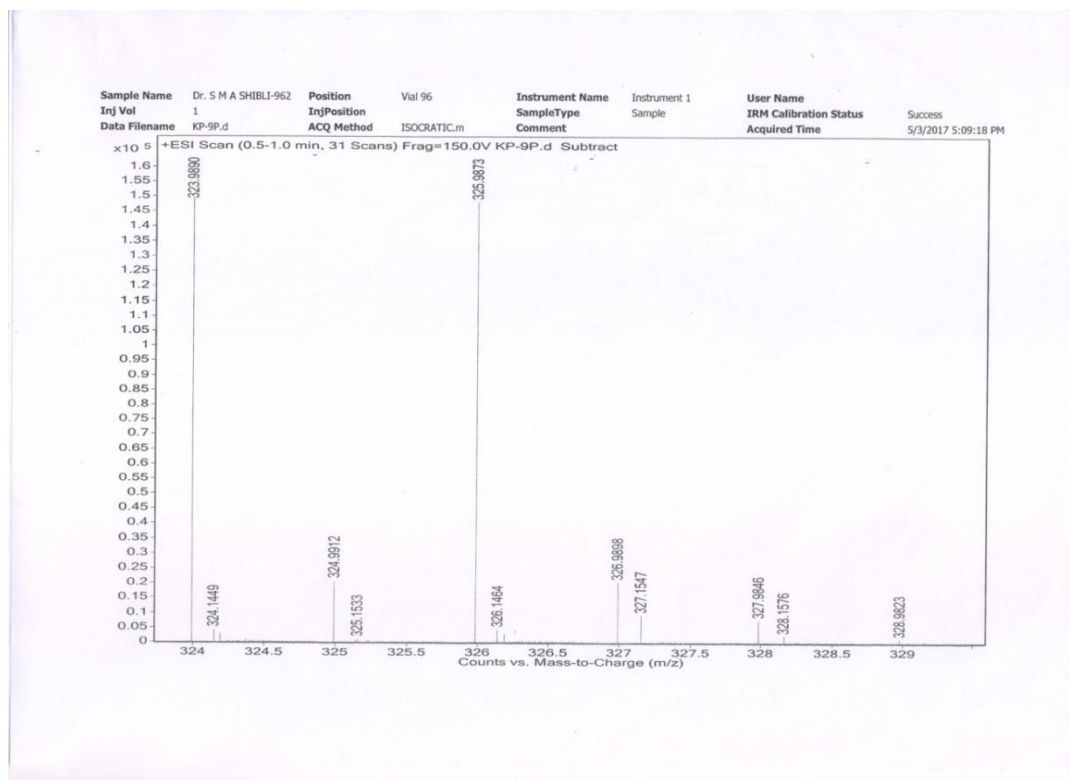


Figure S28. ^1H NMR spectrum of 1-[(N-4-ethoxyphenylthiocarbamoyl)amidino]pyrazole (**2g**) (400 MHz, DMSO)

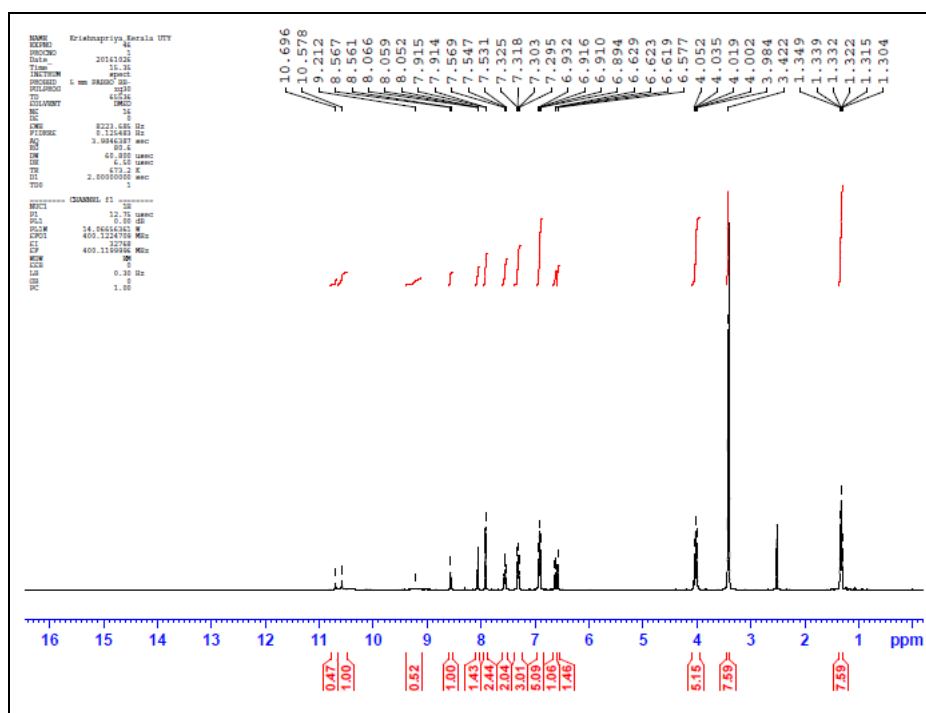


Figure S29. ^1H NMR spectrum (expanded) of 1-[(N-4-ethoxyphenylthiocarbamoyl)amidino]pyrazole (**2g**) (400 MHz, DMSO)

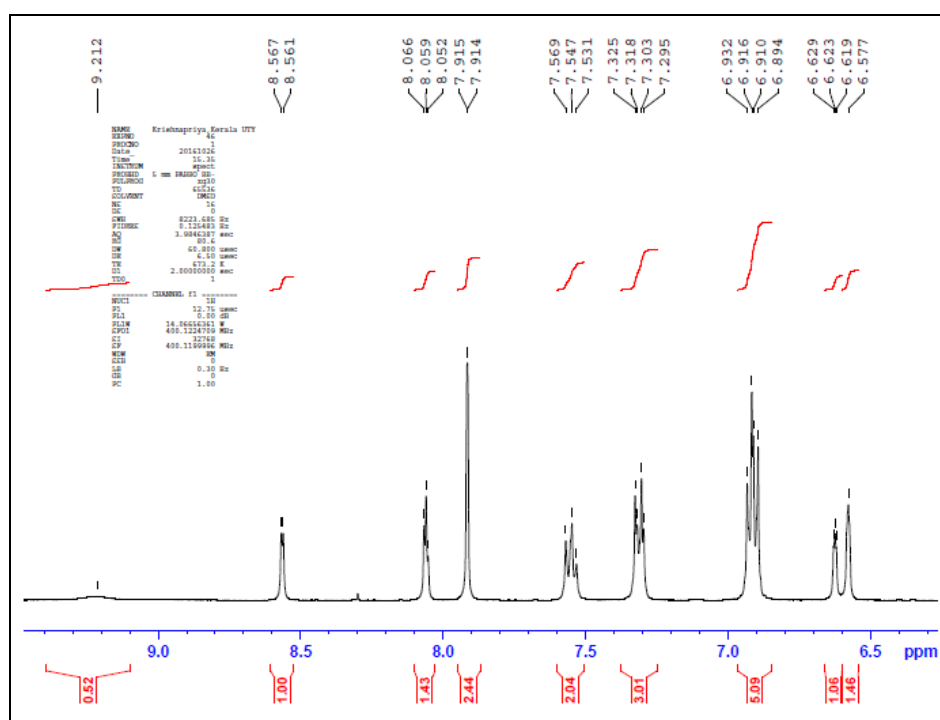


Figure S30. ¹³C NMR spectrum of 1-[(N-4-ethoxyphenylthiocarbamoyl)amidino]pyrazole (**2g**) (100 MHz, DMSO)

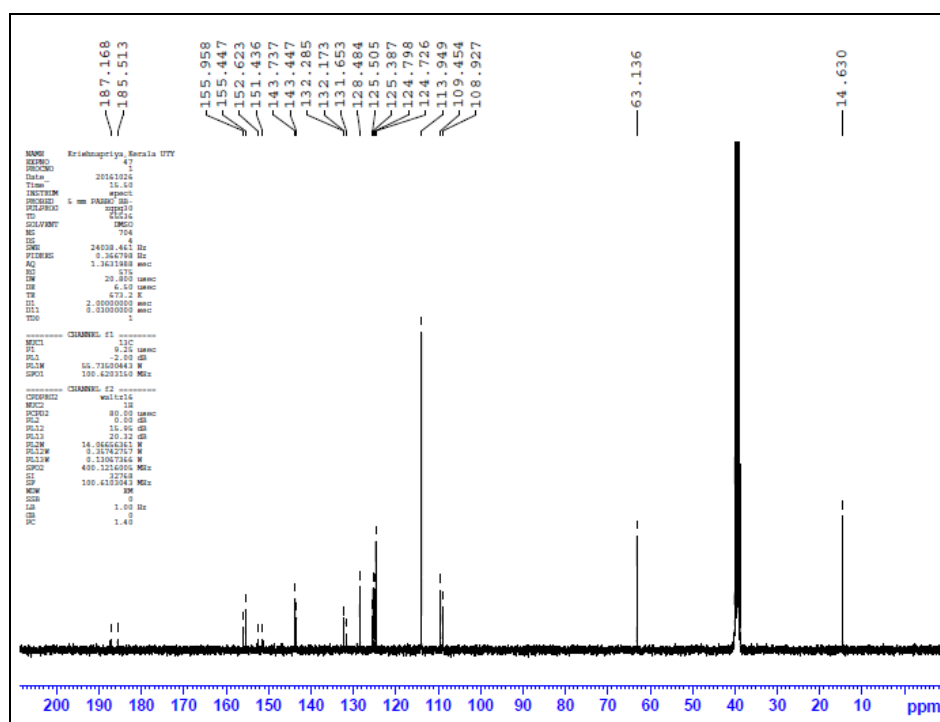


Figure S31. ESI-HRMS spectrum of 1-[(N-4-ethoxyphenylthiocarbamoyl)amidino]pyrazole (**2g**)

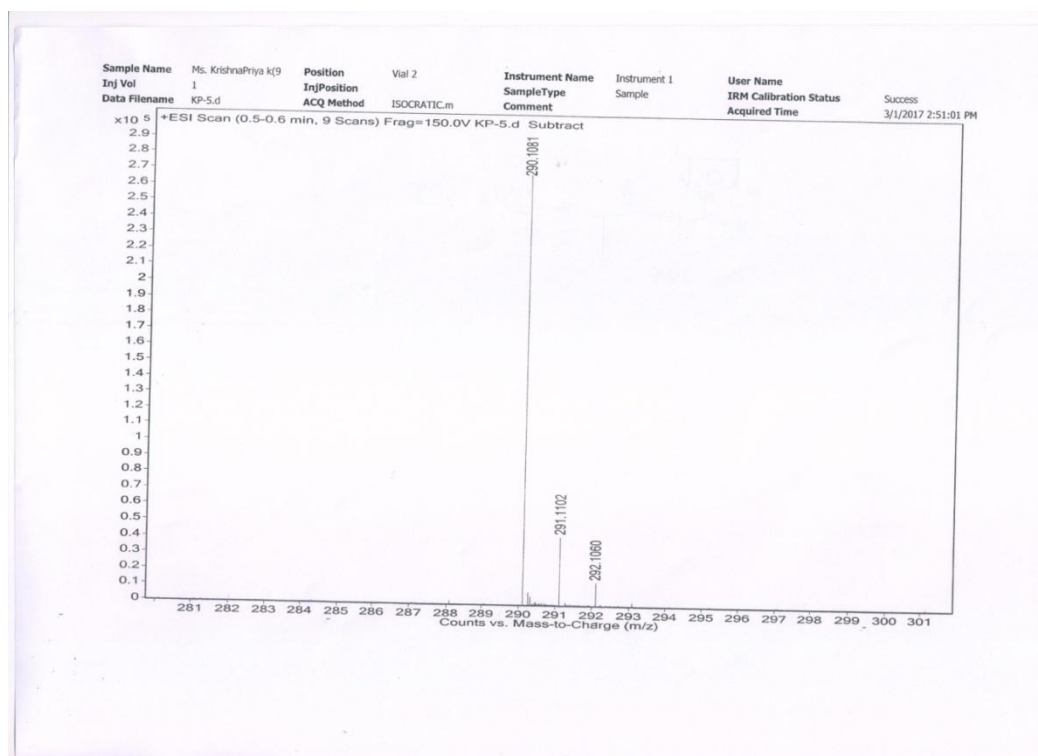


Figure S32. ^1H NMR spectrum of 1-[(*N*-3-methylphenylthiocarbamoyl)amidino]pyrazole (**2h**) (400 MHz, CDCl_3)

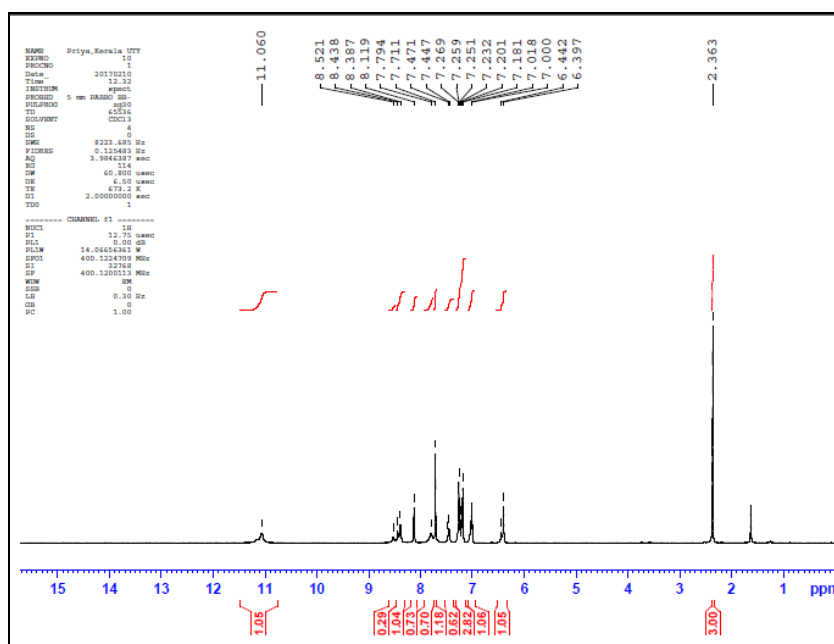


Figure S33. ^1H NMR spectrum (expanded) of 1-[(*N*-3-methylphenylthiocarbamoyl)amidino]pyrazole (**2h**) (400 MHz, CDCl_3)

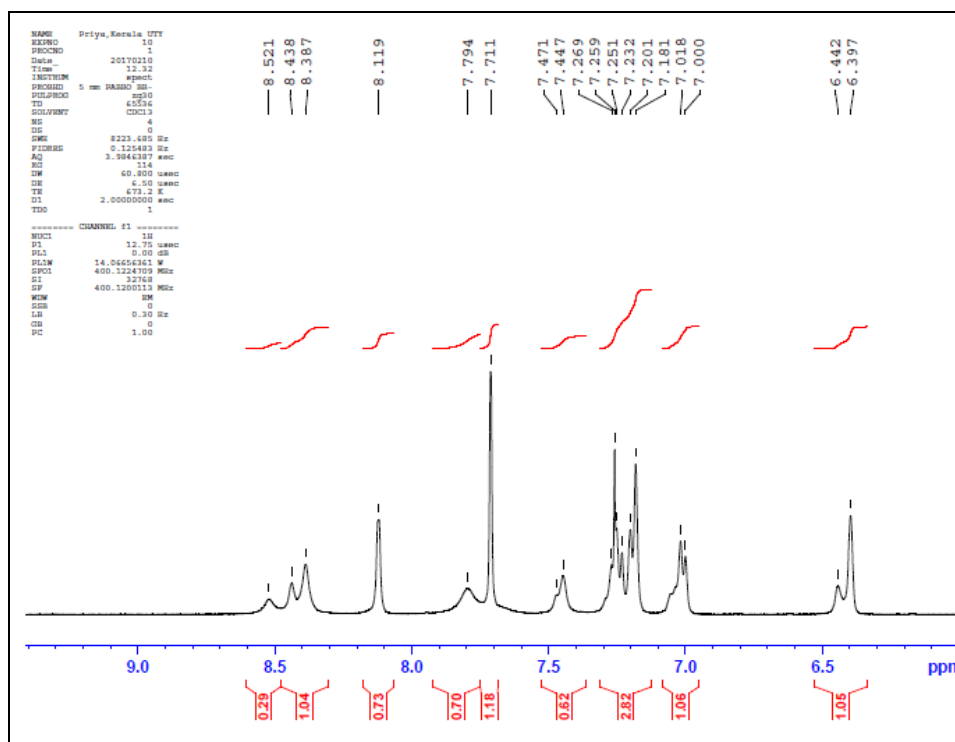


Figure S34. ^{13}C NMR spectrum (of 1-[(N-3-methylphenylthiocarbamoyl)amidino]pyrazole (**2h**) (100 MHz, CDCl_3)

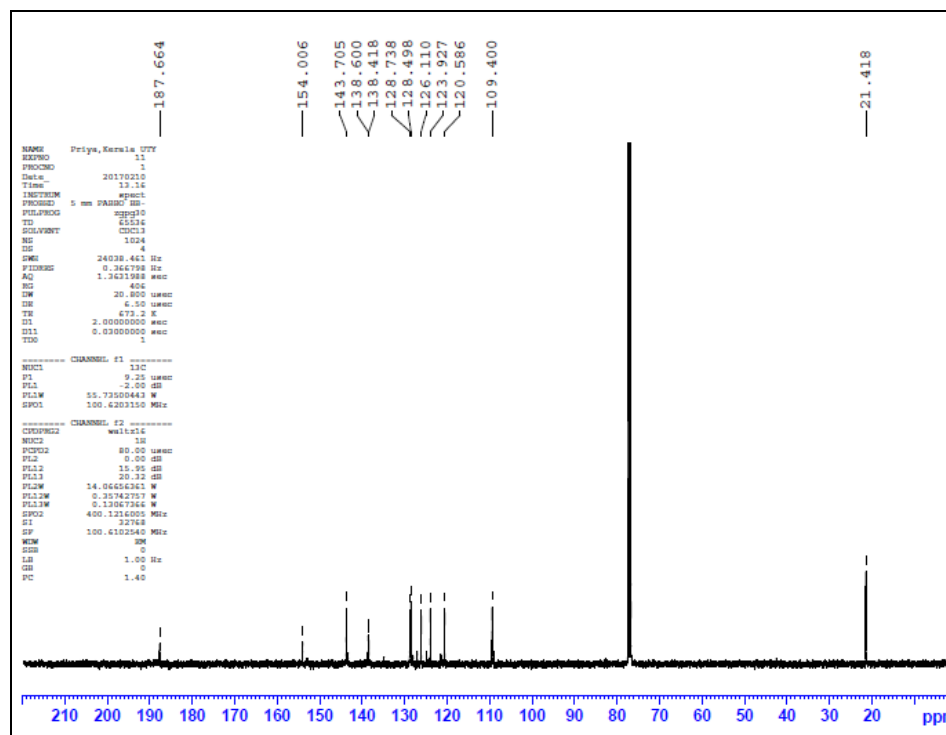


Figure S35. ESI-HRMS spectrum of 1-[(N-3-methylphenylthiocarbamoyl)amidino]pyrazole (**2h**)

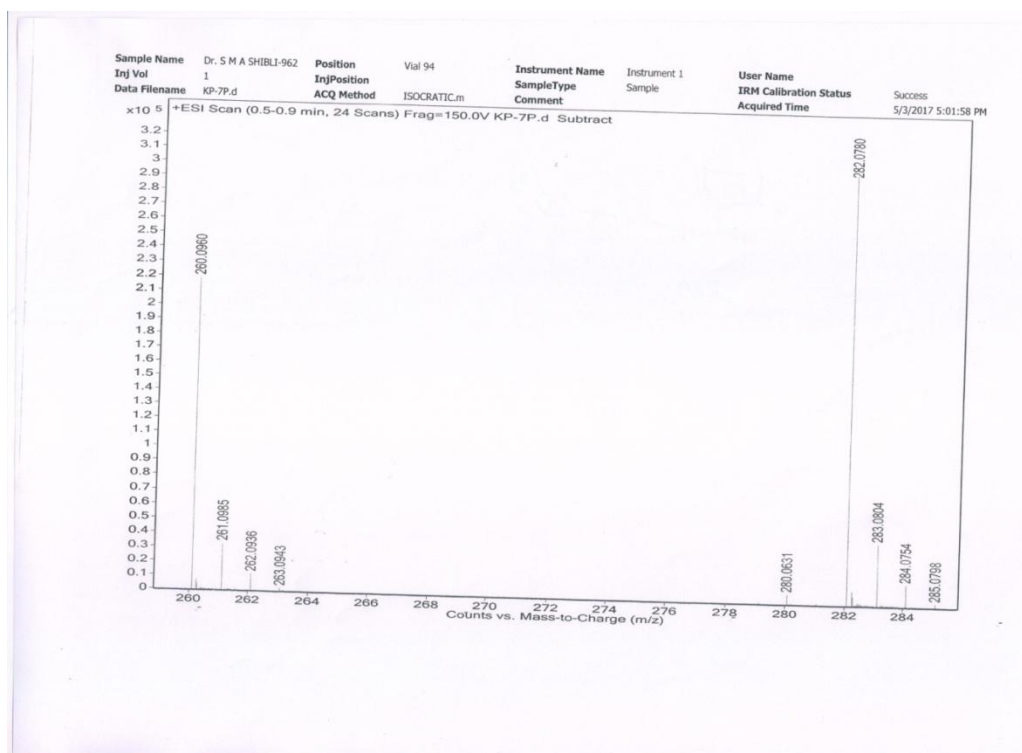


Figure S36. ^1H NMR spectrum of 1-[(*N*-2-chlorophenylthiocarbamoyl)amidino]pyrazole (**2i**) (400 MHz, CDCl_3)

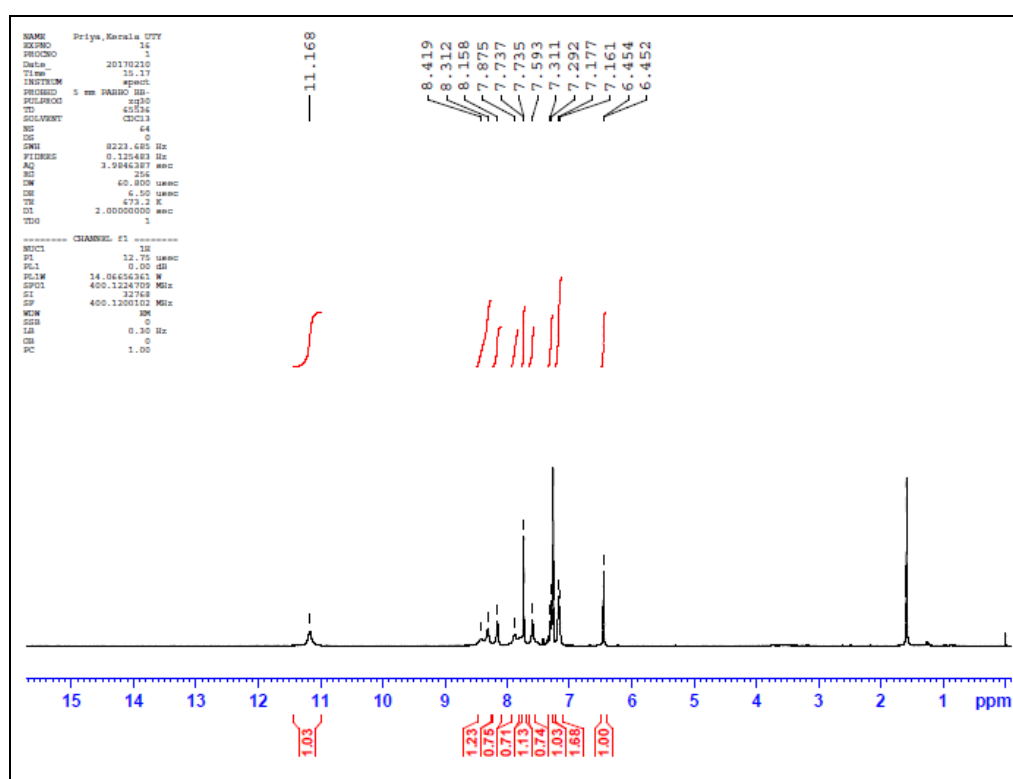


Figure S37. ^1H NMR spectrum (expanded) of 1-[(*N*-2-chlorophenylthiocarbamoyl)amidino]pyrazole (**2i**) (400 MHz, CDCl_3)

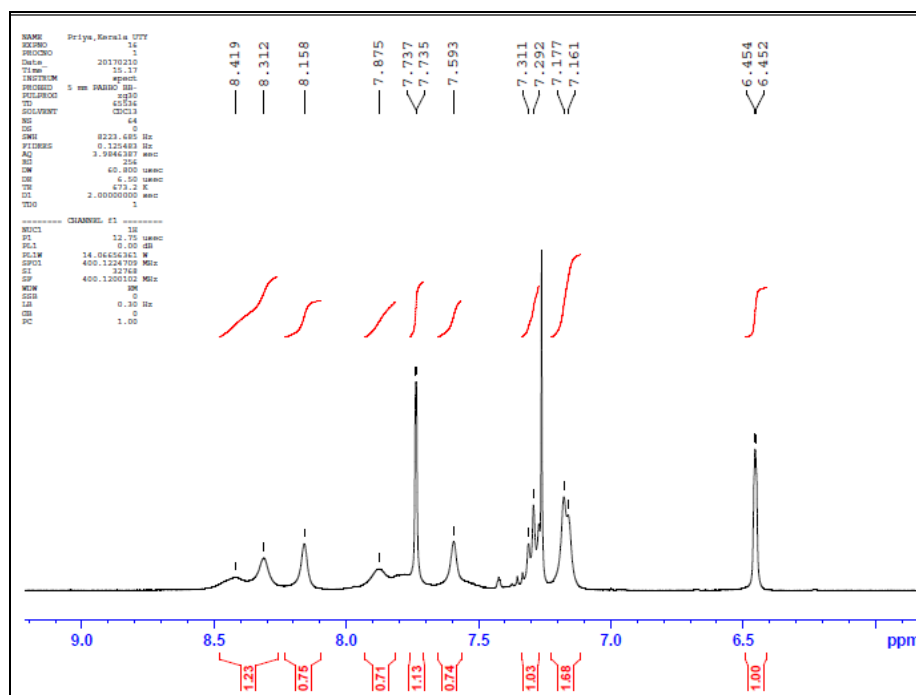


Figure S38. ¹³C NMR spectrum of 1-[(N-2-chlorophenylthiocarbamoyl)amidino]pyrazole (2i) (100 MHz, CDCl₃)

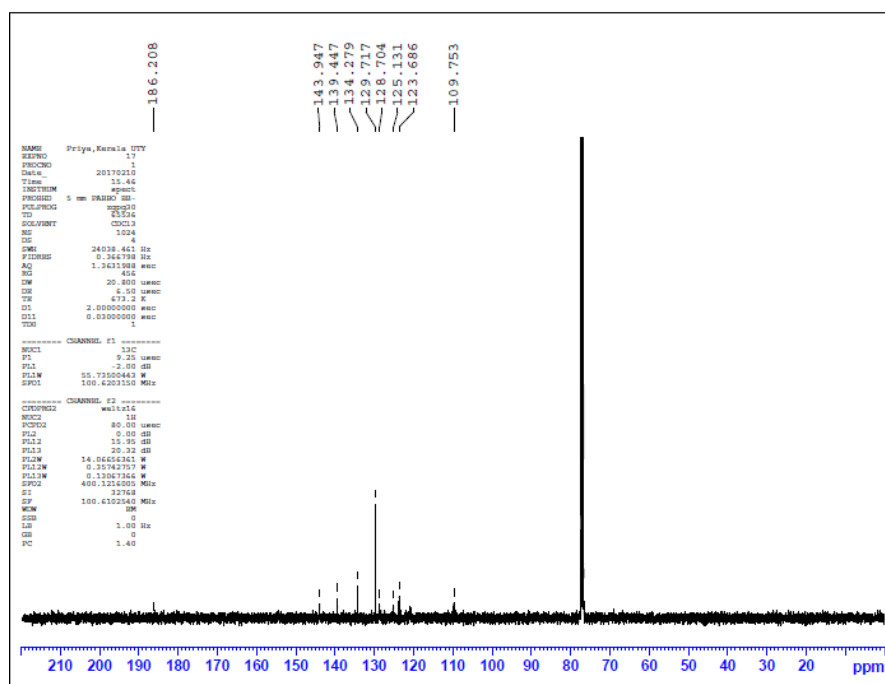


Figure S39. ESI-HRMS spectrum of 1-[(N-2-chlorophenylthiocarbamoyl)amidino]pyrazole (2i)

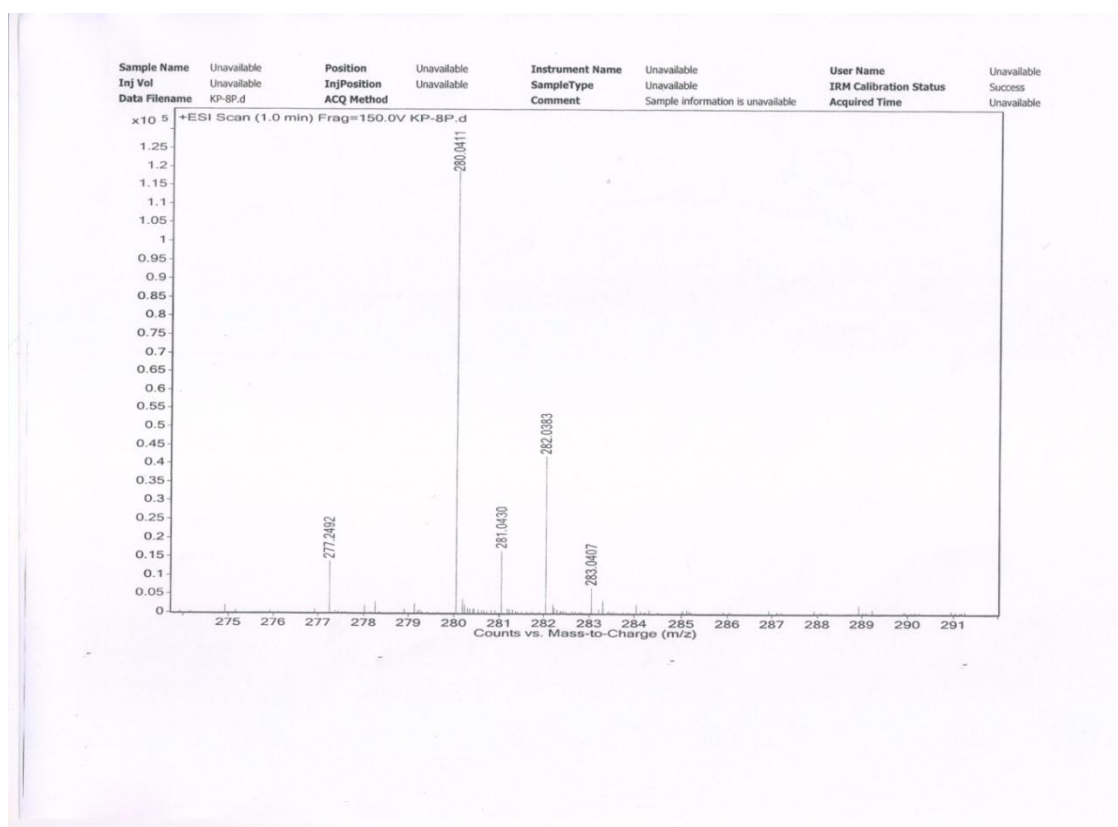


Figure S40. ^1H NMR spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrrolidine (**3a**) (400 MHz, CDCl_3)

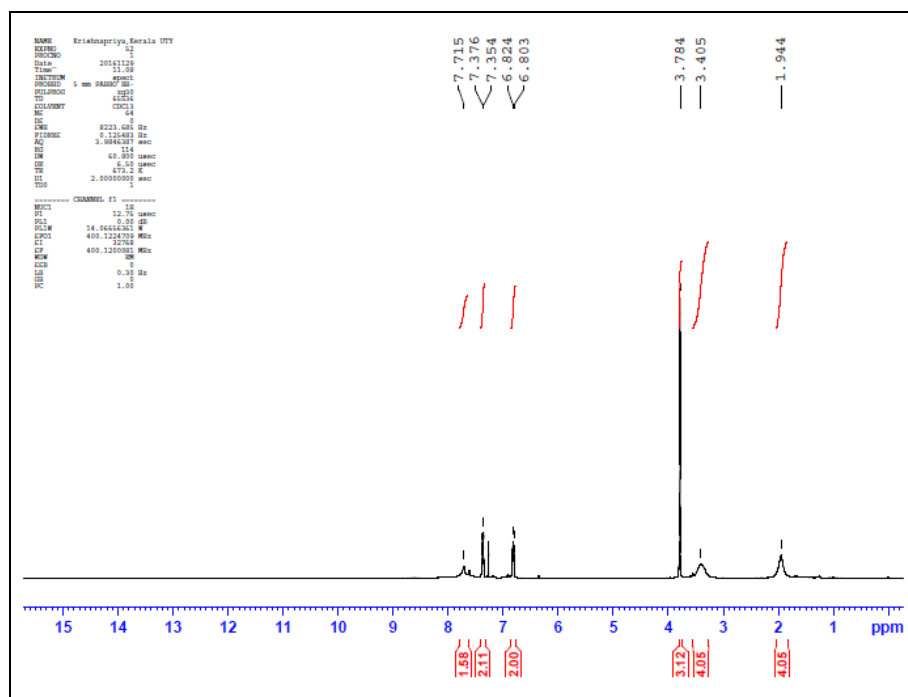


Figure S41. ^1H NMR spectrum (expanded) of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrrolidine (**3a**) (400 MHz, CDCl_3)

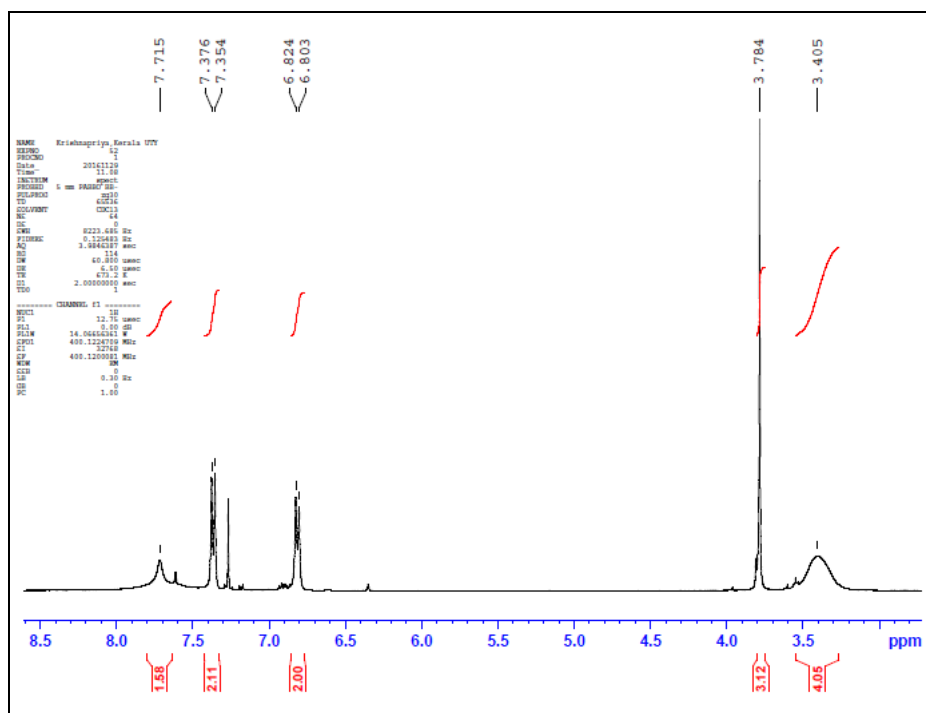


Figure S42. ^{13}C NMR spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrrolidine (3a) (100 MHz, CDCl_3)

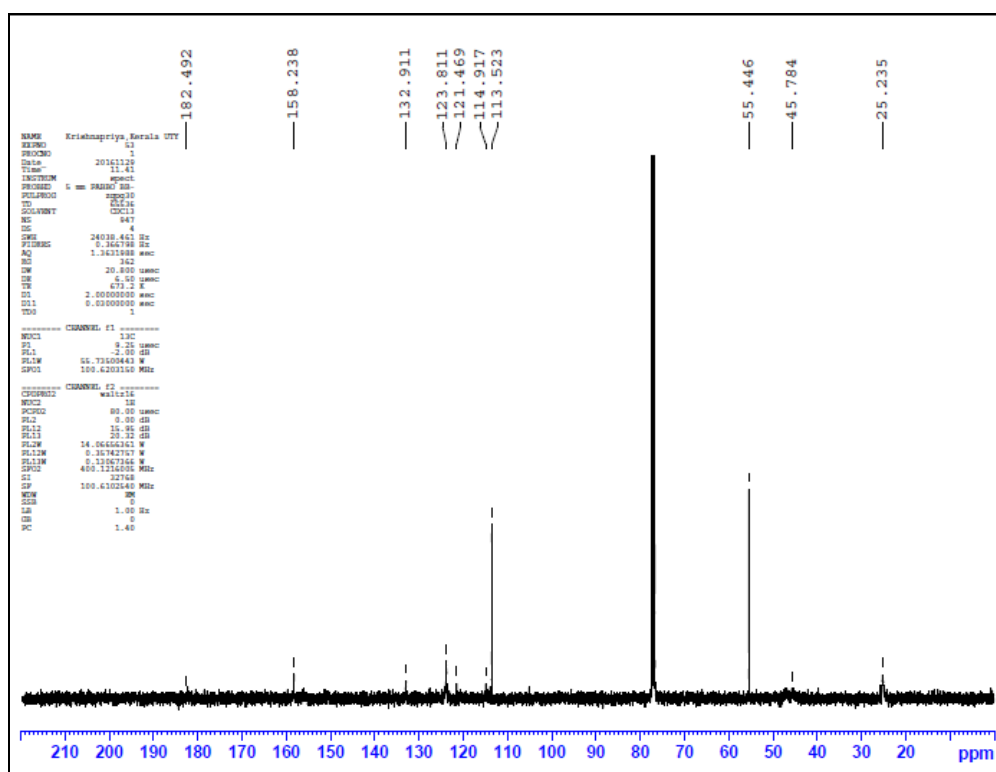


Figure S43. ESI-HRMS spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrrolidine (3a)

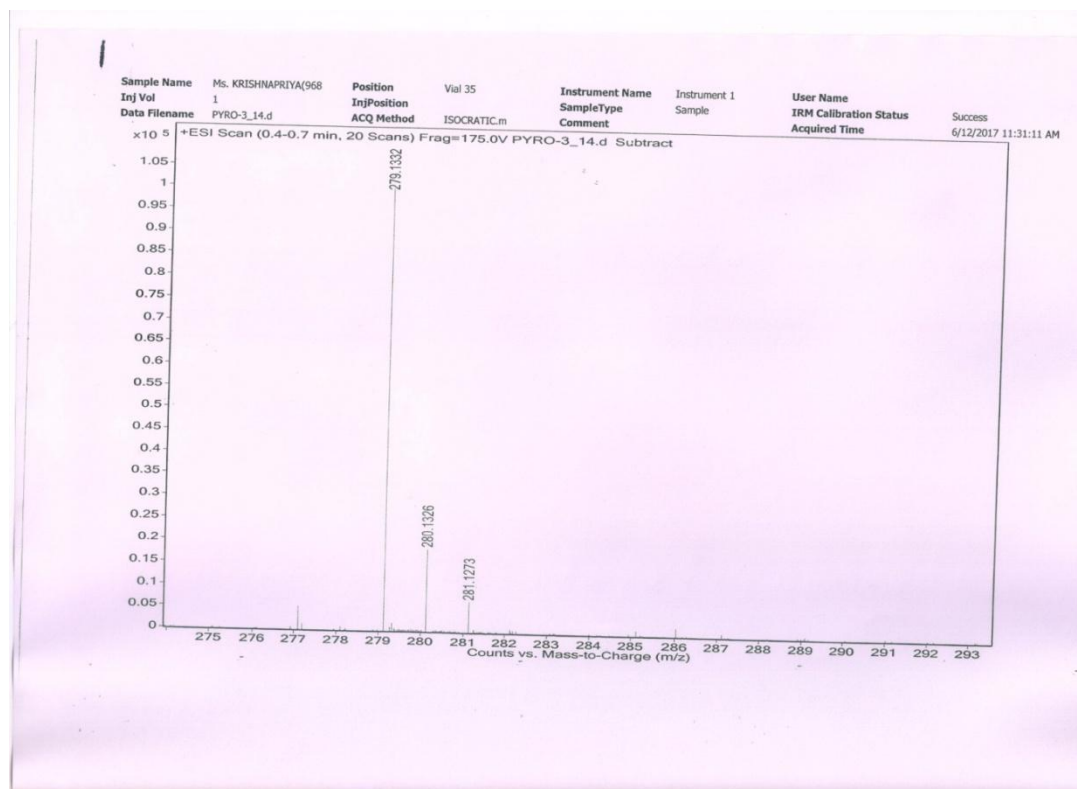


Figure S44. ^1H NMR spectrum 1-[(*N*-4-ethoxyphenylthiocarbamoyl)amidino]pyrrolidine (**3b**) (400 MHz, CDCl_3)

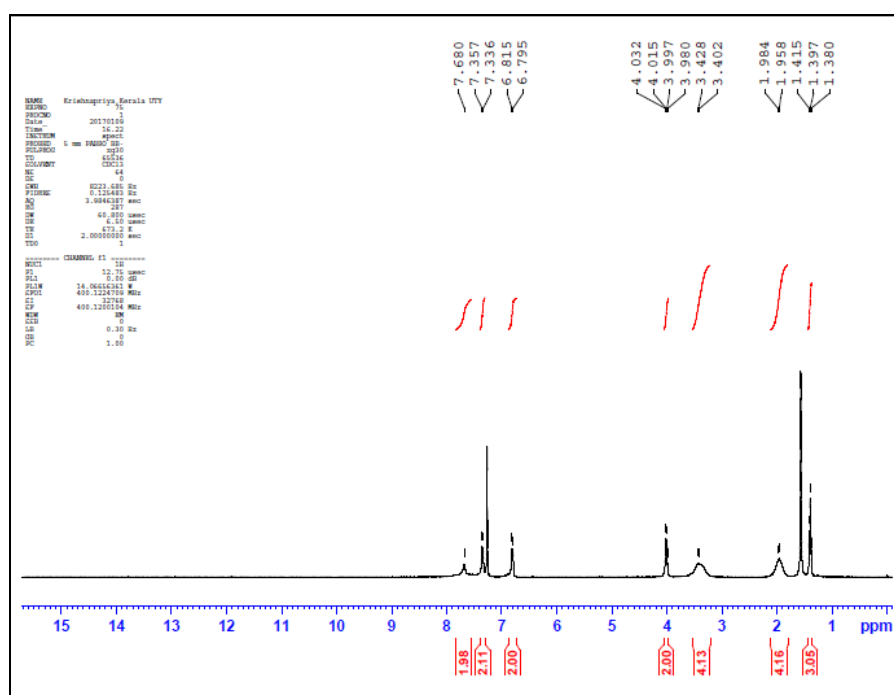


Figure S45. ^1H NMR spectrum (expanded) 1-[(*N*-4-ethoxyphenylthiocarbamoyl)amidino]pyrrolidine (**3b**) (400 MHz, CDCl_3)

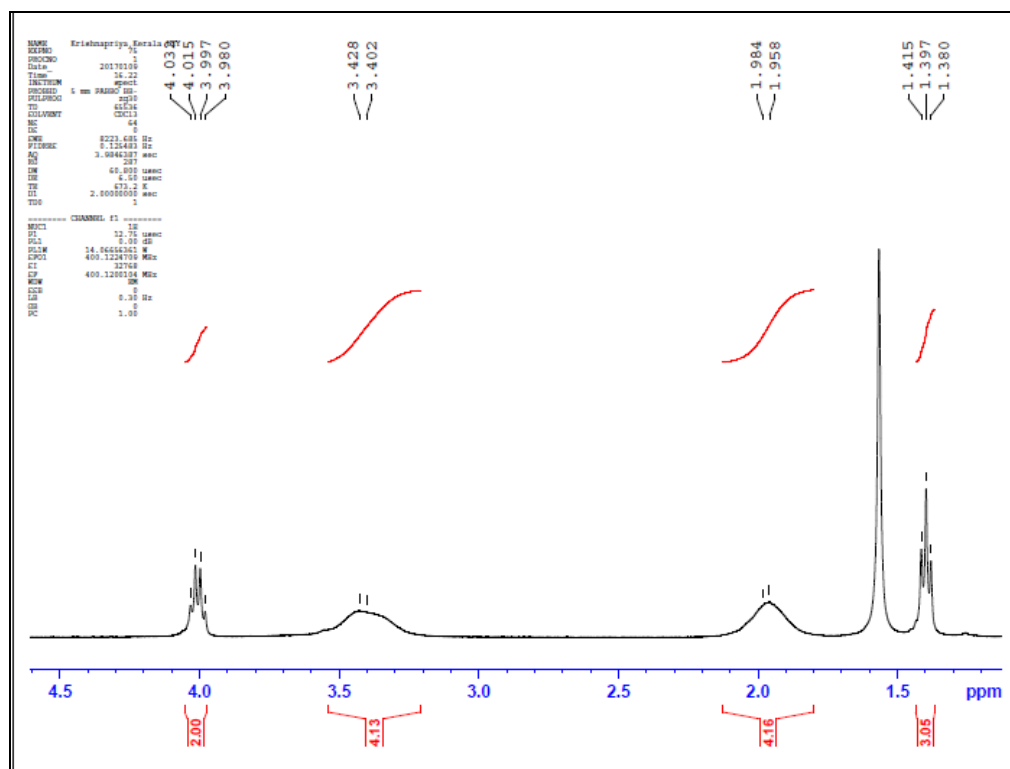


Figure S46. ¹³C NMR spectrum 1-[(N-4-ethoxyphenylthiocarbamoyl)amidino]pyrrolidine (**3b**) (100 MHz, CDCl₃)

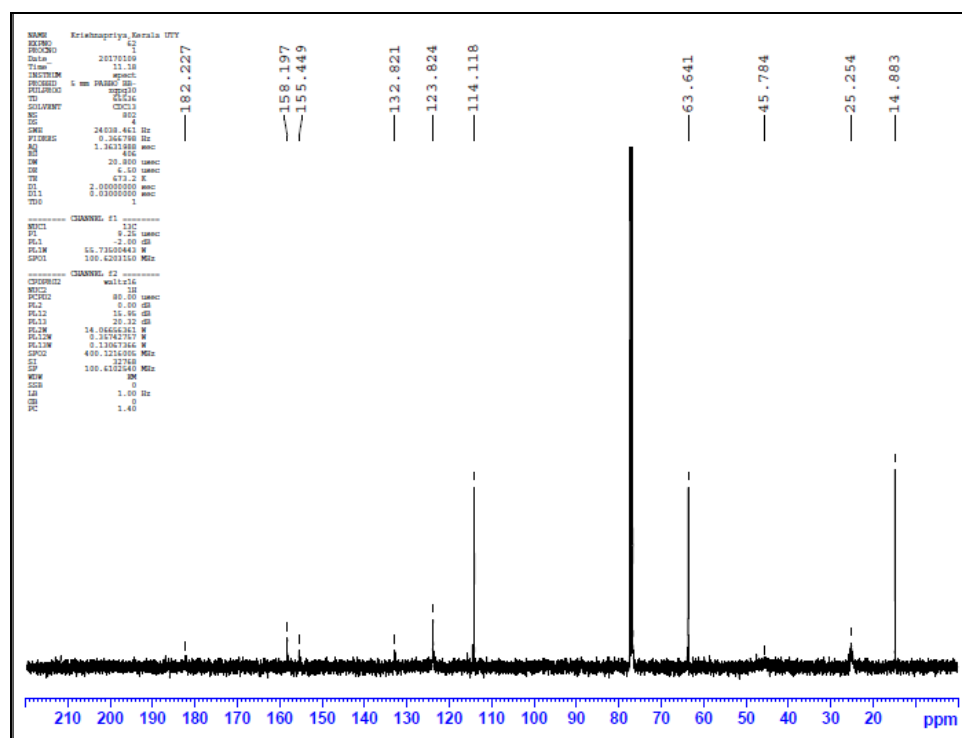


Figure S47. ESI-HRMS spectrum 1-[(N-4-ethoxyphenylthiocarbamoyl)amidino]pyrrolidine (**3b**)

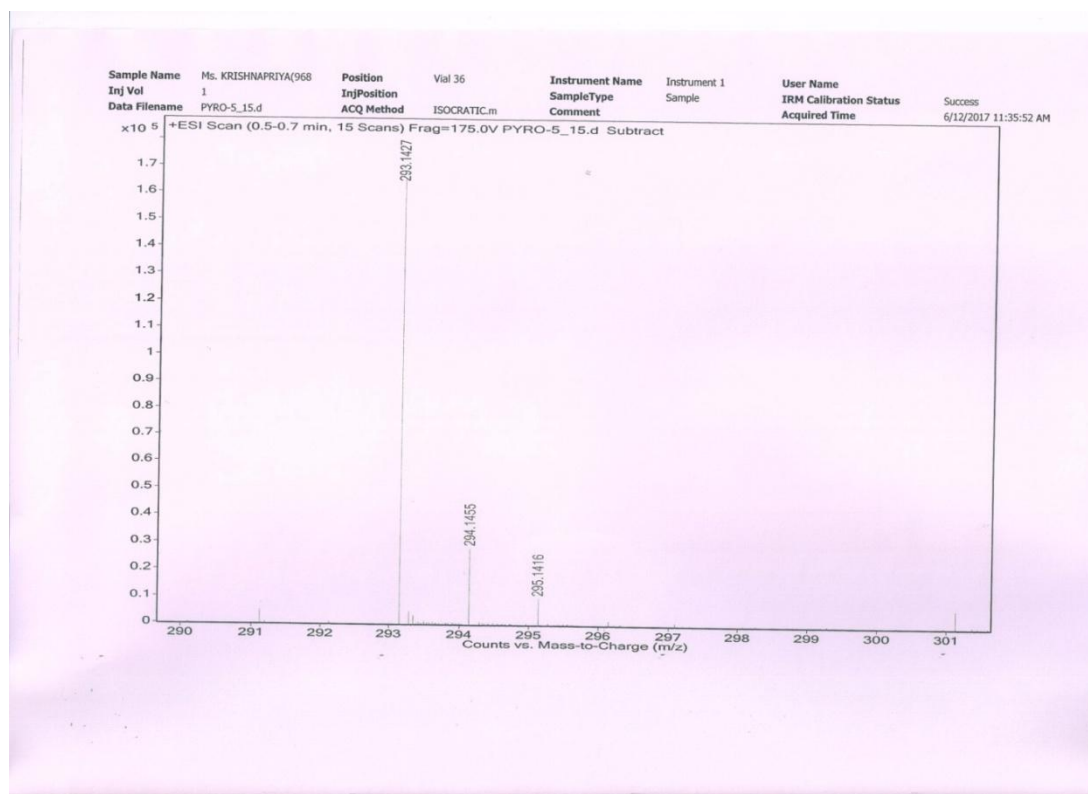


Figure S48. ¹H NMR spectrum 1-[(N-4-methylphenylthiocarbamoyl)amidino]piperidine (**3c**) (400 MHz,

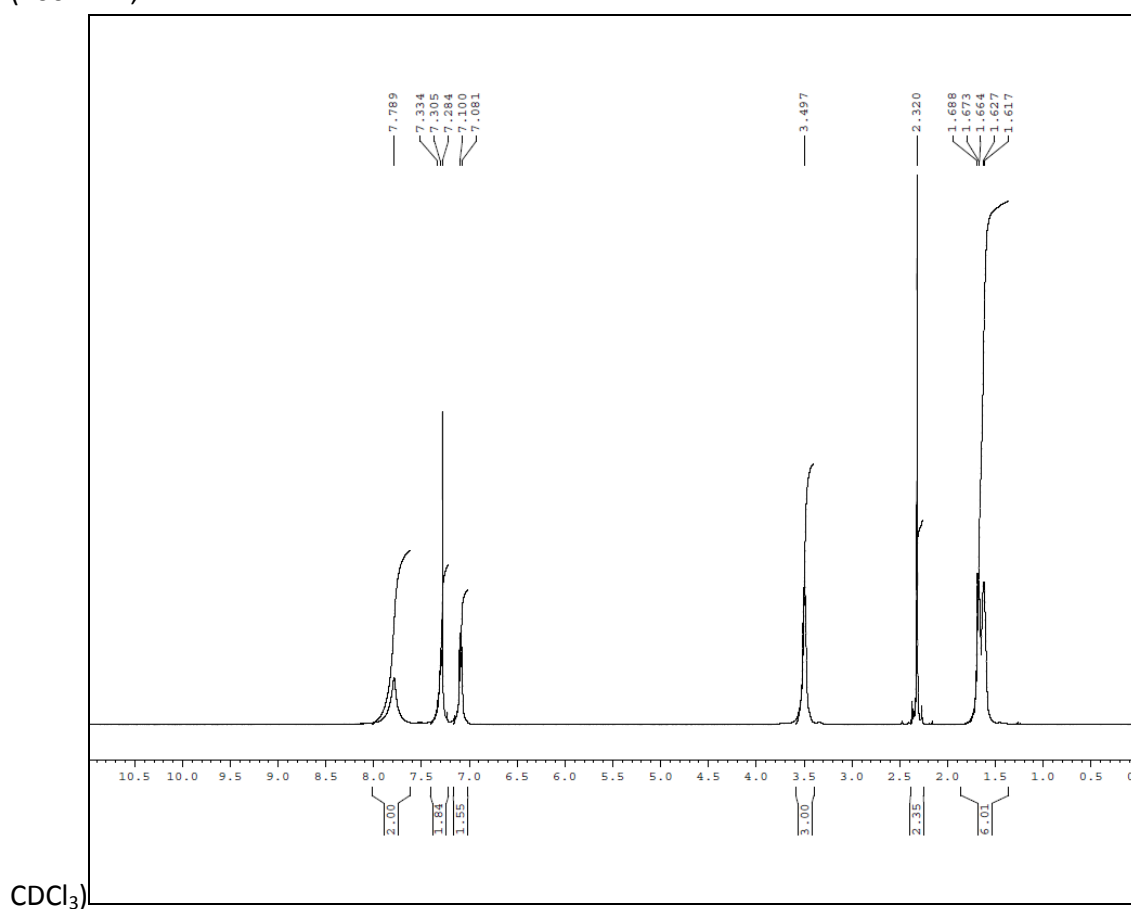


Figure S49. ^{13}C NMR spectrum of 1-[(*N*-4-methylphenylthiocarbamoyl)amidino]piperidine (**3c**) (100 MHz, CDCl_3)

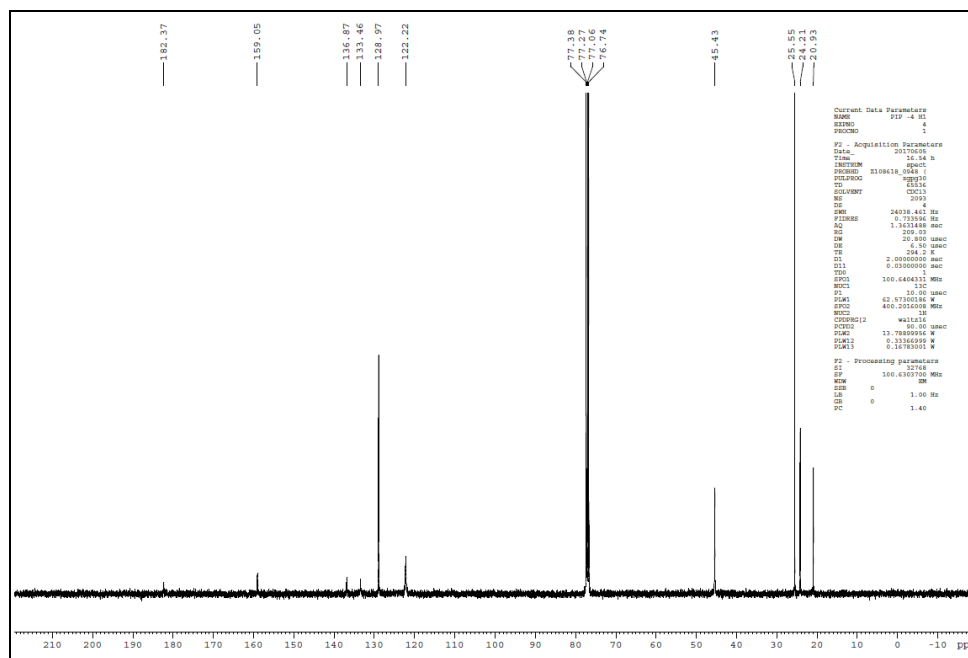


Figure S50. ESI-HRMS spectrum of 1-[(*N*-4-methylphenylthiocarbamoyl)amidino]piperidine (**3c**)

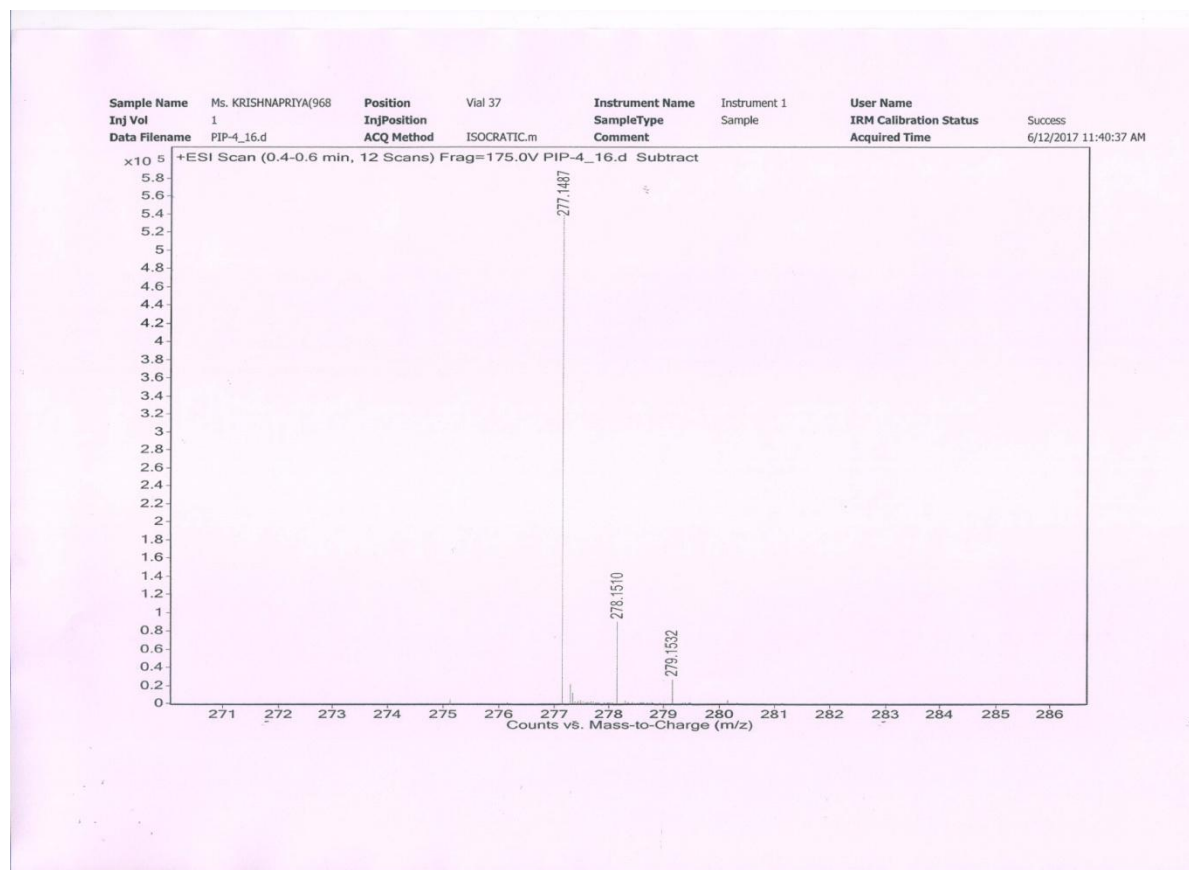


Figure S51. ^1H NMR spectrum of 1-[(*N*-phenylthiocarbamoyl)amidino]-4-methylpiperazine (**3d**) (400 MHz, CDCl_3)

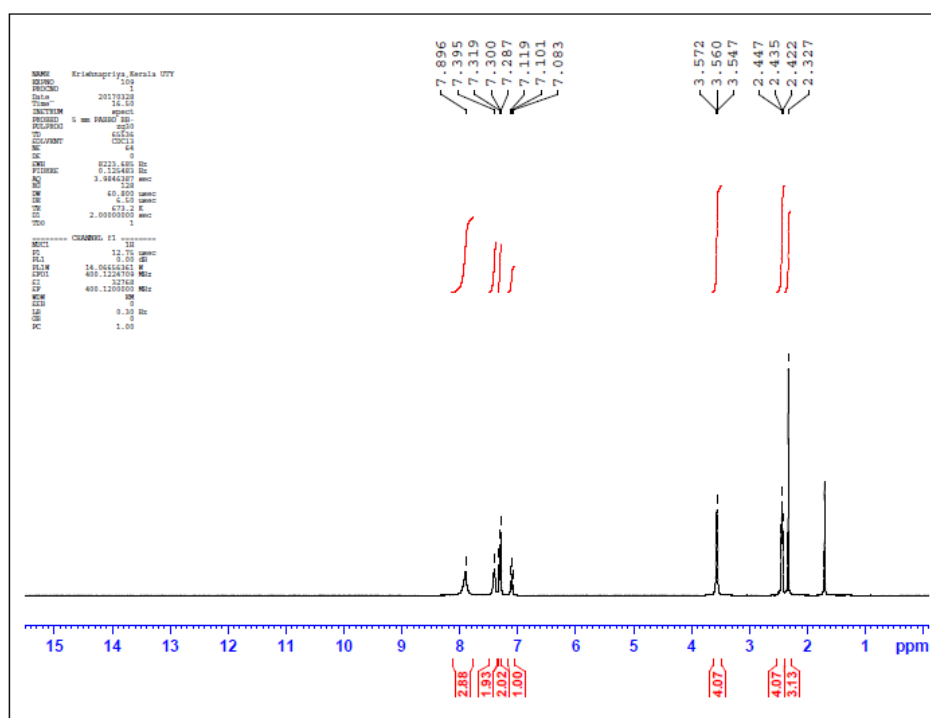


Figure S52. ^1H NMR spectrum (expanded) of 1-[(*N*-phenylthiocarbamoyl)amidino]-4-methylpiperazine (**3d**) (400 MHz, CDCl_3)

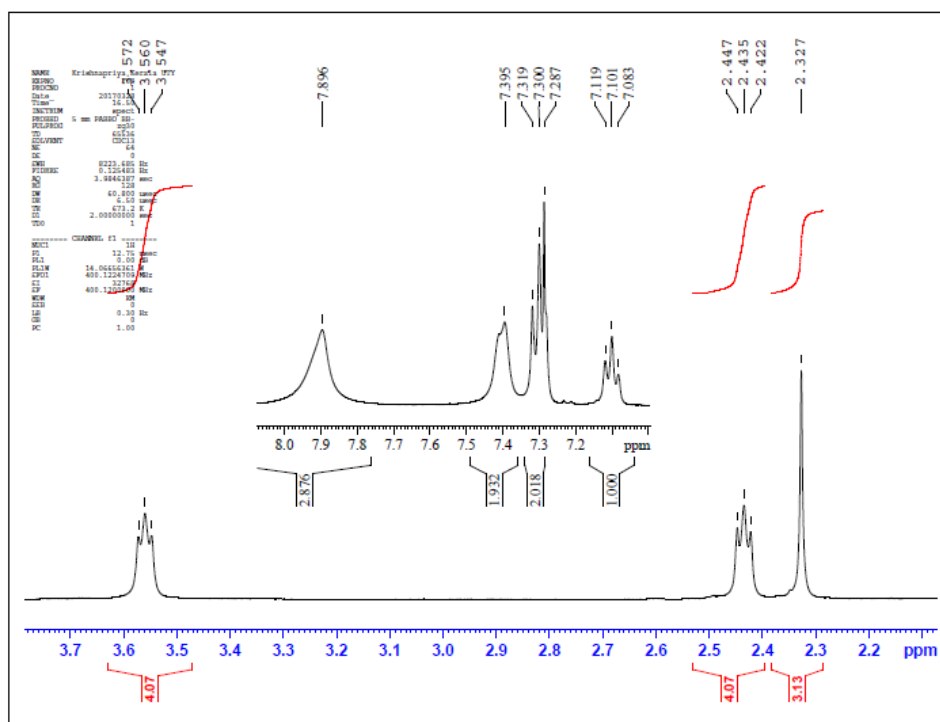


Figure S53. ¹³C NMR spectrum of 1-[(N-phenylthiocarbamoyl)amidino]-4-methylpiperazine (3d) (100 MHz, CDCl₃)

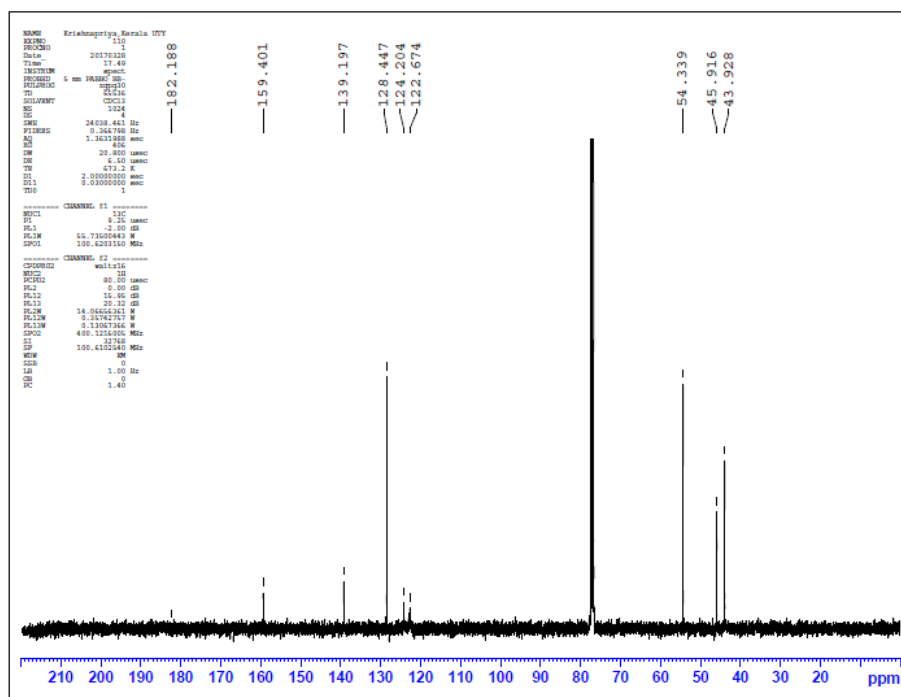


Figure S54. ESI-HRMS spectrum of 1-[(N-Phenylthiocarbamoyl)amidino]-4-methylpiperazine (3d)

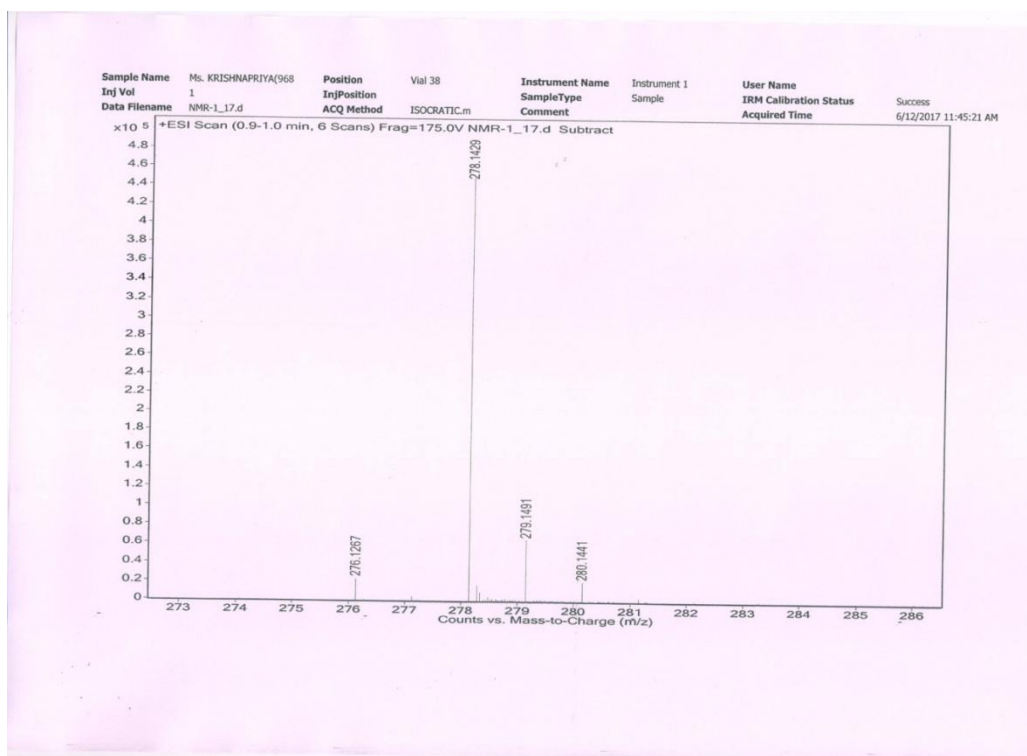


Figure S55. ^1H NMR spectrum of 1-[(*N*-phenylthiocarbamoyl)amidino]morpholine (**3e**) (400 MHz, CDCl_3)

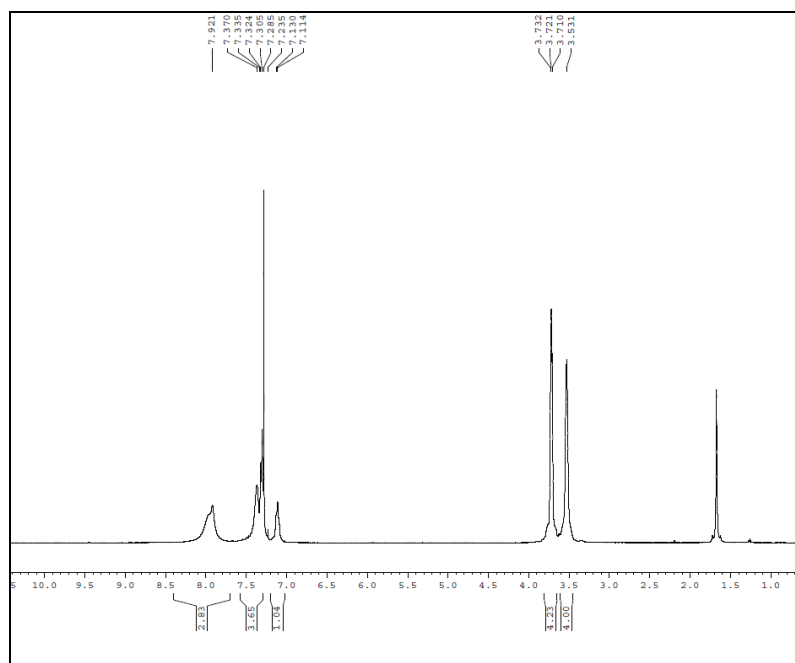


Figure S56. ^1H NMR spectrum (expanded) of 1-[(*N*-phenylthiocarbamoyl)amidino]morpholine (**3e**) (400 MHz, CDCl_3)

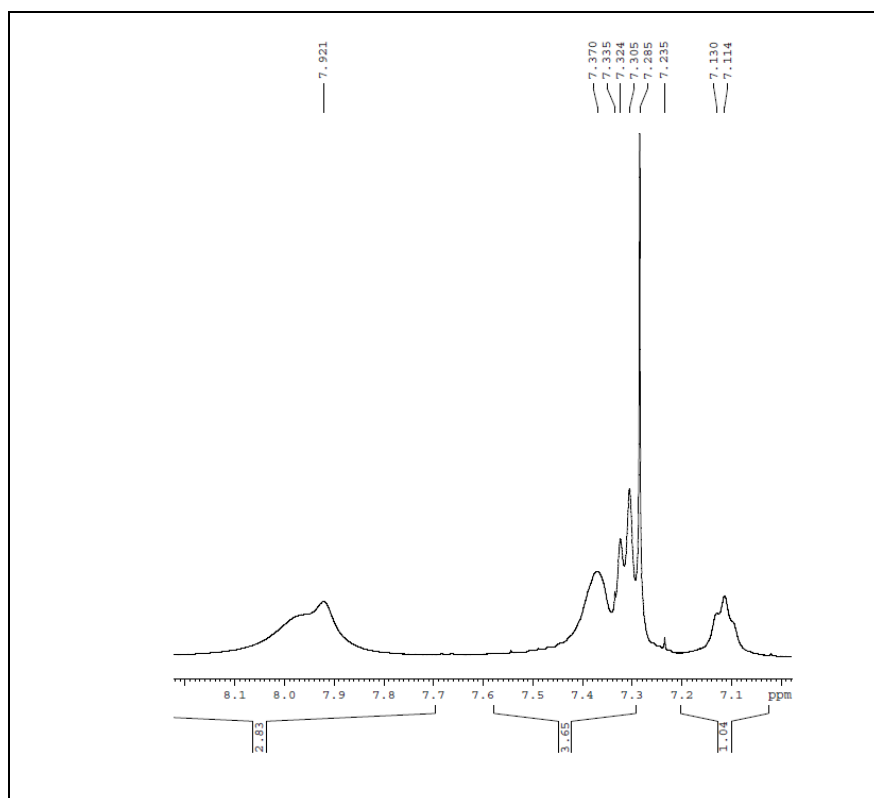


Figure S57. ¹³C NMR spectrum of 1-[(N-phenylthiocarbamoyl)amidino]morpholine (**3e**) (100 MHz, CDCl₃)

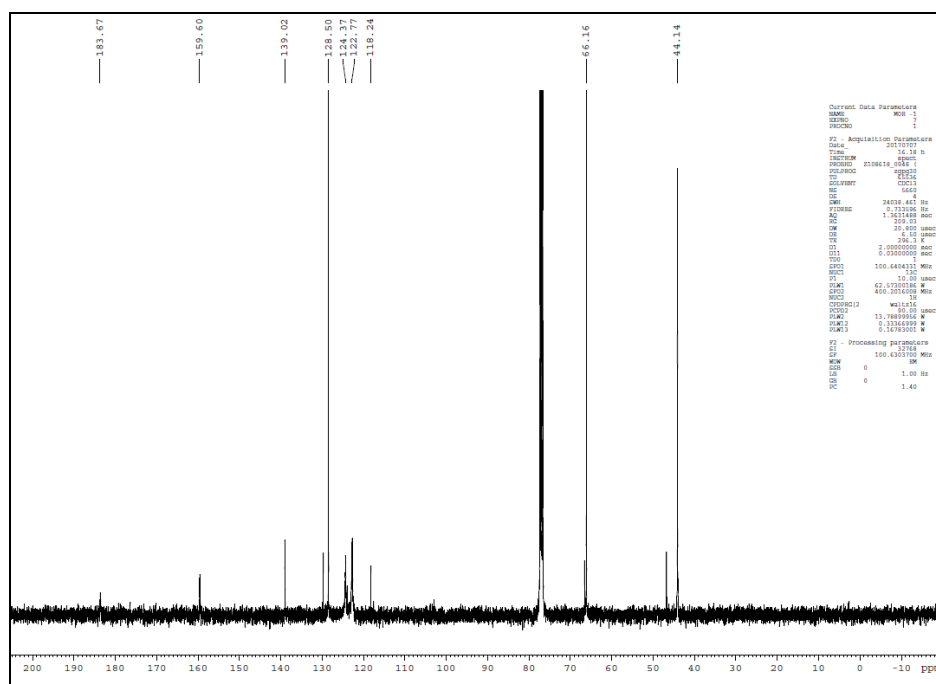


Figure S58. ESI-HRMS spectrum of 1-[(N-phenylthiocarbamoyl)amidino]morpholine (**3e**)

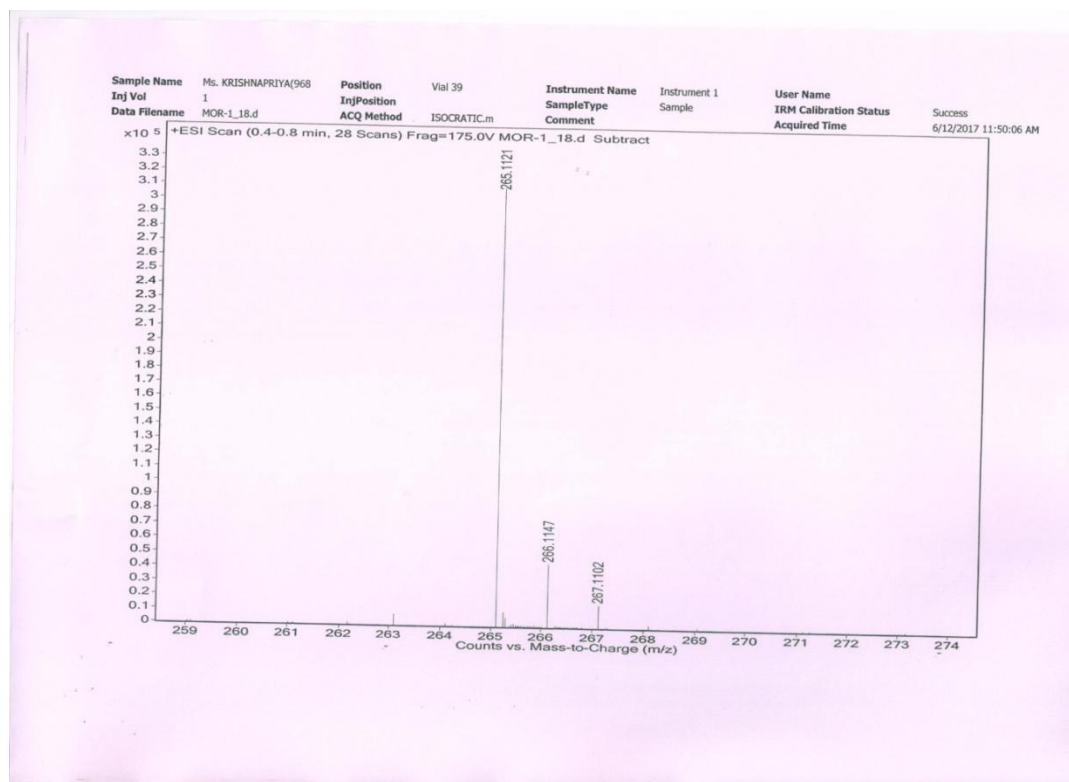


Figure S59. ^1H NMR spectrum of *N*-(phenylthiocarbamoyl)-*N'*-*n*-propylguanidine (**3f**) (400 MHz, CDCl_3)

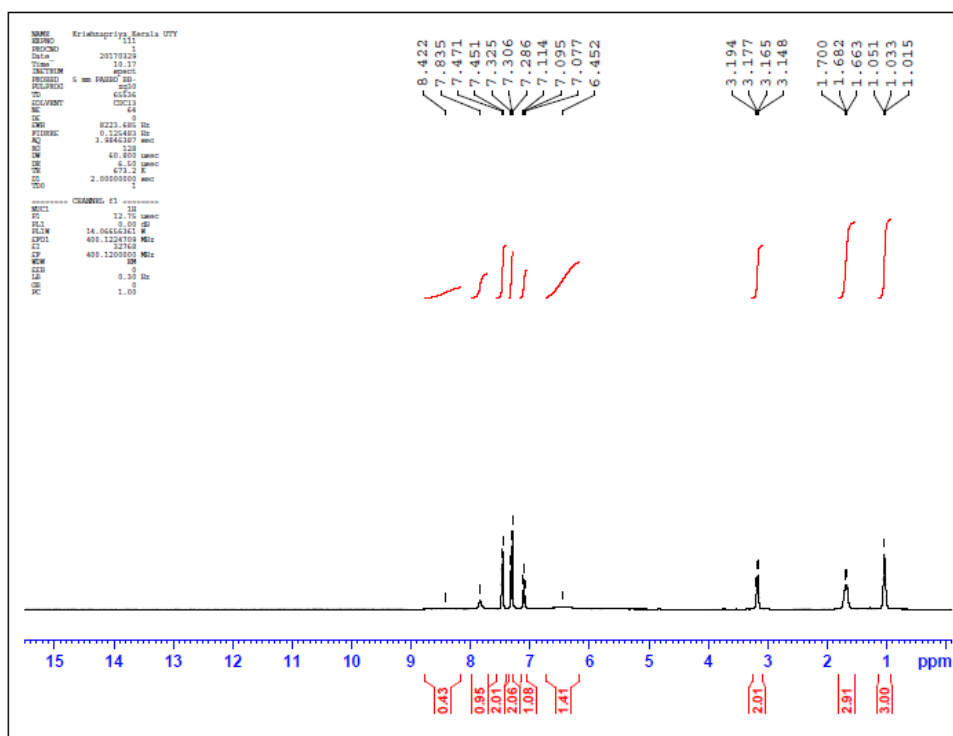


Figure S60. ^1H NMR spectrum (expanded) of *N*-(phenylthiocarbamoyl)-*N'*-*n*-propylguanidine (**3f**) (400 MHz, CDCl_3)

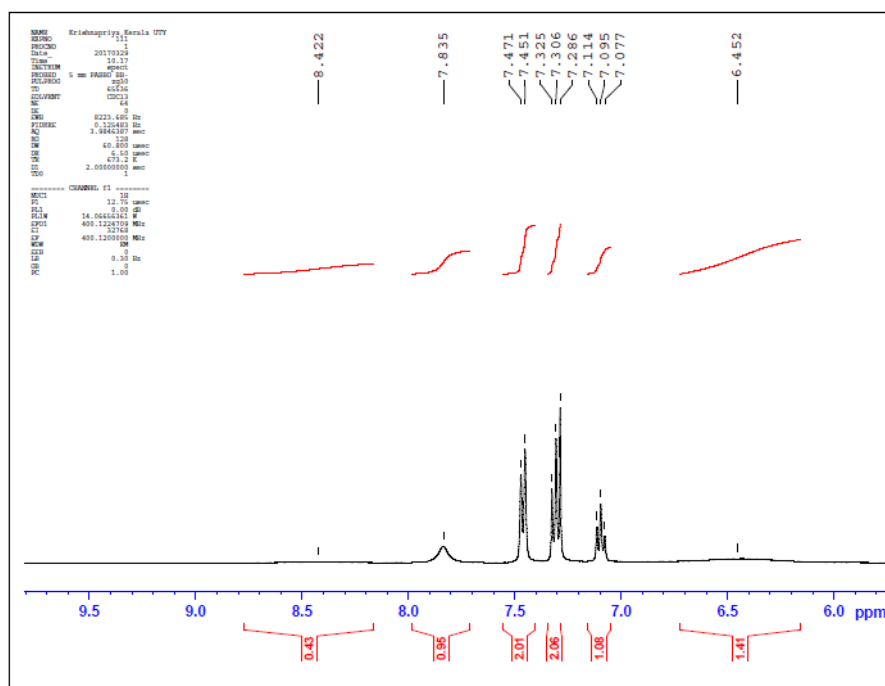


Figure S61. ^1H NMR spectrum (expanded) of *N*-(phenylthiocarbamoyl)-*N'*-*n*-propylguanidine (**3f**) (400 MHz, CDCl_3)

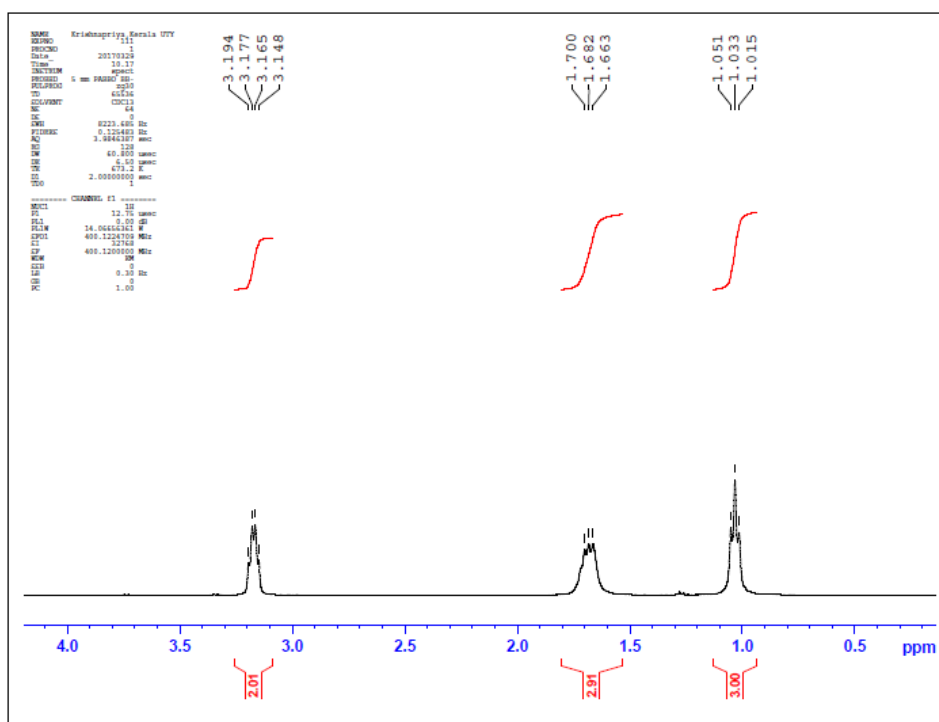


Figure S62. ^{13}C NMR spectrum (of *N*-(phenylthiocarbamoyl)-*N'*-*n*-propylguanidine (**3f**) (100 MHz, CDCl_3)

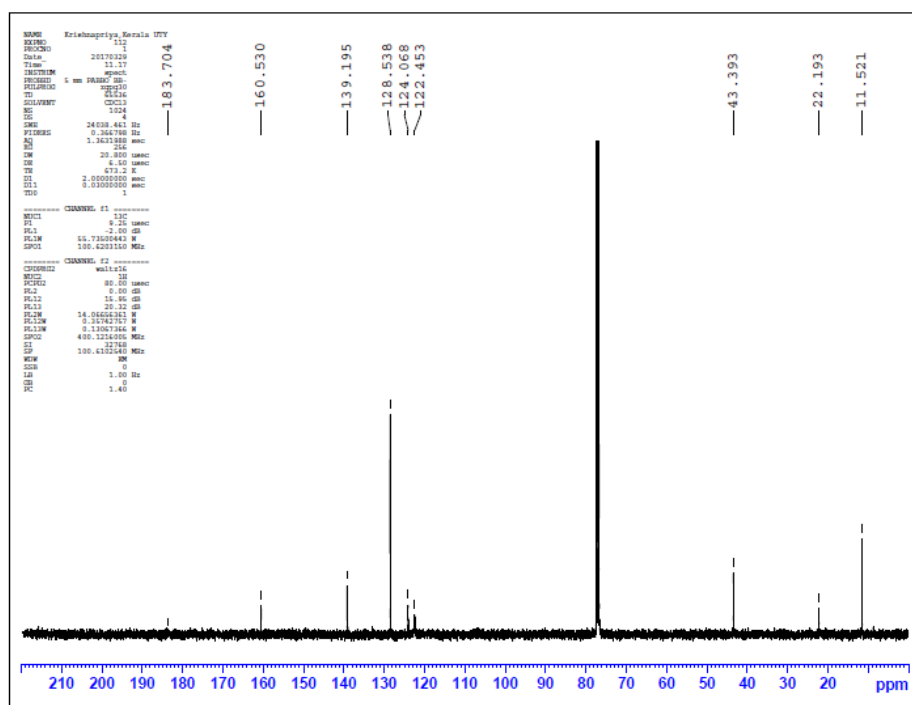


Figure S63. ESI-HRMS spectrum of *N*-(phenylthiocarbamoyl)-*N'*-*n*-propylguanidine (**3f**)

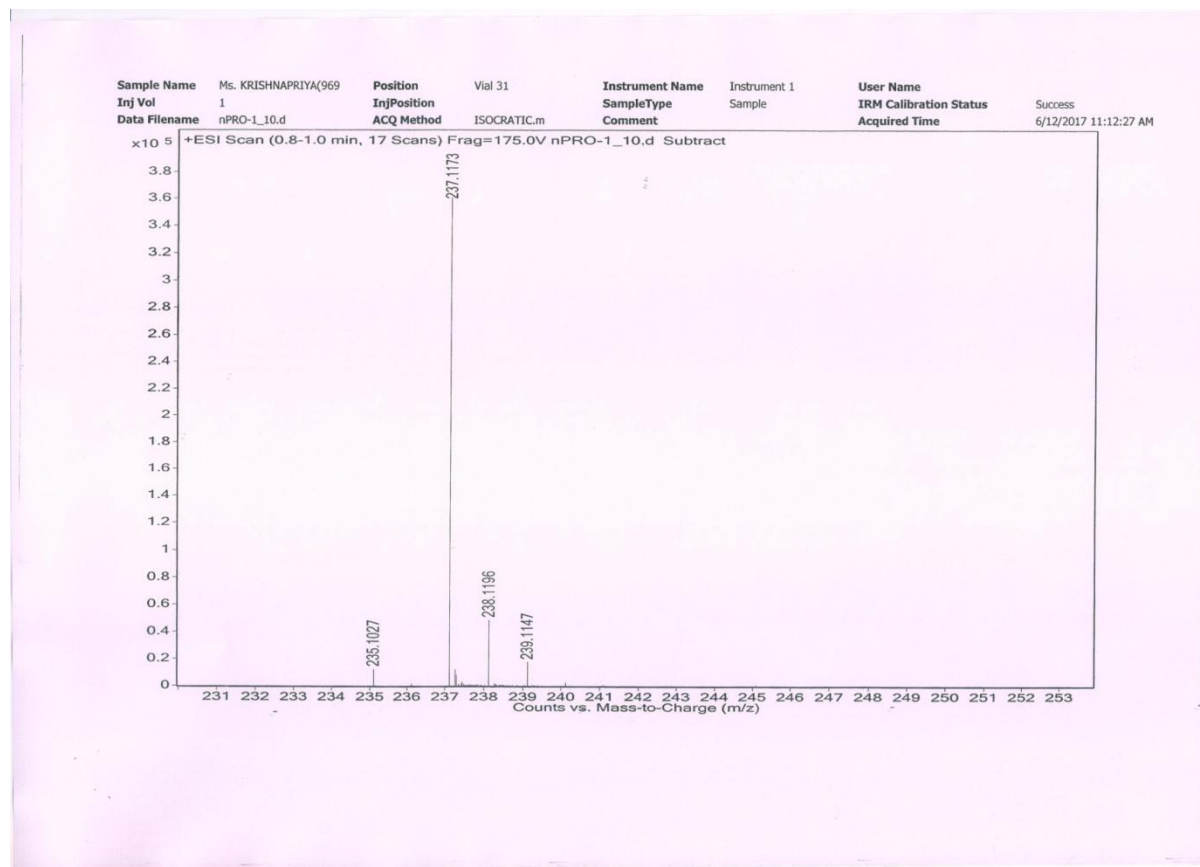


Figure S64. ^1H NMR spectrum of *N*-*n*-butyl)-*N'*-(4-chlorophenylthiocarbamoyl)guanidine (**3g**) (400 MHz, CDCl_3)

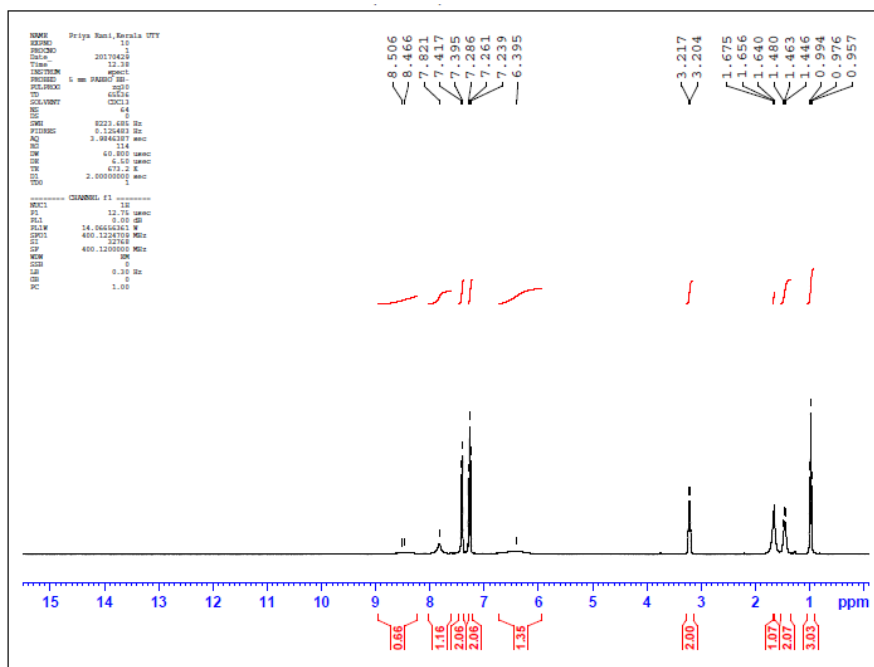


Figure S65. ^1H NMR spectrum (expanded) of *N*-*n*-butyl)-*N'*-(4-chlorophenylthiocarbamoyl)guanidine (**3g**) (400 MHz, CDCl_3)

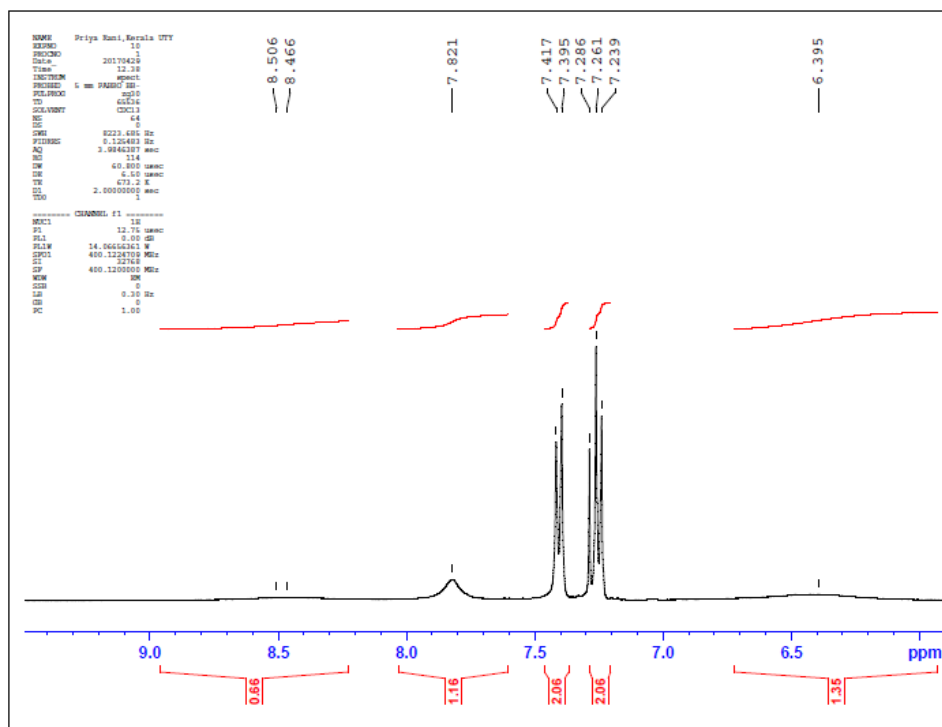


Figure S66. ¹H NMR spectrum (expanded) of *N*-*n*-butyl-*N'*-(4-chlorophenylthiocarbamoyl)guanidine (**3g**) (400 MHz, CDCl₃)

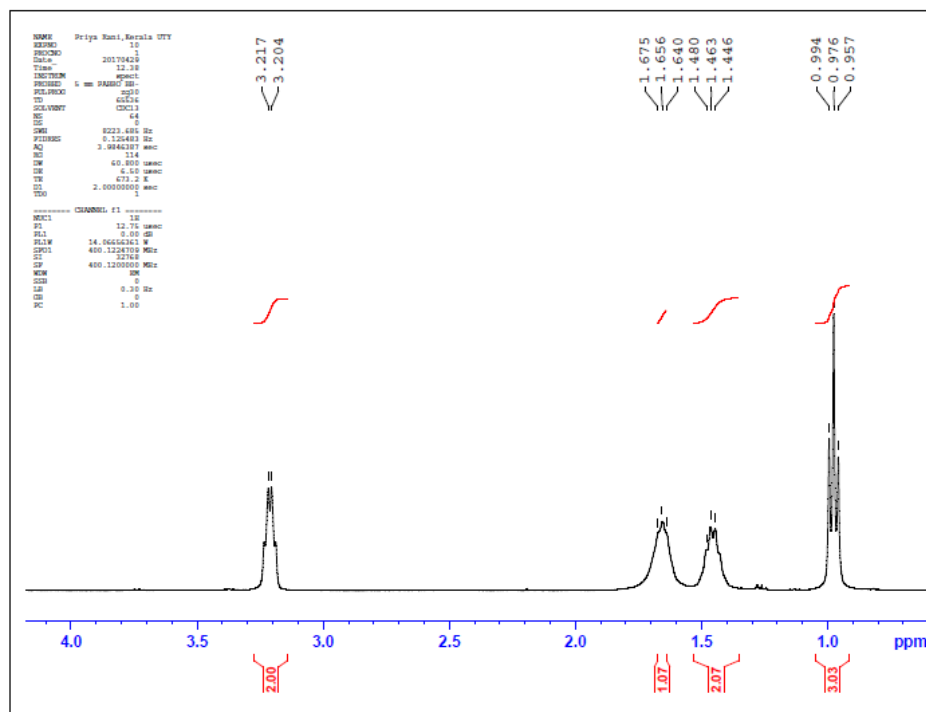


Figure S67. ¹³C NMR spectrum of *N*-*n*-butyl-*N'*-(4-chlorophenylthiocarbamoyl)guanidine (**3g**) (100 MHz, CDCl₃)

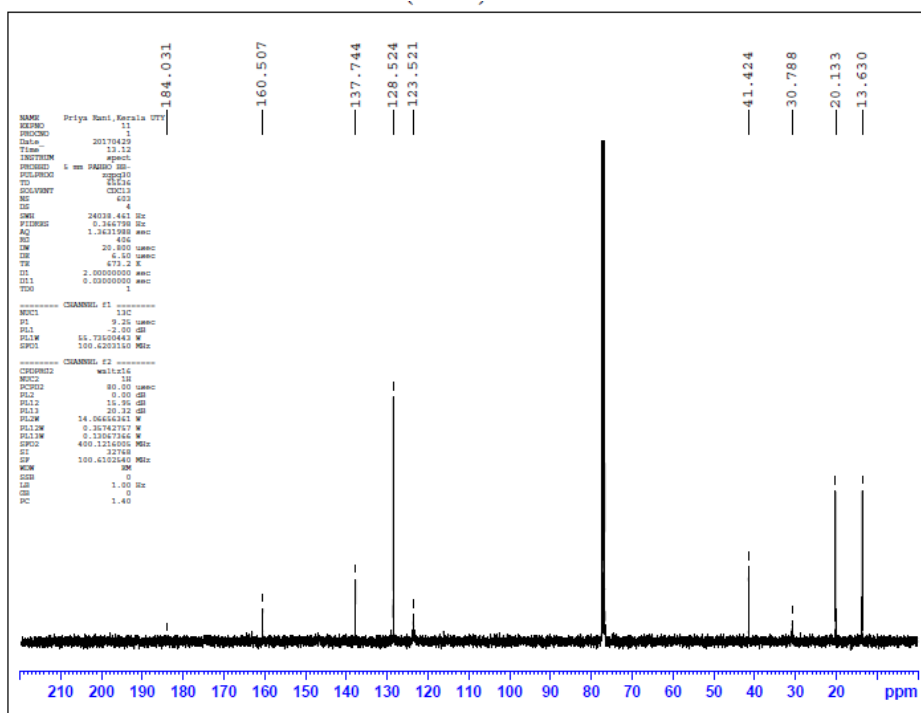


Figure S68. ESI-HRMS spectrum of *N*-n-butyl)-*N'*-(4-chlorophenylthiocarbamoyl)guanidine (3g)

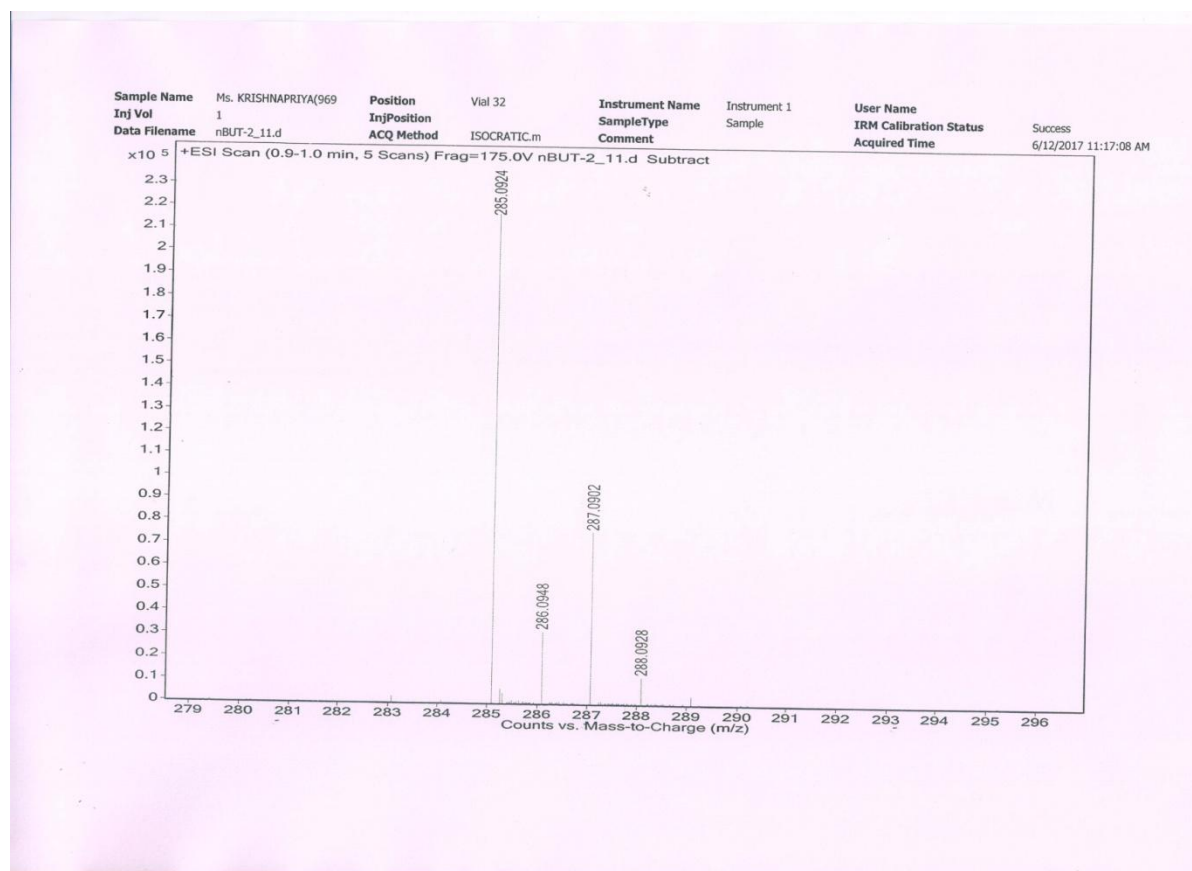


Figure S69. ^1H NMR spectrum of *N*-benzyl-*N'*-(phenylthiocarbamoyl)guanidine (**3h**) (400 MHz, CDCl_3)

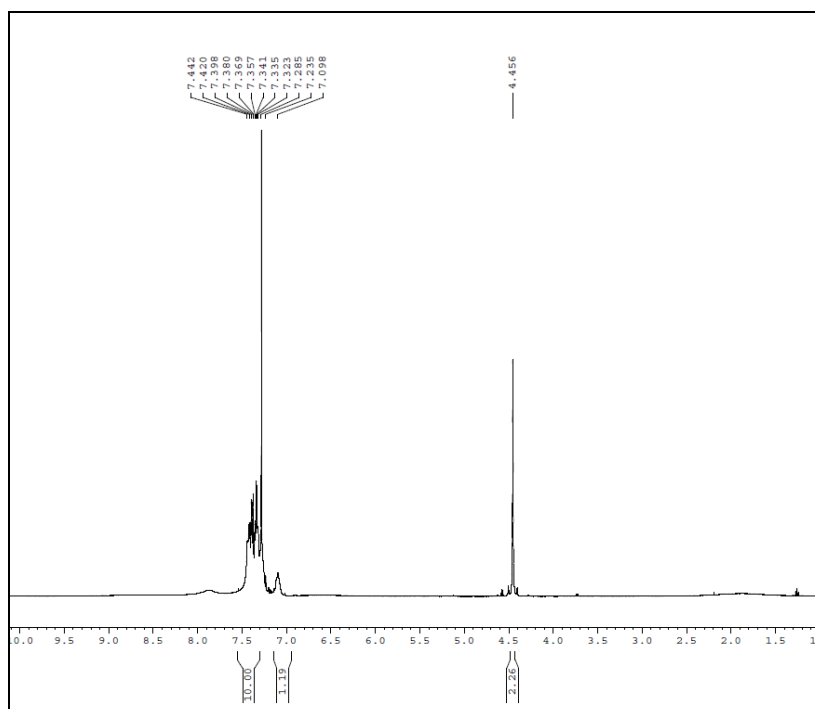


Figure S70. ^1H NMR spectrum (expanded) of *N*-benzyl-*N'*-(phenylthiocarbamoyl)guanidine (**3h**) (400 MHz, CDCl_3)

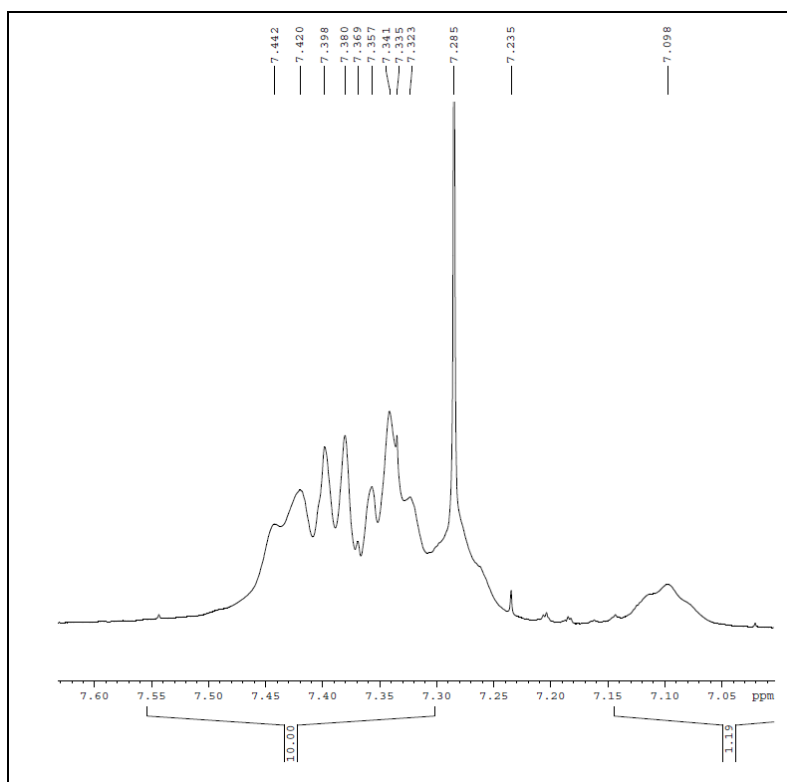


Figure S71. ¹³C NMR spectrum of *N*-benzyl-*N'*-(phenylthiocarbamoyl)guanidine (**3h**) (100 MHz, CDCl₃)

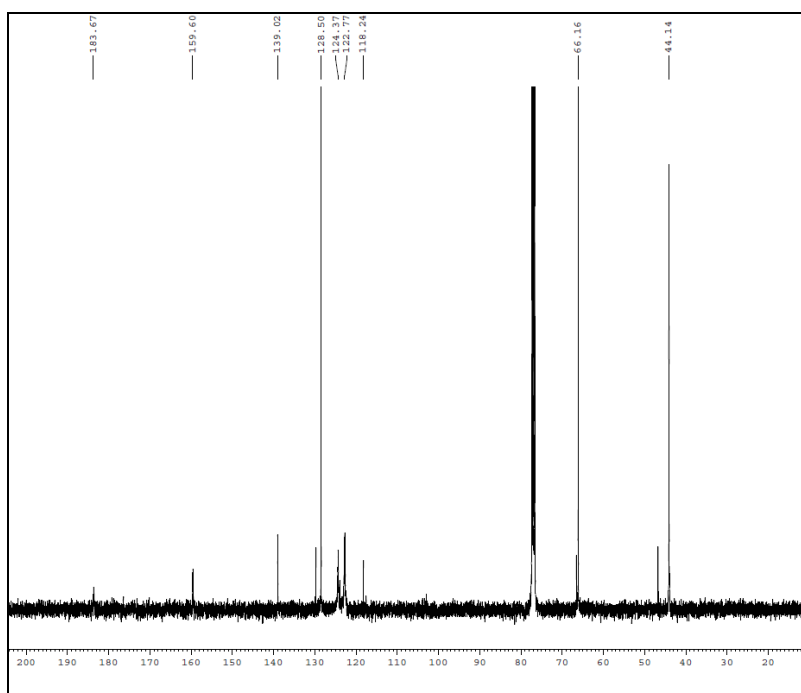


Figure S72. ESI-HRMS spectrum of *N*-benzyl-*N'*-(phenylthiocarbamoyl)guanidine (**3h**)

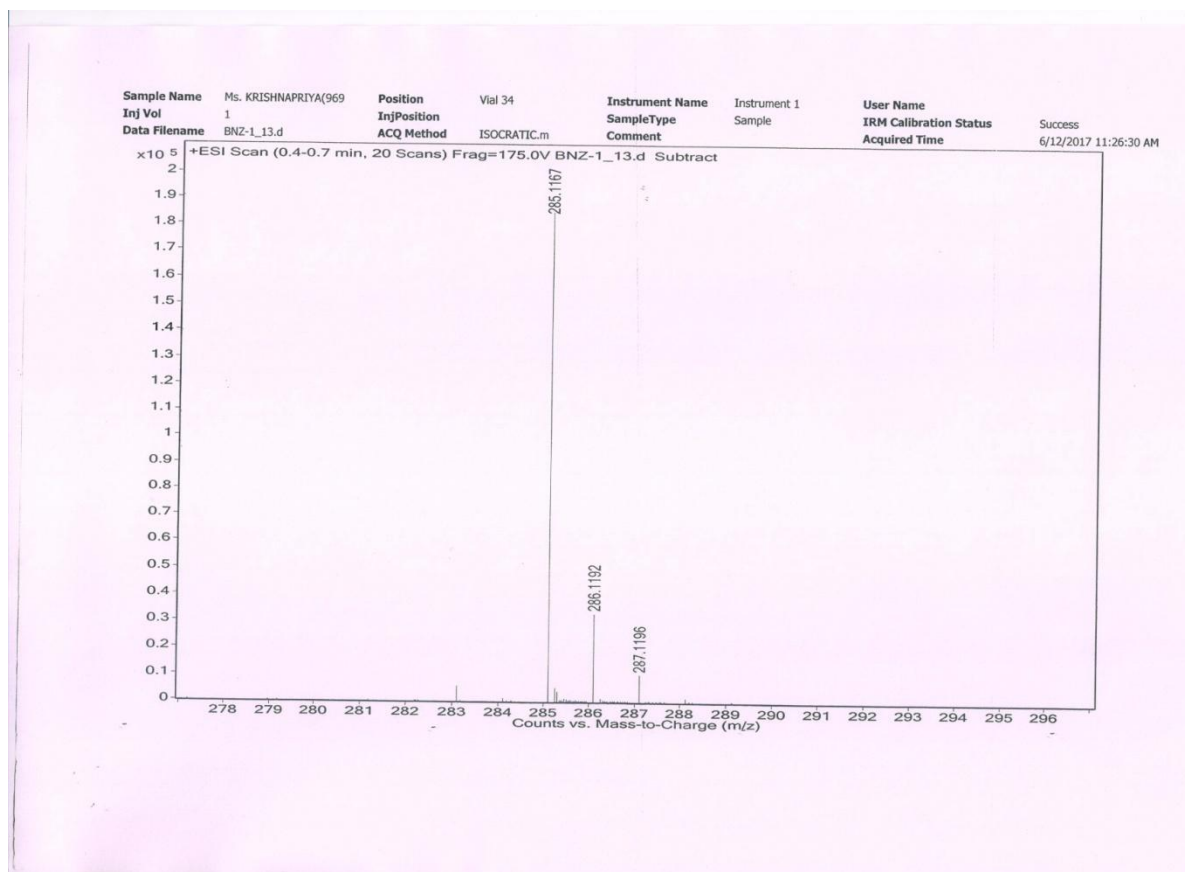


Figure S73. ^1H NMR spectrum of *N*-cyclohexyl-*N'*-(3-methoxyphenylthiocarbamoyl)guanidine (**3i**) (400 MHz, CDCl_3)

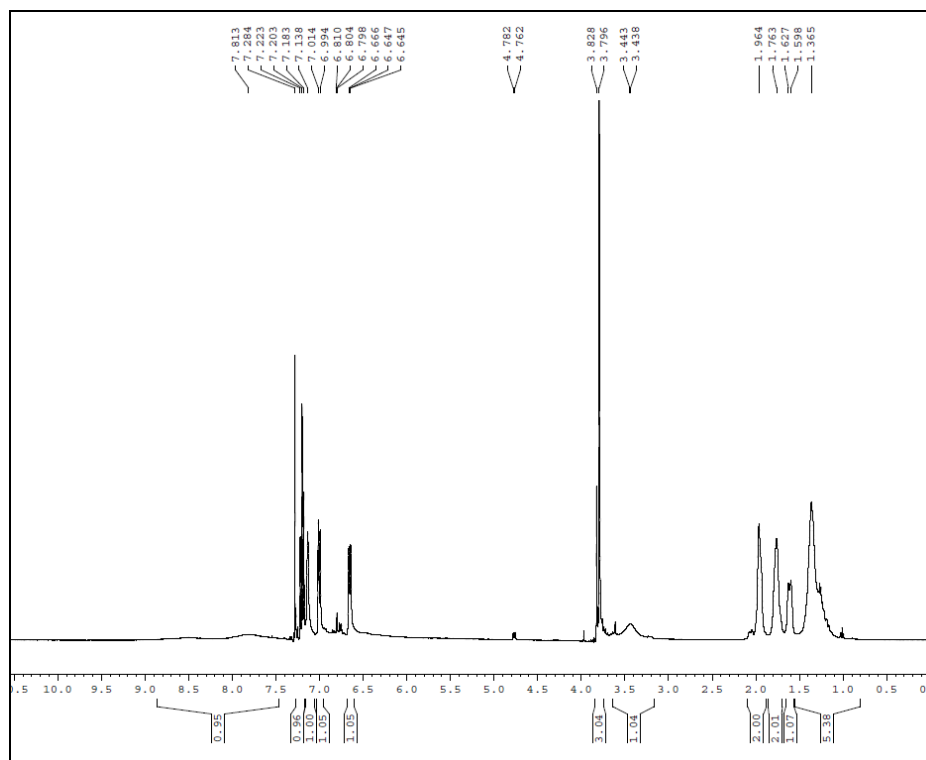


Figure S74. ^1H NMR spectrum (expanded) of *N*-cyclohexyl-*N'*-(3-methoxyphenyl)thiocarbamoylguanidine (**3i**) (400 MHz, CDCl_3)

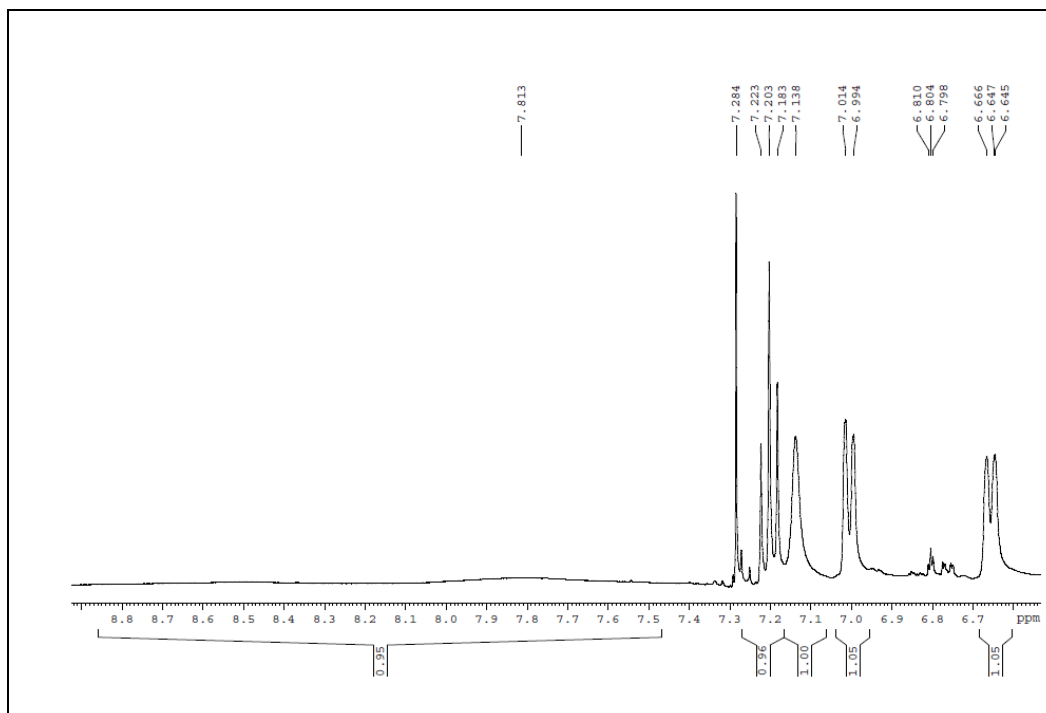


Figure S75. ^{13}C NMR spectrum of *N*-cyclohexyl-*N'*-(3-methoxyphenylthiocarbamoyl)guanidine (**3i**) (100 MHz, CDCl_3)

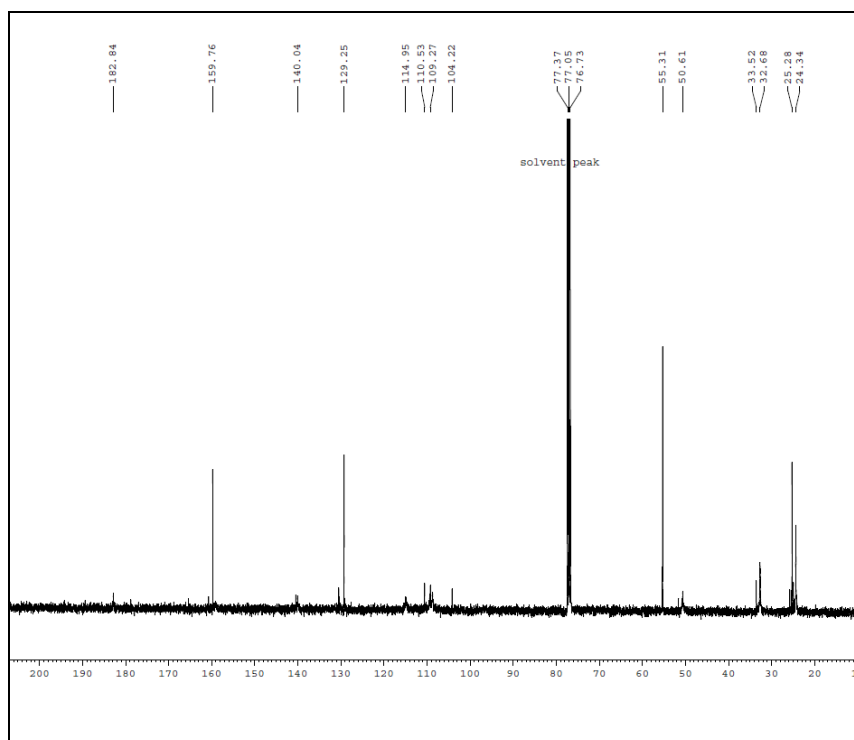


Figure S76. ESI-HRMS spectrum of *N*-cyclohexyl-*N'*-(3-methoxyphenylthiocarbamoyl) guanidine (**3i**)

