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

Table of Contents

1. ^{1}H, ^{13}C and HRMS spectra of compound **2a** S2-S3

2. ^{1}H, ^{13}C and HRMS spectra of compound **2b** S4-S5

3. ^{1}H, ^{13}C and HRMS spectra of compound **2c** S6-S9

4. ^{1}H, ^{13}C and HRMS spectra of compound **2d** S10-S12

5. ^{1}H, ^{13}C and HRMS spectra of compound **2e** S12-S14

6. ^{1}H, ^{13}C and HRMS spectra of compound **2f** S14-S16

7. ^{1}H, ^{13}C and HRMS spectra of compound **2g** S16-S18

8. ^{1}H, ^{13}C and HRMS spectra of compound **2h** S18-S20

9. ^{1}H, ^{13}C and HRMS spectra of compound **2i** S20-S22

10. ^{1}H, ^{13}C and HRMS spectra of compound **3a** S22-S24

11. ^{1}H, ^{13}C and HRMS spectra of compound **3b** S24-S26

12. ^{1}H, ^{13}C and HRMS spectra of compound **3c** S27-S28

13. ^{1}H, ^{13}C and HRMS spectra of compound **3d** S29-S30

14. ^{1}H, ^{13}C and HRMS spectra of compound **3e** S31-S32

15. ^{1}H, ^{13}C and HRMS spectra of compound **3f** S33-S35

16. ^{1}H, ^{13}C and HRMS spectra of compound **3g** S36-S38

17. ^{1}H, ^{13}C and HRMS spectra of compound **3h** S39-S40

18. ^{1}H, ^{13}C and HRMS spectra of compound **3i** S41-S42

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

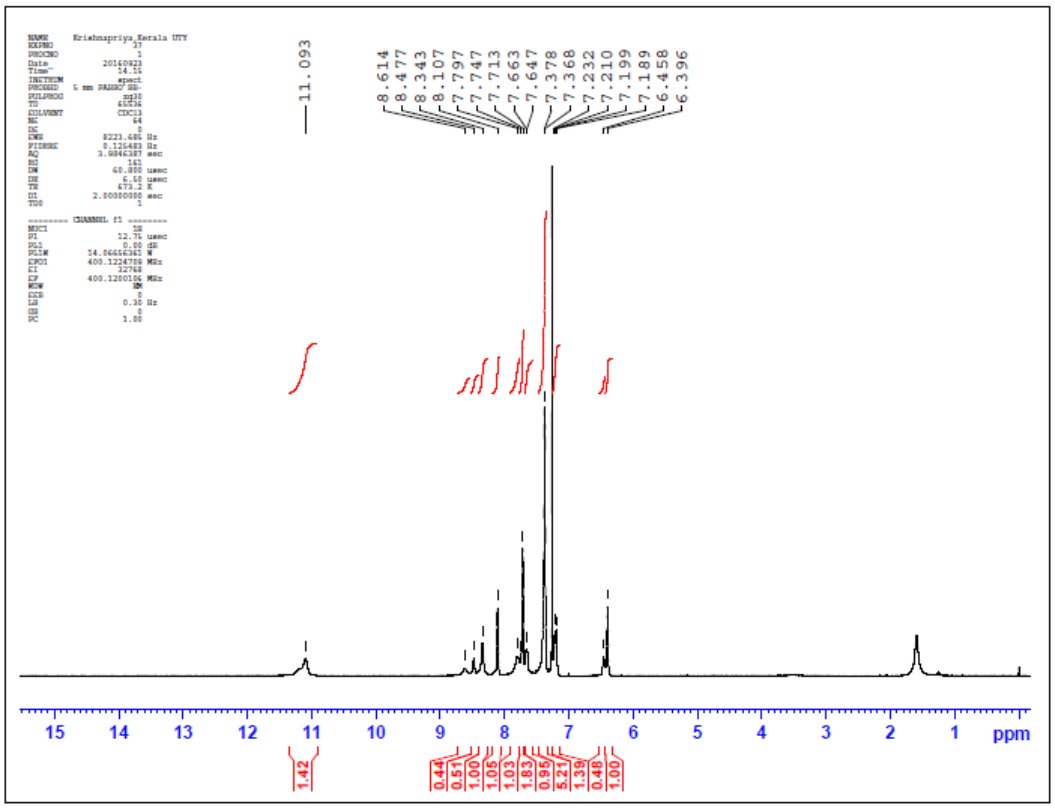
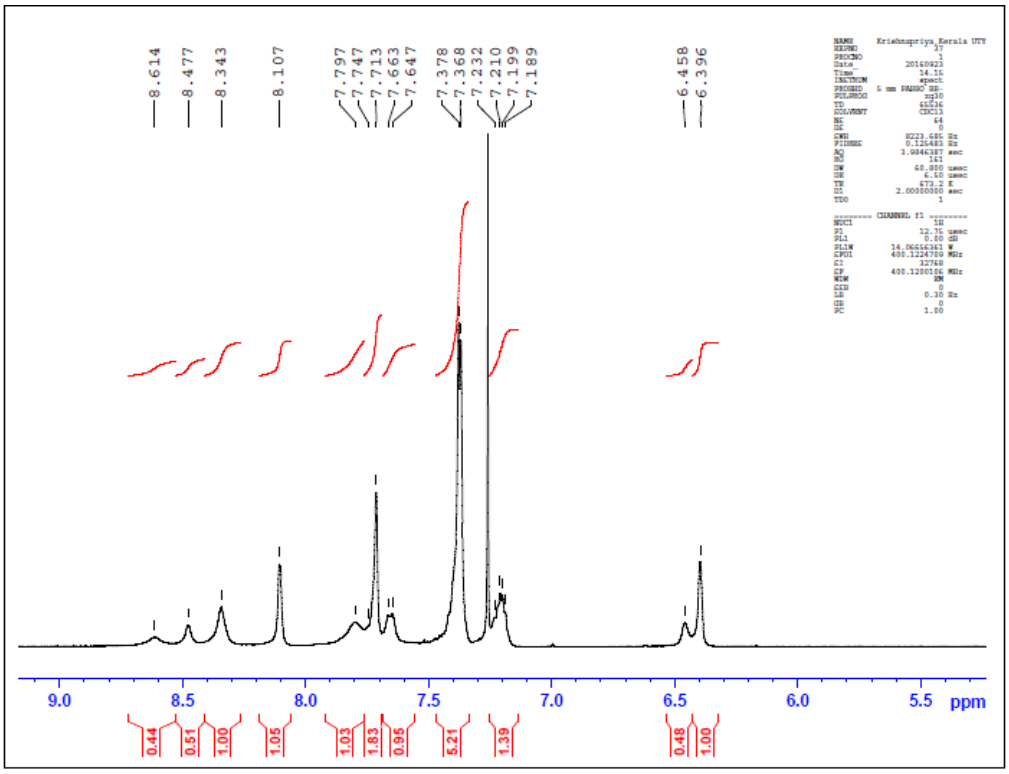


Figure S2. ^{1}H NMR spectrum (expanded) of 1-[(*N*-phenylthiocarbamoyl)amidino]pyrazole **(2a)** (400MHz, $CDCl_3$)



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

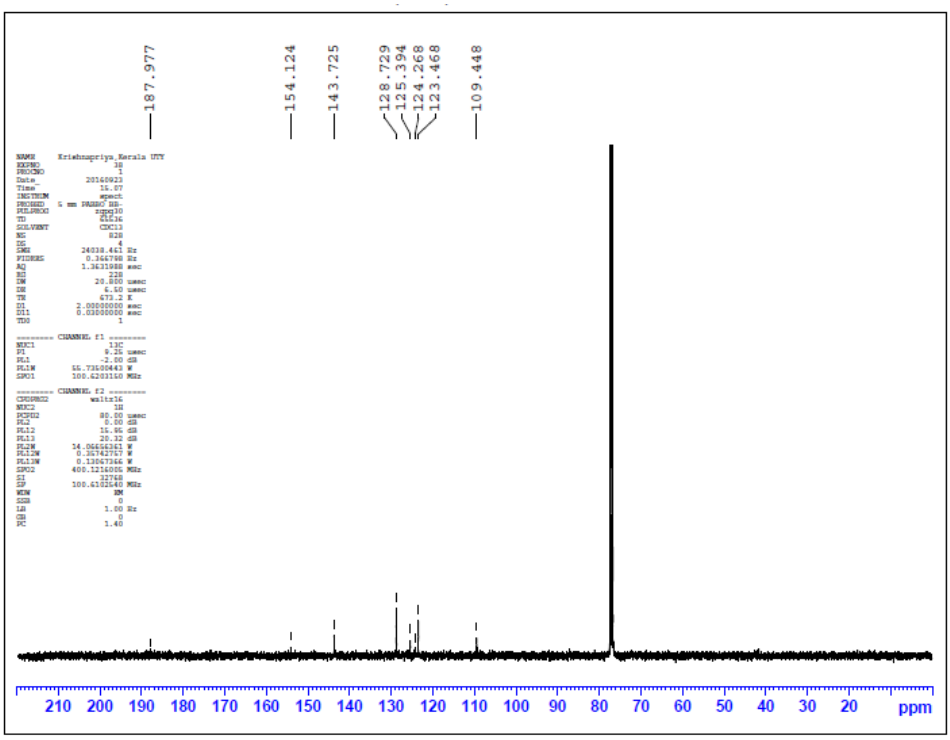
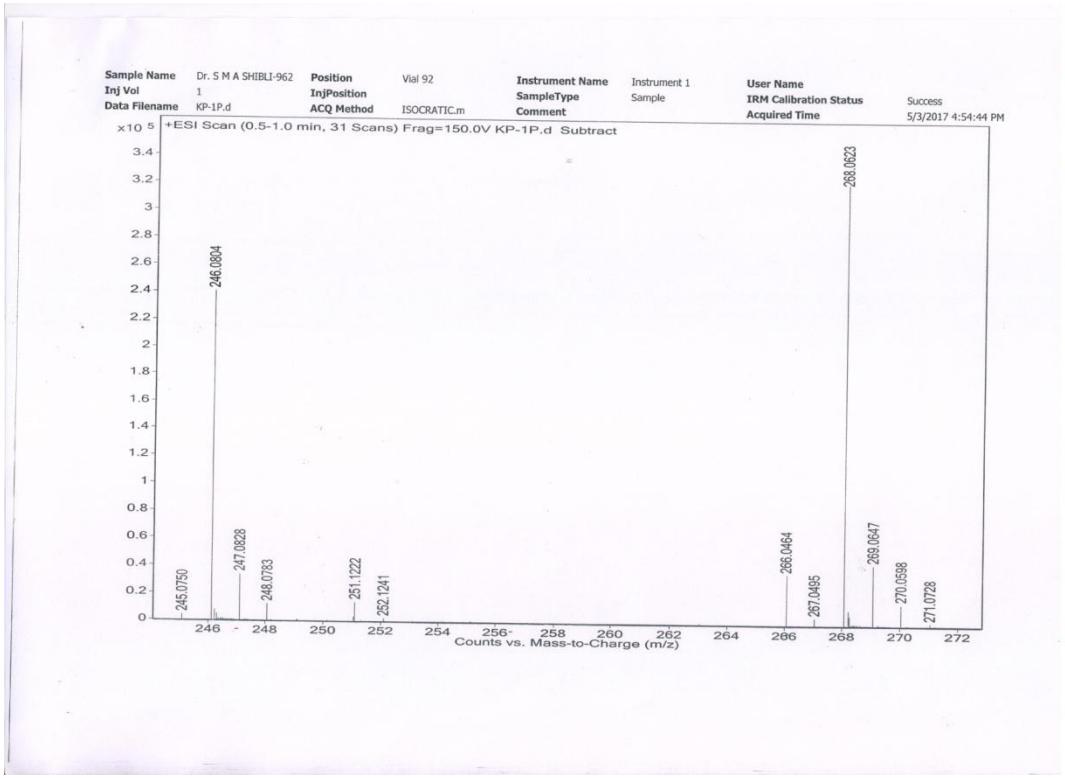


Figure S4. ESI-HRMS spectrum of 1-[(*N*-phenylthiocarbamoyl)amidino]pyrazole **(2a)**



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

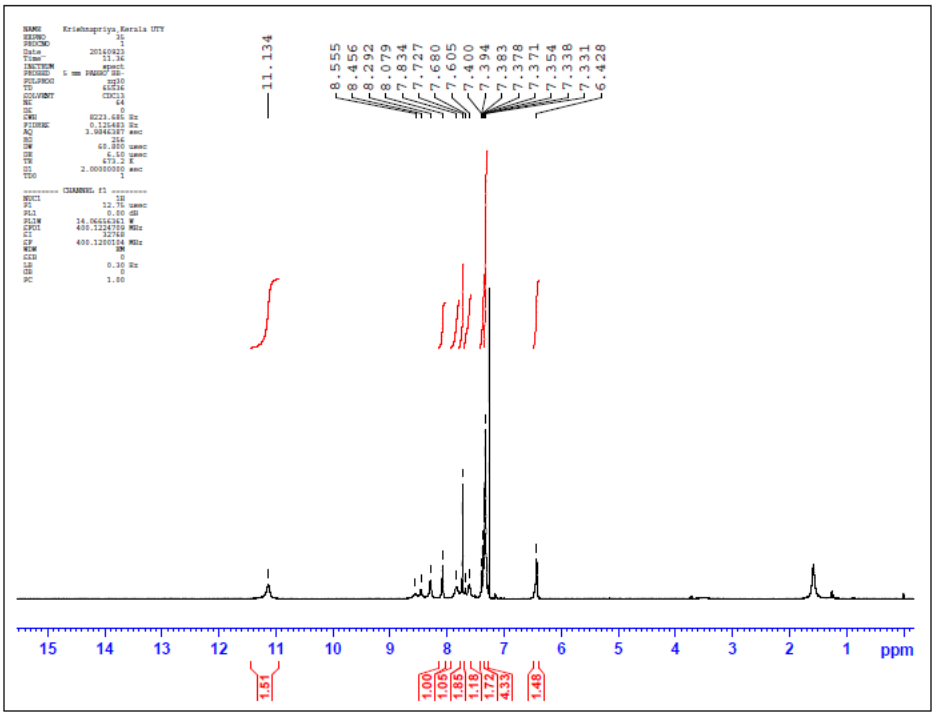
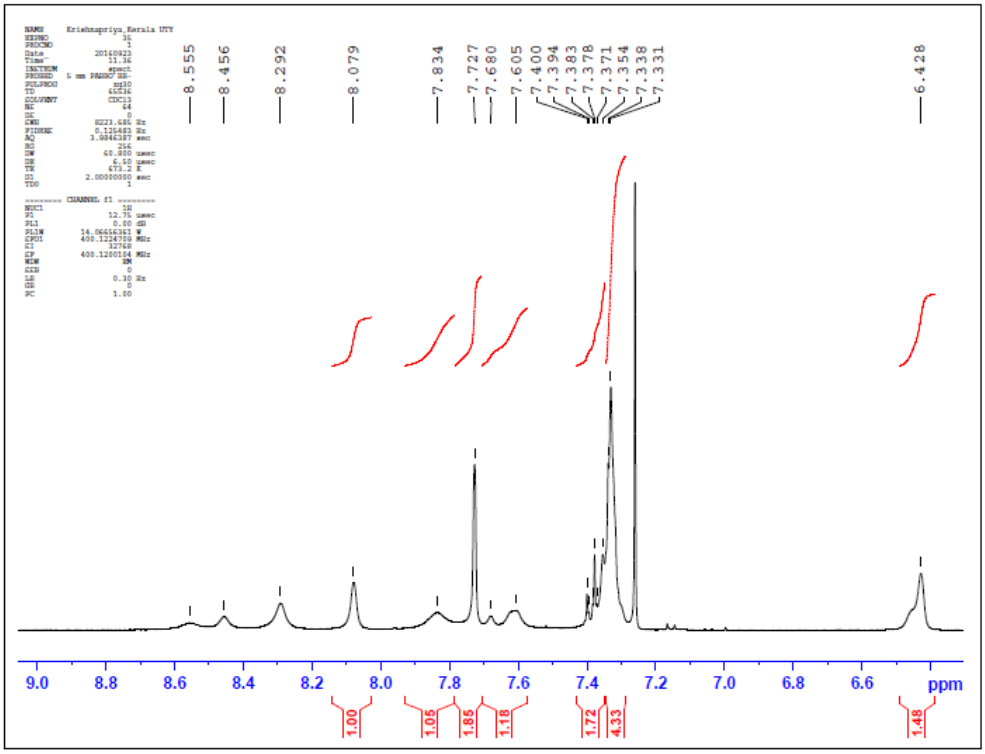


Figure S6. ^{1}H NMR spectrum (expanded) of 1-[(*N*-4-chlorophenylthiocarbamoyl) amidino]pyrazole (**2b)** (400 MHz, $CDCl_3$)



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

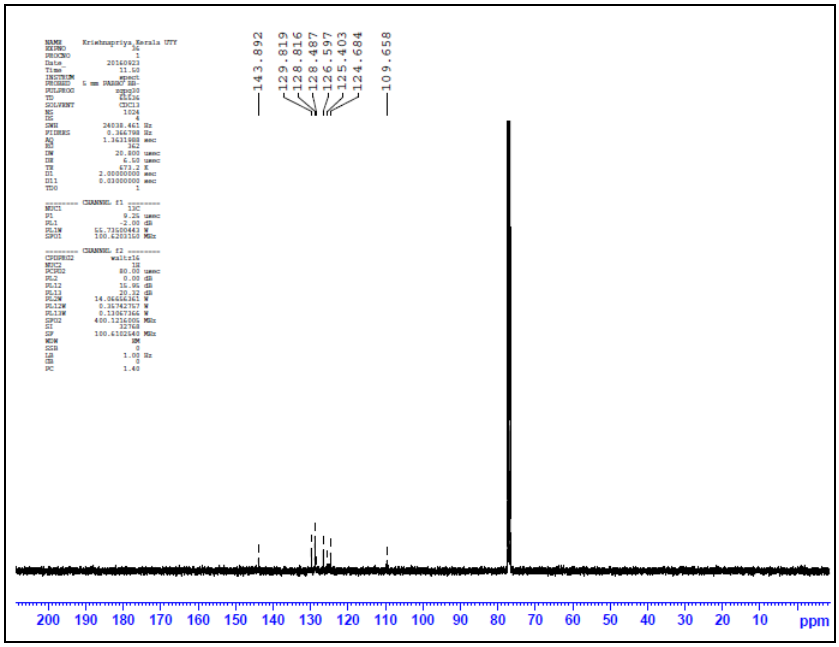
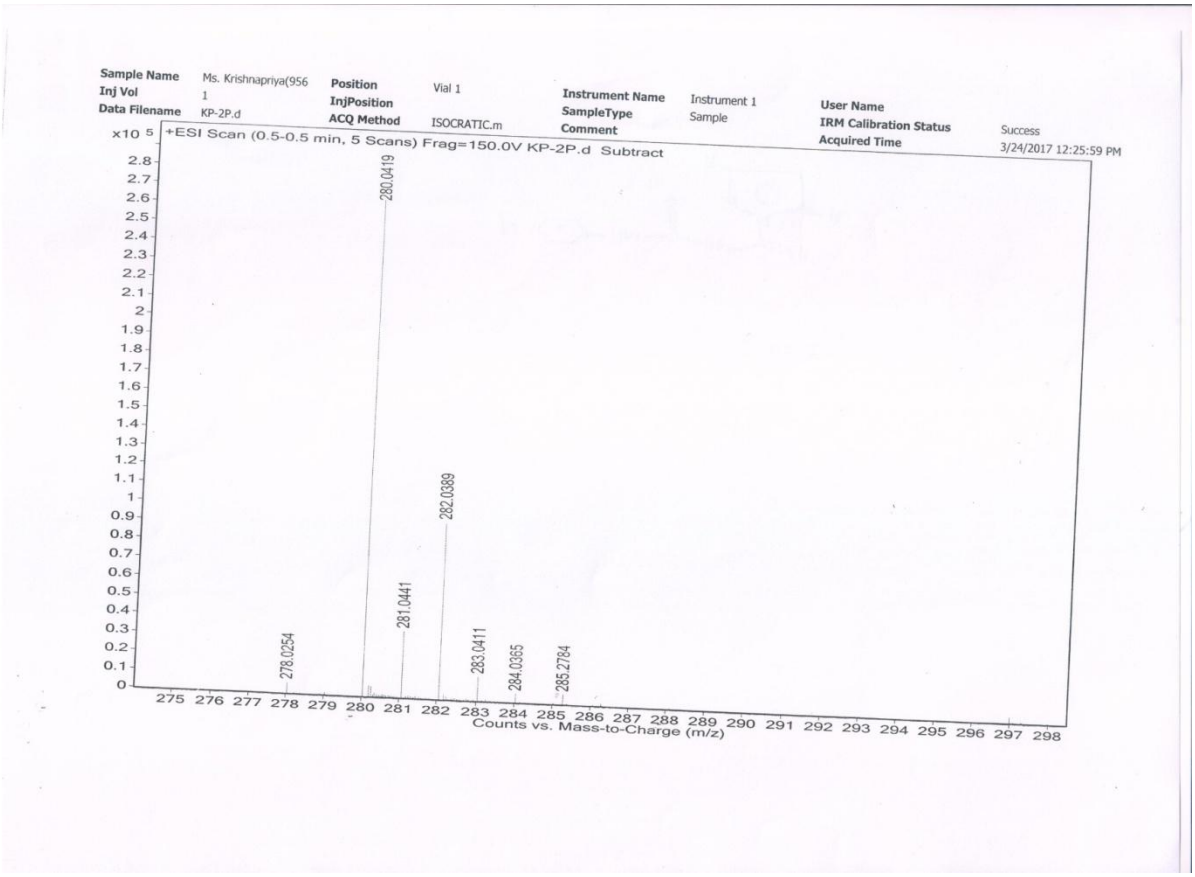


Figure S8. ESI-HRMS spectrum of 1-[(*N*-4-chlorophenylthiocarbamoyl)amidino]pyrazole **(2b)**



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

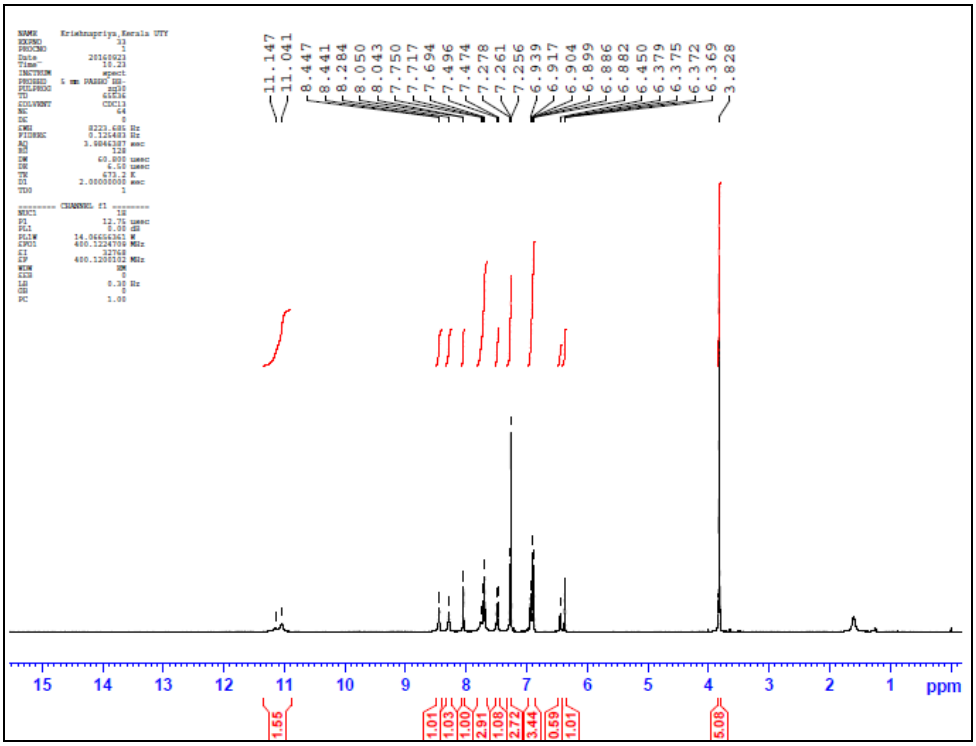
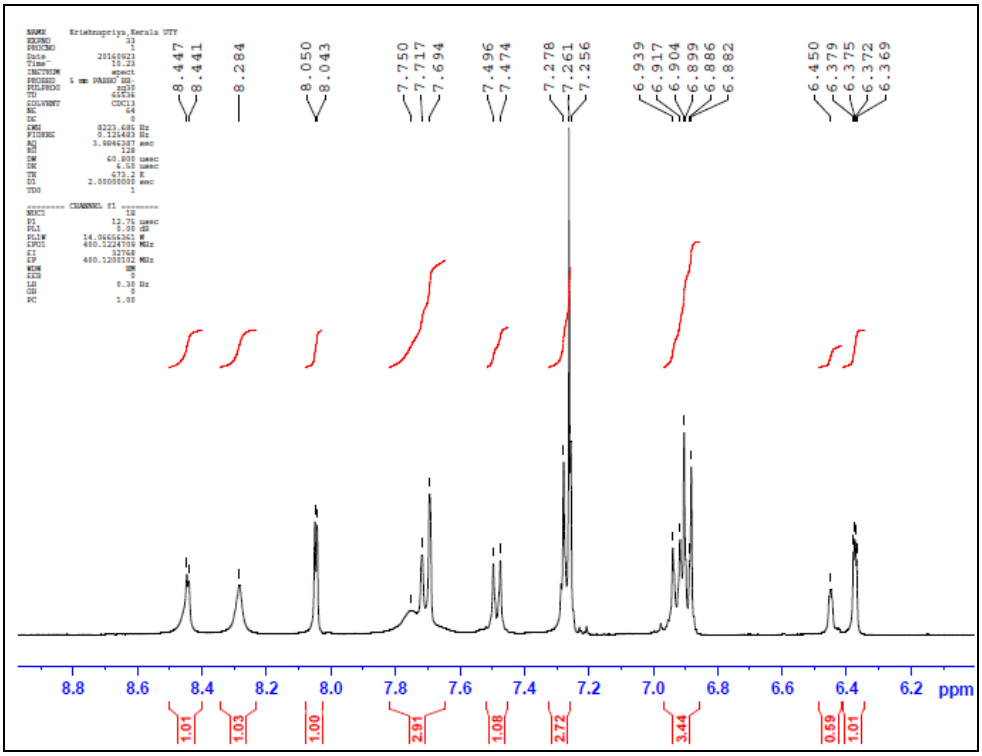


Figure S10. ^{1}H NMR spectrum (expanded) of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino] pyrazole **(2c)** (400 MHz, $CDCl_3$)



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

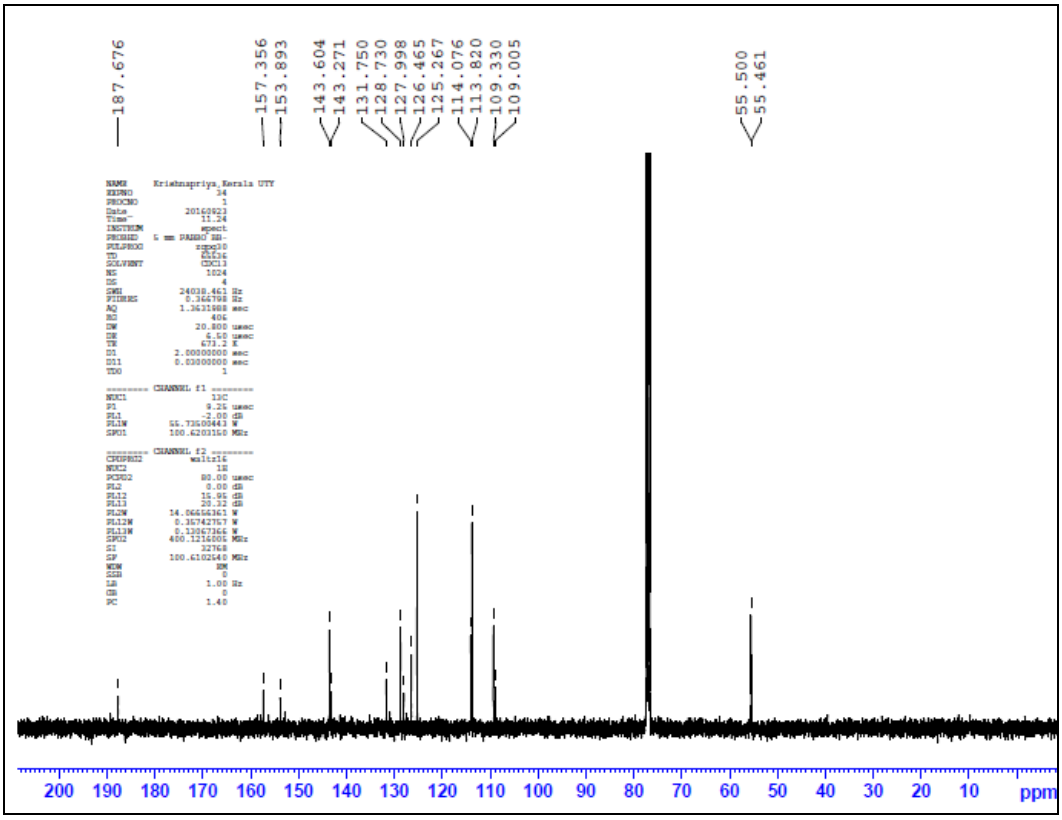
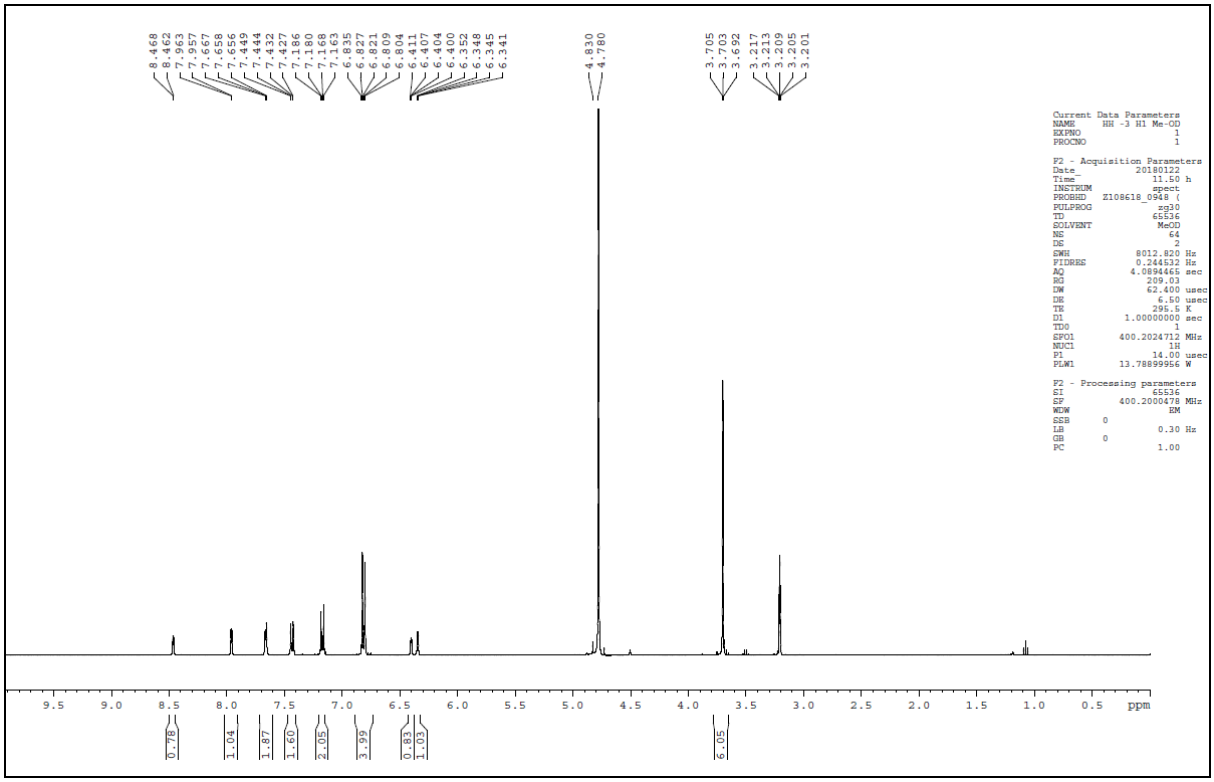


Figure S12. ^{1}H NMR spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrazole **(2c)** (400 MHz, CD_3OD)



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

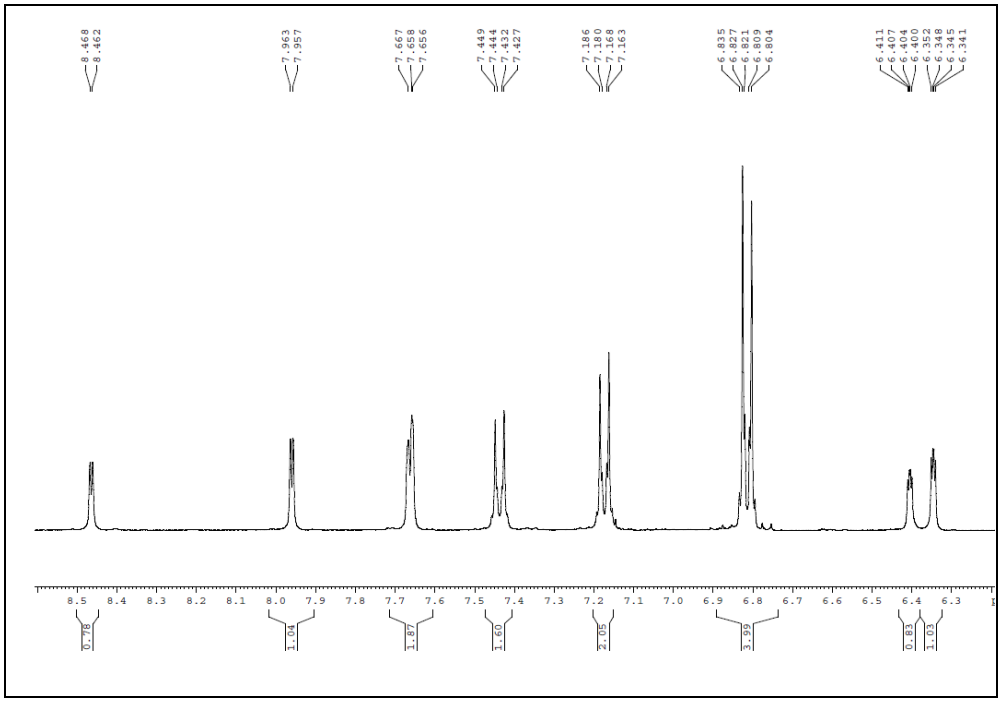
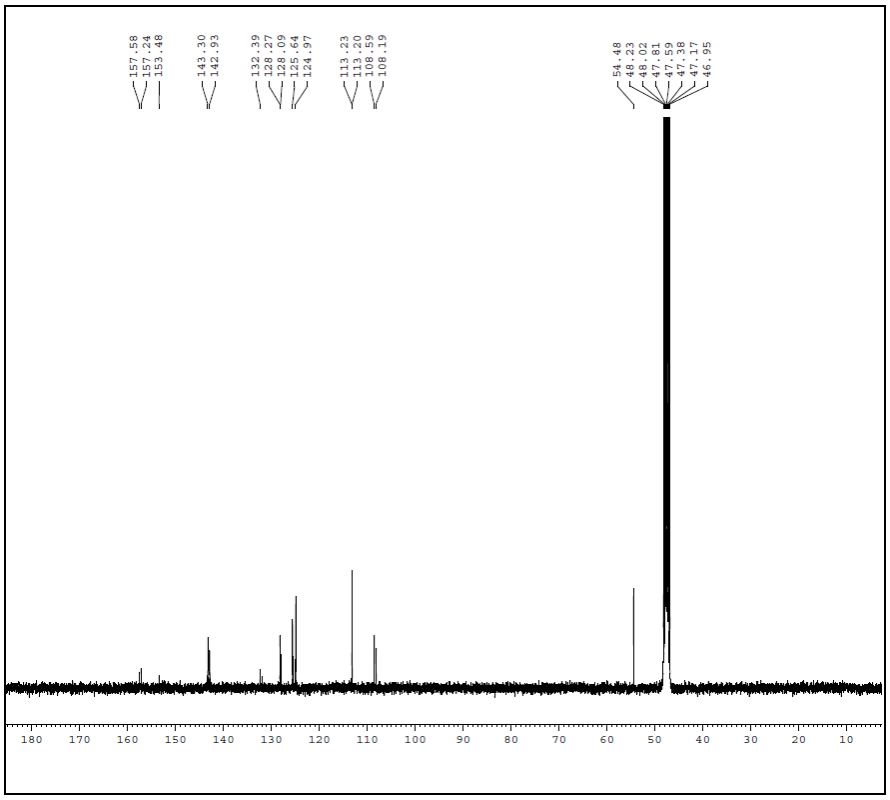
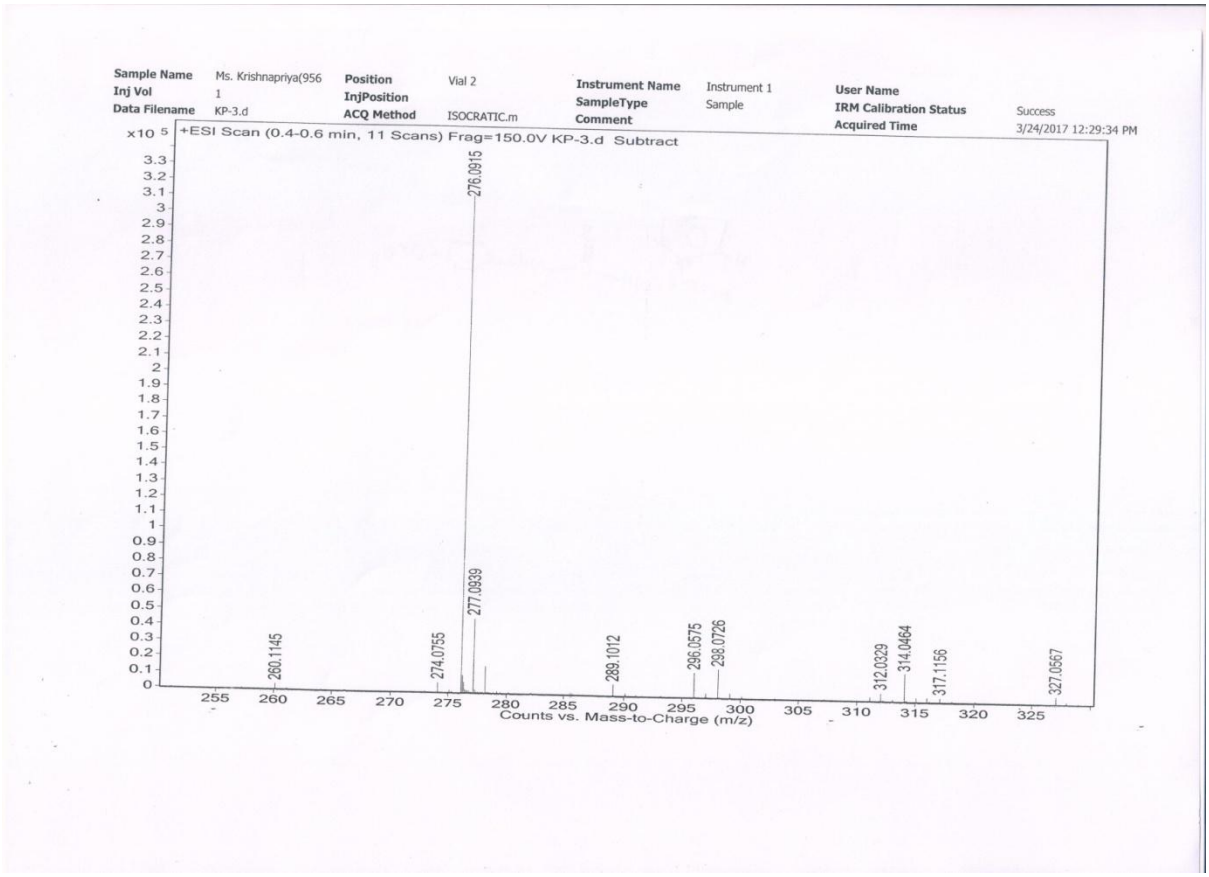


Figure S14. ^{13}C NMR spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrazole **(2c)** (100 MHz, CD_3OD)



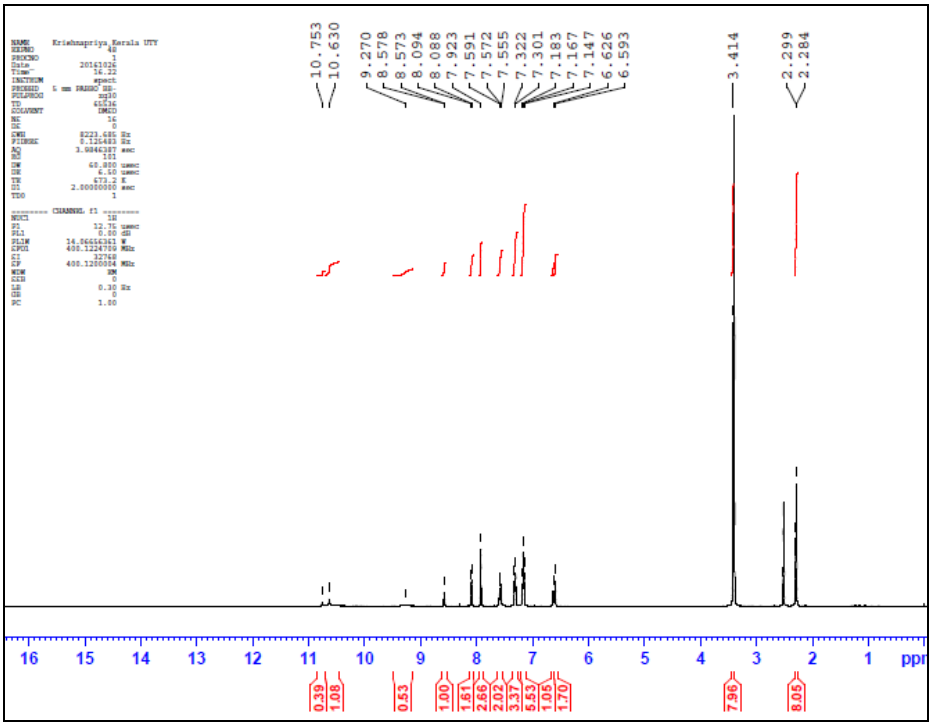
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Figure S15. ESI-HRMS spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrazole **(2c)**



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



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

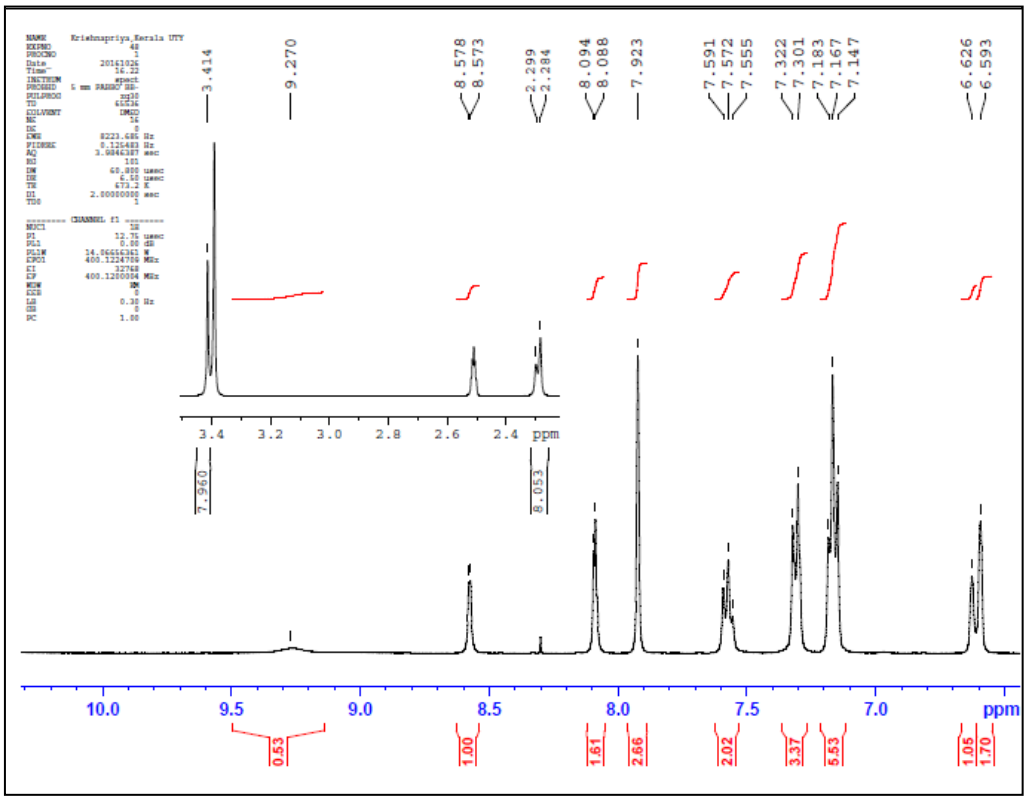


Figure S18. ^{13}C NMR spectrum of 1-[(*N*-4-methylphenylthiocarbamoyl)amidino]pyrazole **(2d**) (100 MHz, DMSO-d_6)

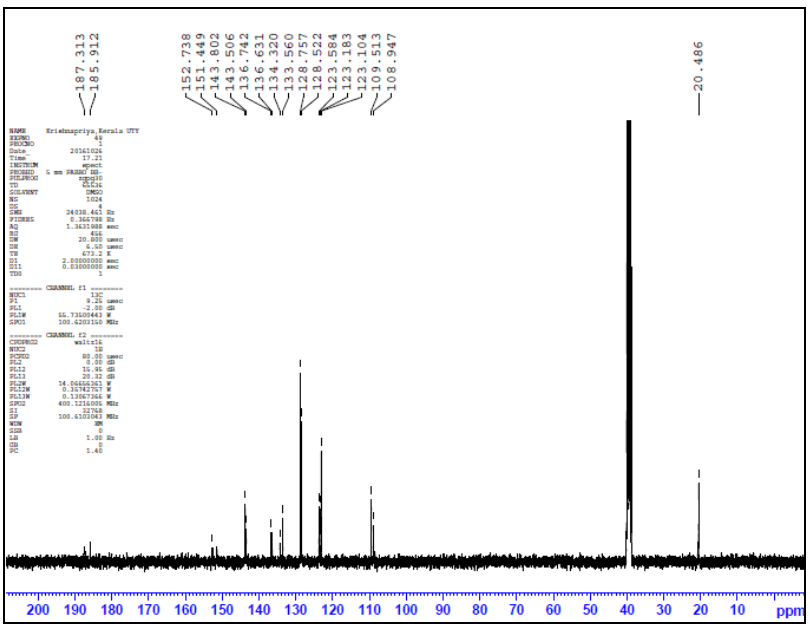


Figure S19. ESI-HRMS spectrum of 1-[(*N*-4-methylphenylthiocarbamoyl)amidino]pyrazole **(2d)**

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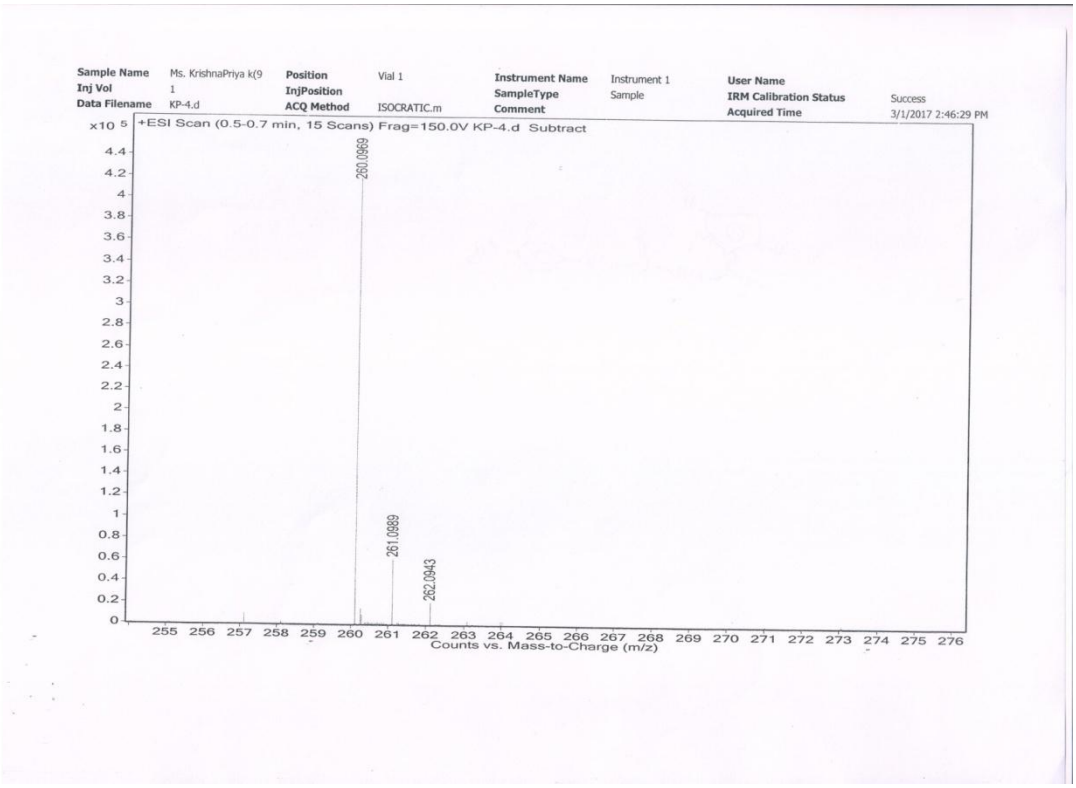


Figure S20. ^{1}H NMR spectrum of 1-[(*N*-3-methoxyphenylthiocarbamoyl)amidino]pyrazole (**2e)** (400 MHz, $CDCl_3$)

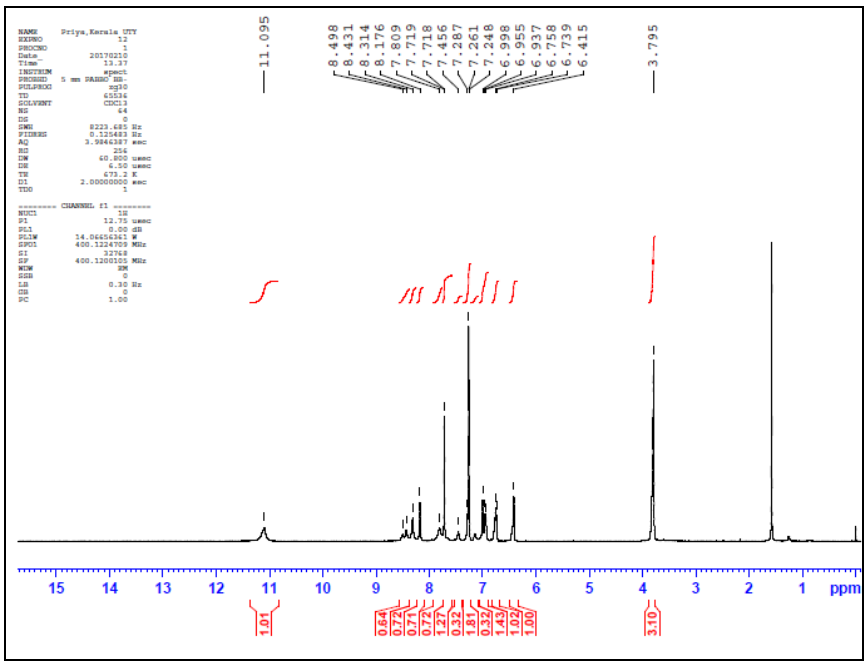


Figure S21. ^{1}H NMR spectrum (expanded) of 1-[(*N*-3-methoxyphenylthiocarbamoyl) amidino]pyrazole (**2e)** (400 MHz, $CDCl_3$)

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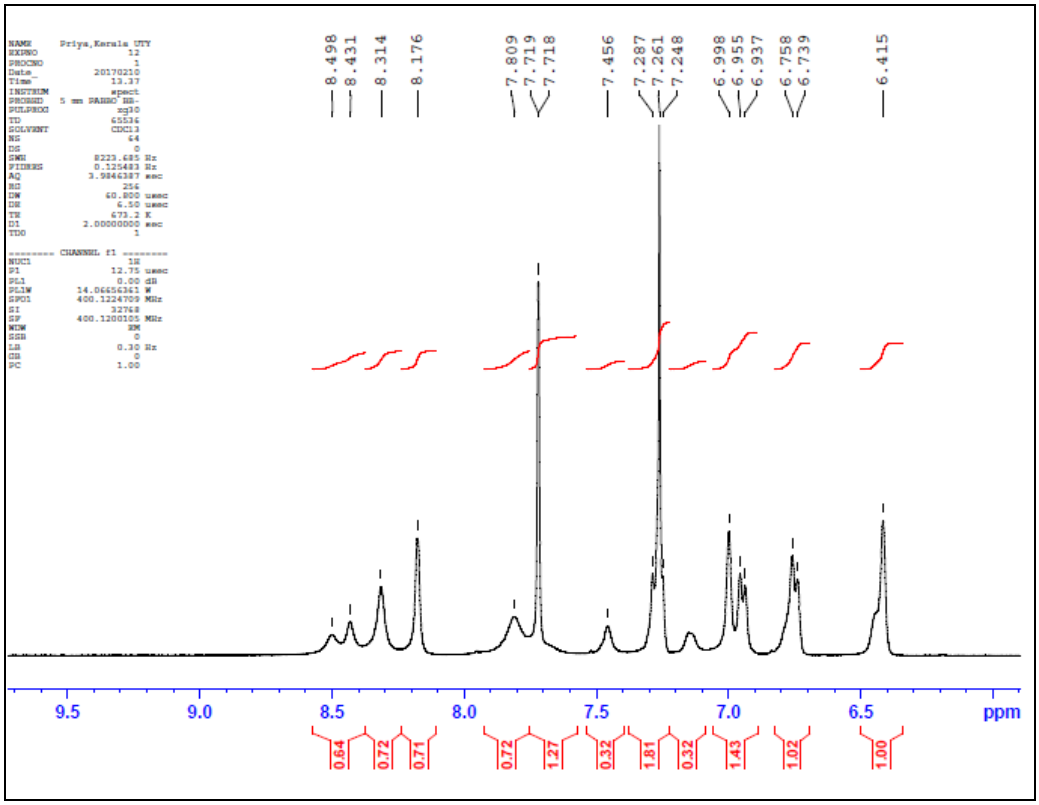


Figure S22. ^{13}C NMR spectrum of 1-[(*N*-3-methoxyphenylthiocarbamoyl)amidino]pyrazole (**2e)** (100 MHz, $CDCl_3$)

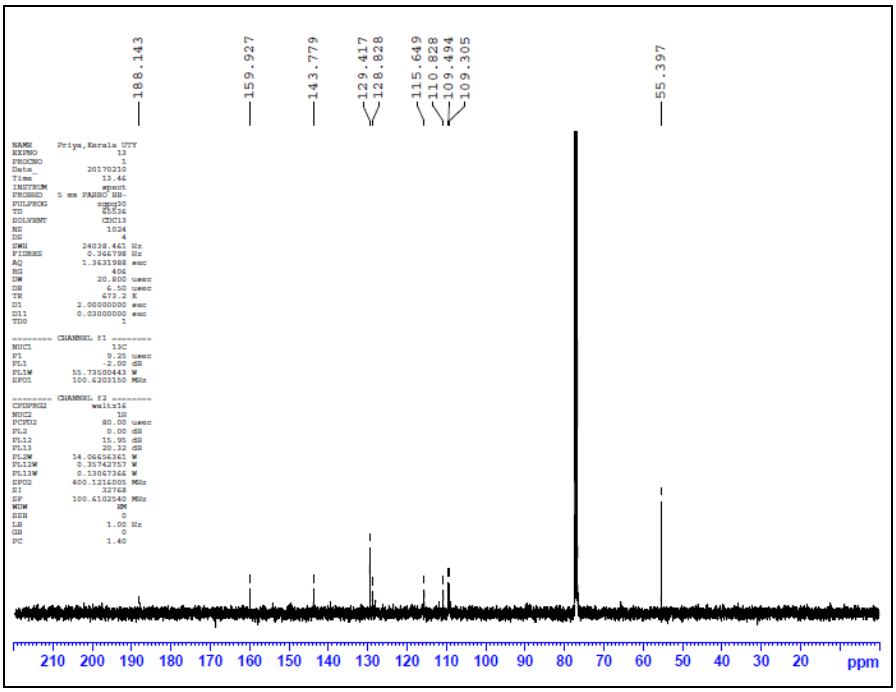


Figure S23. ESI-HRMS spectrum of 1-[(*N*-3-methoxyphenylthiocarbamoyl)amidino]pyrazole (**2e)**

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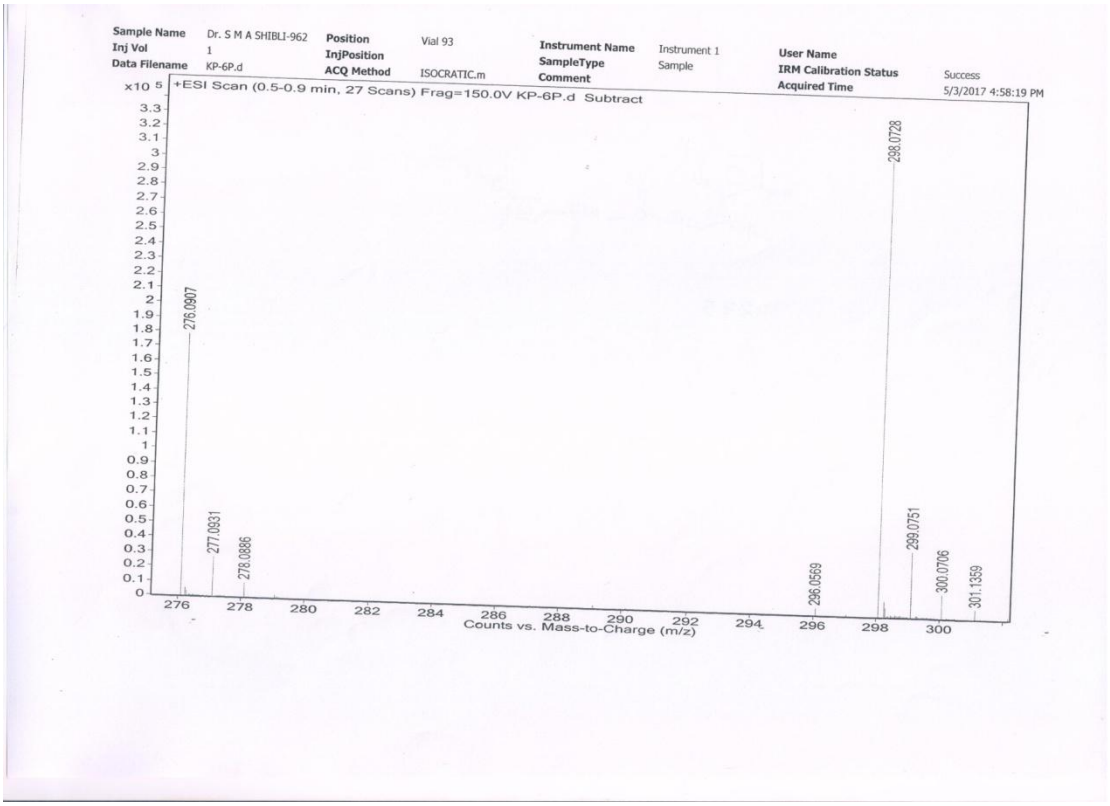


Figure S24. ^{1}H NMR spectrum of 1-[(*N*-4-bromophenylthiocarbamoyl)amidino]pyrazole (**2f)** (400 MHz, $CDCl_3$)

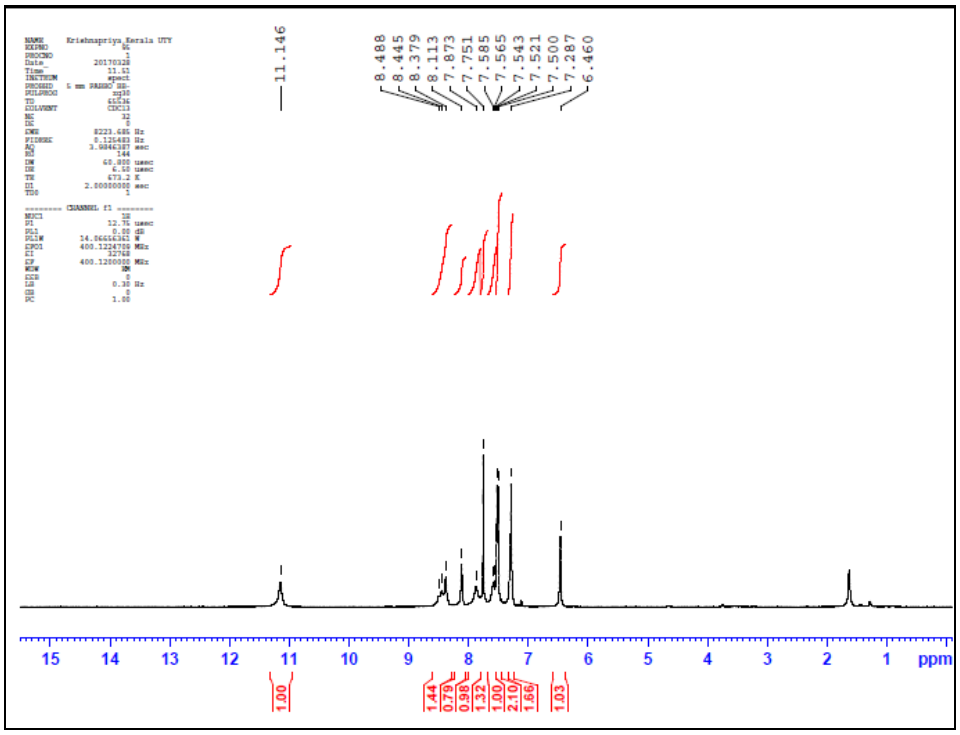


Figure S25. ^{1}H NMR spectrum (expanded) of 1-[(*N*-4-bromophenylthiocarbamoyl) amidino]pyrazole (**2f)** (400 MHz, $CDCl_3$)

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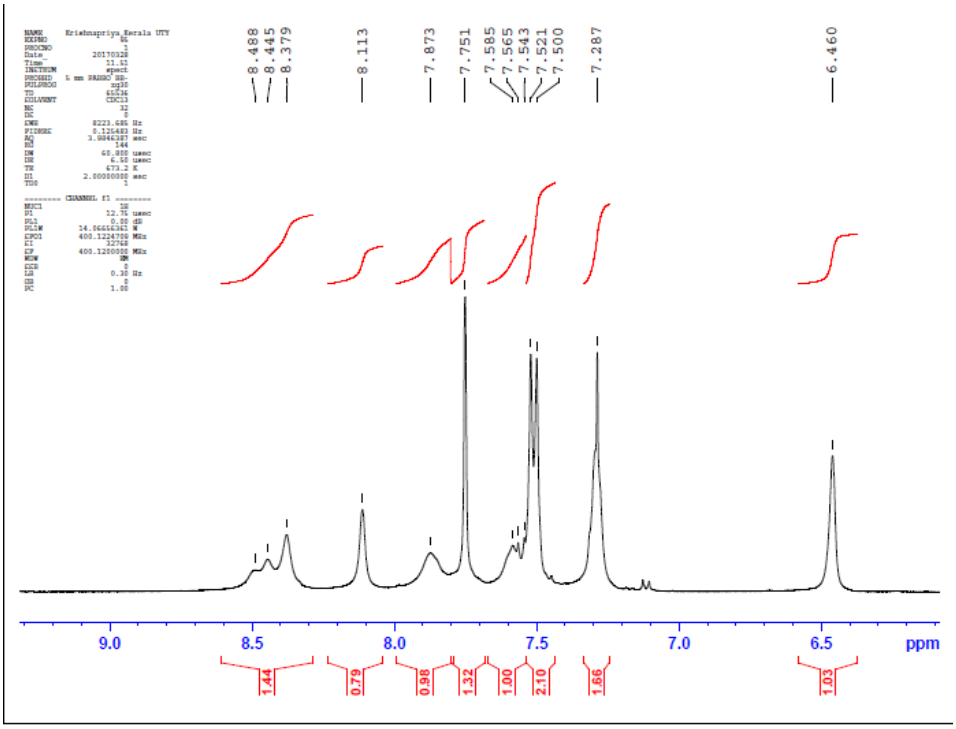


Figure S26. ^{13}C NMR spectrum (expanded) of 1-[(*N*-4-bromophenylthiocarbamoyl) amidino]pyrazole (**2f)** (100 MHz, $CDCl_3$)

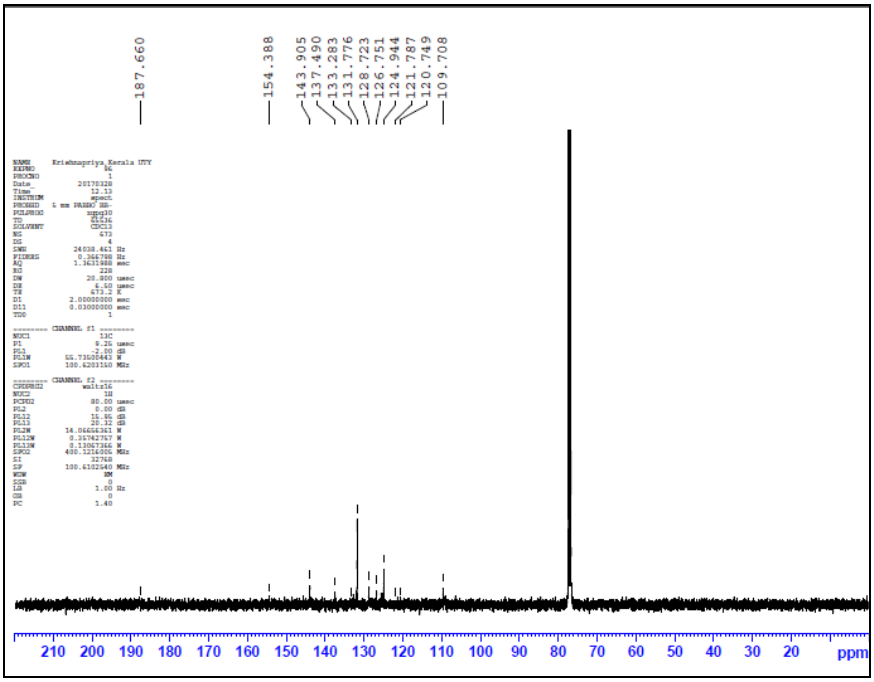


Figure S27. ESI-HRMS spectrum of 1-[(*N*-4-bromophenylthiocarbamoyl)amidino]pyrazole (**2f)**

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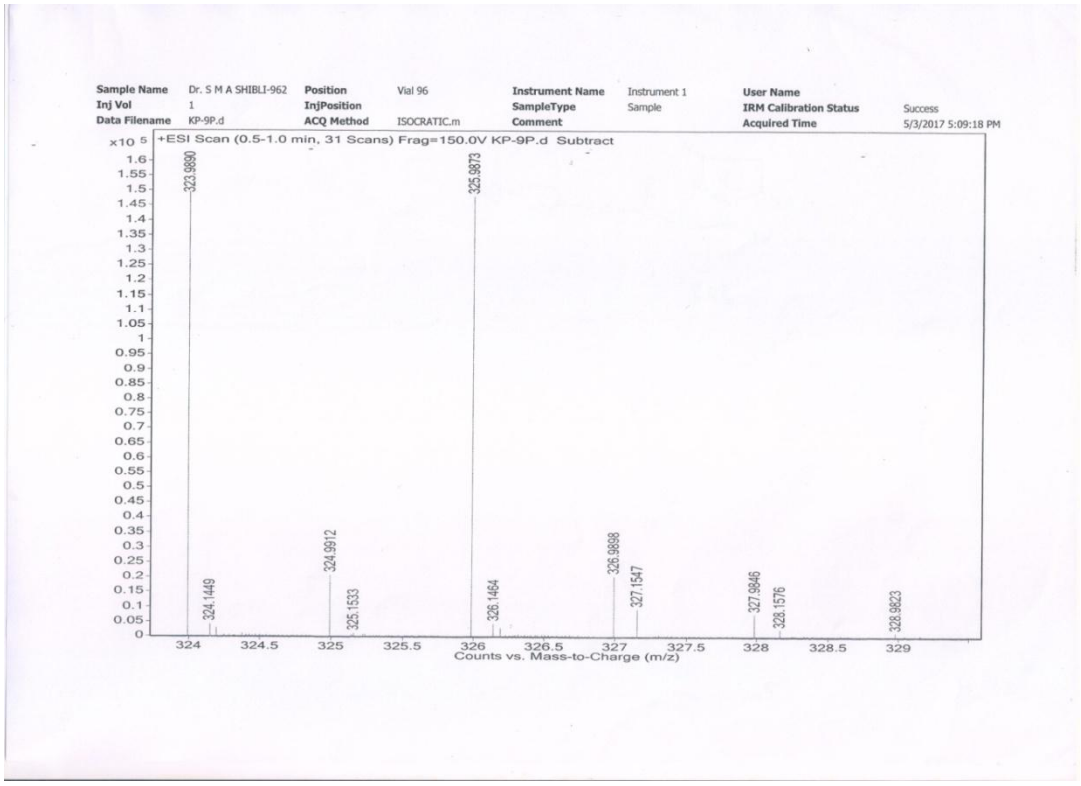


Figure S28. ^{1}H NMR spectrum of 1-[(*N*-4-ethoxyphenylthiocarbamoyl)amidino]pyrazole **(2g)** (400 MHz, DMSO)

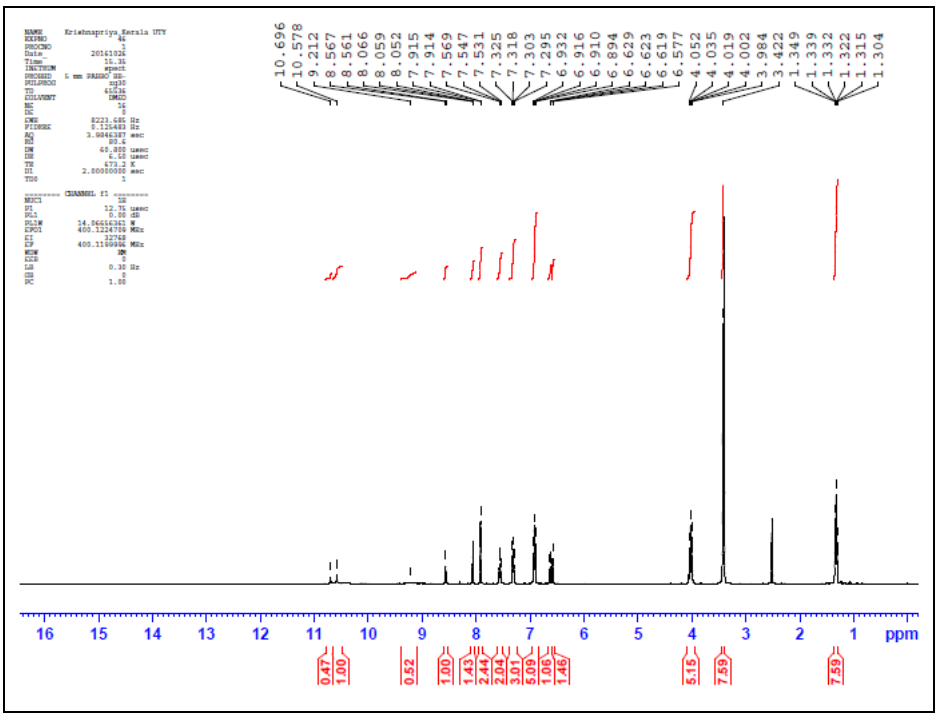


Figure S29. ^{1}H NMR spectrum (expanded) of 1-[(*N*-4-ethoxyphenylthiocarbamoyl) amidino]pyrazole **(2g)** (400 MHz, DMSO)

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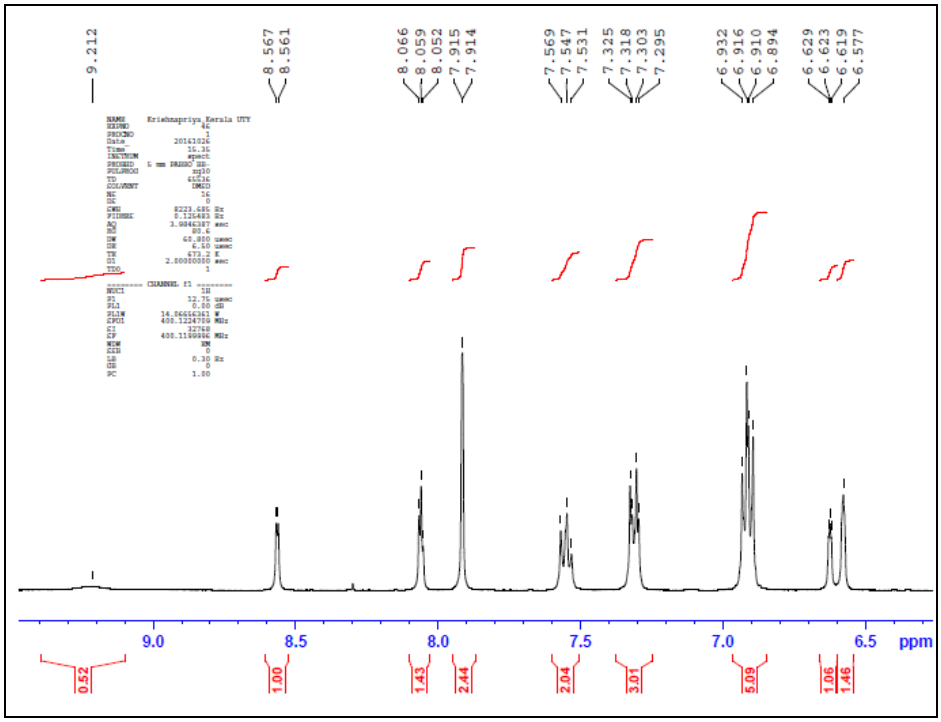


Figure S30. ^{13}C NMR spectrum of 1-[(*N*-4-ethoxyphenylthiocarbamoyl)amidino]pyrazole **(2g)** (100 MHz, DMSO)

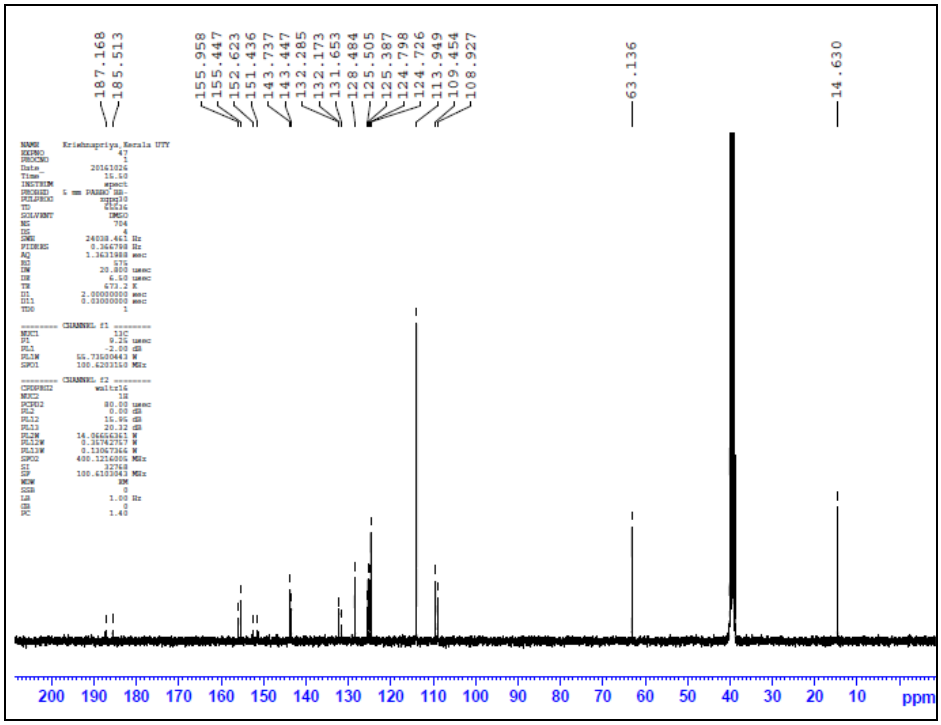


Figure S31. ESI-HRMS spectrum of 1-[(*N*-4-ethoxyphenylthiocarbamoyl)amidino]pyrazole **(2g)**

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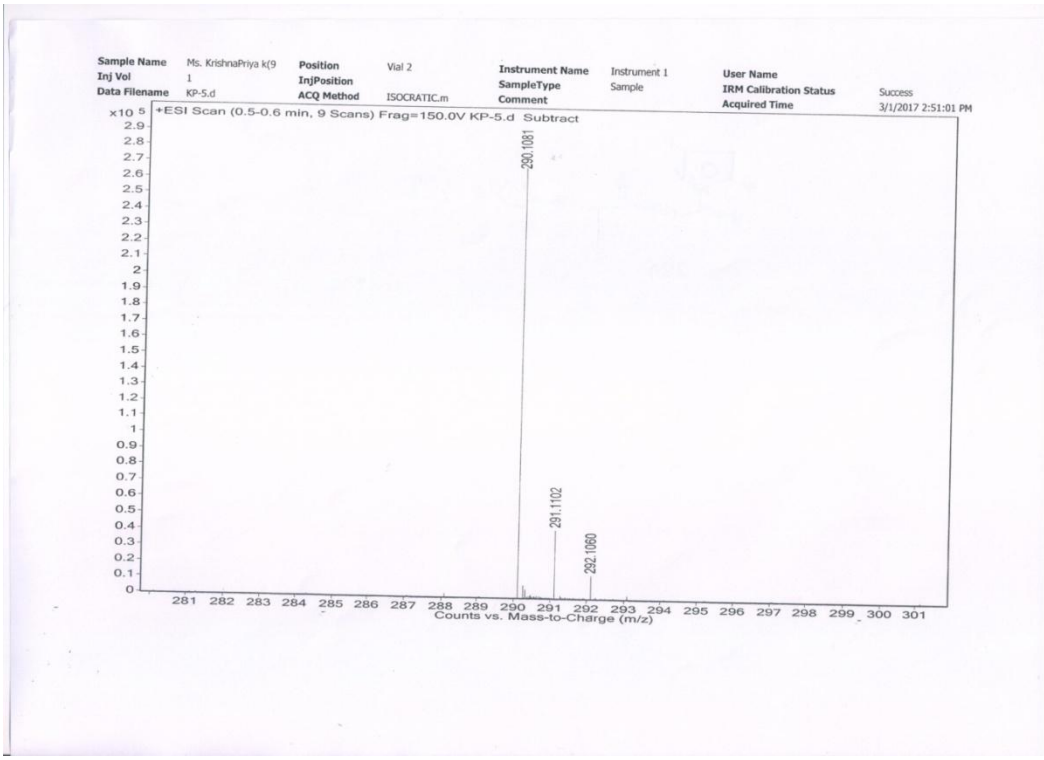


Figure S32. ^{1}H NMR spectrum of 1-[(*N*-3-methylphenylthiocarbamoyl)amidino]pyrazole **(2h)** (400 MHz, $CDCl_3$)

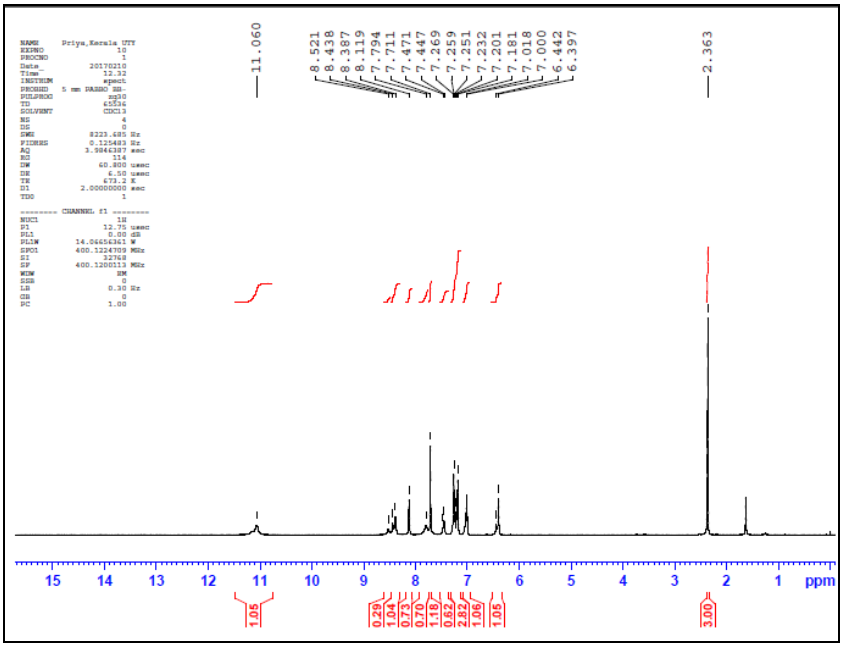


Figure S33. ^{1}H NMR spectrum (expanded) of 1-[(*N*-3-methylphenylthiocarbamoyl) amidino]pyrazole **(2h)** (400 MHz, $CDCl_3$)

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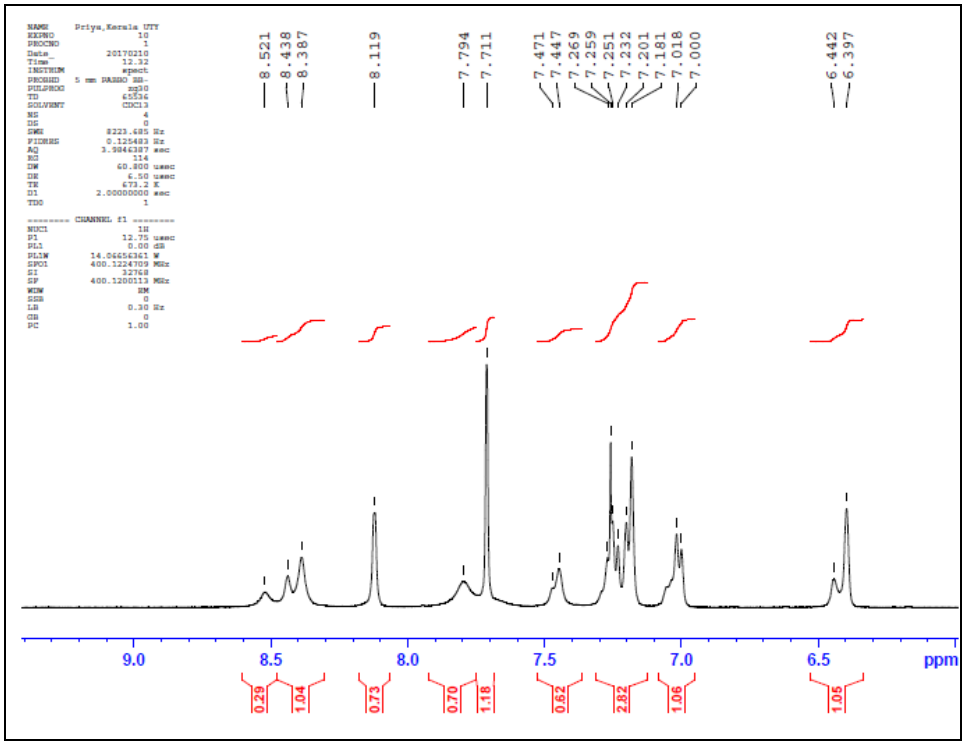


Figure S34. ^{13}C NMR spectrum (of 1-[(*N*-3-methylphenylthiocarbamoyl)amidino]pyrazole **(2h)** (100 MHz, $CDCl_3$)

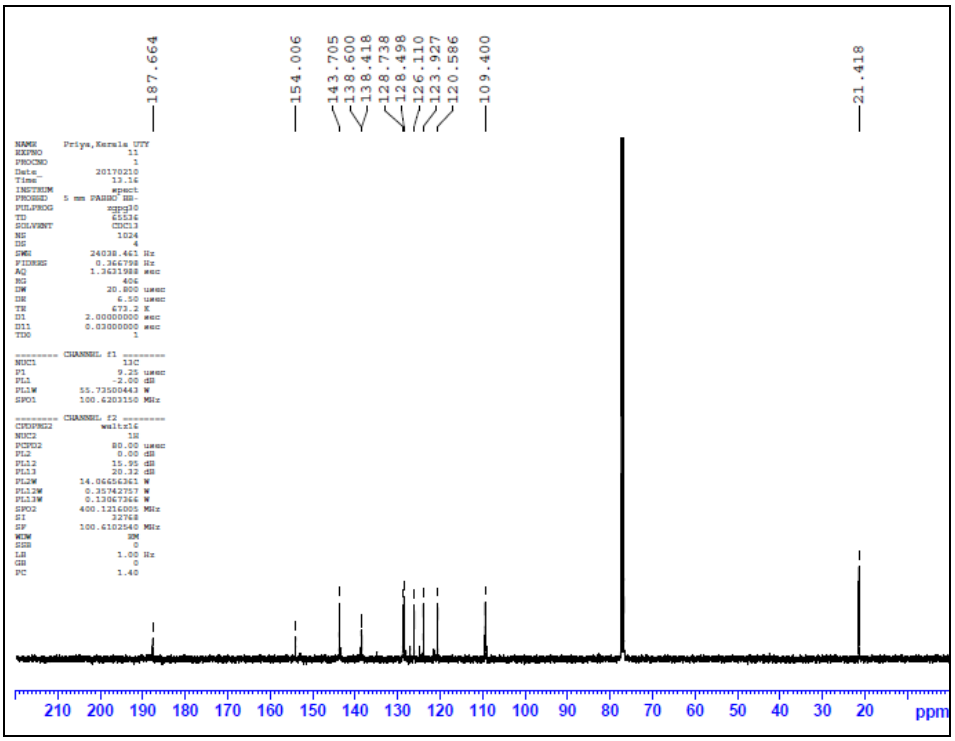


Figure S35. ESI-HRMS spectrum of 1-[(*N*-3-methylphenylthiocarbamoyl)amidino]pyrazole **(2h)**

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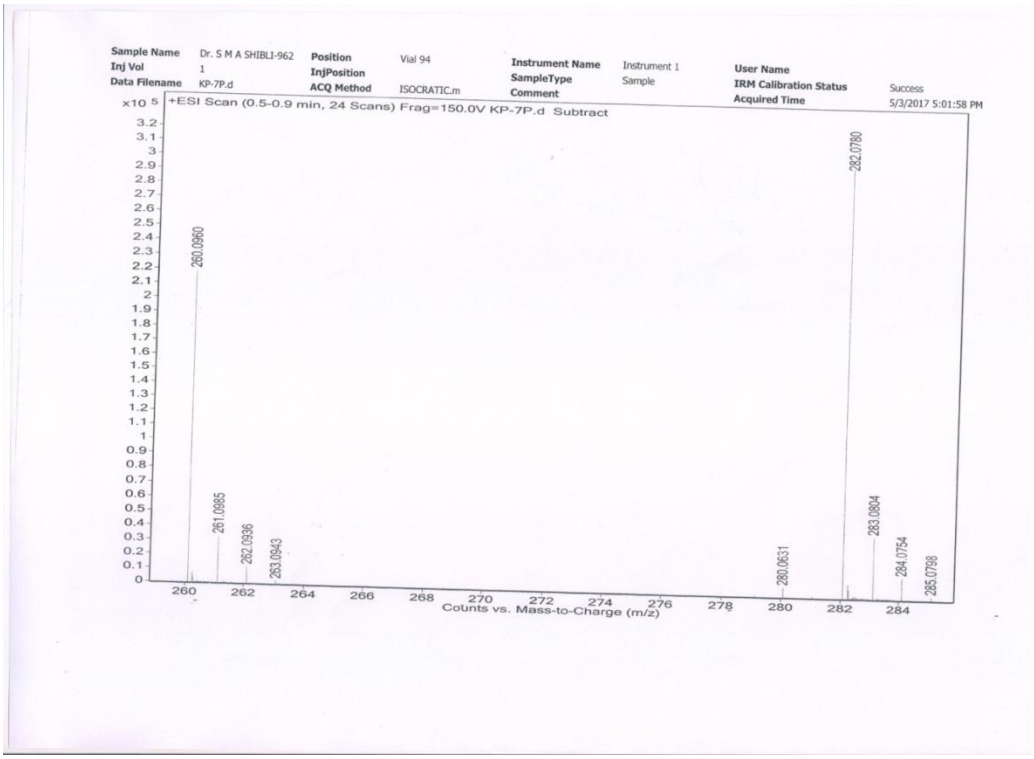


Figure S36. ^{1}H NMR spectrum of 1-[(*N*-2-chlorophenylthiocarbamoyl)amidino]pyrazole **(2i)** (400 MHz, $CDCl_3$)

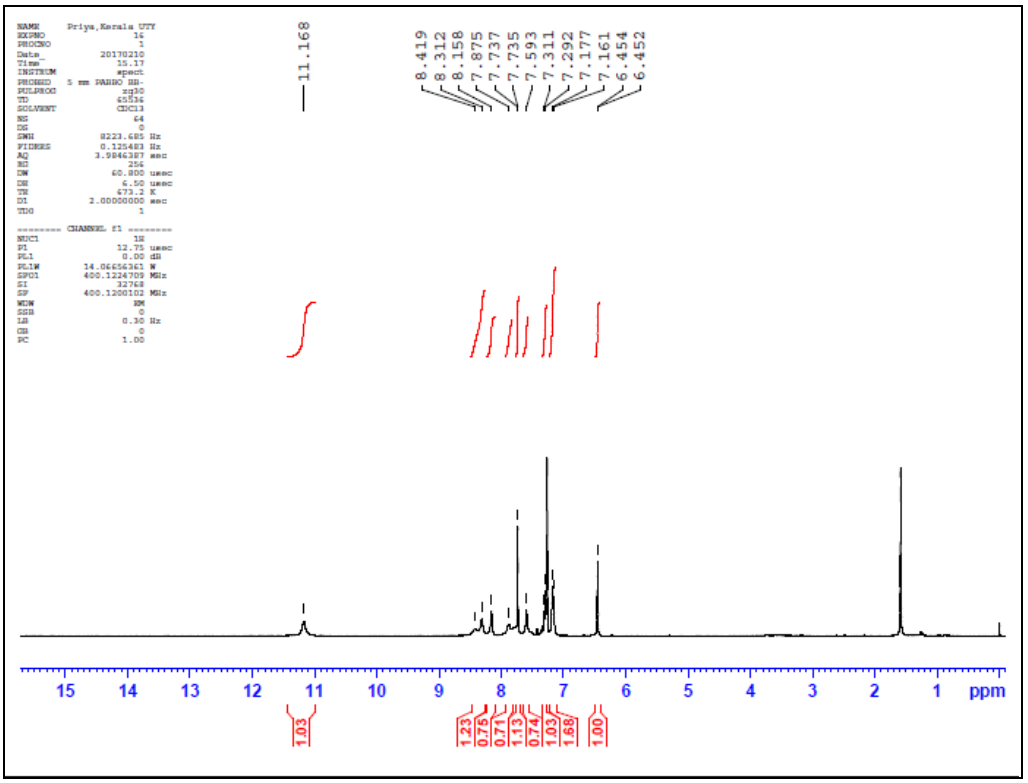


Figure S37. ^{1}H NMR spectrum (expanded) of 1-[(*N*-2-chlorophenylthiocarbamoyl)amidino] pyrazole **(2i)** (400 MHz, $CDCl_3$)

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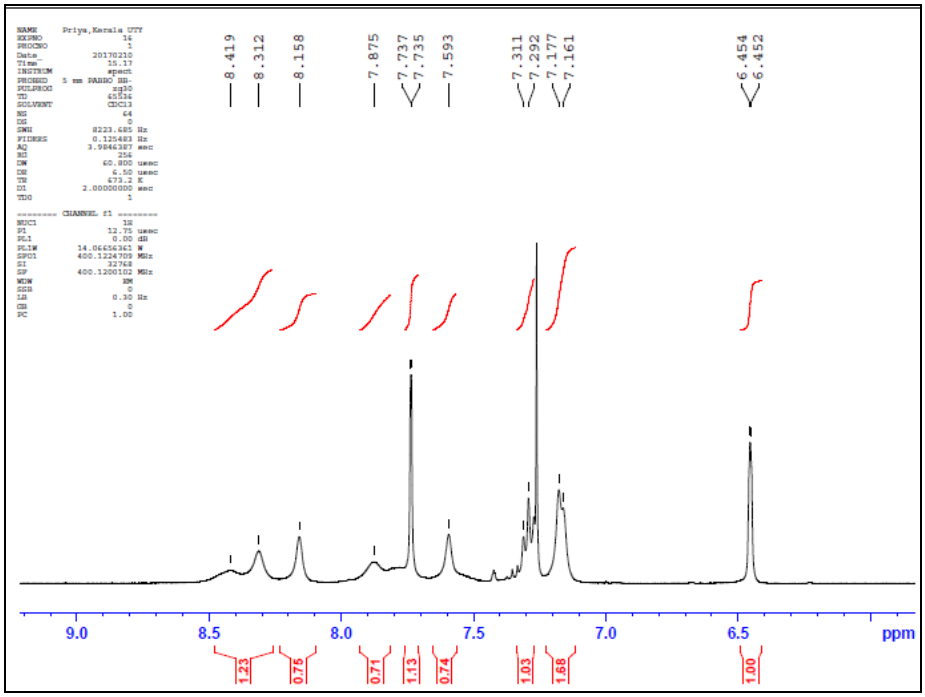


Figure S38. ^{13}C NMR spectrum of 1-[(*N*-2-chlorophenylthiocarbamoyl)amidino] pyrazole **(2i)** (100 MHz, $CDCl_3$)

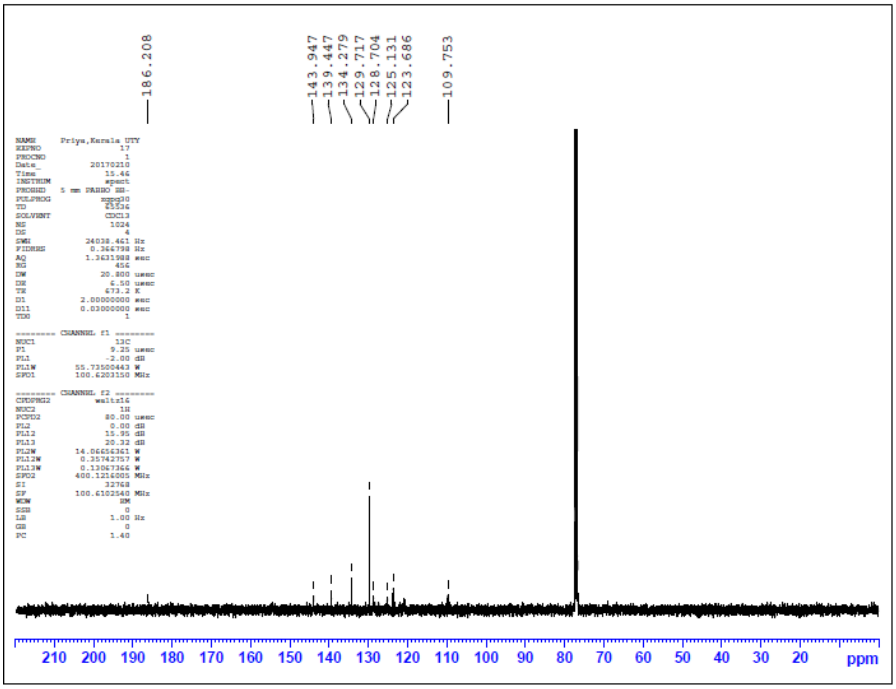


Figure S39. ESI-HRMS spectrum of 1-[(*N*-2-chlorophenylthiocarbamoyl)amidino]pyrazole **(2i)**

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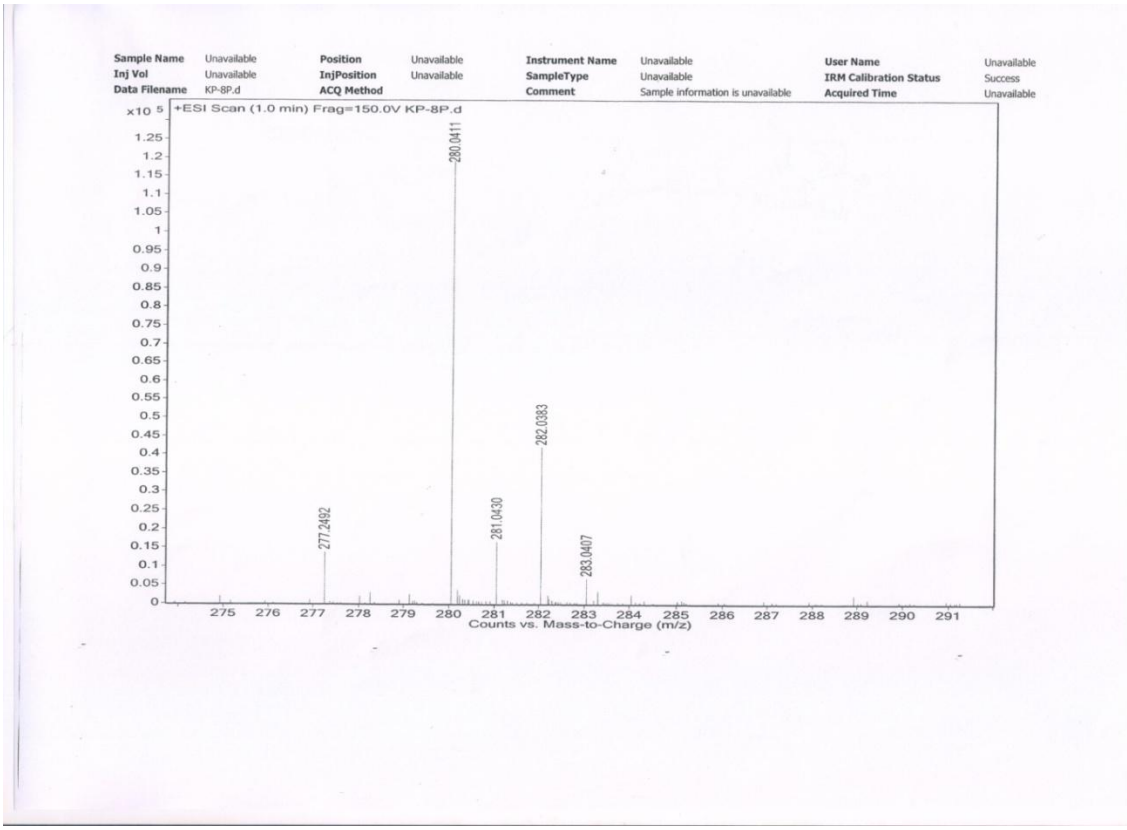


Figure S40. ^{1}H NMR spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrrolidine **(3a)** (400 MHz, $CDCl_3$)

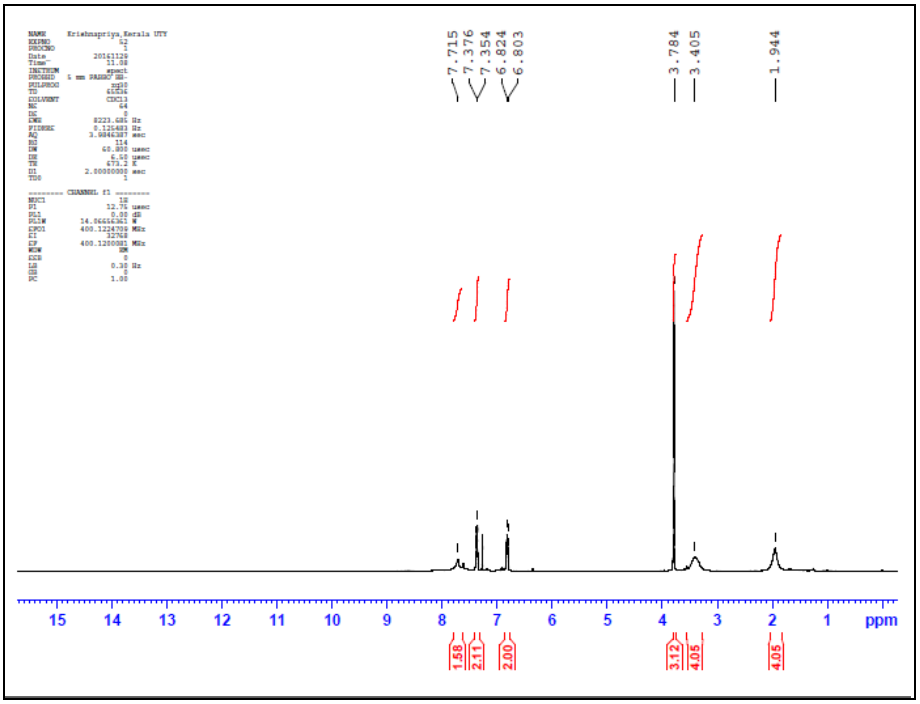


Figure S41. ^{1}H NMR spectrum (expanded) of 1-[(*N*-4-methoxyphenylthiocarbamoyl) amidino]pyrrolidine **(3a)** (400 MHz, $CDCl_3$)

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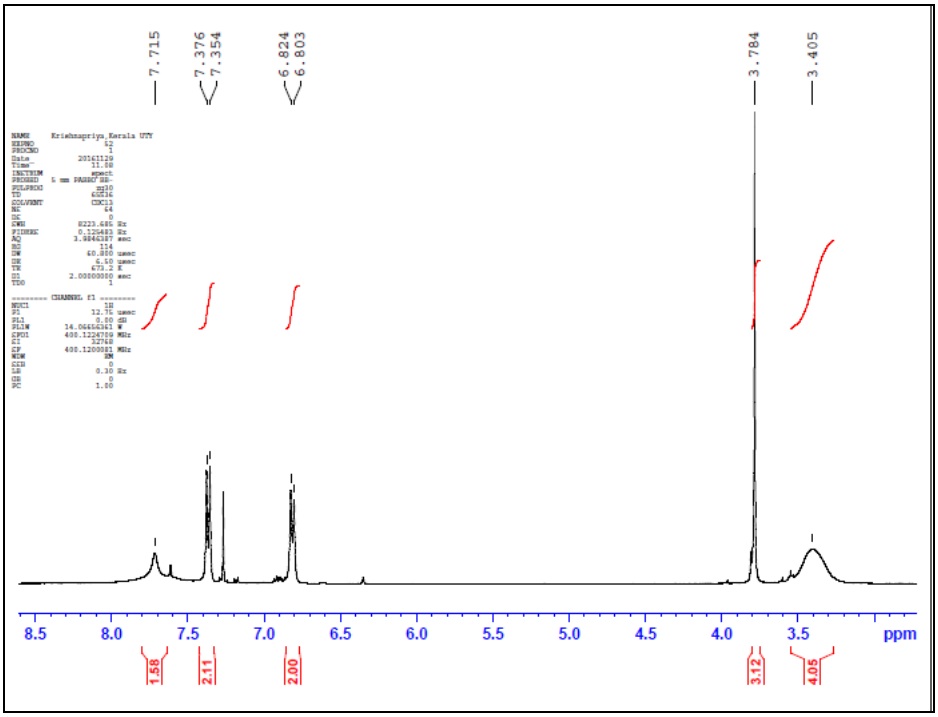


Figure S42. ^{13}C NMR spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl) amidino]pyrrolidine **(3a)** (100 MHz, $CDCl_3$)

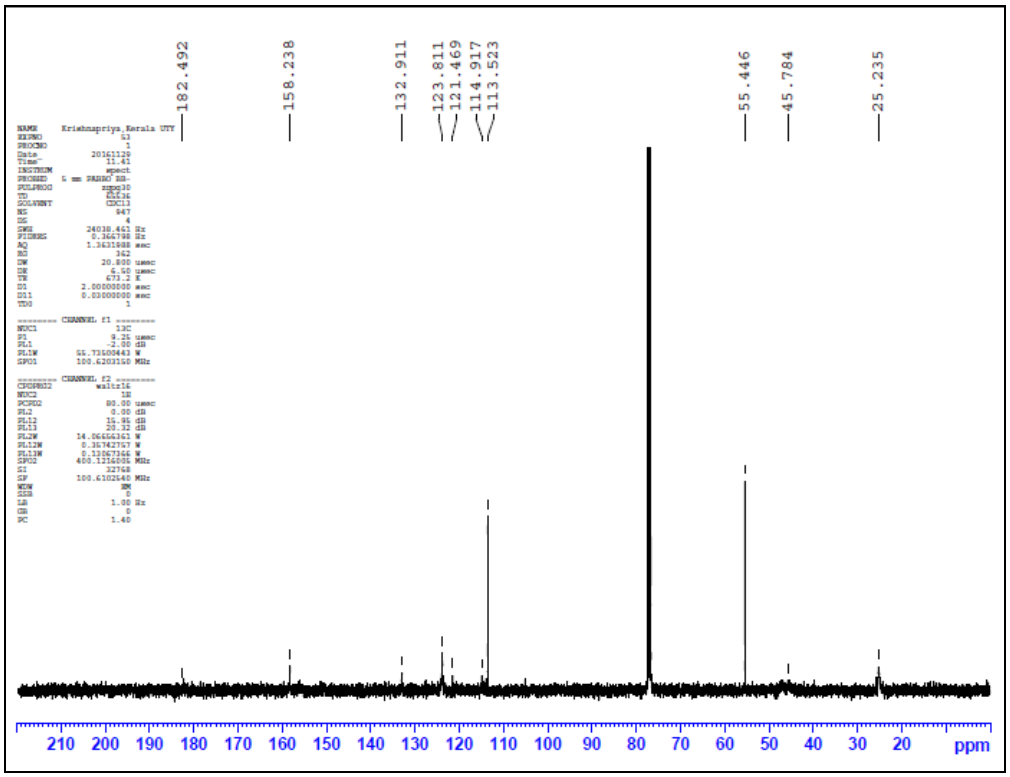


Figure S43. ESI-HRMS spectrum of 1-[(*N*-4-methoxyphenylthiocarbamoyl)amidino]pyrrolidine **(3a)**

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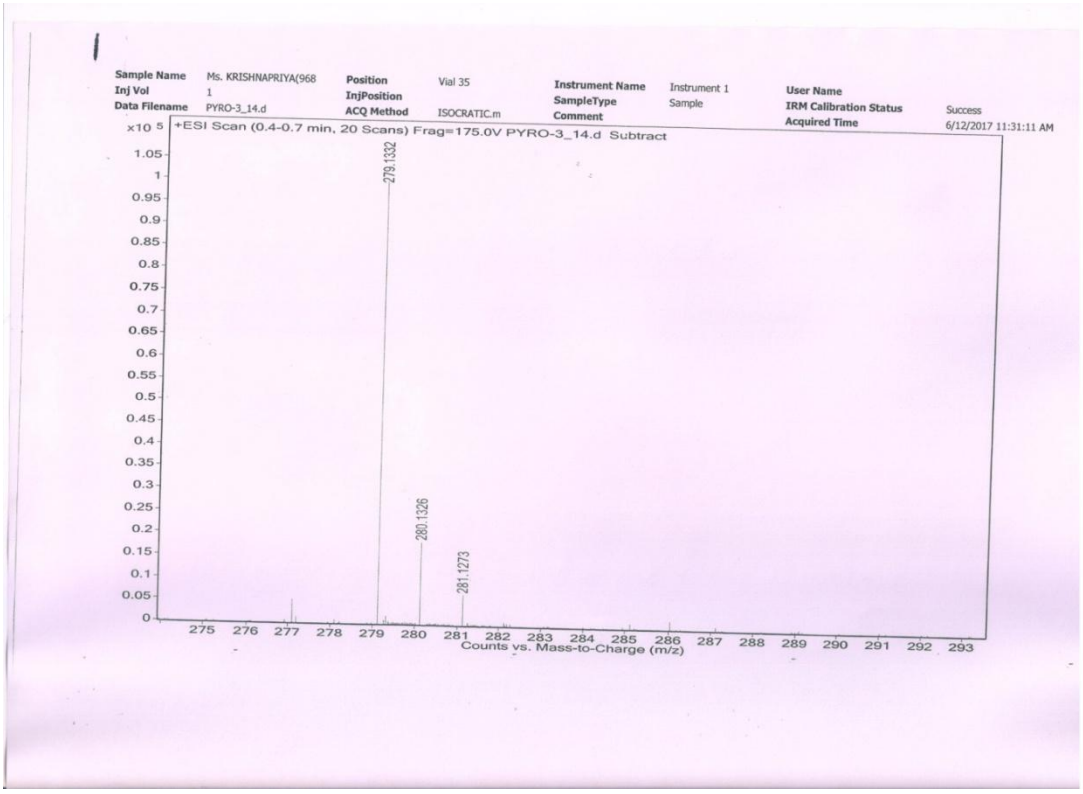


Figure S44. ^{1}H NMR spectrum 1-[(*N*-4-ethoxyphenylthiocarbamoyl)amidino]pyrrolidine **(3b)** (400 MHz, $CDCl_3$)

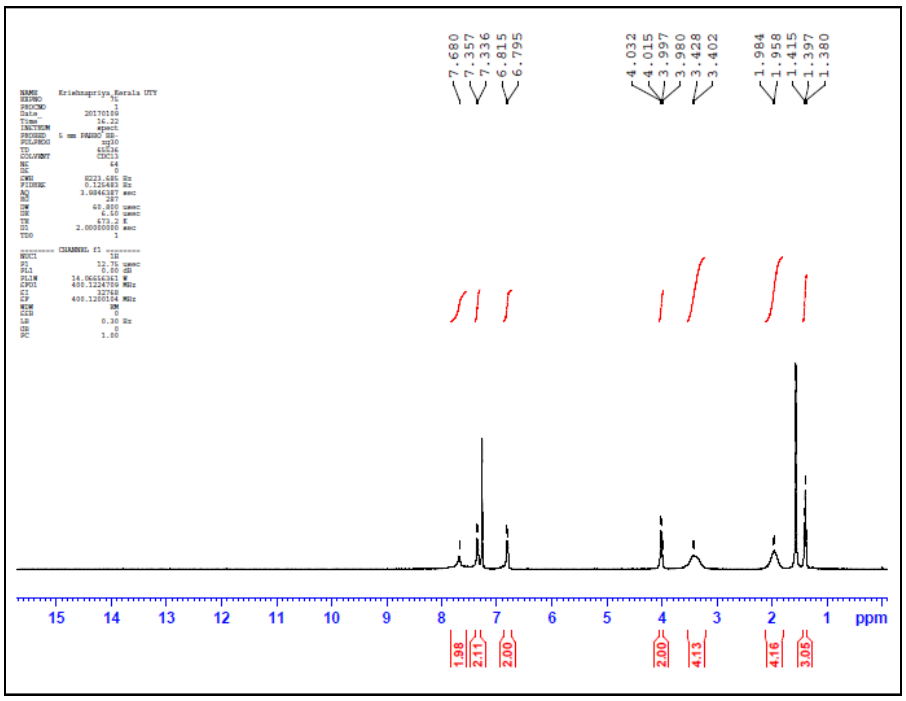


Figure S45. ^{1}H NMR spectrum (expanded) 1-[(*N*-4-ethoxyphenylthiocarbamoyl) amidino]pyrrolidine **(3b)** (400 MHz, $CDCl_3$)

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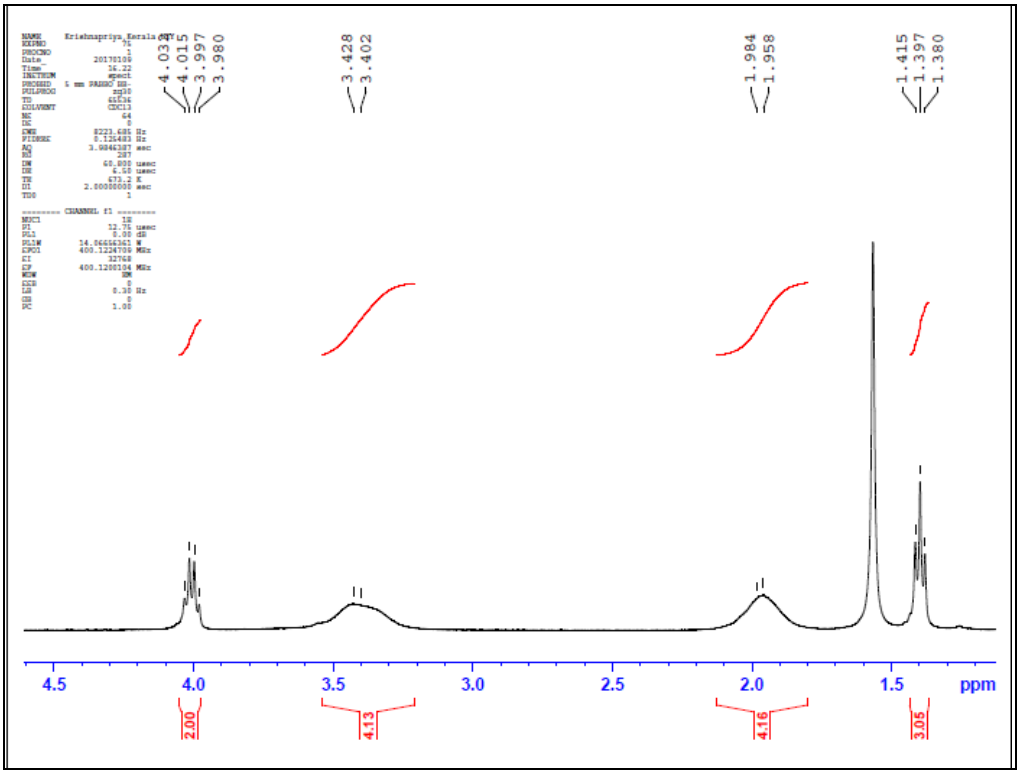


Figure S46. ^{13}C NMR spectrum 1-[(*N*-4-ethoxyphenylthiocarbamoyl)amidino]pyrrolidine **(3b)** (100 MHz, $CDCl_3$)

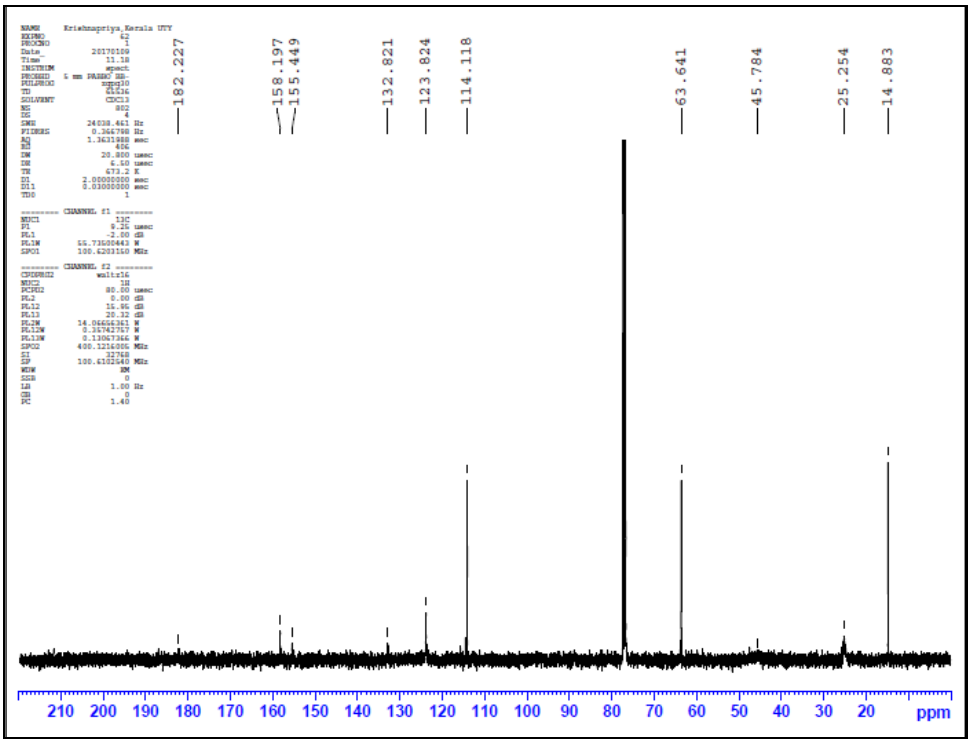


Figure S47. ESI-HRMS spectrum 1-[(*N*-4-ethoxyphenylthiocarbamoyl)amidino]pyrrolidine **(3b)**

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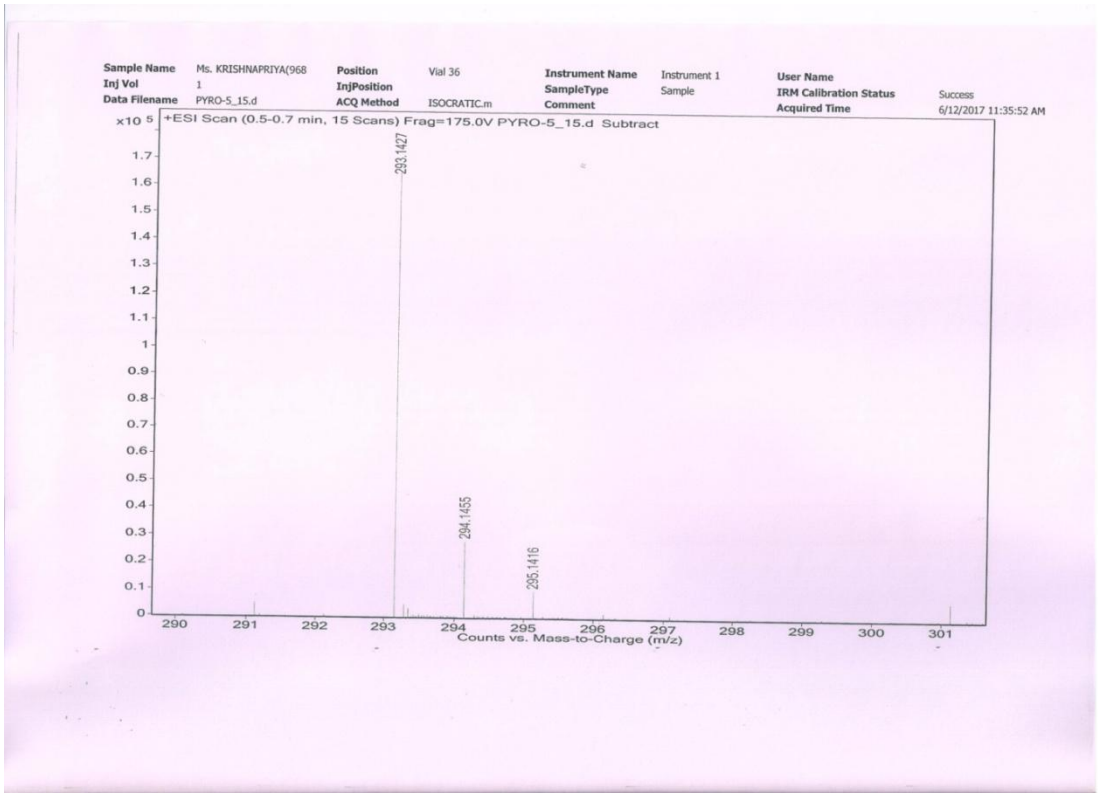
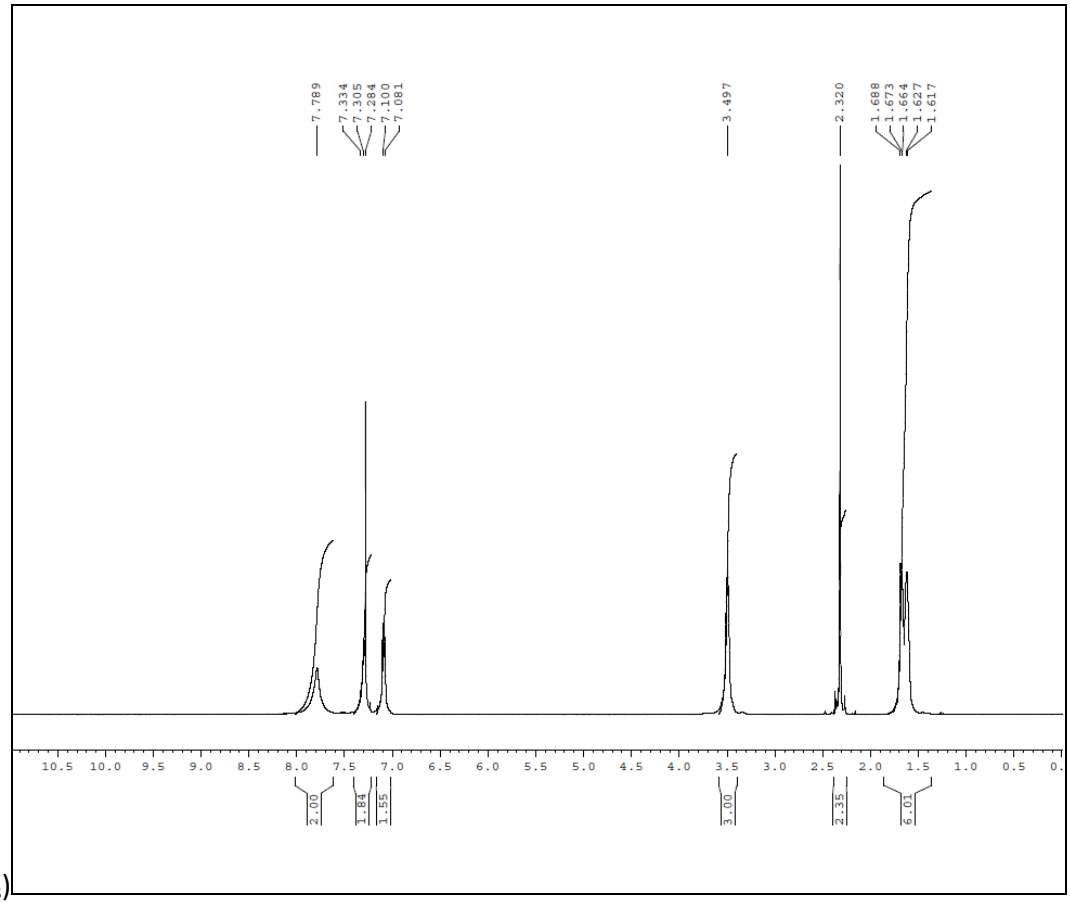


Figure S48. ^{1}H NMR spectrum 1-[(*N*-4-methylphenylthiocarbamoyl)amidino]piperidine **(3c)** (400 MHz, $CDCl_3$)



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

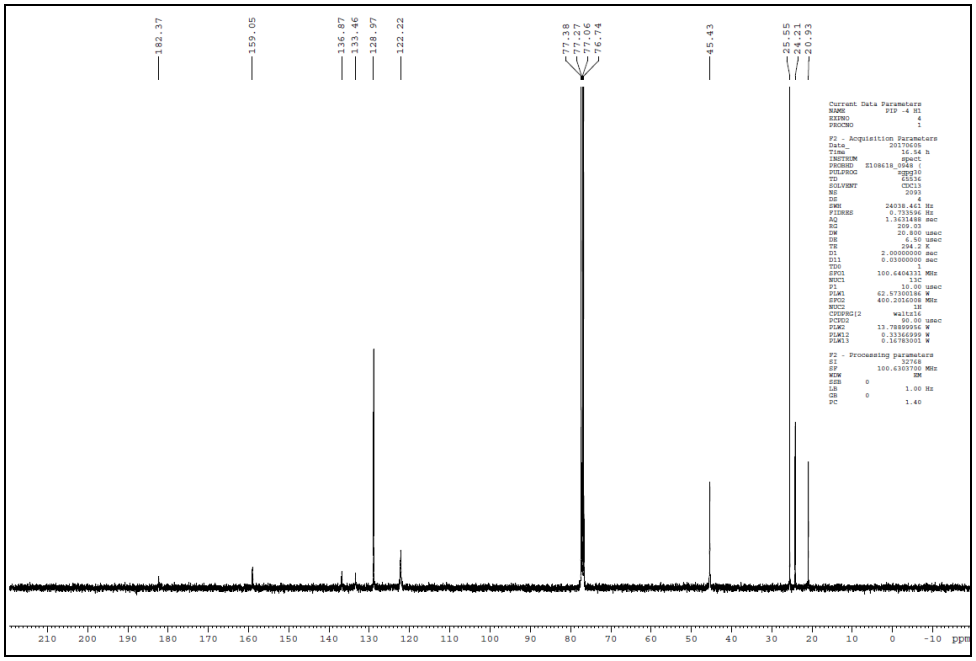
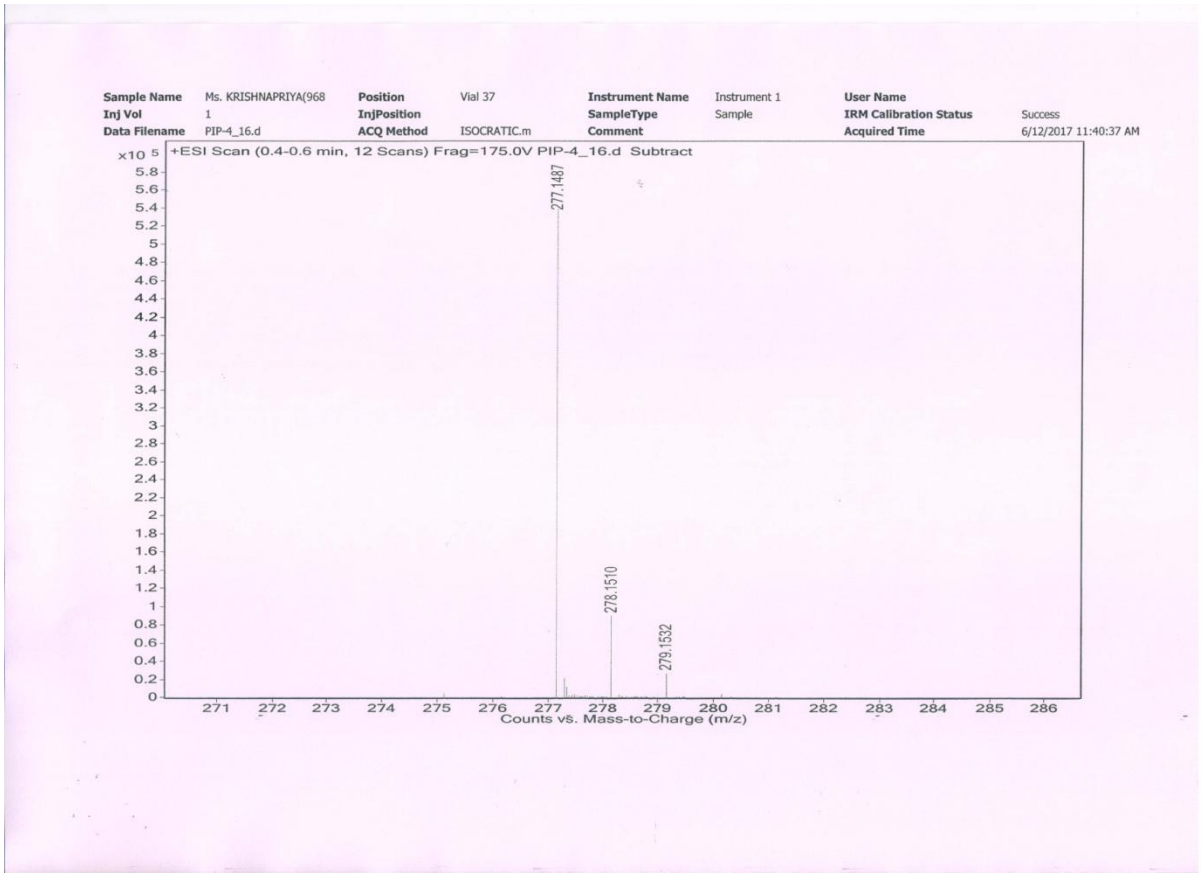


Figure S50. ESI-HRMS spectrum of 1-[(*N*-4-methylphenylthiocarbamoyl)amidino]piperidine **(3c)**



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

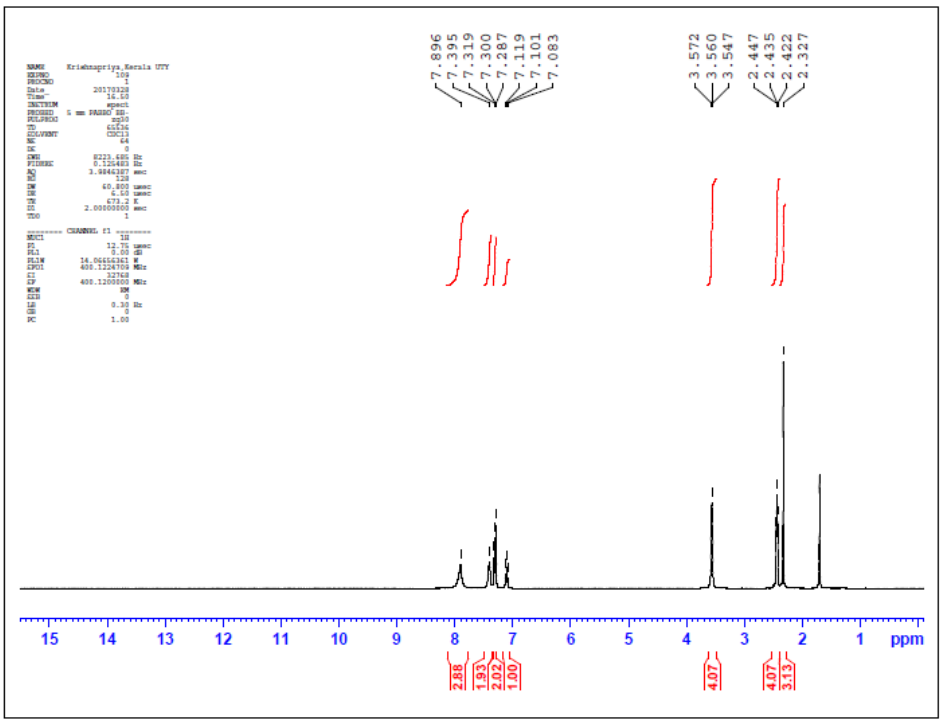


Figure S52. ^{1}H NMR spectrum (expanded) of 1-[(*N*-phenylthiocarbamoyl)amidino]-4-methylpiperazine **(3d)** (400 MHz, $CDCl_3$)

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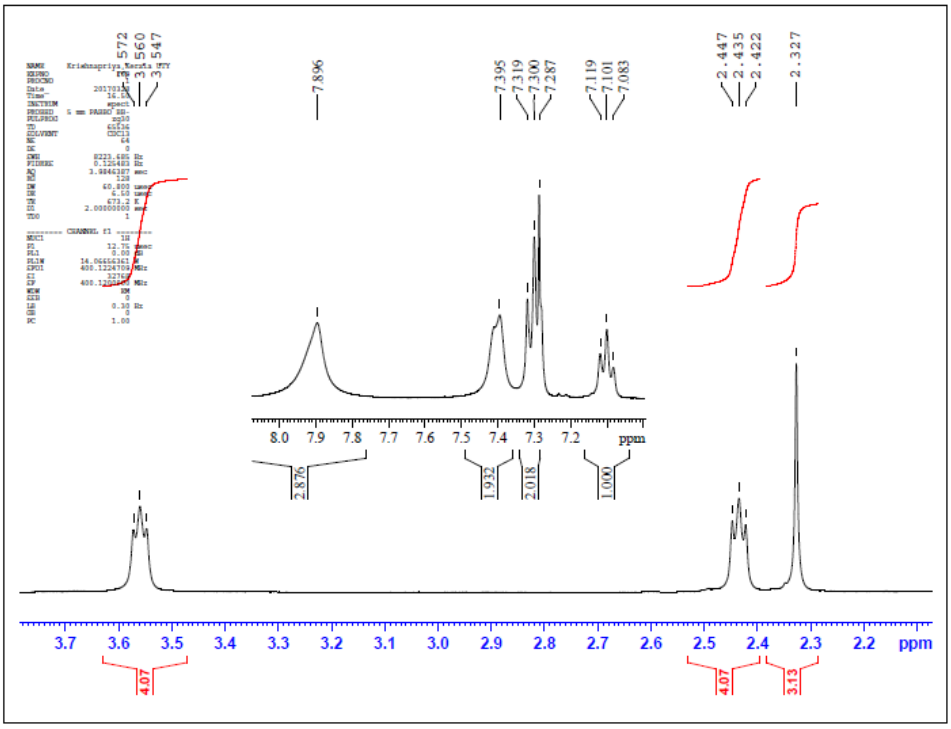


Figure S53. ^{13}C NMR spectrum of 1-[(*N*-phenylthiocarbamoyl)amidino]-4-methylpiperazine **(3d)** (100 MHz, $CDCl_3$)

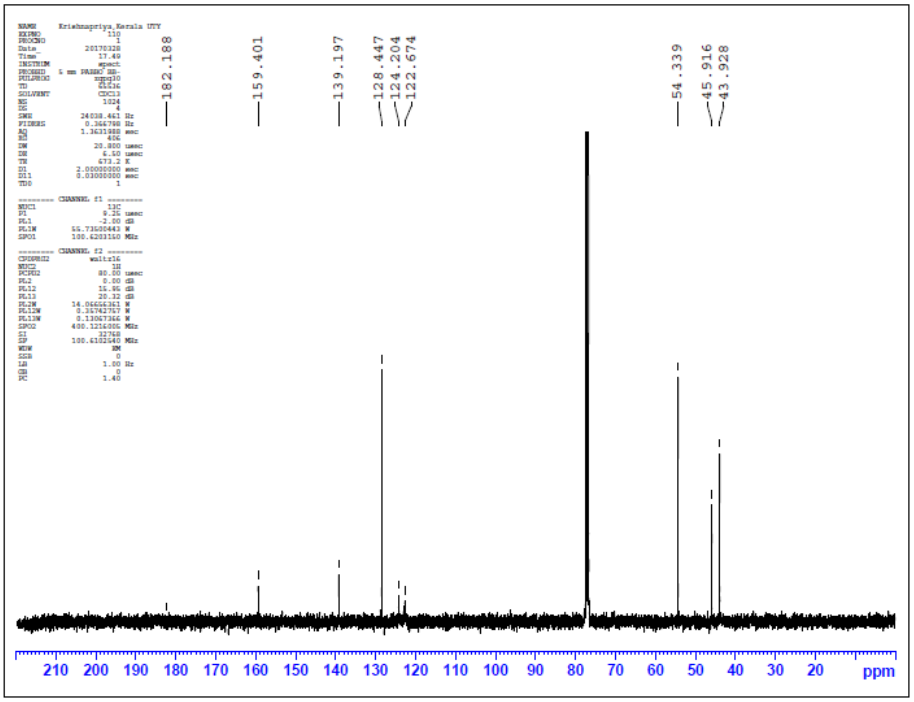


Figure S54. ESI-HRMS spectrum of 1-[(*N*-Phenylthiocarbamoyl)amidino]-4-methylpiperazine **(3d)**

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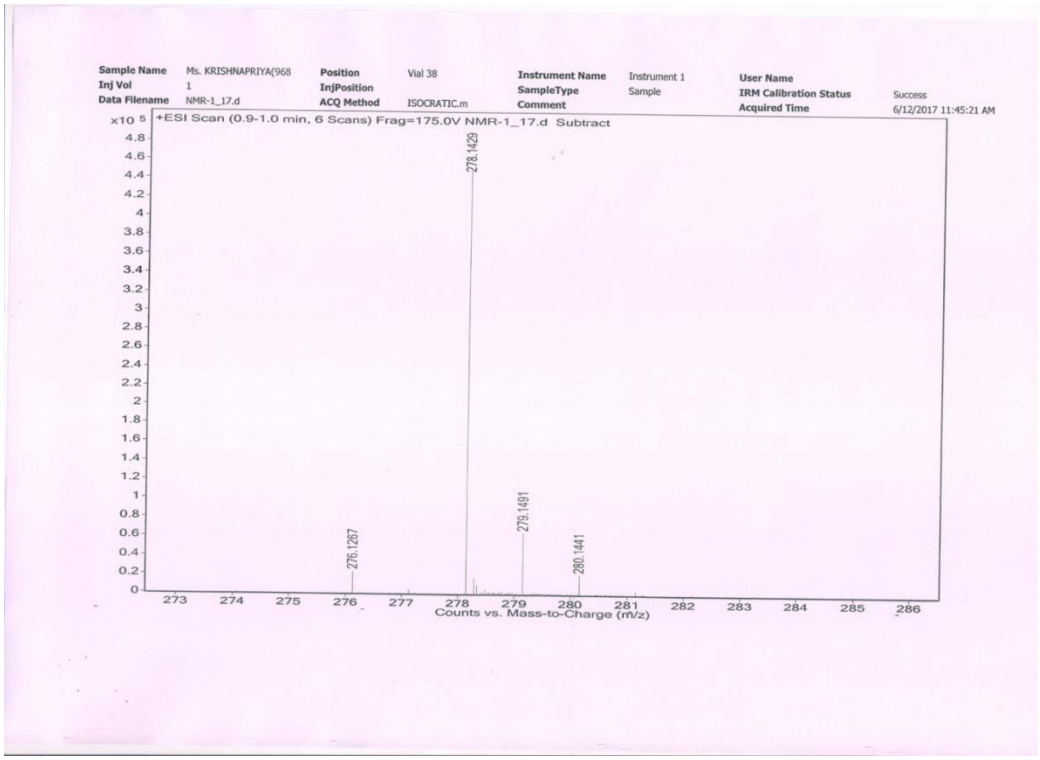


Figure S55. ^{1}H NMR spectrum of 1-[(*N*-phenylthiocarbamoyl)amidino]morpholine **(3e)** (400 MHz, $CDCl_3$)

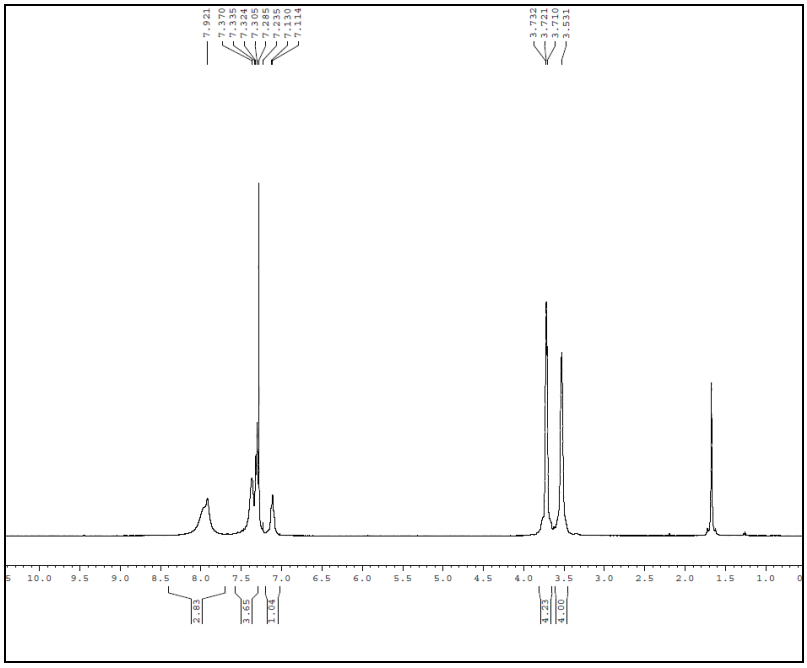


Figure S56. ^{1}H NMR spectrum (expanded) of 1-[(*N*-phenylthiocarbamoyl)amidino]morpholine **(3e)** (400 MHz, $CDCl_3$)

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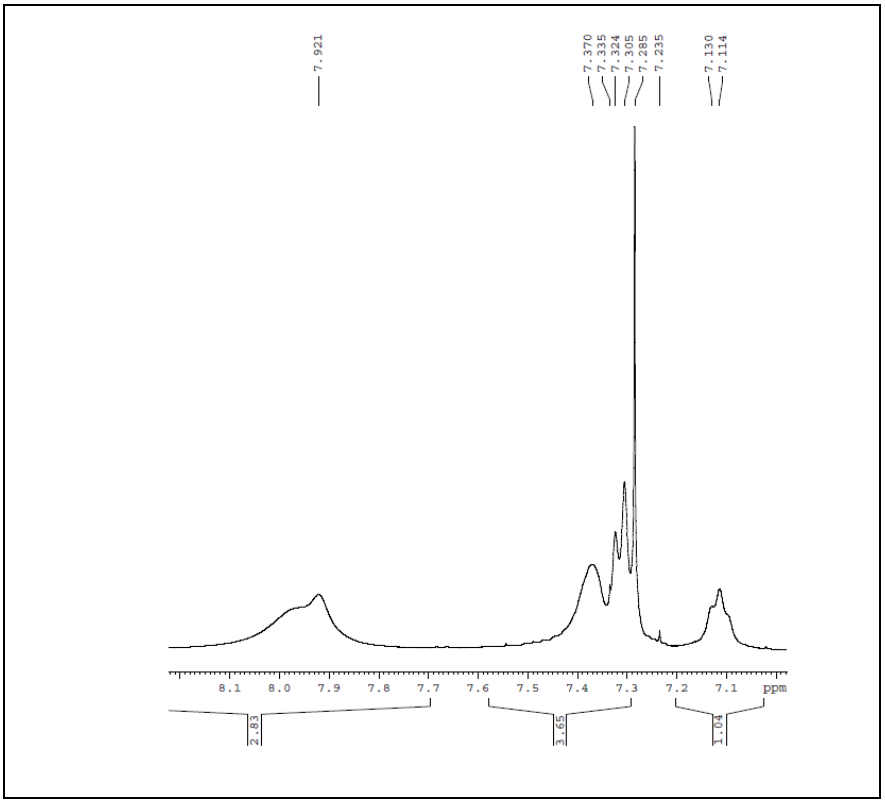


Figure S57. ^{13}C NMR spectrum of 1-[(*N*-phenylthiocarbamoyl)amidino]morpholine **(3e)** (100 MHz, $CDCl_3$)

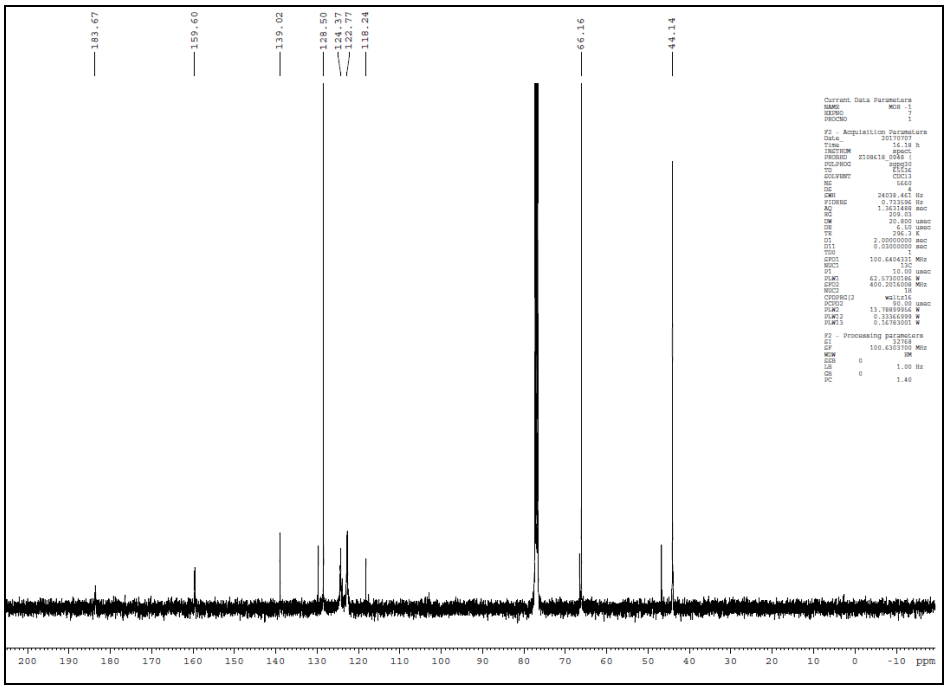


Figure S58. ESI-HRMS spectrum of 1-[(*N*-phenylthiocarbamoyl)amidino]morpholine **(3e)**

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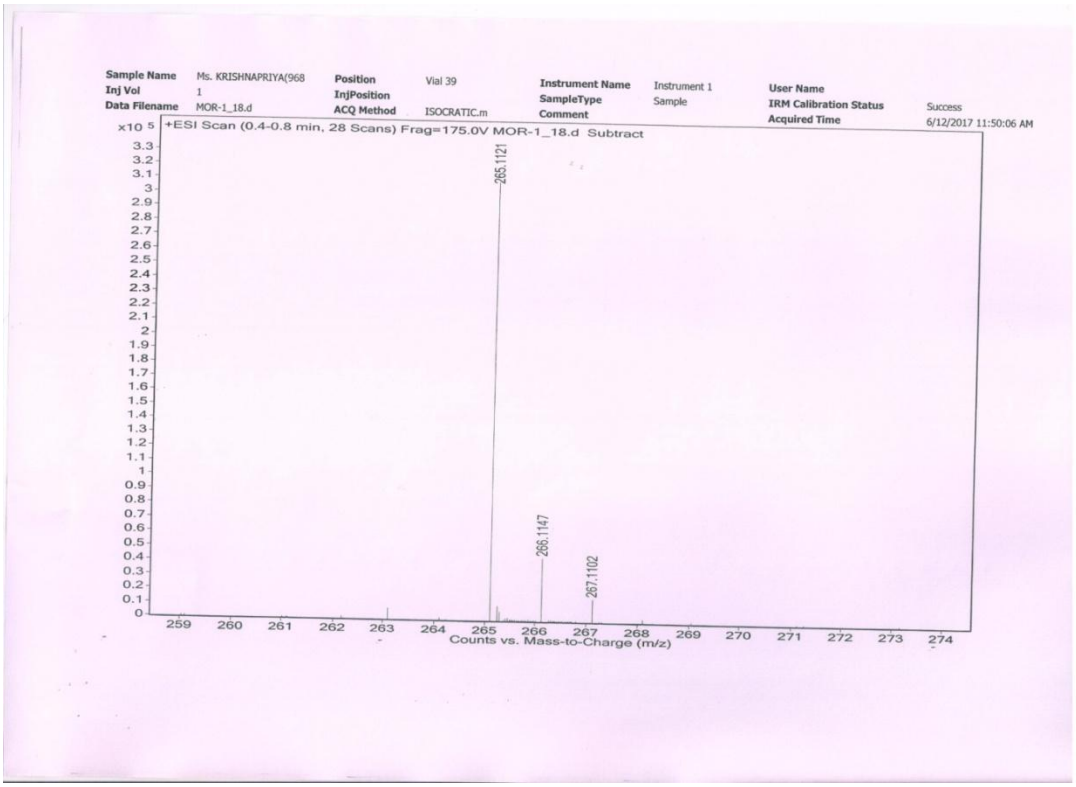


Figure S59. ^{1}H NMR spectrum of *N*-(phenylthiocarbamoyl)-*N*'-n-propylguanidine **(3f)** (400 MHz, $CDCl_3$)

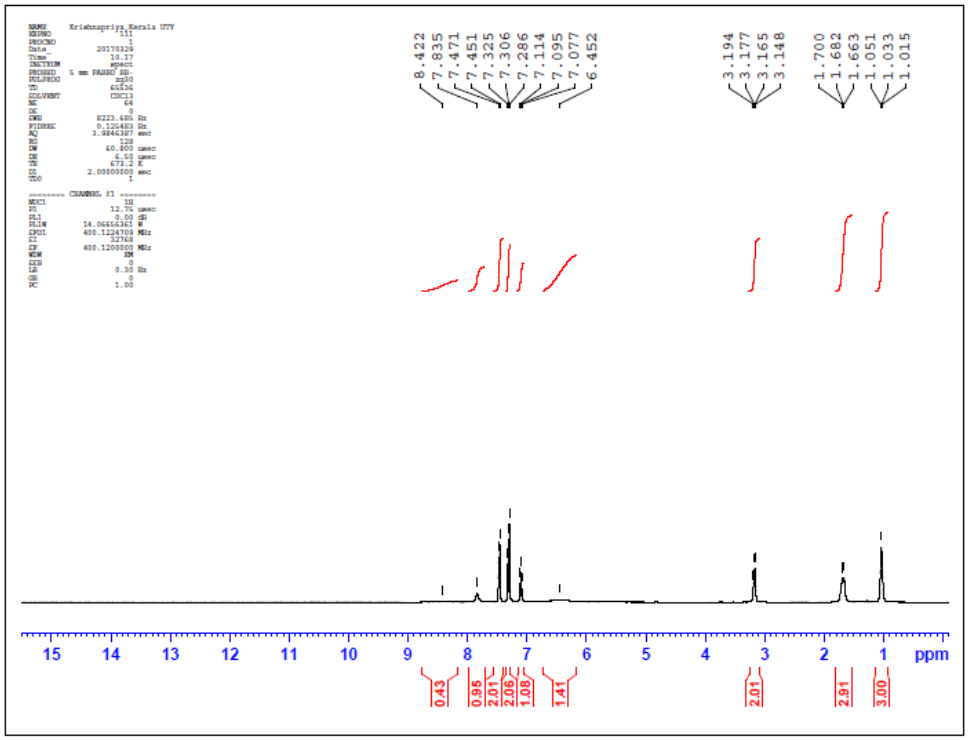


Figure S60. ^{1}H NMR spectrum (expanded) of *N*-(phenylthiocarbamoyl)-*N*'-n-propylguanidine **(3f)** (400 MHz, $CDCl_3$)

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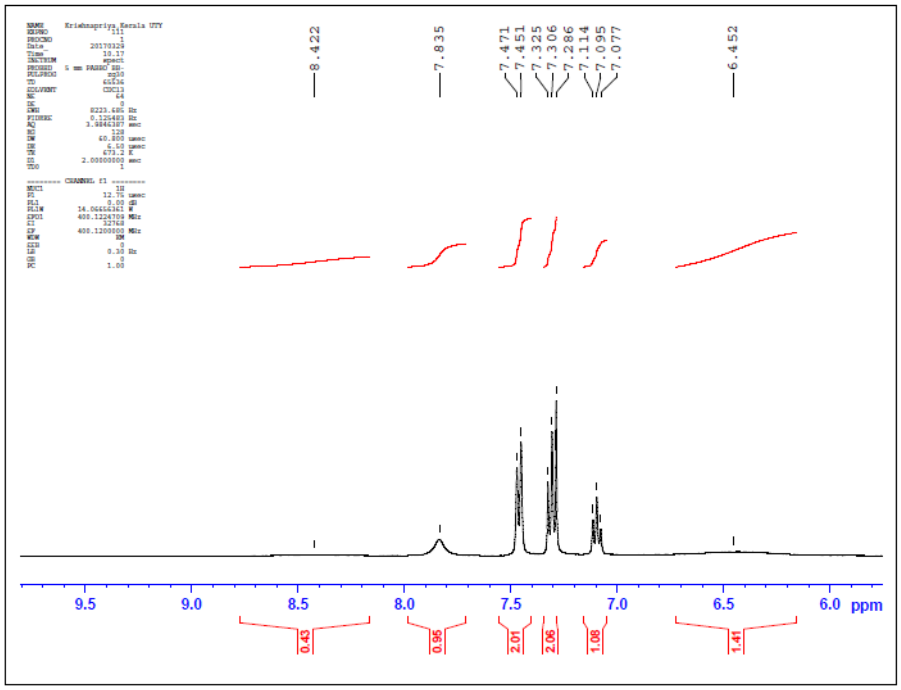


Figure S61. ^{1}H NMR spectrum (expanded) of *N*-(phenylthiocarbamoyl)-*N*'-n-propylguanidine **(3f)** (400 MHz, $CDCl_3$)

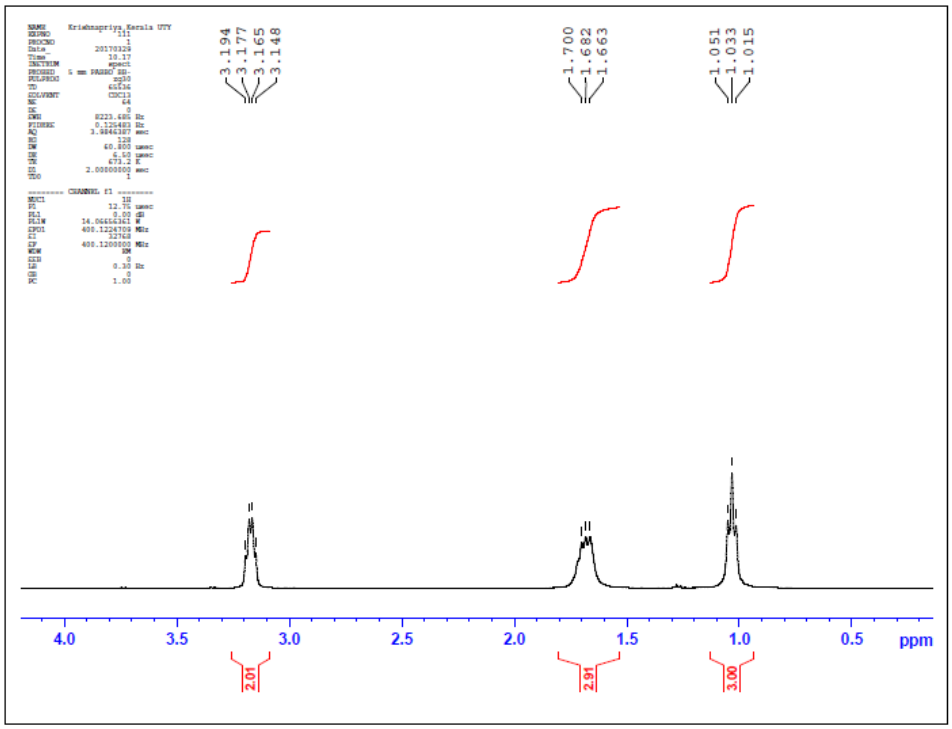


Figure S62. ^{13}C NMR spectrum (of *N*-(phenylthiocarbamoyl)-*N*'-n-propylguanidine **(3f)** (100 MHz, $CDCl_3$)

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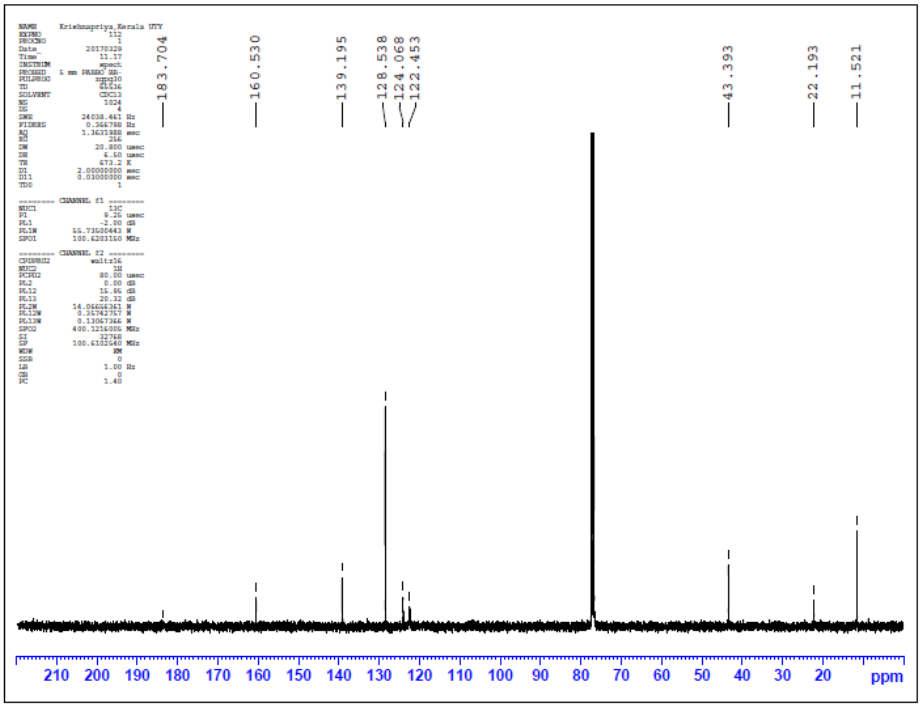
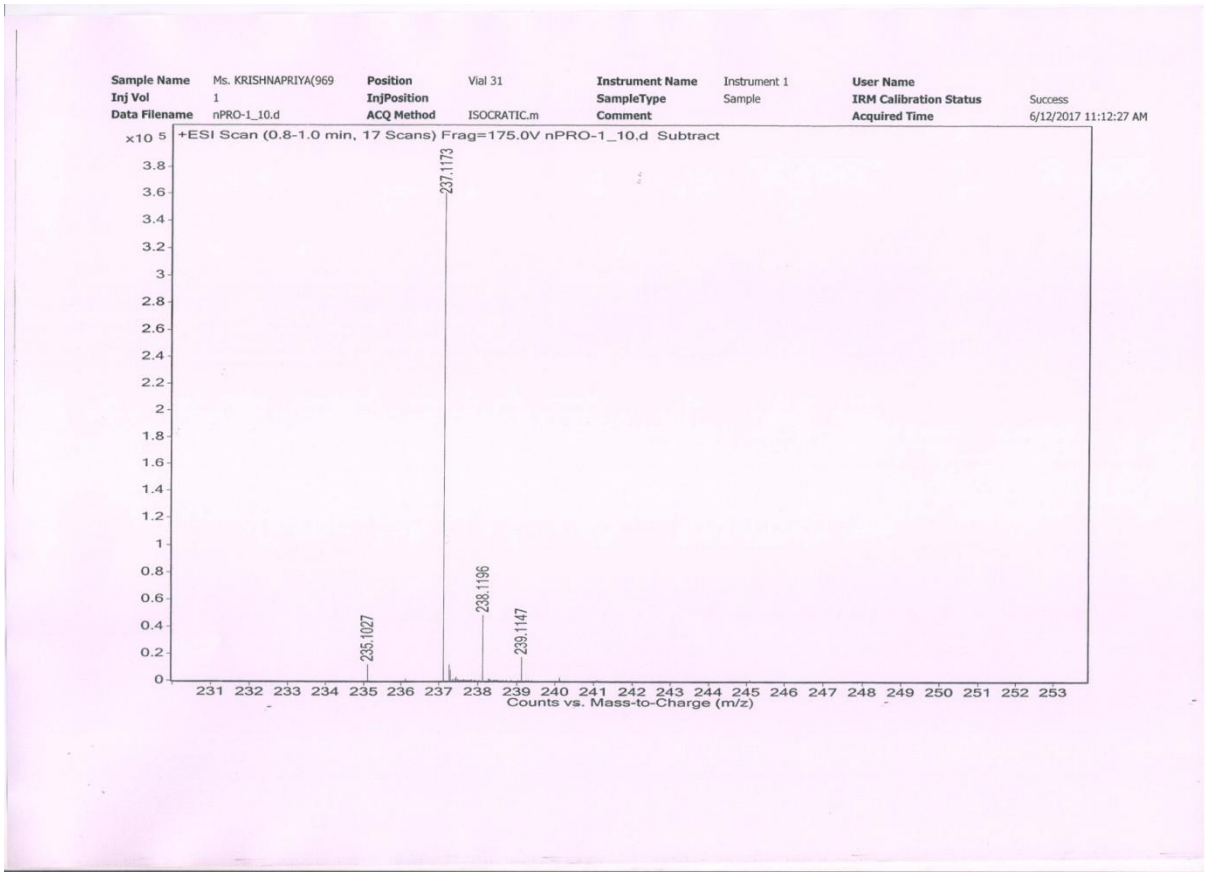


Figure S63. ESI-HRMS spectrum of *N*-(phenylthiocarbamoyl)-*N*'-n-propylguanidine **(3f)**



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

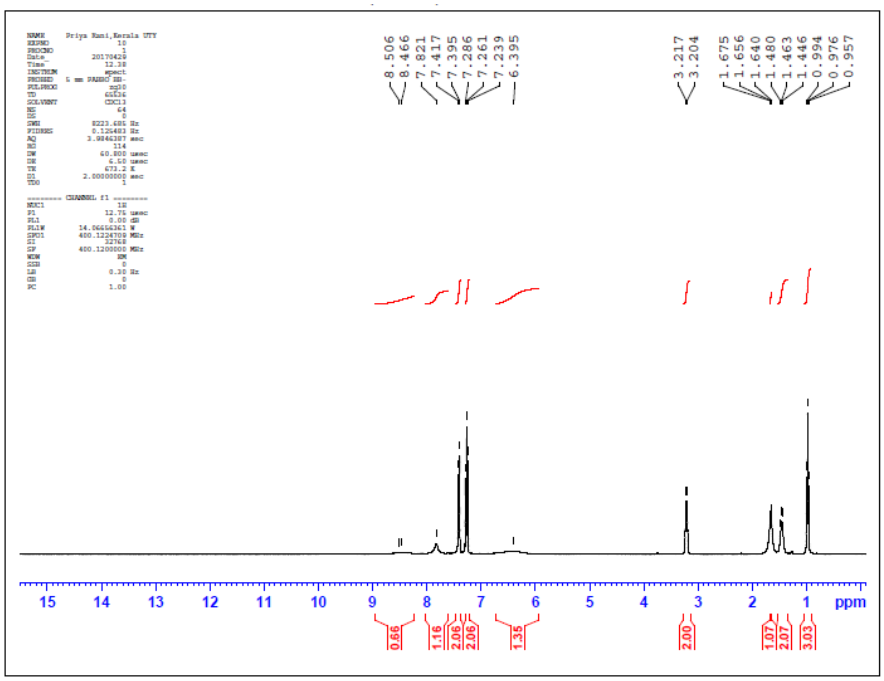


Figure S65. ^{1}H NMR spectrum (expanded) of *N*-n-butyl)-*N'*-(4-chlorophenylthiocarbamoyl)guanidine **(3g)** (400 MHz, $CDCl_3$)

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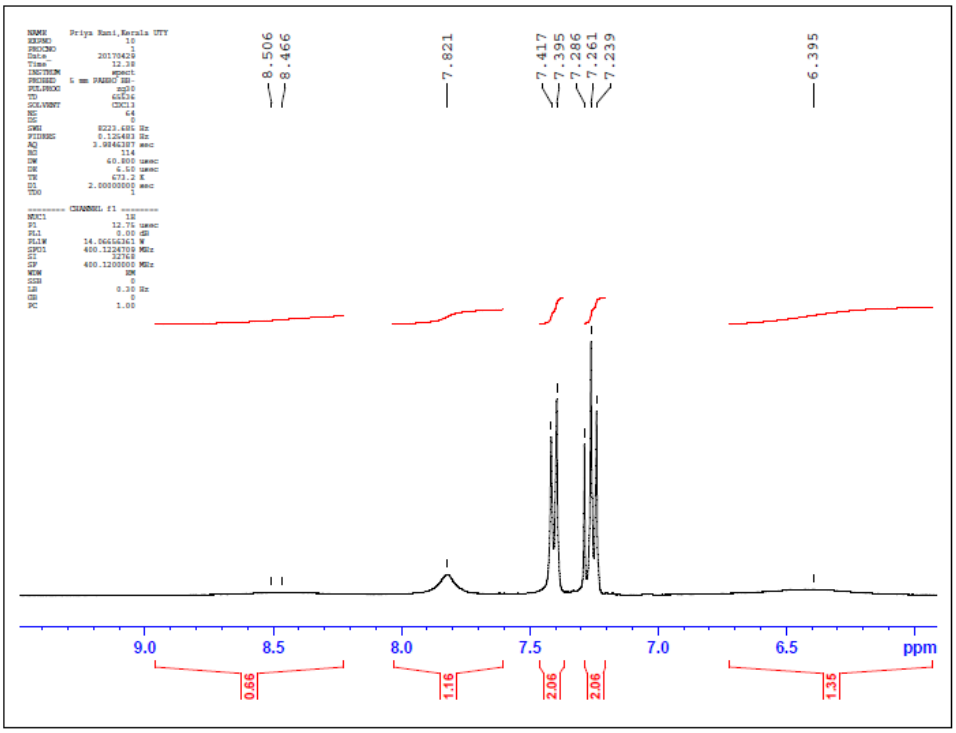


Figure S66. ^{1}H NMR spectrum (expanded) of *N*-n-butyl)-*N'*-(4-chlorophenylthiocarbamoyl)guanidine **(3g)** (400 MHz, $CDCl_3$)

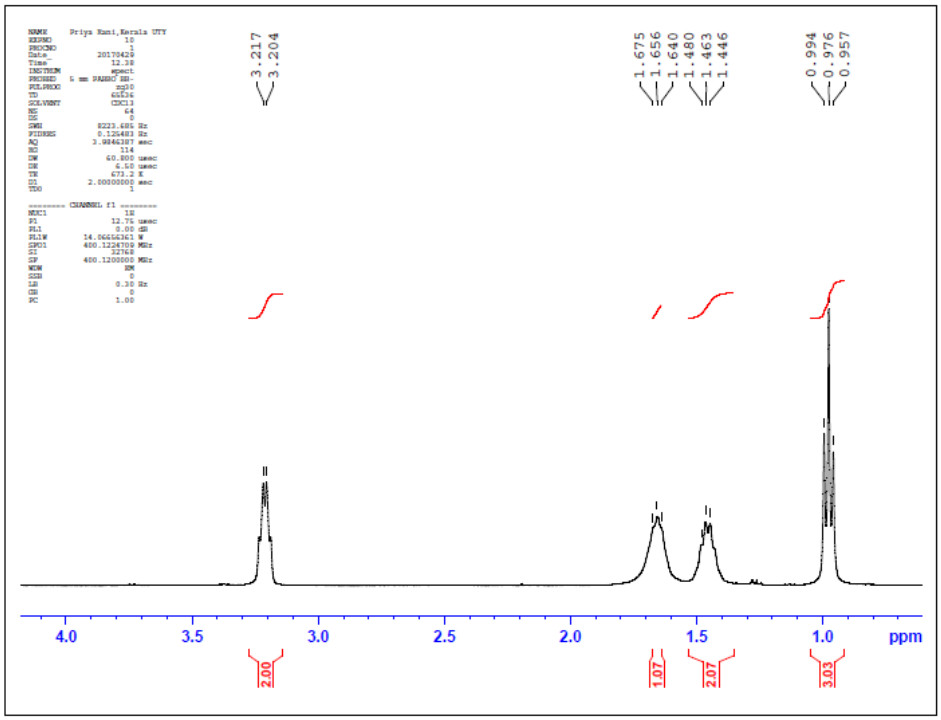


Figure S67. ^{13}C NMR spectrum of *N*-n-butyl)-*N'*-(4-chlorophenylthiocarbamoyl)guanidine **(3g)** (100 MHz, $CDCl_3$)

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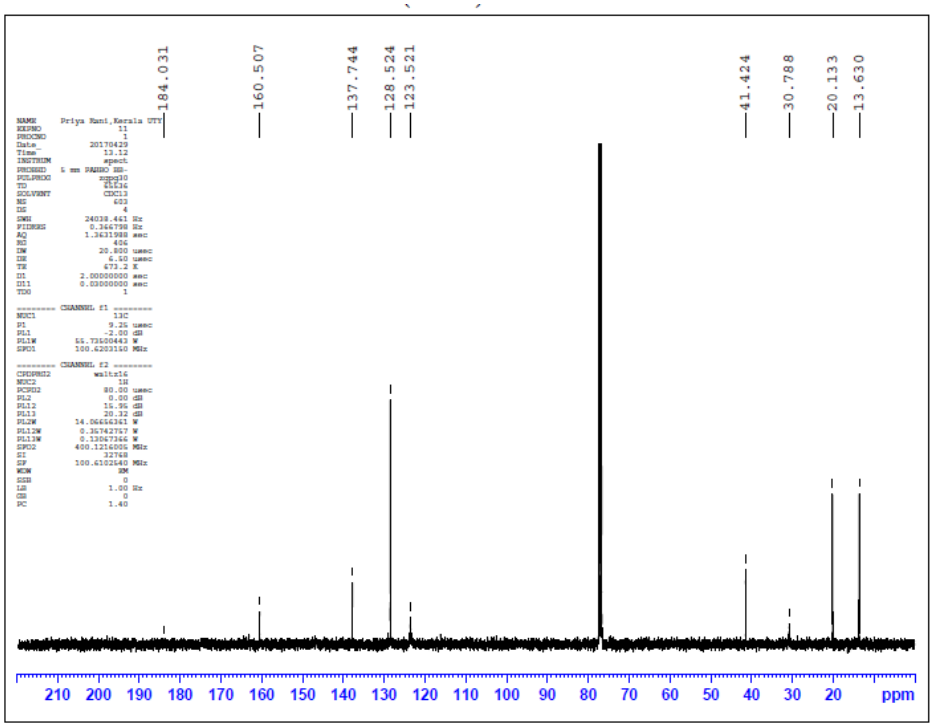
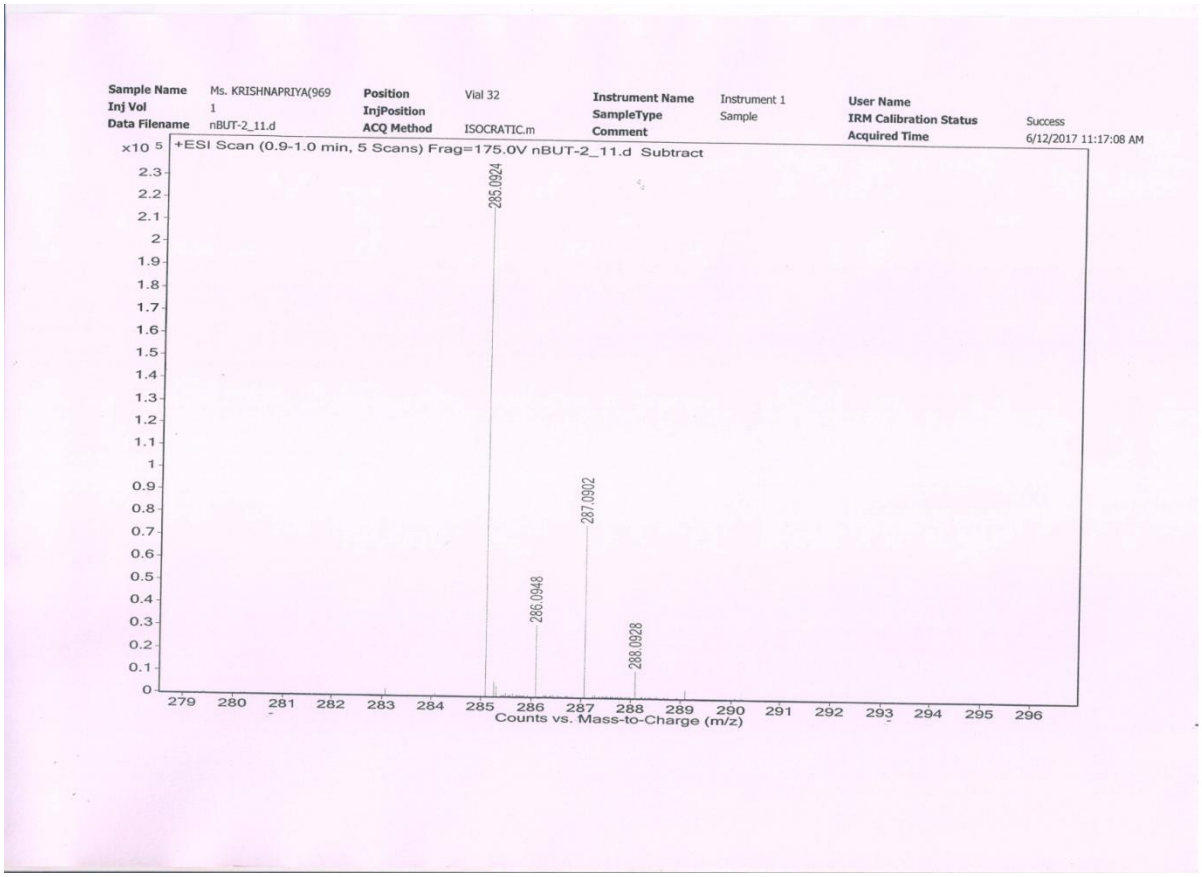


Figure S68. ESI-HRMS spectrum of *N*-n-butyl)-*N'*-(4-chlorophenylthiocarbamoyl)guanidine **(3g)**



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

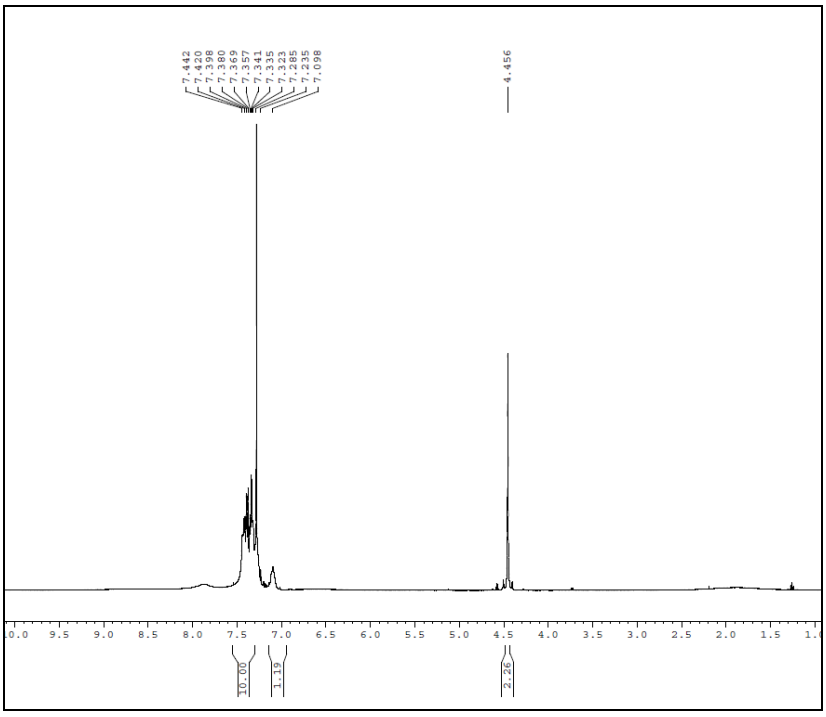


Figure S70. ^{1}H NMR spectrum (expanded) of *N*-benzyl-*N'*-(phenylthiocarbamoyl)guanidine **(3h)** (400 MHz, $CDCl_3$)

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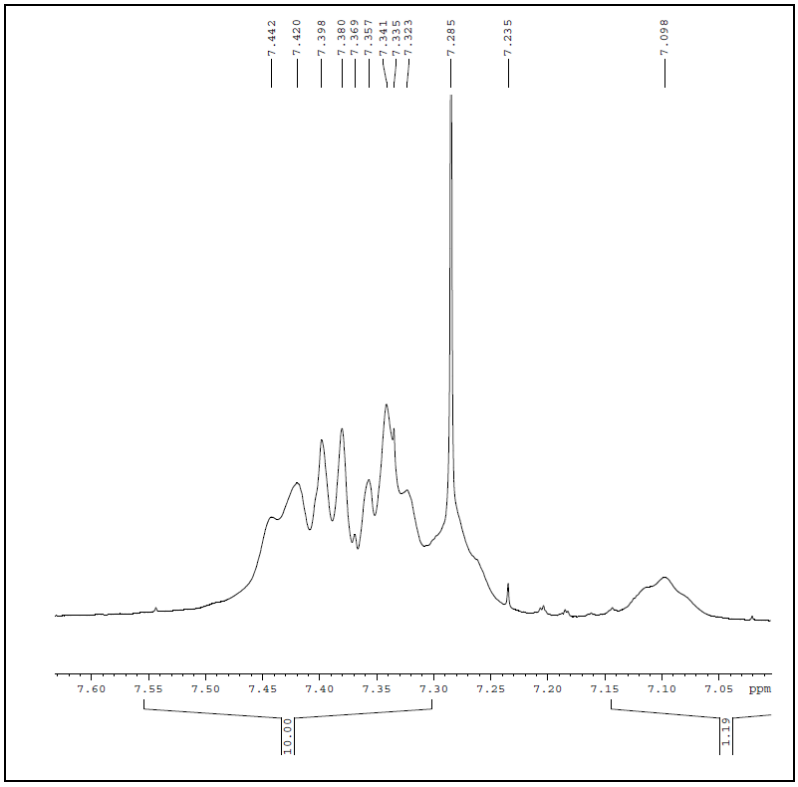


Figure S71. ^{13}C NMR spectrum of *N*-benzyl-*N'*-(phenylthiocarbamoyl)guanidine **(3h)** (100 MHz, $CDCl_3$)

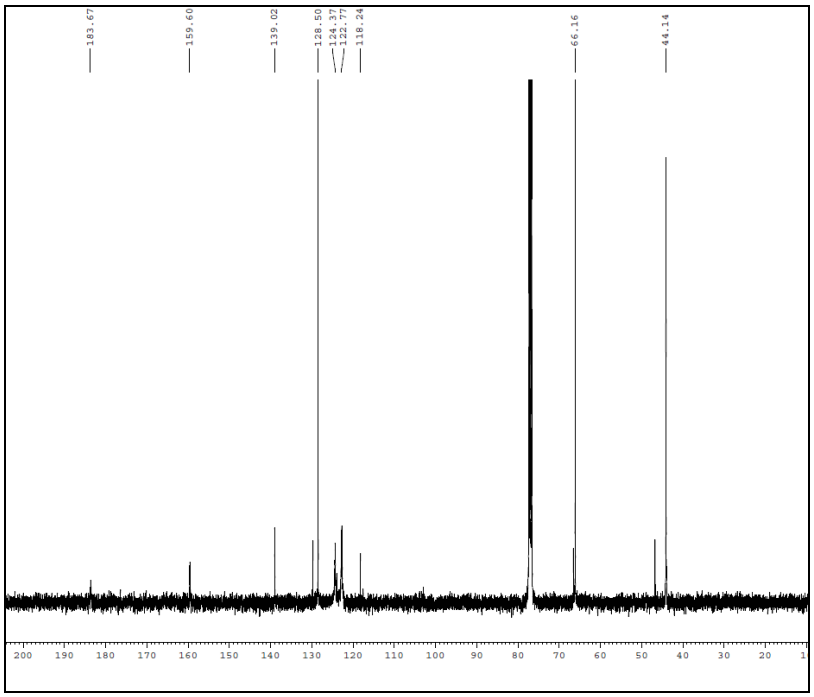


Figure S72. ESI-HRMS spectrum of *N*-benzyl-*N'*-(phenylthiocarbamoyl)guanidine **(3h)**

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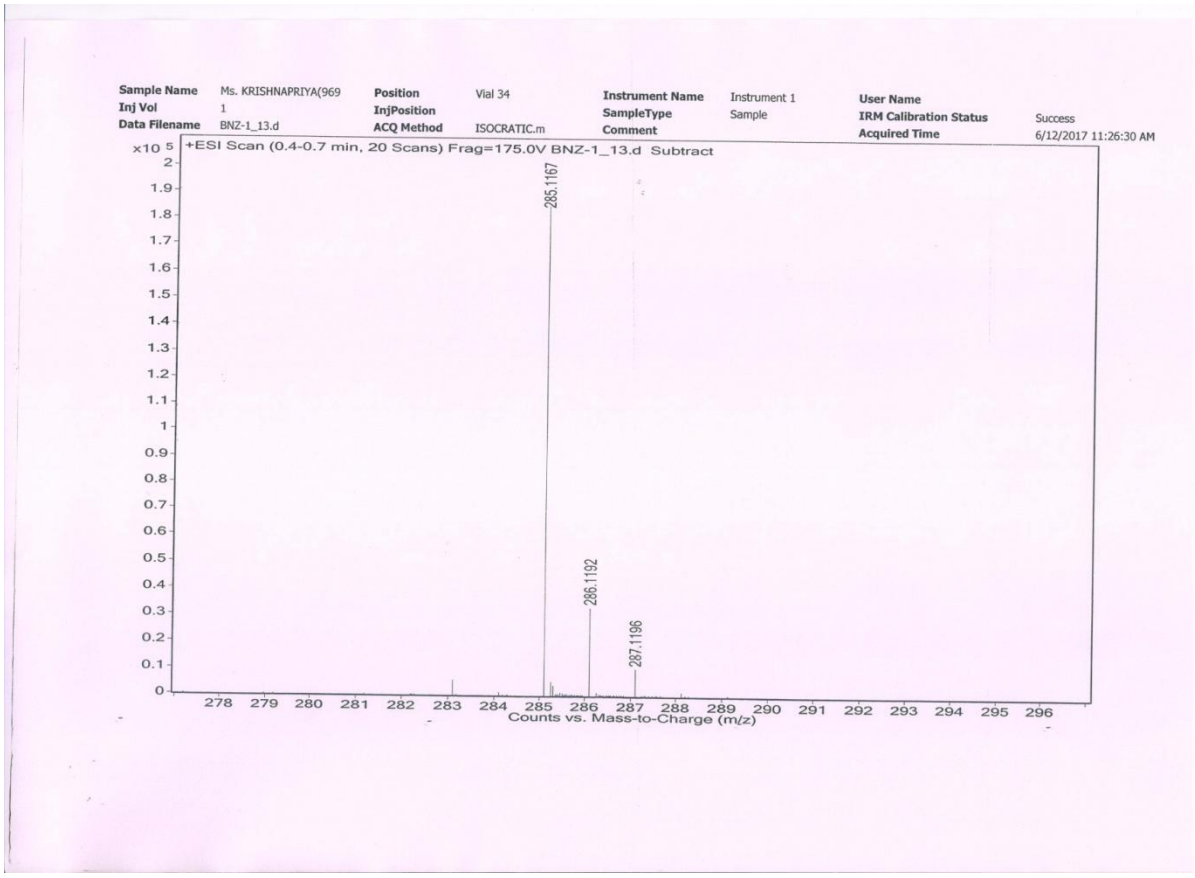
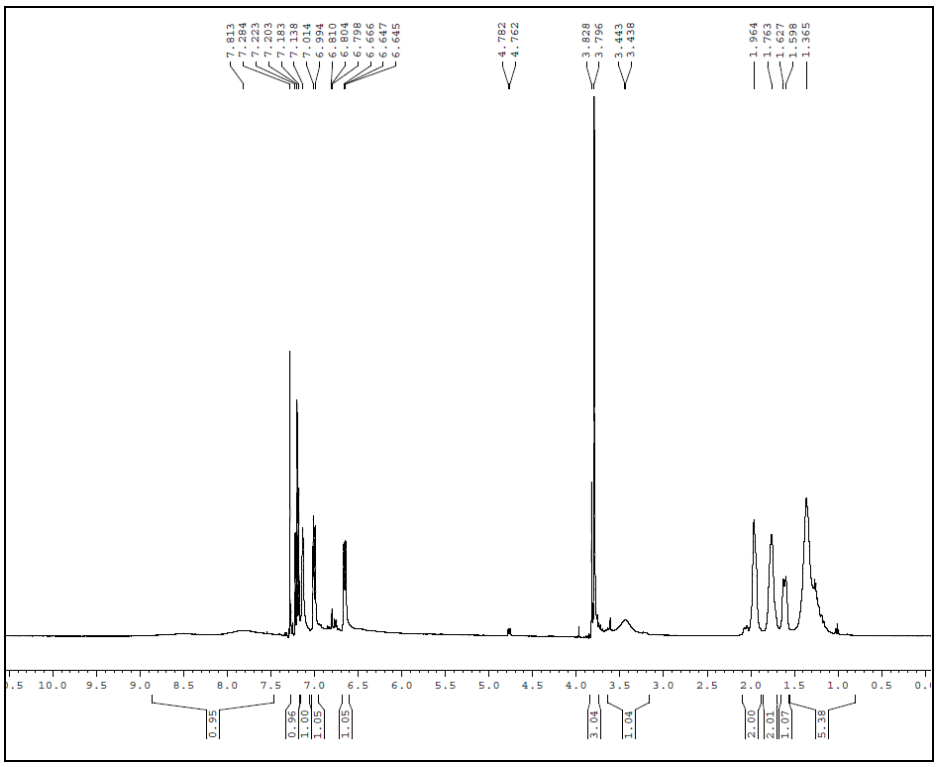


Figure S73. ^{1}H NMR spectrum of *N*-cyclohexyl-*N'*-(3-methoxyphenylthiocarbamoyl)guanidine **(3i)** (400 MHz, $CDCl_3$)



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

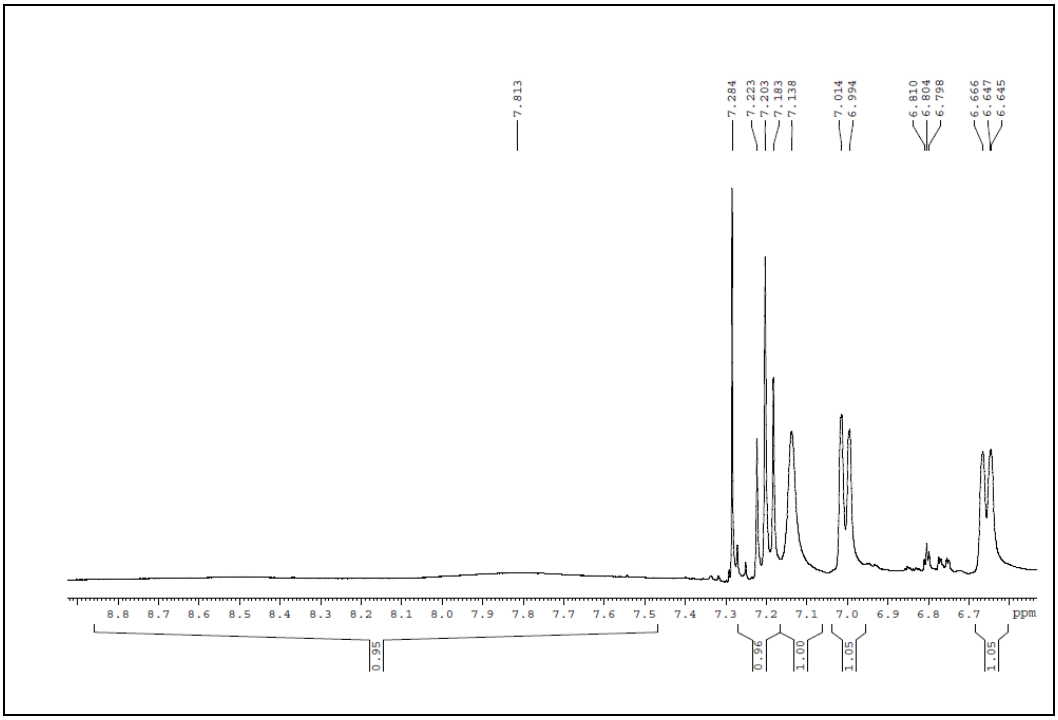
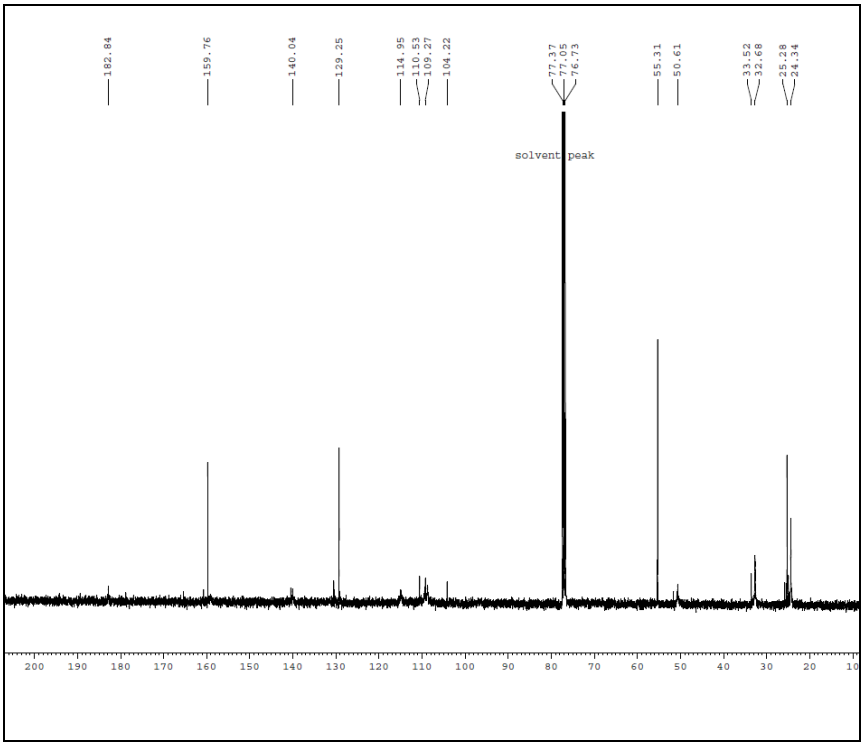
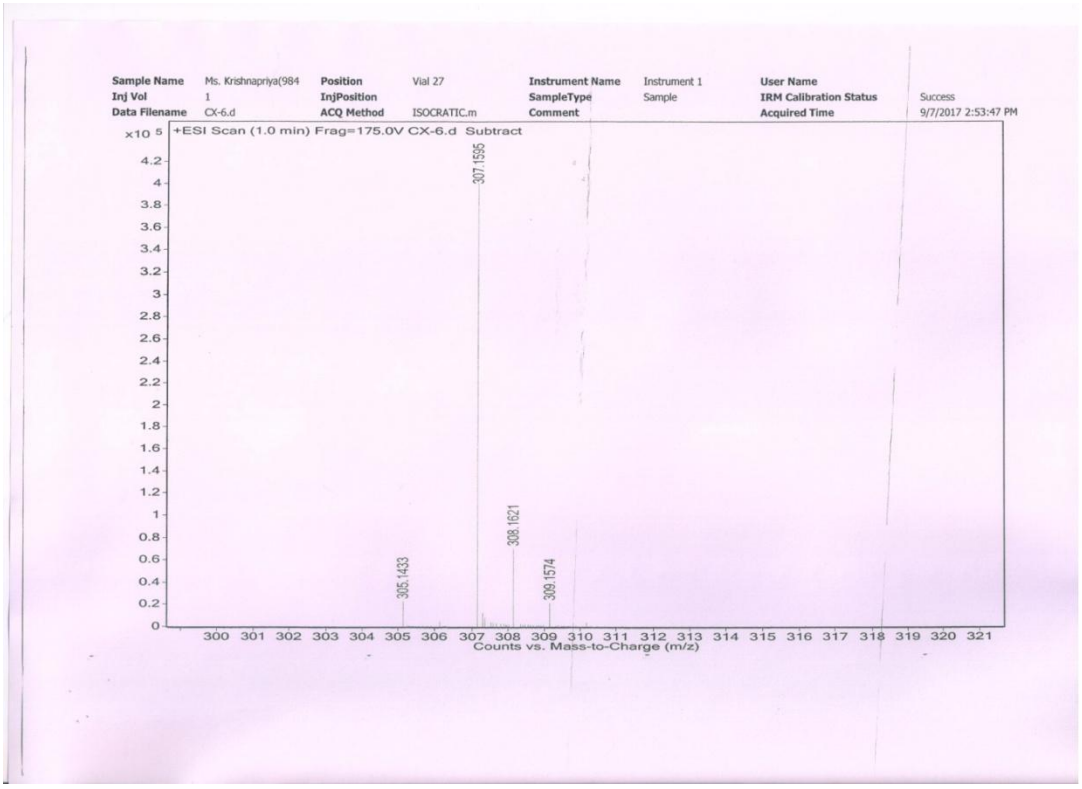


Figure S75. ^{13}C NMR spectrum of *N*-cyclohexyl-*N'*-(3-methoxyphenylthiocarbamoyl)guanidine **(3i)** (100 MHz, $CDCl_3$)



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



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