

Supporting Information

Synthesis and anticancer activity studies of new functionalized pyridine linked thiazole derivatives

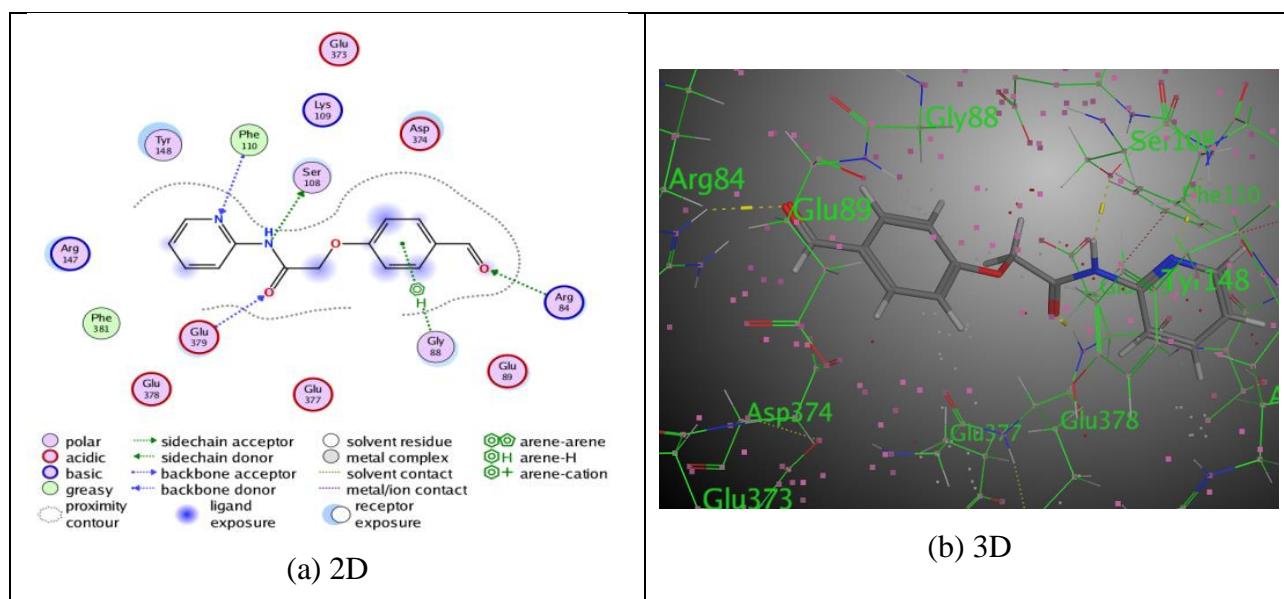


Figure S1. The binding interaction of **2** with Rho-associated protein kinase 1 (PDB ID: 3TWJ).

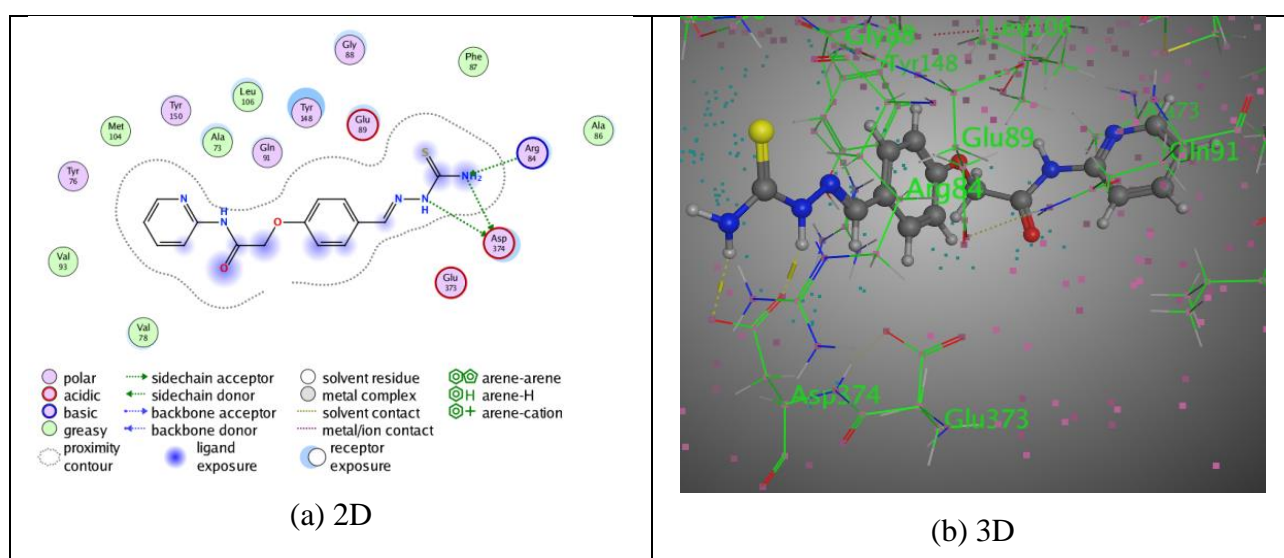


Figure S2. The binding interaction of **3** with Rho-associated protein kinase 1 (PDB ID: 3TWJ).

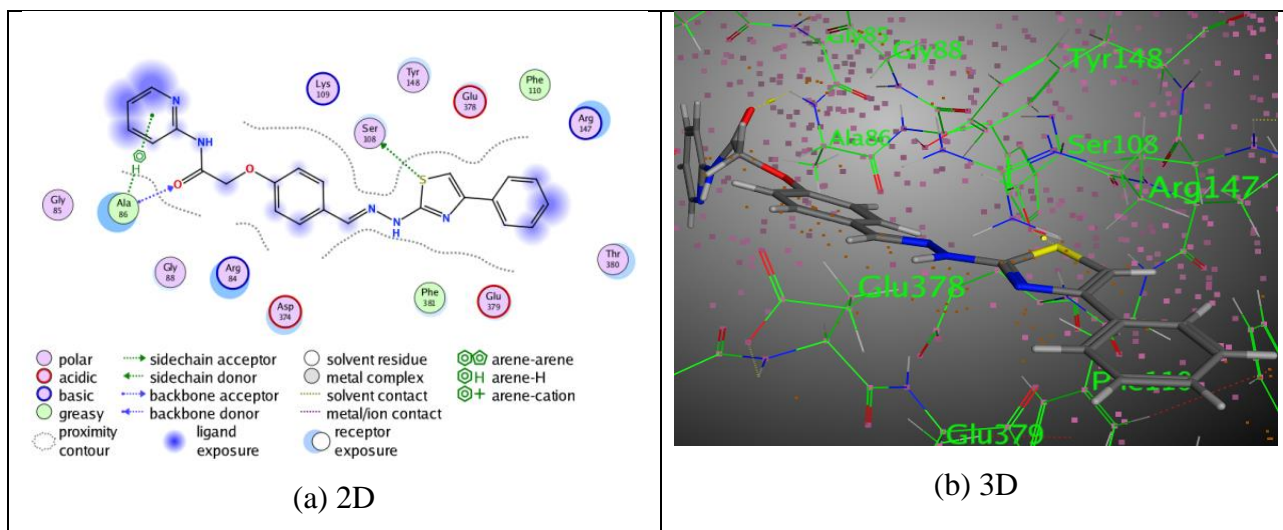


Figure S3. The binding interaction of **4a** with Rho-associated protein kinase 1 (PDB ID: 3TWJ).

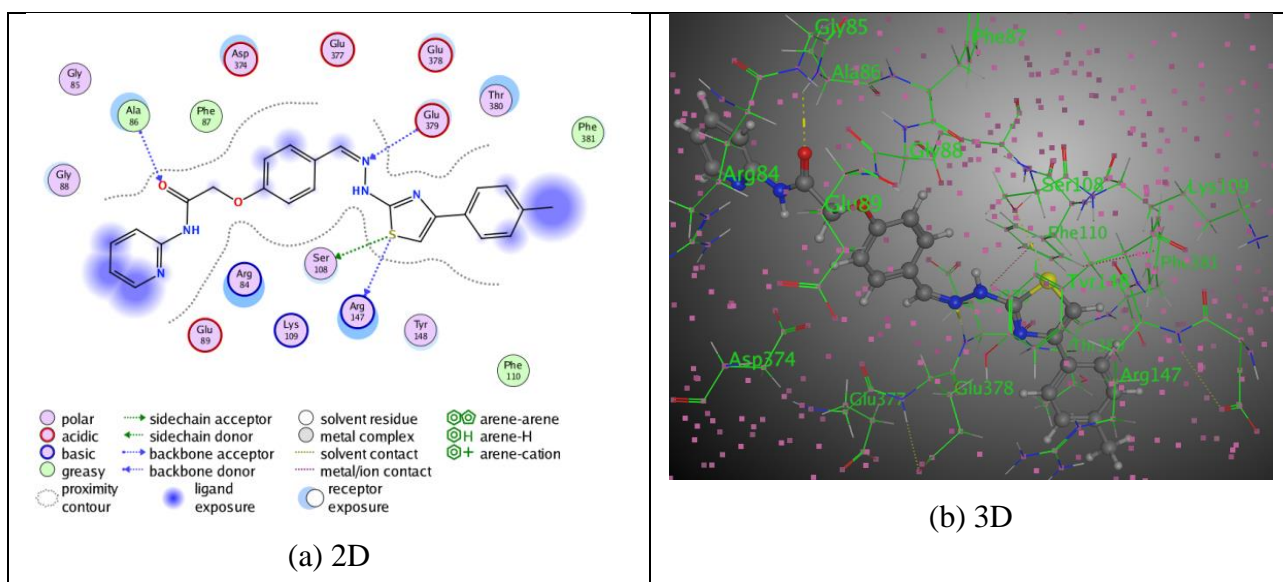


Figure S4. The binding interaction of **4b** Rho-associated protein kinase 1 (PDB ID: 3TWJ).

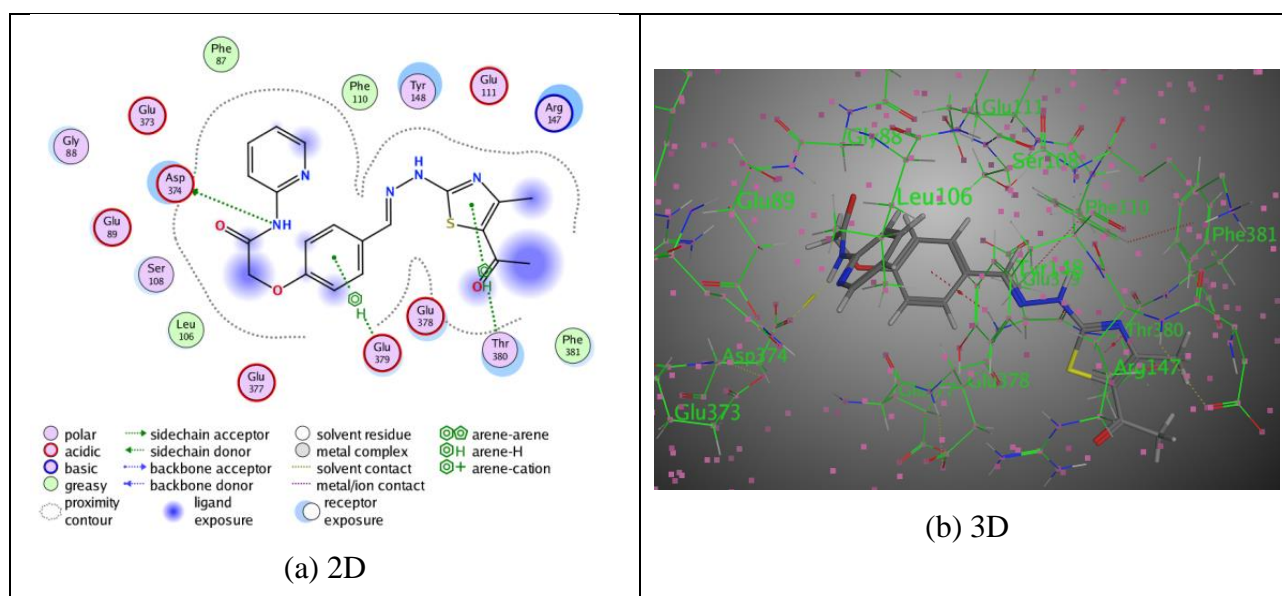


Figure S5. The interaction of **8** with Rho-associated protein kinase 1 (PDB ID: 3TWJ).

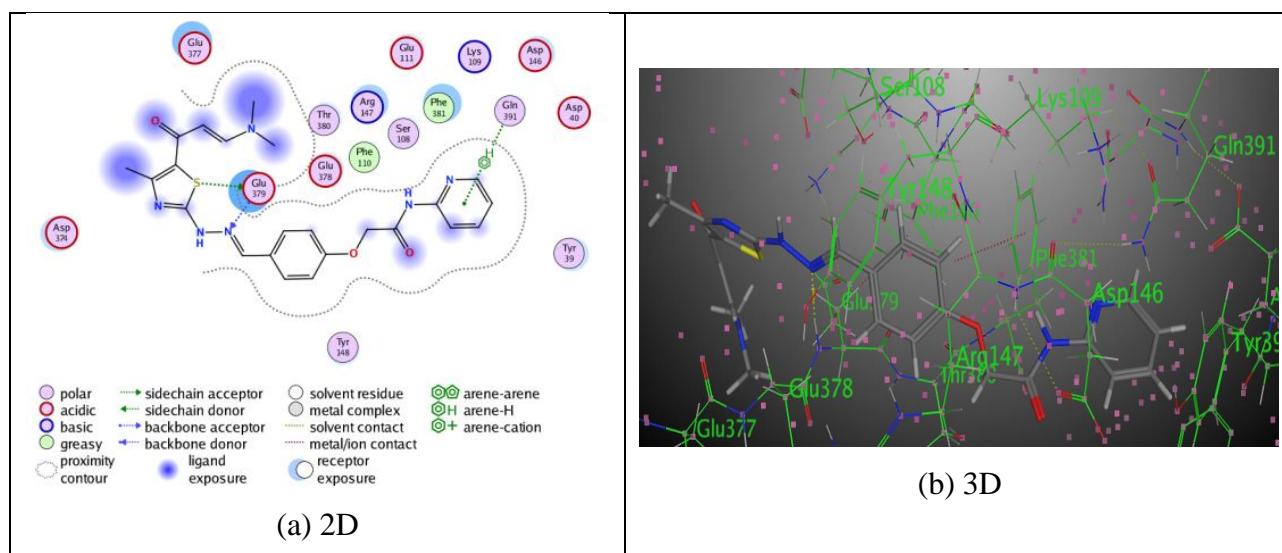


Figure S6. The interaction of **9** with Rho-associated protein kinase 1 (PDB ID: 3TWJ).

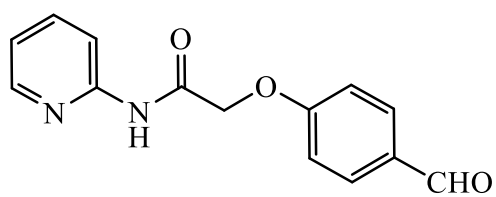
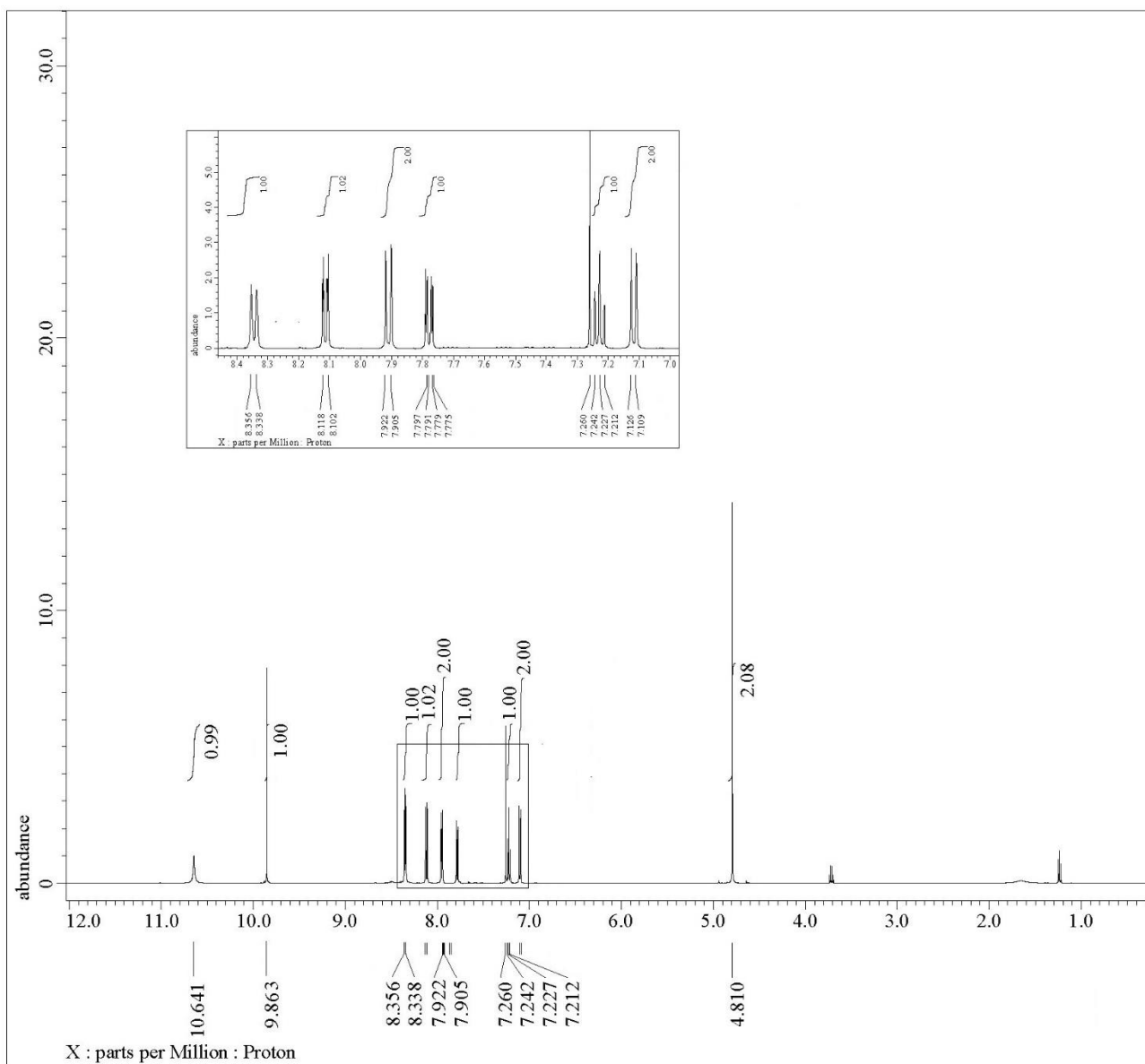


Figure S7. ¹H NMR spectrum of compound (2)

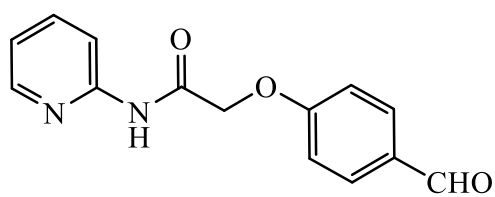
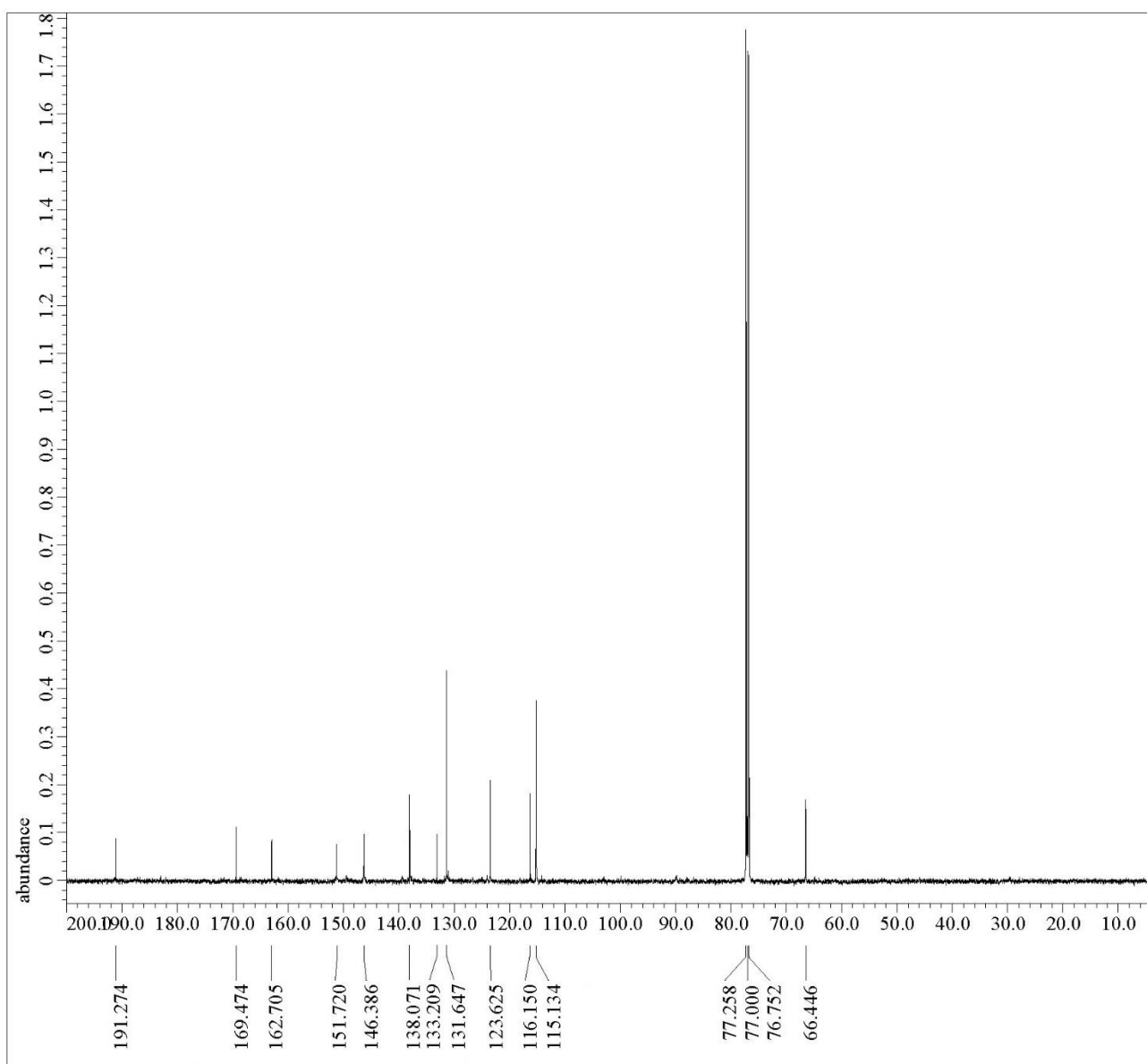
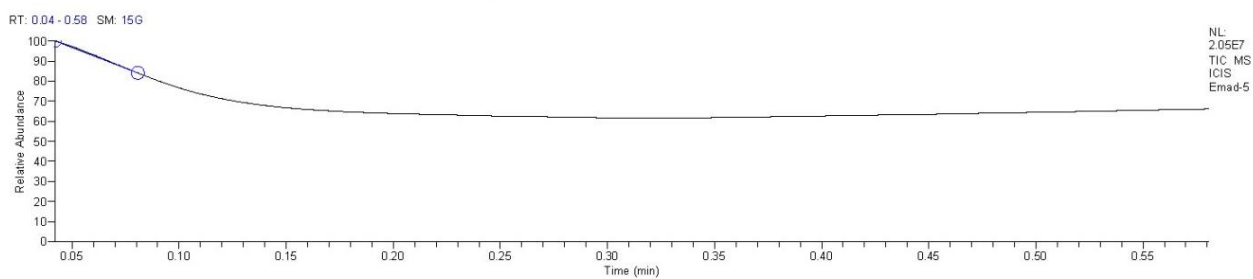


Figure S8. ^{13}C NMR spectrum of compound (2)

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Emad-5 #2 RT: 0.05 AV: 1 TH: 0.01 NL: 2.74E6
T: + c Full ms [50.00-330.00]

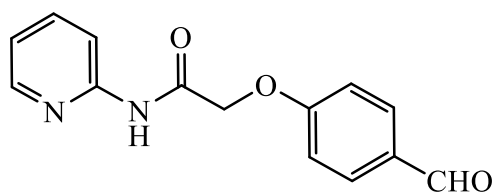
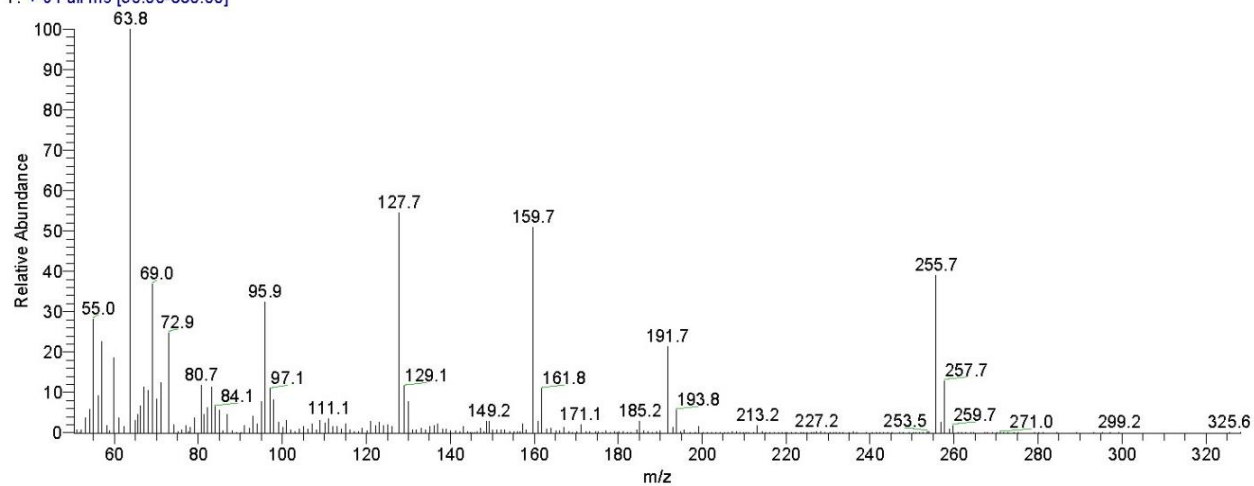


Figure S9. Mass analysis of compound (2)

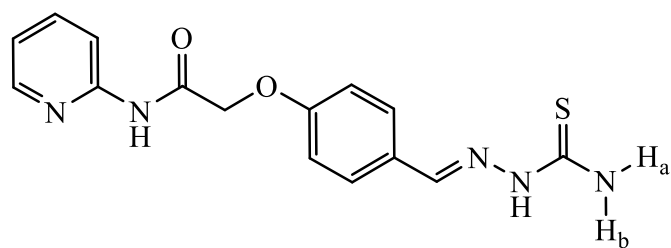
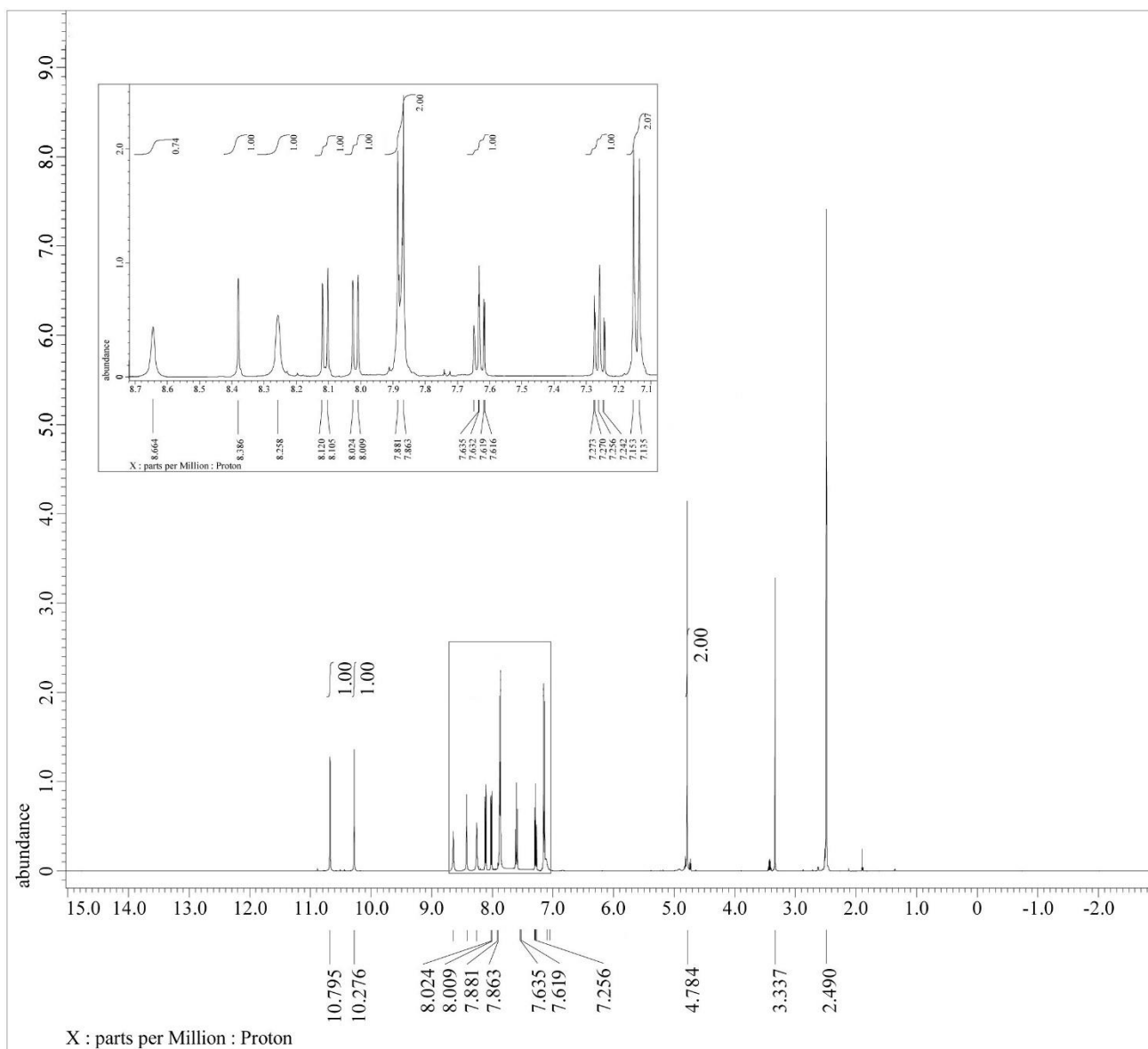


Figure S10. ¹H NMR spectrum of compound (3)

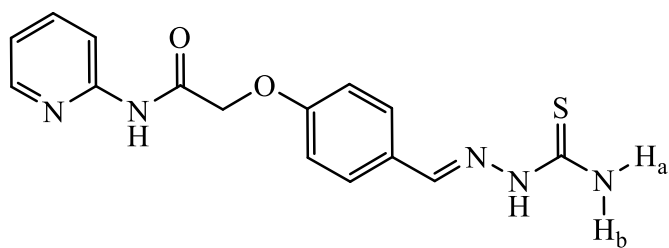
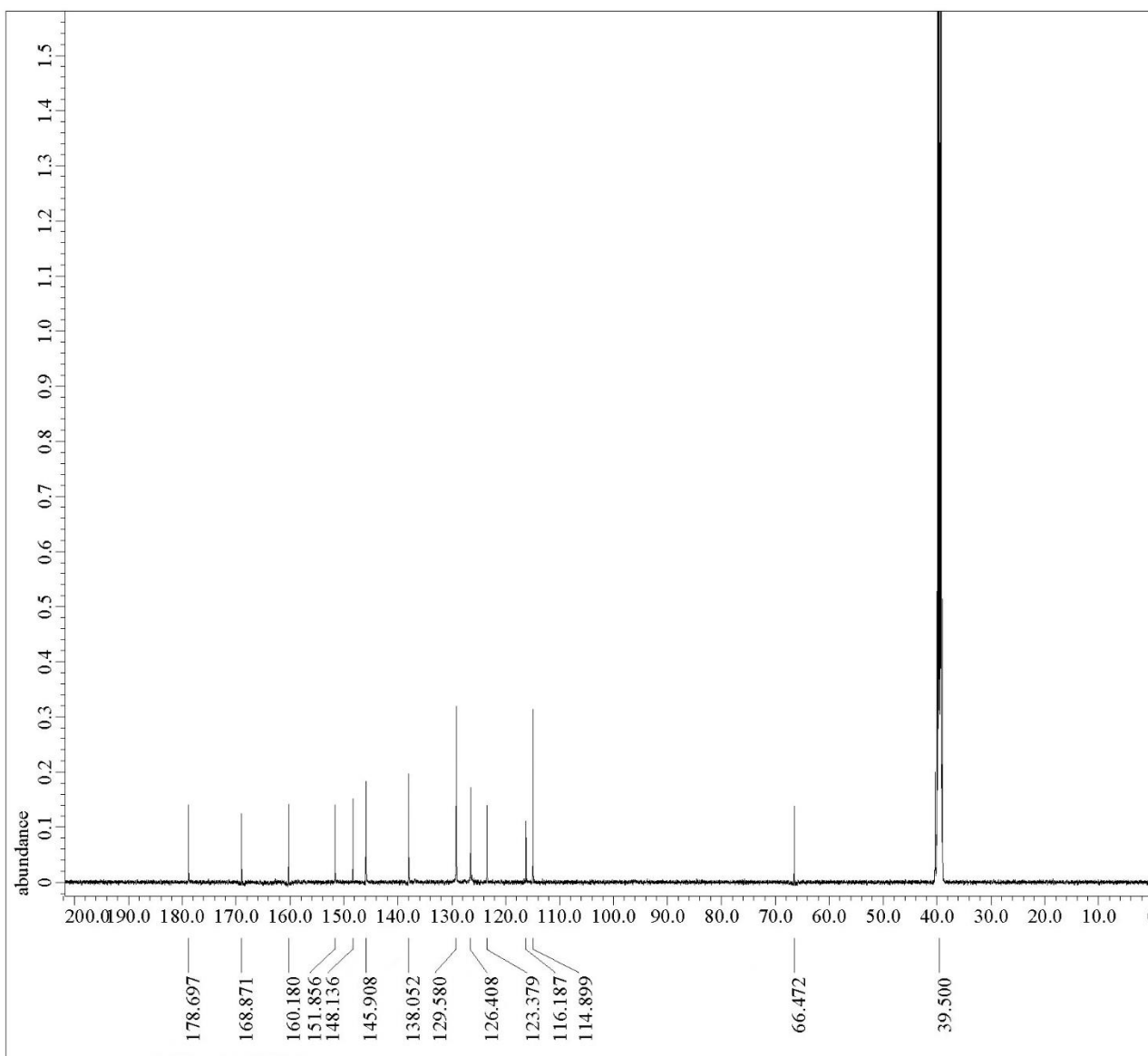
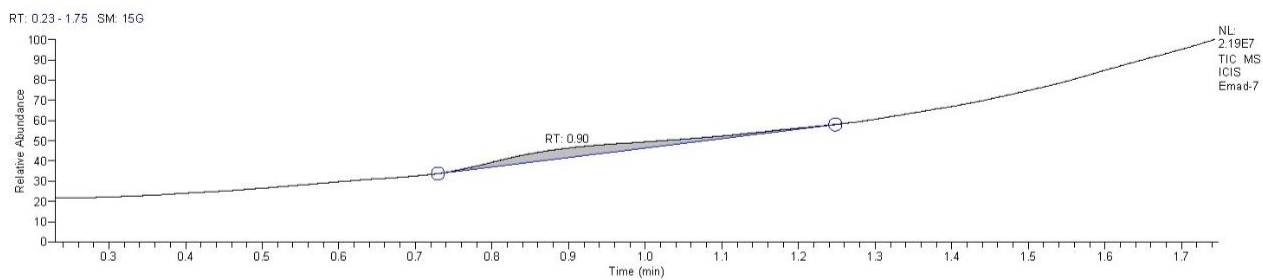


Figure S11. ^{13}C NMR spectrum of compound (3)

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Emad-7 #72 RT: 0.90 AV: 1 TH: 0.01 NL: 1.23E6
T: + c Full ms [50.00-400.00]

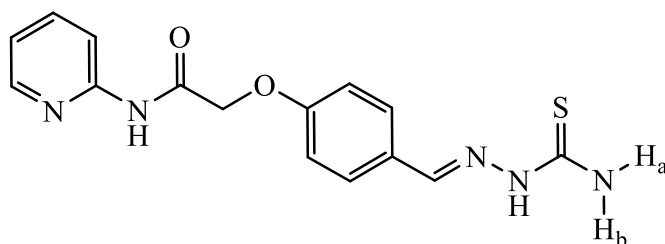
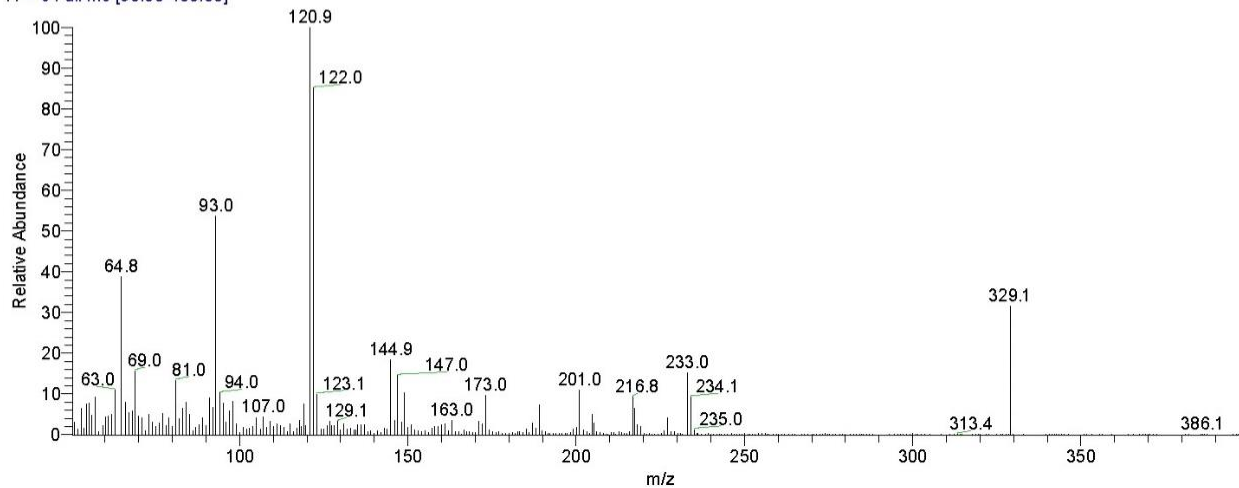


Figure S12. Mass analysis of compound (3)

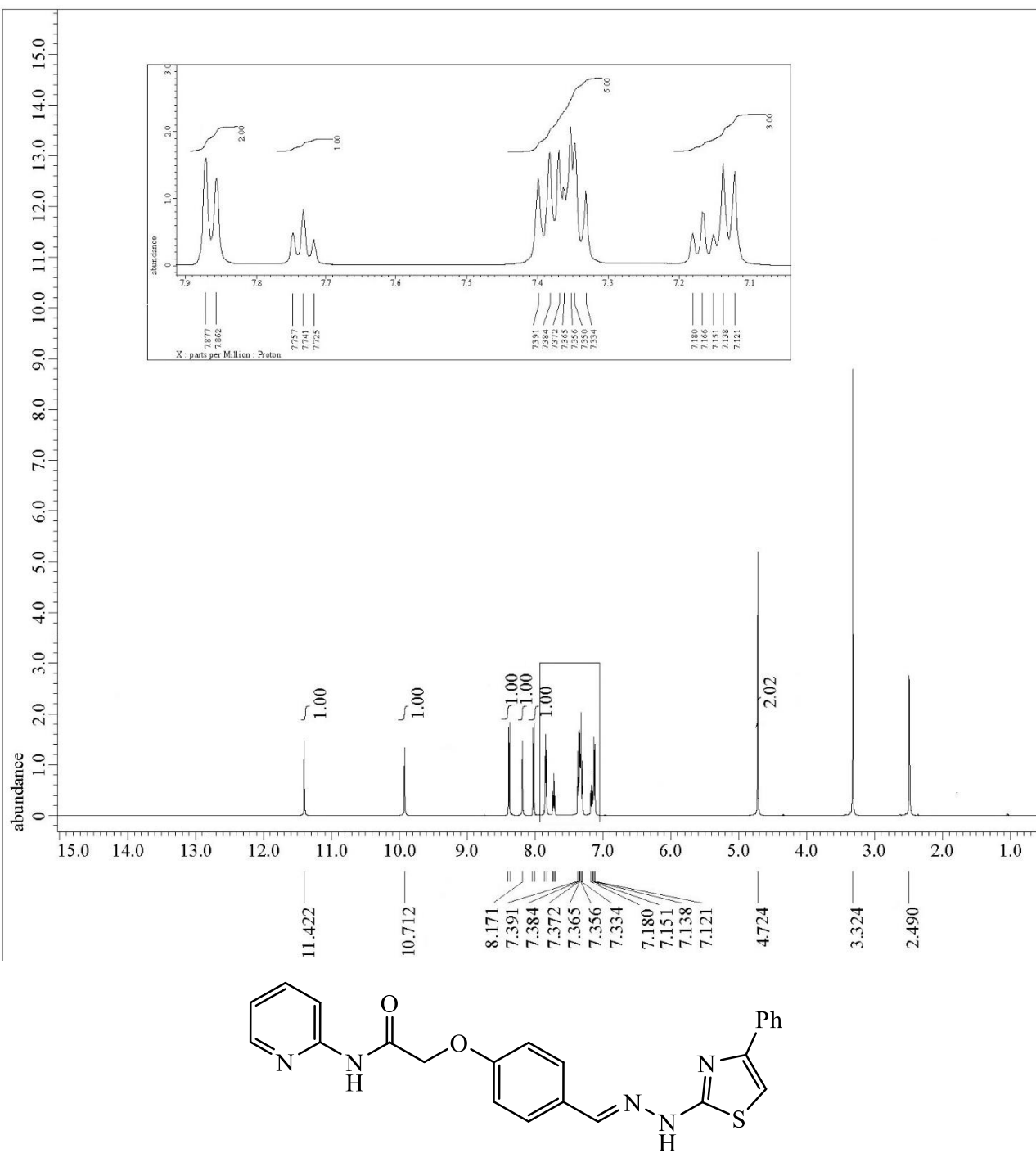


Figure S13. ¹H NMR spectrum of compound (4a)

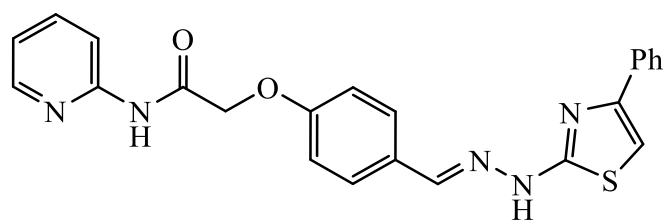
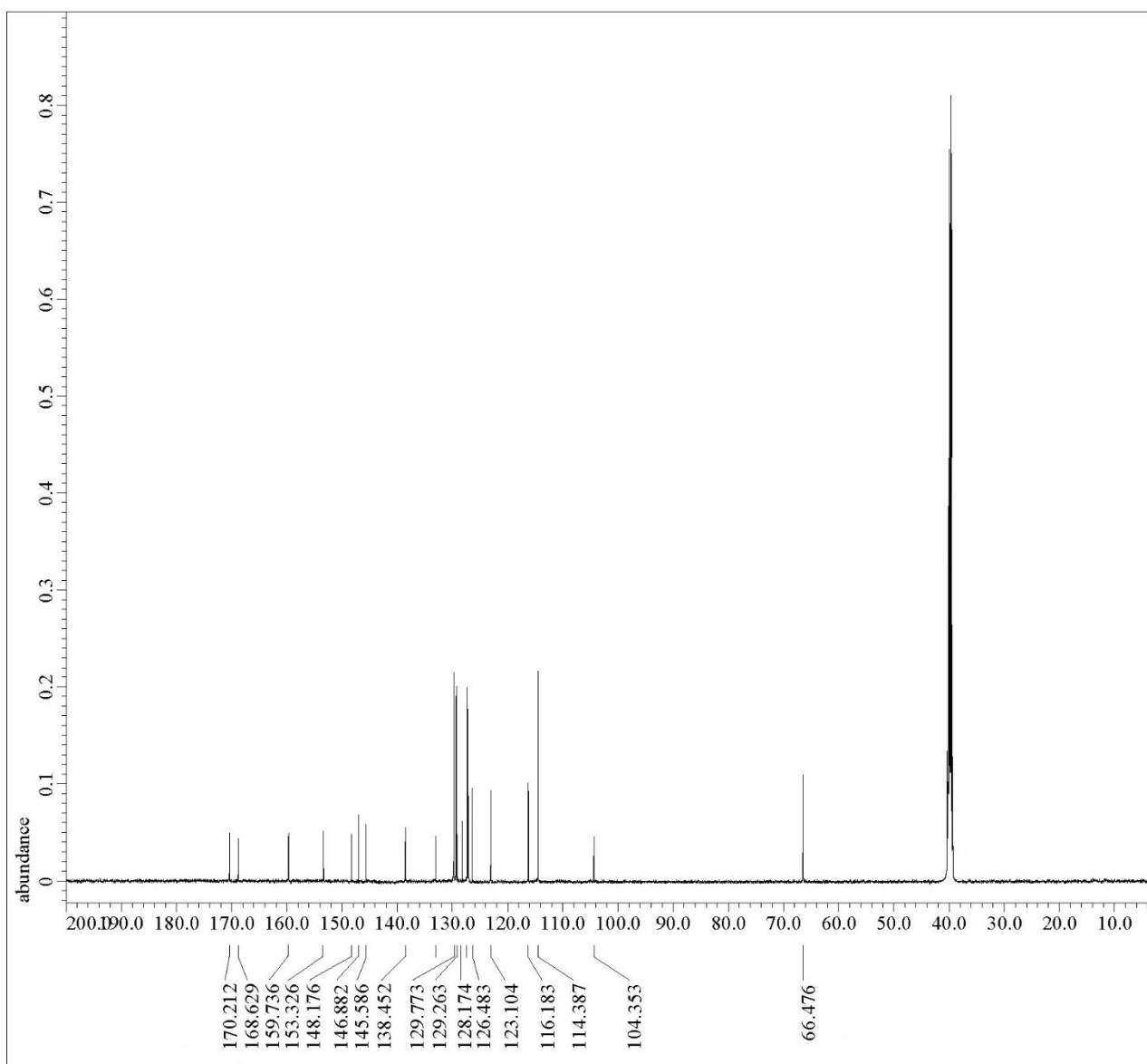
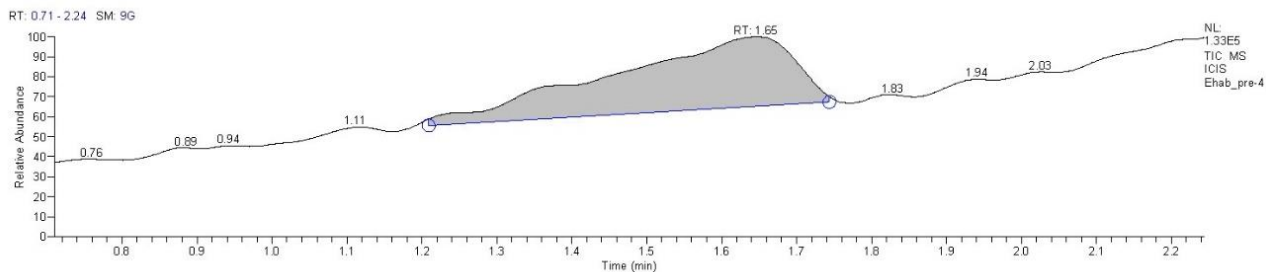


Figure S14. ^{13}C NMR spectrum of compound (4a)

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Ehab_pre-4 #115 RT: 1.65 AV: 1 TH: 0.05 NL: 2.51E4
T: + c Full ms [40.00-450.00]

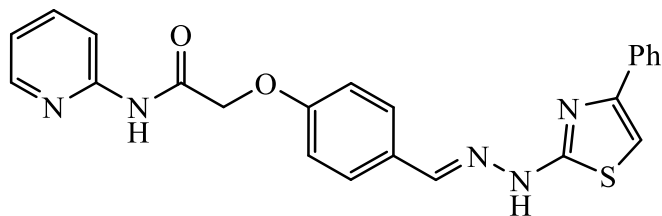
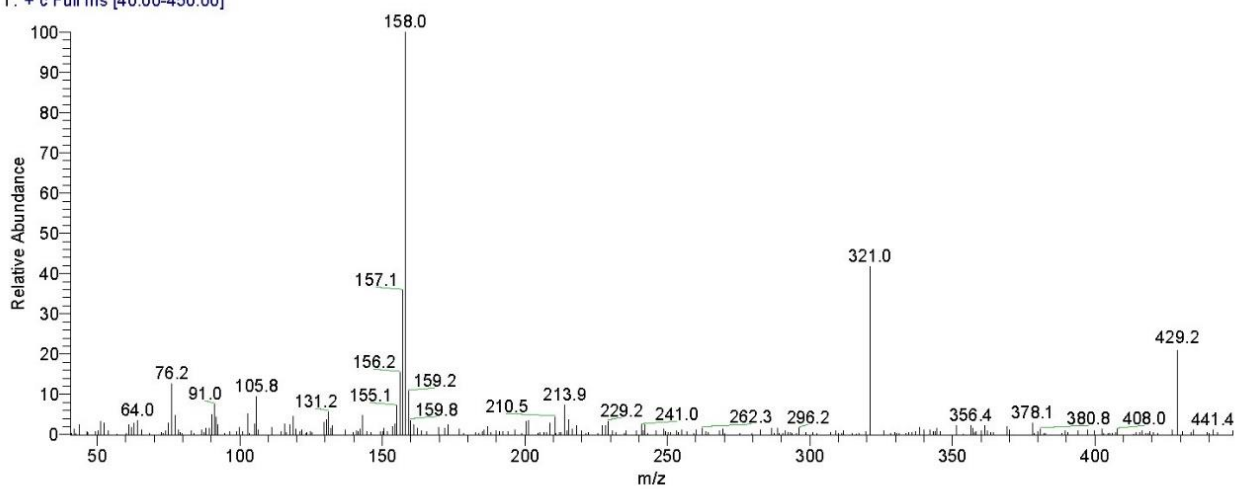


Figure S15. Mass analysis of compound (4a)

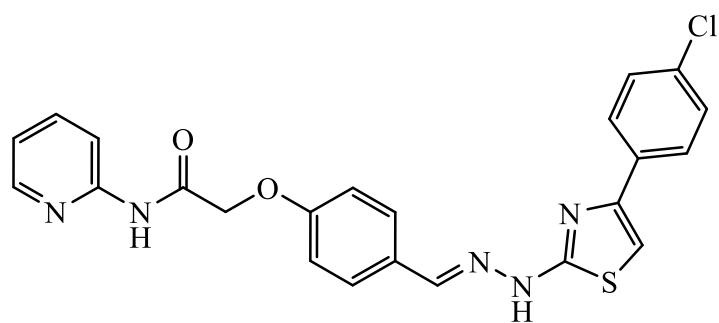
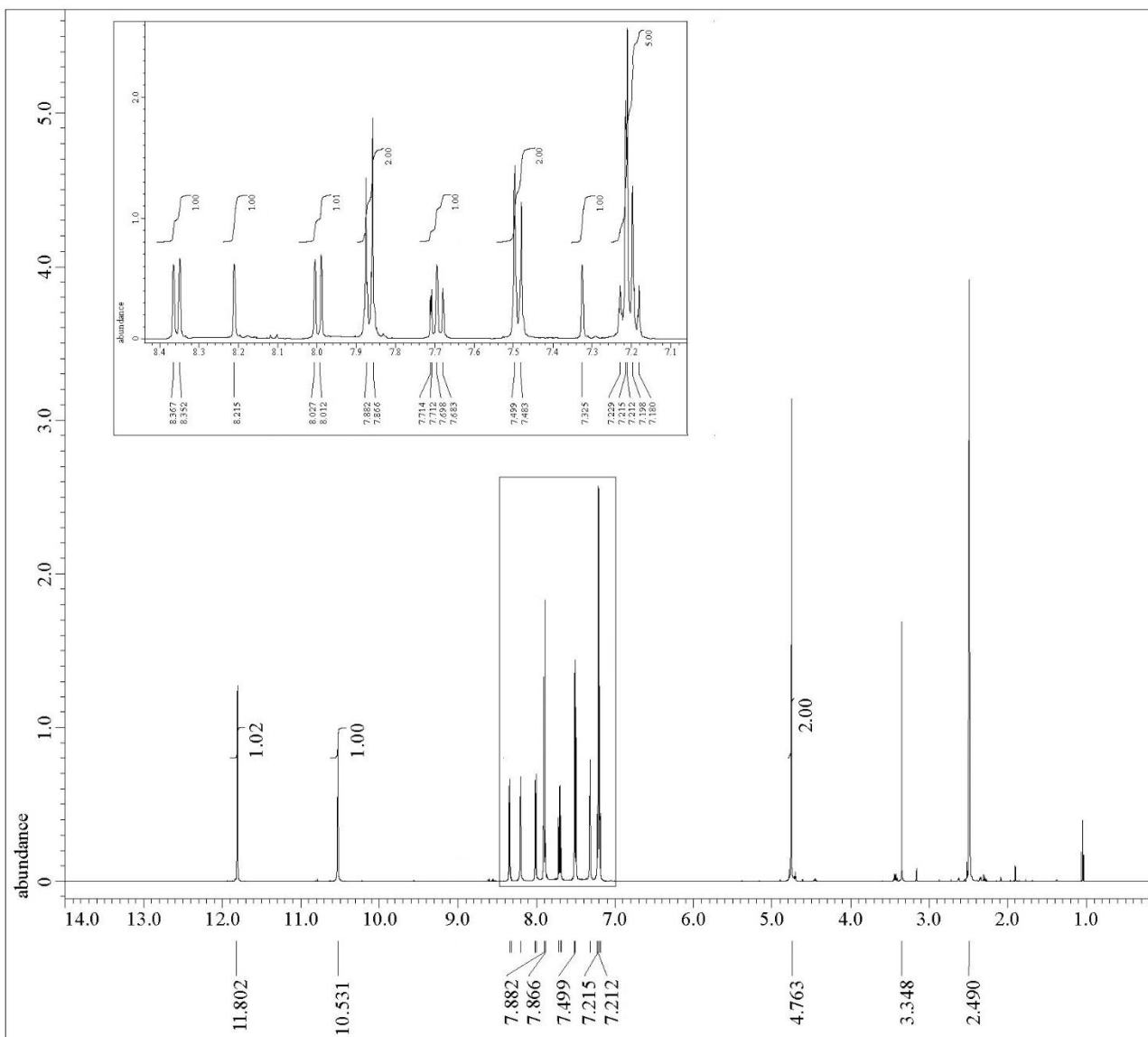


Figure S16. ¹H NMR spectrum of compound (4b)

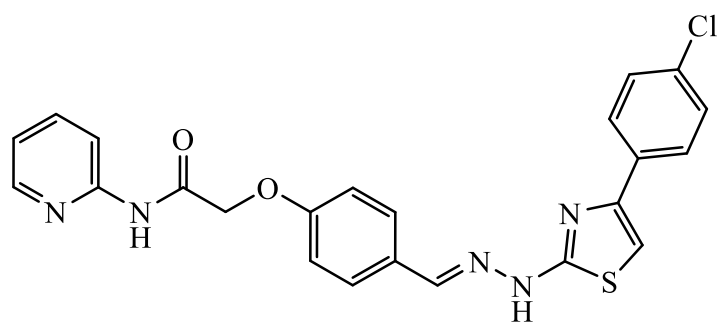
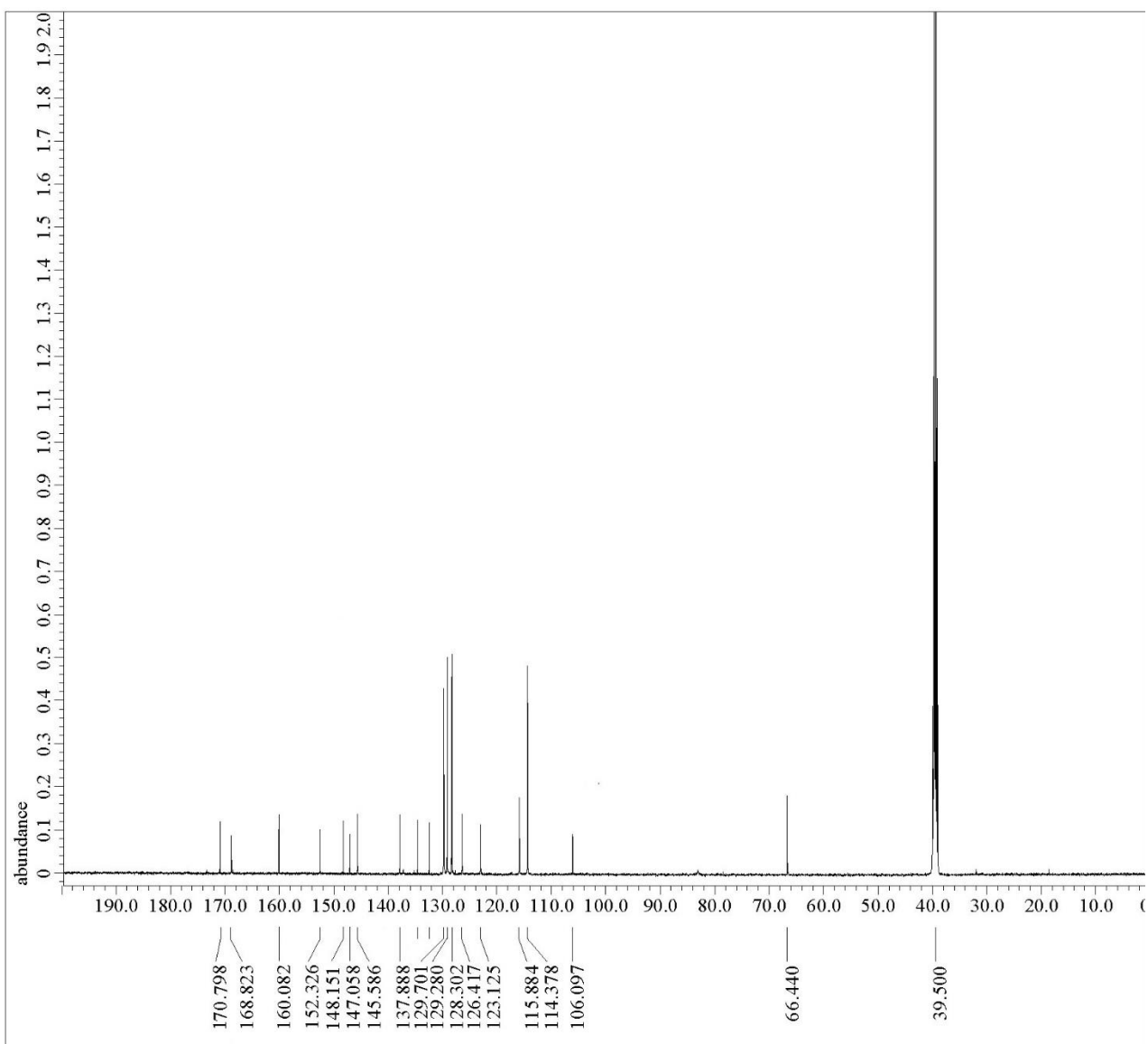
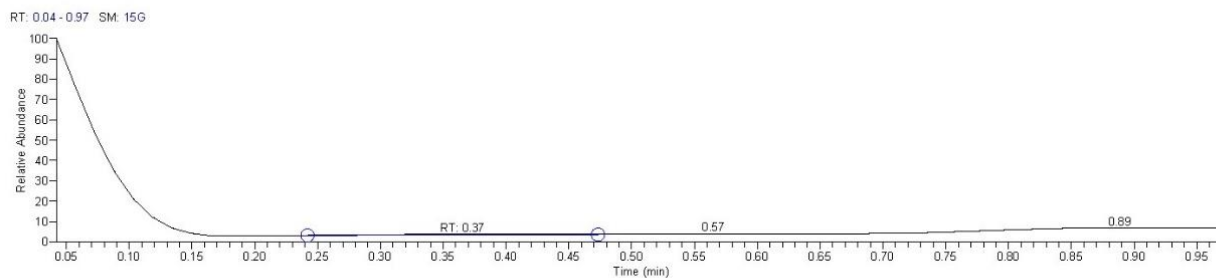


Figure S17. ^{13}C NMR spectrum of compound (4b)

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Fatama-Fat5 #22 RT: 0.37 AV: 1 TH: 0.01 NL: 1.12E3
T: + c Full ms [50.00-500.00]

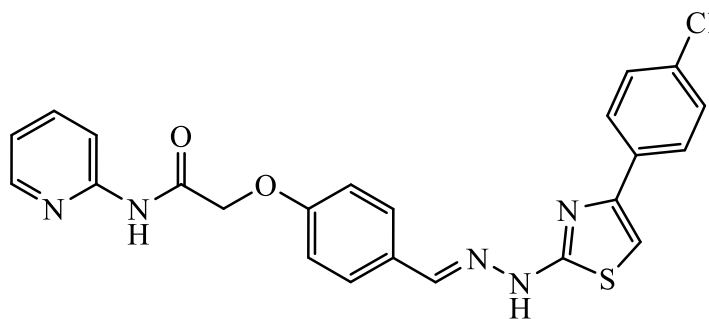
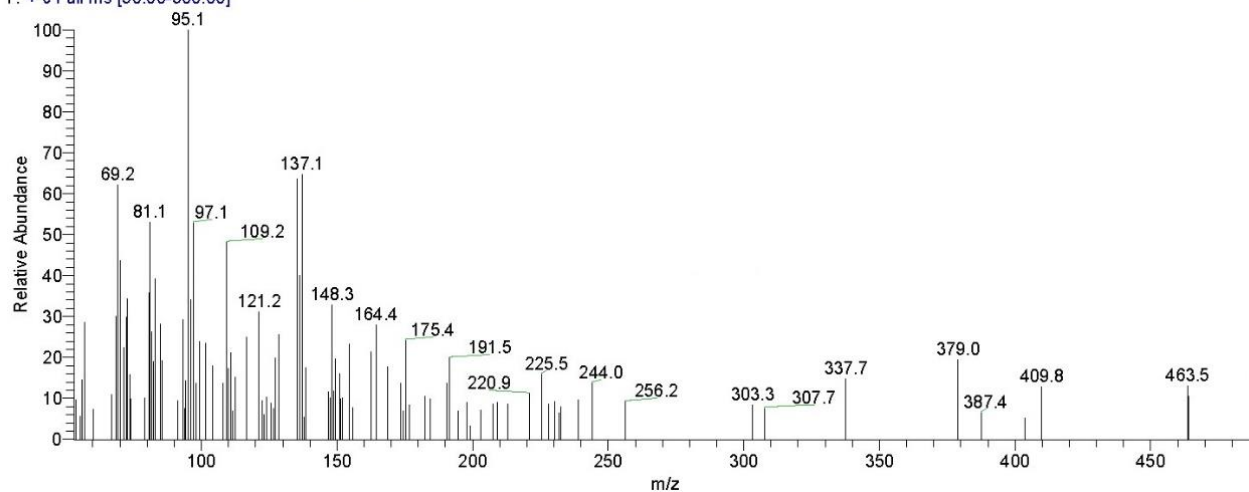


Figure S18. Mass analysis of compound (4b)

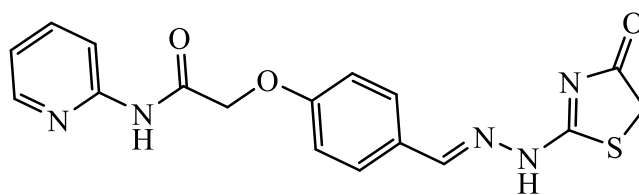
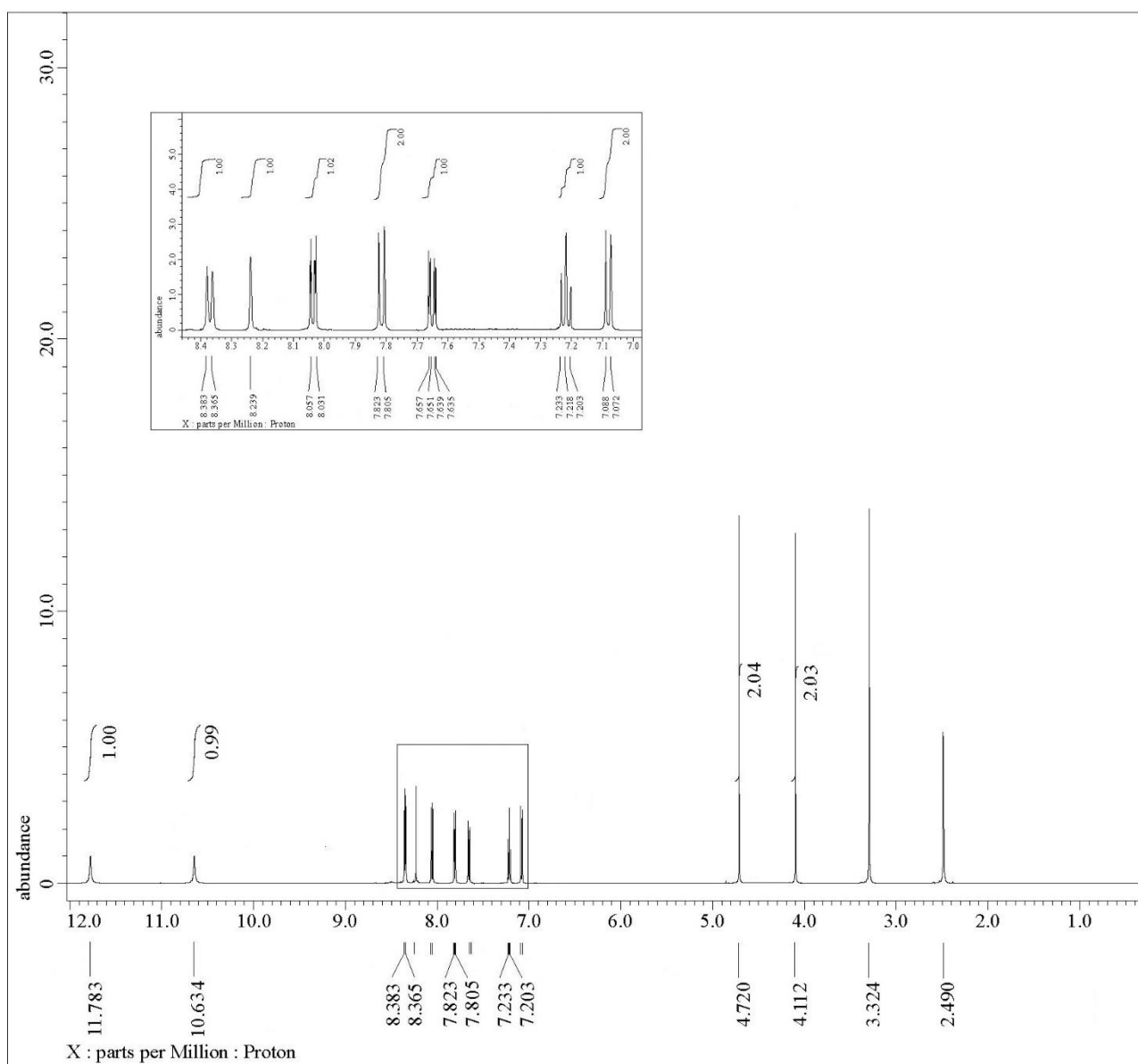


Figure S19. ^1H NMR spectrum of compound (5)

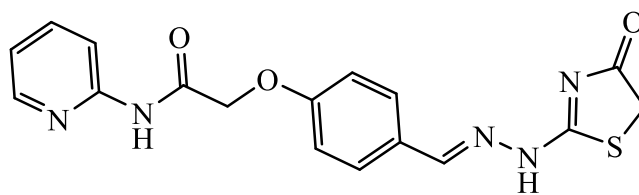
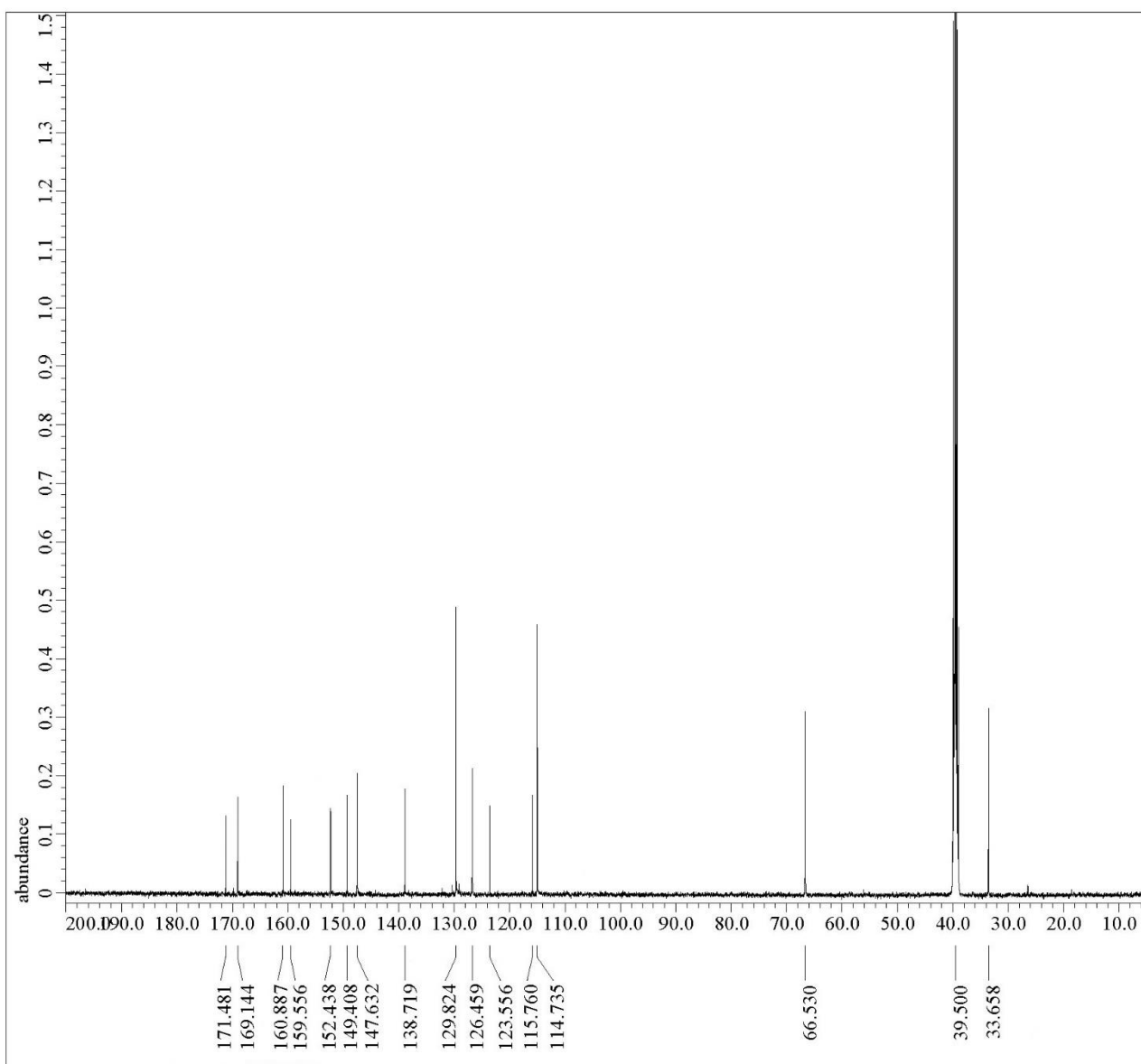


Figure S20. ^{13}C NMR spectrum of compound (5)

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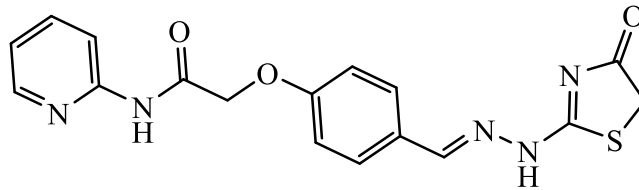
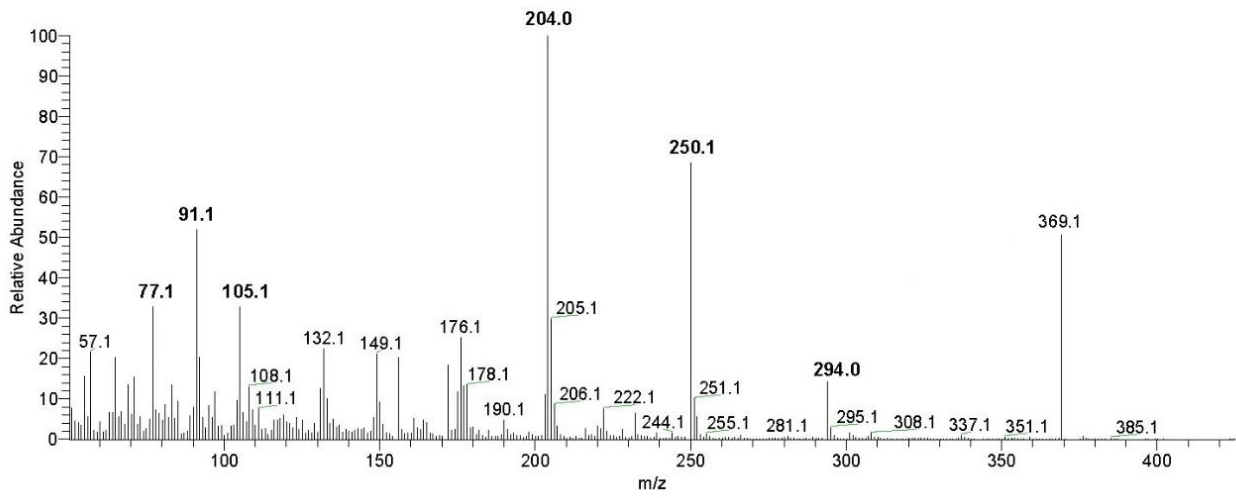
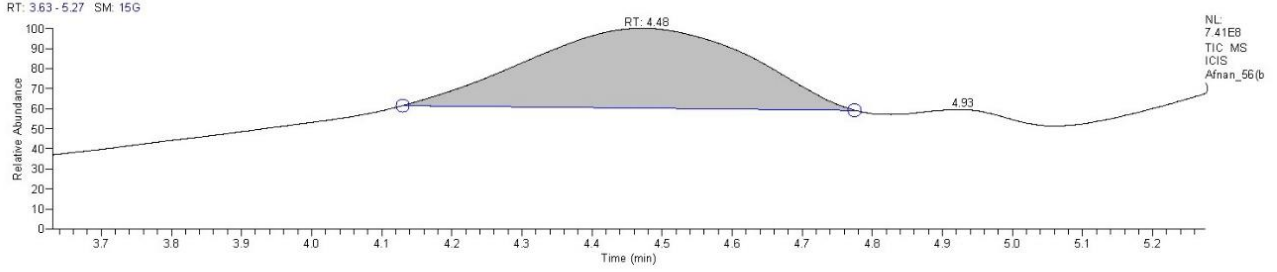


Figure S21. Mass analysis of compound (5)

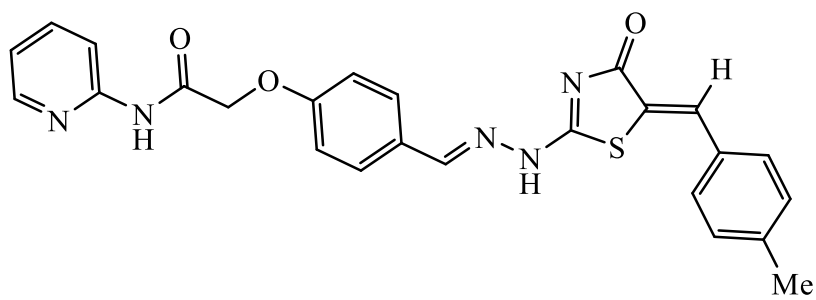
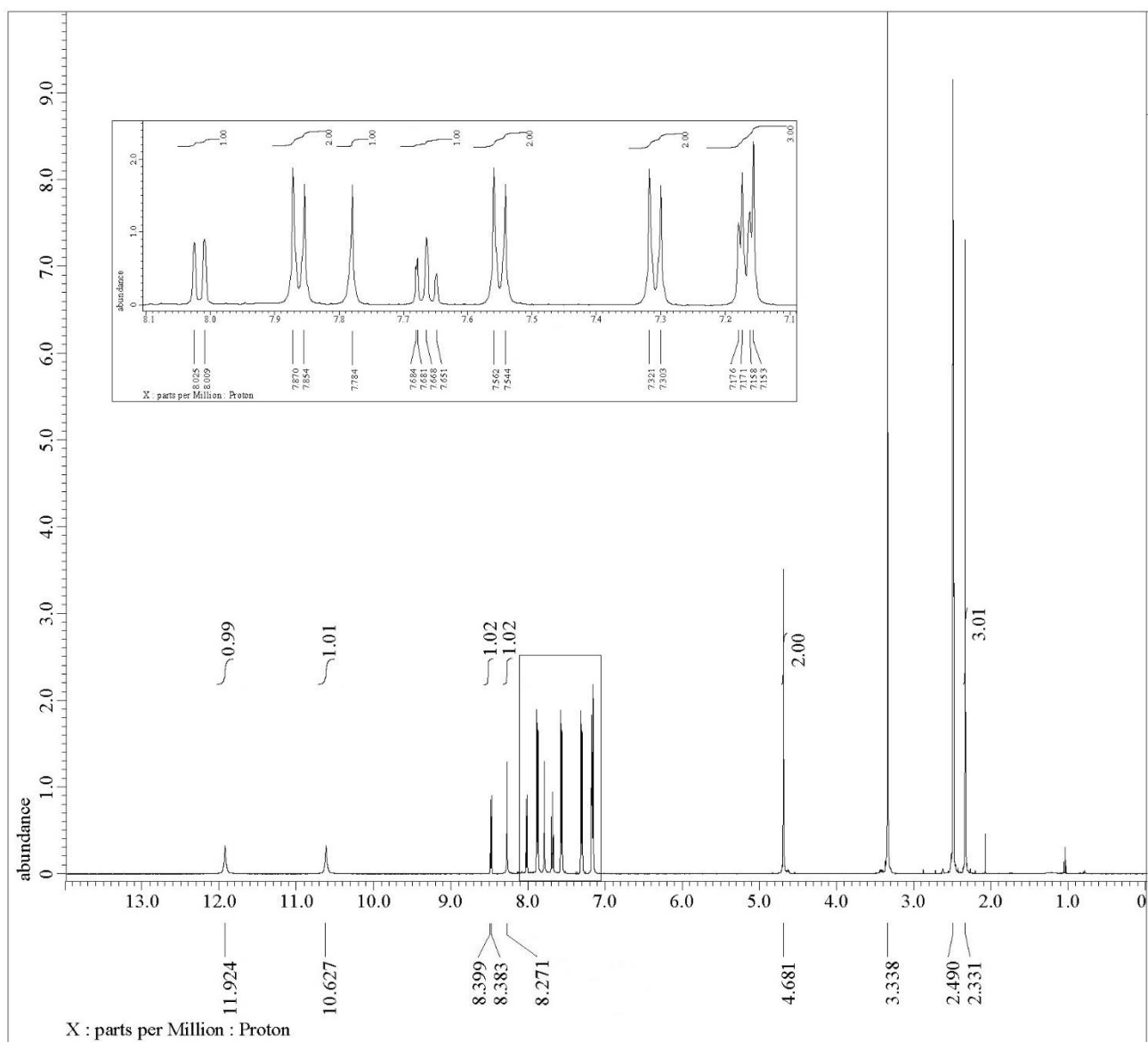


Figure S22. ¹H NMR spectrum of compound (6a)

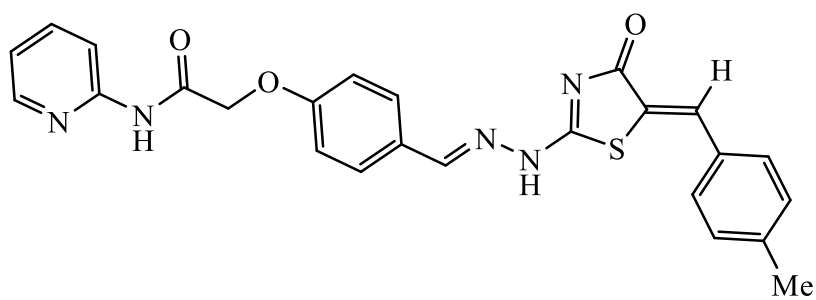
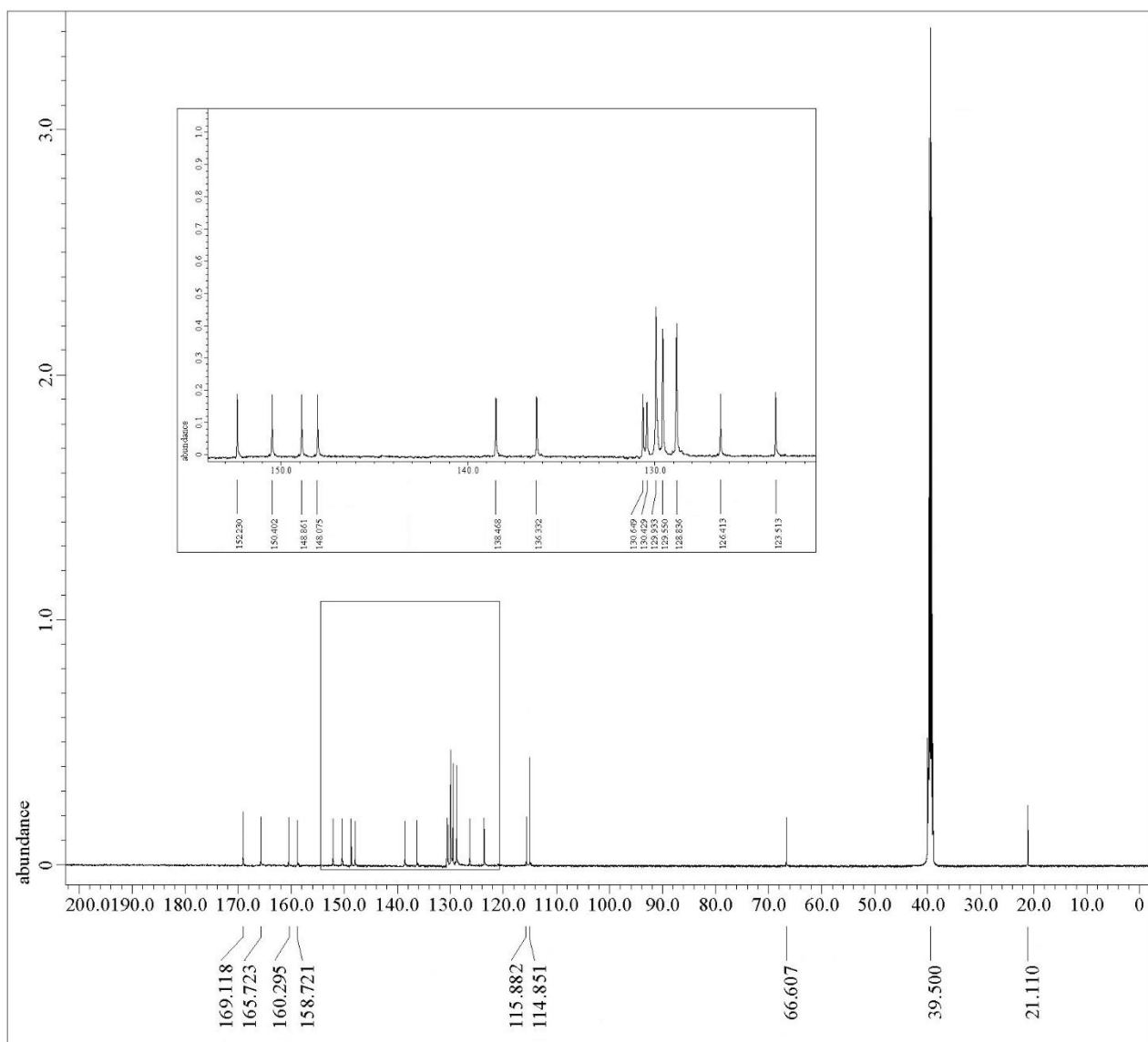
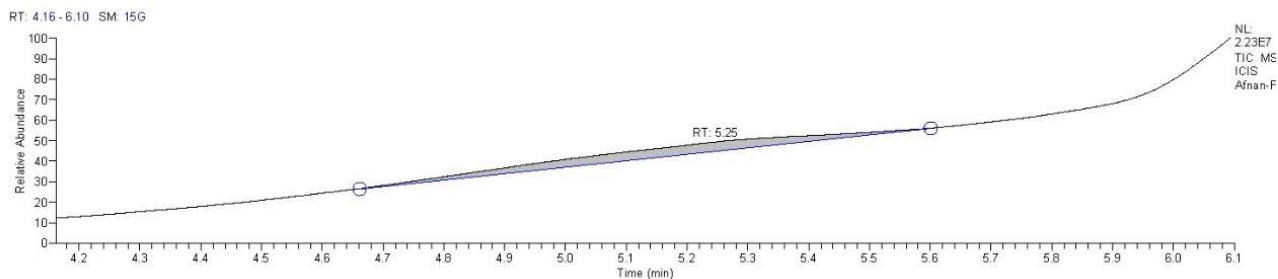


Figure S23. ^{13}C NMR spectrum of compound (6a)

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Afnan-F3 #339 RT: 5.25 AV: 1 TH: 0.05 NL: 1.57E6
T: + c Full ms [50.00-500.00]

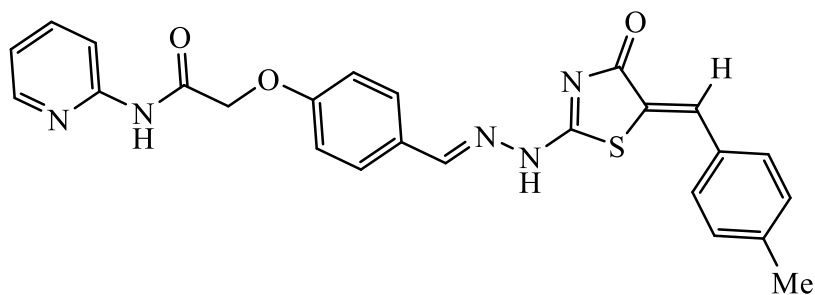
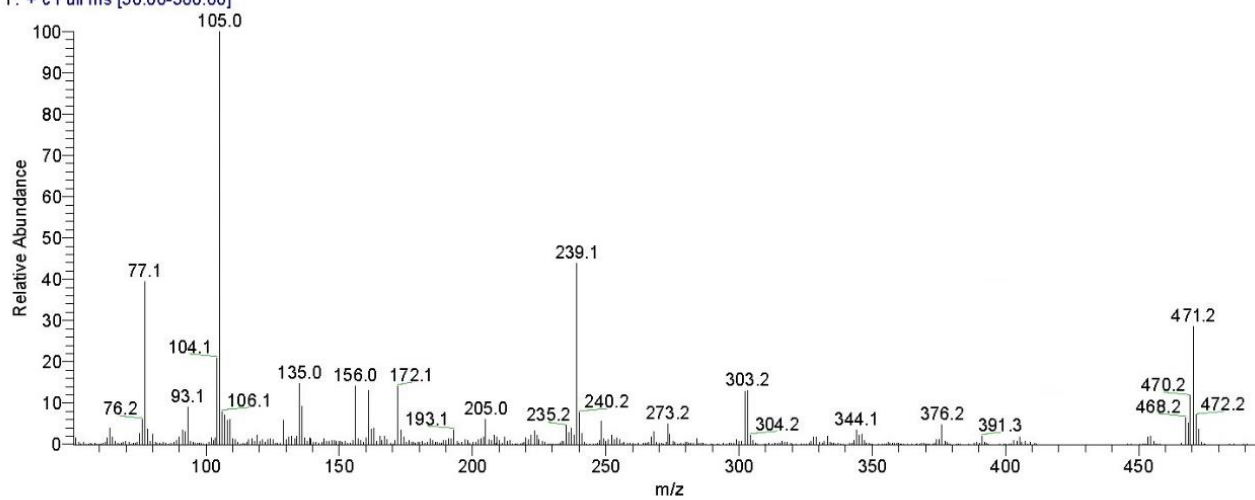


Figure 24. Mass analysis of compound (6a)

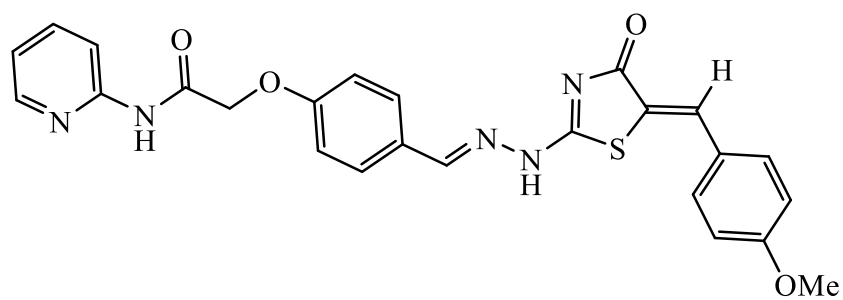
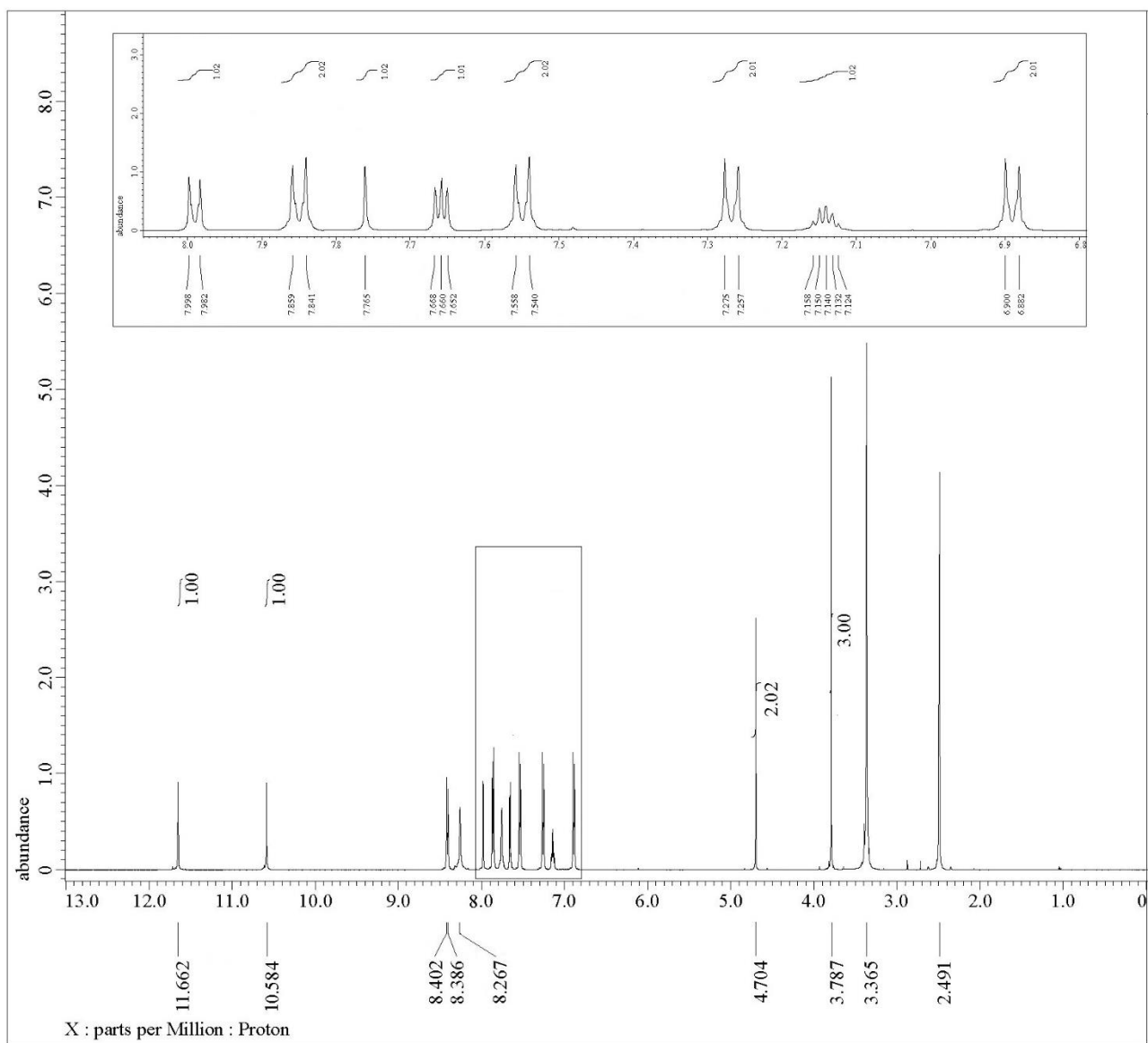


Figure S25. ^1H NMR spectrum of compound (6b)

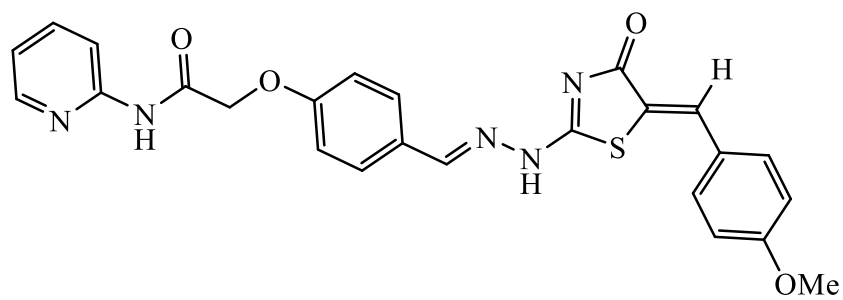
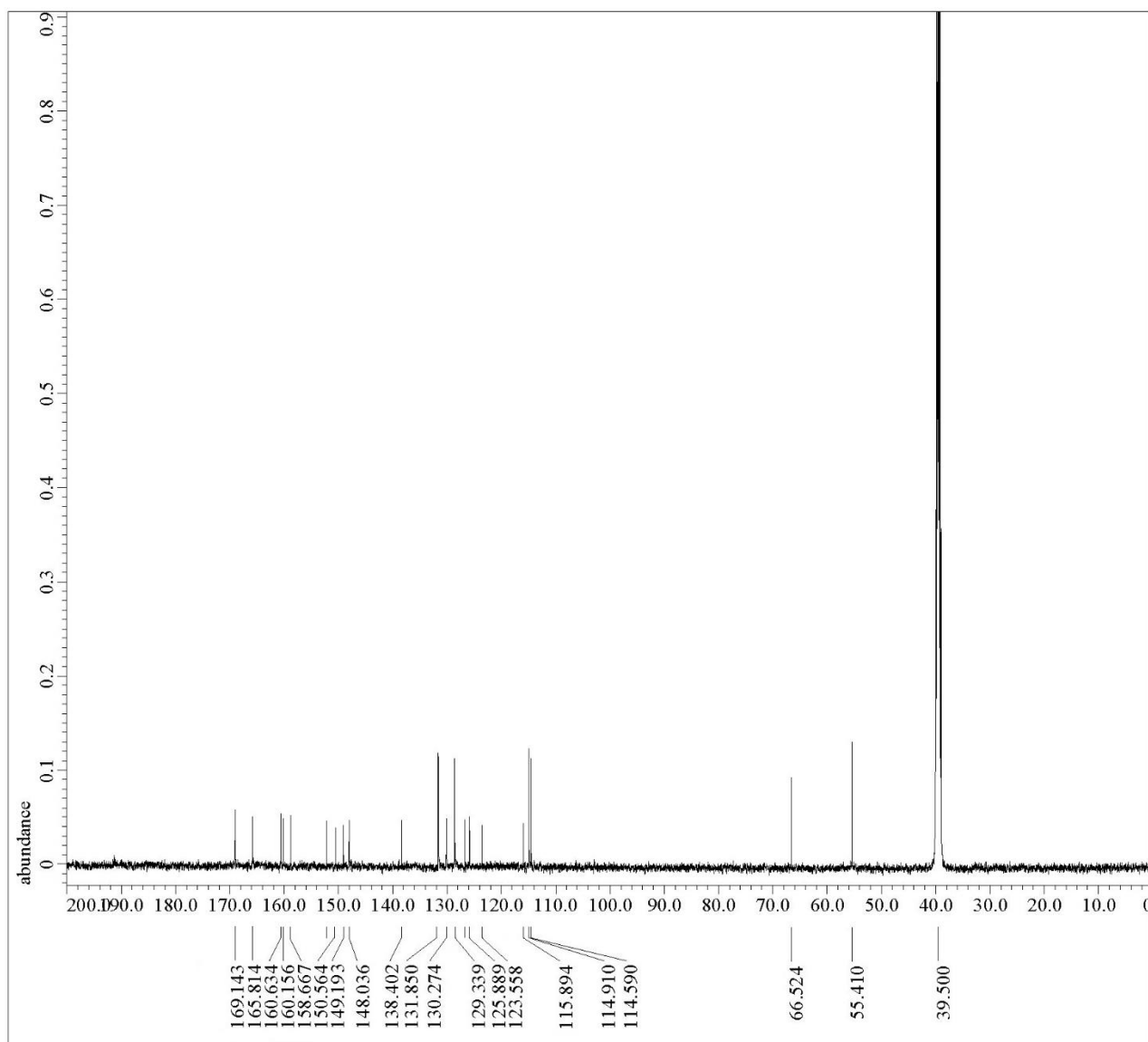
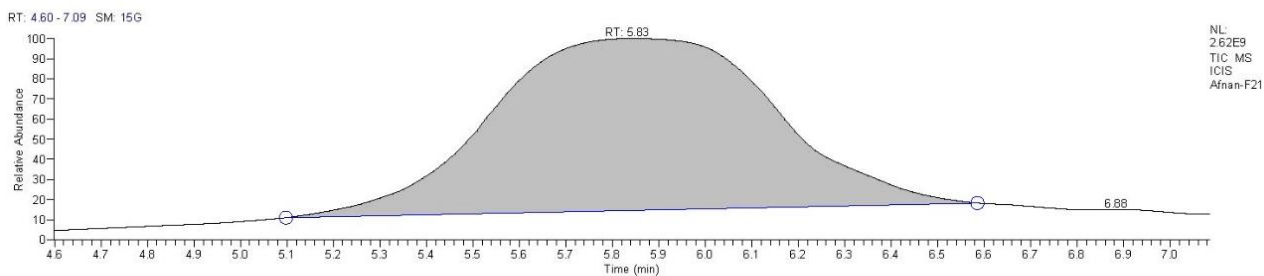


Figure S26. ^{13}C NMR spectrum of compound (6b)

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Afnan-F21 #252 RT: 5.83 AV: 1 TH: 0.05 NL: 2.18E8
T: + c Full ms [50.00-620.00]

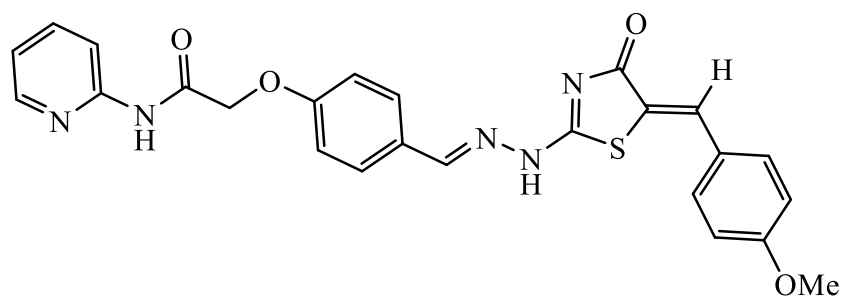
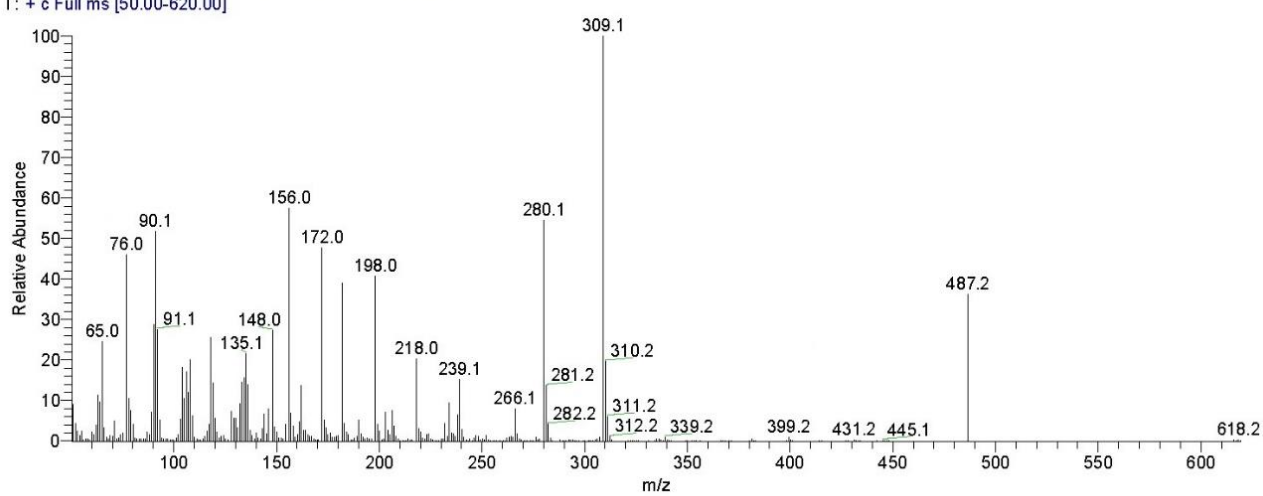


Figure S27. Mass analysis of compound (6b)

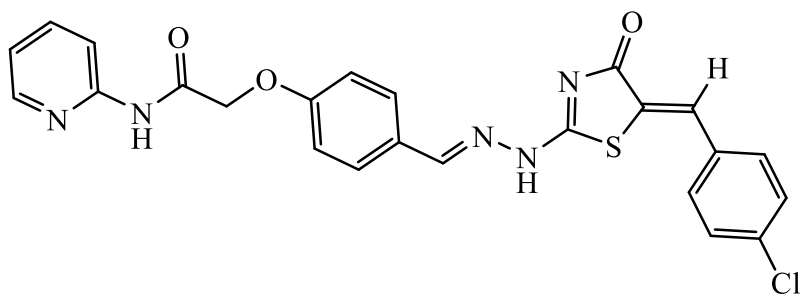
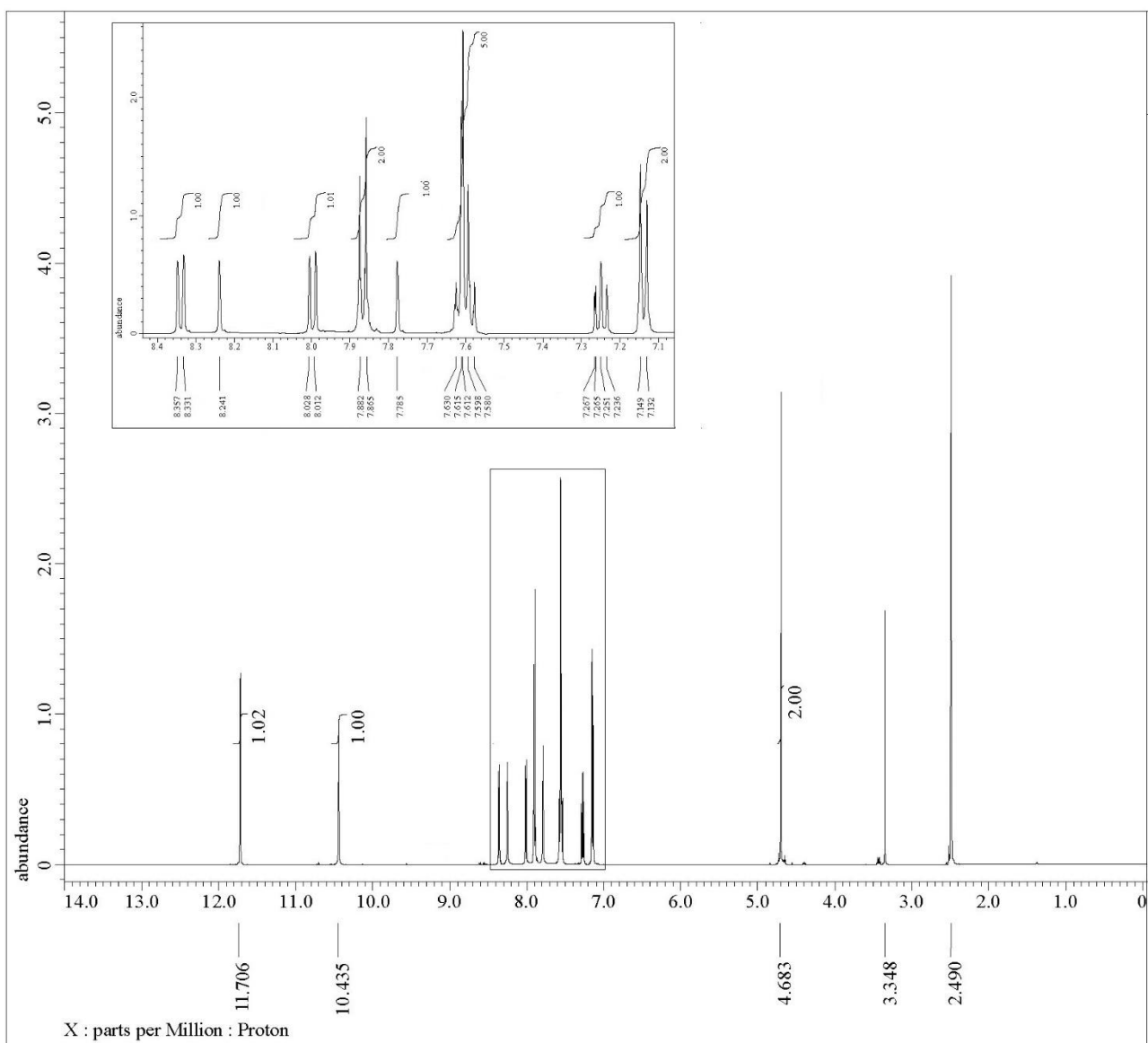


Figure S28. ¹H NMR spectrum of compound (6c)

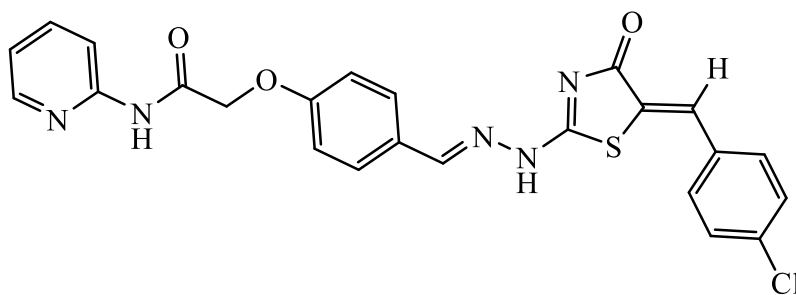
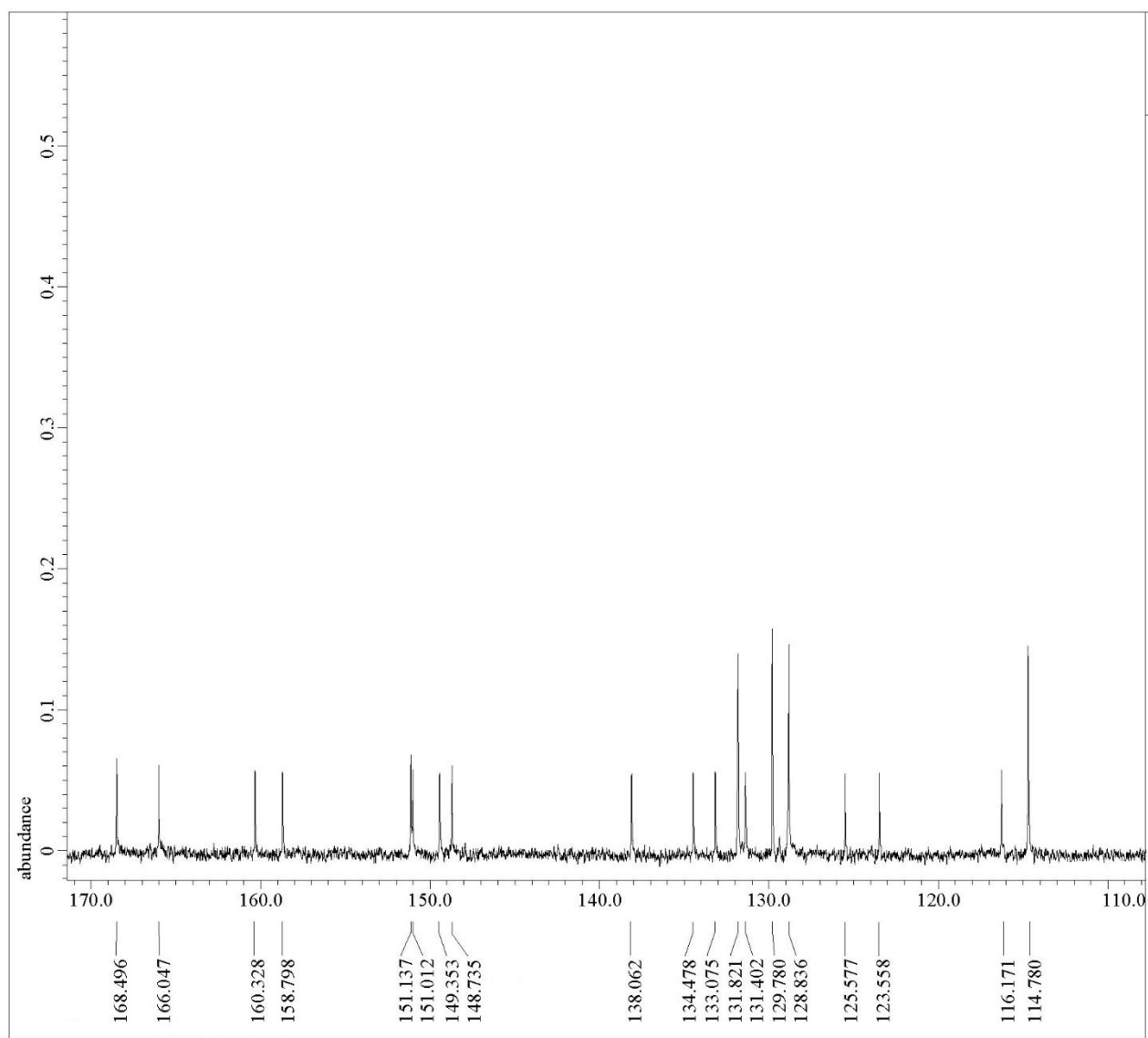
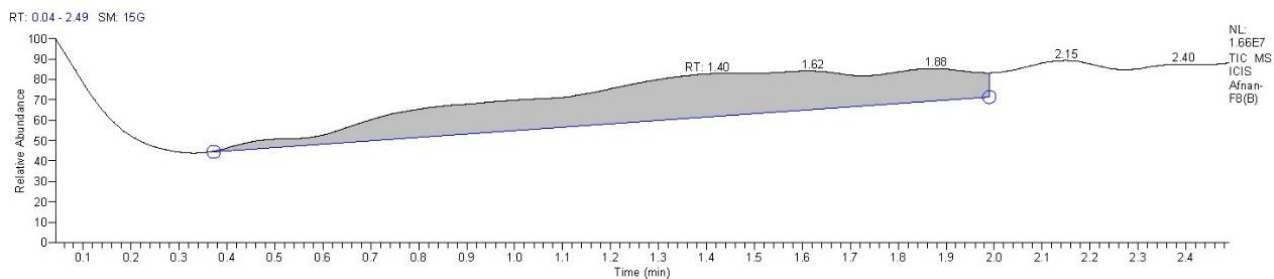


Figure S29. ¹³C NMR spectrum of compound (6c)

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Afnan-F8(B) #61 RT: 1.40 AV: 1 TH: 0.05 NL: 5.60E5
T: + c Full ms [50.00-650.00]

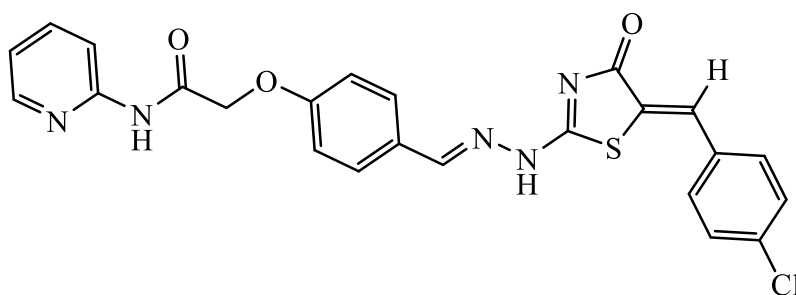
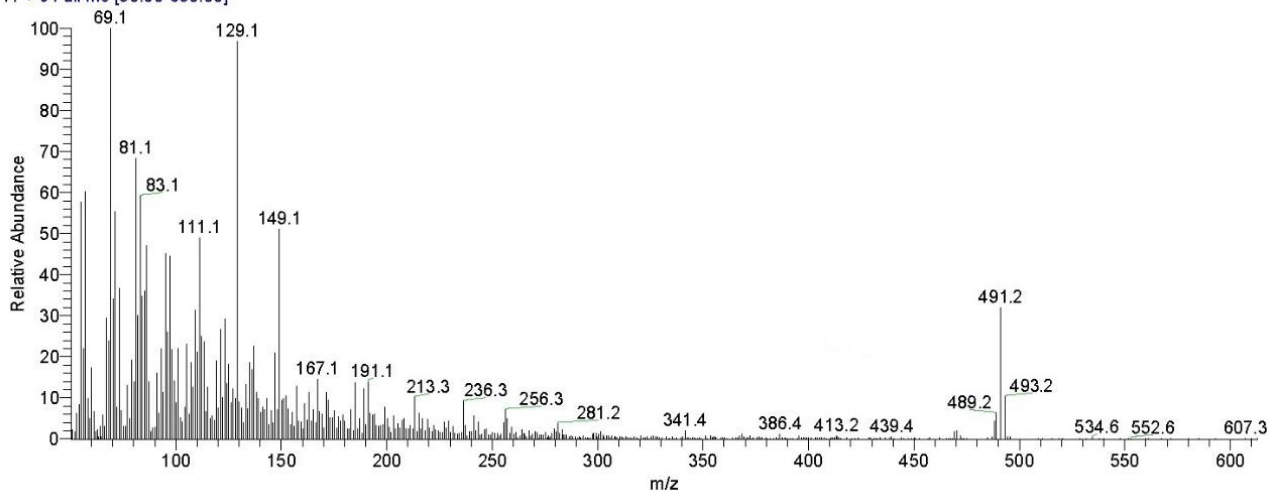


Figure S30. Mass analysis of compound (6c)

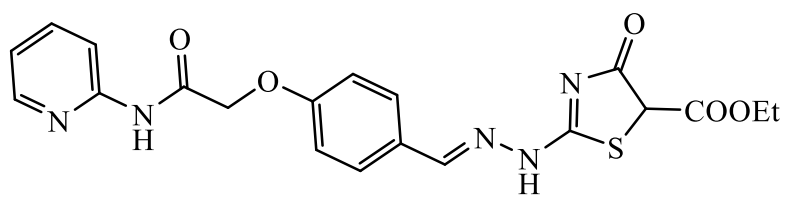
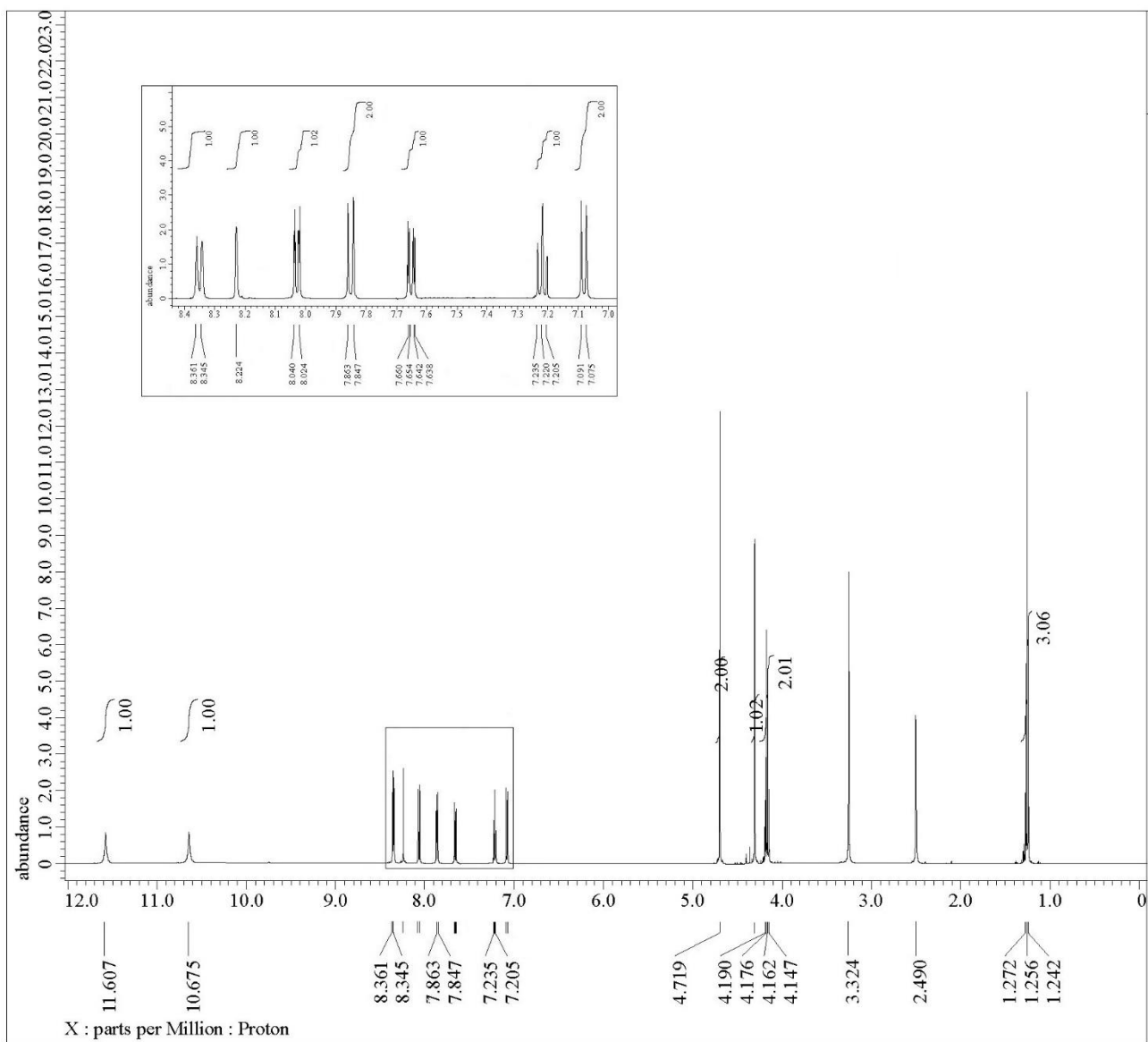


Figure S31. ^1H NMR spectrum of compound (7)

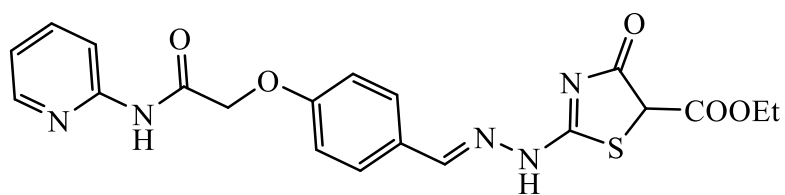
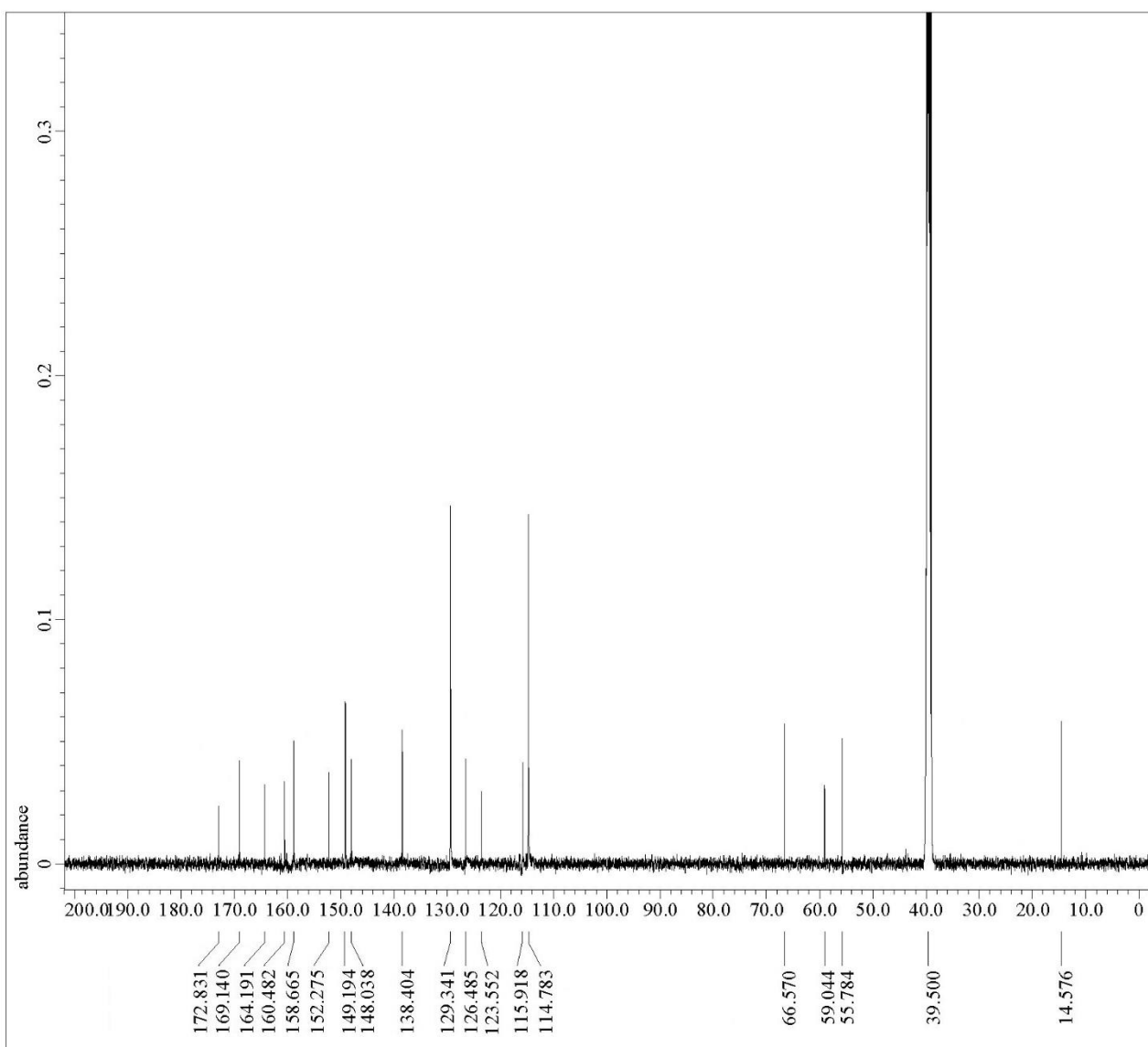
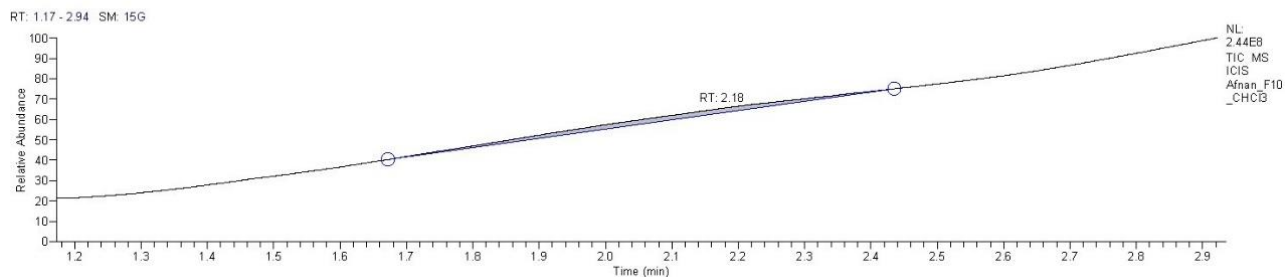


Figure S32. ^{13}C NMR spectrum of compound (7)

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Afnan_F10_CHCl3 #132 RT: 2.18 AV: 1 TH: 0.05 NL: 1.42E7
T: + c Full ms [50.00-525.00]

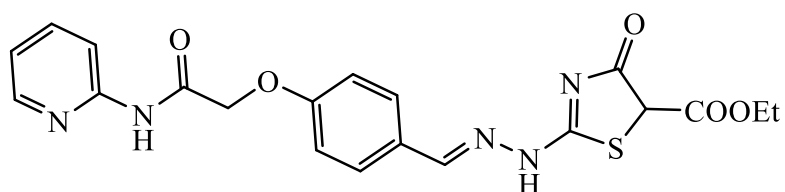
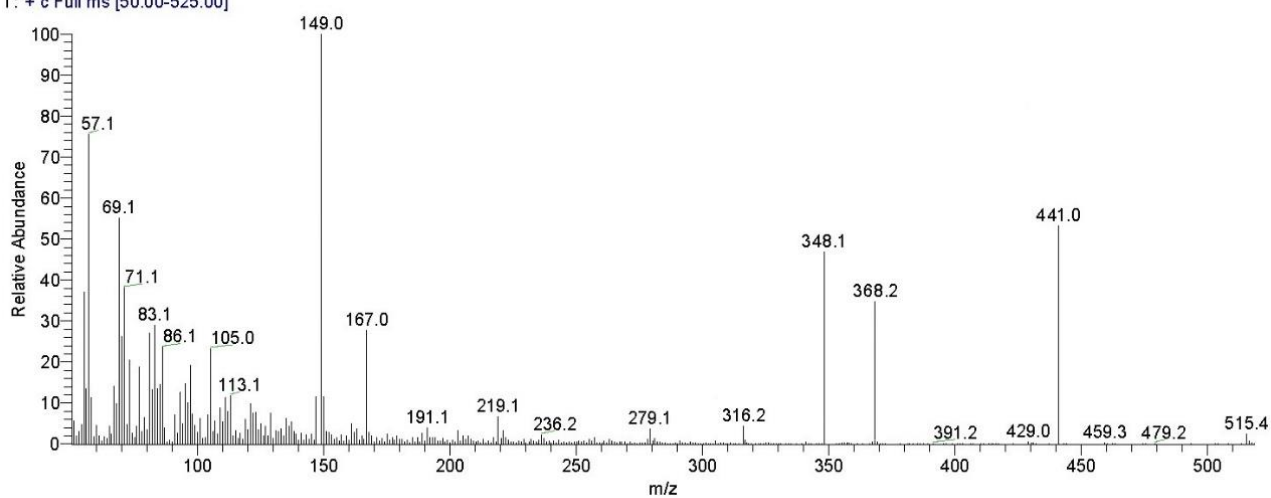


Figure S33. Mass analysis of compound (6c)

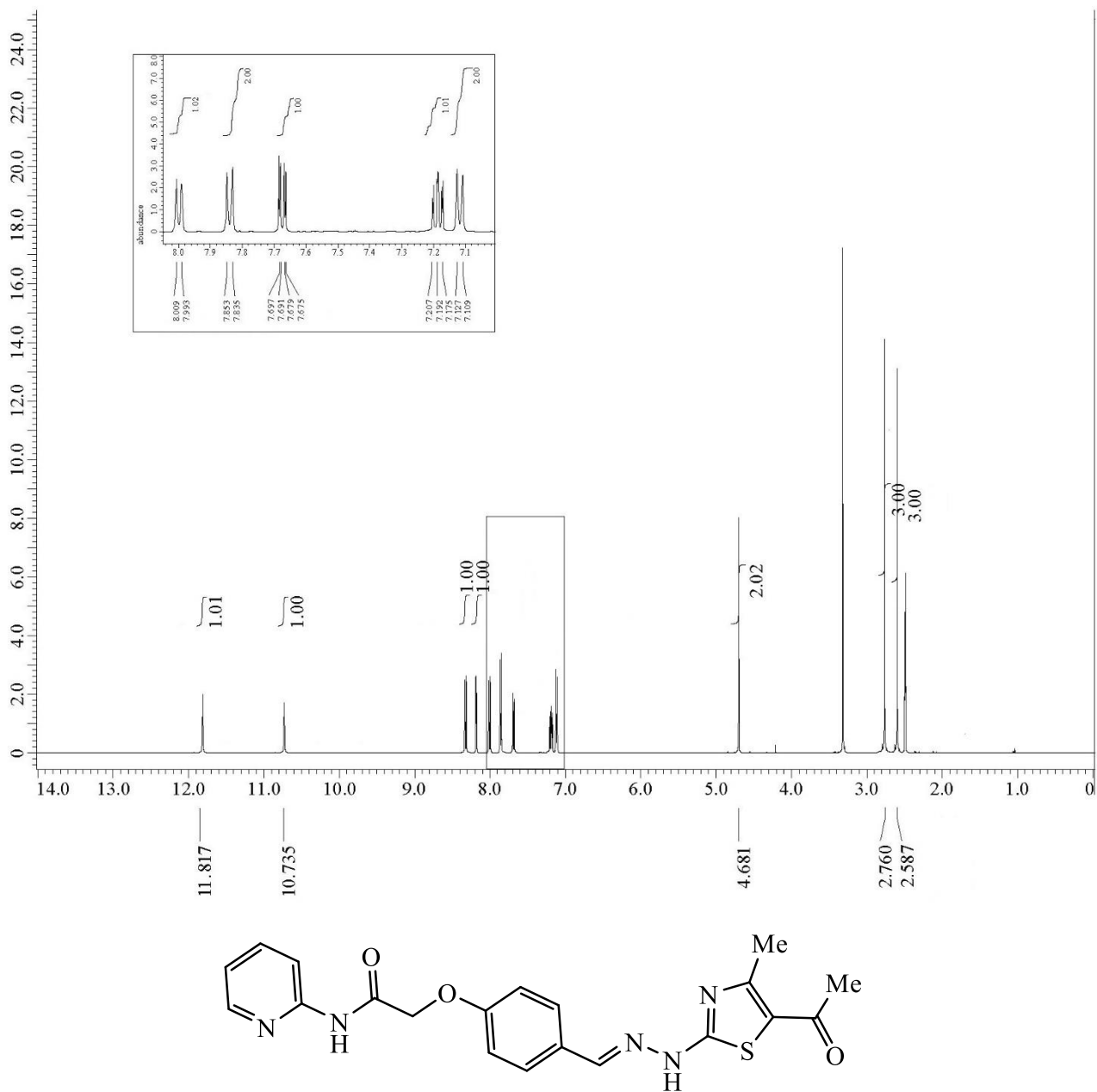


Figure S34. ¹H NMR spectrum of compound (8)

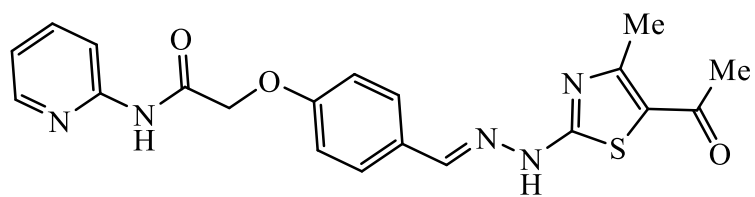
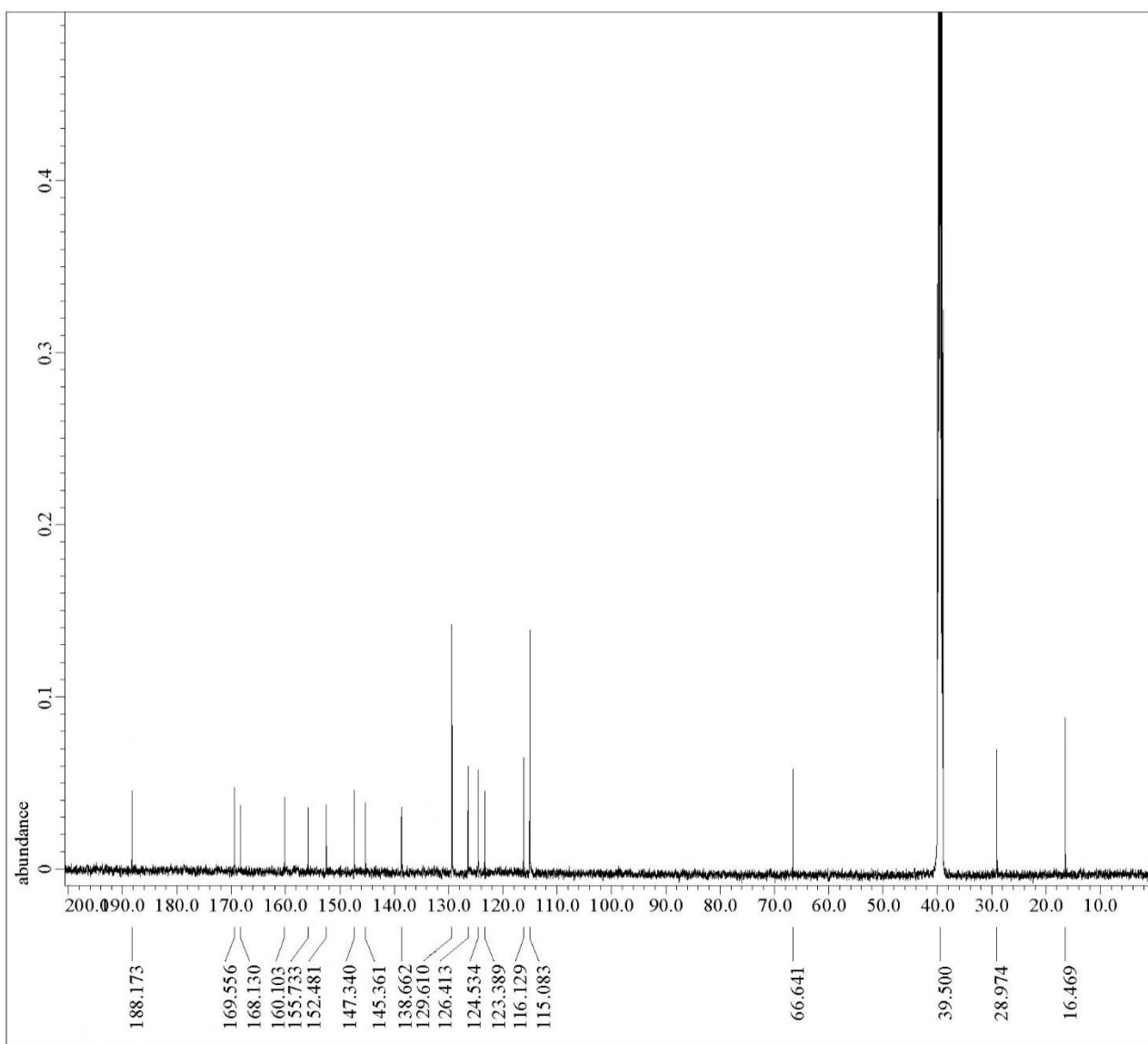
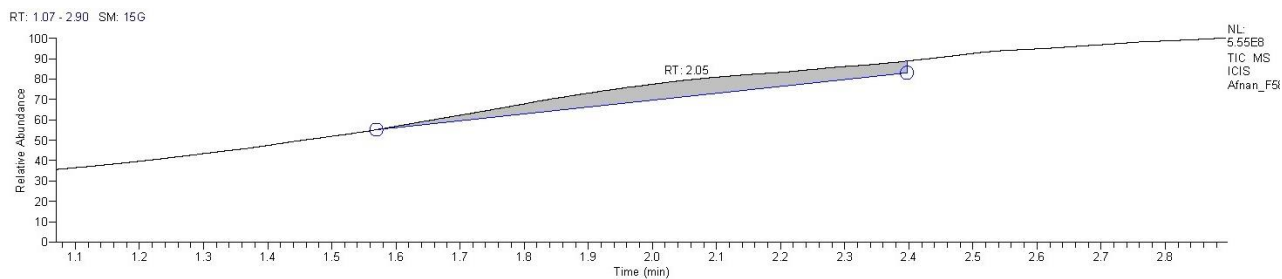


Figure S35. ¹H NMR spectrum of compound (8)

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Afnan_F58 #159 RT: 2.05 AV: 1 TH: 0.05 NL: 3.85E7
T: + c Full ms [50.00-420.00]

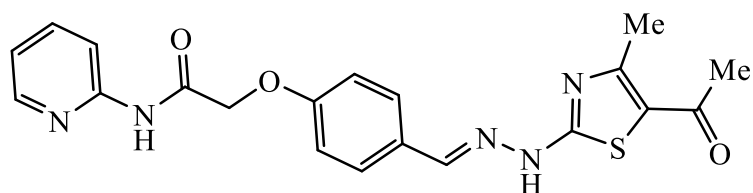
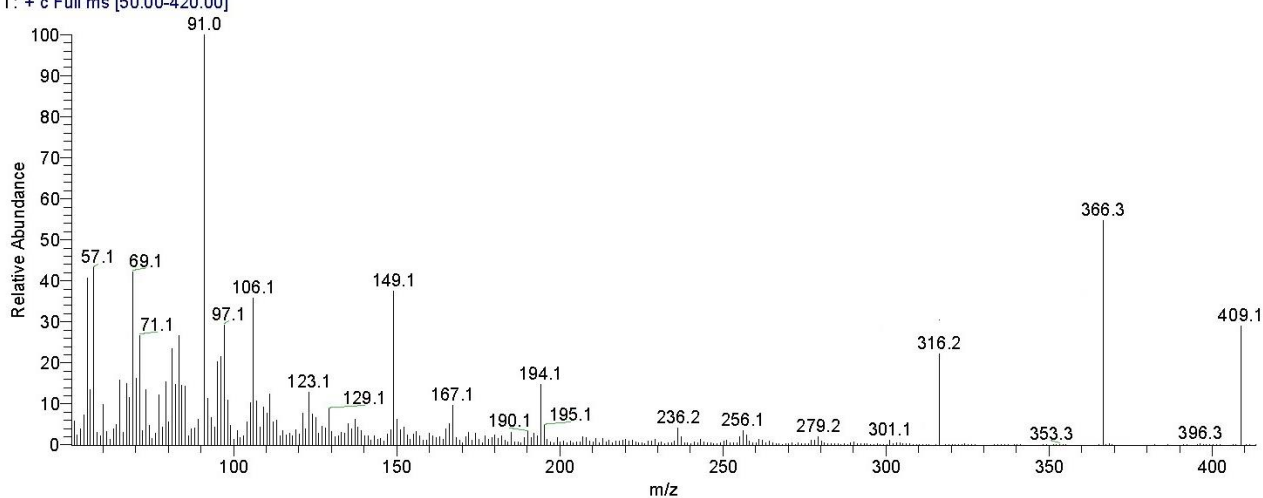


Figure S36. Mass analysis of compound (8)

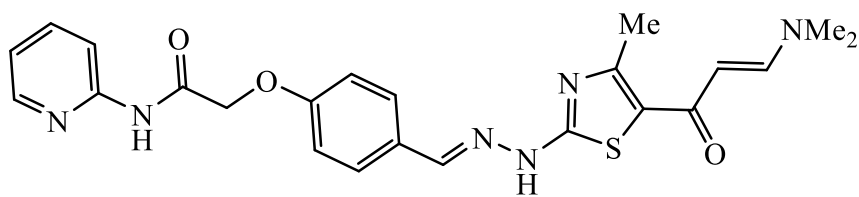
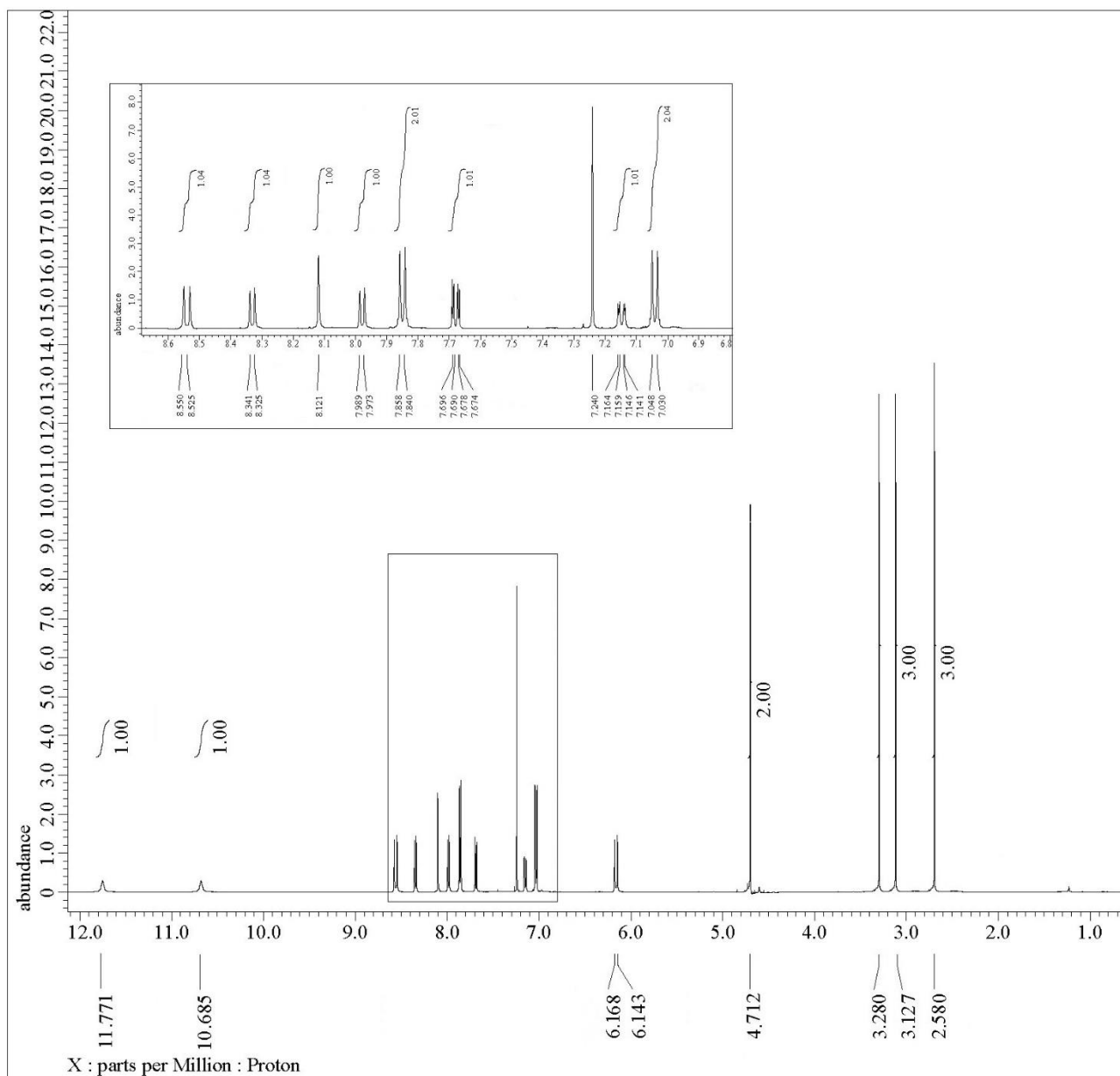


Figure S37. ¹H NMR spectrum of compound (9)

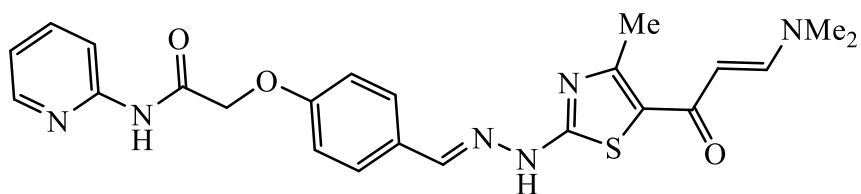
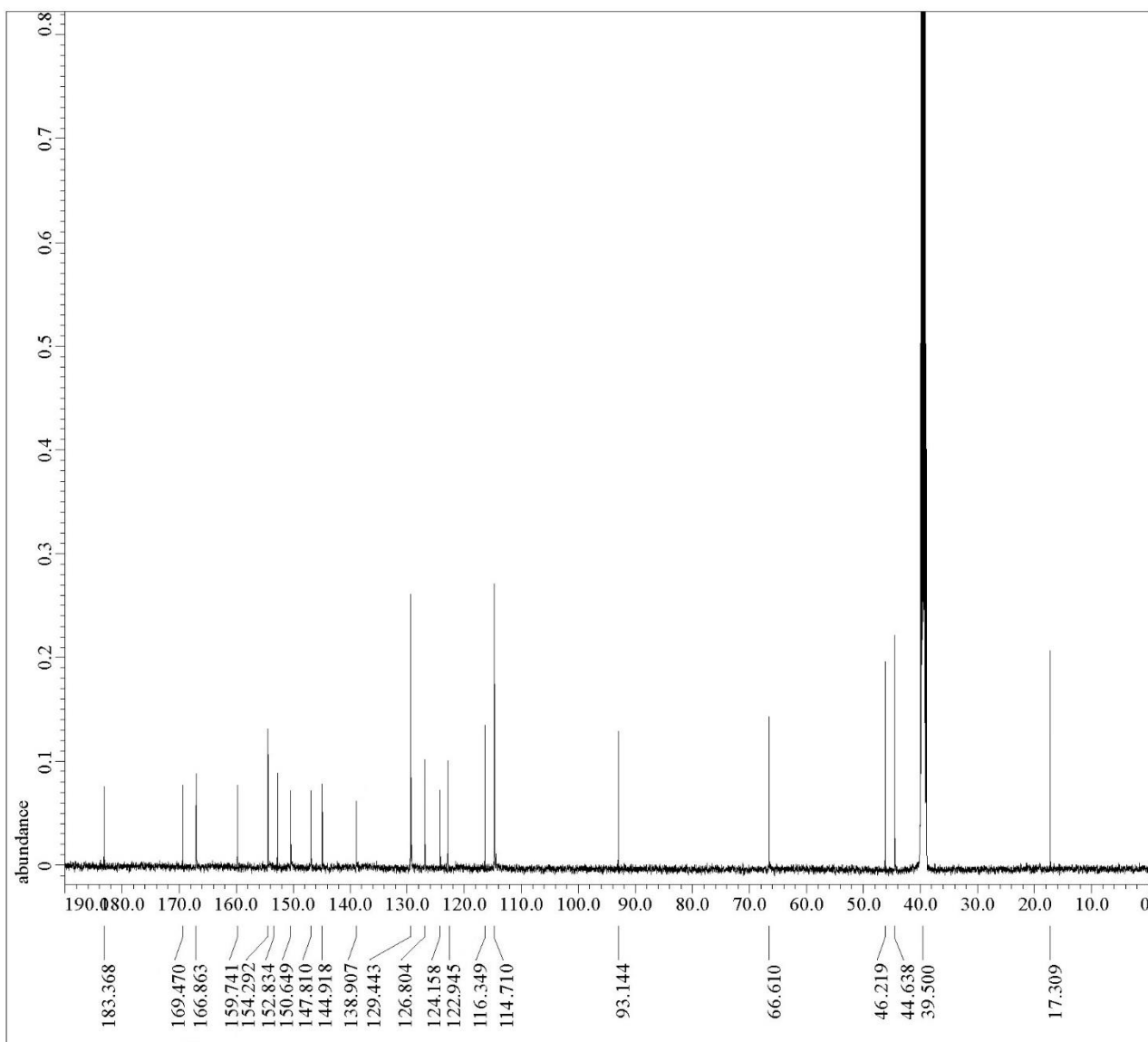
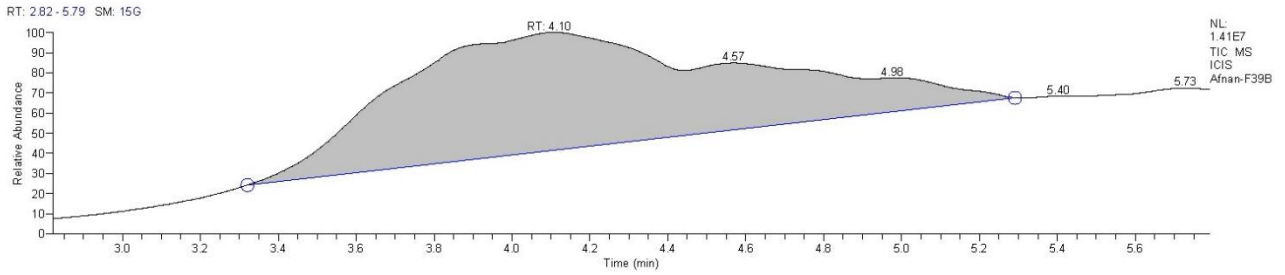


Figure S38. ^1H NMR spectrum of compound (9)

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Afnan-F39B #215 RT: 4.10 AV: 1 TH: 0.05 NL: 3.04E6
T: + c Full ms [50.00-600.00]

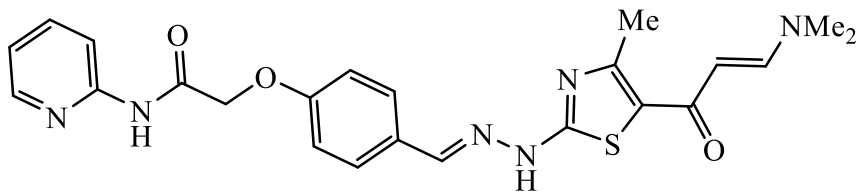
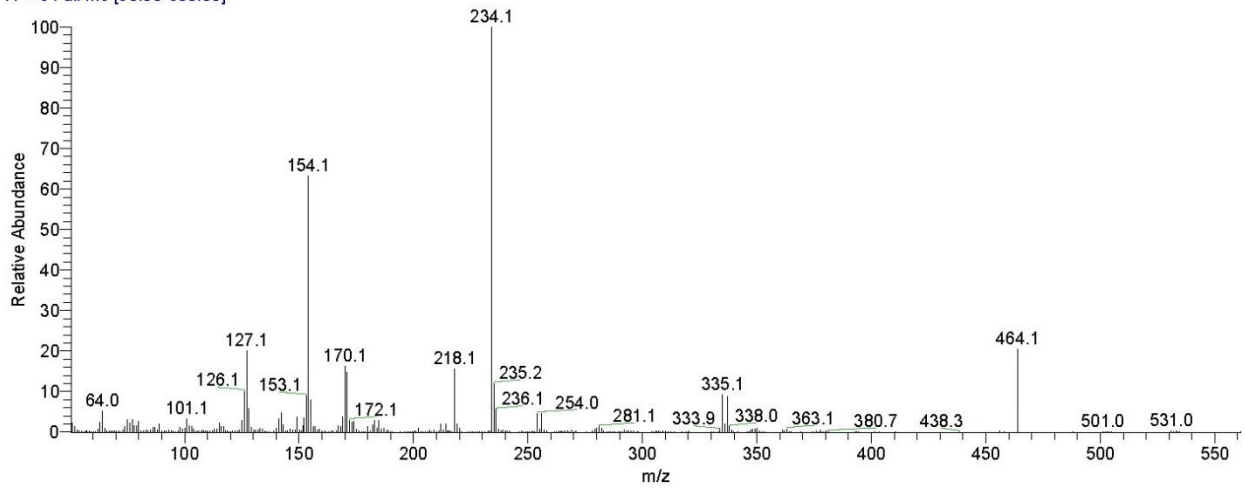


Figure S39. Mass analysis of compound (9)

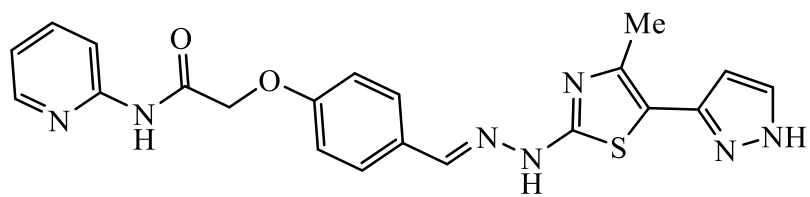
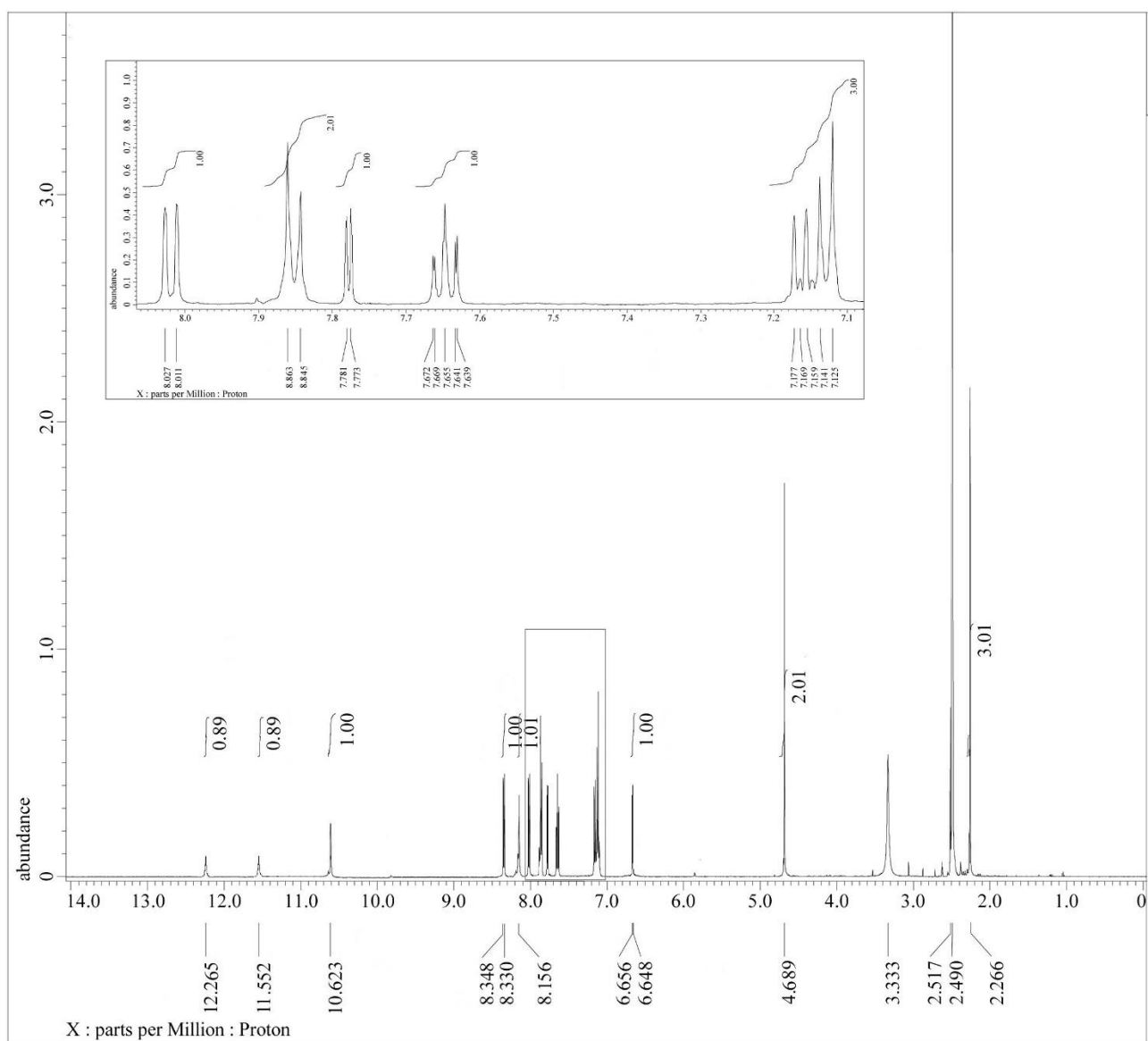


Figure S40. ¹H NMR spectrum of compound (10)

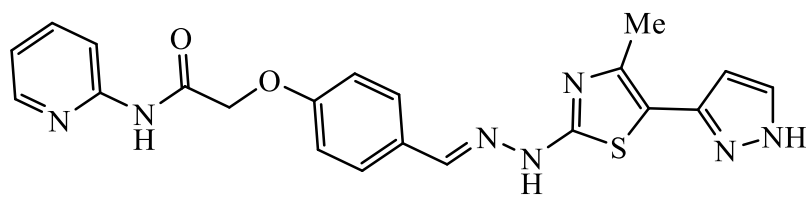
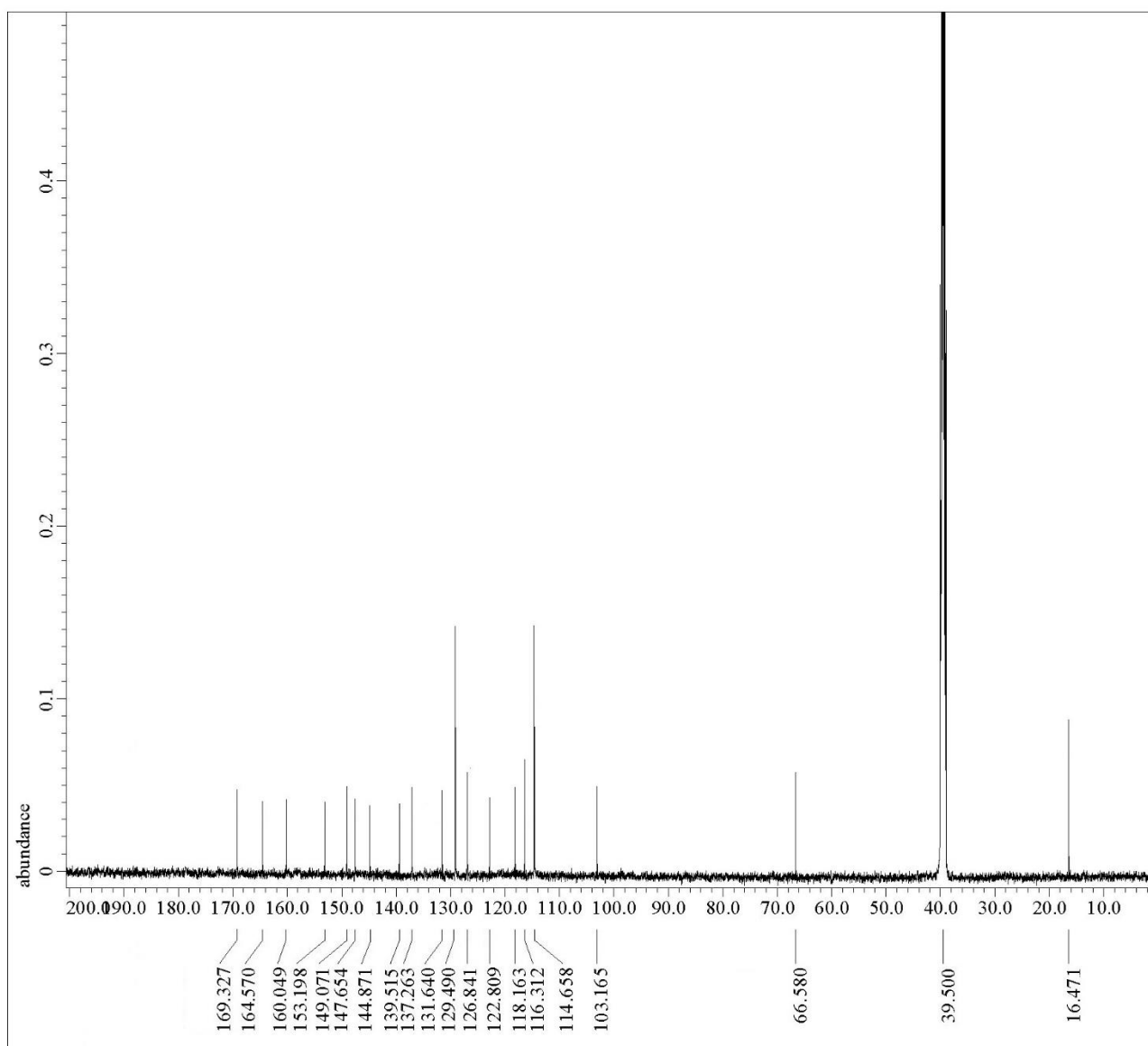
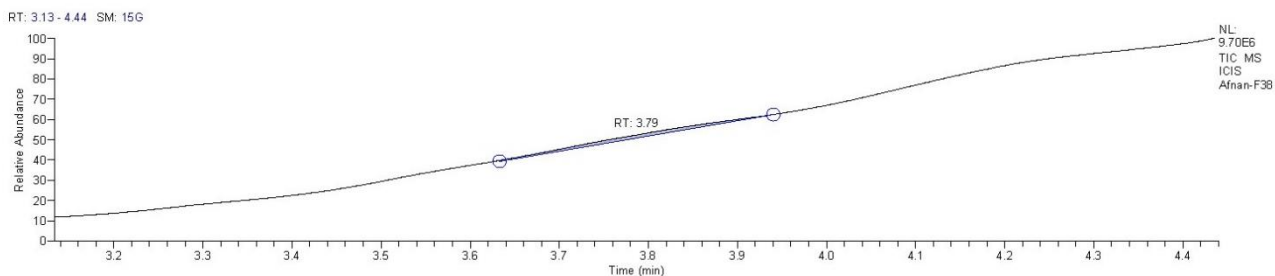


Figure S41. ¹H NMR spectrum of compound (10)

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Central Laboratory



Afnan-F38 #220 RT: 3.79 AV: 1 TH: 0.05 NL: 1.39E6
T: + c Full ms [50.00-550.00]

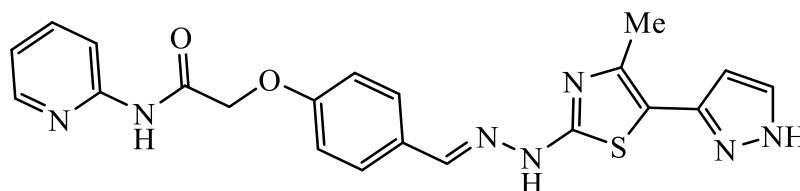
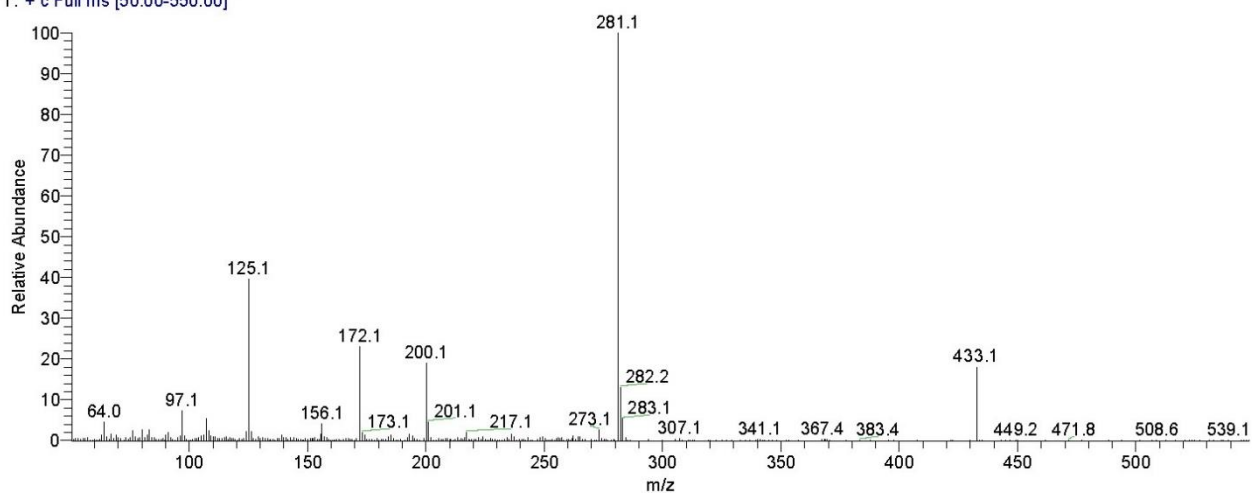


Figure S42. Mass analysis of compound (10)