

Histone Deacetylase Inhibitory Activity and Antiproliferative Potential of New [6]-Shogaol Derivatives

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Supporting Information

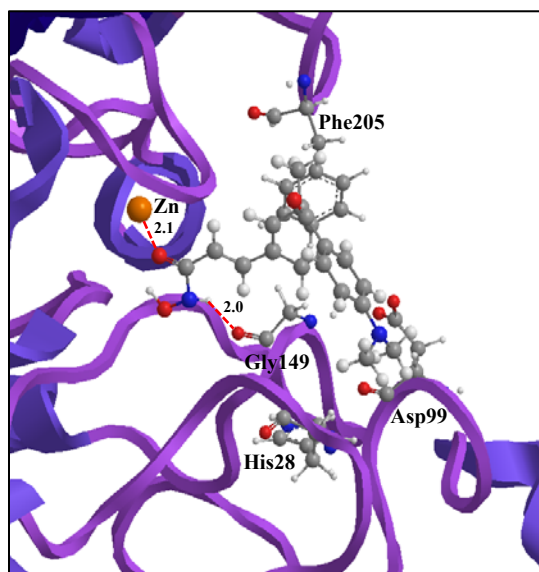


Figure S1. The interaction mode of TSA in the active site of HDAC1.

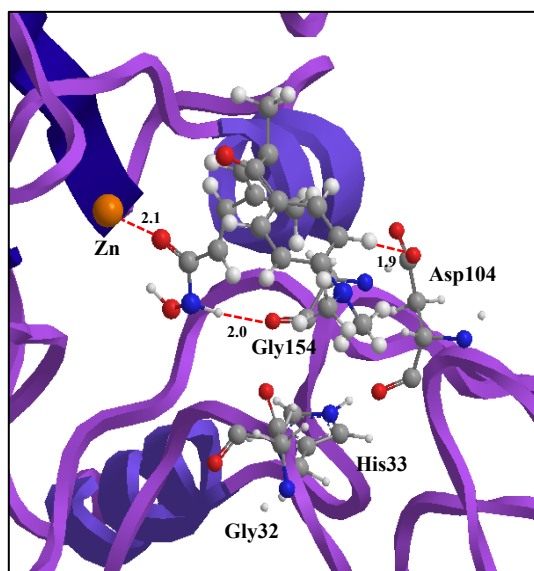


Figure S2. The interaction mode of TSA in the active site of HDAC2.

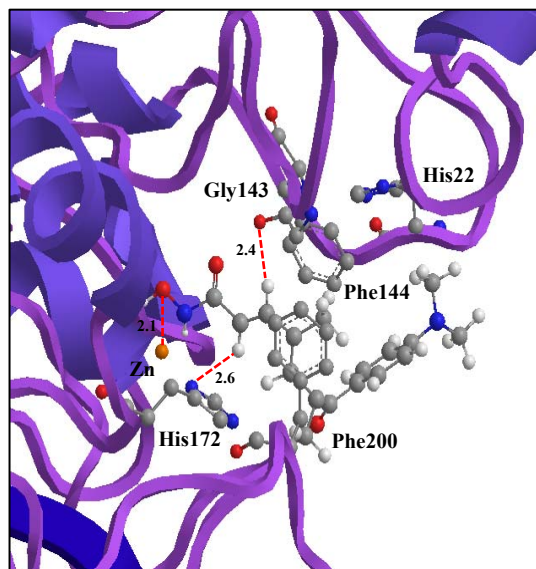


Figure S3. The interaction mode of TSA in the active site of HDAC3.

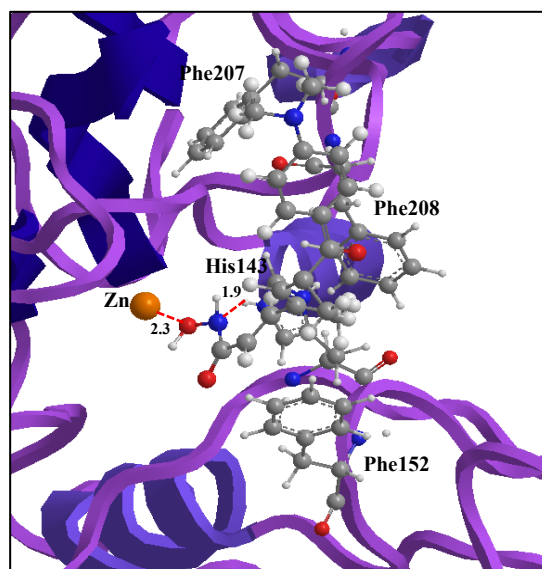


Figure S4. The interaction mode of TSA in the active site of HDAC8.

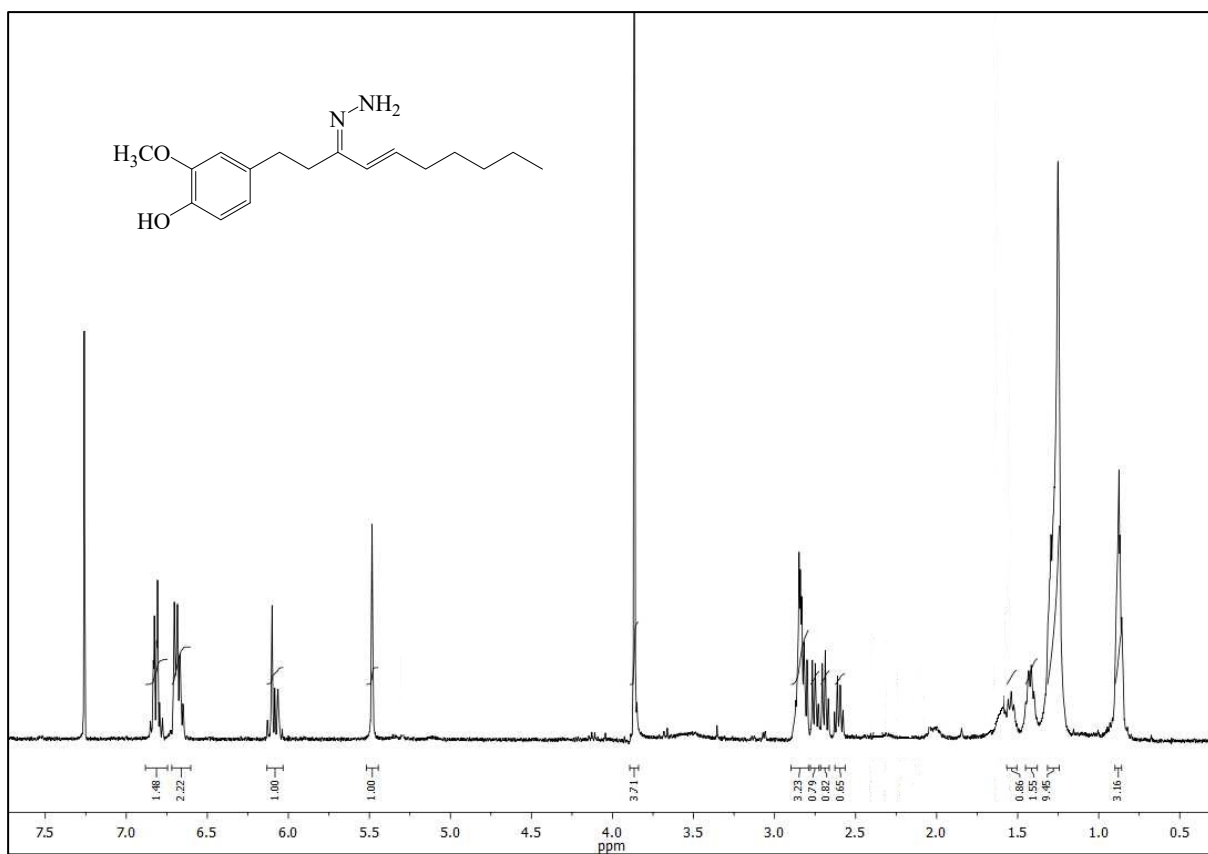


Figure S5. ¹H NMR spectrum of 4a.

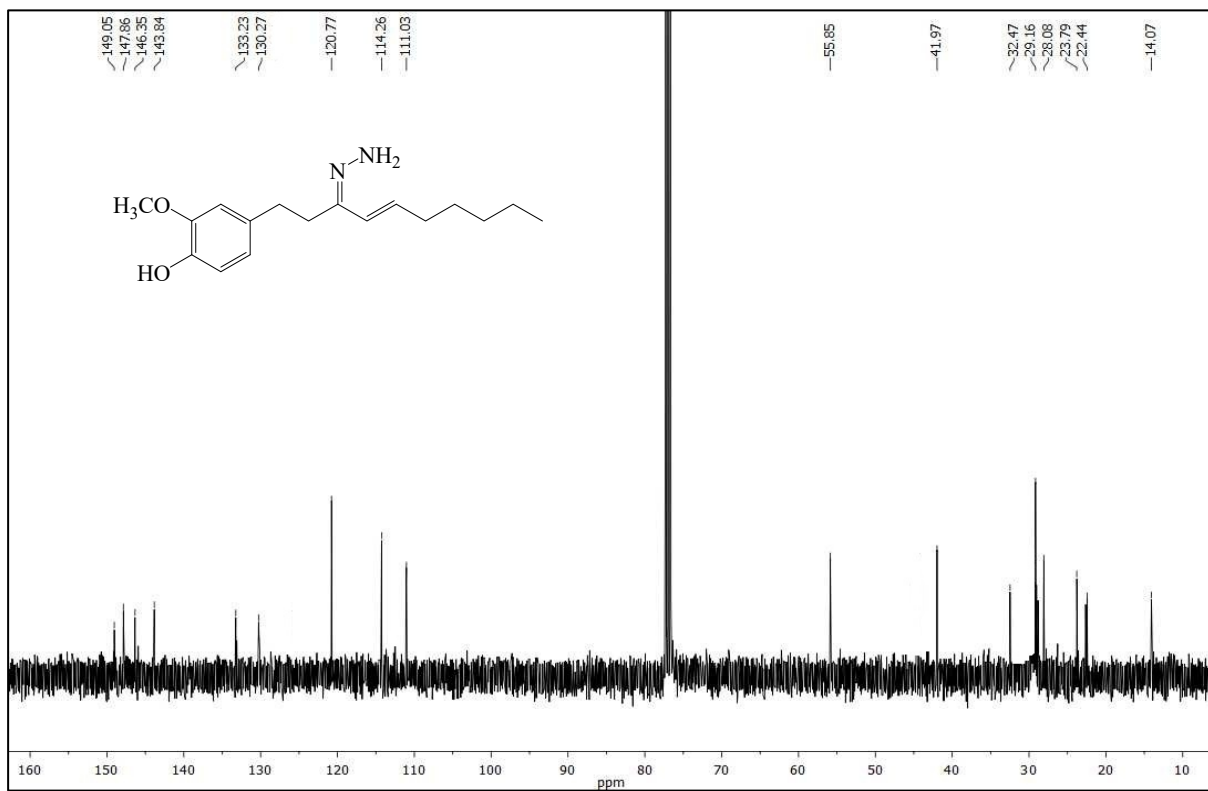


Figure S6. ¹³C NMR spectrum of 4a.

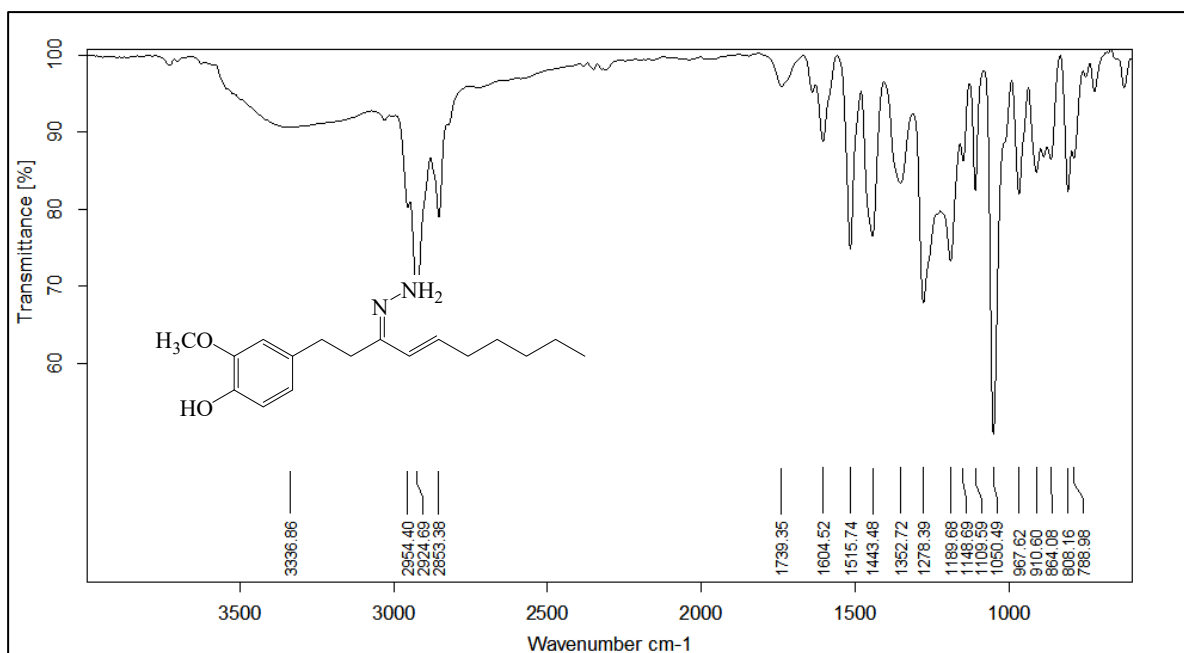


Figure S7. IR spectrum of **4a**.

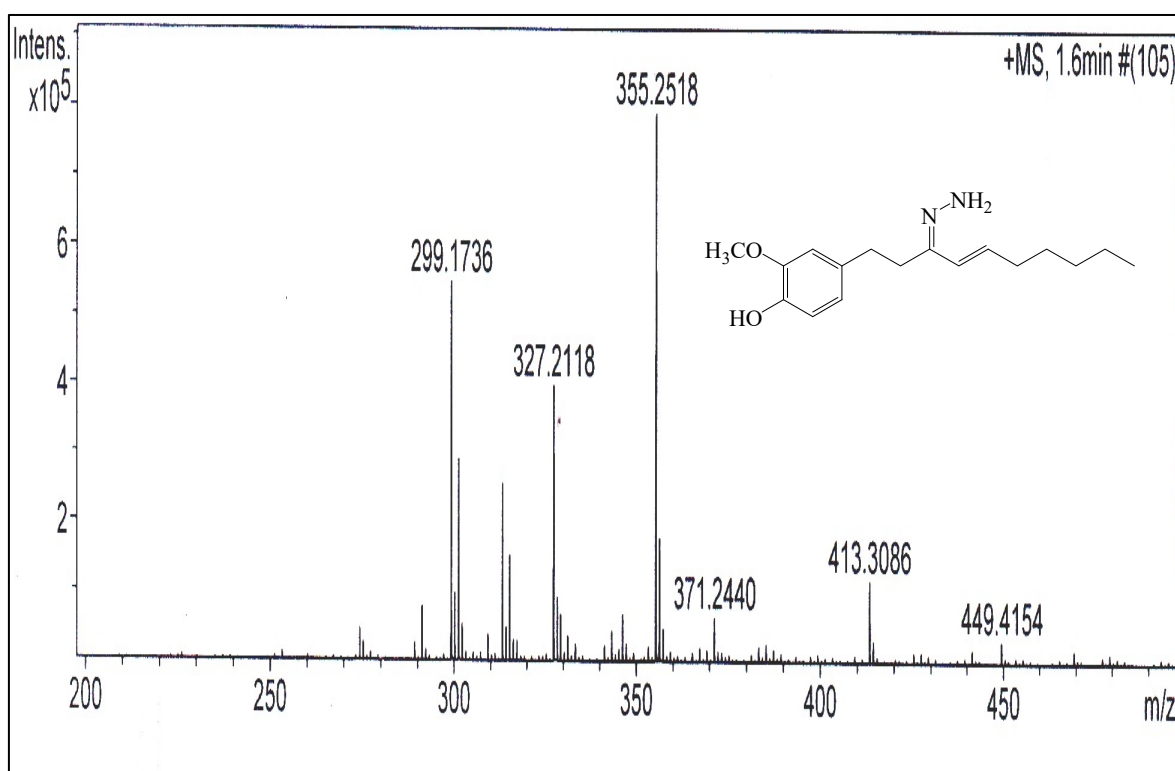


Figure S8. Mass spectrum of **4a**.

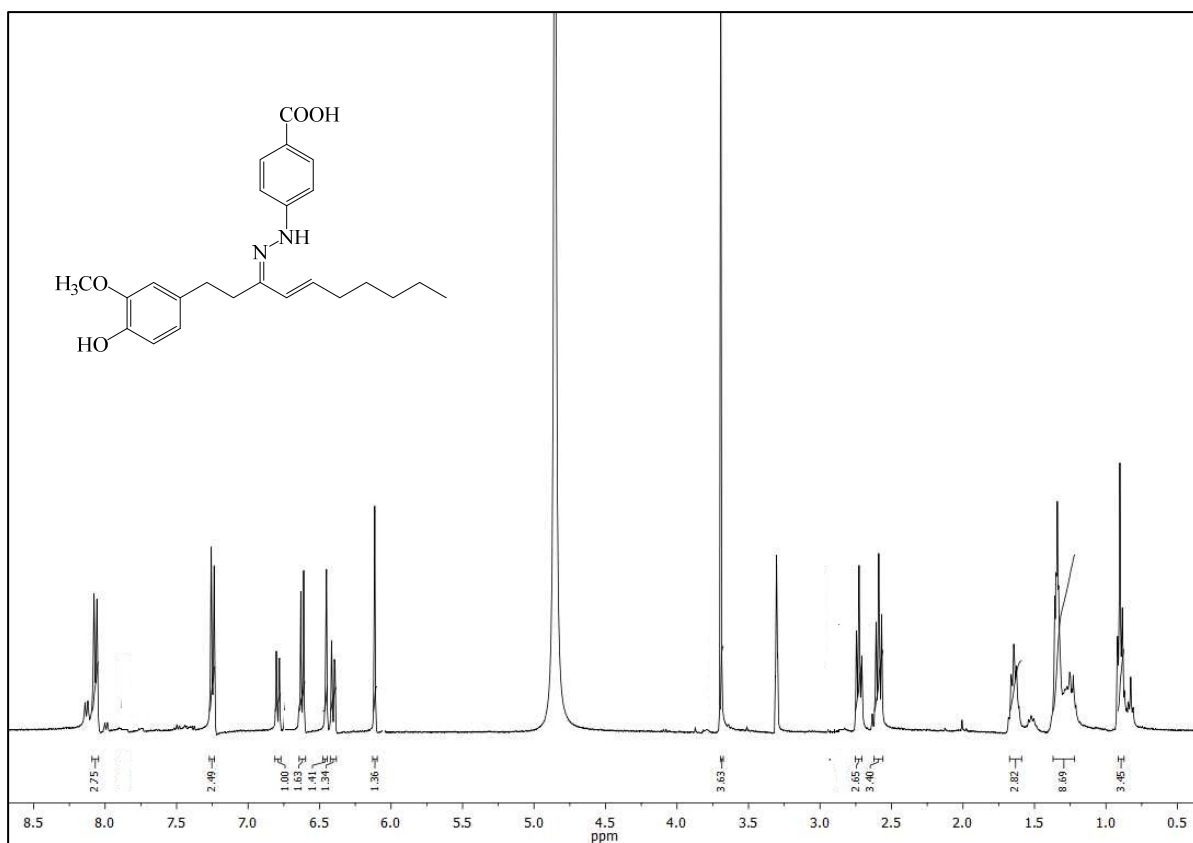


Figure S9. ¹H NMR spectrum of **4b**.

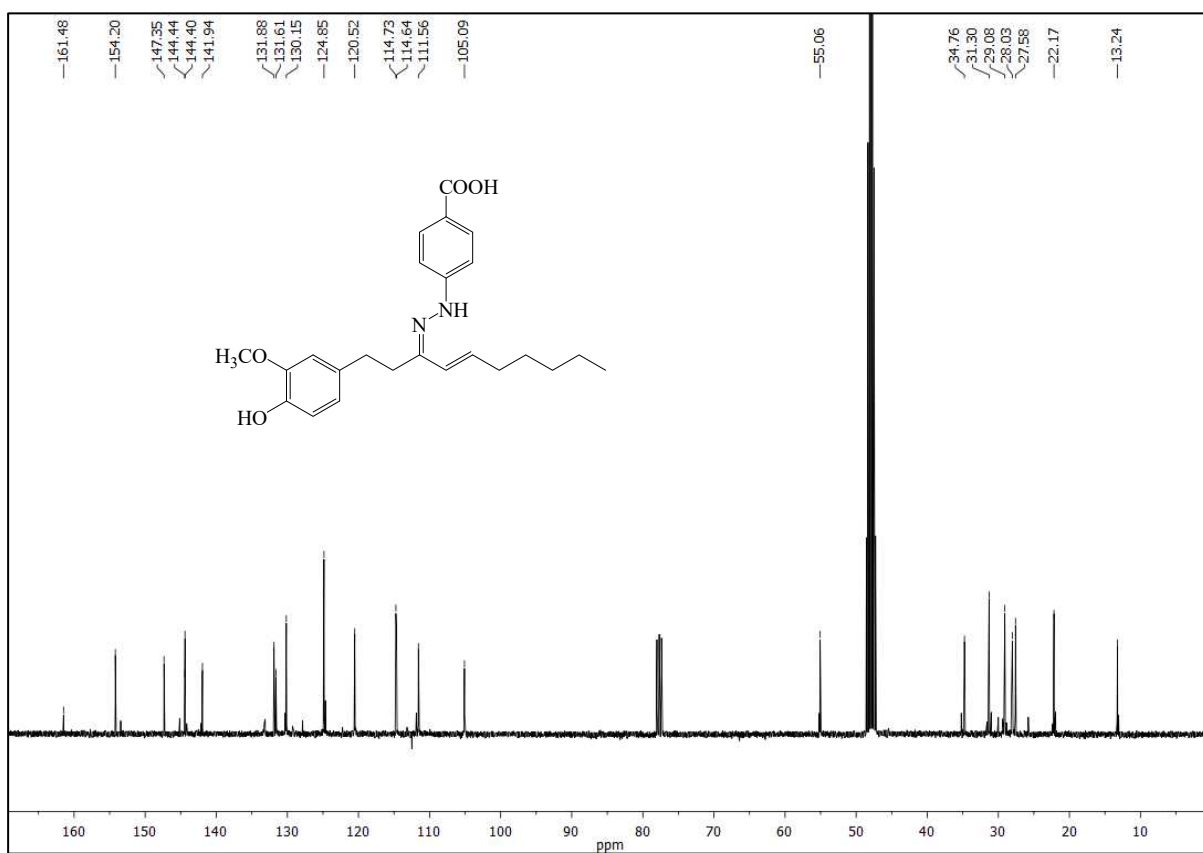


Figure S10. ¹³C NMR spectrum of **4b**.

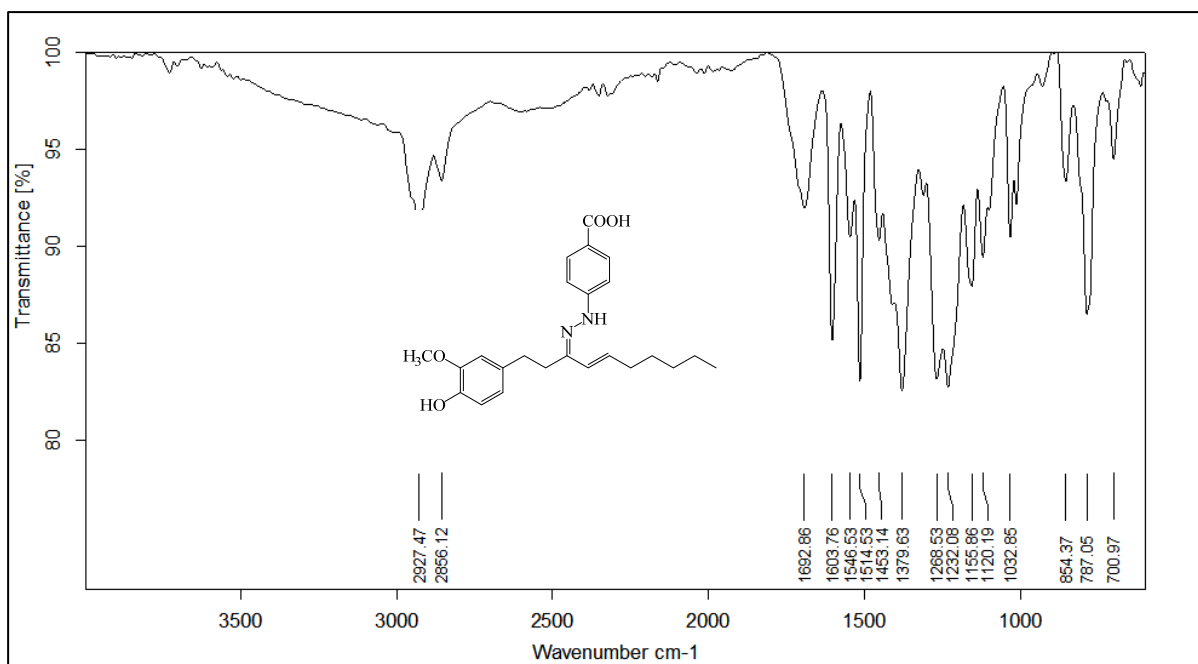


Figure S11. IR spectrum of **4b**.

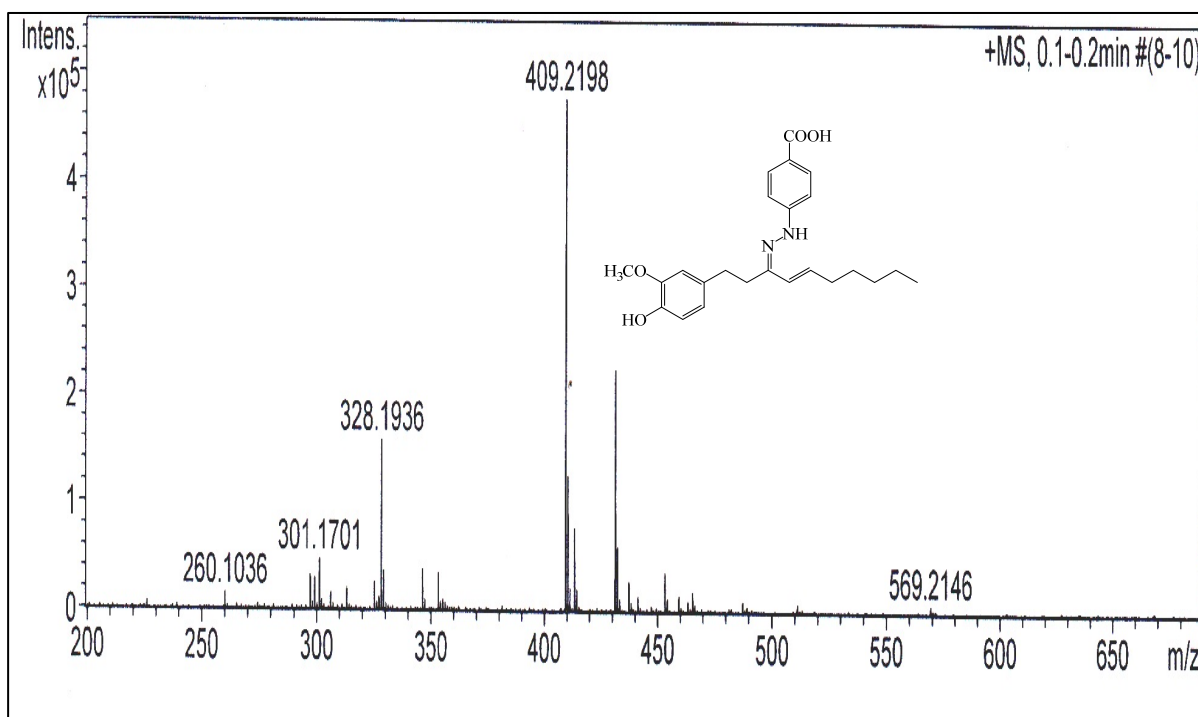


Figure S12. Mass spectrum of **4b**.

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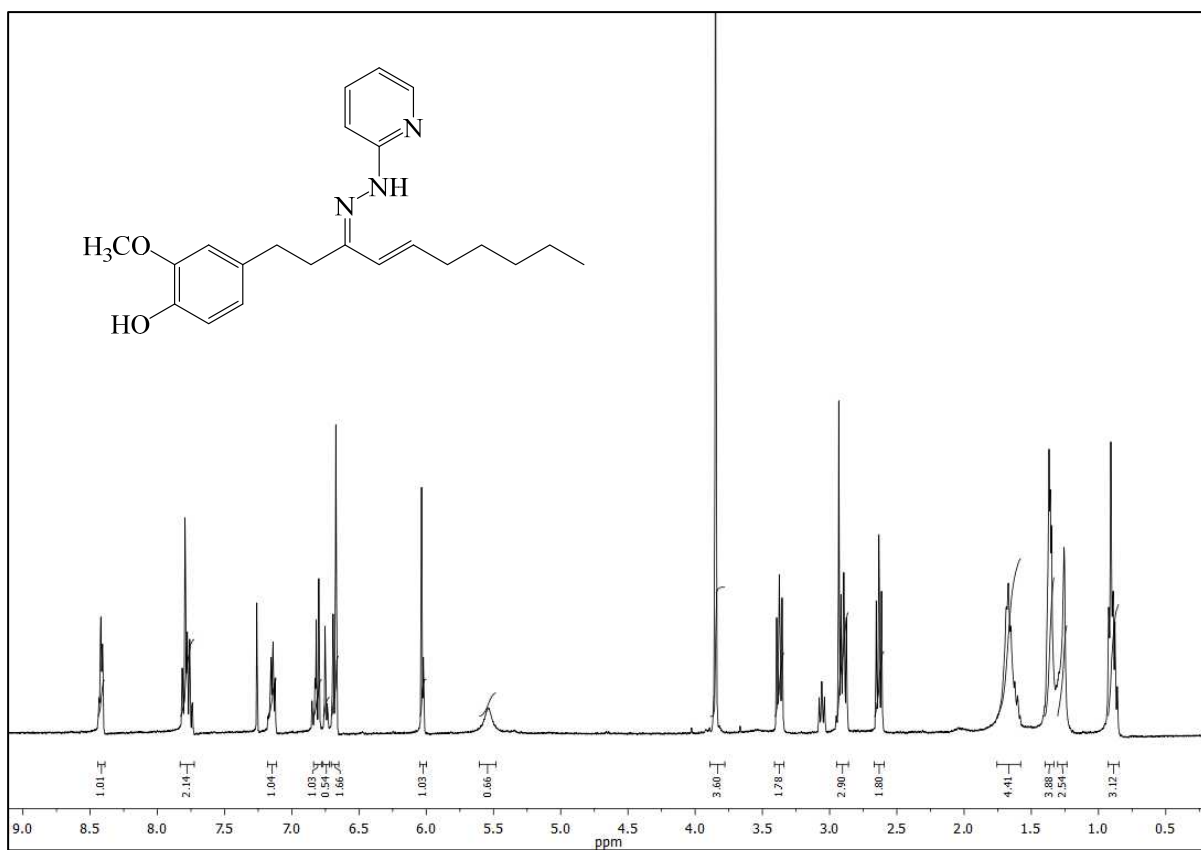


Figure S13. ¹H NMR spectrum of 4c.

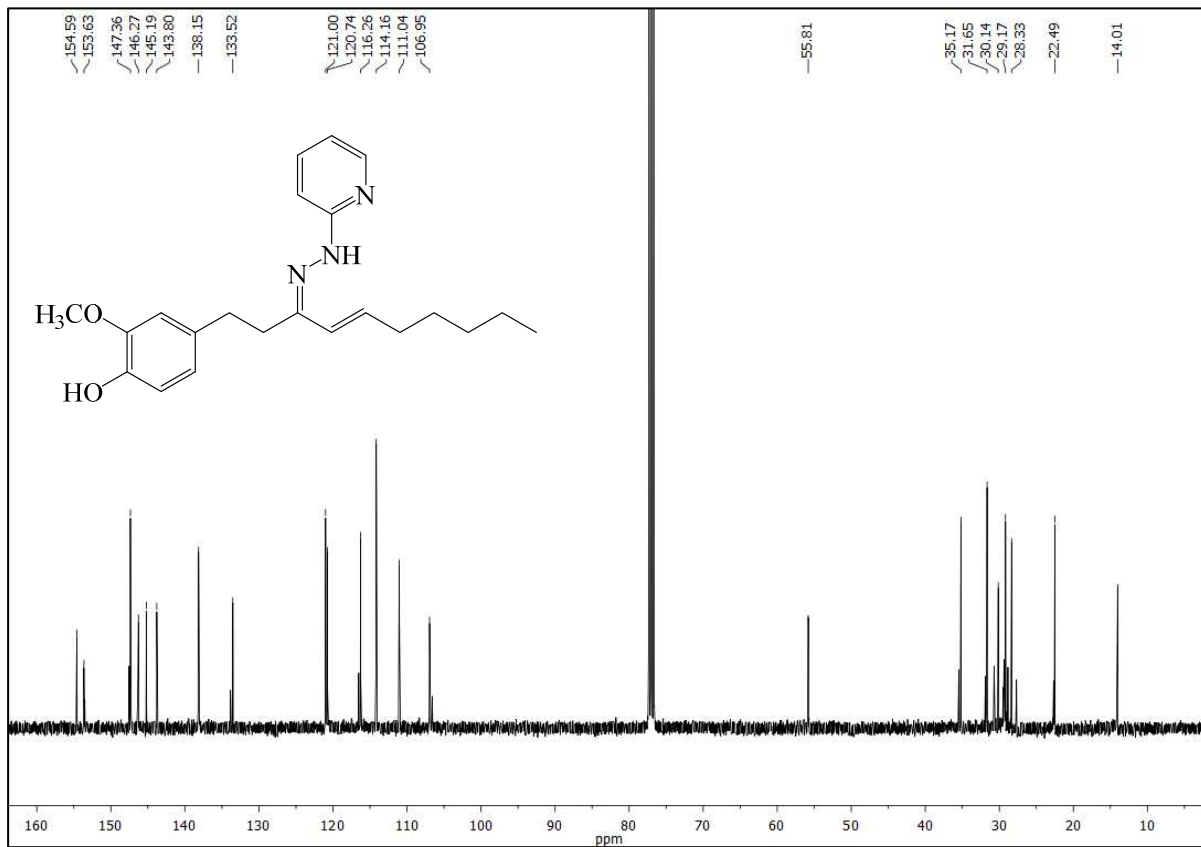


Figure S14. ¹³C NMR spectrum of 4c.

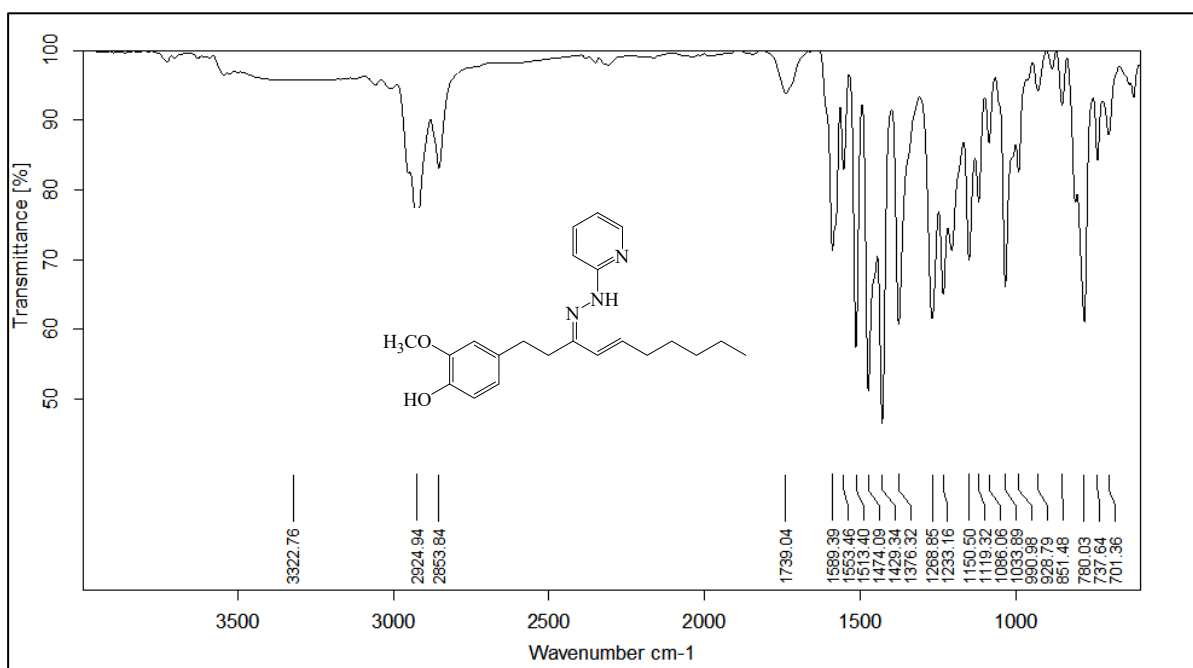


Figure S15. IR spectrum of **4c**.

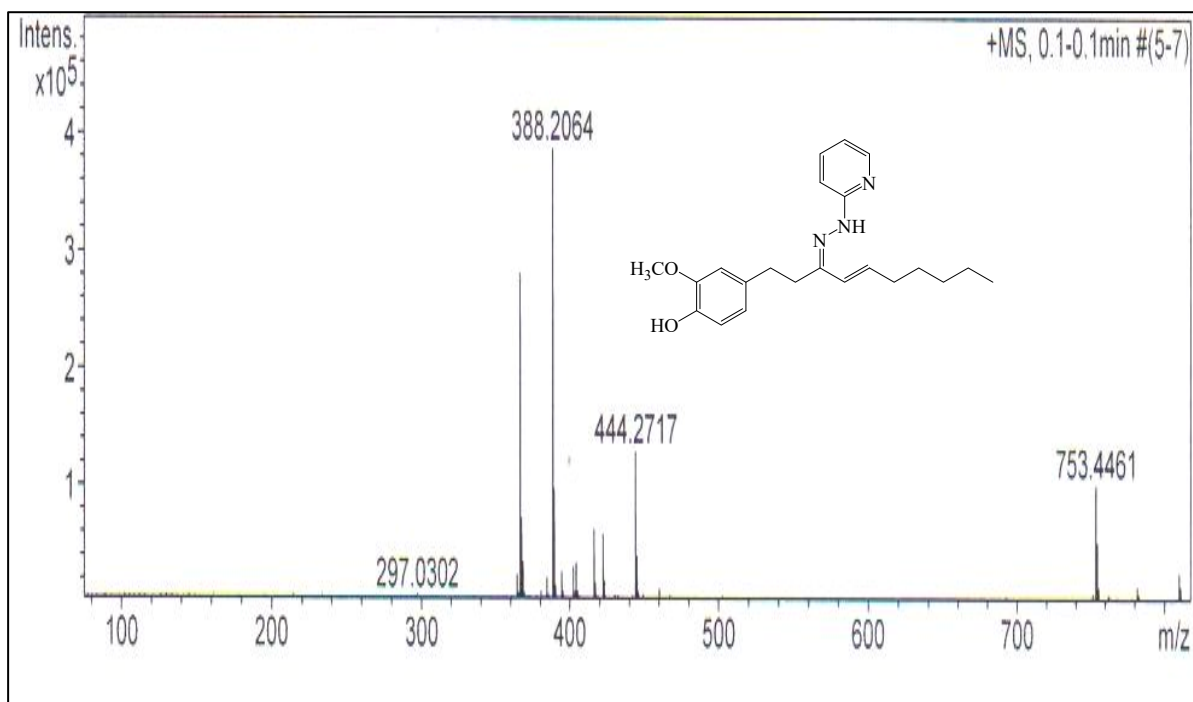


Figure S16. Mass spectrum of **4c**.

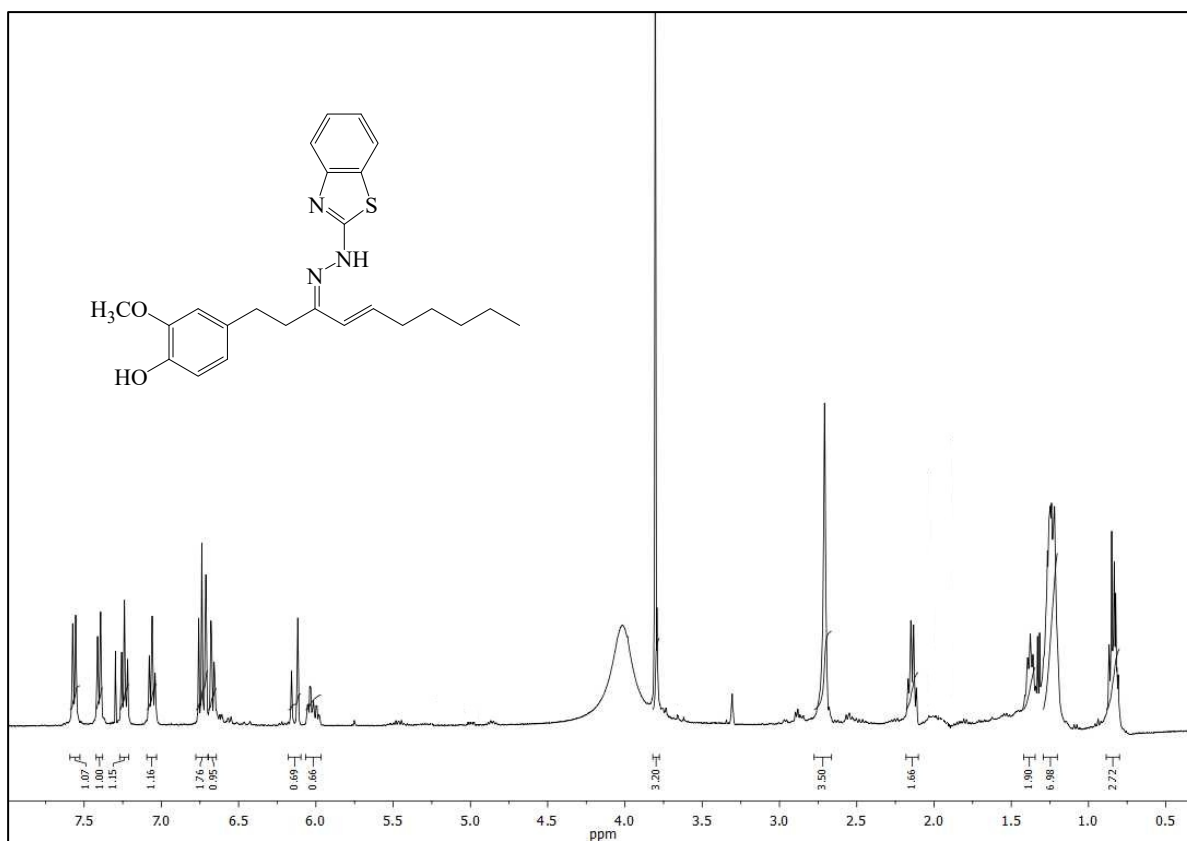


Figure S17. ¹H NMR spectrum of 4d.

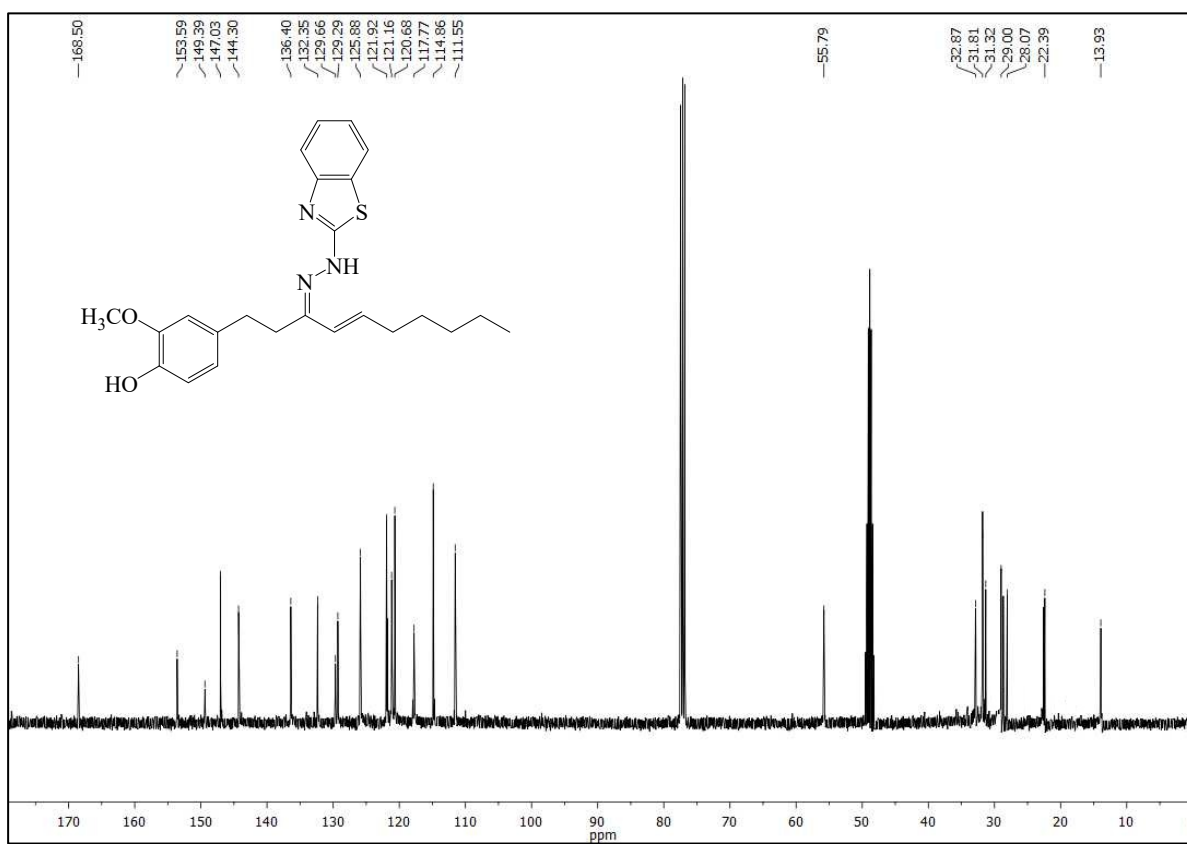


Figure S18. ¹³C NMR spectrum of 4d.

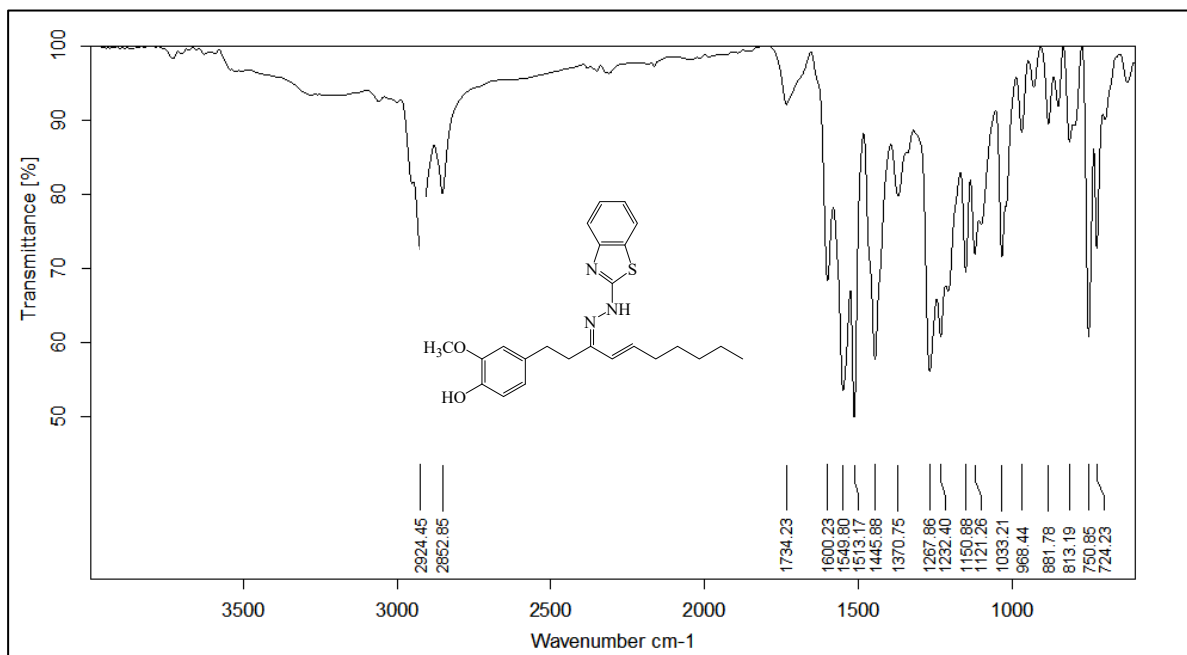


Figure S19. IR spectrum of **4d**.

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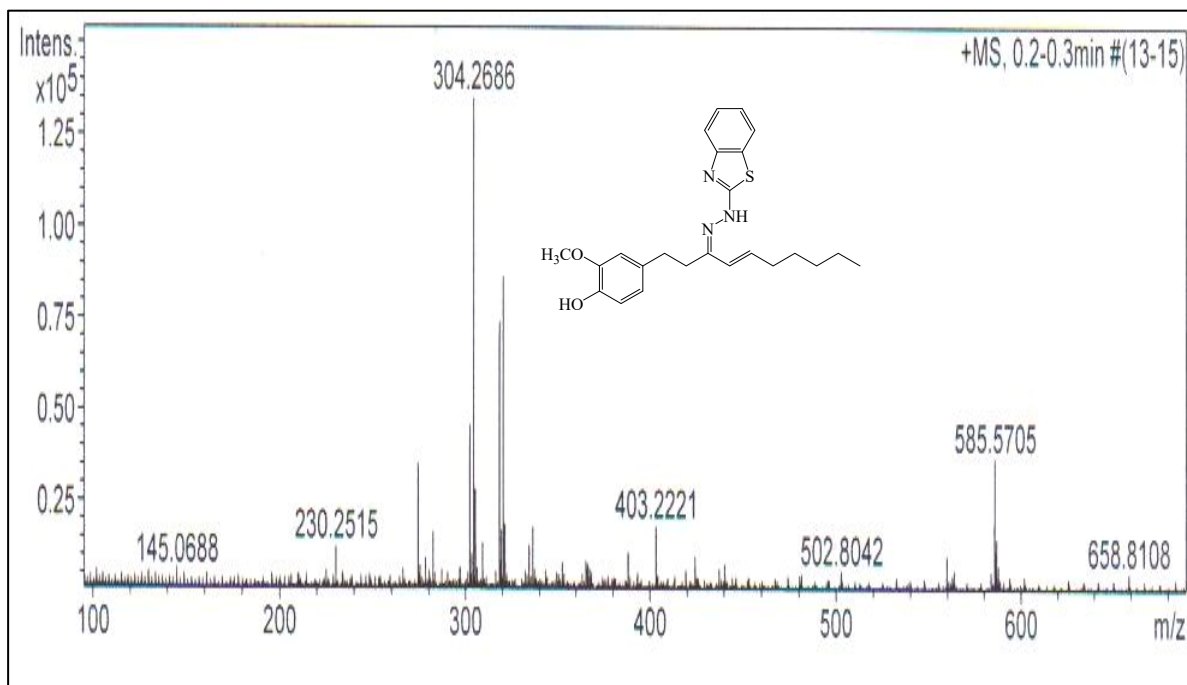


Figure S20. Mass spectrum of **4d**.

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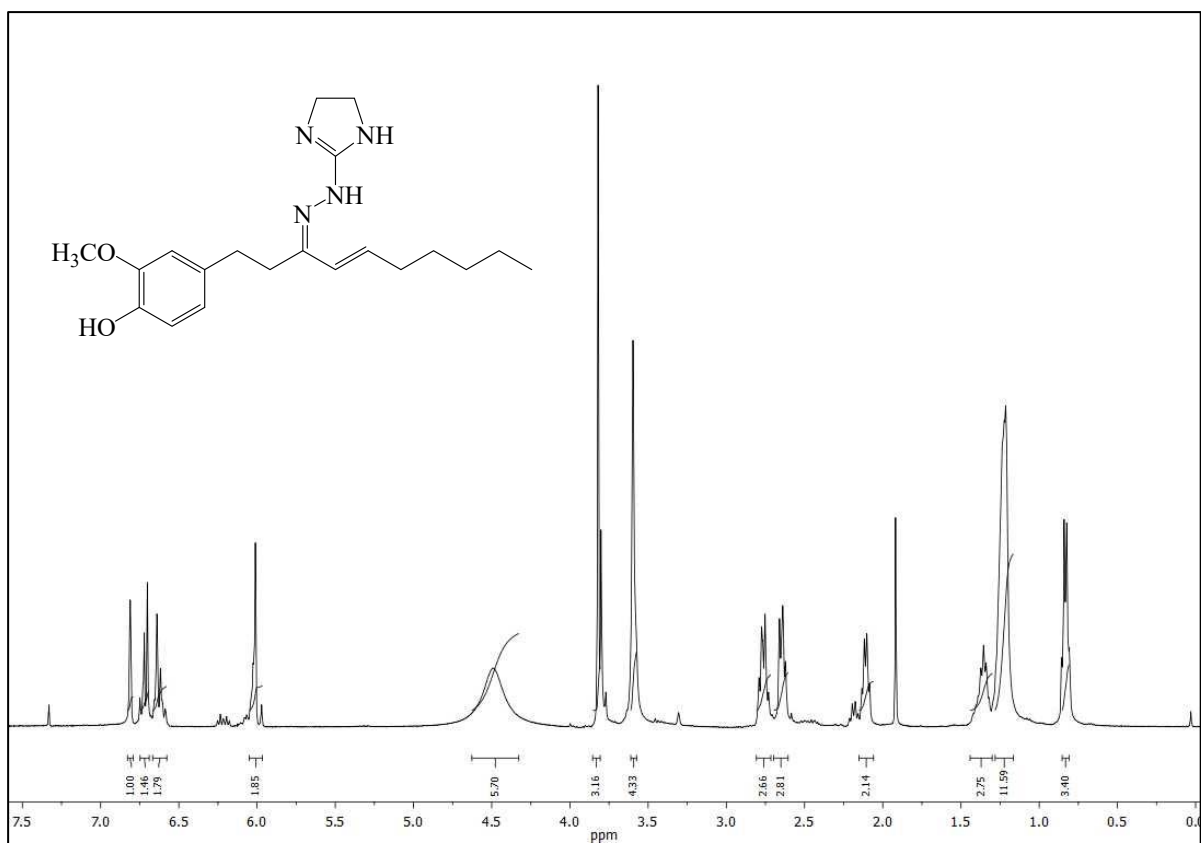


Figure S21. ¹H NMR spectrum of 4e.

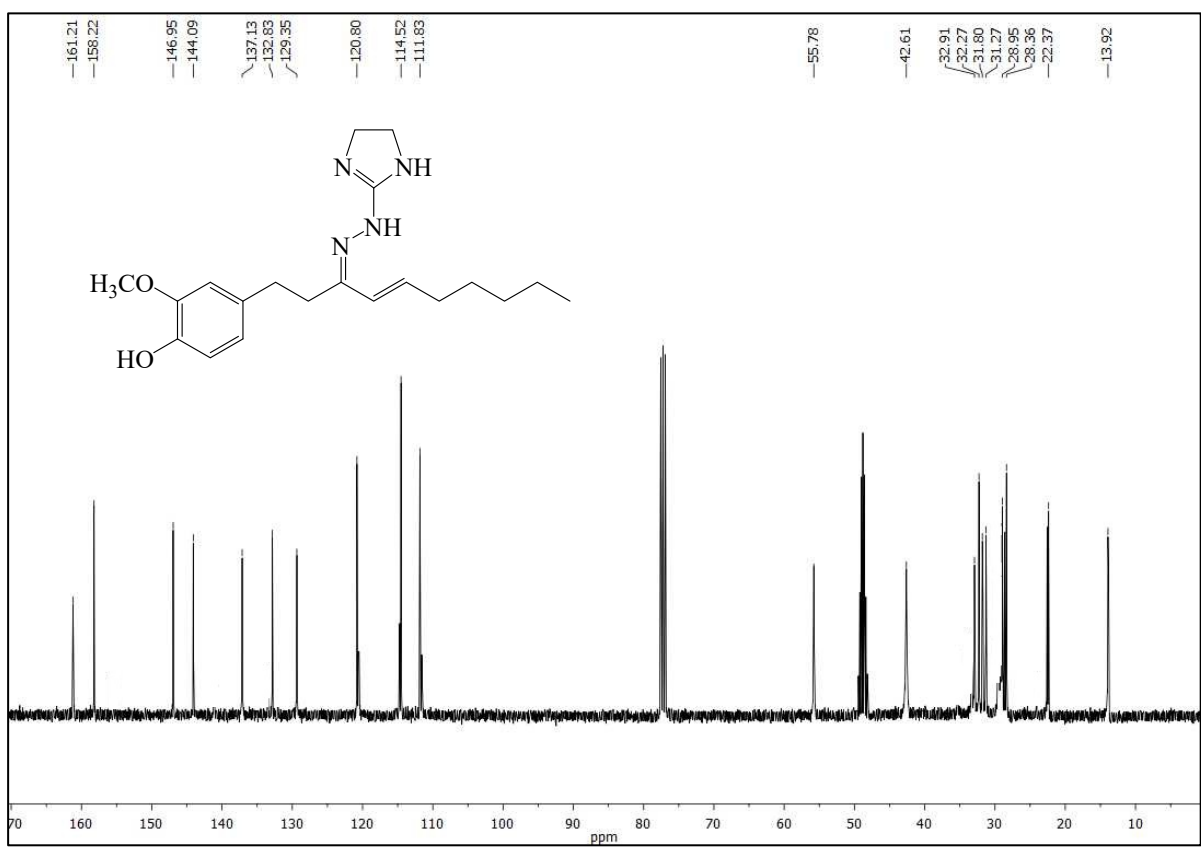


Figure S22. ¹³C NMR spectrum of 4e.

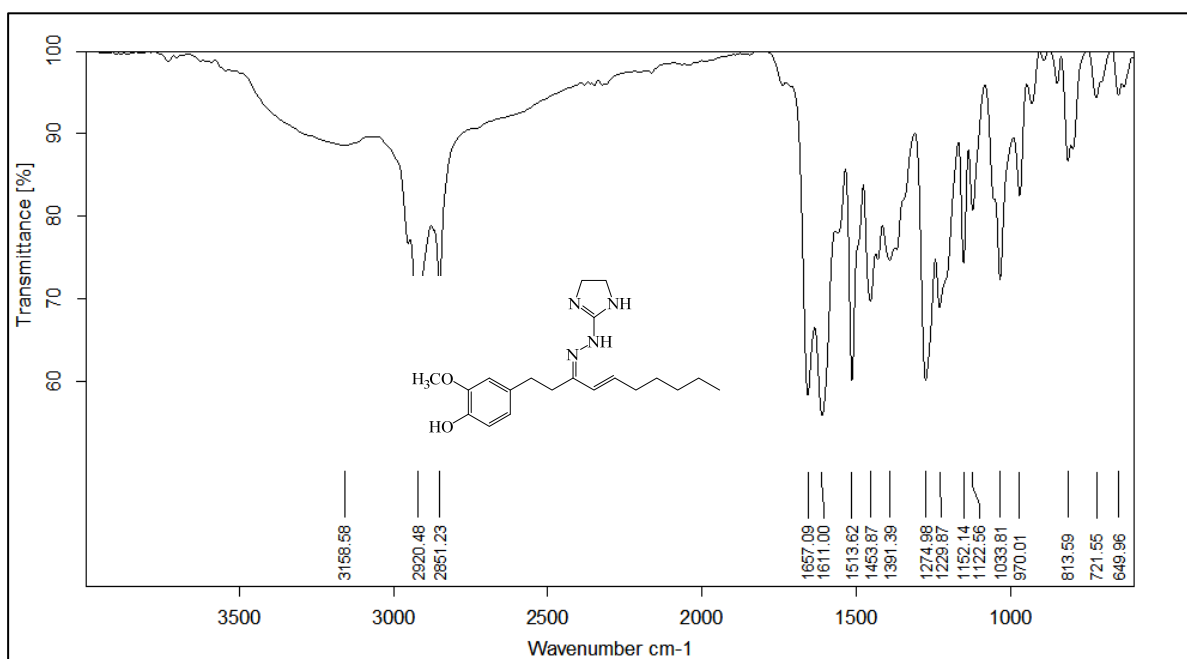


Figure S23. IR spectrum of **4e**.

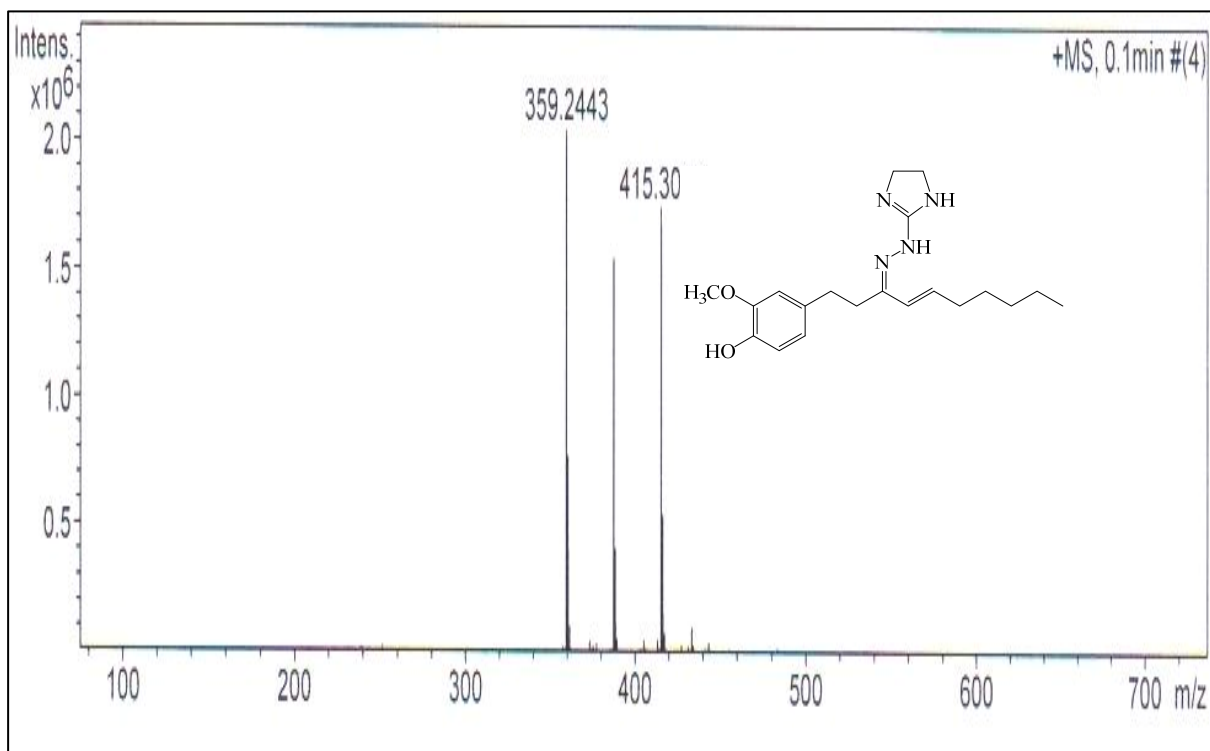


Figure S24. Mass spectrum of **4e**.

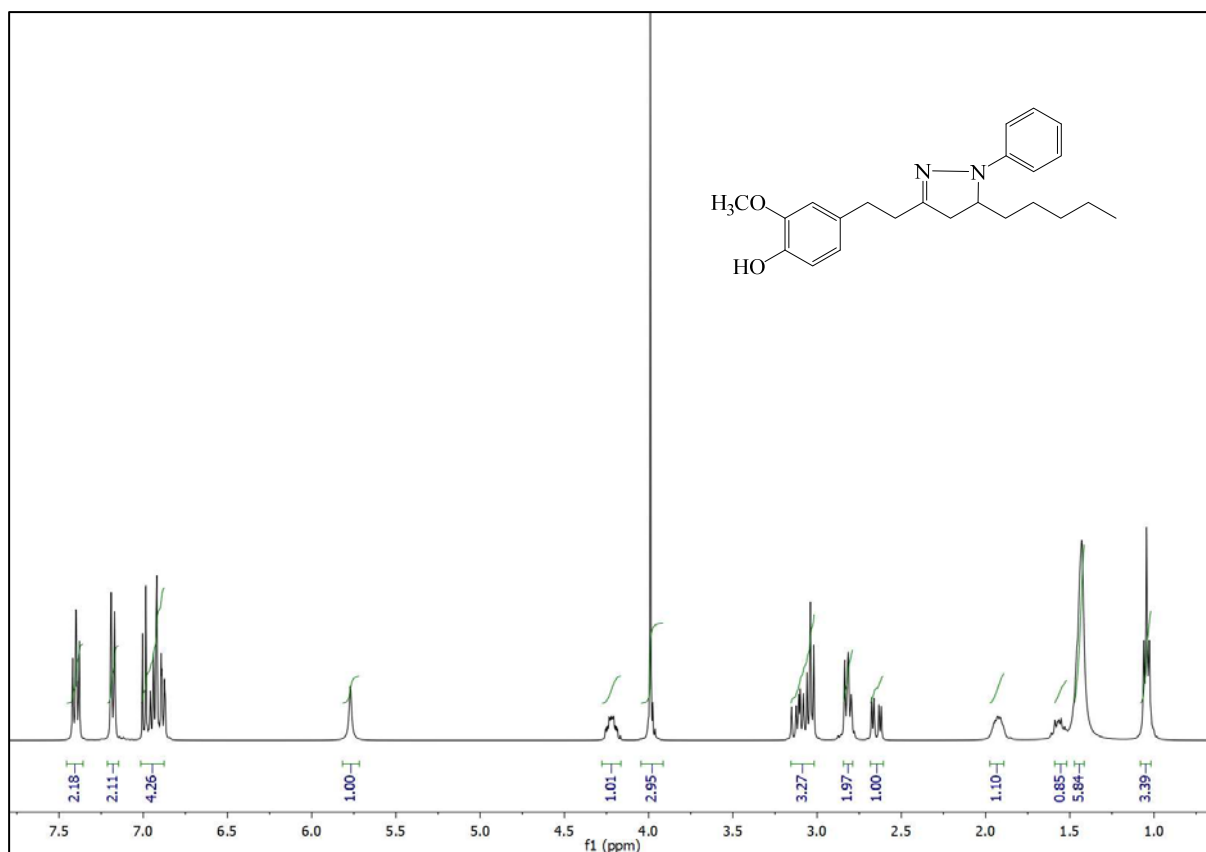


Figure S25. ¹H NMR spectrum of 5a.

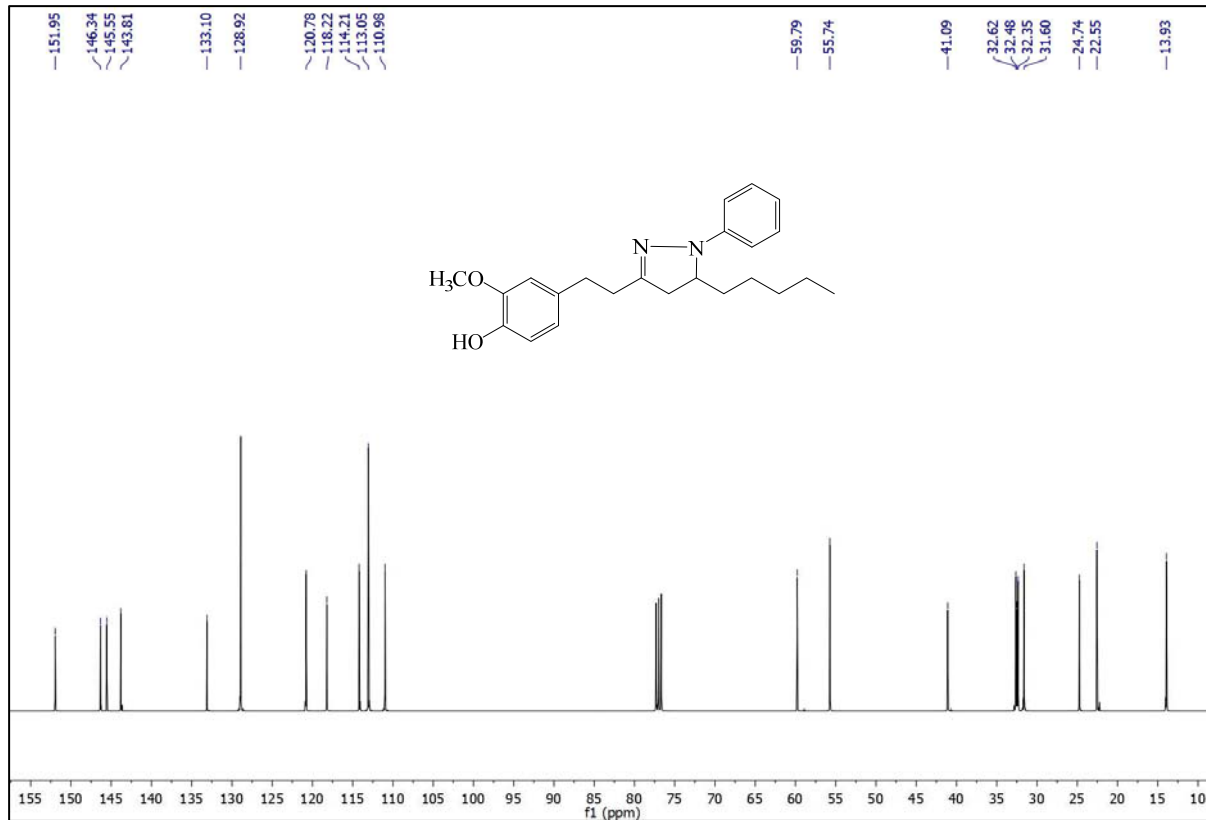


Figure S26. ¹³C NMR spectrum of 5a.

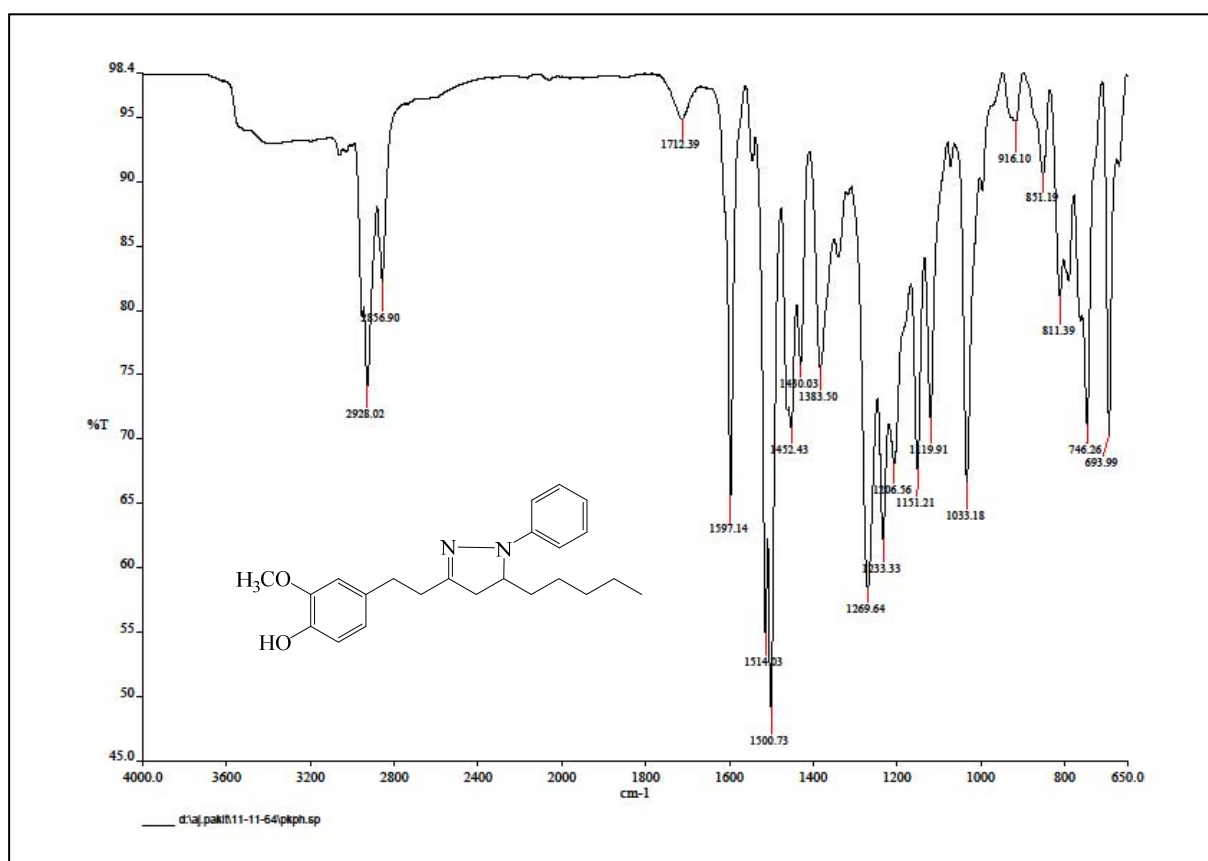


Figure S27. IR spectrum of 5a.

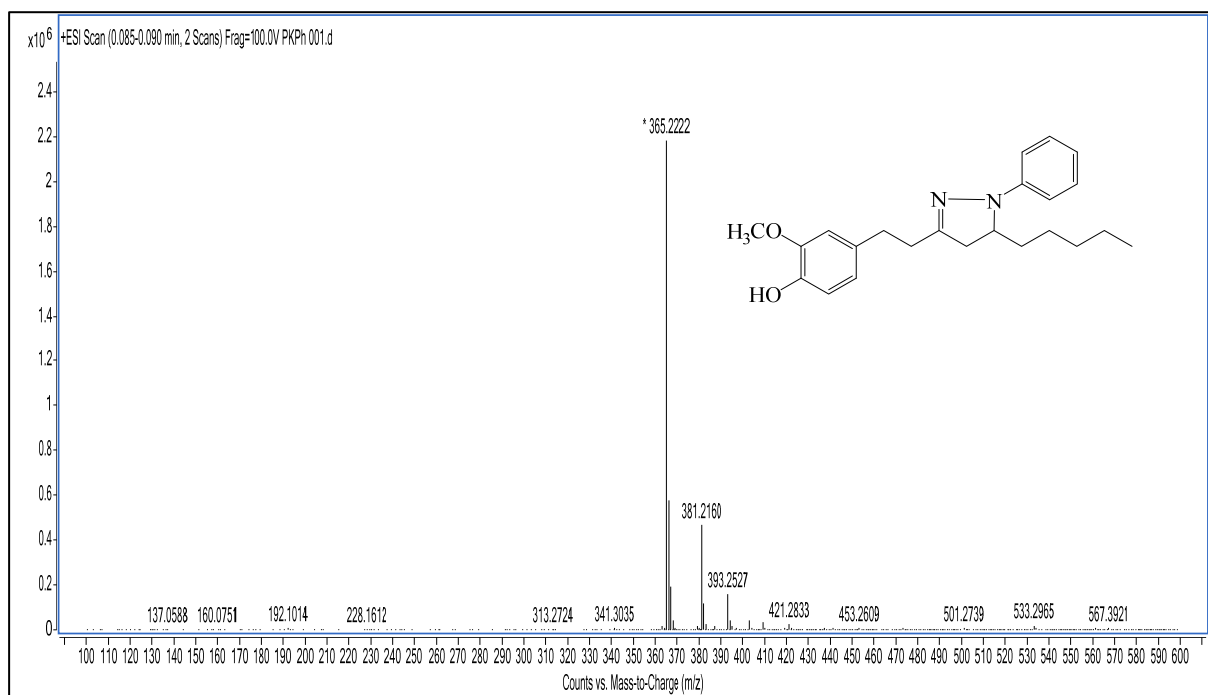


Figure S28. Mass spectrum of 5a.

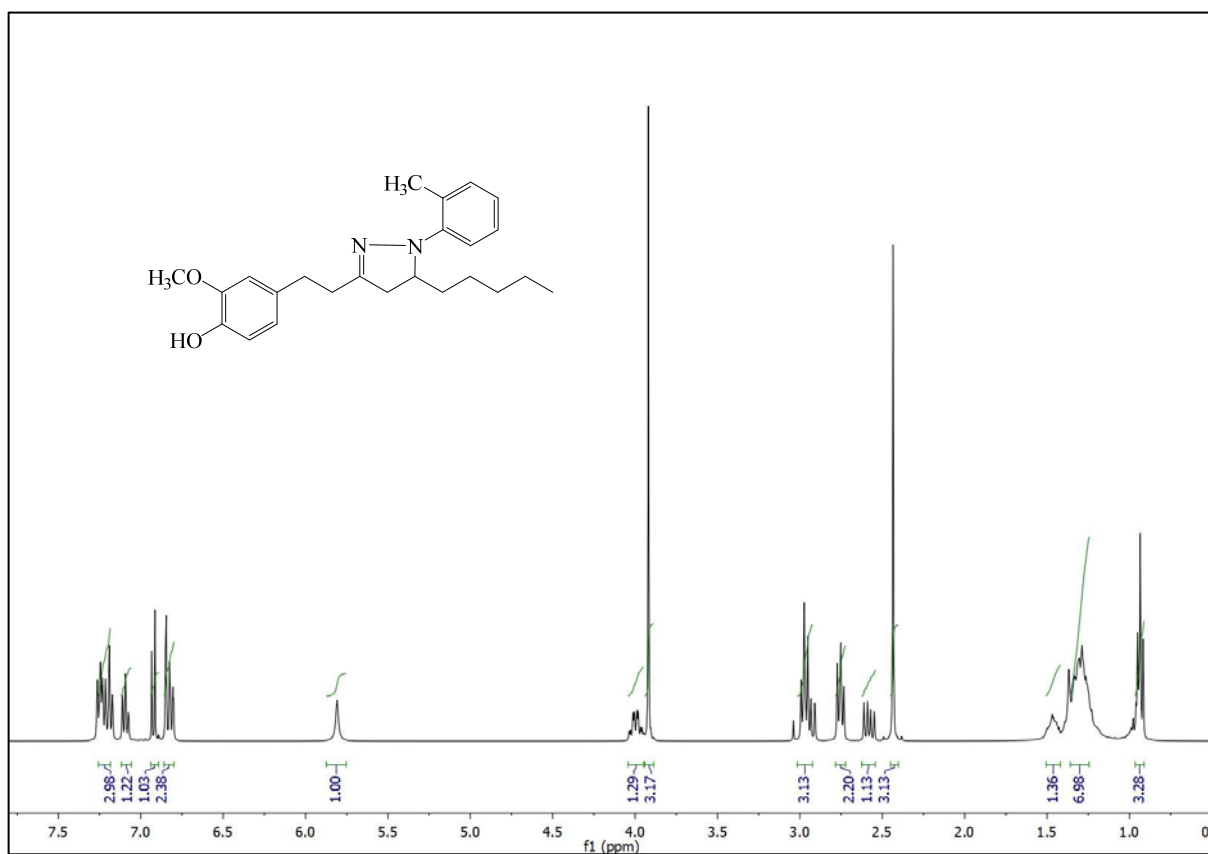


Figure S29. ¹H NMR spectrum of **5b**.

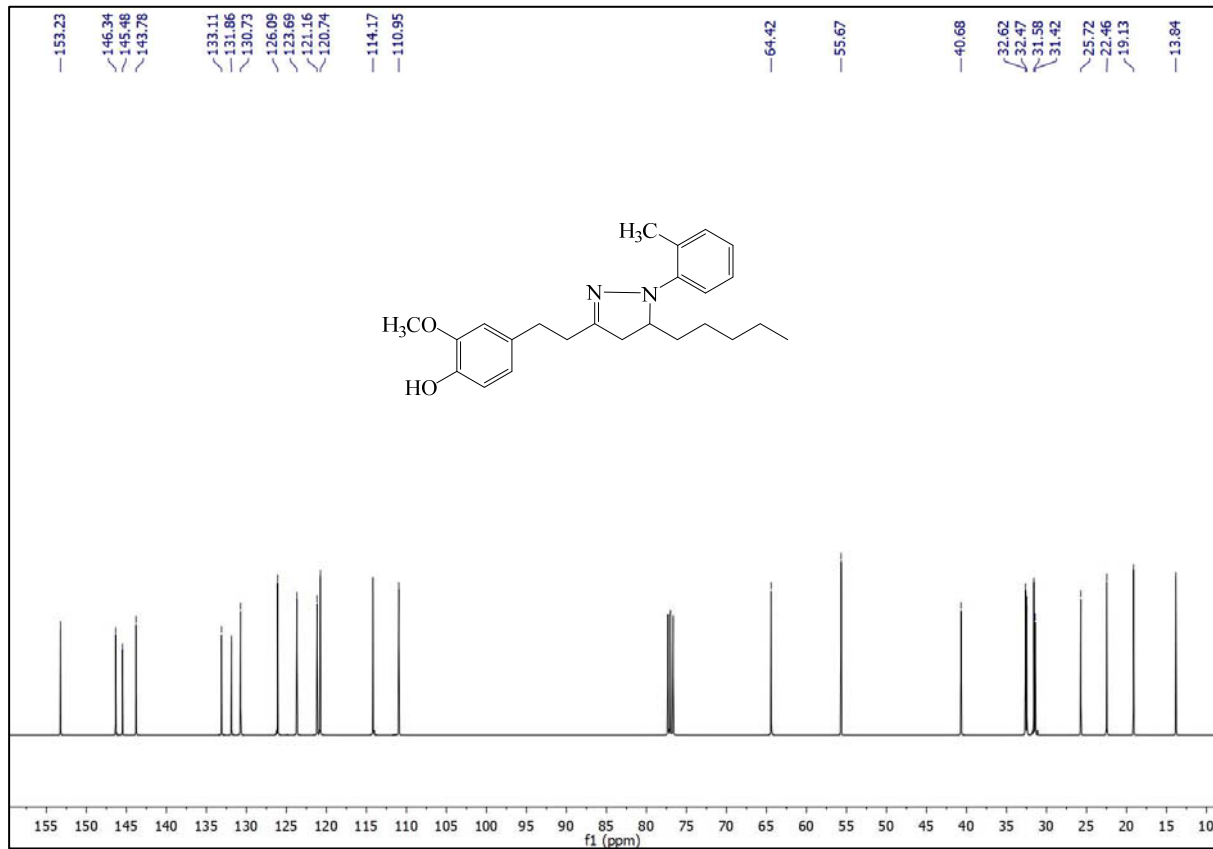


Figure S30. ¹³C NMR spectrum of **5b**.

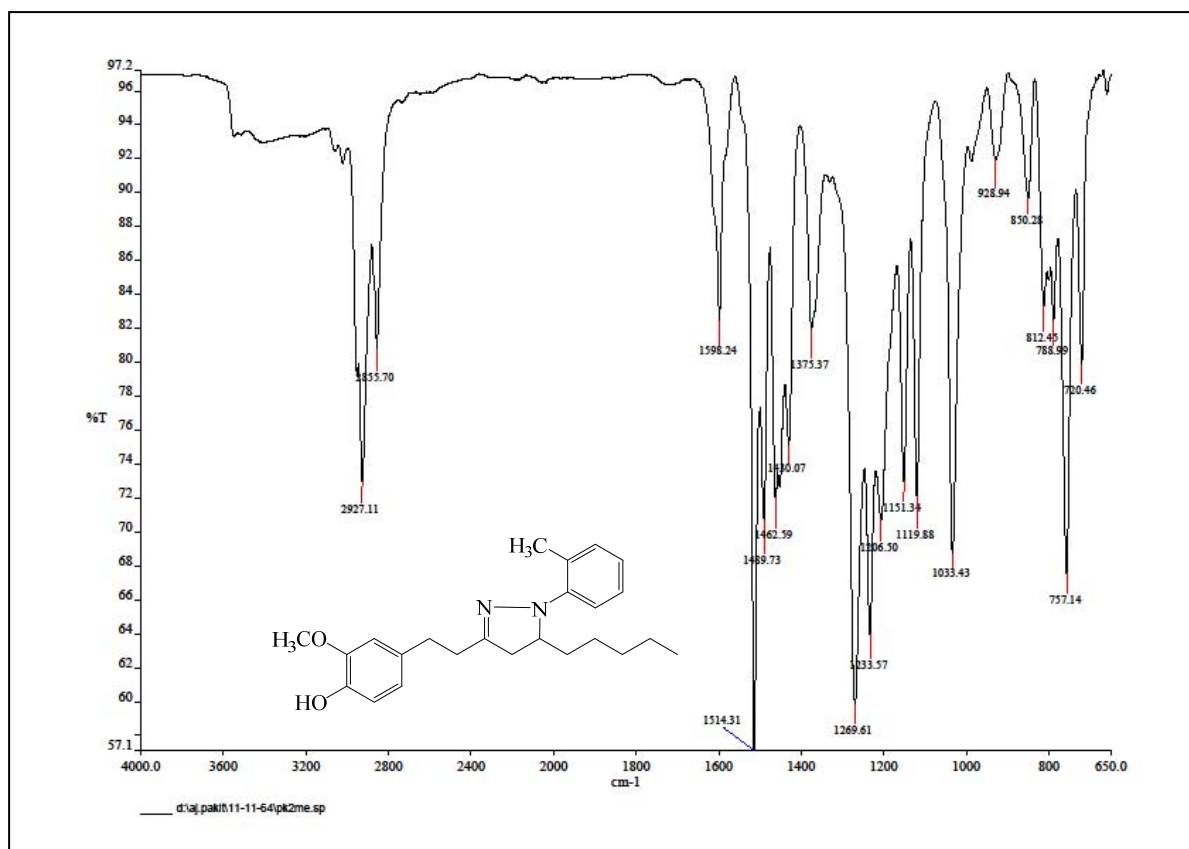


Figure S31. IR spectrum of **5b**.

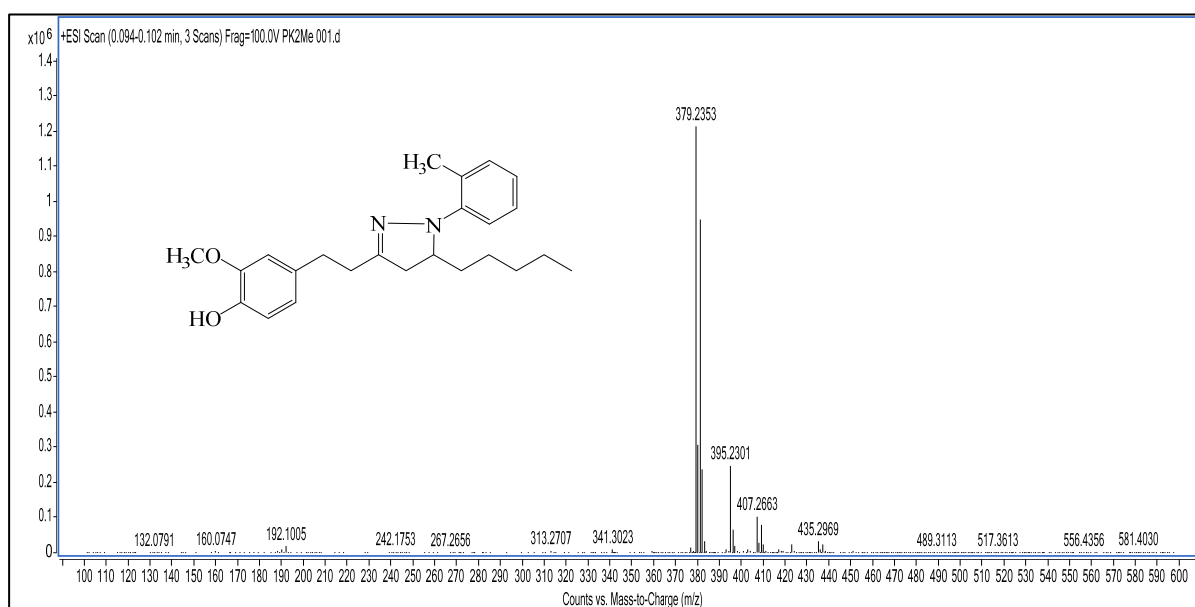


Figure S32. Mass spectrum of **5b**.

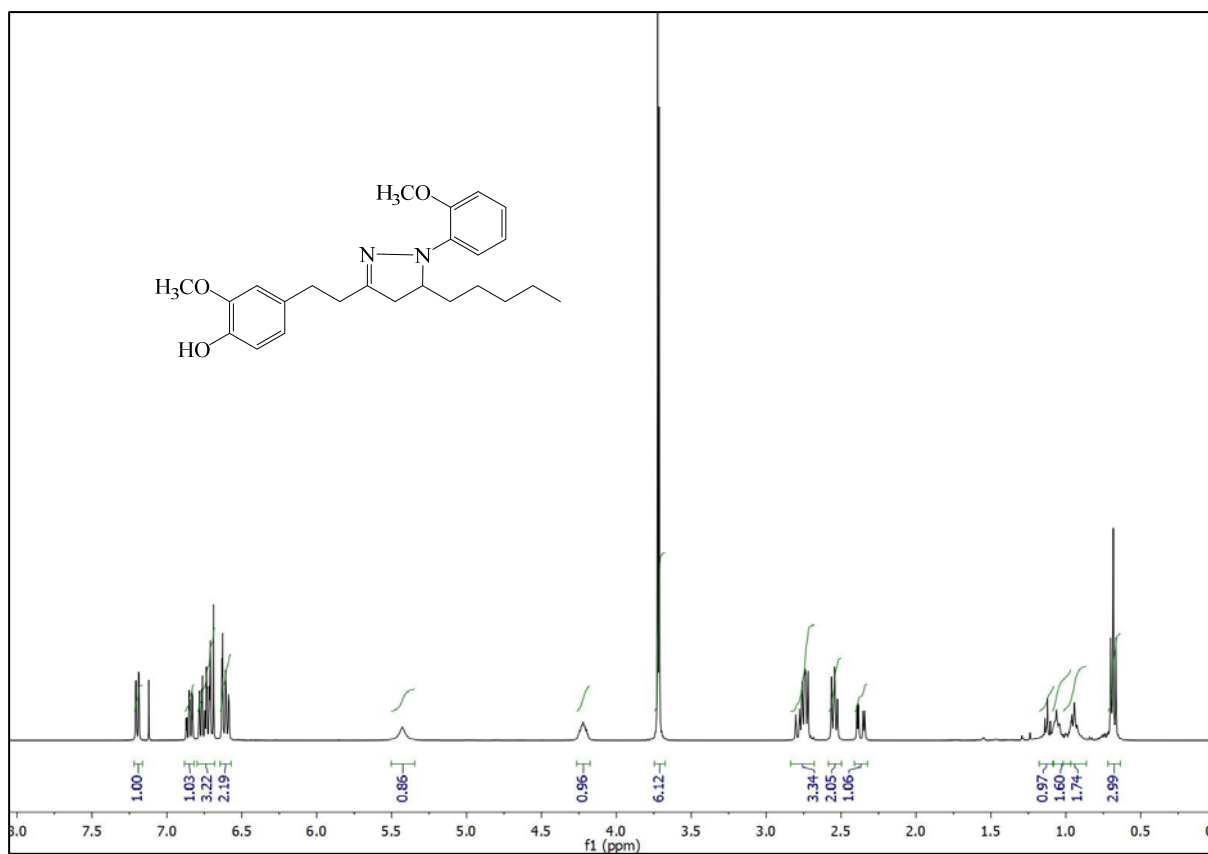


Figure S33. ^1H NMR spectrum of **5c**.

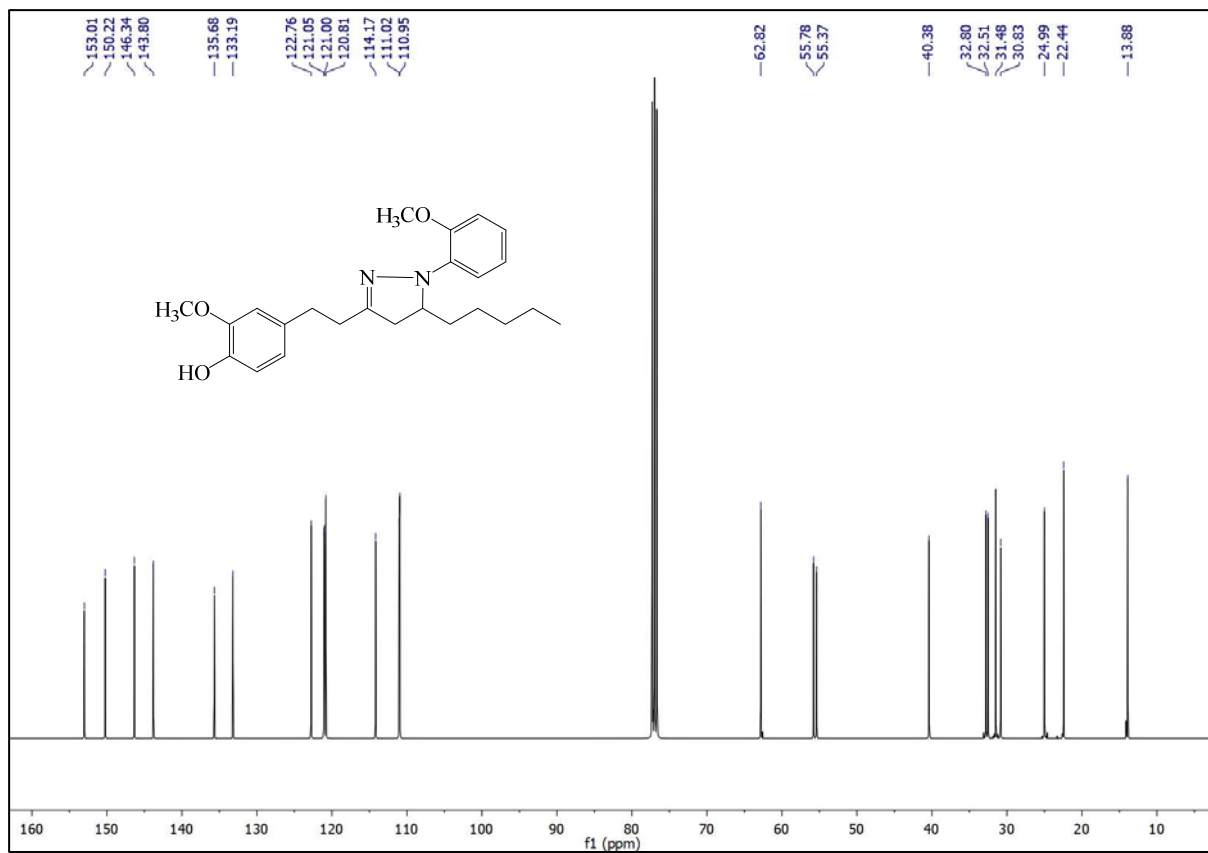


Figure S34. ^{13}C NMR spectrum of **5c**.

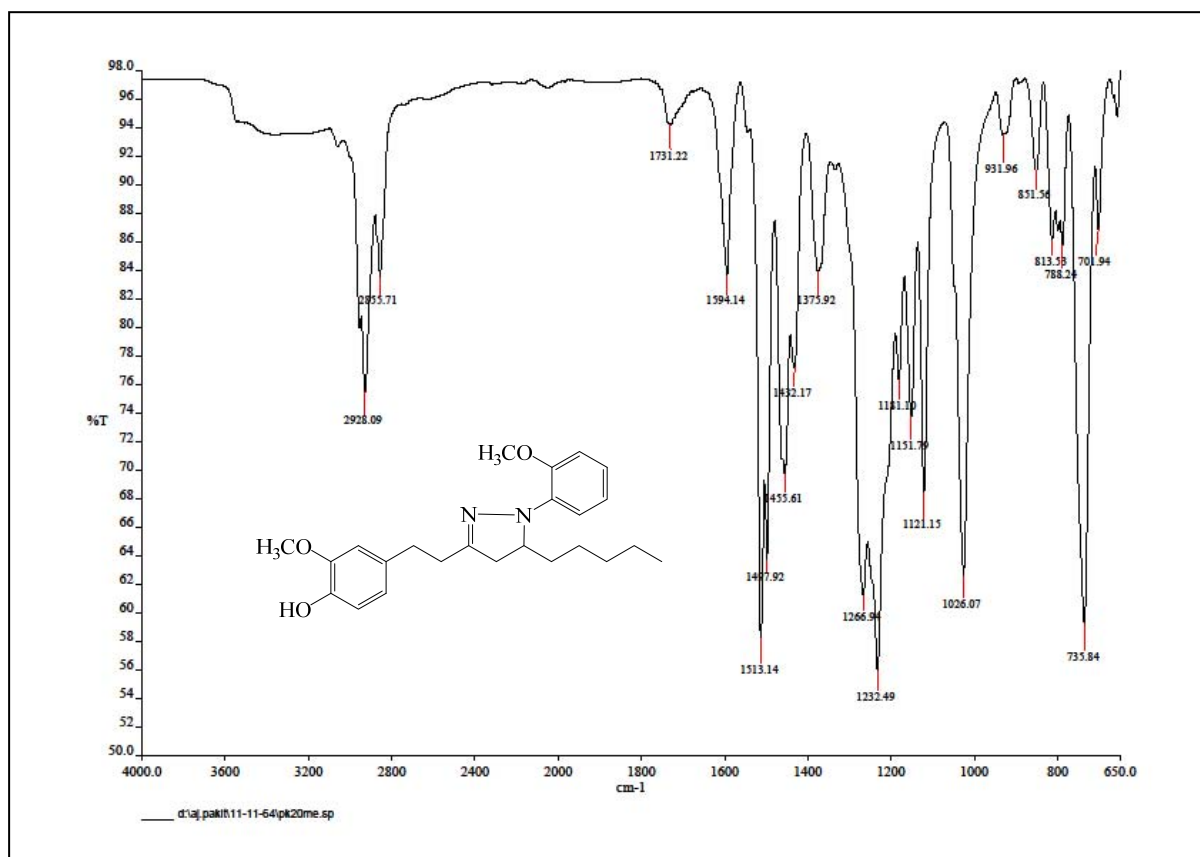


Figure S35. IR spectrum of 5c.

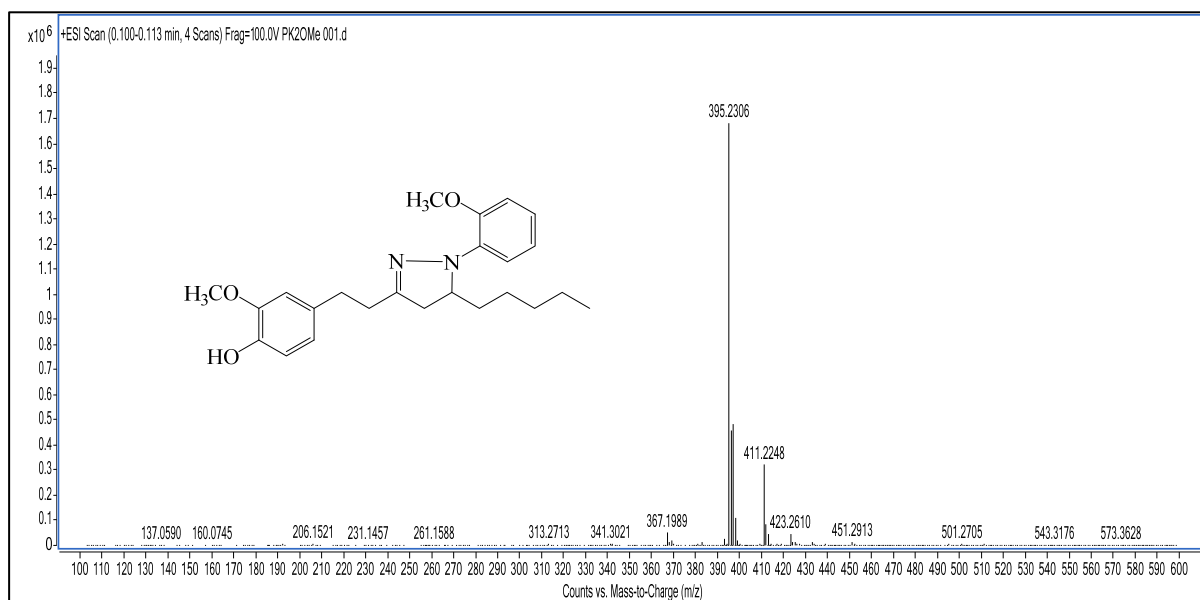


Figure S36. Mass spectrum of 5c.

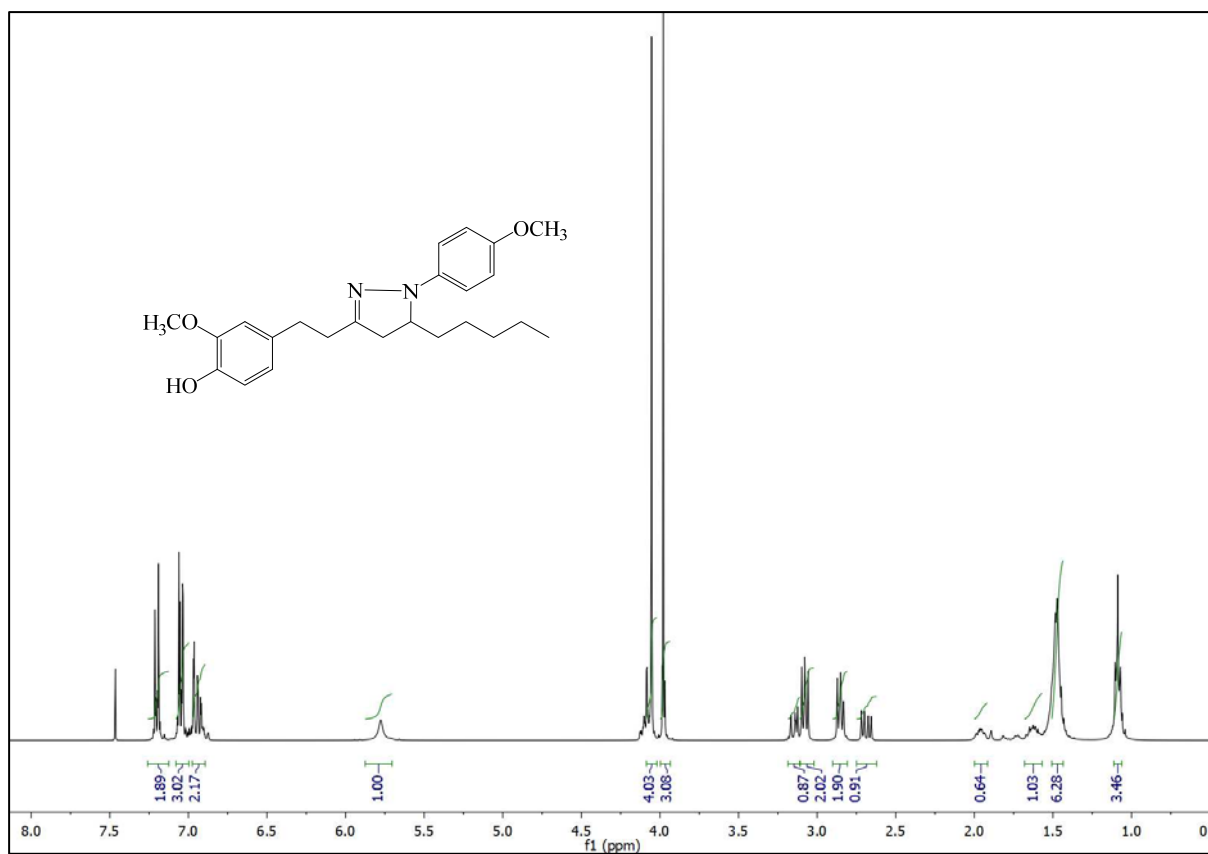


Figure S37. ¹H NMR spectrum of **5d**.

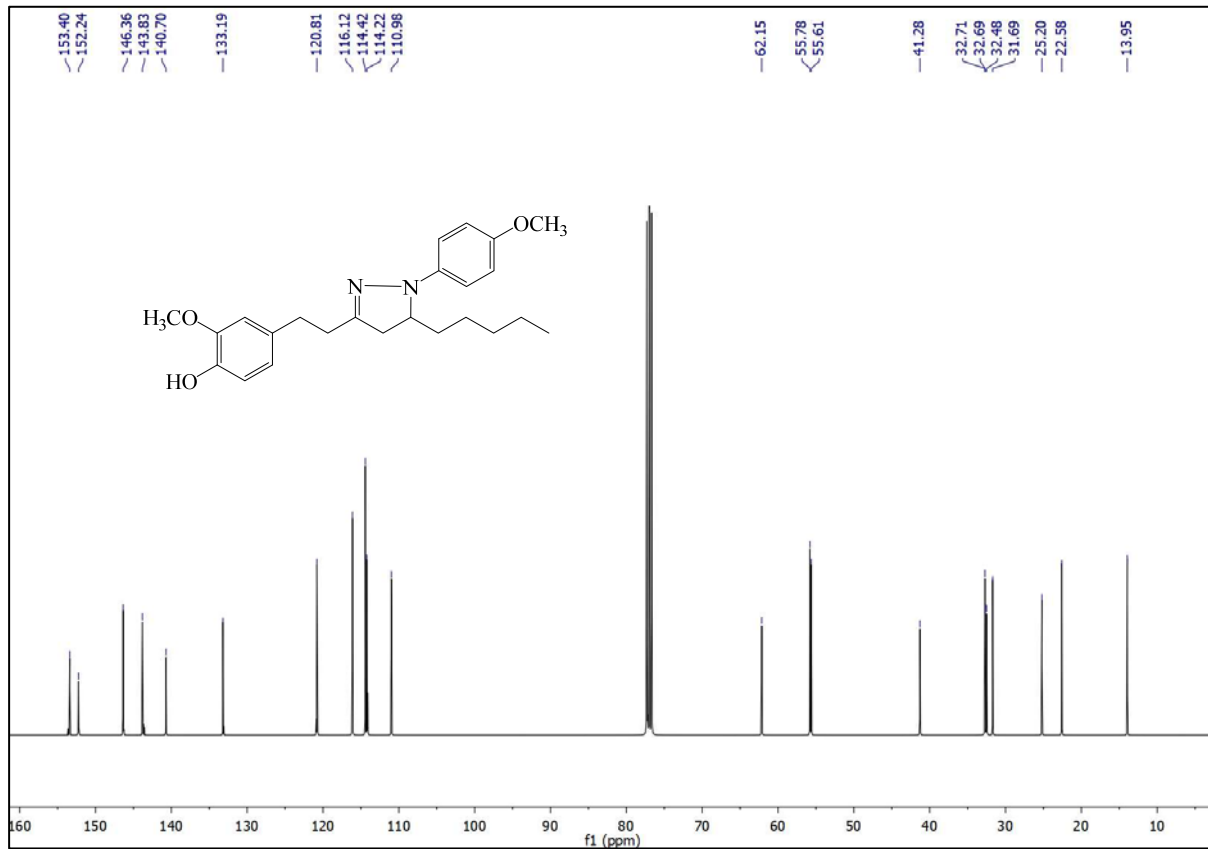


Figure S38. ¹³C NMR spectrum of **5d**.

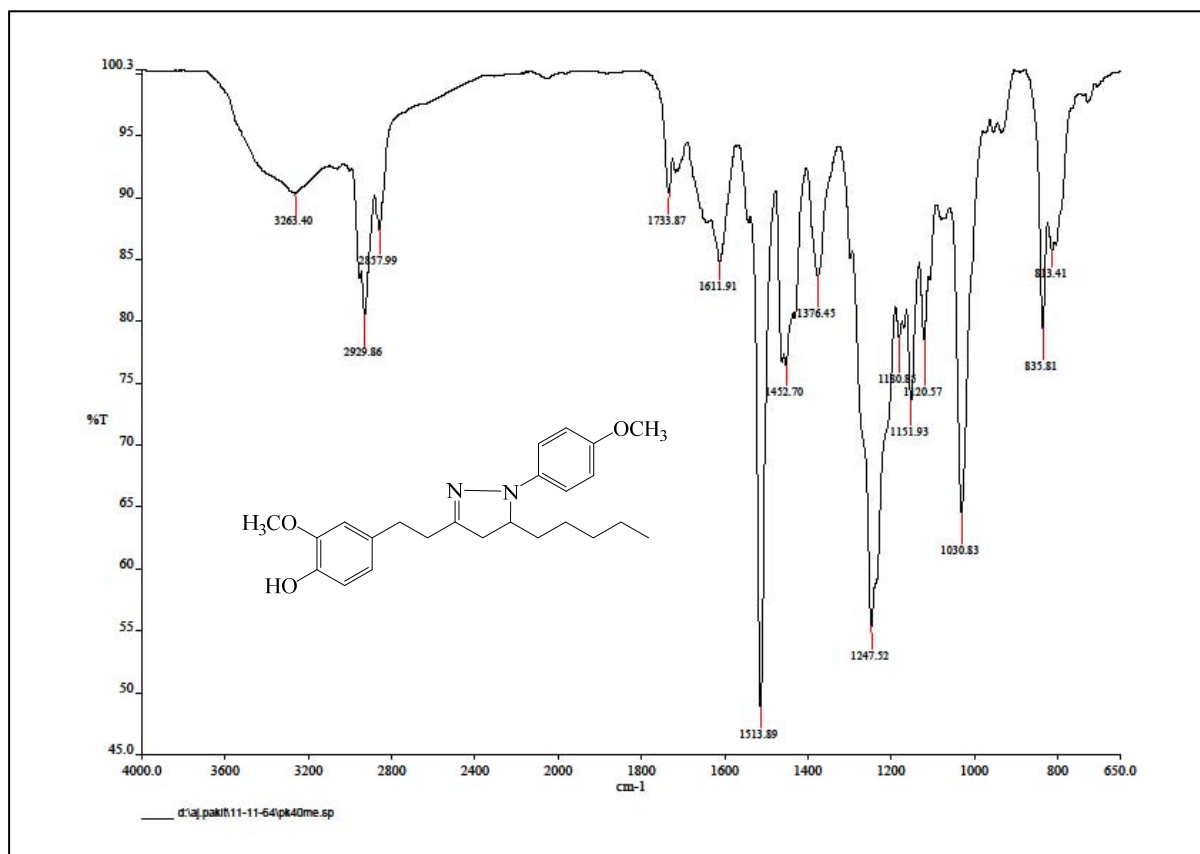


Figure S39. IR spectrum of 5d.

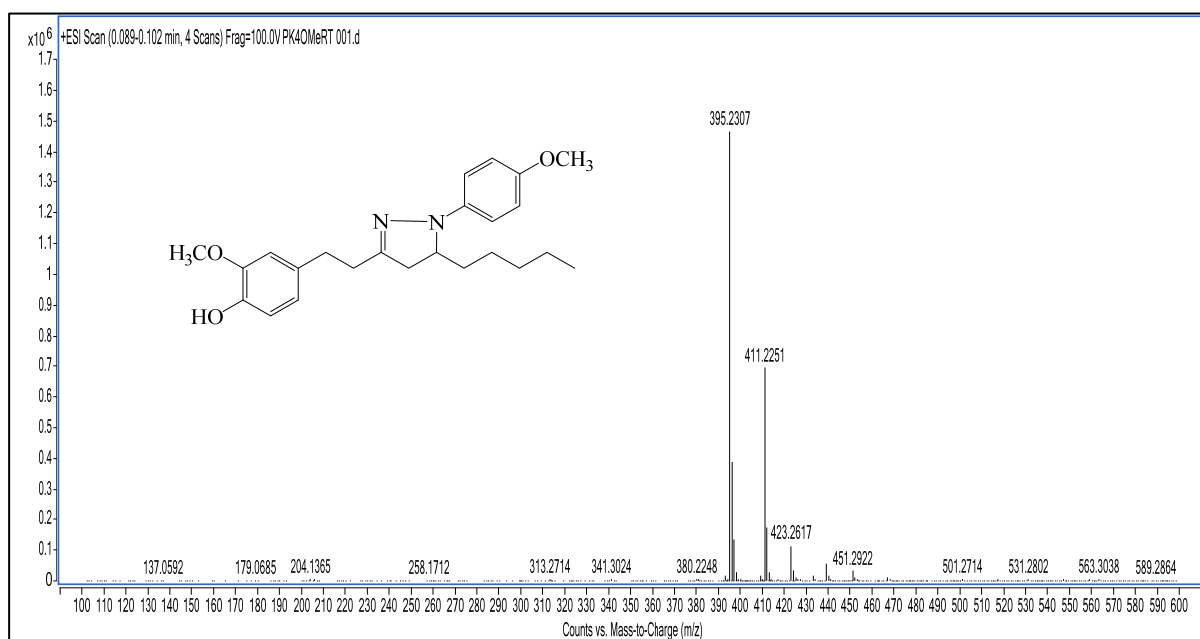


Figure S40. Mass spectrum of 5d.

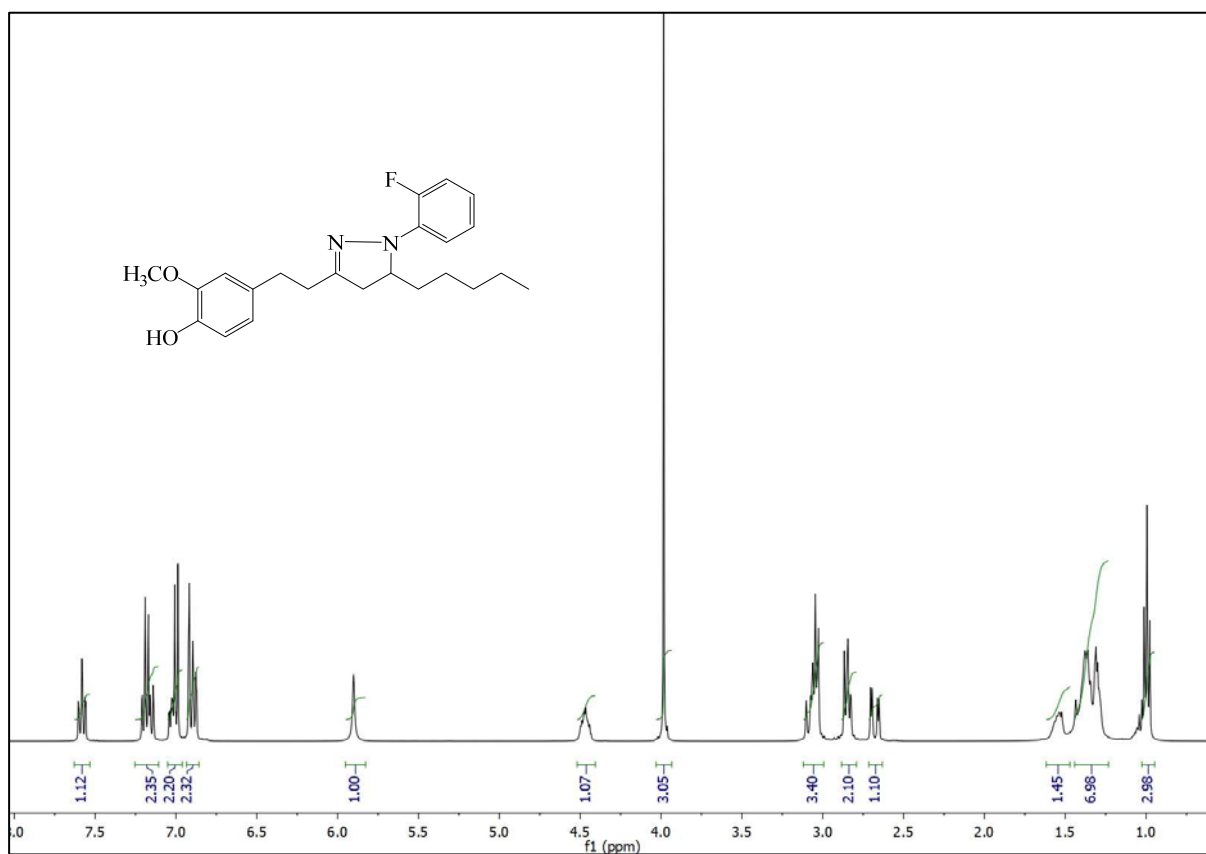


Figure S41. ¹H NMR spectrum of 5e.

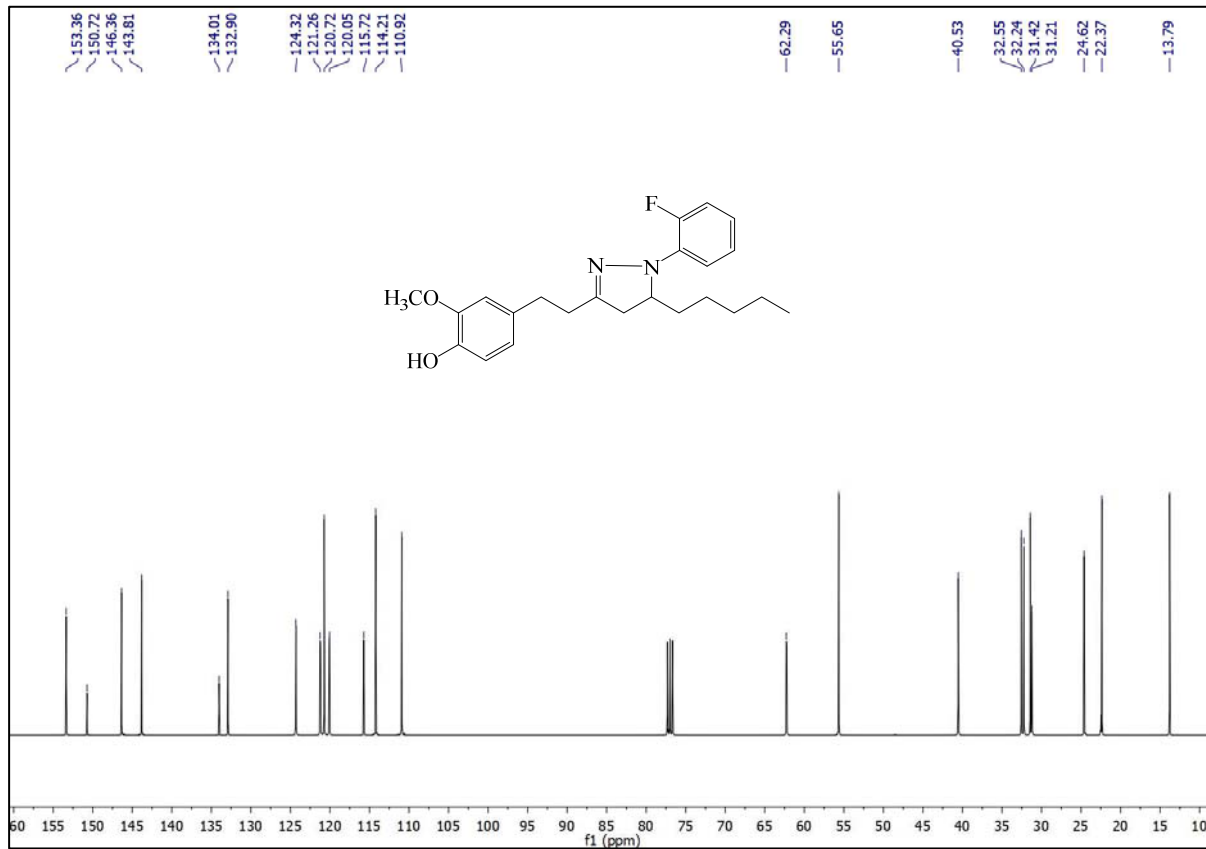


Figure S42. ¹³C NMR spectrum of 5e.

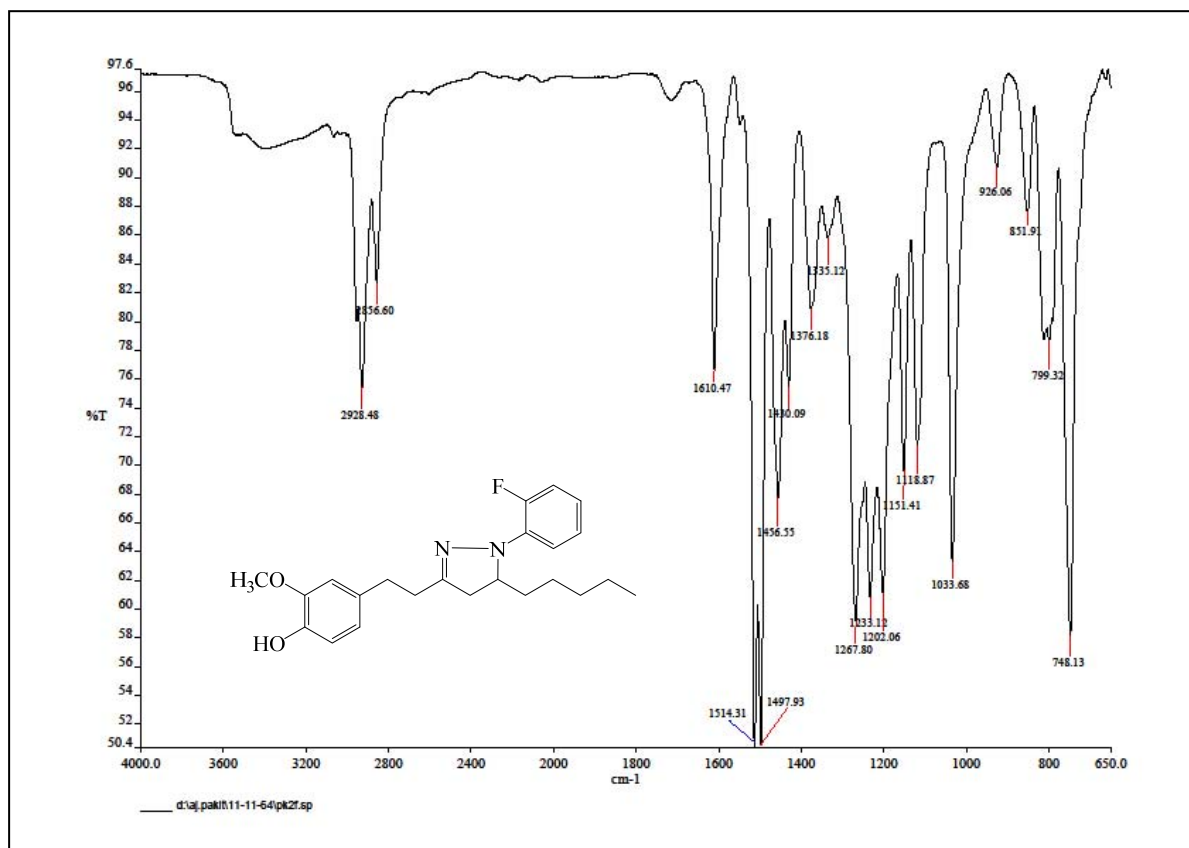


Figure S43. IR spectrum of 5e.

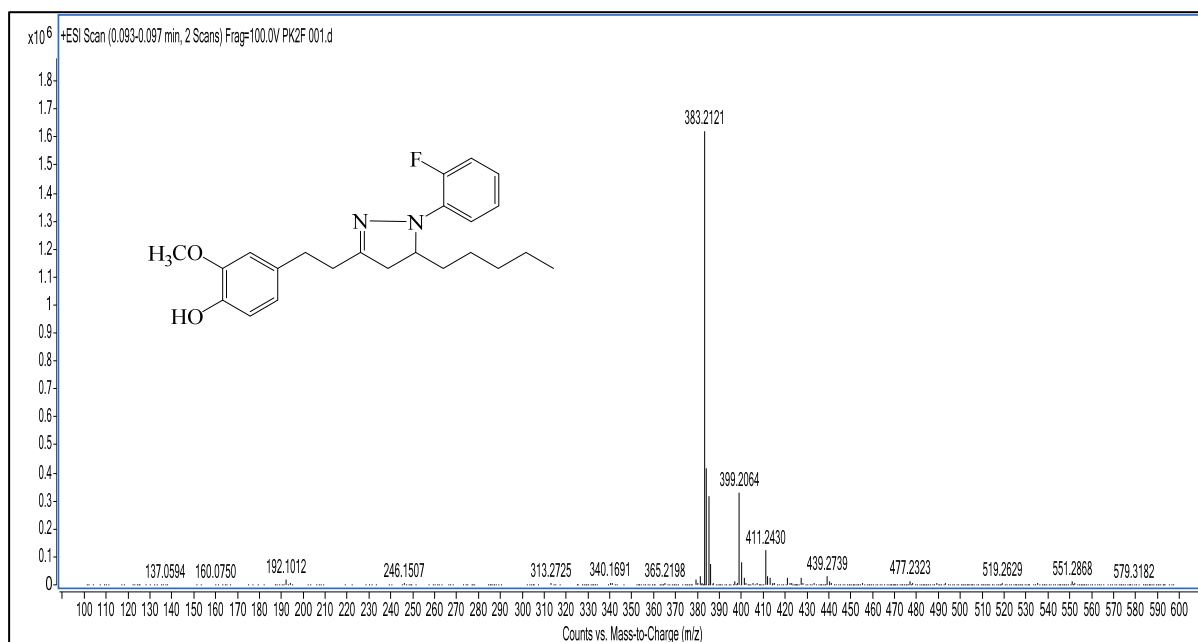


Figure S44. Mass spectrum of 5e.

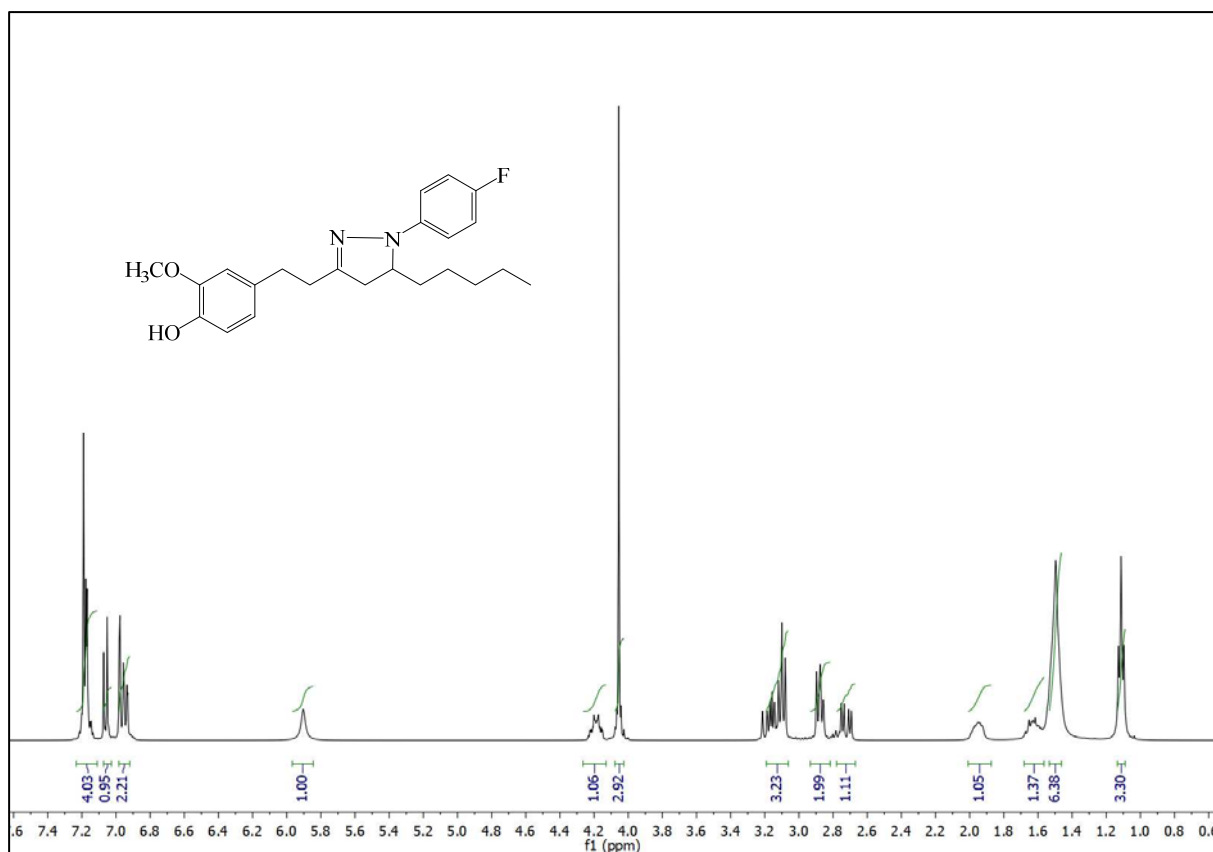


Figure S45. ¹H NMR spectrum of **5f**.

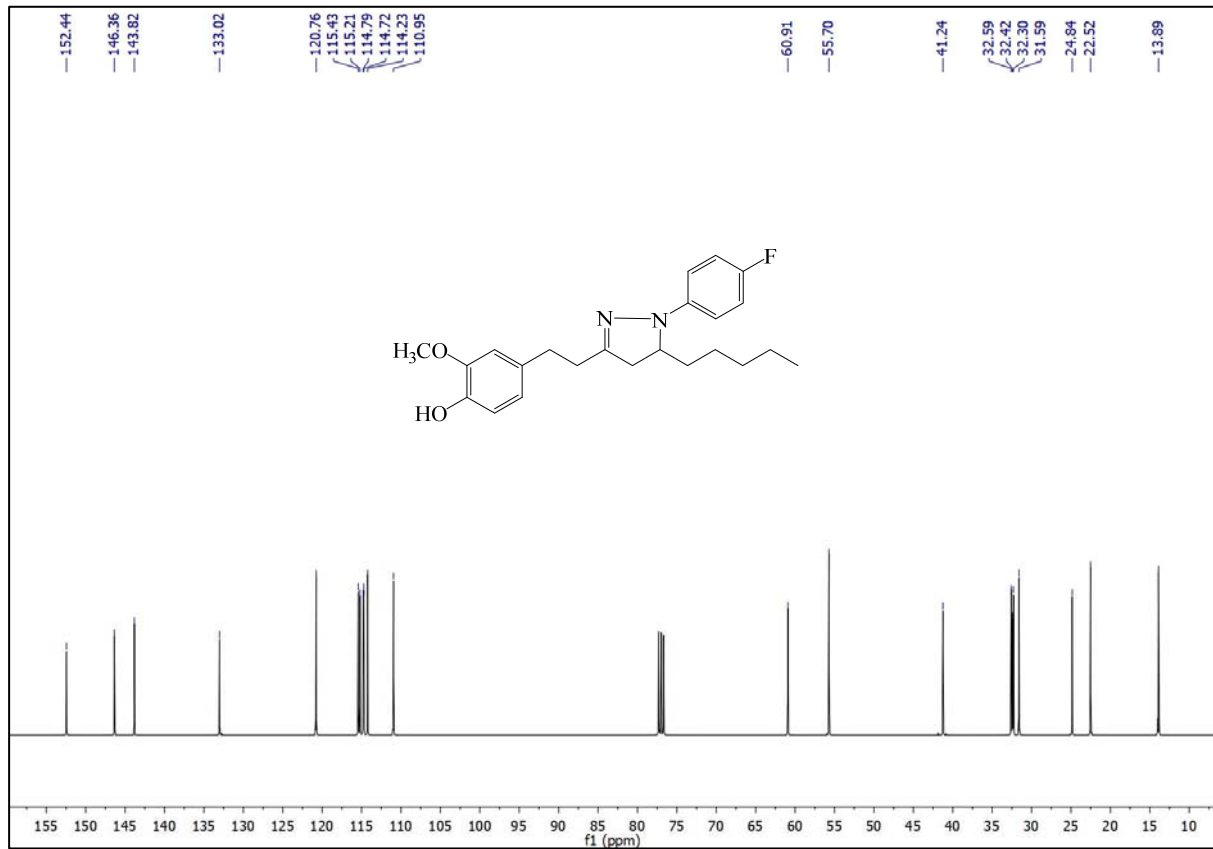


Figure S46. ¹³C NMR spectrum of **5f**.

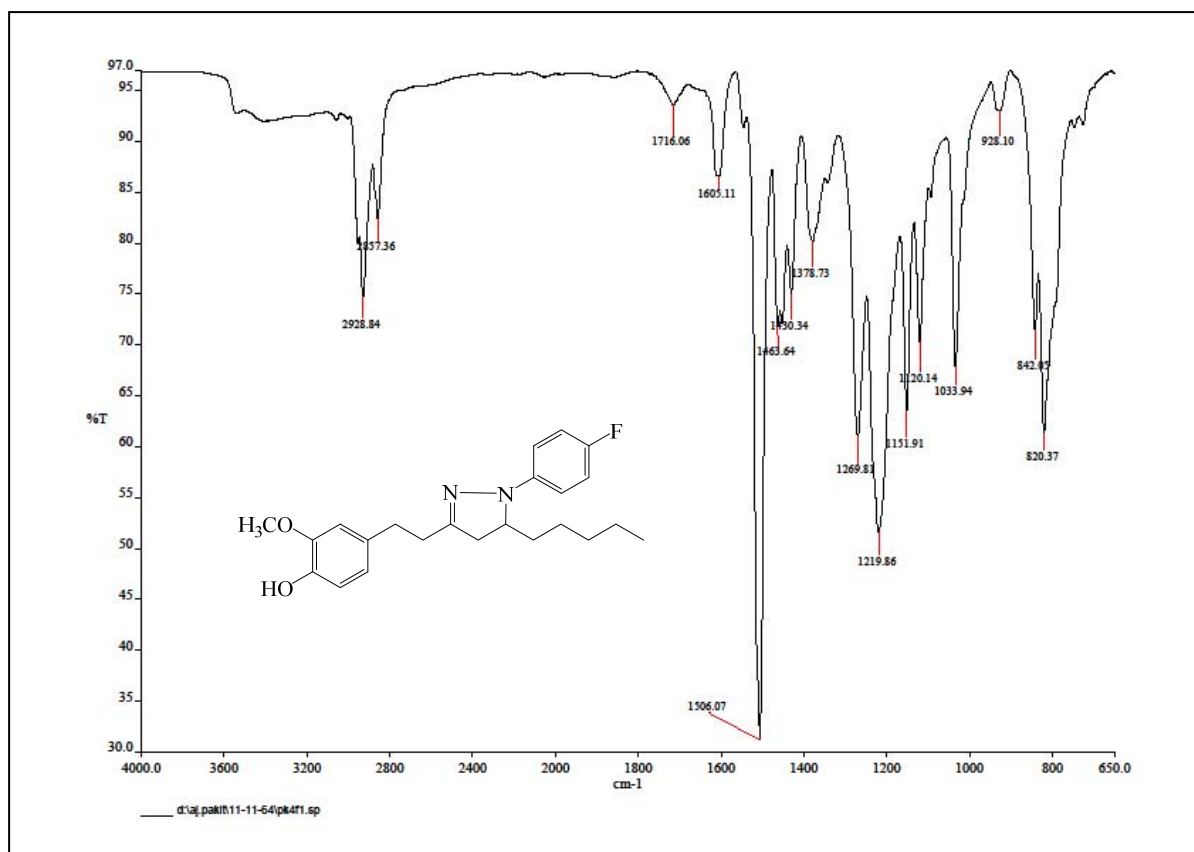


Figure S47. IR spectrum of **5f**.

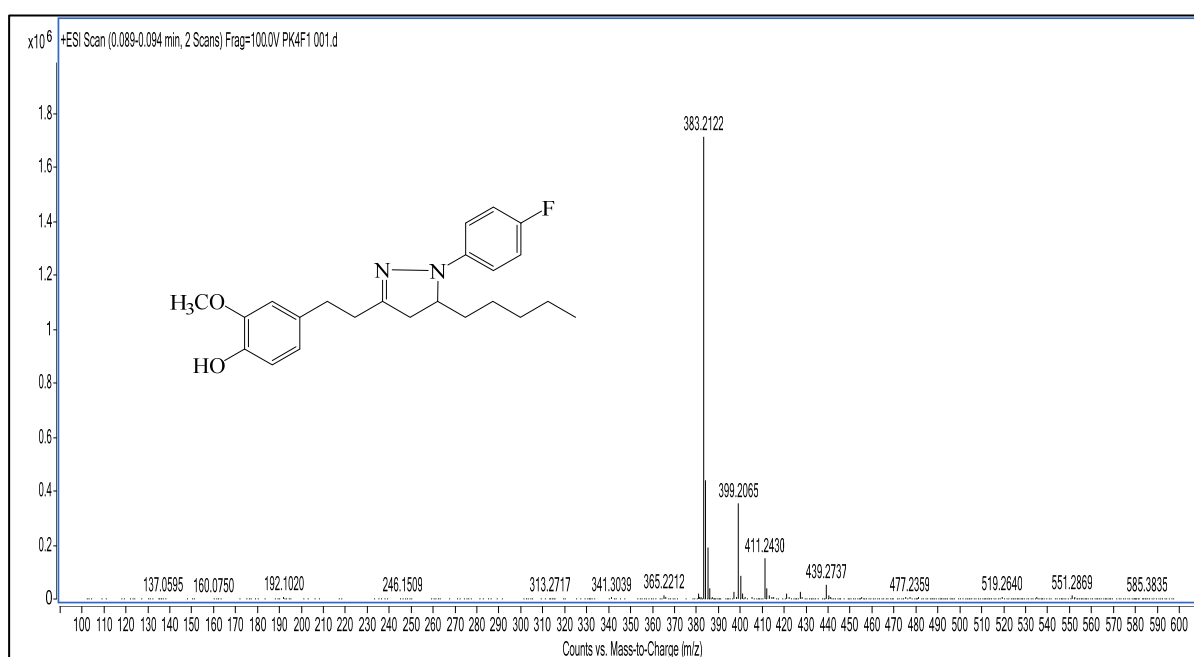


Figure S48. Mass spectrum of **5f**.

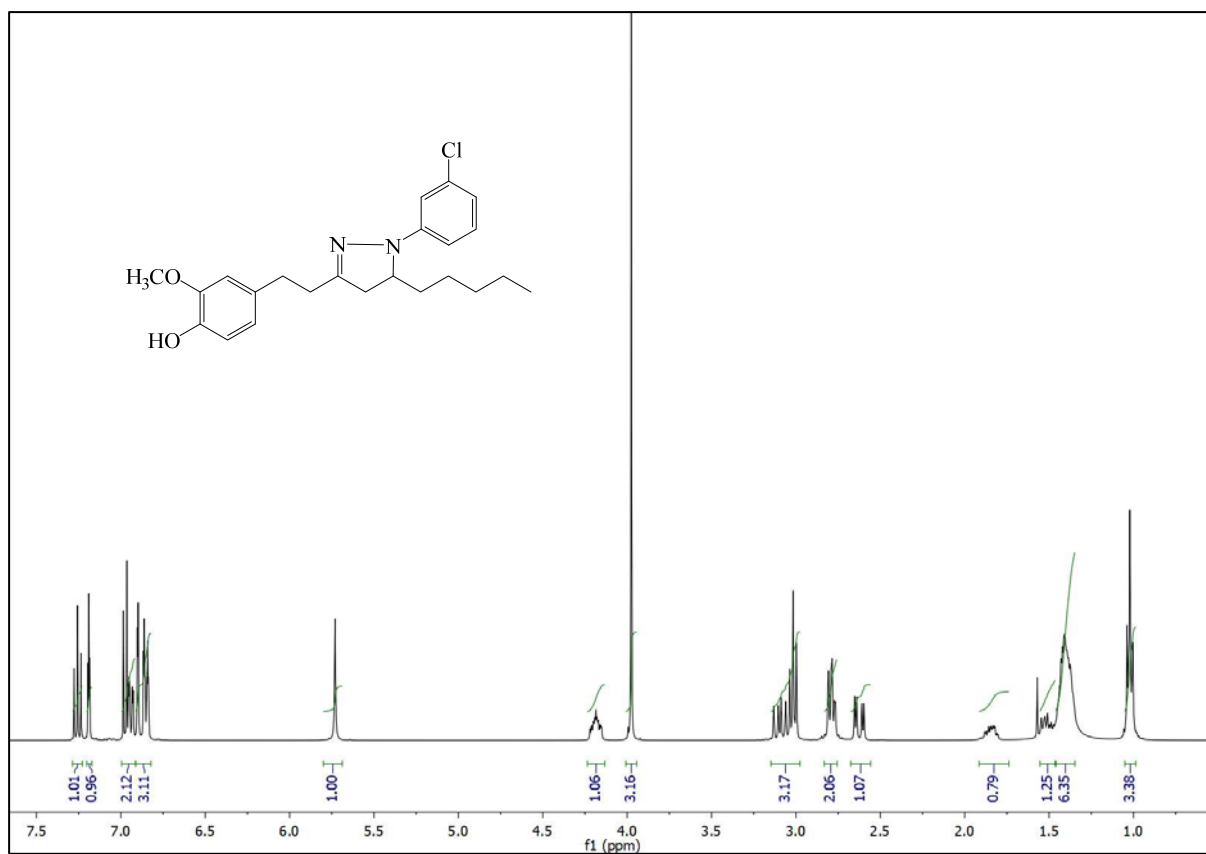


Figure S49. ¹H NMR spectrum of **5g**.

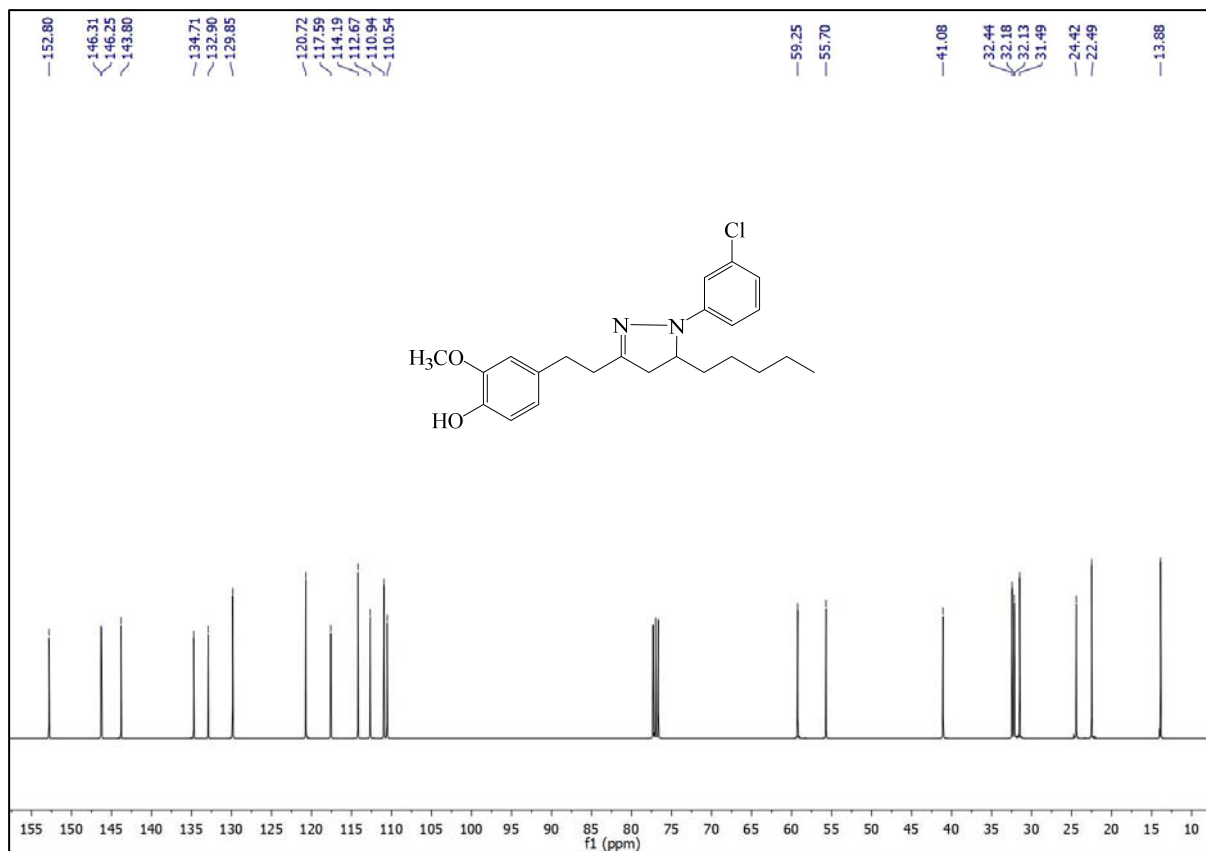


Figure S50. ¹³C NMR spectrum of **5g**.

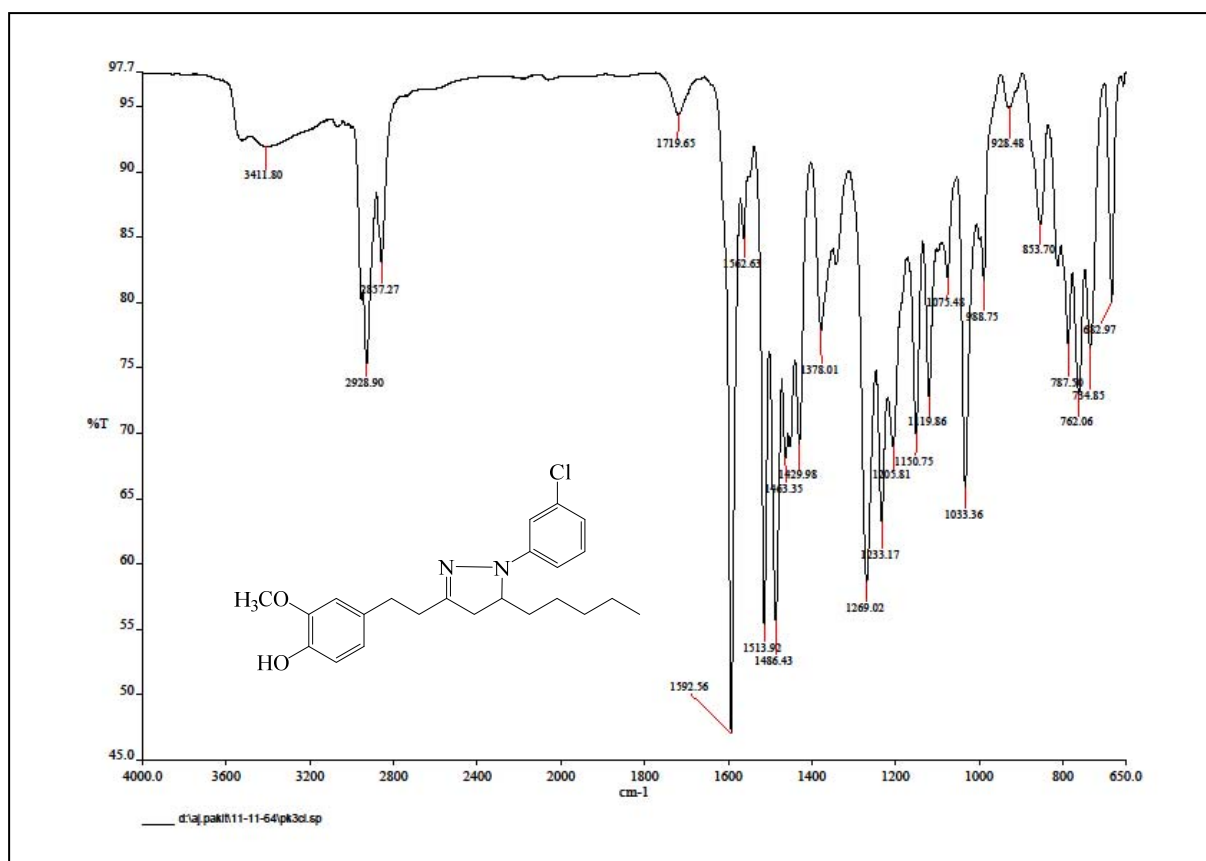


Figure S51. IR spectrum of **5g**.

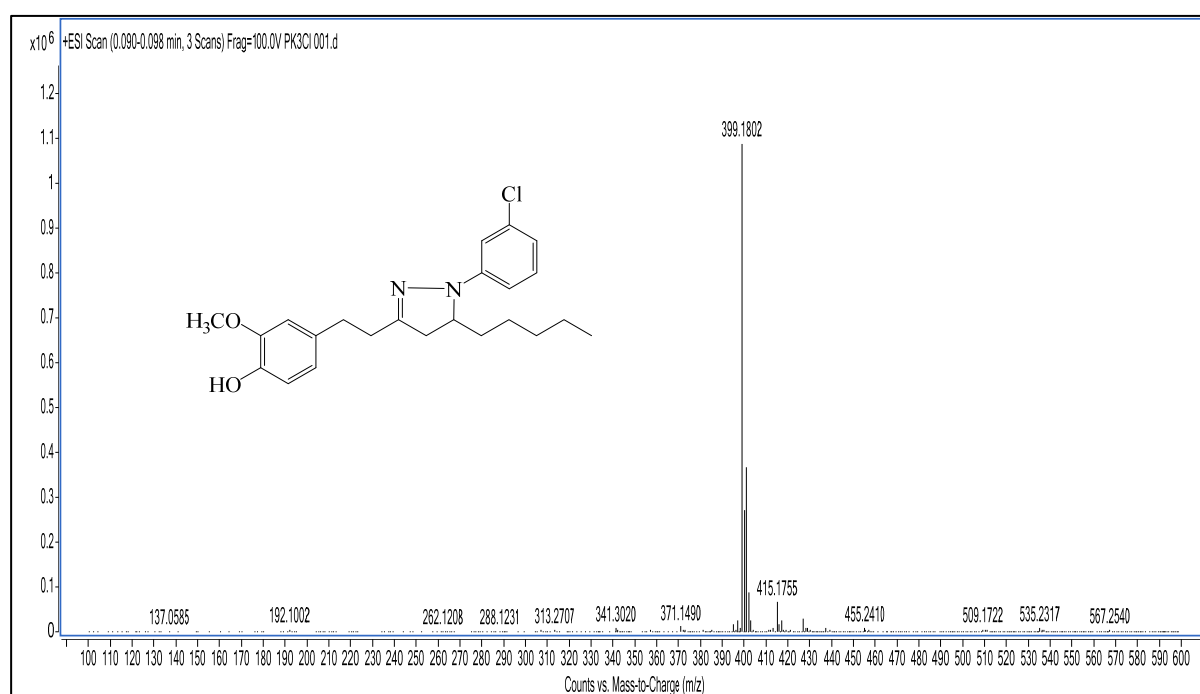


Figure S52. Mass spectrum of **5g**.

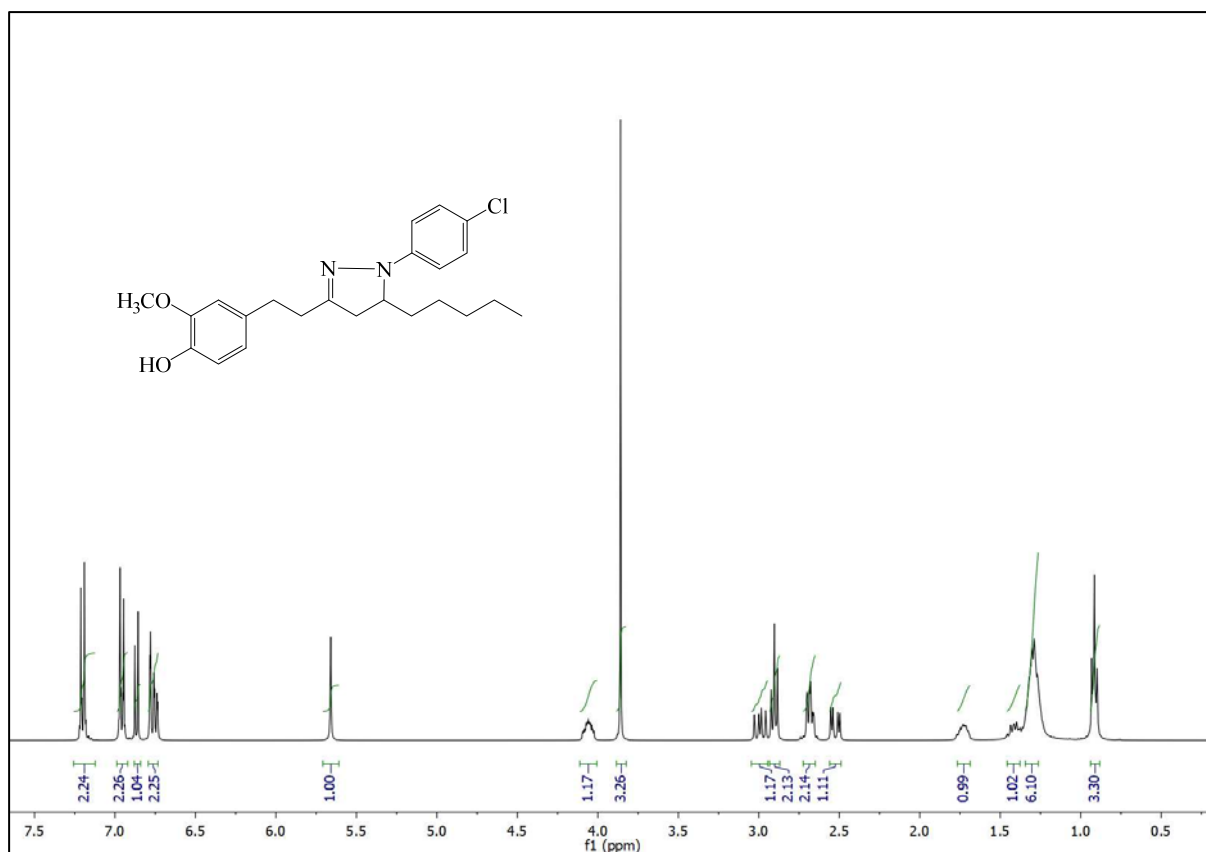


Figure S53. ¹H NMR spectrum of **5h**.

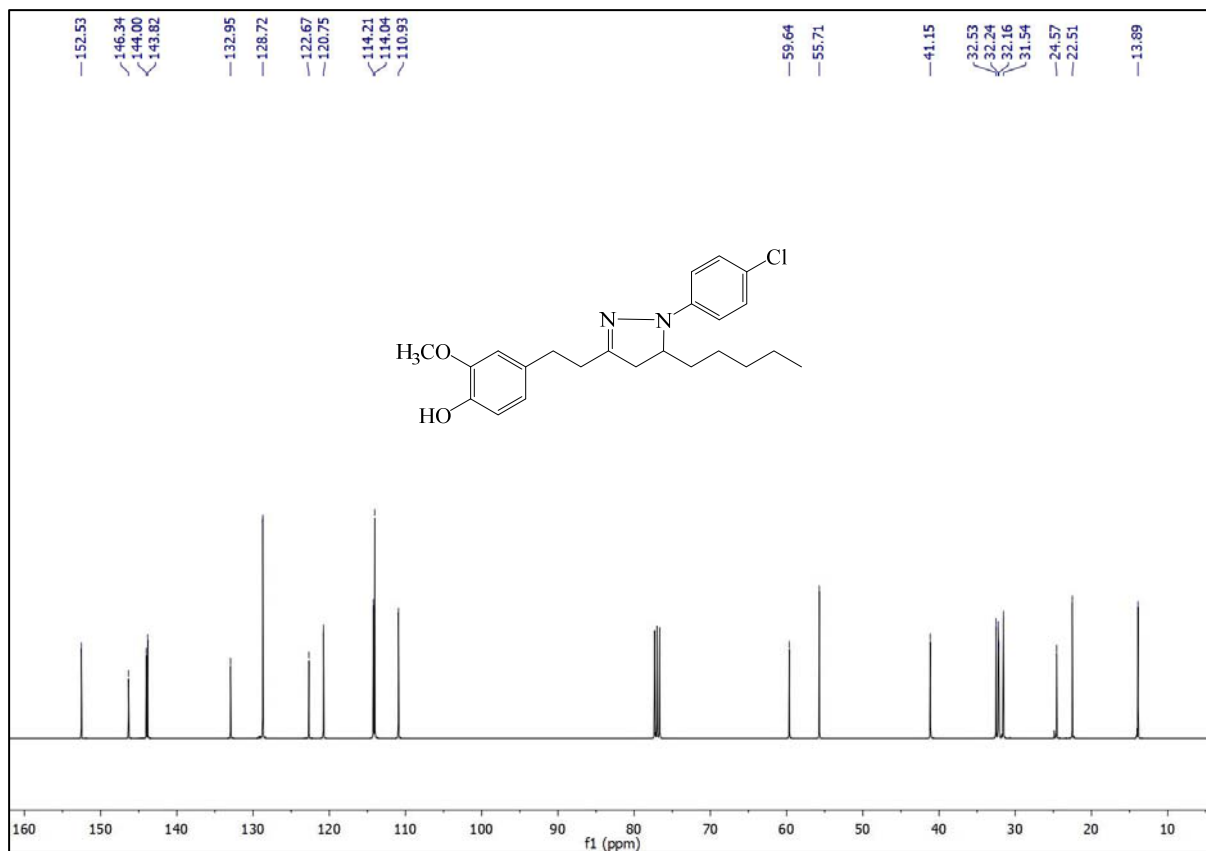


Figure S54. ¹³C NMR spectrum of **5h**.

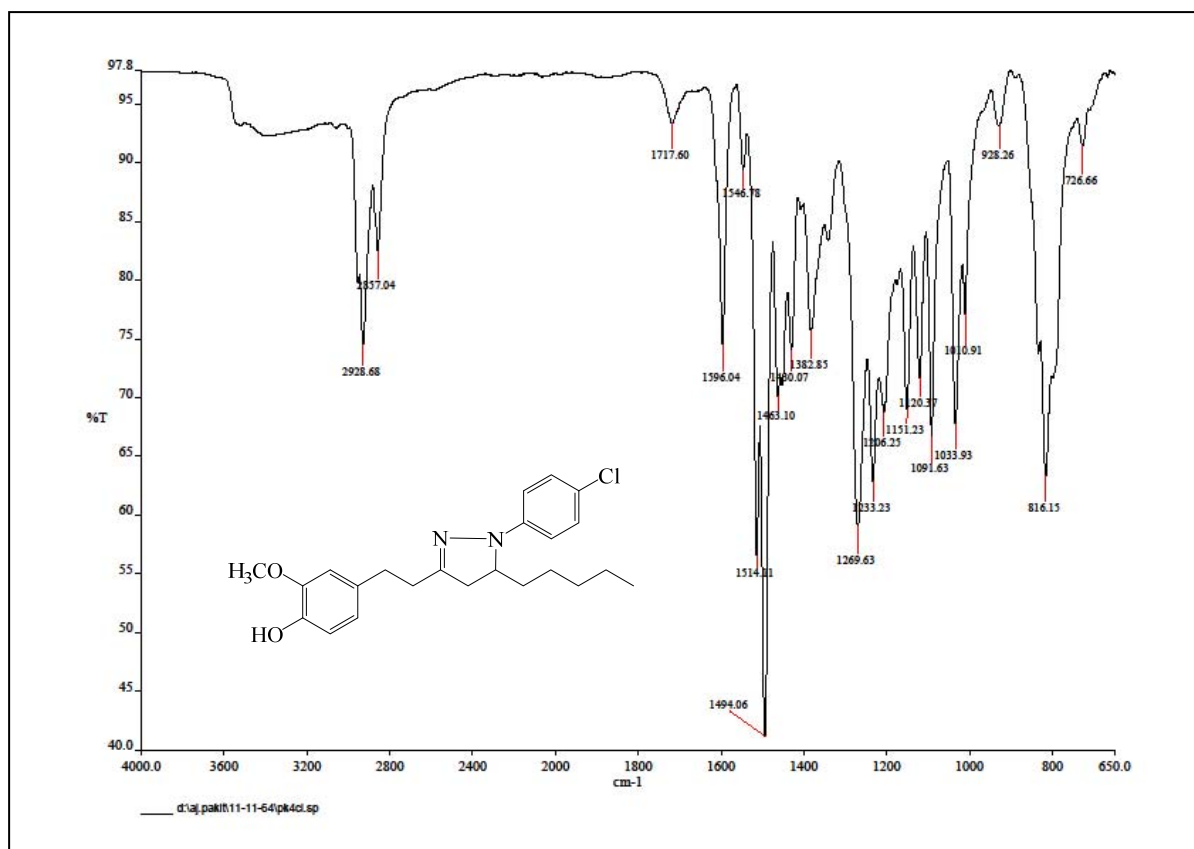


Figure S55. IR spectrum of **5h**.

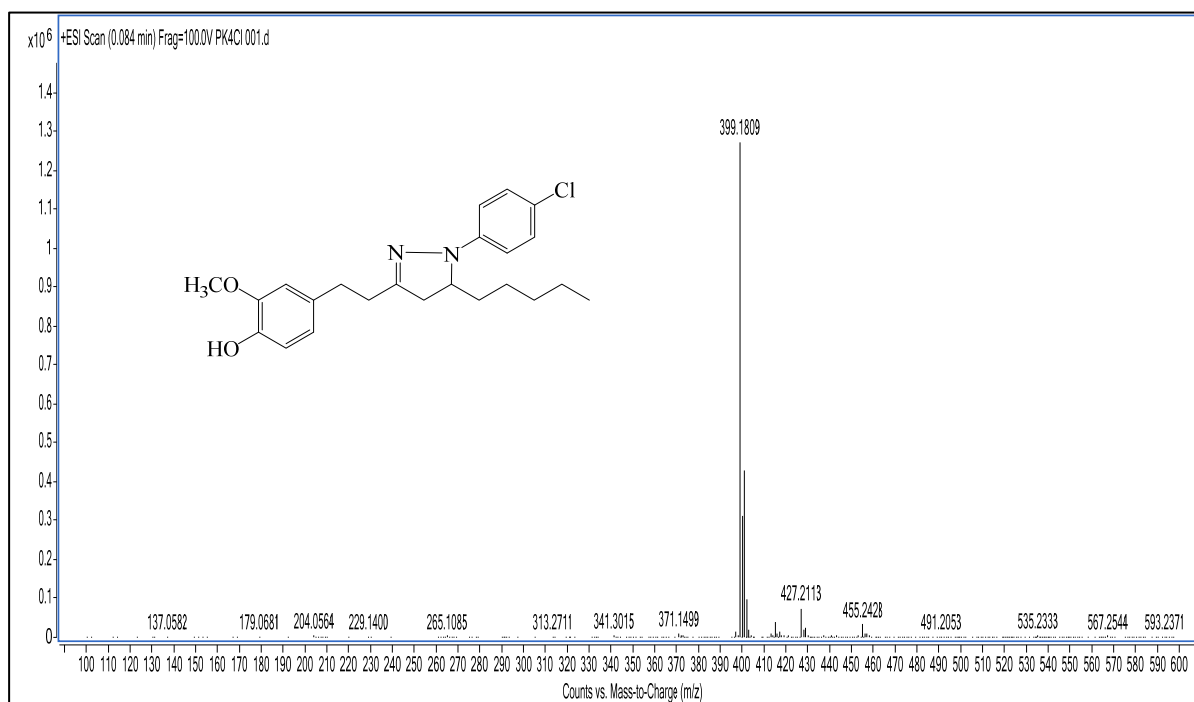


Figure S56. Mass spectrum of **5h**.

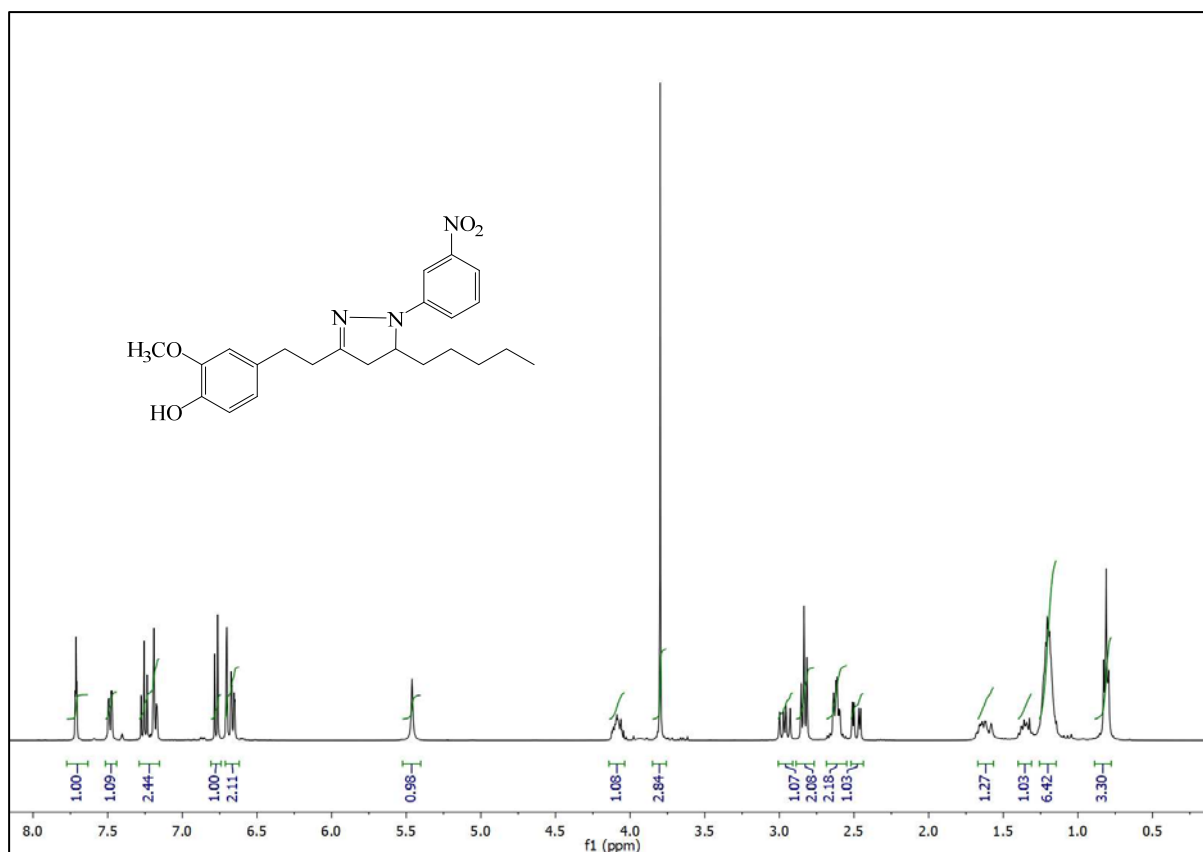


Figure S57. ¹H NMR spectrum of **5i**.

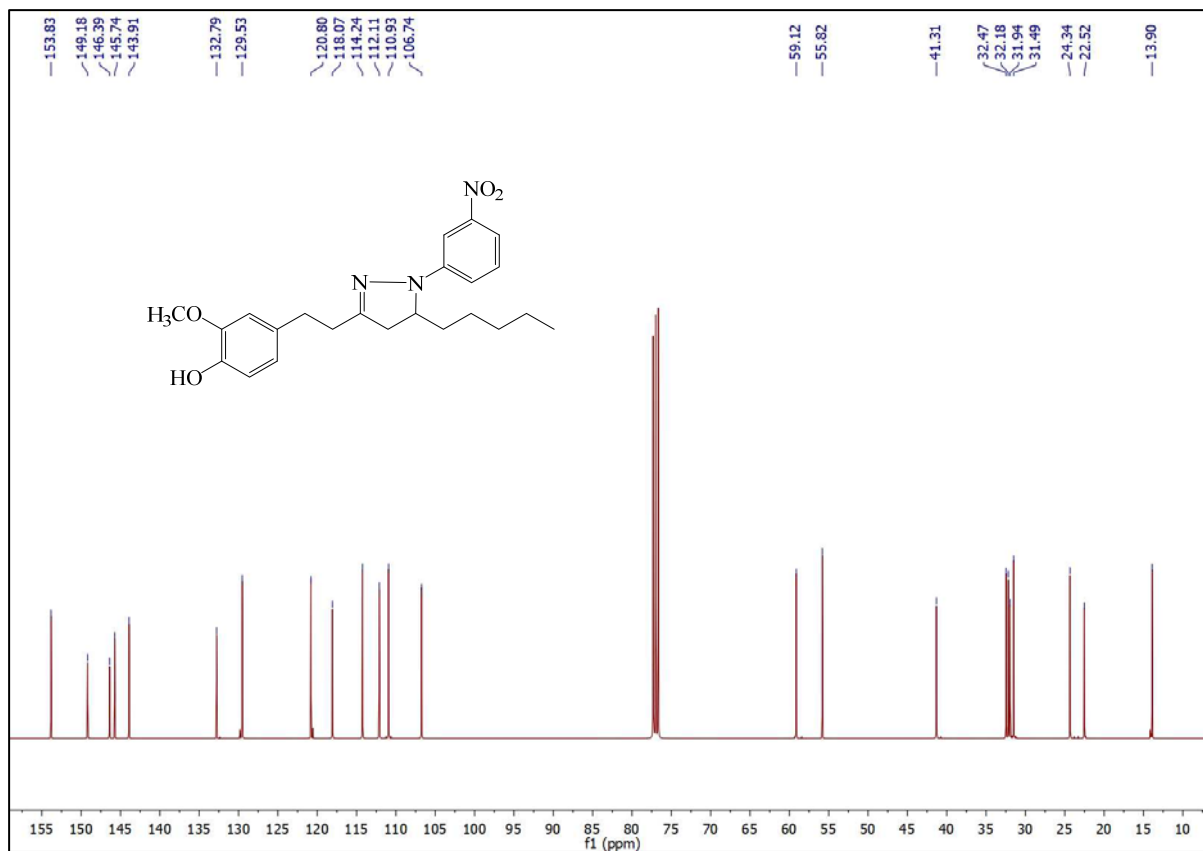


Figure S58. ¹³C NMR spectrum of **5i**.

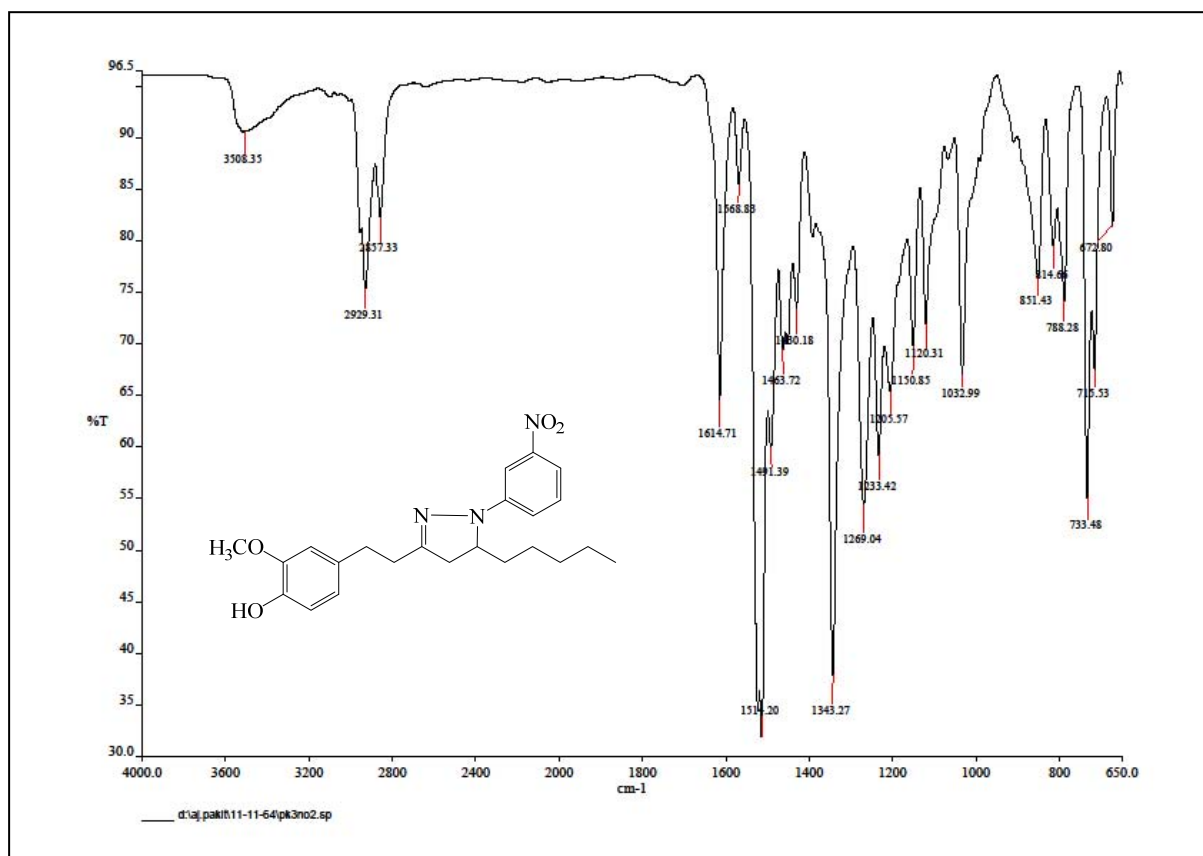


Figure S59. IR spectrum of **5i**.

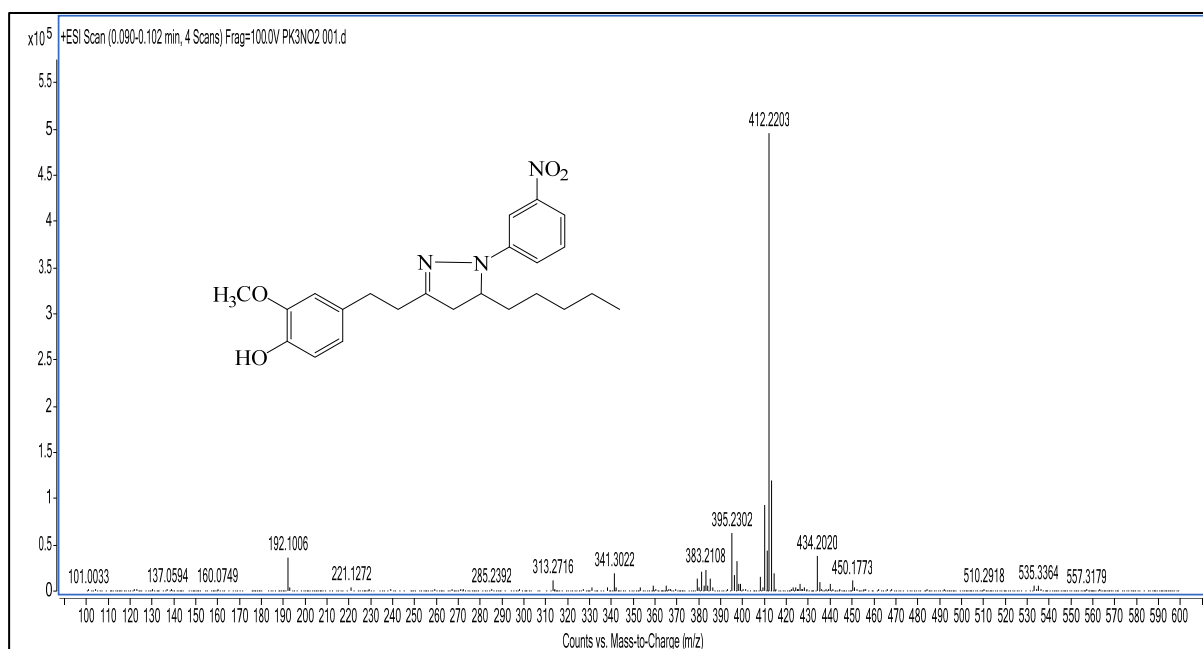


Figure S60. Mass spectrum of **5i**.

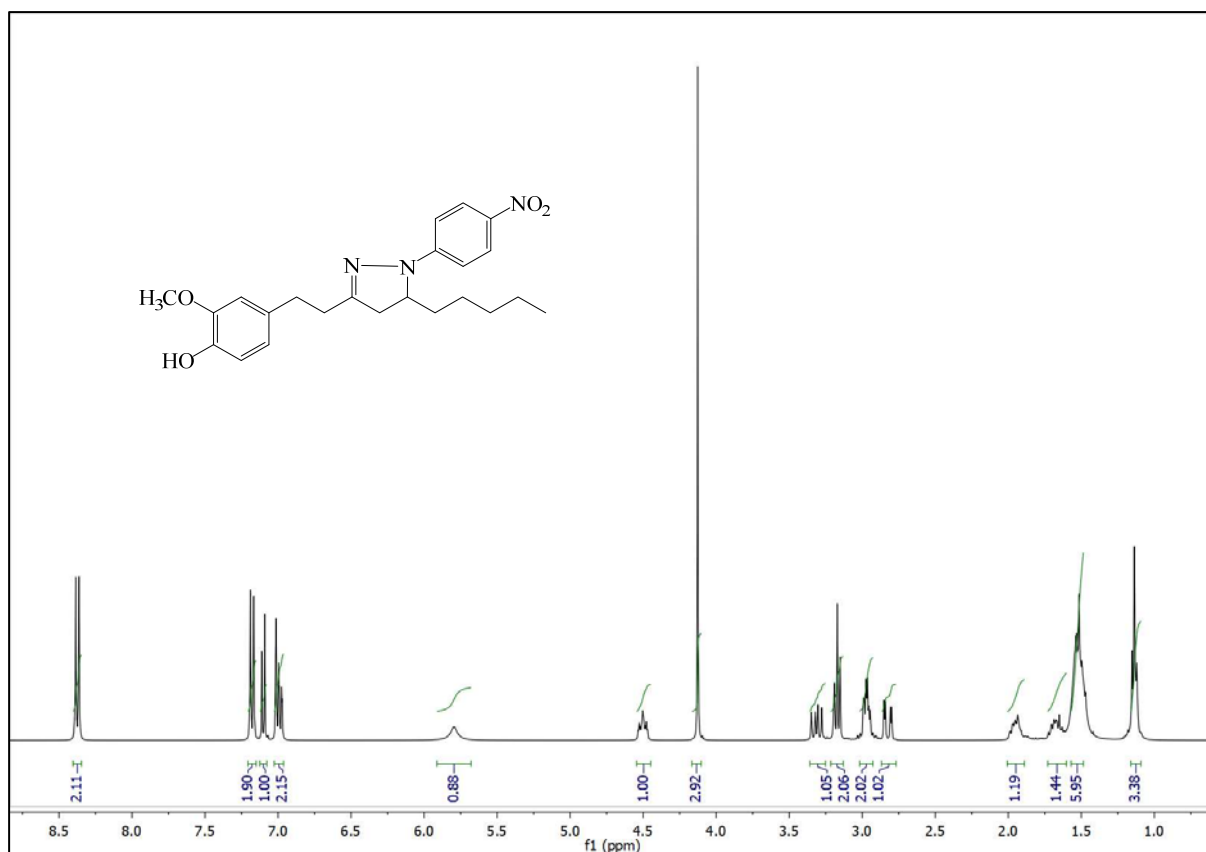


Figure S61. ¹H NMR spectrum of **5j**.

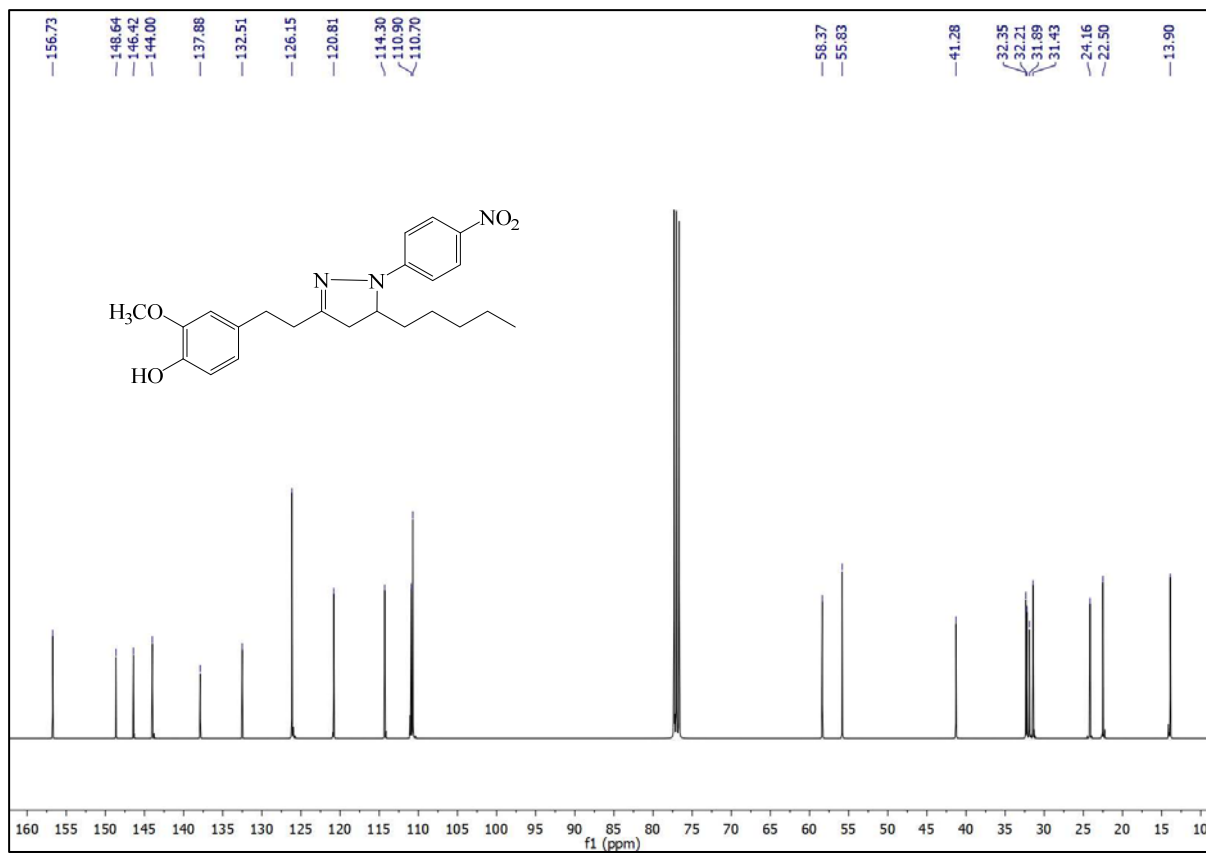


Figure S62. ¹³C NMR spectrum of **5j**.

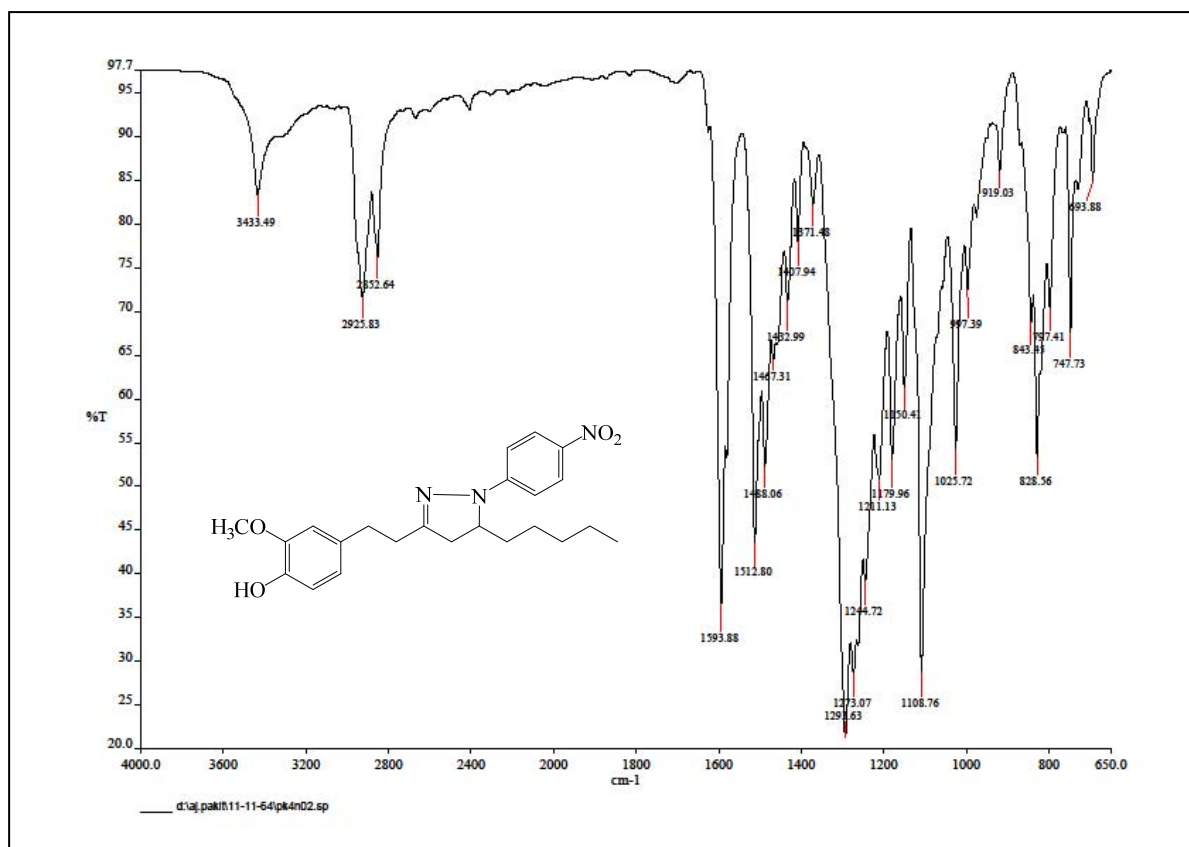


Figure S63. IR spectrum of **5j**.

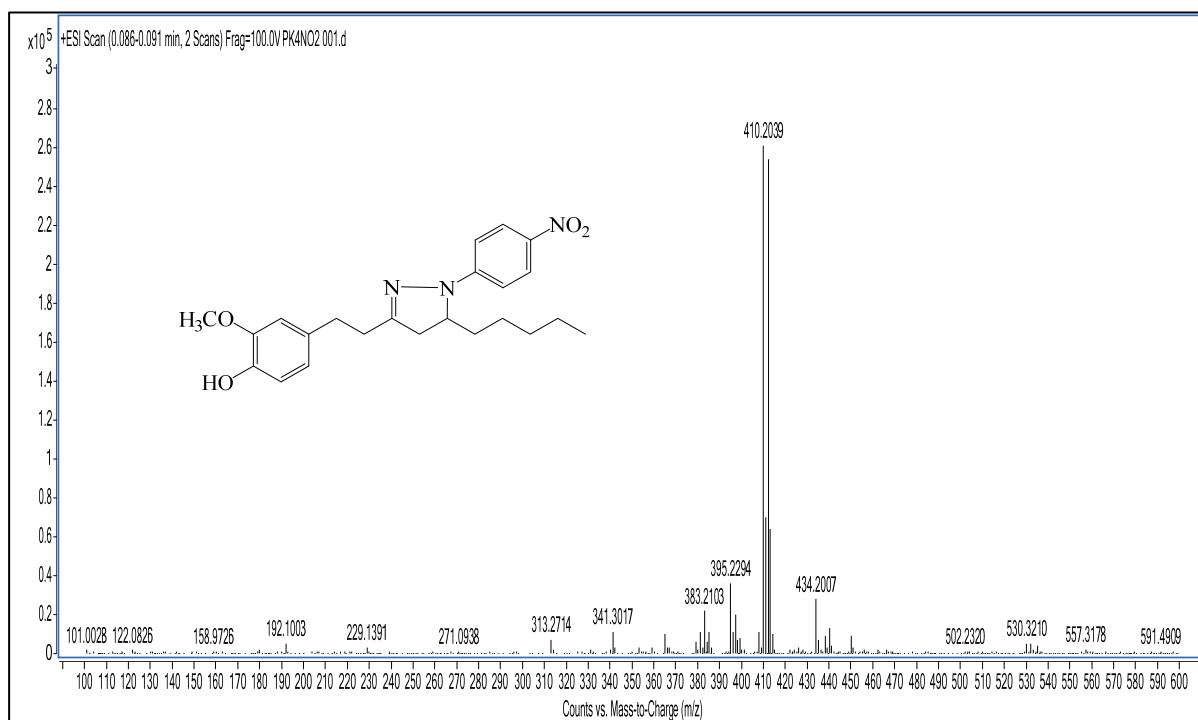


Figure S64. Mass spectrum of **5j**.

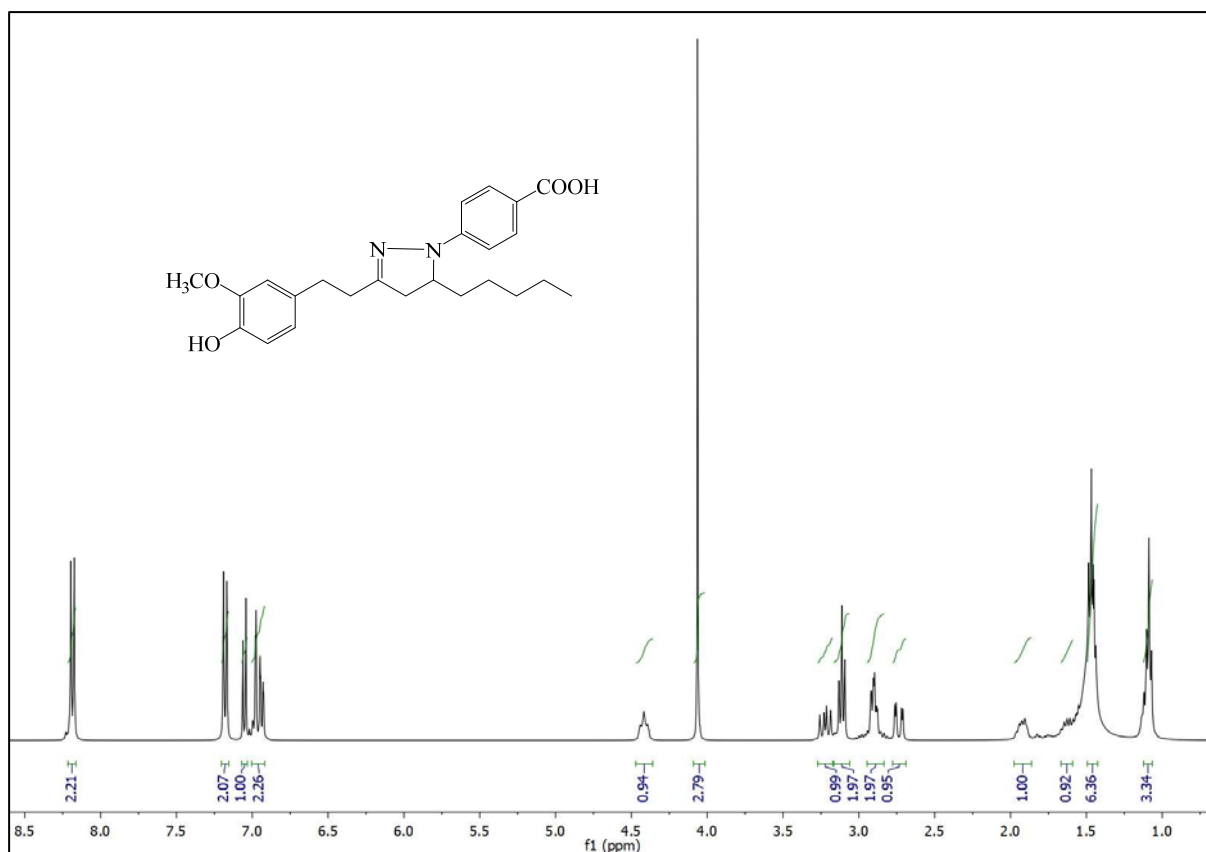


Figure S65. ¹H NMR spectrum of **5k**.

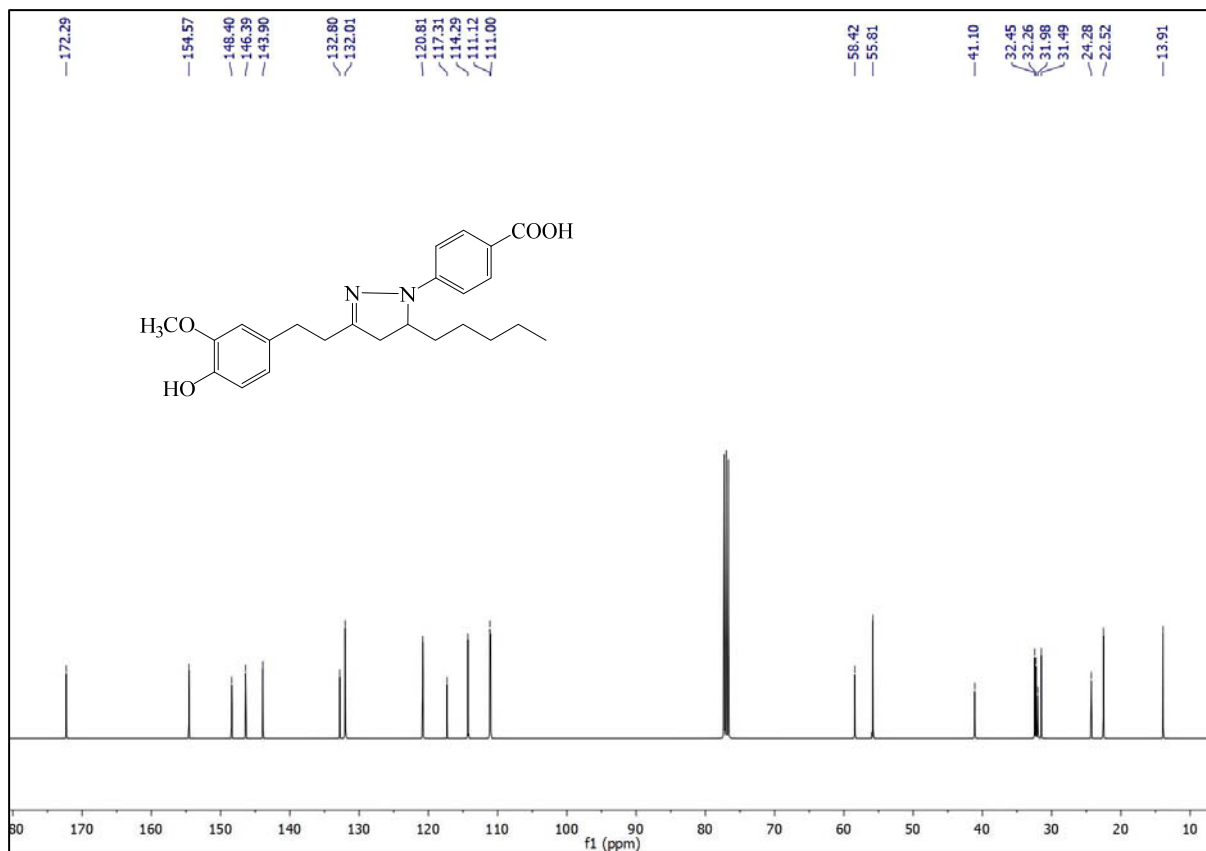


Figure S66. ¹³C NMR spectrum of **5k**.

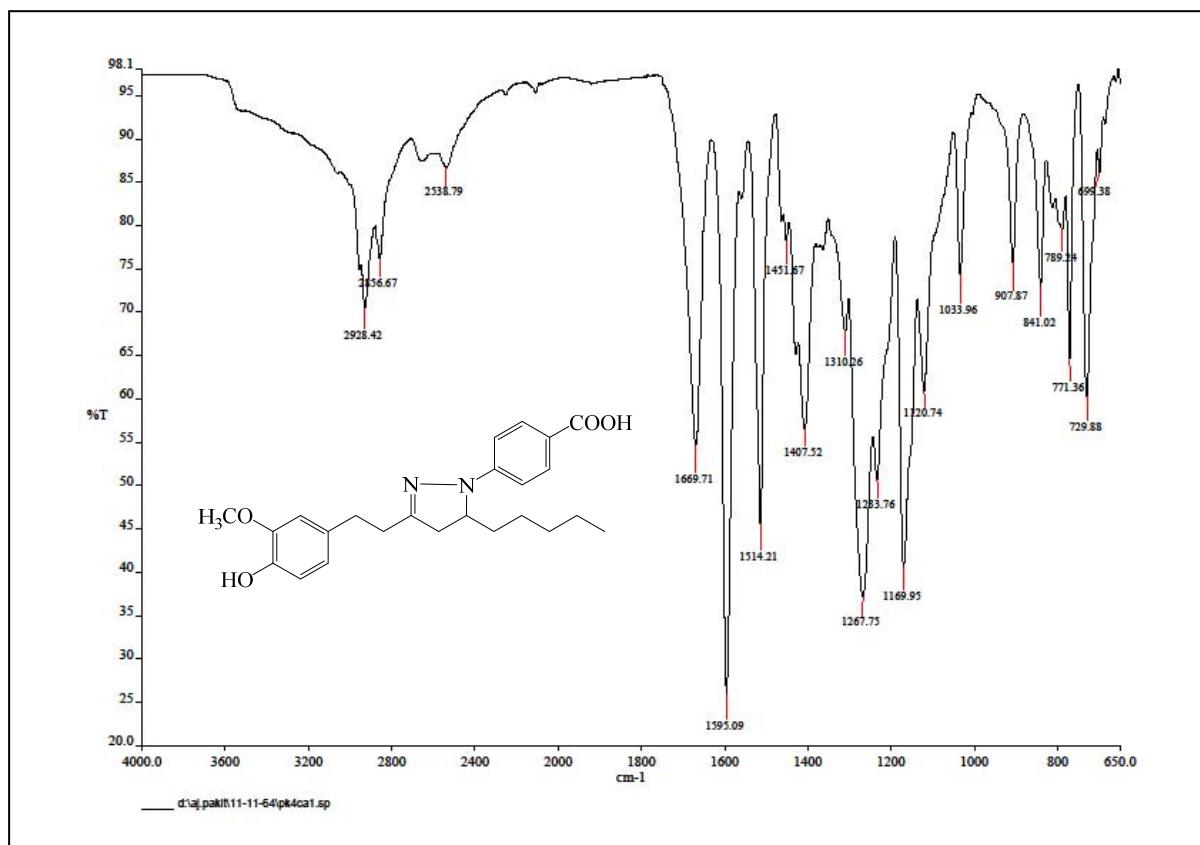


Figure S67. IR spectrum of 5k.

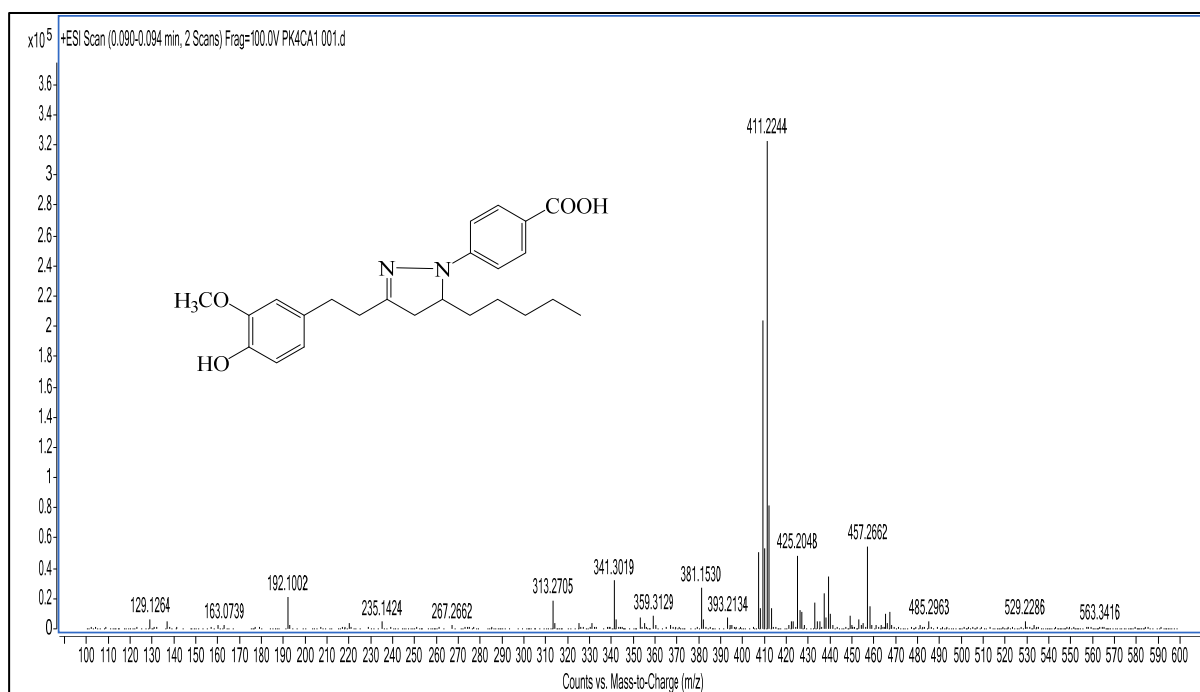


Figure S68. Mass spectrum of 5k.

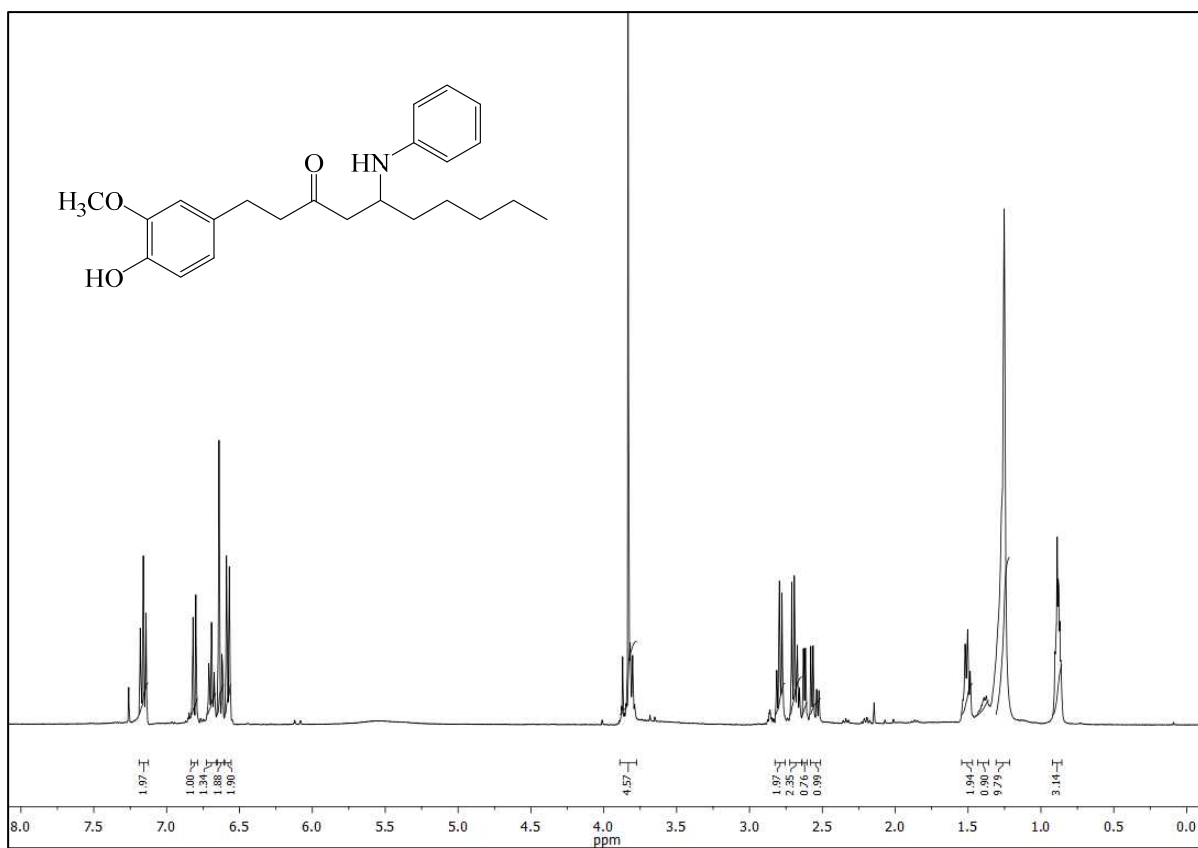


Figure S69. ¹H NMR spectrum of 6a.

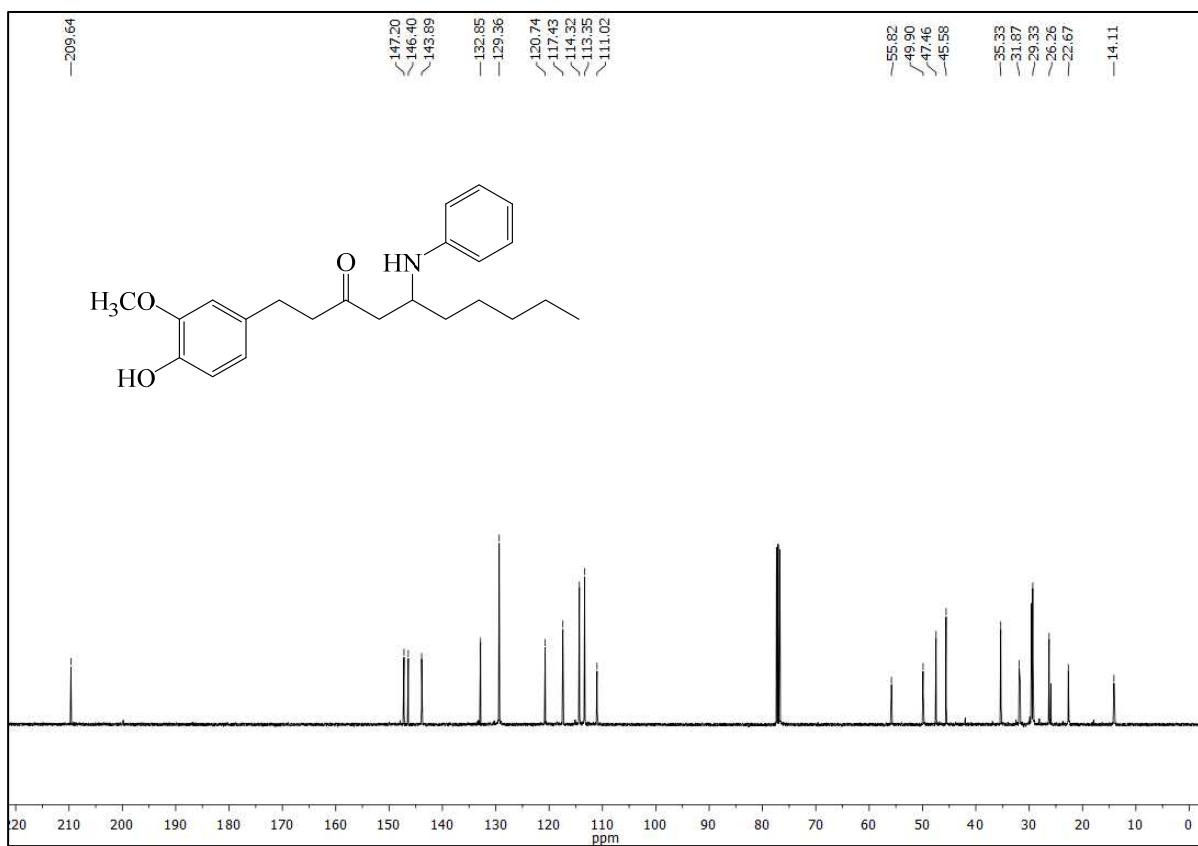


Figure S70. ¹³C NMR spectrum of 6a.

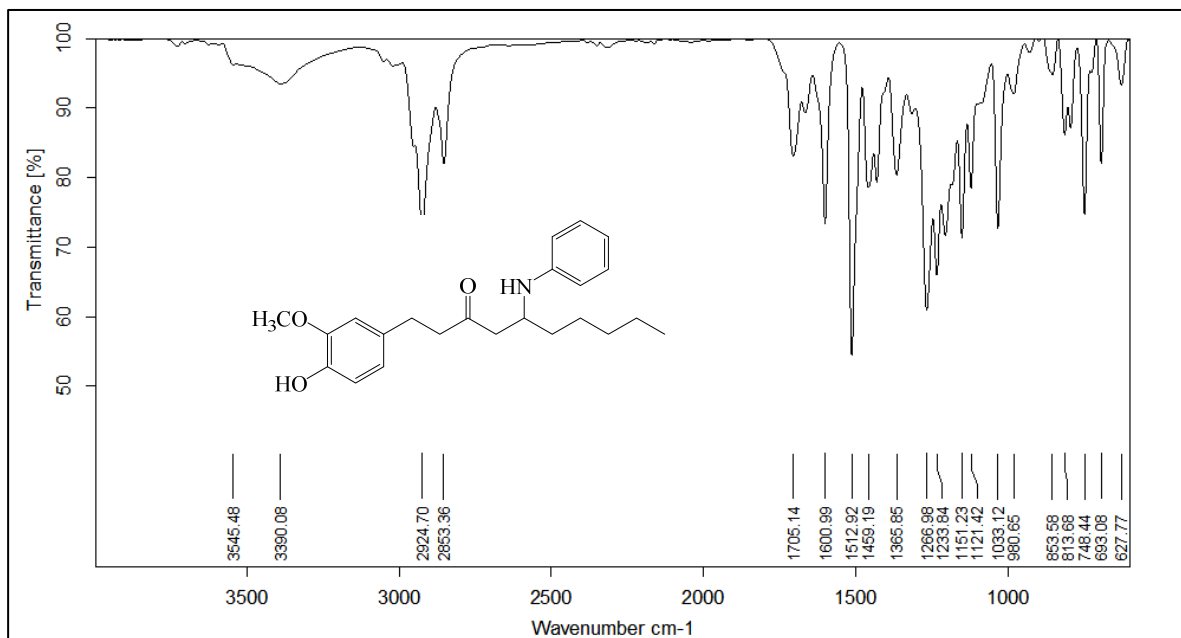


Figure S71. IR spectrum of 6a.

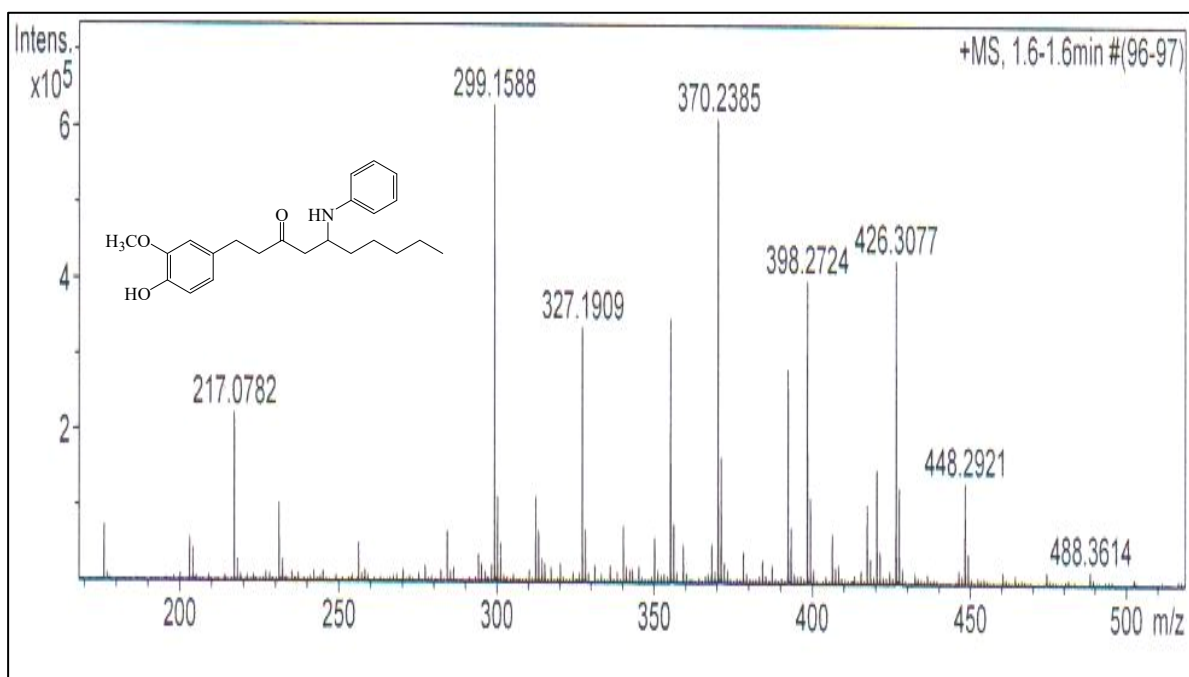


Figure S72. Mass spectrum of 6a.

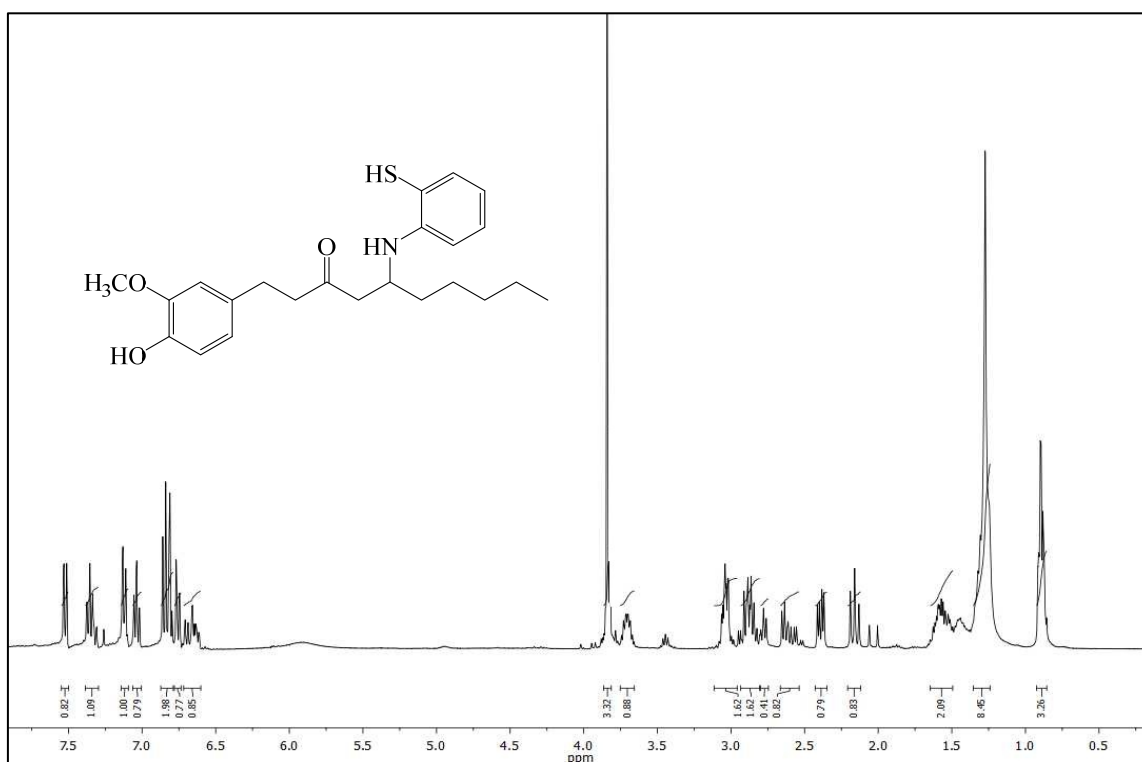


Figure S73. ¹H NMR spectrum of **6b**.

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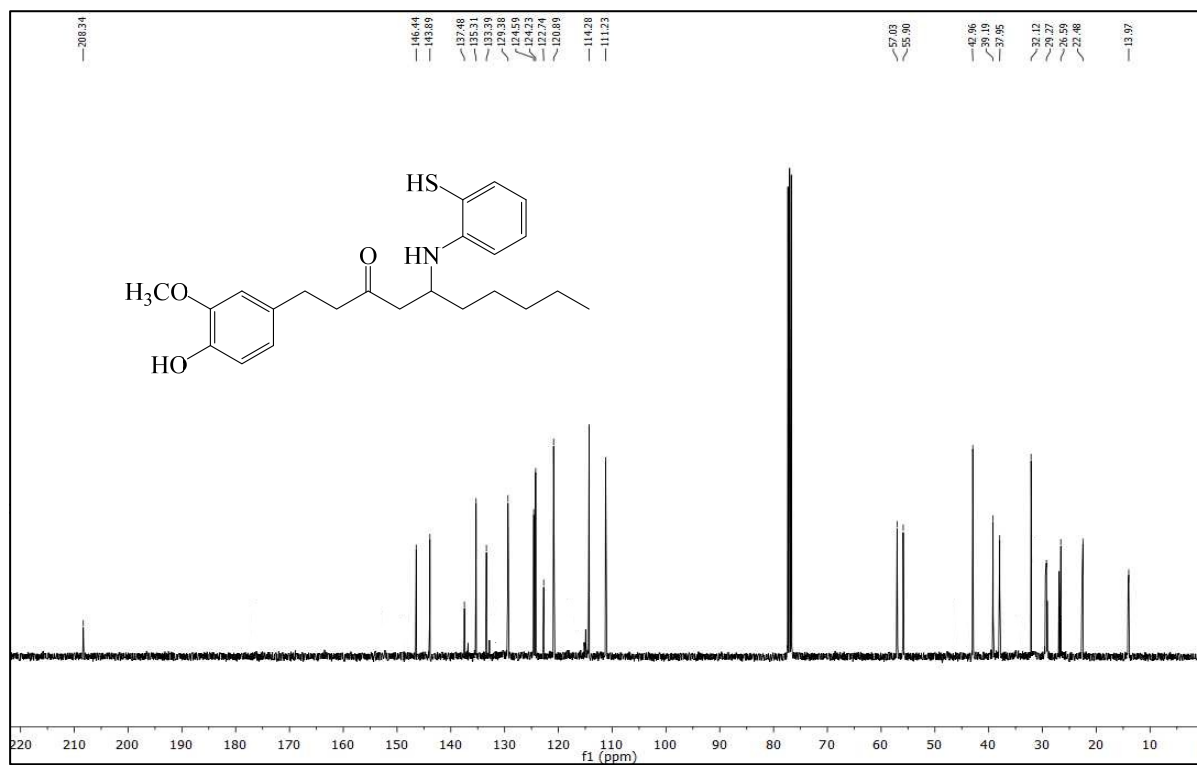


Figure S74. ¹³C NMR spectrum of **6b**.

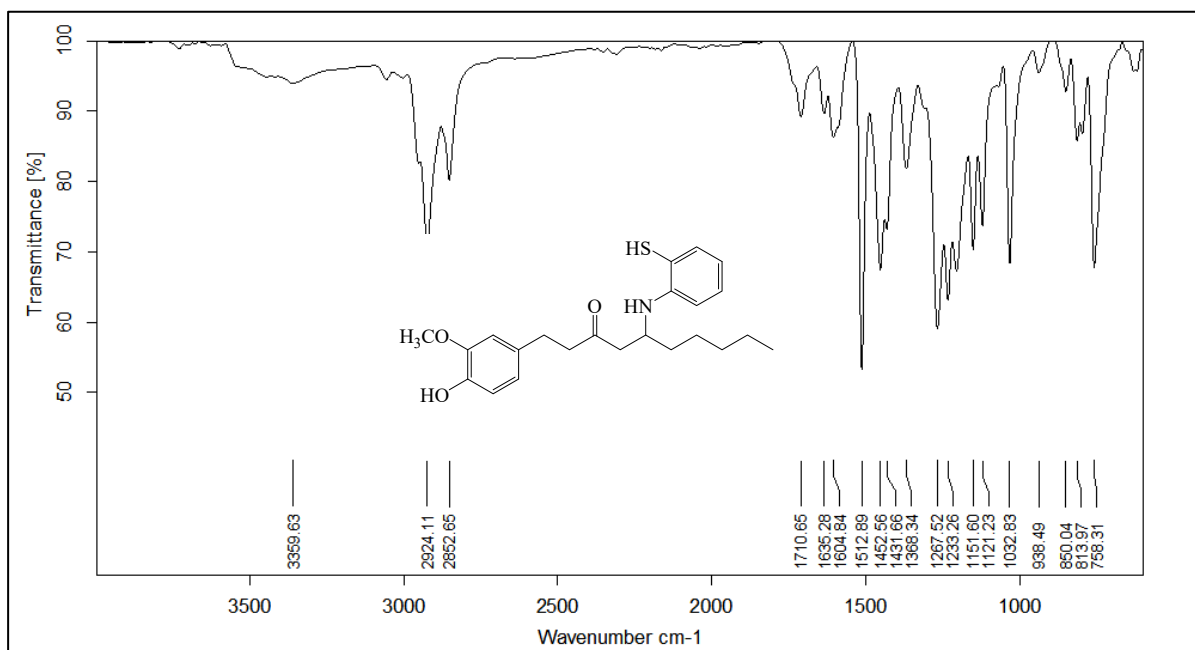


Figure S75. IR spectrum of **6b**.

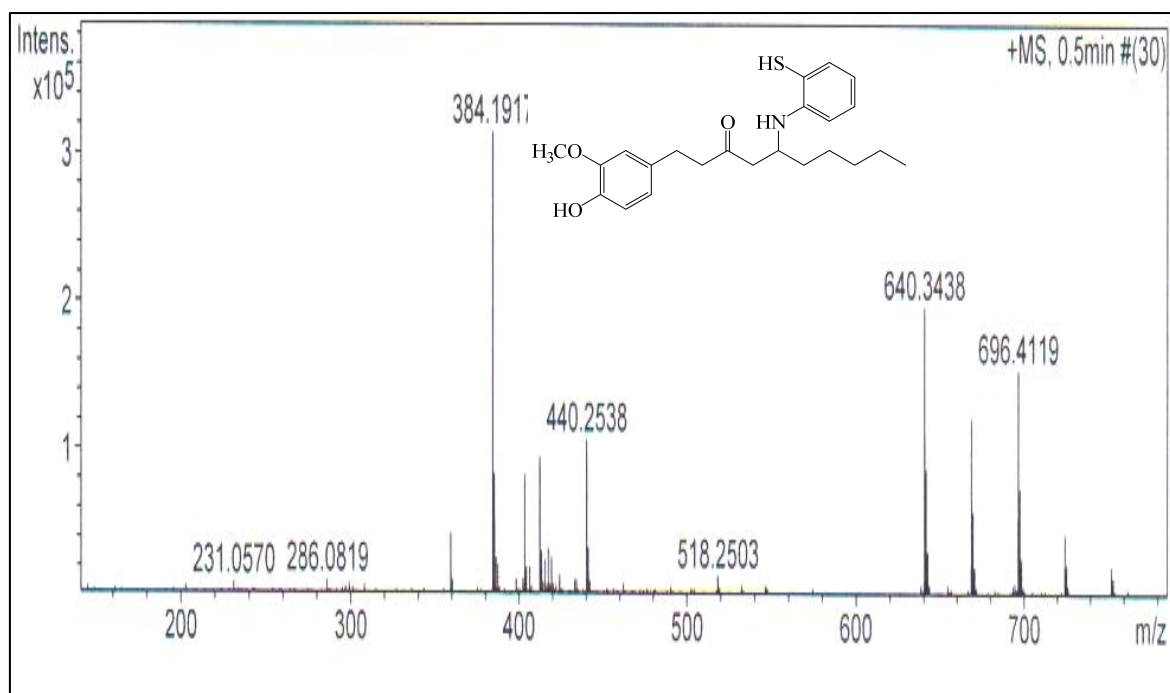


Figure S76. Mass spectrum of **6b**.

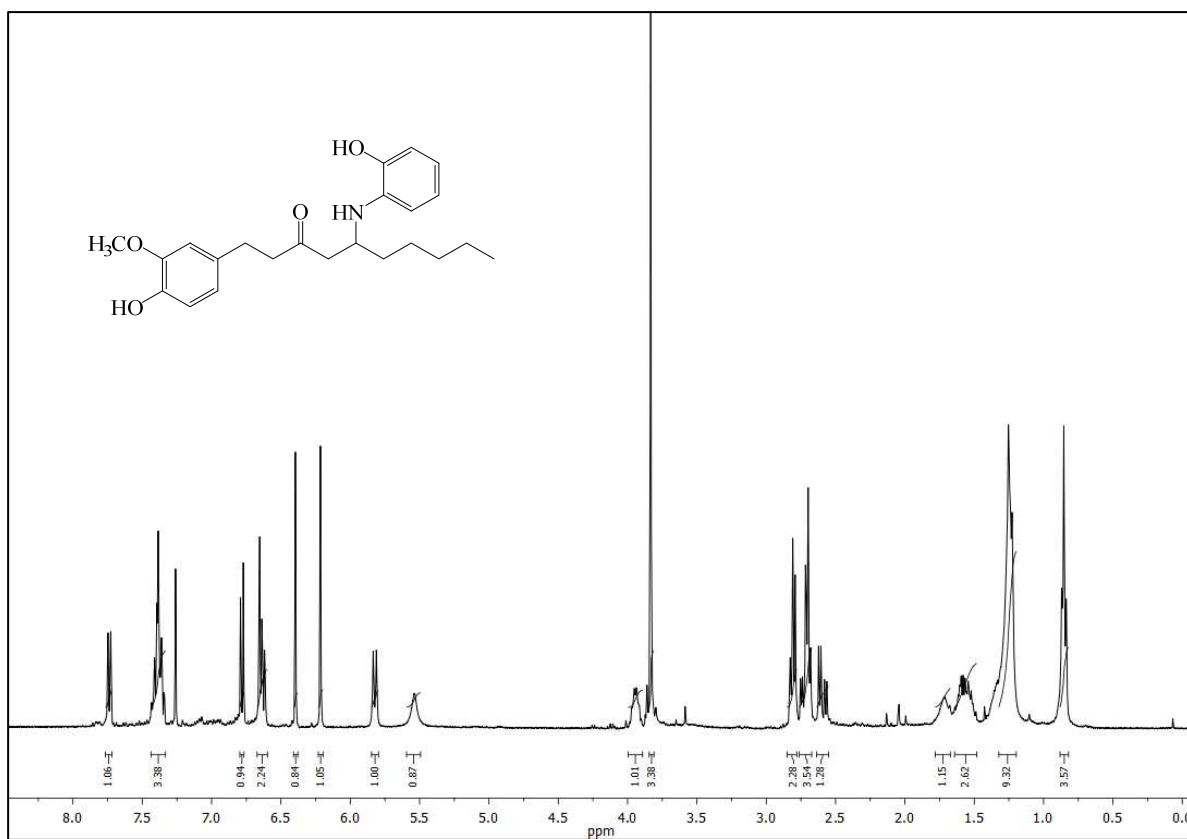


Figure S77. ¹H NMR spectrum of 6c.

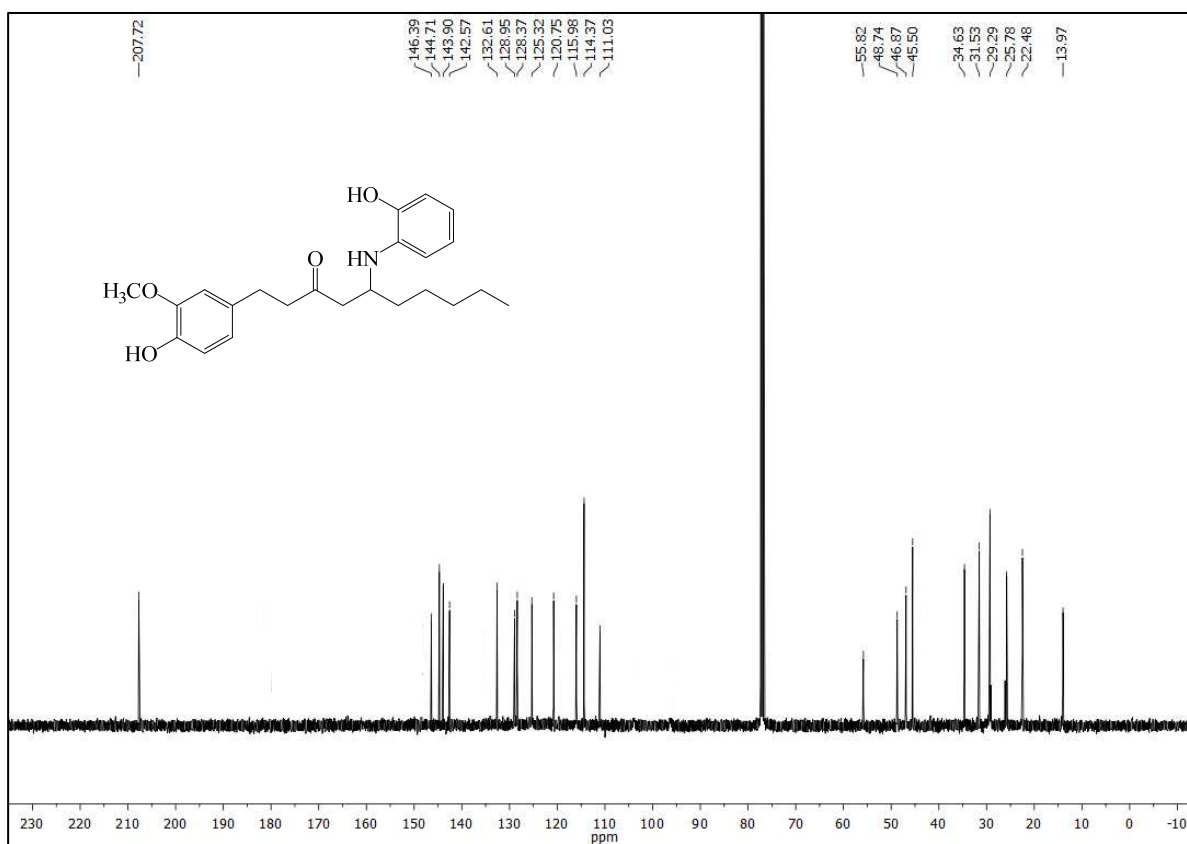


Figure S78. ¹³C NMR spectrum of 6c.

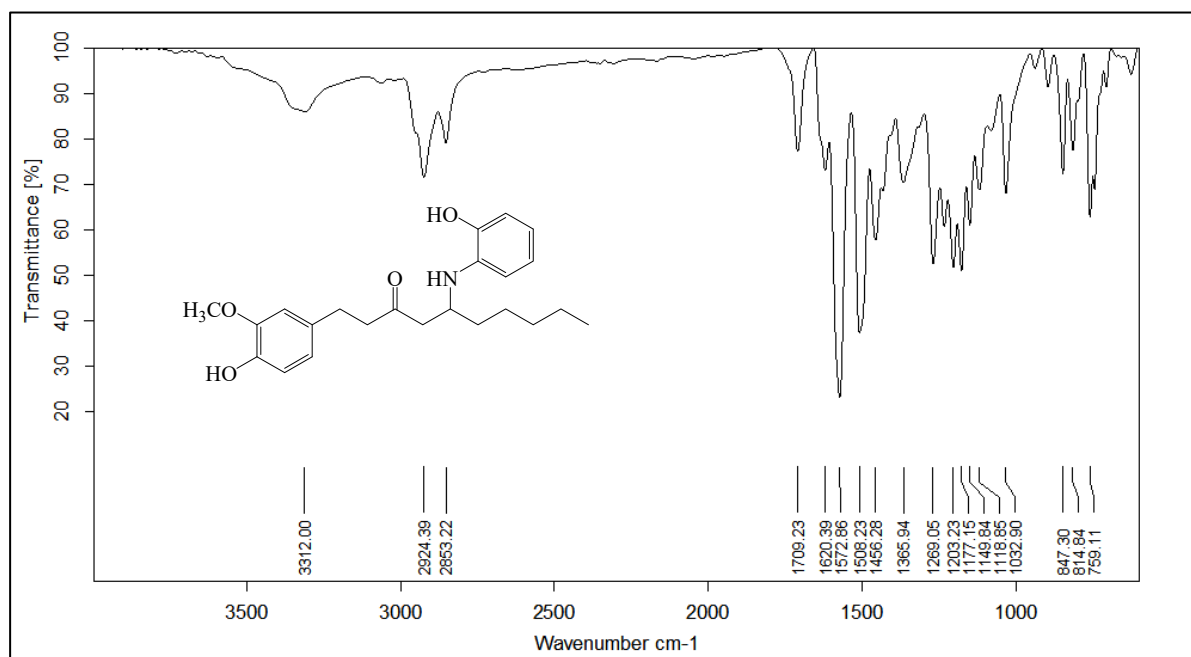


Figure S79. IR spectrum of **6c**.

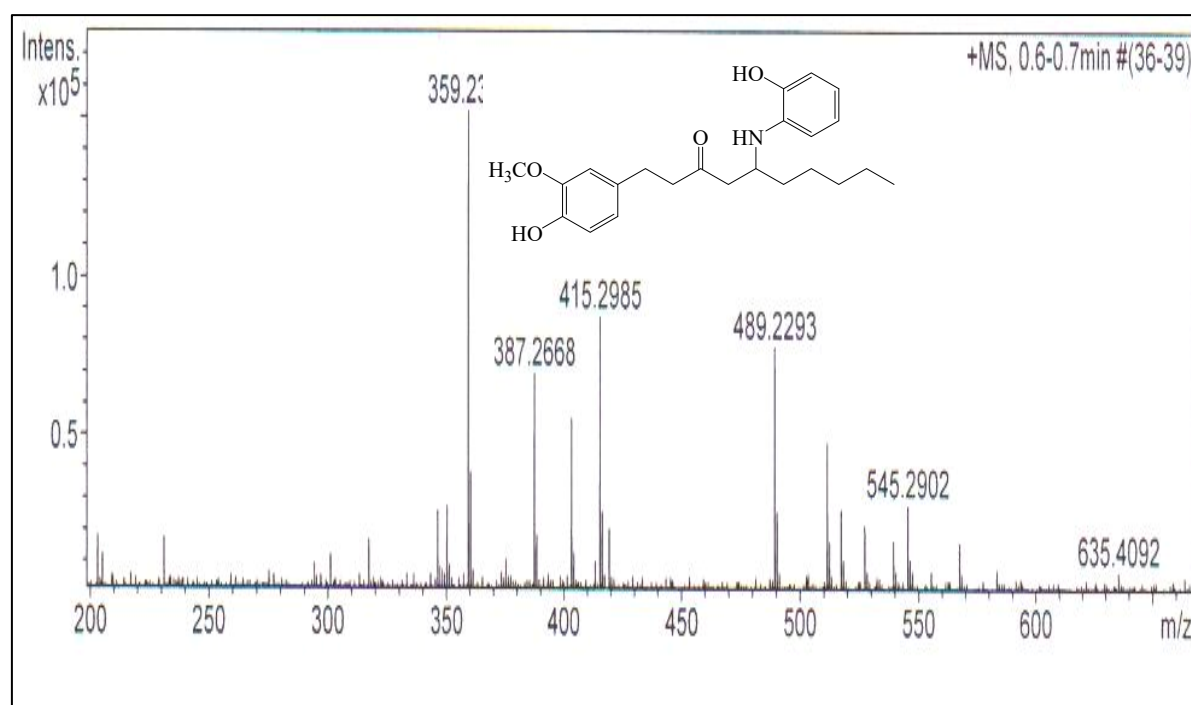


Figure S80. Mass spectrum of **6c**.

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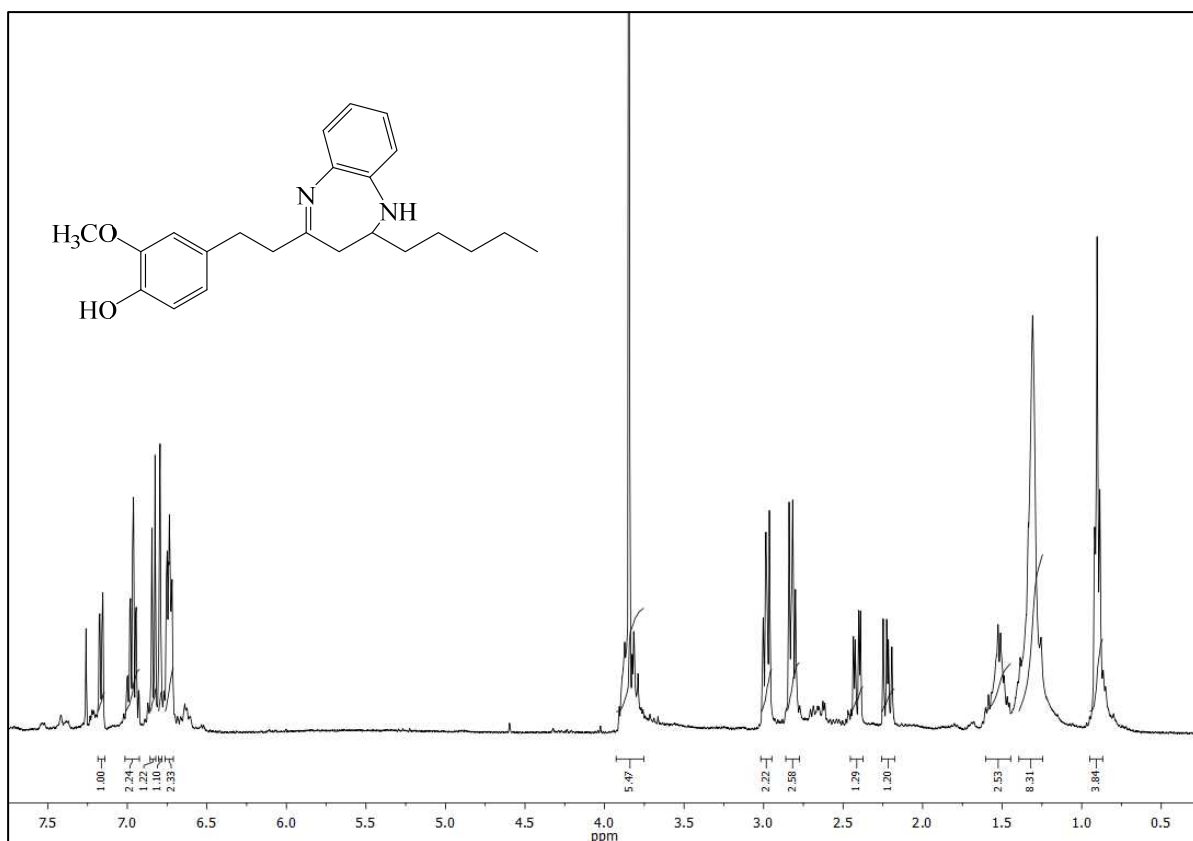


Figure S81. ¹H NMR spectrum of 7.

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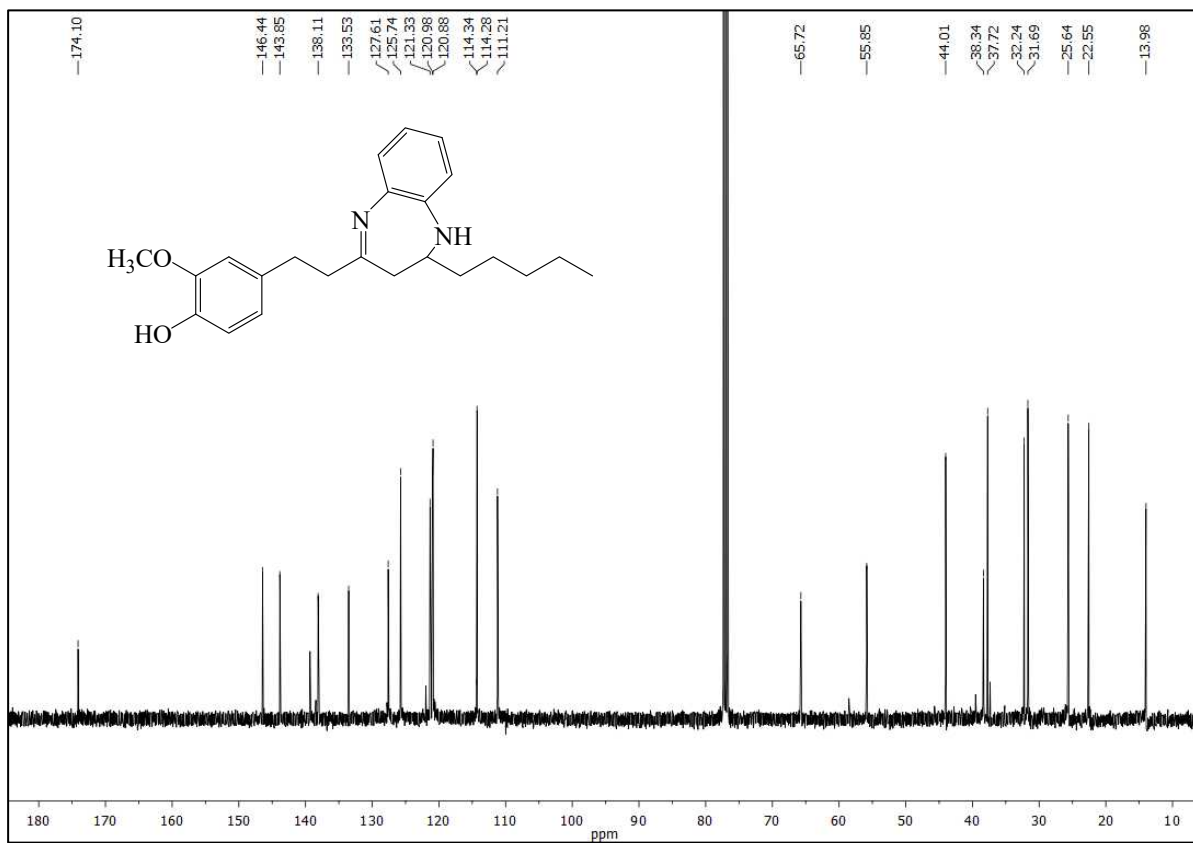


Figure S82. ¹³C NMR spectrum of 7.

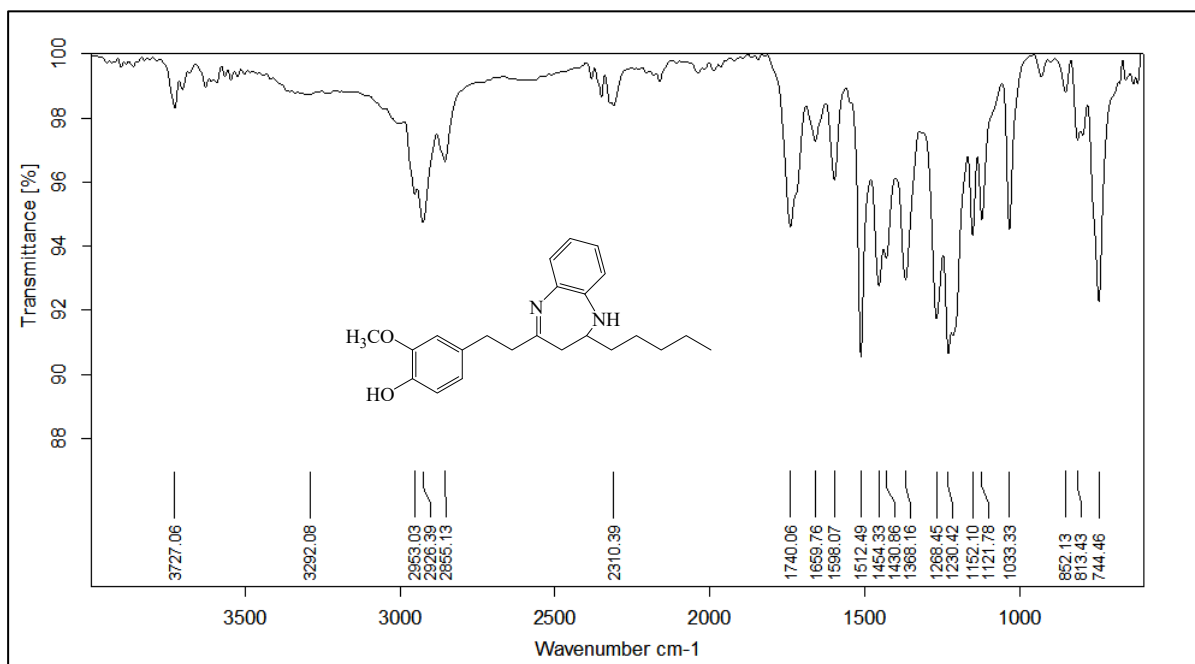


Figure S83. IR spectrum of 7.

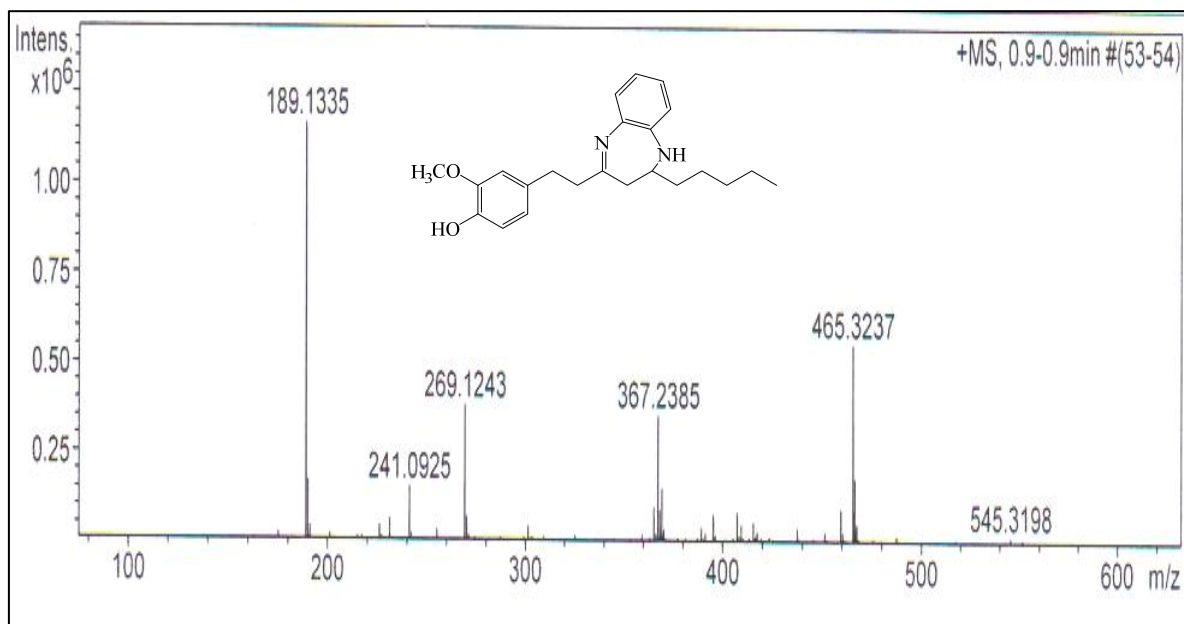


Figure S84. Mass spectrum of 7.