

Supplementary Material

Synthesis, anticancer activity and molecular docking studies of new 4-nitroimidazole derivatives

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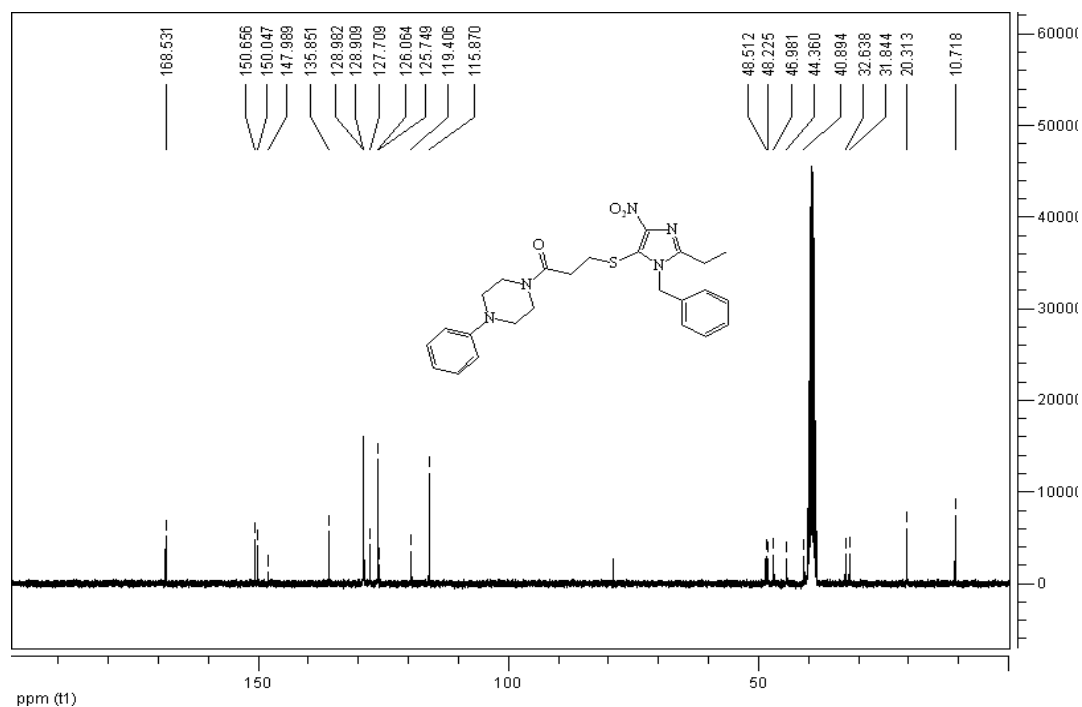


Figure 1. ¹³C-NMR spectrum for compound **(5a)** in DMSO-*d*₆.

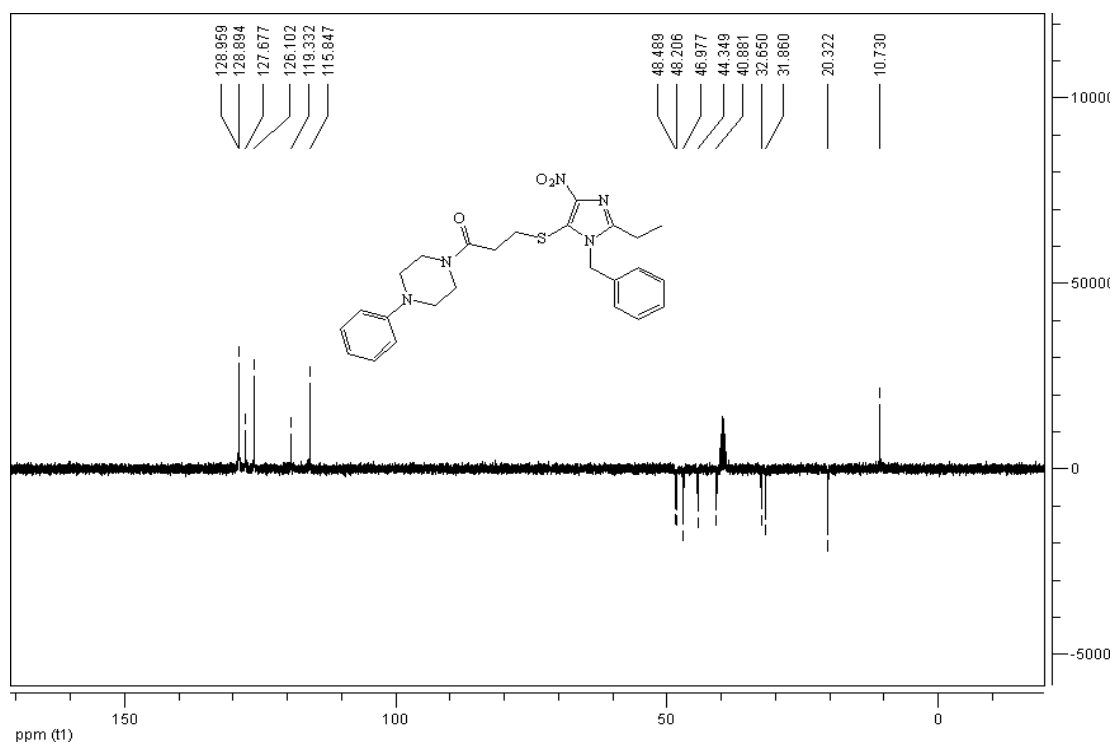


Figure 2. DEPT-135° spectrum for compound **(5a)** in DMSO-*d*₆.

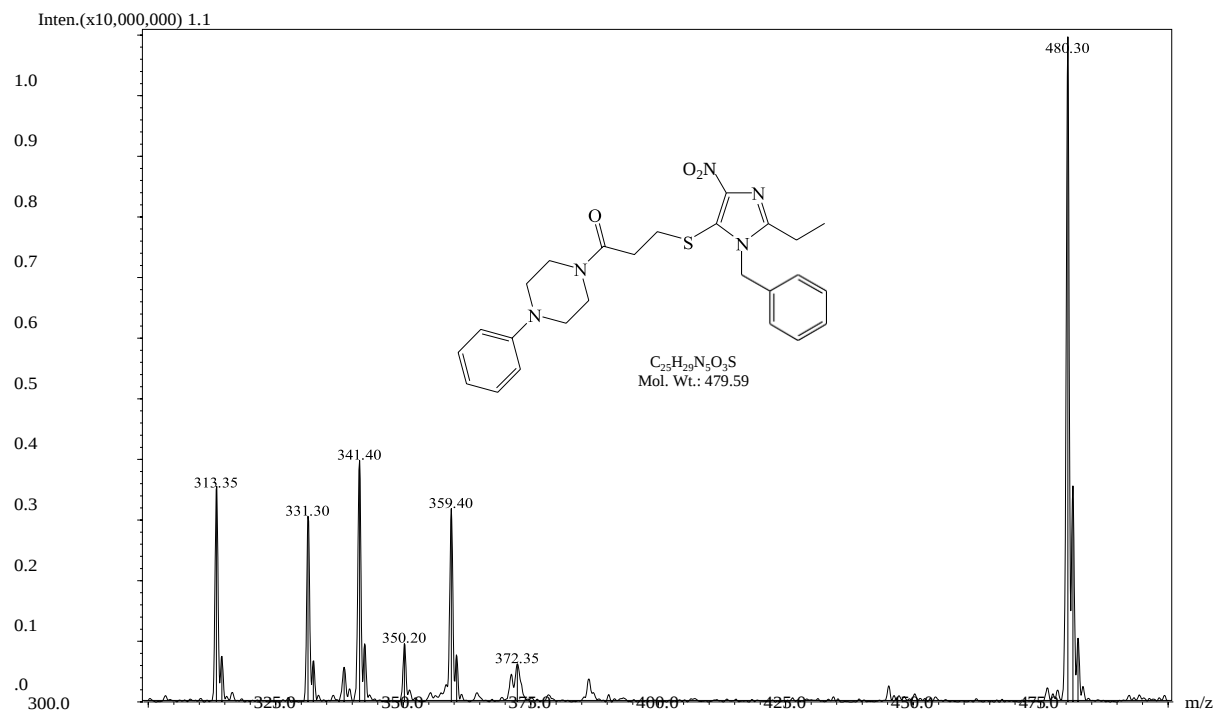


Figure 3. Mass spectrum for compound (5a), $[M+H]^+$.

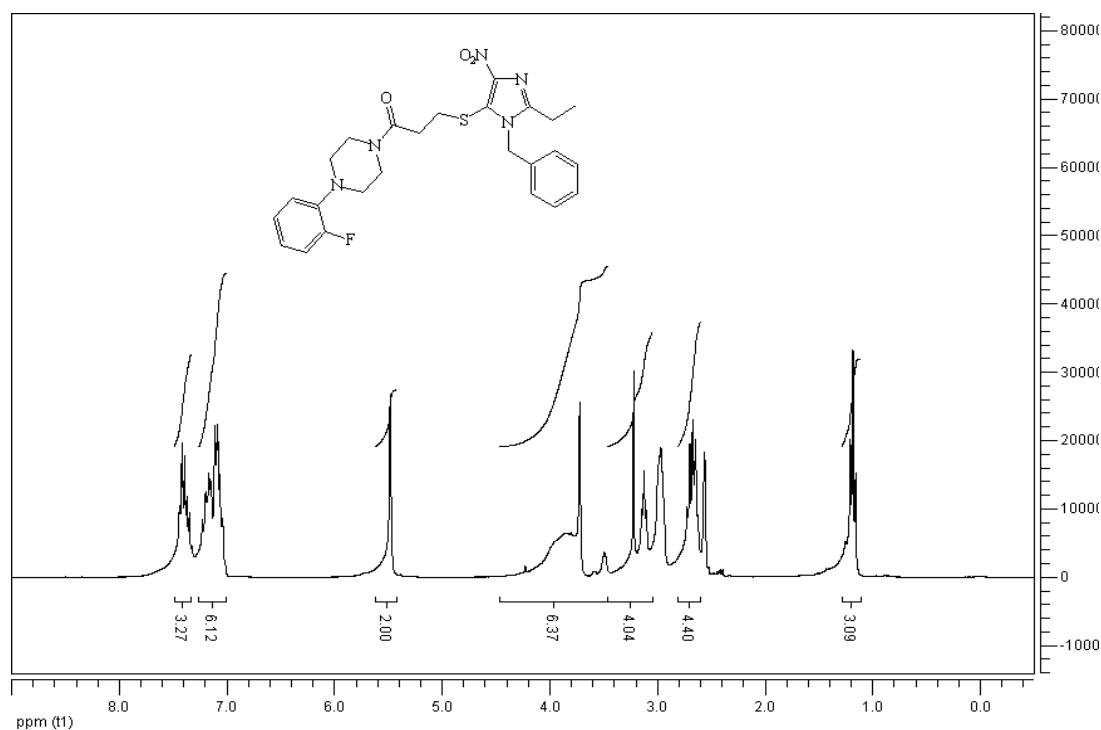


Figure 4. 1H -NMR spectrum for compound (5b) in $DMSO-d_6$.

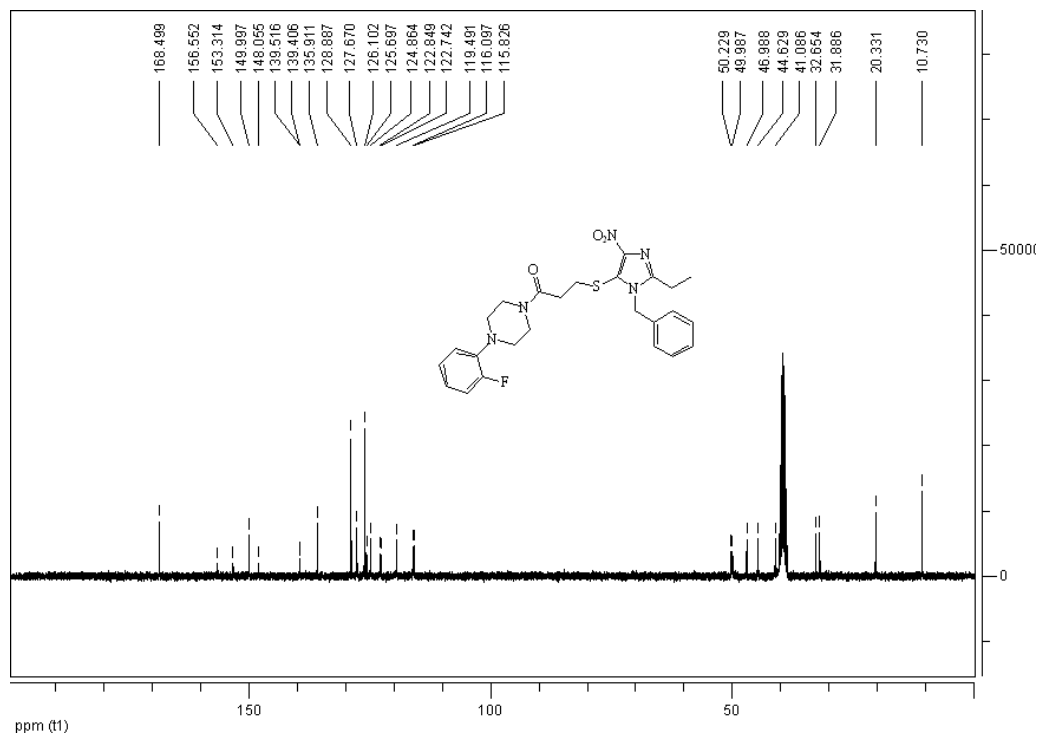


Figure 5.: ¹³C-NMR spectrum for compound **(5b)** in DMSO-*d*₆.

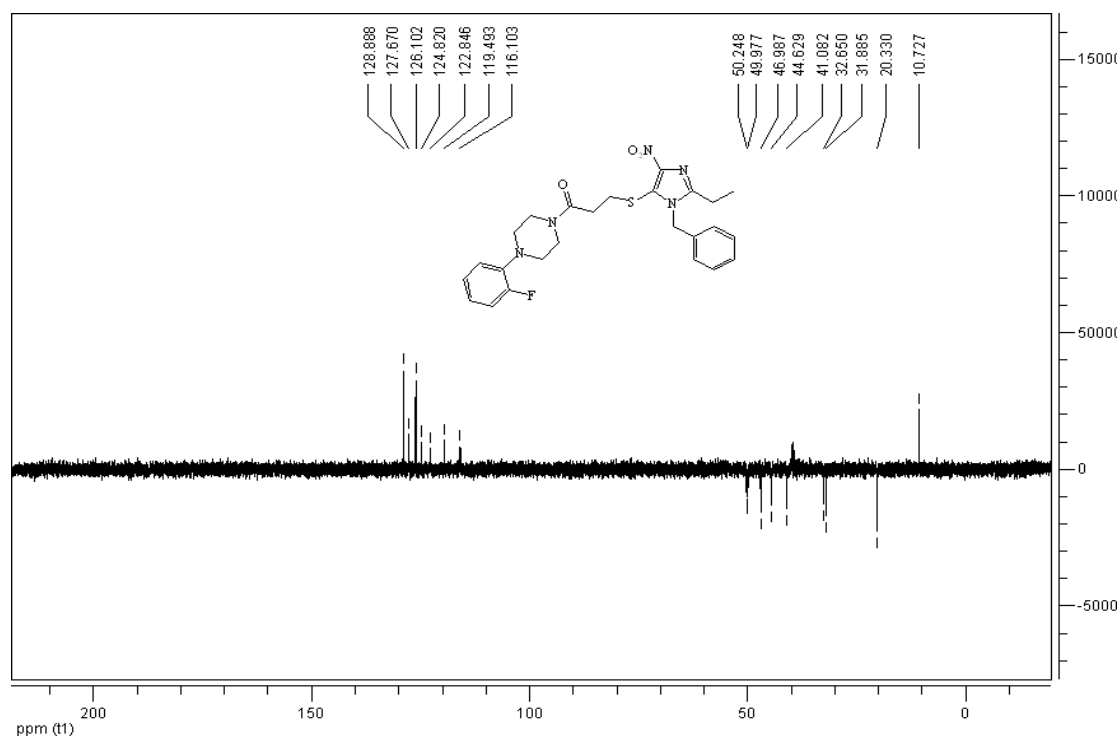


Figure 6. DEPT-135° spectrum for compound **(5b)** in DMSO-*d*₆.

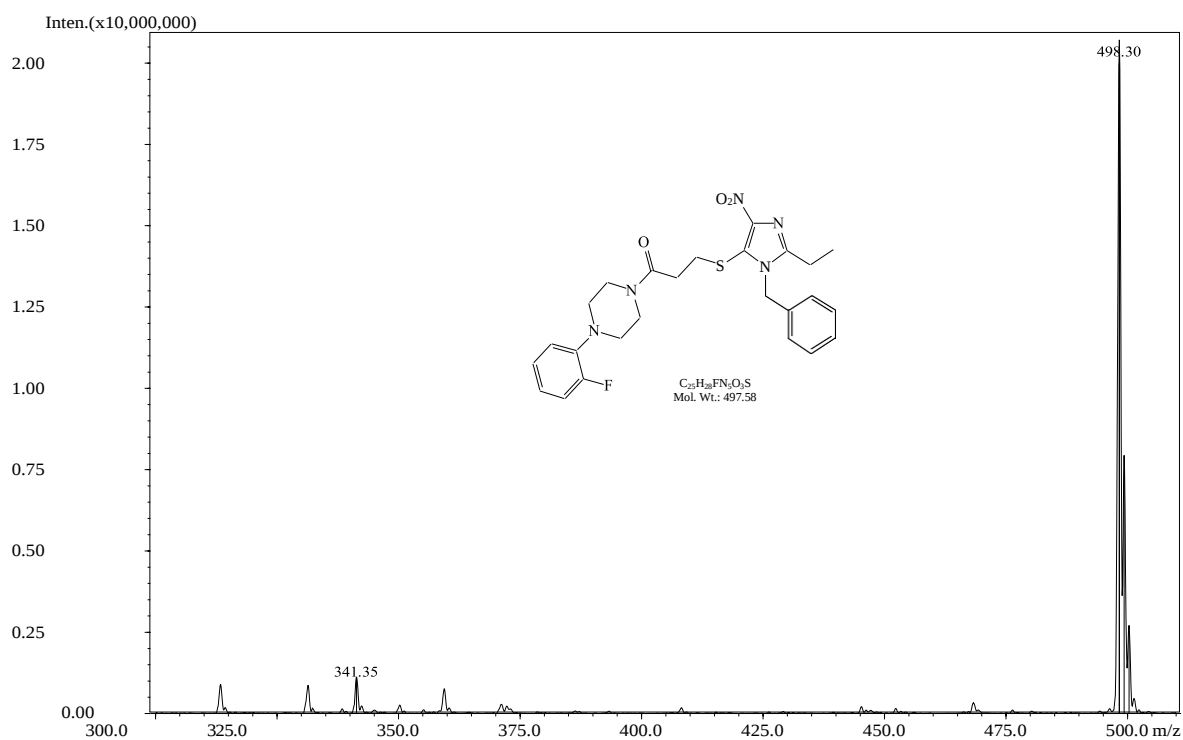


Figure 7. Mass spectrum for compound **(5b)**, $[M+H]^+$.

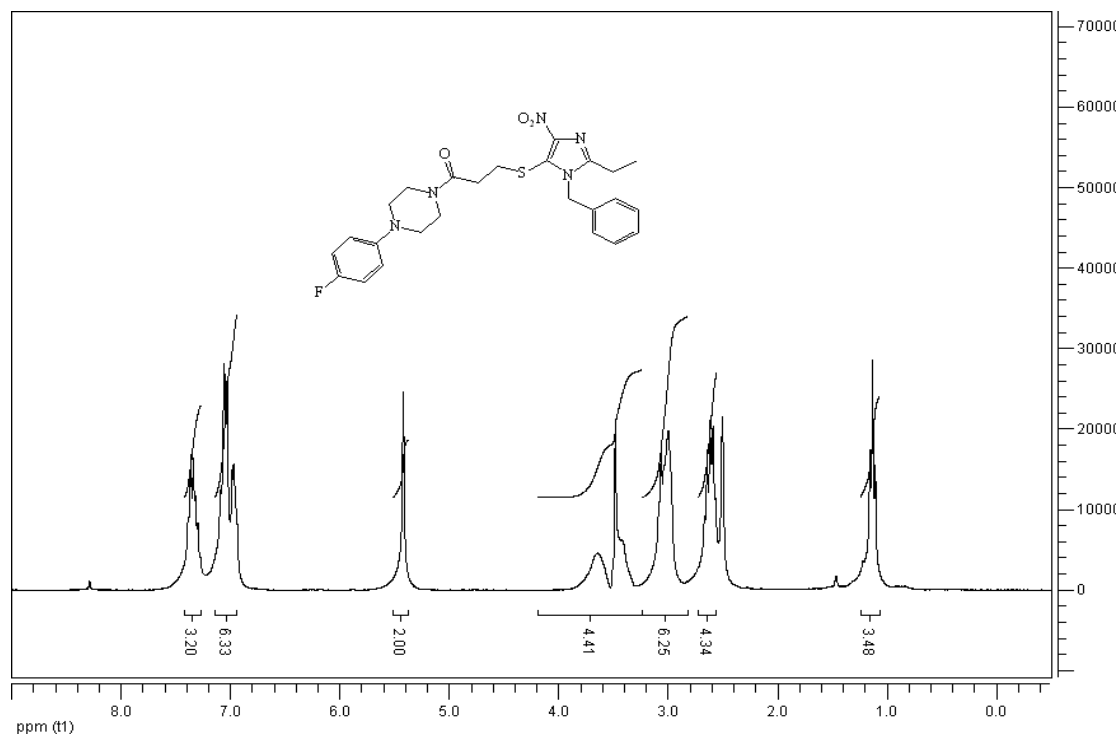


Figure 8. 1H -NMR spectrum for compound **(5c)** in $DMSO-d_6$.

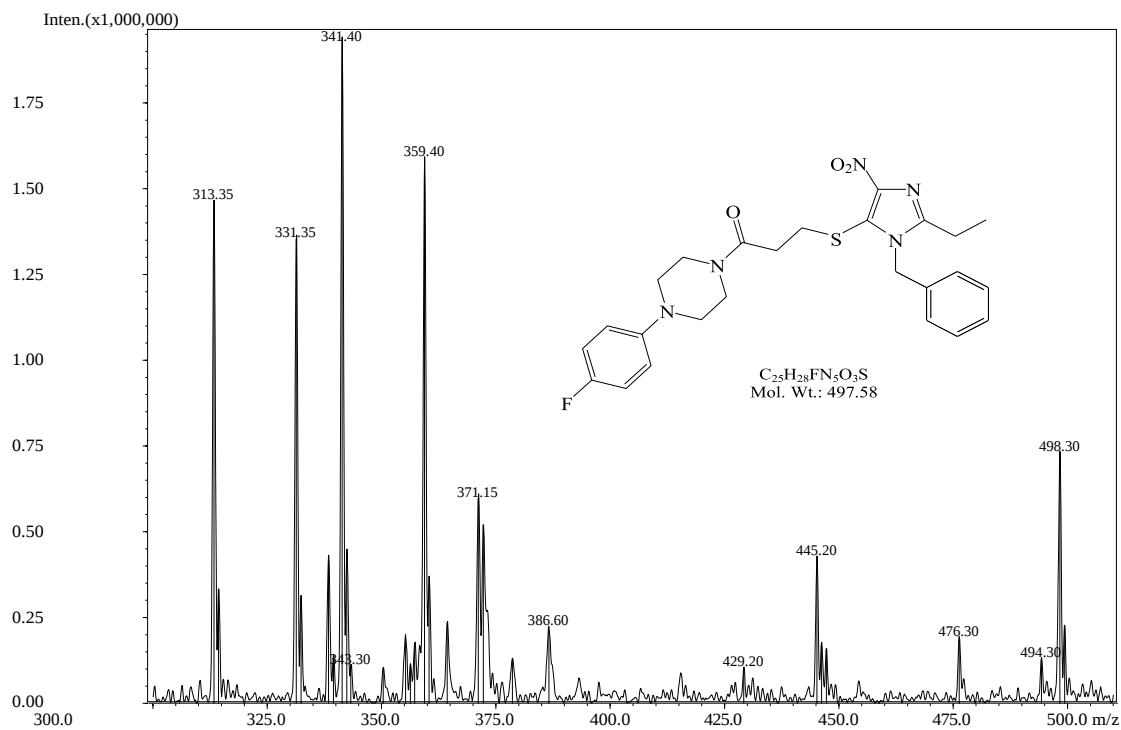


Figure 9. Mass spectrum for compound **(5c)**, $[M+H]^+$.

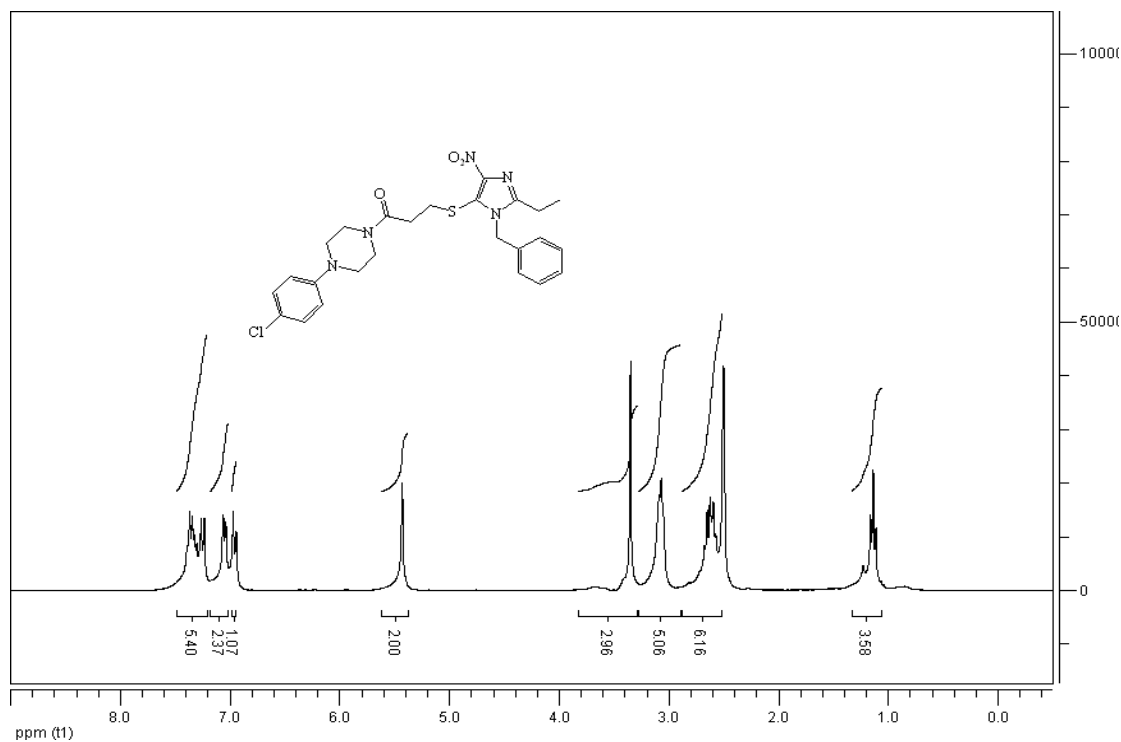


Figure 10. 1H -NMR spectrum for compound **(5d)** in $DMSO-d_6$.

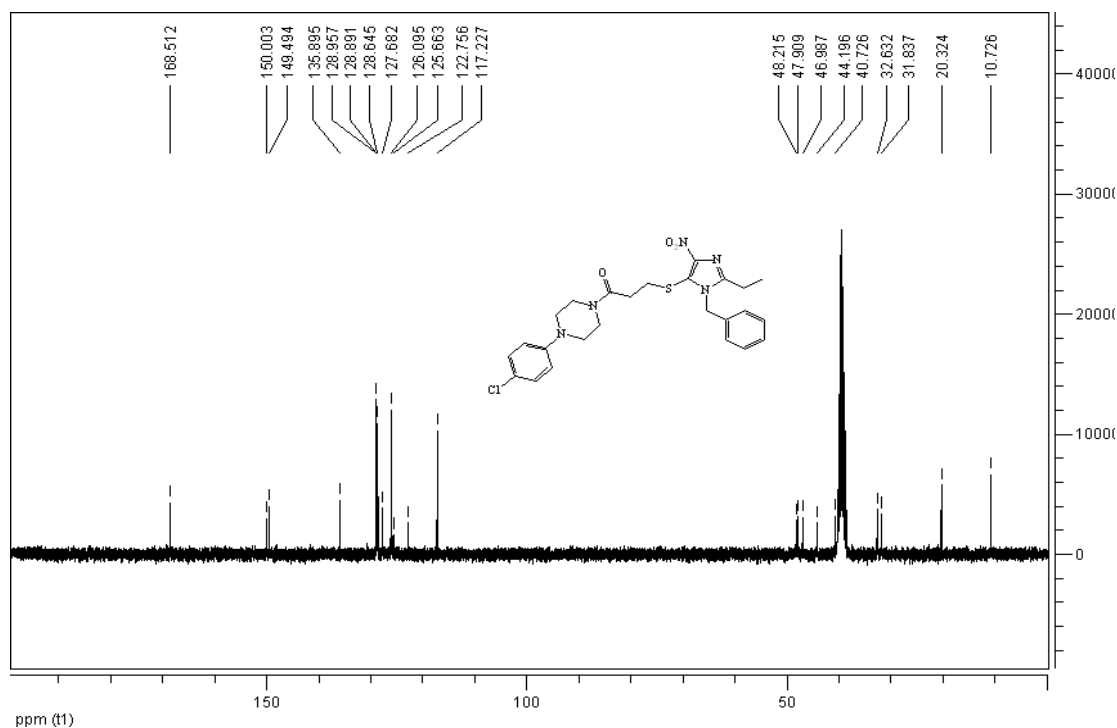


Figure 11. ¹³C-NMR spectrum for compound (**5d**) in DMSO-*d*₆.

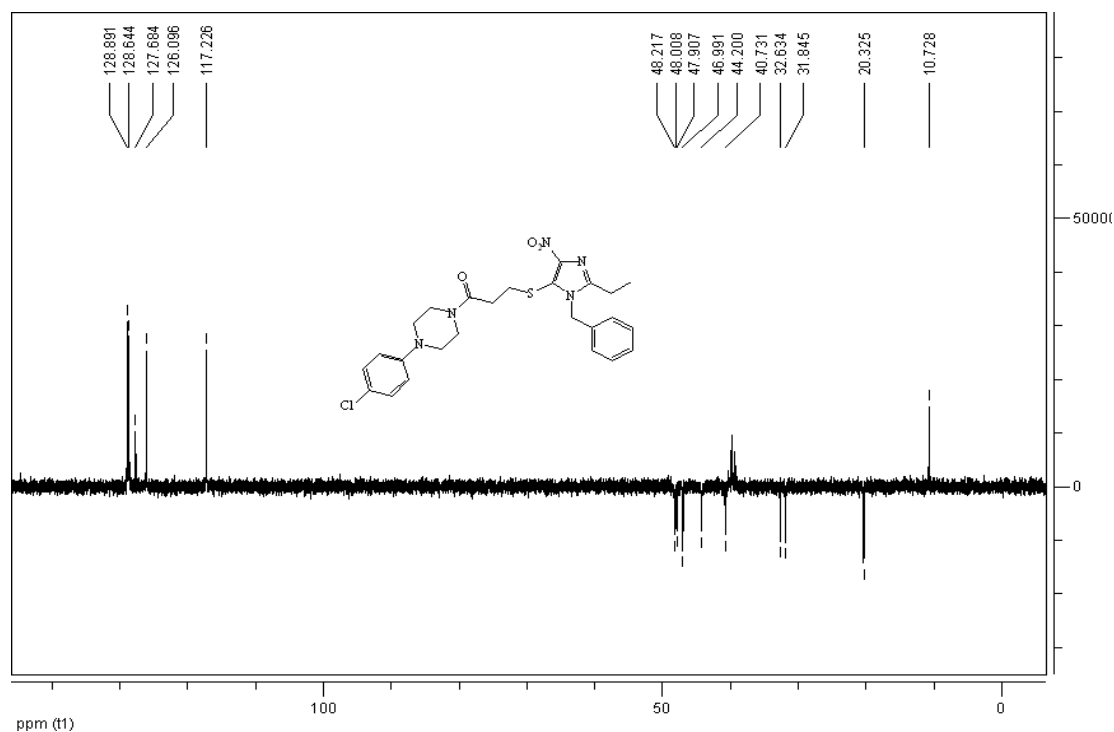


Figure 12. DEPT-135° spectrum for compound (**5d**) in DMSO-*d*₆.

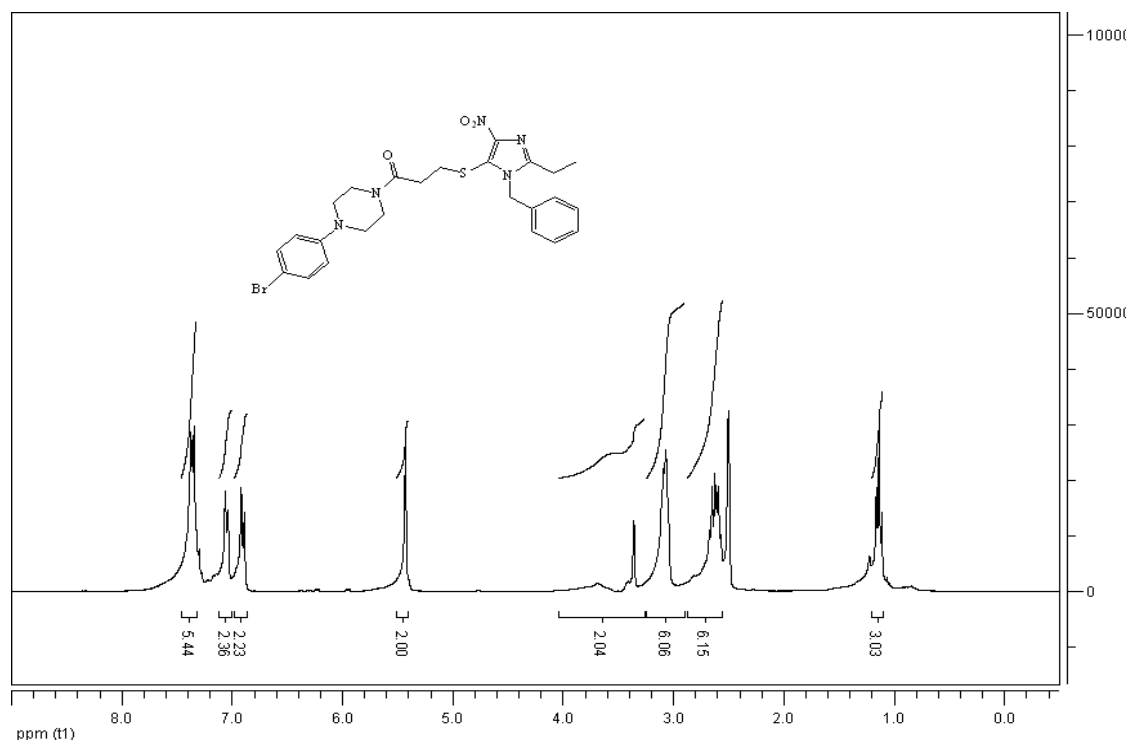


Figure 13. ¹H-NMR spectrum for compound (5e) in DMSO-*d*₆.

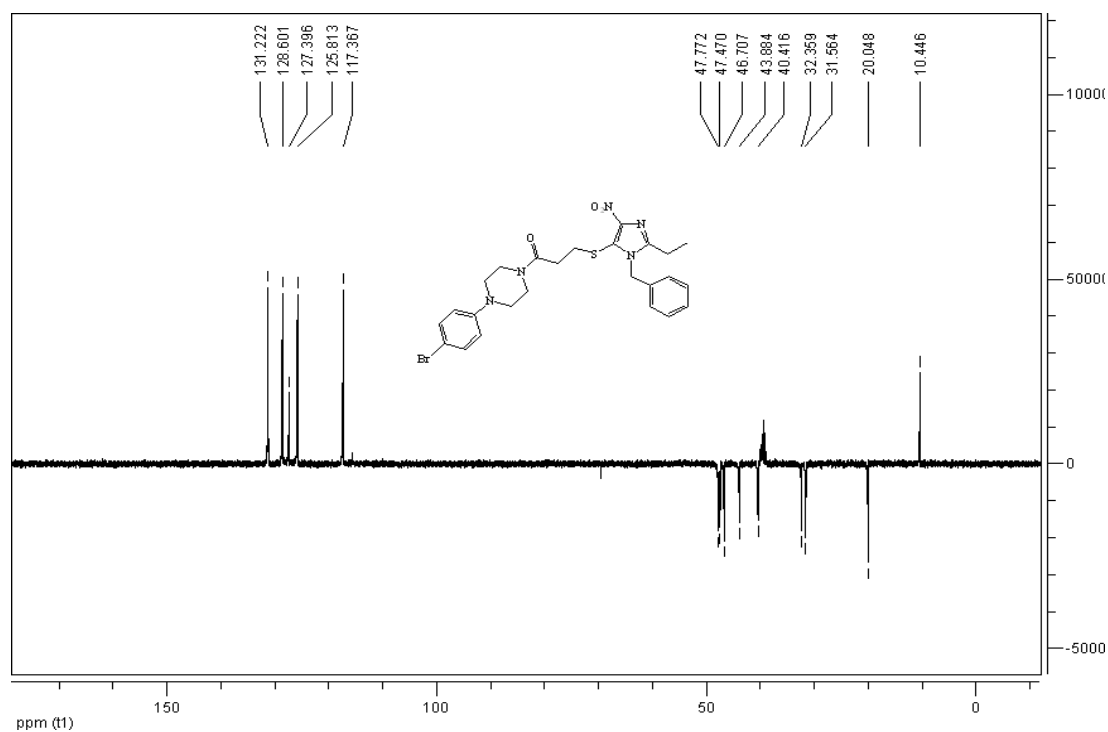


Figure 14. DEPT-135° spectrum for compound (5e) in DMSO-*d*₆.

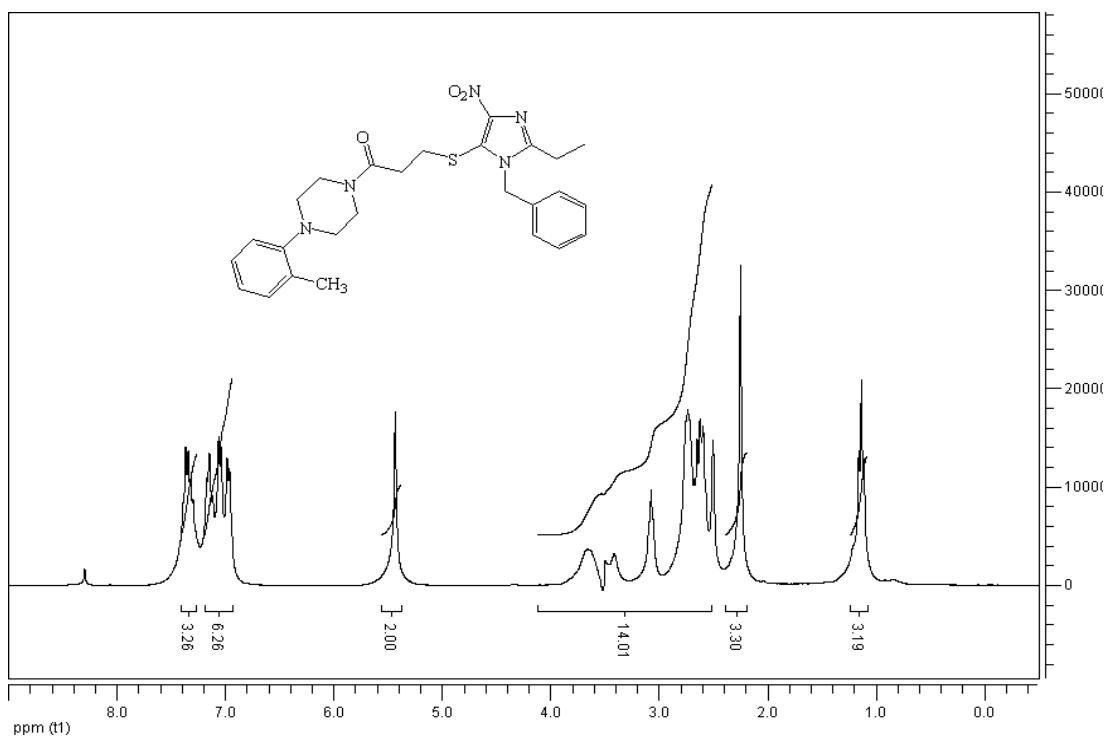


Figure 15. ¹H-NMR spectrum for compound (**5f**) in DMSO-*d*₆.

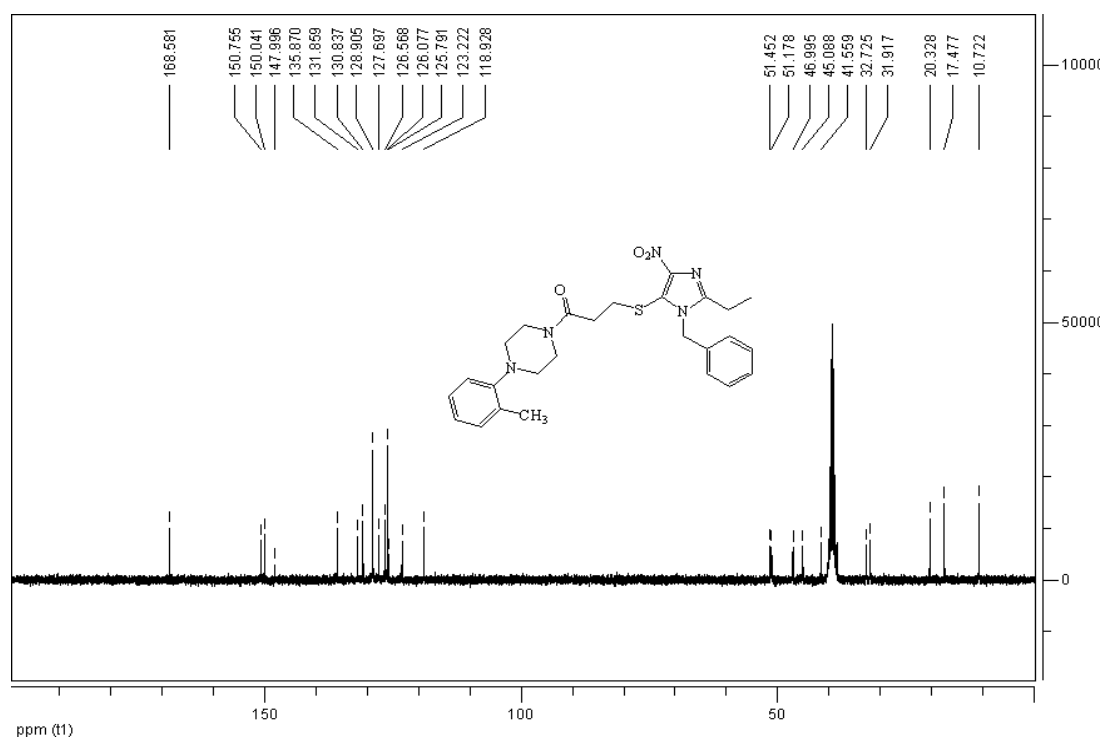


Figure 16. ¹³C-NMR spectrum for compound (**5f**) in DMSO-*d*₆.

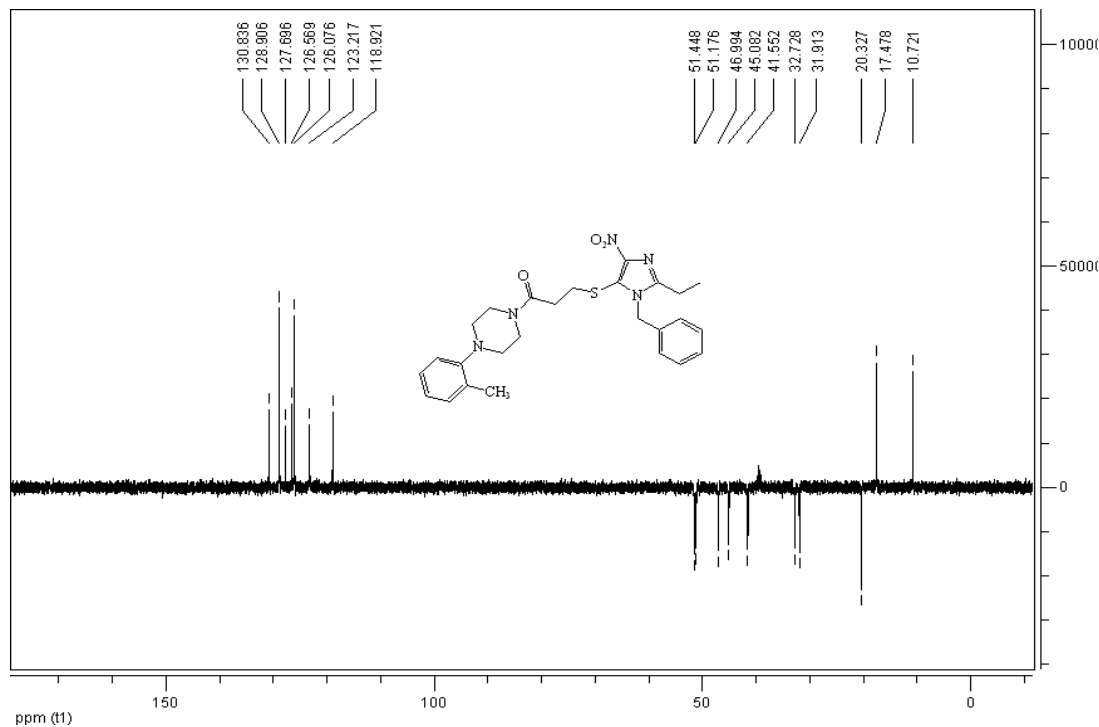


Figure 17. DEPT-135° spectrum for compound (**5f**) in DMSO-*d*₆.

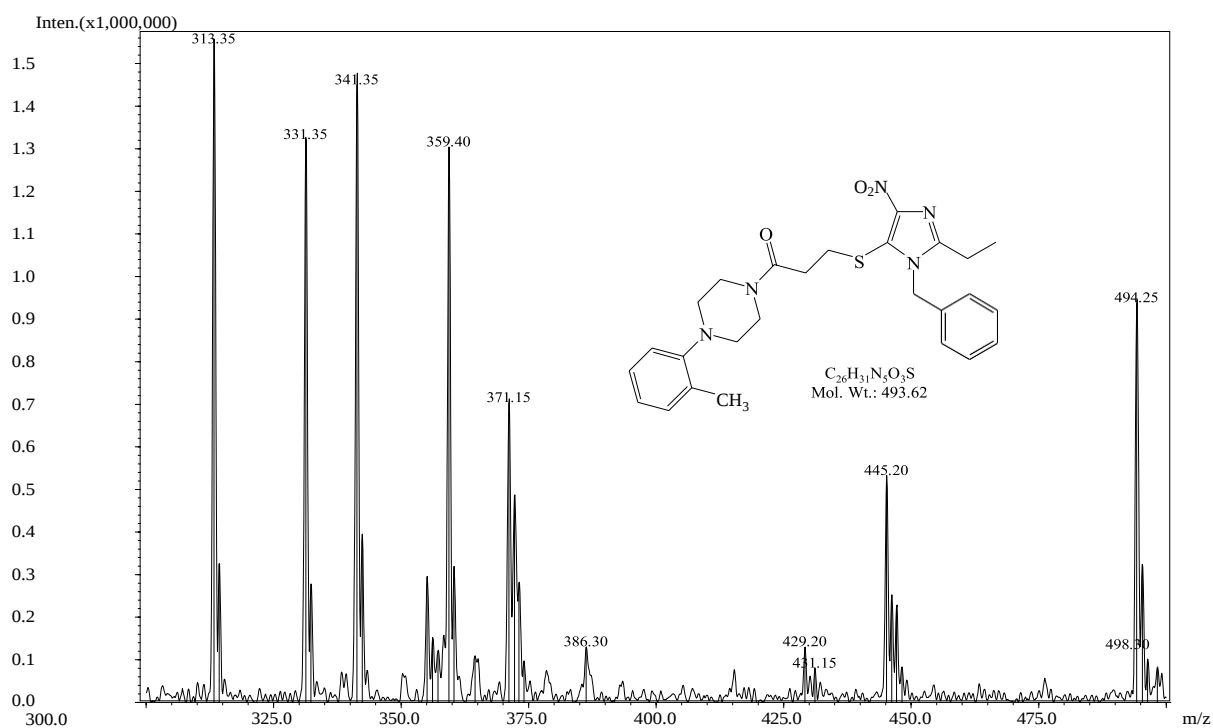


Figure 18. Mass spectrum for compound (**5f**), [M+H]⁺.

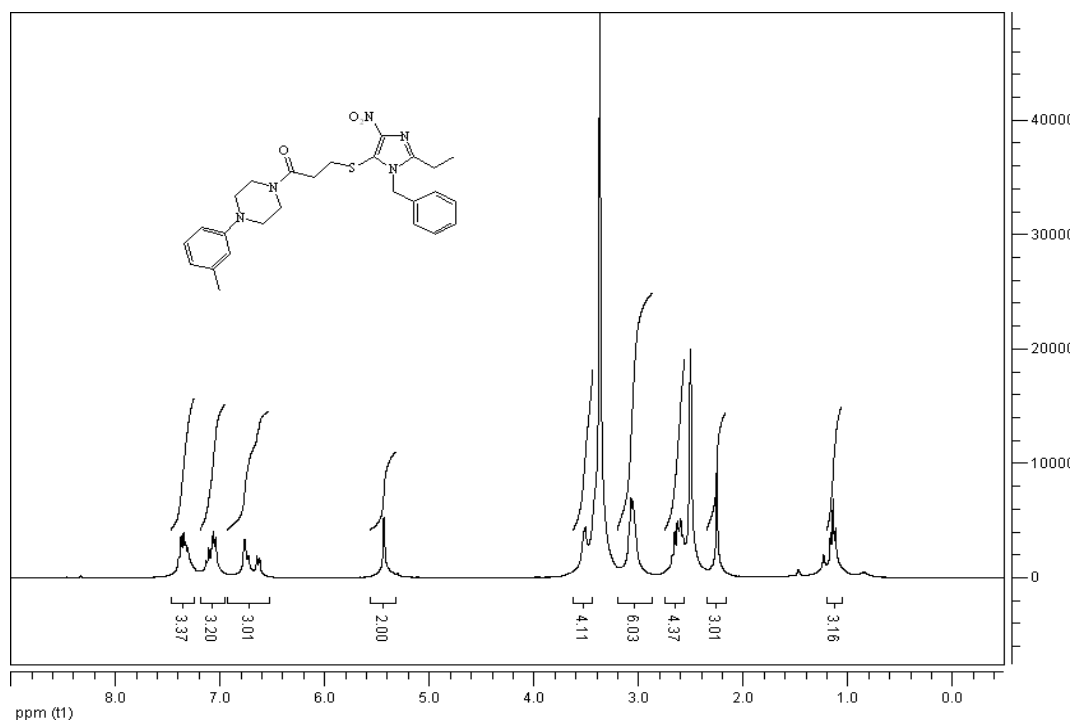


Figure 19. ¹H-NMR spectrum for compound (**5g**) in DMSO-*d*₆.

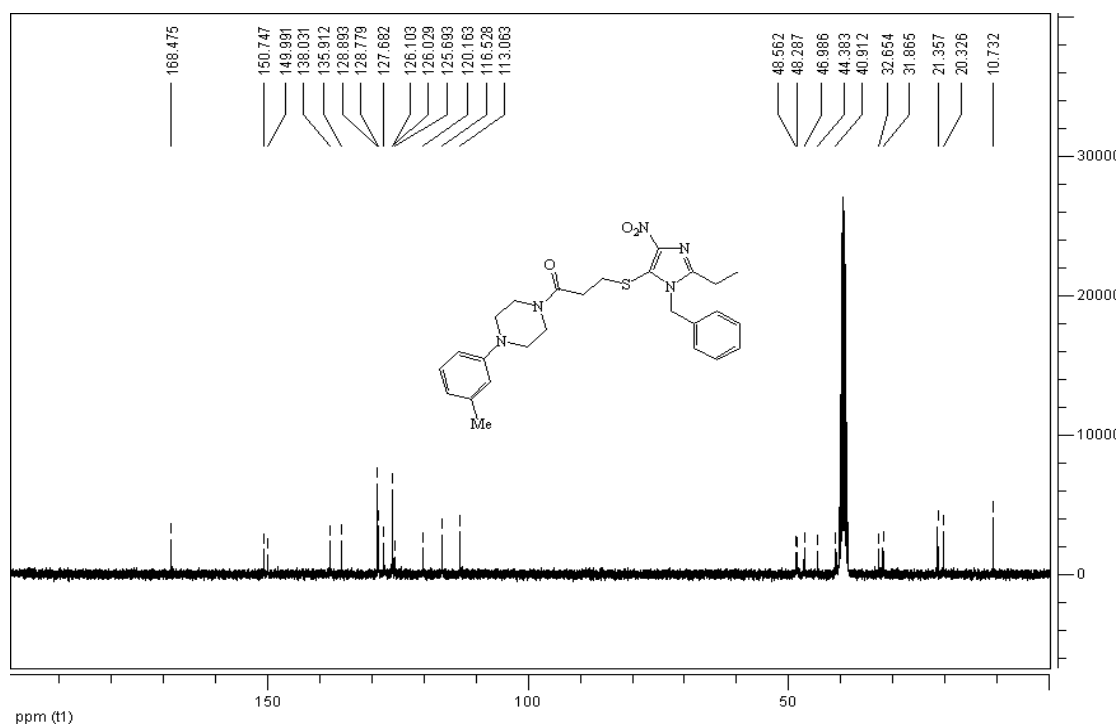


Figure 20. ¹³C-NMR spectrum for compound (**5g**) in DMSO-*d*₆.

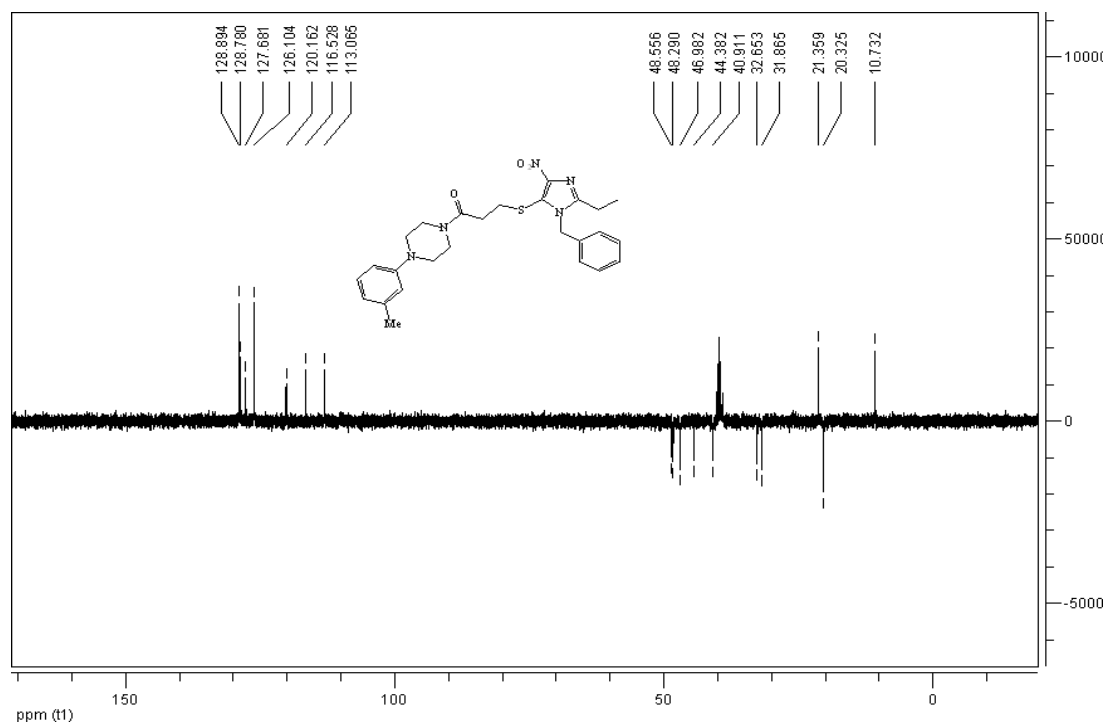


Figure 21. DEPT-135° spectrum for compound (**5g**) in DMSO-*d*₆.

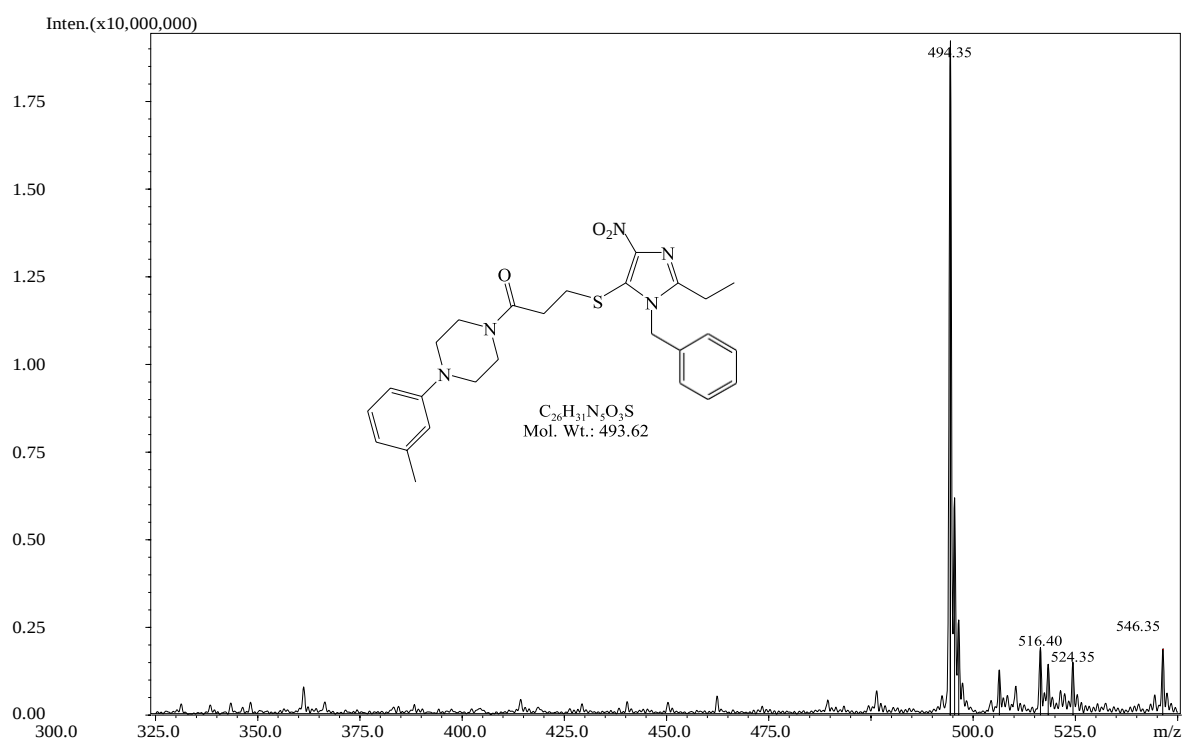


Figure 22. Mass spectrum for compound (**5g**), [M+H]⁺.

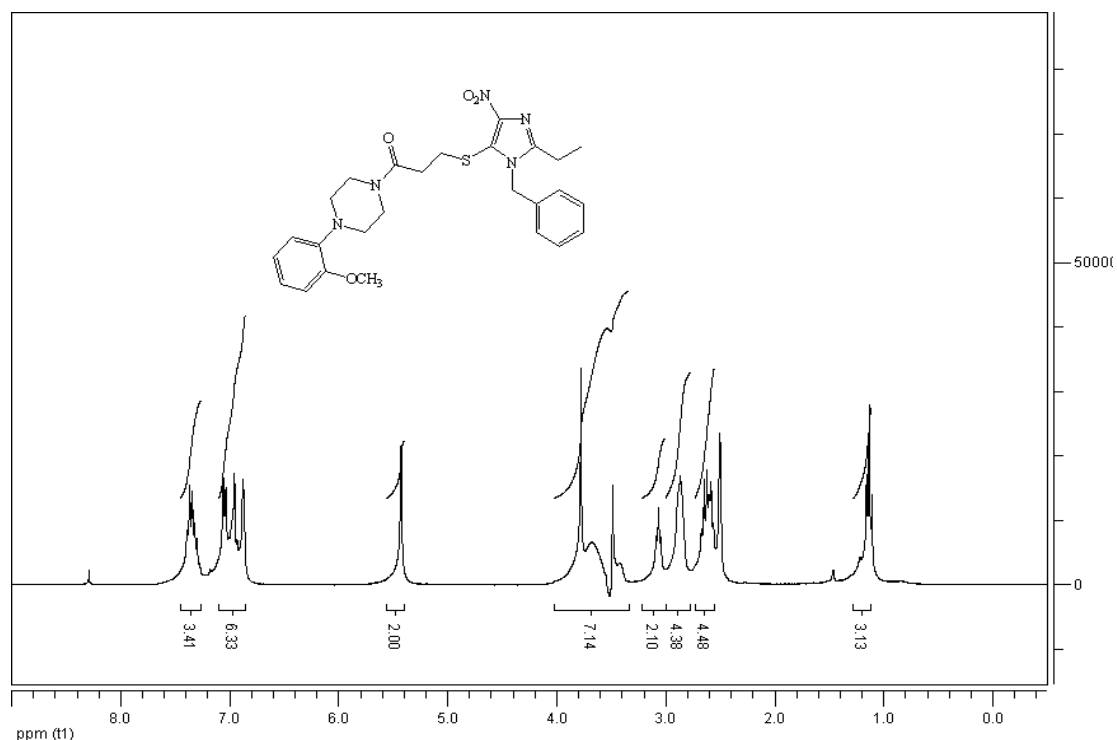


Figure 23. ¹H-NMR spectrum for compound (5h) in DMSO-*d*₆.

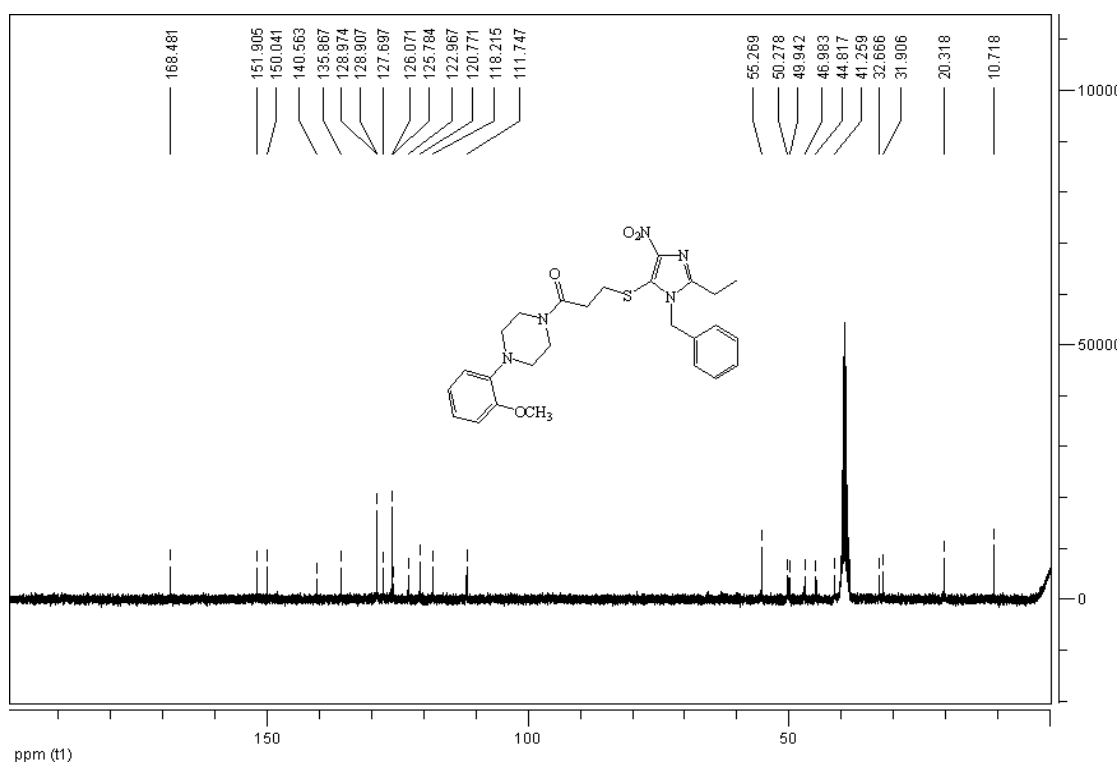


Figure 24. ¹³C-NMR spectrum for compound (5h) in DMSO-*d*₆.

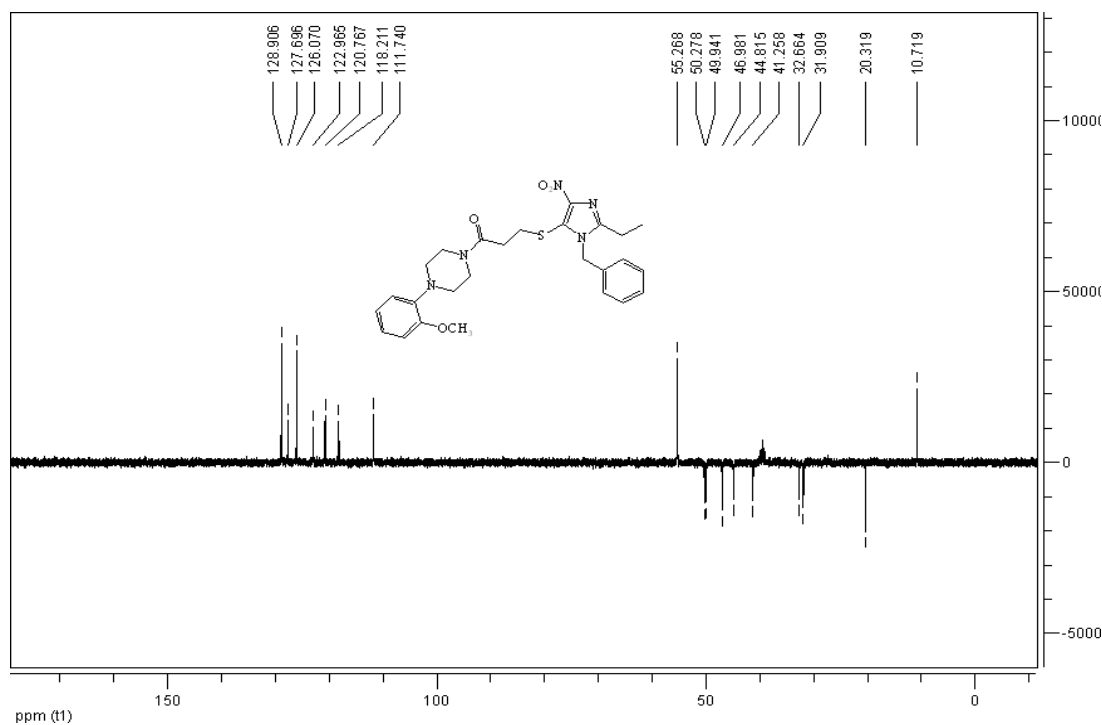


Figure 25. DEPT-135° spectrum for compound (**5h**) in DMSO-*d*₆.

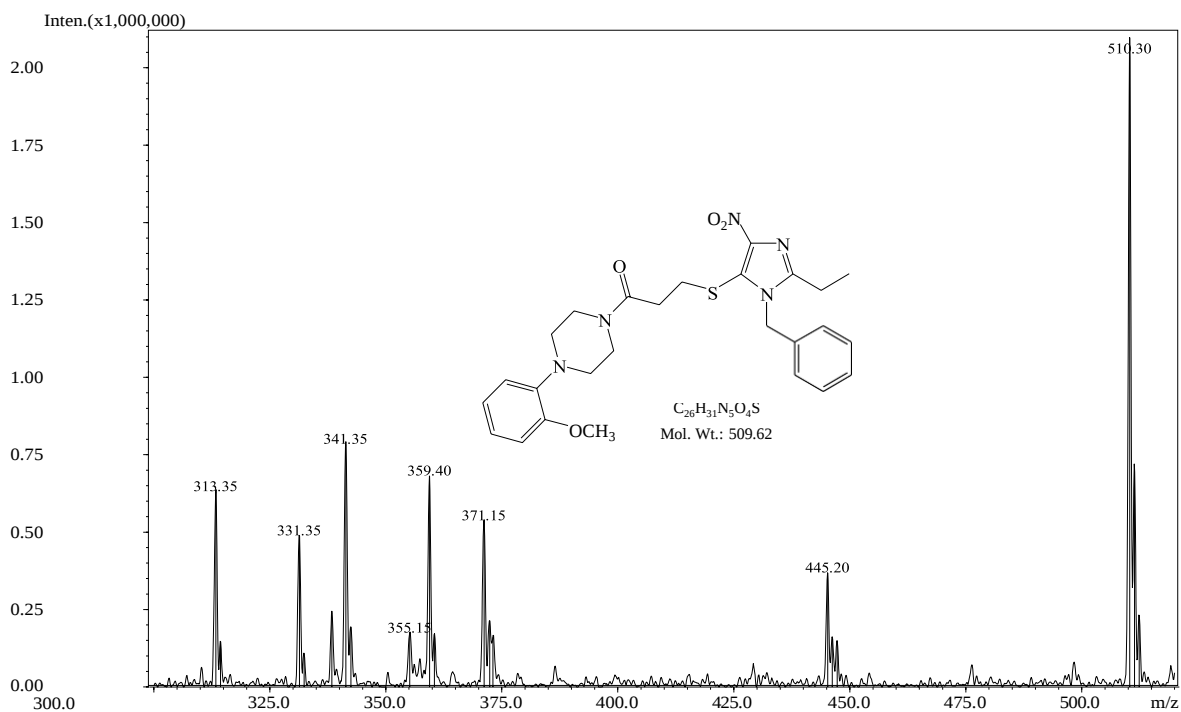


Figure 26. Mass spectrum for compound (**5h**), [M+H]⁺.

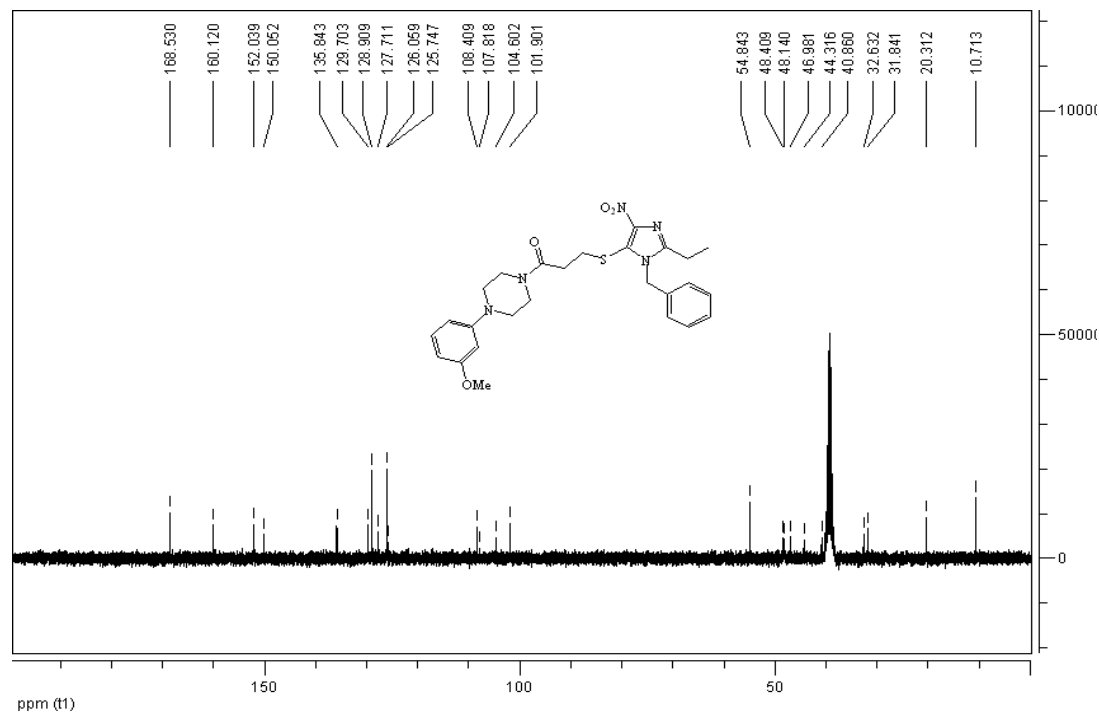


Figure 27. ¹³C-NMR spectrum for compound (5i) in DMSO-*d*₆.

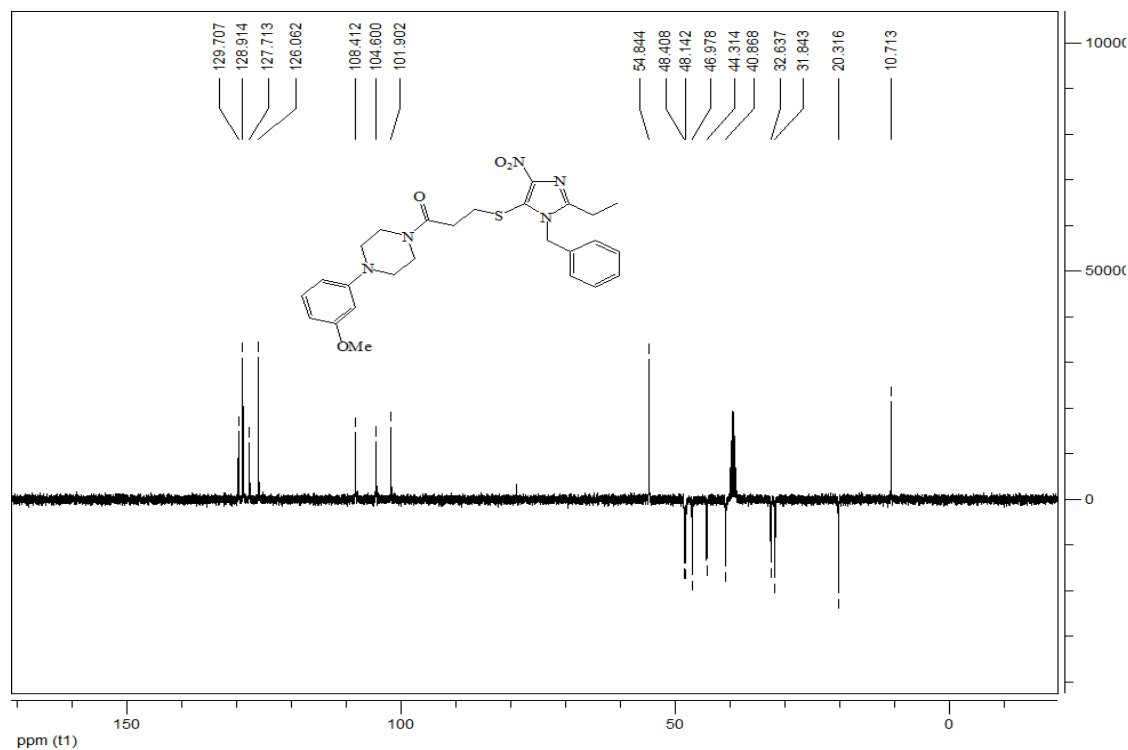


Figure 28. DEPT-135° spectrum for compound (5i) in DMSO-*d*₆.

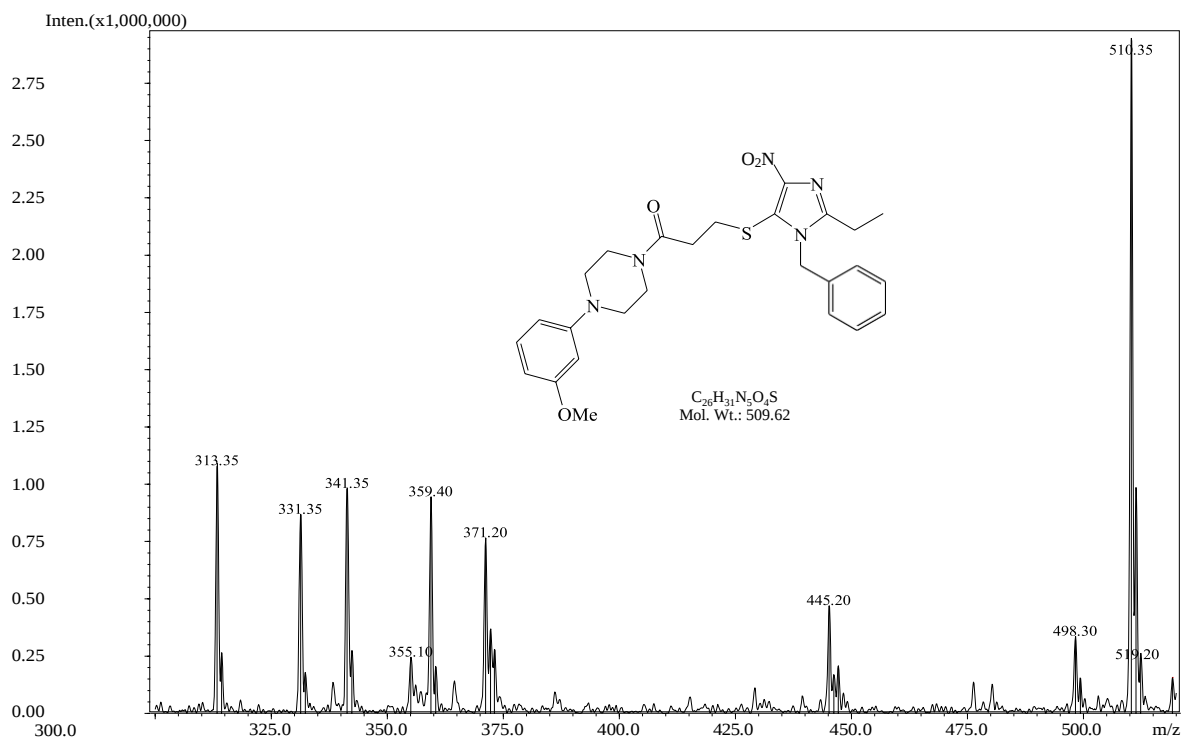


Figure 29. Mass spectrum for compound (5i), $[M+H]^+$.

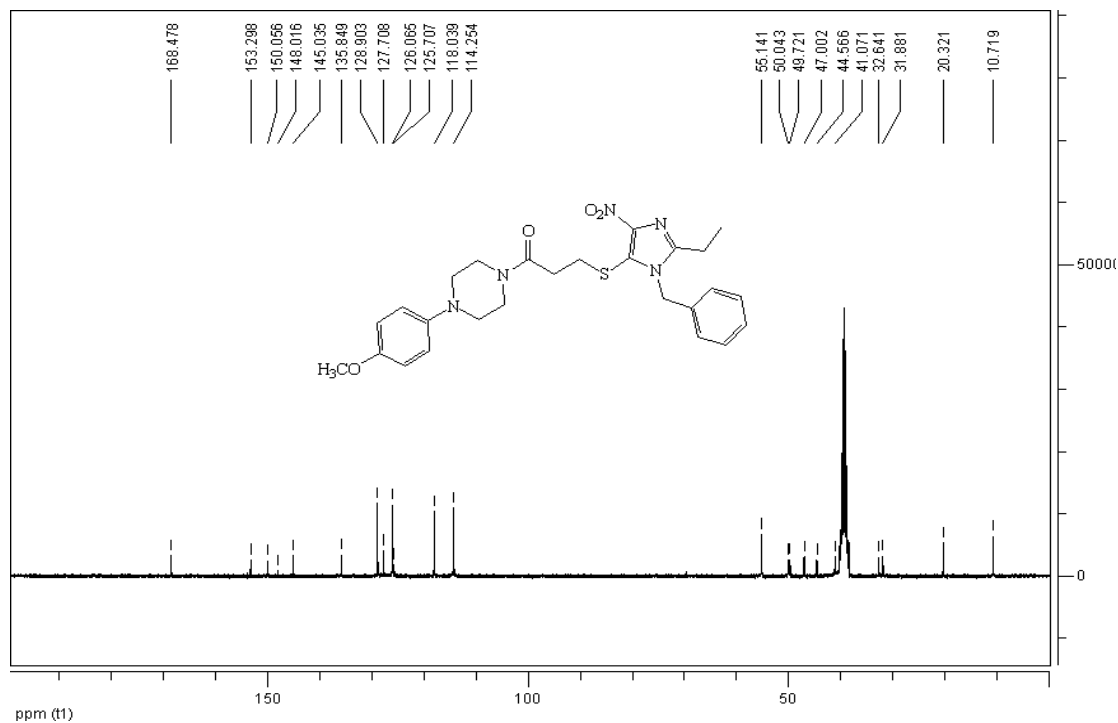


Figure 30. ^{13}C -NMR spectrum for compound (5j) in $DMSO-d_6$.

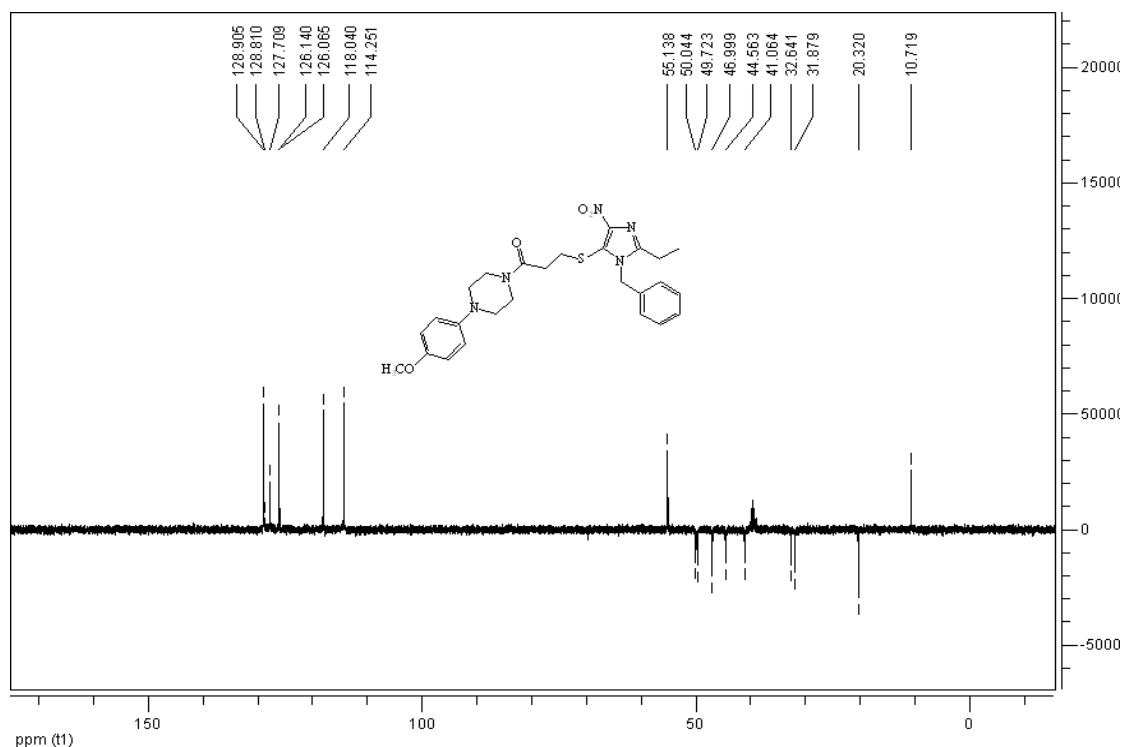


Figure 31. DEPT-135° spectrum for compound (5j) in DMSO-*d*₆.

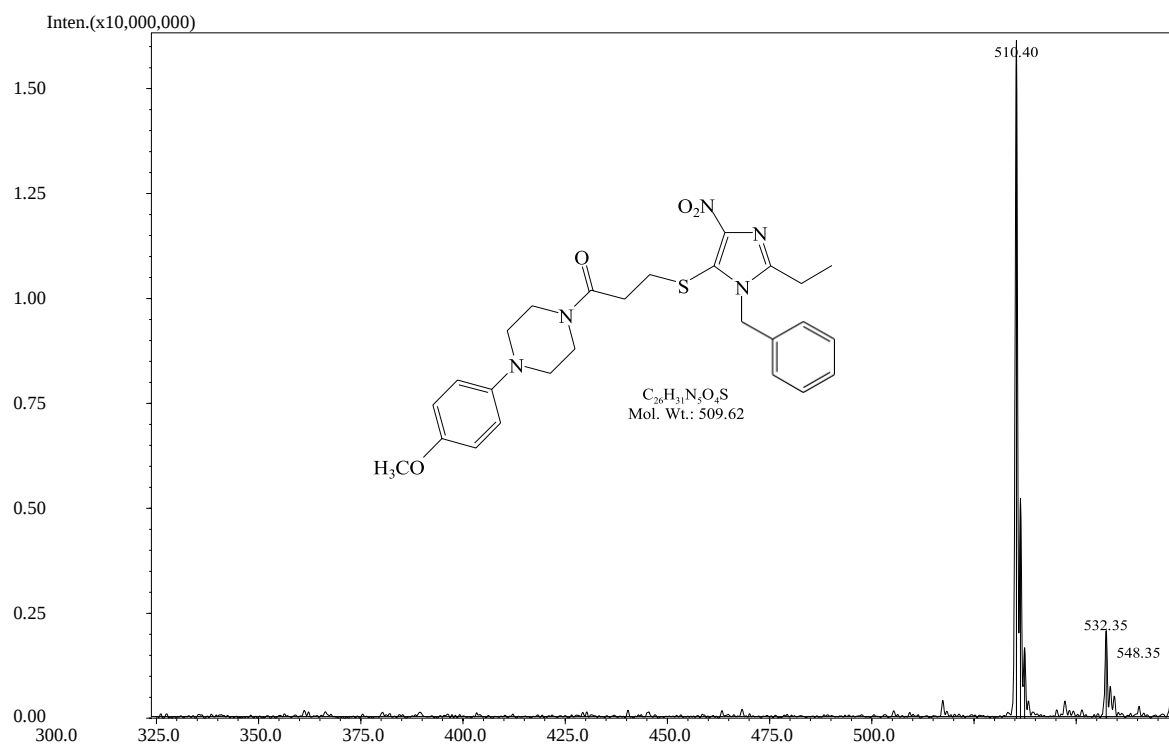


Figure 32. Mass spectrum for compound (5j), [M+H]⁺.

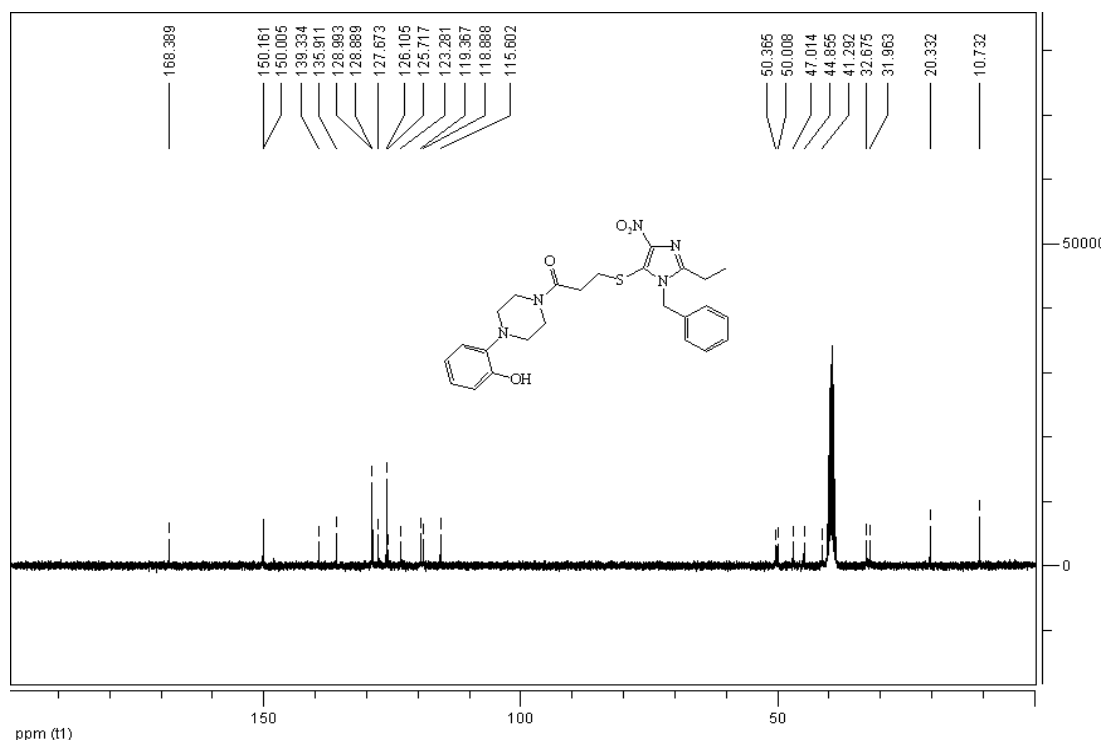


Figure 33. ¹³C-NMR spectrum for compound **(5k)** in DMSO-*d*₆.

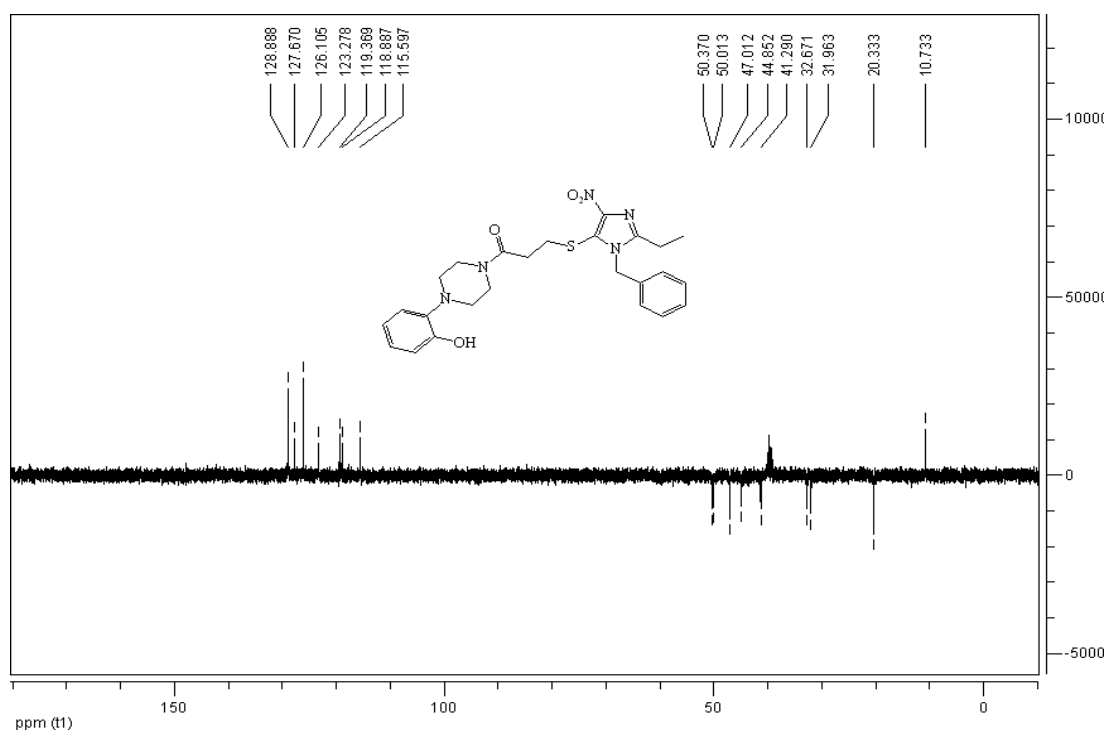


Figure 34. DEPT-135° spectrum for compound **(5k)** in DMSO-*d*₆.

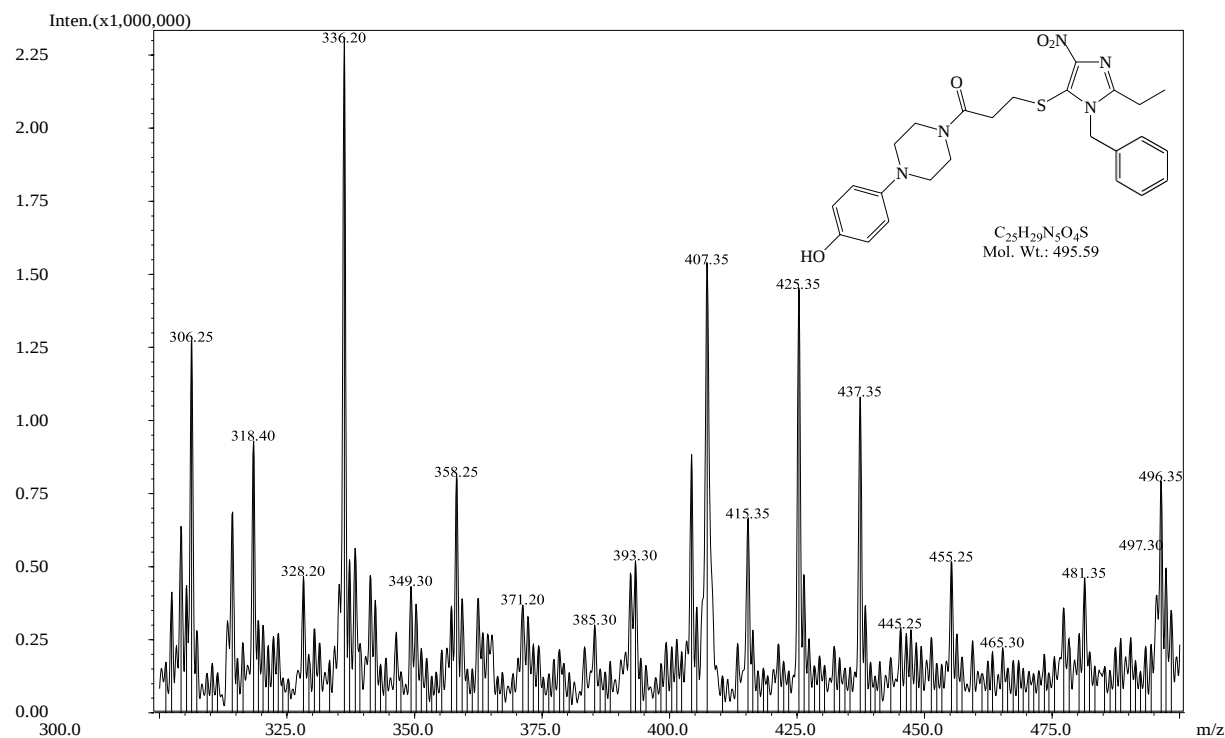


Figure 35. Mass spectrum for compound (5I), $[M+H]^+$.

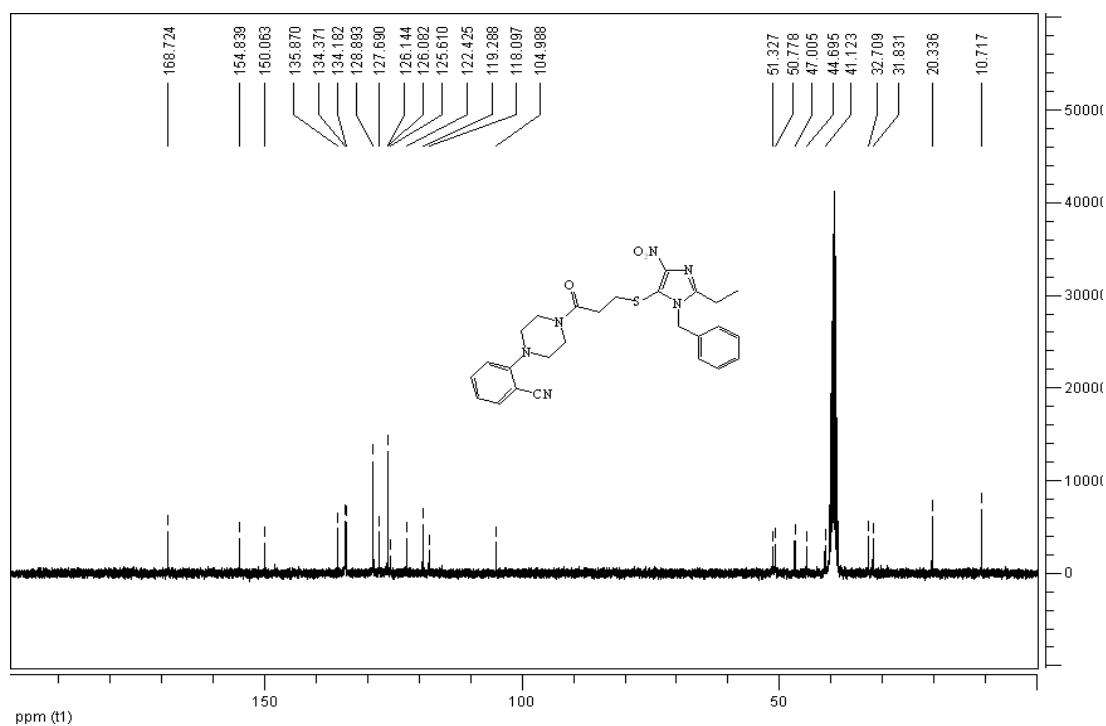


Figure 36. ^{13}C -NMR spectrum for compound (5m) in $DMSO-d_6$.

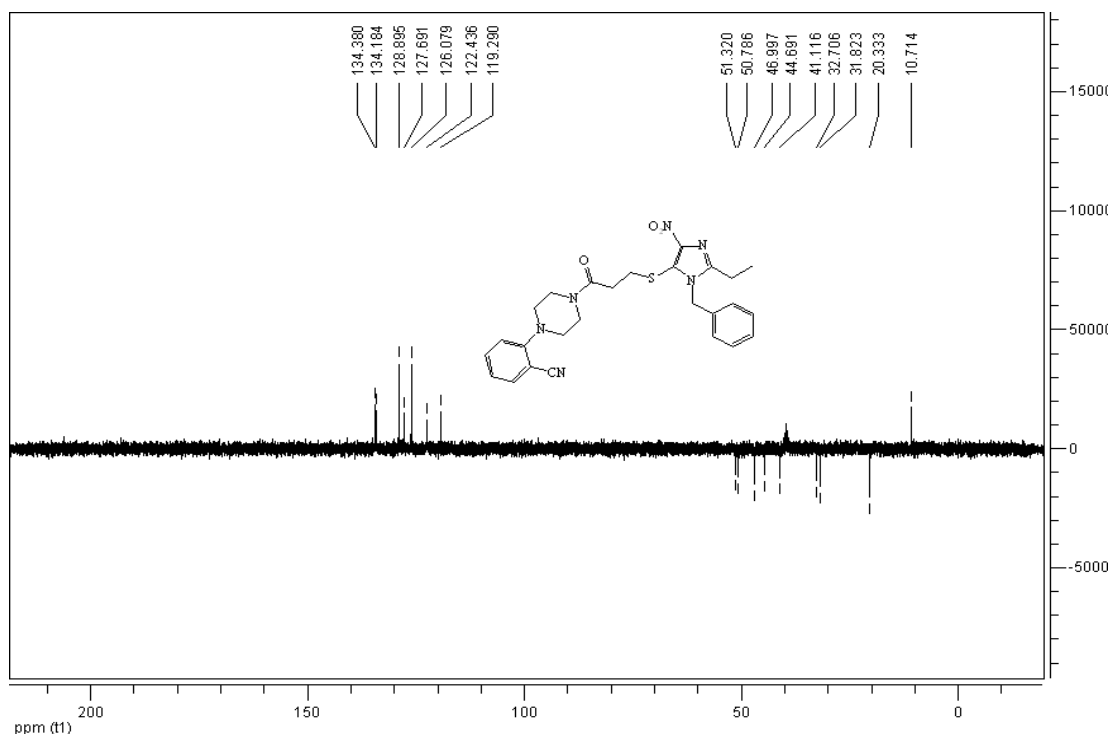


Figure 37. DEPT-135° spectrum for compound (5m) in DMSO- d_6 .

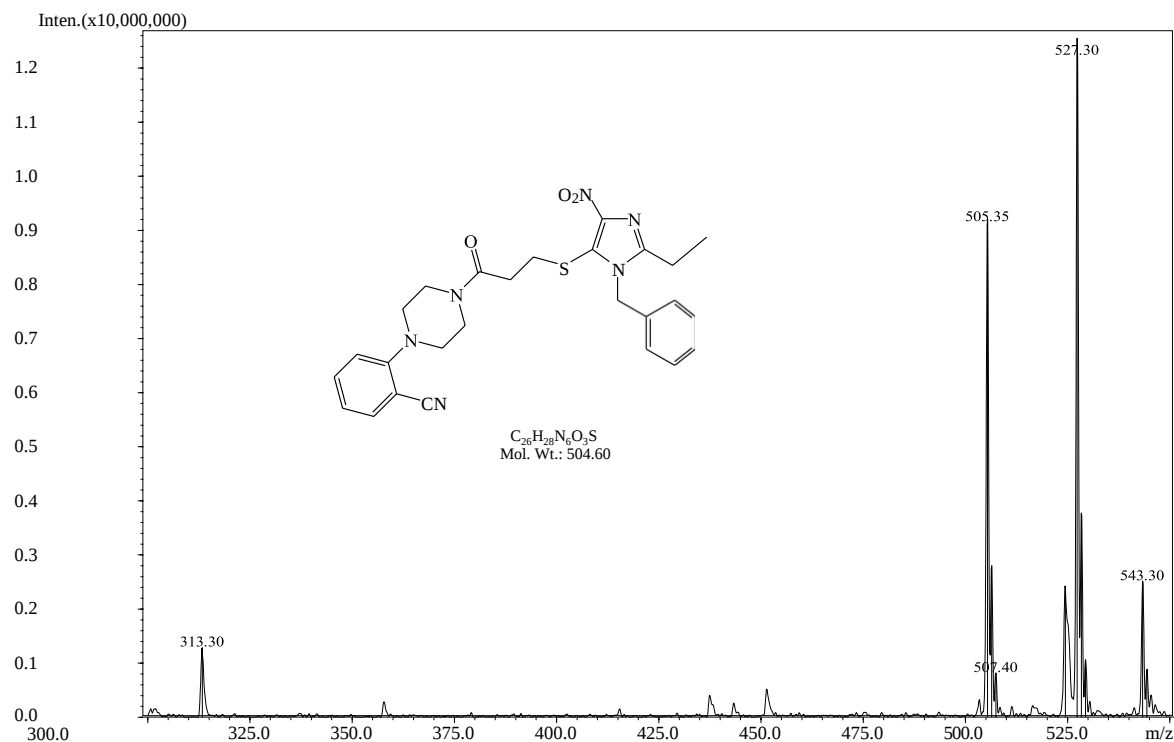


Figure 38. Mass spectrum for compound (5m), $[M+H]^+$.

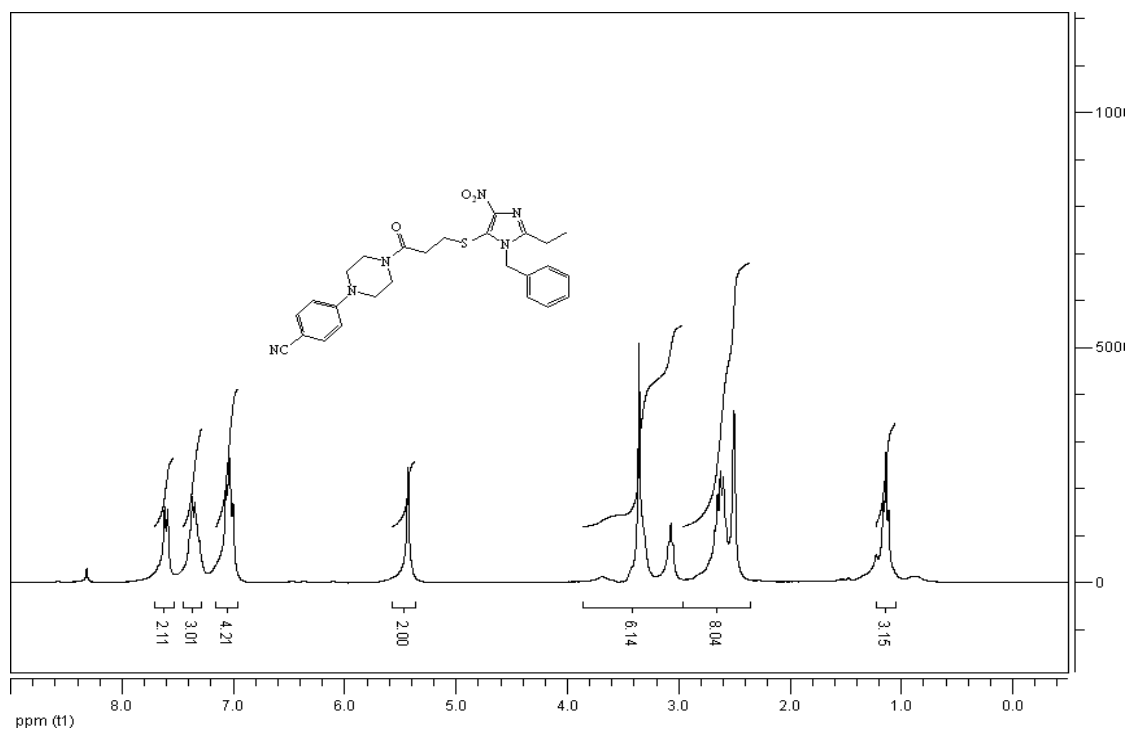


Figure 39. ¹H-NMR spectrum for compound (5n) in DMSO-*d*₆.

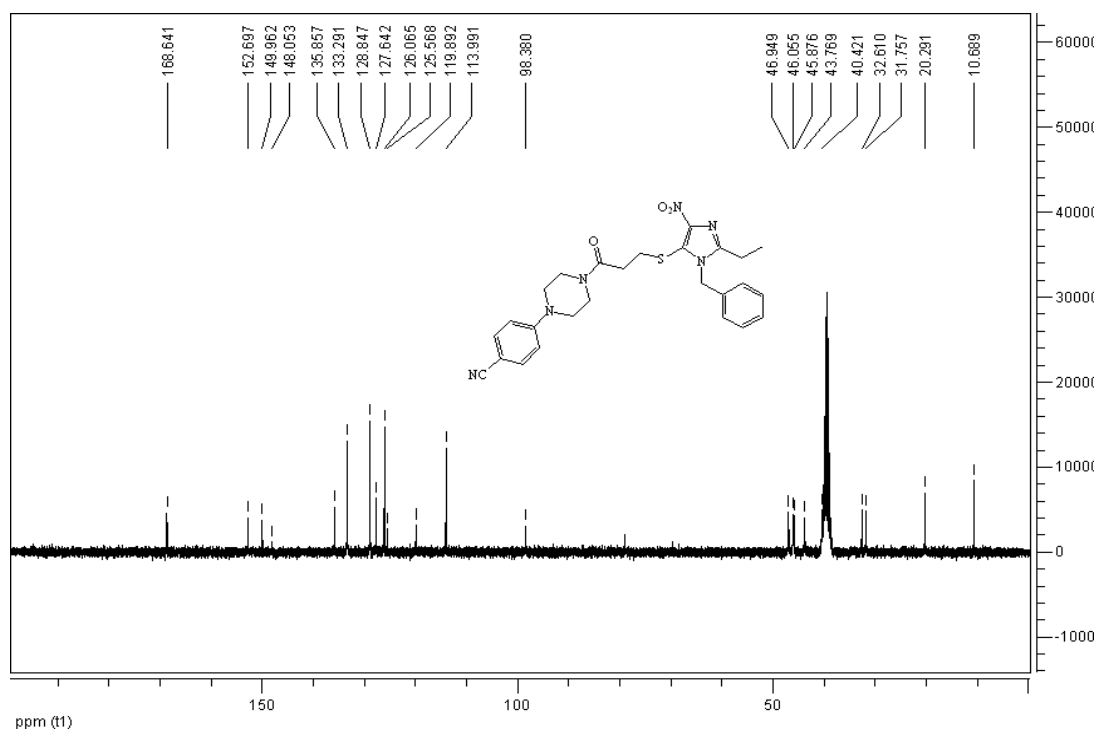


Figure 40. ¹³C-NMR spectrum for compound (5n) in DMSO-*d*₆.

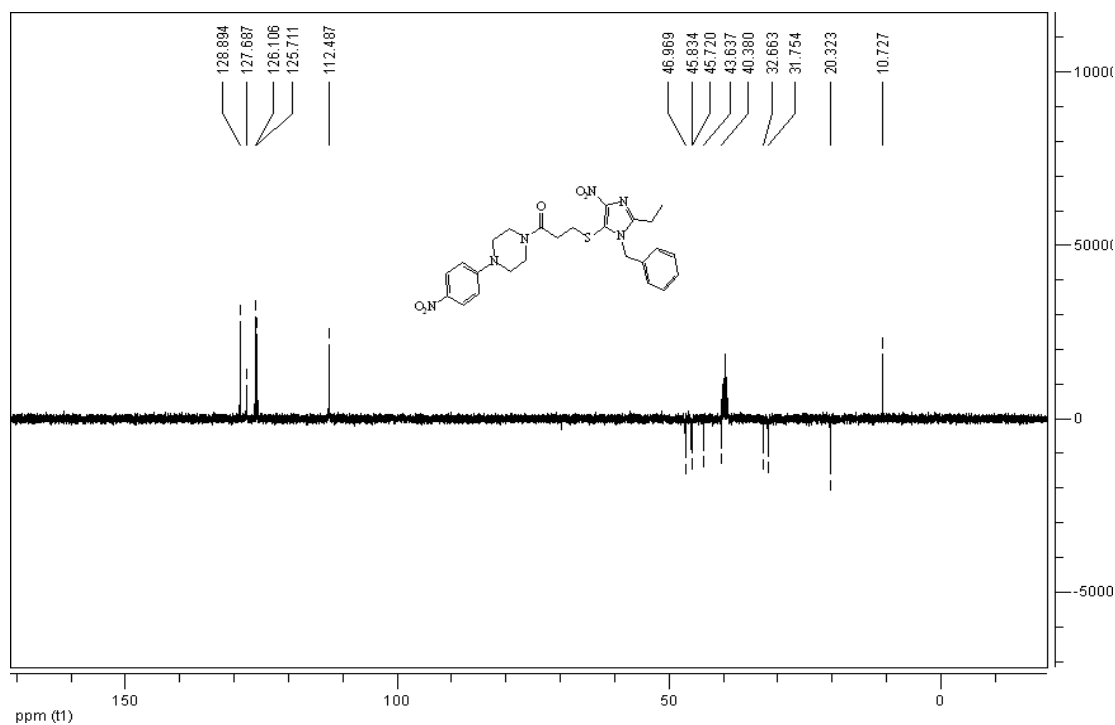


Figure 41. ¹³C-NMR spectrum for compound **(5o)** in DMSO-*d*₆.

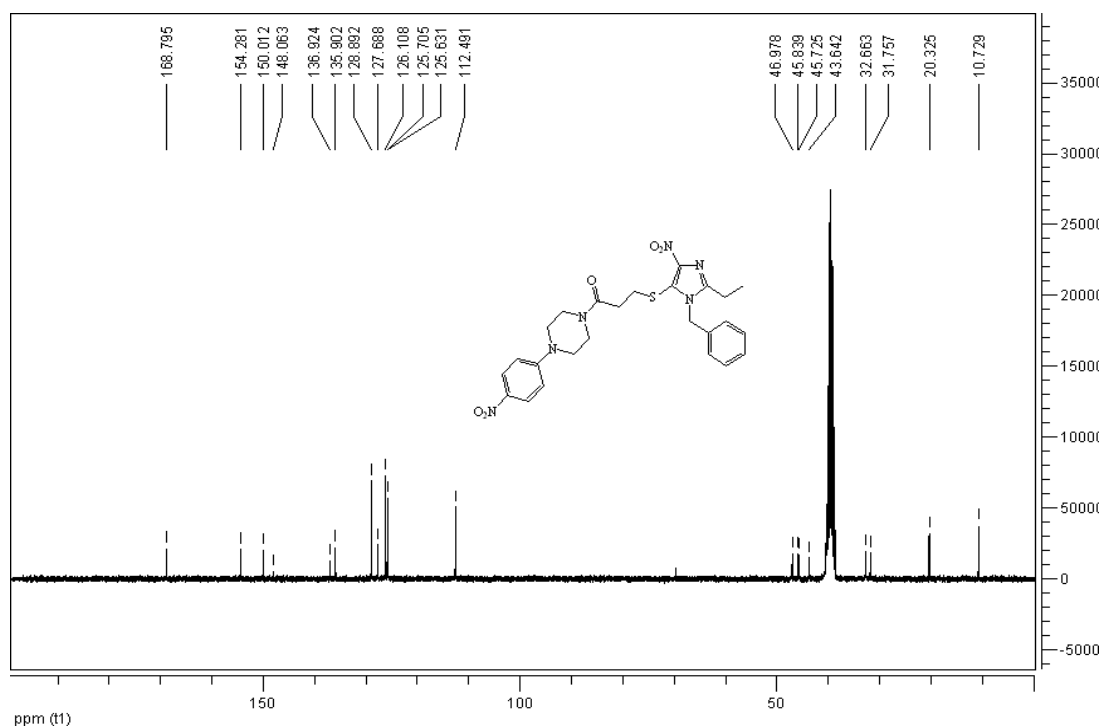


Figure 42. DEPT-135° spectrum for compound **(5o)** in DMSO-*d*₆.

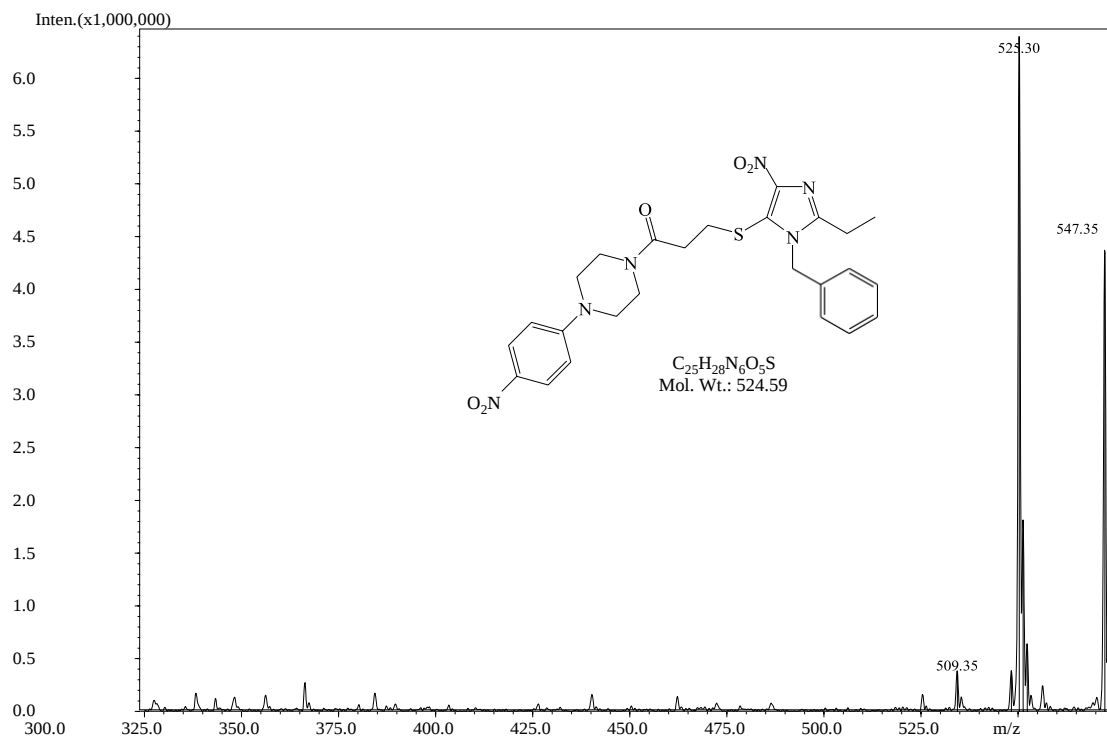


Figure 43. Mass spectrum for compound (5o), $[M+H]^+$.

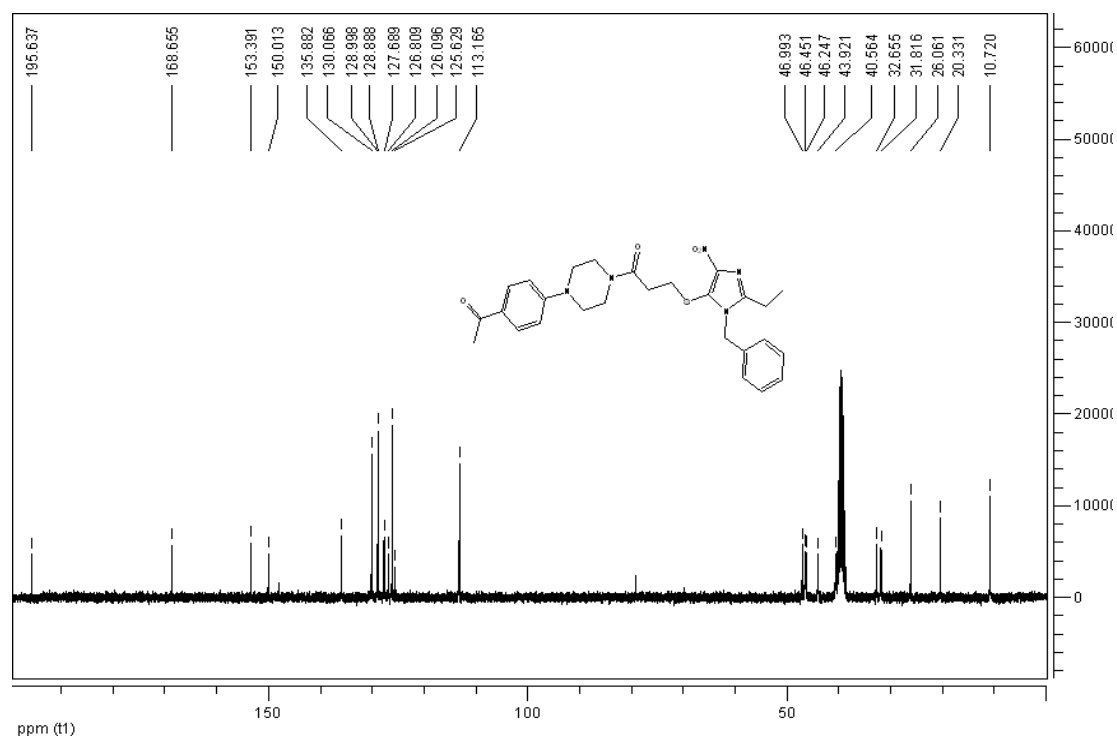


Figure 44. ^{13}C -NMR spectrum for compound (5p) in $DMSO-d_6$.

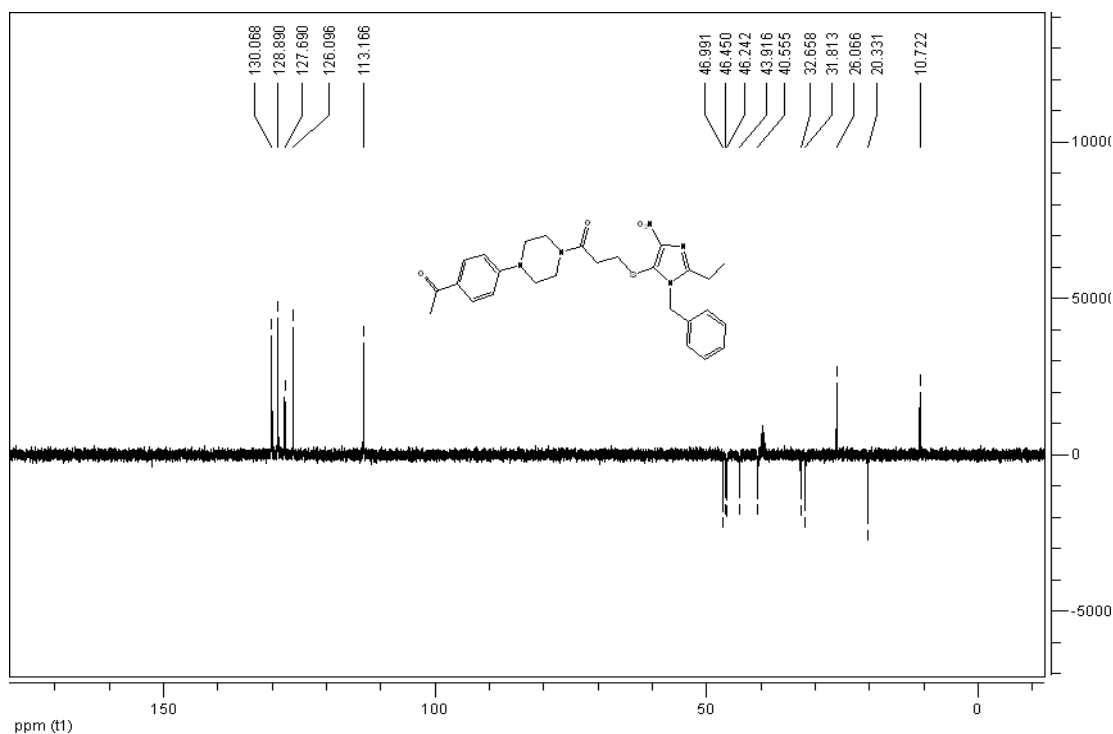


Figure 45. DEPT-135° spectrum for compound (5p) in DMSO-*d*₆.

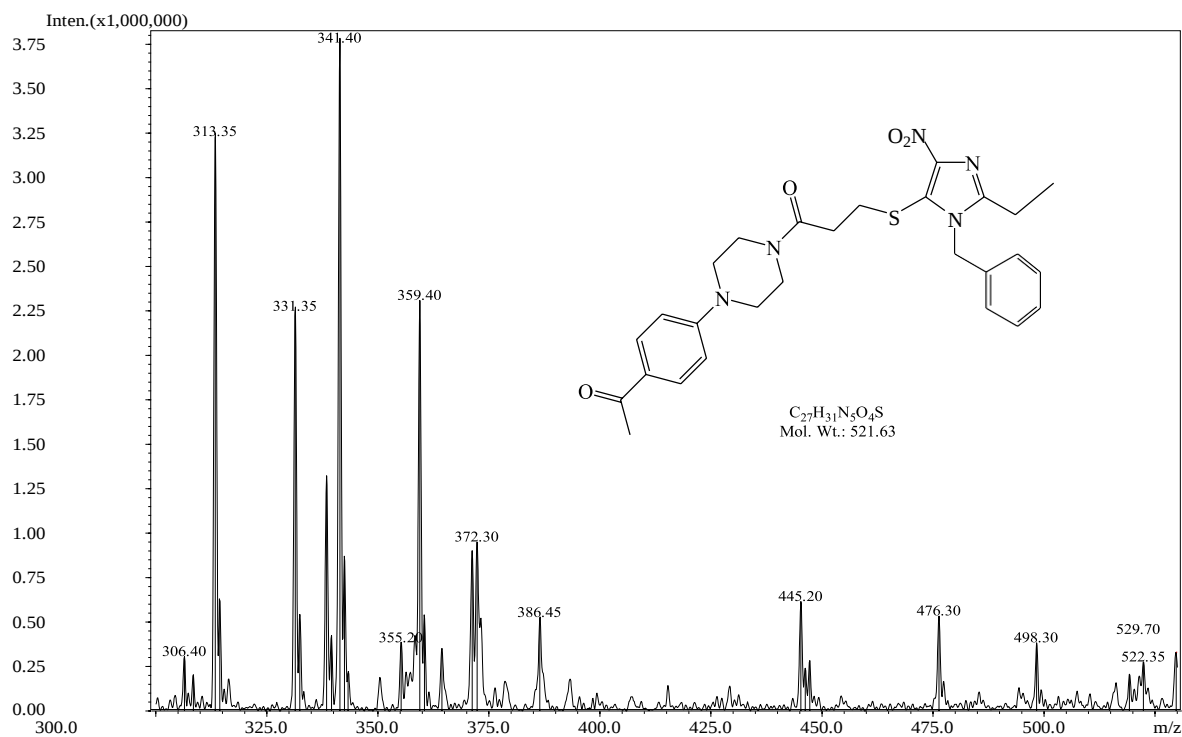


Figure 46. Mass spectrum for compound (5p), [M+H]⁺.

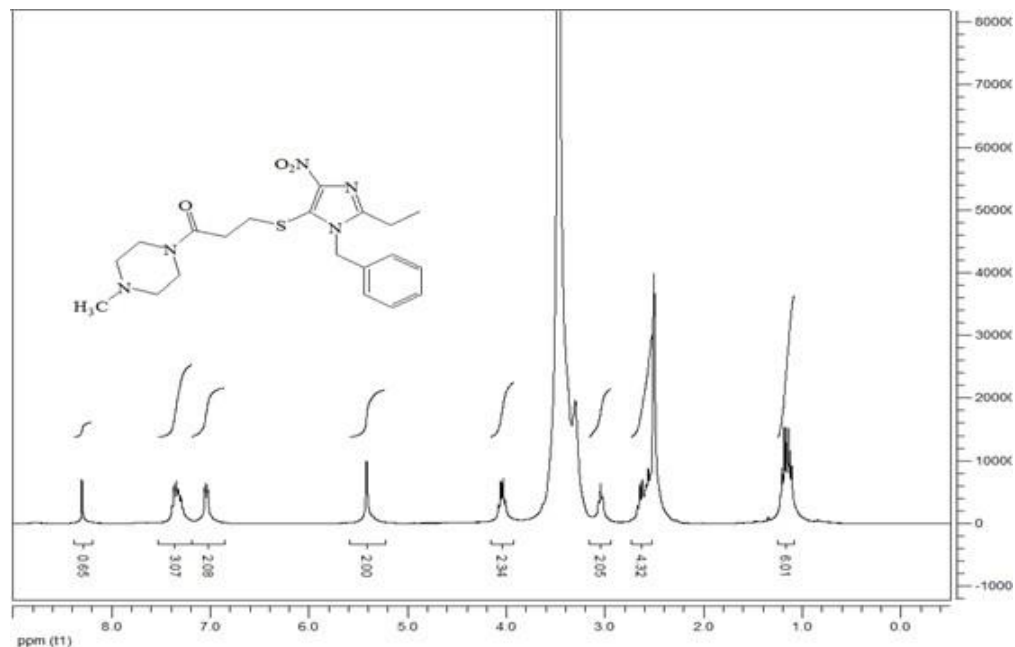


Figure 47. ¹H-NMR spectrum for compound (**5q**) in DMSO-*d*₆.

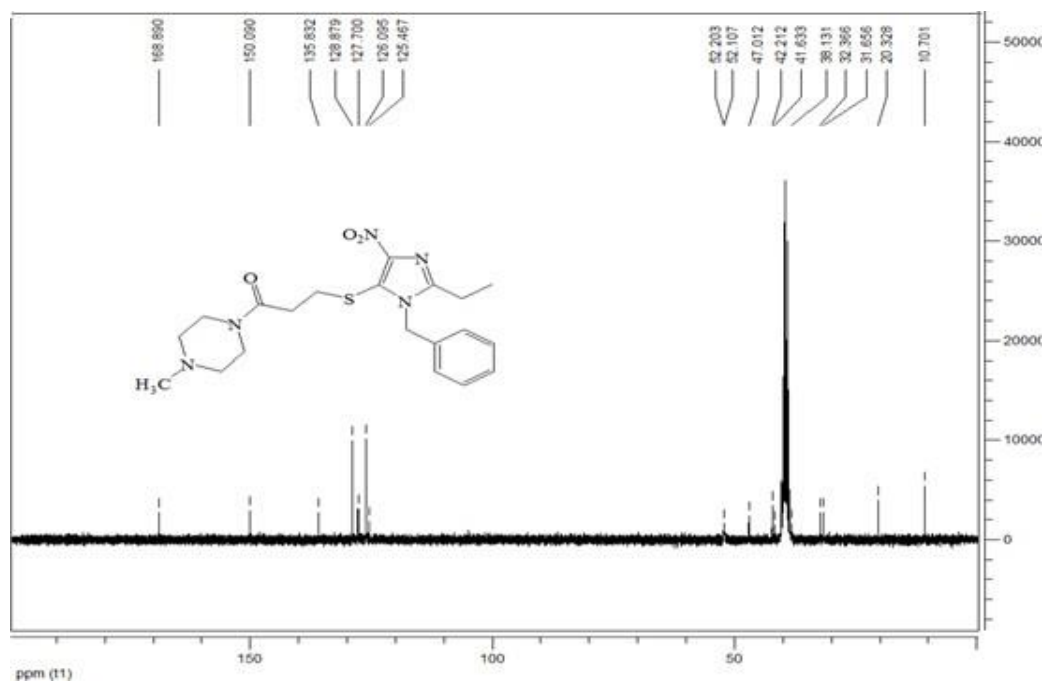


Figure 48. ¹³C-NMR spectrum for compound (**5q**) in DMSO-*d*₆.

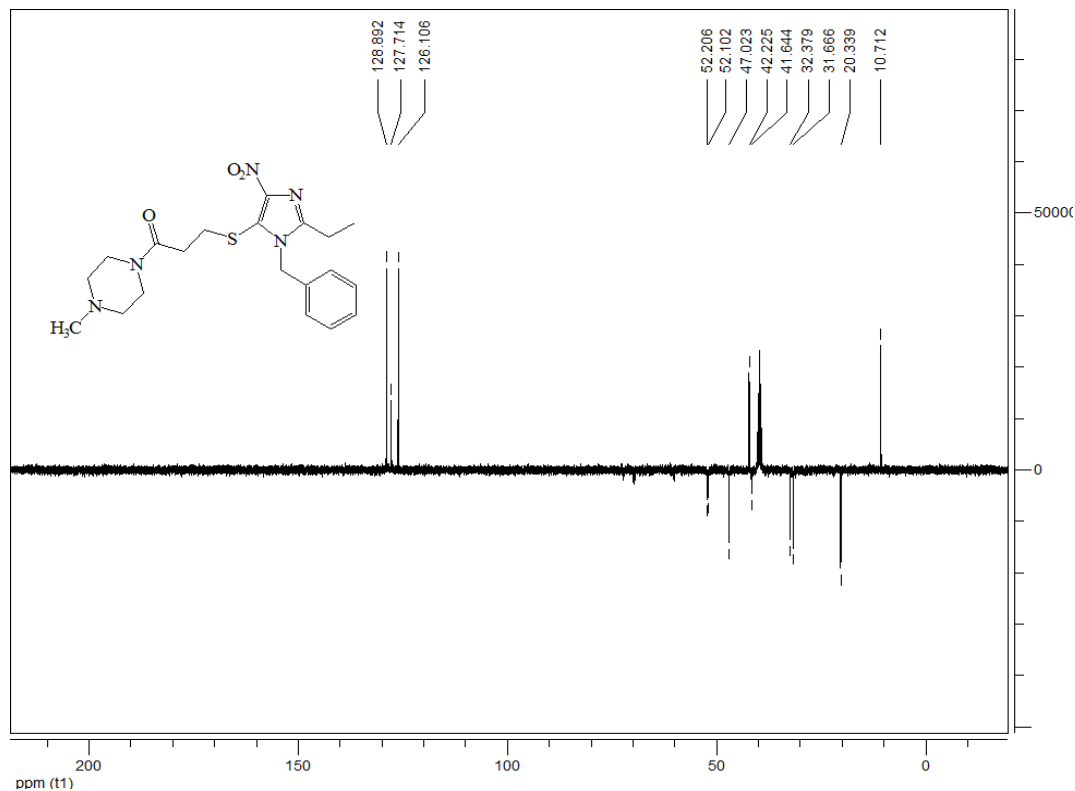


Figure 49. DEPT-135 spectrum for compound (**5q**) in DMSO-*d*₆.

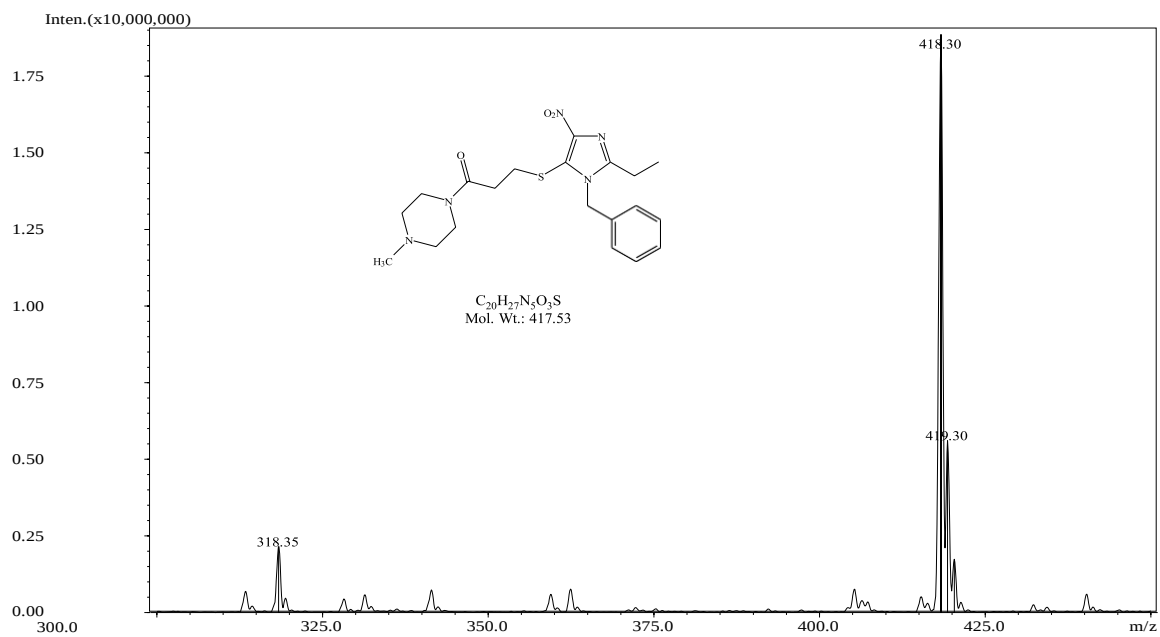


Figure 50. Mass spectrum for compound (**5q**), [M+H]⁺.

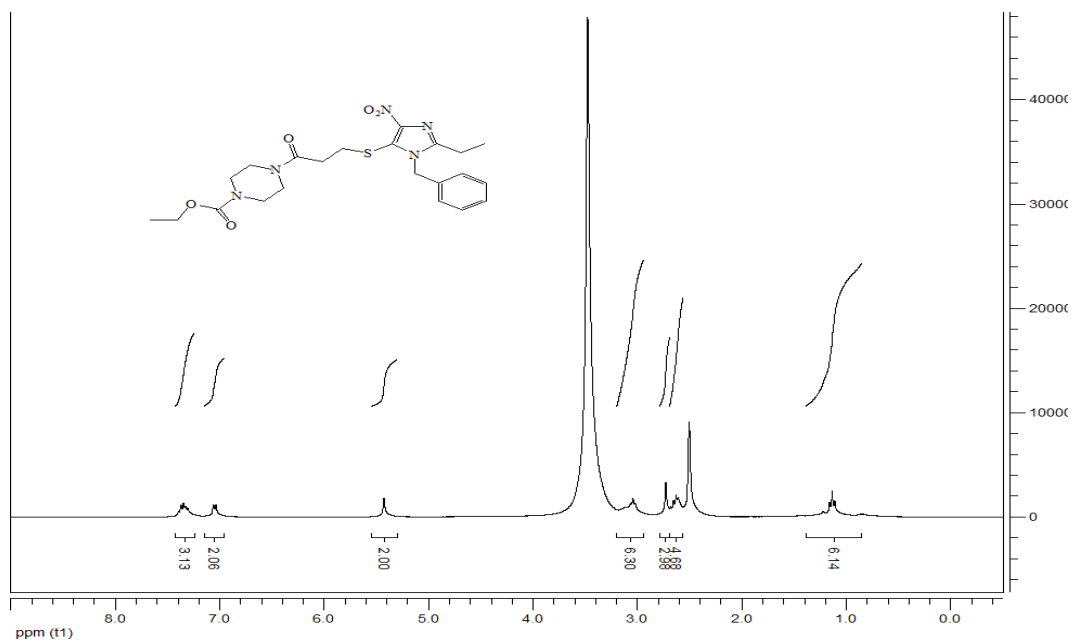


Figure 51. ¹H-NMR spectrum for compound (**5r**) in DMSO-*d*₆.

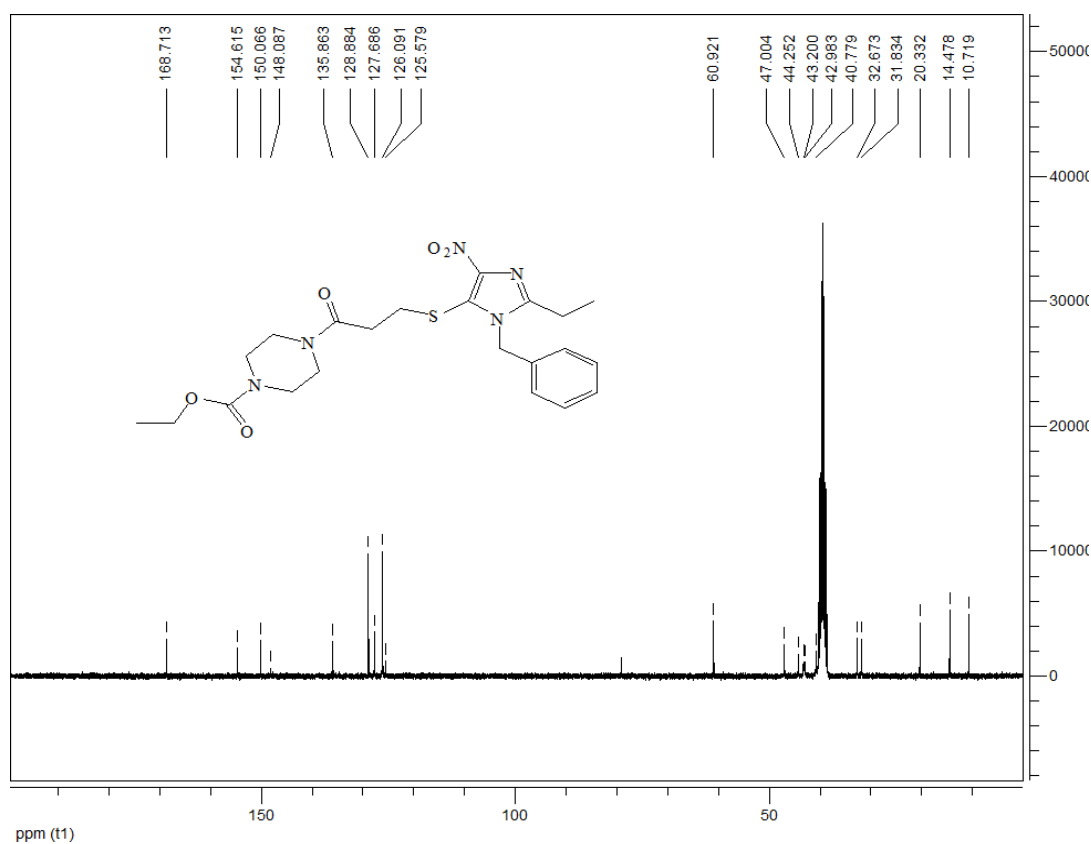


Figure 52. ¹³C-NMR spectrum for compound (**5r**) in DMSO-*d*₆.

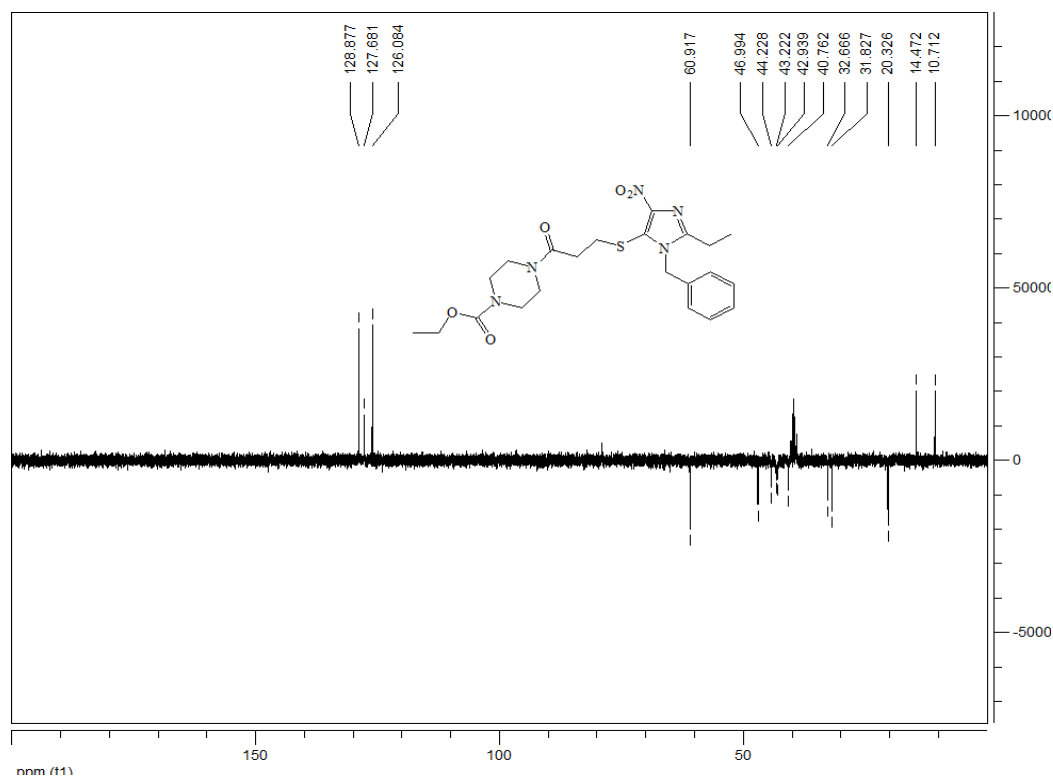


Figure 53. DEPT-135 spectrum for compound (**5r**) in DMSO- d_6 .

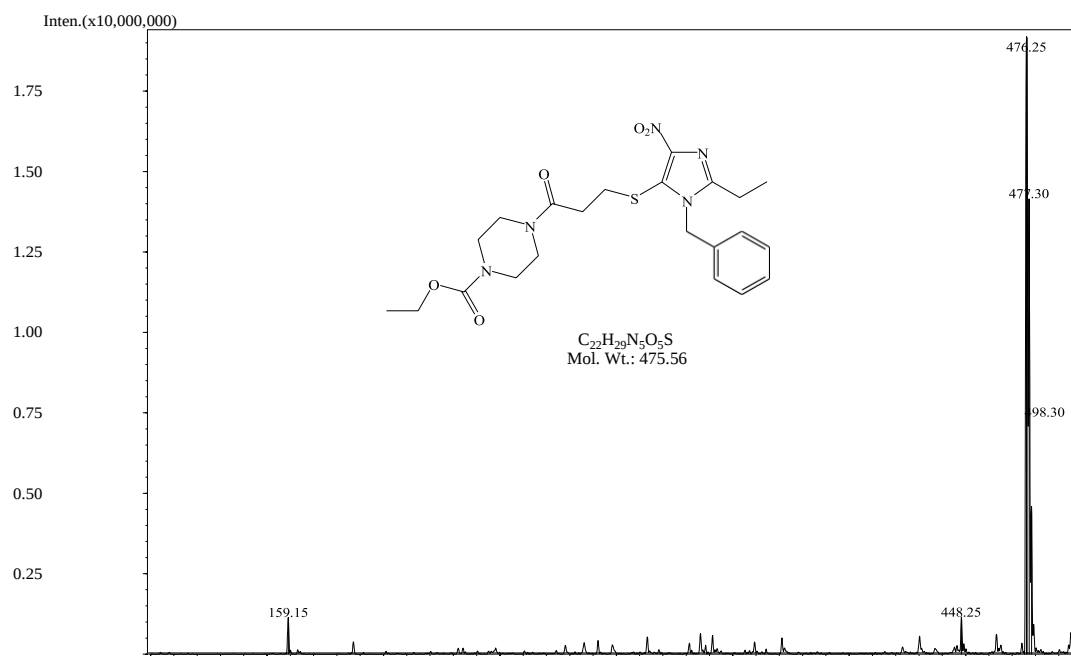


Figure 54. Mass spectrum of (**5r**), $[M+H]^+$