

Supporting Information

Reaction of diphenacylaniline and diphenacyl sulfide under Gewald condition: Generation of enamine / thioamide

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Experimental

General

Melting points were measured in open capillary tubes and are uncorrected. The ^1H , ^{13}C and 2D NMR were recorded on a Bruker (Avance) 300 MHz NMR instrument using TMS as internal standard and CDCl_3 as solvent. Standard Bruker software was used throughout. Chemical shifts are given in parts per million (δ -scale) and the coupling constants are given in Hertz. Silica gel-G plates (Merck) were used for TLC analysis with a mixture of petroleum ether (60–80 °C) and ethylacetate as eluant. Electrospray ionisation mass spectrometry (ESI-MS) analysis was performed in the positive ion mode on a liquid chromatography-ion trap mass spectrometer (LCQ Fleet, Thermo Fisher Instruments Limited, US). Elemental analyses were performed on a Perkin Elmer 2400 Series II Elemental CHNS analyzer.

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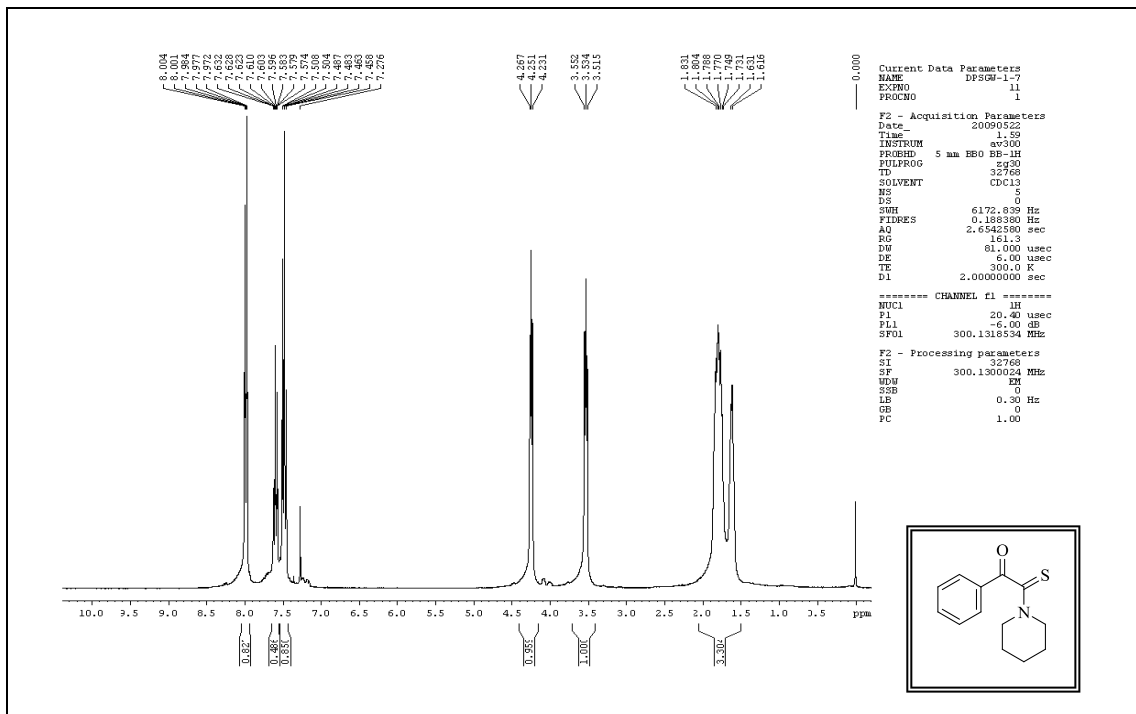


Figure 1. ¹H NMR Spectrum of **8a** (CDCl₃)

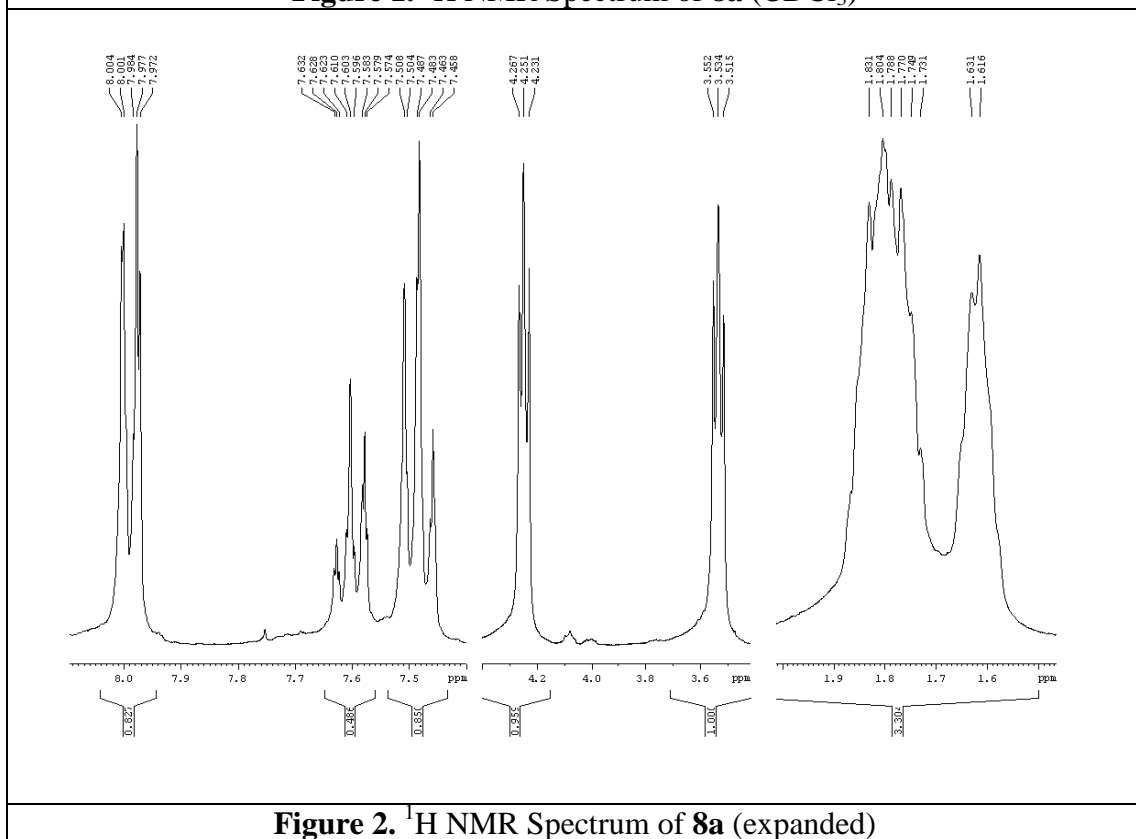


Figure 2. ¹H NMR Spectrum of **8a** (expanded)

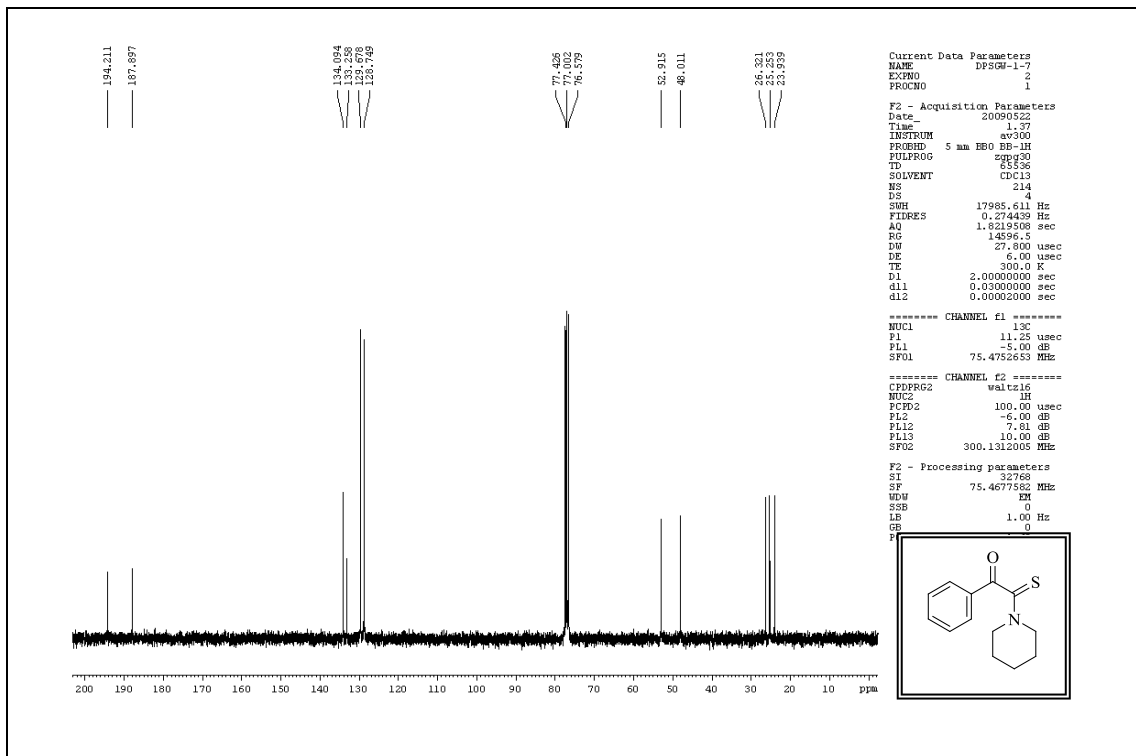


Figure 3. ¹³C NMR Spectrum of 8a (CDCl₃)

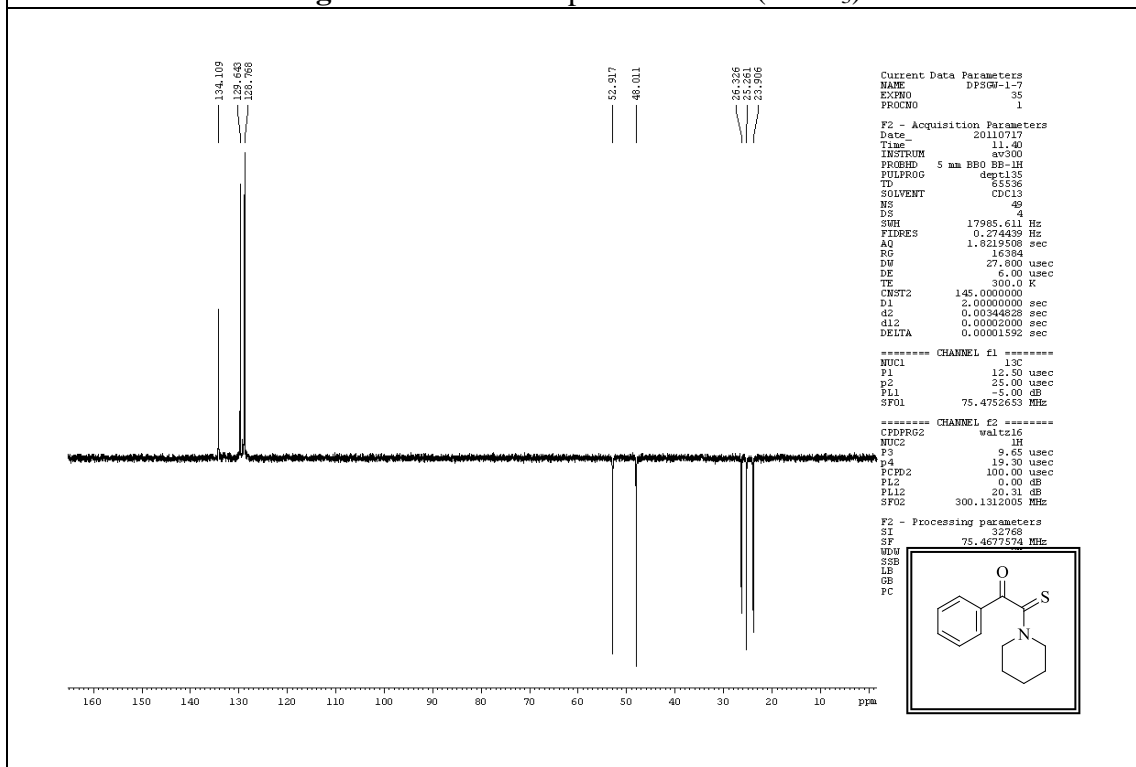


Figure 4. DEPT-135 Spectrum of 8a (CDCl₃)

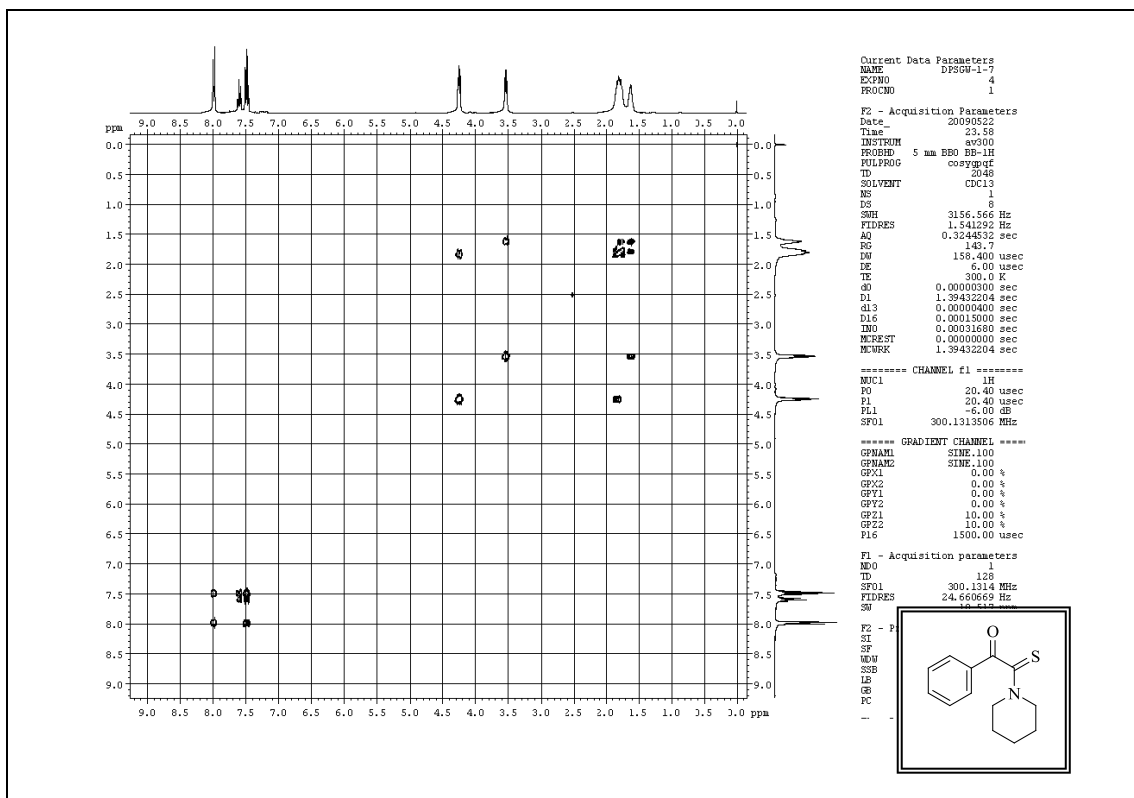


Figure 5. H,H-COSY Spectrum of 8a

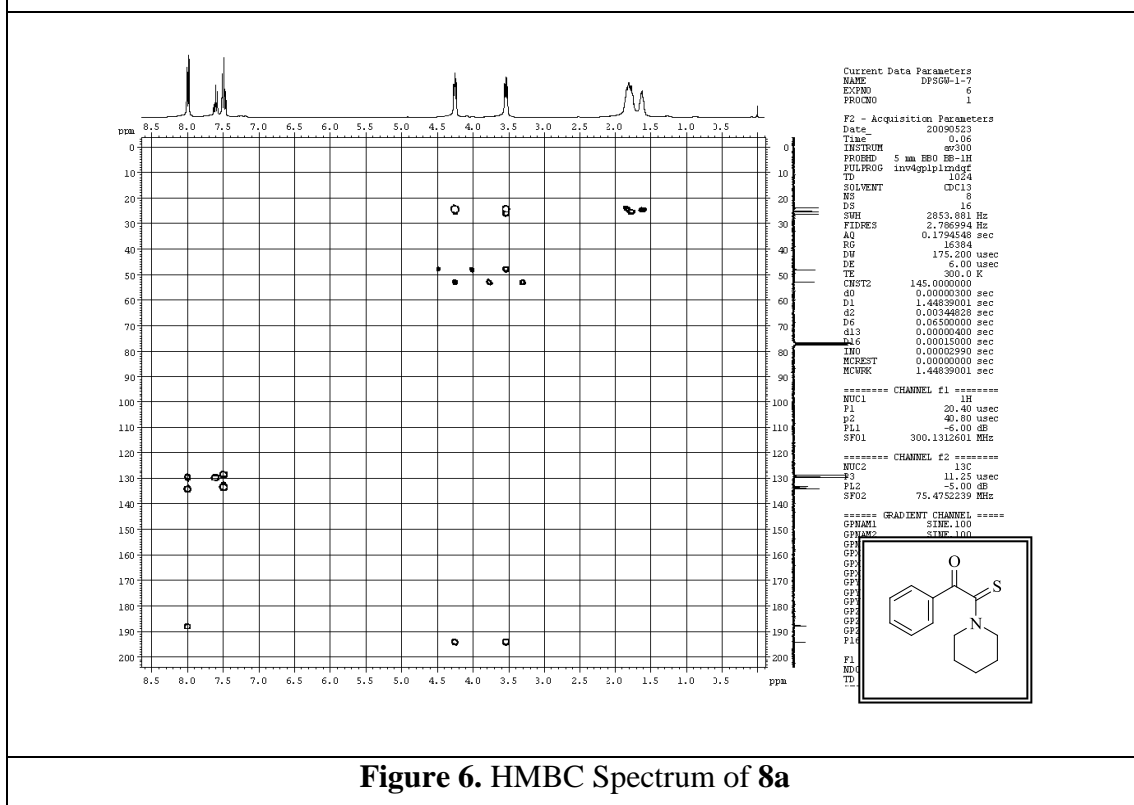


Figure 6. HMBC Spectrum of 8a

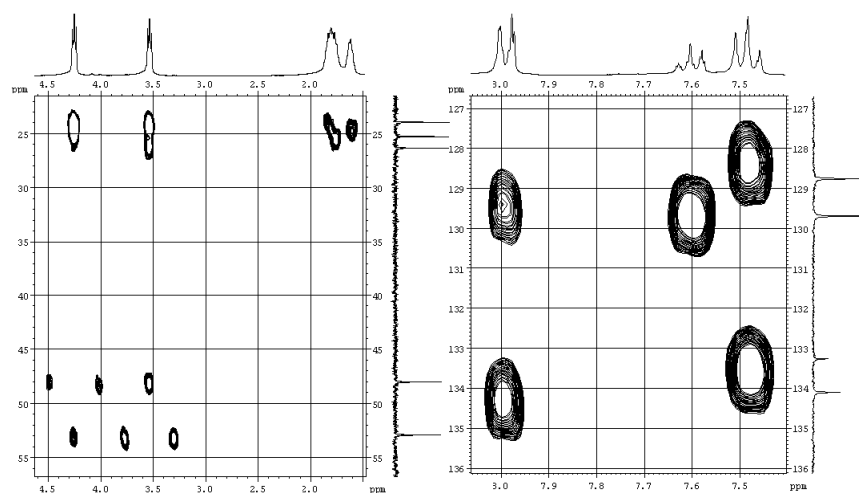


Figure 7. HMBC Spectrum of **8a** (expanded)

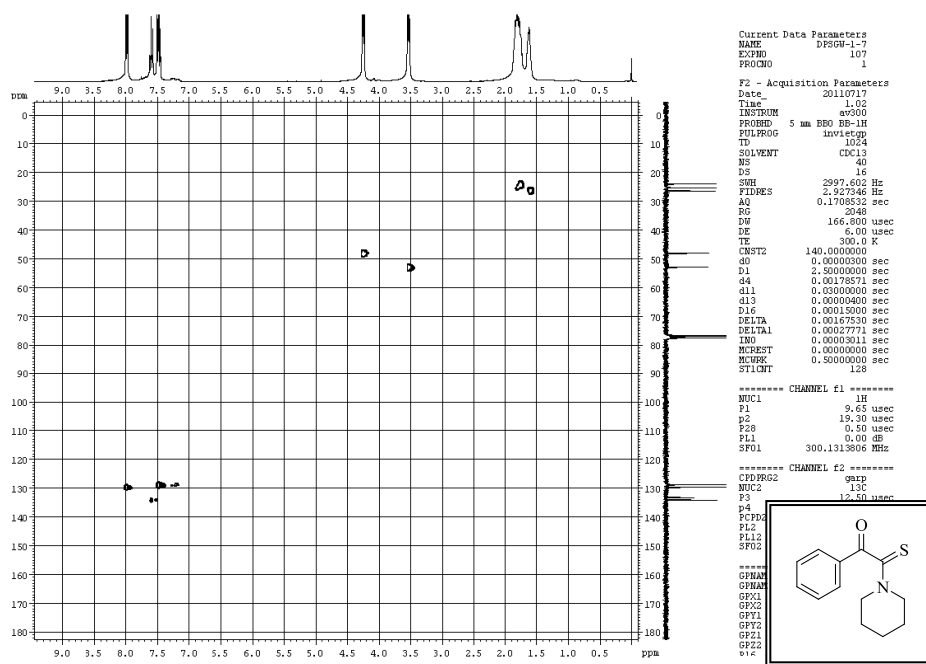


Figure 8. C,H-COSY Spectrum of **8a**

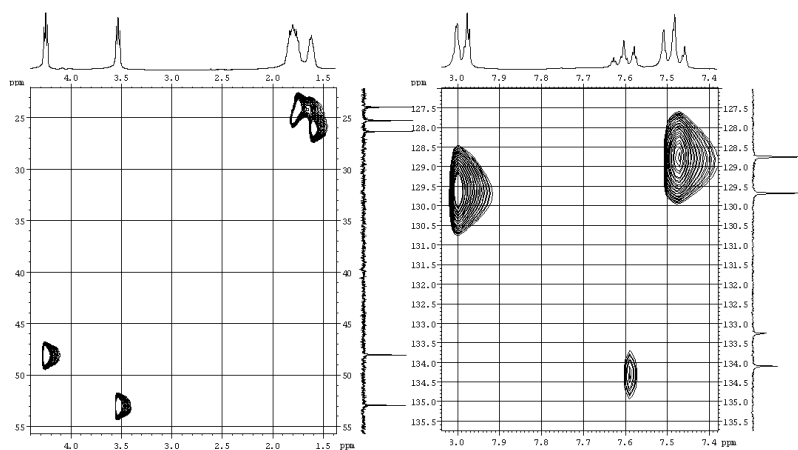


Figure 9. C,H-COSY Spectrum of **8a** (expanded)

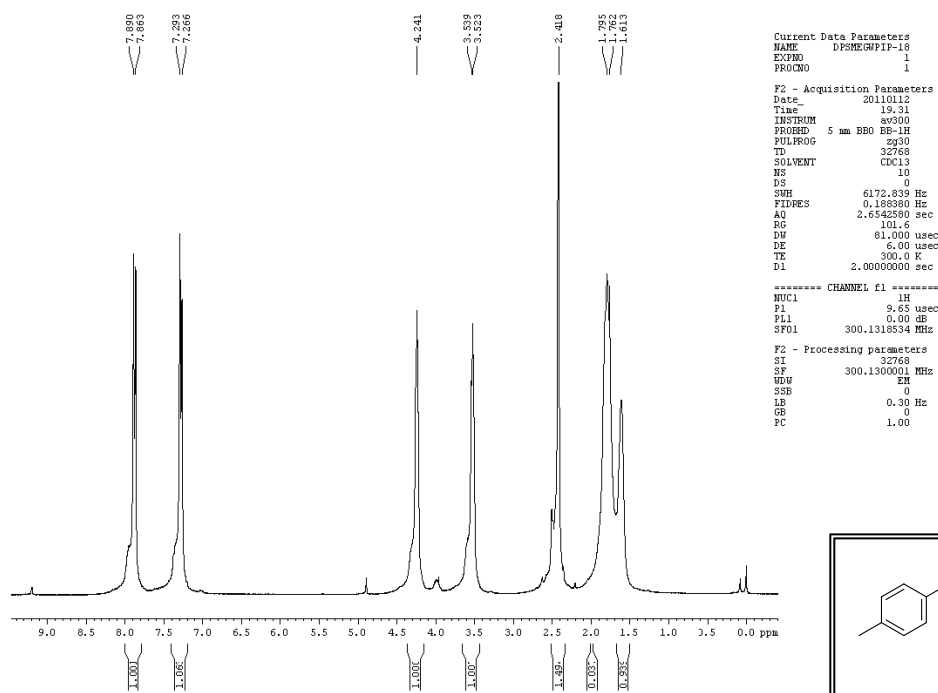


Figure 10. ^1H NMR Spectrum of **8b** (CDCl_3)

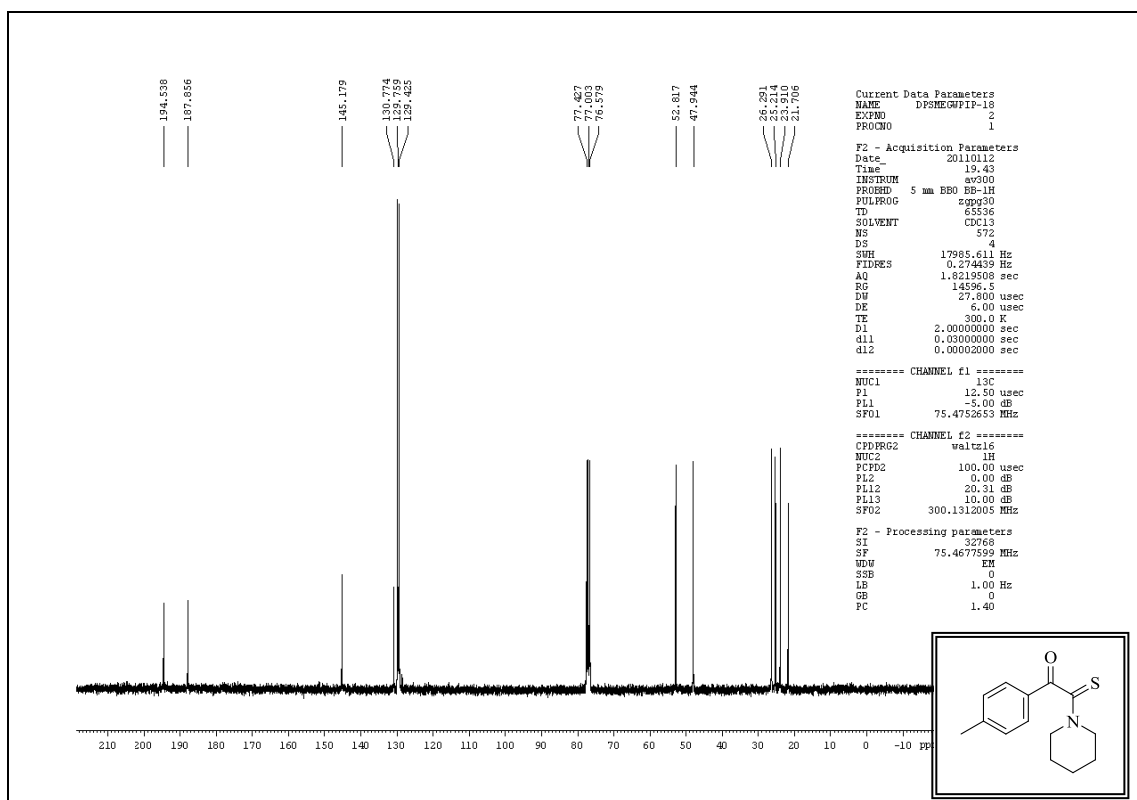


Figure 11. ^{13}C NMR Spectrum of **8b** (CDCl_3)

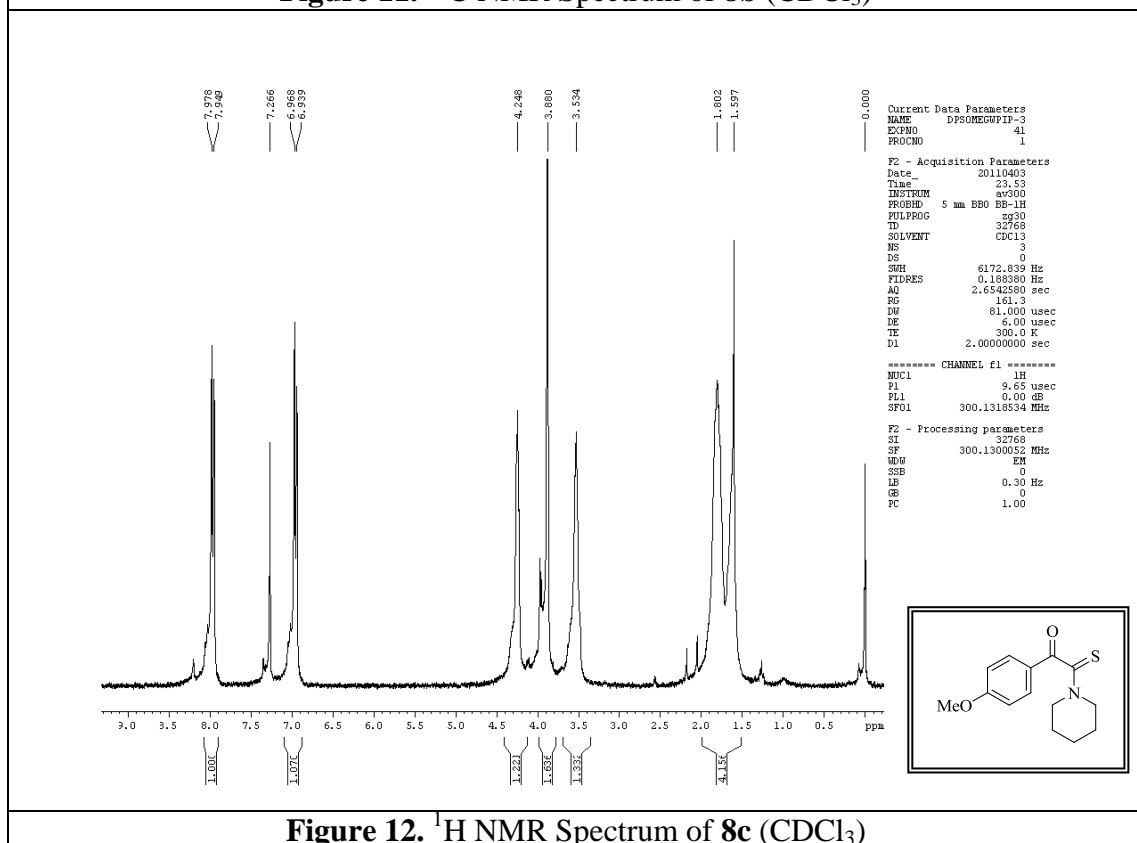


Figure 12. ^1H NMR Spectrum of **8c** (CDCl_3)

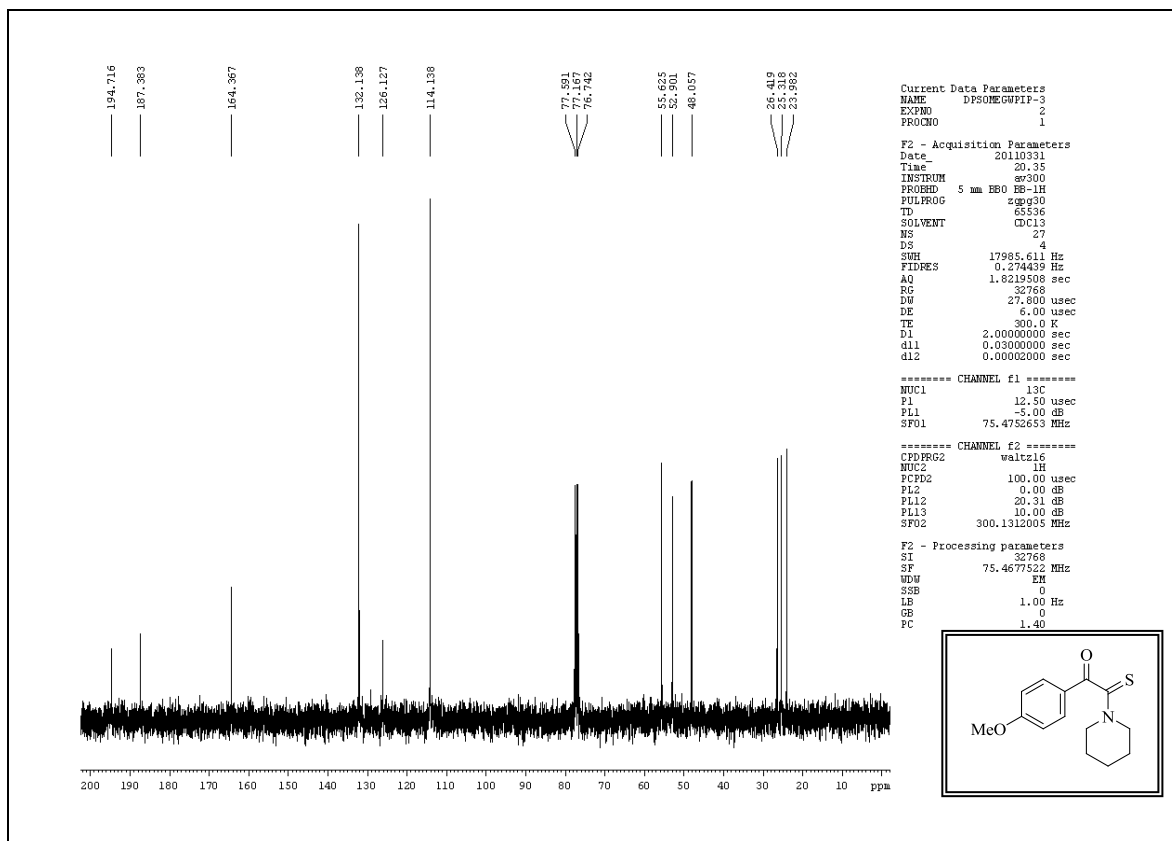


Figure 13. ^{13}C NMR Spectrum of **8c** (expanded)

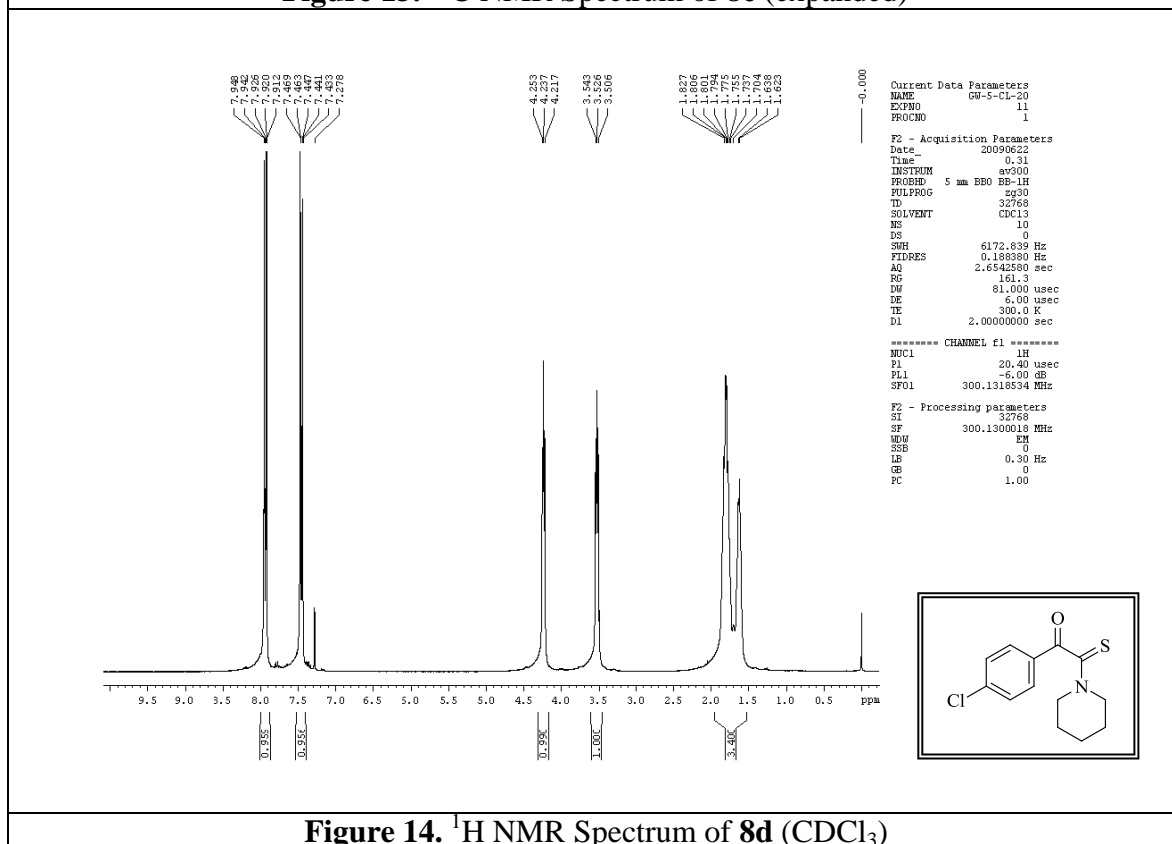


Figure 14. ^1H NMR Spectrum of **8d** (CDCl_3)

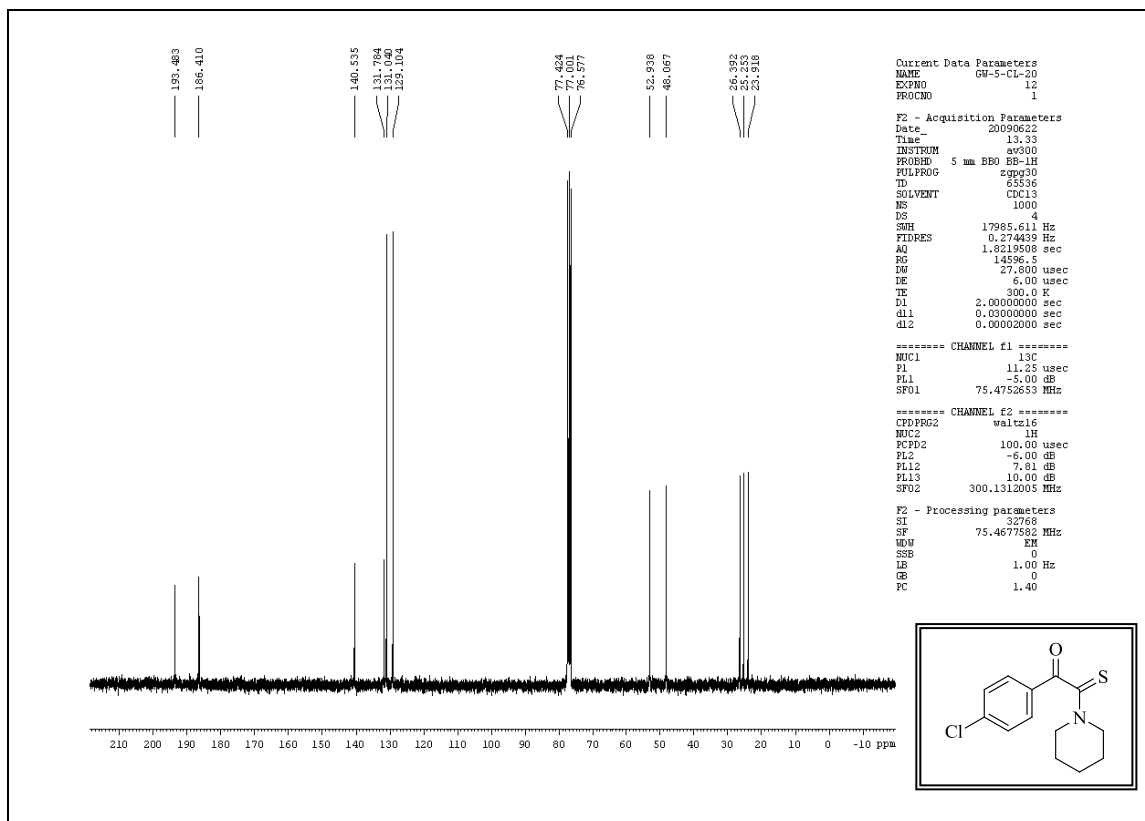


Figure 15. ^{13}C NMR Spectrum of **8d** (expanded)

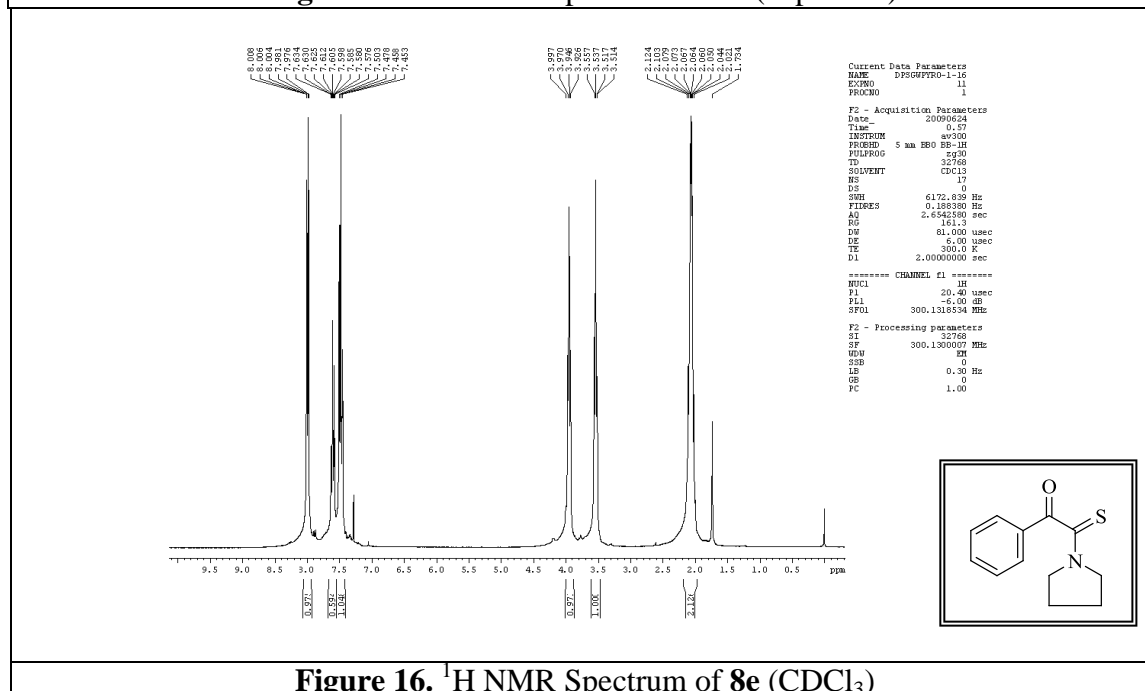


Figure 16. ^1H NMR Spectrum of **8e** (CDCl_3)

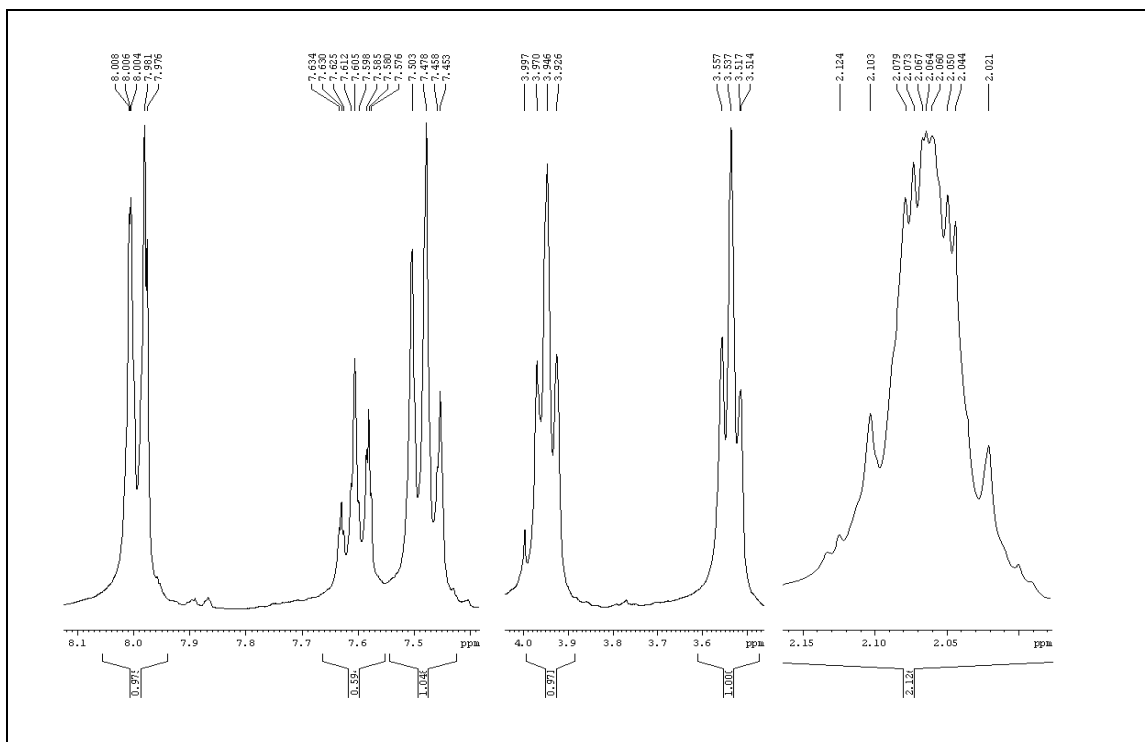


Figure 17. ^1H NMR Spectrum of **8e** (expanded)

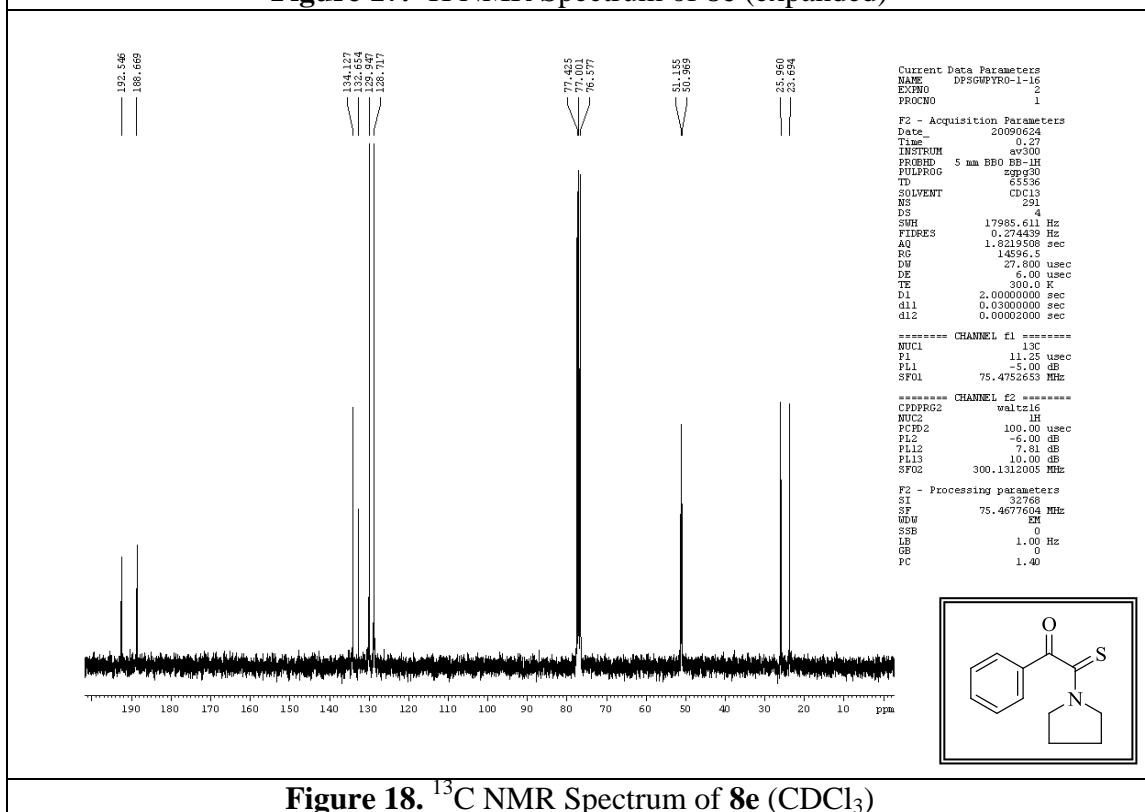


Figure 18. ^{13}C NMR Spectrum of **8e** (CDCl_3)

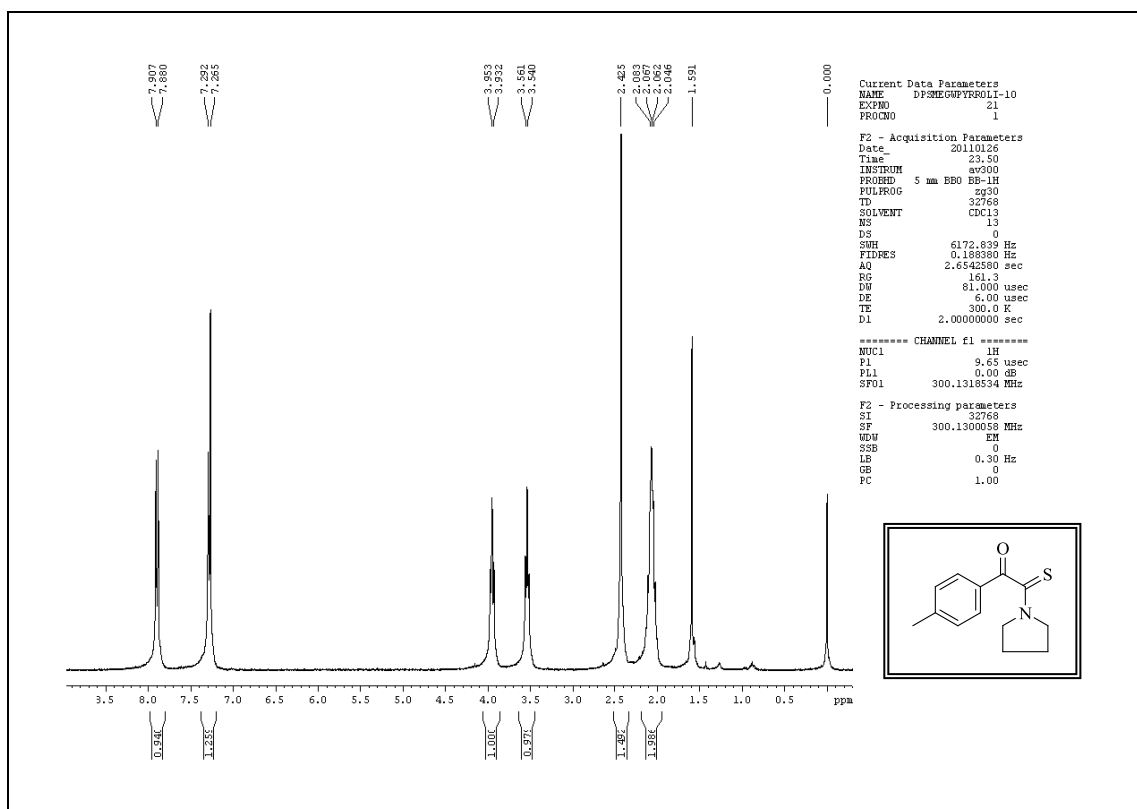


Figure 19. ¹H NMR Spectrum of **8f** (CDCl₃)

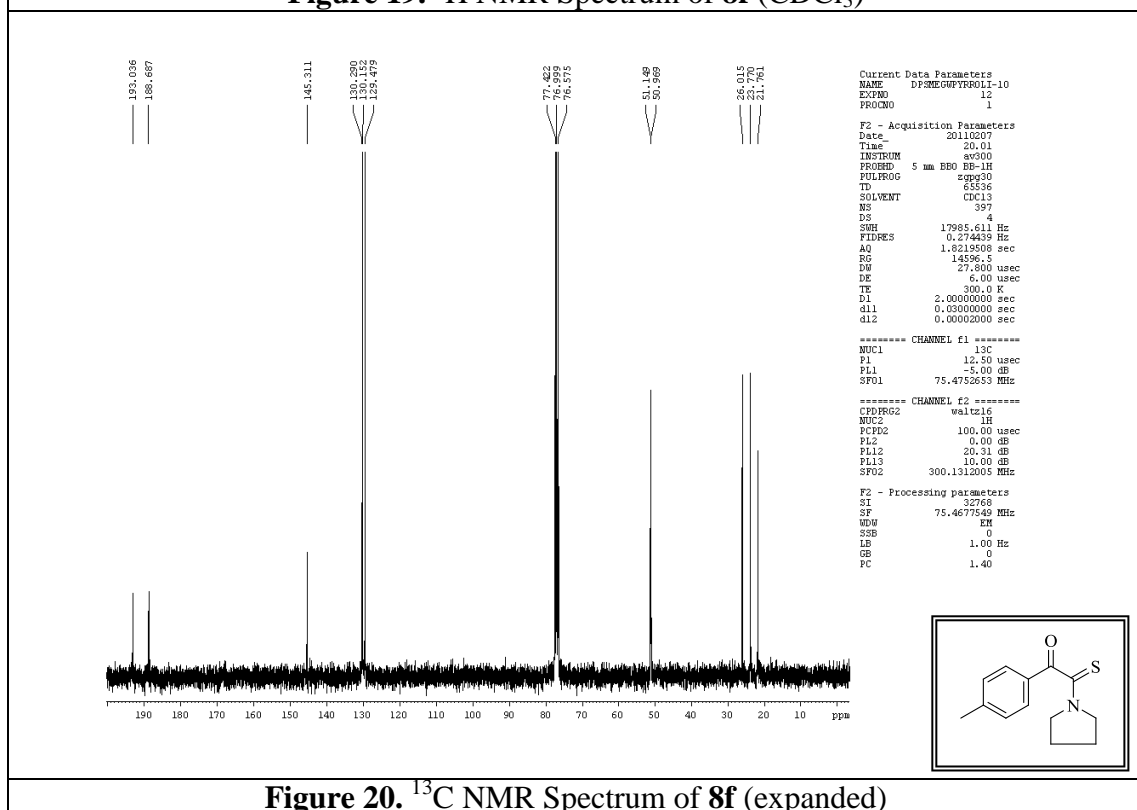


Figure 20. ¹³C NMR Spectrum of **8f** (expanded)

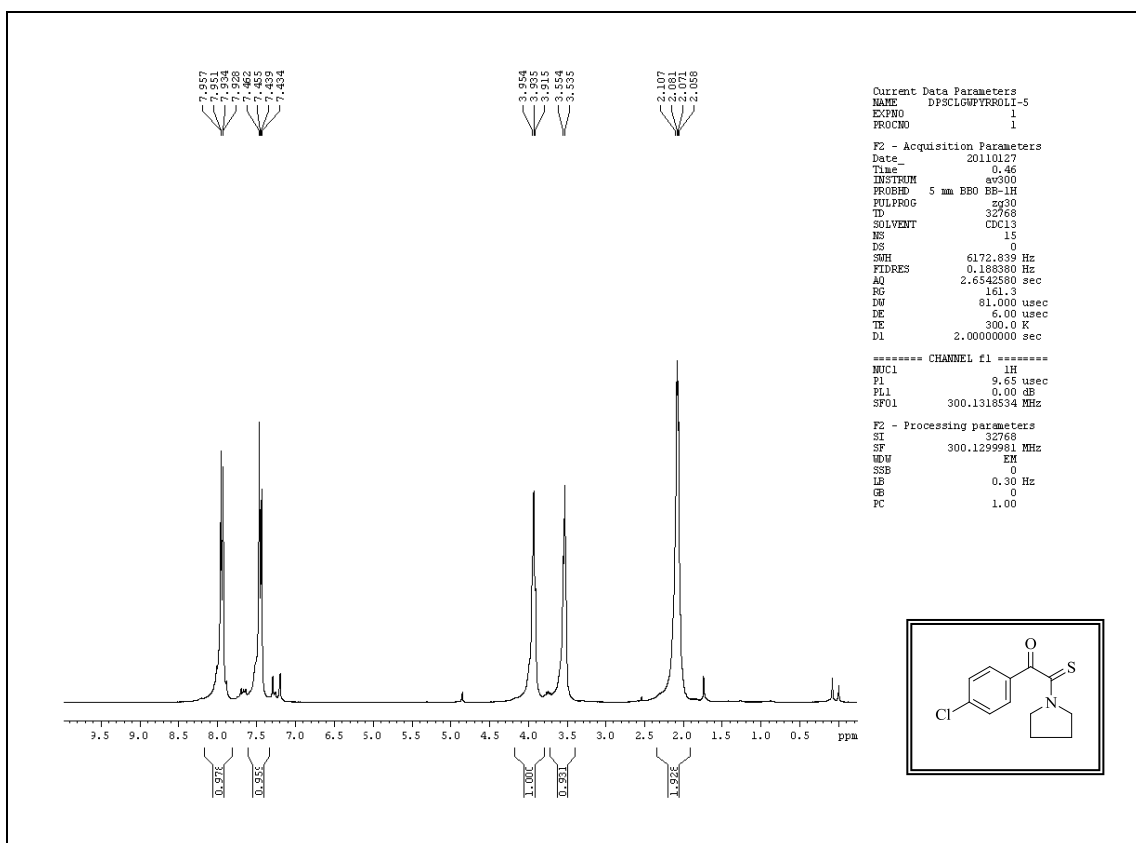


Figure 21. ¹H NMR Spectrum of **8g** (CDCl₃)

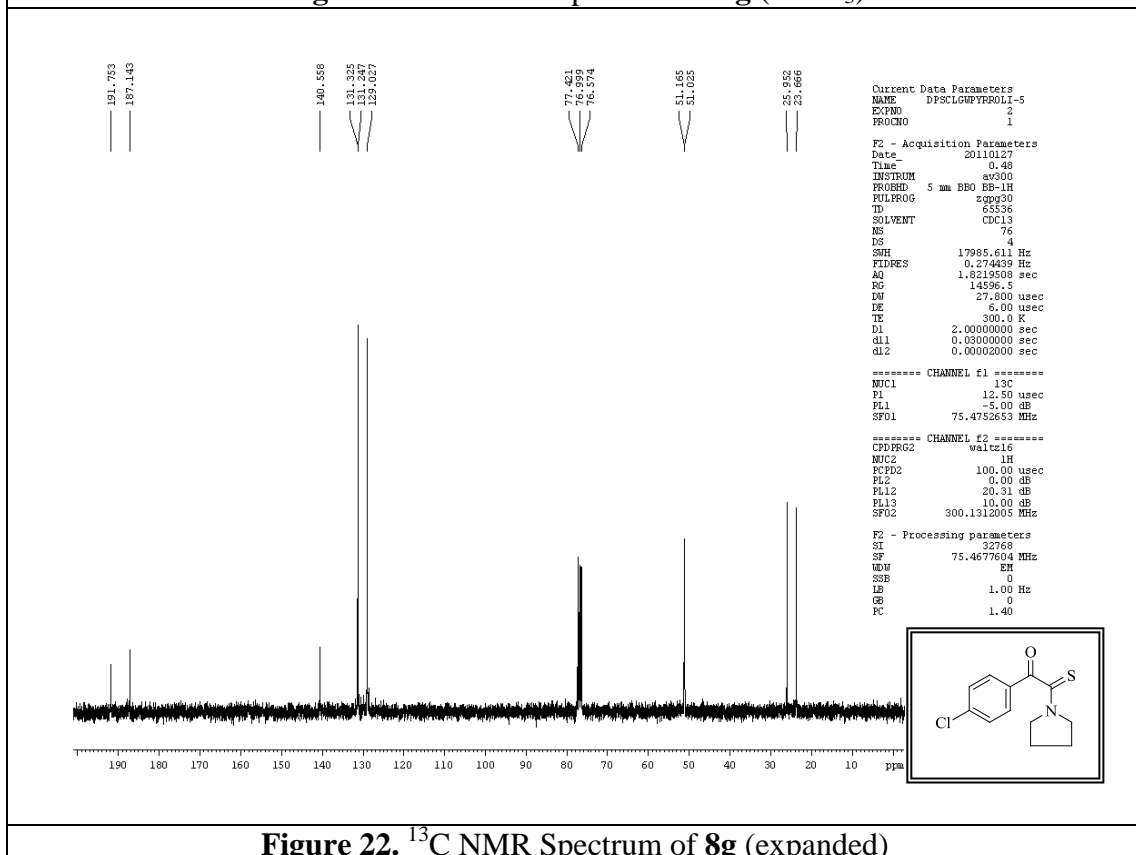


Figure 22. ¹³C NMR Spectrum of **8g** (expanded)

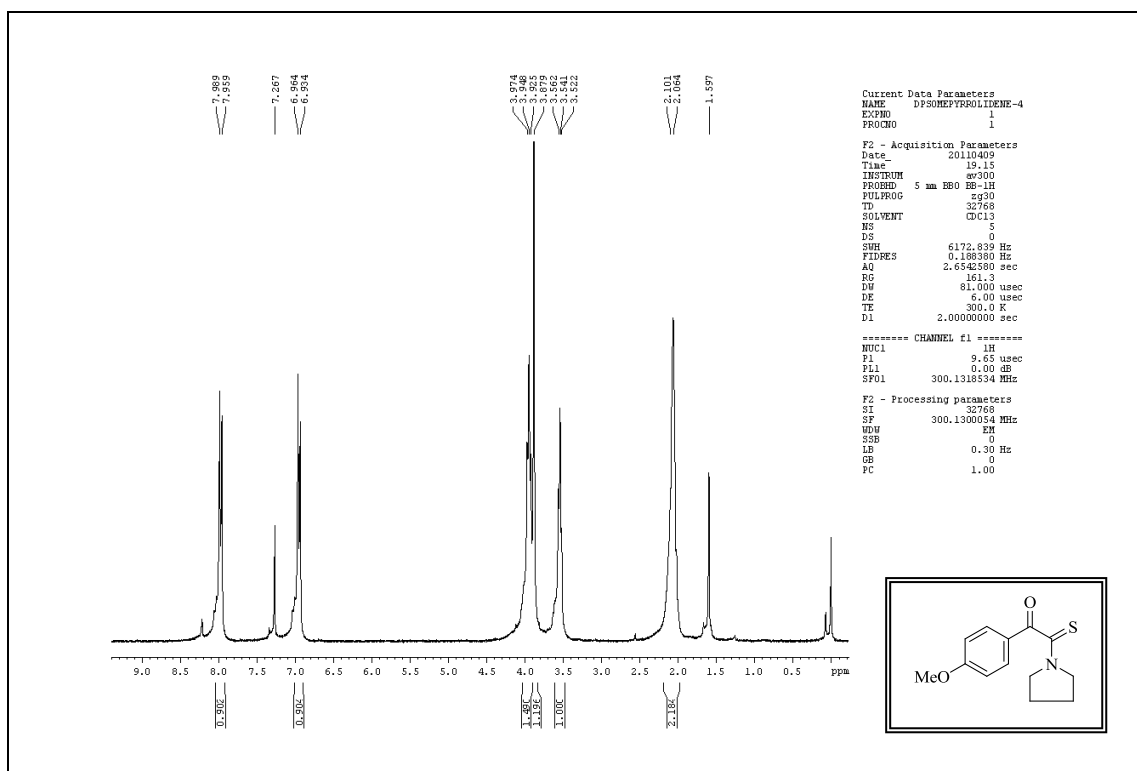


Figure 23. ^1H NMR Spectrum of **8h** (CDCl_3)

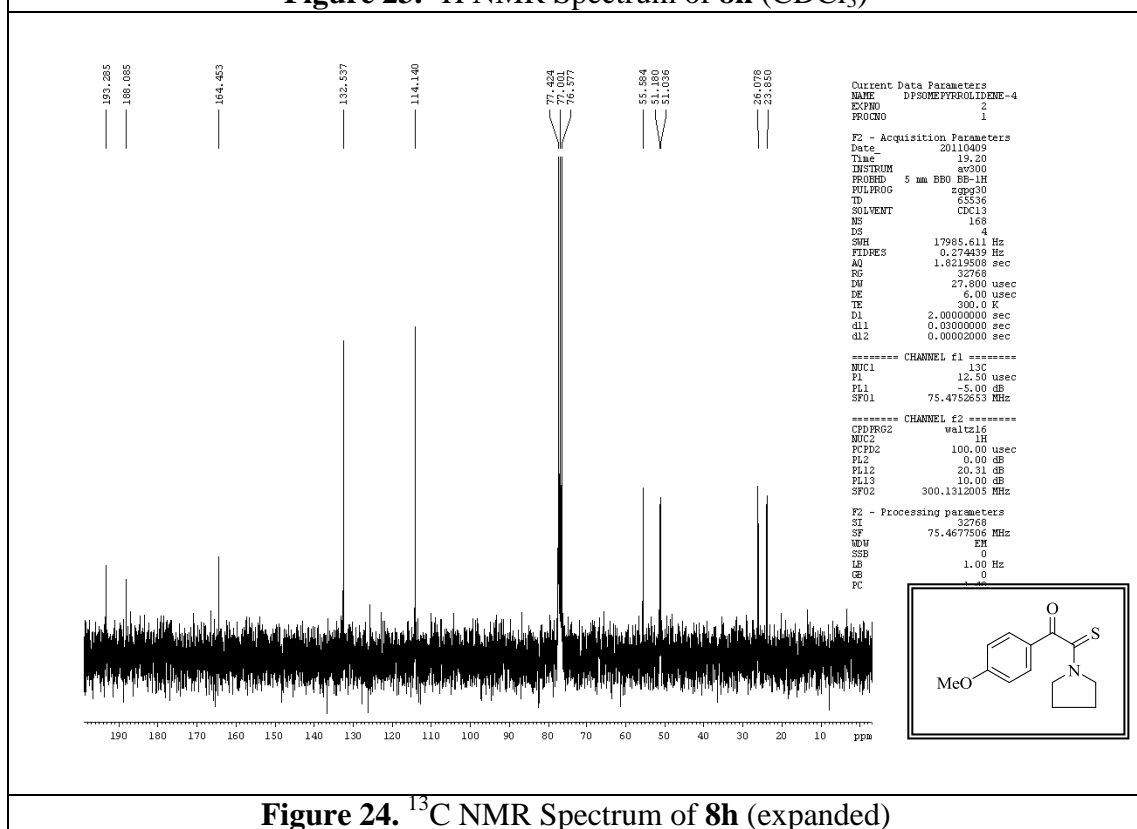


Figure 24. ^{13}C NMR Spectrum of **8h** (expanded)

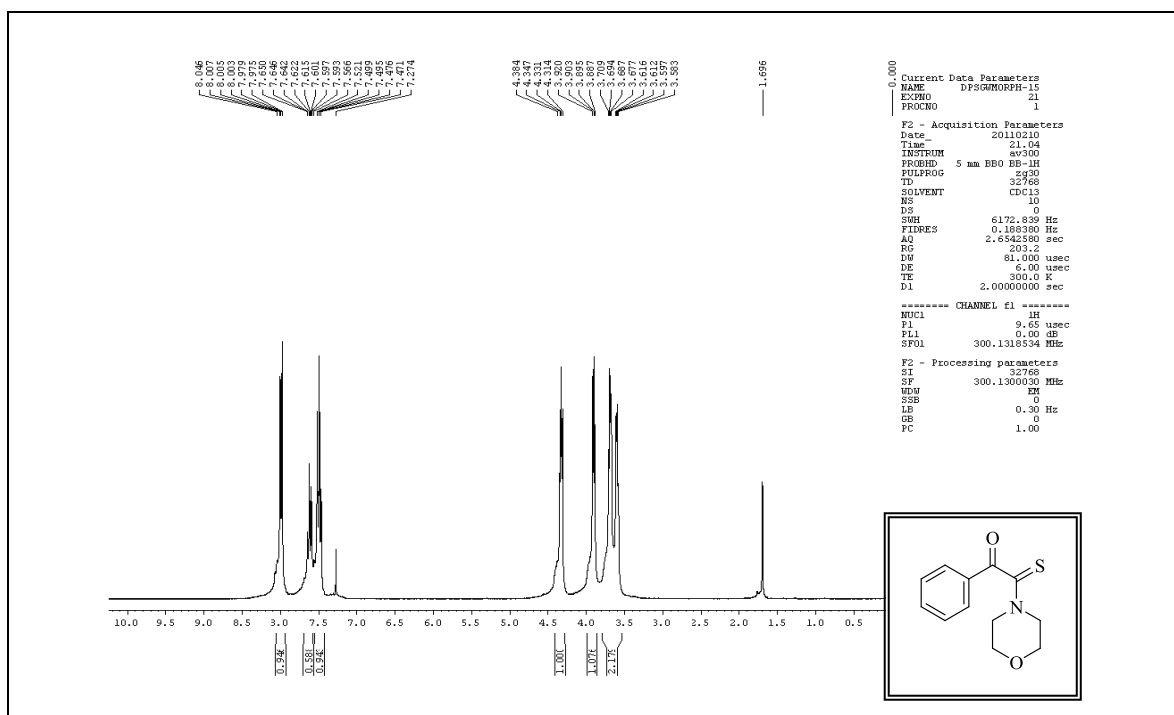


Figure 25. ^1H NMR Spectrum of **8i** (CDCl_3)

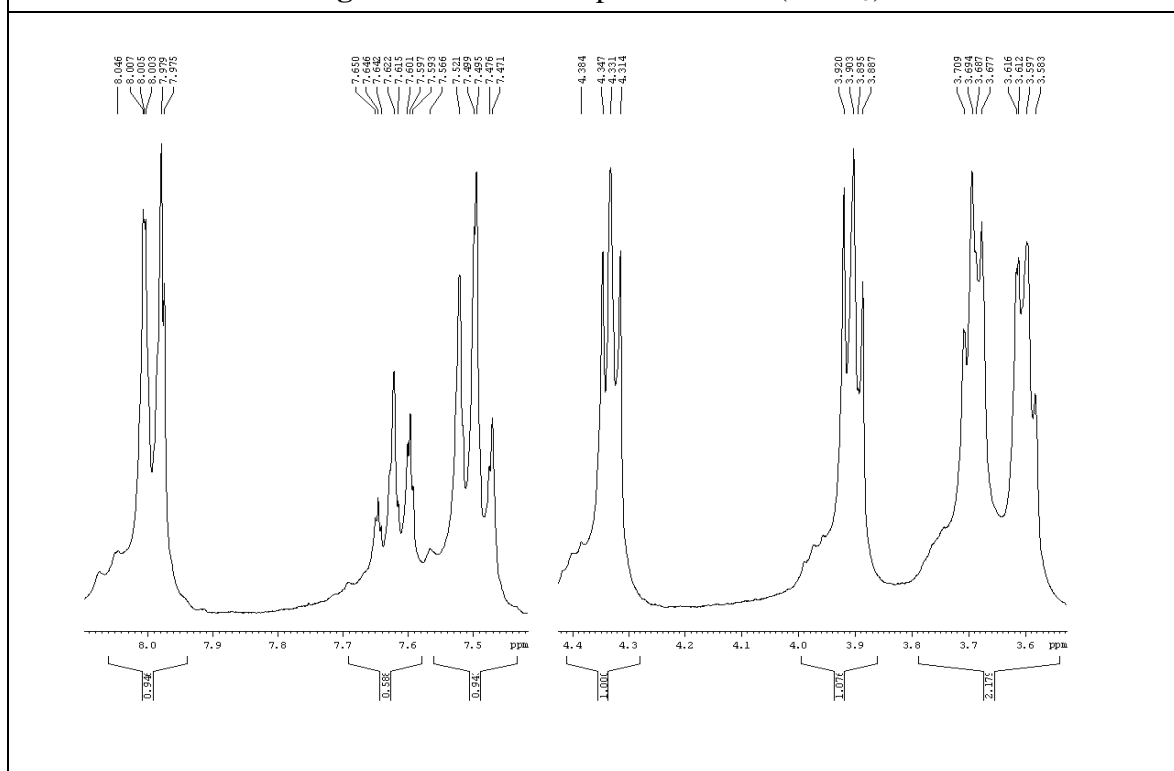


Figure 26. ^1H NMR Spectrum of **8i** (expanded)

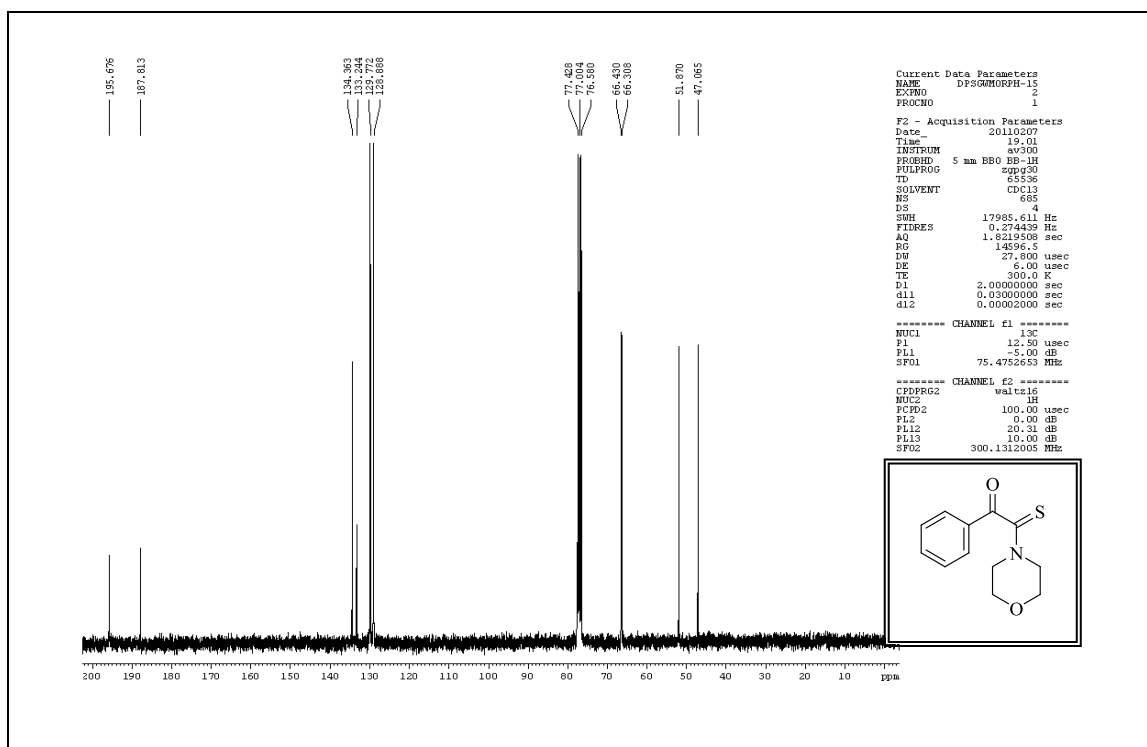


Figure 27. ^{13}C NMR Spectrum of **8i** (CDCl_3)

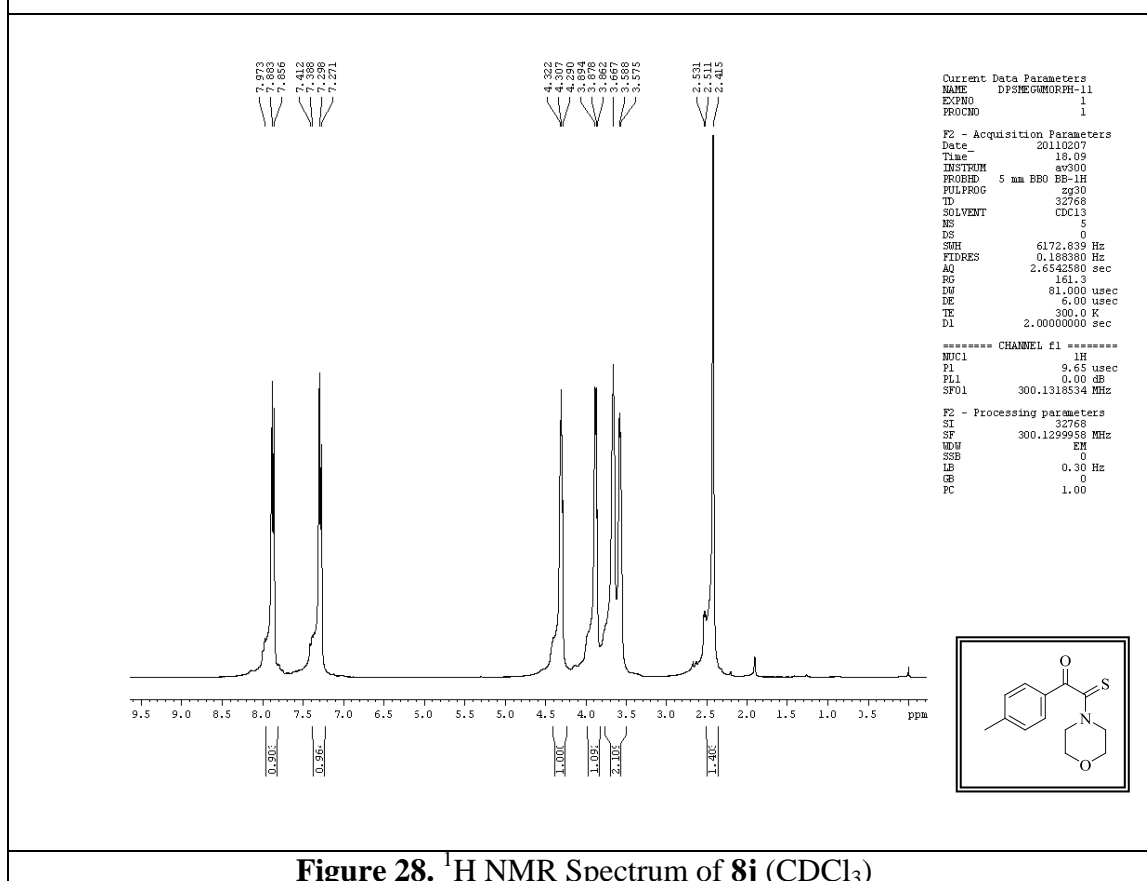


Figure 28. ^1H NMR Spectrum of **8j** (CDCl_3)

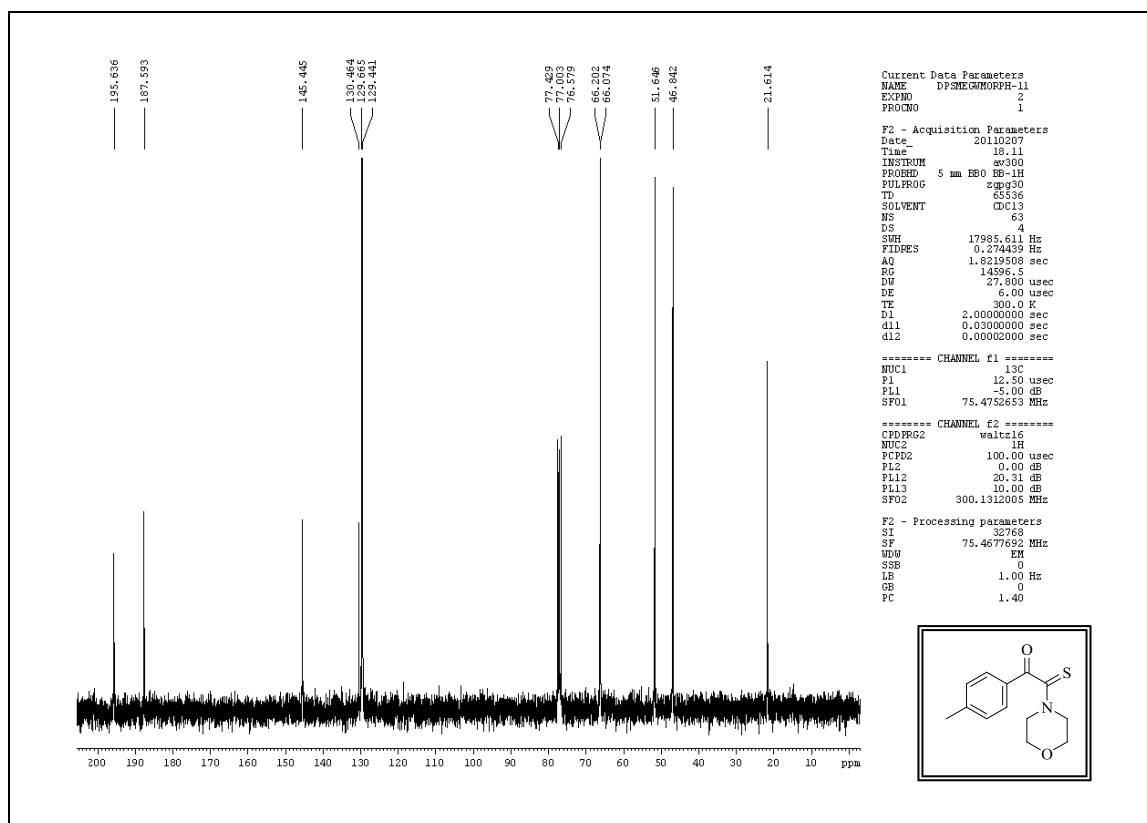


Figure 29. ^{13}C NMR Spectrum of **8j**

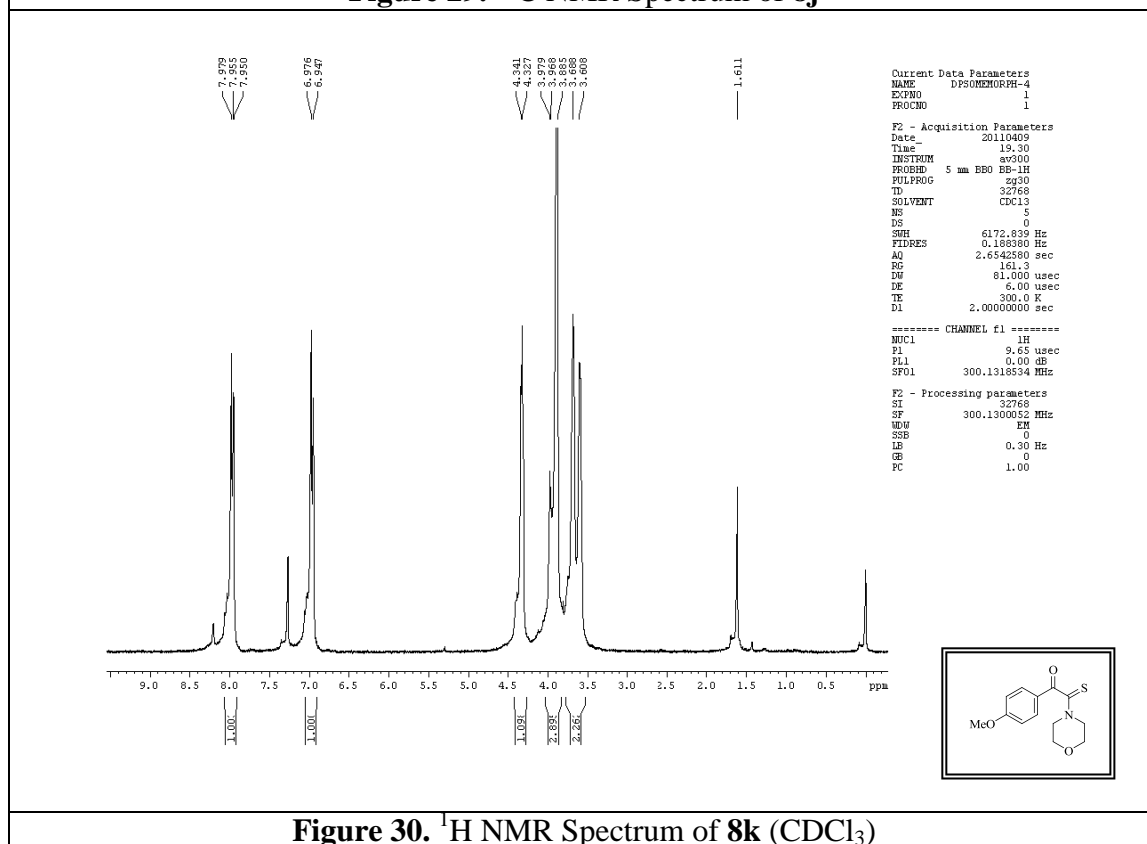


Figure 30. ^1H NMR Spectrum of **8k** (CDCl_3)

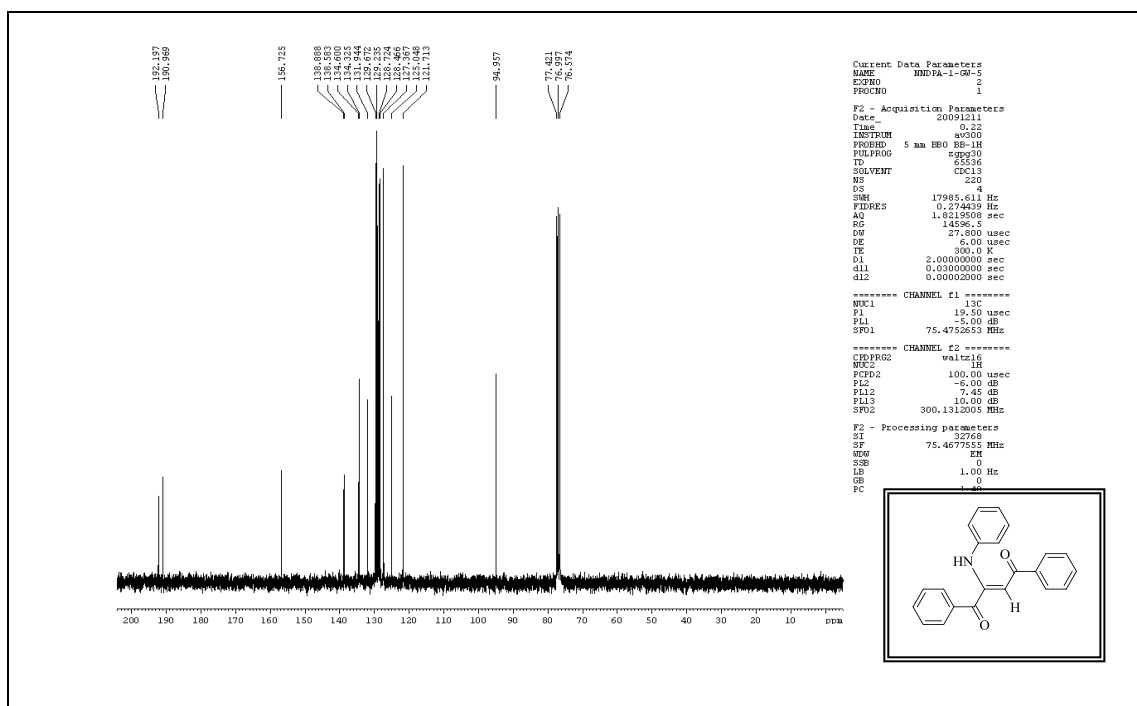


Figure 33. ^{13}C NMR Spectrum of 5a (CDCl_3)

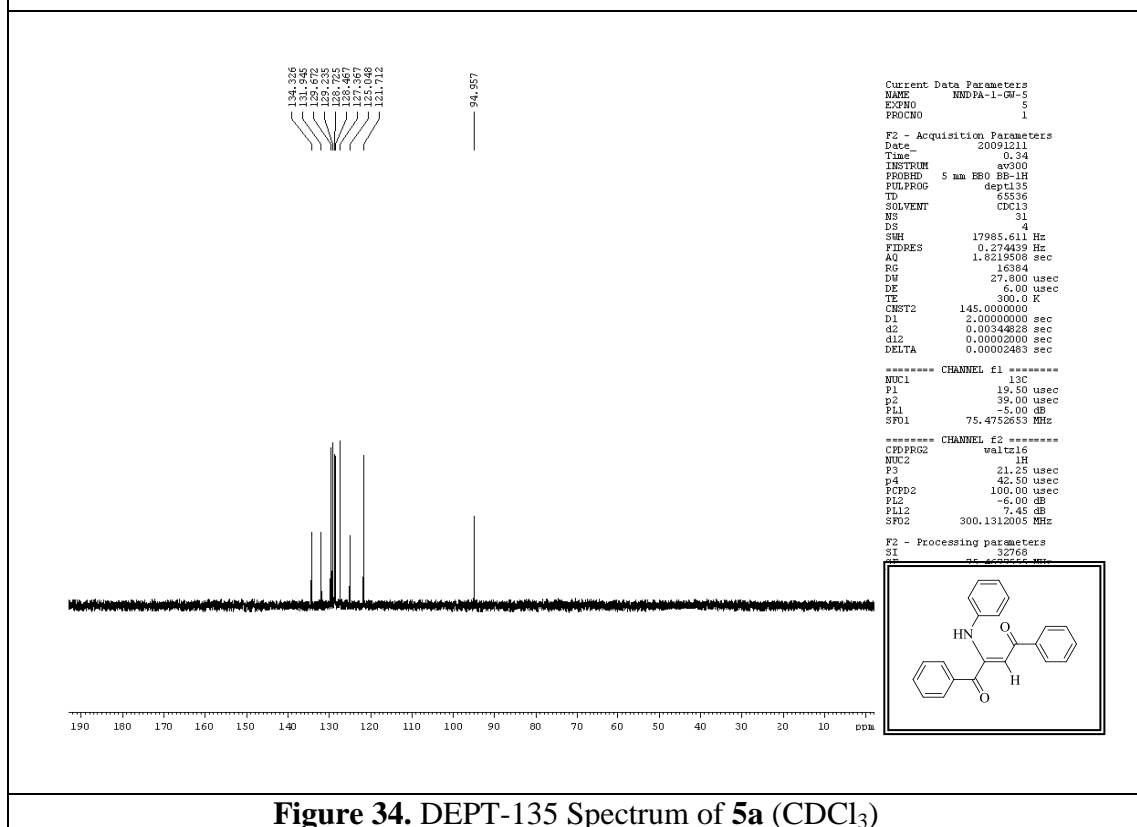


Figure 34. DEPT-135 Spectrum of 5a (CDCl_3)

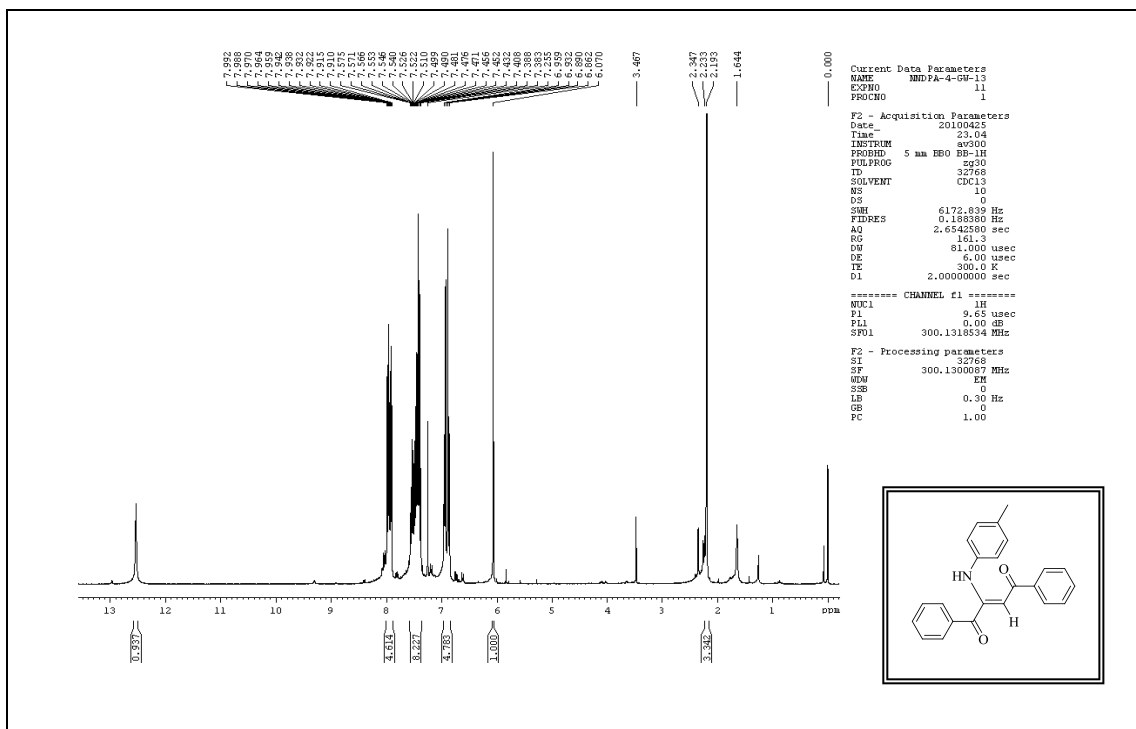


Figure 35. ¹H NMR Spectrum of 5b

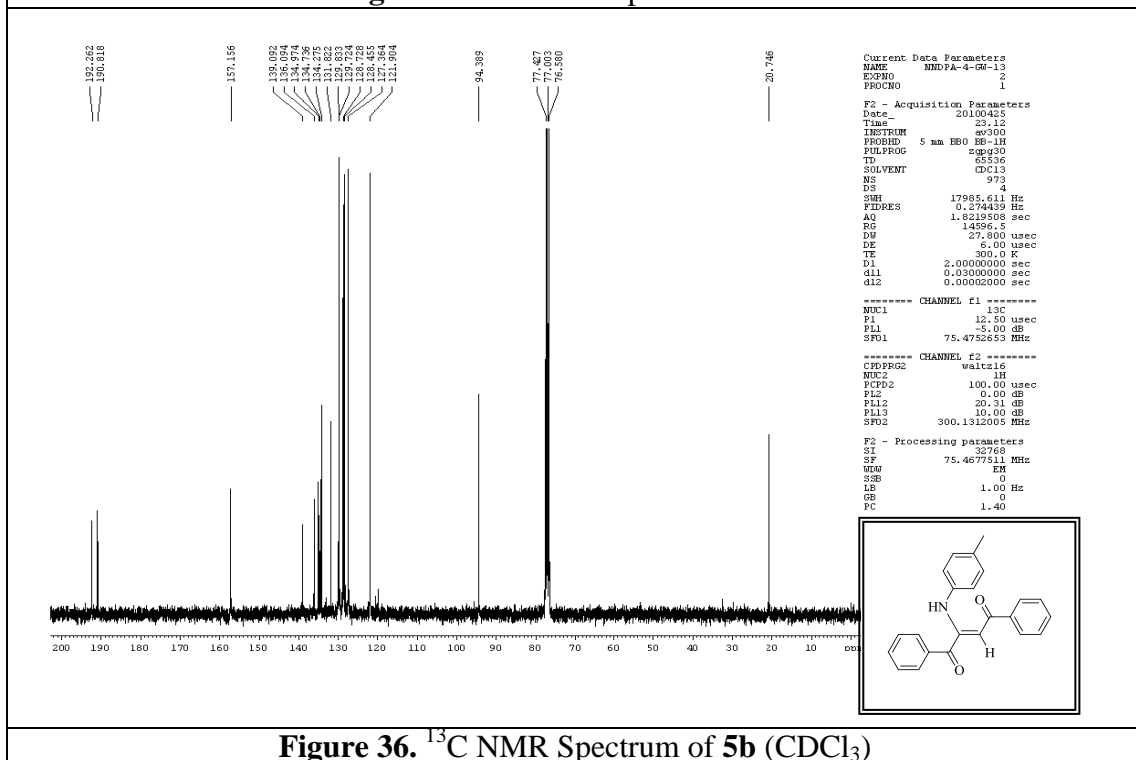


Figure 36. ¹³C NMR Spectrum of 5b (CDCl₃)

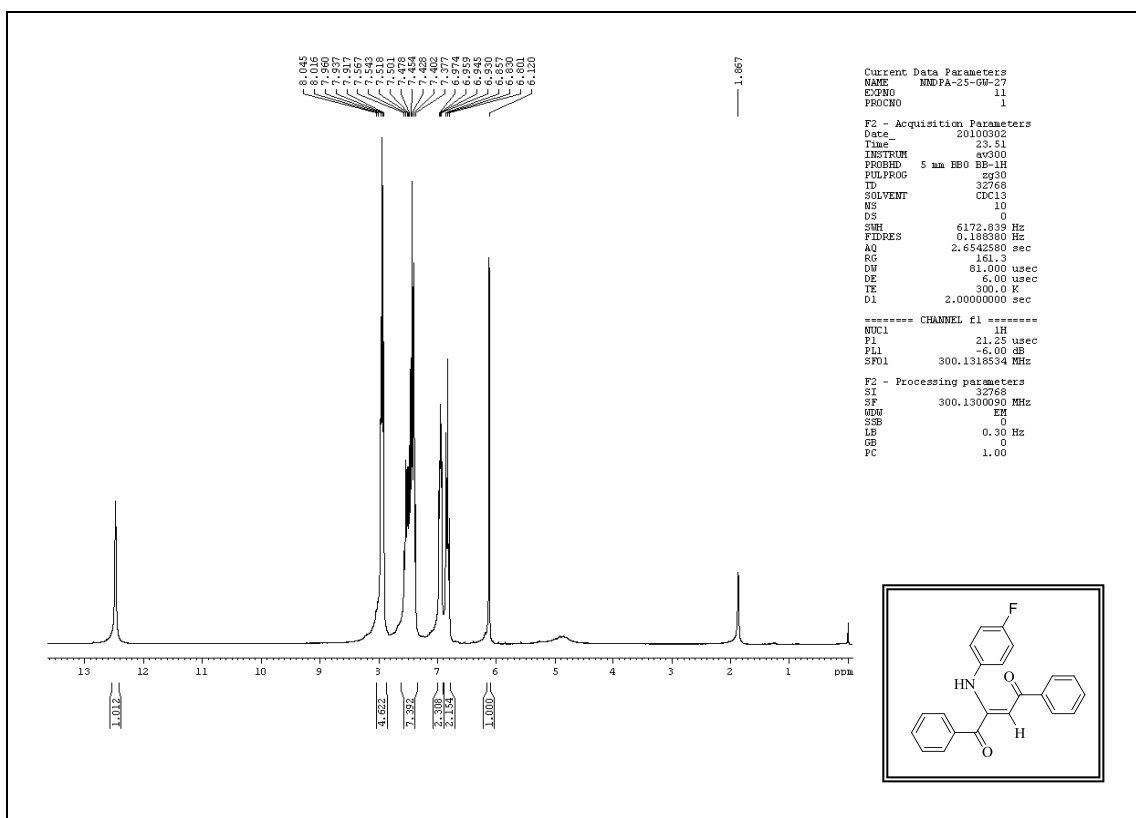


Figure 37. ¹H NMR Spectrum of 5c

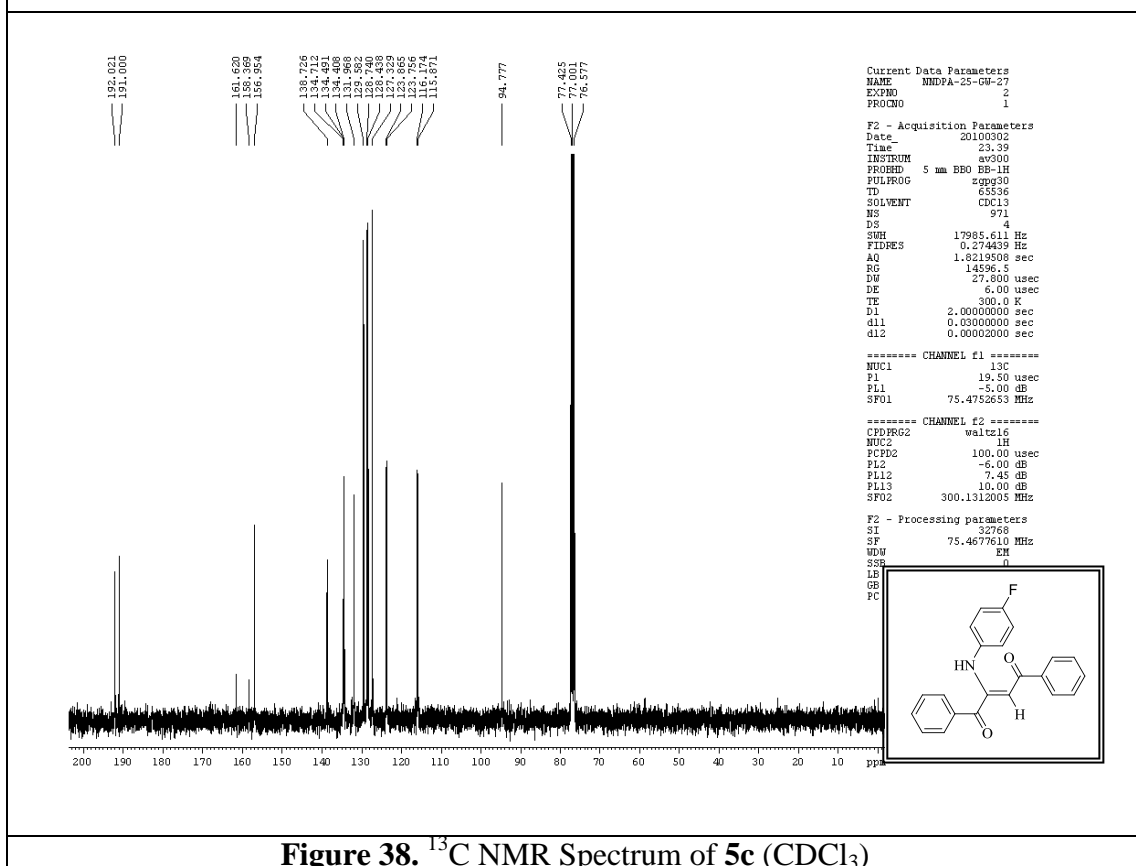


Figure 38. ¹³C NMR Spectrum of 5c (CDCl₃)

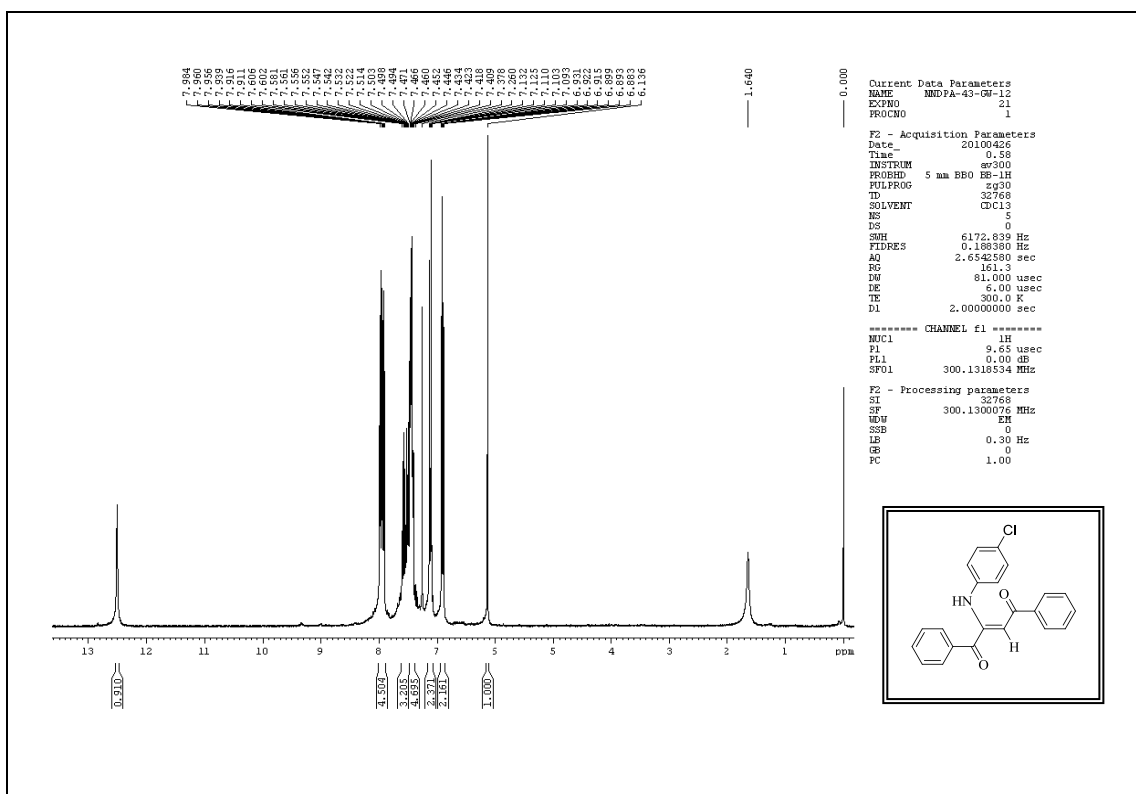


Figure 39. ¹H NMR Spectrum of 5d

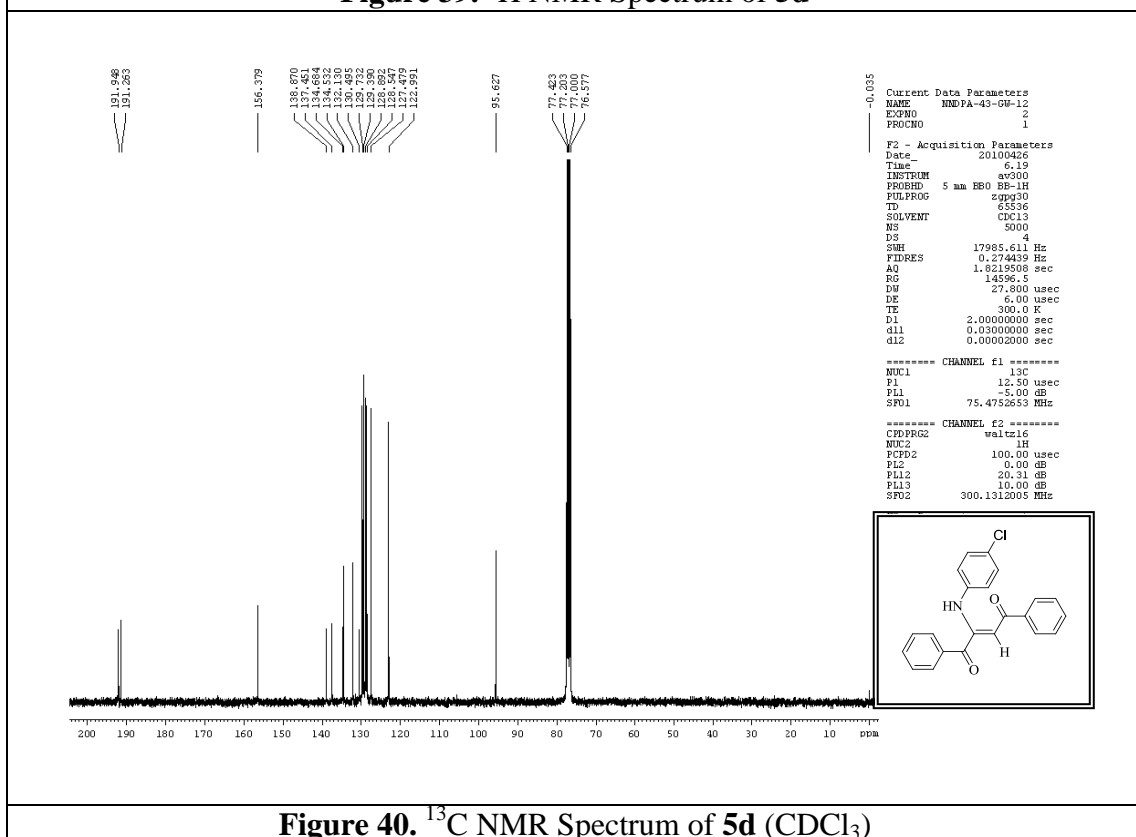


Figure 40. ¹³C NMR Spectrum of 5d (CDCl₃)

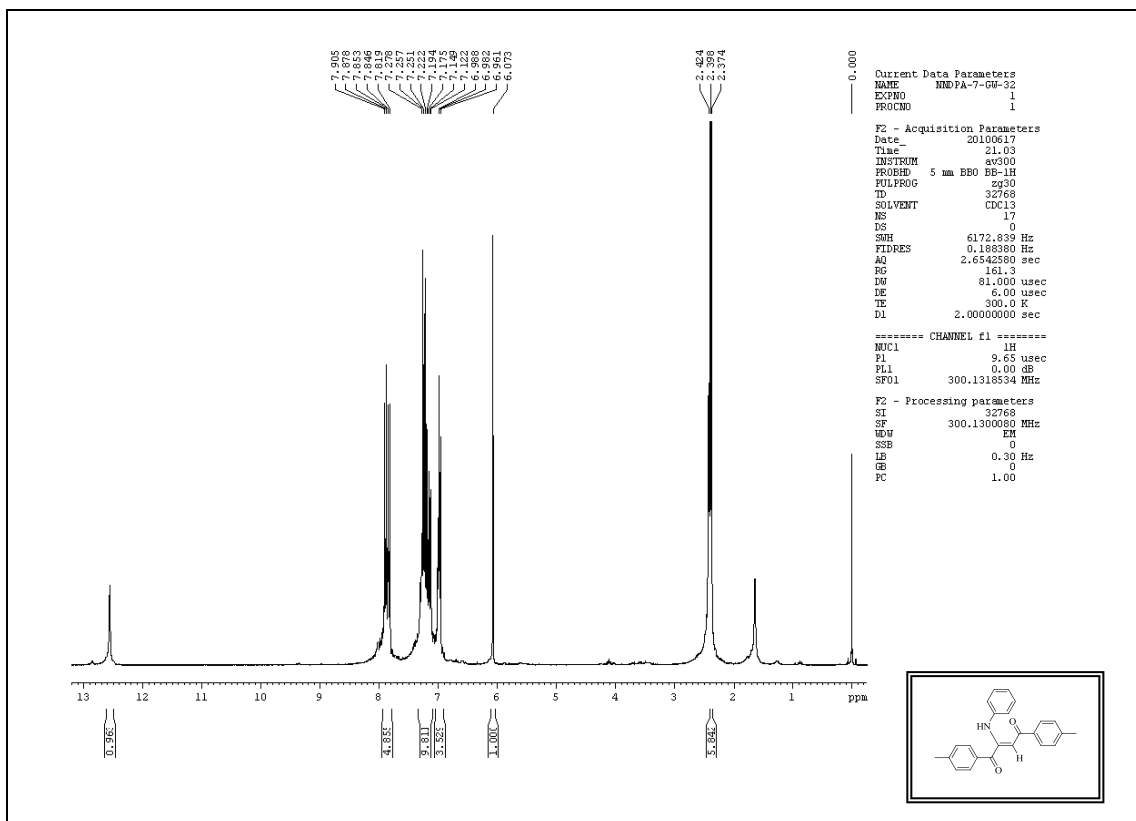


Figure 41. ^1H NMR Spectrum of **5e** (CDCl_3)

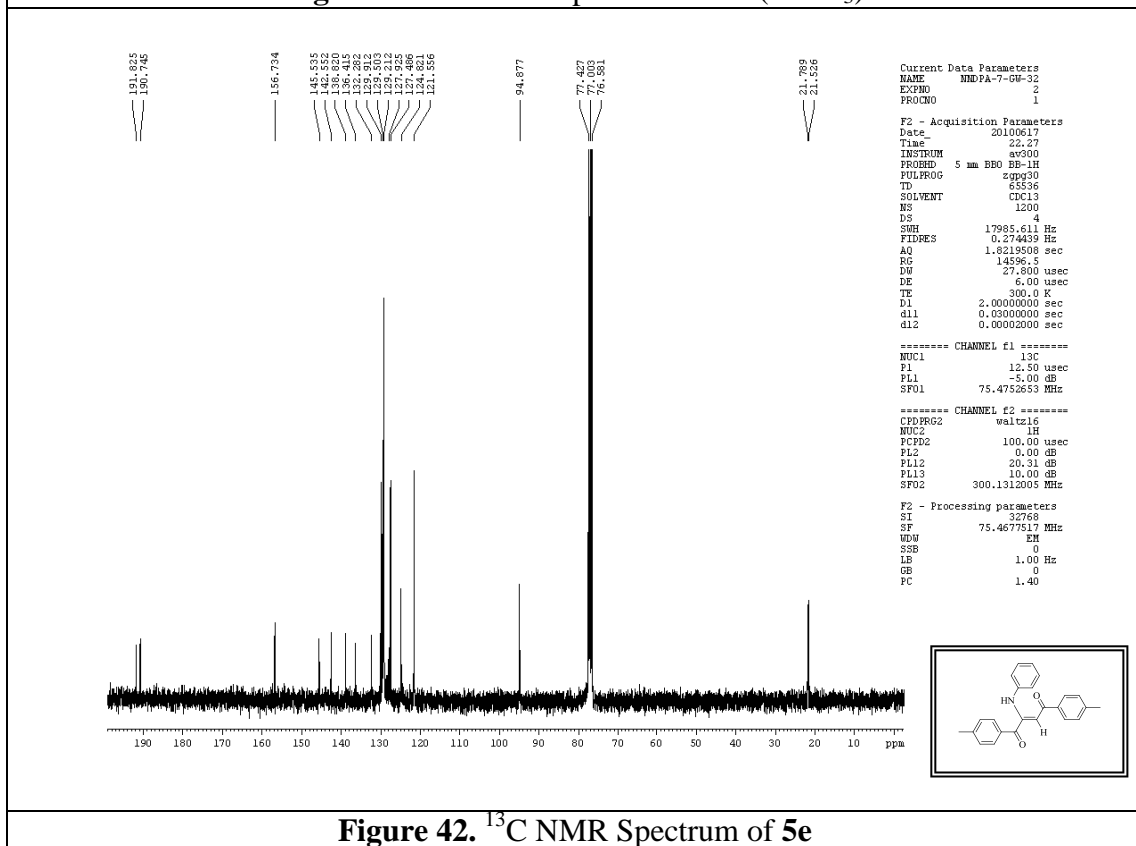


Figure 42. ^{13}C NMR Spectrum of **5e**

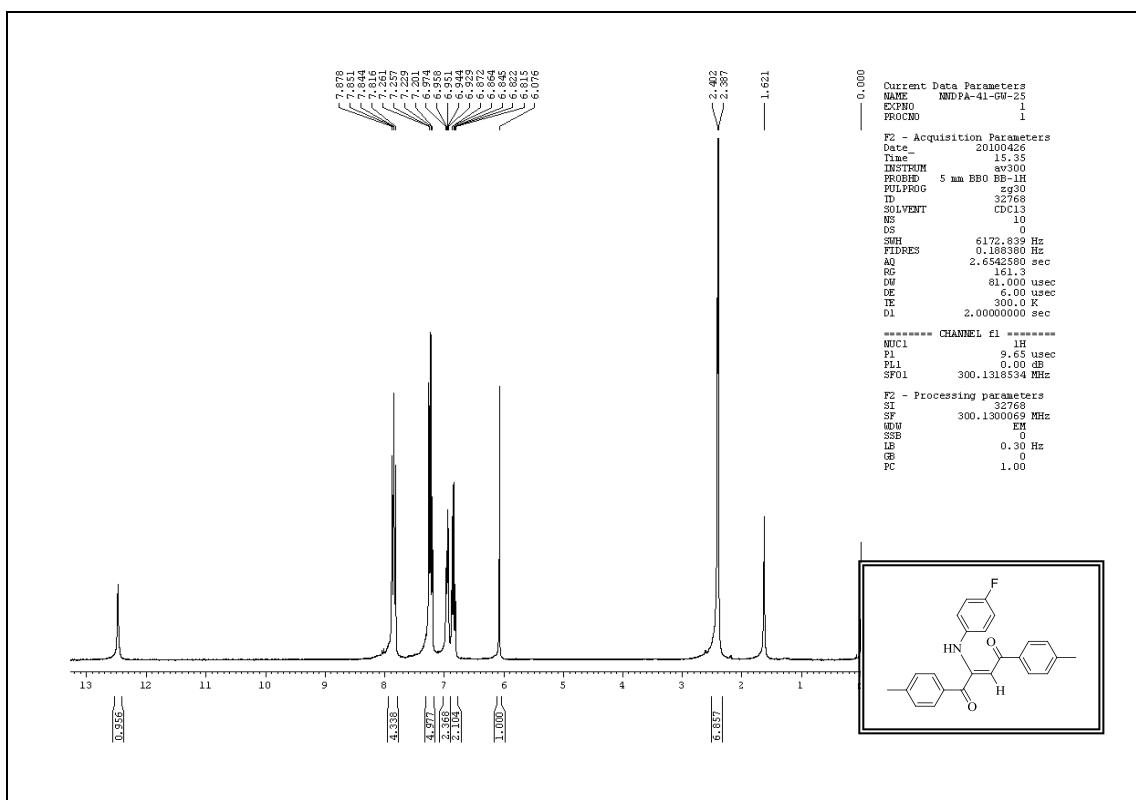


Figure 43. ¹H NMR Spectrum of 5f

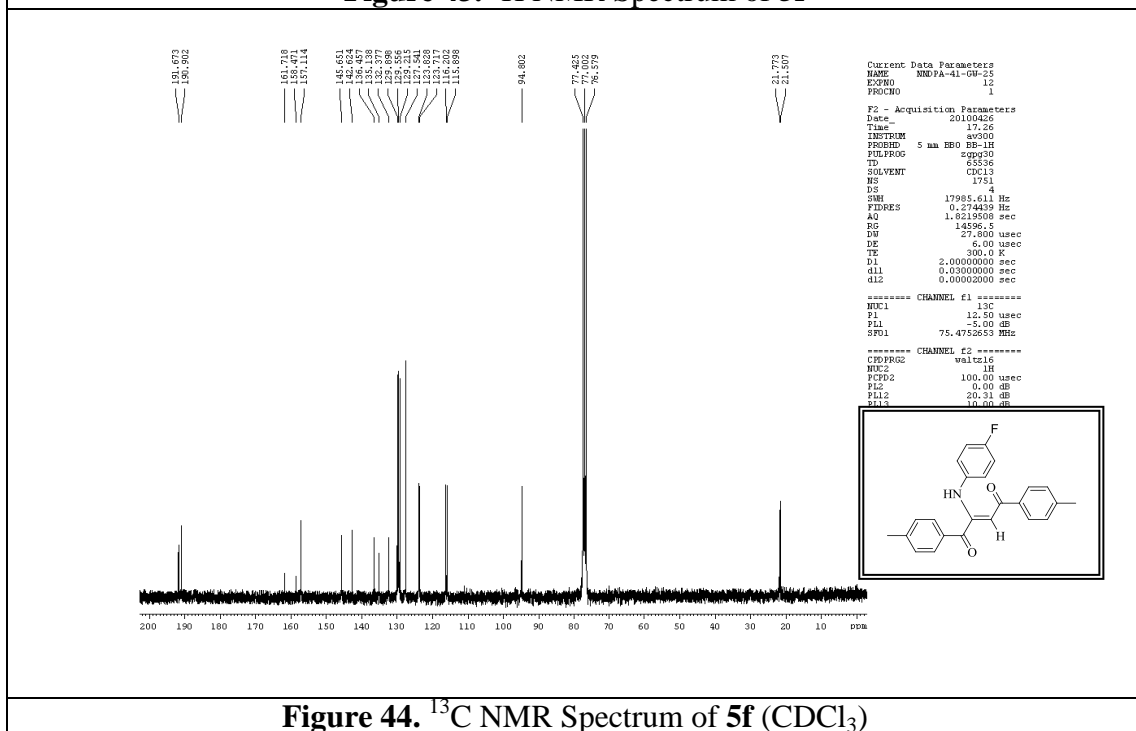


Figure 44. ¹³C NMR Spectrum of 5f (CDCl₃)

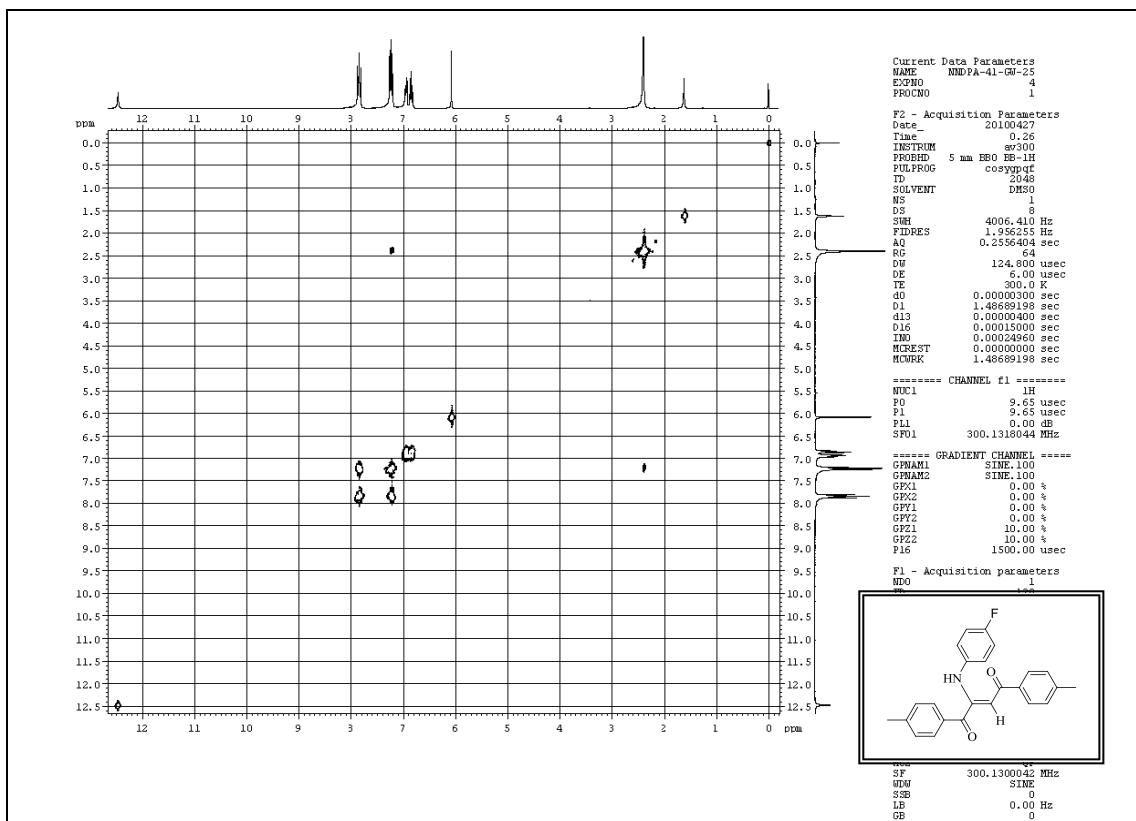


Figure 45. H,H-COSY Spectrum of **5f**

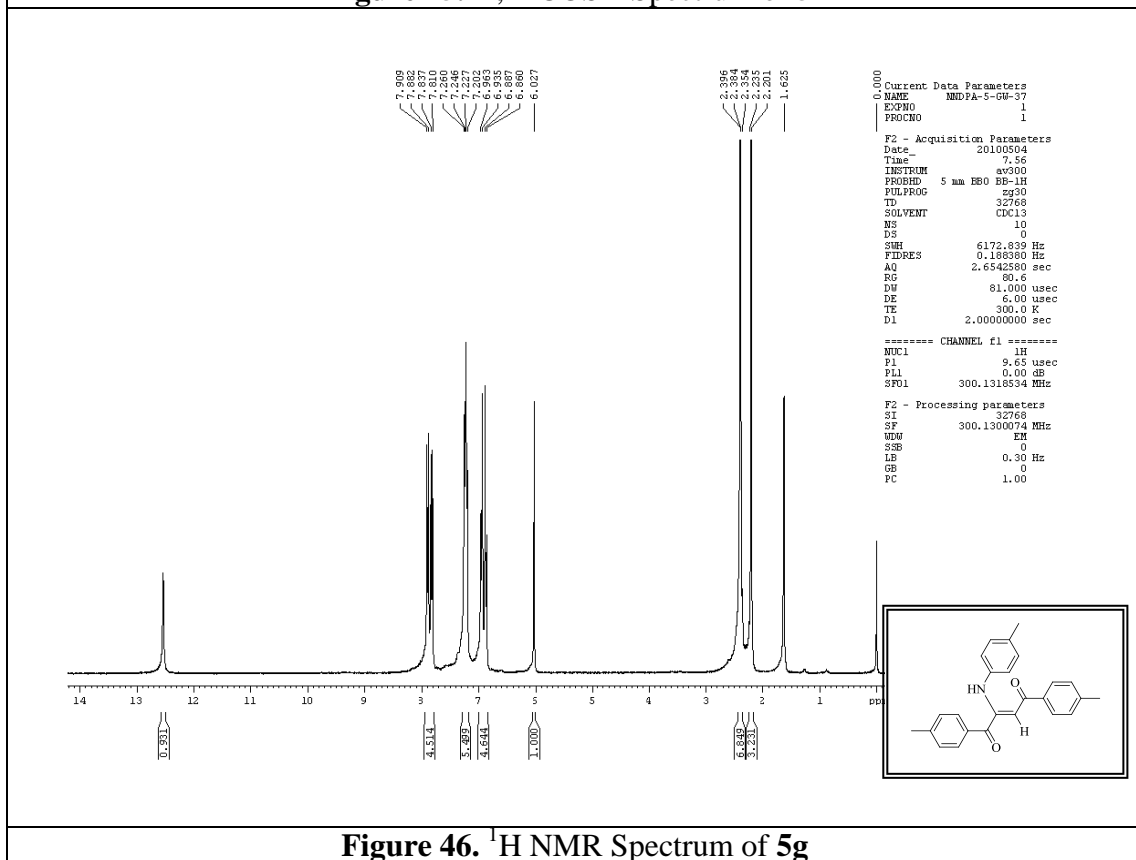


Figure 46. ¹H NMR Spectrum of **5g**

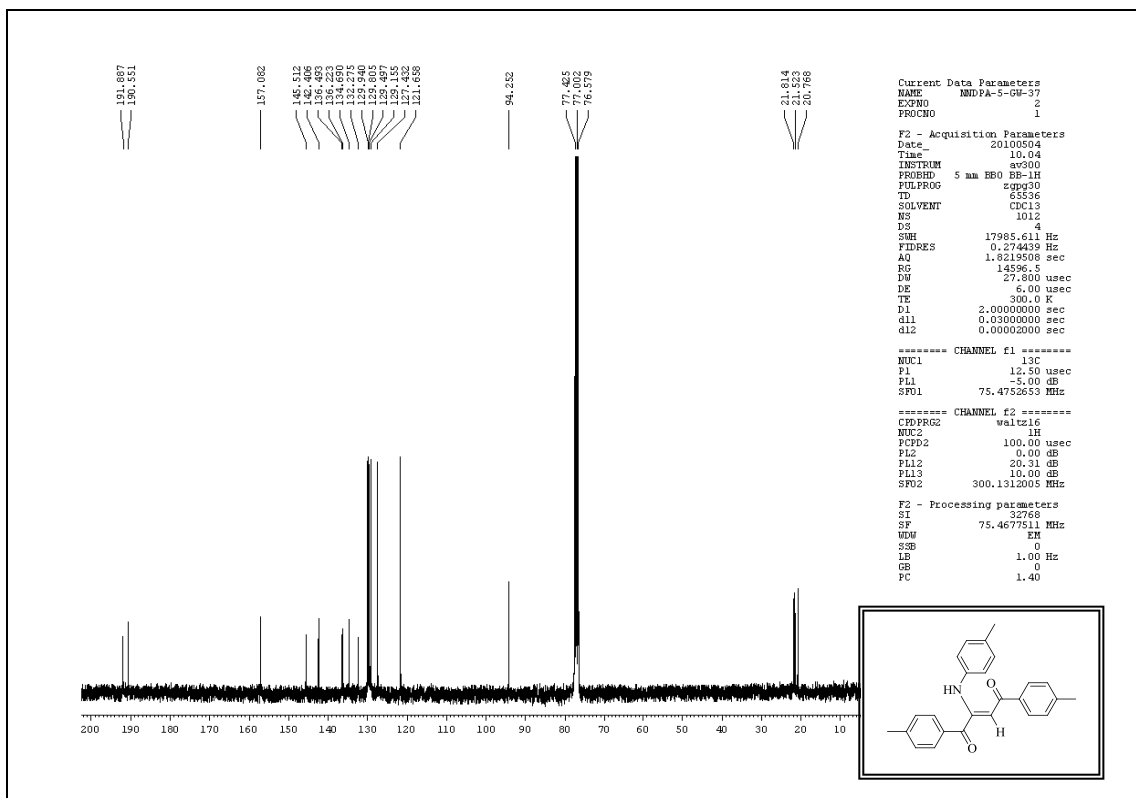


Figure 47. ¹³C NMR Spectrum of **5g** (CDCl₃)

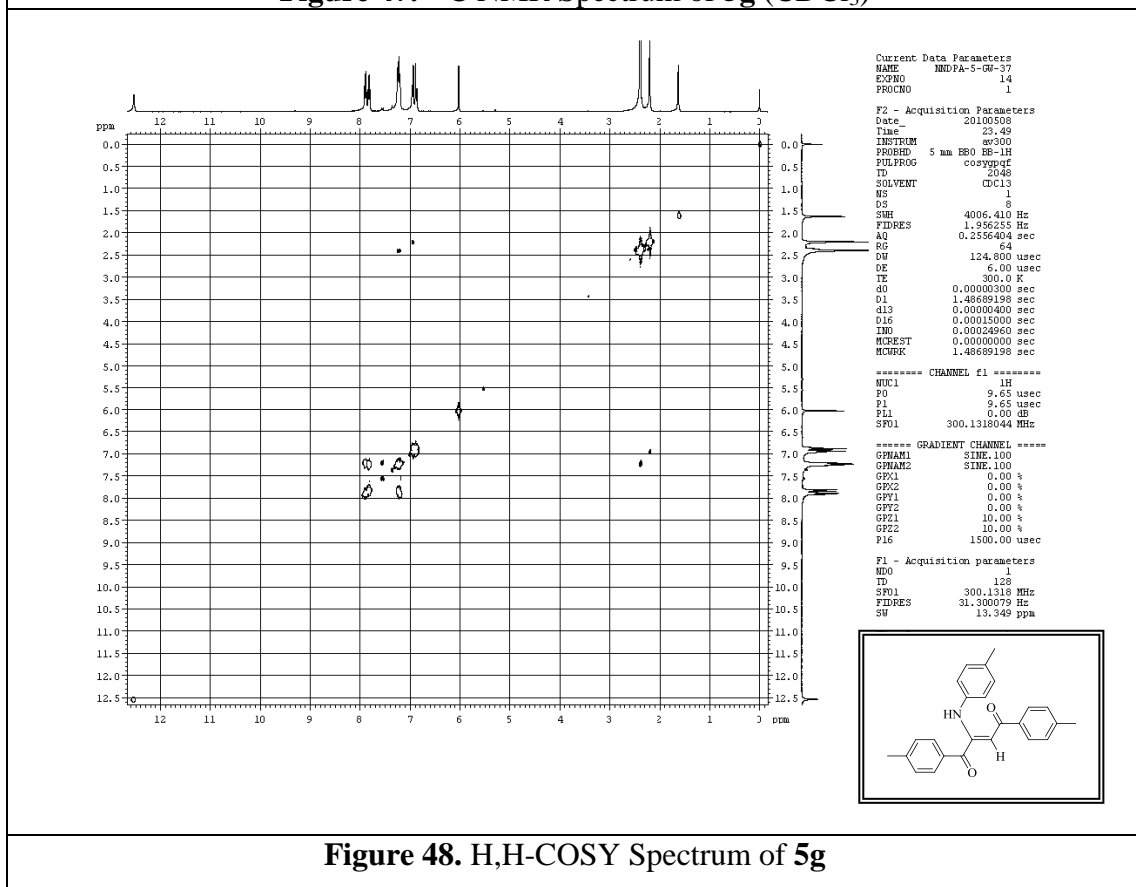


Figure 48. H,H-COSY Spectrum of **5g**

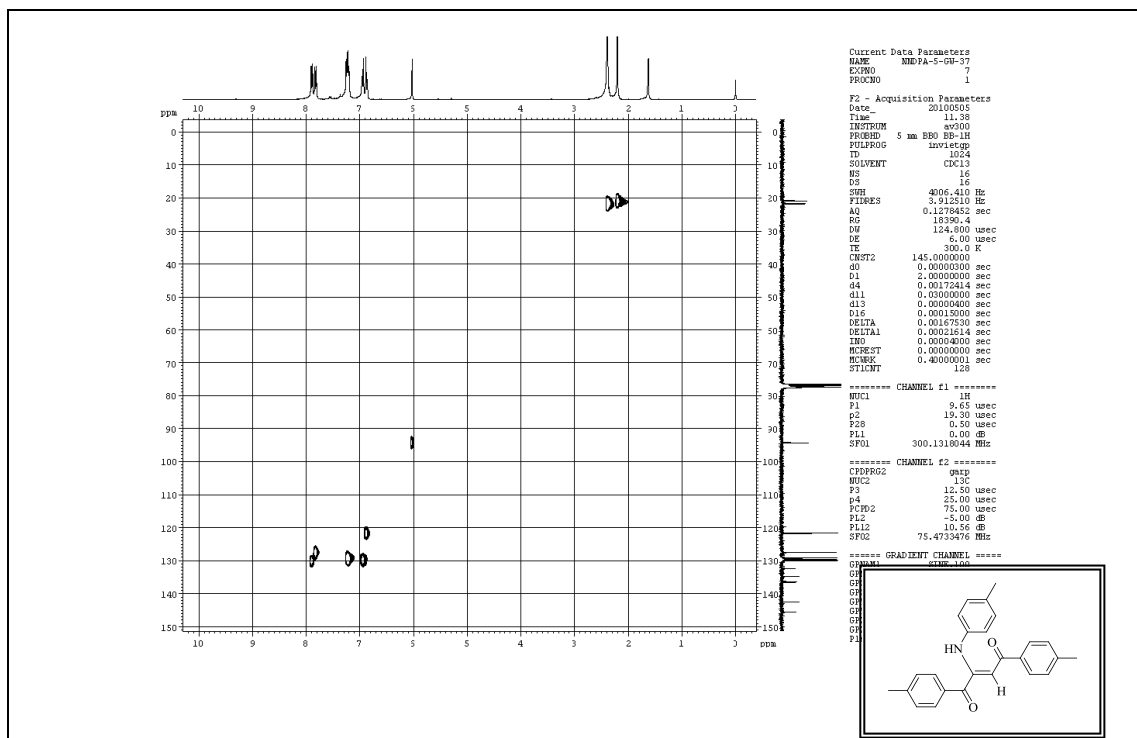


Figure 49. C,H-COSY Spectrum of **5g**

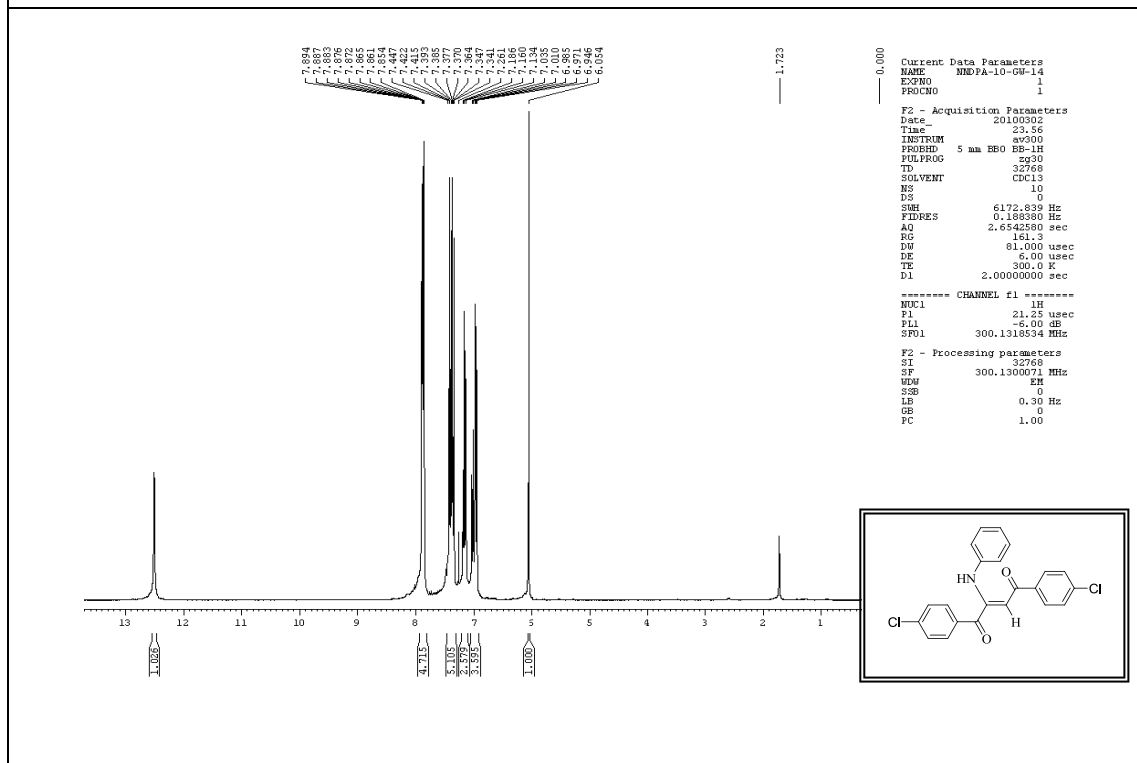


Figure 50. ¹H NMR Spectrum of **5h**

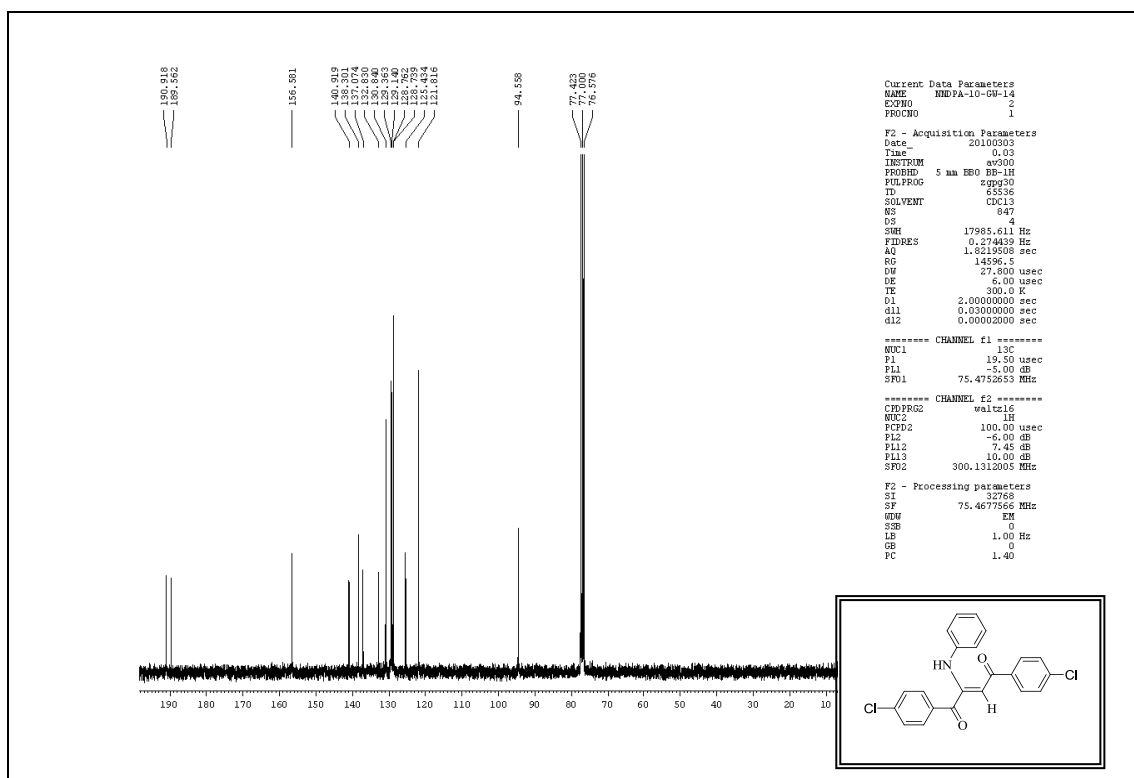


Figure 51. ^{13}C NMR Spectrum of **5h** (CDCl_3)

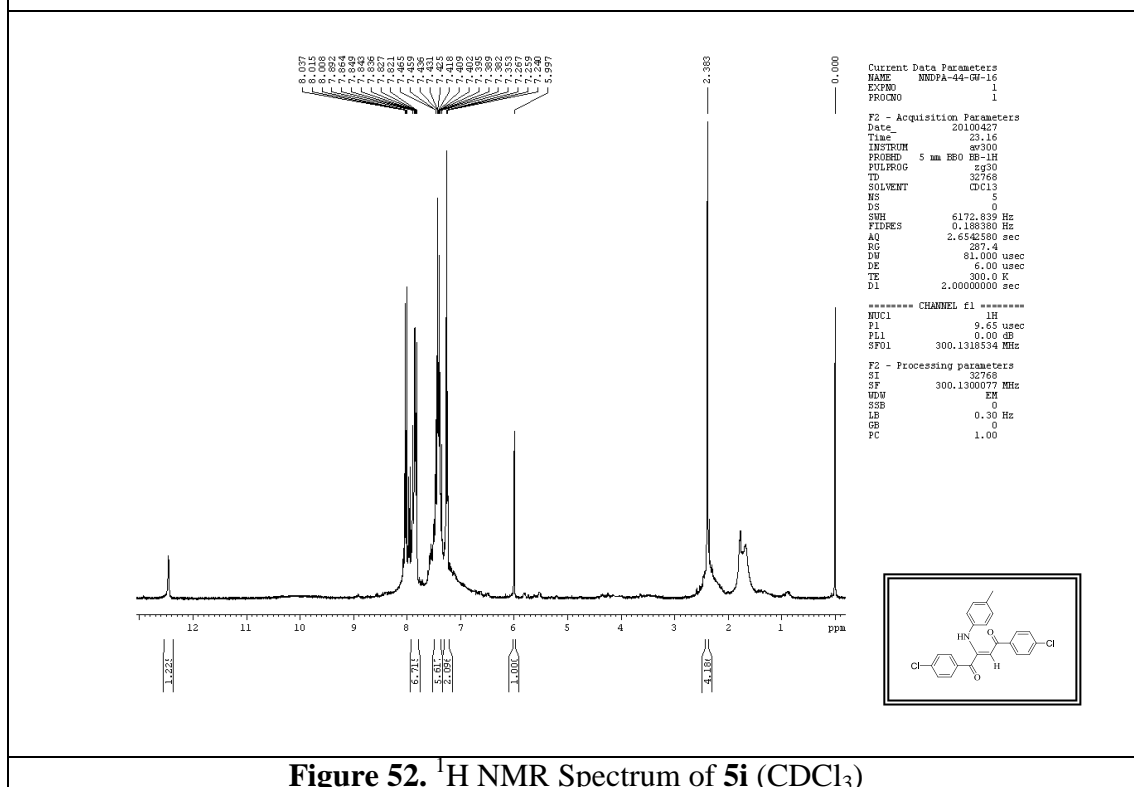


Figure 52. ^1H NMR Spectrum of **5i** (CDCl_3)

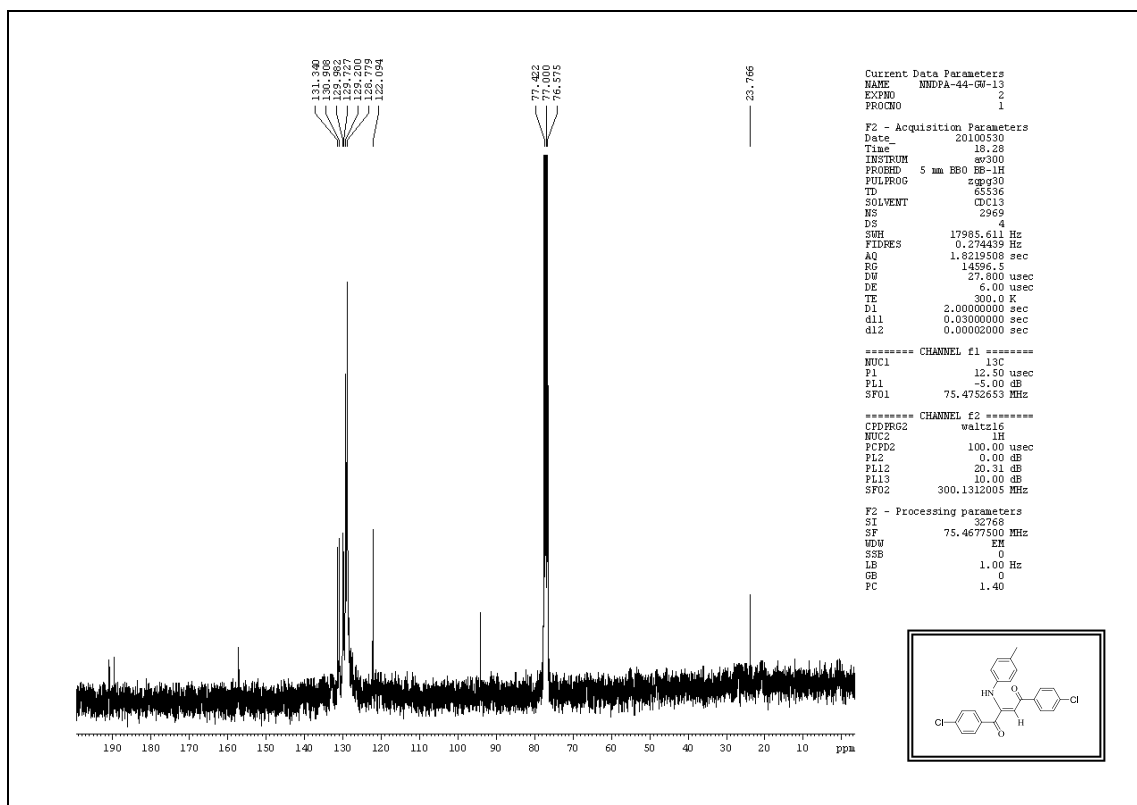


Figure 53. ^{13}C NMR Spectrum of **5i**

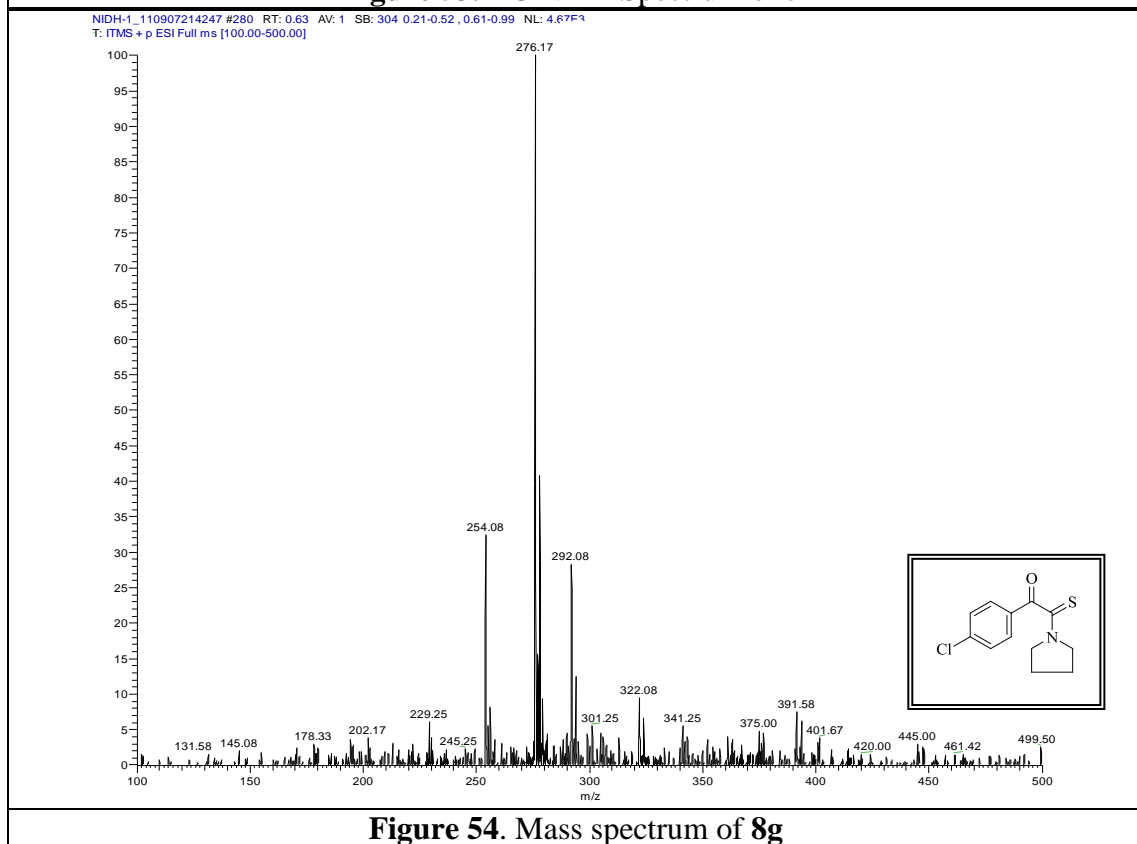


Figure 54. Mass spectrum of **8g**

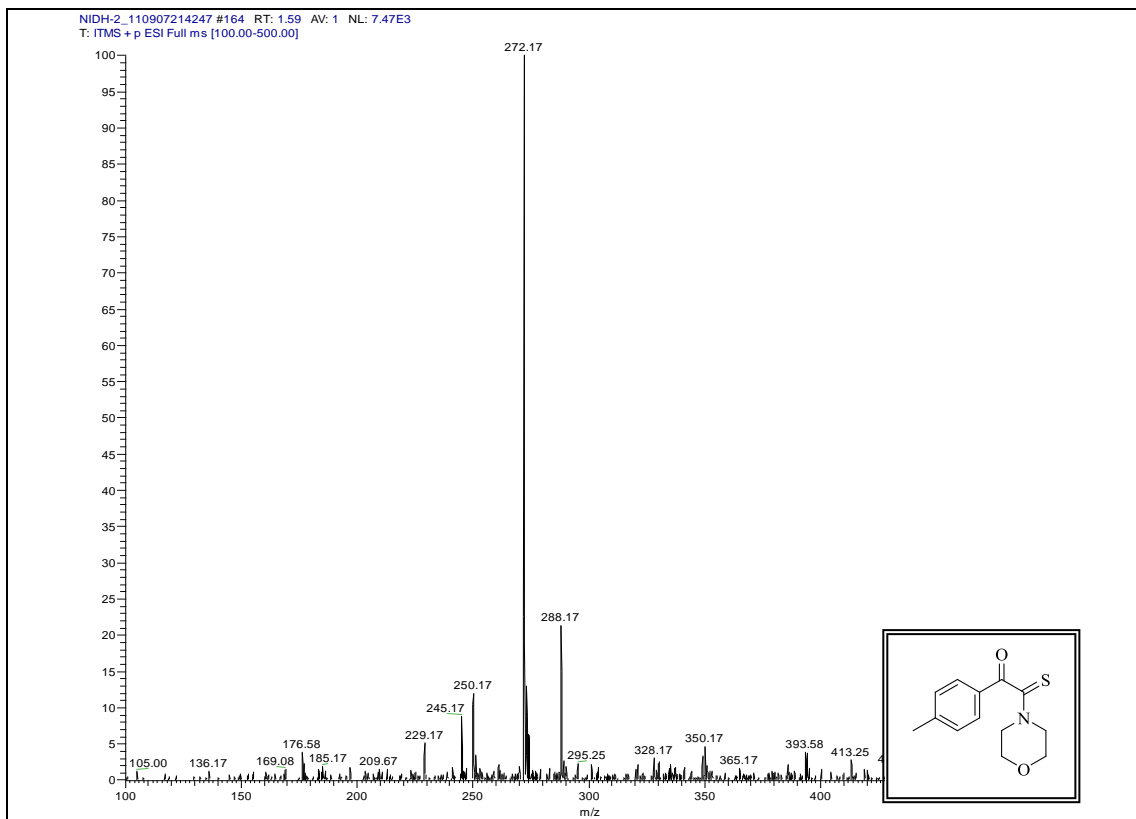


Figure 55. Mass spectrum of 8j

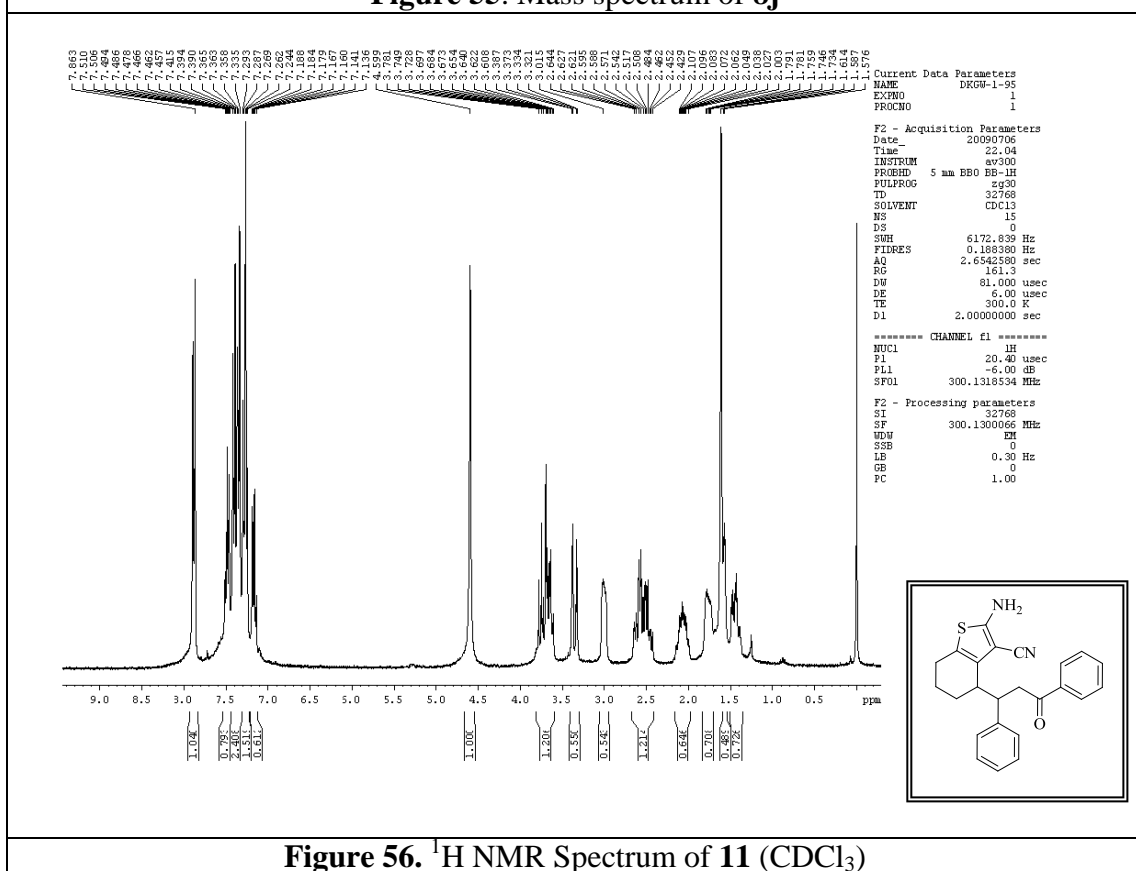


Figure 56. ¹H NMR Spectrum of 11 (CDCl₃)

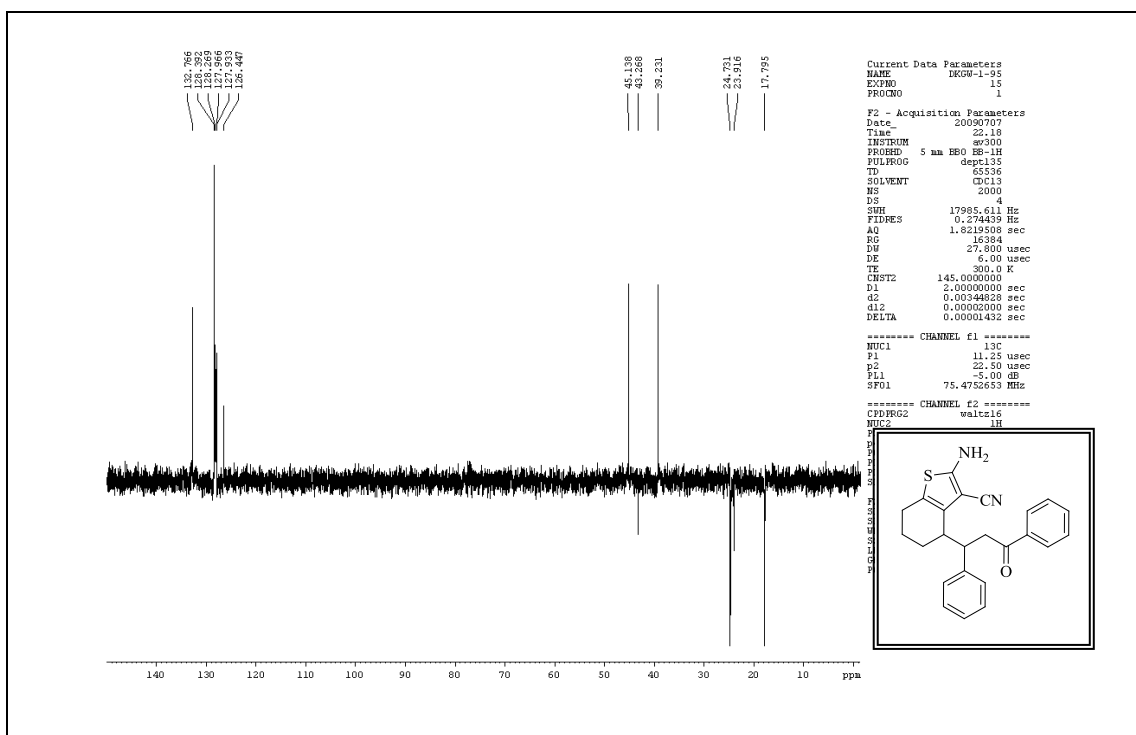


Figure 59. DEPT Spectrum of 11 (CDCl₃)

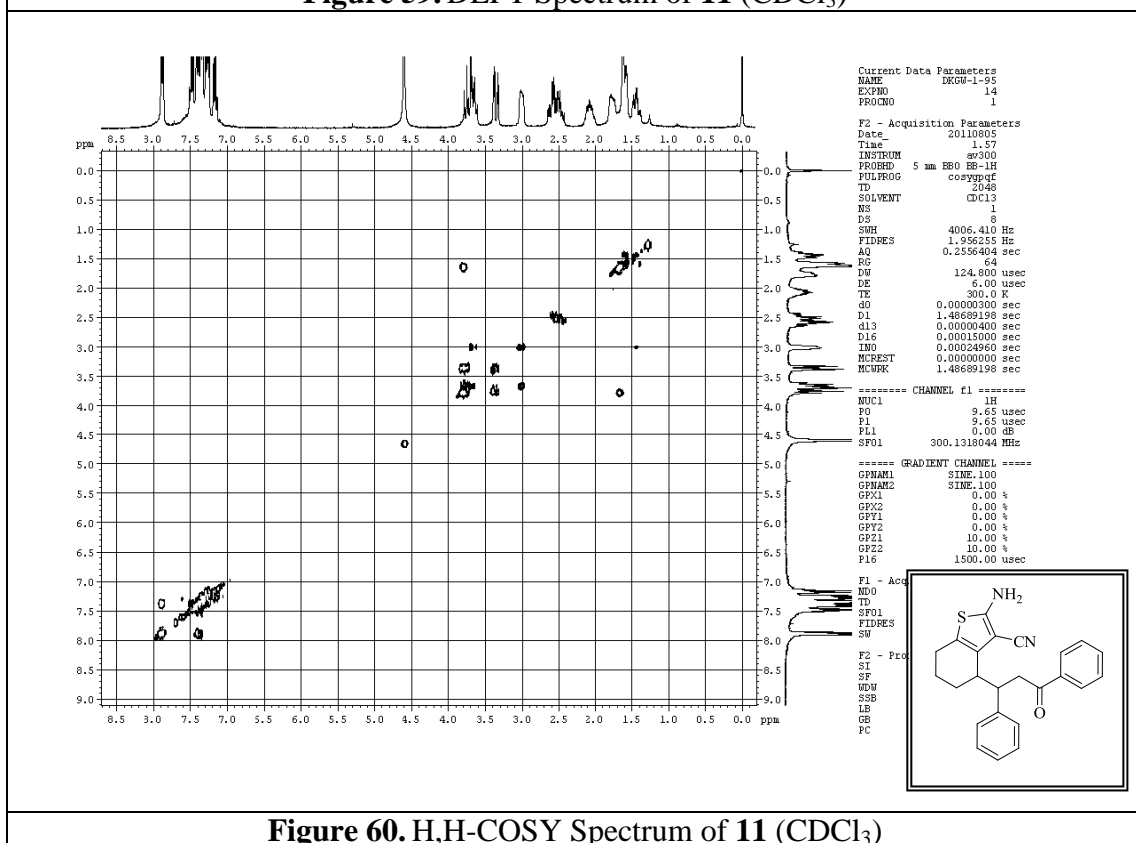


Figure 60. H,H-COSY Spectrum of 11 (CDCl₃)

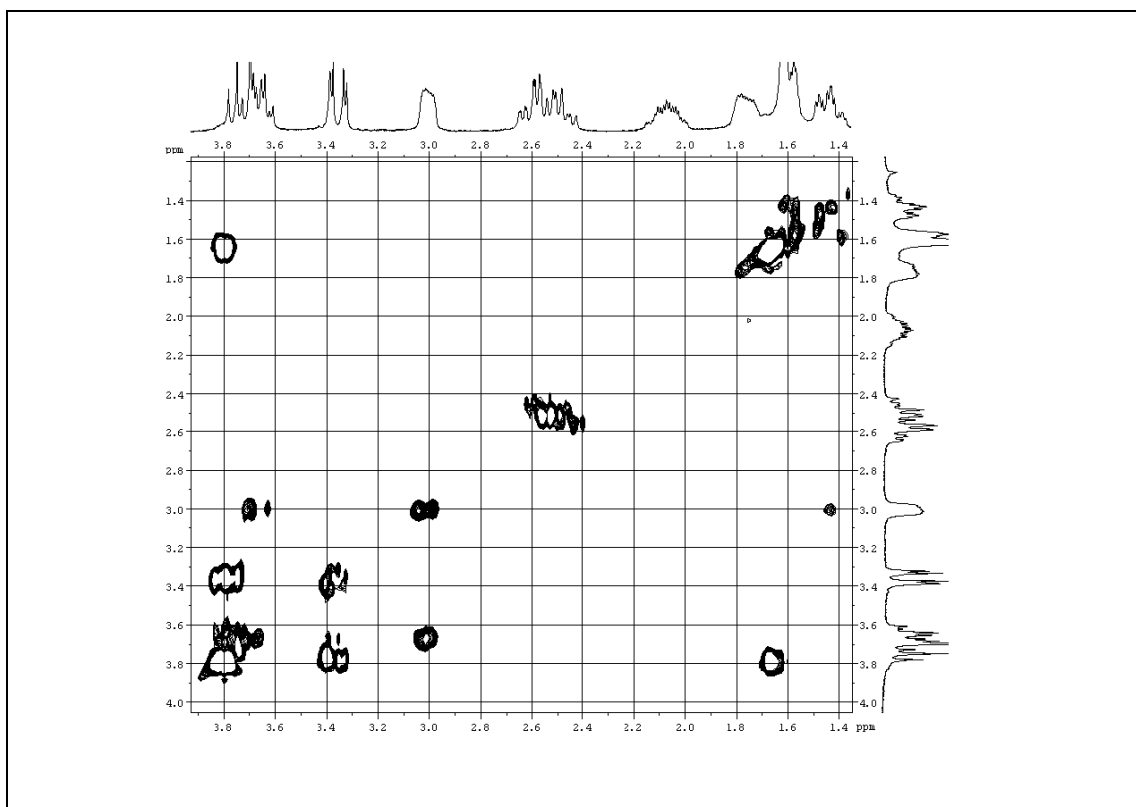


Figure 61. H,H-COSY Spectrum of 11 (expanded)

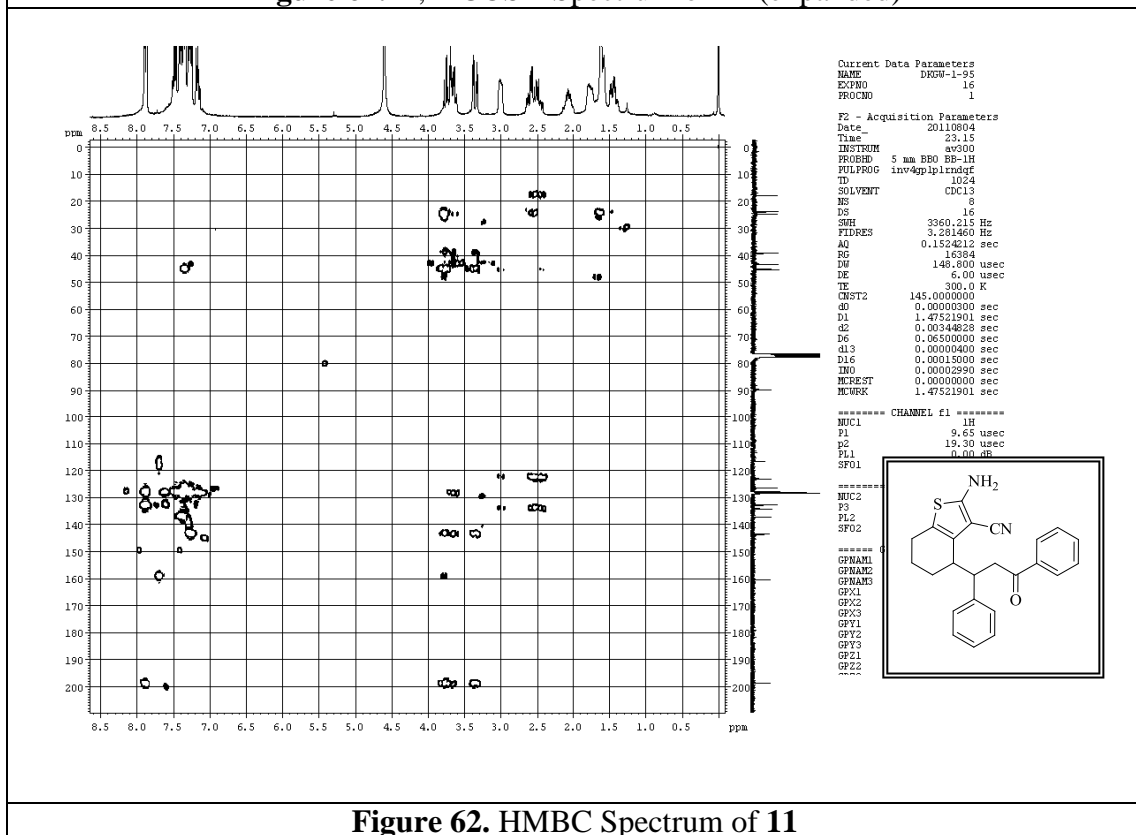


Figure 62. HMBC Spectrum of 11

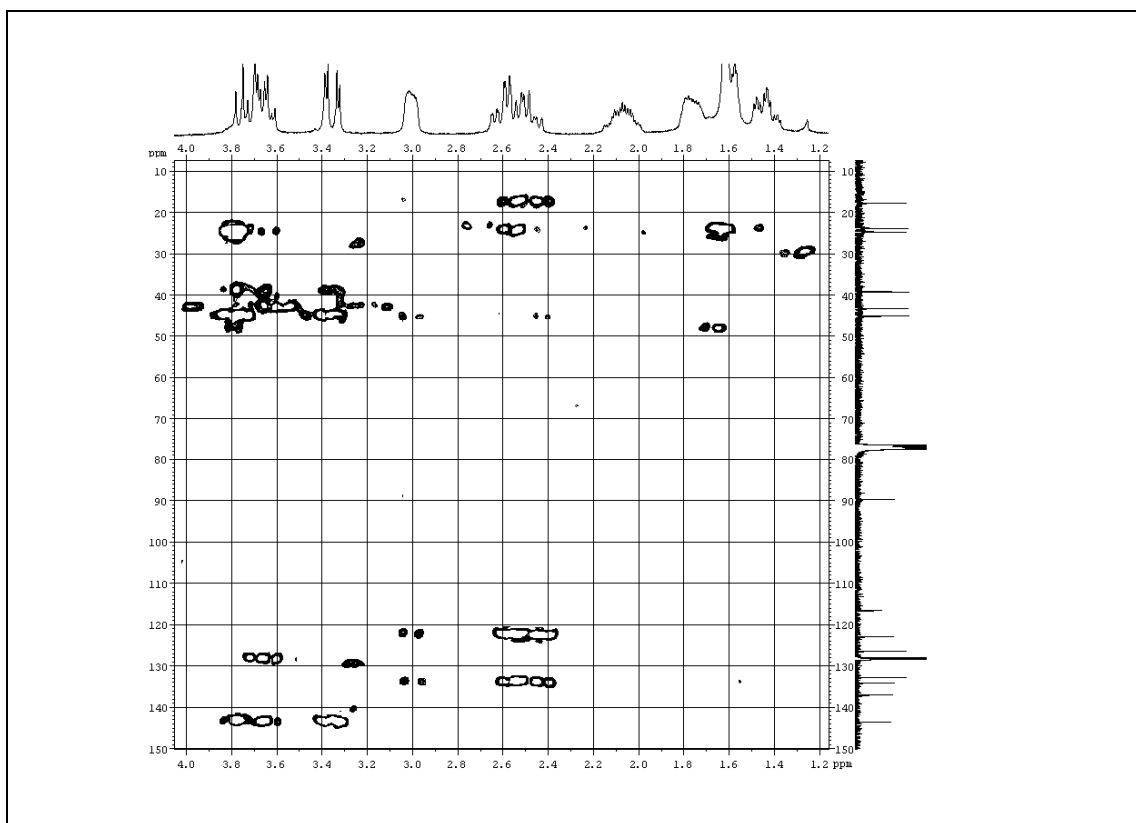


Figure 63. HMBC Spectrum of 11 (expanded)

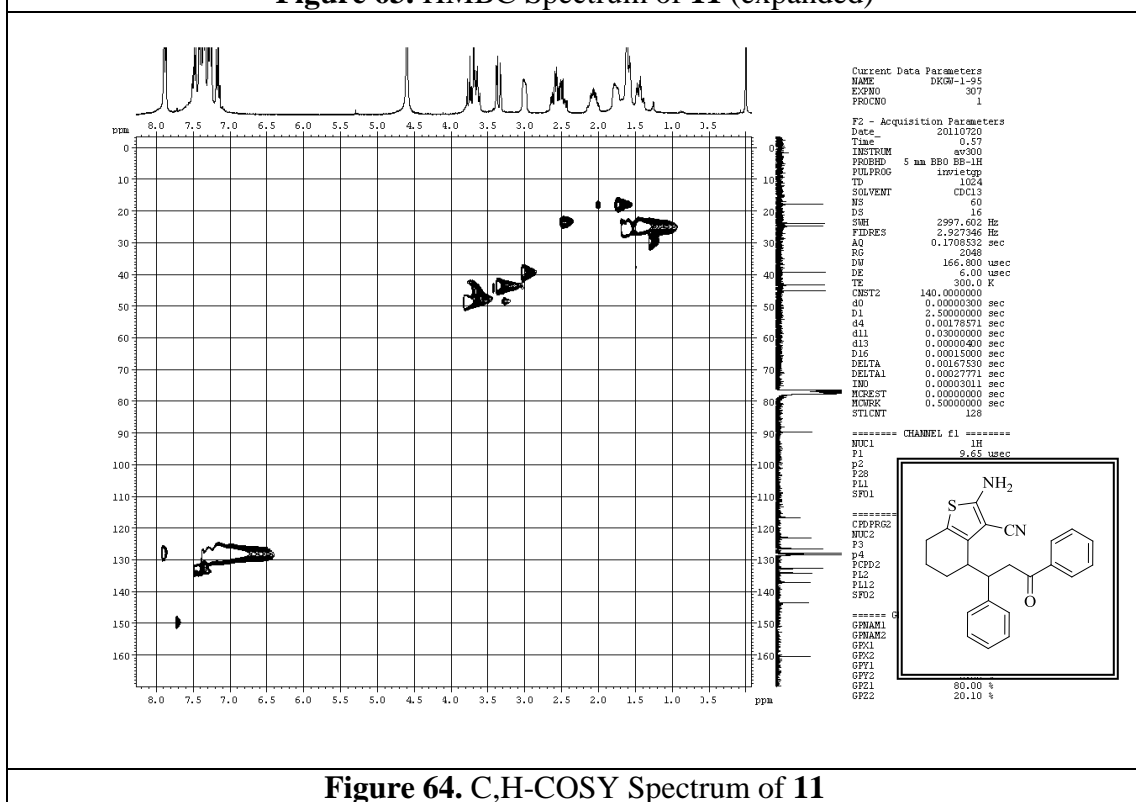


Figure 64. C,H-COSY Spectrum of 11

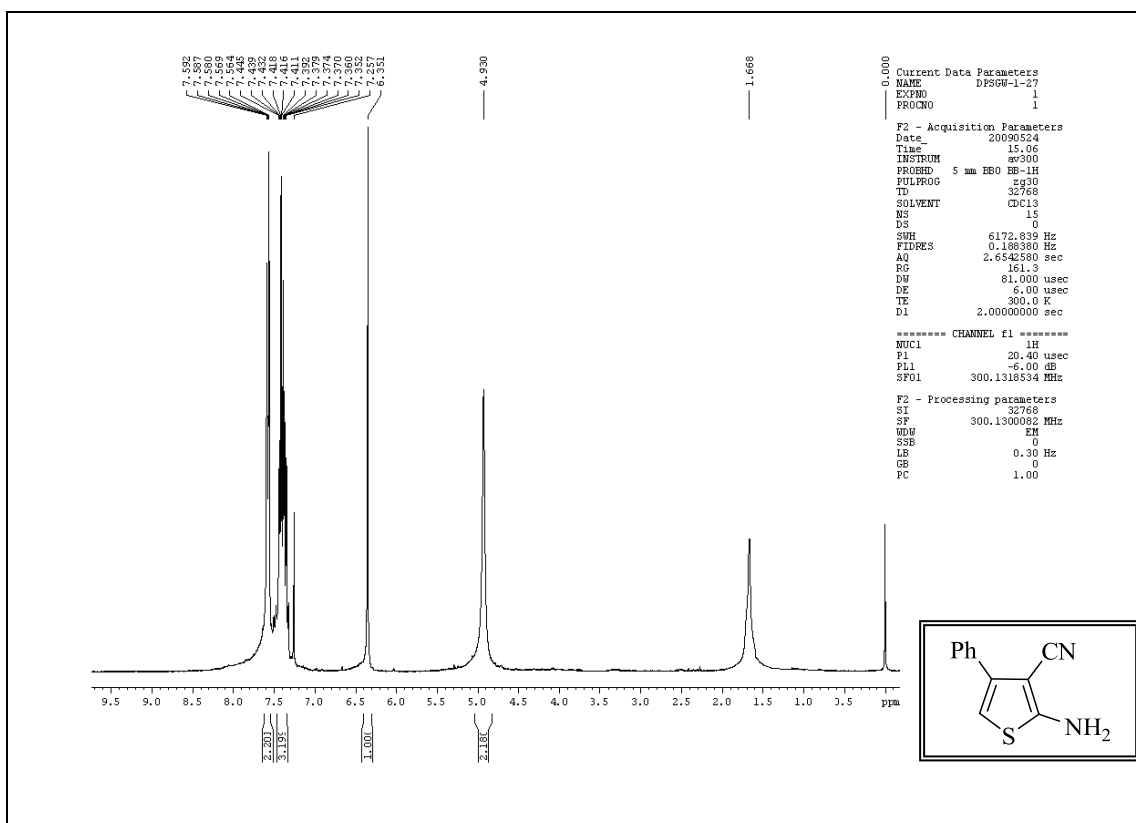


Figure 65. ¹H NMR Spectrum of 9 (CDCl₃)

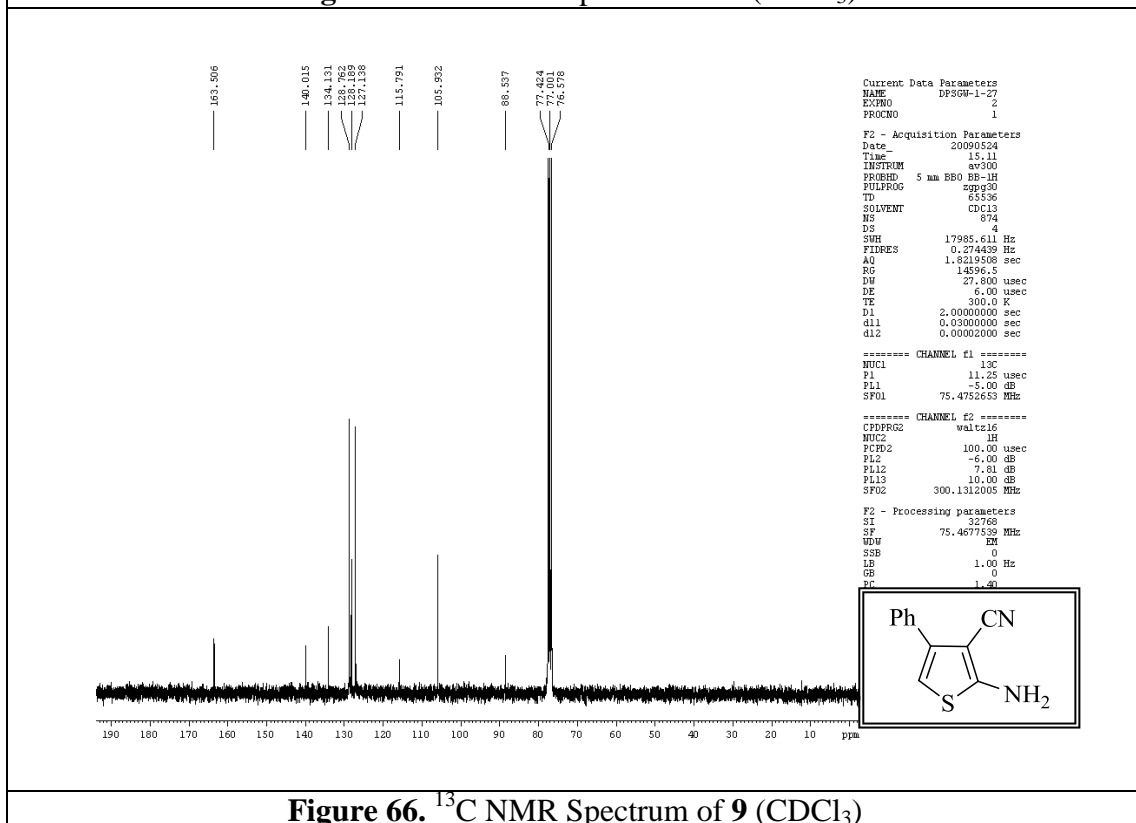


Figure 66. ¹³C NMR Spectrum of 9 (CDCl₃)

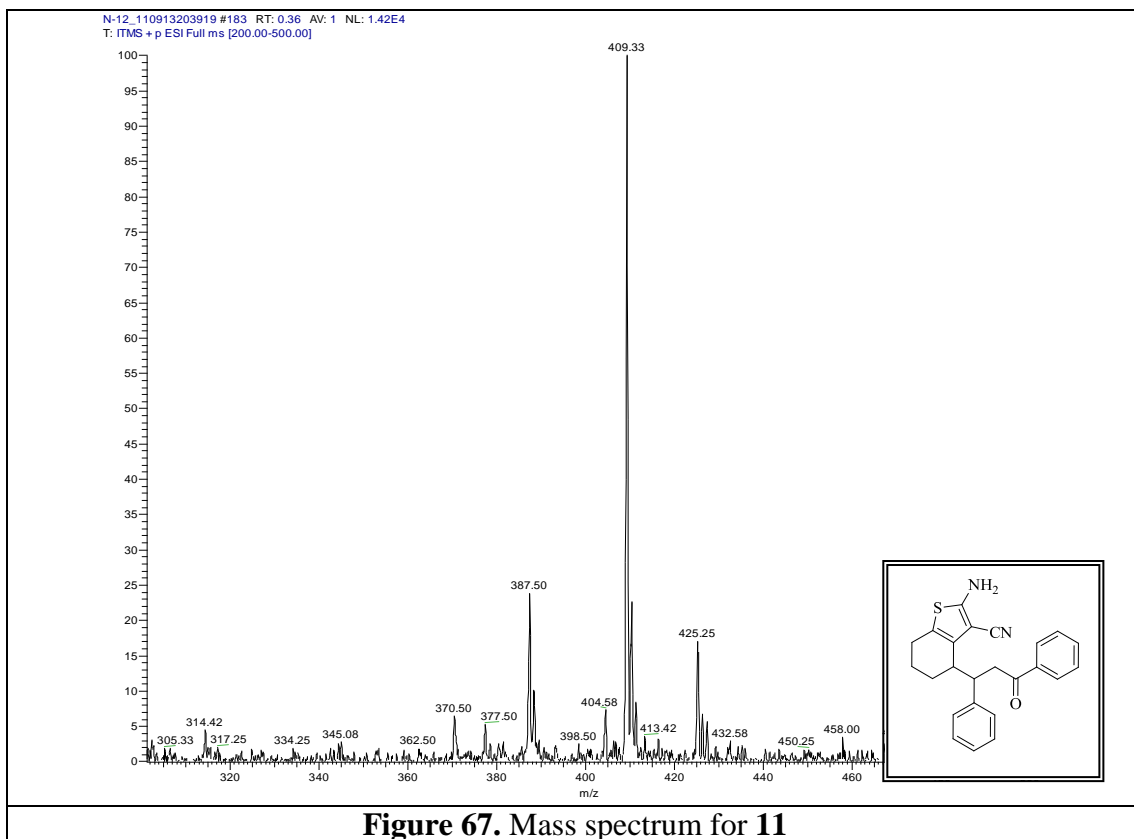


Figure 67. Mass spectrum for **11**

Crystal Data for compound 5b

Compound	5b
Empirical formula	C ₂₃ H ₁₉ N O ₂
Formula weight	341.39
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 2 1/c
Unit cell dimensions	a = 10.0504(7) Å α = 90.00°. b = 8.6750(7) Å β = 103.066(6)°. c = 21.4200(12) Å γ = 90.00°.
Volume	1819.2(2) Å ³
Z	4
Density (calculated)	1.246 Mg/m ³
Absorption coefficient	0.079 mm ⁻¹
F(000)	720
Crystal size	0.4 x 0.3 x 0.2 mm ³
Theta range for data collection	3.05 to 25.00°.
Index ranges	-11 ≤ h ≤ 11, -10 ≤ k ≤ 9, -25 ≤ l ≤ 24
Reflections collected	11790
Independent reflections	3197 [R(int) = 0.0331]
Completeness to theta = 60.00°	99.9 %
Max. and min. transmission	0.9902 and 0.9797
Data / restraints / parameters	3197 / 0 / 236
Goodness-of-fit on F ²	1.018
Final R indices [I > 2σ(I)]	R1 = 0.0477, wR2 = 0.1407
R indices (all data)	R1 = 0.0695, wR2 = 0.1626
Largest diff. peak and hole	0.158 and -0.193 e.Å ⁻³