

Supplementary Material

Malic acid as an effective and valuable bioorganocatalyst for one-pot, three-component synthesis of pyrrolidinone derivatives

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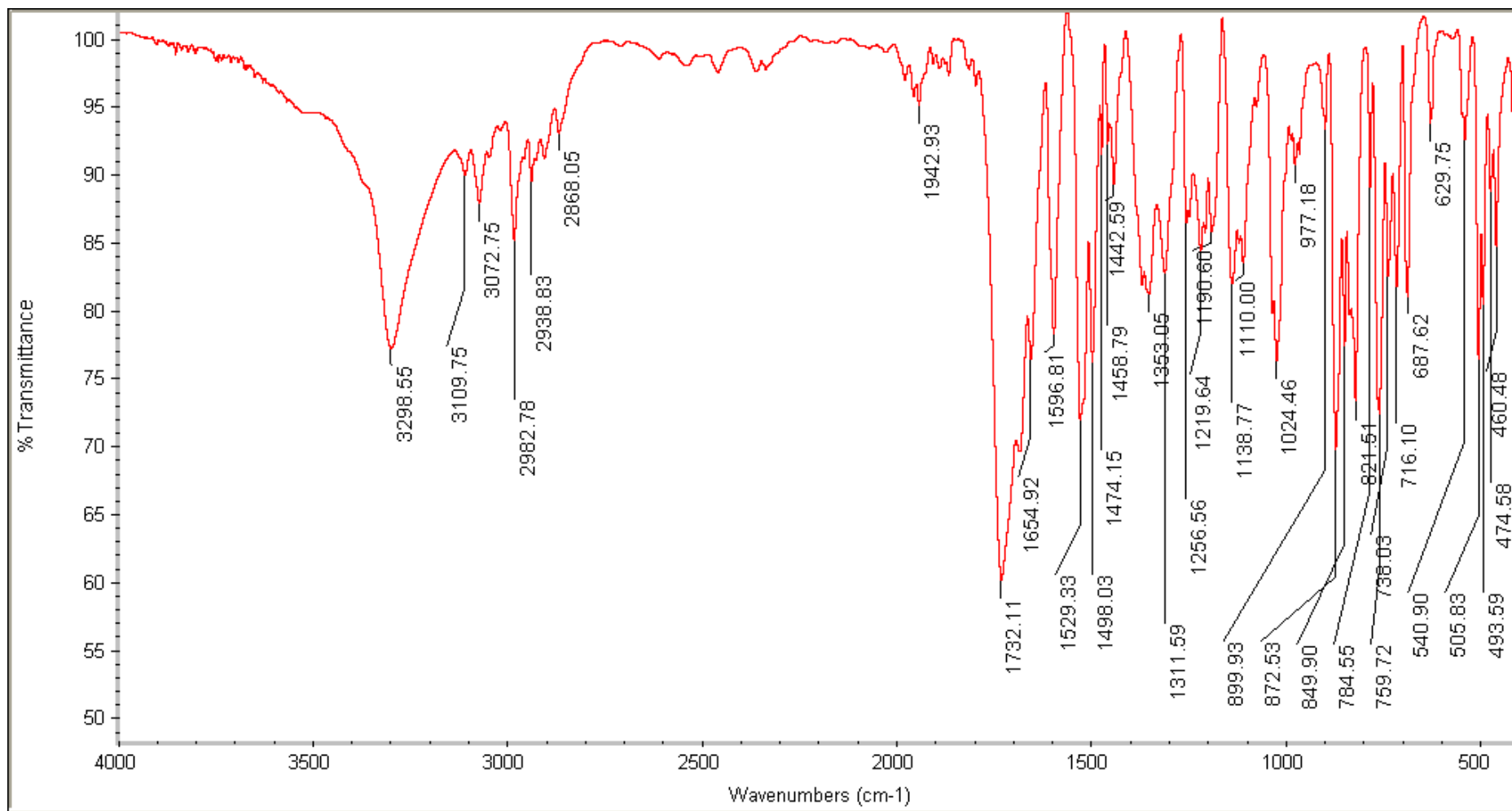


Figure 1. FT-IR spectrum of Ethyl 2-(4-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4a**).

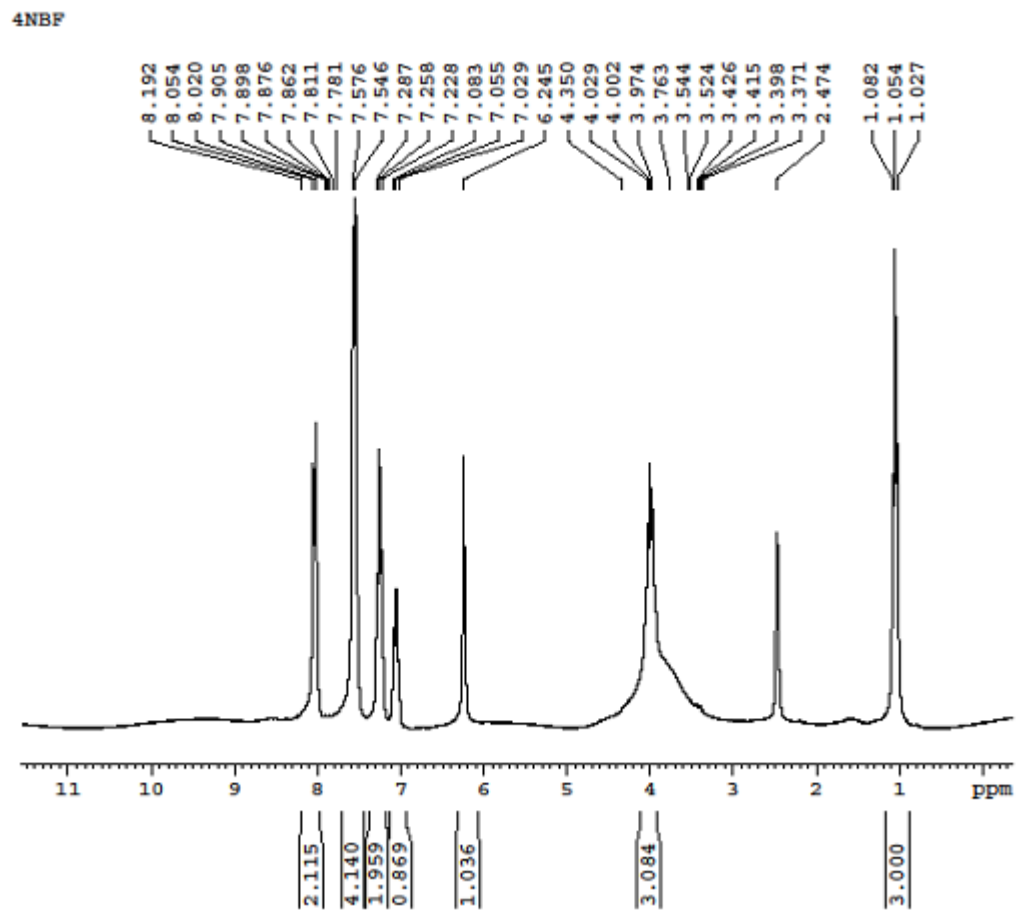


Figure 2. ^1H NMR (250.13 MHz, DMSO-d_6) of Ethyl 2-(4-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4a**).

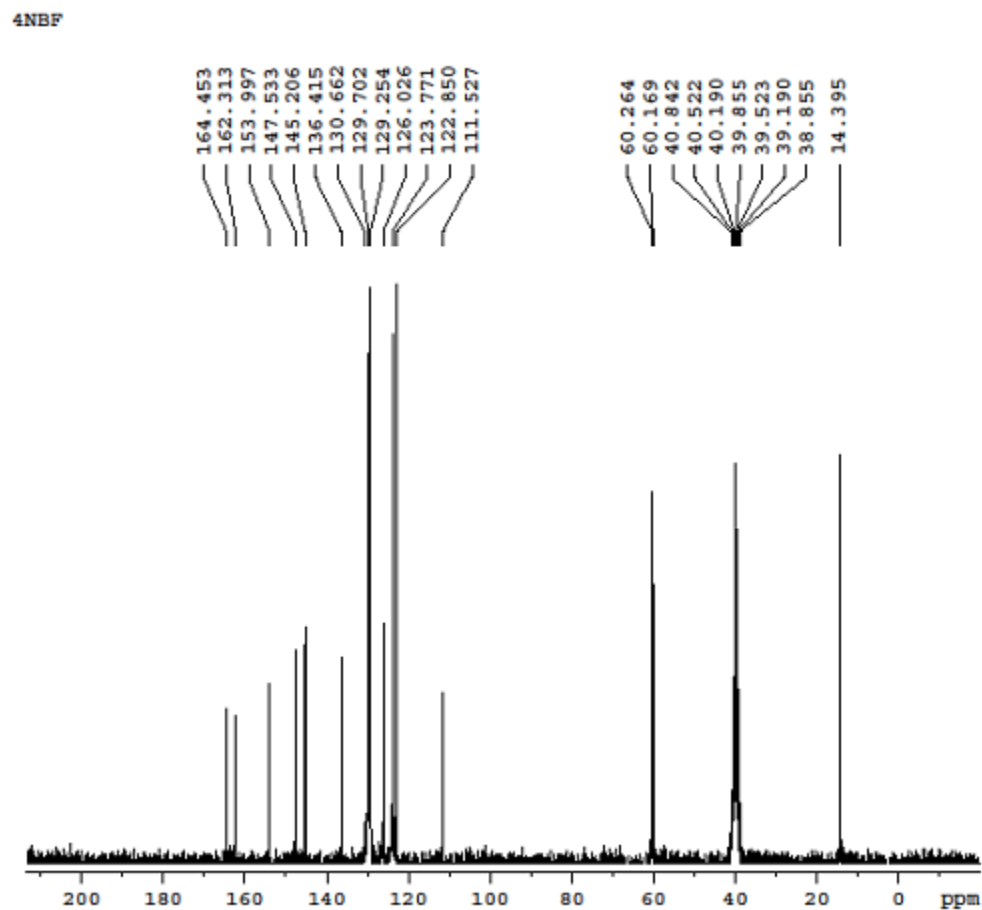


Figure 3. ^{13}C NMR (62.90 MHz, DMSO- d_6) of Ethyl 2-(4-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4a**).

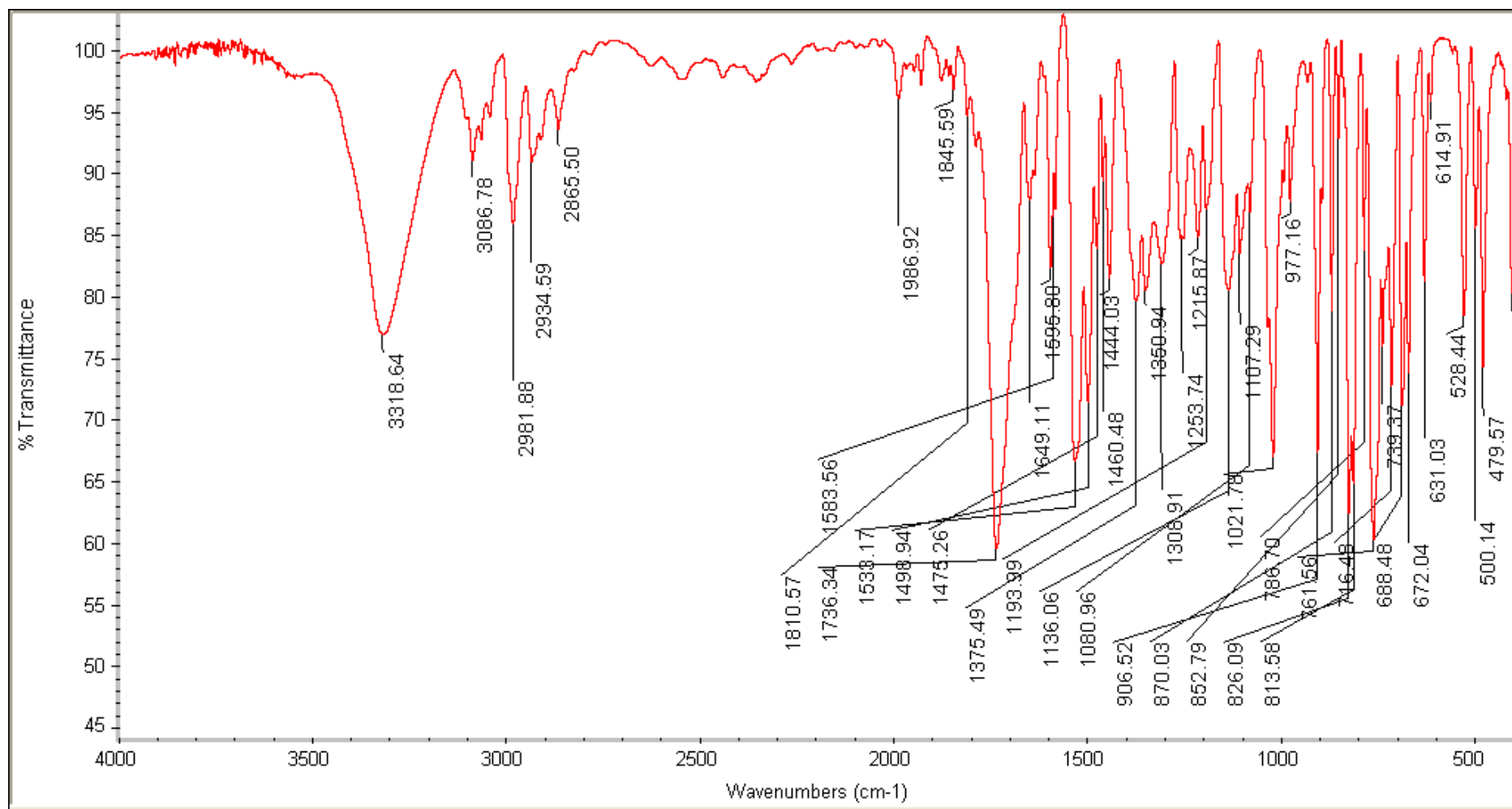


Figure 4. FT-IR spectrum of Ethyl 2-(3-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4b**).

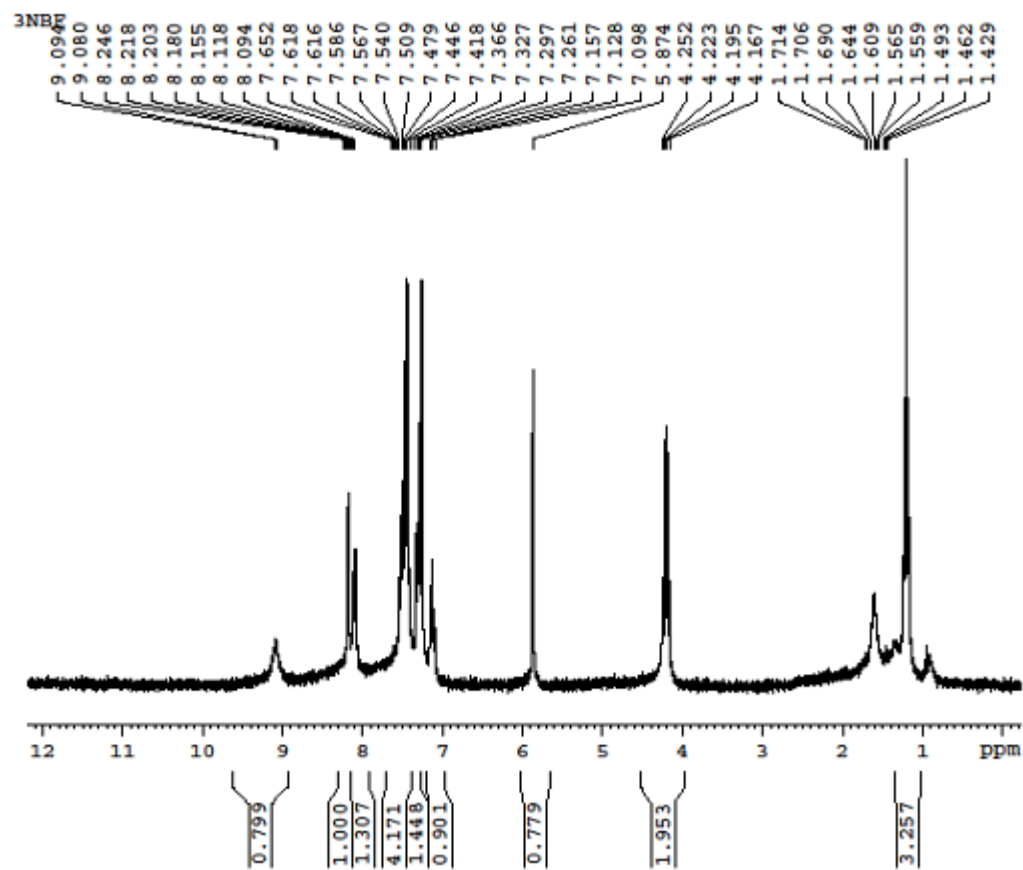


Figure 5. ¹H NMR (250.13 MHz, CDCl₃) spectrum of Ethyl 2-(3-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4b**).

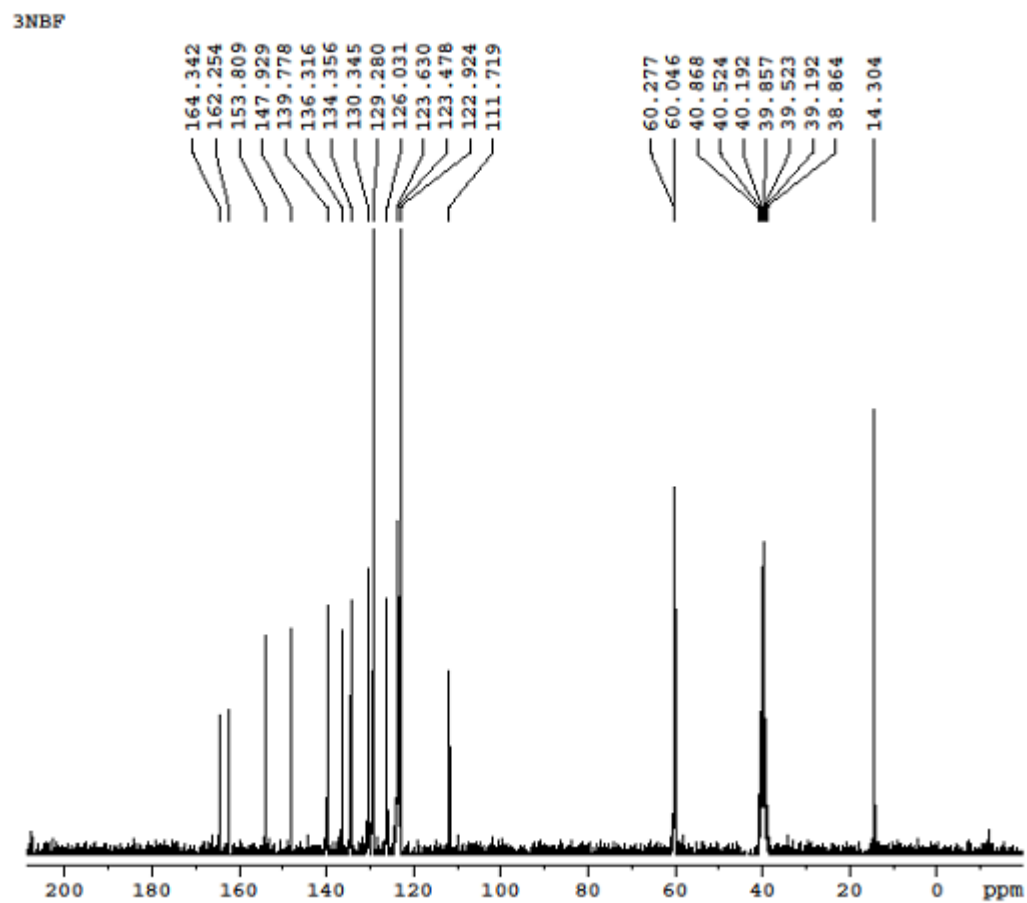


Figure 6. ^{13}C NMR (62.90 MHz, DMSO-d_6) spectrum of Ethyl 2-(3-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4b**).

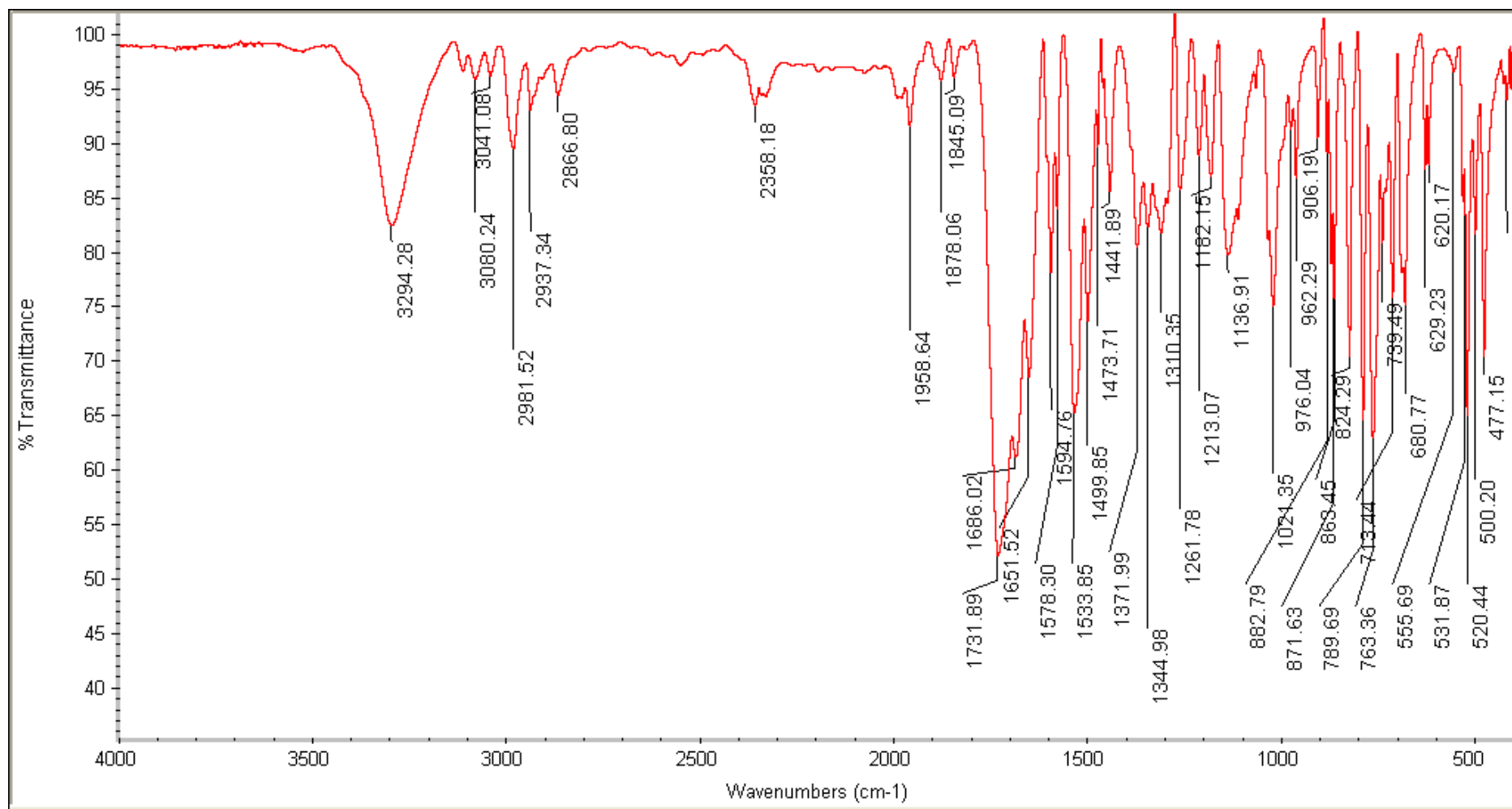


Figure 7. FT-IR spectrum of Ethyl 2-(2-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4c**).

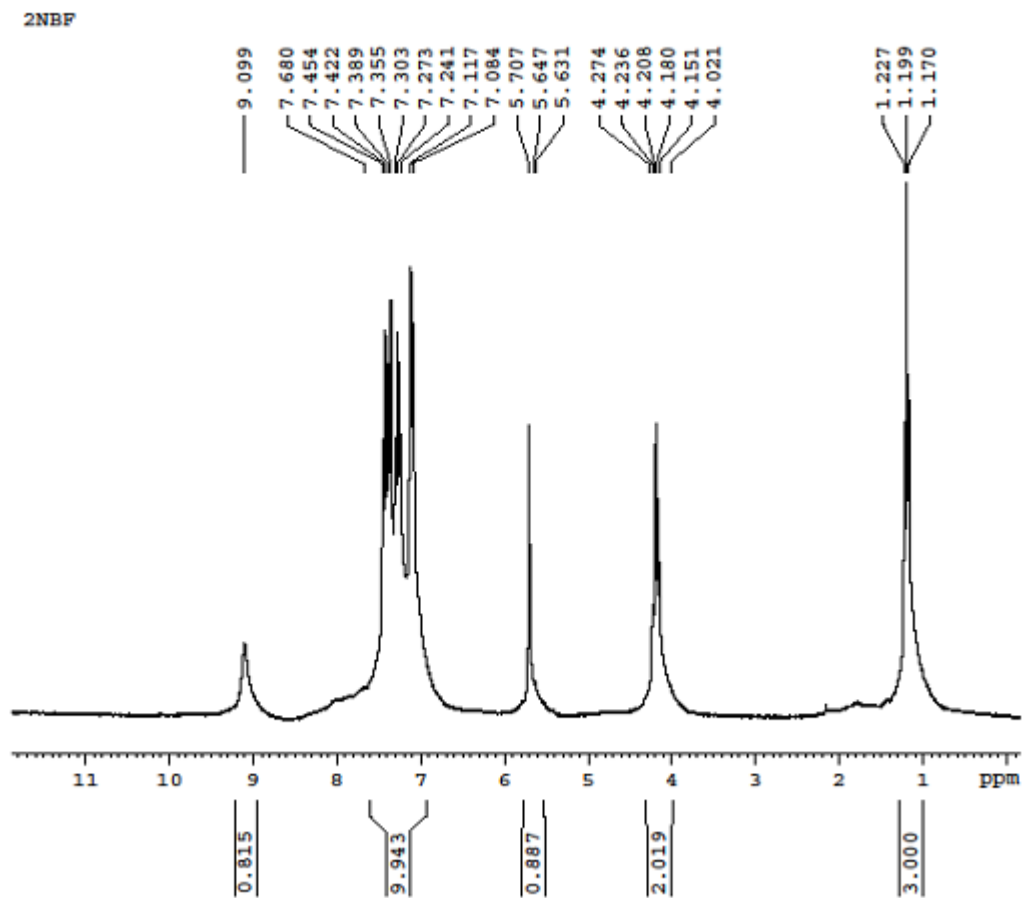


Figure 8. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 2-(2-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4c**).

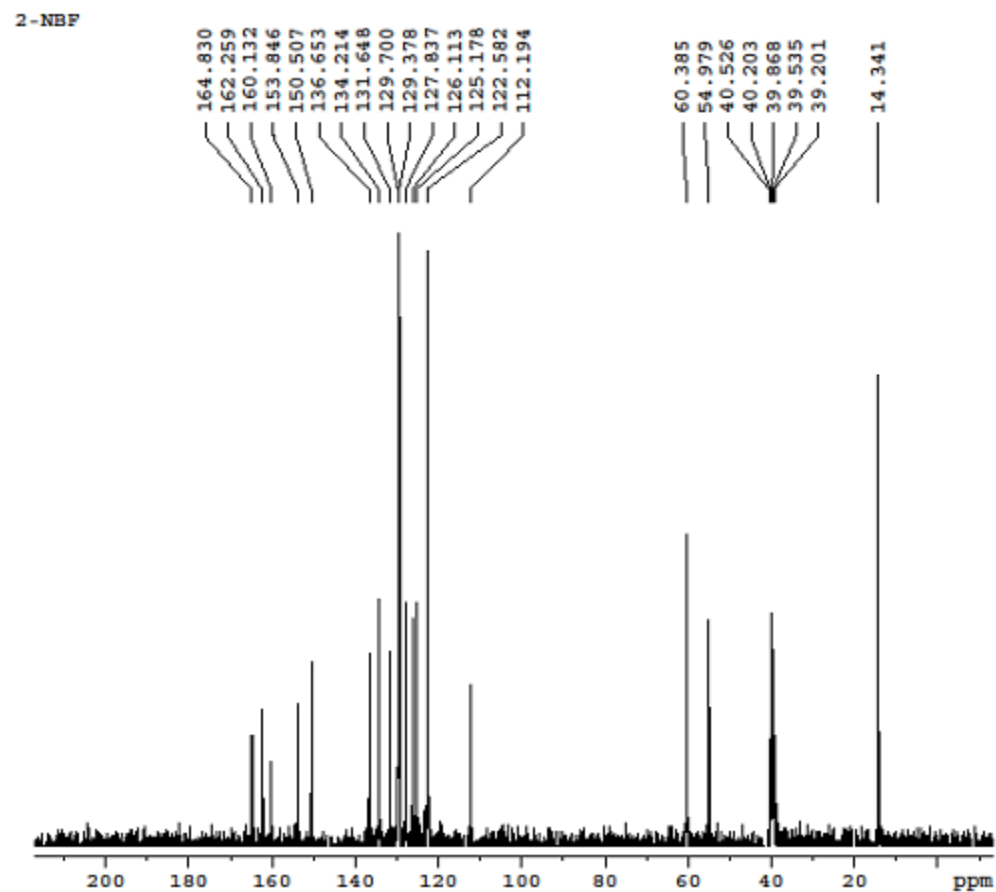


Figure 9. ^{13}C NMR (62.90 MHz, DMSO-d_6) spectrum of Ethyl 2-(2-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4c**).

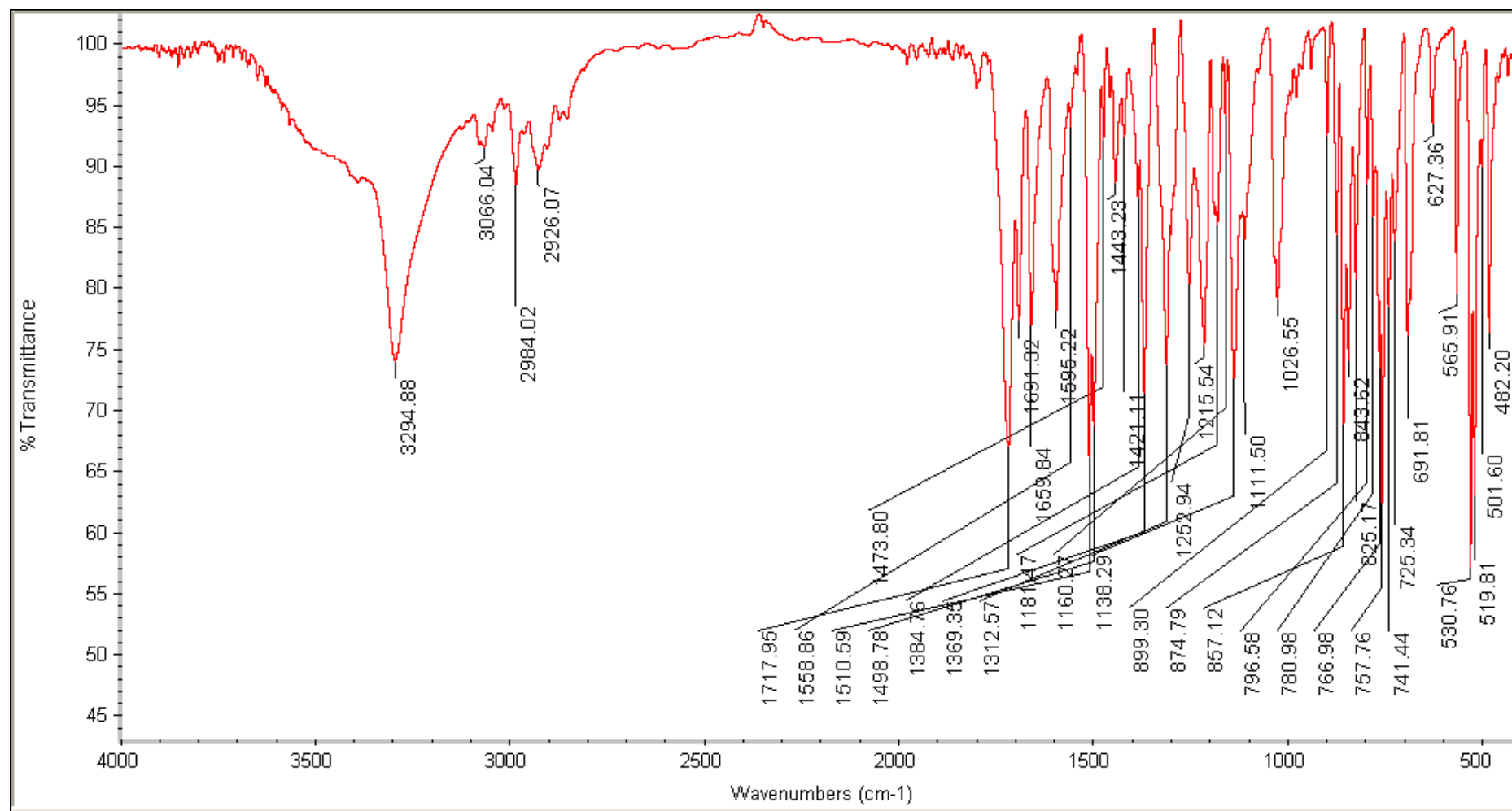


Figure 10. FT-IR spectrum of Ethyl 2-(4-fluorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4d**).

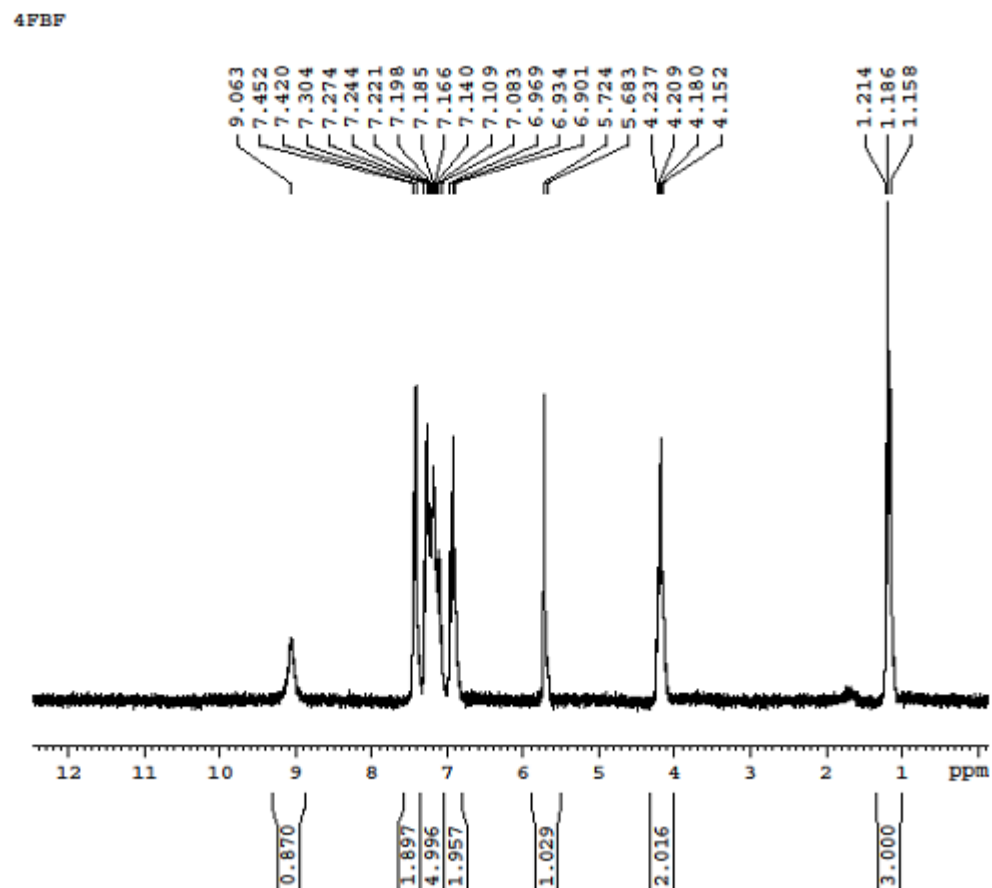


Figure 11. ¹H NMR (250.13 MHz, CDCl₃) spectrum of Ethyl 2-(4-fluorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4d**).

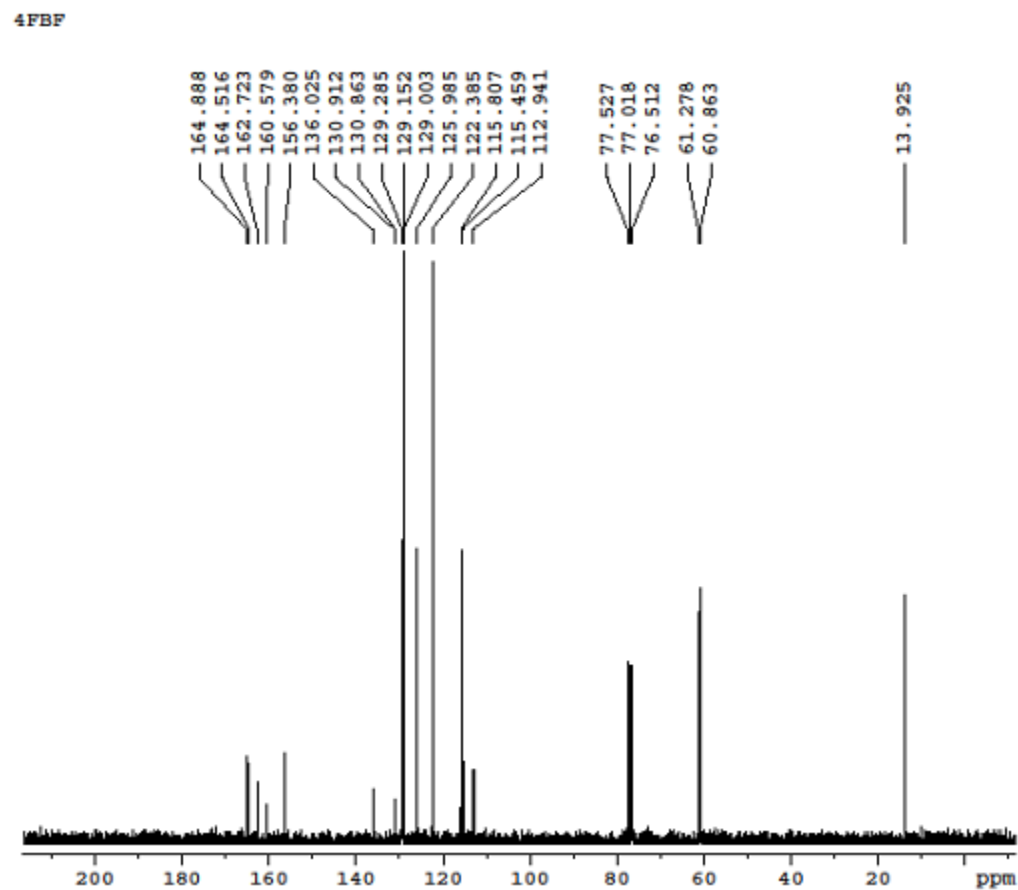


Figure 12. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 2-(4-fluorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4d**).

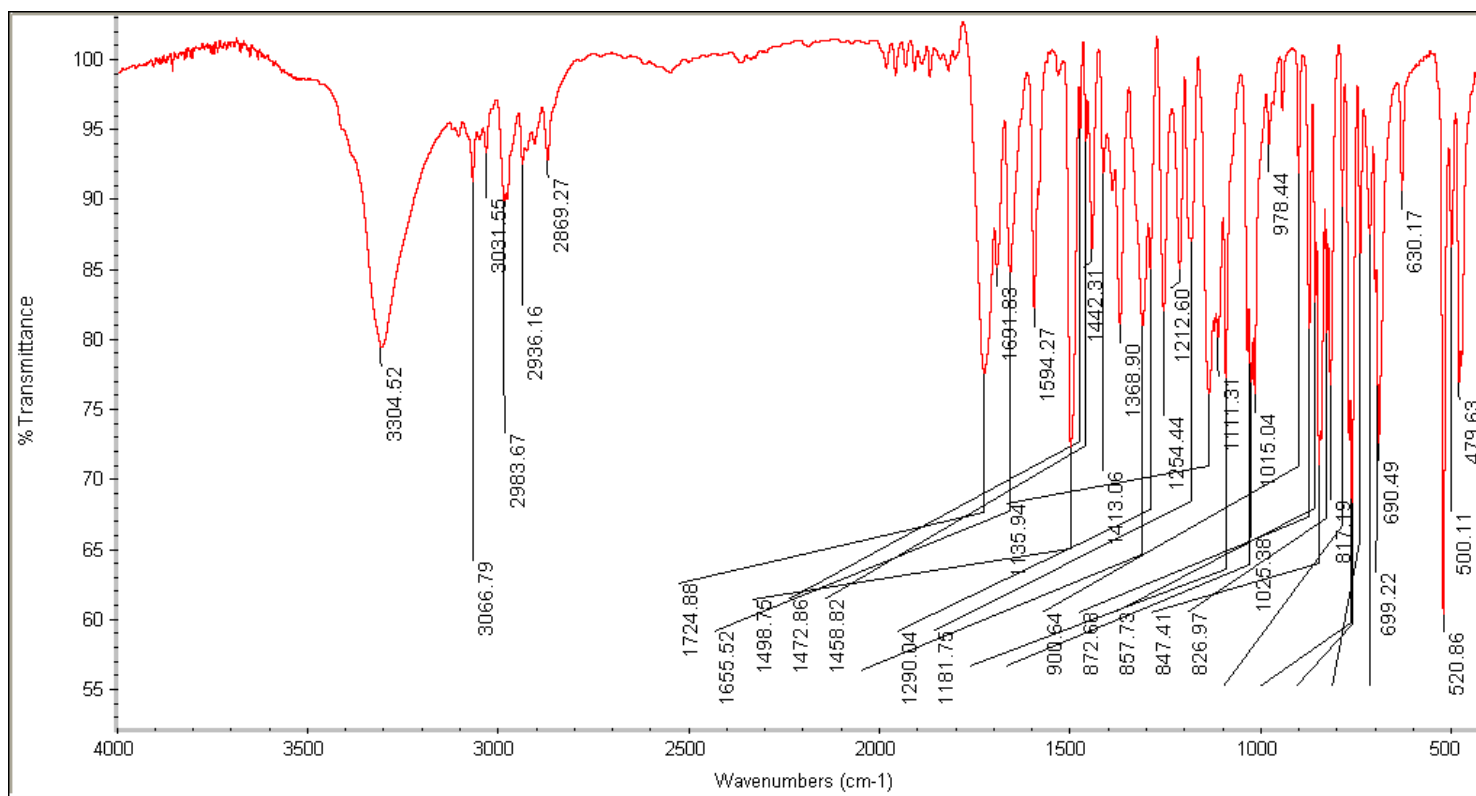


Figure 13. FT-IR spectrum of Ethyl 2-(4-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4e**).

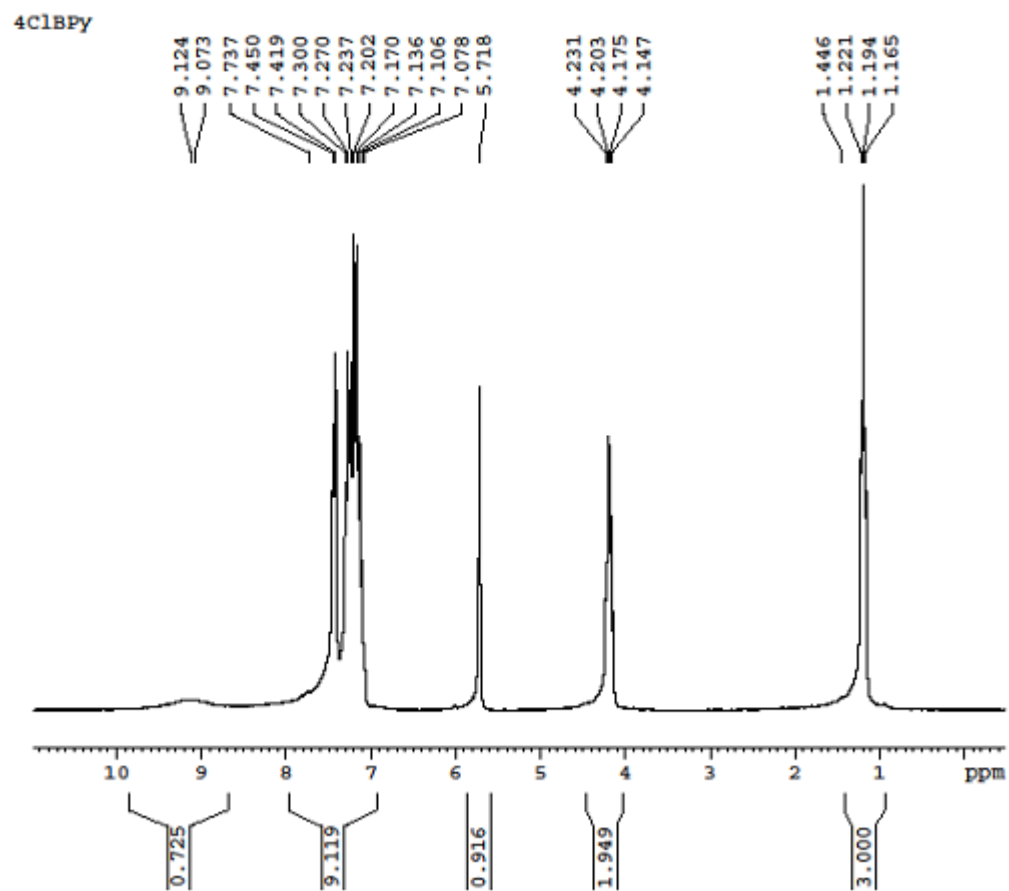


Figure 14. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 2-(4-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4e**).

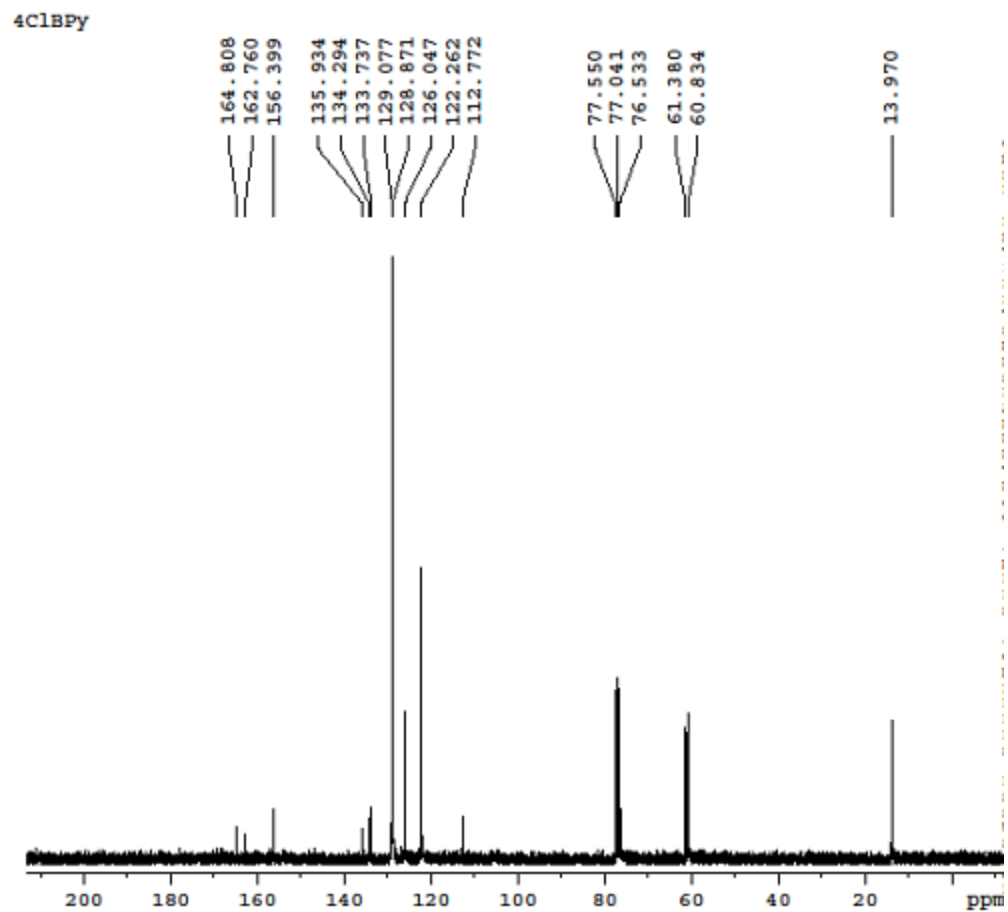


Figure 15. ¹³C NMR (62.90 MHz, CDCl₃) spectrum of Ethyl 2-(4-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4e**).

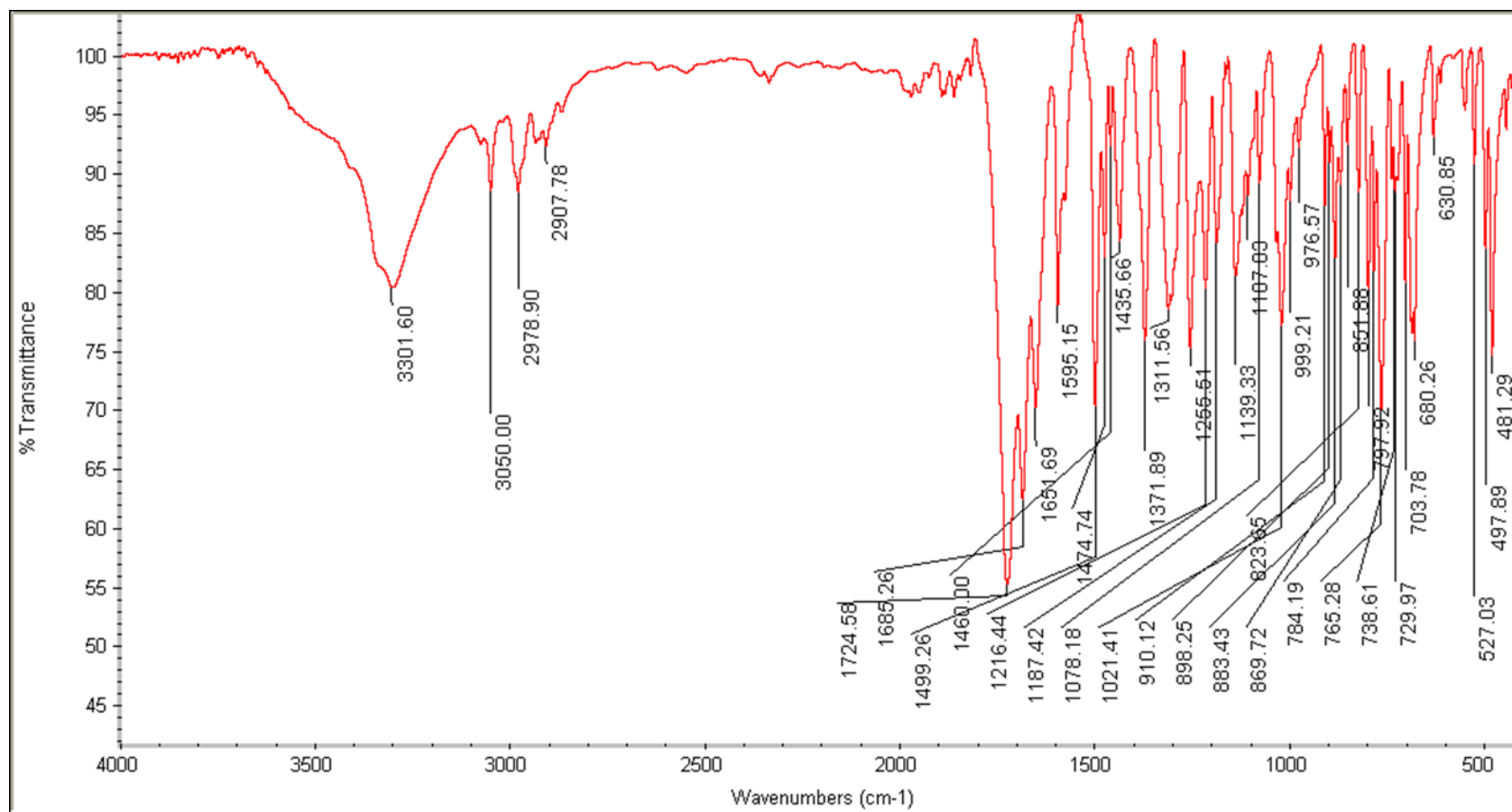
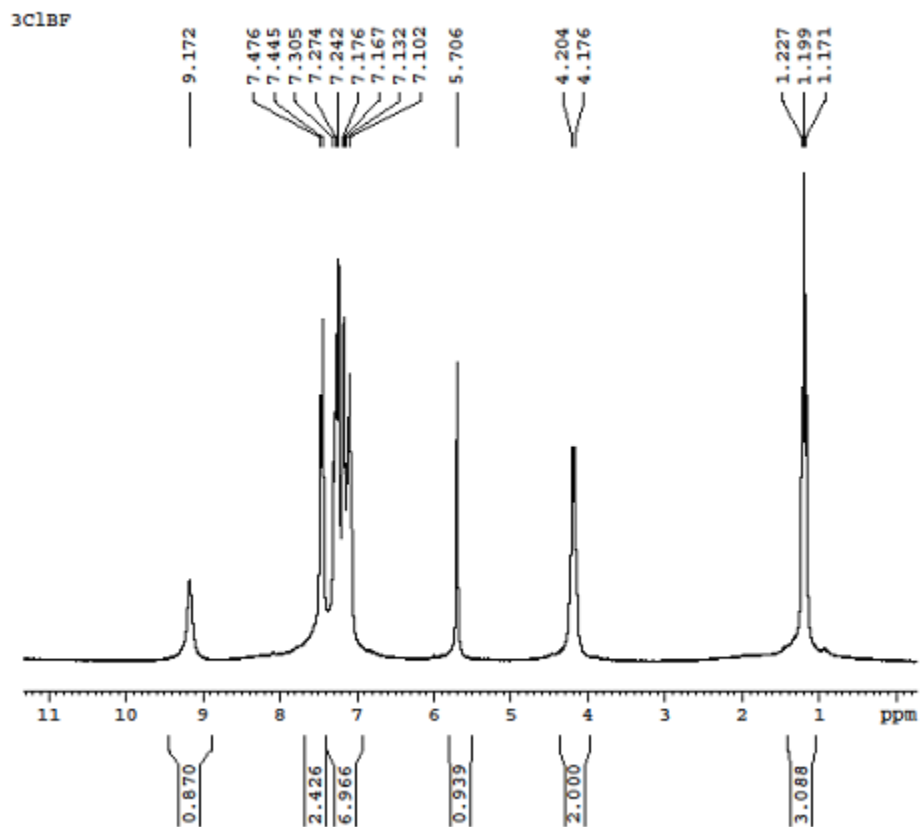


Figure 16. FT-IR spectrum of Ethyl 2-(3-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (4f)



Figur 17. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 2-(3-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4f**).

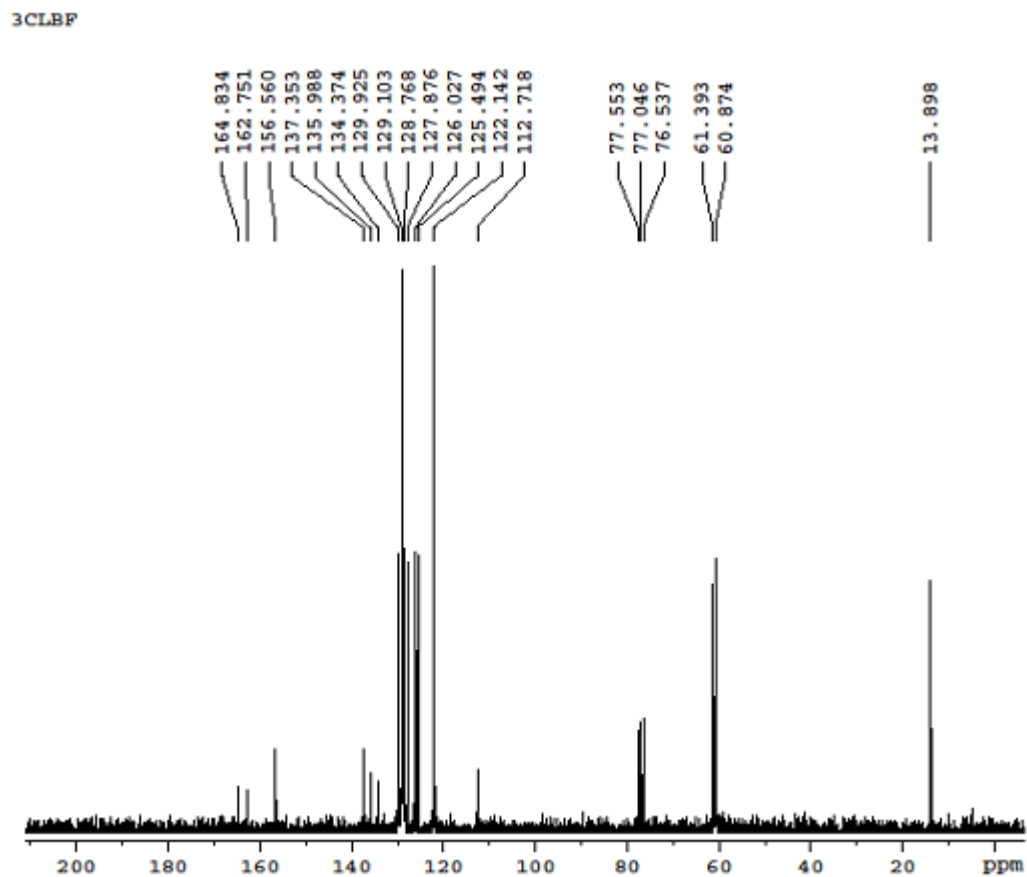


Figure 18. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 2-(3-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4f**).

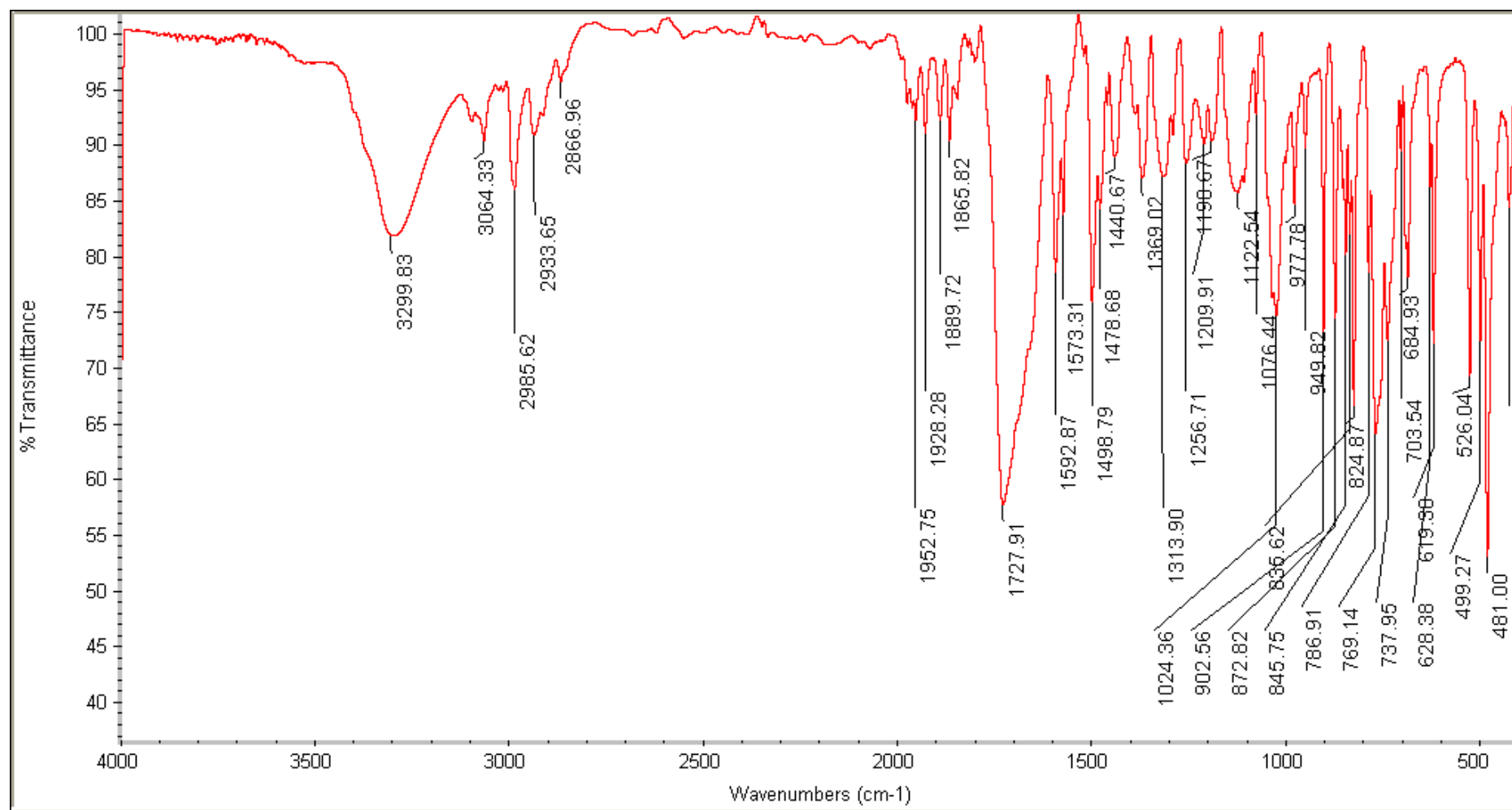


Figure 19. FT-IR spectrum of Ethyl 2-(2-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4g**)

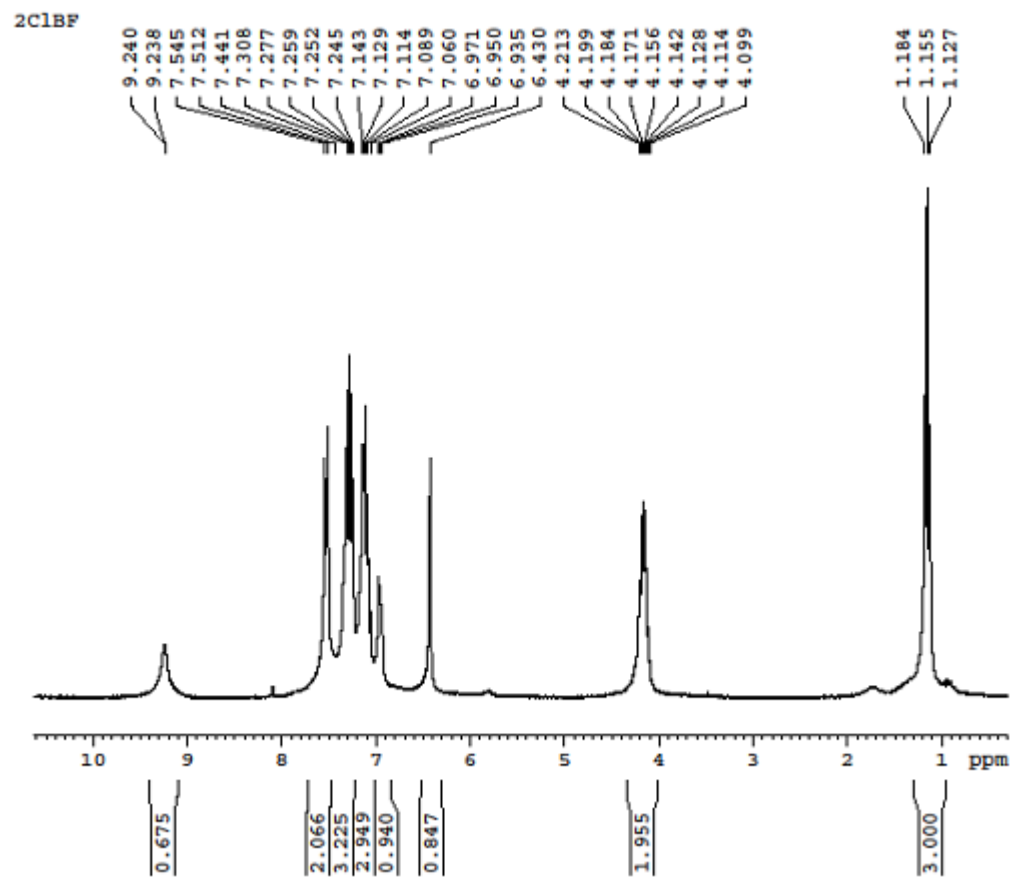


Figure 20. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 2-(2-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4g**)

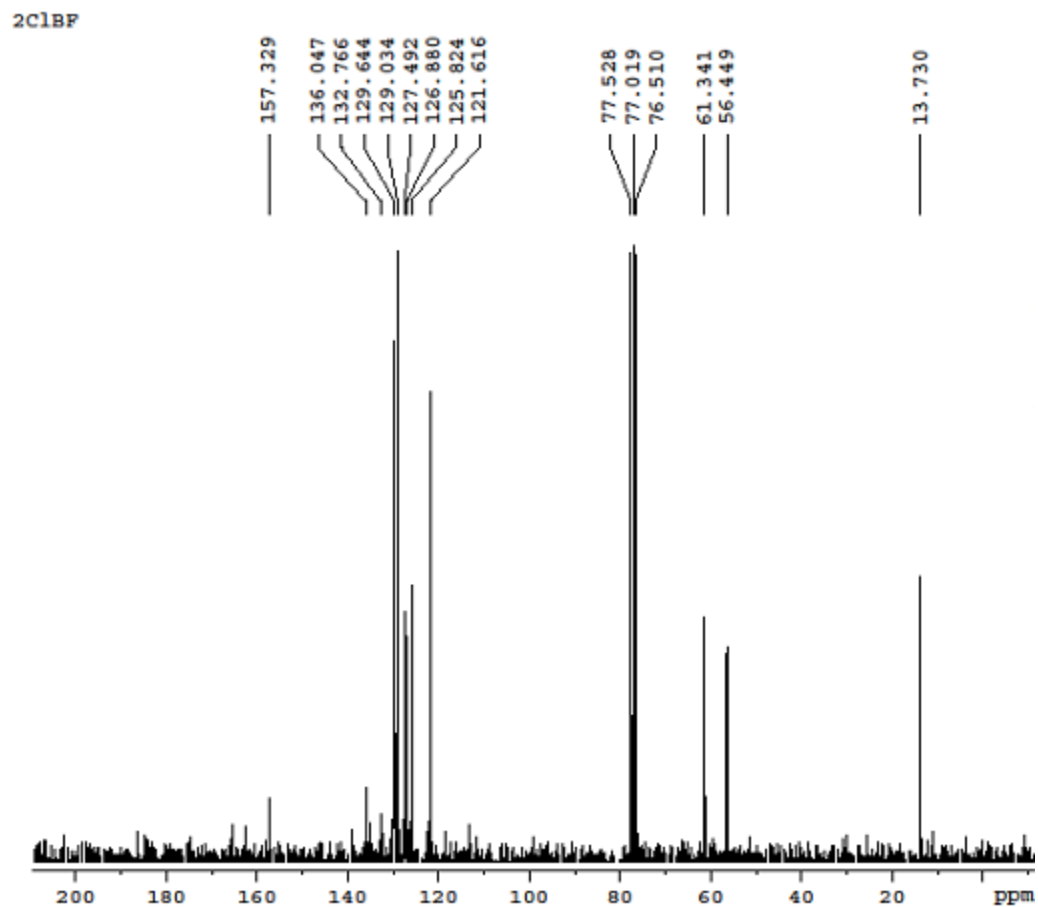


Figure 21. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 2-(2-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4g**)

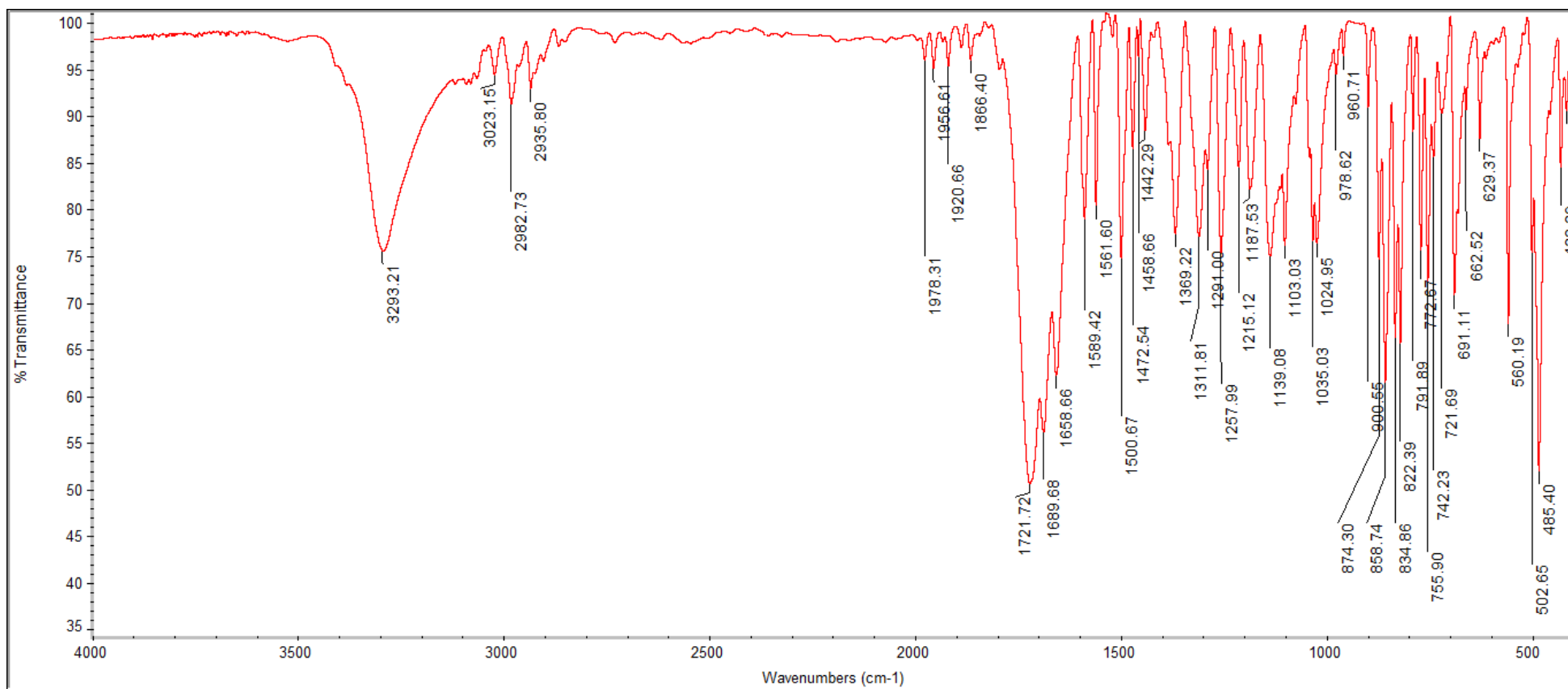


Figure 22. FT-IR spectrum of Ethyl 2-(2,4-dichlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4h**)

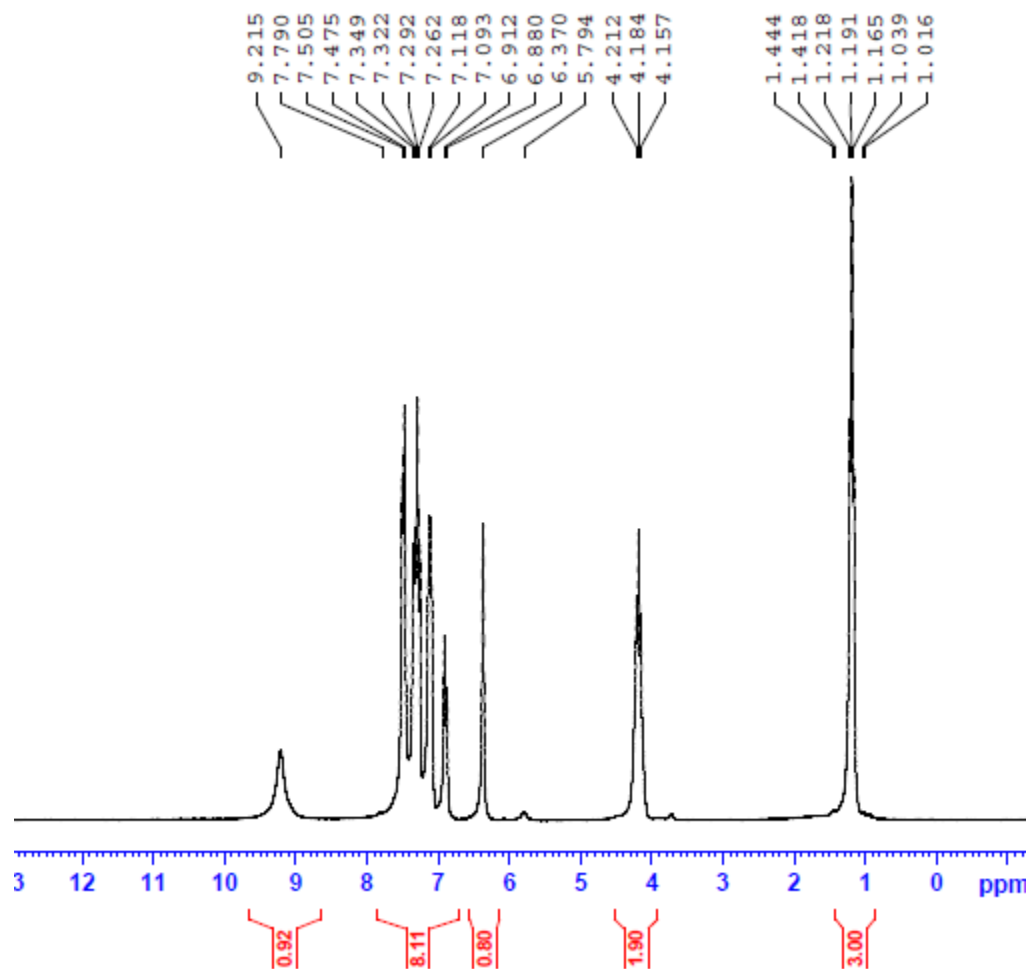


Figure 23. ¹H NMR (250.13 MHz, CDCl₃) spectrum of Ethyl 2-(2,4-dichlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (4h)

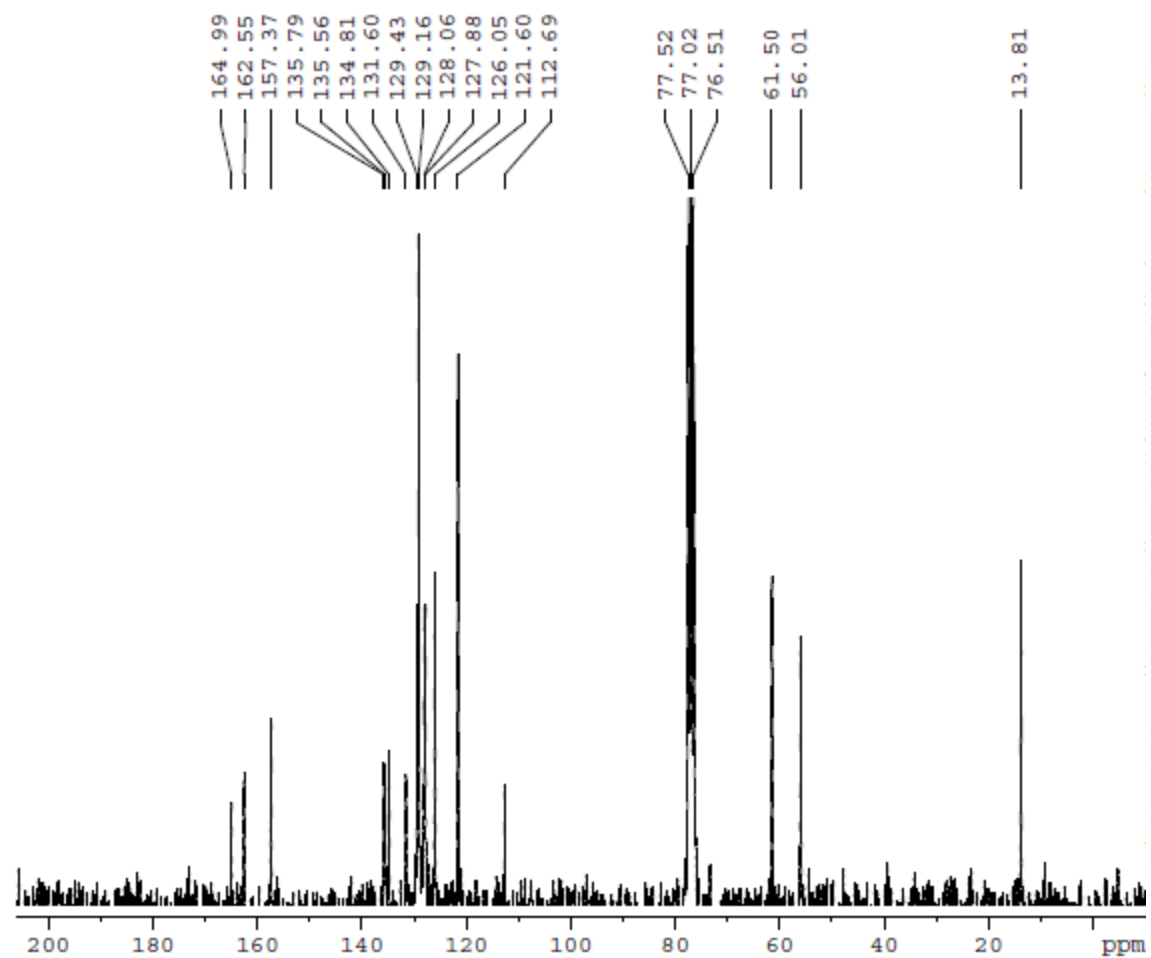


Figure 24. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 2-(2,4-dichlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4h**)

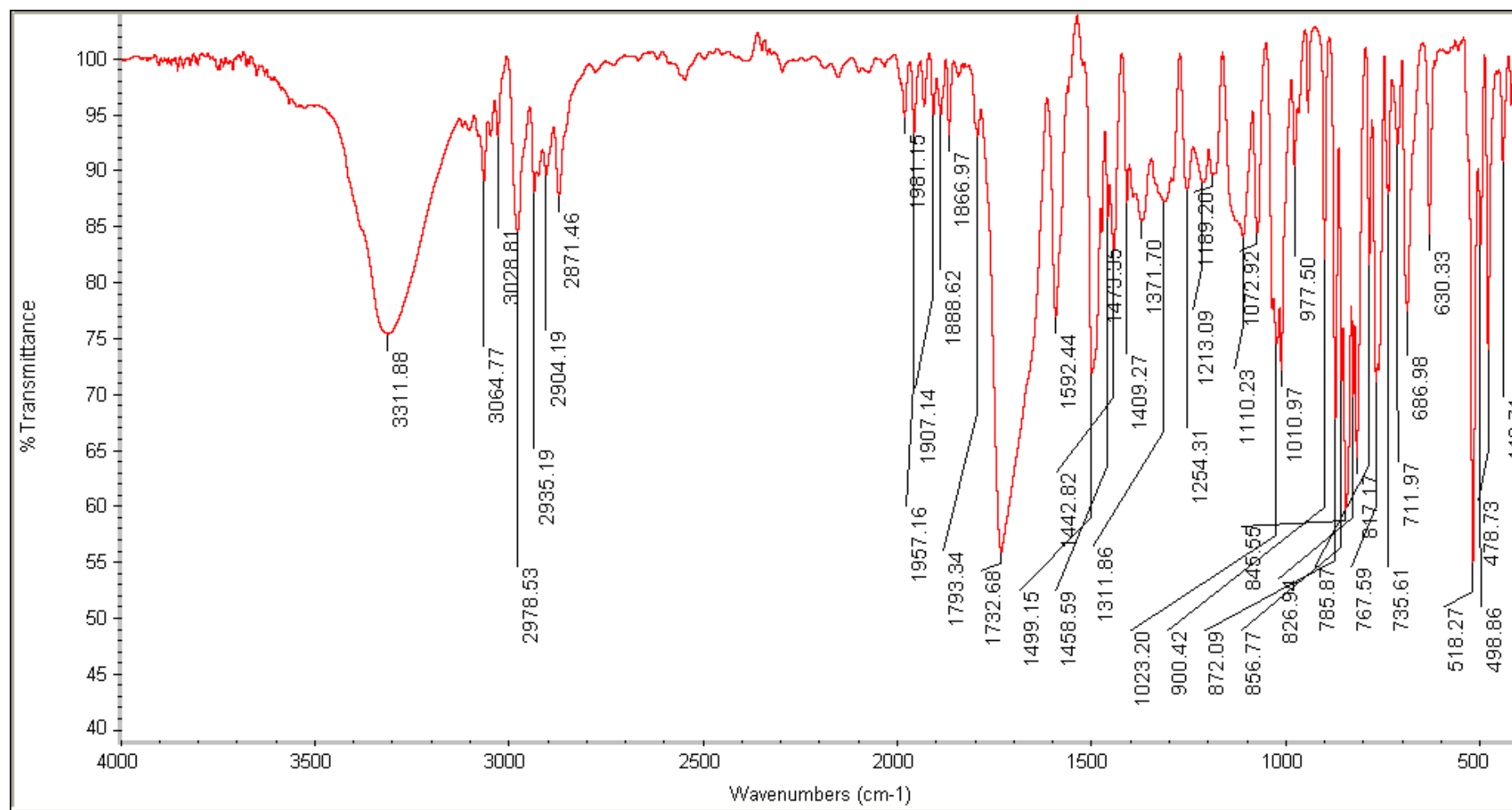


Figure 25. FT-IR spectrum of Ethyl 2-(4-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4i**)

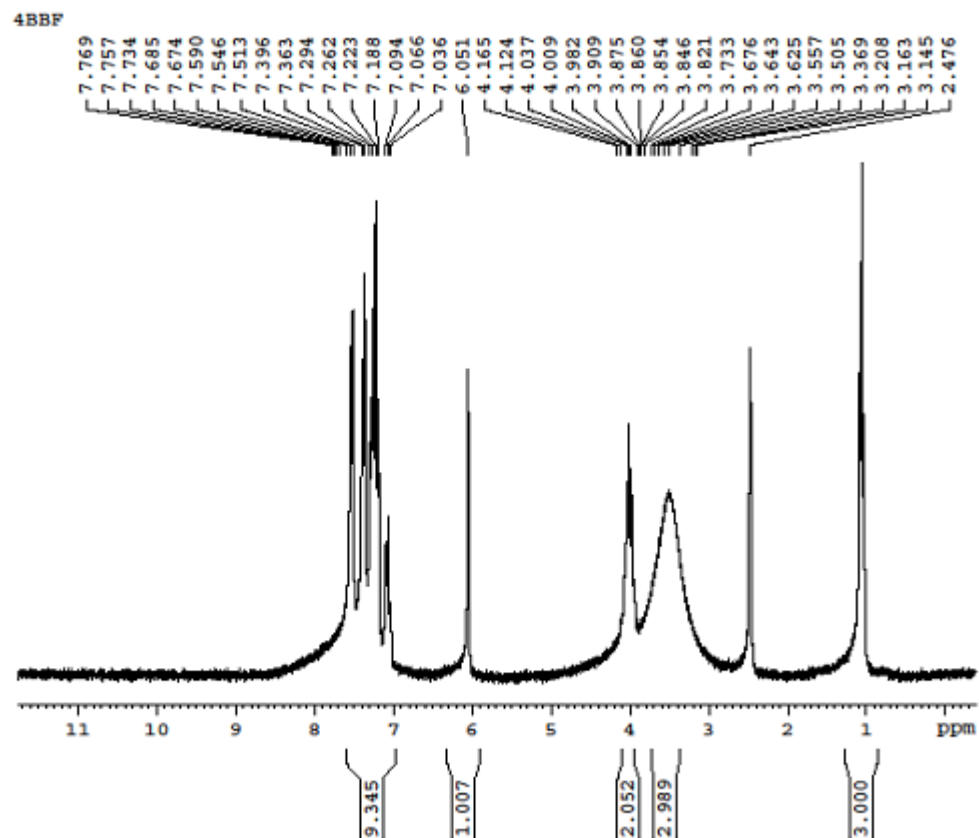


Figure 26. ^1H NMR (250.13 MHz, DMSO-d_6) spectrum of Ethyl 2-(4-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4i**)

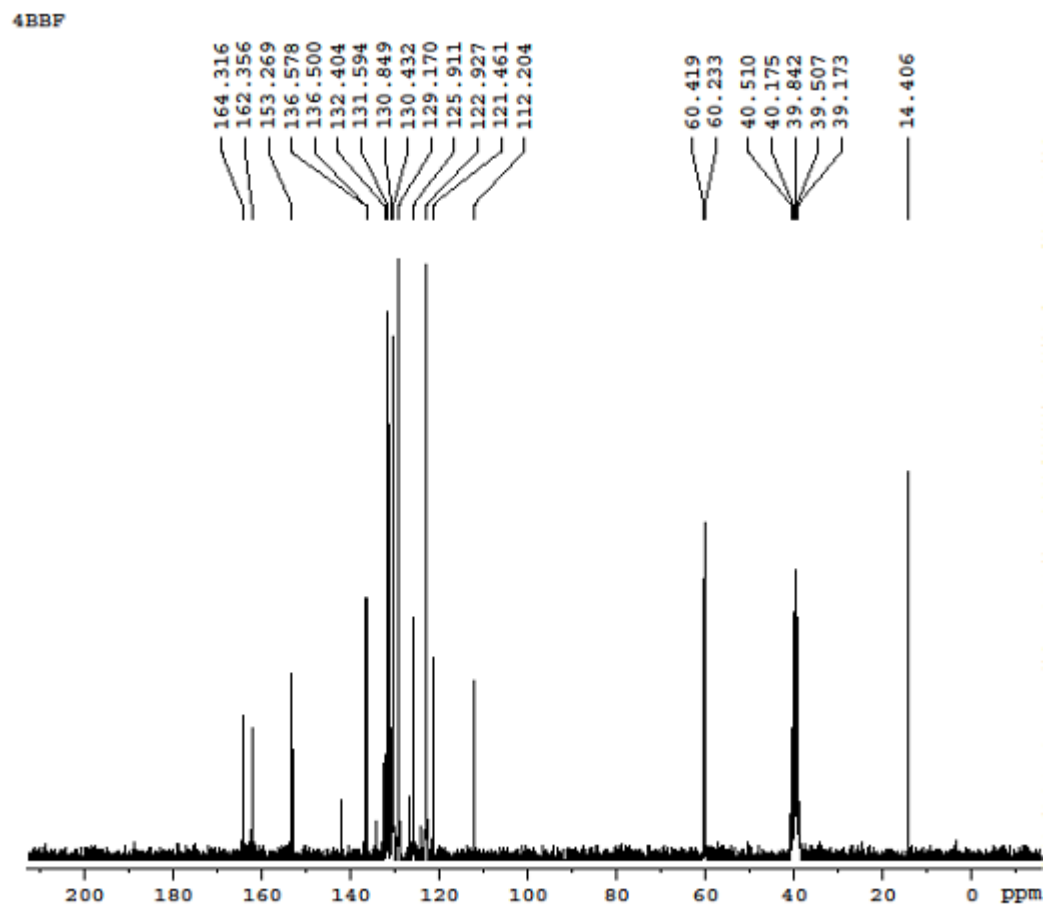


Figure 27. ^{13}C NMR (62.90 MHz, DMSO-d_6) spectrum of Ethyl 2-(4-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4e**)

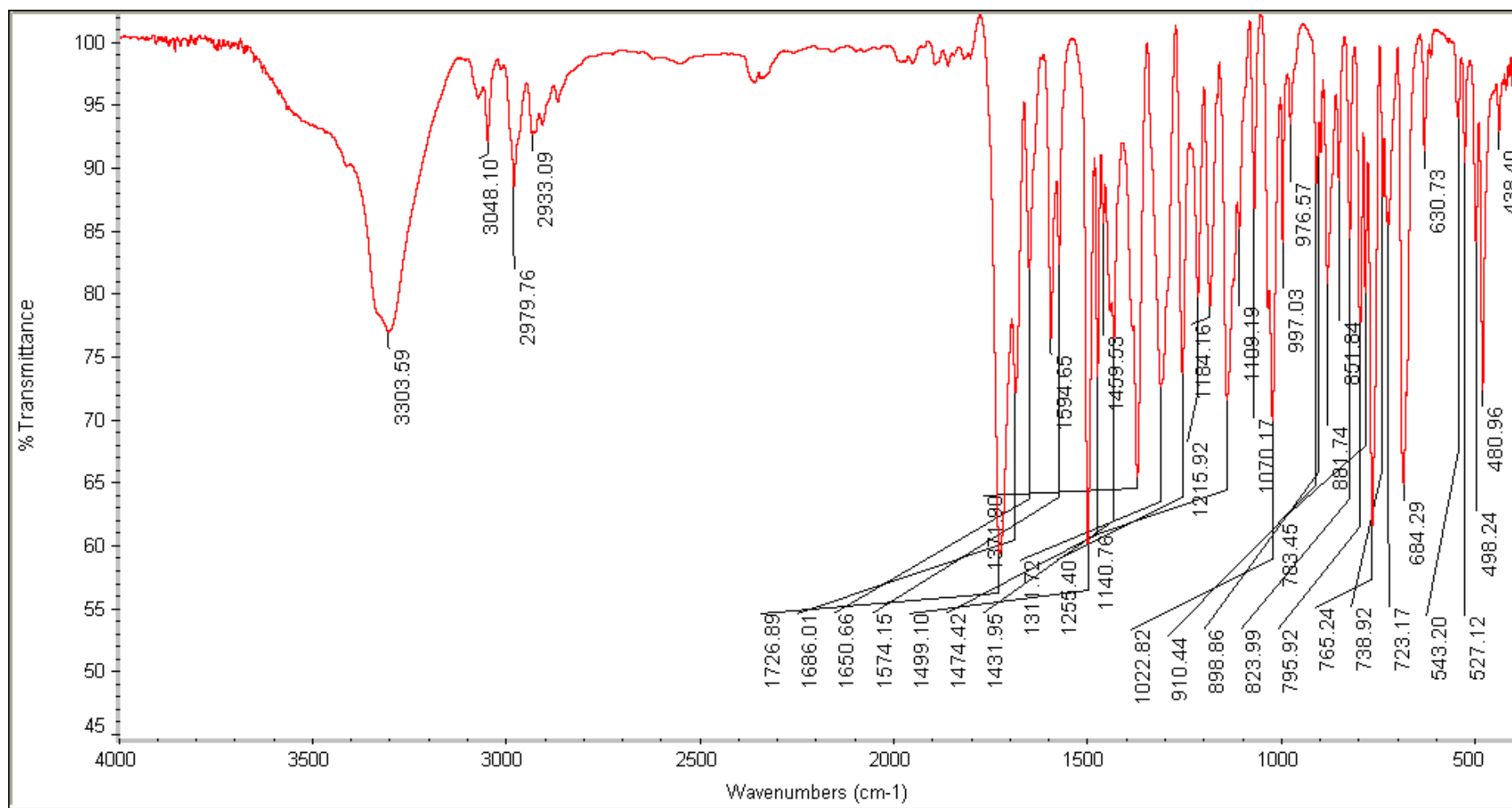


Figure 28. FT-IR spectrum of Ethyl 2-(3-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4j**)

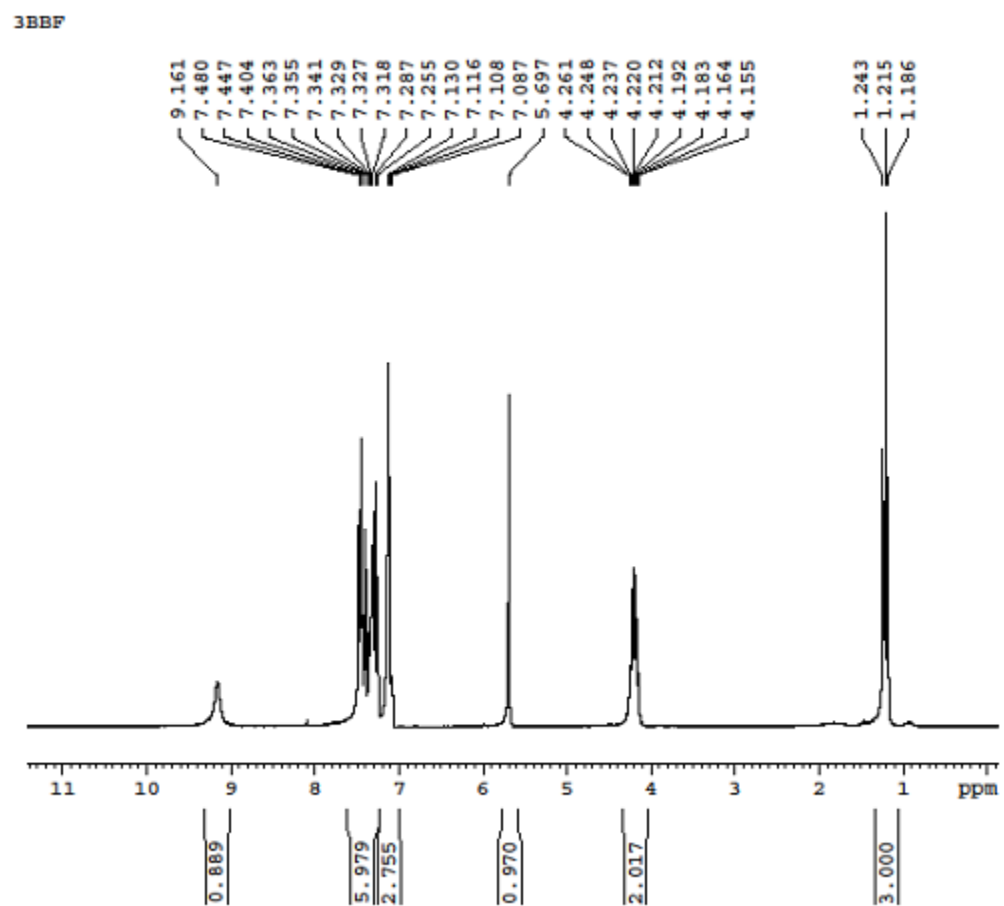


Figure 29. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 2-(3-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4j**)

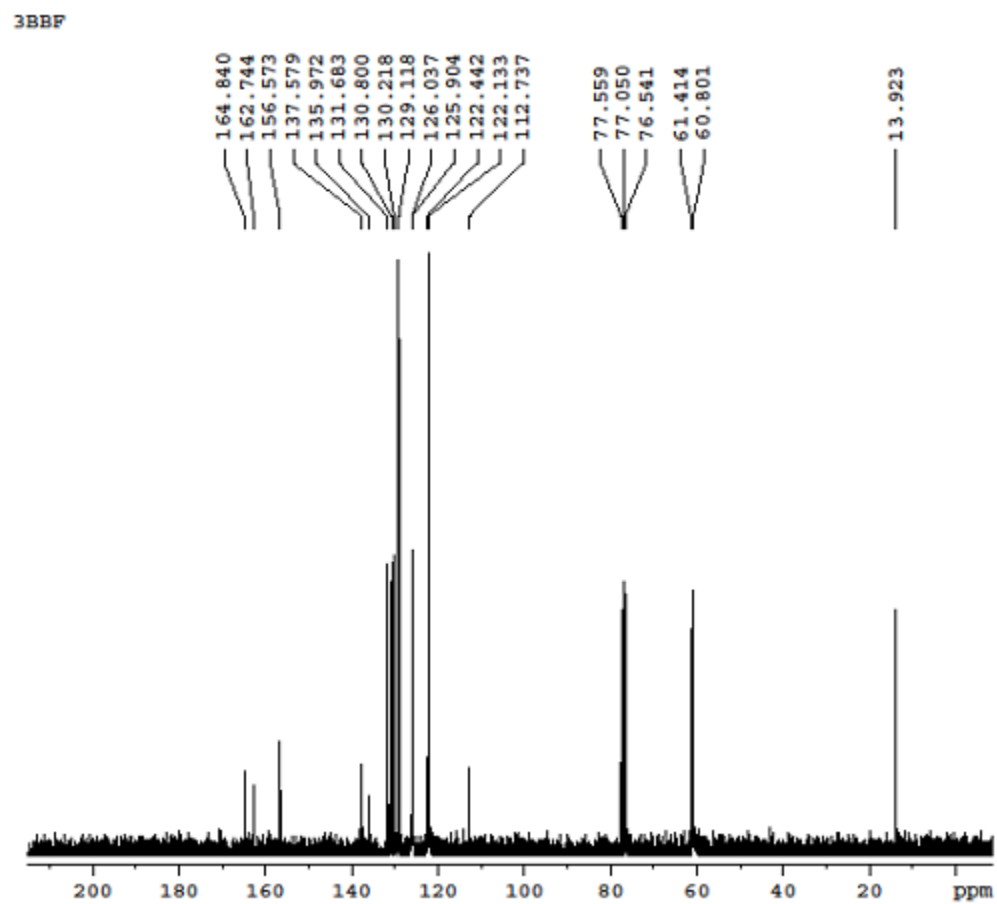


Figure 30. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 2-(4-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4j**)

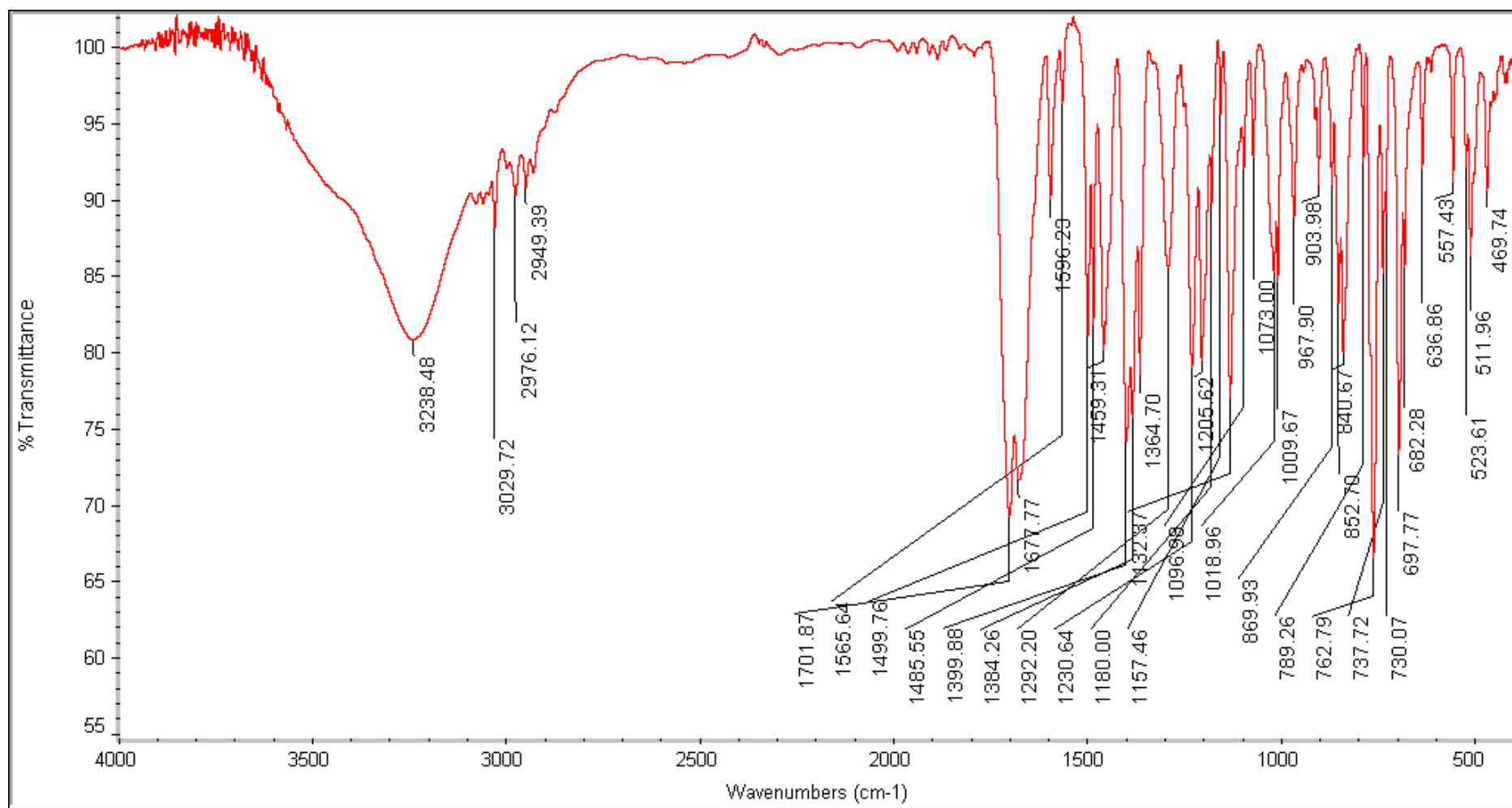


Figure 31. FT-IR spectrum of Ethyl 2-([1, 1'-biphenyl]-4-yl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4k**).

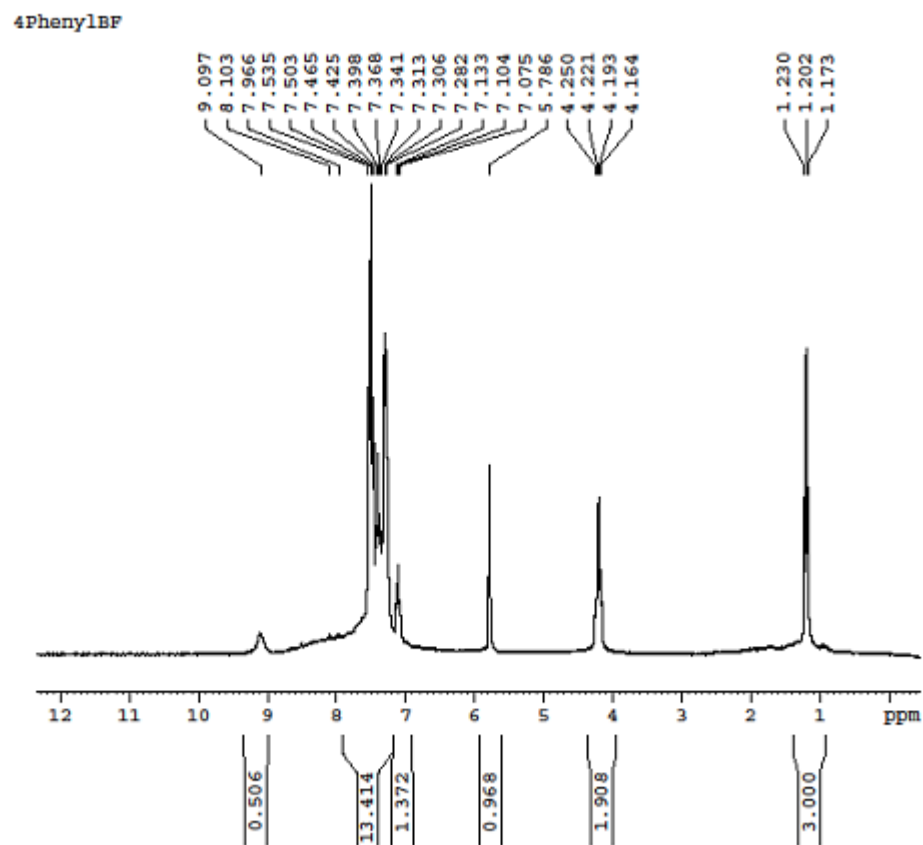


Figure 32. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 2-([1,1'-biphenyl]-4-yl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4k**)

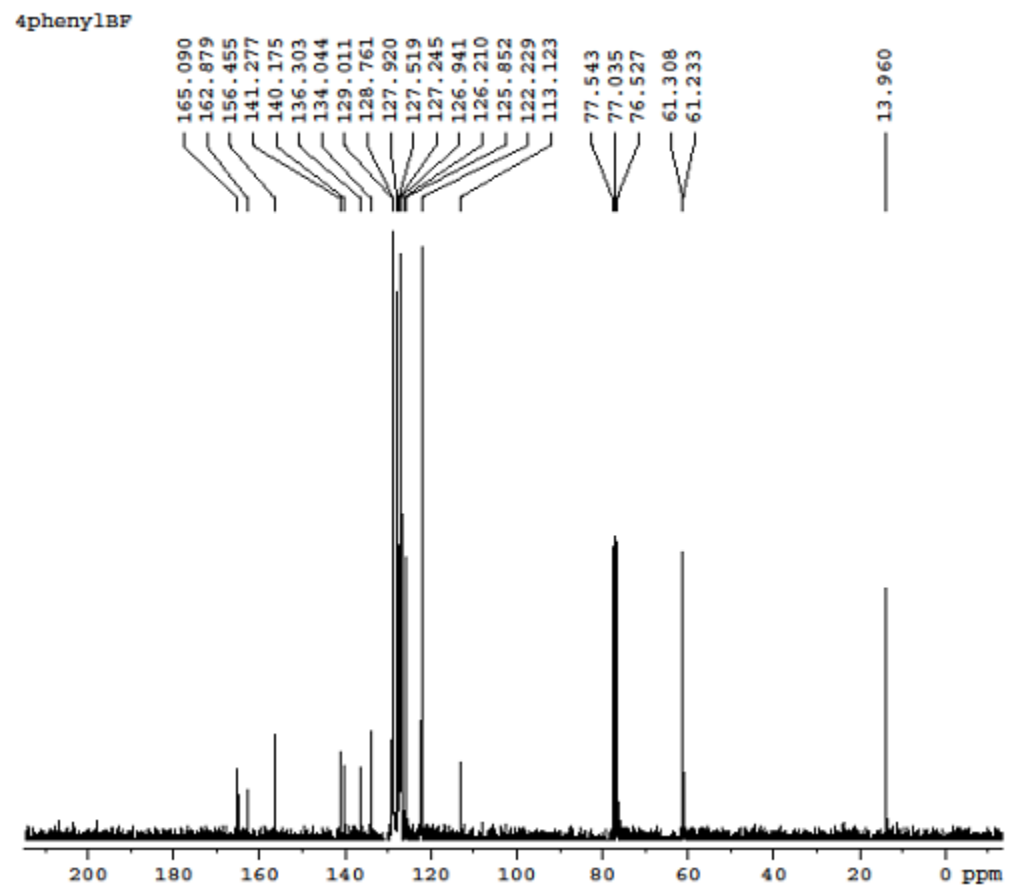


Figure 33. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 2-([1,1'-biphenyl]-4-yl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (4k)

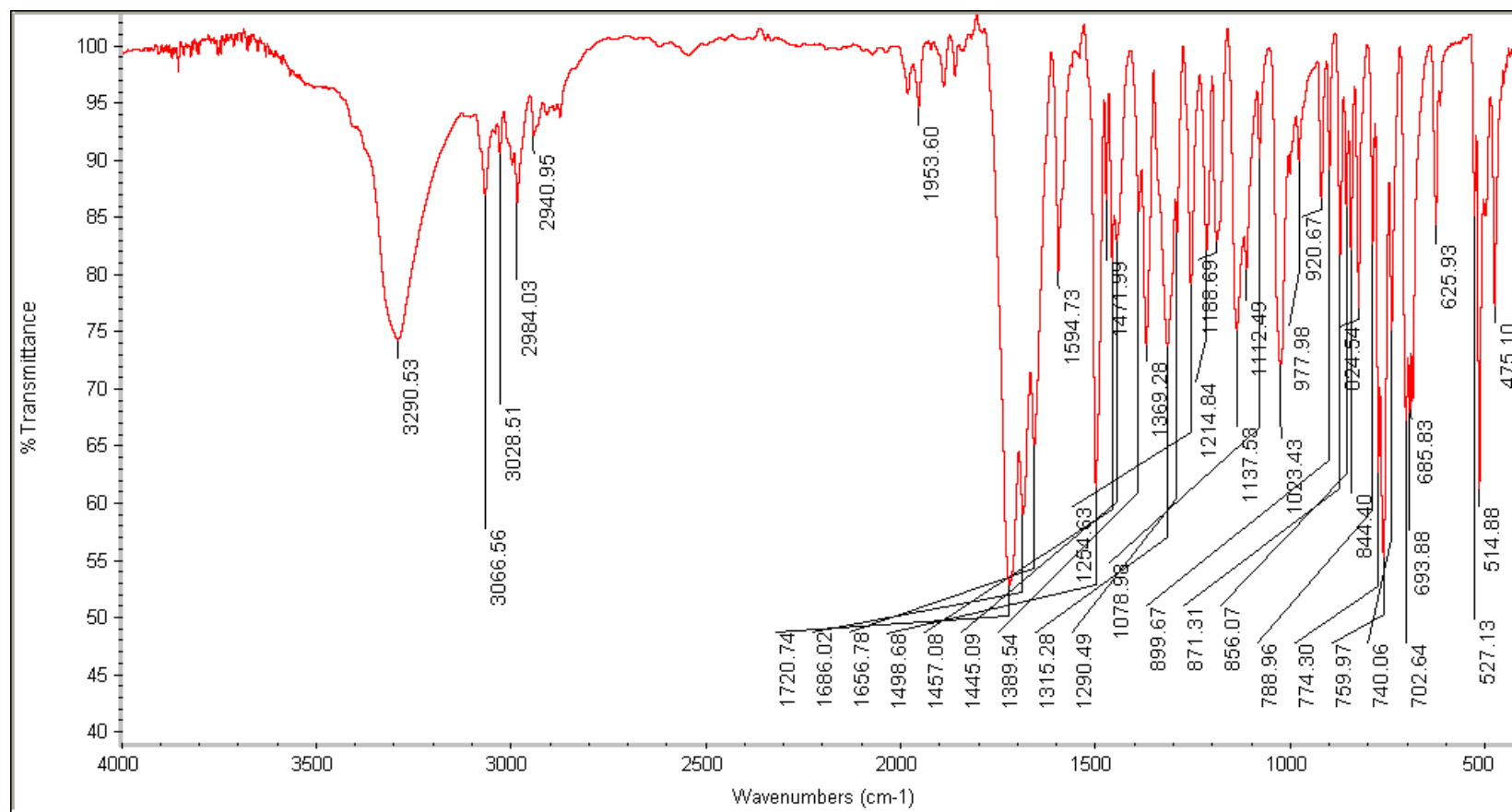


Figure 34. FT-IR spectrum of Ethyl 4-hydroxy-5-oxo-1,2-diphenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4I**)

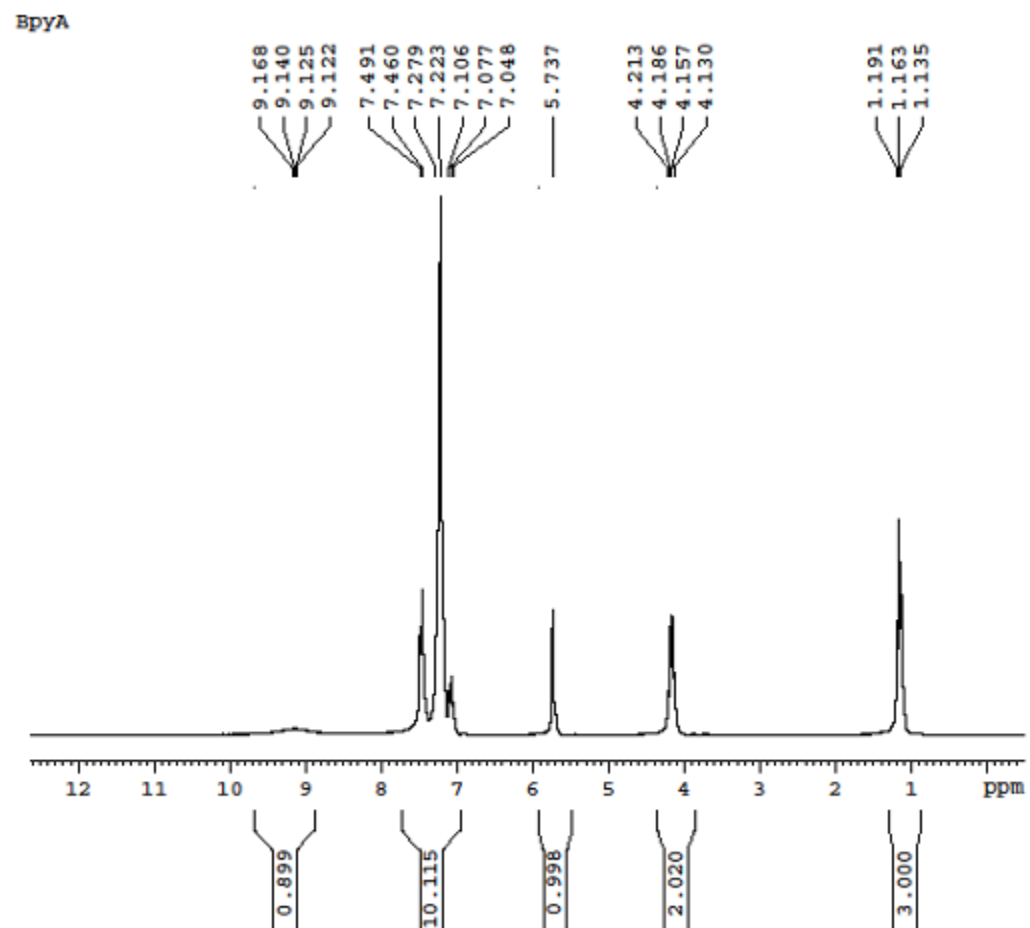


Figure 35. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-5-oxo-1,2-diphenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4l**)

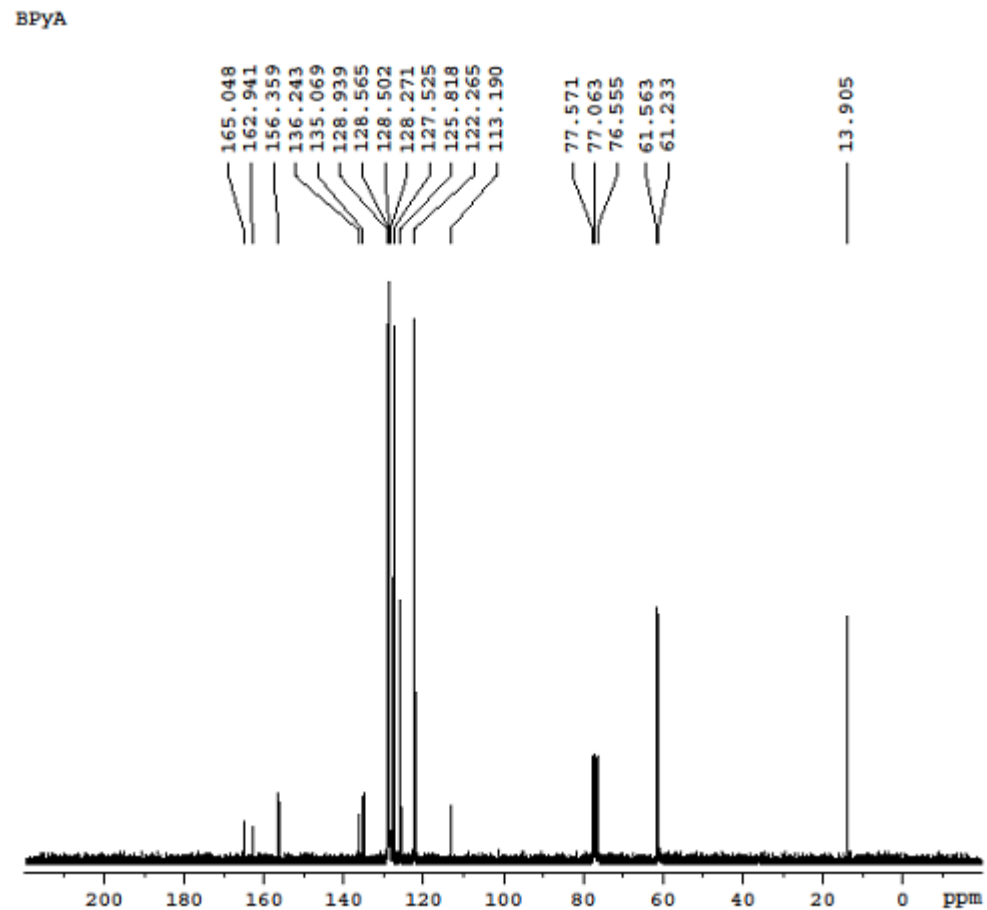


Figure 36. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-5-oxo-1,2-diphenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4I**)

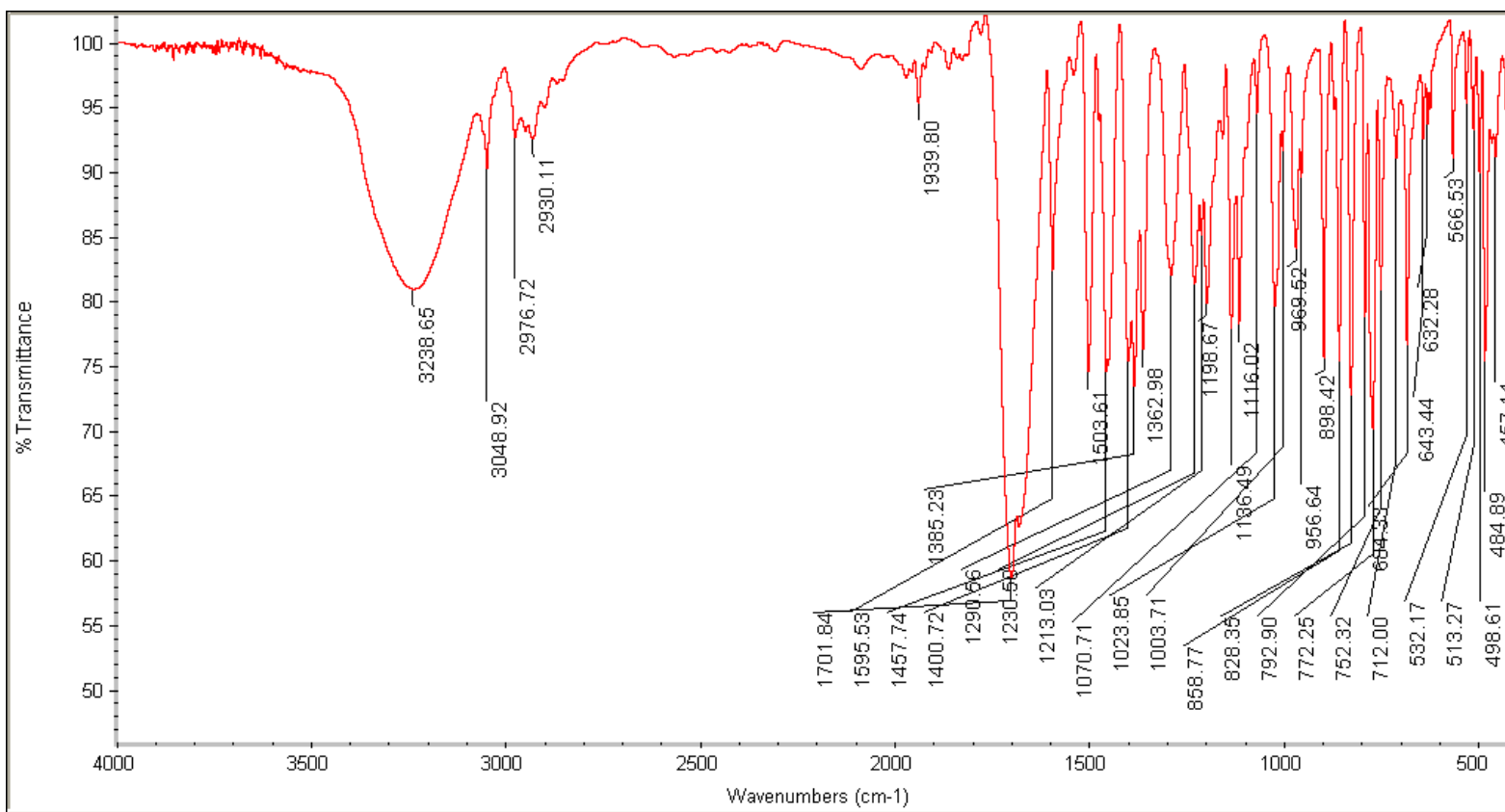


Figure 37. FT-IR spectrum of Ethyl 4-hydroxy-2-(naphthalen-2-yl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4m**)

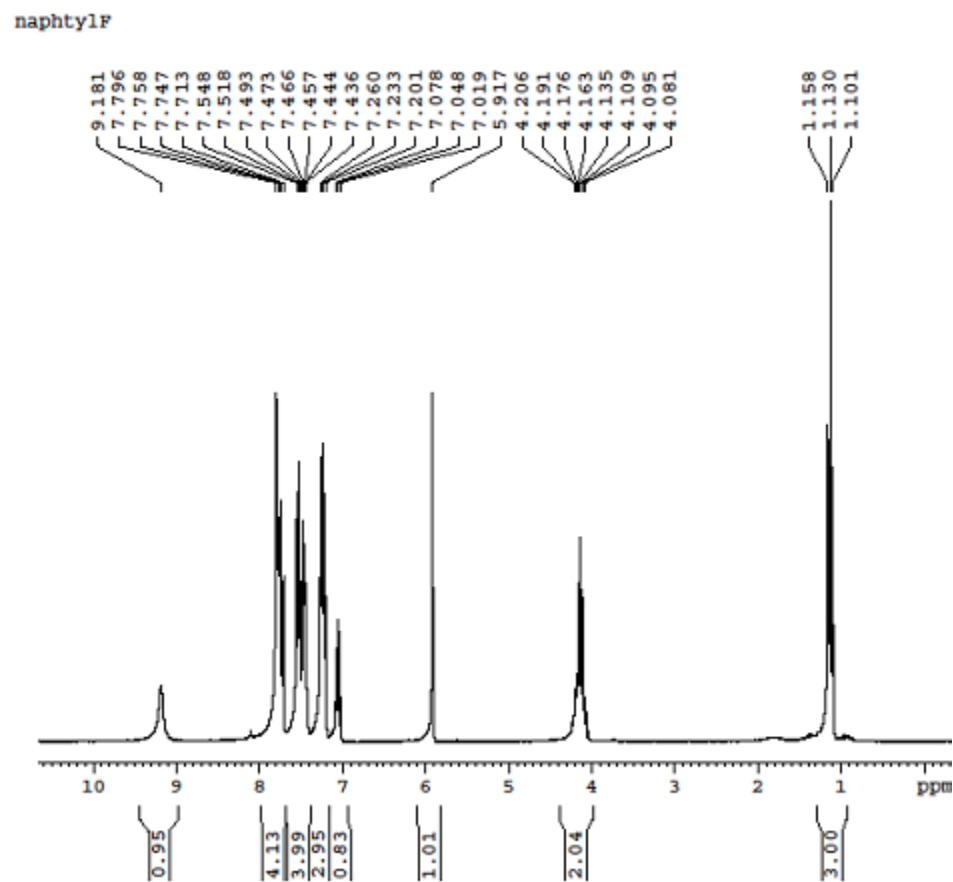


Figure 38. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-2-(naphthalen-2-yl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4m**)

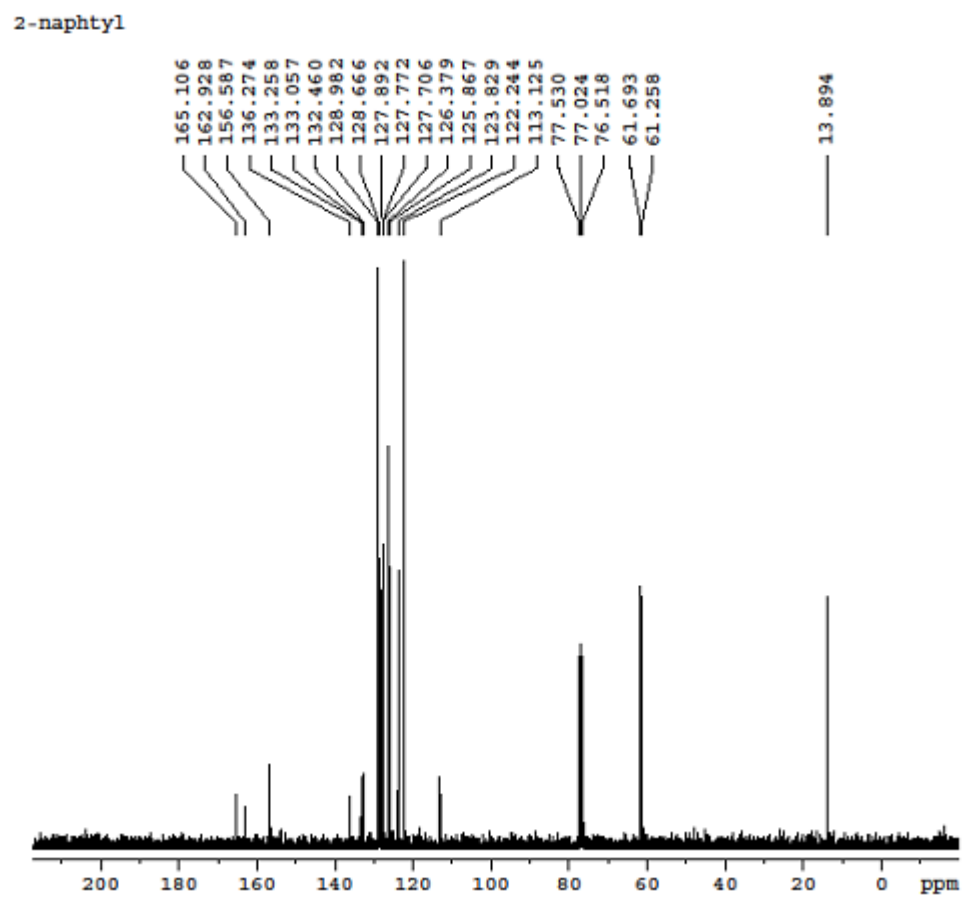


Figure 39. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-2-(naphthalen-2-yl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4m**)

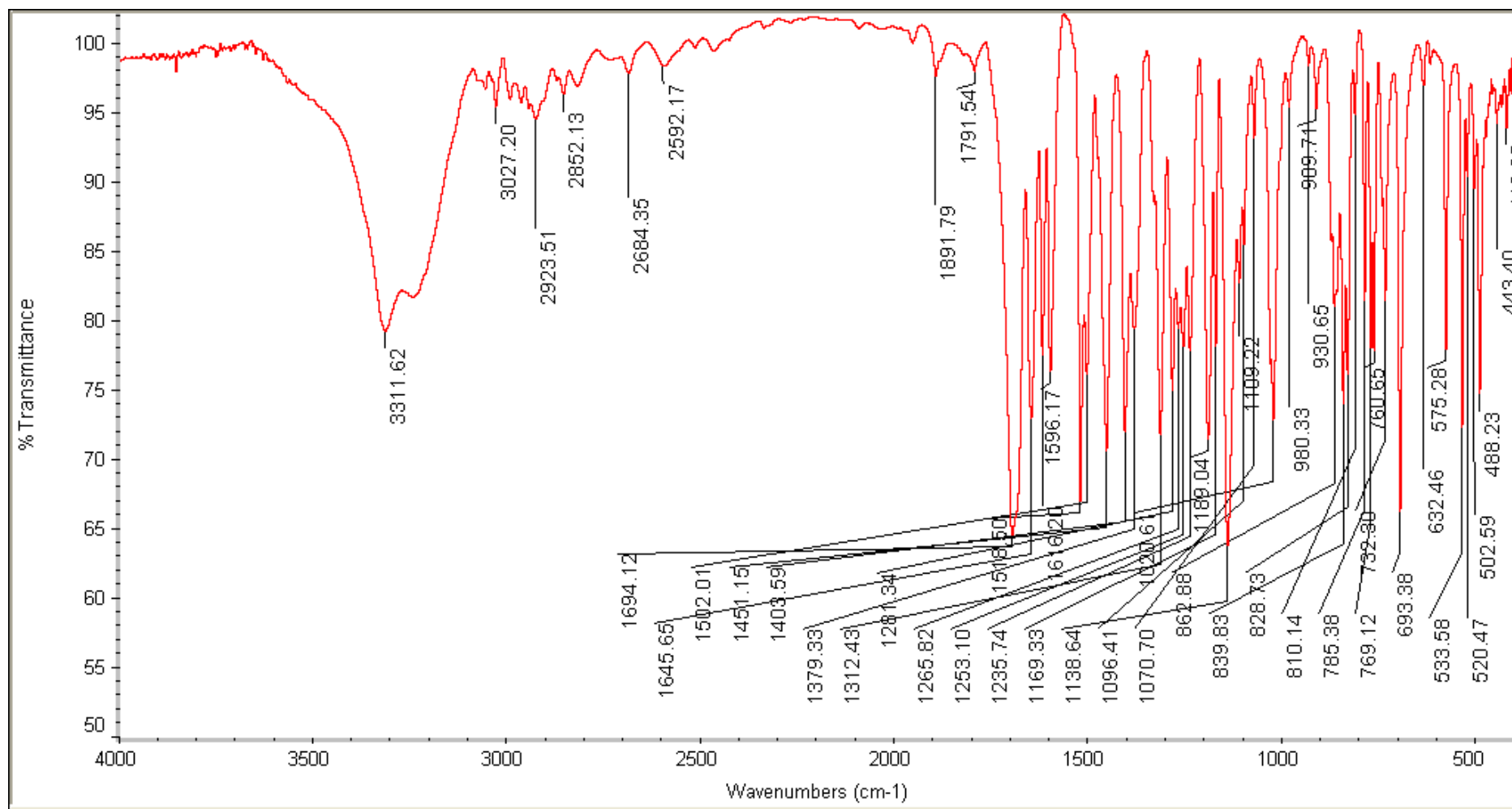


Figure 40. FT-IR spectrum of Ethyl 4-hydroxy-2-(4-hydroxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4n**)

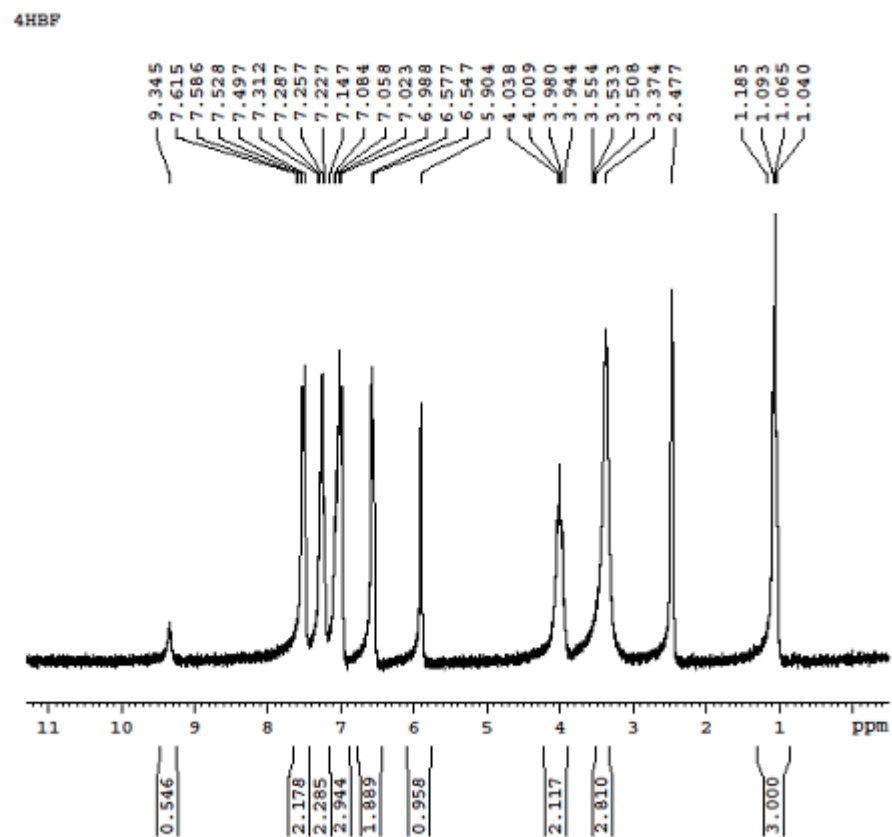


Figure 41. ¹H NMR (250.13 MHz, DMSO-d₆) spectrum of Ethyl 4-hydroxy-2-(4-hydroxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4n**)

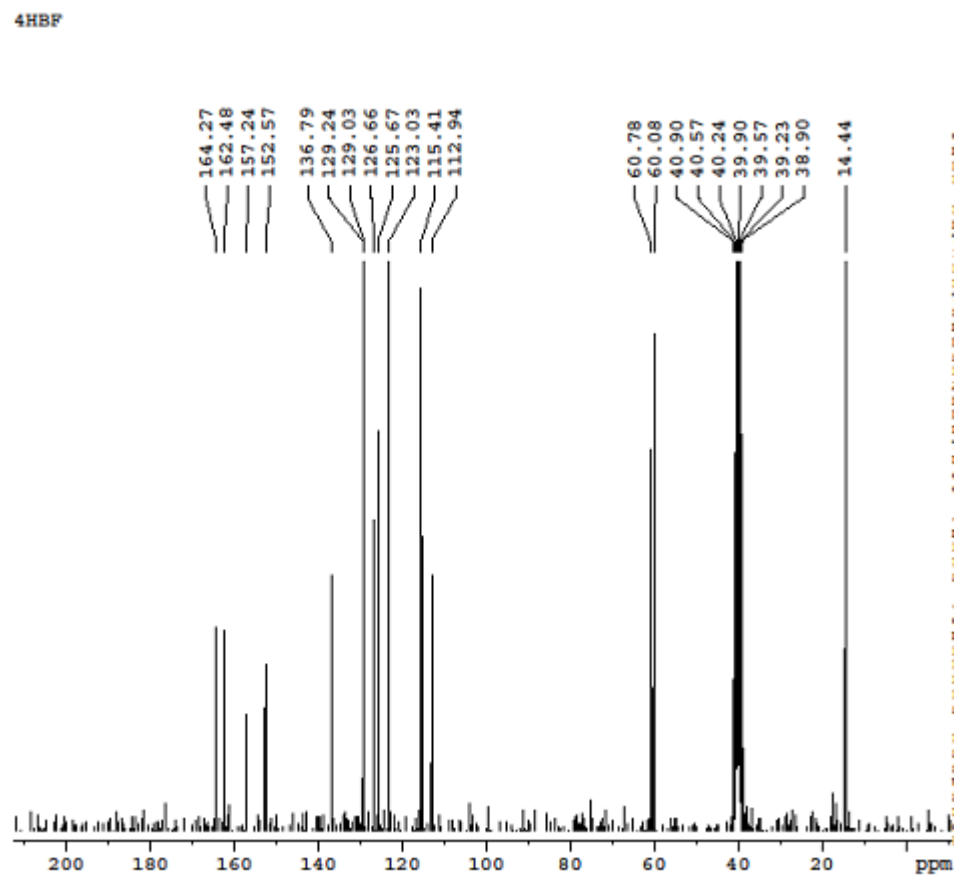


Figure 42. ^1H NMR (62.90 MHz, DMSO-d_6) spectrum of Ethyl 4-hydroxy-2-(4-hydroxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4n**)

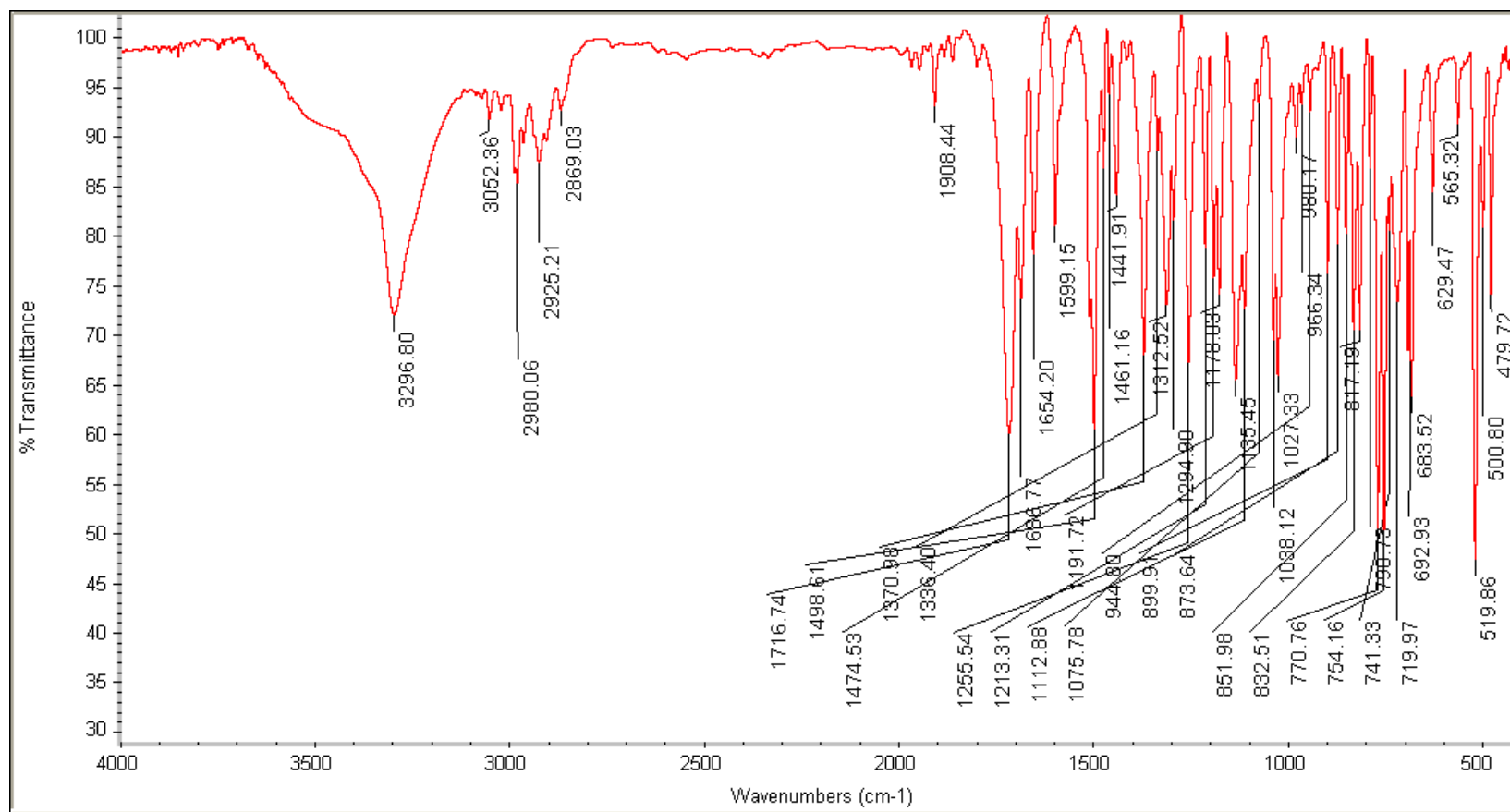


Figure 43. FT-IR spectrum of Ethyl 4-hydroxy-5-oxo-1-phenyl-2-(p-tolyl)-2,5-dihydro-1H-pyrrole-3-carboxylate (**4o**)

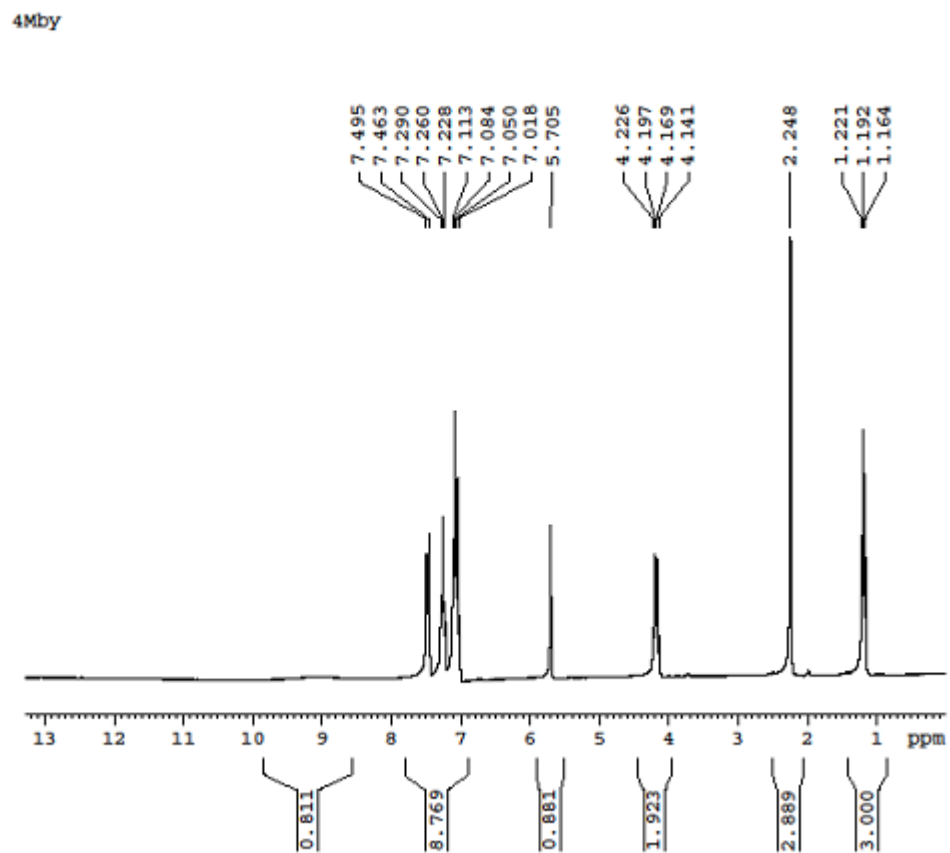


Figure 44. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-5-oxo-1-phenyl-2-(p-tolyl)-2,5-dihydro-1H-pyrrole-3-carboxylate (**4o**)

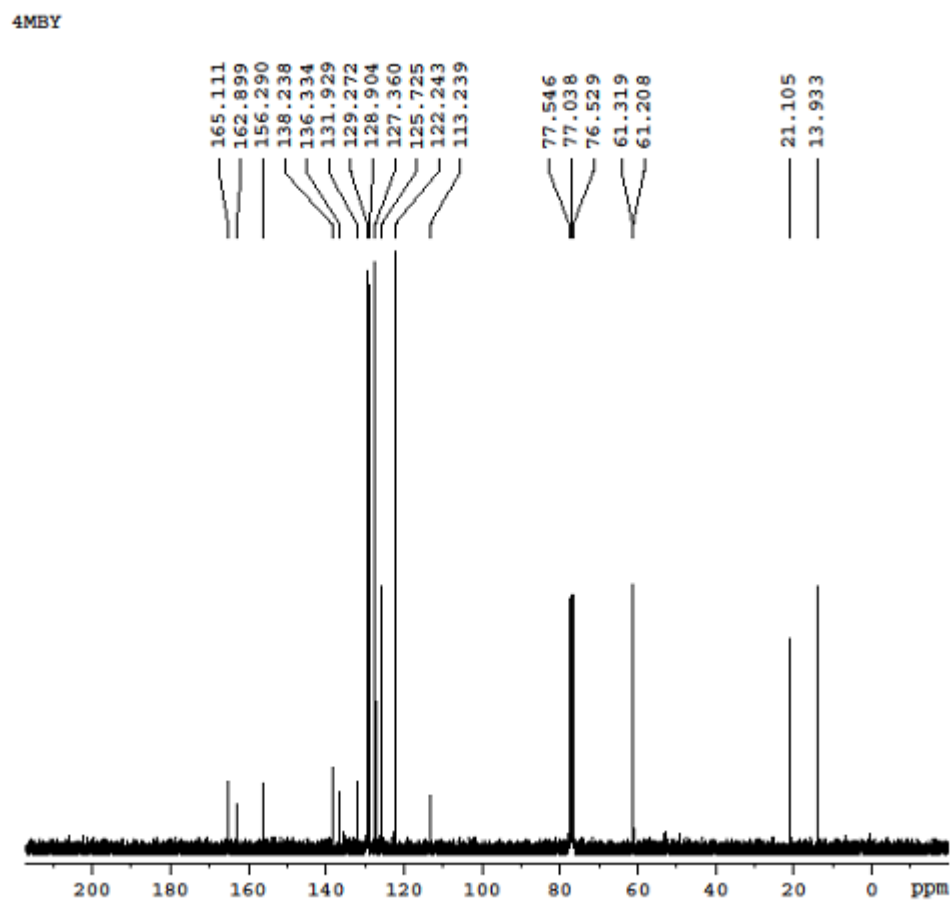


Figure 45. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-5-oxo-1-phenyl-2-(p-tolyl)-2,5-dihydro-1H-pyrrole-3-carboxylate (**4o**).

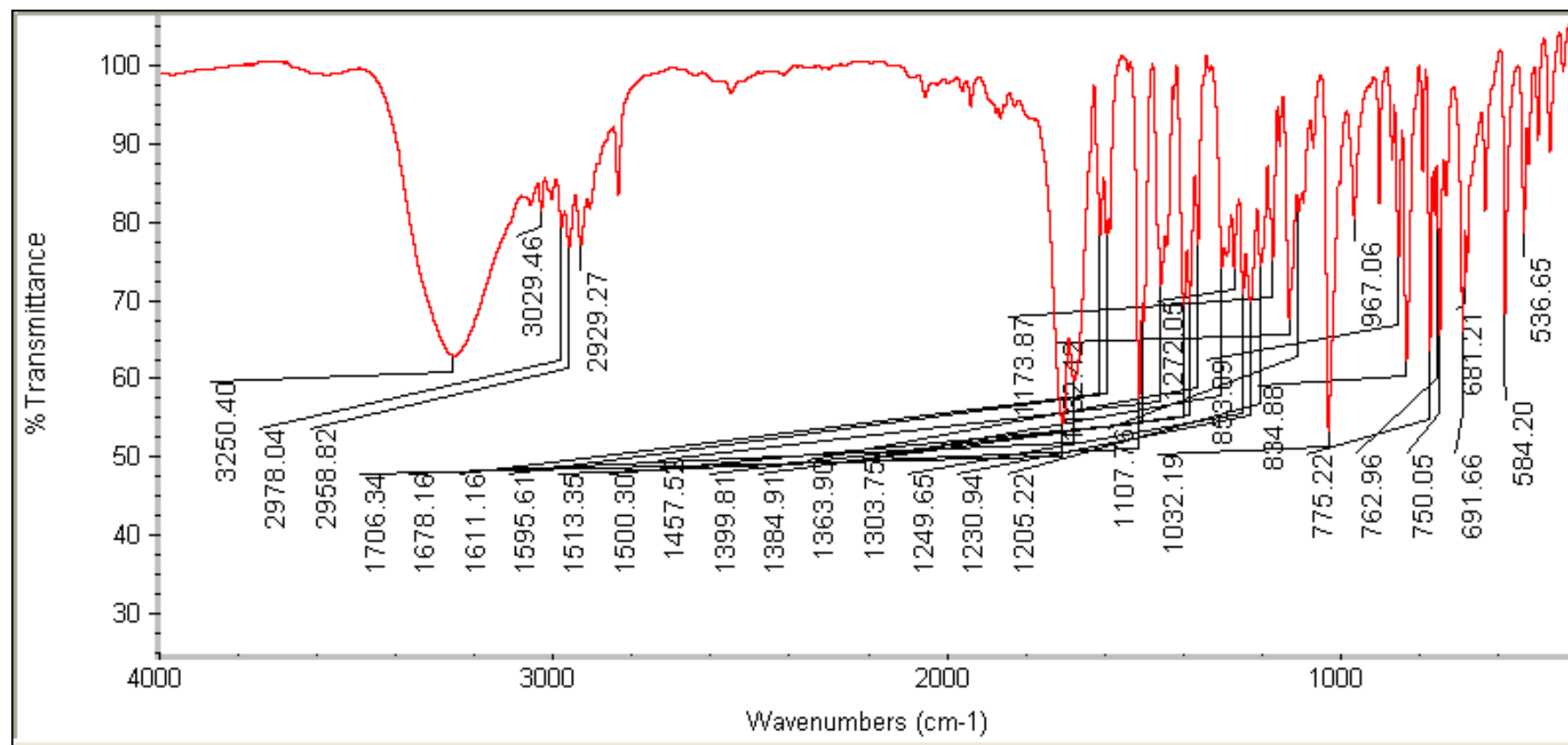


Figure 46. FT-IR spectrum of Ethyl 4-hydroxy-2-(4-methoxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4p**).

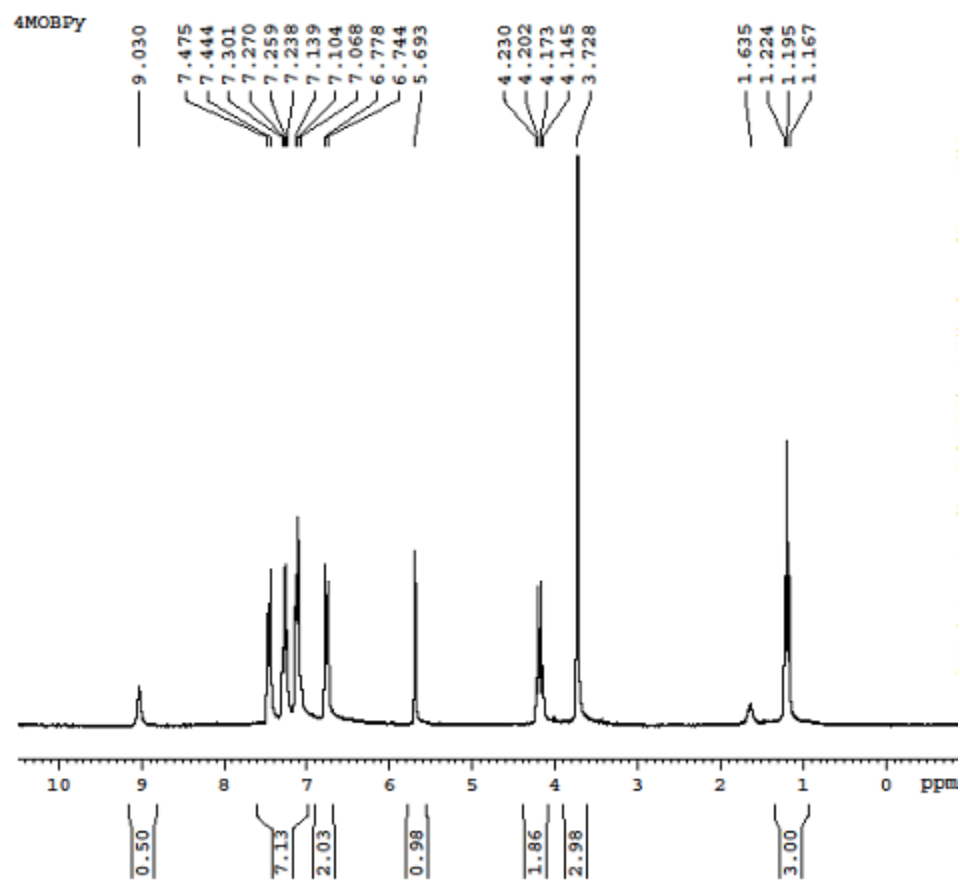


Figure 47. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-2-(4-methoxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4p**)

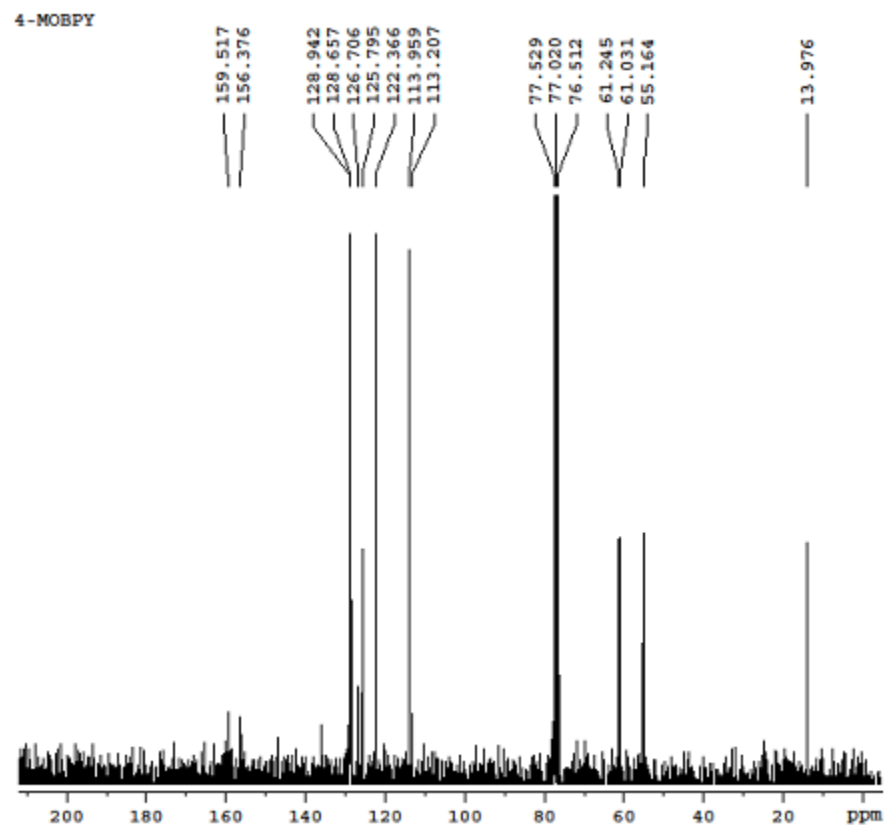


Figure 48. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-2-(4-methoxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4p**)

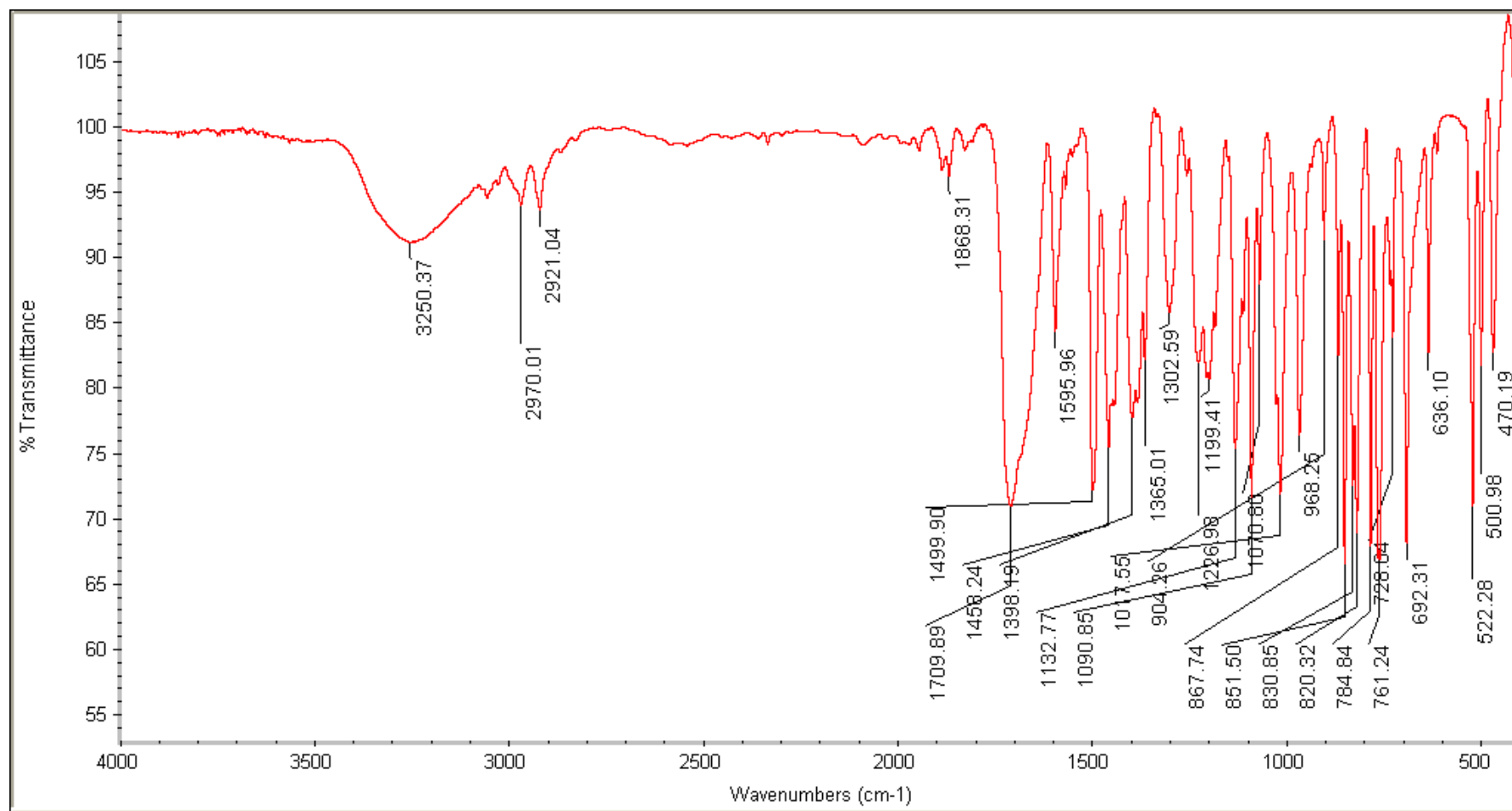


Figure 49. FT-IR spectrum of Ethyl 4-hydroxy-2-(4-(methylthio)phenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4q**)

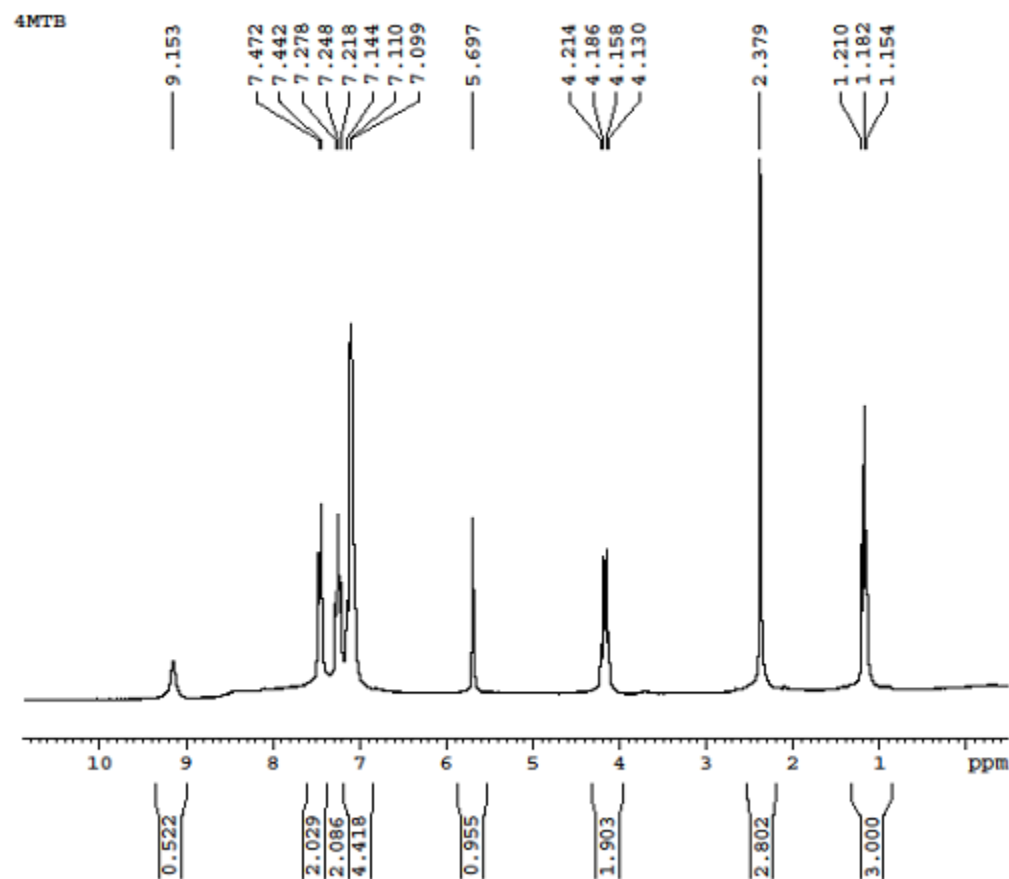


Figure 50. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-2-(4-(methylthio)phenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4q**)

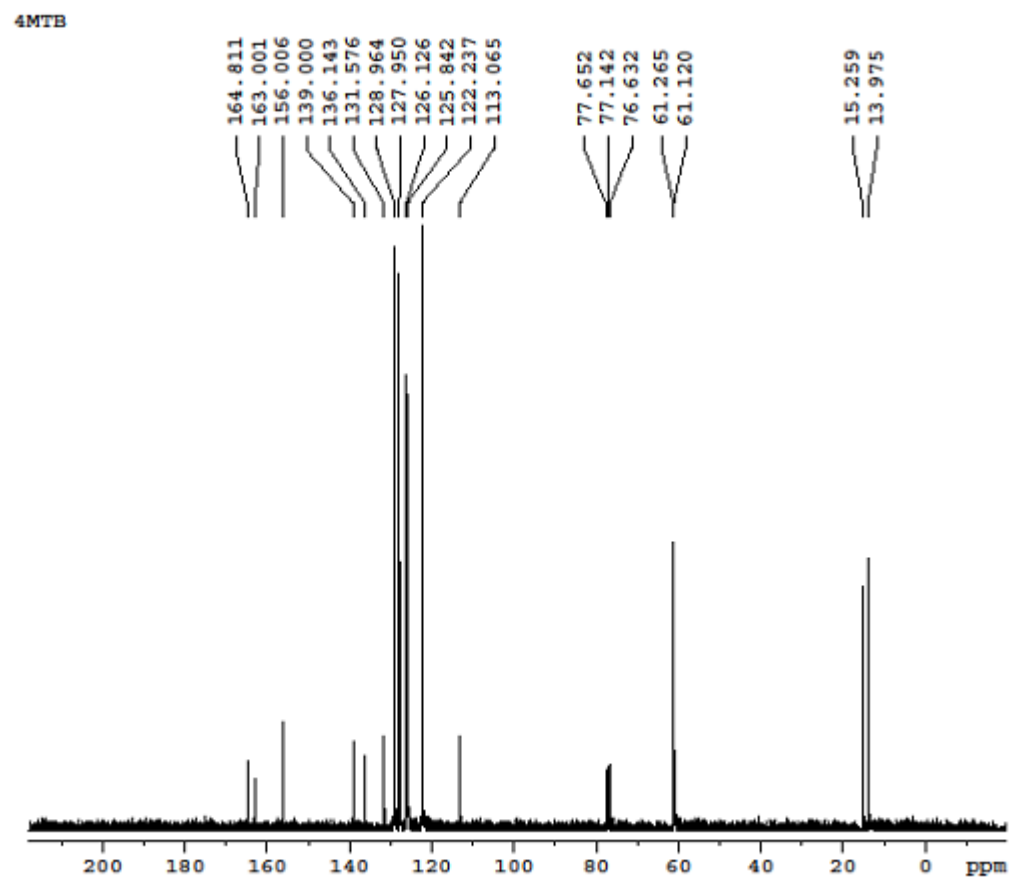


Figure 51. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-2-(4-(methylthio)phenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4q**)

Table1. X-ray diffraction study details for Ethyl 4-hydroxy-2-(4-(methylthio)phenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4q**)

CCDC No.	2021152
Chemical formula	C ₂₀ H ₁₉ NO ₄ S
M_r	369.42
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	9.922 (3), 6.156 (2), 28.905 (9)
β (°)	92.68 (3)
V (Å ³)	1763.6 (10)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.21
Crystal size (mm)	0.43 × 0.22 × 0.11
Diffractometer	Agilent Technologies Xcalibur R diffractometer
Absorption correction	Multi-scan
T_{\min}, T_{\max}	0.991, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10885, 5008, 4131
R_{int}	0.025
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.720
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.039, 0.099, 1.03
No. of reflections	5008
No. of parameters	241
No. of restraints	0
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.45, -0.31