

Supplementary Material

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

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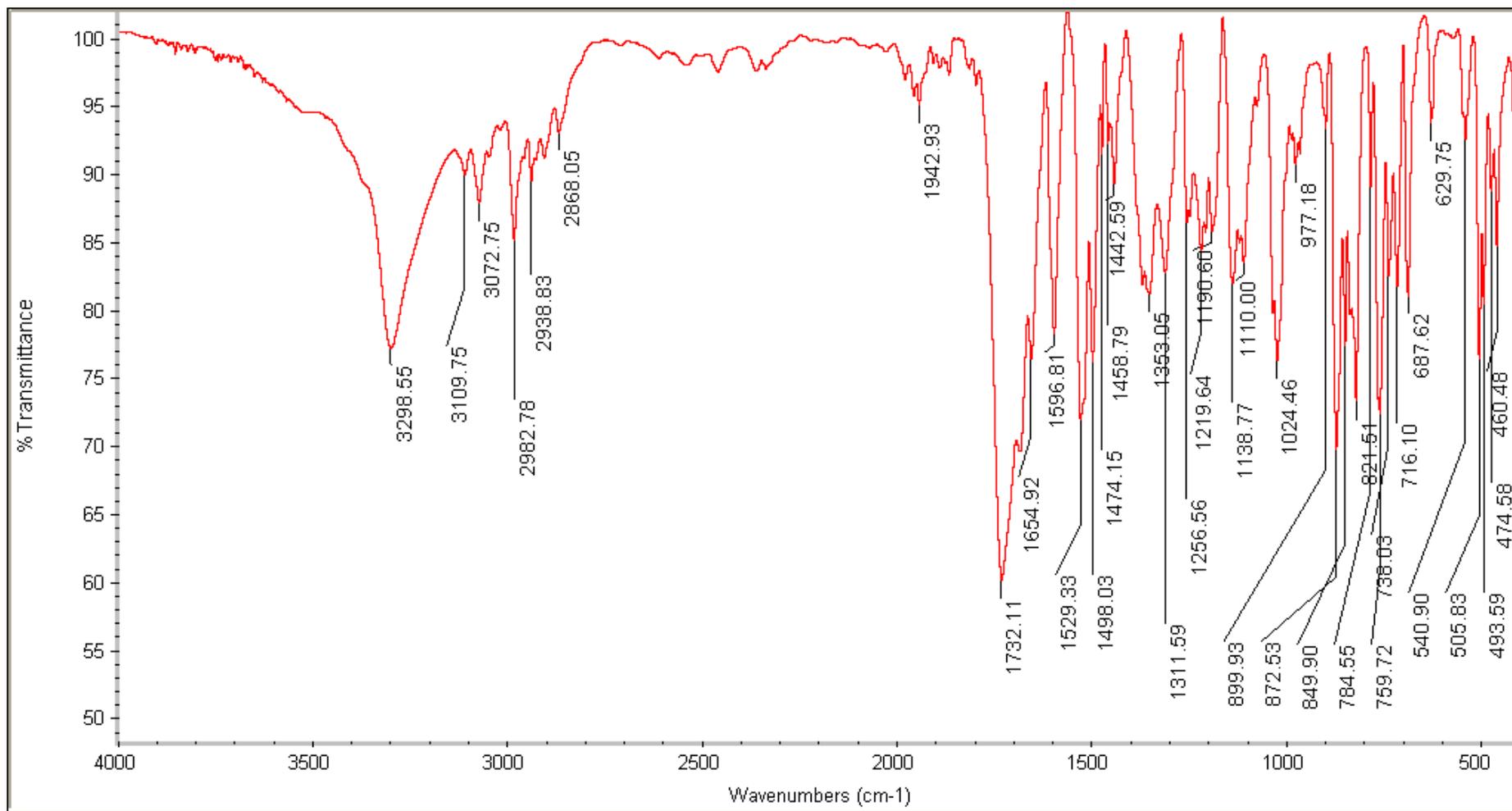


Figure 1. FT-IR spectrum of Ethyl 2-(4-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4a**).

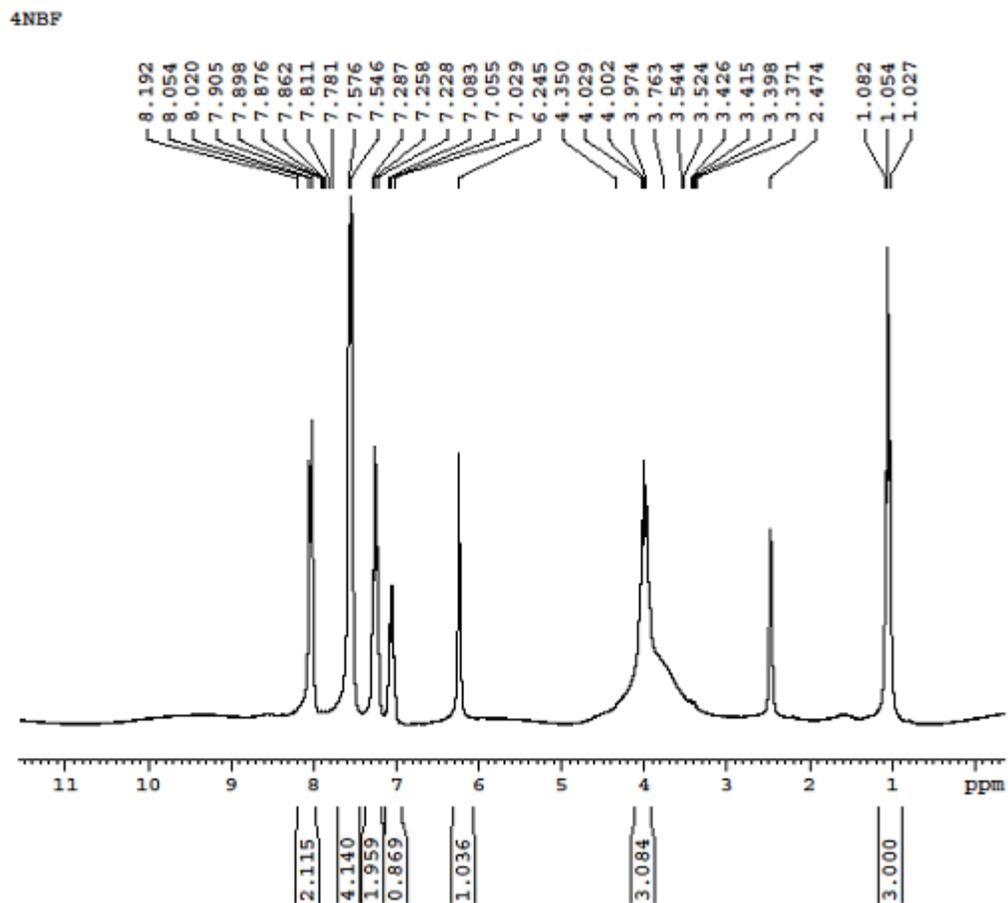


Figure 2. ^1H NMR (250.13 MHz, DMSO-d_6) of Ethyl 2-(4-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4a**).

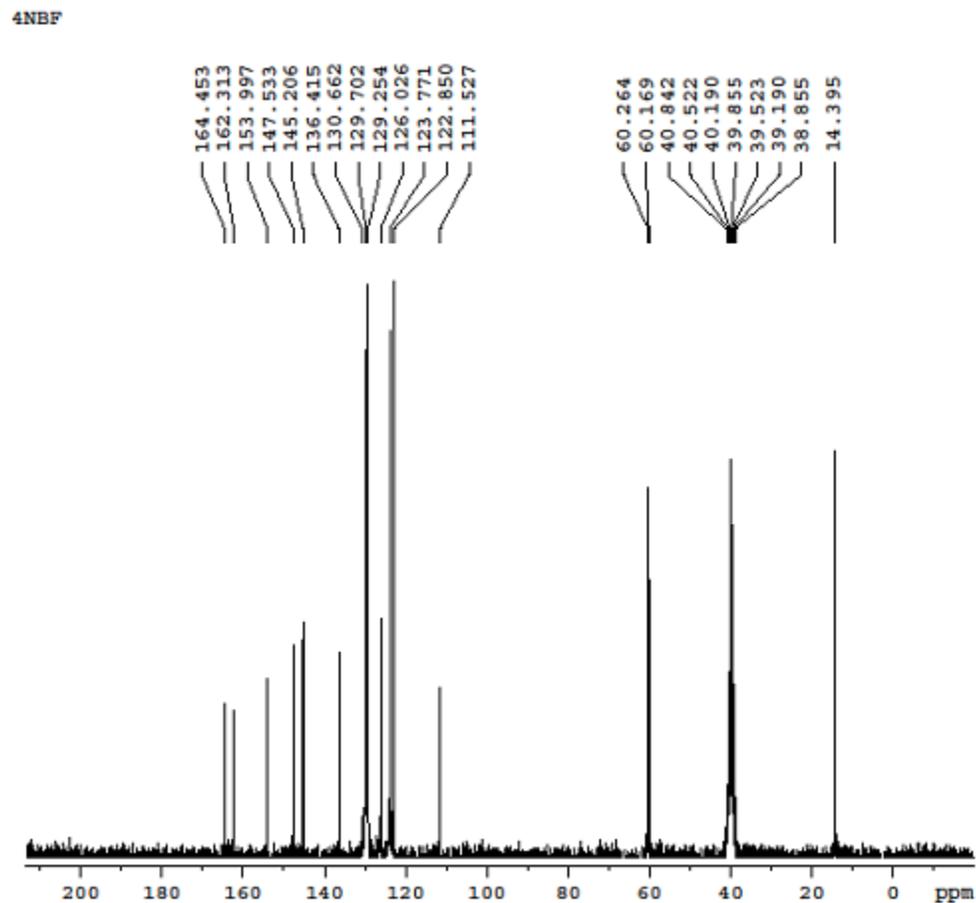


Figure 3. ^{13}C NMR (62.90 MHz, DMSO- d_6) of Ethyl 2-(4-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4a**).

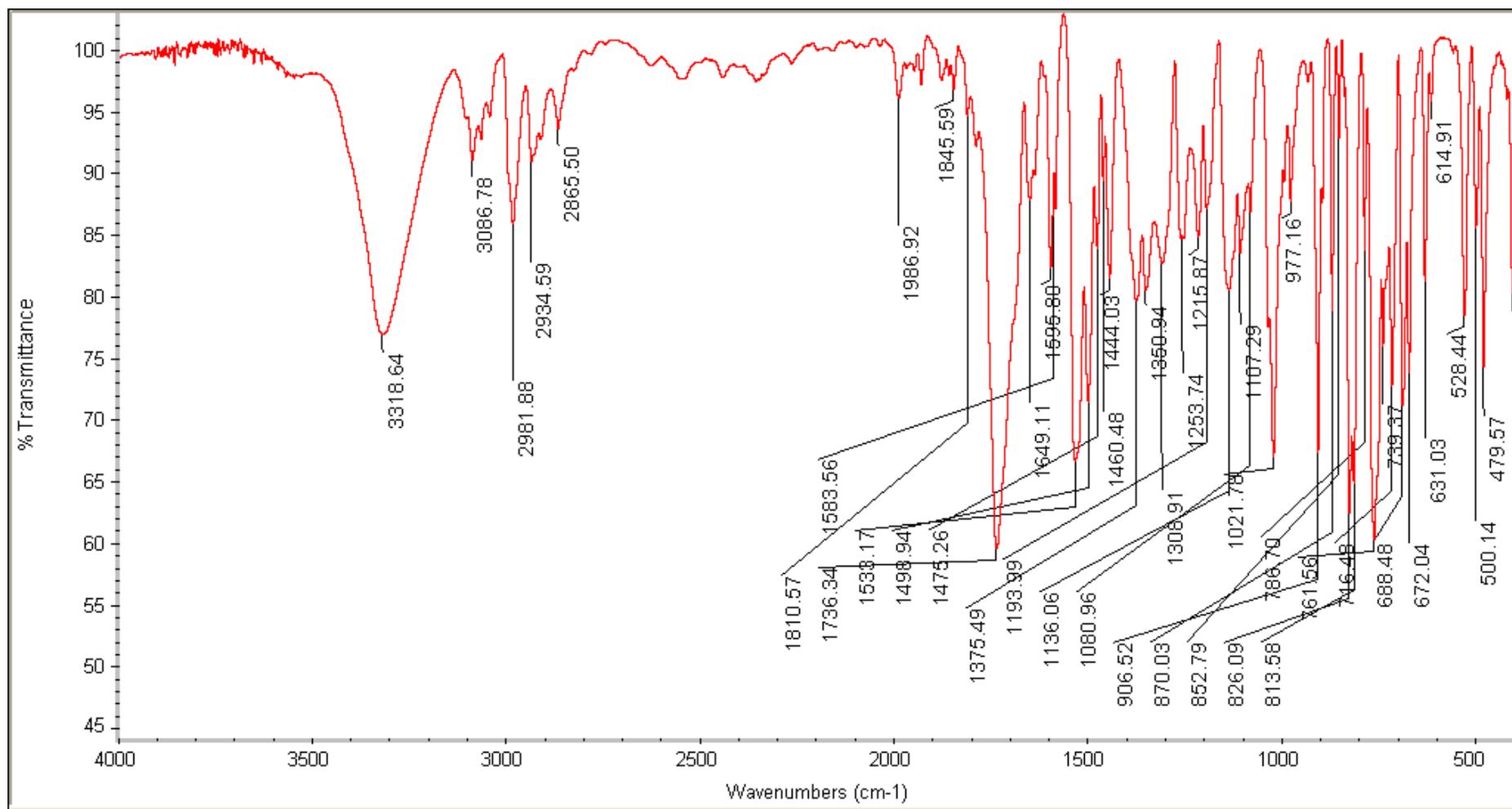


Figure 4. FT-IR spectrum of Ethyl 2-(3-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4b**).

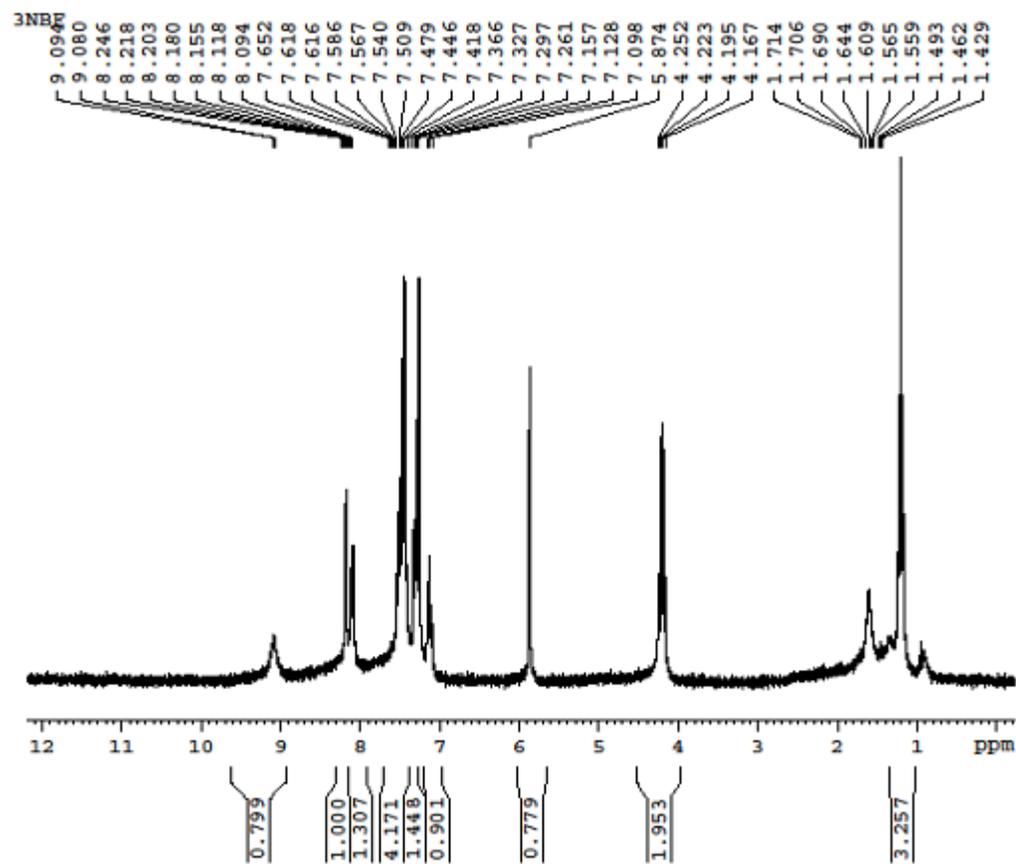


Figure 5. ¹H NMR (250.13 MHz, CDCl₃) spectrum of Ethyl 2-(3-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4b**).

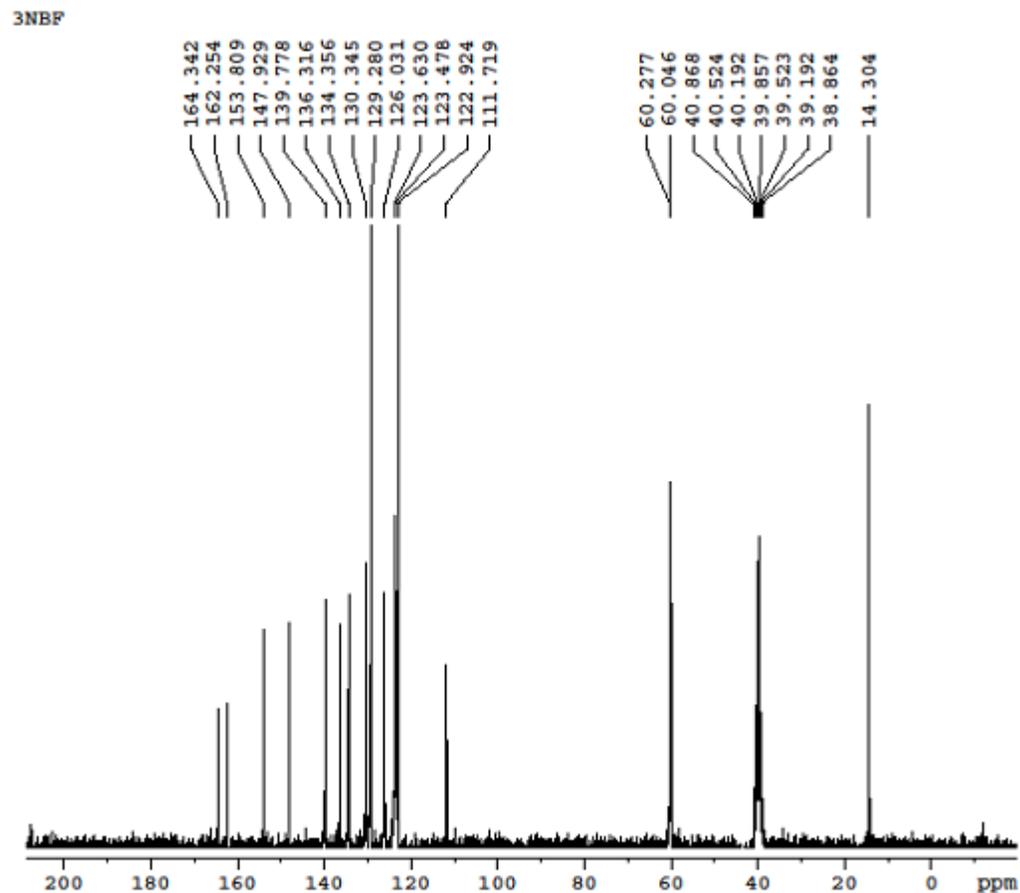


Figure 6. ^{13}C NMR (62.90 MHz, DMSO-d_6) spectrum of Ethyl 2-(3-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4b**).

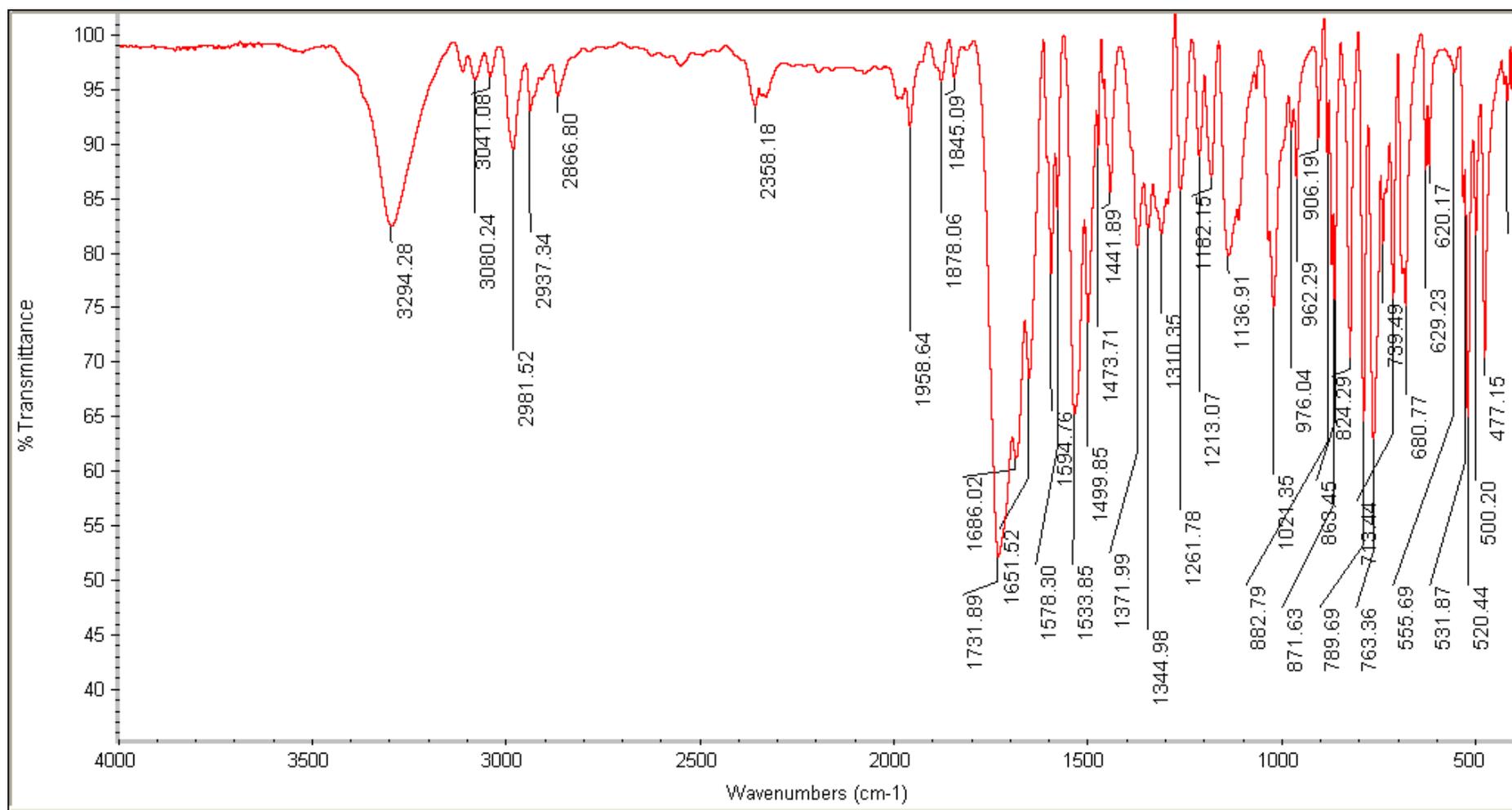


Figure 7. FT-IR spectrum of Ethyl 2-(2-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4c**).

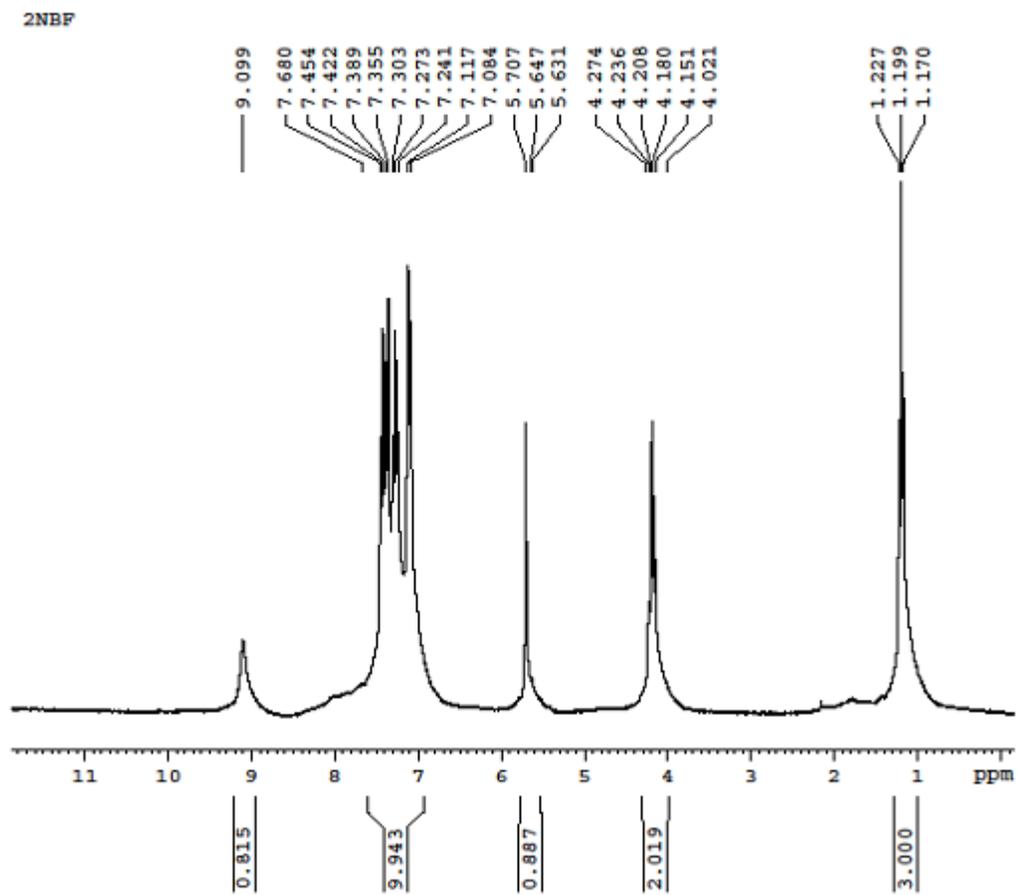


Figure 8. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 2-(2-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4c**).

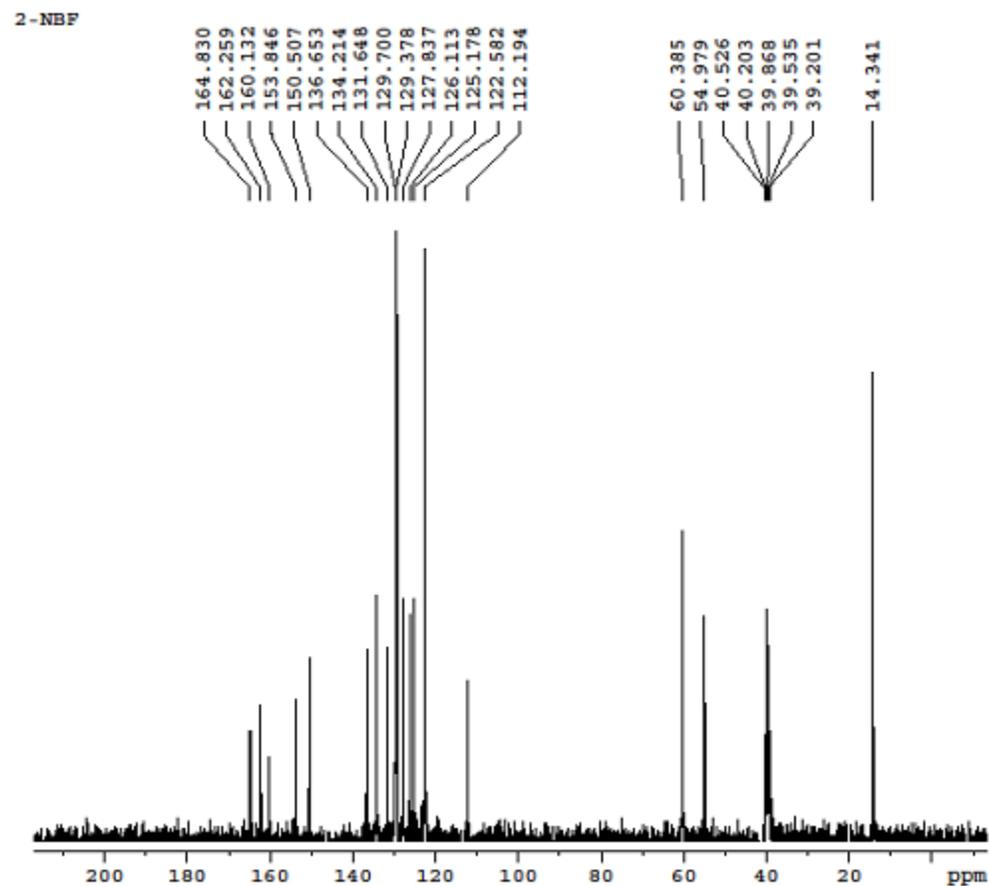


Figure 9. ^{13}C NMR (62.90 MHz, DMSO-d_6) spectrum of Ethyl 2-(2-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4c**).

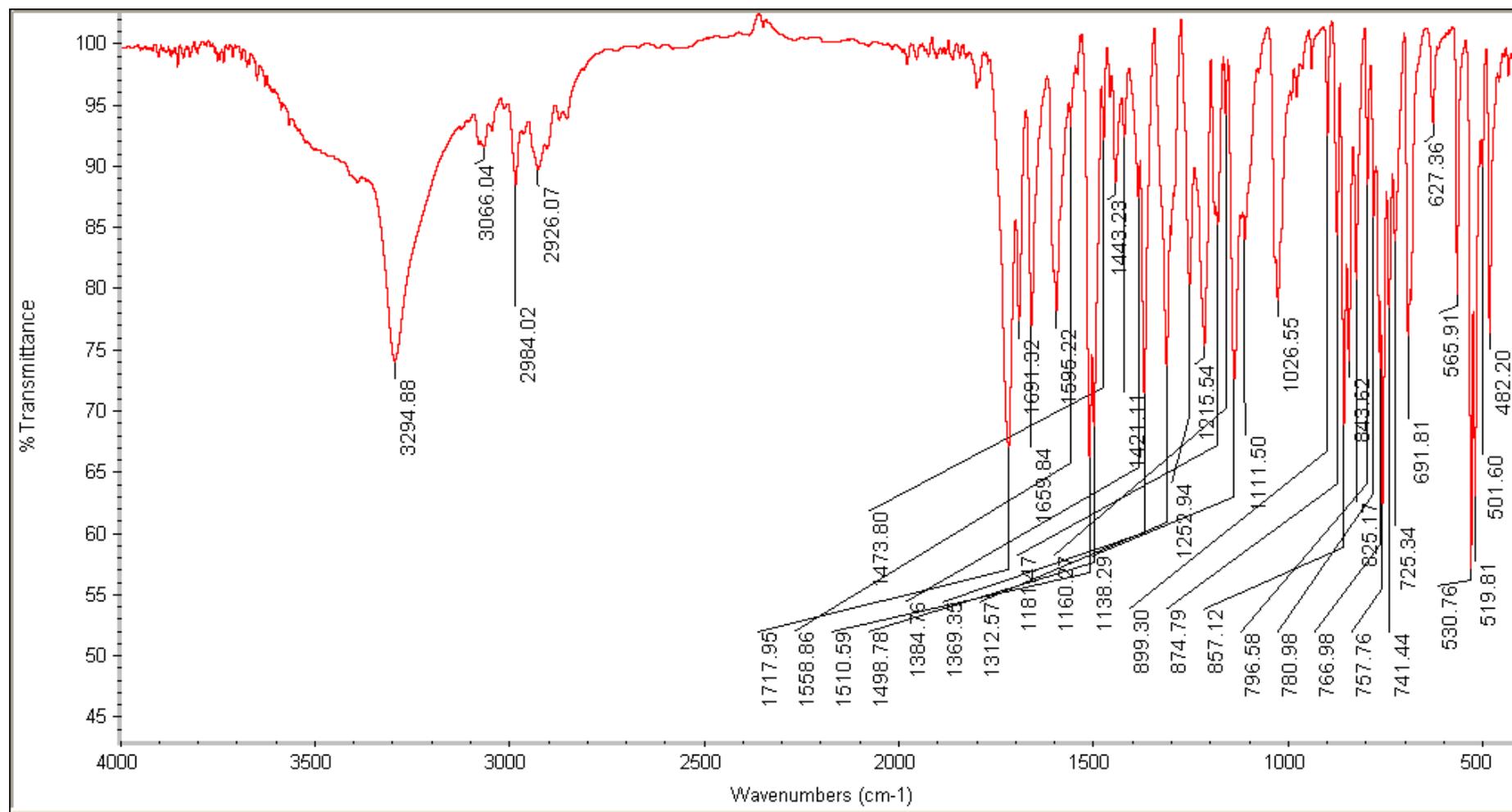


Figure 10. FT-IR spectrum of Ethyl 2-(4-fluorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4d**).

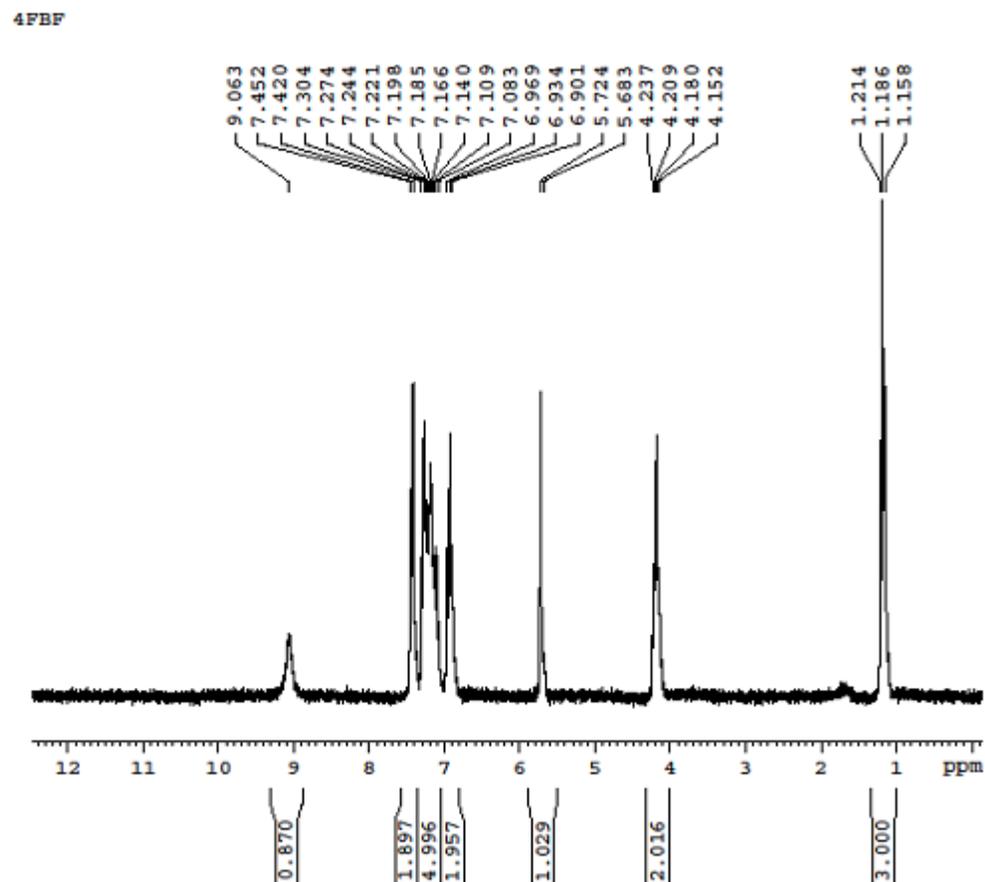


Figure 11. ¹H NMR (250.13 MHz, CDCl₃) spectrum of Ethyl 2-(4-fluorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4d**).

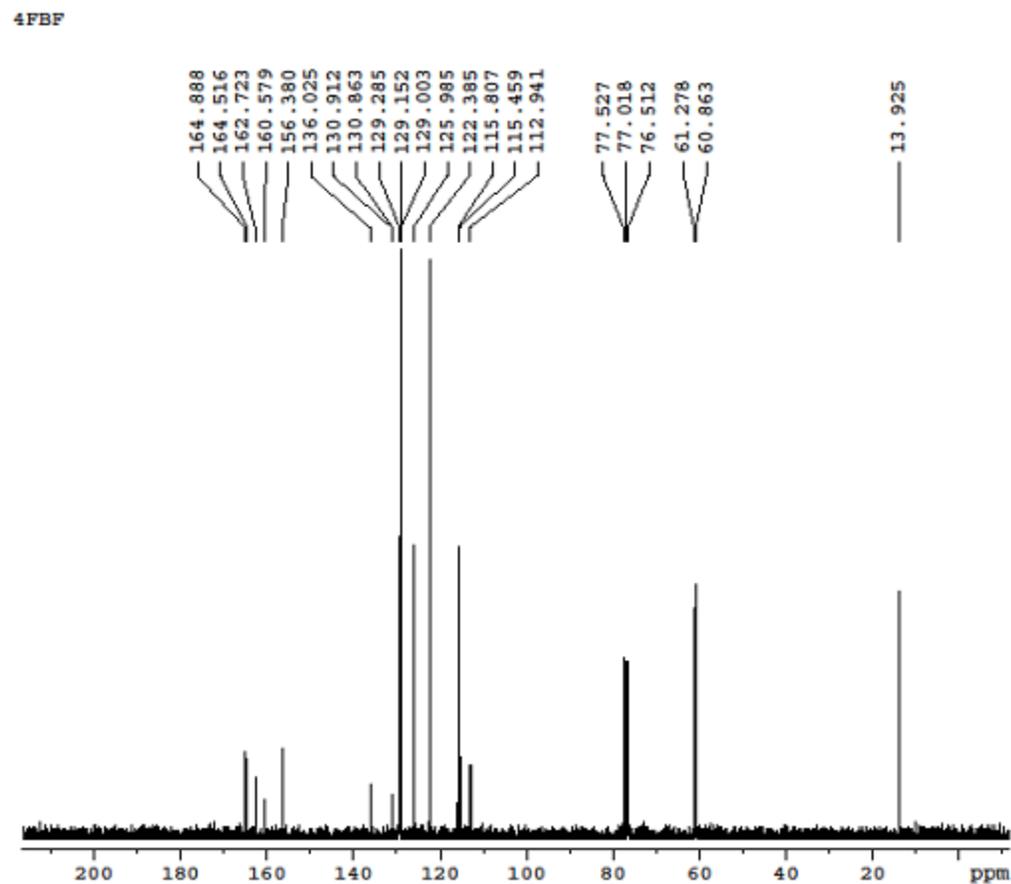


Figure 12. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 2-(4-fluorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4d**).

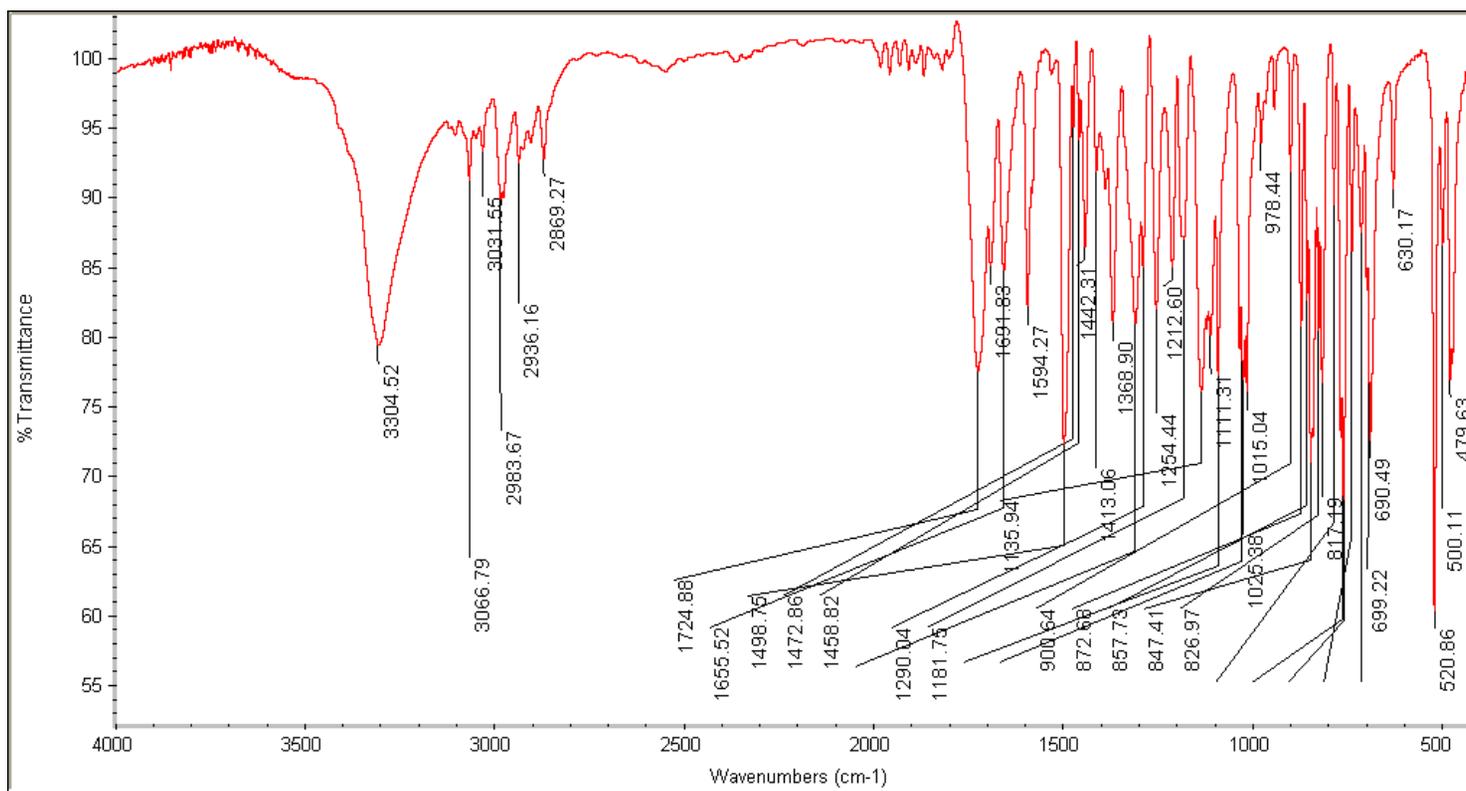


Figure 13. FT-IR spectrum of Ethyl 2-(4-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4e**).

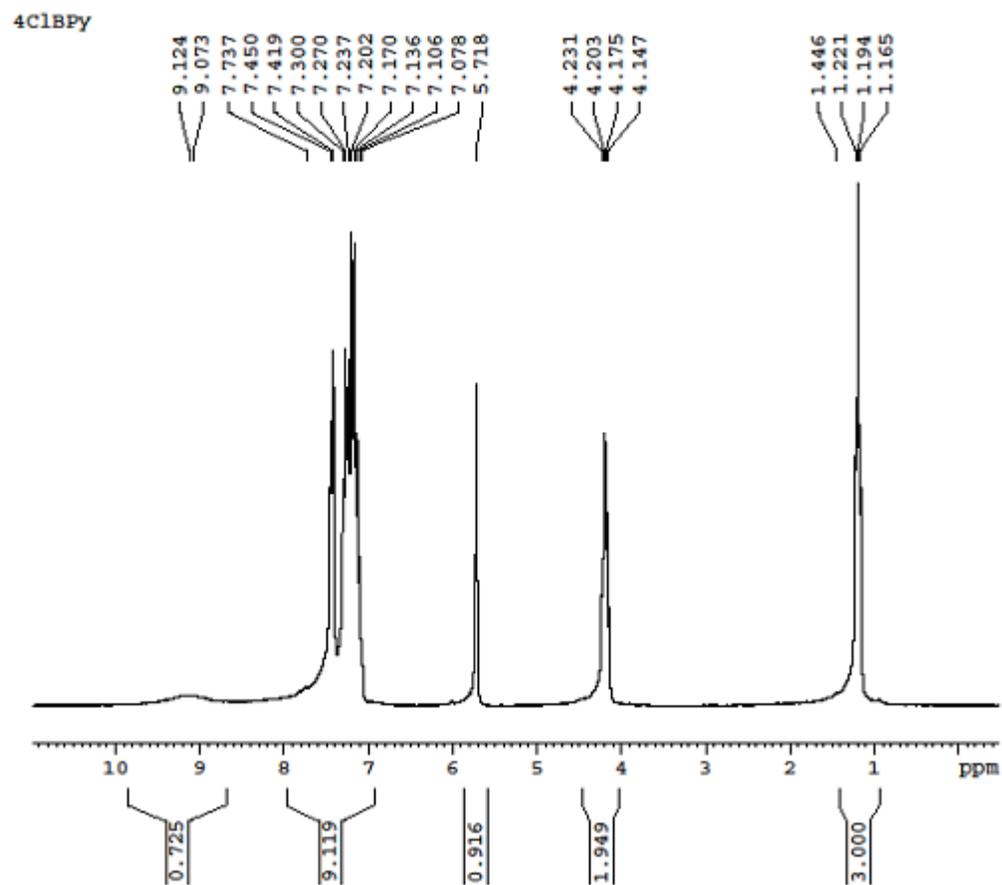


Figure 14. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 2-(4-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4e**).

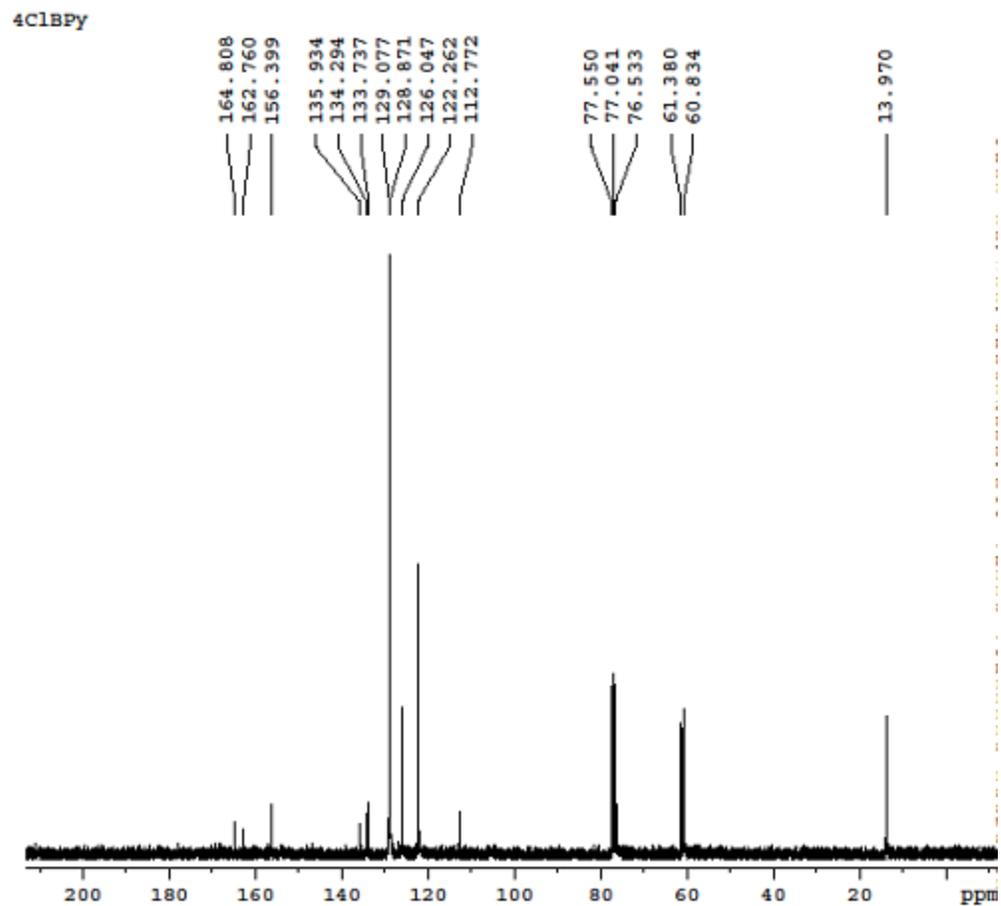


Figure 15. ¹³C NMR (62.90 MHz, CDCl₃) spectrum of Ethyl 2-(4-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4e**).

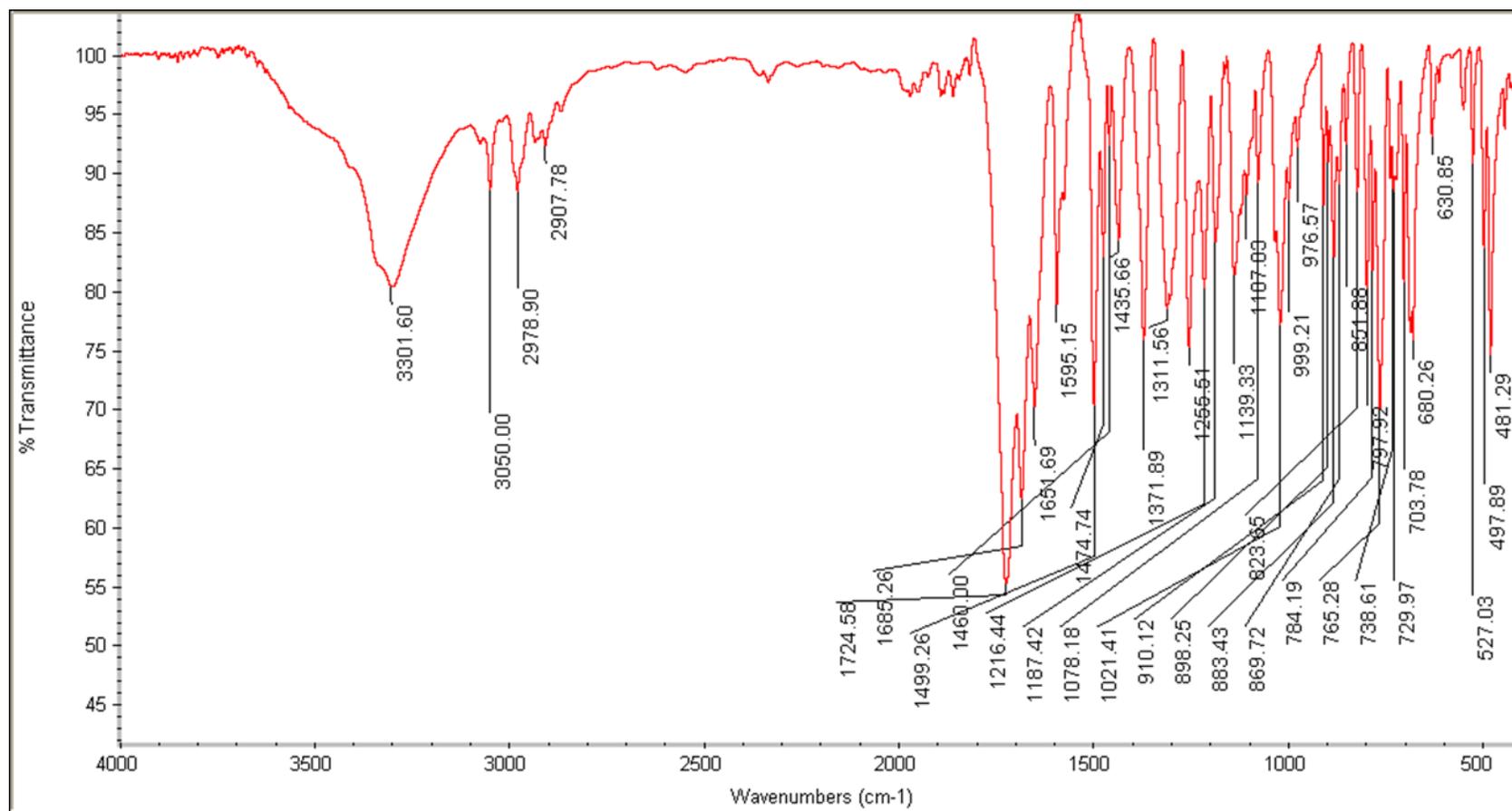
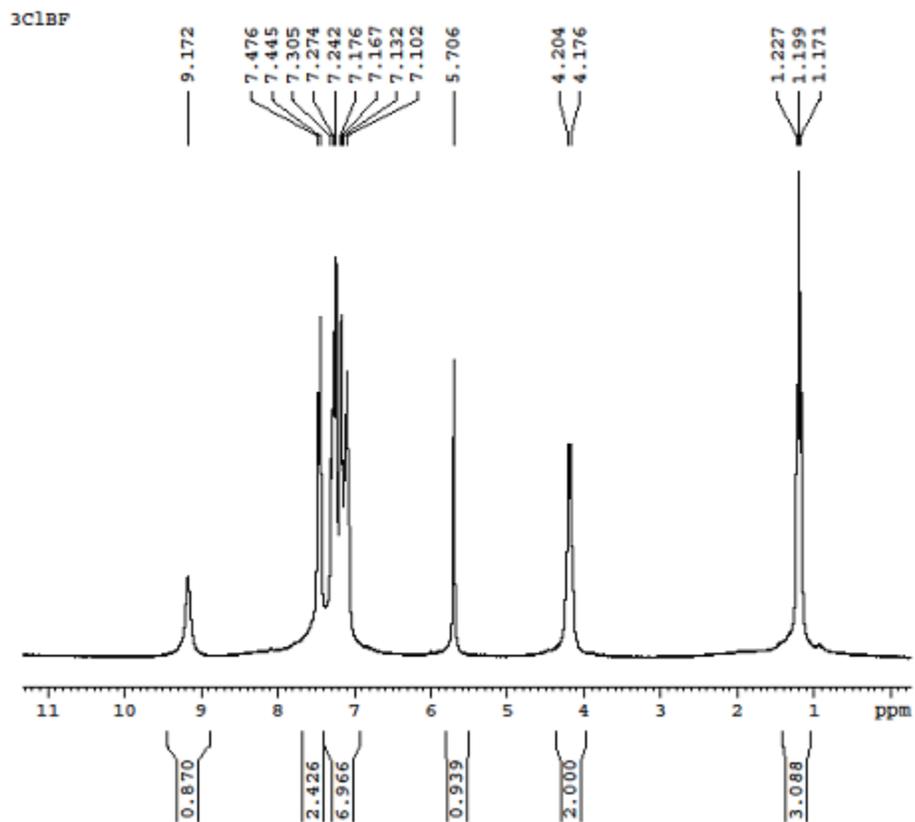


Figure 16. FT-IR spectrum of Ethyl 2-(3-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (4f)



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**).

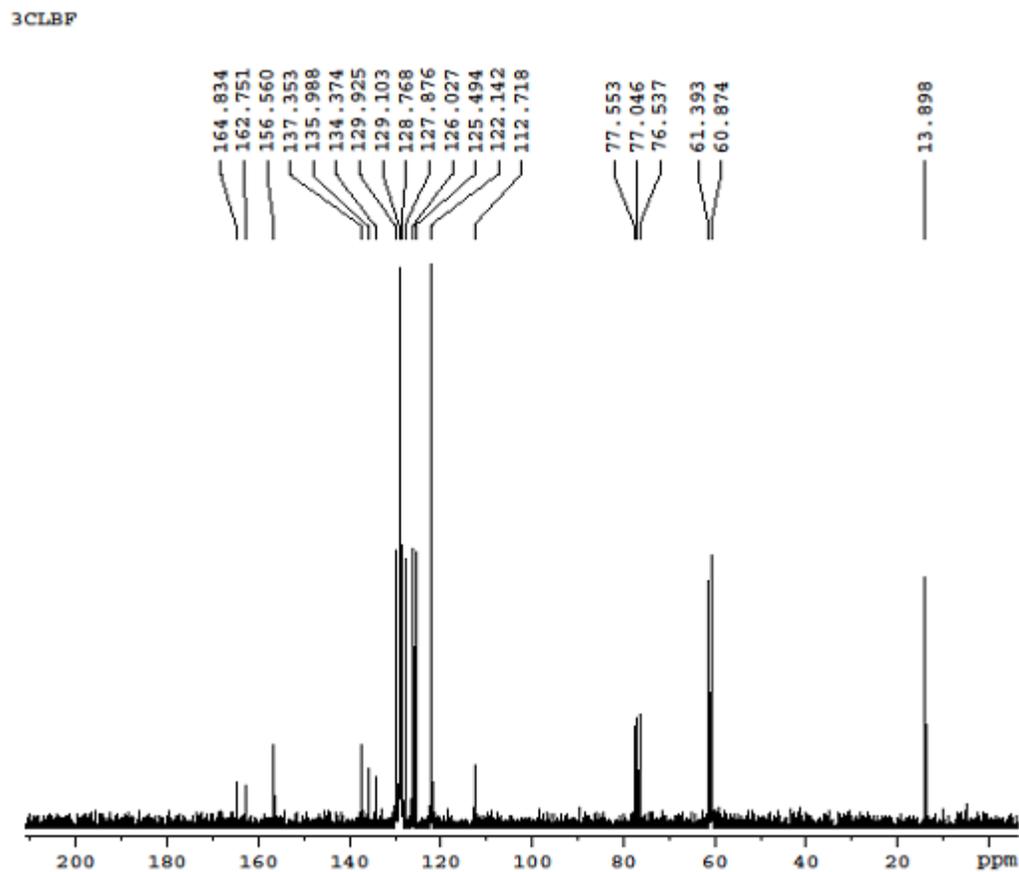


Figure 18. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 2-(3-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4f**).

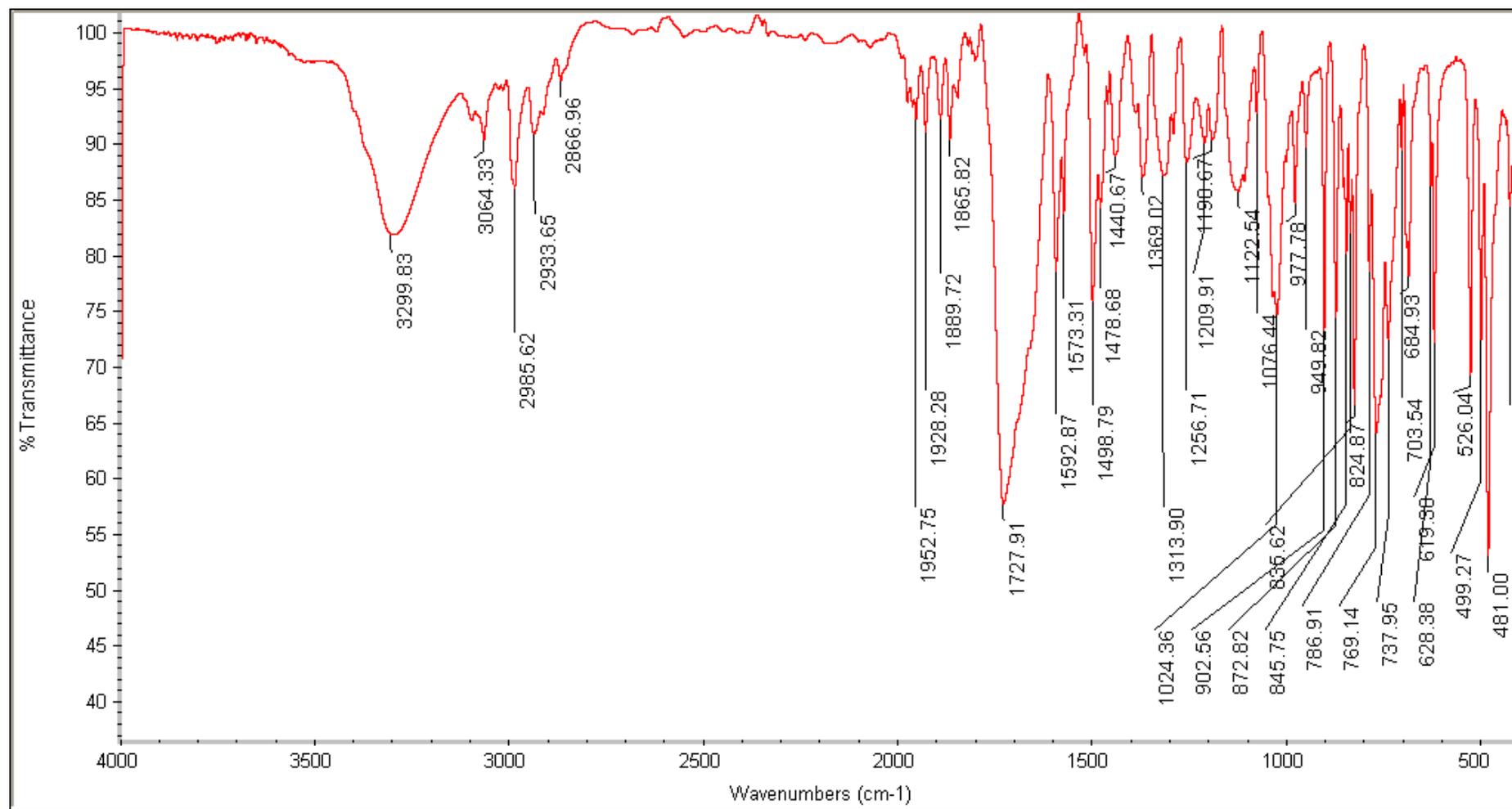


Figure 19. FT-IR spectrum of Ethyl 2-(2-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4g**)

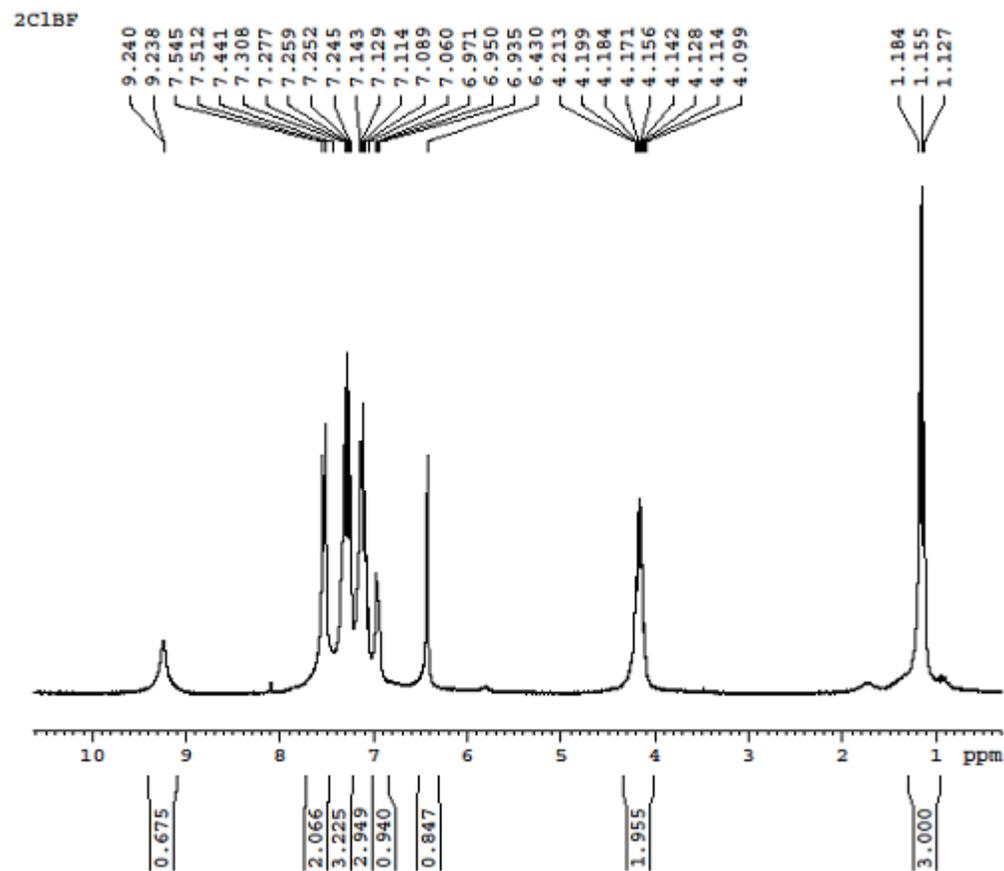


Figure 20. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 2-(2-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4g**)

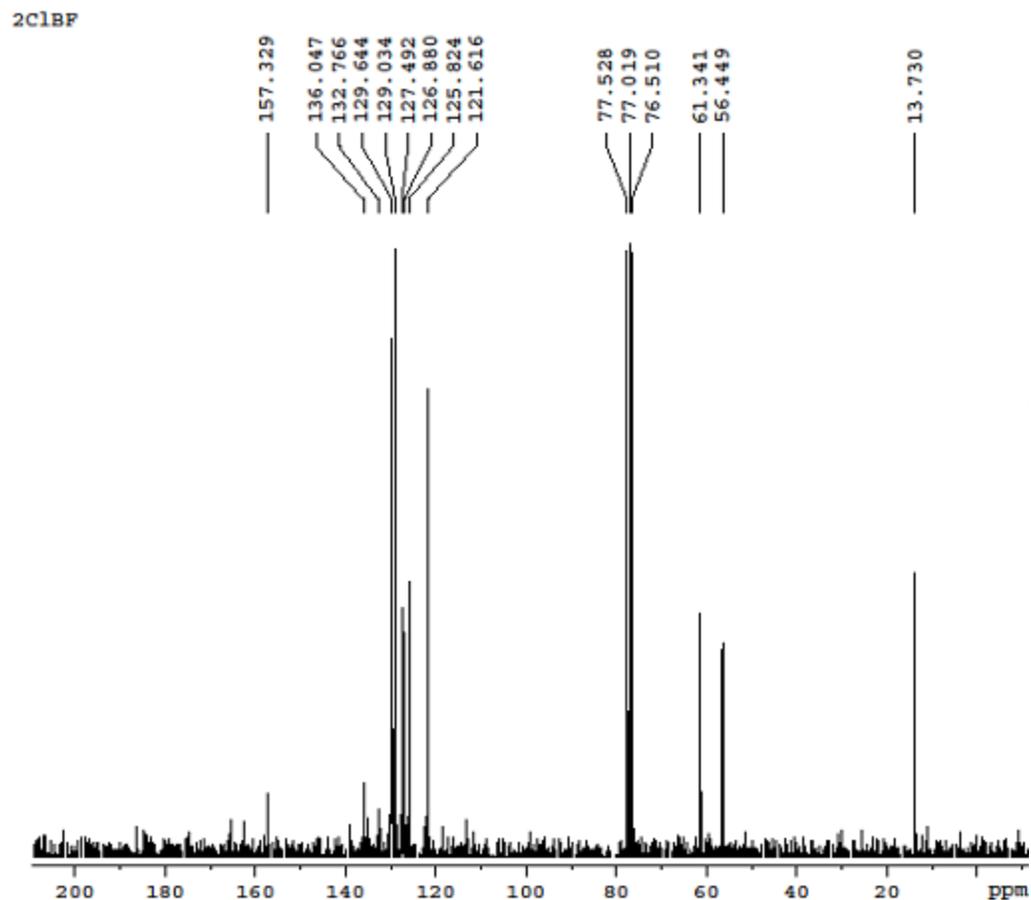


Figure 21. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 2-(2-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4g**)

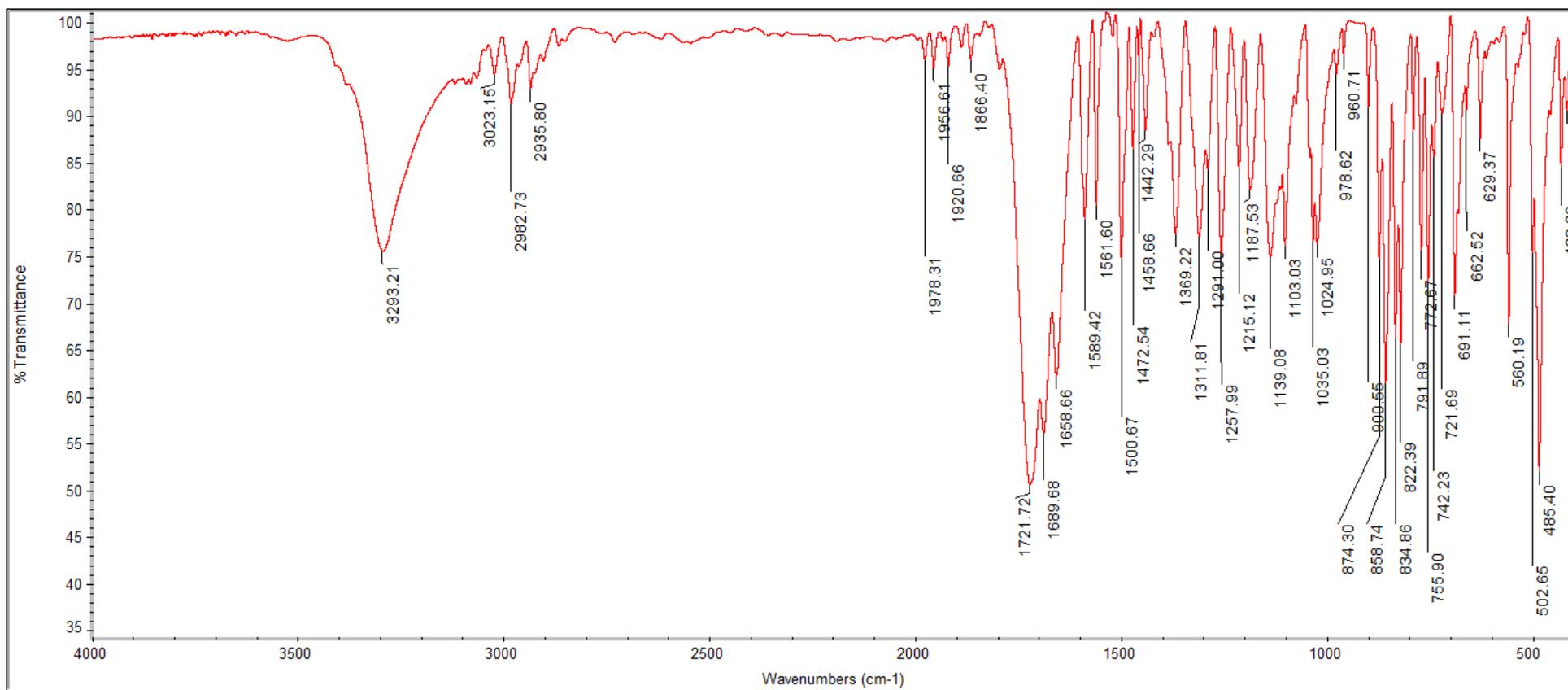


Figure 22. FT-IR spectrum of Ethyl 2-(2,4-dichlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4h**)

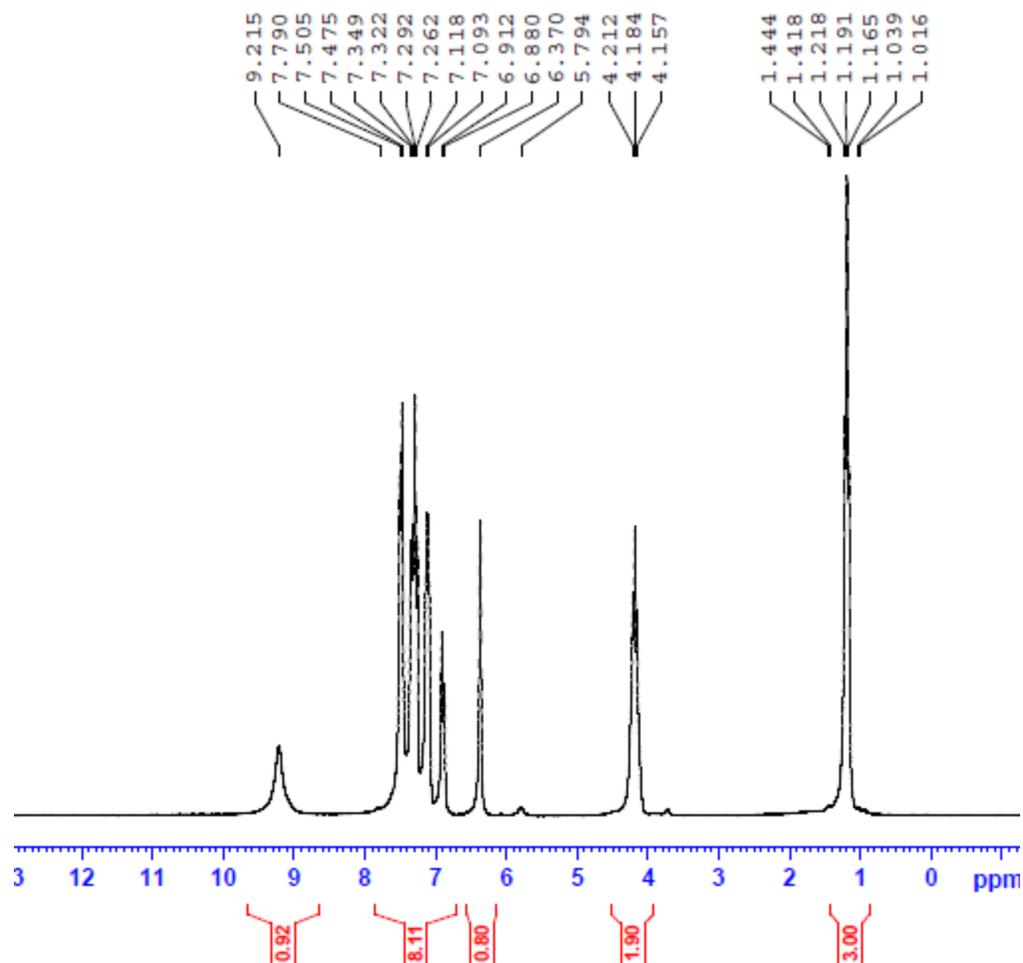


Figure 23. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 2-(2,4-dichlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4h**)

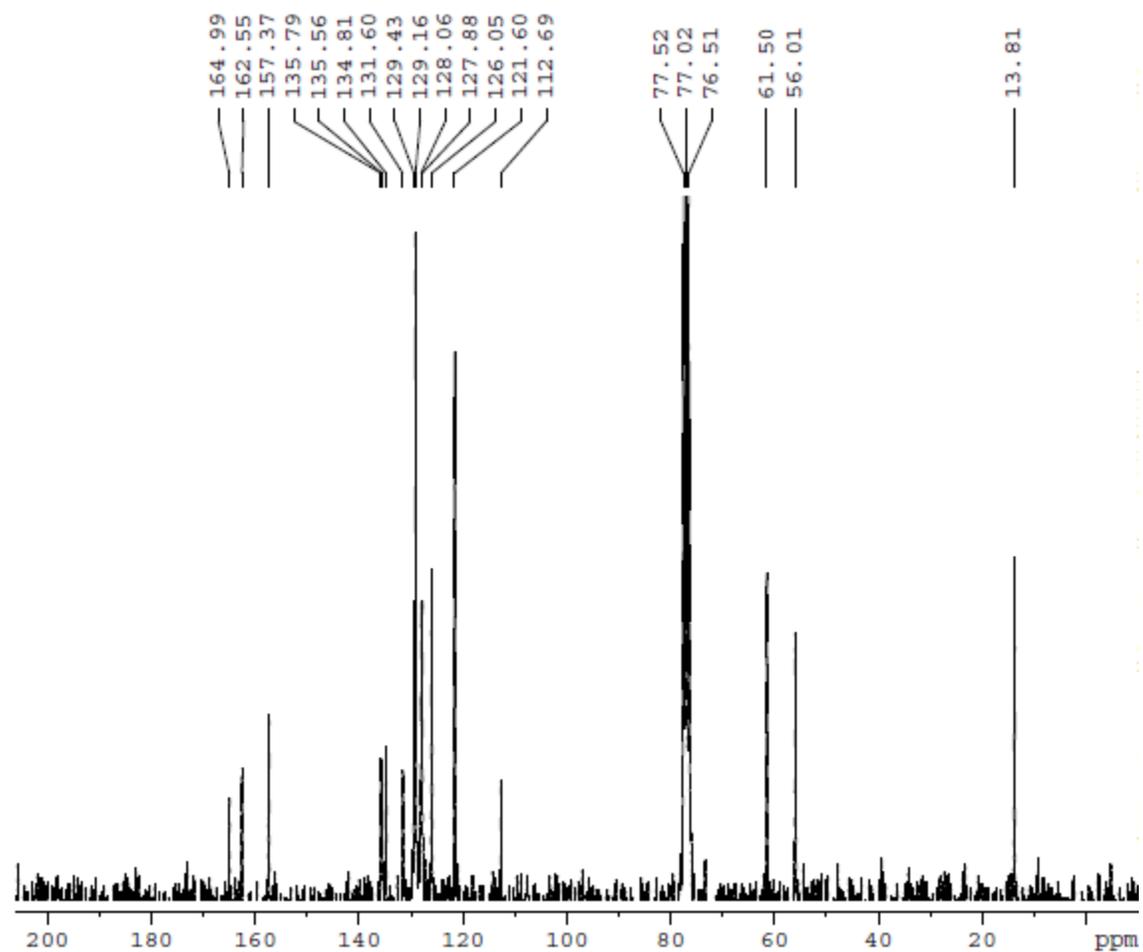


Figure 24. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 2-(2,4-dichlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4h**)

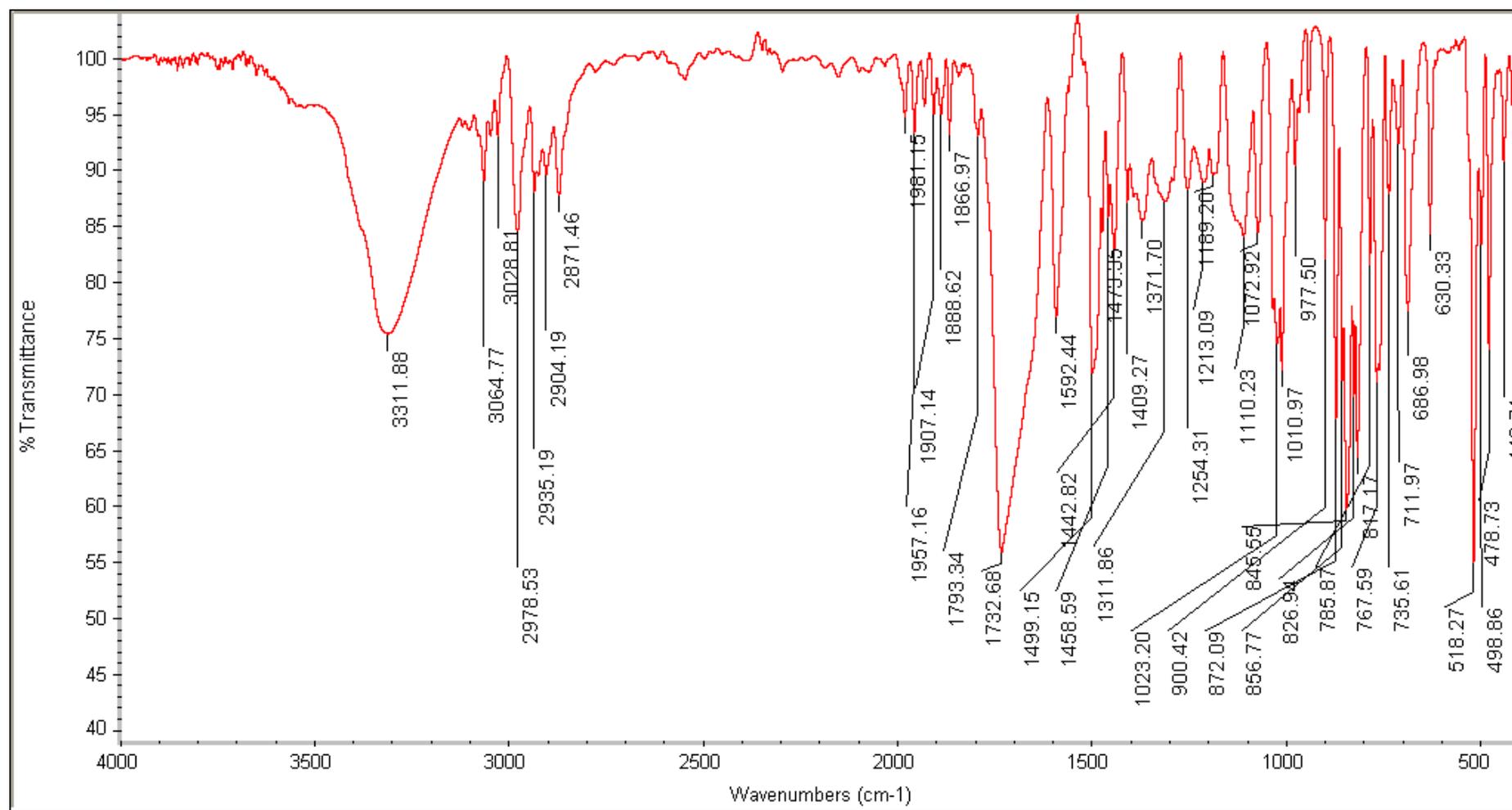


Figure 25. FT-IR spectrum of Ethyl 2-(4-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4i**)

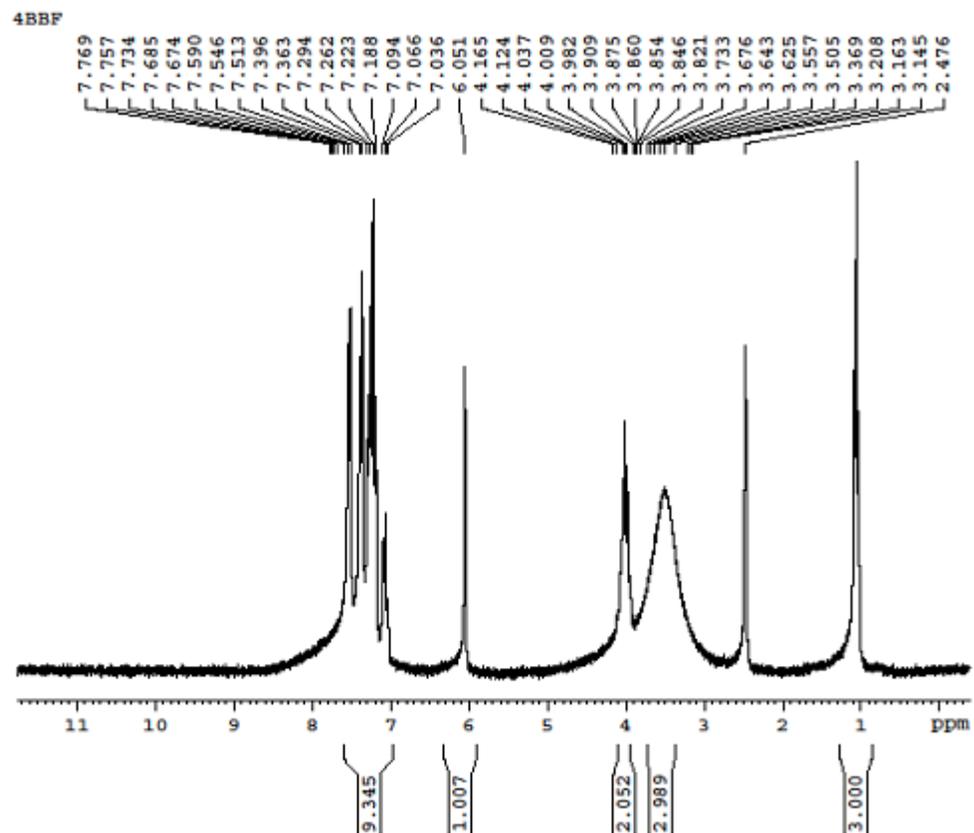


Figure 26. ^1H NMR (250.13 MHz, DMSO-d_6) spectrum of Ethyl 2-(4-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4i**)

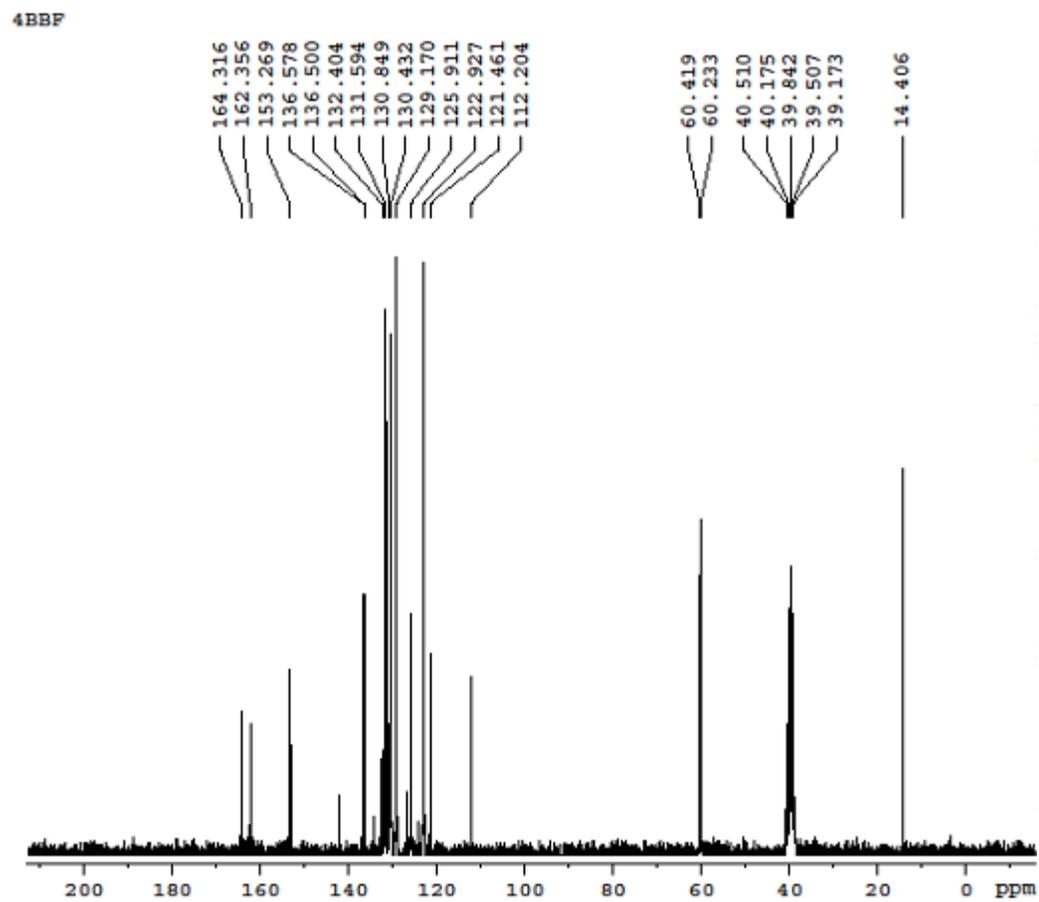


Figure 27. ^{13}C NMR (62.90 MHz, DMSO-d_6) spectrum of Ethyl 2-(4-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4e**)

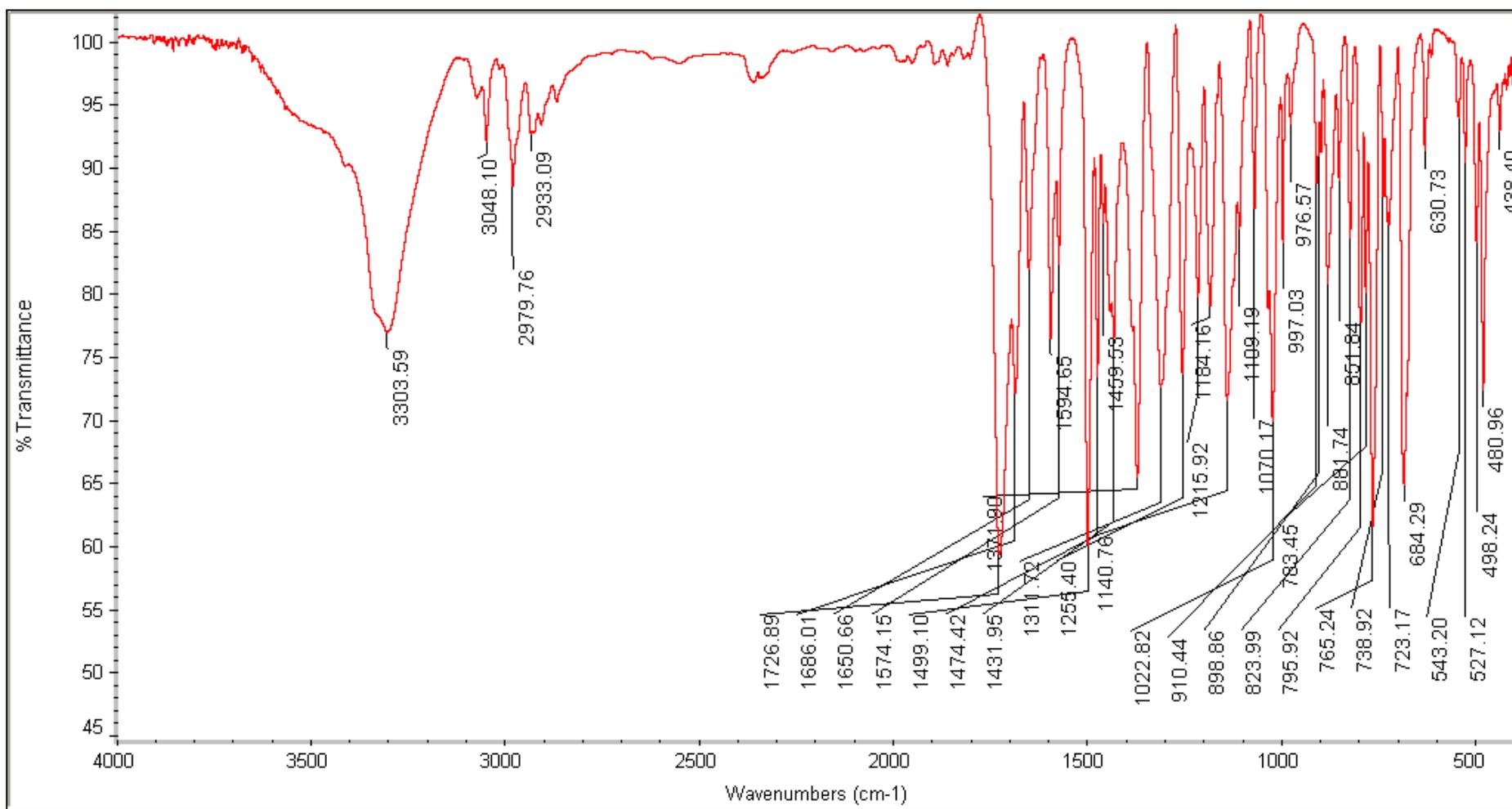


Figure 28. FT-IR spectrum of Ethyl 2-(3-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4j**)

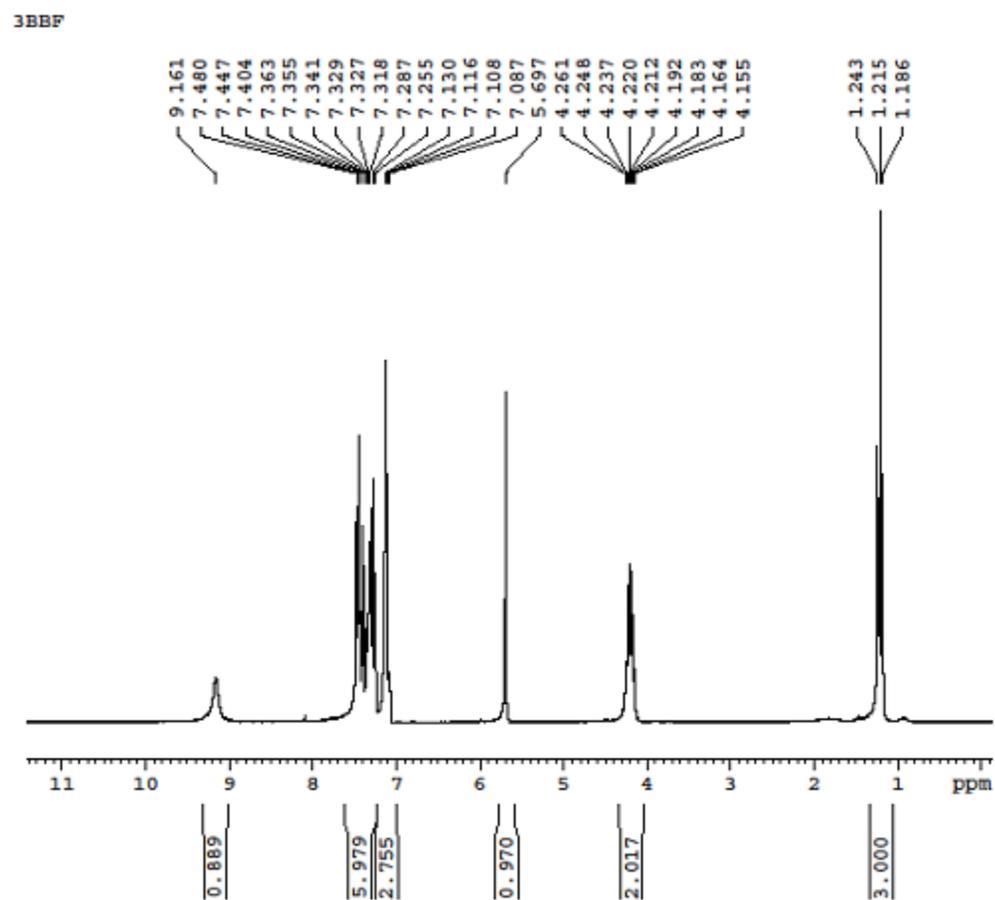


Figure 29. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 2-(3-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4j**)

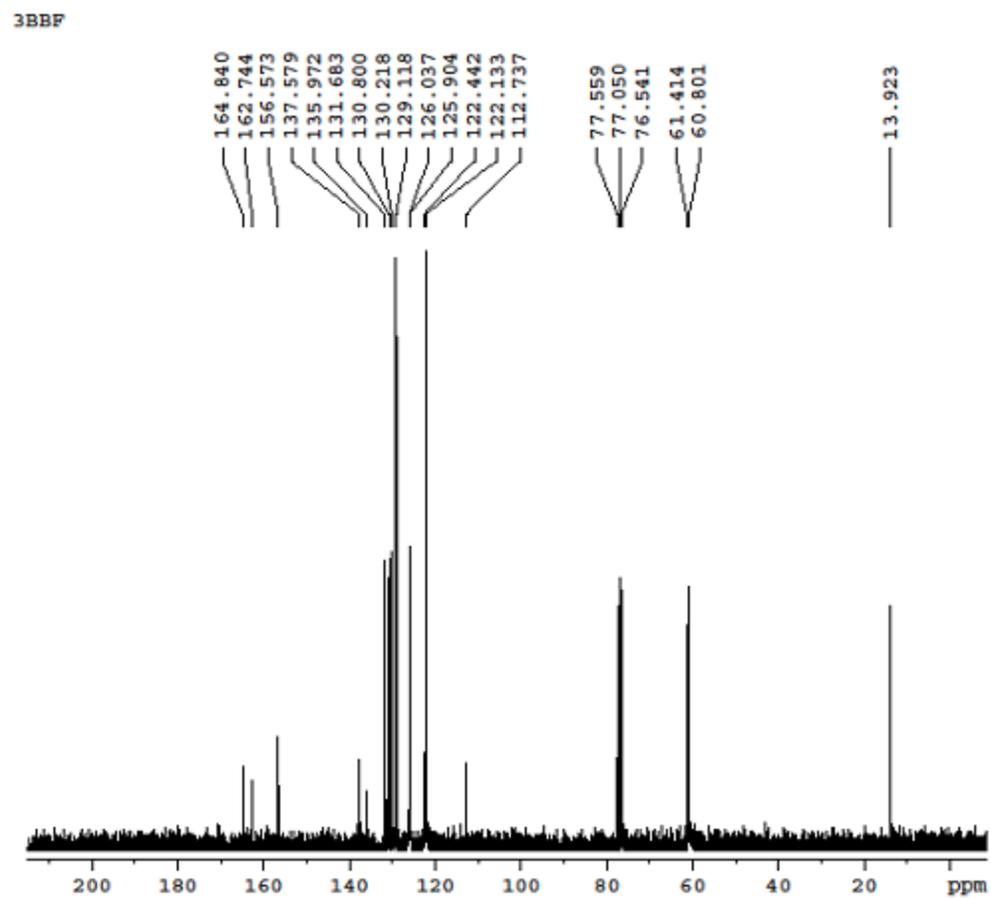


Figure 30. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 2-(4-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4j**)

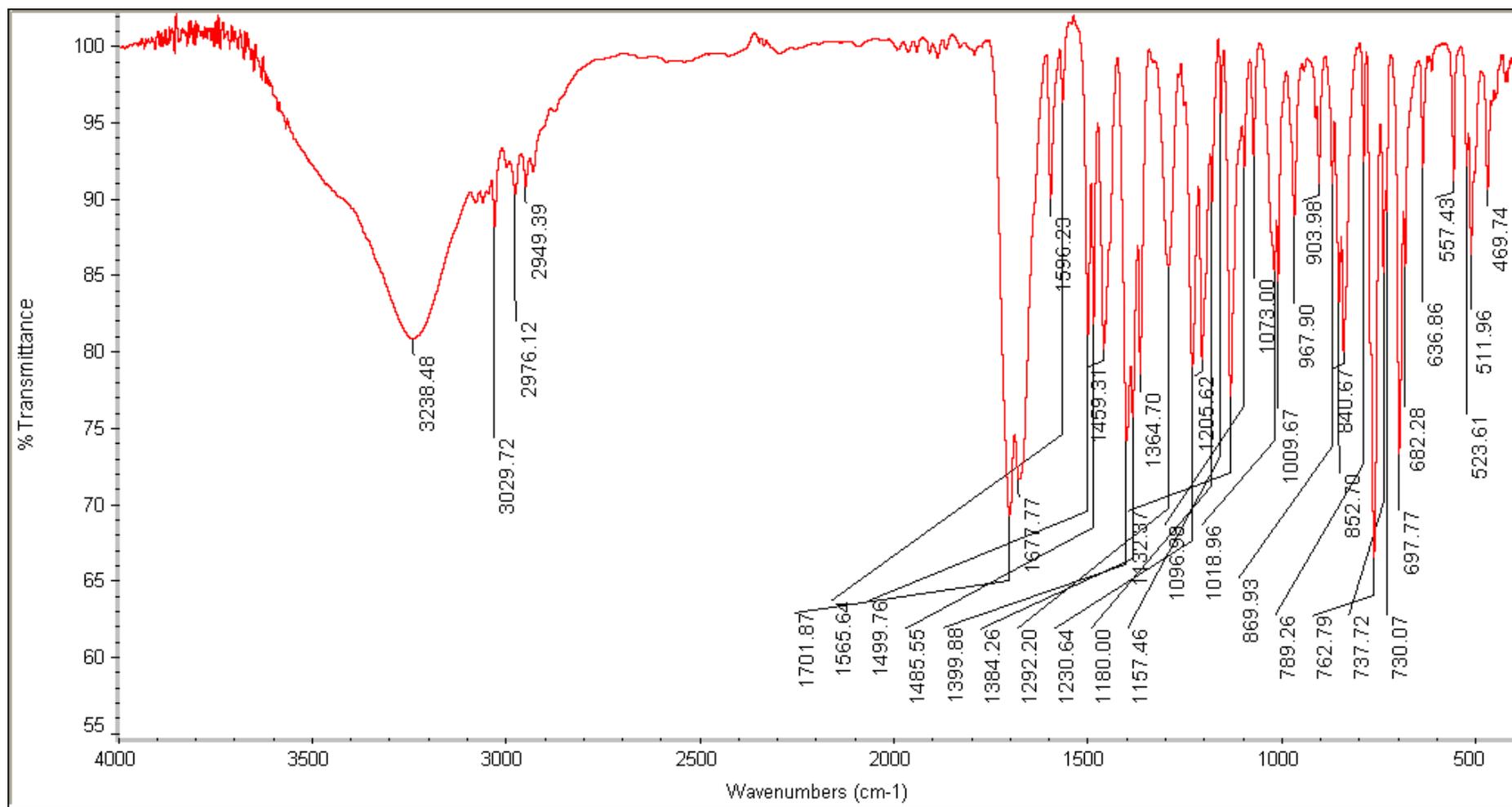


Figure 31. FT-IR spectrum of Ethyl 2-([1, 1'-biphenyl]-4-yl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4k**).

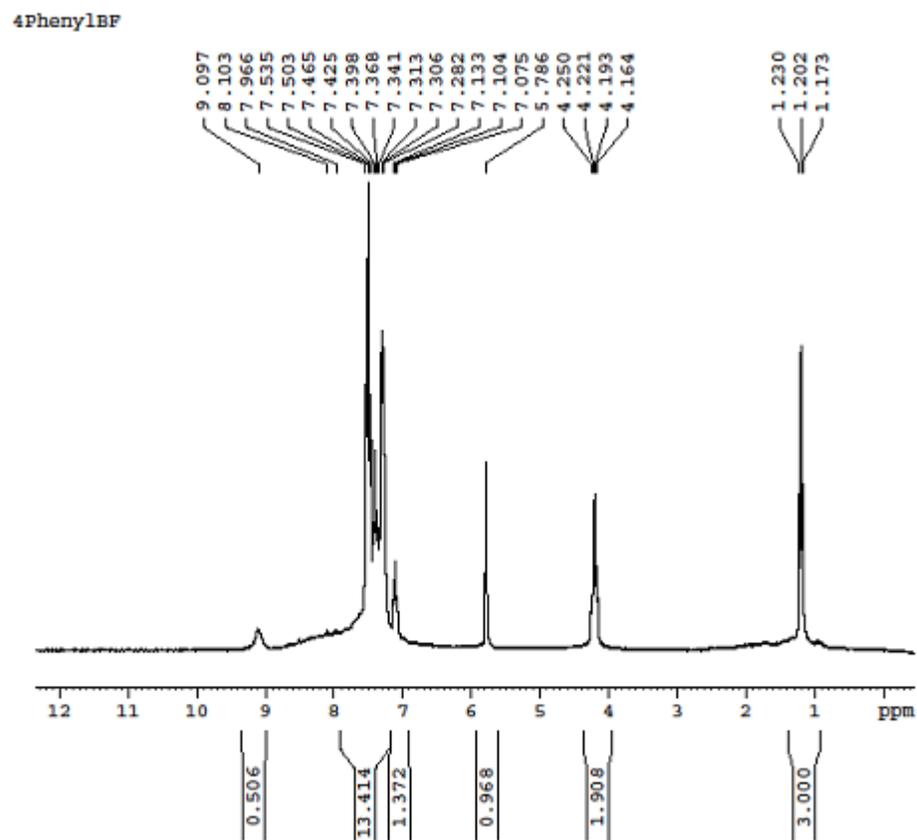


Figure 32. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 2-([1,1'-biphenyl]-4-yl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4k**)

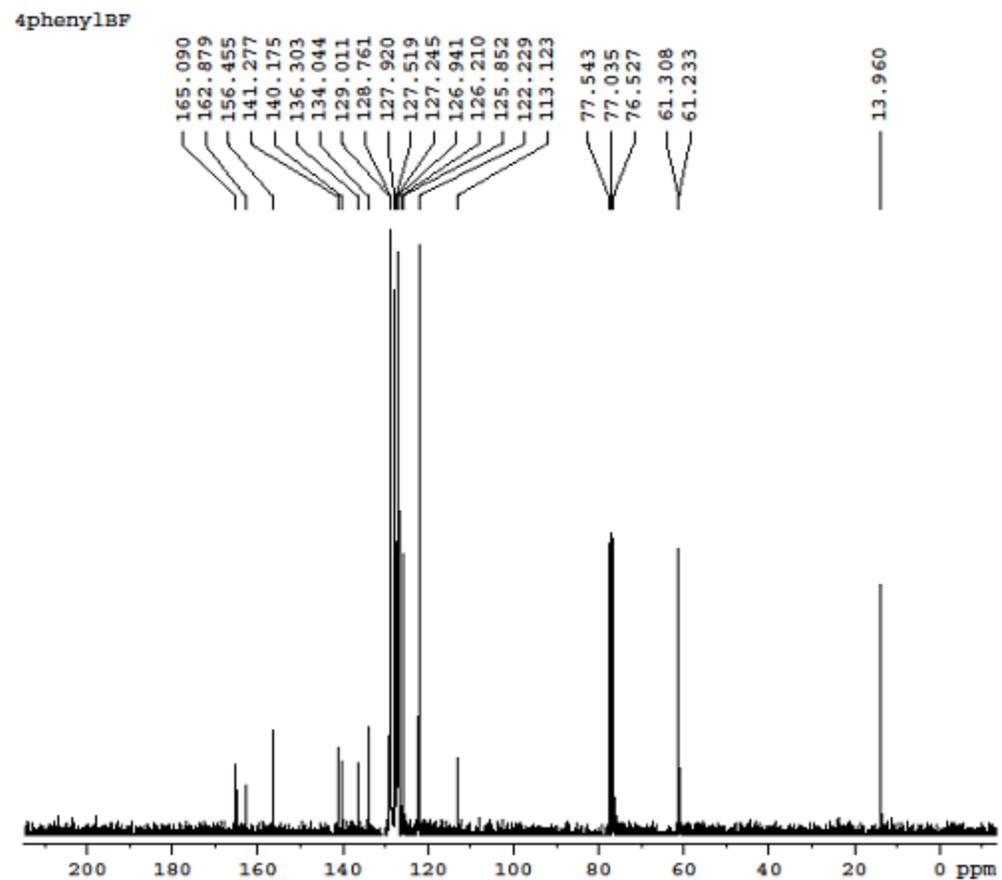


Figure 33. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 2-([1,1'-biphenyl]-4-yl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (4k)

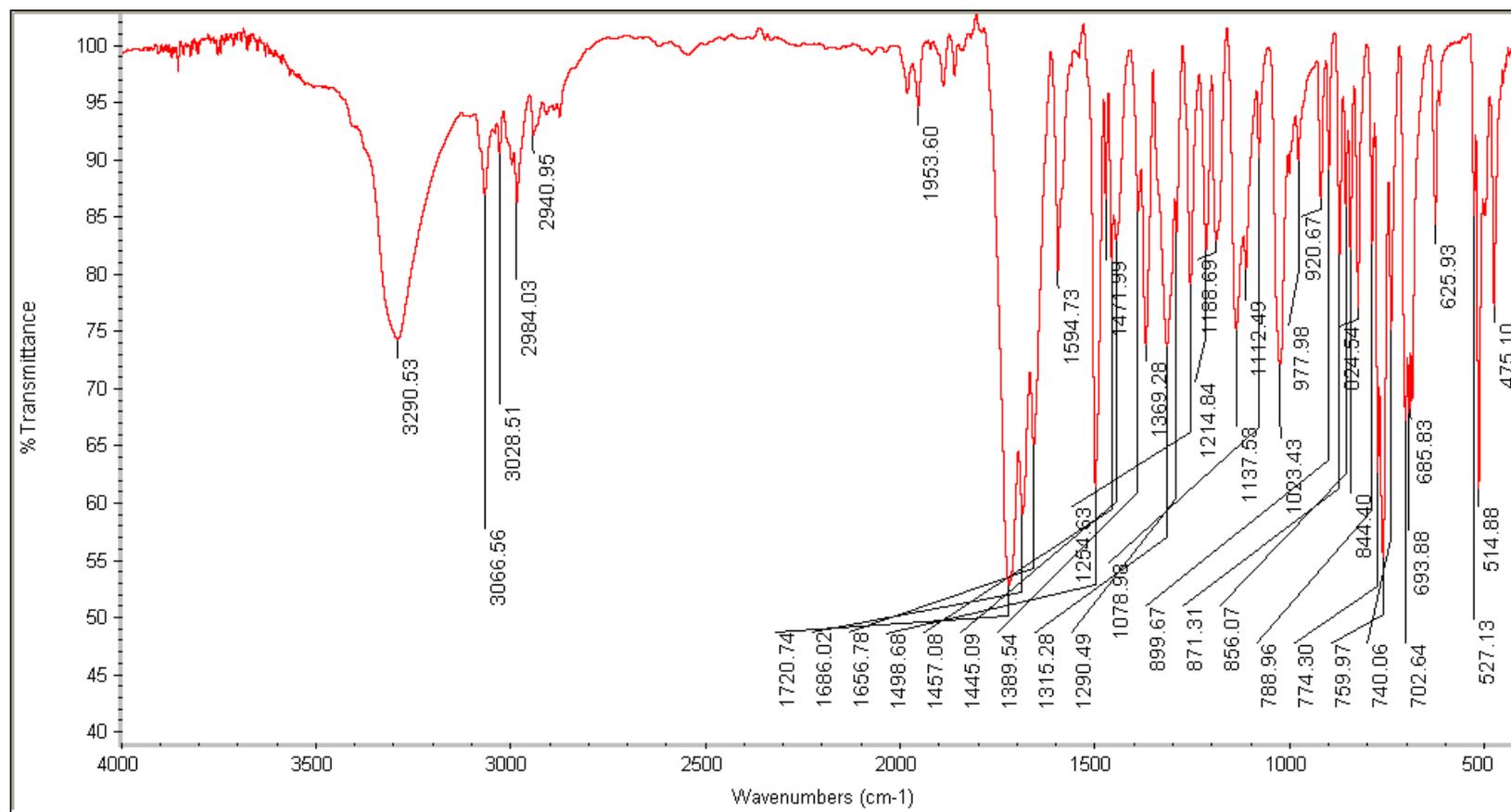


Figure 34. FT-IR spectrum of Ethyl 4-hydroxy-5-oxo-1,2-diphenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4I**)

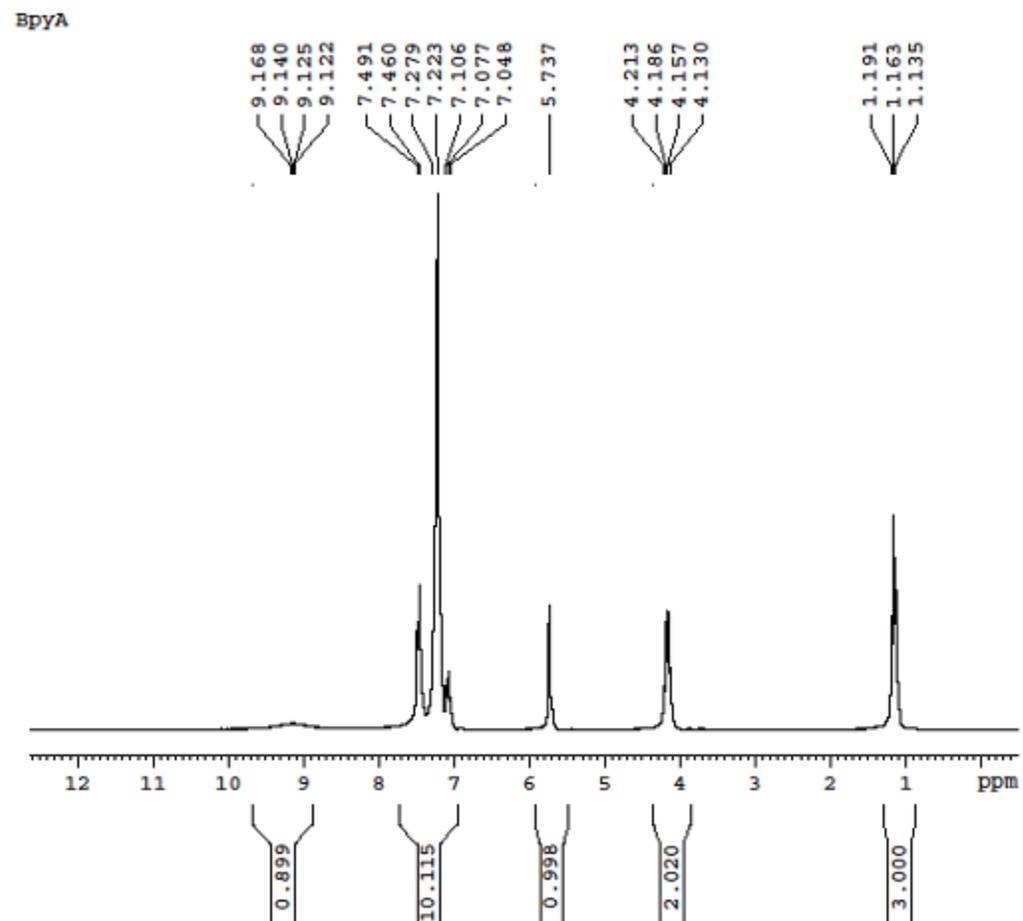


Figure 35. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-5-oxo-1,2-diphenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4l**)

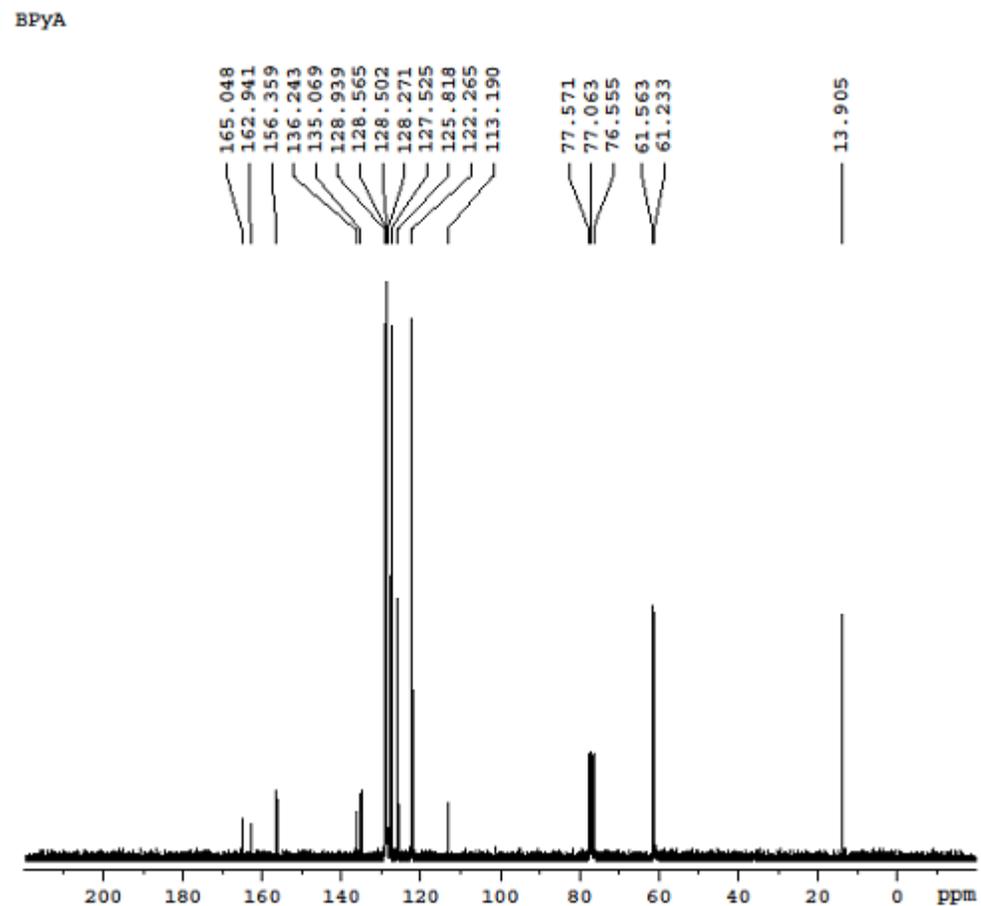


Figure 36. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-5-oxo-1,2-diphenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4I**)

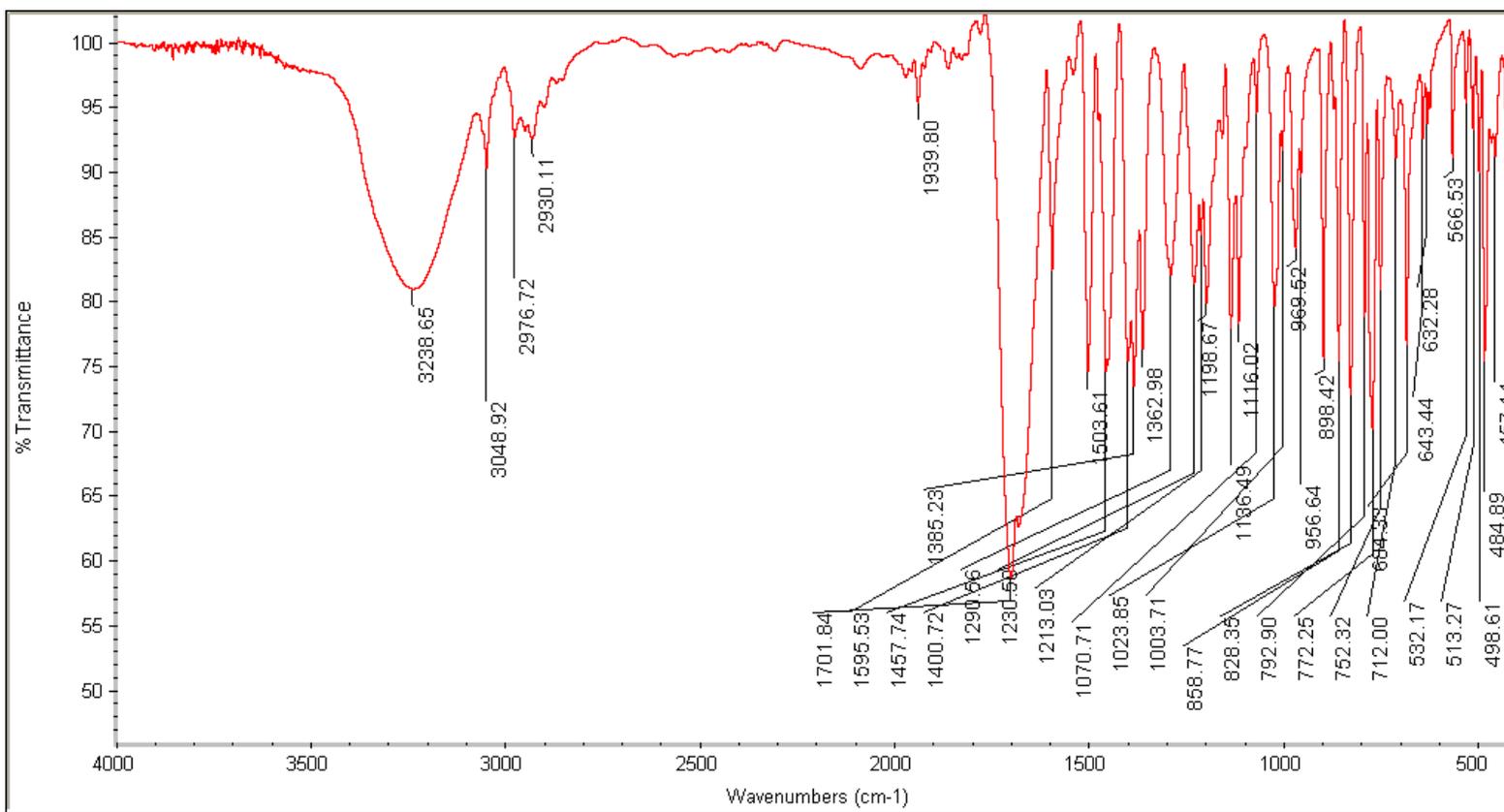


Figure 37. FT-IR spectrum of Ethyl 4-hydroxy-2-(naphthalen-2-yl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4m**)

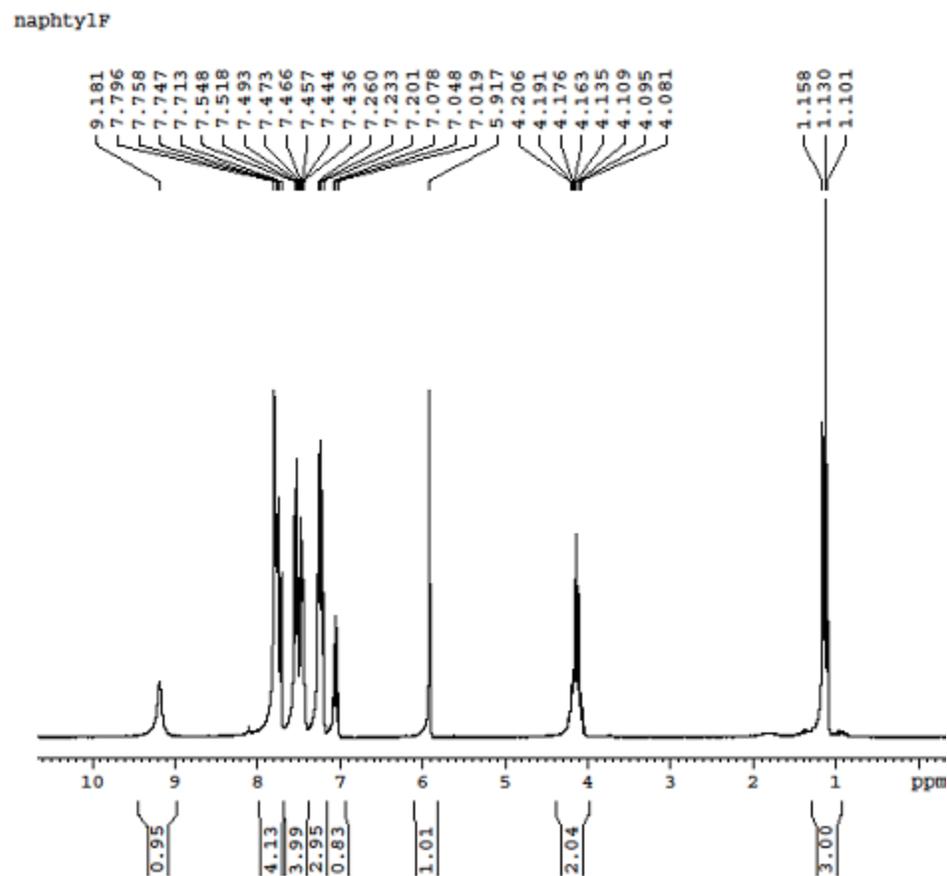


Figure 38. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-2-(naphthalen-2-yl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4m**)

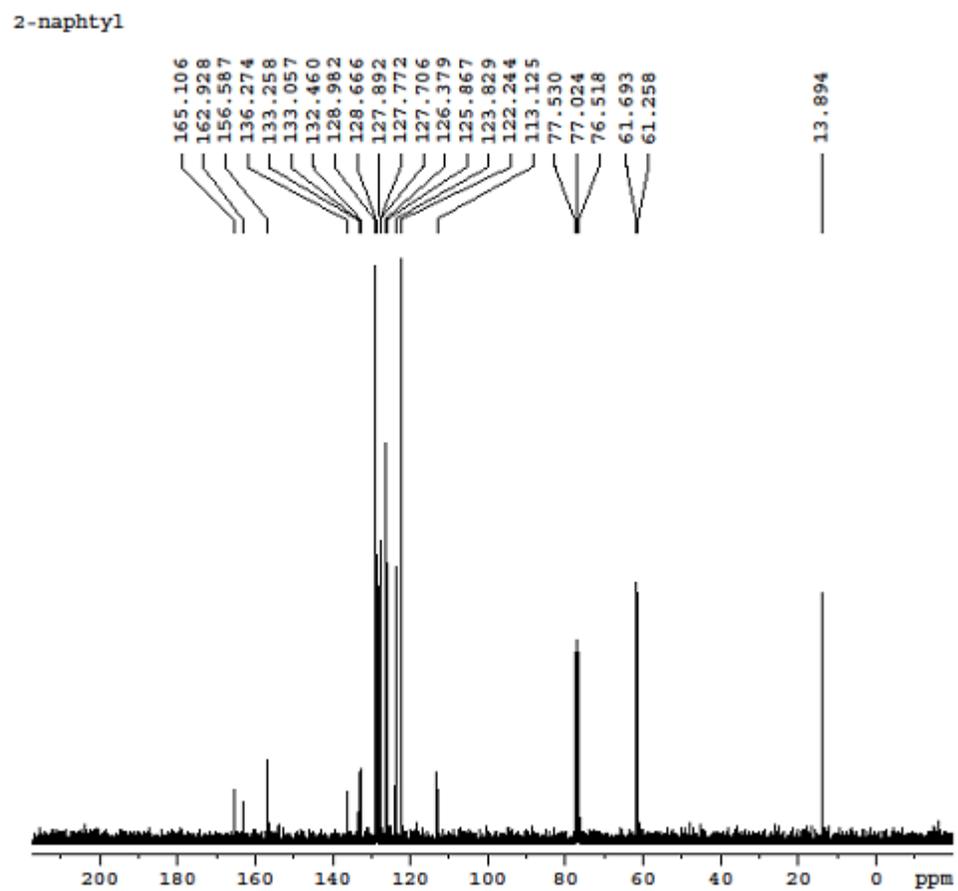


Figure 39. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-2-(naphthalen-2-yl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4m**)

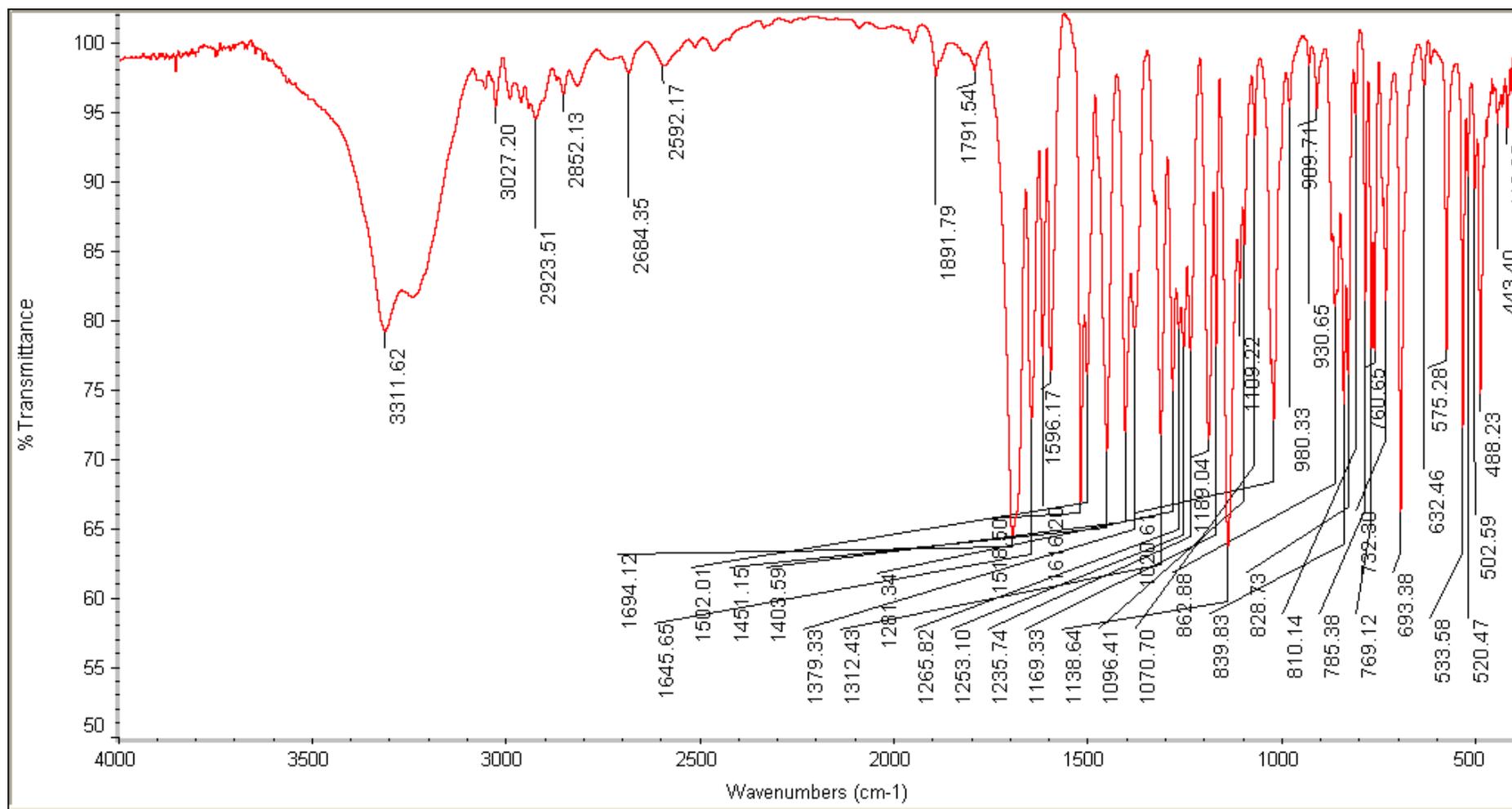


Figure 40. FT-IR spectrum of Ethyl 4-hydroxy-2-(4-hydroxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4n**)

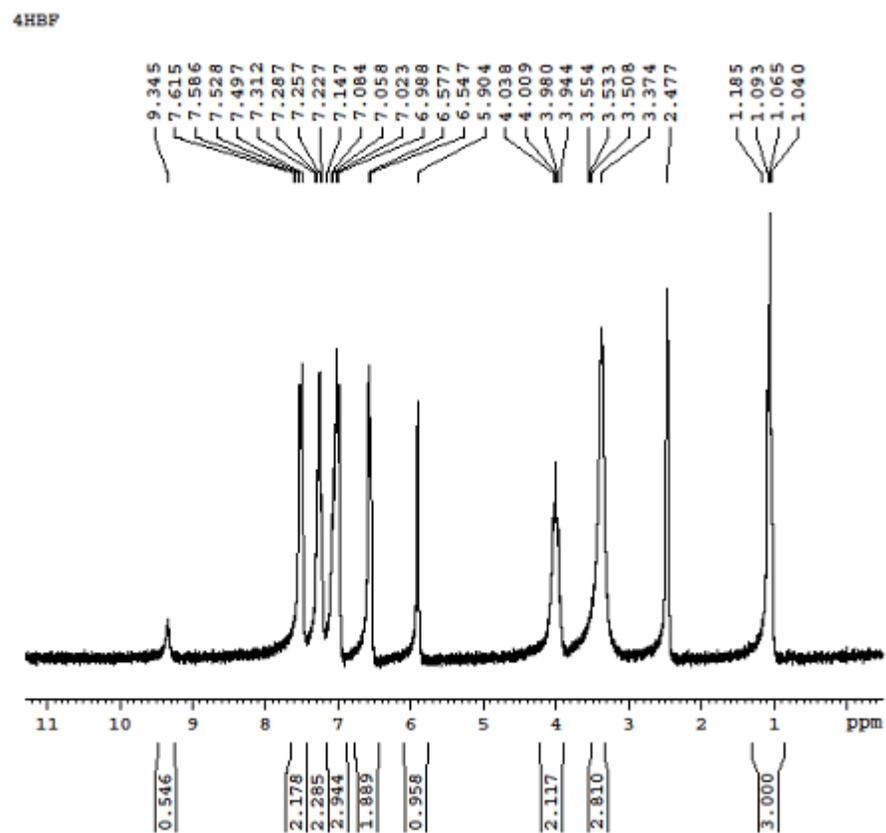


Figure 41. ^1H NMR (250.13 MHz, DMSO-d_6) spectrum of Ethyl 4-hydroxy-2-(4-hydroxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4n**)

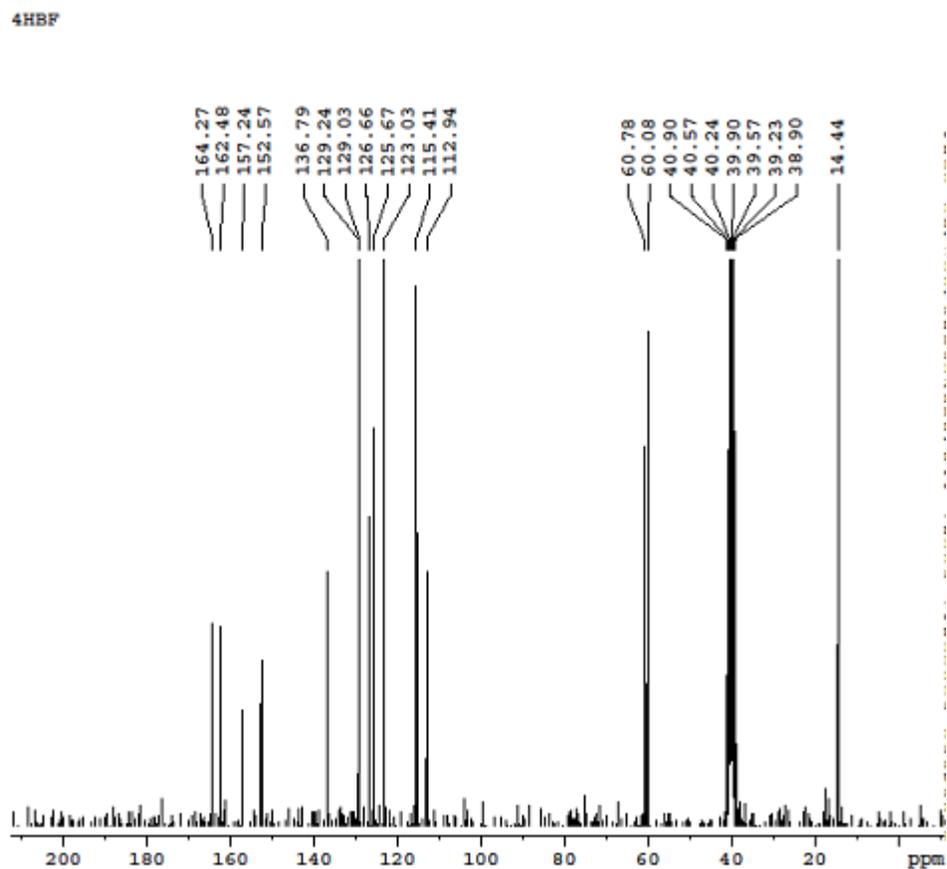


Figure 42. ^1H NMR (62.90 MHz, DMSO-d_6) spectrum of Ethyl 4-hydroxy-2-(4-hydroxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4n**)

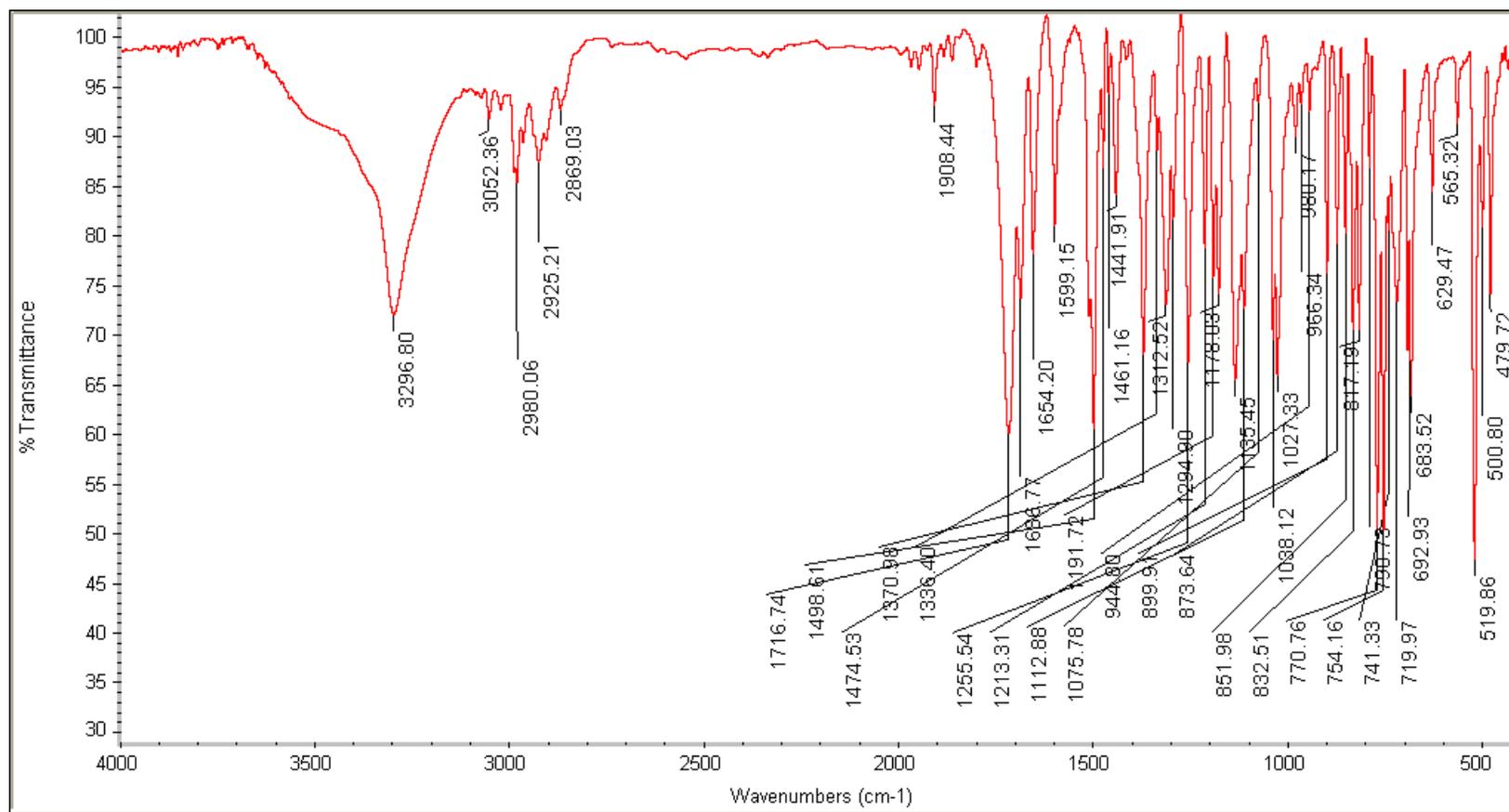


Figure 43. FT-IR spectrum of Ethyl 4-hydroxy-5-oxo-1-phenyl-2-(p-tolyl)-2,5-dihydro-1H-pyrrole-3-carboxylate (**4o**)

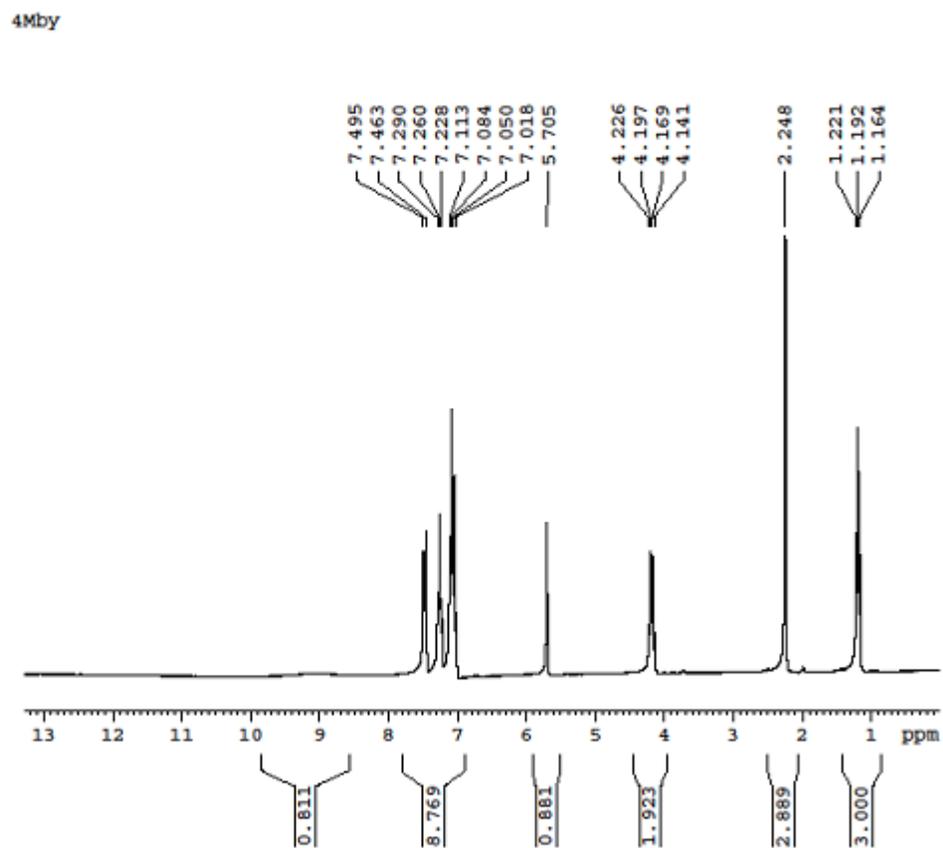


Figure 44. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-5-oxo-1-phenyl-2-(p-tolyl)-2,5-dihydro-1H-pyrrole-3-carboxylate (**4o**)

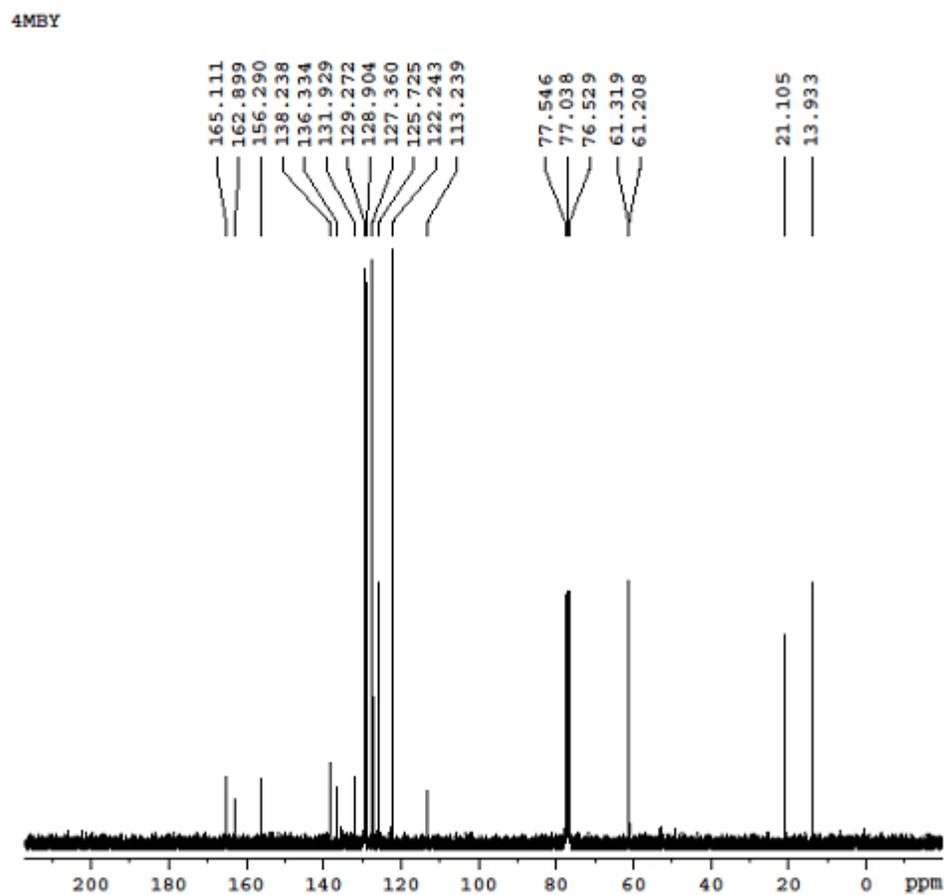


Figure 45. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-5-oxo-1-phenyl-2-(p-tolyl)-2,5-dihydro-1H-pyrrole-3-carboxylate (**4o**).

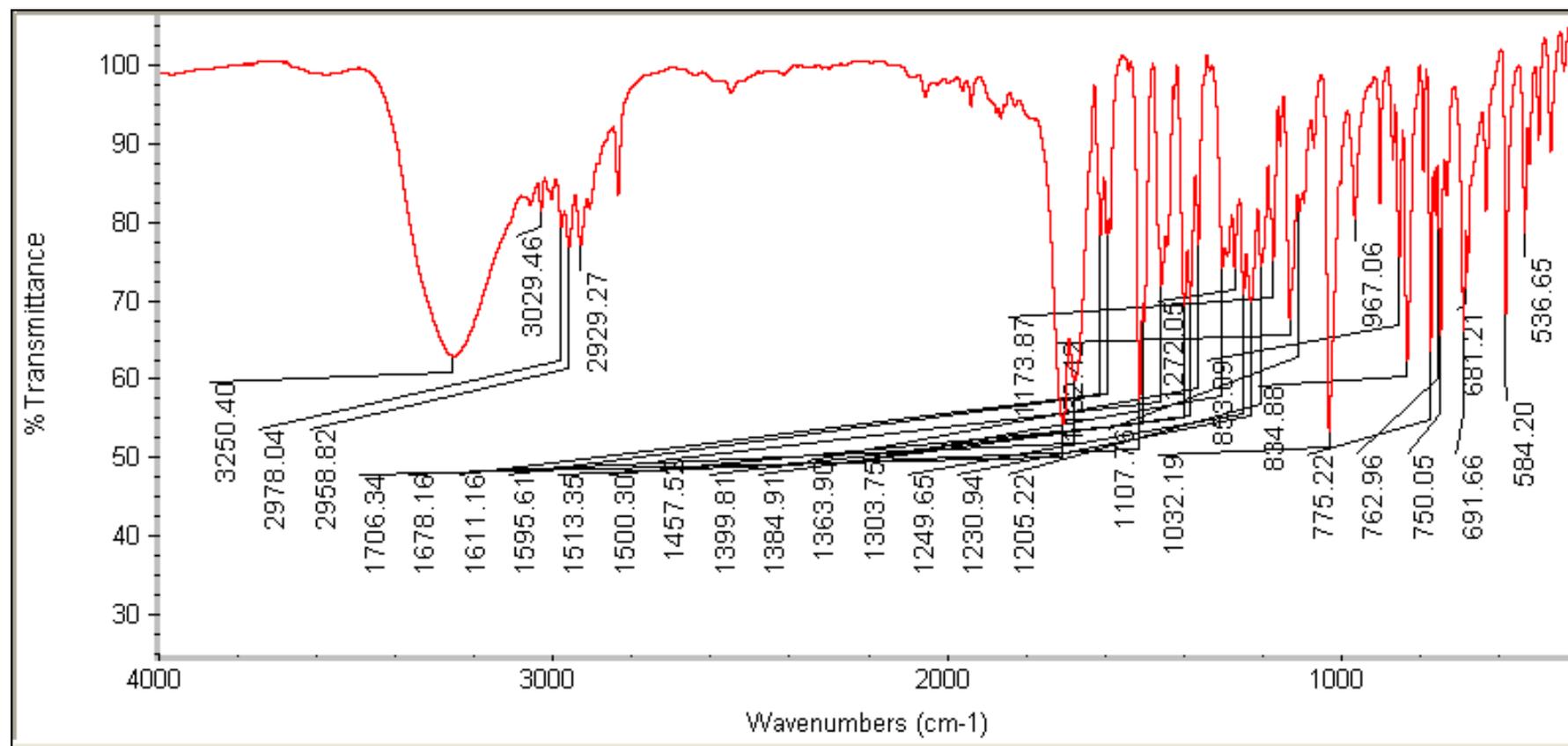


Figure 46. FT-IR spectrum of Ethyl 4-hydroxy-2-(4-methoxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4p**).

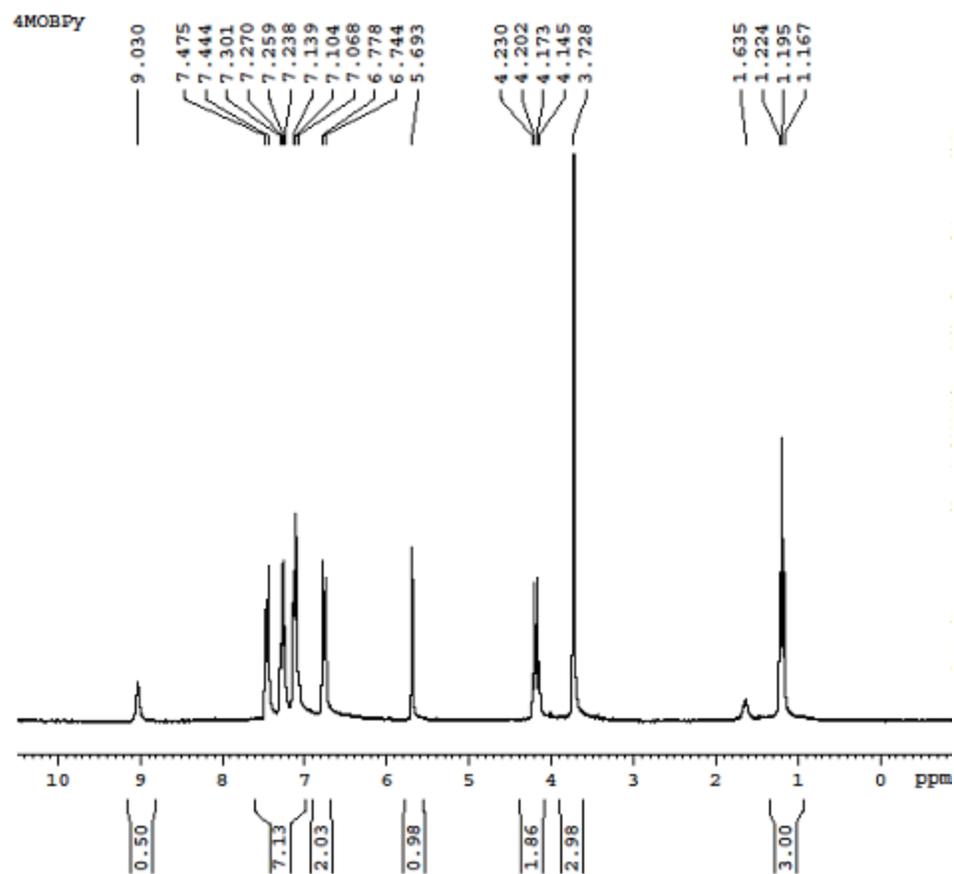


Figure 47. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-2-(4-methoxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4p**)

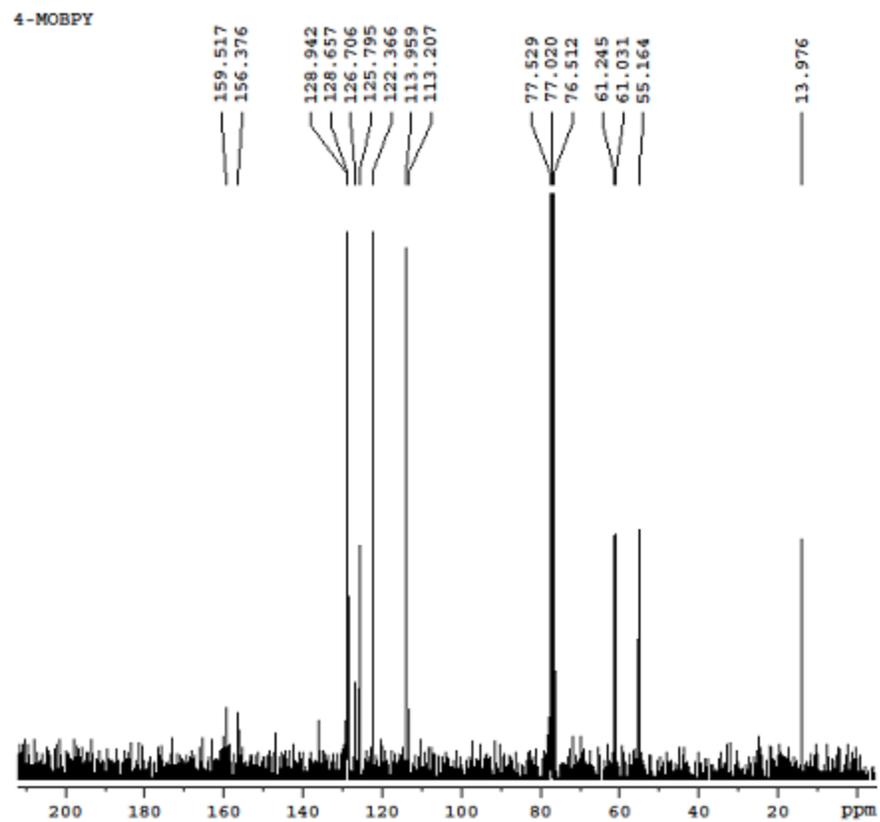


Figure 48. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-2-(4-methoxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4p**)

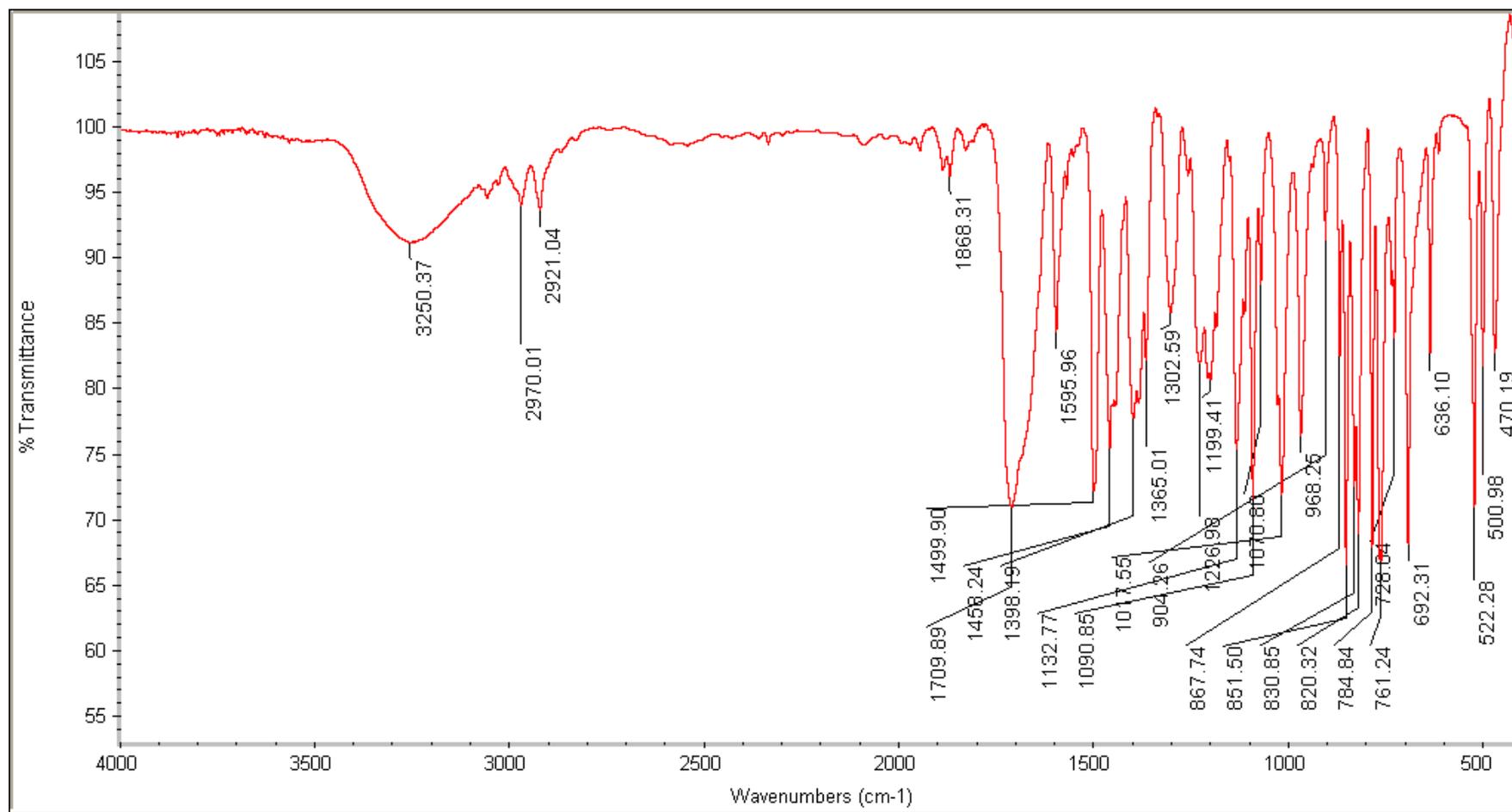


Figure 49. FT-IR spectrum of Ethyl 4-hydroxy-2-(4-(methylthio)phenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4q**)

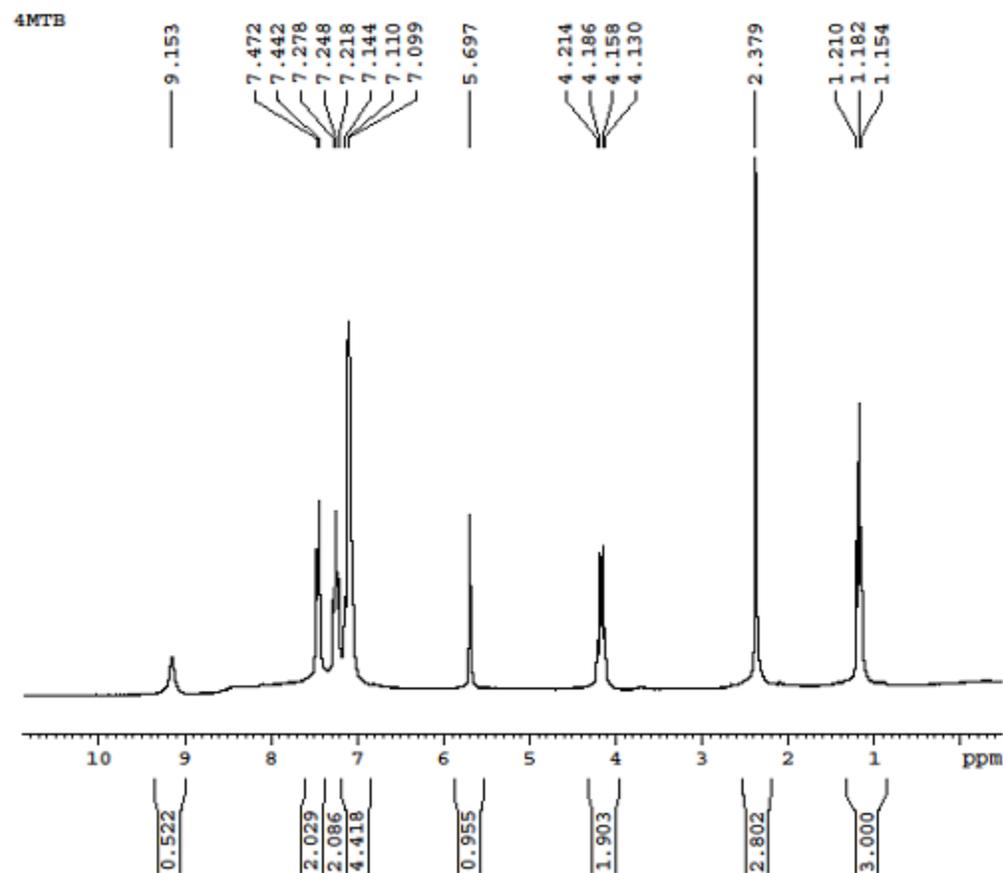


Figure 50. ^1H NMR (250.13 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-2-(4-(methylthio)phenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4q**)

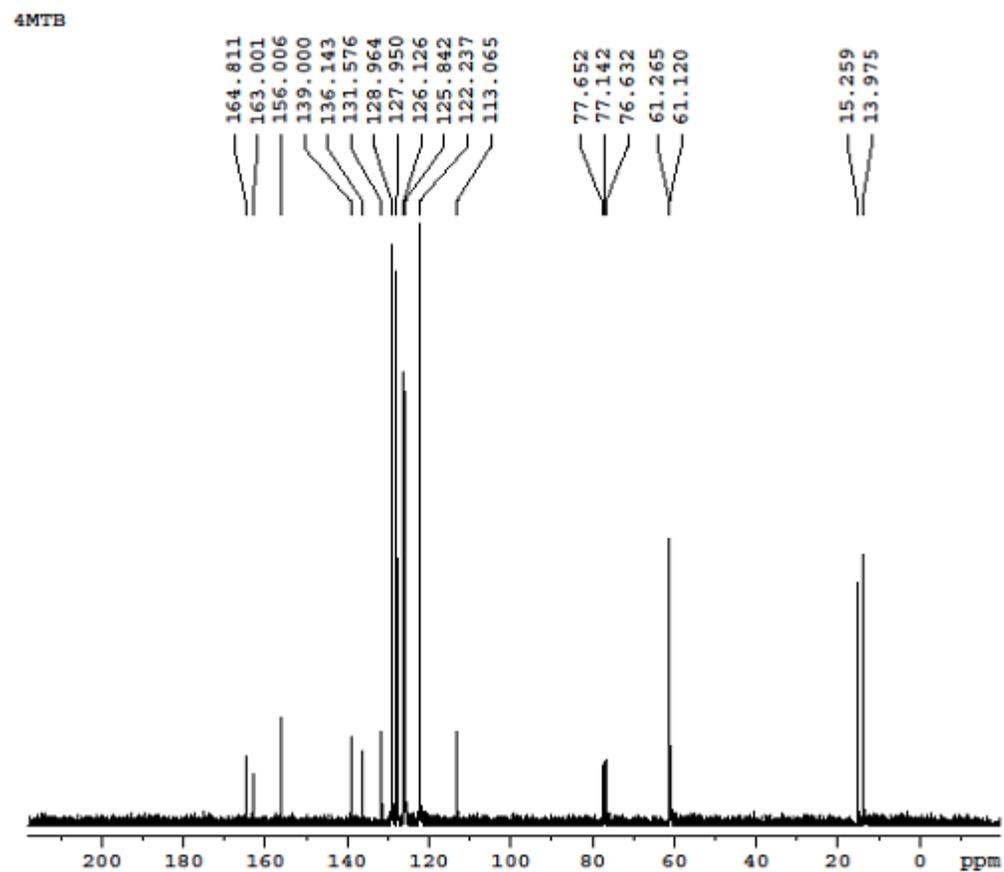


Figure 51. ^{13}C NMR (62.90 MHz, CDCl_3) spectrum of Ethyl 4-hydroxy-2-(4-(methylthio)phenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4q**)

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 |
| <i>M_r</i> | 369.42 |
| Crystal system, space group | Monoclinic, <i>P</i> 2 ₁ / <i>n</i> |
| Temperature (K) | 100 |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 9.922 (3), 6.156 (2), 28.905 (9) |
| <i>β</i> (°) | 92.68 (3) |
| <i>V</i> (Å ³) | 1763.6 (10) |
| <i>Z</i> | 4 |
| Radiation type | Mo <i>K</i> α |
| <i>μ</i> (mm ⁻¹) | 0.21 |
| Crystal size (mm) | 0.43 × 0.22 × 0.11 |
| Diffractometer | Agilent Technologies Xcalibur R diffractometer |
| Absorption correction | Multi-scan |
| <i>T_{min}</i> , <i>T_{max}</i> | 0.991, 1.000 |
| No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections | 10885, 5008, 4131 |
| <i>R_{int}</i> | 0.025 |
| (sin θ/λ) _{max} (Å ⁻¹) | 0.720 |
| <i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i> | 0.039, 0.099, 1.03 |
| No. of reflections | 5008 |
| No. of parameters | 241 |
| No. of restraints | 0 |
| Δρ _{max} , Δρ _{min} (e Å ⁻³) | 0.45, -0.31 |