

Supplementary Material

Synthesis of styryl pyrazolones and evaluation of their potential antioxidant activities

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1 | Experimental section

In Vitro Antioxidant Assay

The sample's antioxidant activity was assessed and compared with the standard Trolox using the two assays, DPPH and FRAP [2]. The experiments were conducted in a Microplate Spectrophotometer, and the results were averaged. The IC₅₀ values for the sample and the standard were found using the DPPH test. The percentage of DPPH free radical scavenging was calculated using the following method, which was based on the measured absorbance:

$$\text{DPPH scavenging activity (\%)} = \frac{A_{\text{control}} - A_{\text{sample}}}{A_{\text{control}}} * 100$$

where A_{control} is the absorbance (DPPH + methanol) of the control and A_{sample} is the absorbance of the sample. To assess the antioxidant activity, the IC₅₀ values were employed.

For DPPH assay, 0.1 mM solution of Trolox was prepared in 1000 ml ethanol and the synthesized compounds were dissolved in ethanol solvent. For the preparation of DPPH, 0.5 mM solution of DPPH was prepared in methanol.

In the FRAP assay, a Microplate Spectrophotometer was used to measure the absorbance of the reaction mixture at 700 nm. Increased absorbance values signified stronger reducing potential and, consequently, higher antioxidant activity. For FRAP studies, 0.1 mM solution of Trolox was prepared in ethanol. Similarly, 1g of potassium ferricyanide was dissolved in 100 ml of distilled water. The synthesized styryl pyrazolones were dissolved in ethanol solvent.

2 Figures of DPPH and FRAP

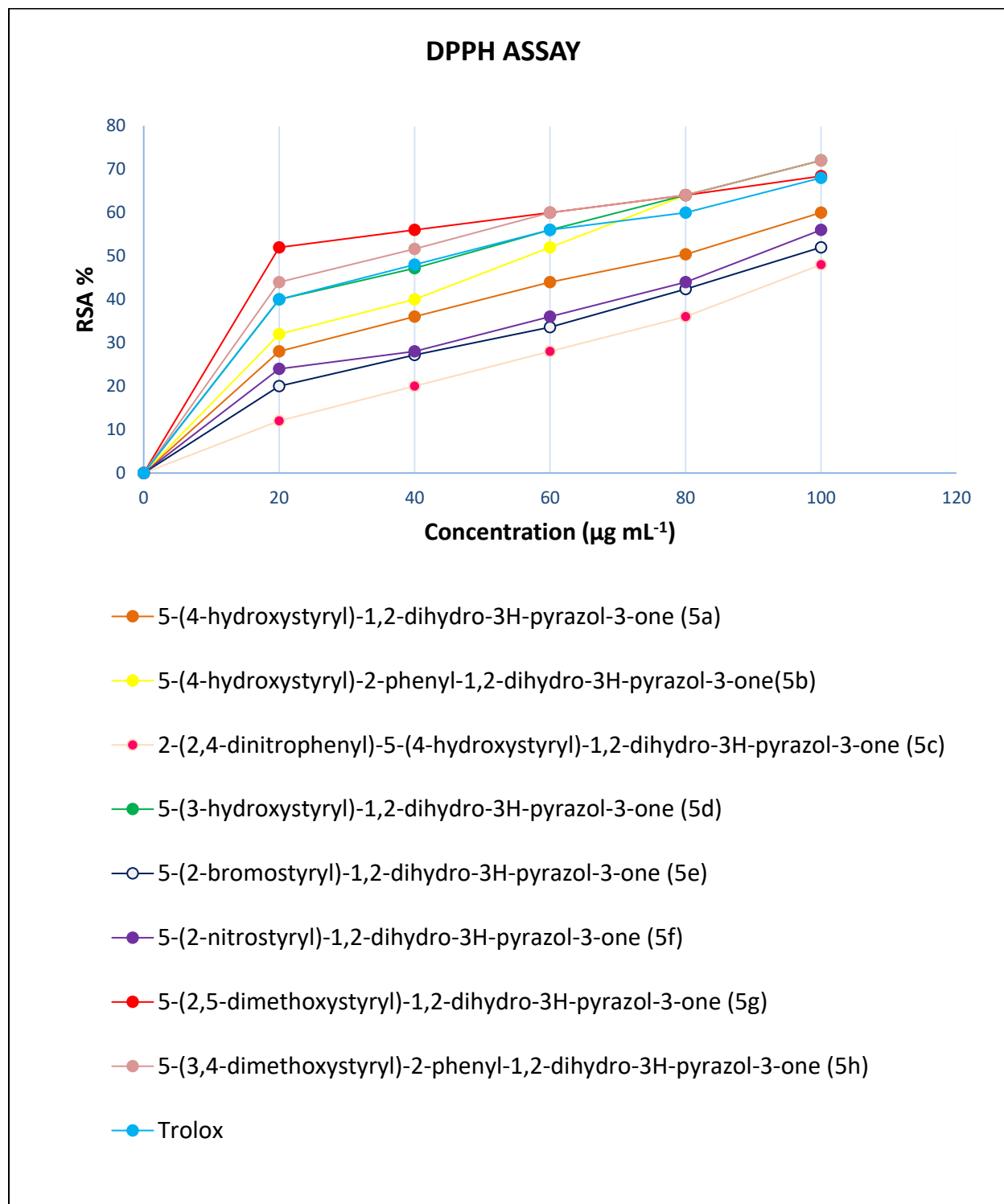


Figure 1. Activity of DPPH free radical scavenging in the presence of various synthesized pyrazole and Trolox concentrations.

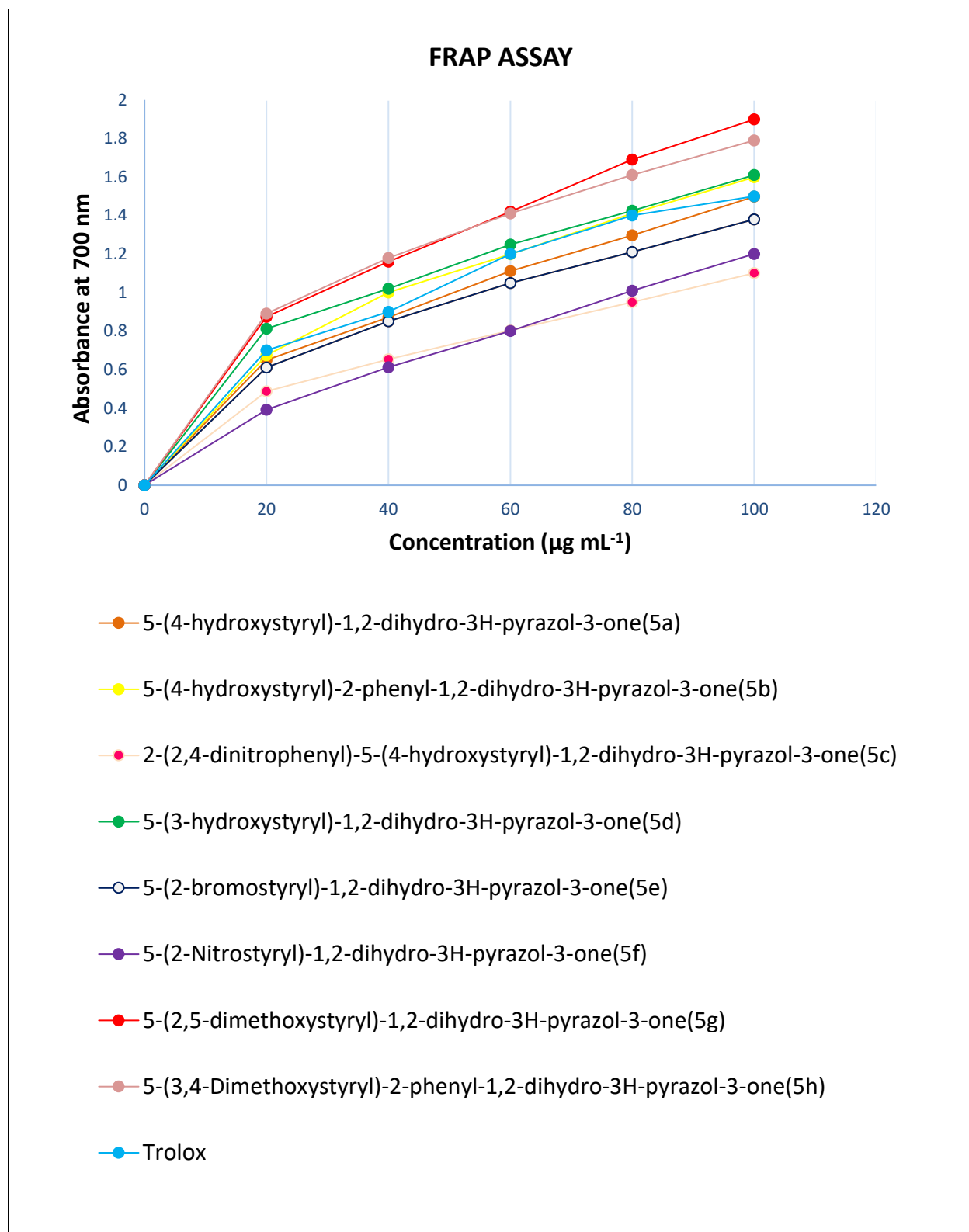


Figure 2. Antioxidant activity of standard Trolox and synthesized compounds using FRAP assay.

3 | Supplementary Data of IR, Mass, ^{13}C and ^1H NMR of styryl pyrazolone derivatives

3.1 | 5-(4-hydroxystyryl)-1,2-dihydro-3H-pyrazol-3-one (5a)

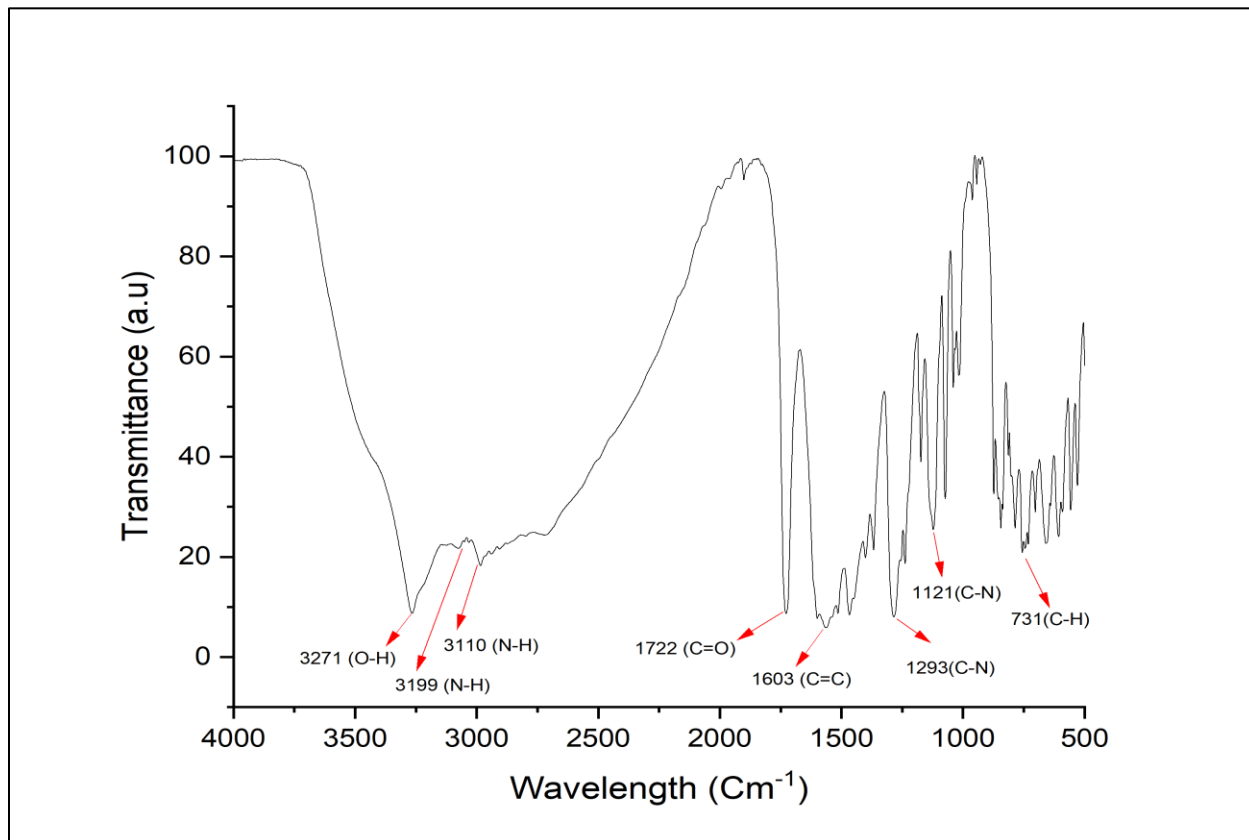


Figure 3. IR Spectra of 5a.

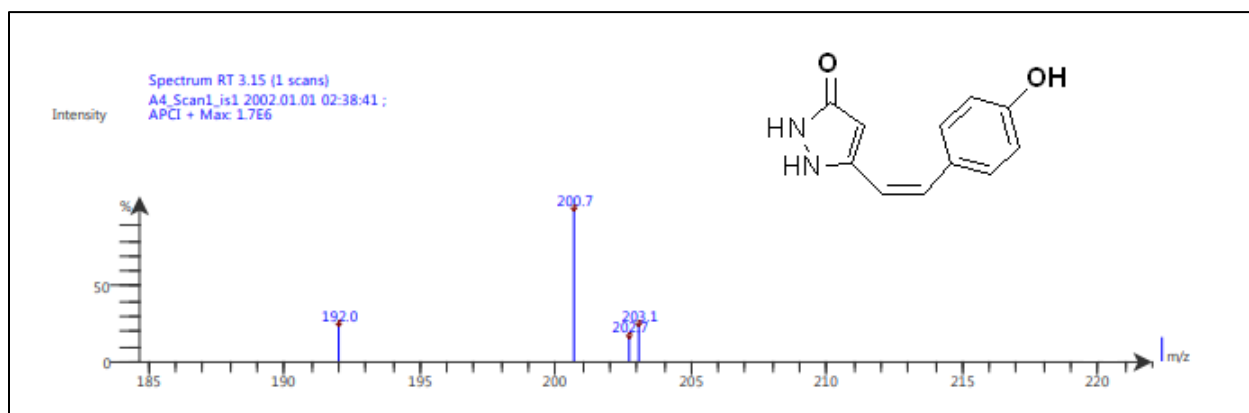
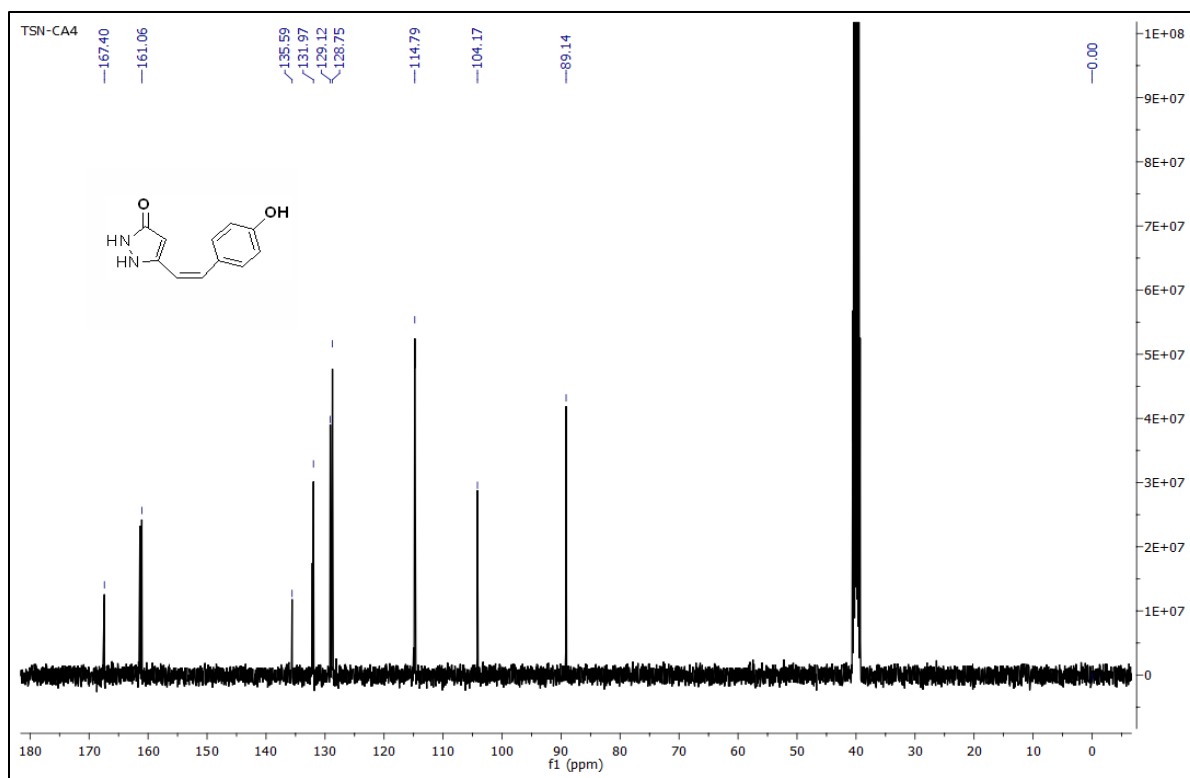
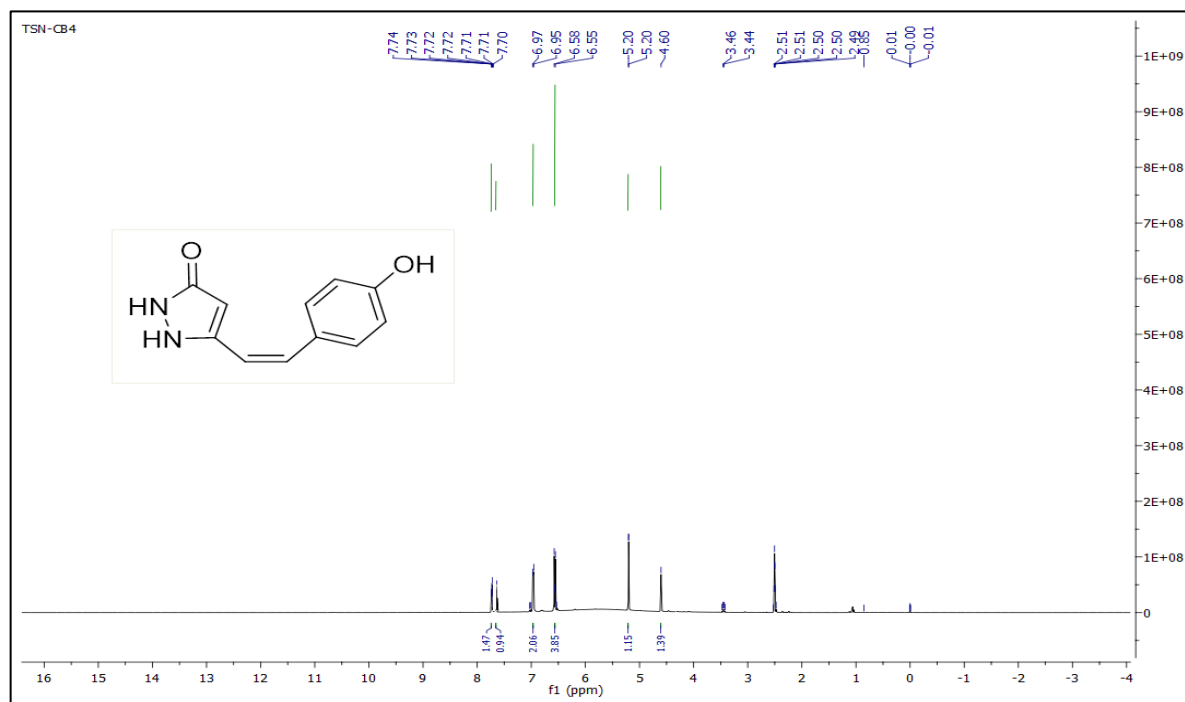


Figure 4. Mass Spectra of 5a.

Figure 5. ^{13}C NMR data of 5a.Figure 6. ^1H NMR data of 5a.

3.2 | 5-(4-hydroxystyryl)-2-phenyl-1,2-dihydro-3H-pyrazol-3-one (5b)

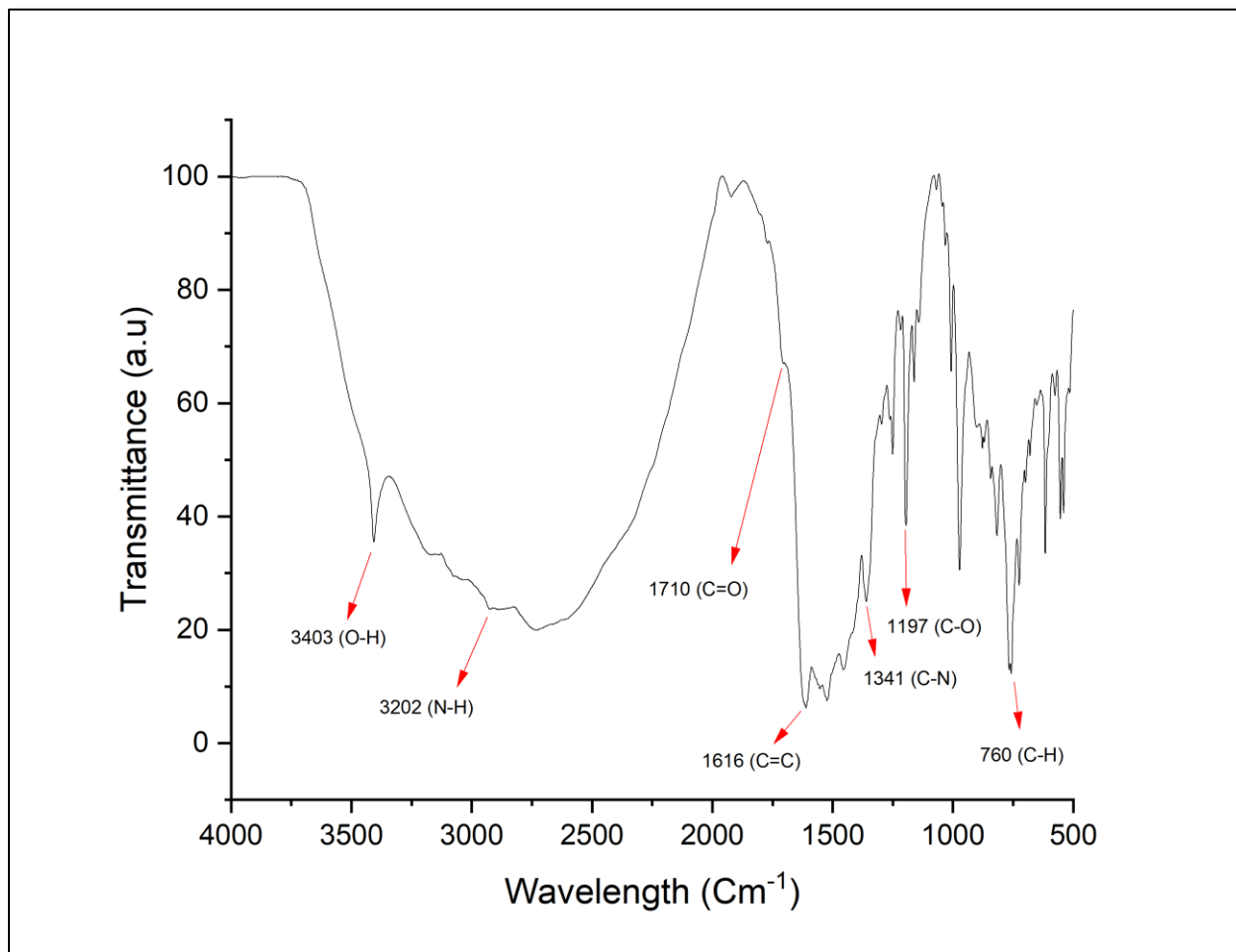


Figure 7. IR Spectra of 5b.

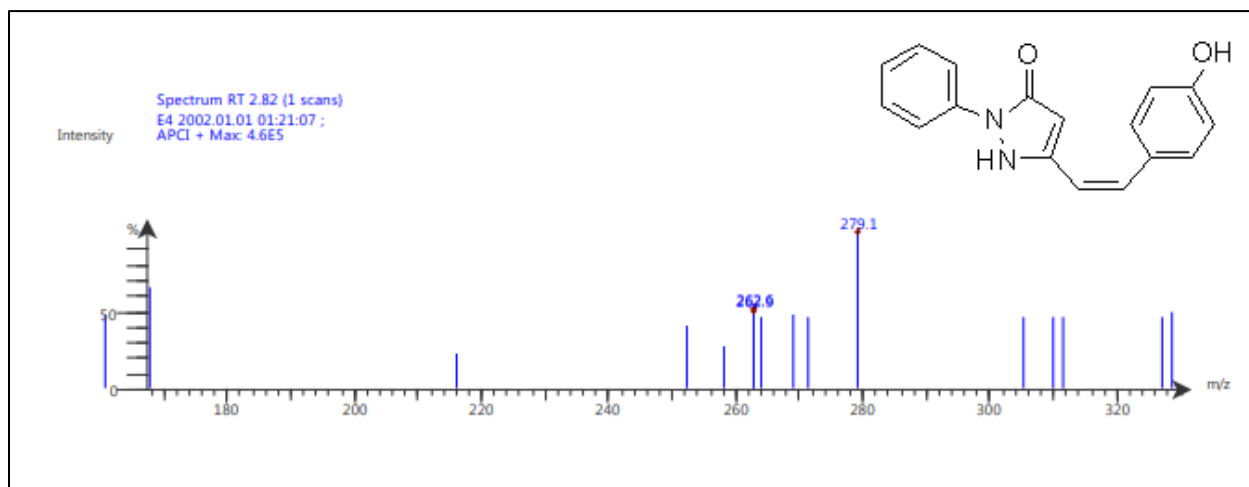
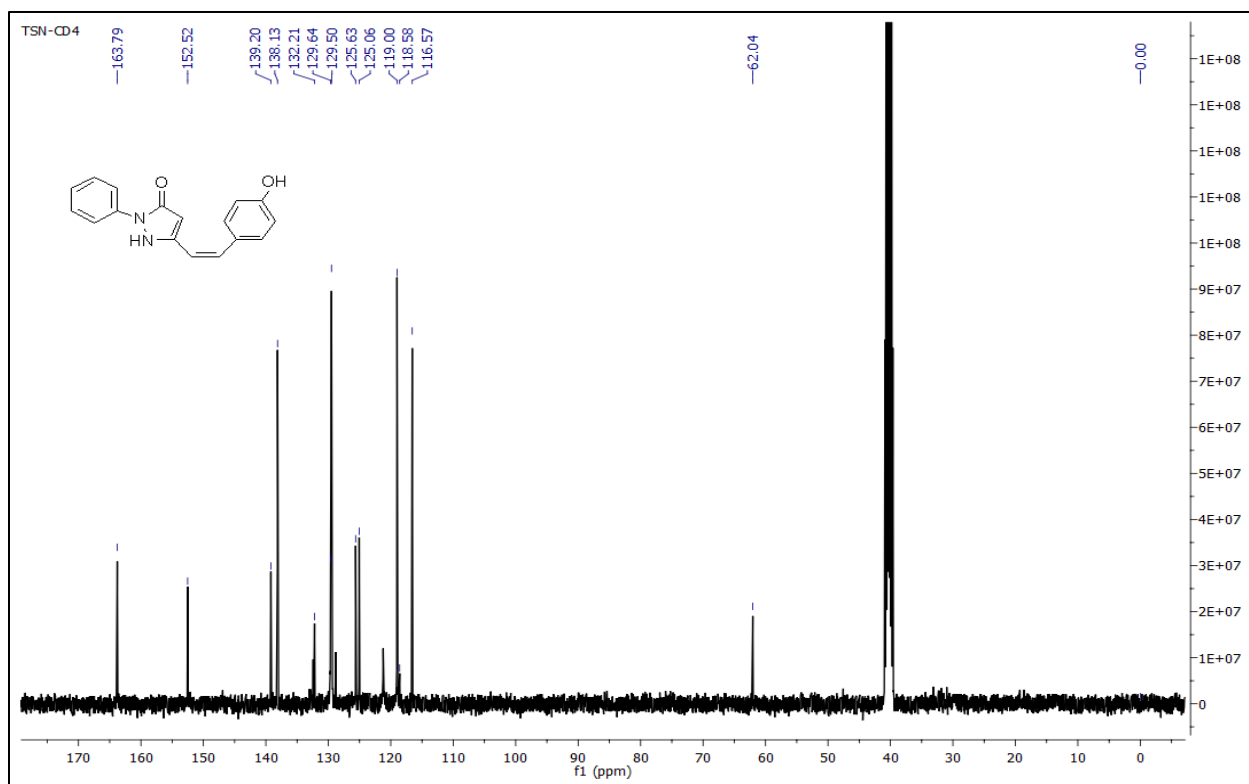
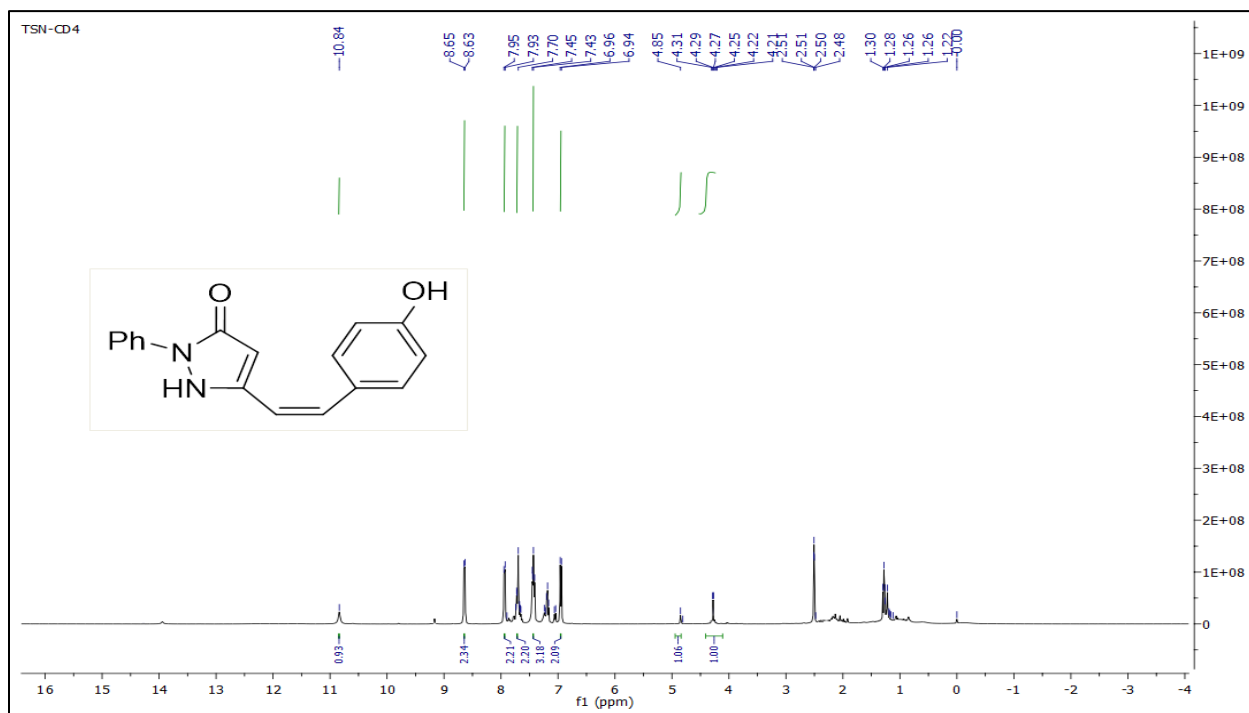


Figure 8. Mass Spectra of 5b.

Figure 9. ^{13}C NMR data of 5b.Figure 10. ^1H NMR data of 5b.

3.3 | 2-(2,4-dinitrophenyl)-5-(4-hydroxystyryl)-1,2-dihydro-3H-pyrazol-3-one (5c)

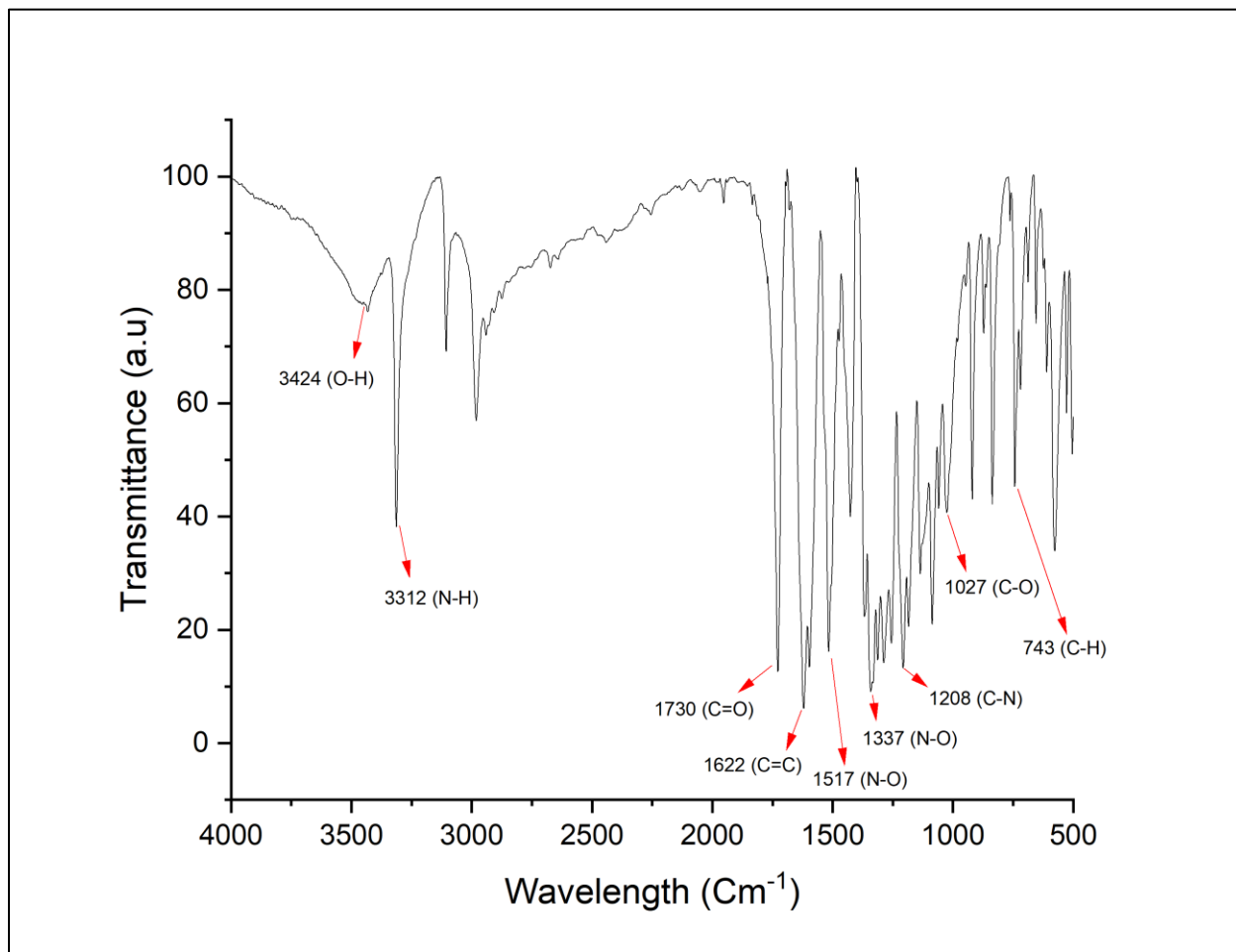


Figure 11. IR Spectra of 5c.

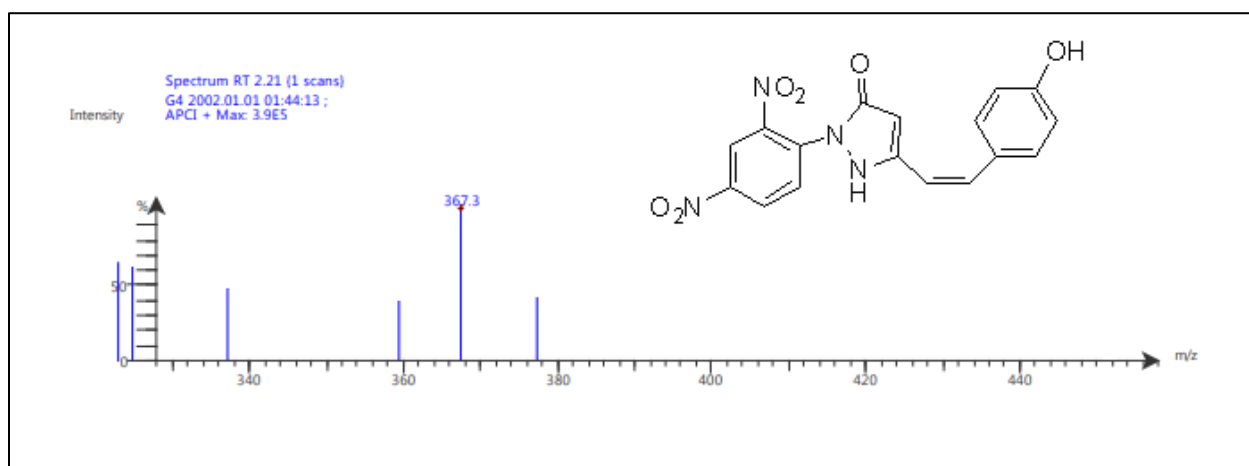


Figure 12. Mass Spectra of 5c.

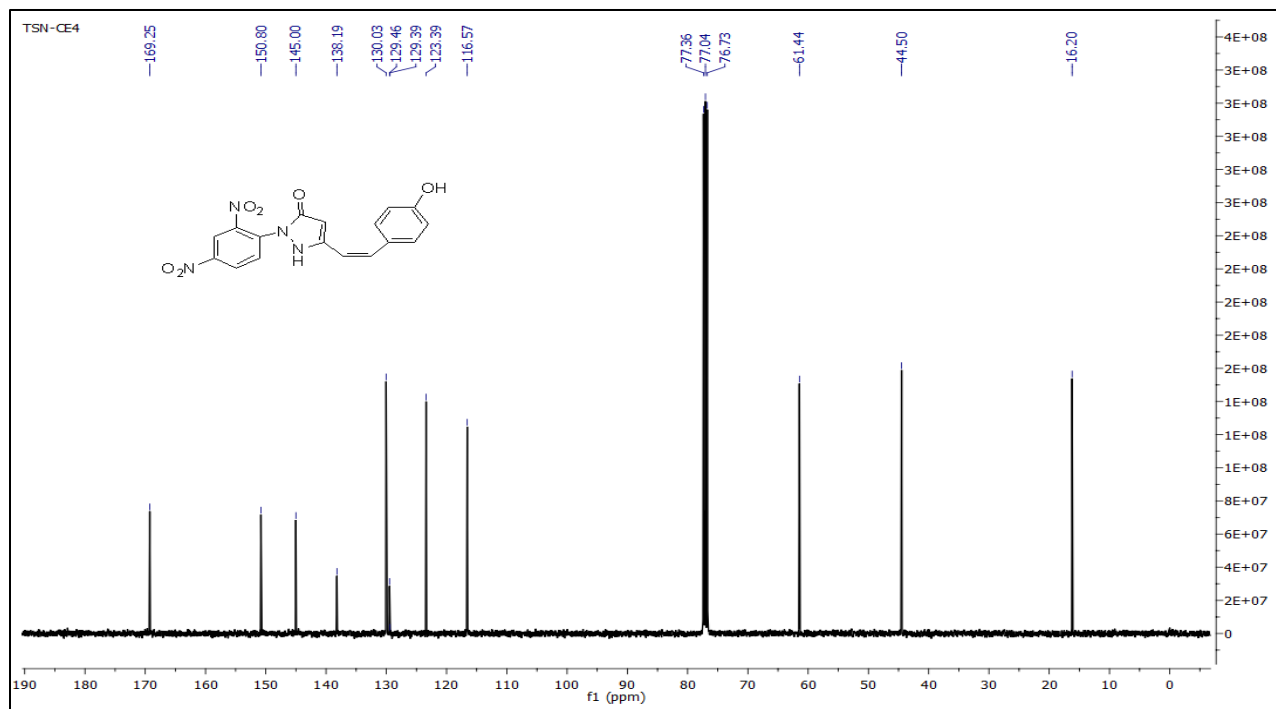


Figure 13. ¹³C NMR data of 5c.

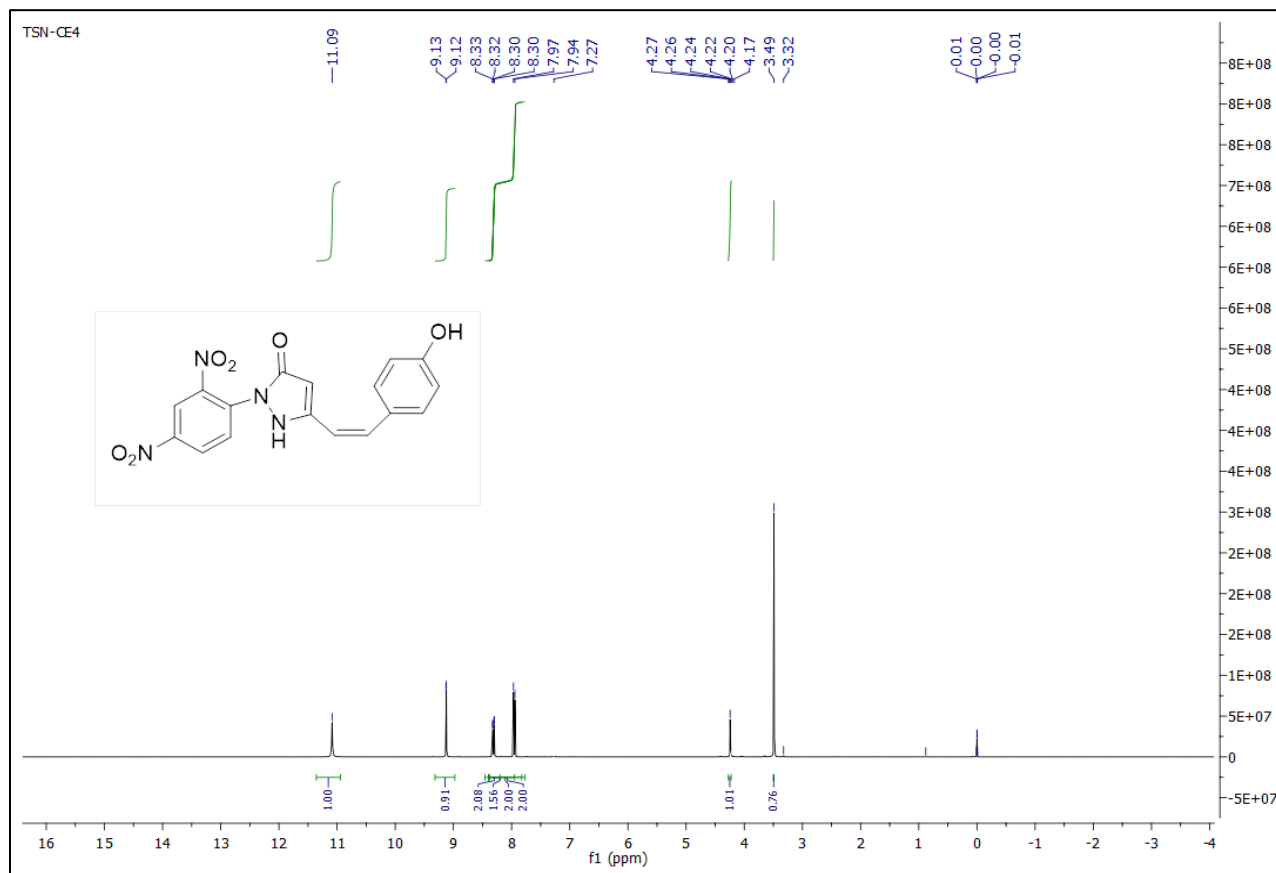


Figure 14. ¹H NMR data of 5c.

3.4 | 5-(3-hydroxystyryl)-2,4-dihydro-3H-pyrazol-3-one (5d)

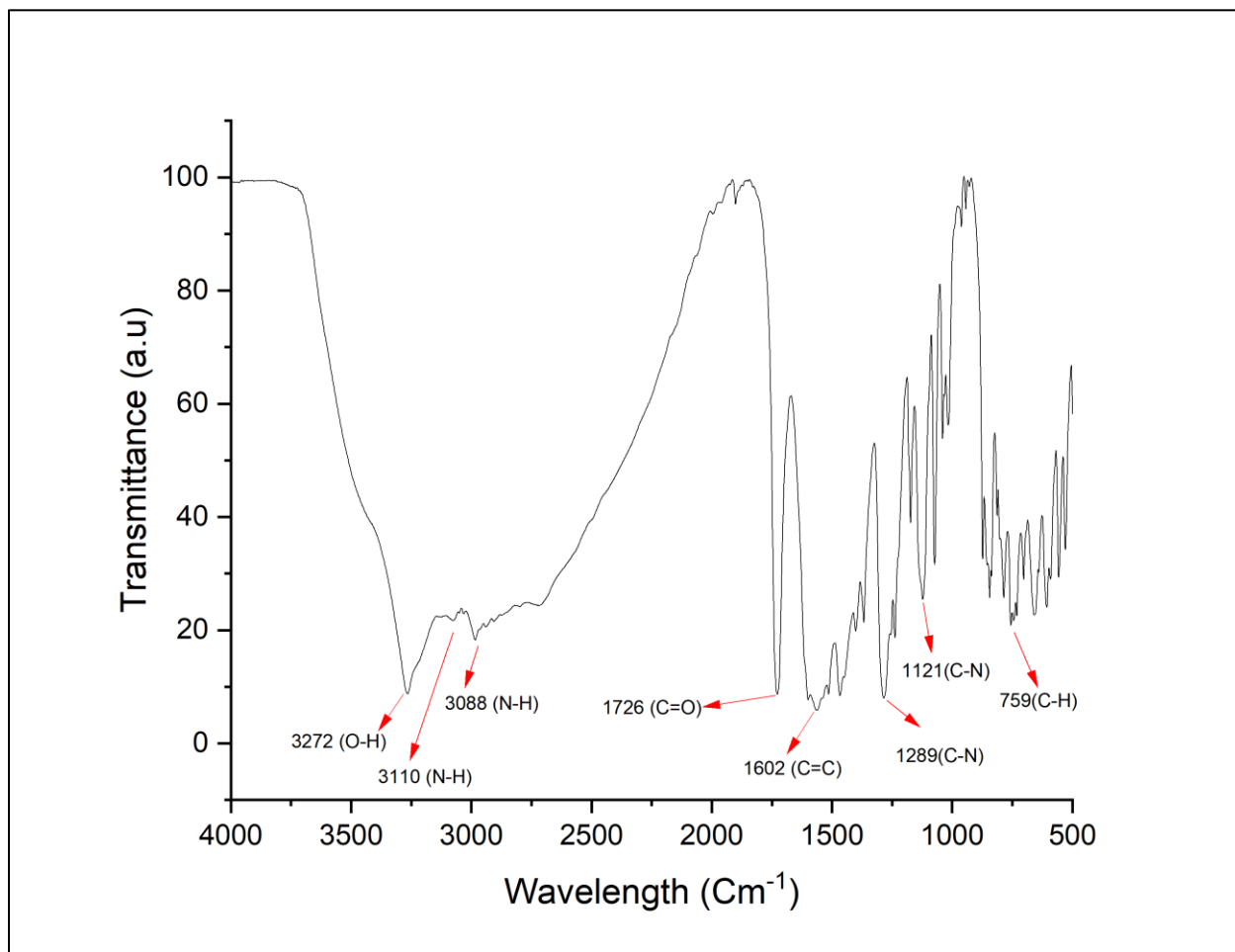


Figure 15. IR Spectra of 5d.

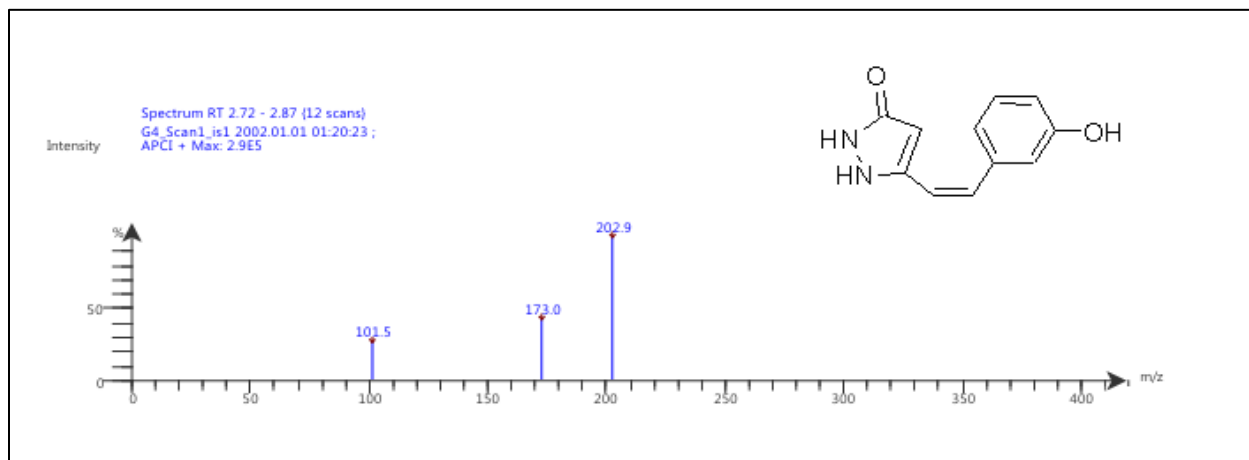
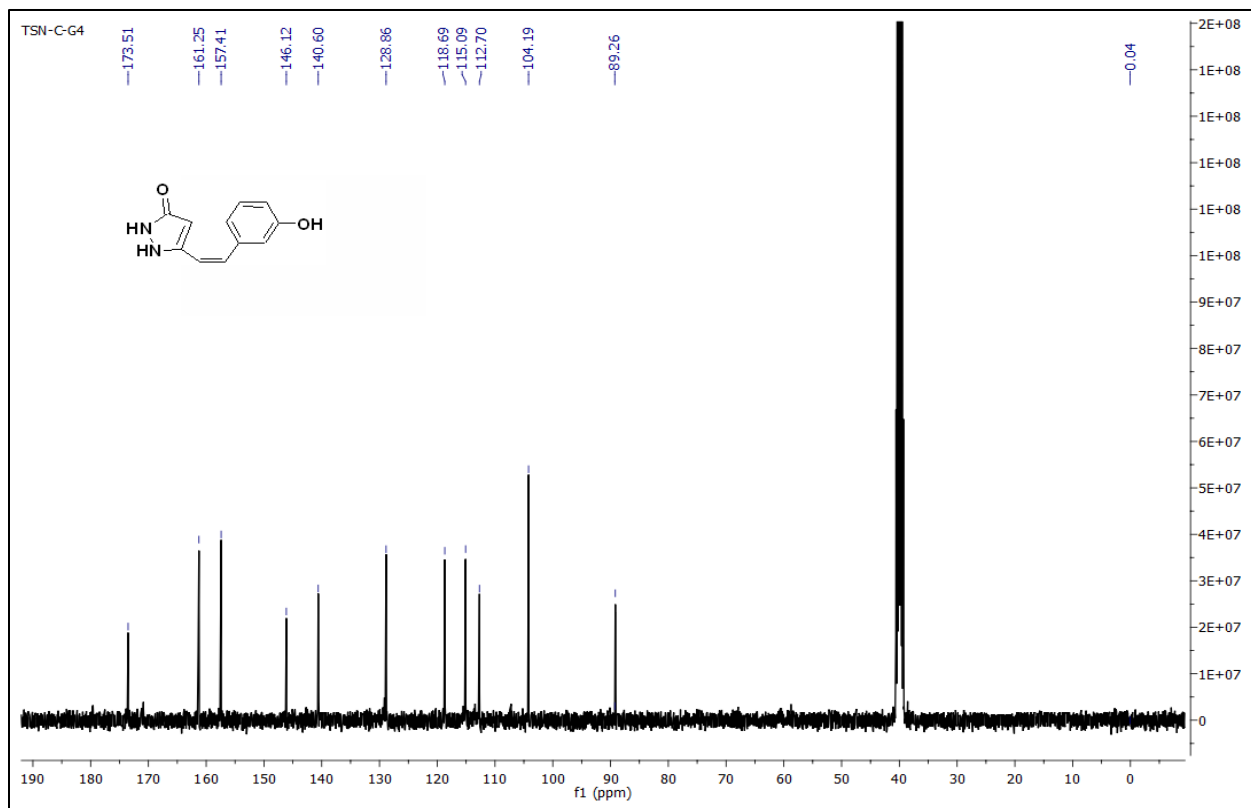
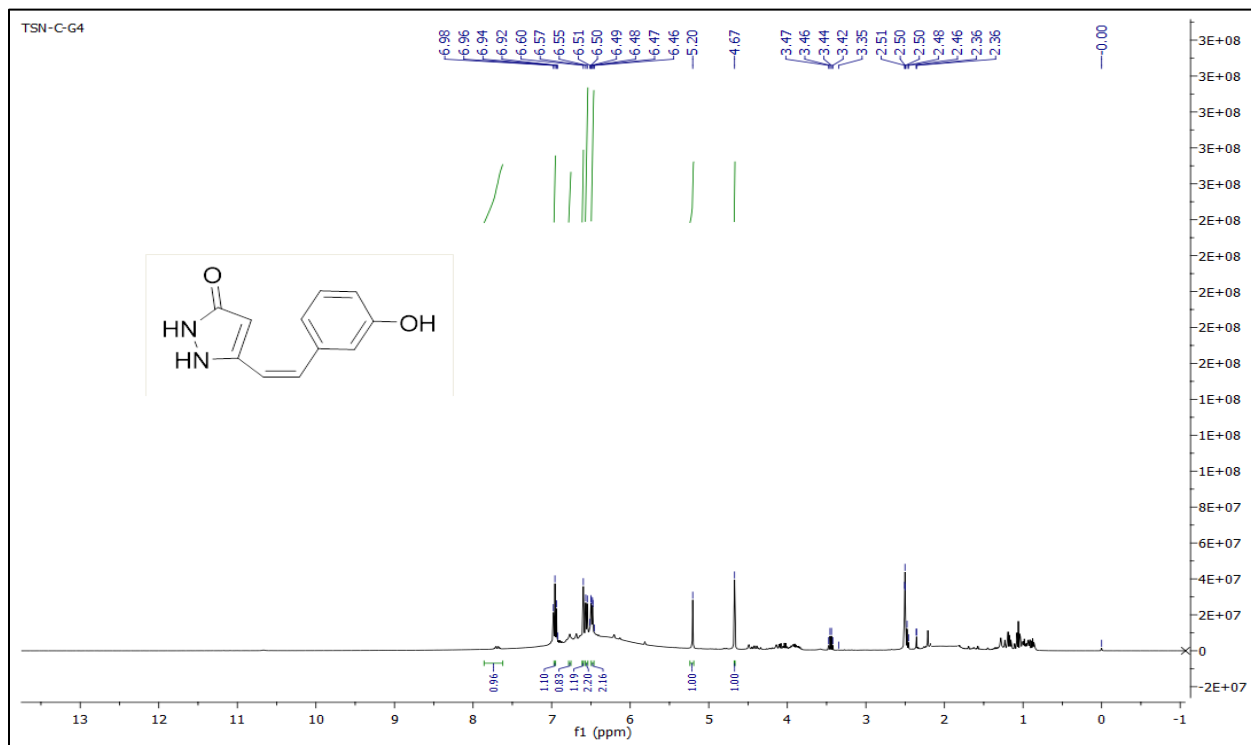


Figure 16. Mass Spectra of 5d.

Figure 17. ^{13}C NMR data of 5d.Figure 18. ^1H NMR data of 5d.

3.5 | 5-(2-bromostyryl)-1,2-dihydro-3H-pyrazol-3-one (5e)

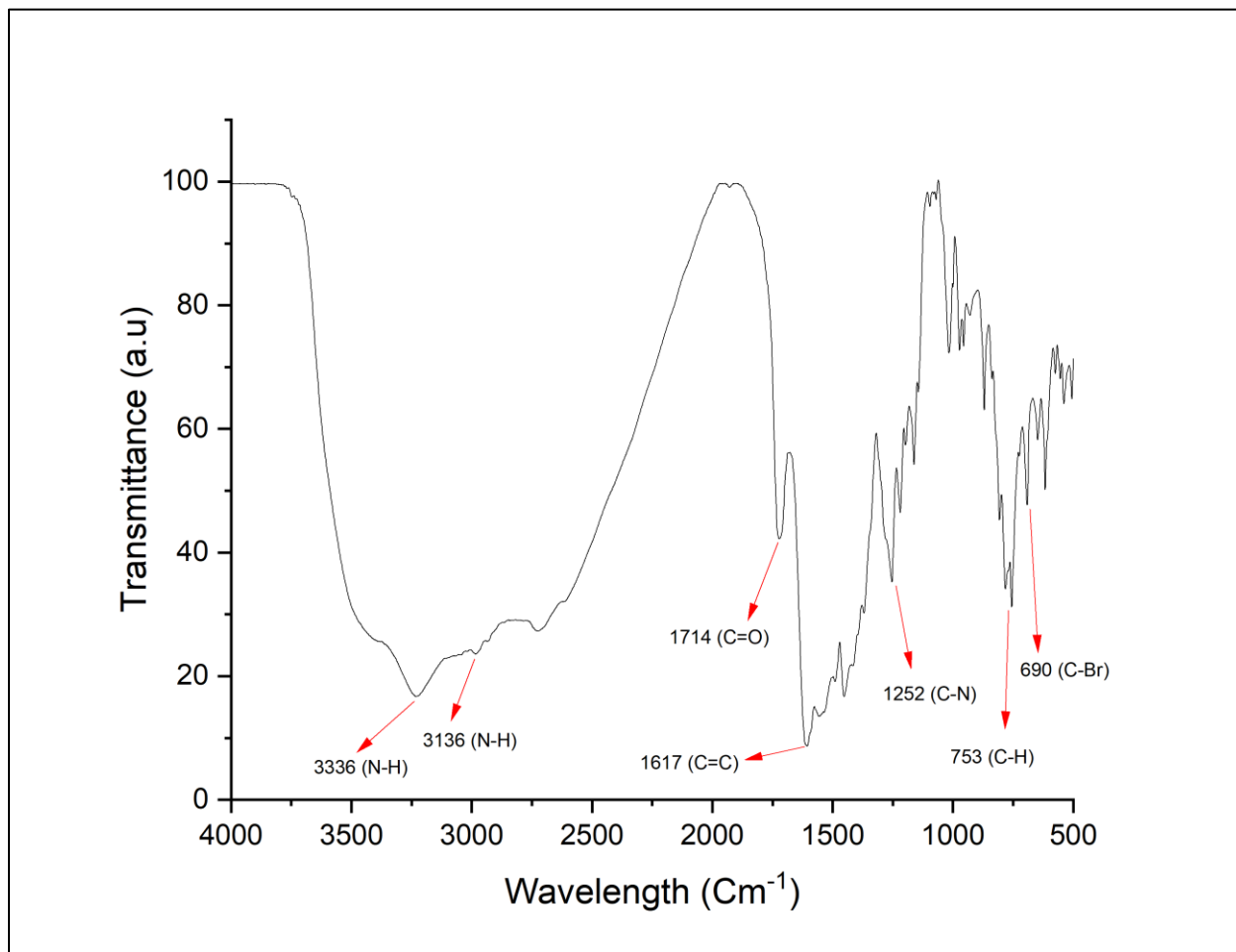


Figure 19. IR Spectra of 5e.

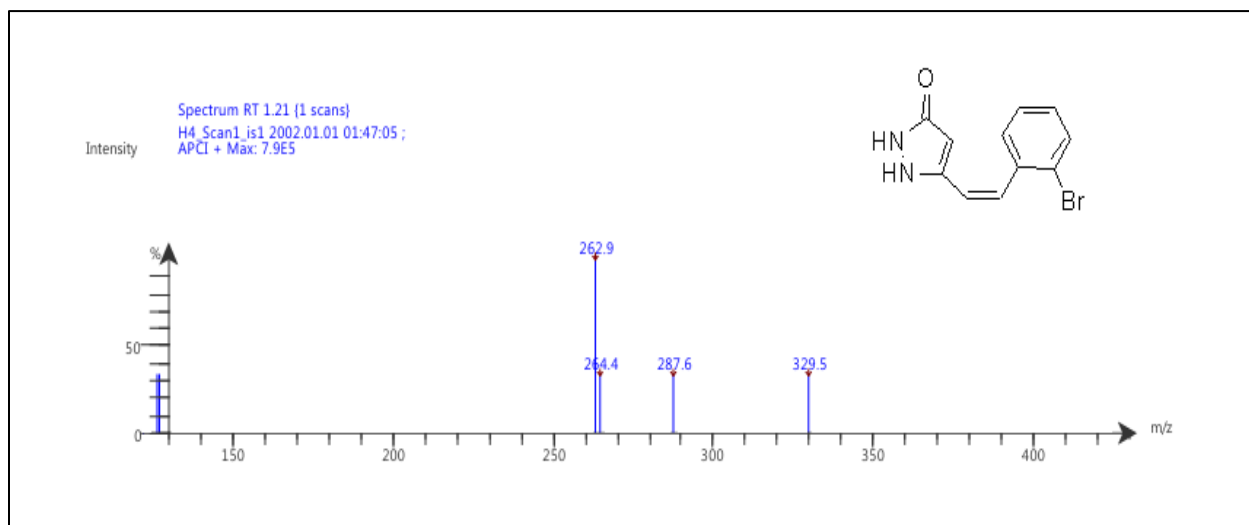
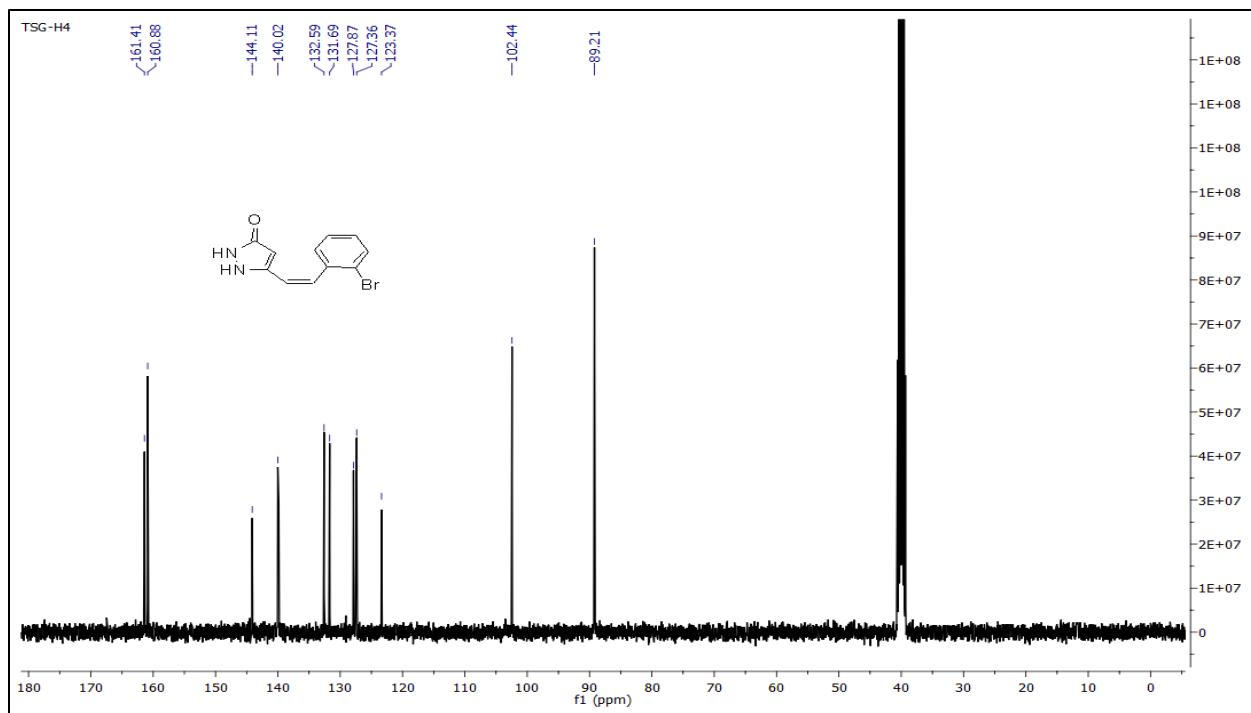
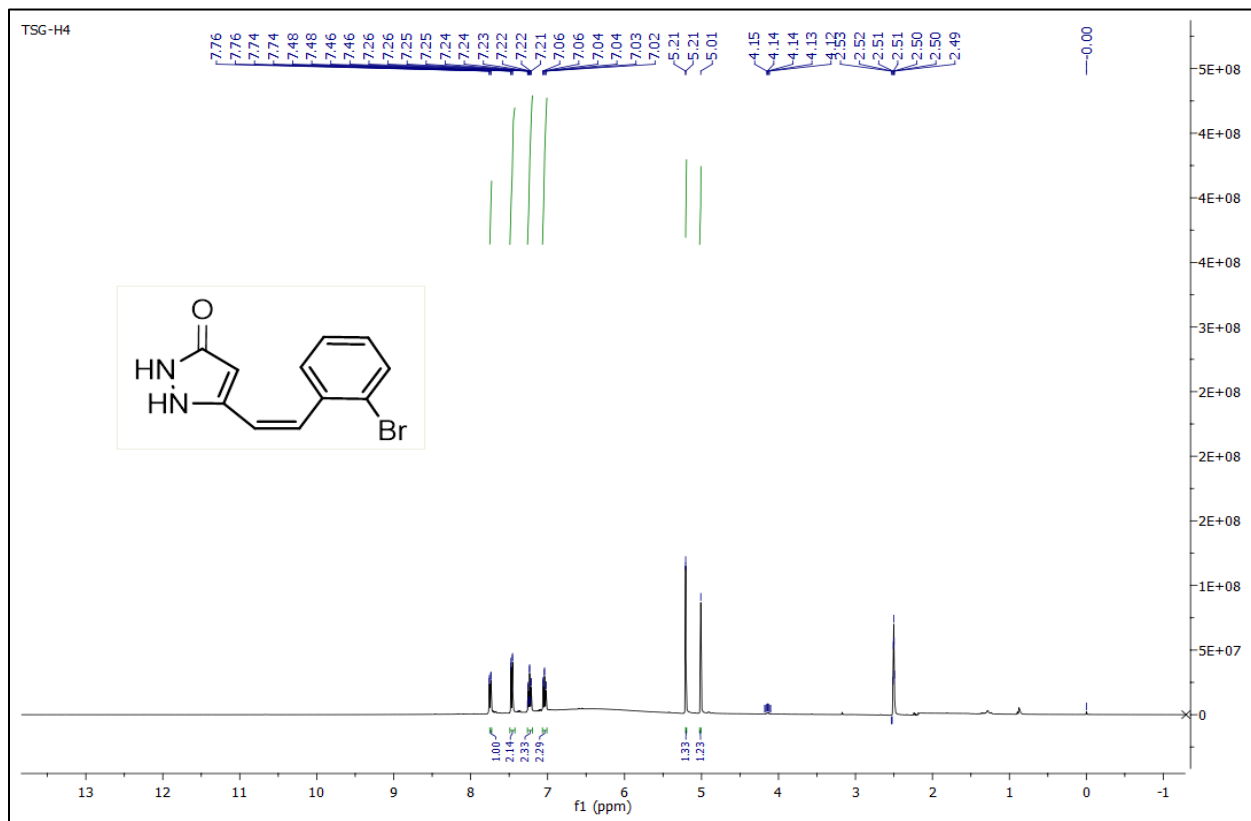


Figure 20. Mass Spectra of 5e.

Figure 21. ¹³C NMR data of 5e.Figure 22. ¹H NMR data of 5e.

3.6 | 5-(2-nitrostyryl)-1,2-dihydro-3H-pyrazol-3-one (5f)

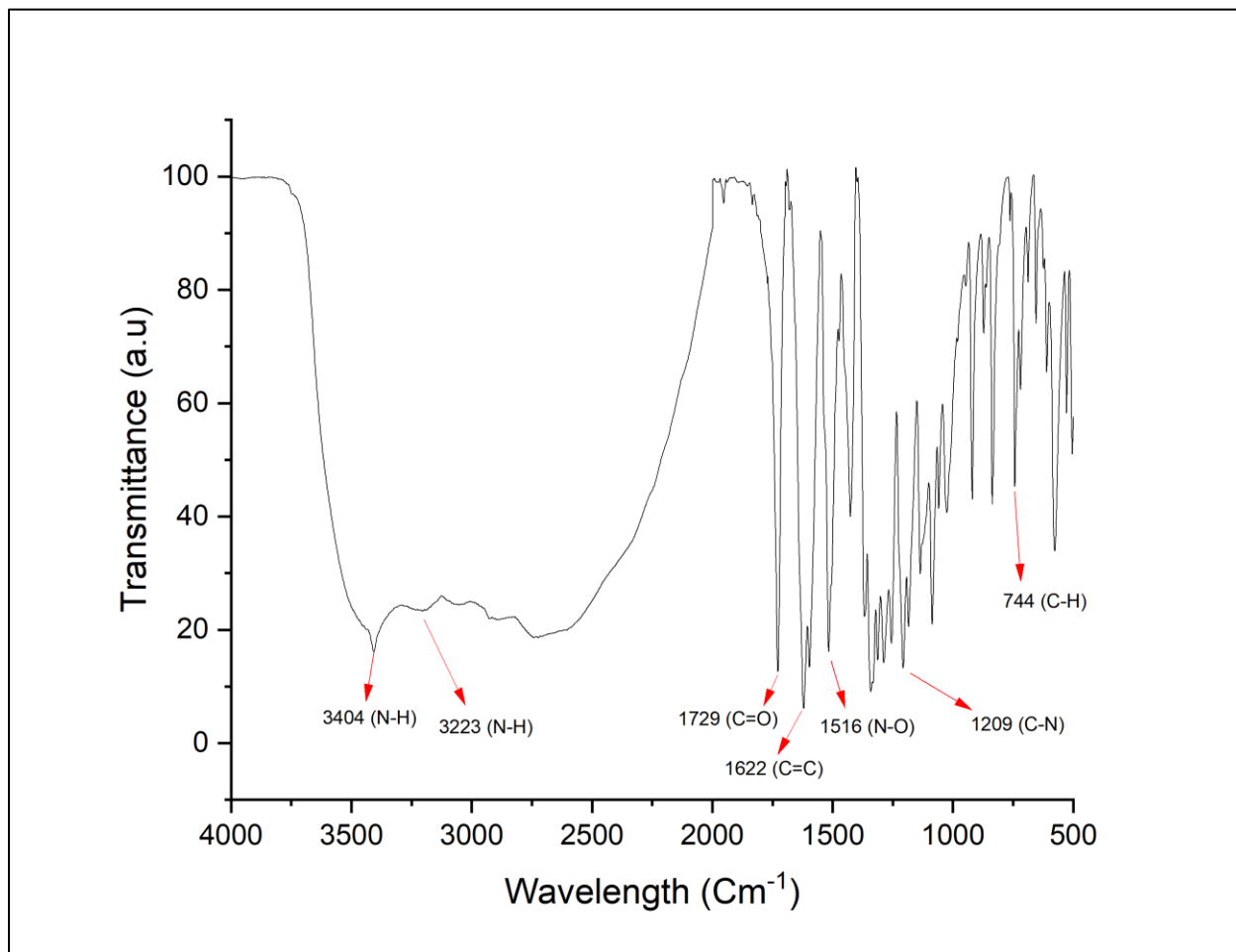


Figure 23. IR Spectra of 5f.

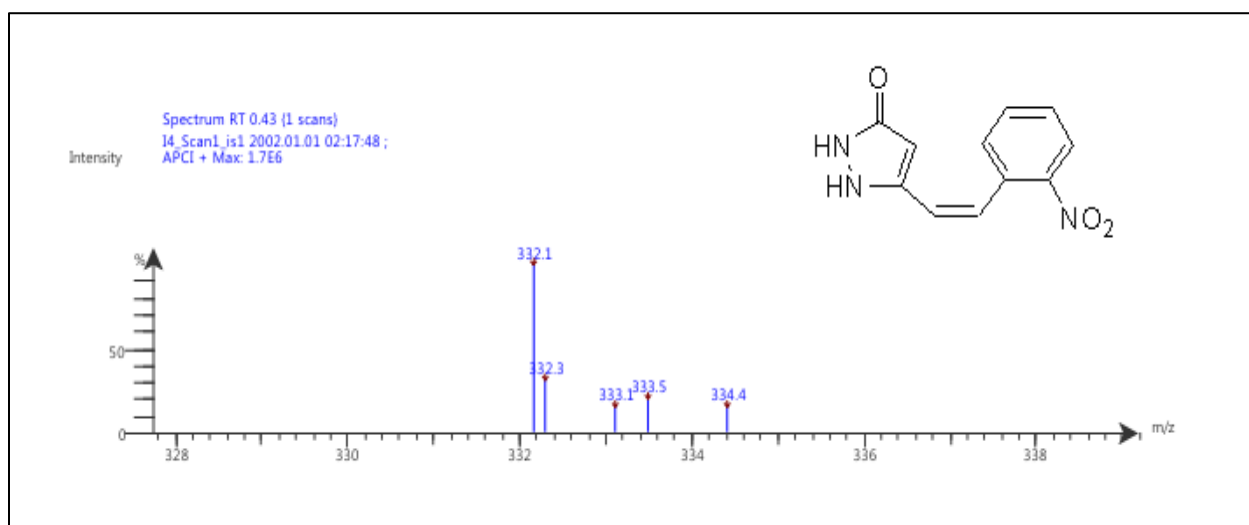
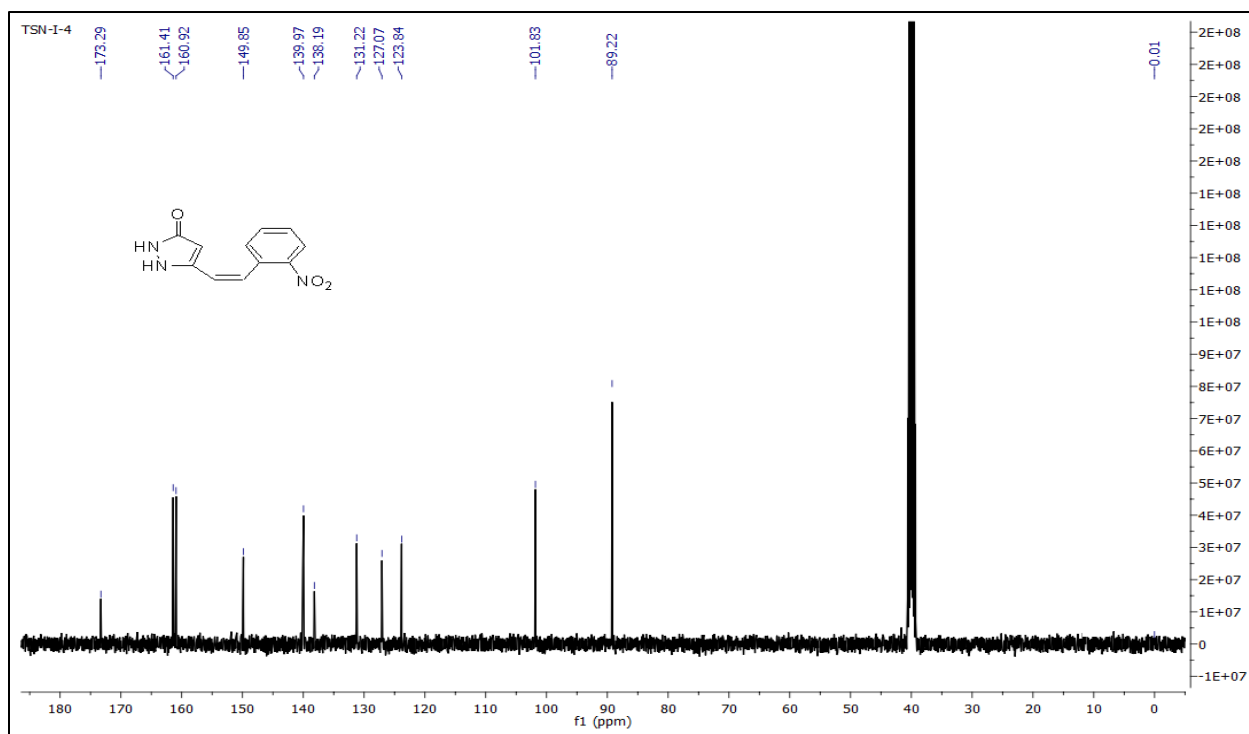
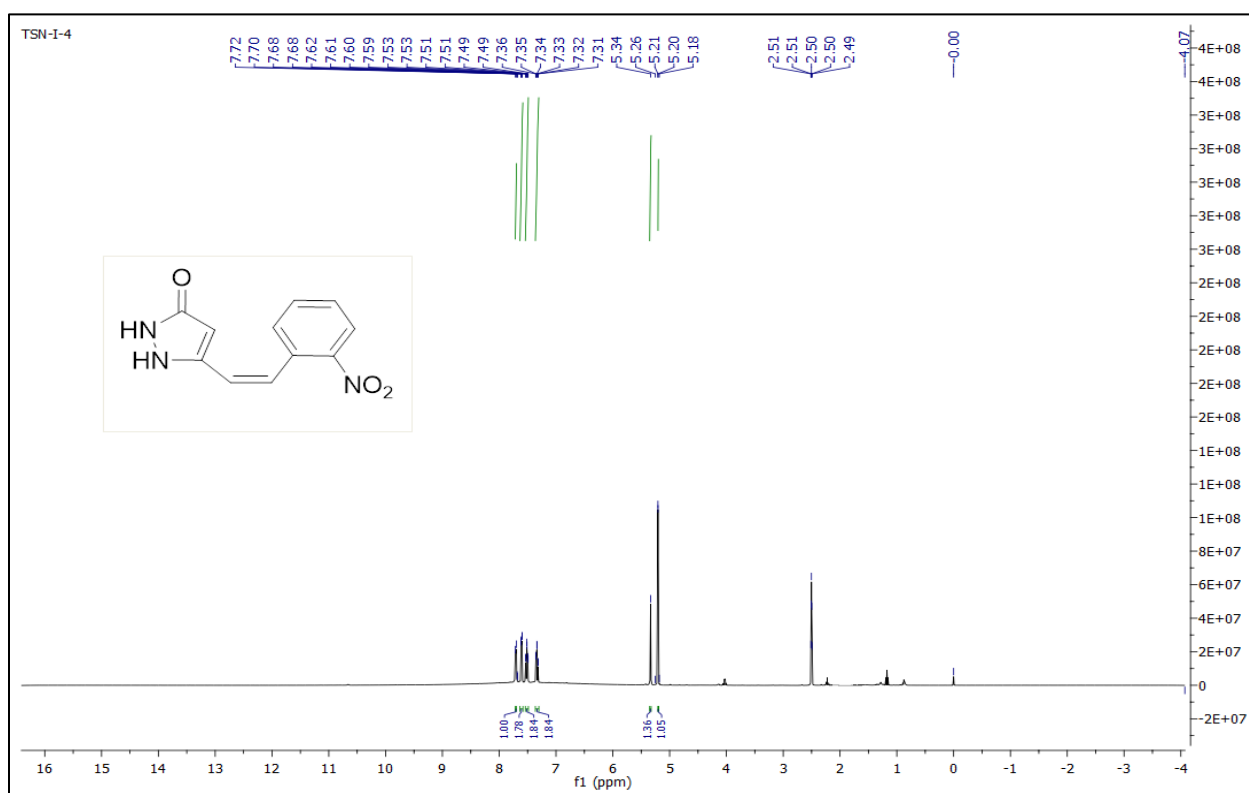


Figure 24. Mass Spectra of 5f.

Figure 25. ^{13}C NMR data of 5f.Figure 26. ^1H NMR data of 5f.

3.7 | 5-(2,5- dimethoxystyryl)-1,2-dihydro-3H-pyrazol-3-one (5g)

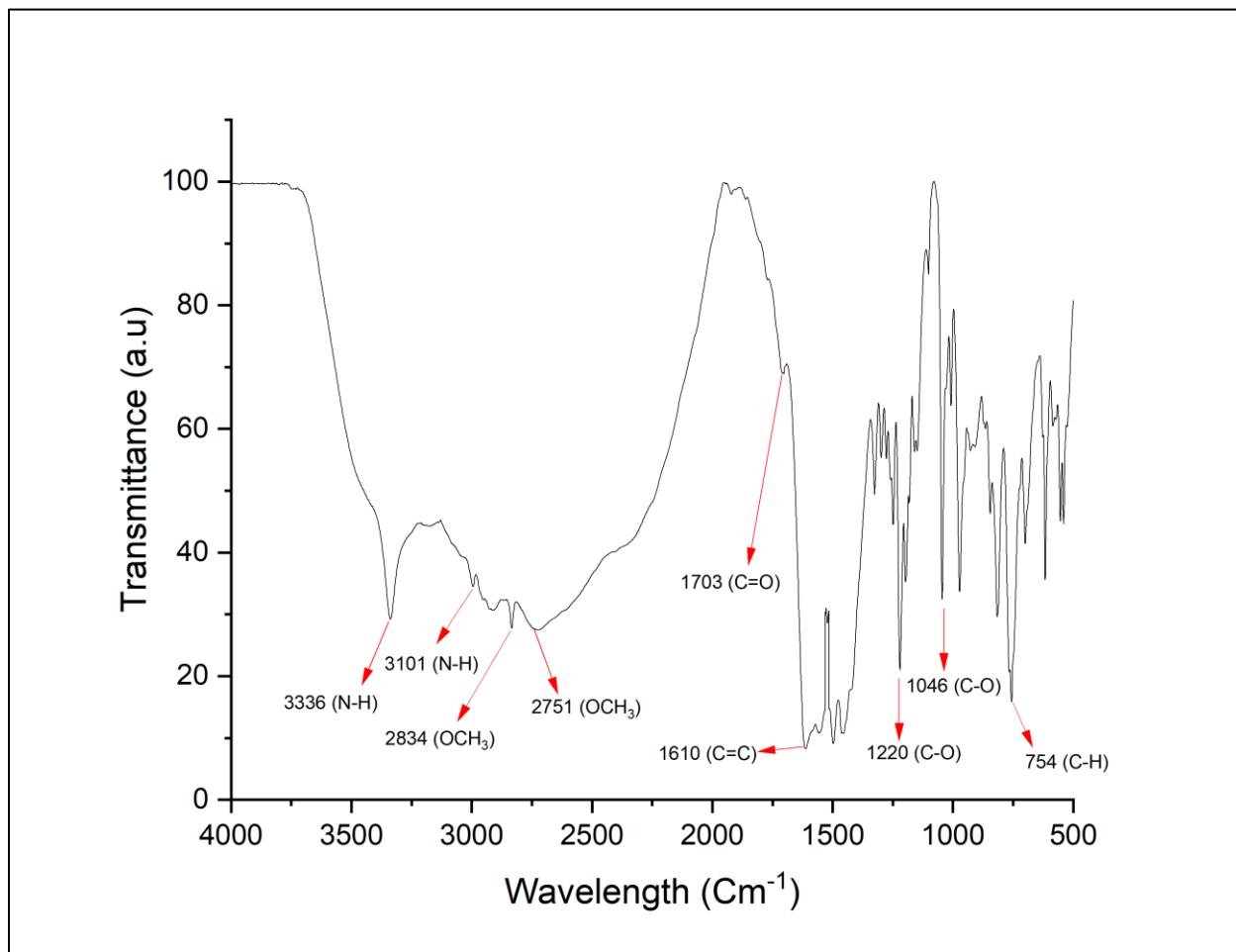


Figure 27. IR Spectra of 5g.

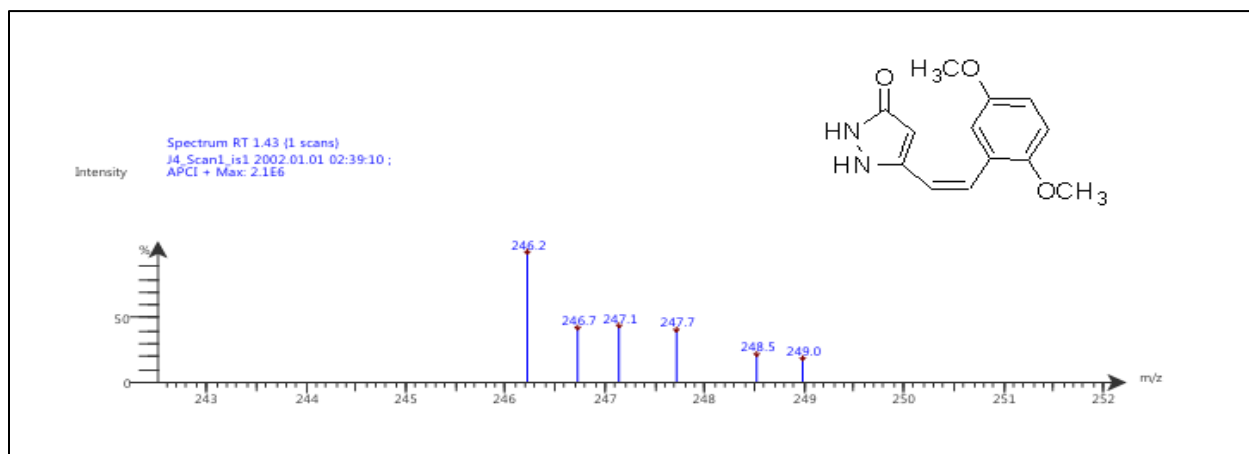


Figure 28. Mass Spectra of 5g.

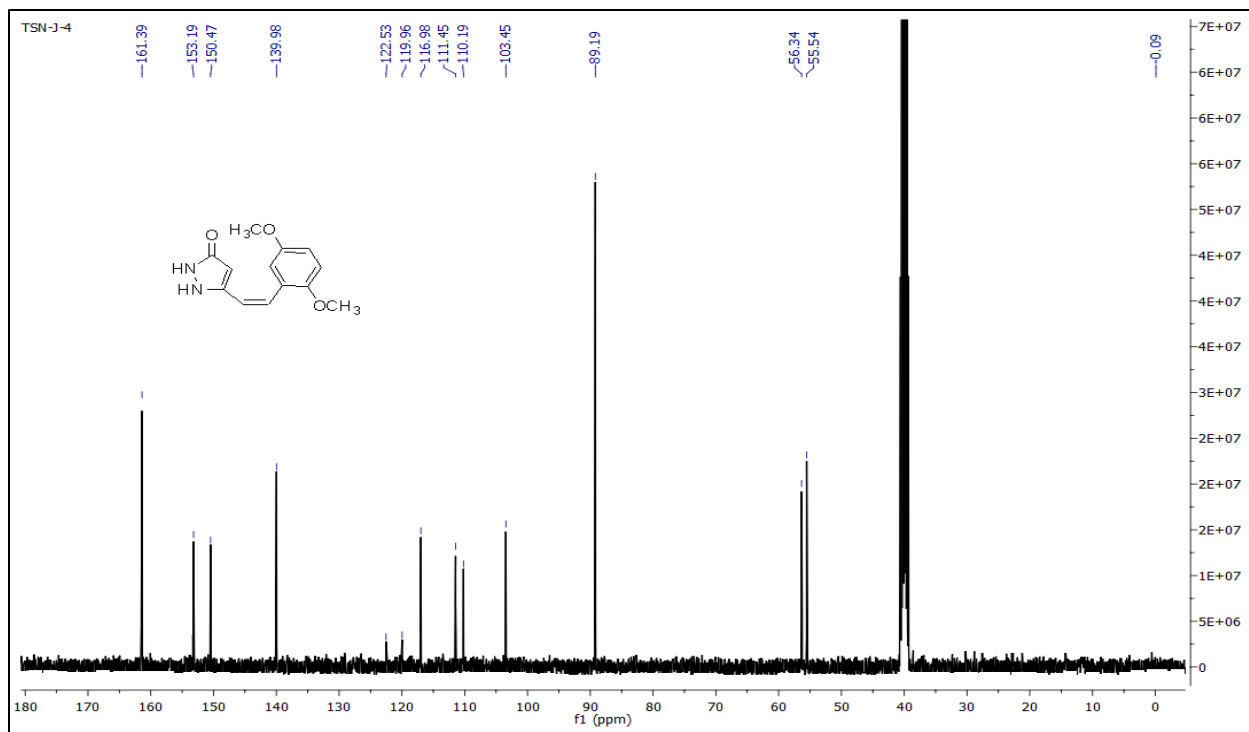


Figure 29. ¹³C NMR data of 5g.

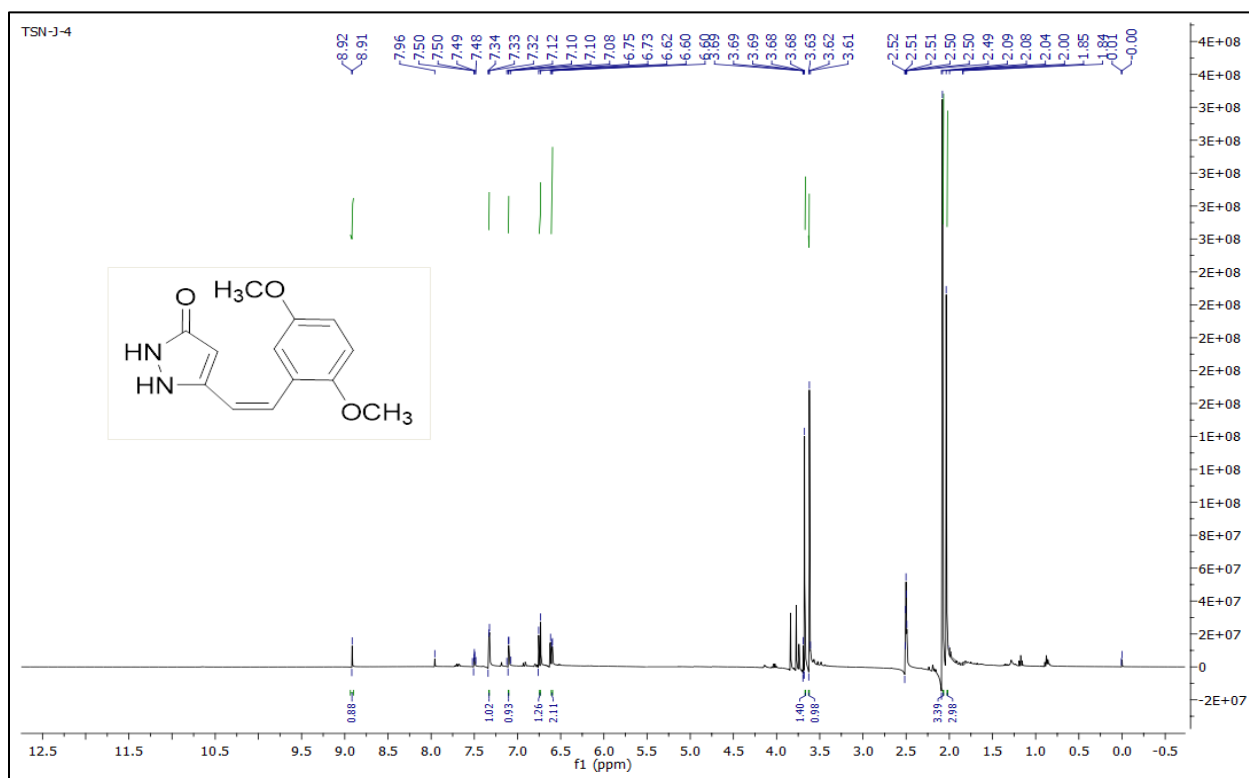


Figure 30. ¹H NMR data of 5g.

3.8 | 5-(3,4-dimethoxystyryl)-2-phenyl-2,4-dihydro-3H-pyrazol-3-one (5h)

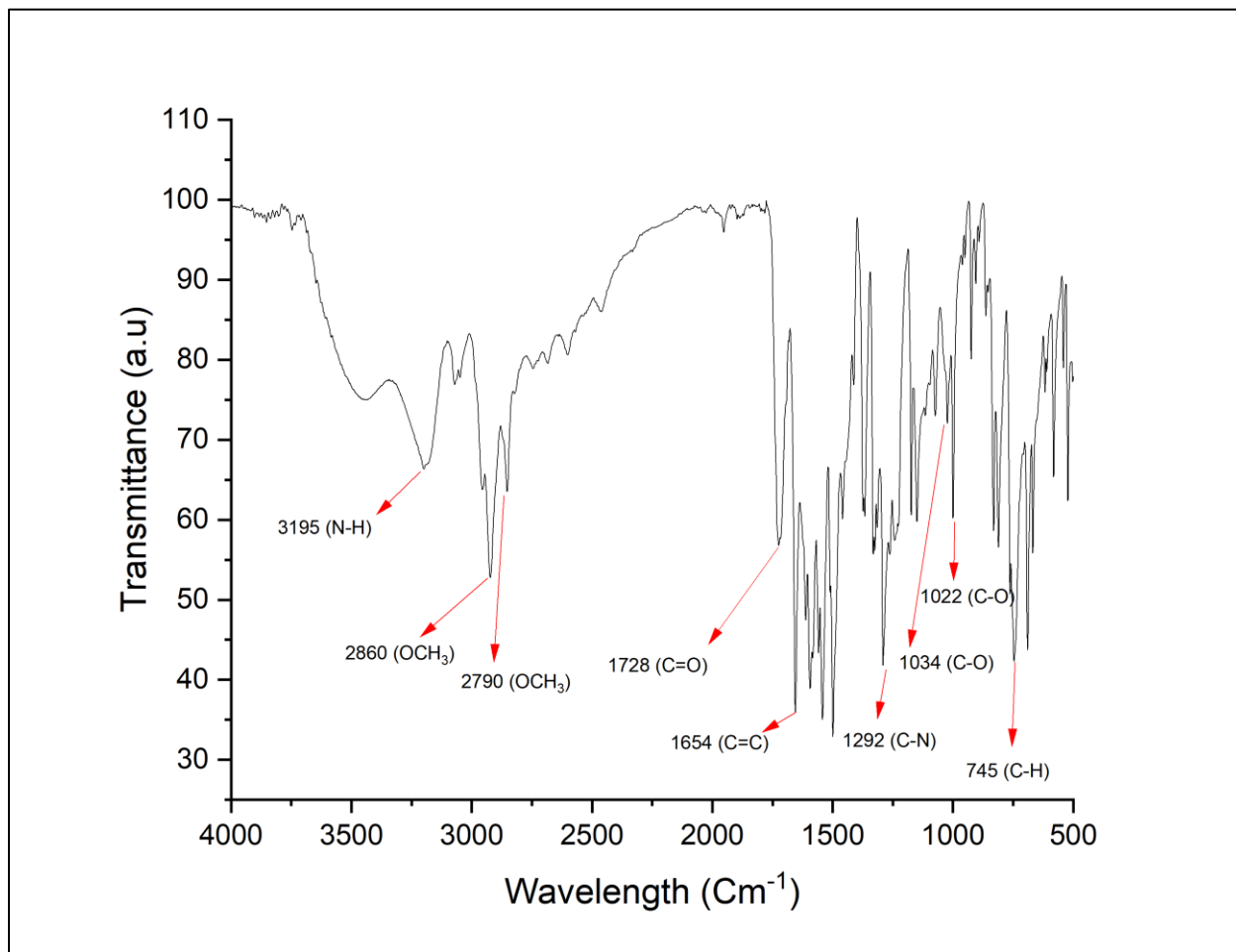


Figure 31. IR Spectra of 5h.

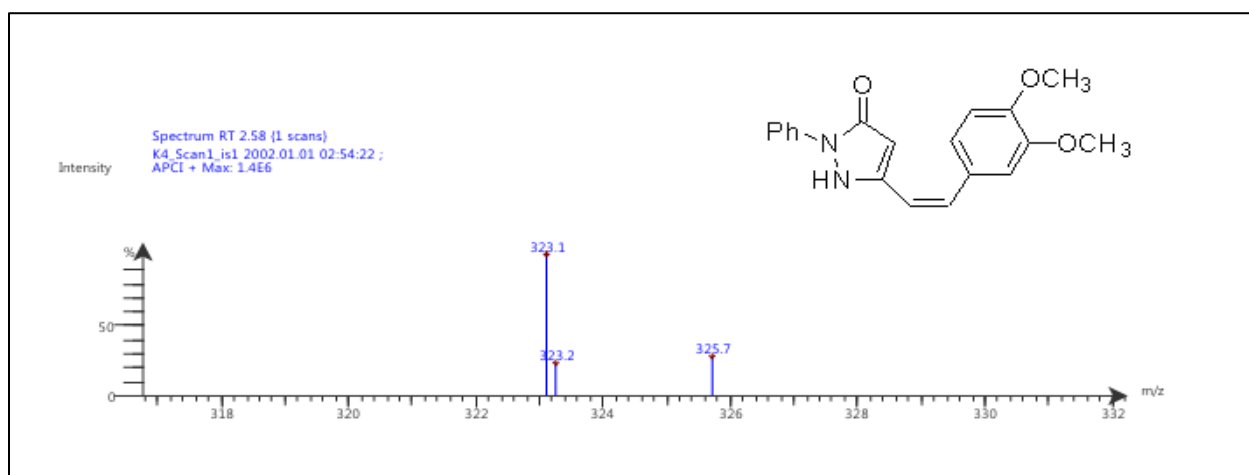
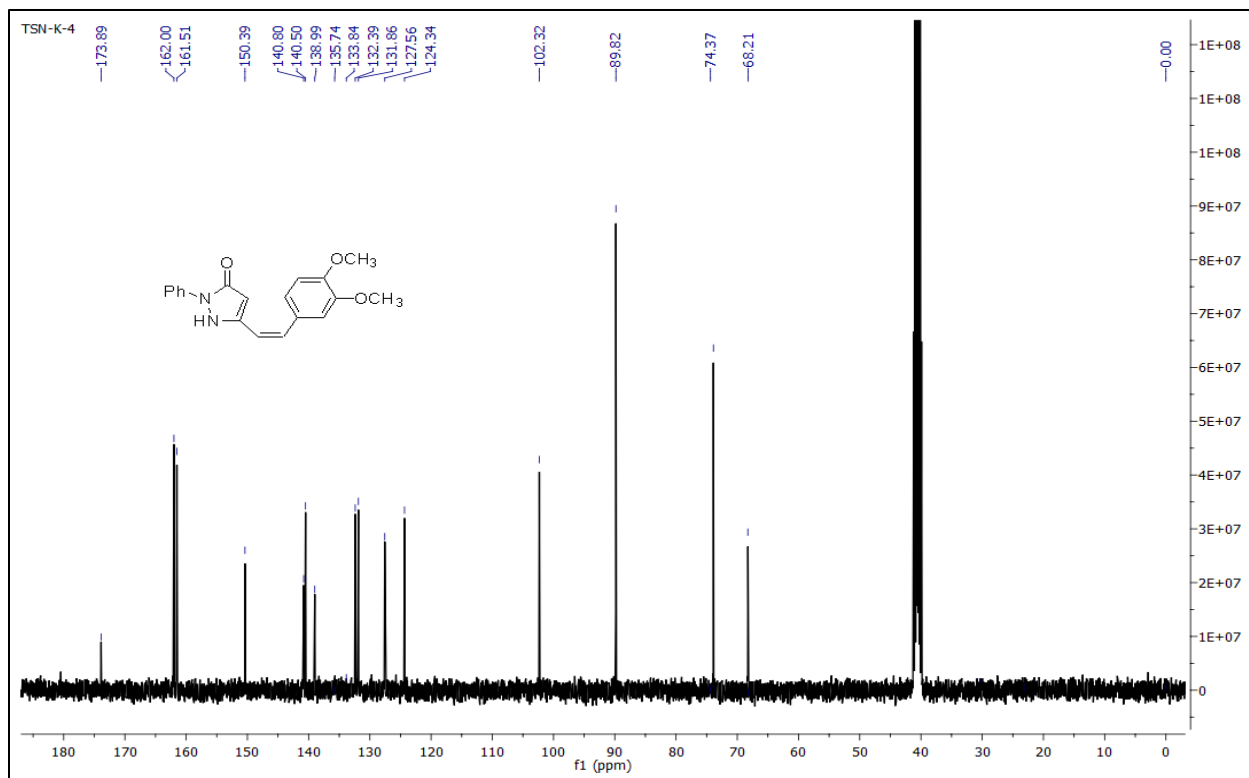
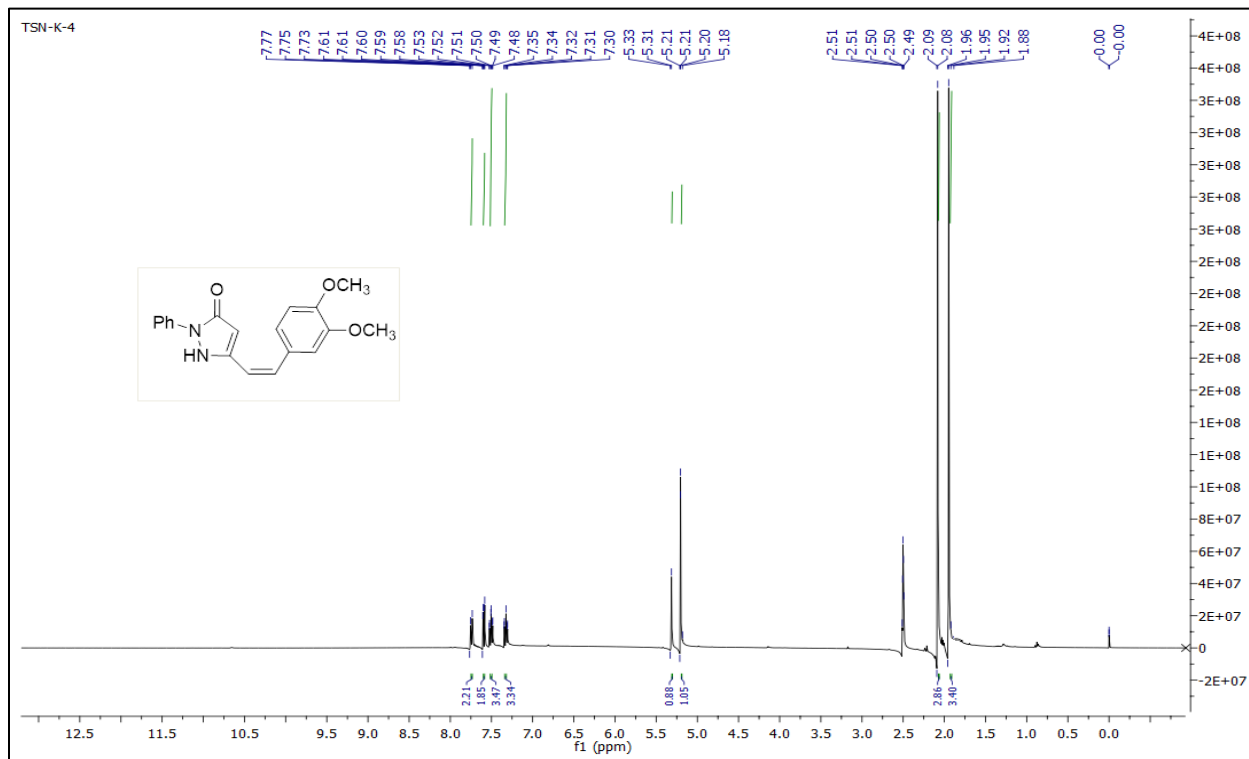


Figure 32. Mass Spectra of 5h.

Figure 33. ^{13}C NMR data of 5h.Figure 34. ^1H NMR data of 5h.