Electronic Supplementary Information (ESI)

Photophysical Investigation of Green Vitamin C Adducts as Synthetic pH Indicators: Solvatochromism, Halochromism, and DFT Calculations Integrating Optical Band Gap and Electronic Transition Analysis

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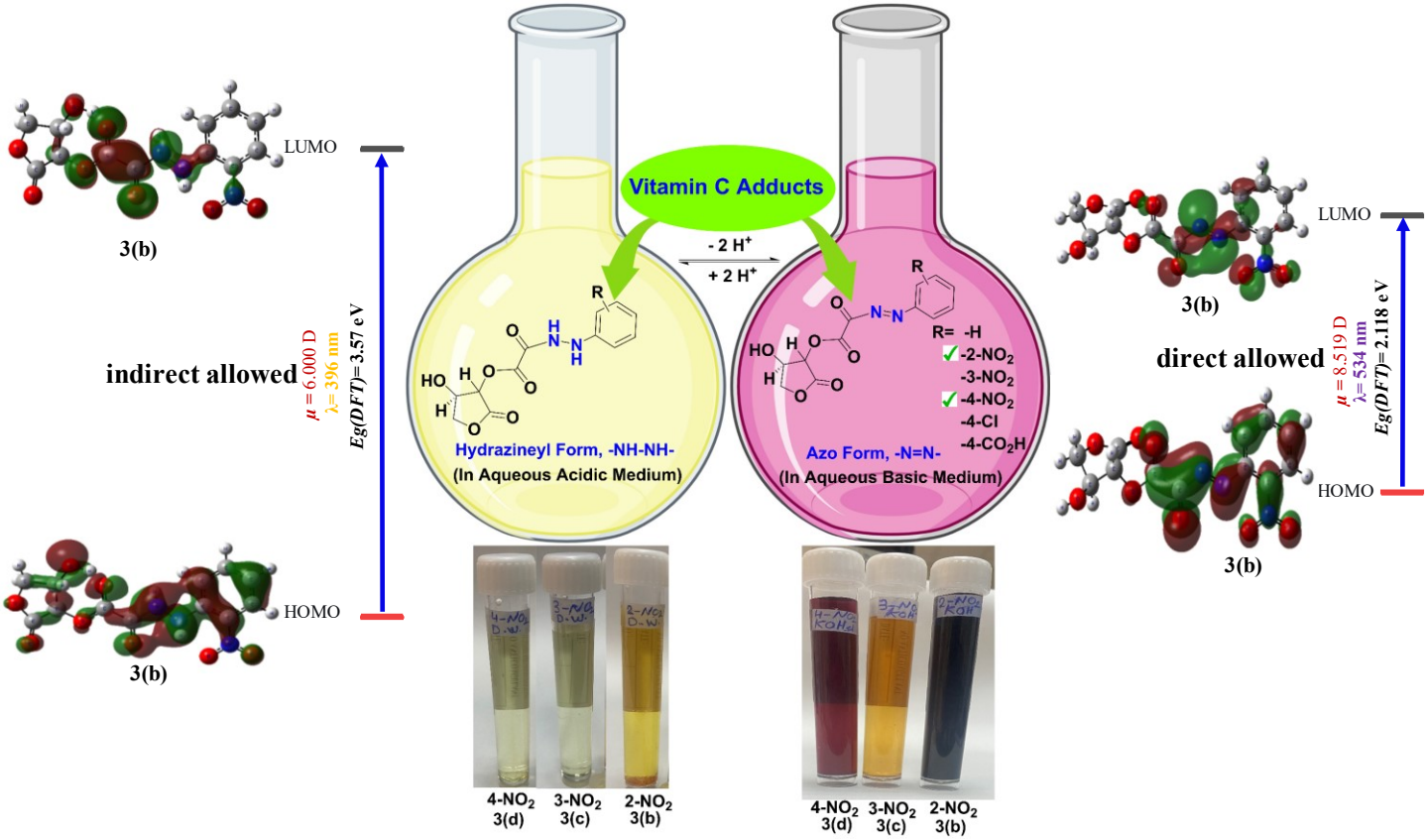

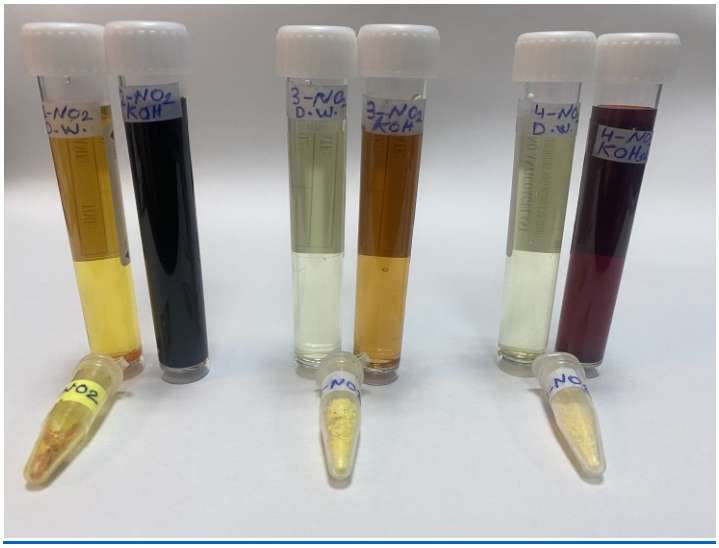

B3LYP /6-311+G (d, p)

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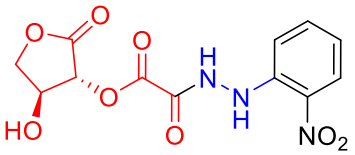
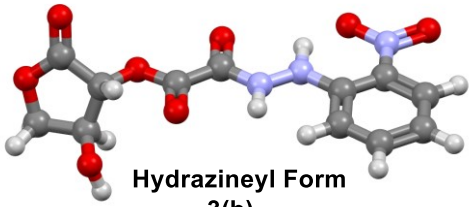
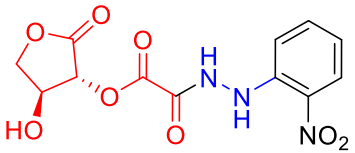
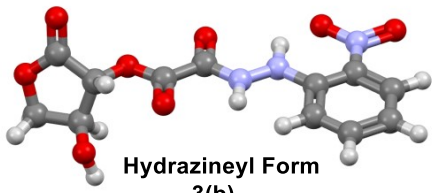
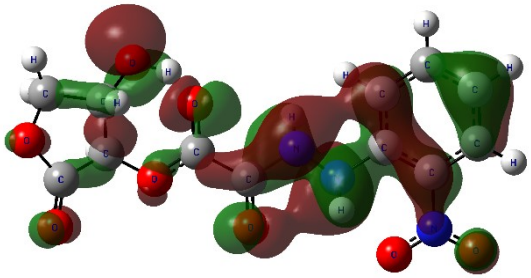
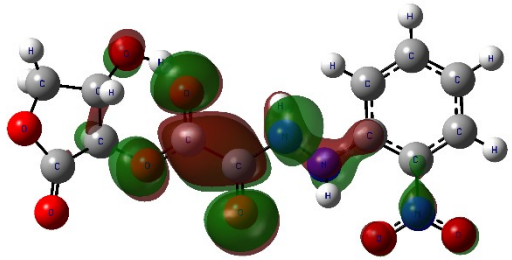
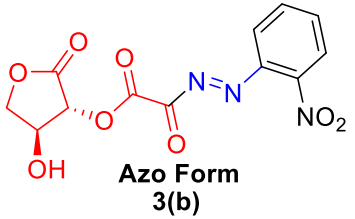
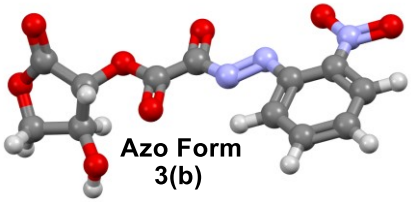
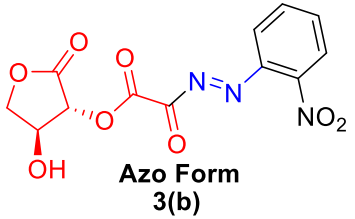
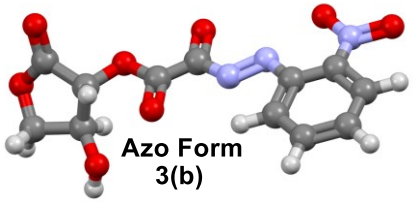
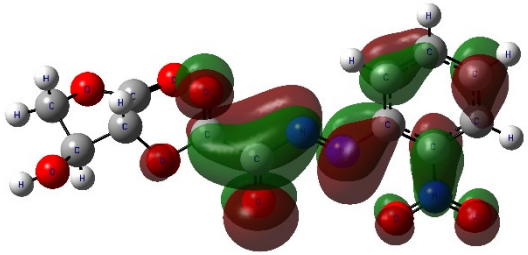
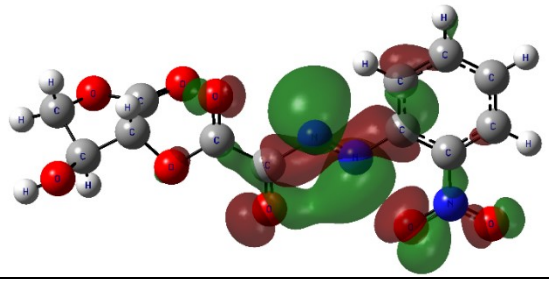
 Hydrazineyl Form 3(b)	 Hydrazineyl Form 3(b)	 Hydrazineyl Form 3(b)	 Hydrazineyl Form 3(b)
			
 Azo Form 3(b)	 Azo Form 3(b)	 Azo Form 3(b)	 Azo Form 3(b)
			

B3LYP /6-311+G (d, p)

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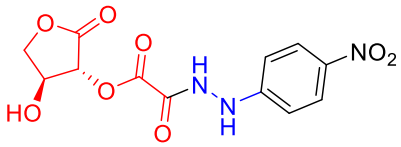
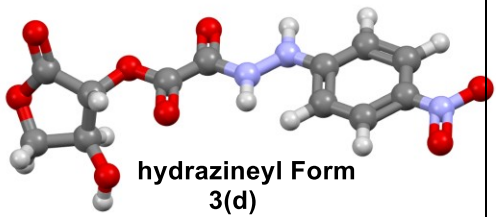
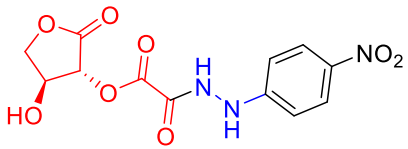
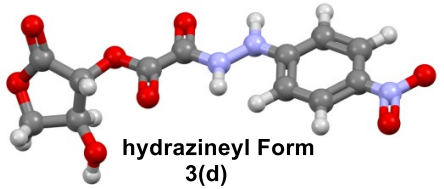
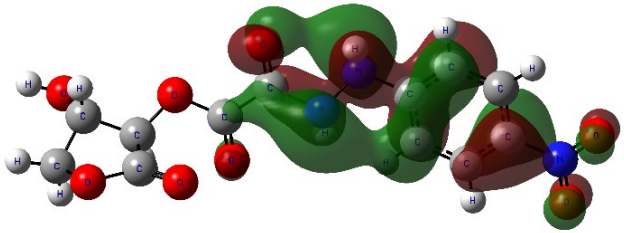
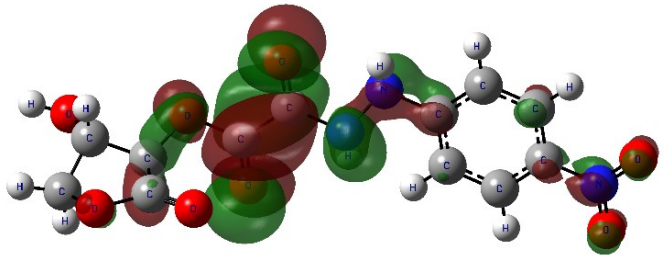
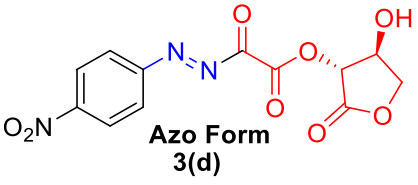
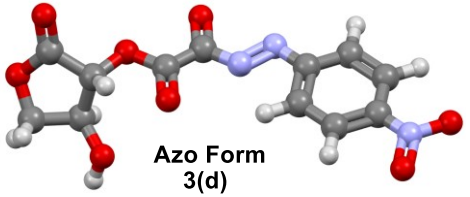
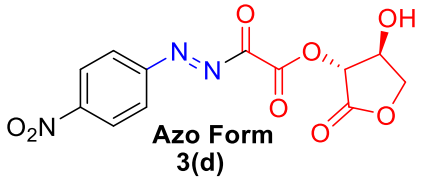
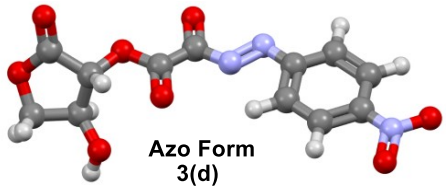
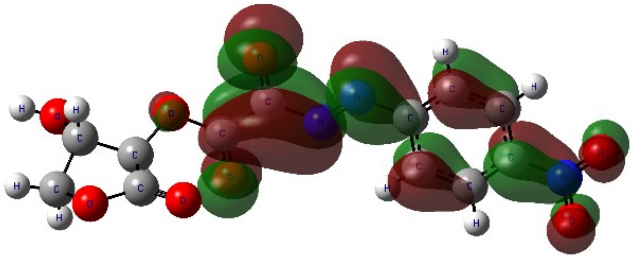
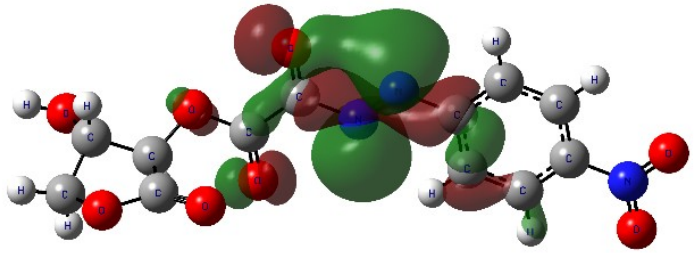
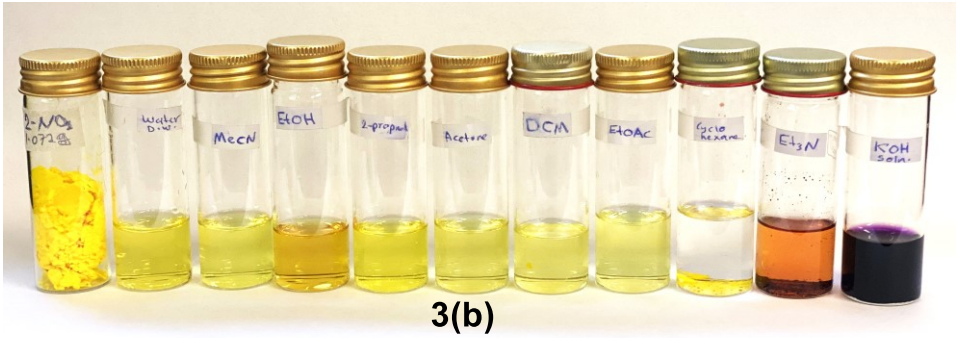
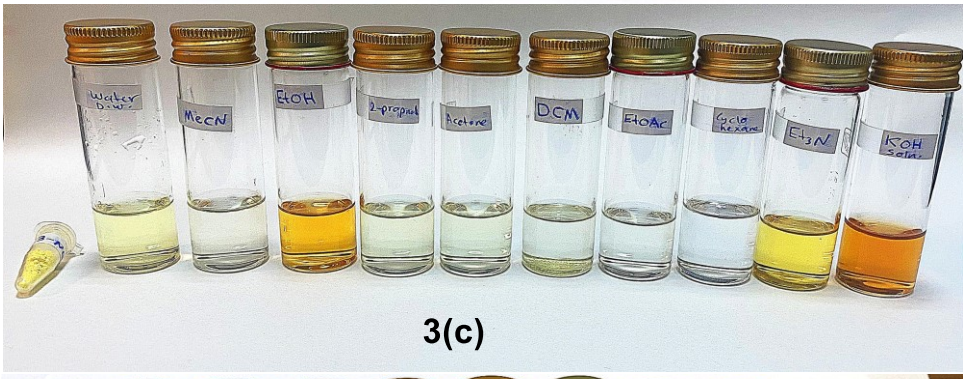
 hydrazineyl Form 3(d)	 hydrazineyl Form 3(d)	 hydrazineyl Form 3(d)	 hydrazineyl Form 3(d)
			
 Azo Form 3(d)	 Azo Form 3(d)	 Azo Form 3(d)	 Azo Form 3(d)
			



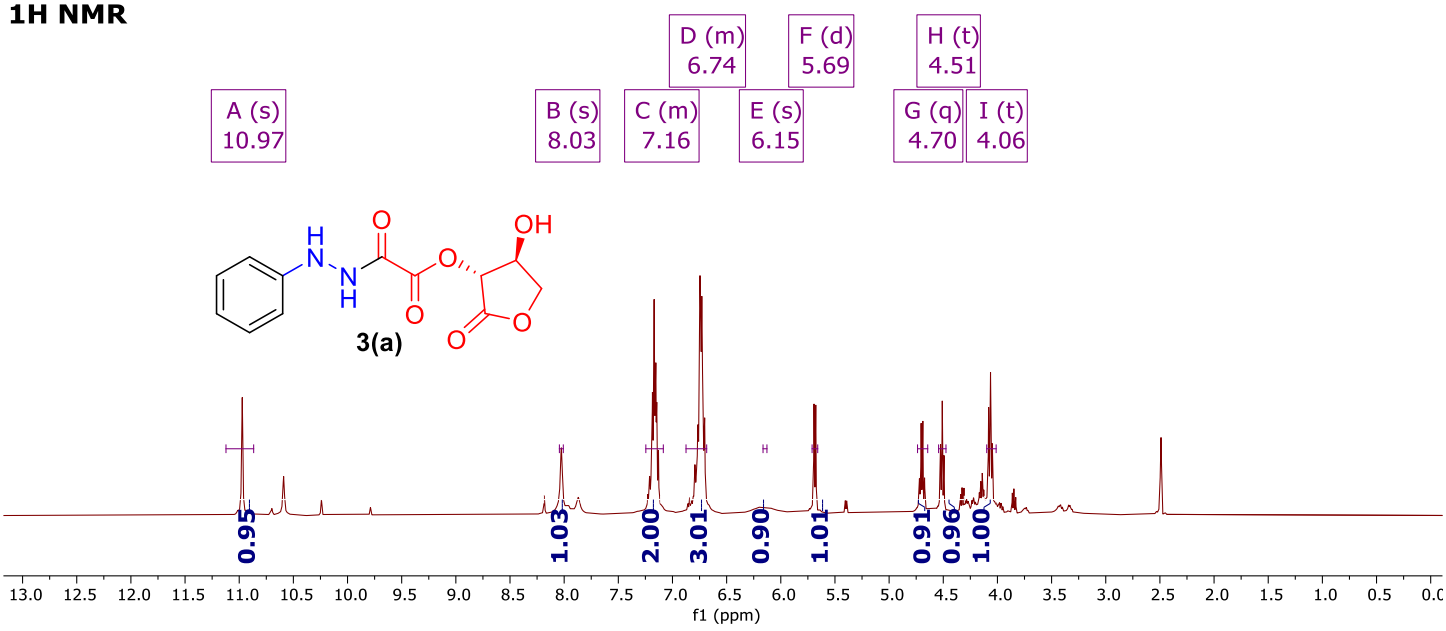
3(b)



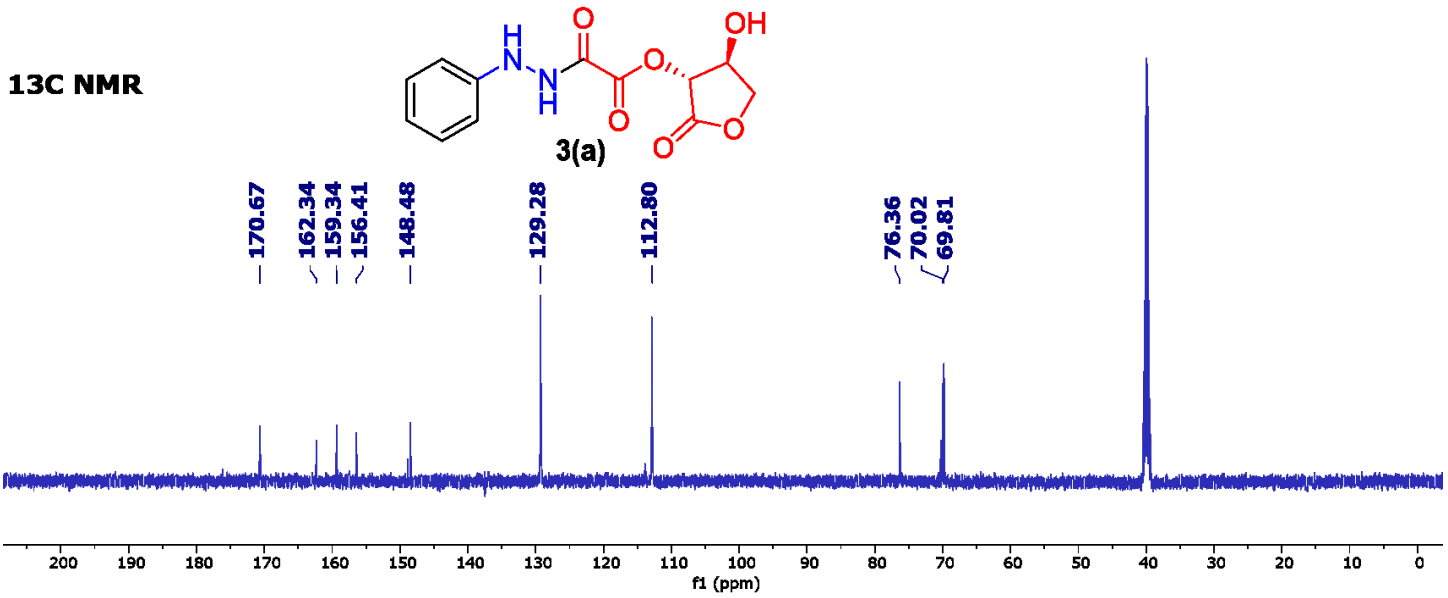
3(c)

3(d)

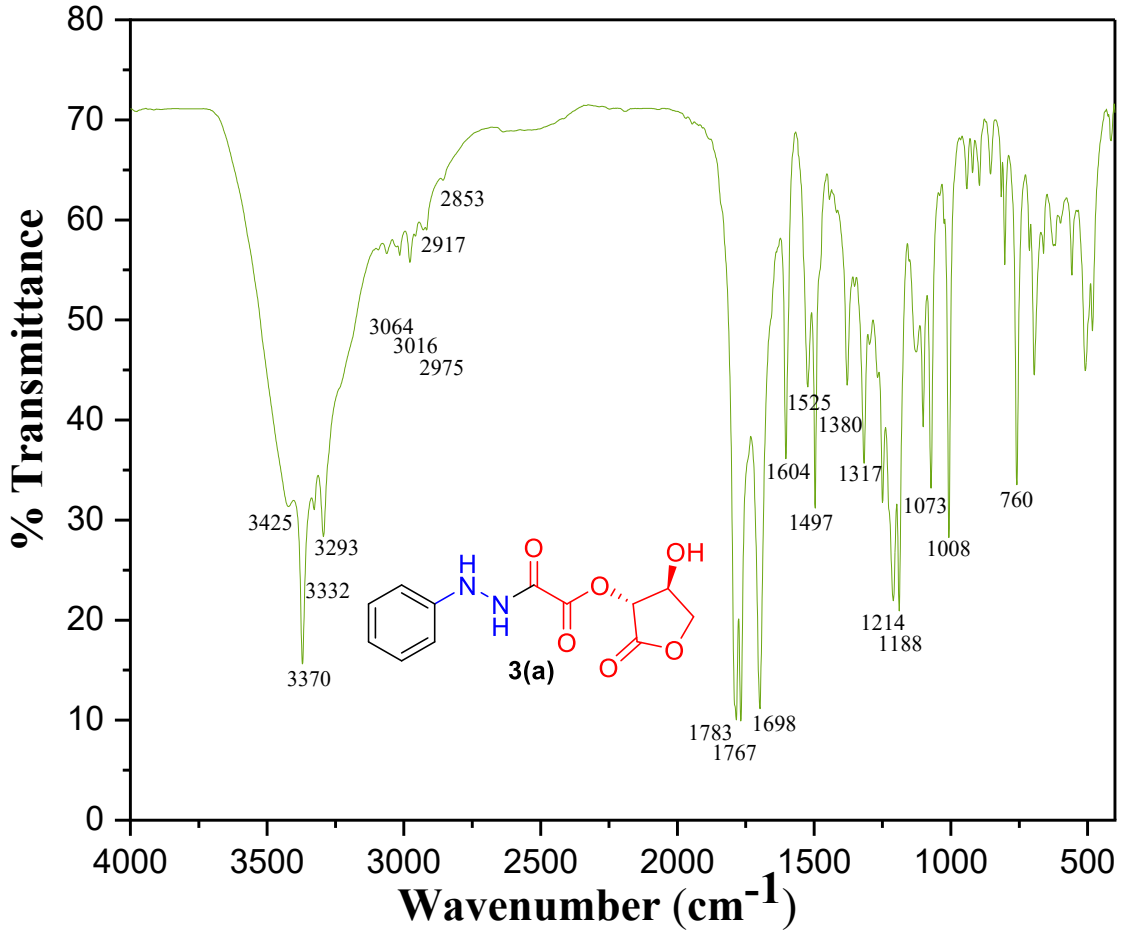
1H NMR



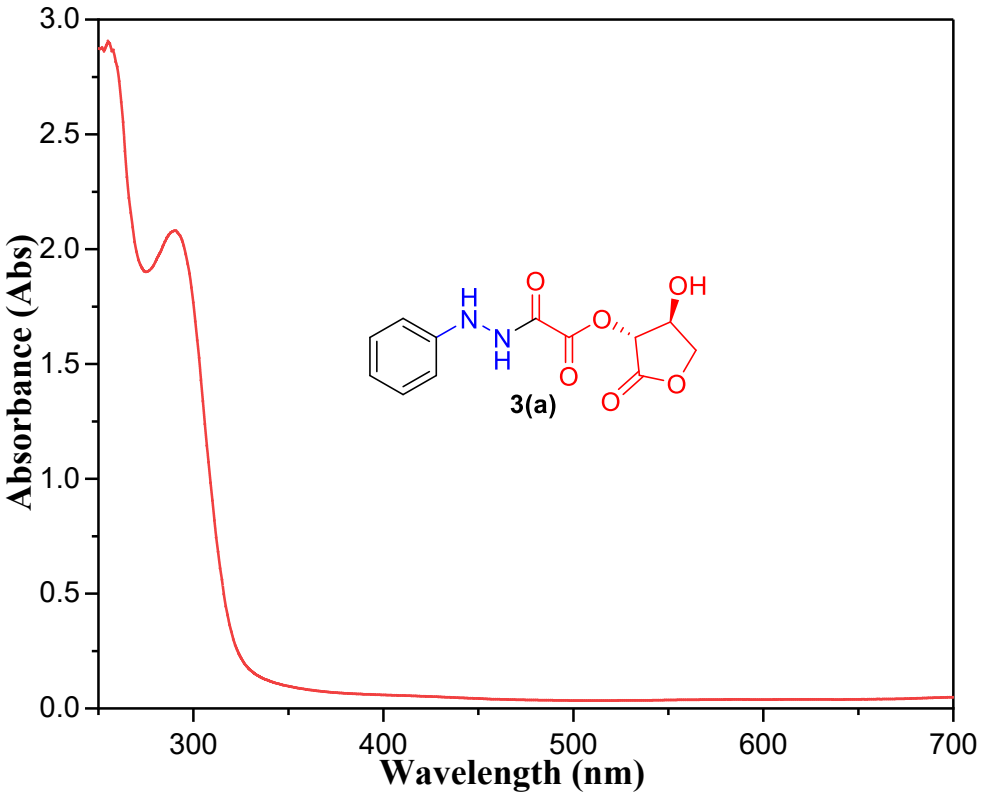
S. Figure 1. ^{1}H NMR spectrum of Adduct **3(a)**.



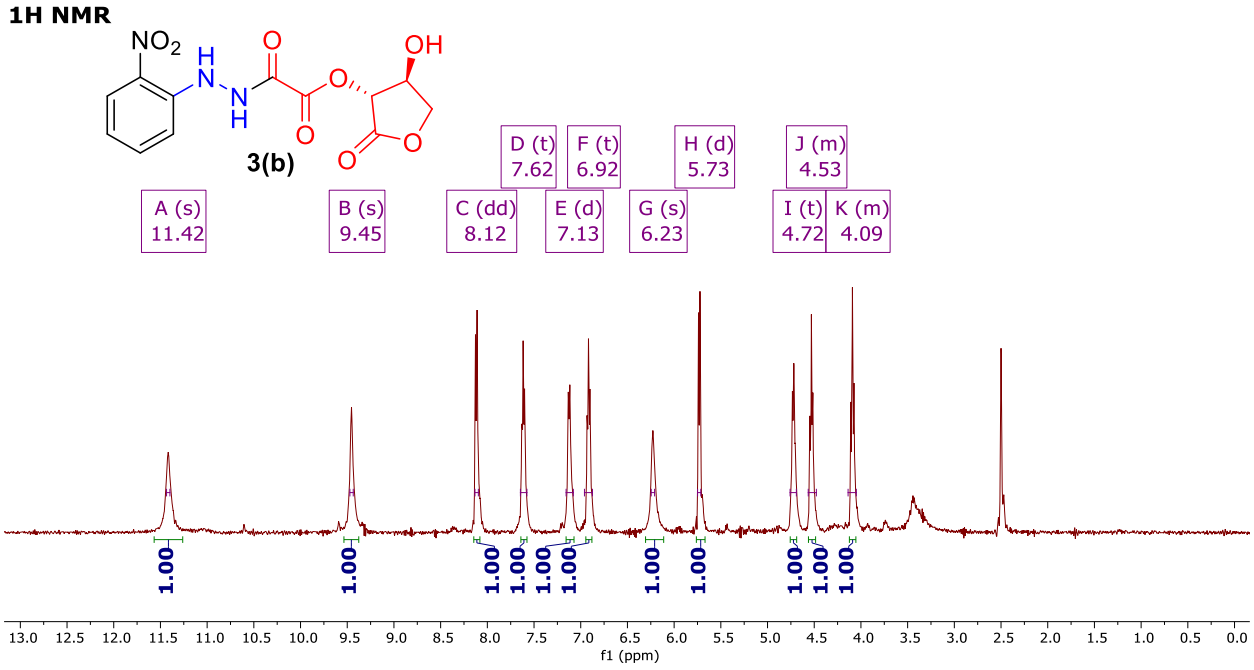
S. Figure 2. ^{13}C NMR spectrum of Adduct **3(a)**.



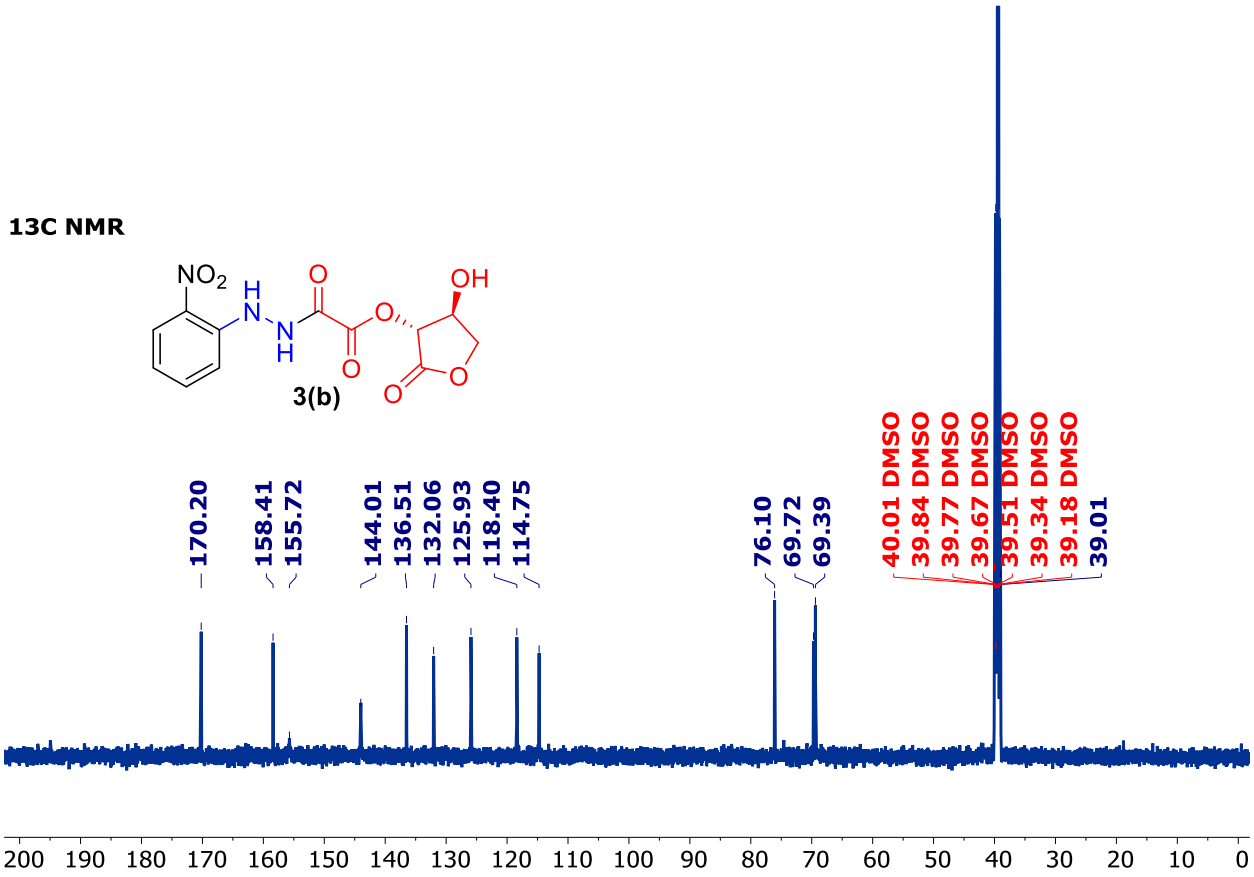
S. Figure 3. IR spectrum of Adduct **3(a)**.



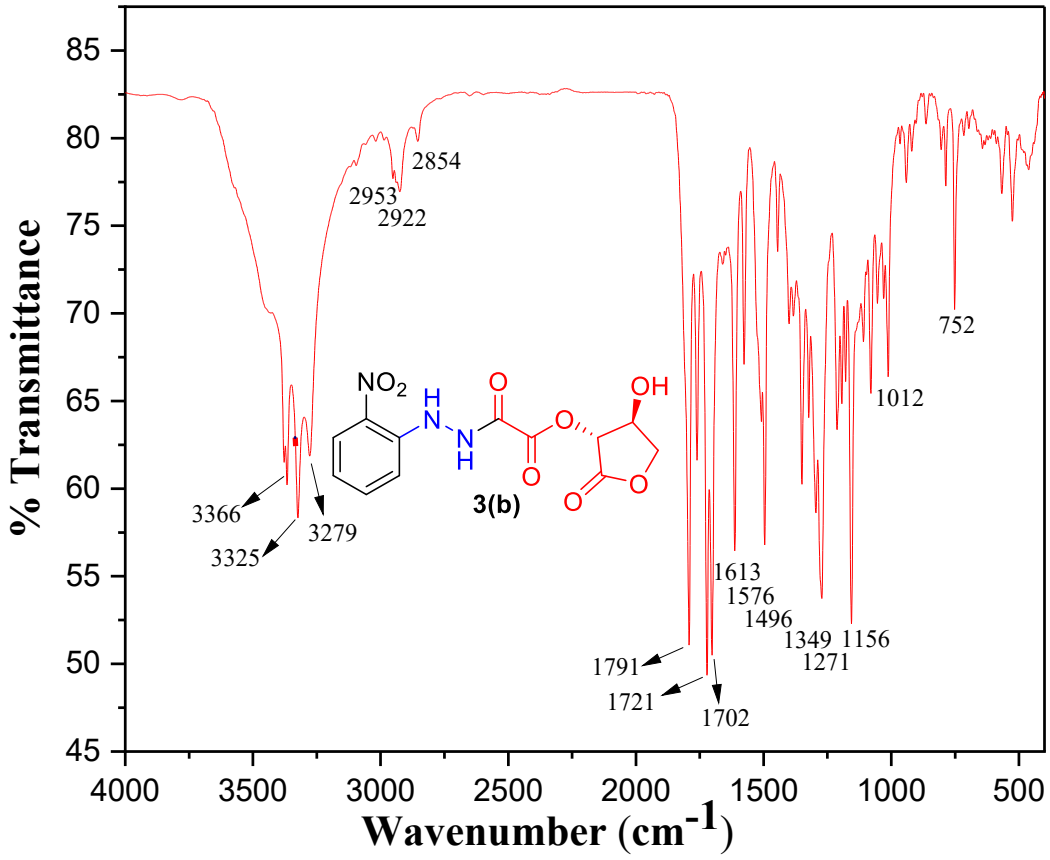
S. Figure 4. UV-vis. spectrum of Adduct **3(a)** in DW.



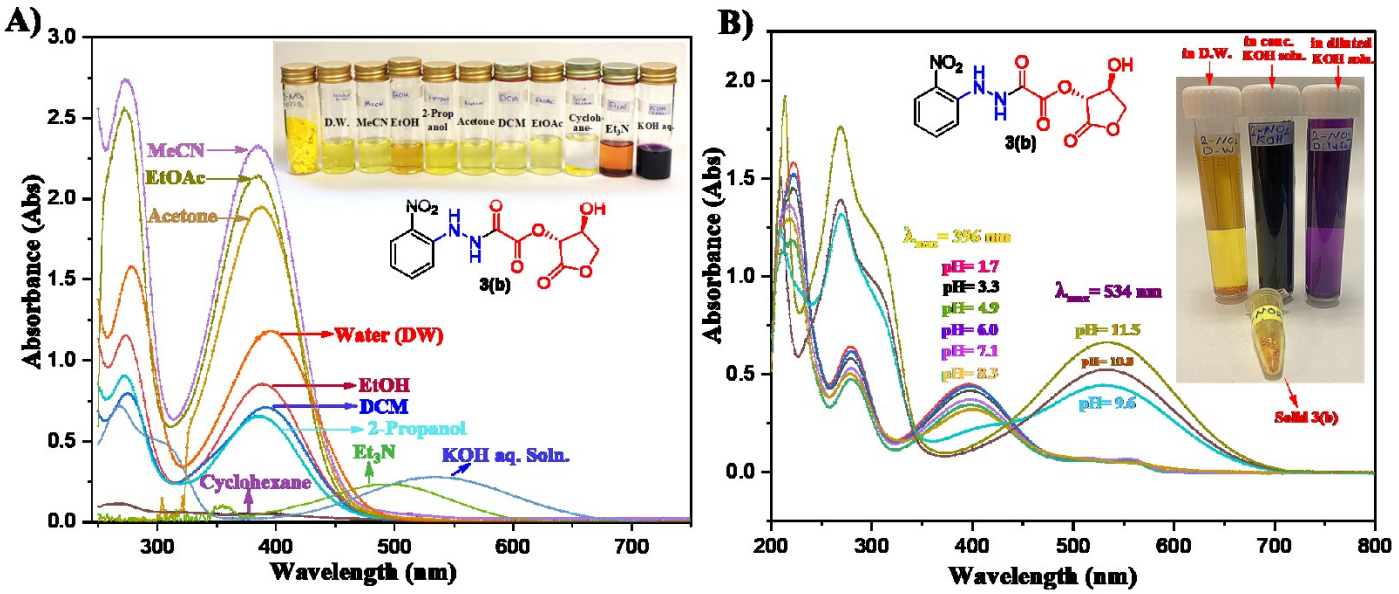
S. Figure 5. ^{1}H NMR spectrum of Adduct **3(b)**.



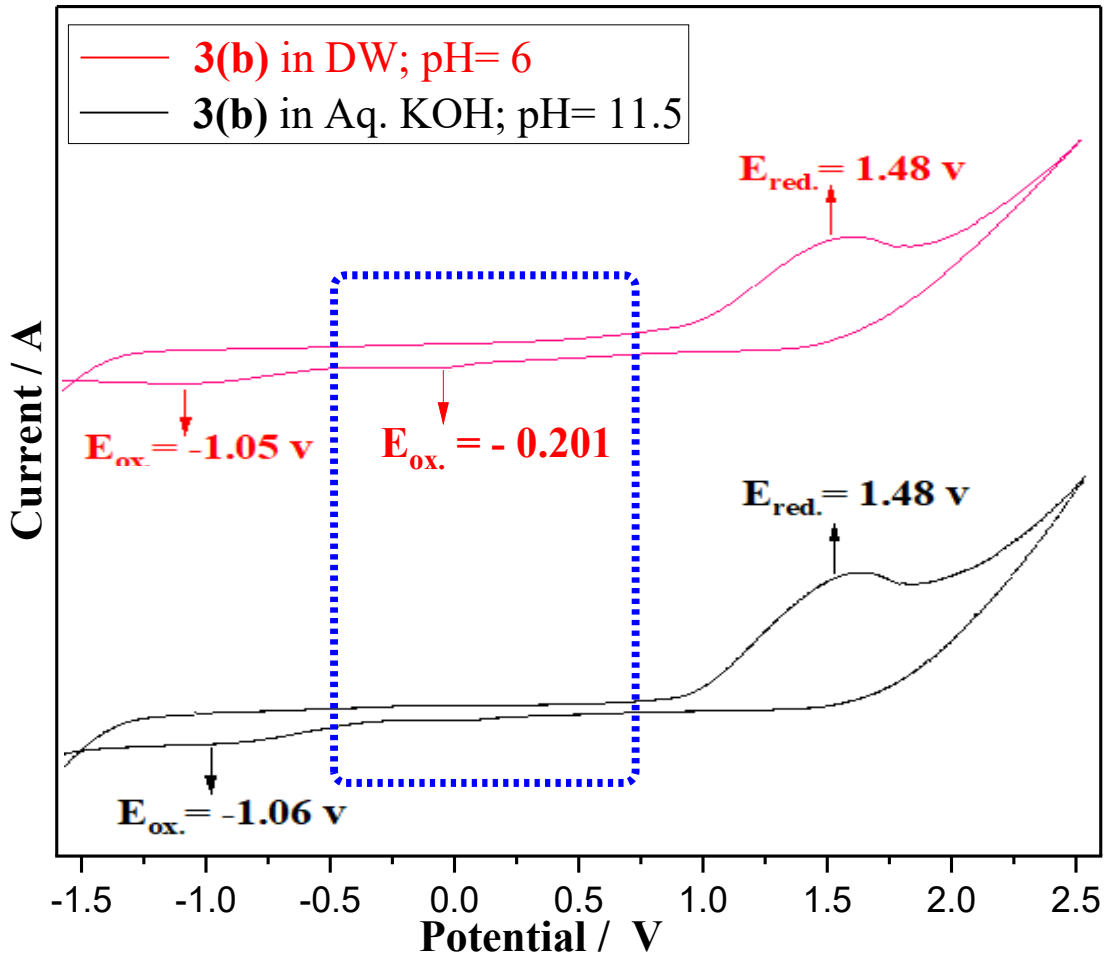
S. Figure 6. ^{13}C NMR spectrum of Adduct **3(b)**.



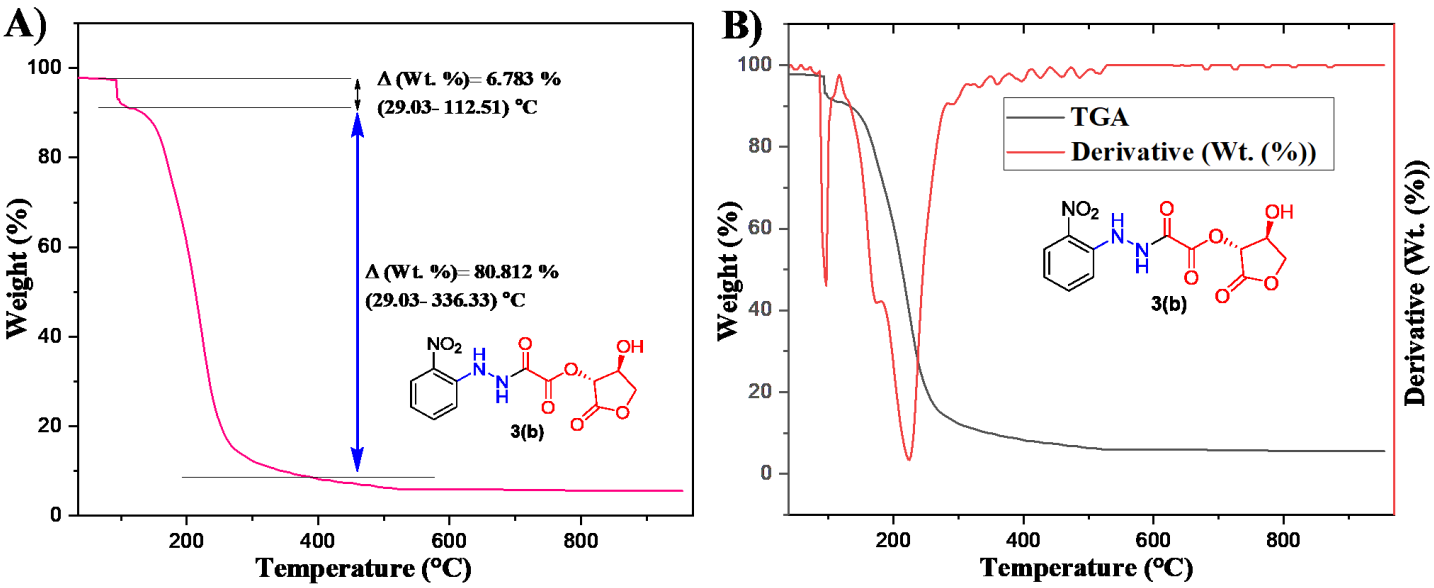
S. Figure 7. IR spectrum of Adduct **3(b)**.



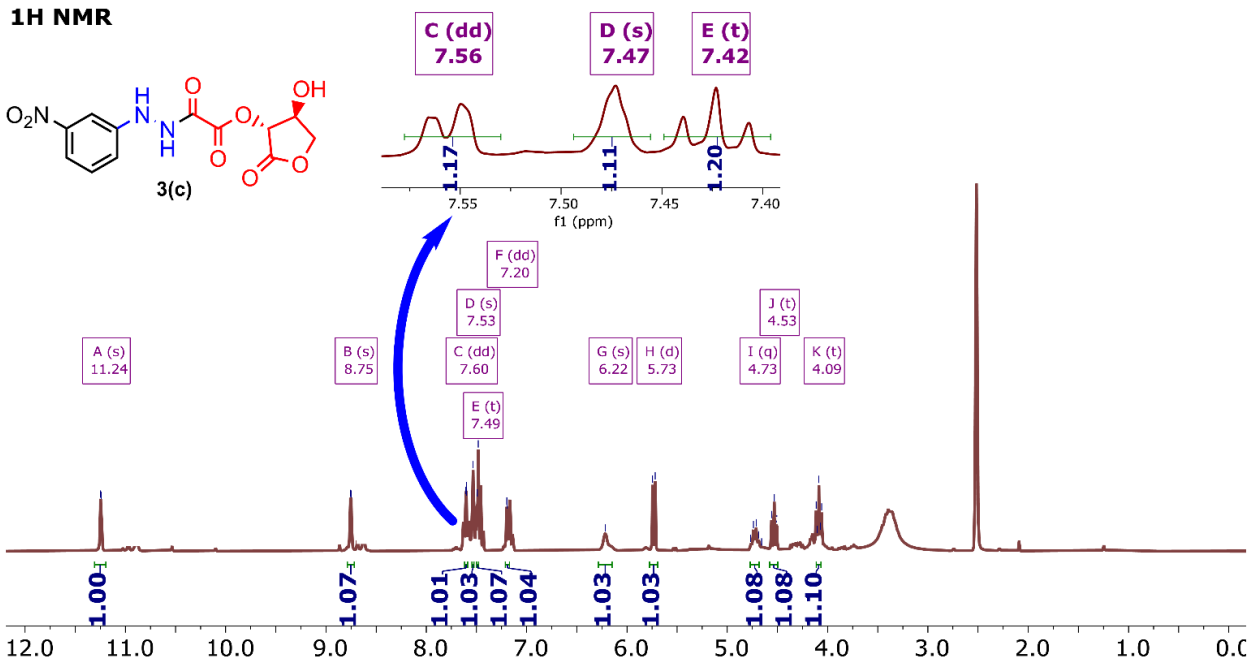
S. Figure 8. UV-Vis Spectra of the Adduct **3(b)**. **(A)**: in various solvents; **(B)**: in aqueous solution at different pHs.



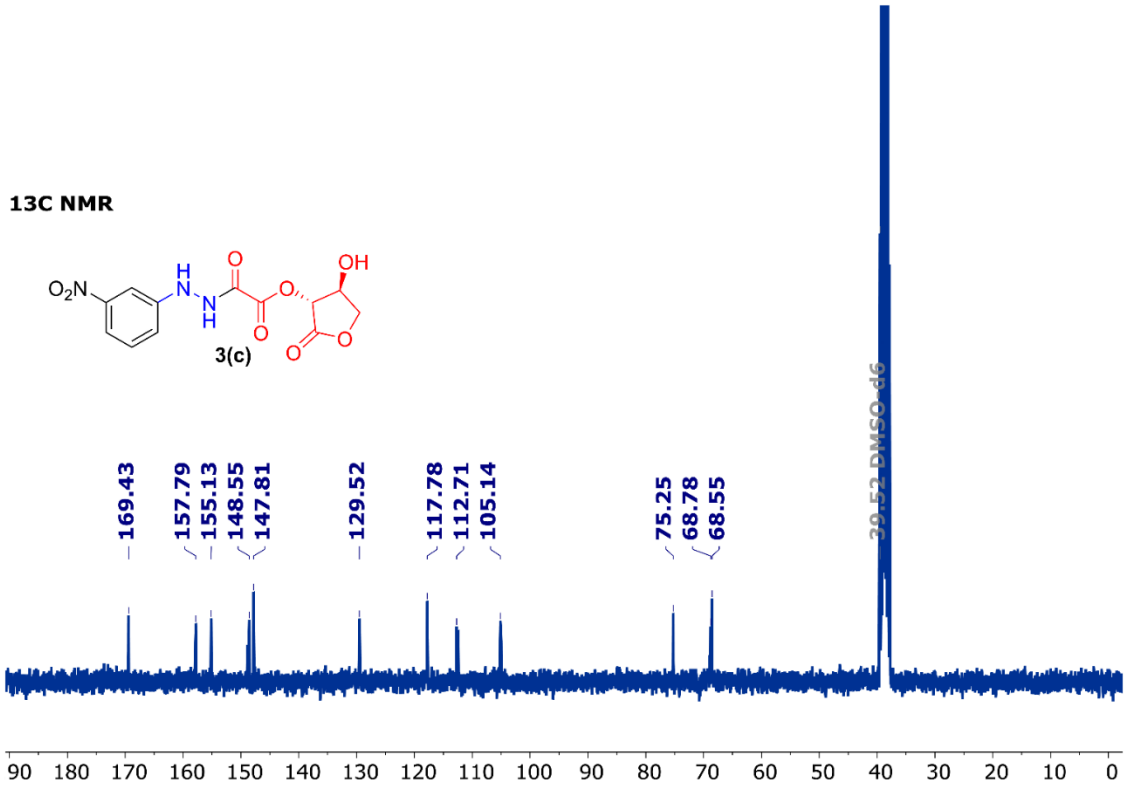
S. Figure 9. Cyclic Voltammetry (CV) outcomes of adduct **3(b)** in acidic and basic media.



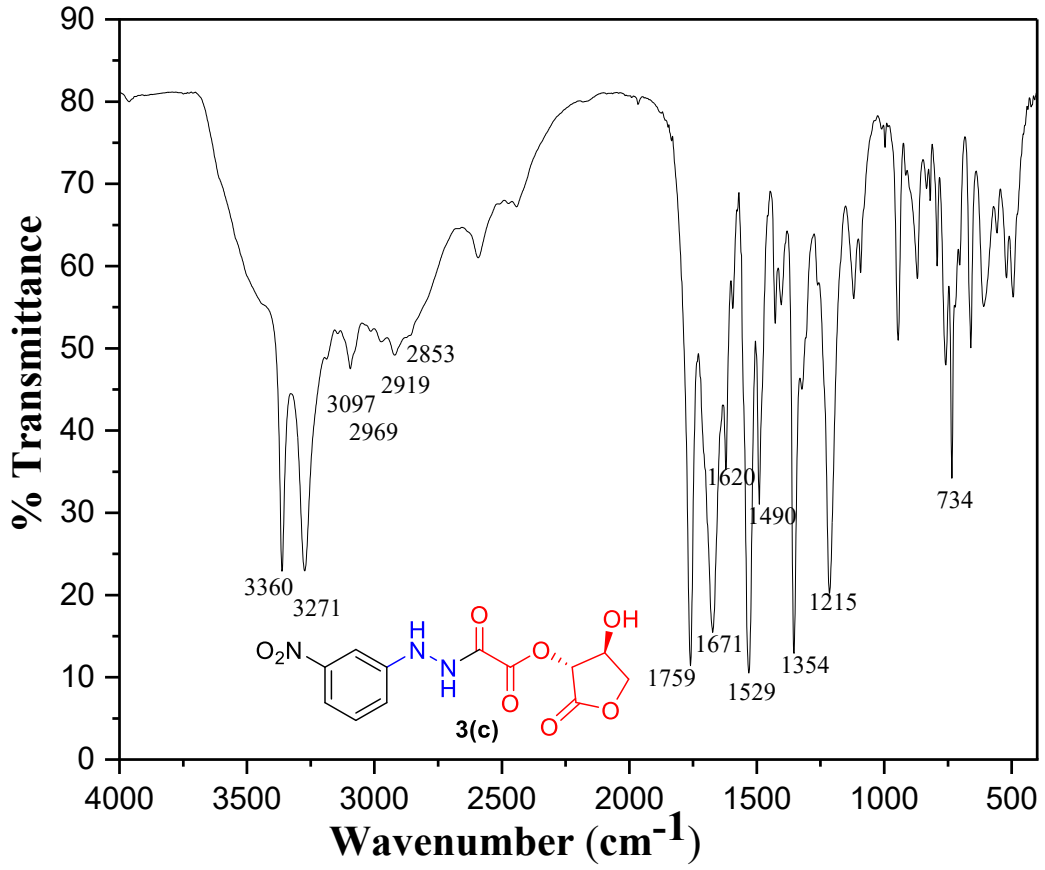
S. Figure 10. TGA thermogram of **3(b)**.



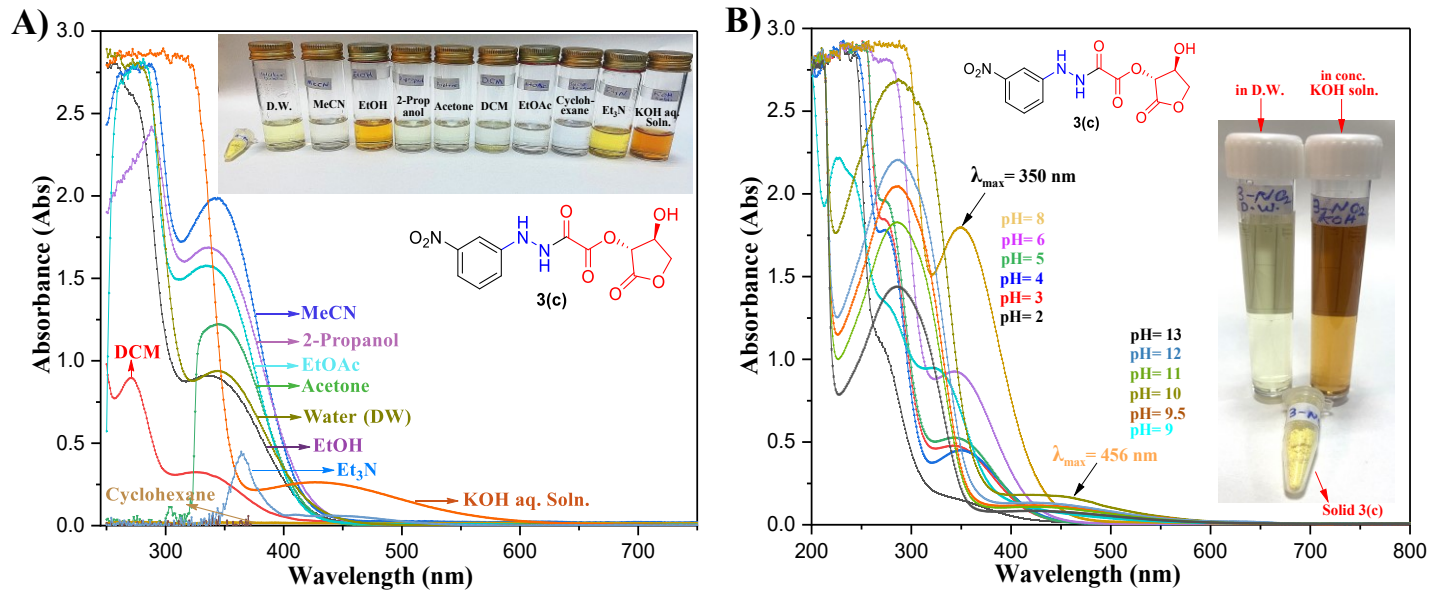
S. Figure 11. ^{1}H NMR spectrum of Adduct **3(c)**.



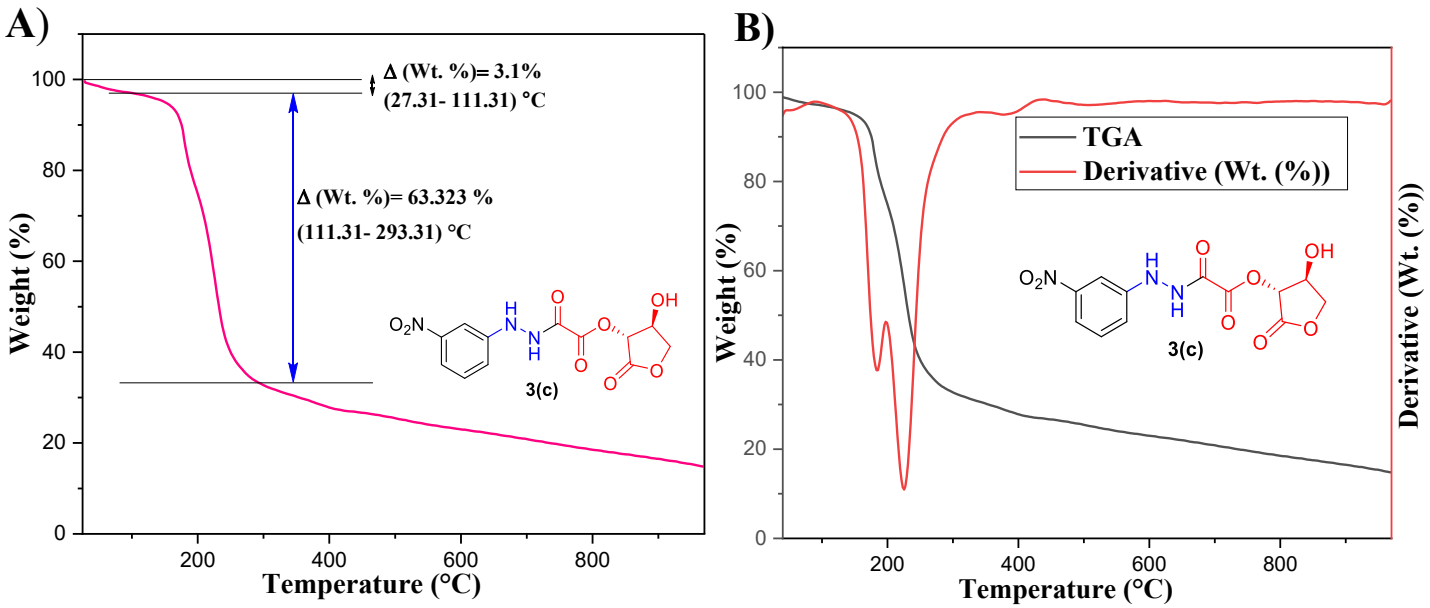
S. Figure 12. ^{13}C NMR spectrum of Adduct **3(c)**.



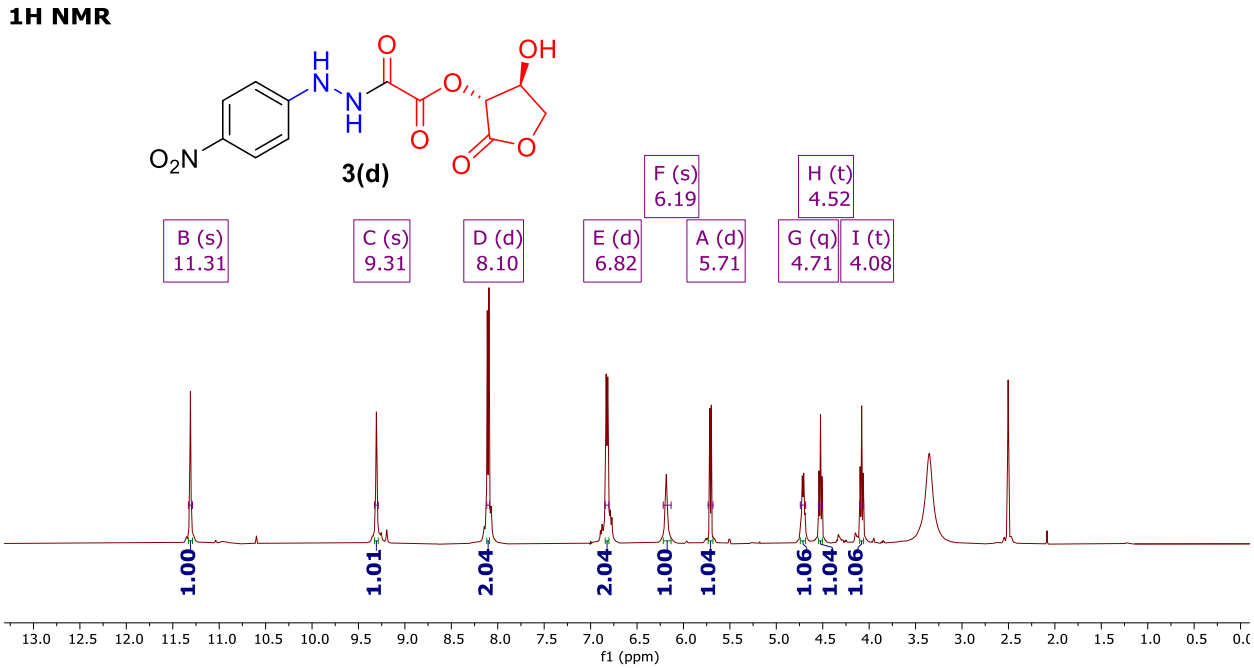
S. Figure 13. IR spectrum of Adduct **3(c)**.



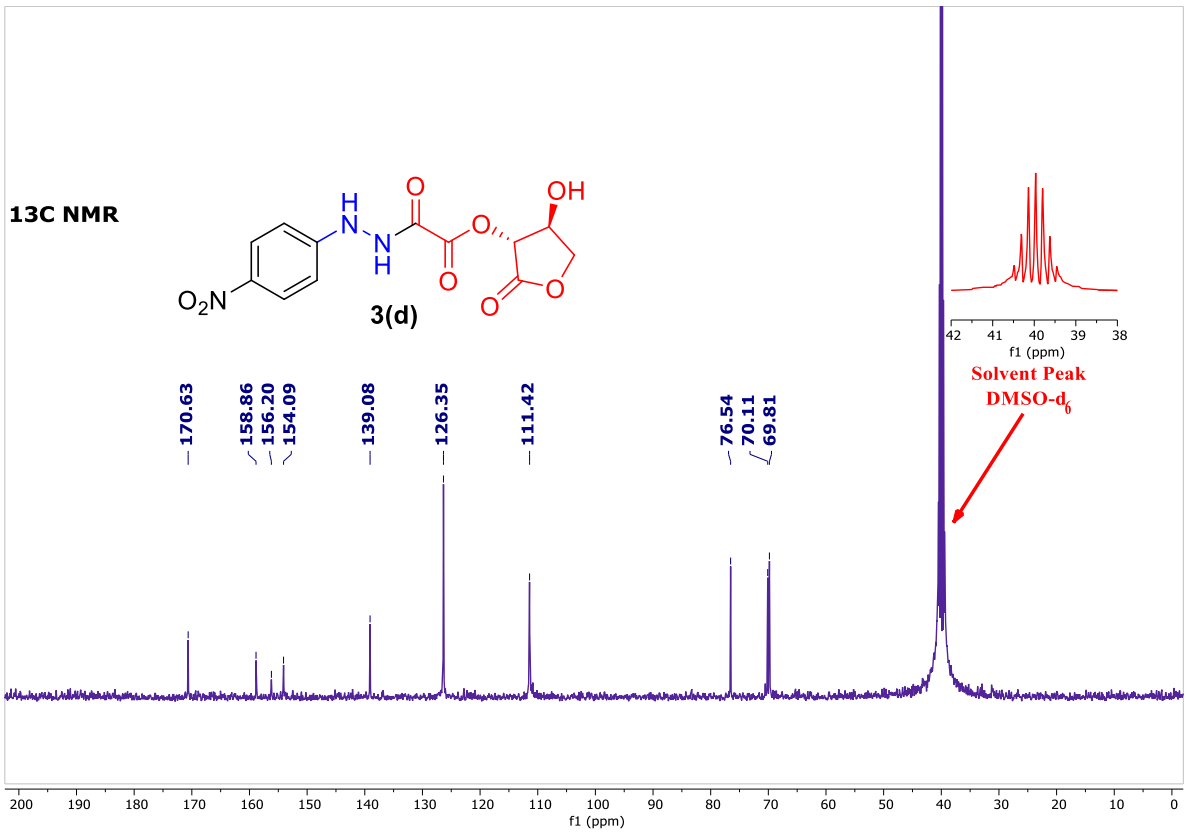
S. Figure 14. UV-Vis Spectra of the Adduct **3(c)**. **(A)**: in various solvents; **(B)**: in aqueous solution at different pHs.



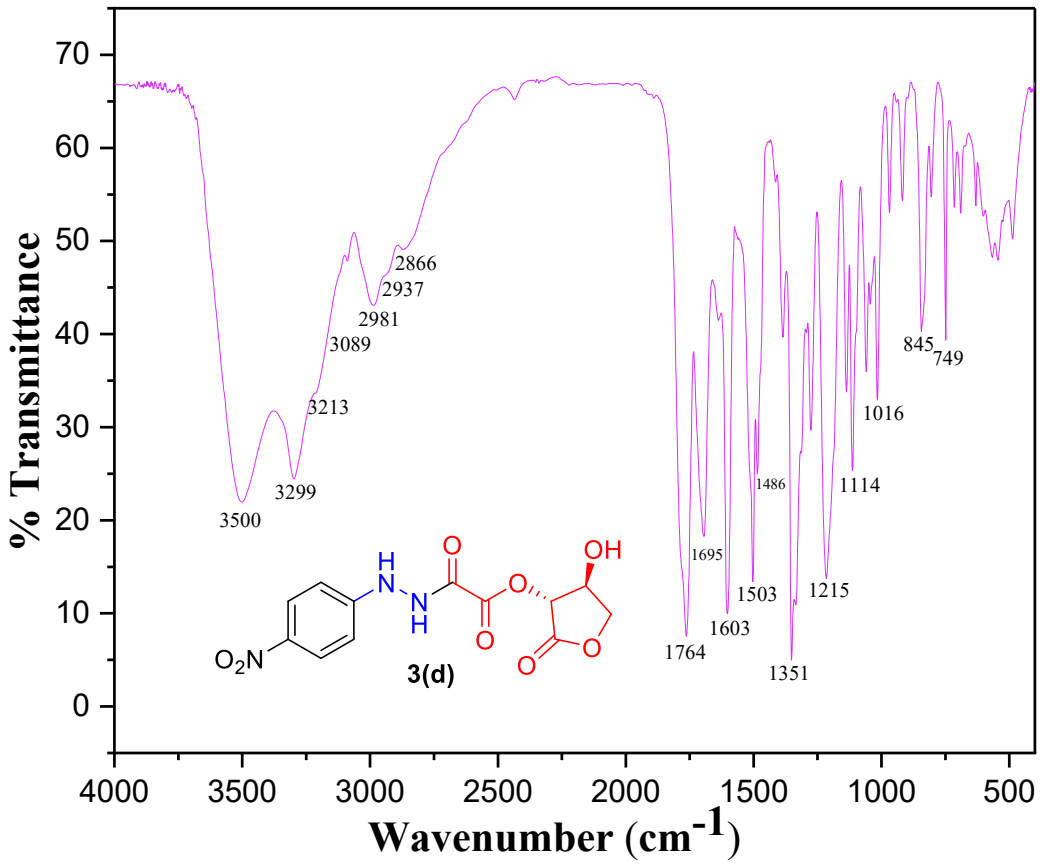
S. Figure 15. TGA thermogram of **3(c)**.



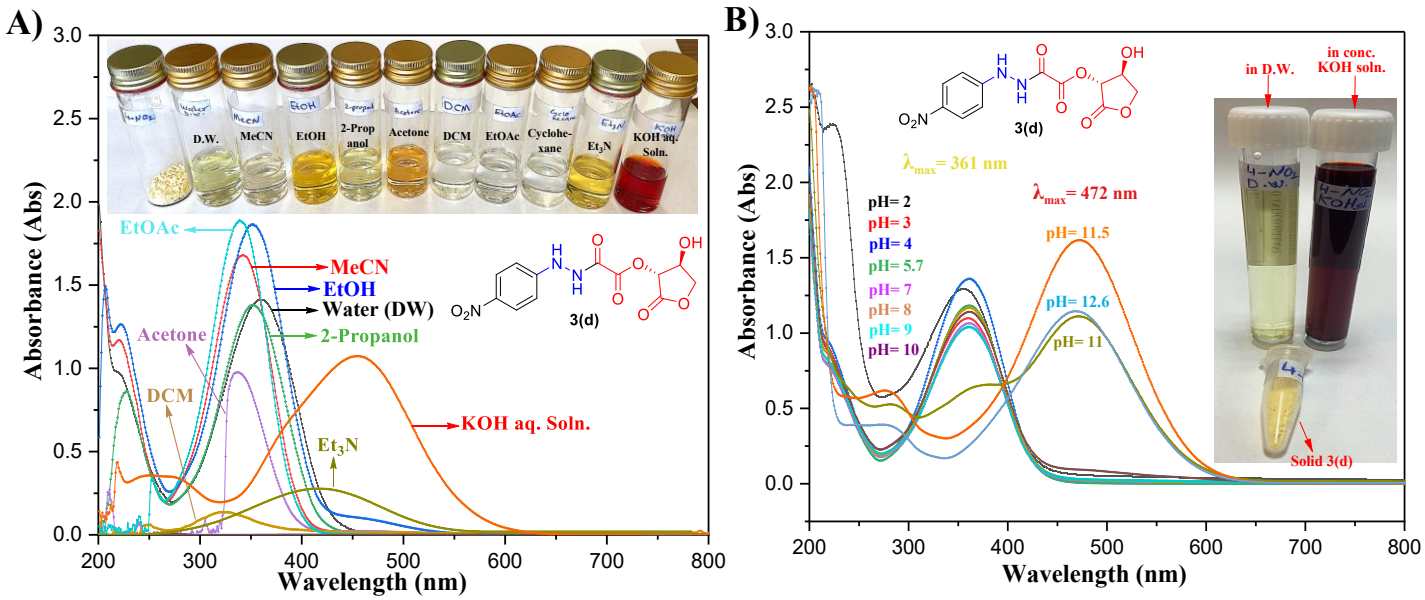
S. Figure 16. ^{1}H NMR spectrum of Adduct **3(d)**.



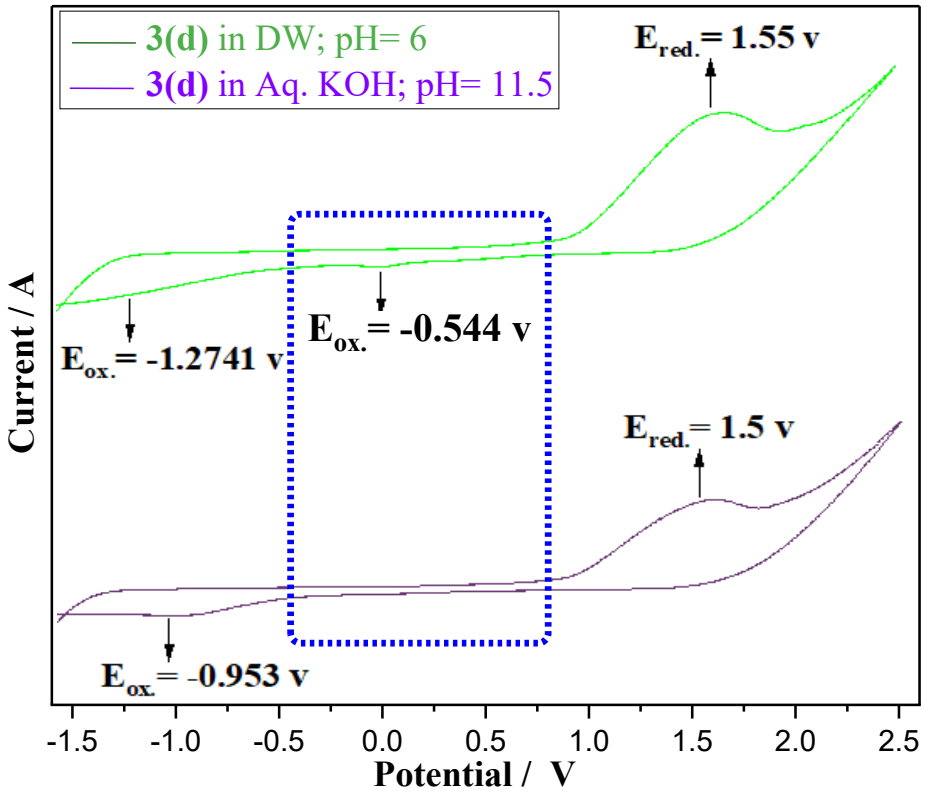
S. Figure 17. ^{13}C NMR spectrum of Adduct **3(d)**.



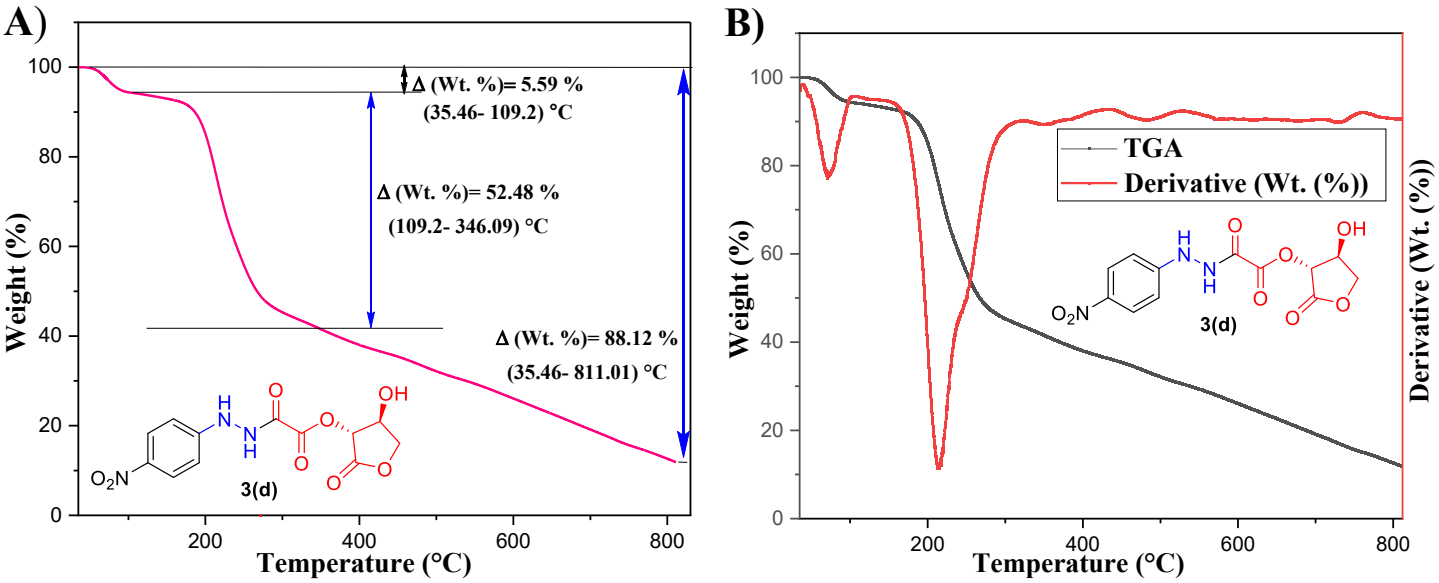
S. Figure 18. IR spectrum of Adduct **3(d)**.



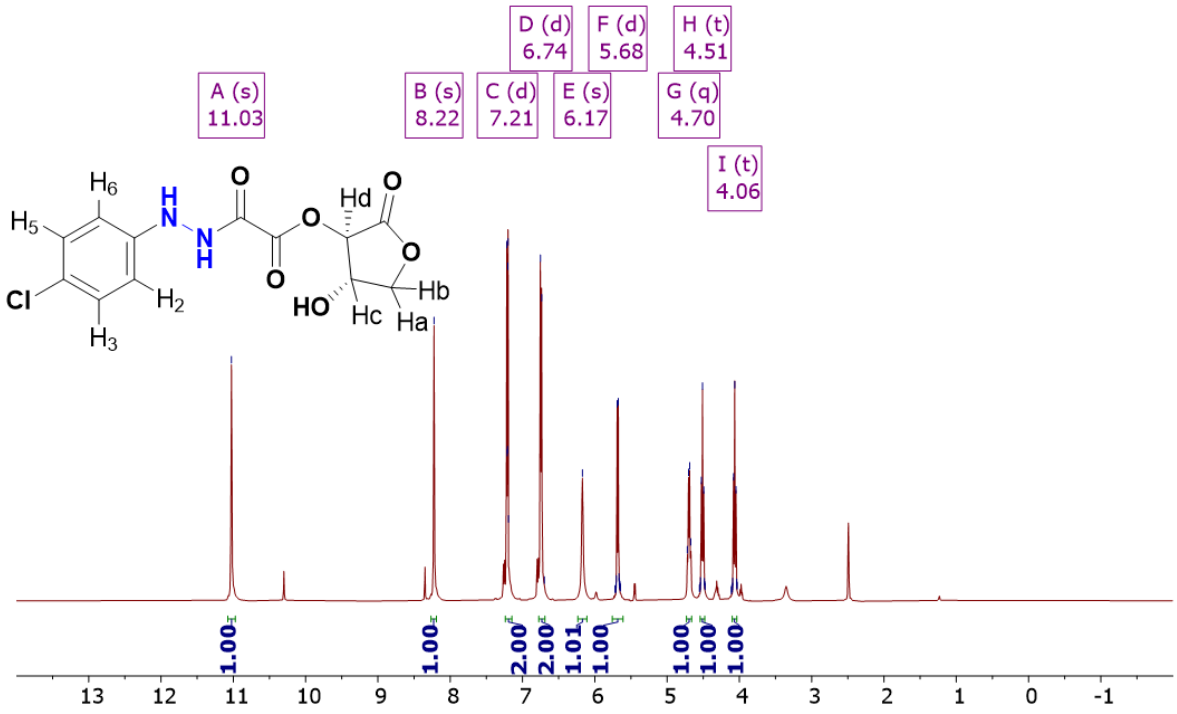
S. Figure 19. UV-Vis Spectra of the Adduct **3(d)**. **(A)**: in various solvents; **(B)**: in aqueous solution at different pHs.



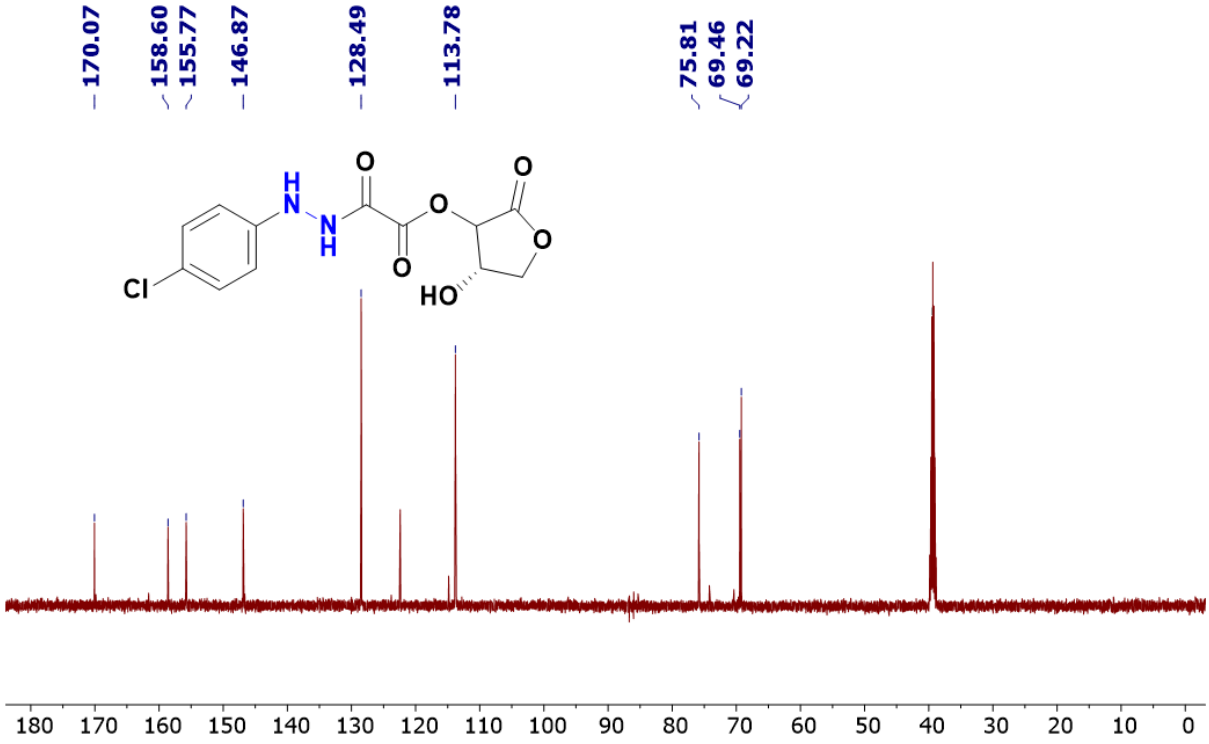
S. Figure 20. Cyclic Voltammetry (CV) outcomes of adduct **3(d)** in acidic and basic media.



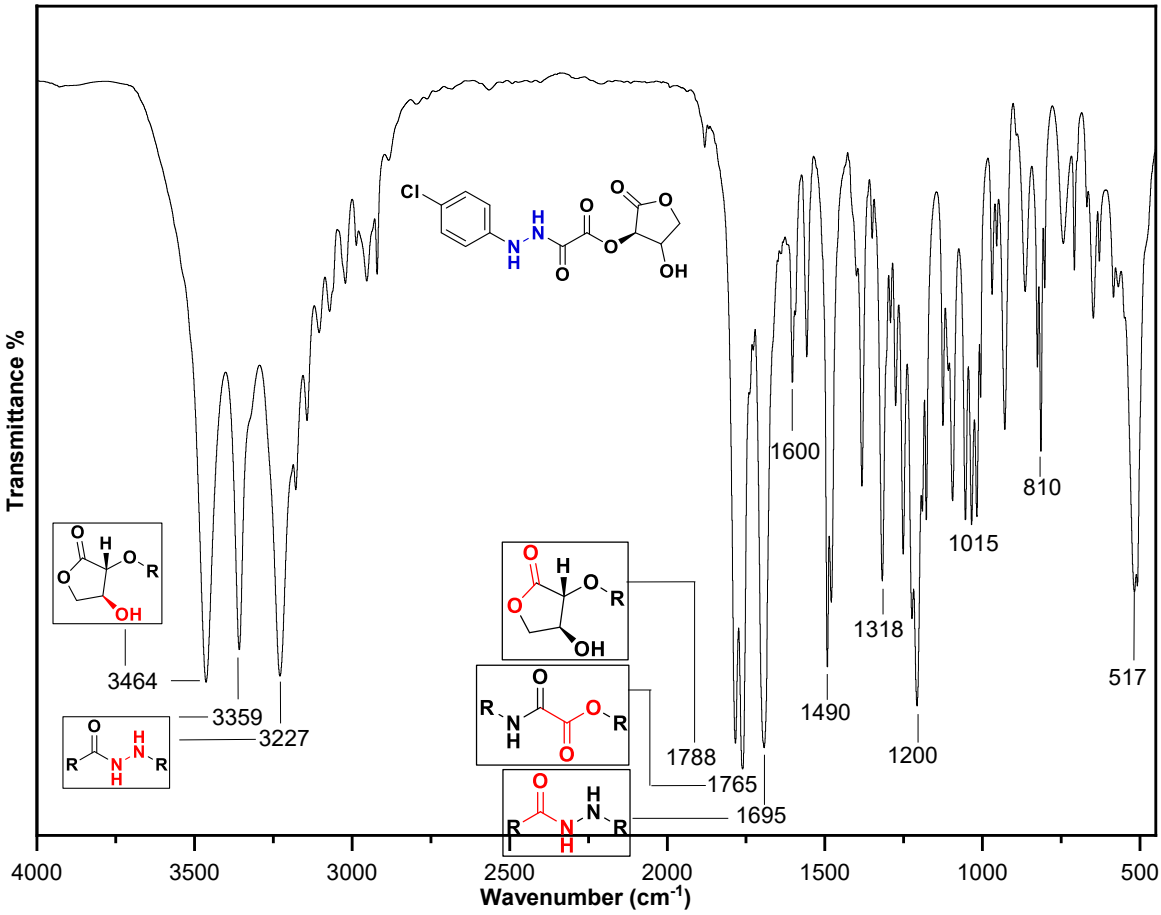
S. Figure 21. TGA thermogram of **3(d)**.



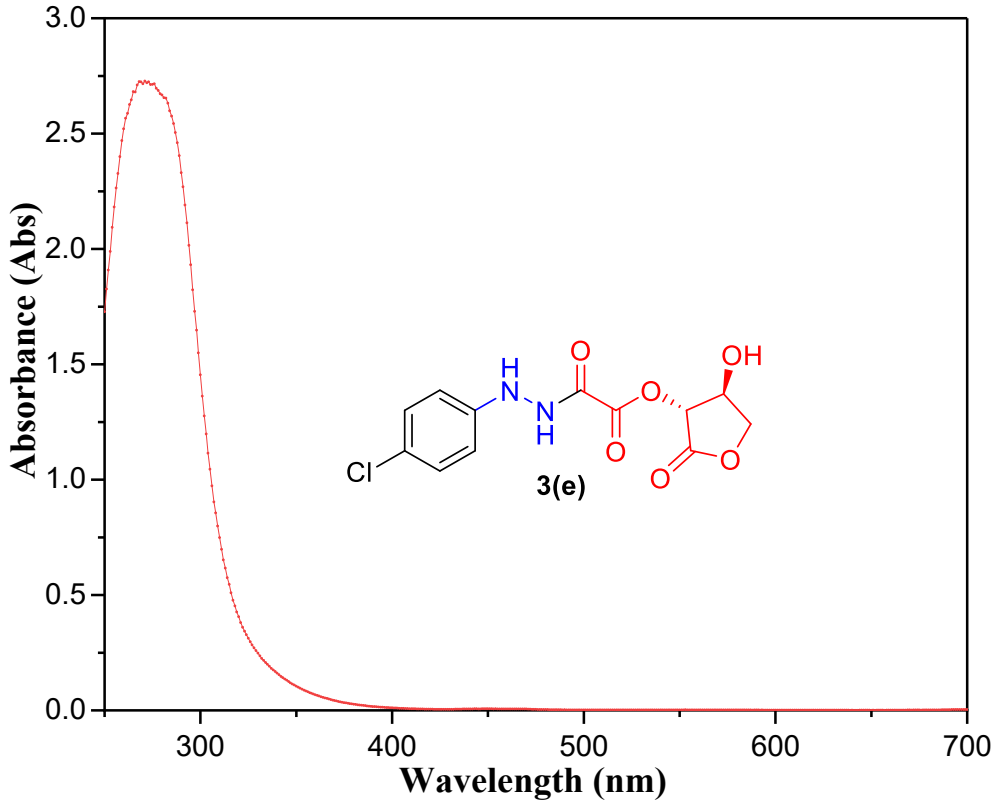
S. Figure 22. ^{1}H NMR spectrum of Adduct **3(e)**.



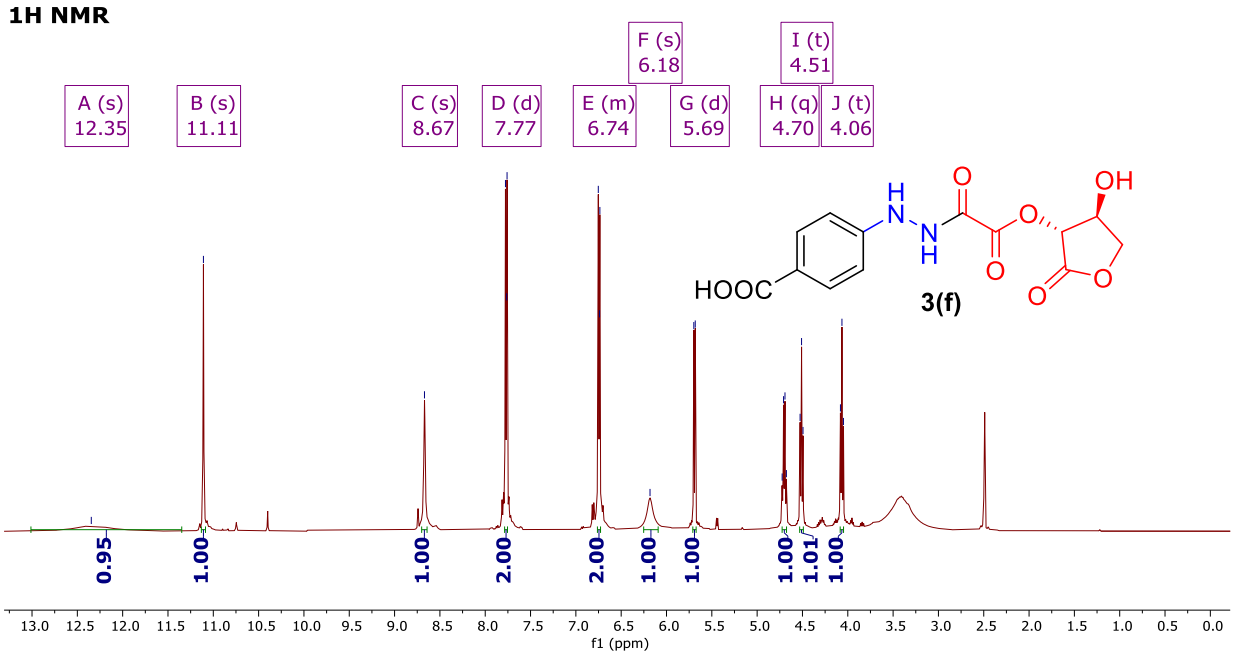
S. Figure 23. ^{13}C NMR spectrum of Adduct **3(e)**.



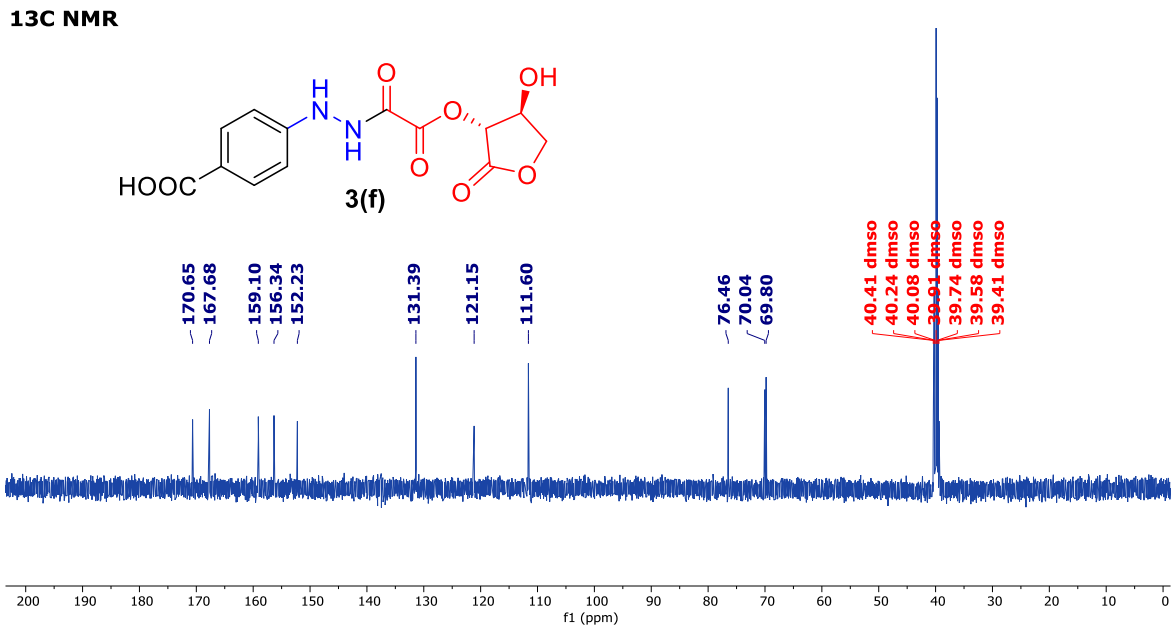
S. Figure 24. IR spectrum of Adduct **3(e)**.



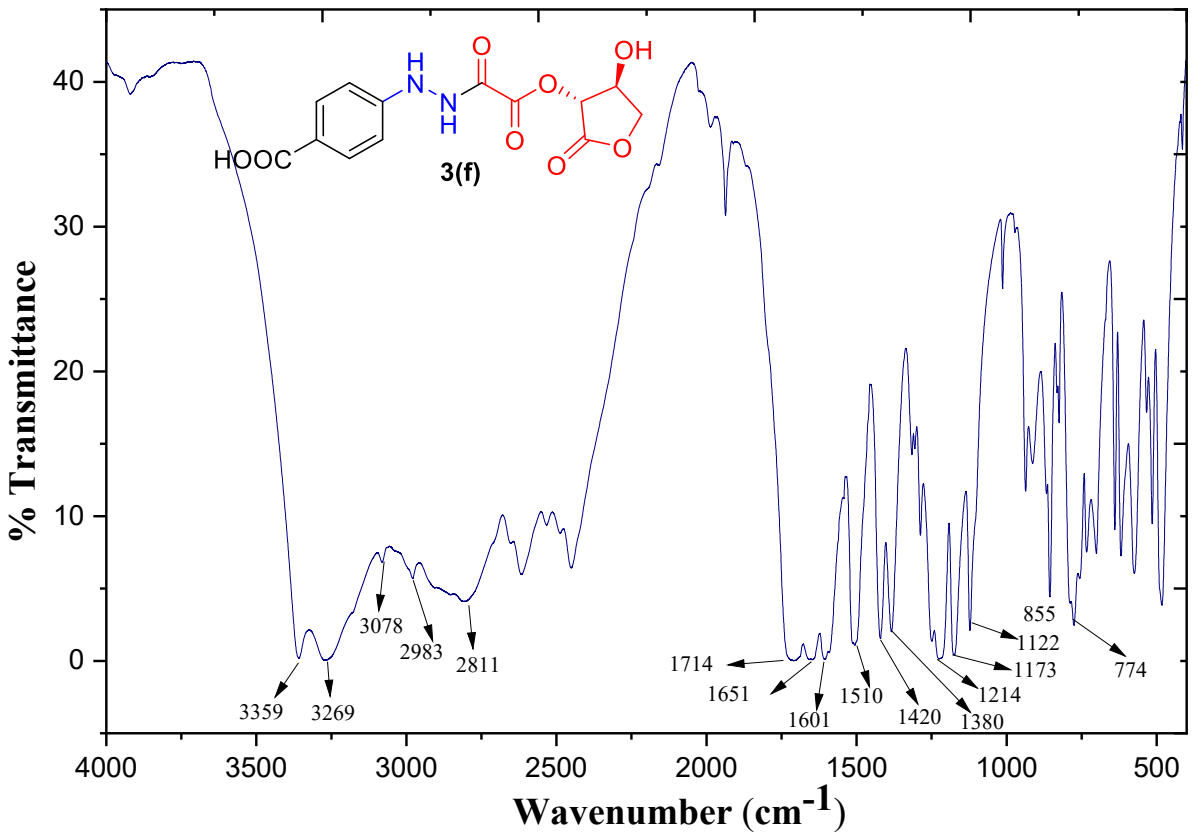
S. Figure 25. UV-vis. spectrum of Adduct **3(e)** in DW.



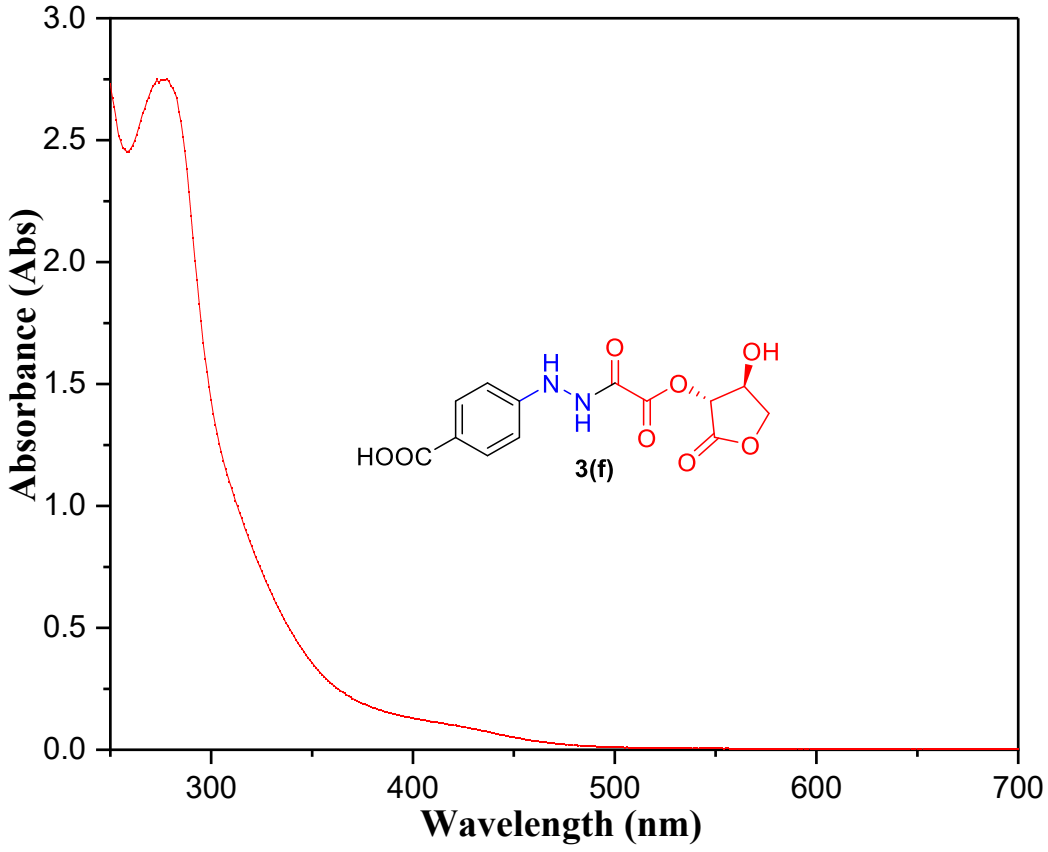
S. Figure 26. ^{1}H NMR spectrum of Adduct **3(f)**.



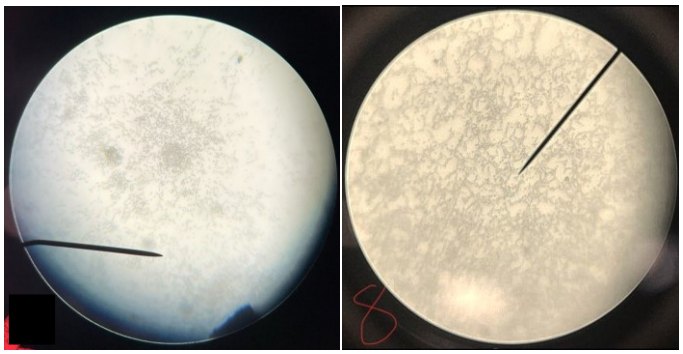
S. Figure 27. ^{13}C NMR spectrum of Adduct **3(f)**.



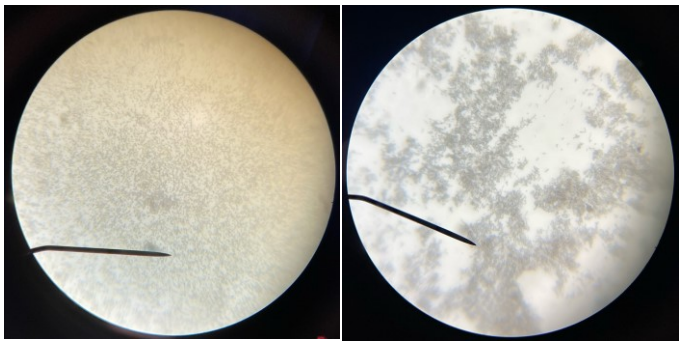
S. Figure 28. IR spectrum of Adduct **3(f)**.



S. Figure 29. UV-vis. spectrum of Adduct **3(f)** in DW.



3(b)/ H_2O/ pH= 6 **3(b)**/ Aq. KOH/ pH= 11

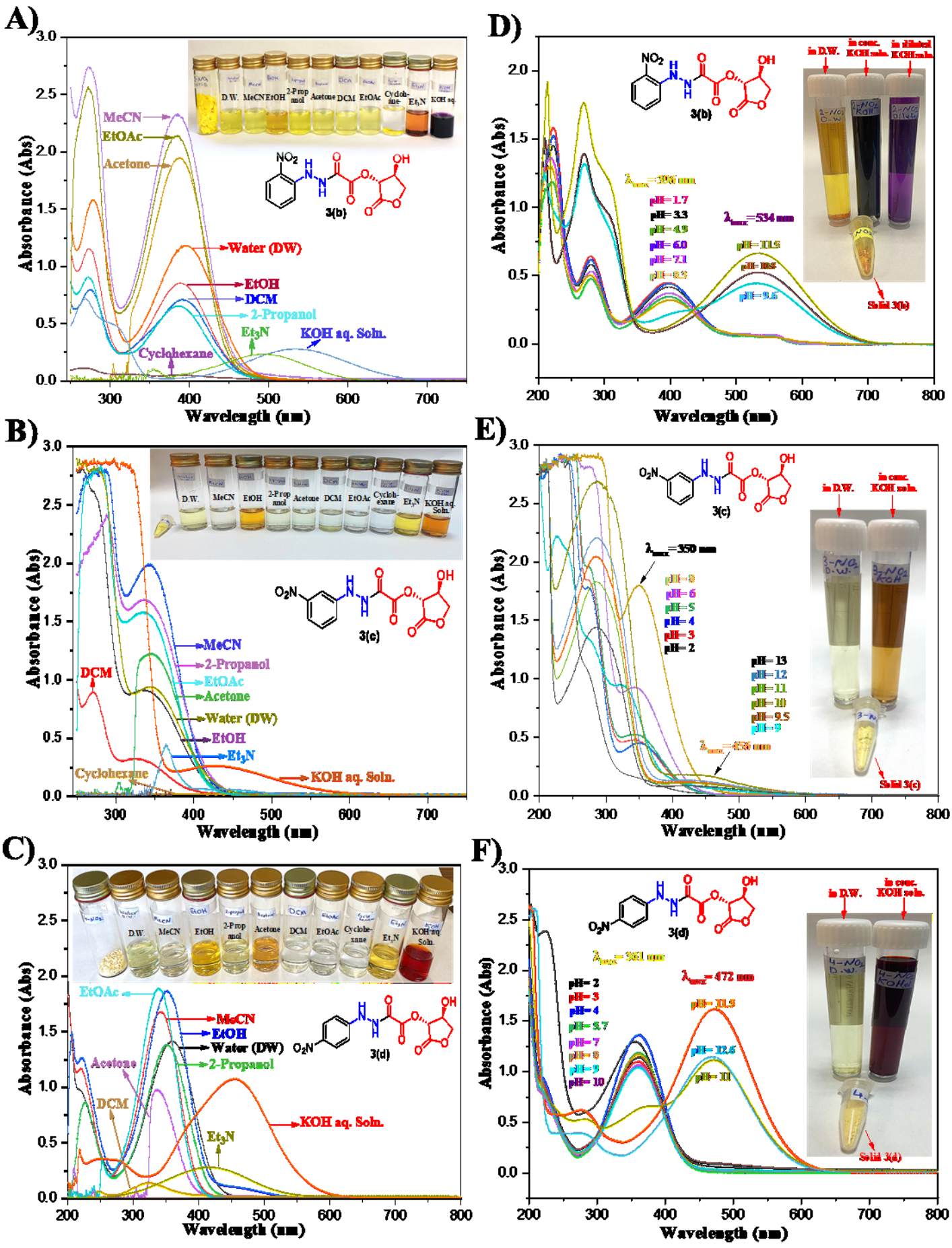


3(d)/ H_2O/ pH= 6 **3(d)**/ Aq. KOH/ pH= 11

Deep staining

Crystal Violet/ H_2O/ pH= 6

S. Figure 30. Microscopic visualization of Gram-positive *B. cereus* staining results using dyes **3(b)**, **3(d)**, and crystal violet.


A)
B)
C)
D)
E)
F)
Absorbance (Abs)
Wavelength (nm)
MeCN
EtOAc
Acetone
Water (DW)
EtOH
DCM
2-Propanol
Et3N
KOH aq. Soln.
Cyclohexane
3(b)
3(c)
3(d)
λmax=396 nm
λmax=534 nm
λmax=350 nm
λmax=458 nm
λmax=361 nm
λmax=472 nm
Solid 3(b)
Solid 3(c)
Solid 3(d)
in D.W.
in conc. KOH soln.
in diluted KOH soln.