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# Supporting Information

## Catalyst-free approach to a novel imidazo [4,5-f][1,10] phenanthroline ligand and its corresponding ruthenium(II) complex: insights into their applications in colorimetric anion sensing

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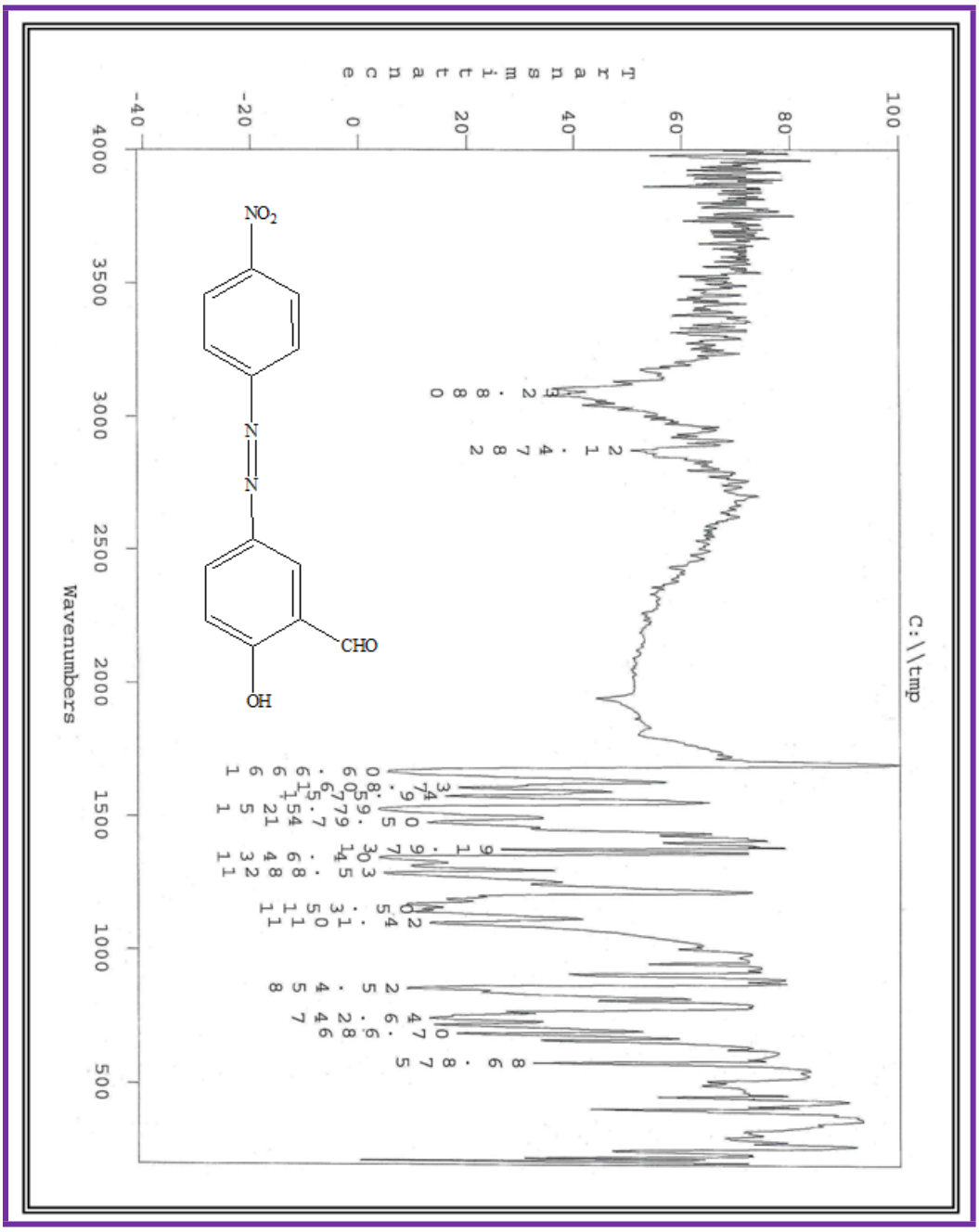



**Figure S1.** IR spectrum of 1-(3-Formyl-4-hydroxyphenylazo)-4-nitrobenzene

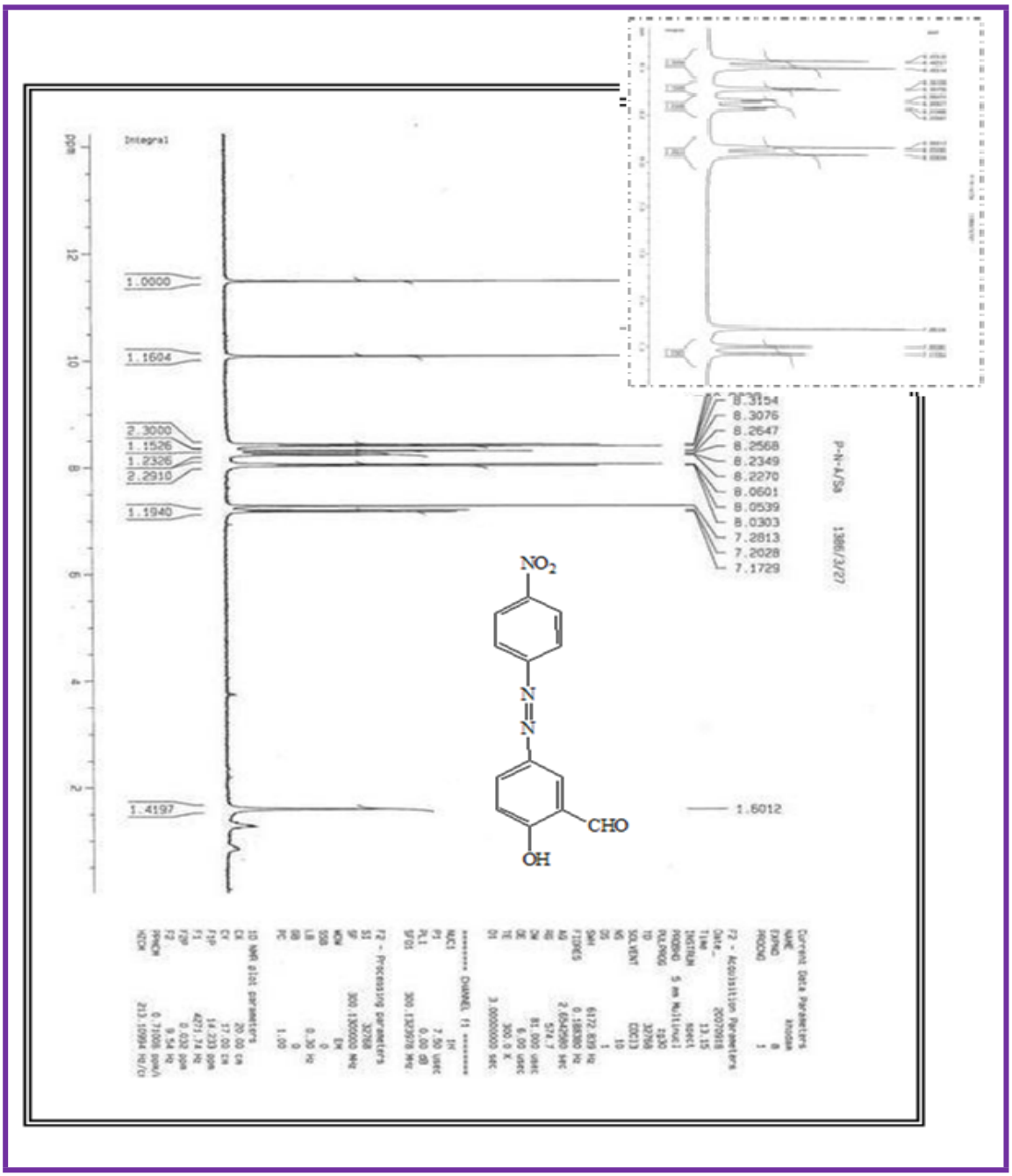



**Figure S2.** $^{1}$H NMR spectrum of 1-(3-Formyl-4-hydroxyphenylazo)-4-nitrobenzene

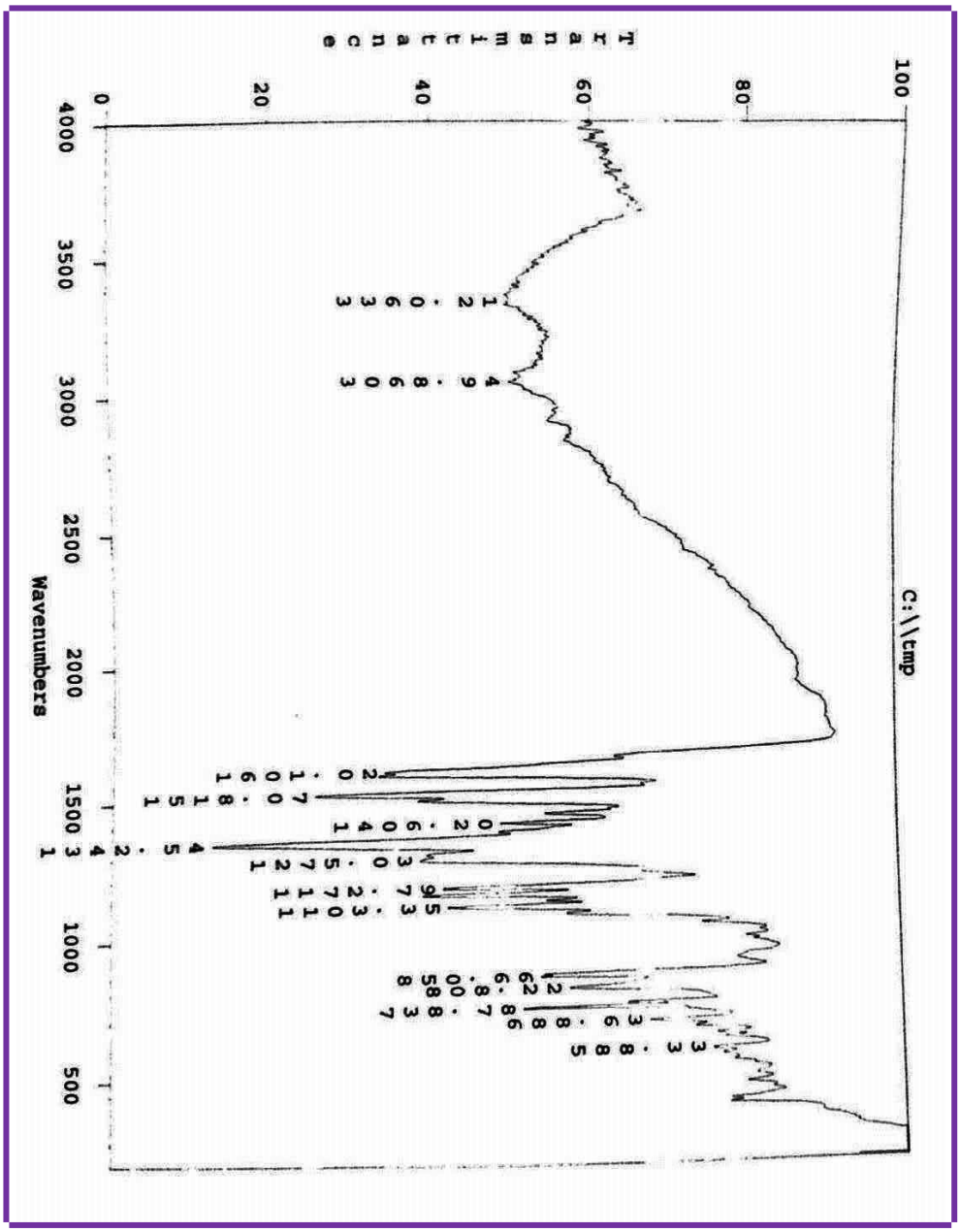



**Figure S3.** IR spectrum of **L**

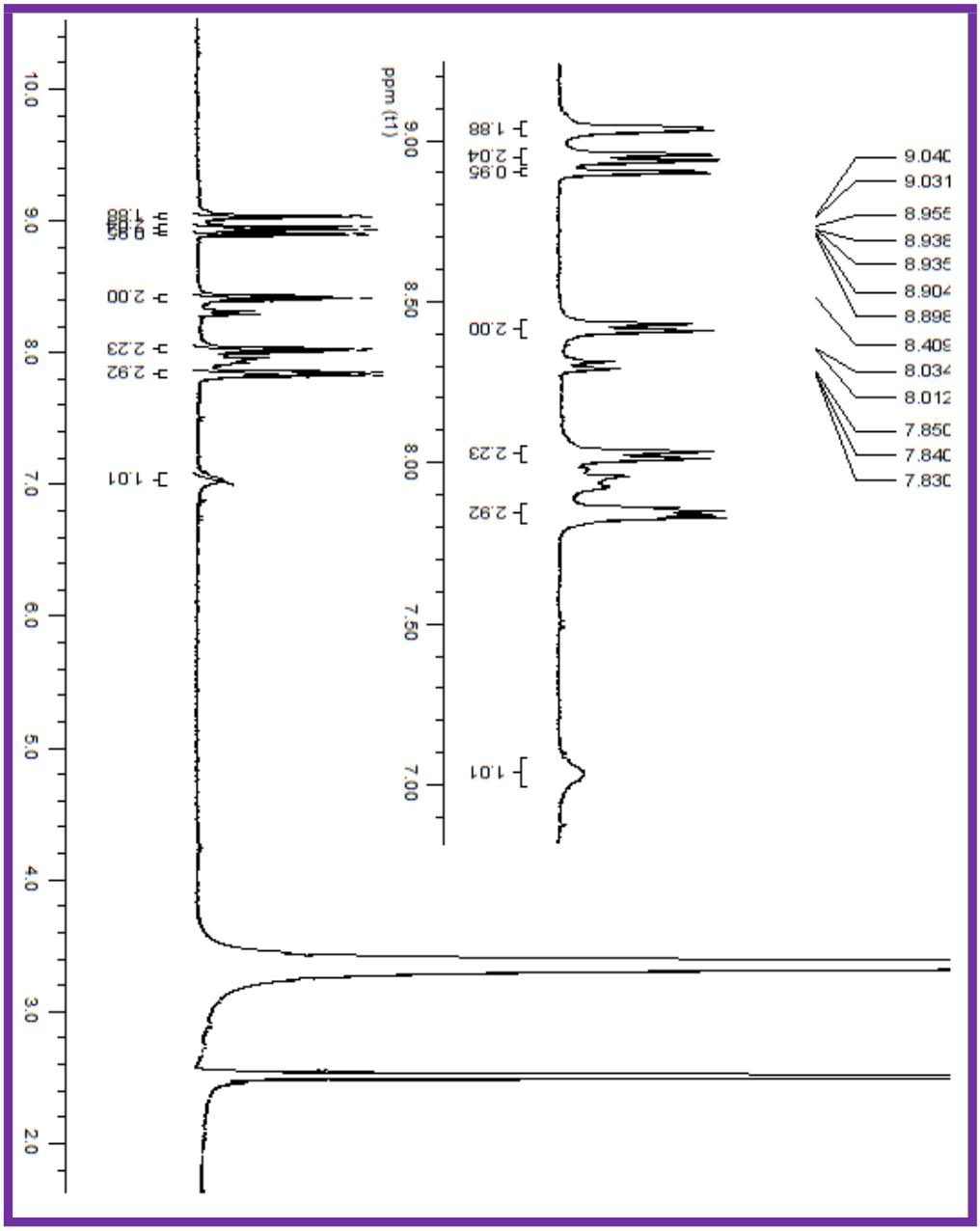



**Figure S4.** $^{1}$H NMR spectrum of **L**

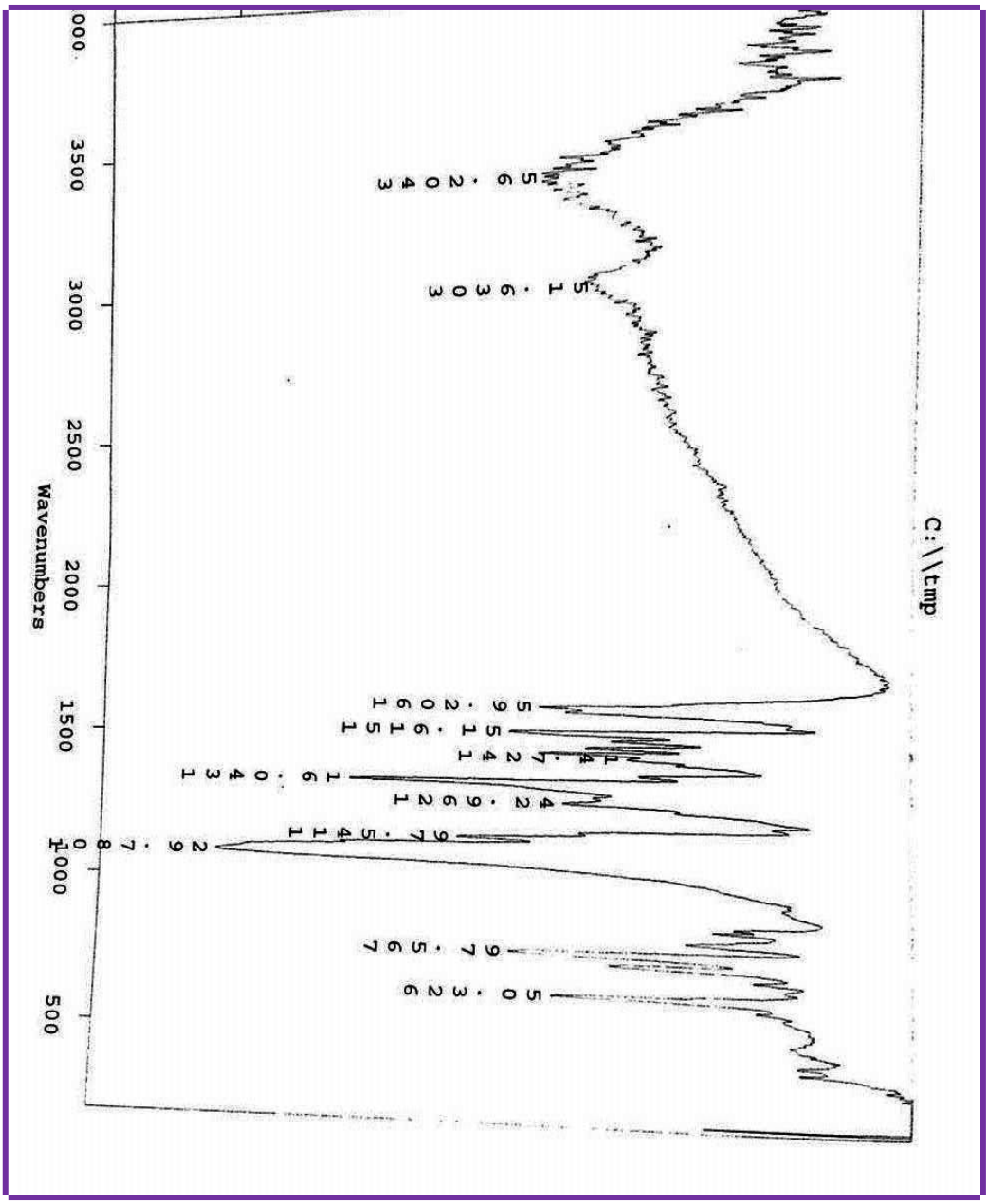



**Figure S5.** IR spectrum of **1**

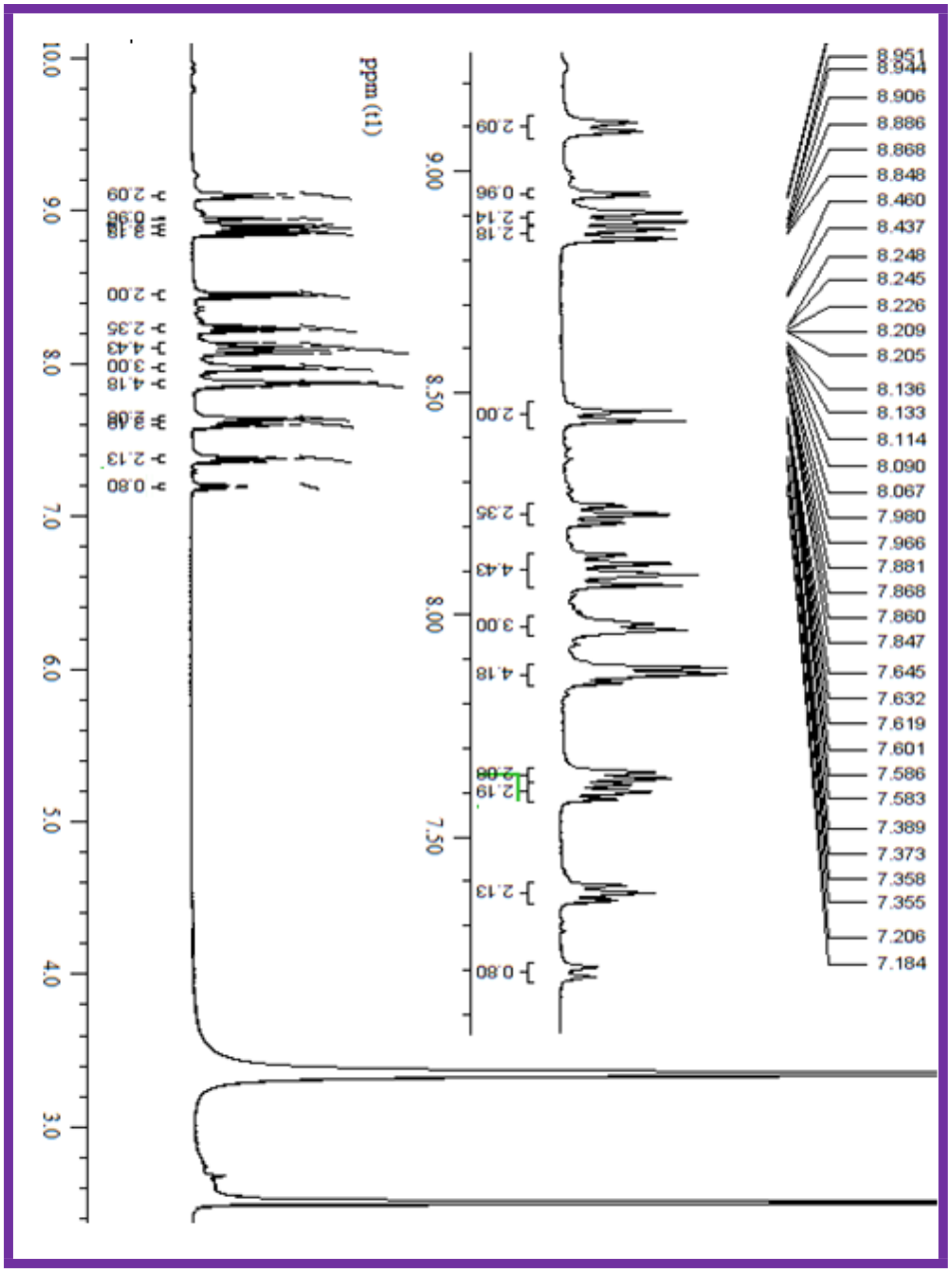



**Figure S6.** $^{1}$H NMR spectrum of **1**

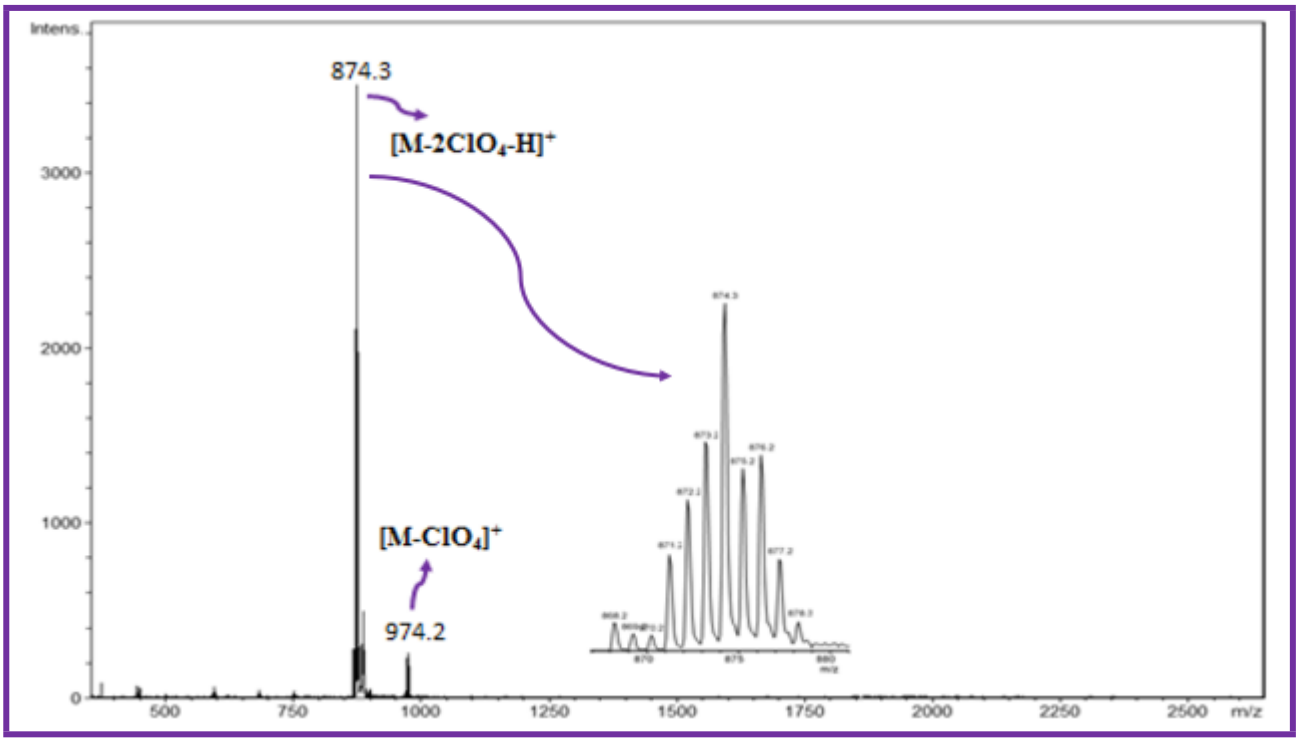



**Figure S7.** MALDI-TOF mass spectrum of **1**

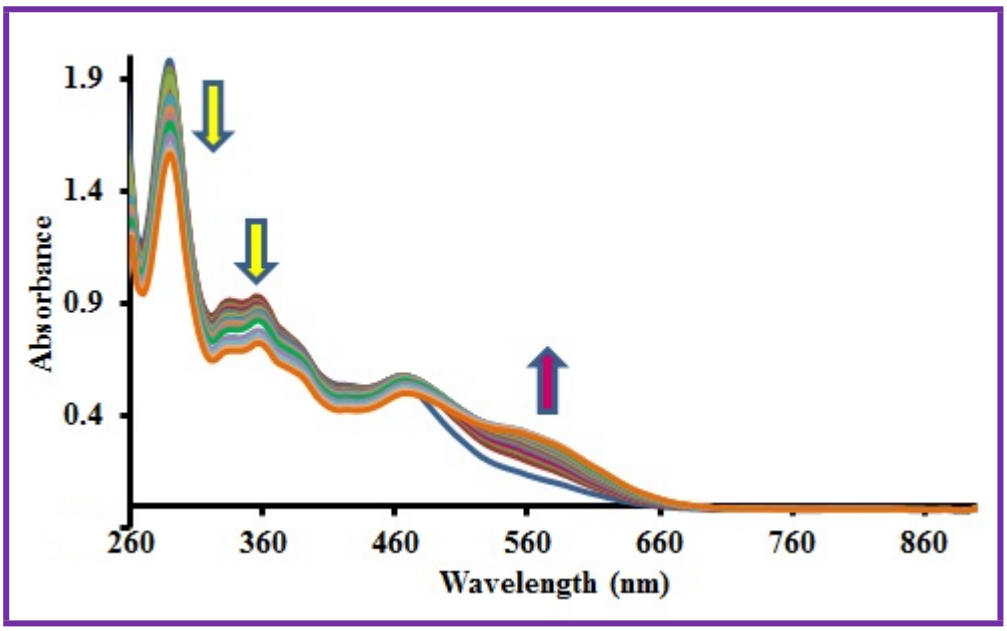



**Figure S8.** UV-Vis absorption spectra of sensor **1** ($2\times10^{-5}$ mol $L^{-1}$) in dry DMSO upon addition of $H_2PO_4$ (0-5 equiv.).

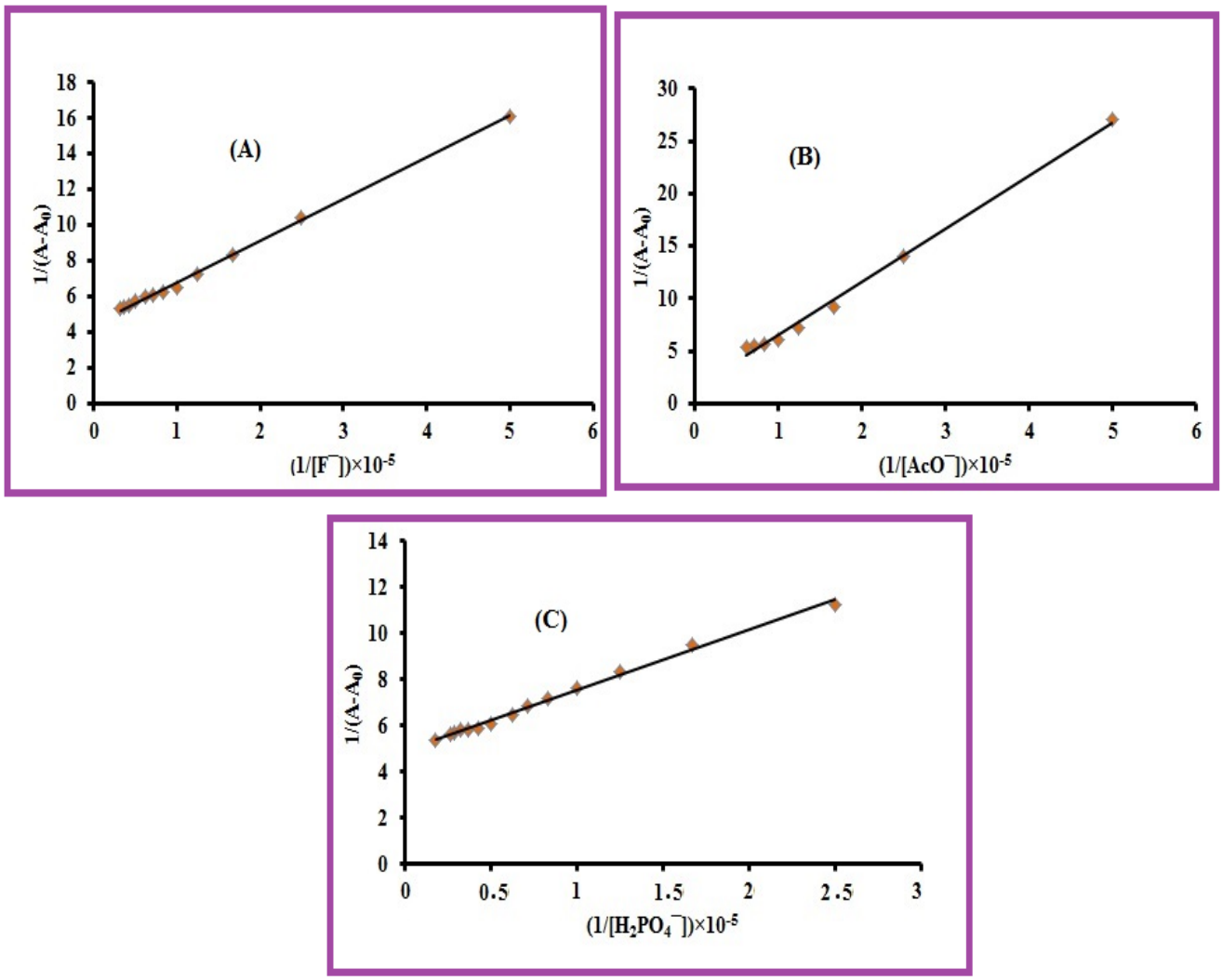



**Figure S9.** Benesi–Hildebrand plots of sensor **1** with (A) $F^-$, (B) $AcO^-$ and (C) $H_2PO_4^-$ anions associated with absorbance change at 560 nm in DMSO.

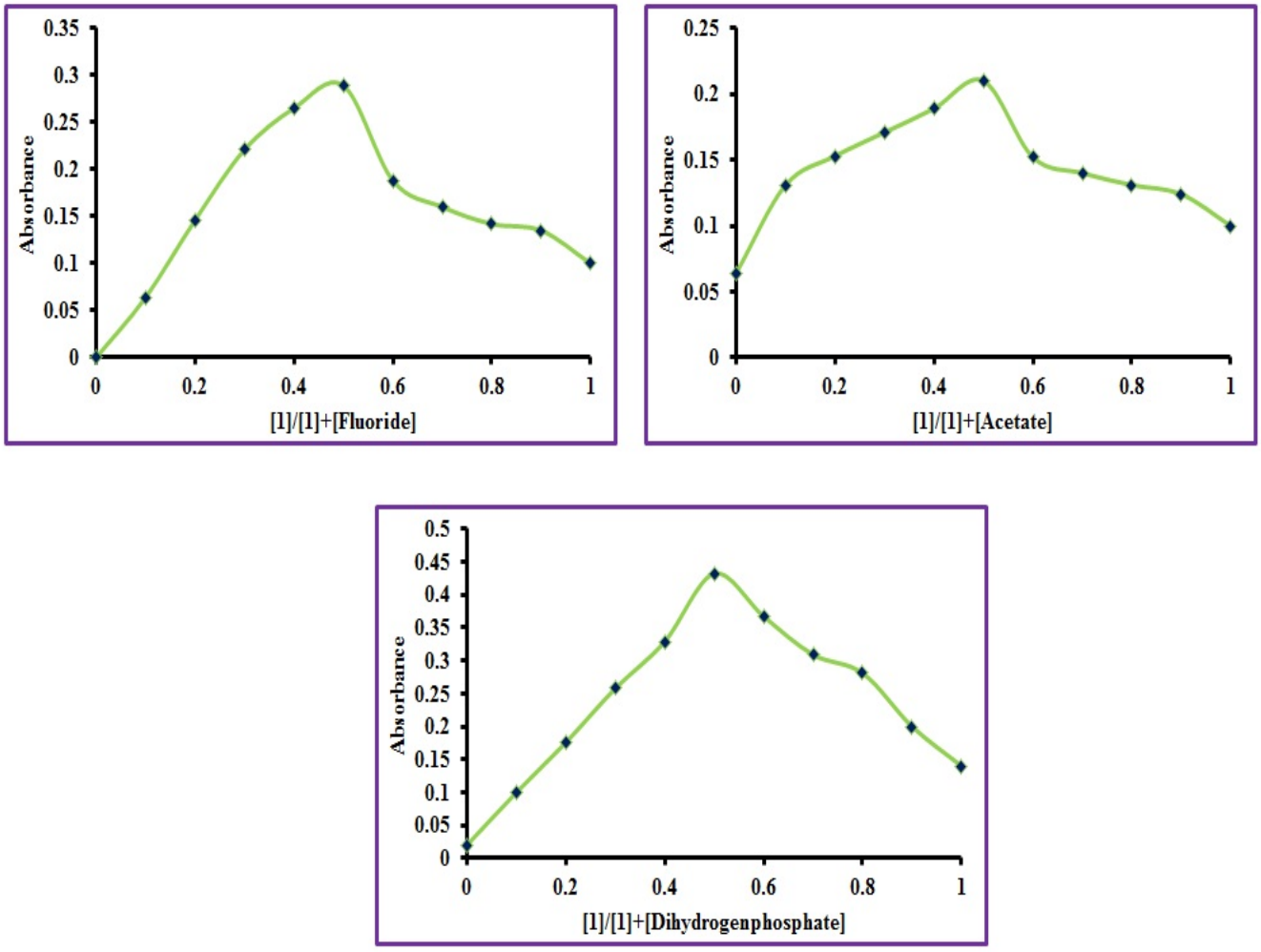



**Figure S10.** Job's plot for sensor **1** and anions with a total concentration of $2.0\times10^{-5}$ M in DMSO at 560 nm.

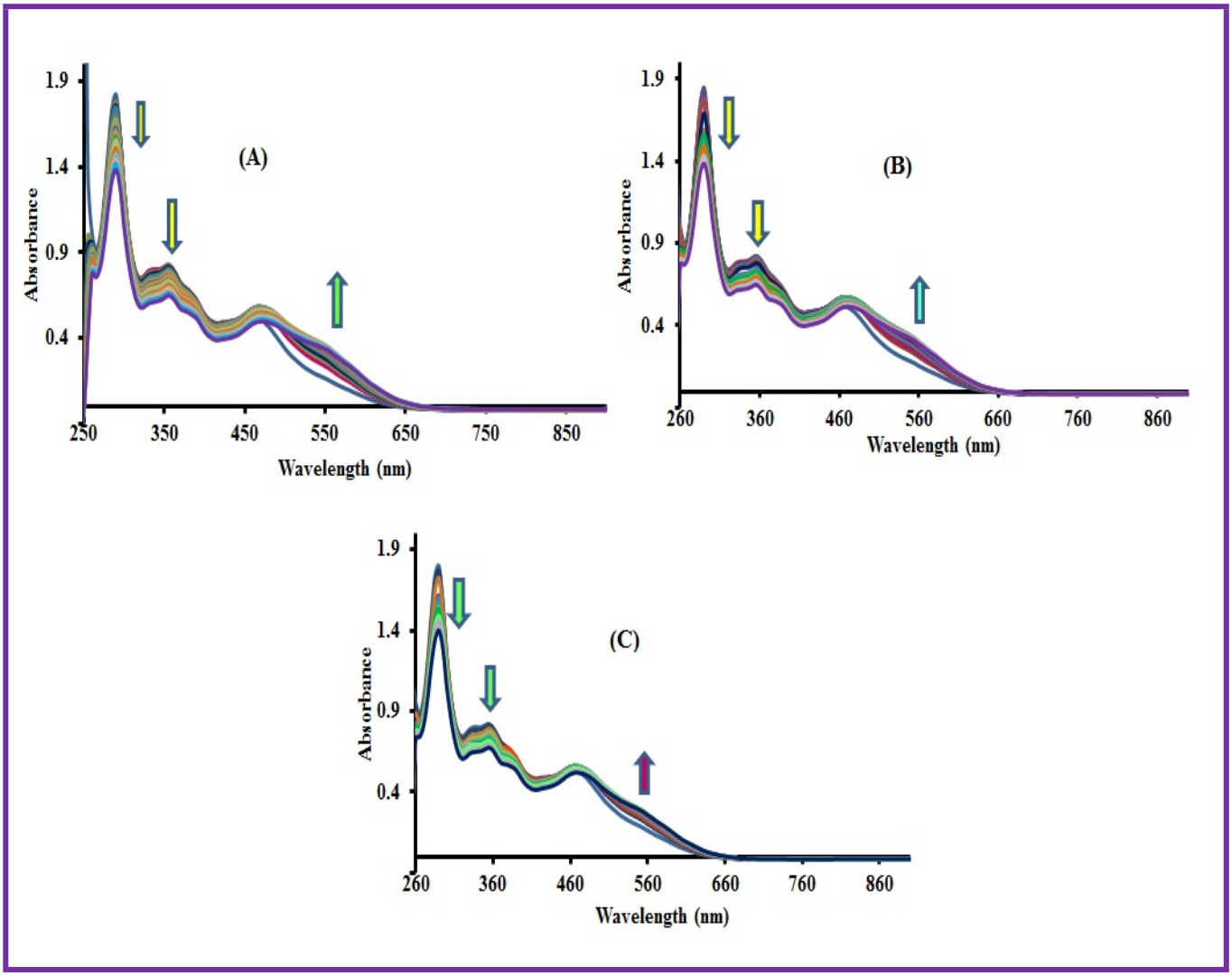



**Figure S11.** UV-Vis absorption spectra of sensor **1** ($2\times10^{-5}$ mol $L^{-1}$) in 9:1, DMSO-water upon addition of (A) TBAF, (B) TBAOAc and (C) $TBAH_2PO_4$ (0-5 equiv.).

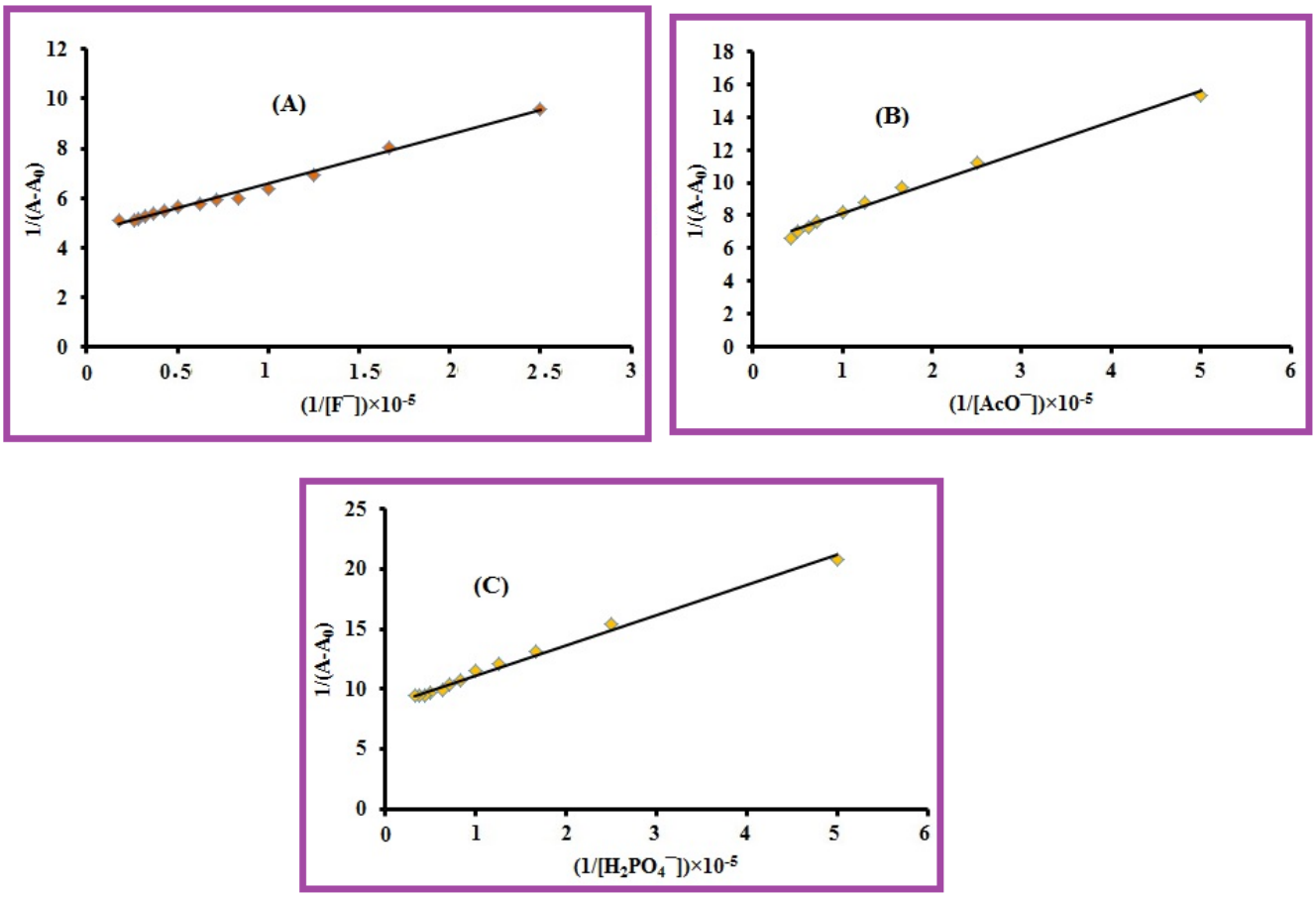
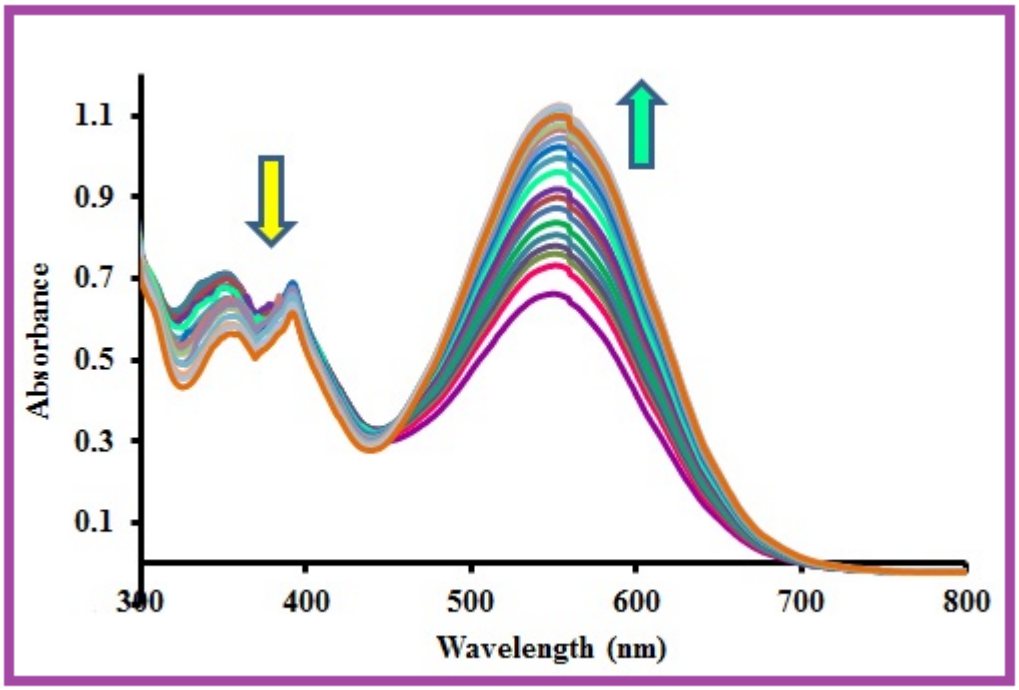
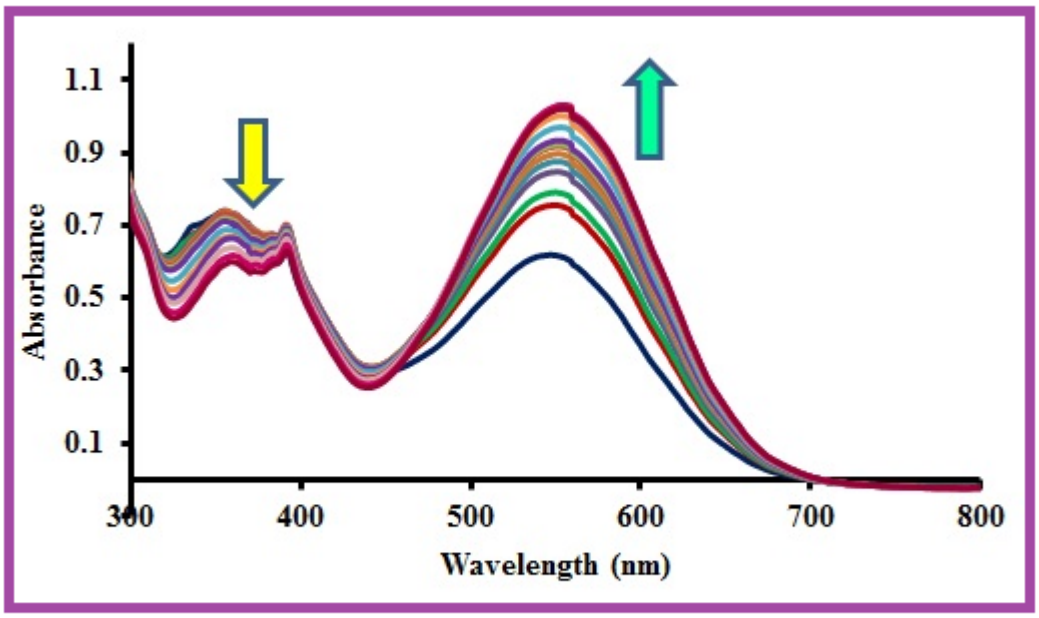



**Figure S12.** Benesi–Hildebrand plots of sensor **1** with (A) TBAF, (B) TBAOAc and (C) $TBAH_2PO_4$ associated with absorbance change at 560 nm in 9:1, DMSO-water.

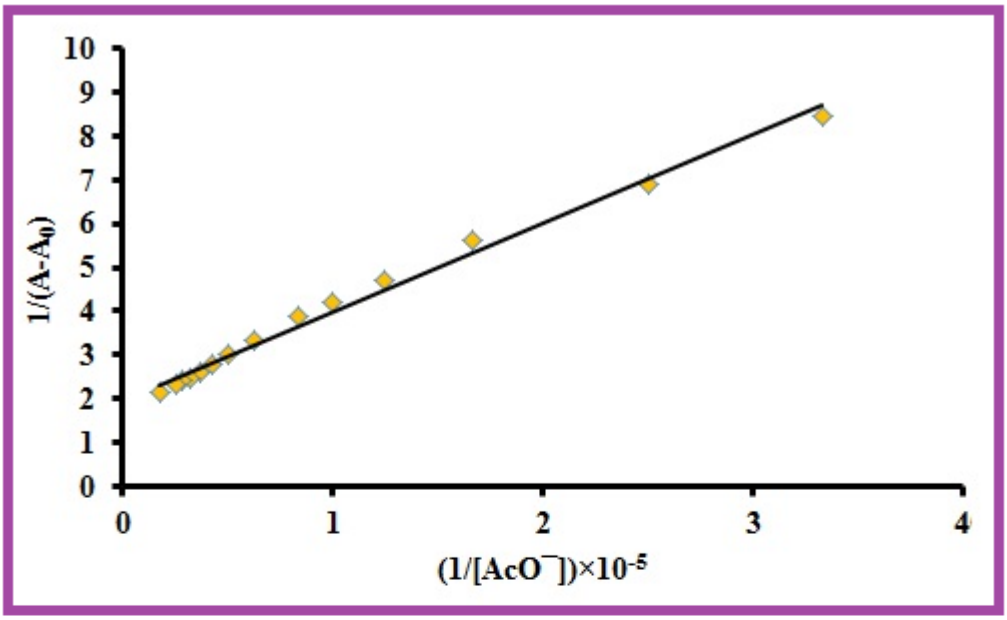



(A)

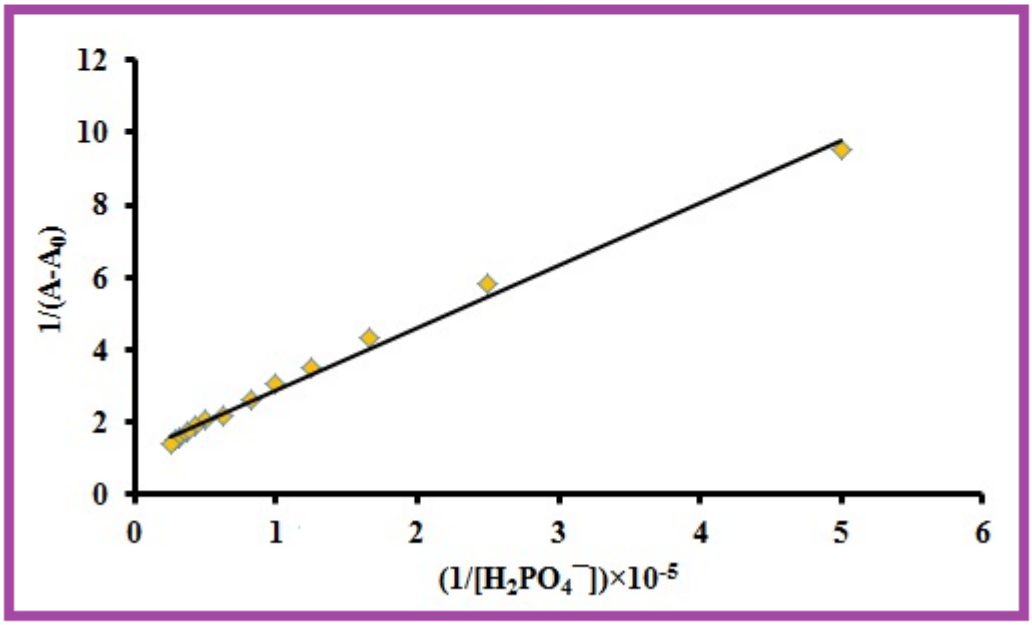



(B)

**Figure S13.** UV-Vis absorption spectra of sensor **L** ($2\times10^{-5}$ mol $L^{-1}$) in DMSO upon addition of (A) TBAOAc and (B) $TBAH_2PO_4$ (0-5 equiv.).




(A)




(B)

**Figure S14.** Benesi–Hildebrand plots of sensor **L** with (A) TBAOAc and (B) $TBAH_2PO_4$ anions associated with absorbance change at 552 nm in DMSO.

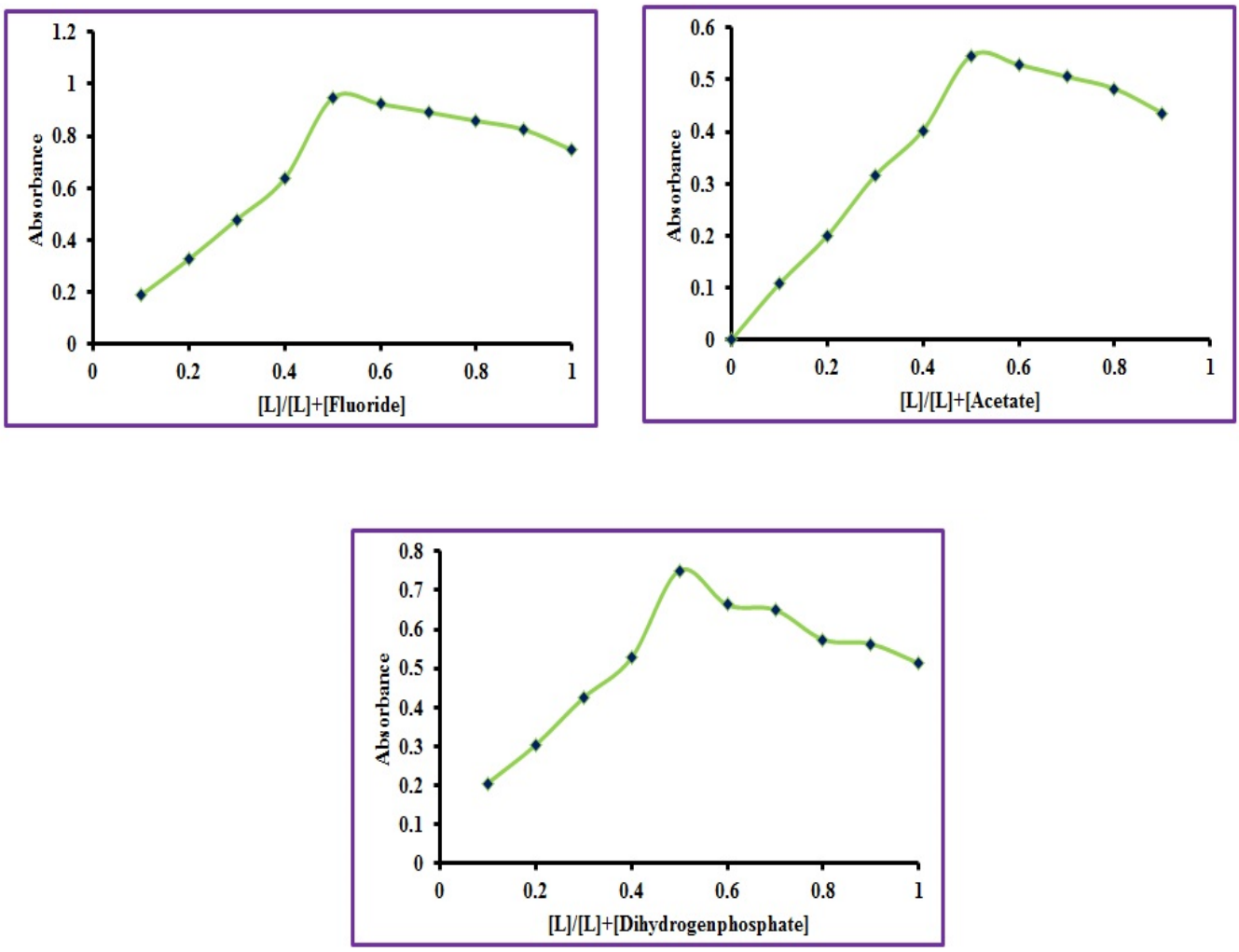



**Figure S15.** Job's plot for sensor **L** and anions with a total concentration of $2.0\times10^{-5}$ M in DMSO at 552 nm.

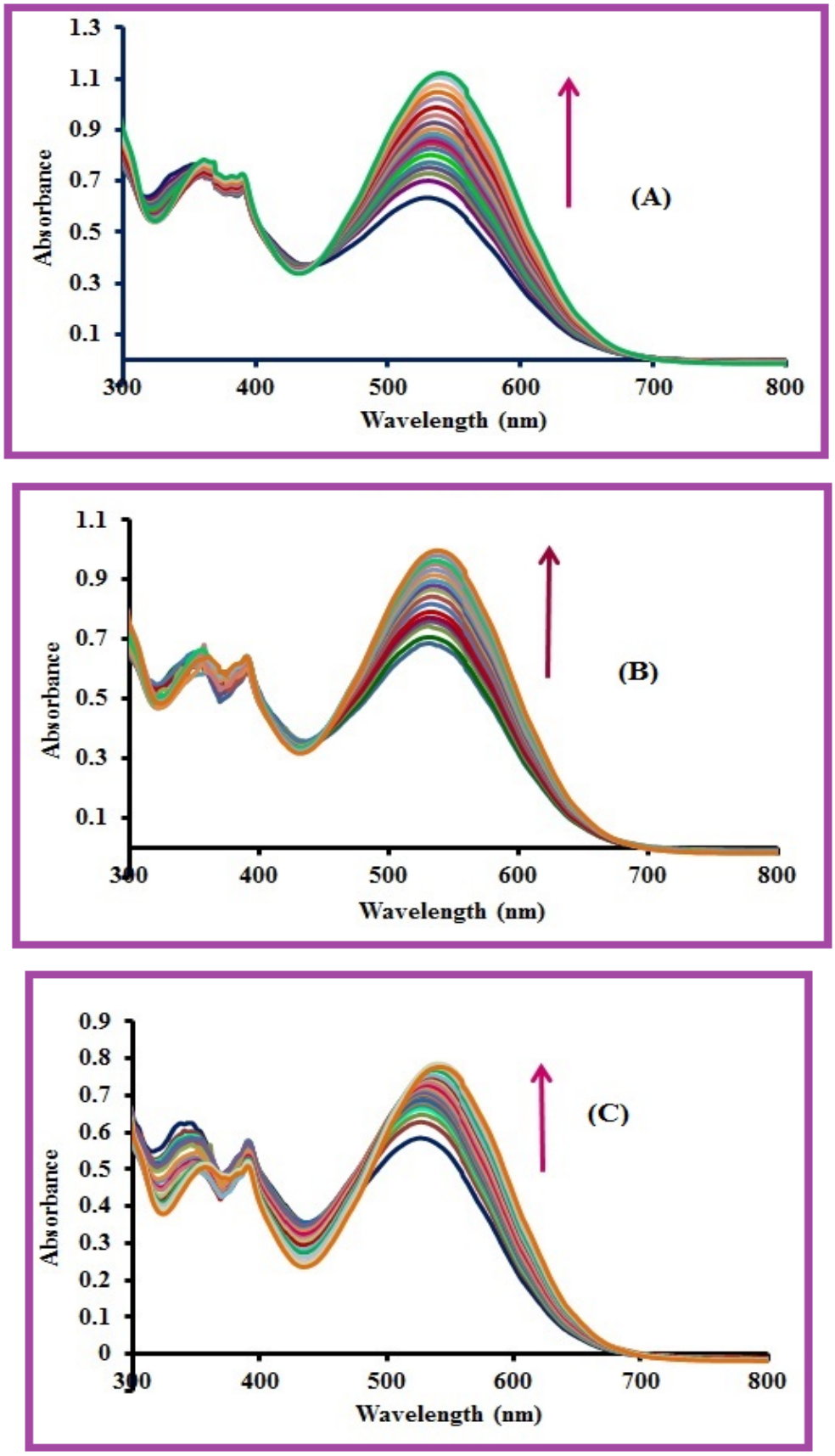



**Figure S16.** UV-Vis absorption spectra of sensor **L** ($2\times10^{-5}$ mol $L^{-1}$) in 9:1, DMSO-water upon addition of (A) TBAF, (B) TBAOAc and (C) $TBAH_2PO_4$ (0-5 equiv.).

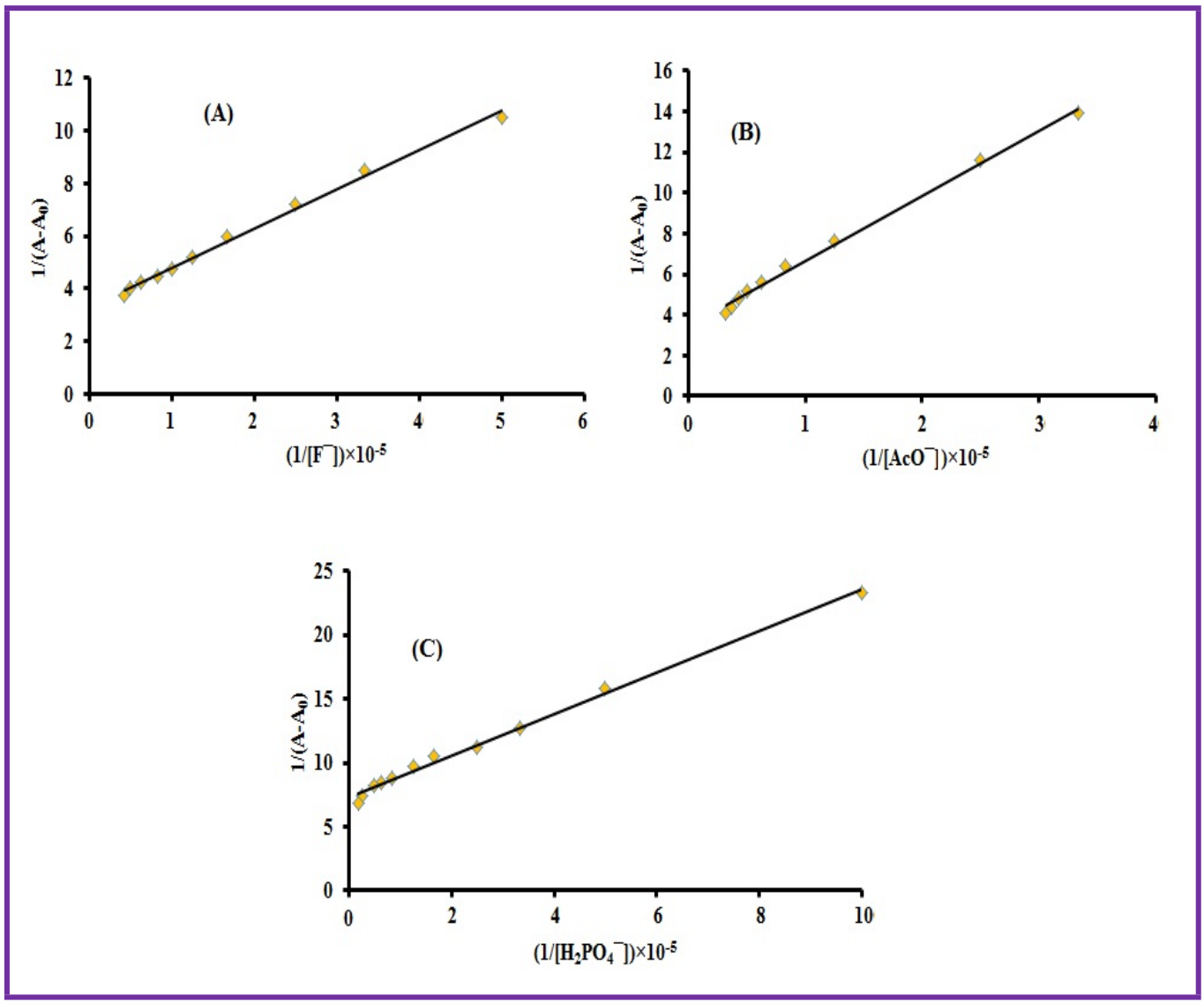



**Figure S17.** Benesi–Hildebrand plots of sensor **L** with (A) TBAF, (B) TBAOAc and (C) $TBAH_2PO_4$ associated with absorbance change at 529 nm in 9:1, DMSO-water.

**Determination of the p$K_a$ value:**

To determine the p$K_a$ values of **L** and **1**, the spectrophotometric pH titrations were carried out in 9:1 DMSO-Water. The values were assigned as the maxima of the first derivative of the data shown in **Figure S18** (The inset shows the plot of the derivatives of the titrations).

(*J. Am. Chem. Soc.* ***2000****, 122, 6769-6770*)

The p*K*a values were determined to be ~ 10.25 for **L** and 8.33 for **1** (on the basis of new band formed at 552 and 560 nm for **L** and **1**, respectively) indicating that **L** and **1** likely are deprotonated with relatively basic anions.

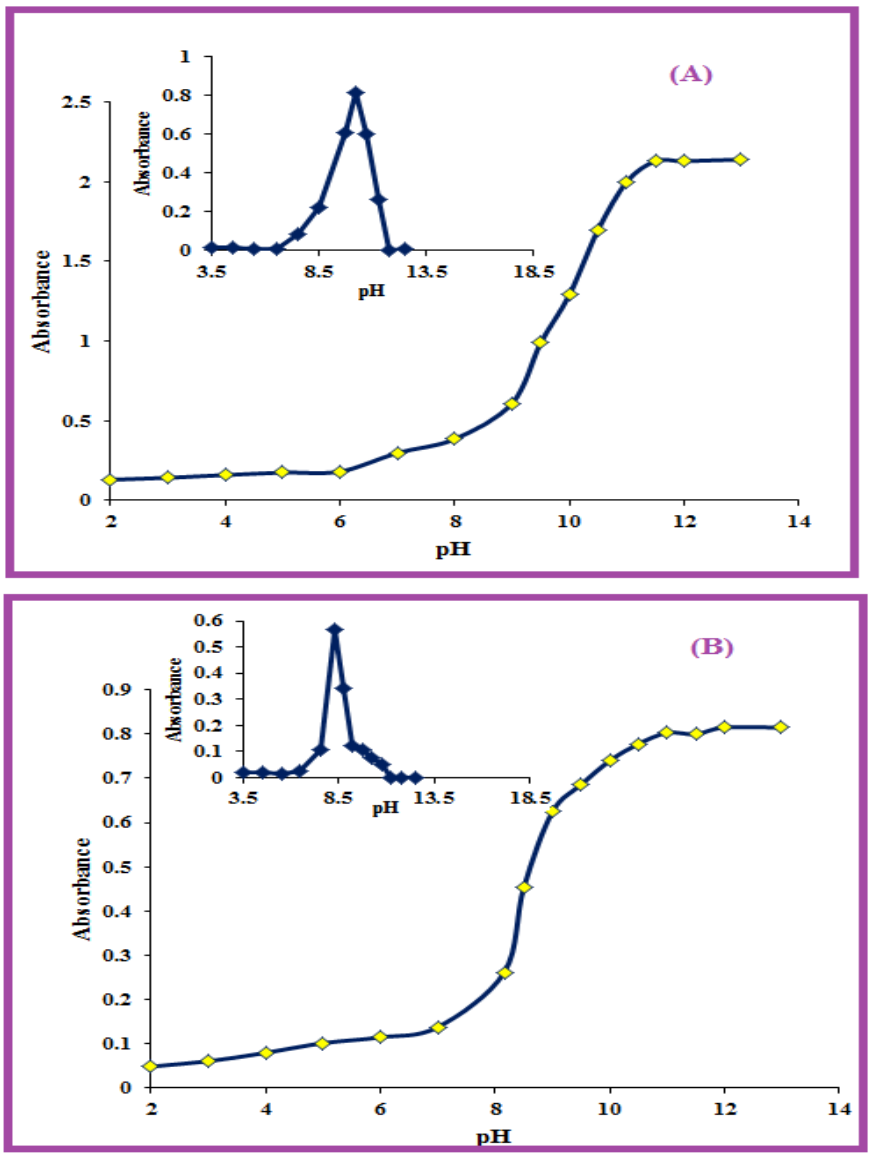



**Figure S18. (A) L and (B) 1**

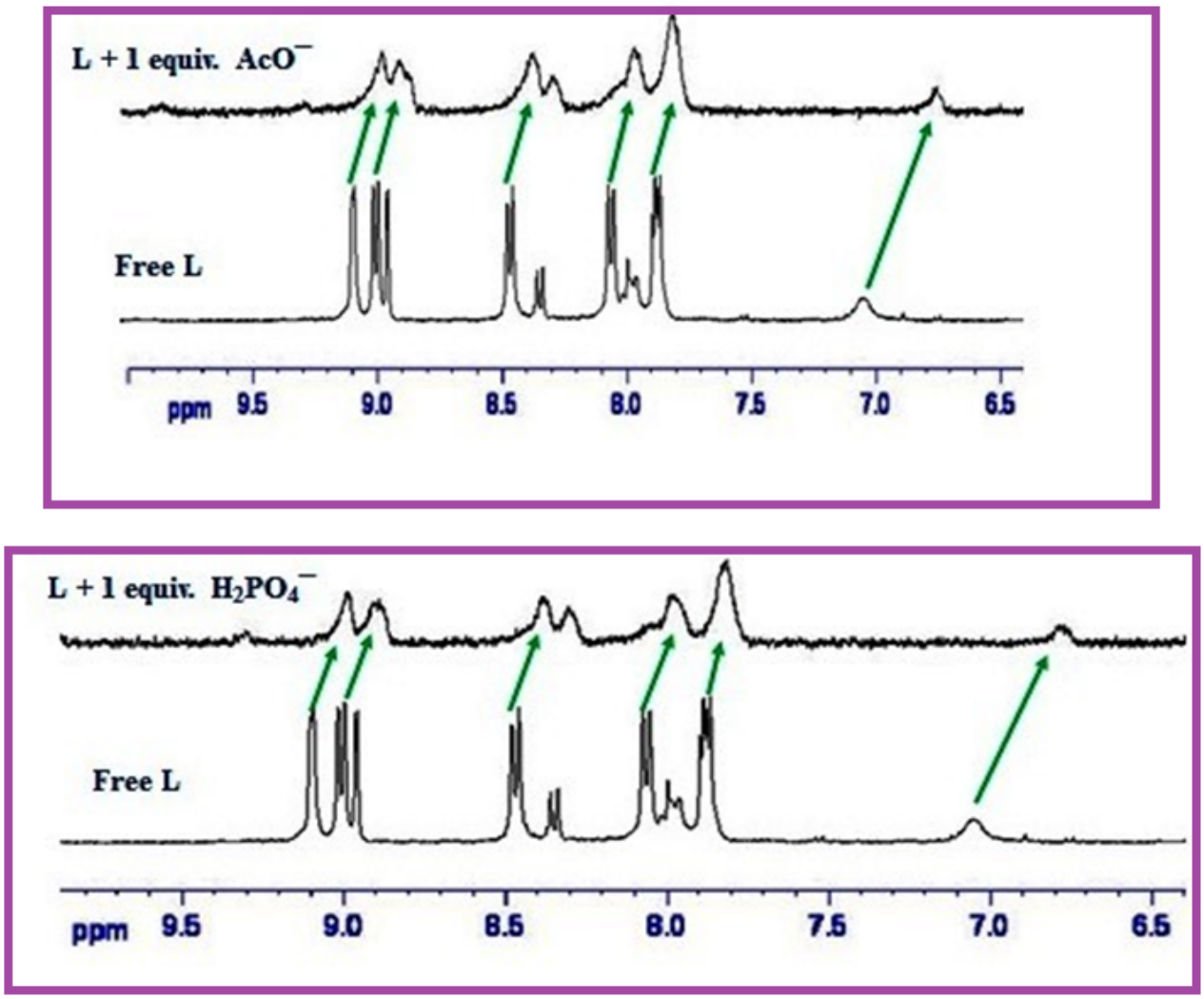



**Figure S19.** $^{1}$H NMR spectra of **L** in DMSO-$d_6$ ($2\times10^{-2}$ mol $L^{-1}$) in the absence and presence of TBAOAc and $TBAH_2PO_4$

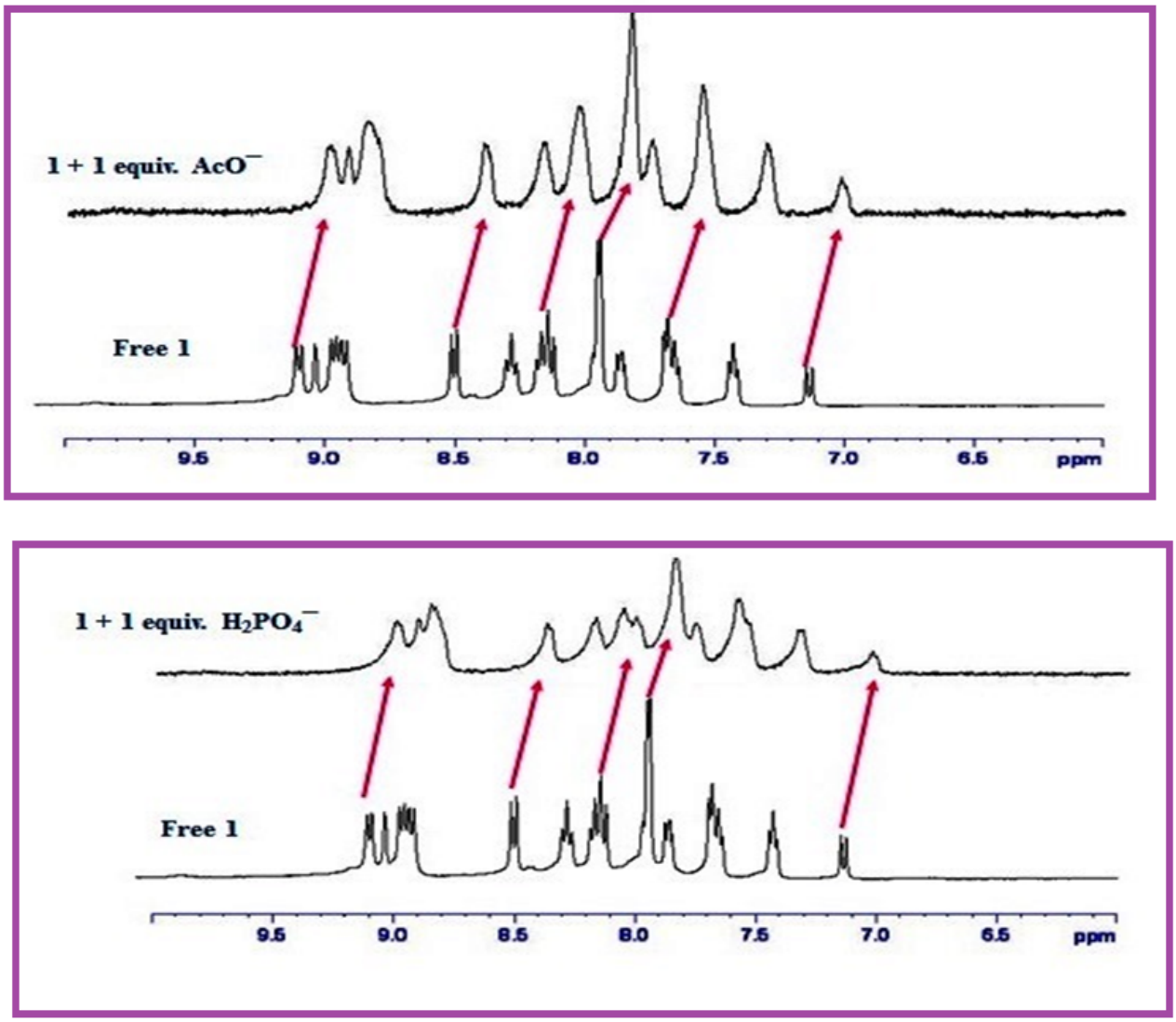



**Figure S20.** $^{1}$H NMR spectra of **1** in DMSO-$d_6$ ($2\times10^{-2}$ mol $L^{-1}$) in the absence and presence of TBAOAc and $TBAH_2PO_4$

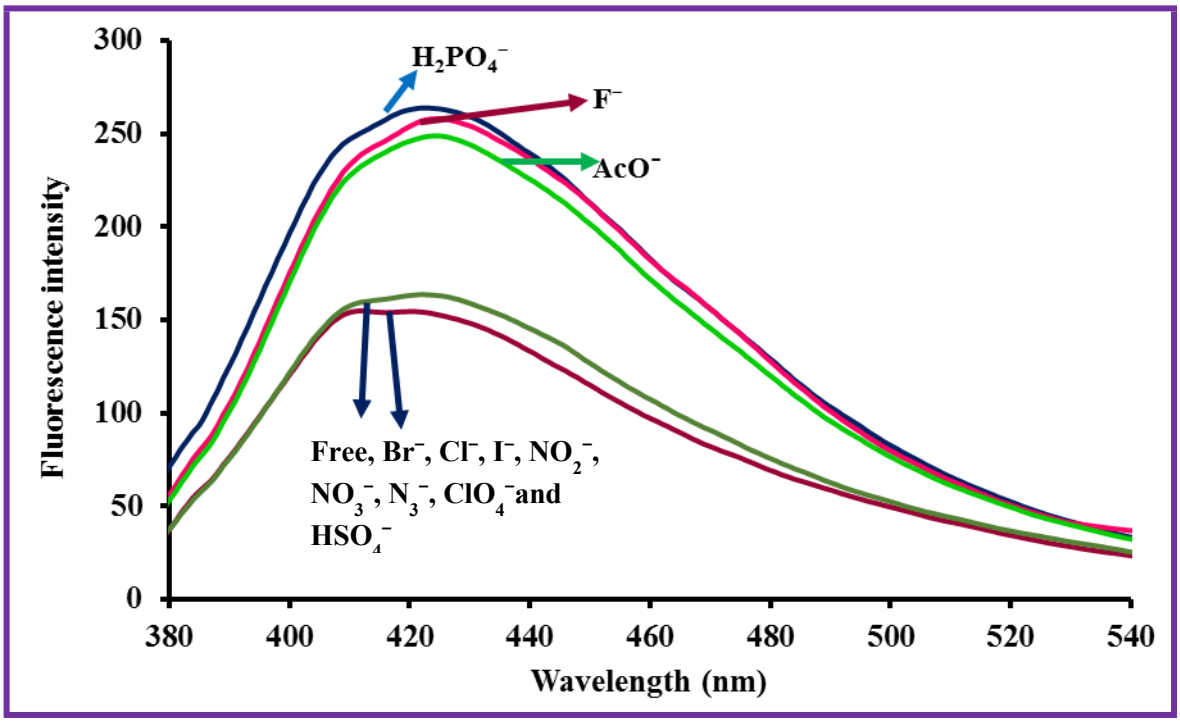



**Figure S21.** Fluorescence spectra of **L** ($2\times10^{-5}$ mol $L^{-1}$) in the presence of the different anions