

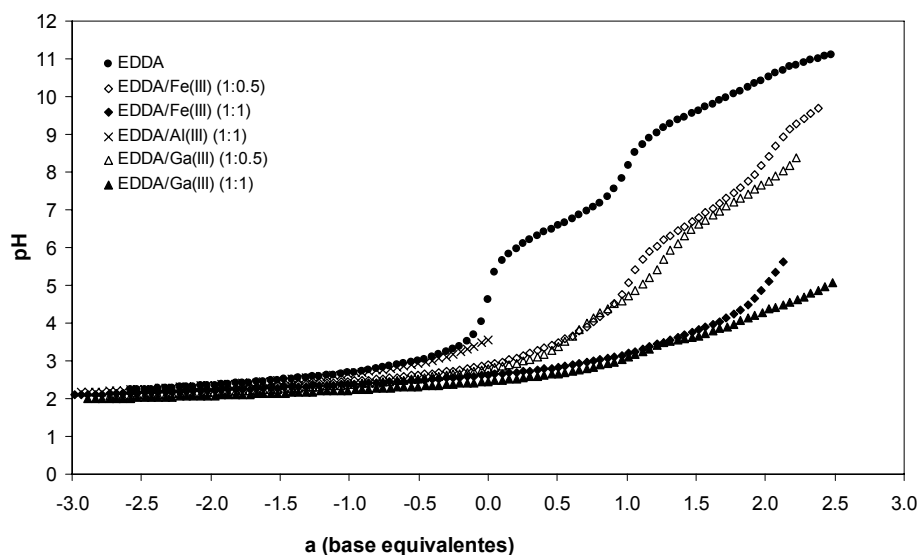


Fig. S1 – Potentiometric titration curves of aqueous solutions containing EDDA, alone (●) with $C_L = 3.91 \times 10^{-3}$ M, and in presence of the three-charged metal ions (M^{3+}), at conditions of: ca. 1:1 ligand-to-metal molar ratio and $C_{Fe} = 3.91 \times 10^{-3}$ M (◆), $C_{Ga} = 3.91 \times 10^{-3}$ M (▲) and $C_{Al} = 3.84 \times 10^{-3}$ M (×); ca. 1:0.5 ligand-to-metal molar ratio and $C_{Fe} = 1.96 \times 10^{-3}$ M (◇) and $C_{Ga} = 1.92 \times 10^{-3}$ M (△). $I = 0.2$ M KCl, $T = 25.0$ °C.

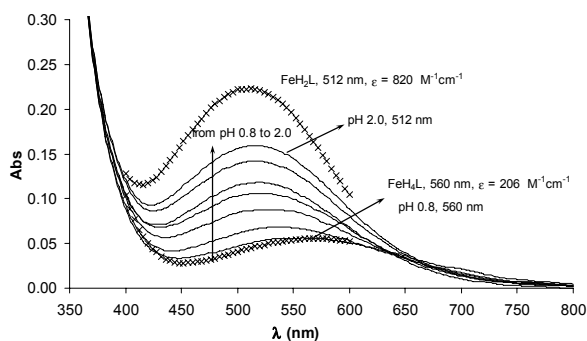


Fig. S2 – Absorption spectra registered at different pH values and 1:1 ligand-to-metal molar ratio for the EDTAPr(3,4-HP)₂/Fe(III) system with experimental (–) and calculated (×) absorption spectra for the EDTAPr(3,4-HP)₂/Fe(III) system, for pH from 0.8 and 2, with $C_L = 2.75 \times 10^{-4}$ M, $C_{Fe^{3+}} = 2.71 \times 10^{-4}$ M. $I = 0.2$ M (KCl, HCl), $T = 25.0$ °C.

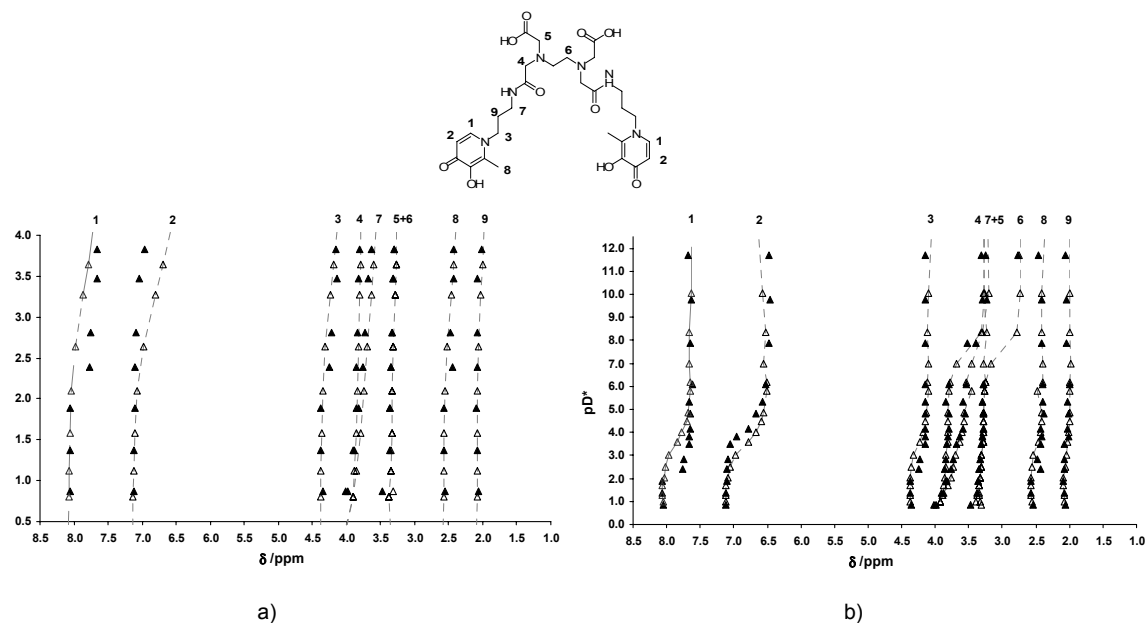


Fig. S3 – Graphical representation of the chemical shifts as a function of pD of the spectra obtained for the ligand EDTAPr(3,4-HP)₂ alone (▲) and for the EDTAPr(3,4-HP)₂/Al(III) system (△) at a) 1:1 and b) 3:1 ligand-to-metal molar ratio.

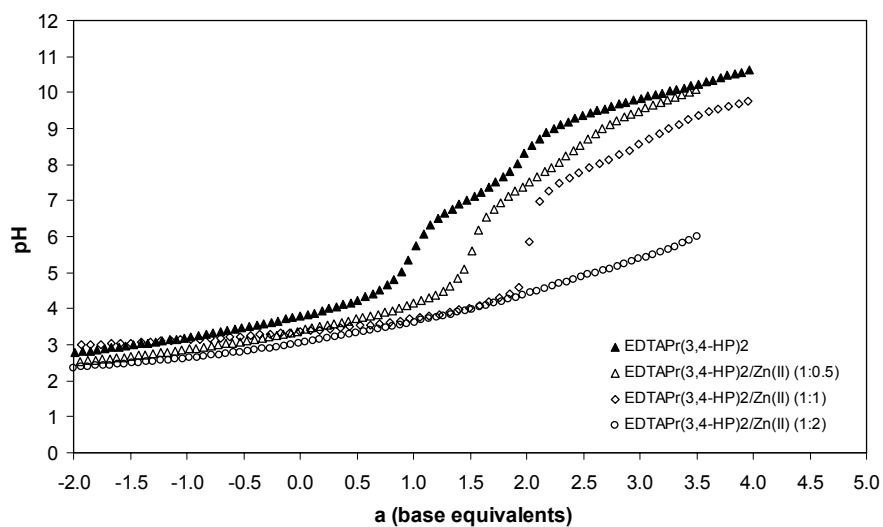


Fig. S4 – Potentiometric titration curves of aqueous solutions containing EDTAPr(3,4-HP)₂, alone (▲), and in presence of the Zn²⁺ metal ion, at: 1:0.5 (△), 1:1 (◇) and 1:2 (○) ligand-to-metal molar ratio, $C_L = 3.09 \times 10^{-3}$ M, $I = 0.2$ M KCl, $T = 25.0$ °C.

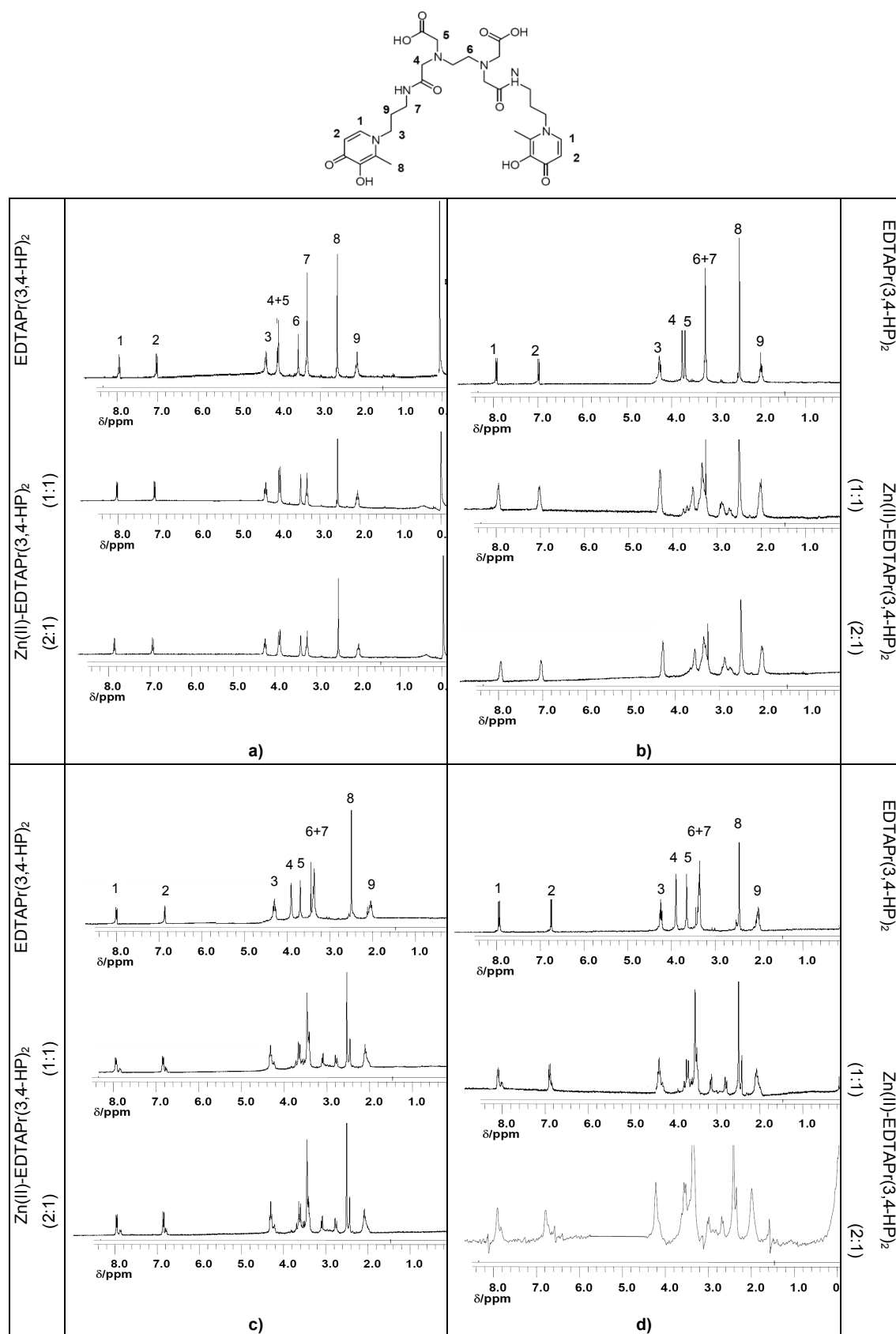


Fig. S5 – Detailed and comparative representation of the ¹H NMR spectra of the ligand EDTAPr(3,4-HP)₂ free and in the presence of Zn(II), at 1:1 and 1:2 ligand-to-metal, and at the indicated pH.