

Supplementary Materials

Sensing Zn²⁺ in aqueous solution with a fluorescent scorpian macrocyclic ligand decorated with an anthracene bearing tail.

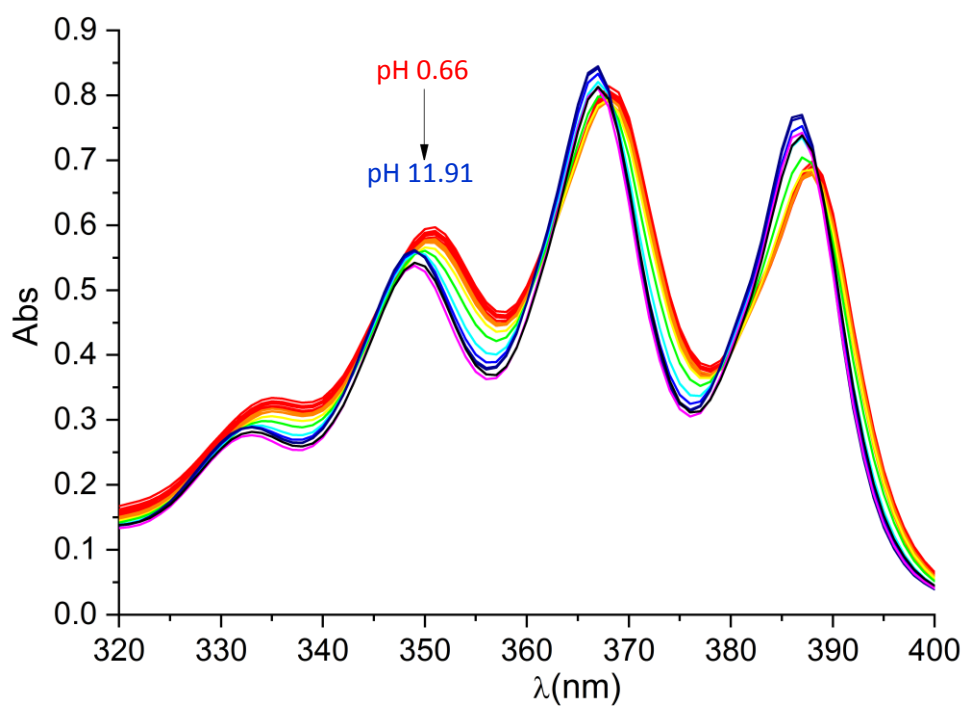
Matteo Savastano¹, Matteo Fiaschi¹, Giovanni Ferraro,¹ Paola Gratteri², Palma Mariani¹, Antonio Bianchi^{1,*}, Carla Bazzicalupi¹

¹ Department of Chemistry “Ugo Schiff”, University of Florence, Via della Lastruccia, 3-13, 50019 Sesto Fiorentino (Italy).

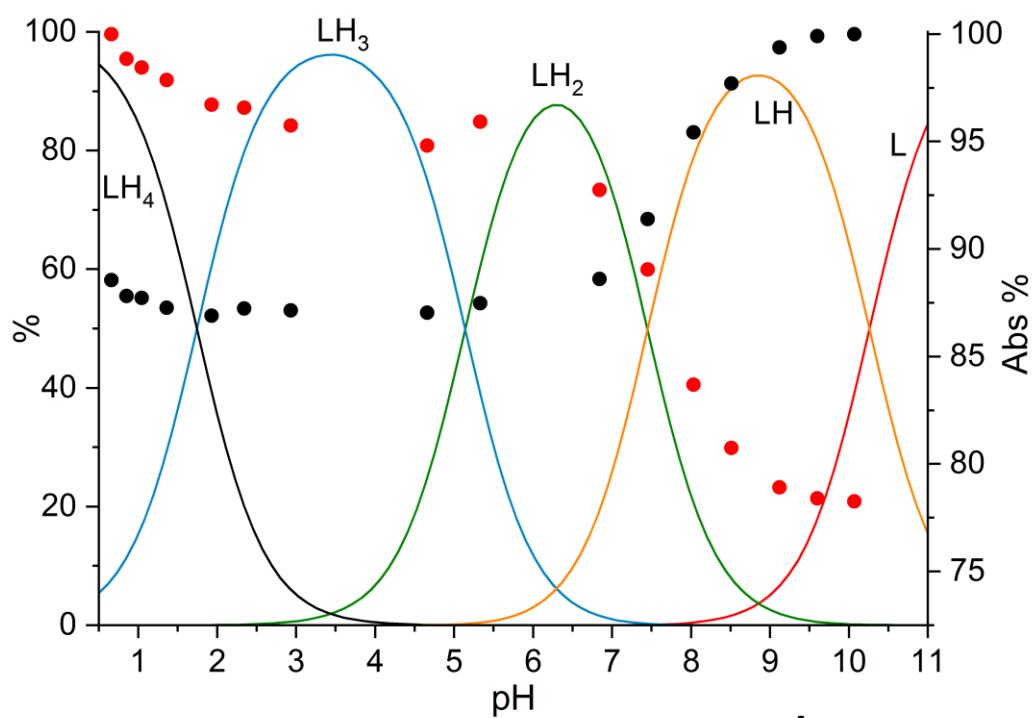
² Department of NEUROFARBA- Pharmaceutical and Nutraceutical section, and Laboratory of Molecular Modeling Cheminformatics & QSAR, University of Florence, Via Ugo Schiff 6, 50019 Sesto Fiorentino (Italy).

Content

Figure S1. Absorption spectra of L at different pH values.	S3
Figure S2. Plot of the fluorescence intensity at 413 nm versus the concentration of Zn^{2+} and data fitting for the determination of the limit of detection (LOD).	S4
Figure S3. Absorption spectra of the Zn^{2+} /L system at different pH values.	S5
Figure S4. Emission spectra of the system L/phosphate at different pH values.	S6
Figure S5. Emission spectra of the system L/benzoate at different pH values.	S7
Figure S6. Emission spectra of the system L/ Zn^{2+} /phosphate at different pH values.	S8
Figure S7. Emission spectra of the system L/ Zn^{2+} /benzoate at different pH values.	S9
Figure S8. Distribution diagram of the species formed by L as a function of pH.	S10
Figure S9. Distribution diagram of the species formed by L with Zn^{2+} as a function of pH. ..	S11
Figure S10. Distribution diagram of the species formed by L with phosphate as a function of pH.	S12
Figure S11. Distribution diagram of the species formed by L with benzoate as a function of pH.	S13
Figure S12. Distribution diagram of the species formed by L with Zn^{2+} and phosphate as a function of pH.	S14
Figure S13. Distribution diagram of the species formed by L with Zn^{2+} and benzoate as a function of pH.	S15



a



b

Figure S1. a) Absorption spectra of L at different pH values. $[L] = 1 \times 10^{-4}$ M. b) Absorbances at 387 nm (black dots) and 356 nm (red dots) superimposed to the distribution diagram of the species formed by L as a function of pH. $[L] = 1 \times 10^{-4}$ M).

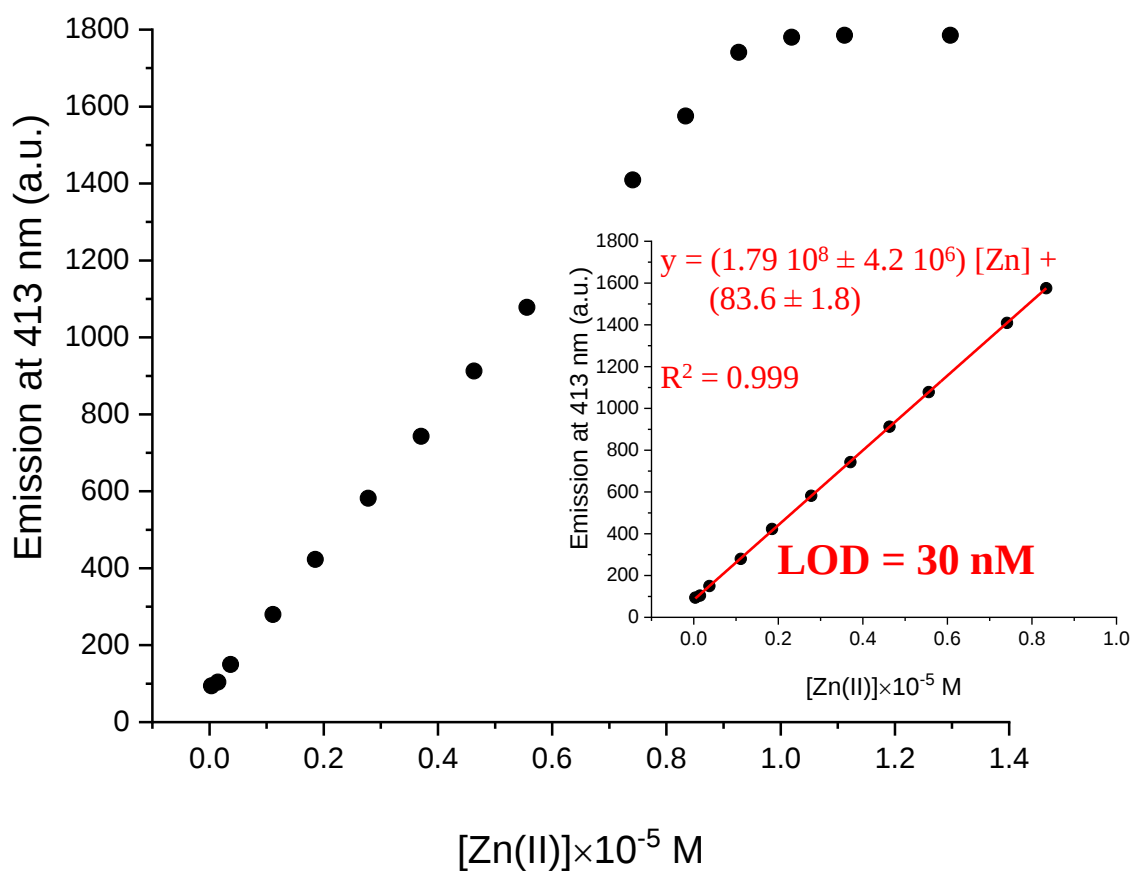


Figure S2. Plot of the fluorescence intensity at 413 nm (λ_{exc} 362 nm) of L (1×10^{-5} M, pH 9) versus the concentration of Zn^{2+} . Inset: data fitting for the determination of the limit of detection (LOD) based on the $3\sigma/\text{slope}$.

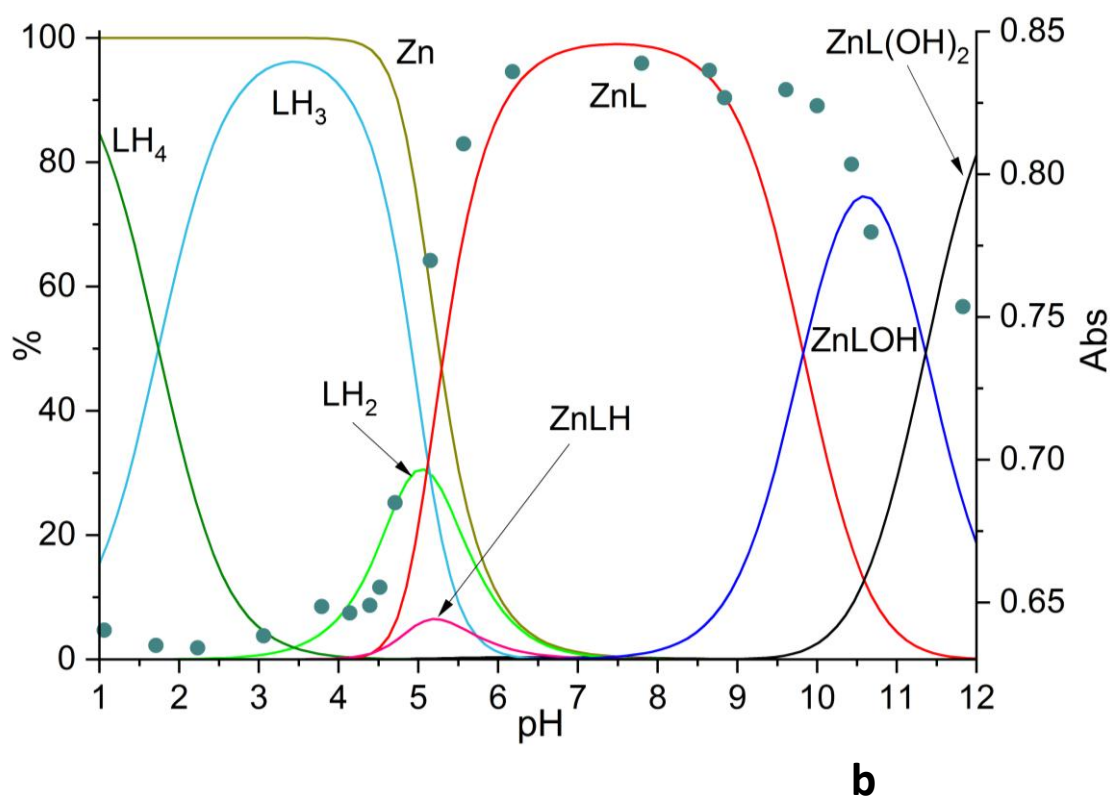
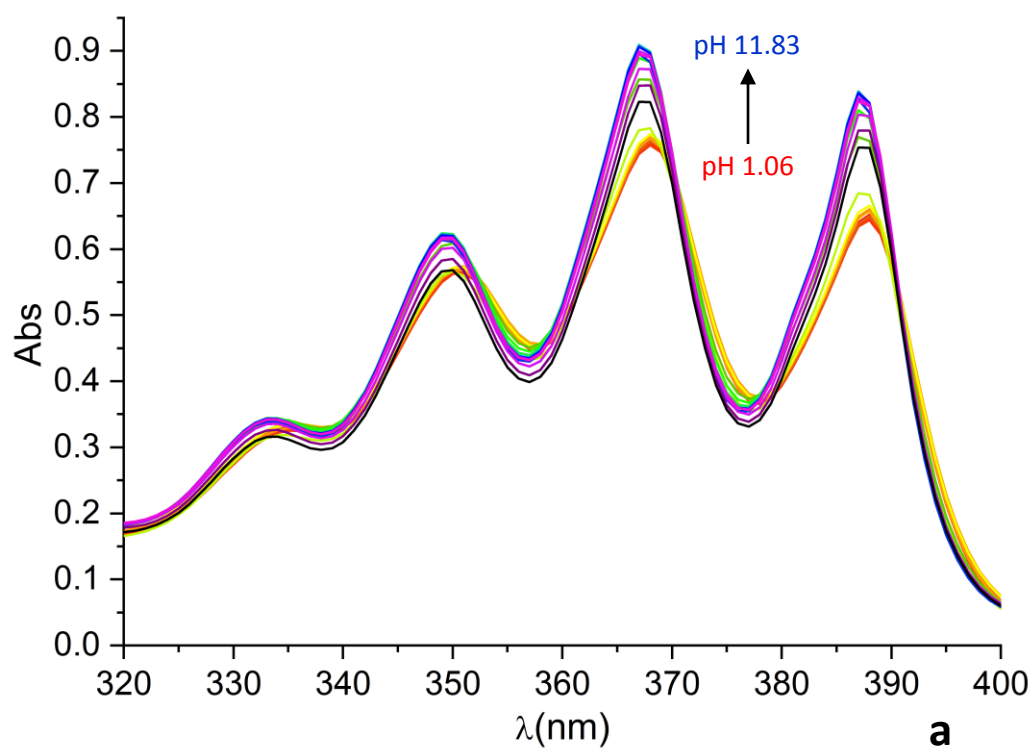


Figure S3. a) Absorption spectra of the Zn^{2+}/L system at different pH values. $[\text{L}] = [\text{Zn}^{2+}] = 1 \times 10^{-4} \text{ M}$. b) Absorbance at 367 nm (green dots) superimposed to the distribution diagram of the species formed in the Zn^{2+}/L system ($[\text{L}] = [\text{Zn}^{2+}] = 1 \times 10^{-4} \text{ M}$).

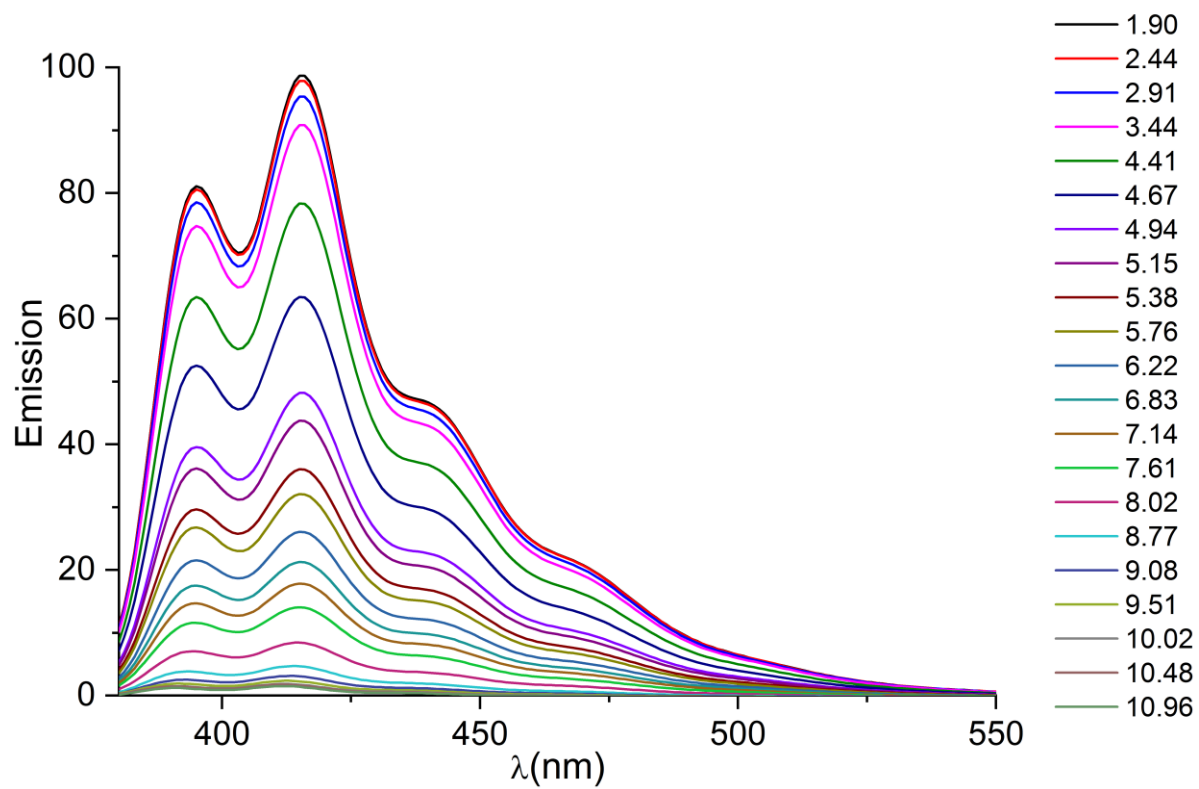


Figure S4. Emission spectra of the system L/phosphate at different pH values. $[L] = [\text{phosphate}] = 1 \times 10^{-5} \text{ M}$. λ_{exc} 362 nm.

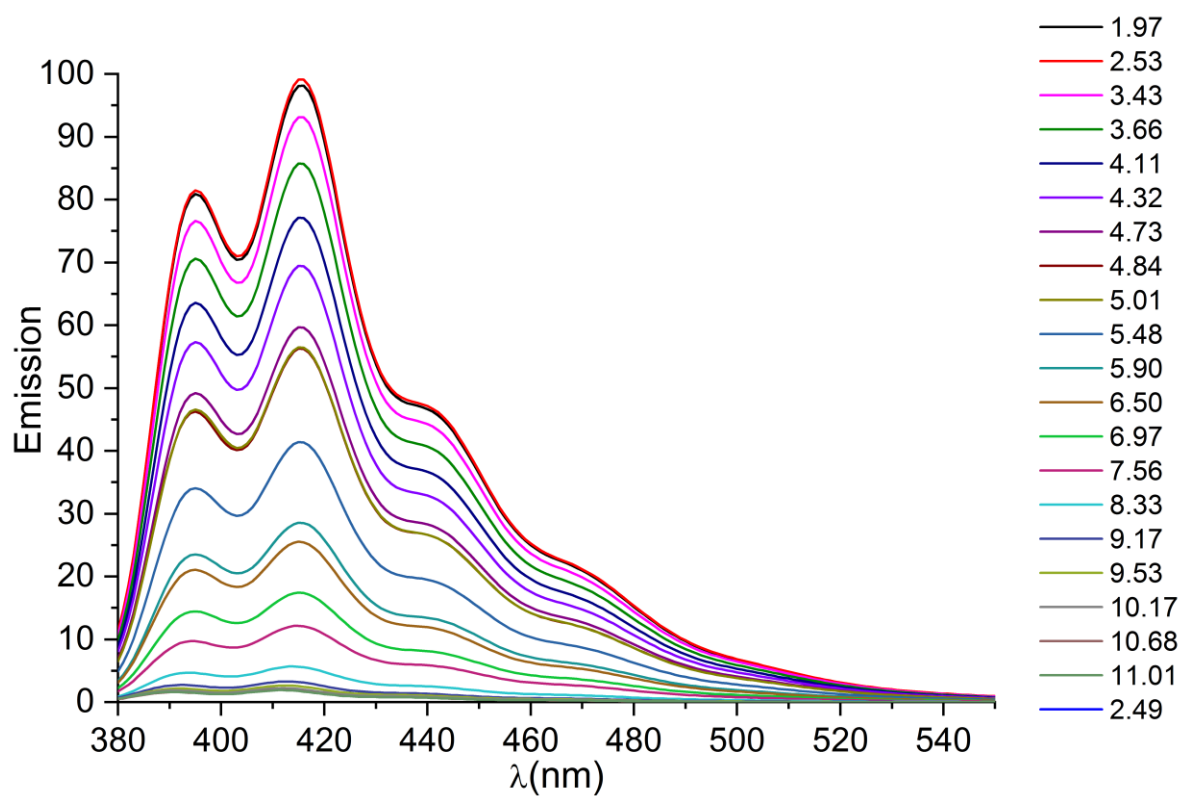


Figure S5. Emission spectra of the system L/benzoate at different pH values. $[L] = [\text{benzoate}] = 1 \times 10^{-5} \text{ M}$. λ_{exc} 362 nm.

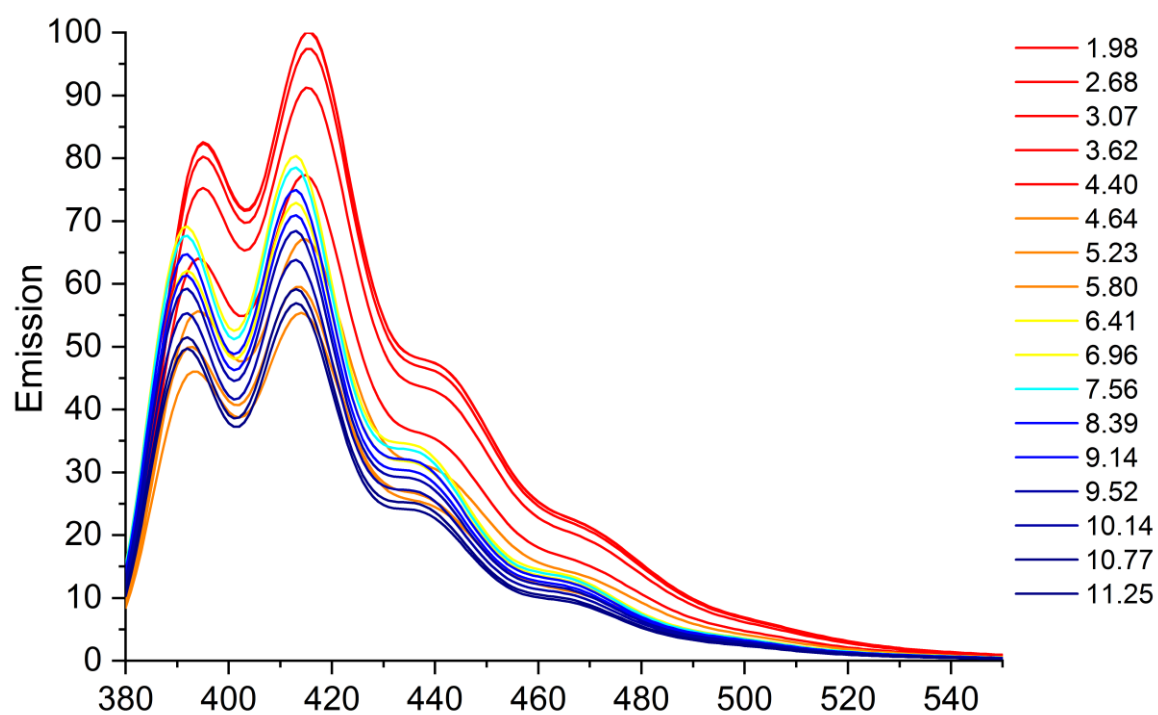


Figure S6. Emission spectra of the system L/Zn²⁺/phosphate at different pH values. [L] = [Zn²⁺] = [phosphate] = 1×10⁻⁵ M. λ_{exc} 362 nm.

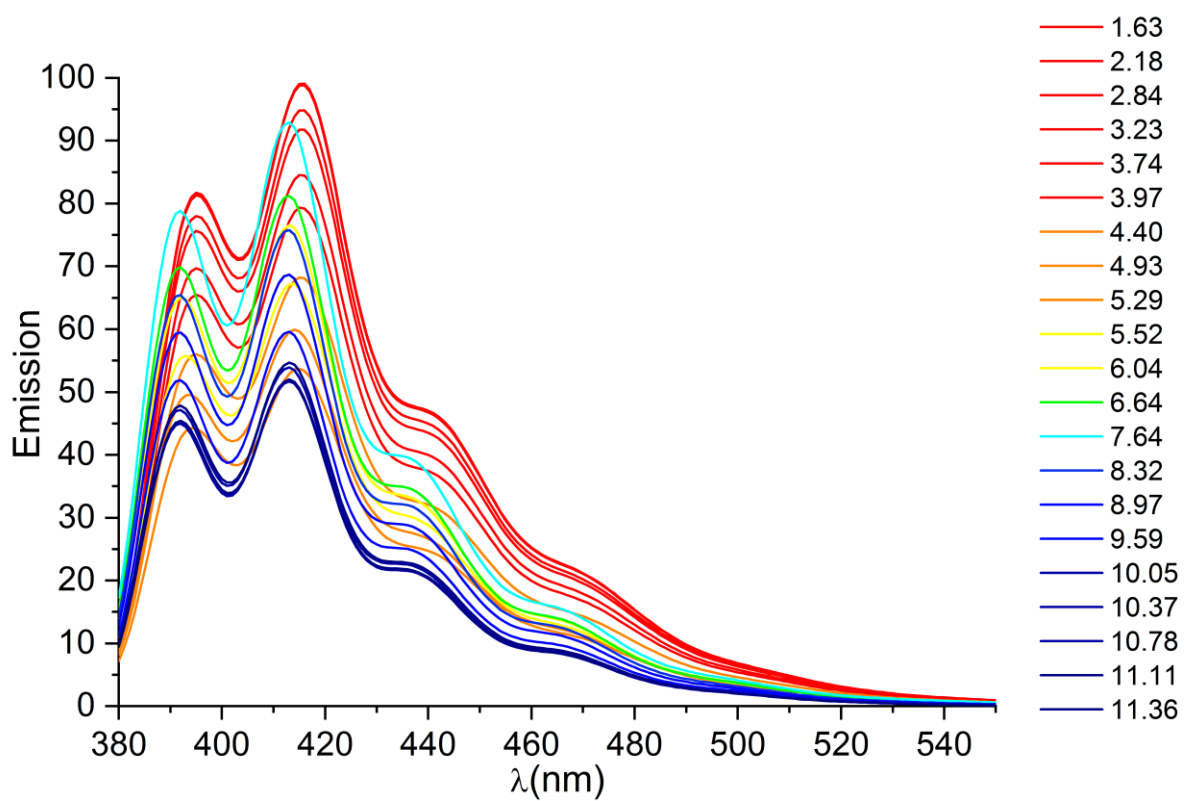


Figure S7. Emission spectra of the system L/Zn²⁺/benzoate at different pH values. [L] = [Zn²⁺] = [benzoate] = 1×10⁻⁵ M. λ_{exc} 362 nm.

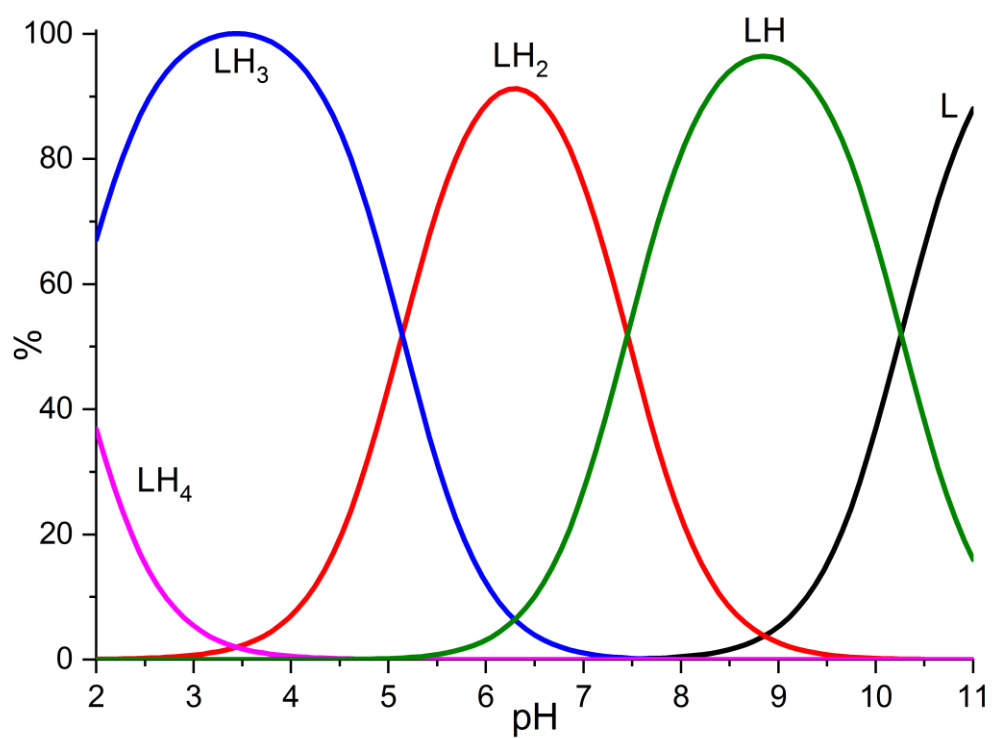


Figure S8. Distribution diagram of the species formed by L as a function of pH. $[L] = 1 \times 10^{-3}$ M. Charges omitted.

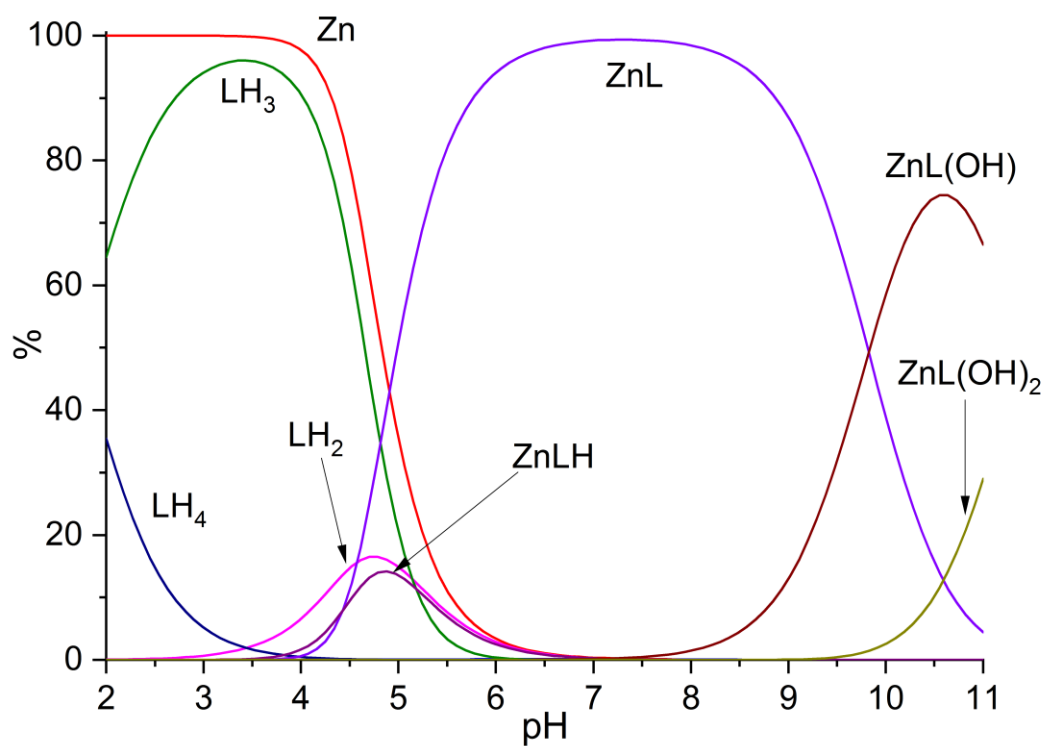


Figure S9. Distribution diagram of the species formed by L with Zn^{2+} as a function of pH. $[\text{L}] = [\text{Zn}^{2+}] = 1 \times 10^{-3}$ M. Charges omitted.

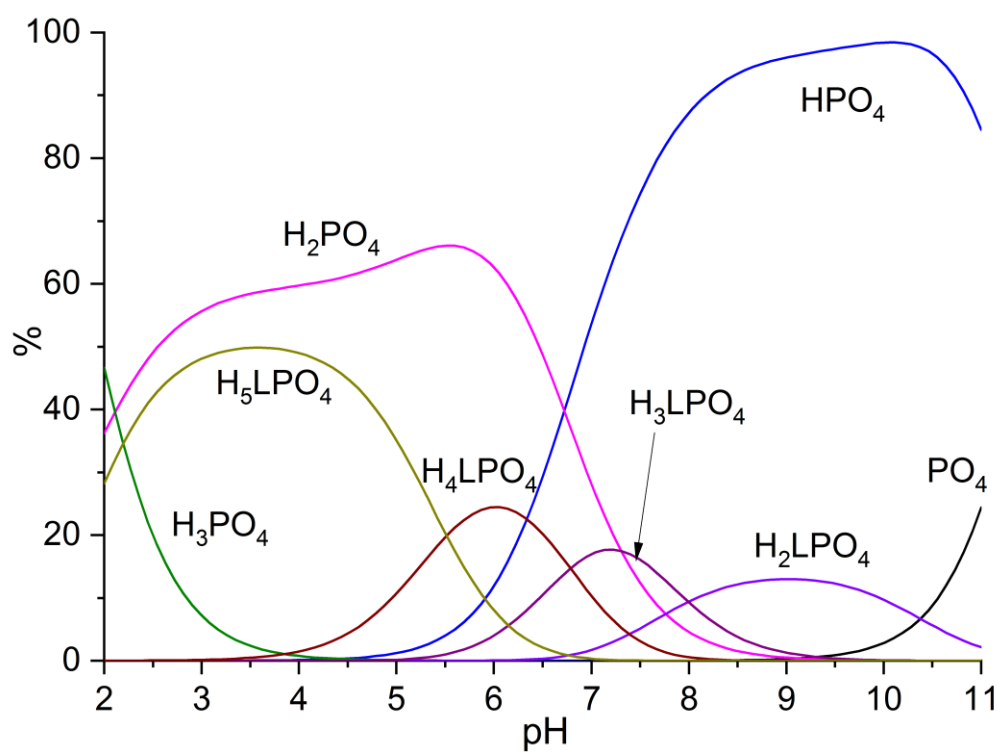


Figure S10. Distribution diagram of the species formed by L with phosphate as a function of pH. $[\text{L}] = [\text{phosphate}] = 1 \times 10^{-3} \text{ M}$. Charges omitted.

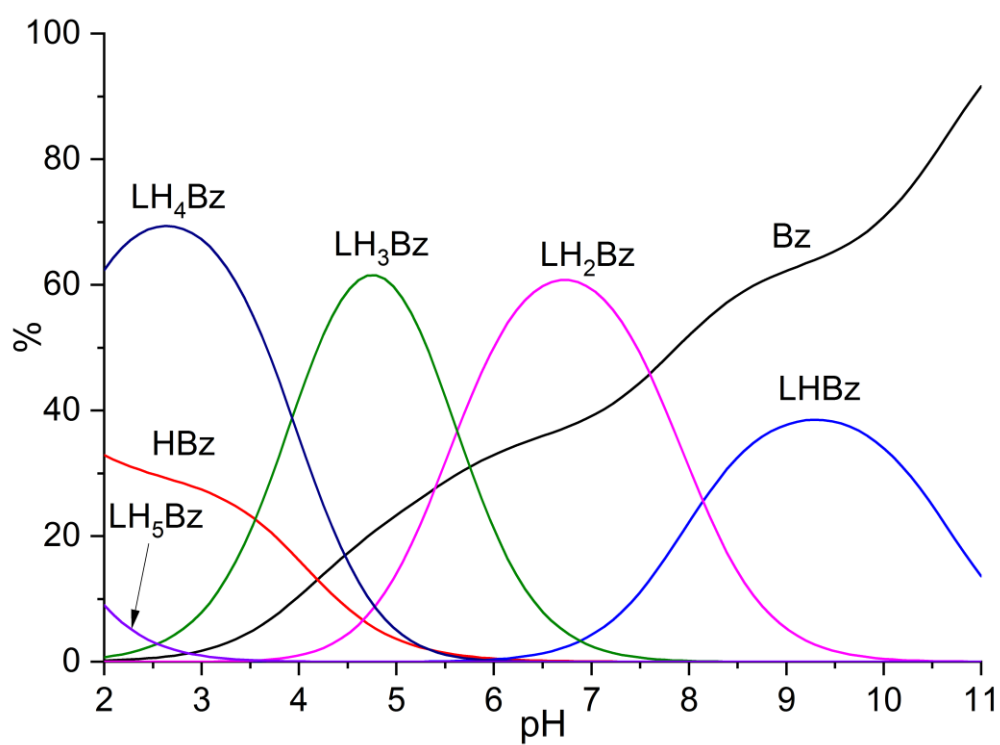


Figure S11. Distribution diagram of the species formed by L with benzoate as a function of pH. $[L] = [benzoate] = 1 \times 10^{-3} \text{ M}$. Charges omitted.

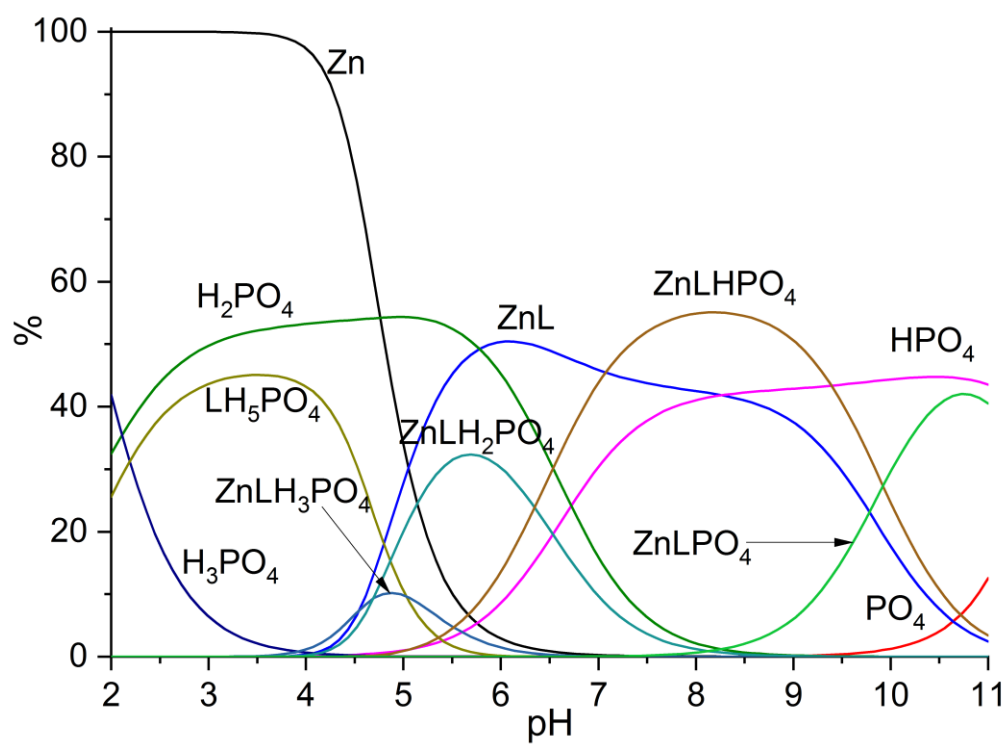


Figure S12. Distribution diagram of the species formed by L with Zn^{2+} and phosphate as a function of pH. $[\text{L}] = [\text{Zn}^{2+}] = [\text{phosphate}] = 1 \times 10^{-3} \text{ M}$. Charges omitted.

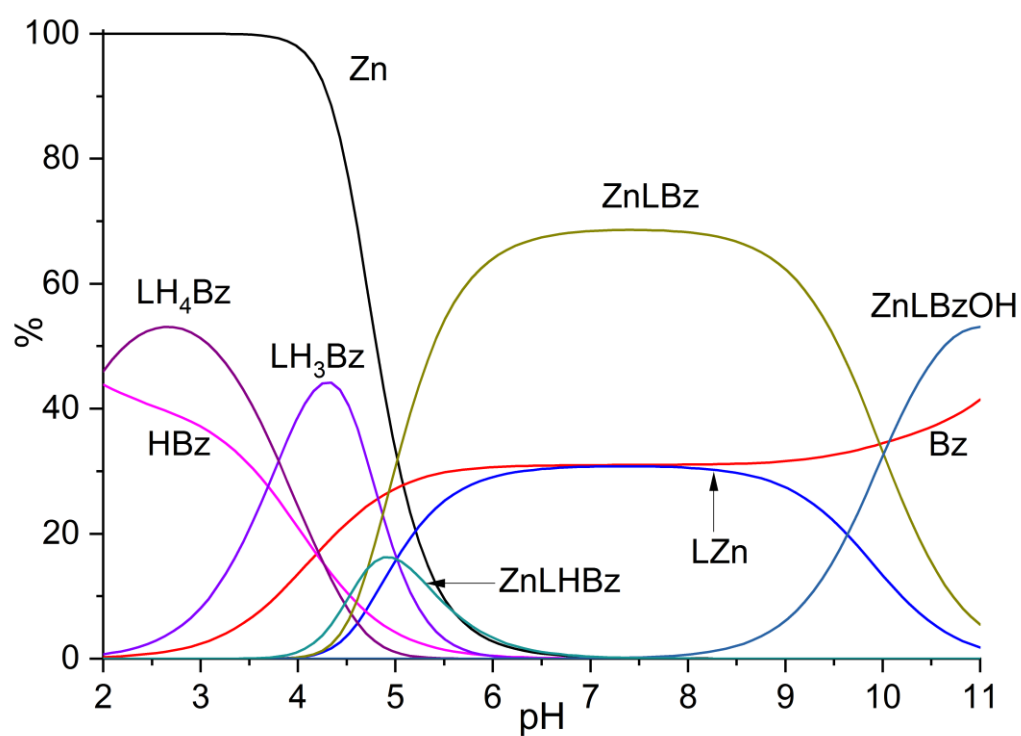


Figure S13. Distribution diagram of the species formed by L with Zn^{2+} and benzoate as a function of pH. $[\text{L}] = [\text{Zn}^{2+}] = [\text{benzoate}] = 1 \times 10^{-3} \text{ M}$. Charges omitted.