

Supporting information for:

Zinc-mediated diastereoselective assembly of a trinuclear circular helicate

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1. Characterization of the triptycene-based ligand H_2L

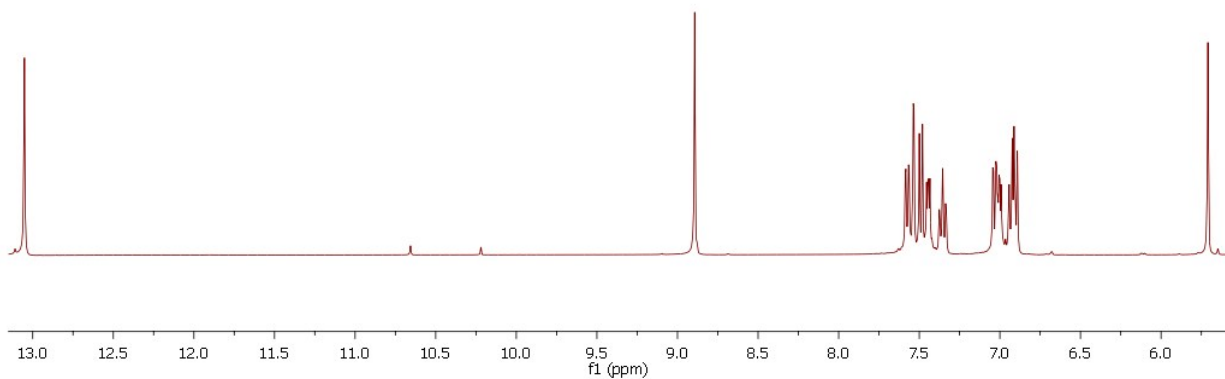


Fig. S1. ^1H NMR spectrum of H_2L in dms0-d_6

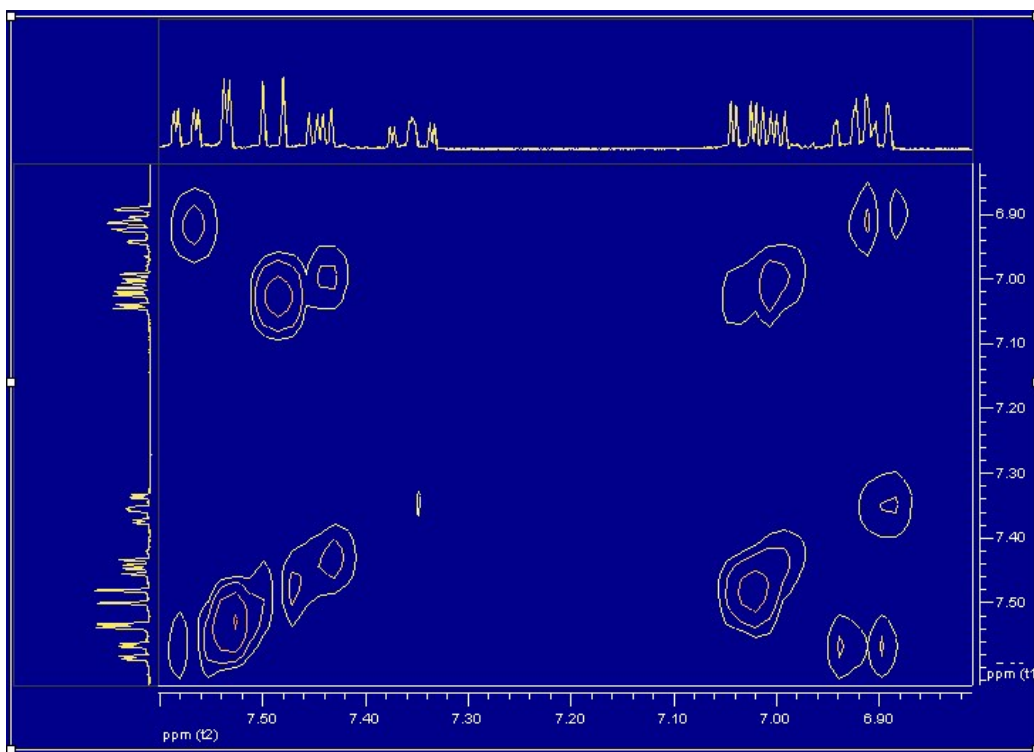


Fig. S2. Partial view (aromatic region) of the COSY spectrum (H-H correlation) of H_2L in dms0-d_6

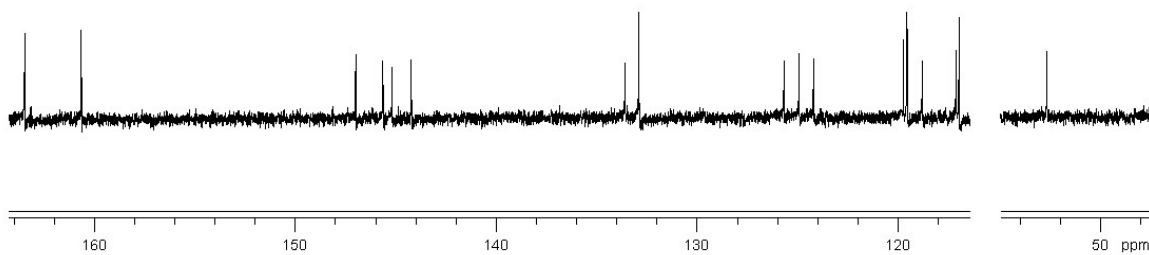


Fig. S3. ^{13}C NMR spectrum of H_2L in dms0-d_6

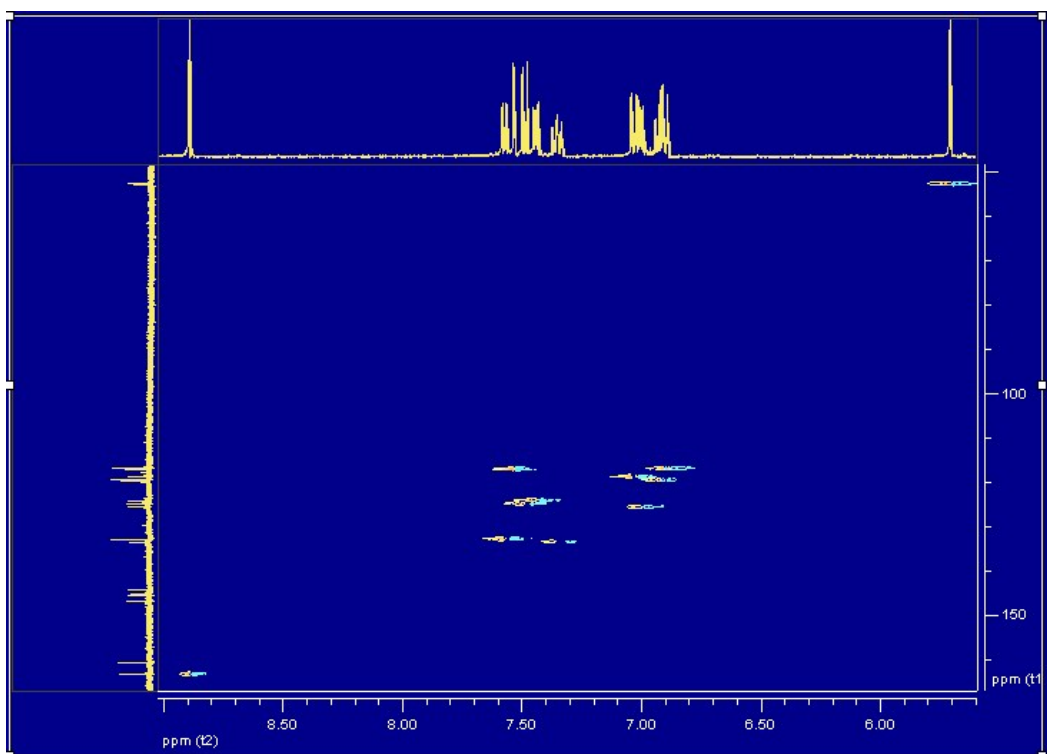


Fig. S4. HMBC spectrum (C-H correlation) of H₂L in dms0-*d*₆

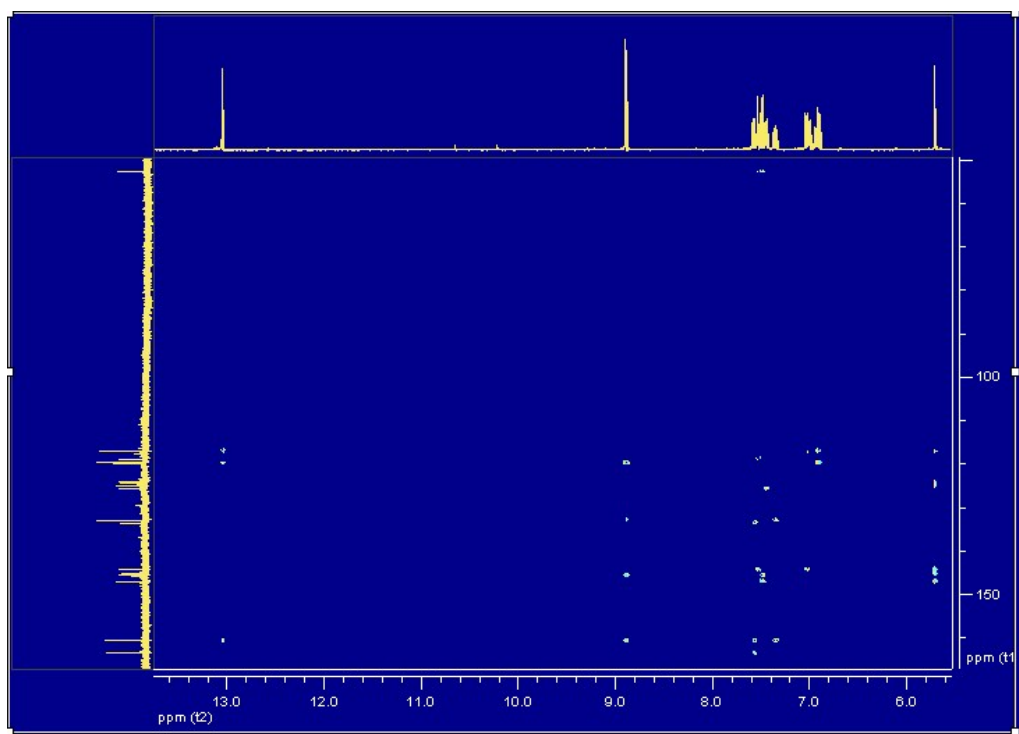


Fig. S5. HMBC spectrum (C-H correlation) of H₂L in dms0-*d*₆

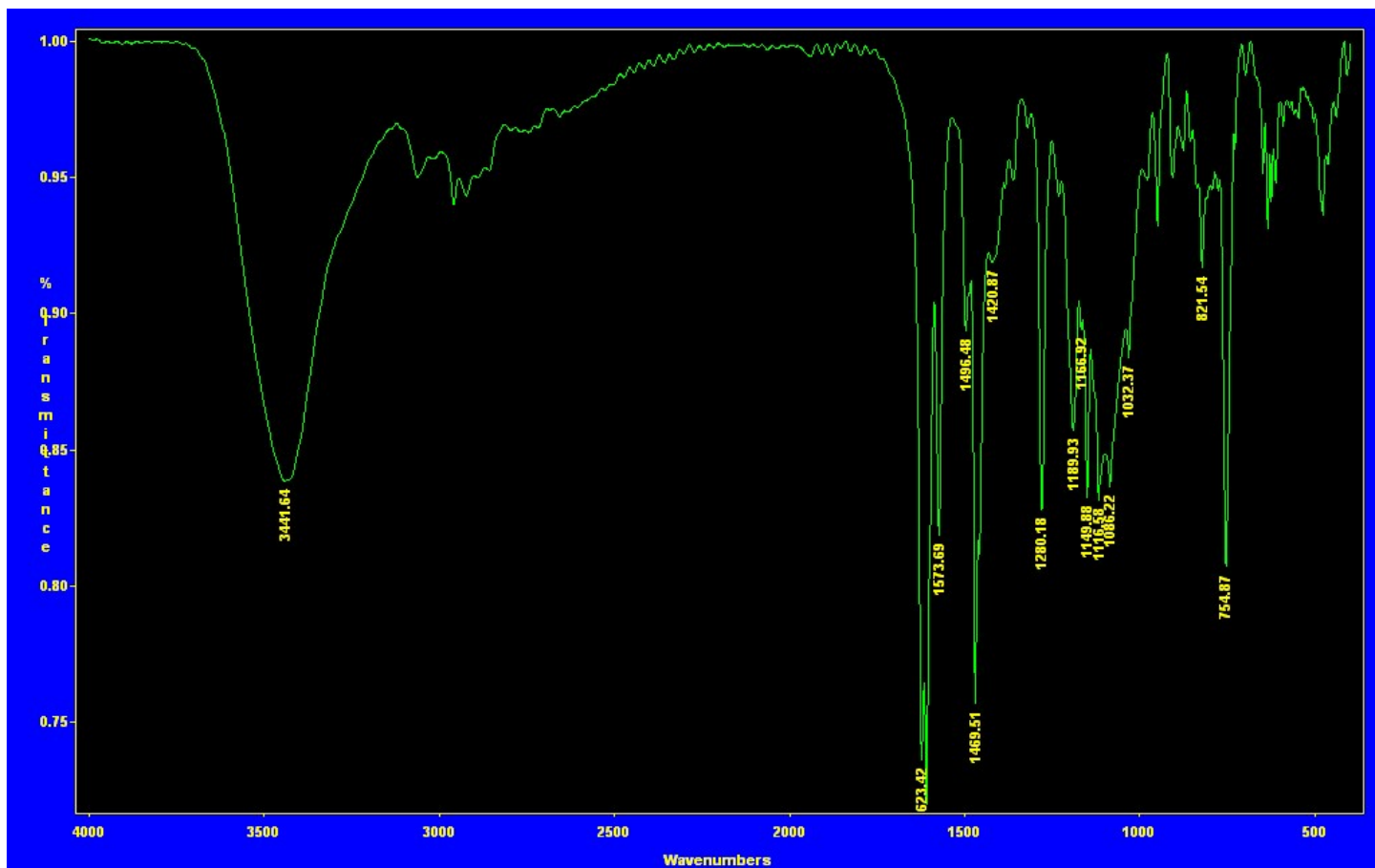


Fig. S6. IR spectrum of H₂L

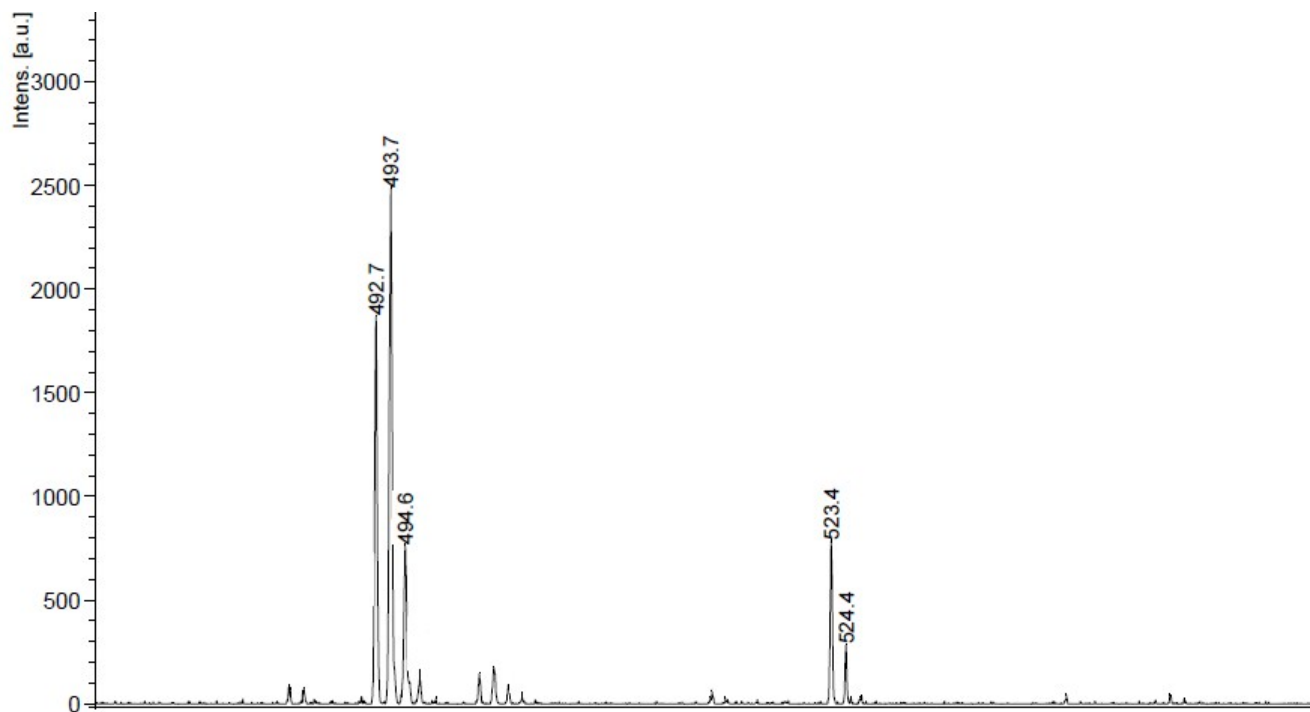


Fig. S7. Mass spectrum (MALDI-TOF) of H₂L

2 Characterization of $Zn_3L_3 \cdot 8H_2O$

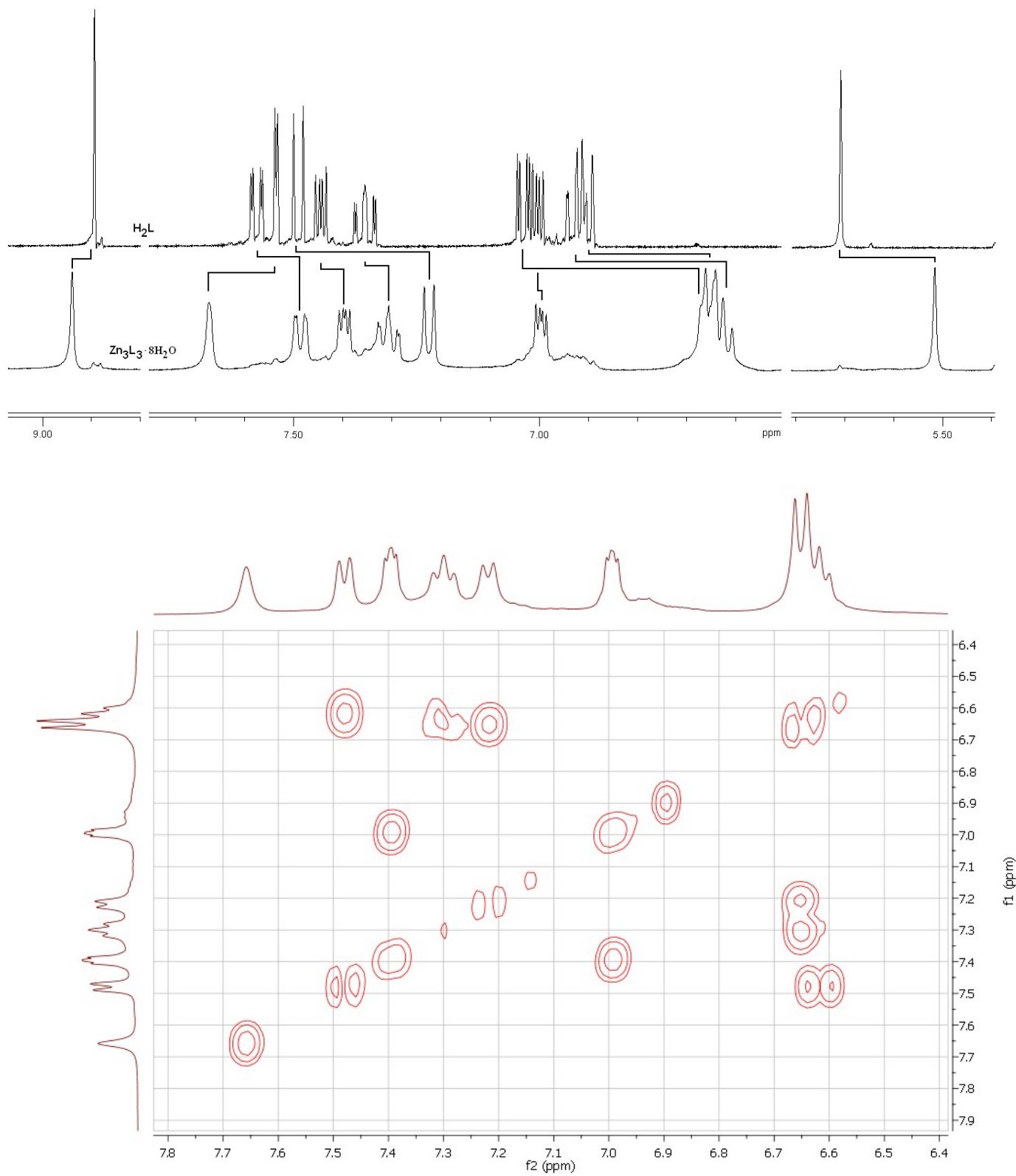


Fig. S9. Partial view (aromatic region) of the COSY spectrum of $Zn_3L_3 \cdot 8H_2O$ in $dms0-d_6$

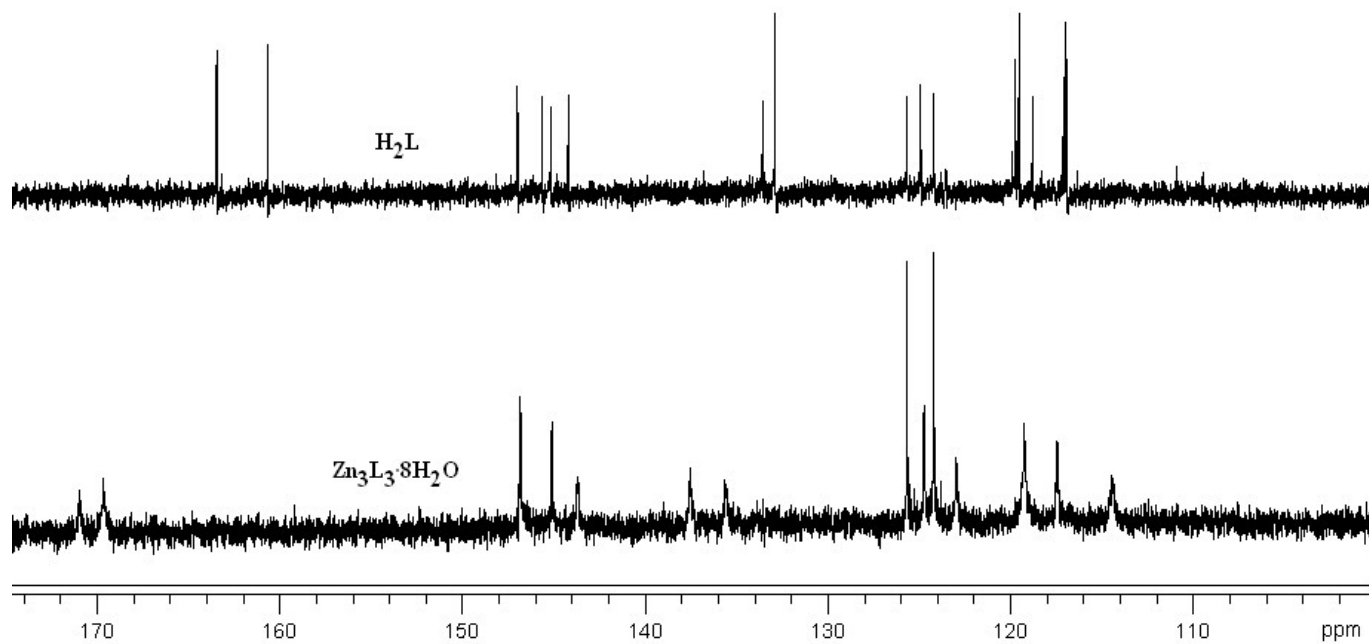


Fig. S10. Superposition of ^{13}C NMR spectra of $\text{Zn}_3\text{L}_3 \cdot 8\text{H}_2\text{O}$ and H_2L in $\text{dmsO}-d_6$ showing the influence of complexation in chemical shifts of the proton signals.

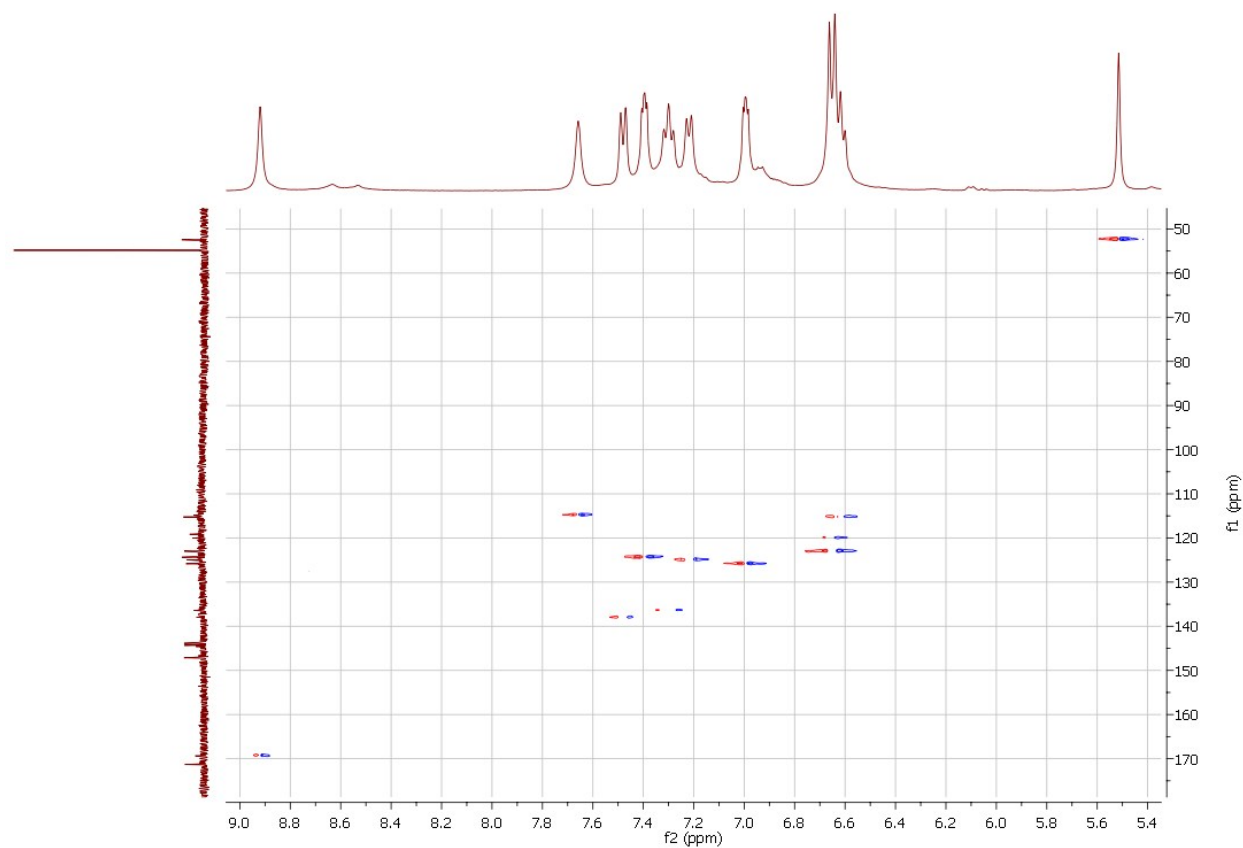


Fig. S11. HMQC spectrum of $\text{Zn}_3\text{L}_3 \cdot 8\text{H}_2\text{O}$ in $\text{dmsO}-d_6$

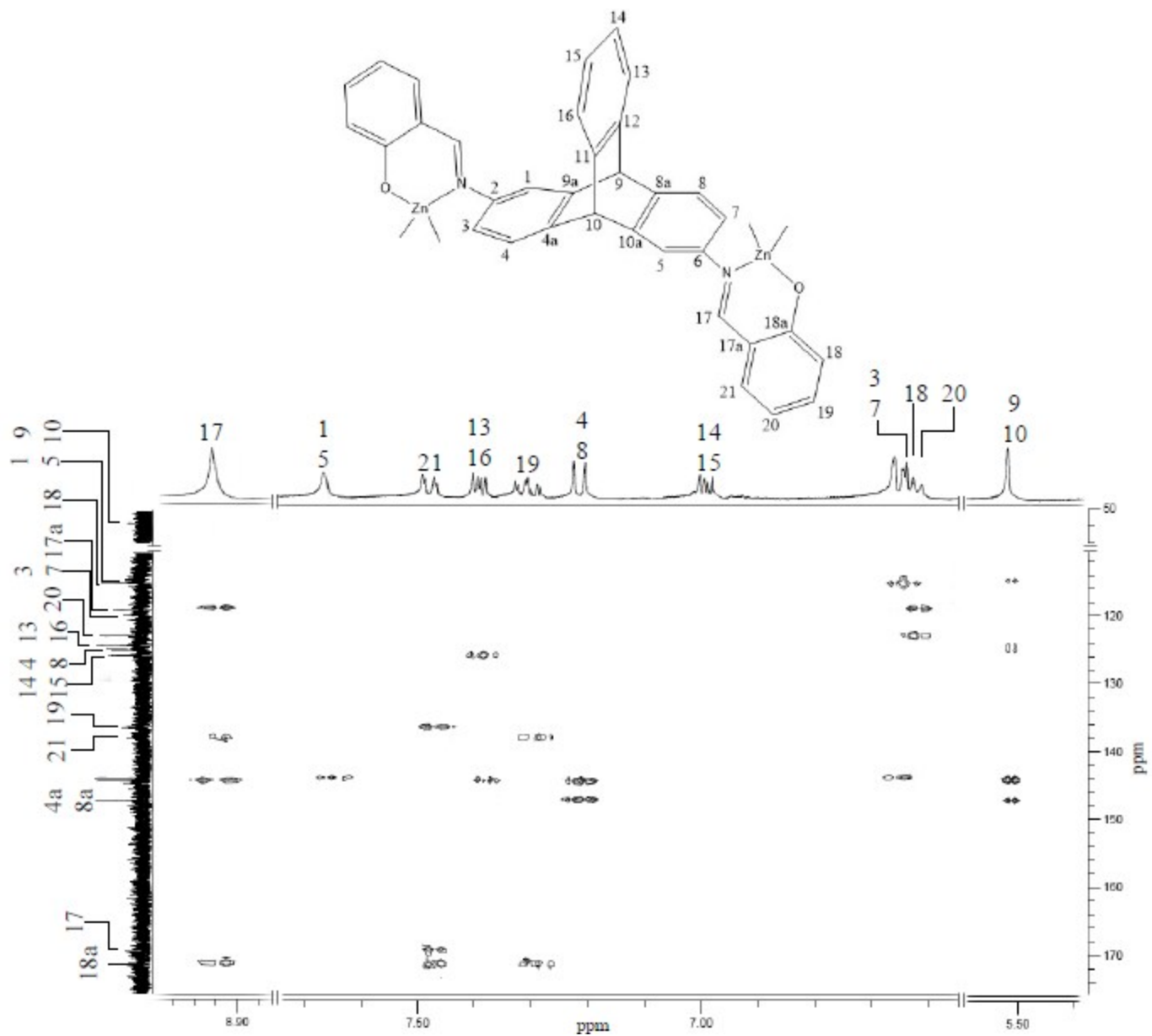


Fig. S12. HMBC spectrum of $Zn_3L_3 \cdot 8H_2O$ in $dms0-d_6$

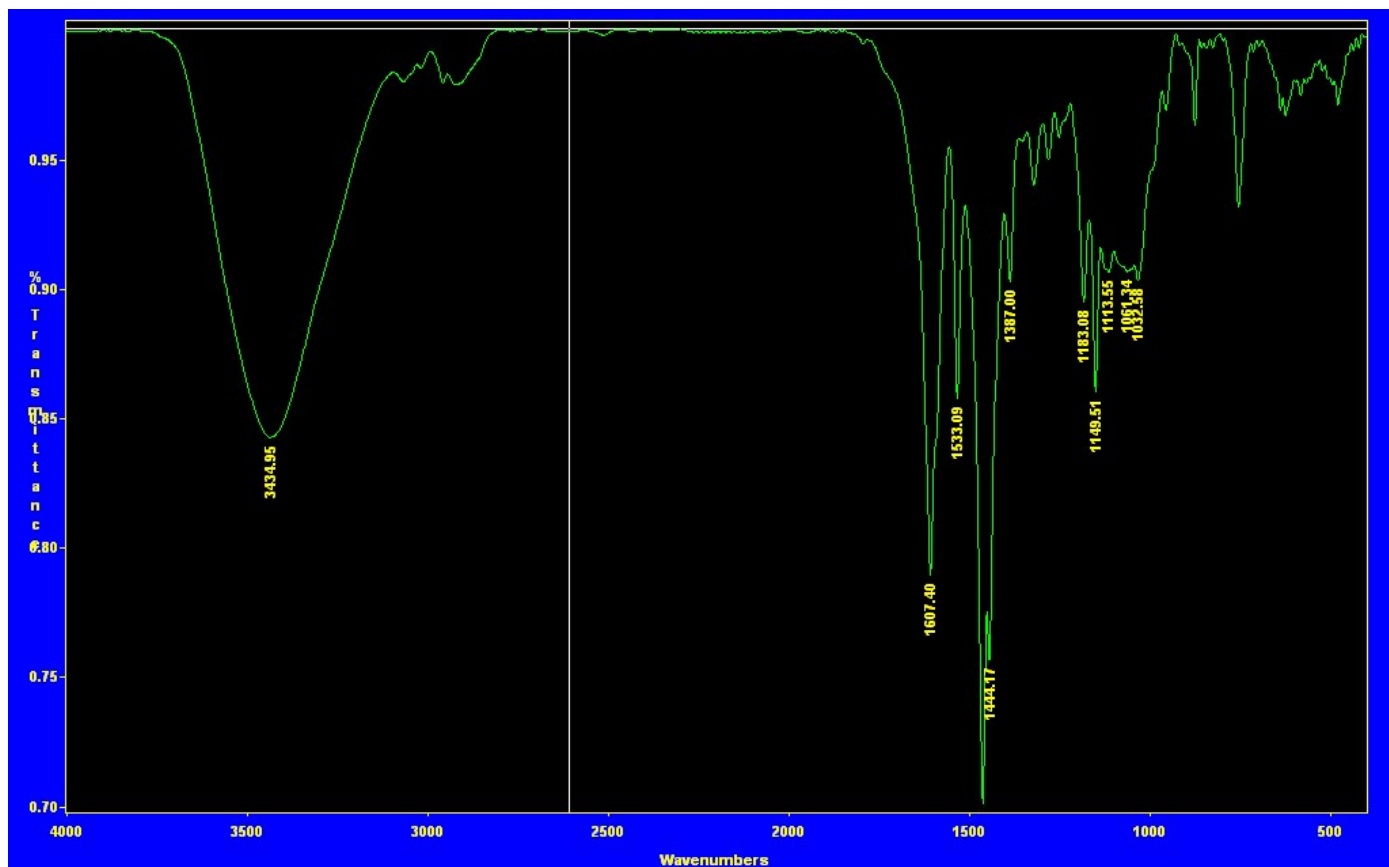


Fig. S13. IR spectrum of $Zn_3L_3 \cdot 8H_2O$

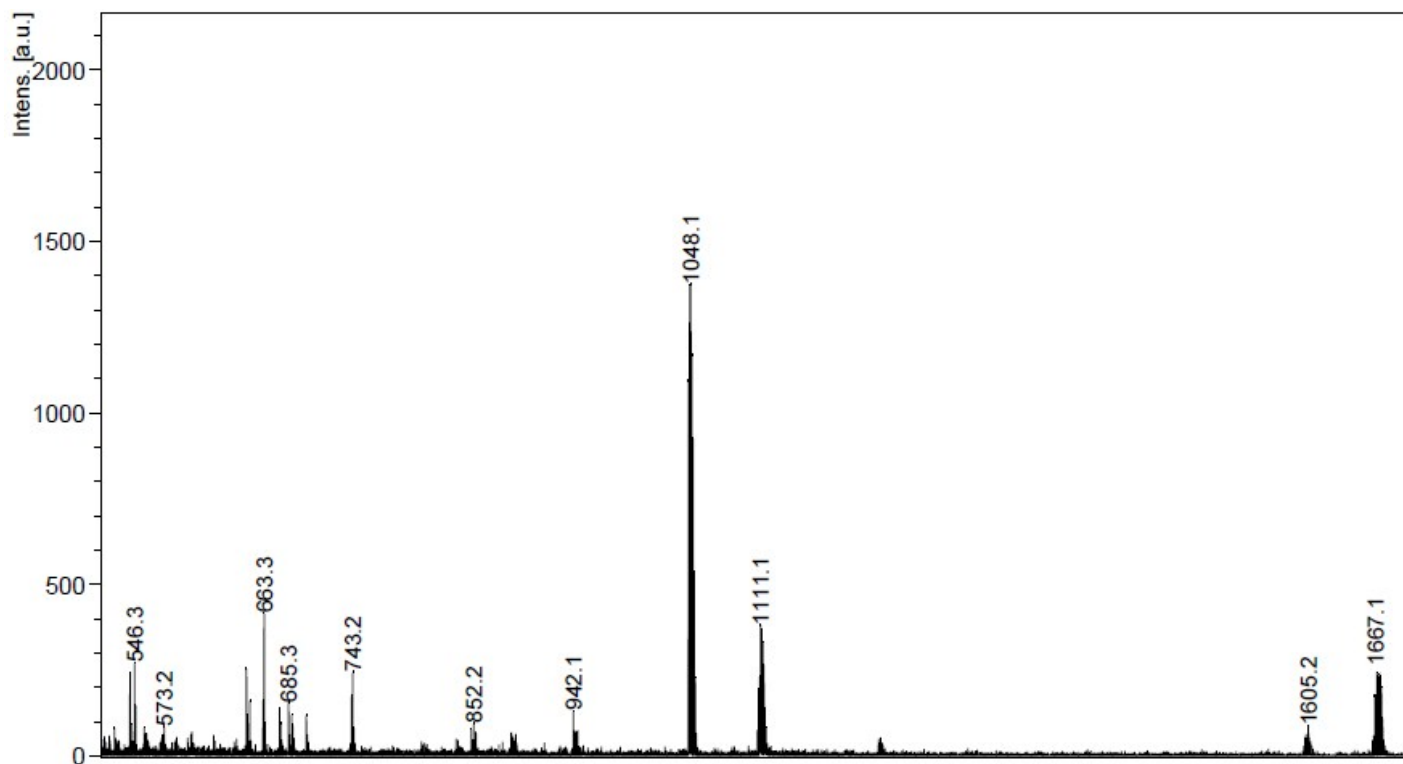


Fig. S14. Partial view of the mass spectrum of $Zn_3L_3 \cdot 8H_2O$

3. Optical studies on the compounds

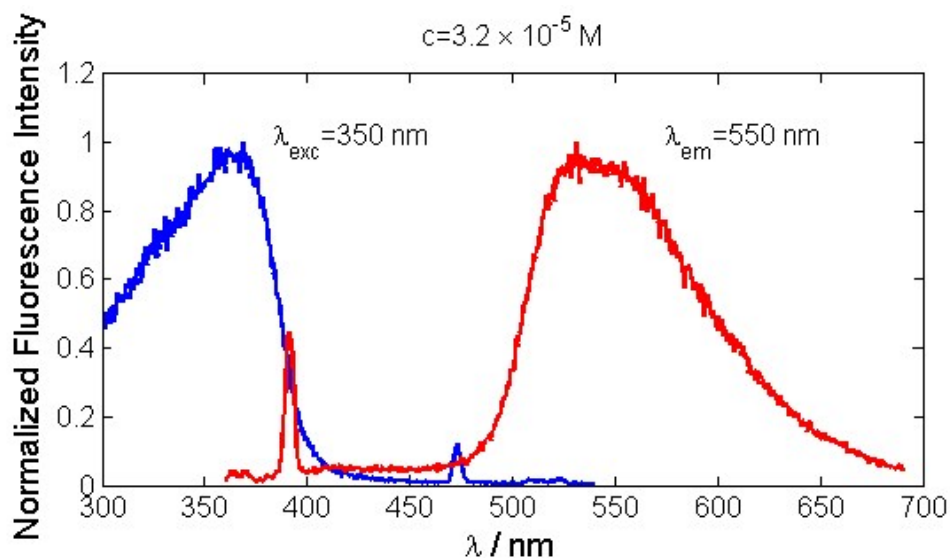


Fig. S15. Excitation (blue line) and emission (red line) spectra of H₂L (in THF, 3.2×10^{-5} M).

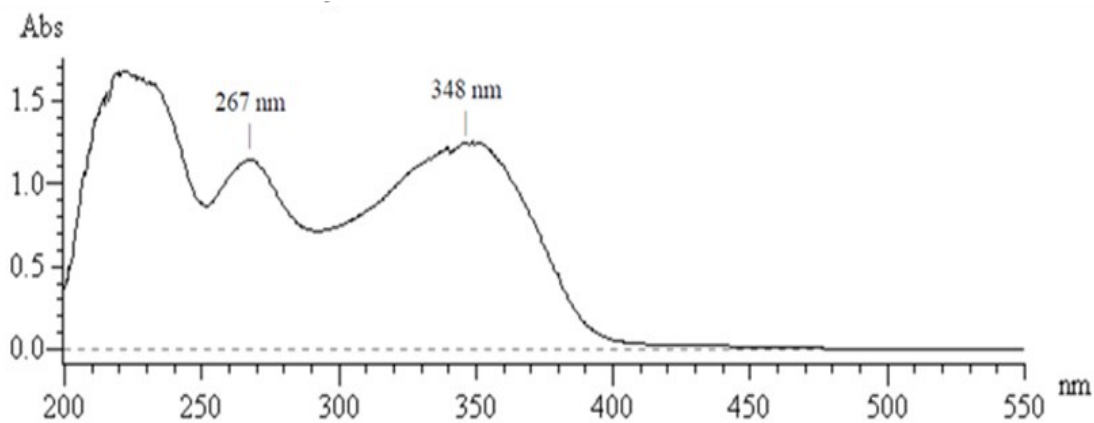


Fig. S16. UV-Vis absorption spectrum of H₂L/tetramethylammonium hydroxide in acetonitrile/methanol

Table S1. Instrumental parameters of the UV-Vis absorption measurements

Data mode	Abs	Delay	0 sec
Start Wavelength	550 nm	Path Length	10.0 nm
End Wavelength	200 nm	Response	Fast
Scan speed	800 nm/min	Light Source	WI/D ₂
Baseline correction	System	Lamp Change	340 nm

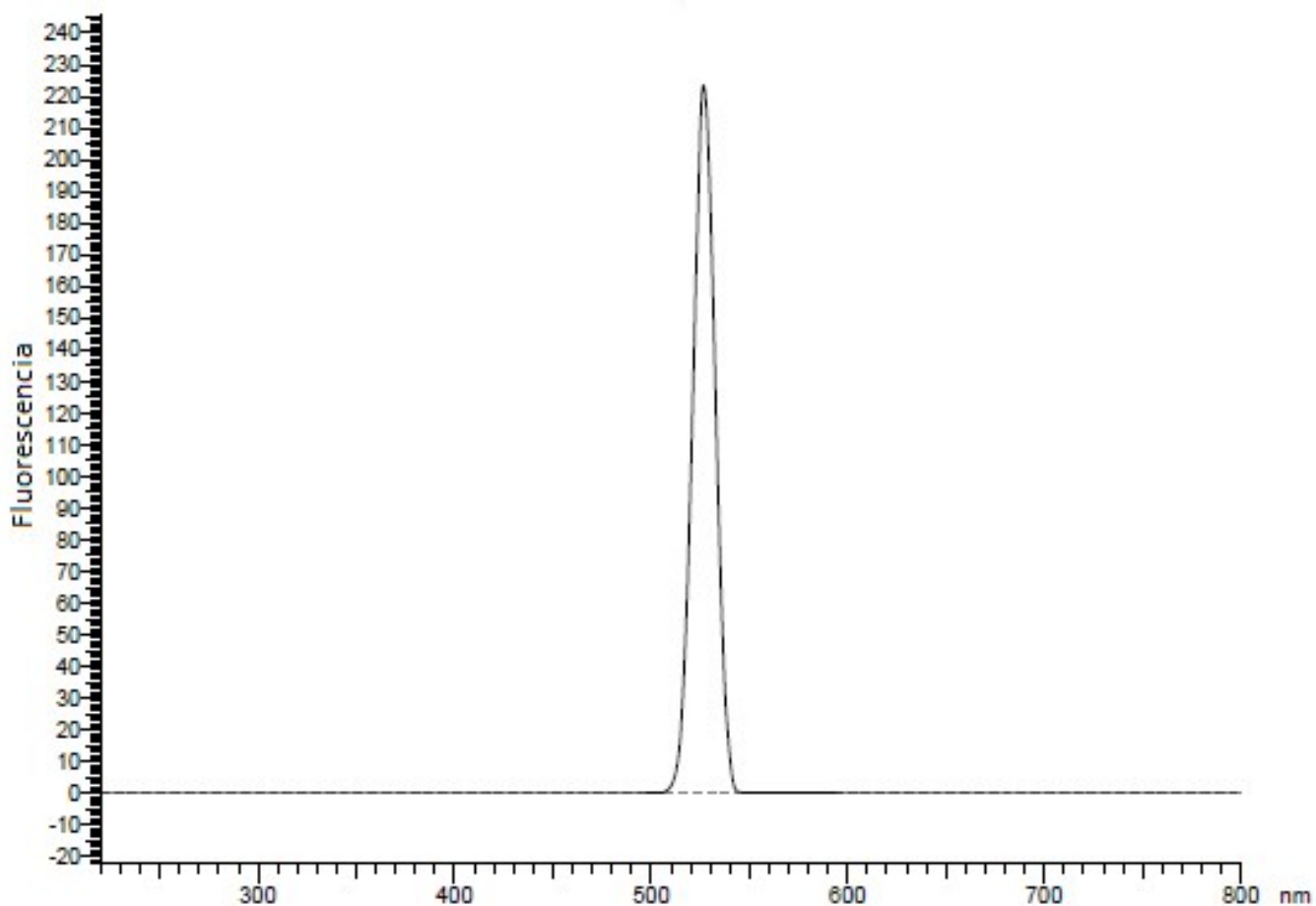


Fig. S17. Fluorescence emission spectrum of H₂L/tetramethylammonium hydroxide in acetonitrile/methanol

Table S2. Instrumental parameters of the fluorescence emission measurements.

Measurement Type	Wavelength scan	Scan speed	1500 nm/min
Scan mode	Emission	Delay	0 sec
Data mode	Fluorescence	EX Slit/ EM Slit	10.0 nm/10.0 nm
EX WL	350.0 nm	PMT Voltage	400 V
EM Start WL	220.0 nm	Response	0.08 sec
EM End WL	800.0 nm	Corrected spectra	Off

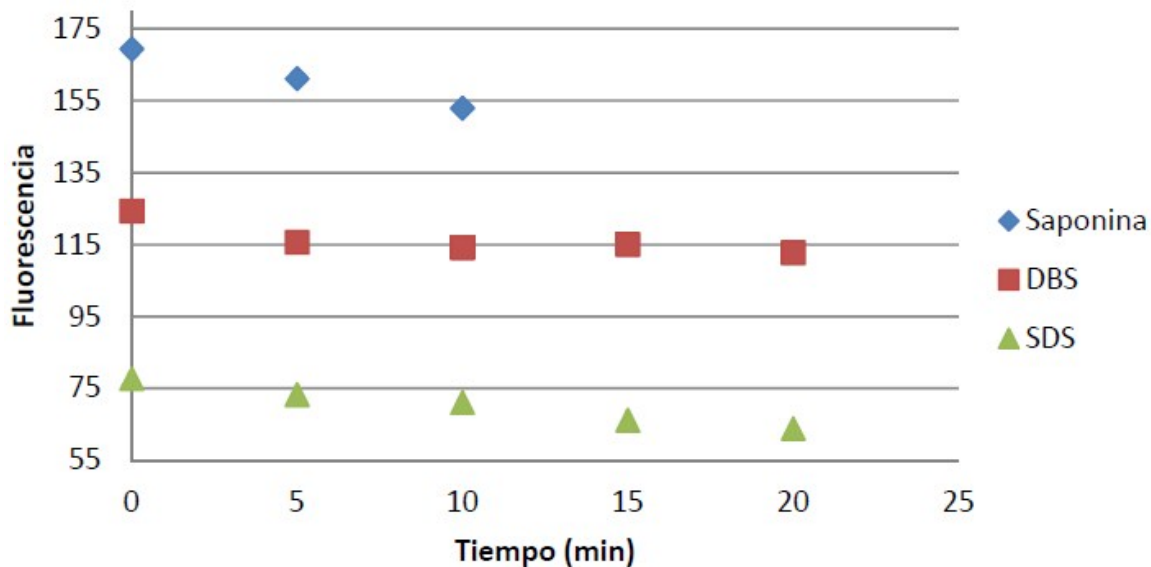


Fig. S18. Variation of the fluorescence emission spectrum with time for $\lambda = 525$ nm at $\lambda_{exc} = 350$ nm of H_2L /tetramethylammonium hydroxide in the presence of 50 μL of Saponina, sodium dodecylbenzenesulfonate (SDBS) and sodium dodecylsulfate (SDS) using acetonitrile/methanol as solvent

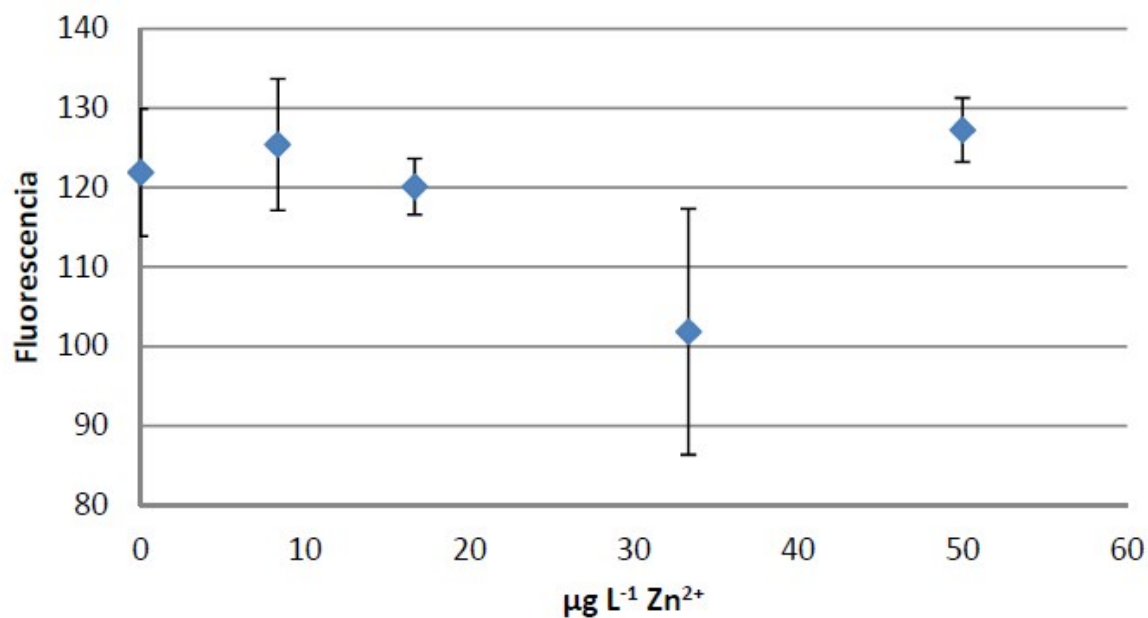


Fig. S19. Variation of the fluorescence emission spectrum of H_2L /tetramethylammonium with the addition of Zn^{2+} in the presence of SDBS

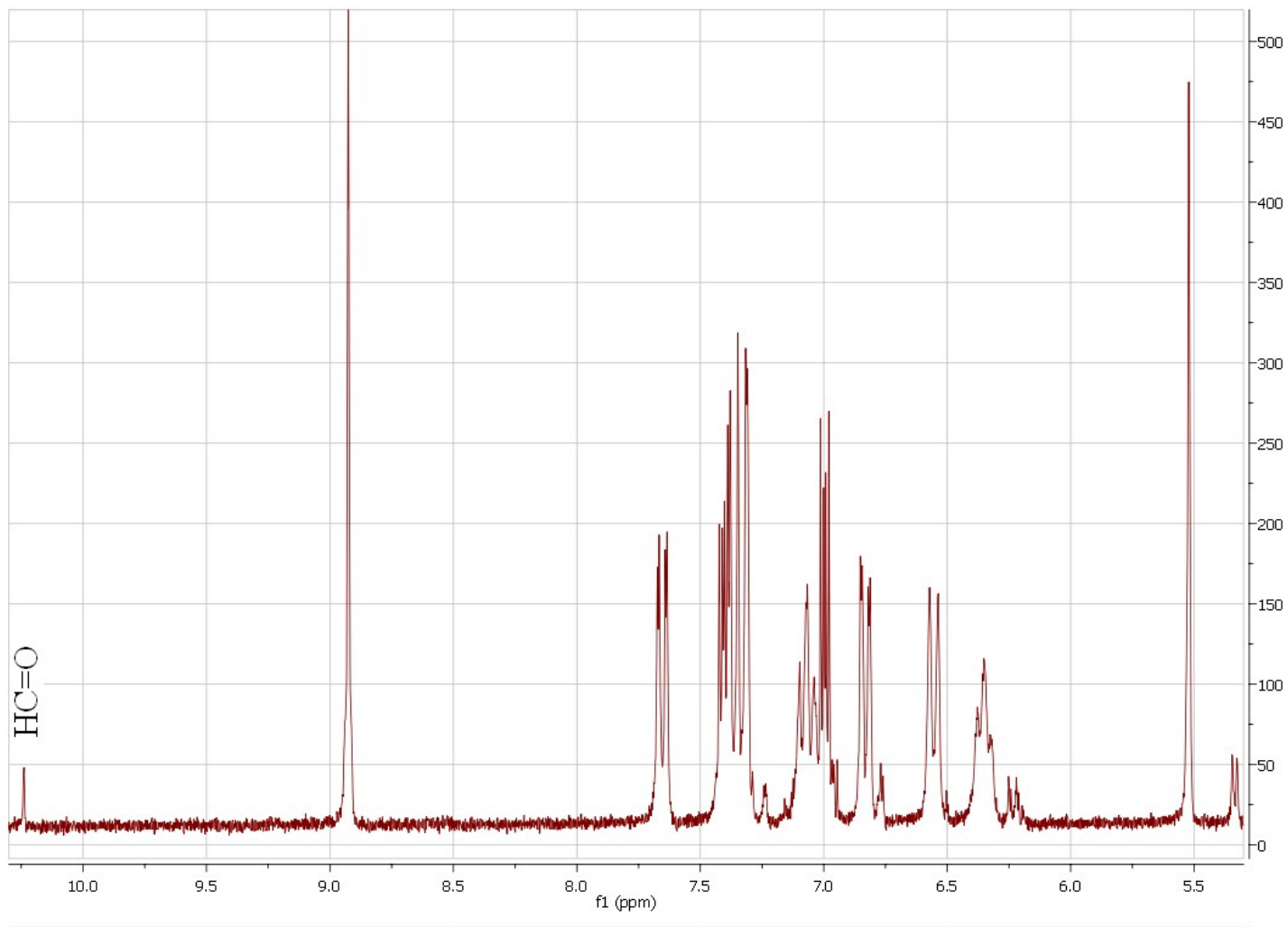


Fig. S20. ^1H NMR spectrum of H_2L /tetramethylammonium hydroxide after 3 h in an acetonitrile- d_3 /methanol- d_4 solution. Low-intensity signals attributed to 2-hydroxybenzaldehyde and 2,6-diaminotriptycene can be observed. The signal attributed to $\text{HC}=\text{O}$ of 2-hydroxybenzaldehyde has been marked