Comparative Biological Activity of Manganese(II) and Zinc(II) Hydrazone Complexes

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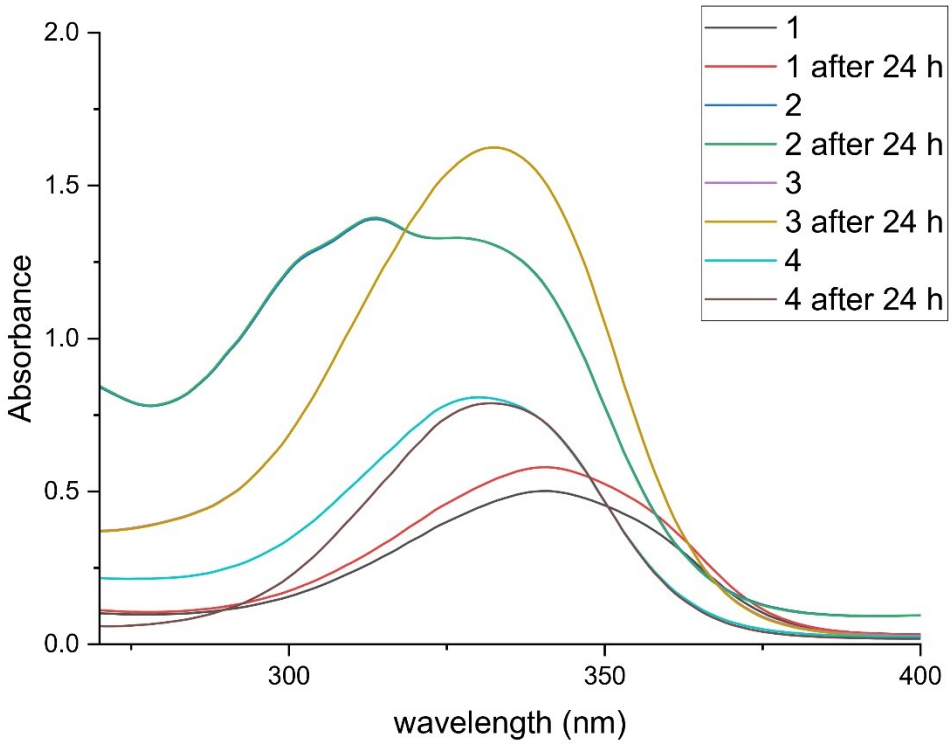

Figure S1. The UV–Vis spectra of all complexes were recorded in DMSO (10^{-5} M), immediately upon preparation and repeated after 24 h

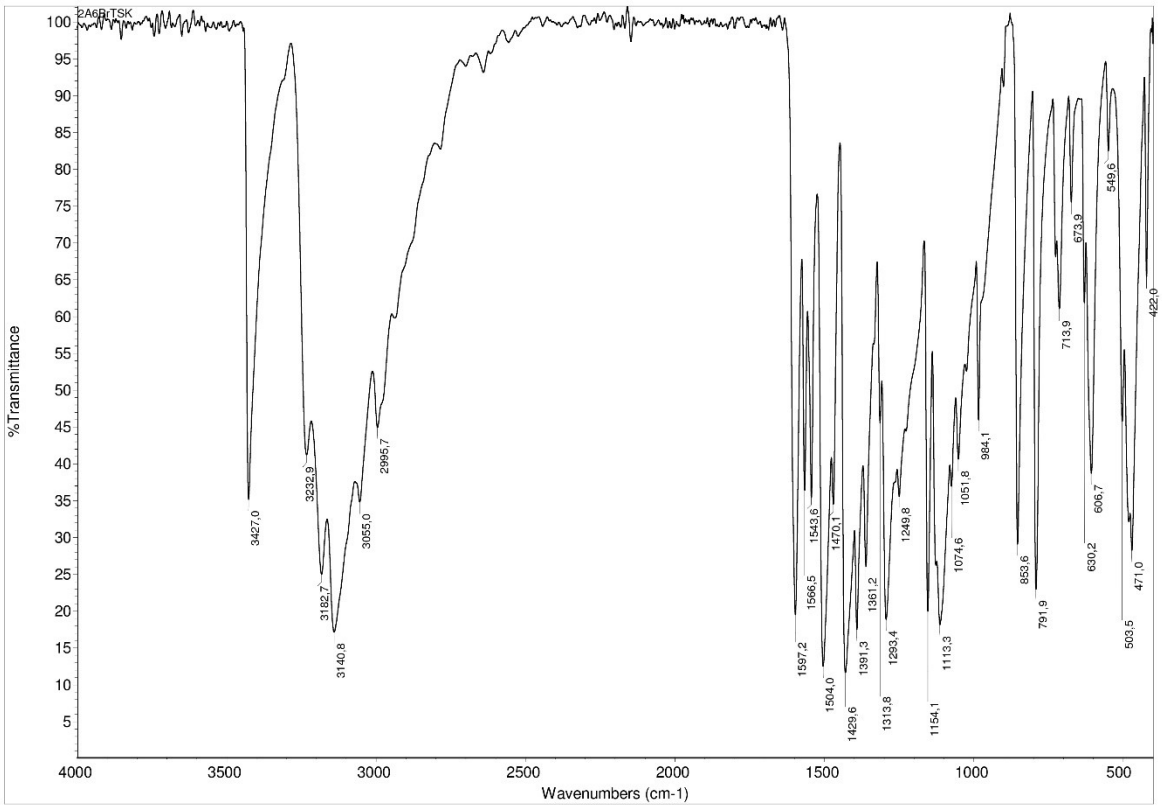

Figure S2. IR spectrum of **HL2** ligand (*E*)-2-(1-(6-bromopyridin-2-yl)ethylidene)hydrazine-1-carbothioamide

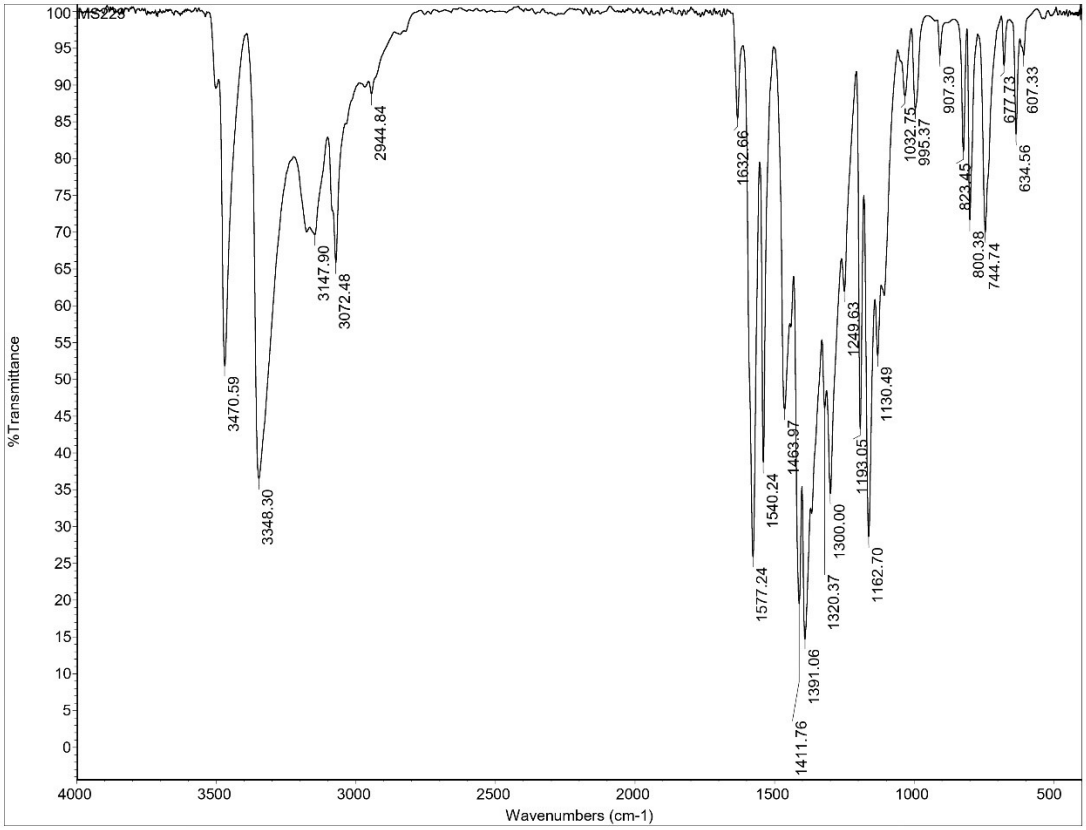

Figure S3. IR spectrum of [Zn(**L2**)$_2$] complex

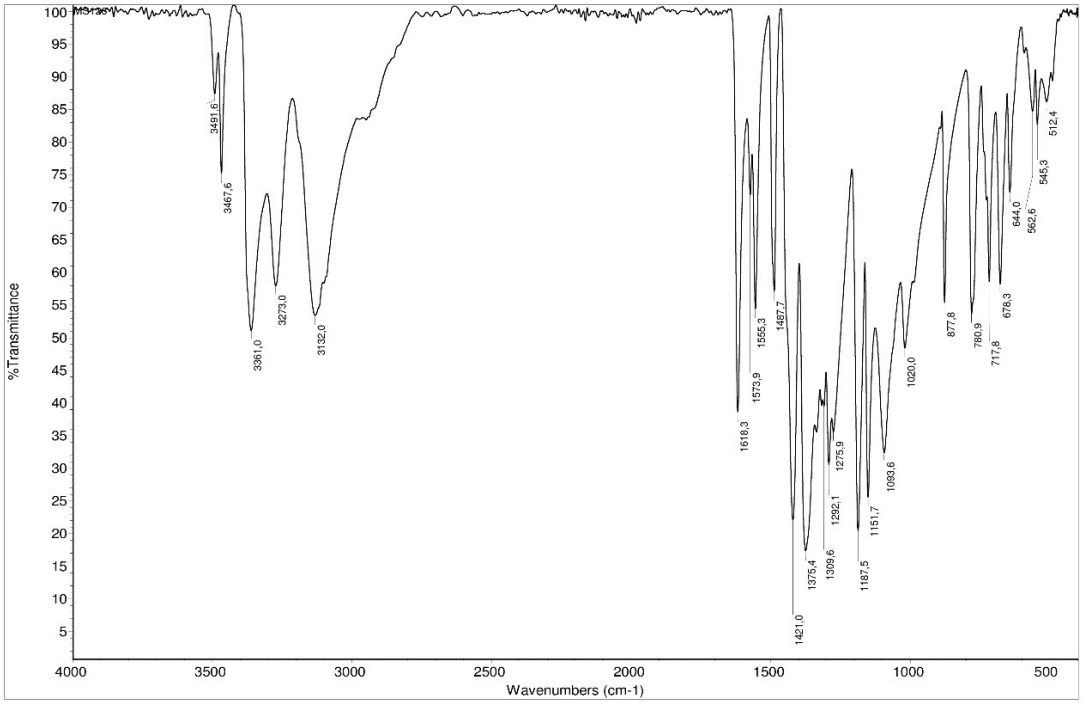

Figure S4. IR spectrum of [Mn(**L1**)$_2$] complex

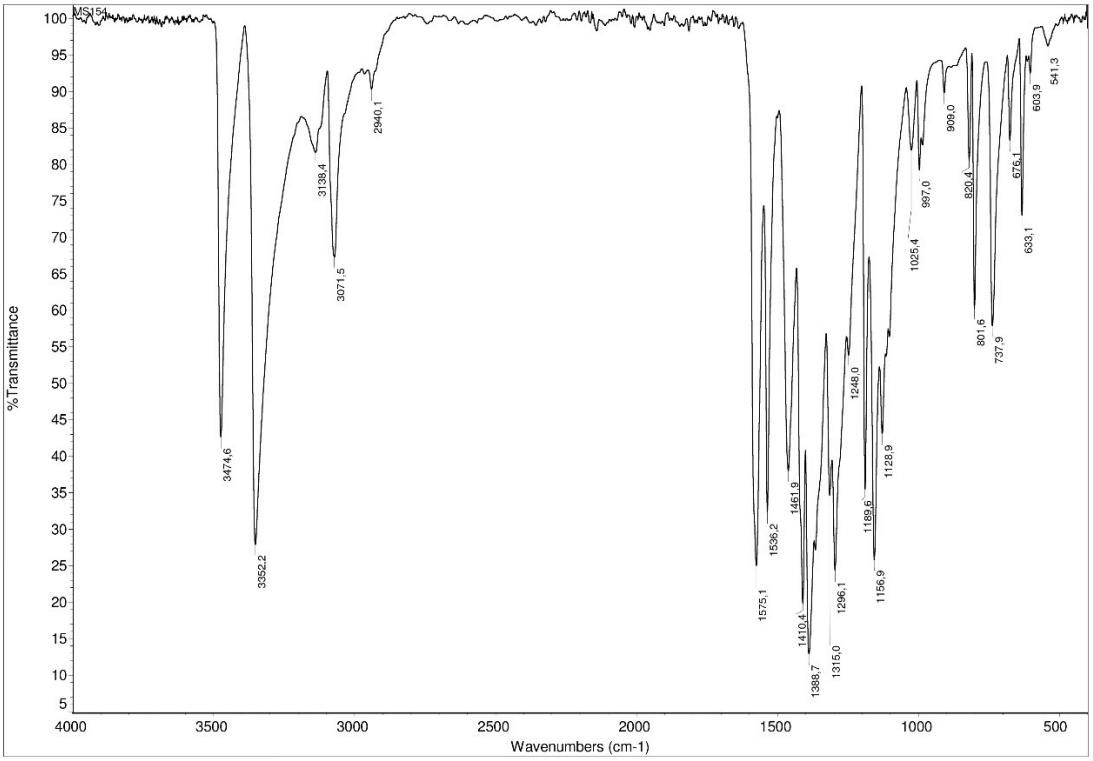

Figure S5. IR spectrum of [Mn(**L2**)$_2$] complex

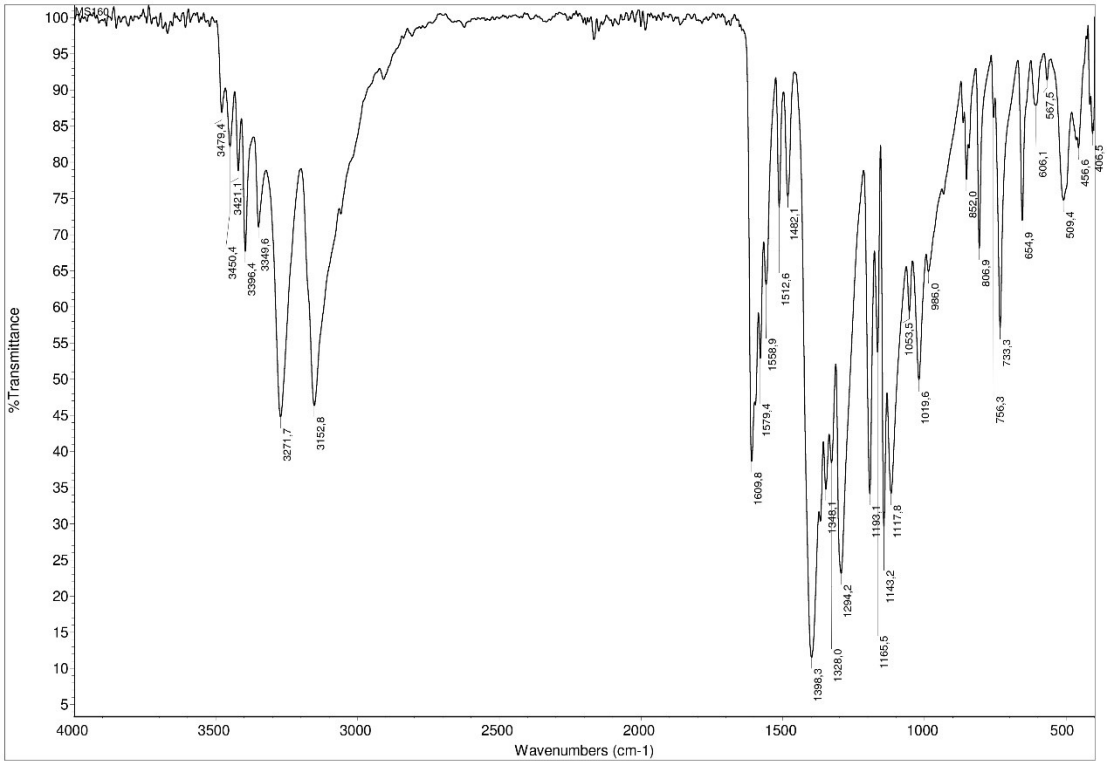

Figure S6. IR spectrum of [Mn(**L3**)$_2$] complex

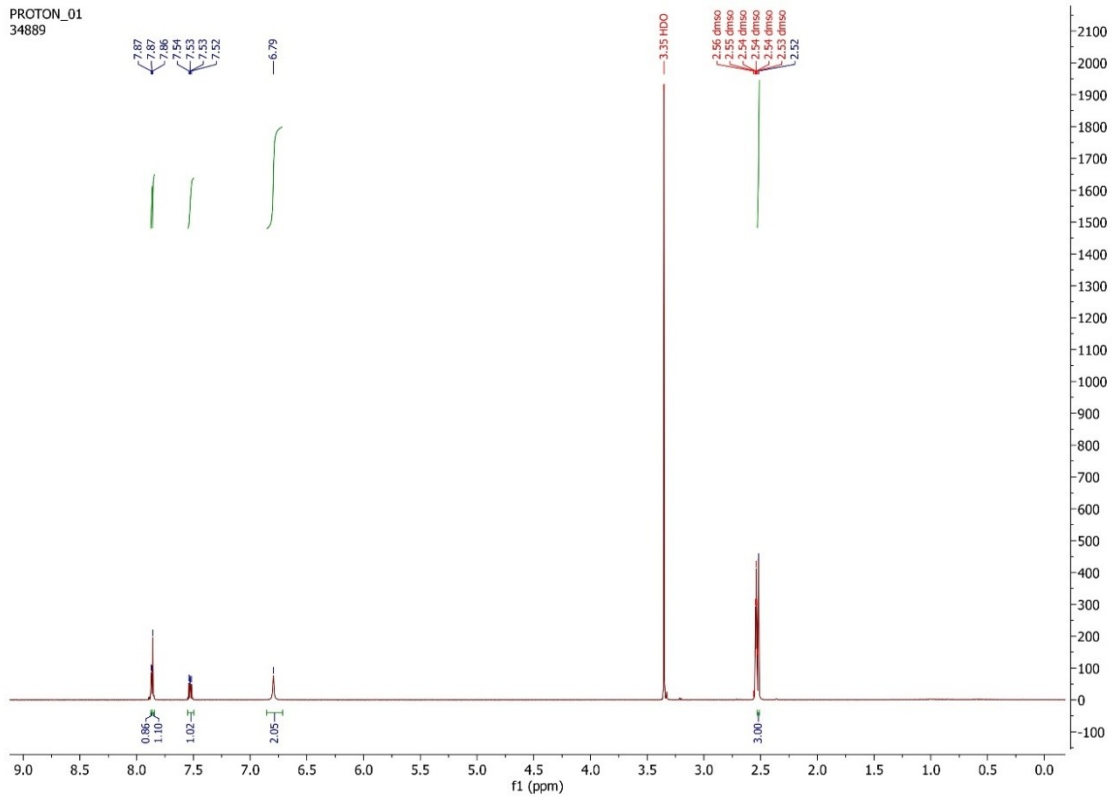

Figure S7. ^{1}H NMR spectrum of [Zn(**L2**)$_2$] complex

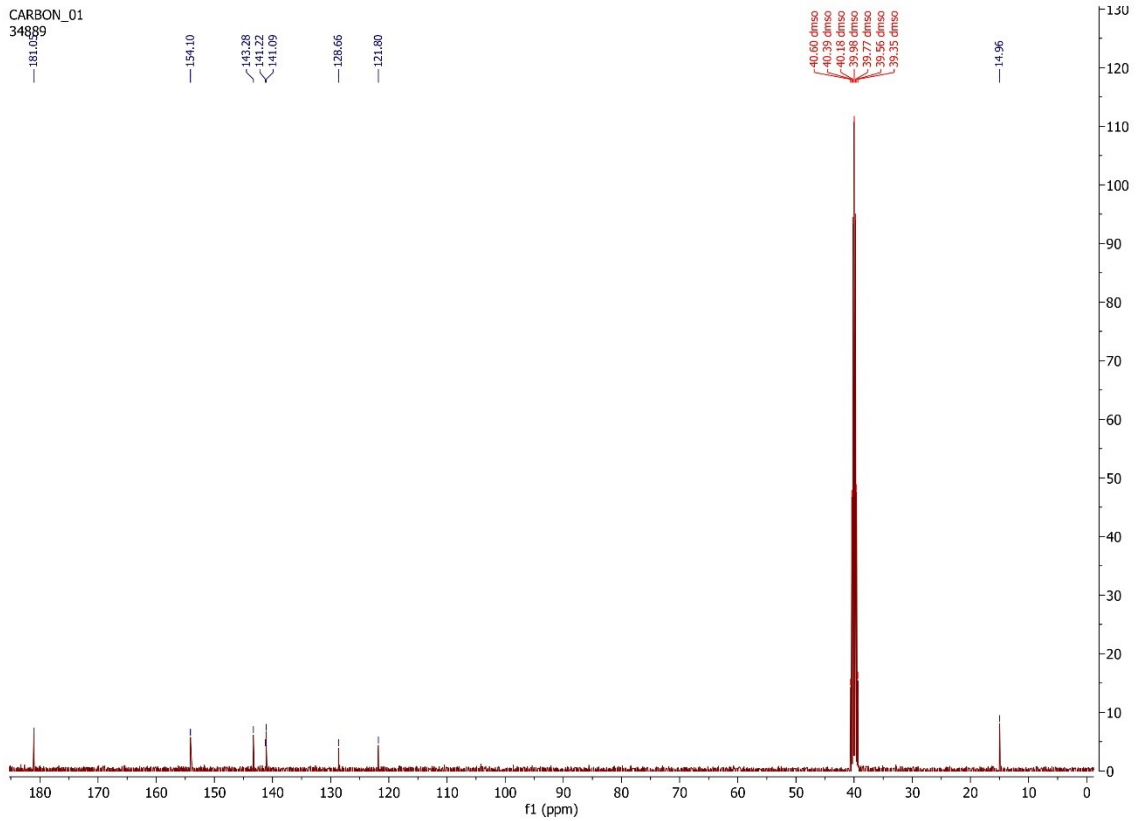

Figure S8. ^{13}C NMR spectrum of [Zn(**L2**)$_2$] complex

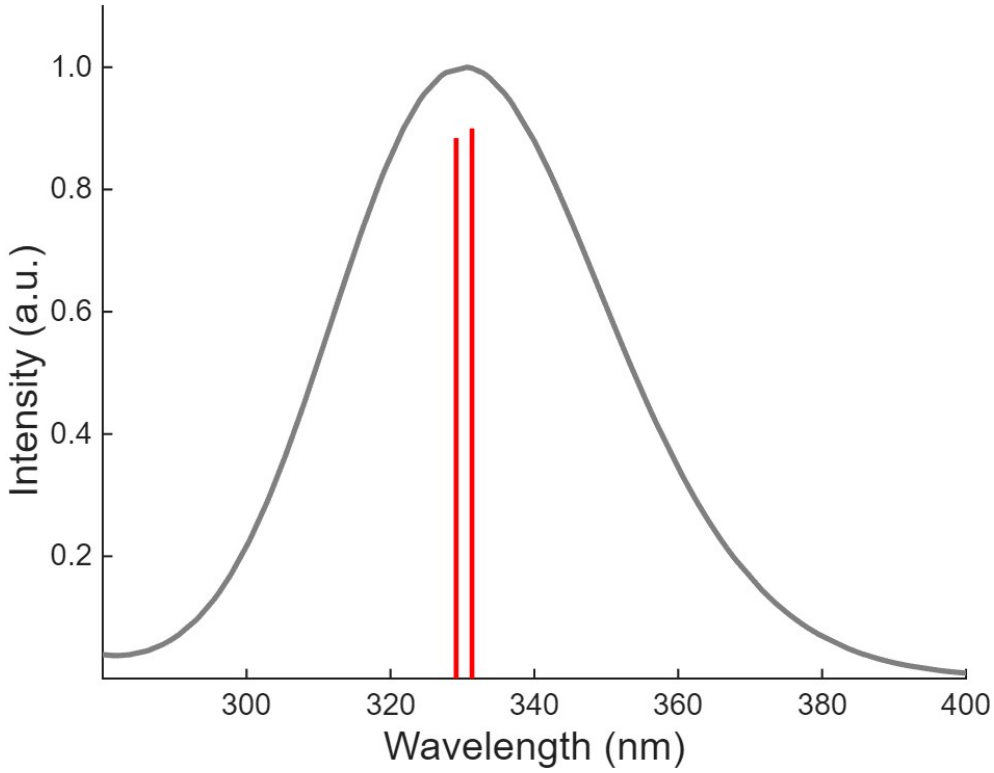

Figure S9. TD-DFT calculated (WB97X D4rev/def2 TZVP(−f)–SMD(DMSO) level of theory) absorption spectrum of Zn(II) complex. The Gaussian-broadened profile (FWHM = 0.5 eV, grey) and the corresponding stick spectrum (red) are shown

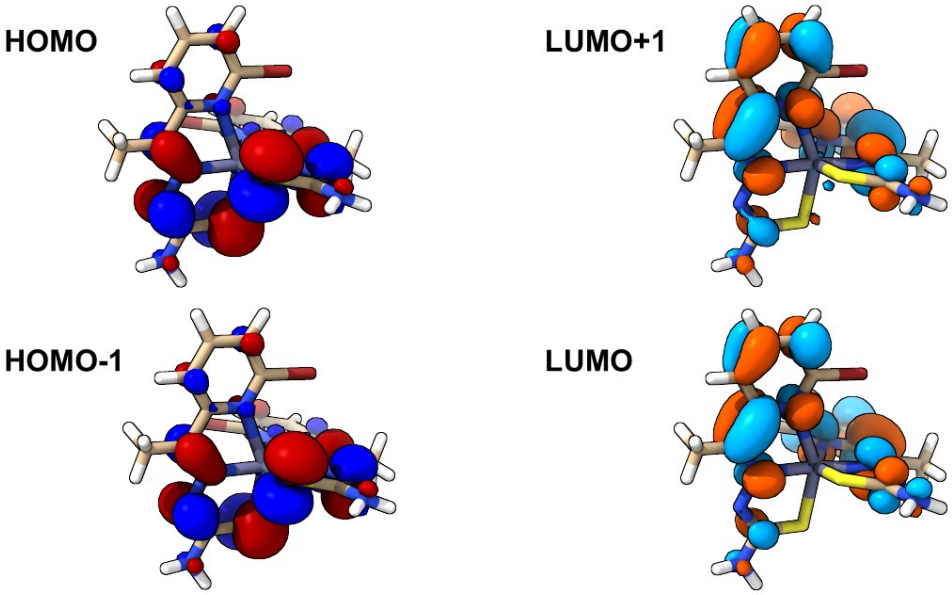

Figure S10. Frontier molecular orbitals (HOMO–1, HOMO, LUMO, and LUMO+1; isovalue 0.03) of the Zn(II) complex calculated at the WB97X-D4rev/def2-TZVP(−f)–SMD(DMSO) level of theory

Table S1. Crystal data and details of the structure refinement for [Zn(**L2**)$_2$].

formula	$C_{16}H_{16}Br_2N_8S_2Zn$
Fw (g mol^{-1})	609.68
crystal size (mm)	0.40×0.15×0.10
crystal color	yellow
crystal system	orthorhombic
space group	*Pbcn*
a (Å)	13.7666(9)
b (Å)	9.7475(8)
c (Å)	15.4591(9)
β (º)	90
V (Å^3)	2074.5(2)
Z	4
calcd density (g cm^{-3})	1.952
F(000)	1200
no. of collected reflns	8996
no. of independent reflns	2377
R_{int}	0.0316
no. of reflns observed	2020
no. parameters	139
$R[I > 2\sigma(I)]^a$	0.0266
wR_2(all data)^b	0.0638
Goof, S^c	1.121
$\Delta\rho_{max}/\Delta\rho_{min}$ (eÅ^3) (e Å^{-3})	+0.36/–0.65

$^a R = \sum||F_o| - |F_c||/\sum|F_o|$. $^b wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$.

$^c S = \{\sum[(F_o^2 - F_c^2)^2]/(n/p)\}^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.