Exploring the Structural Design, Antibacterial Activity, and Molecular Docking of Newly Synthesized Zn(II) Complexes with *NNO*-Donor Carbazate Ligands

Supporting Information

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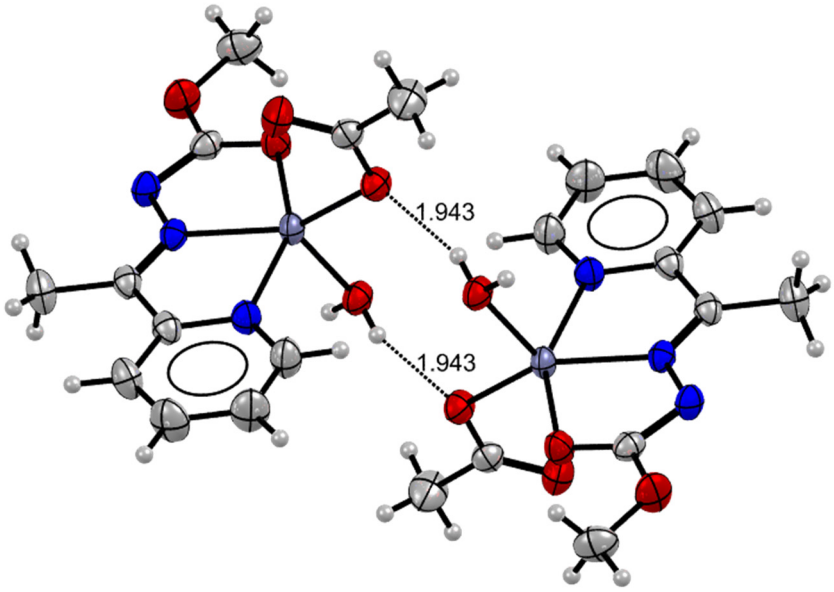

Figure S1: Intermolecular hydrogen interactions present in the Complex (1).

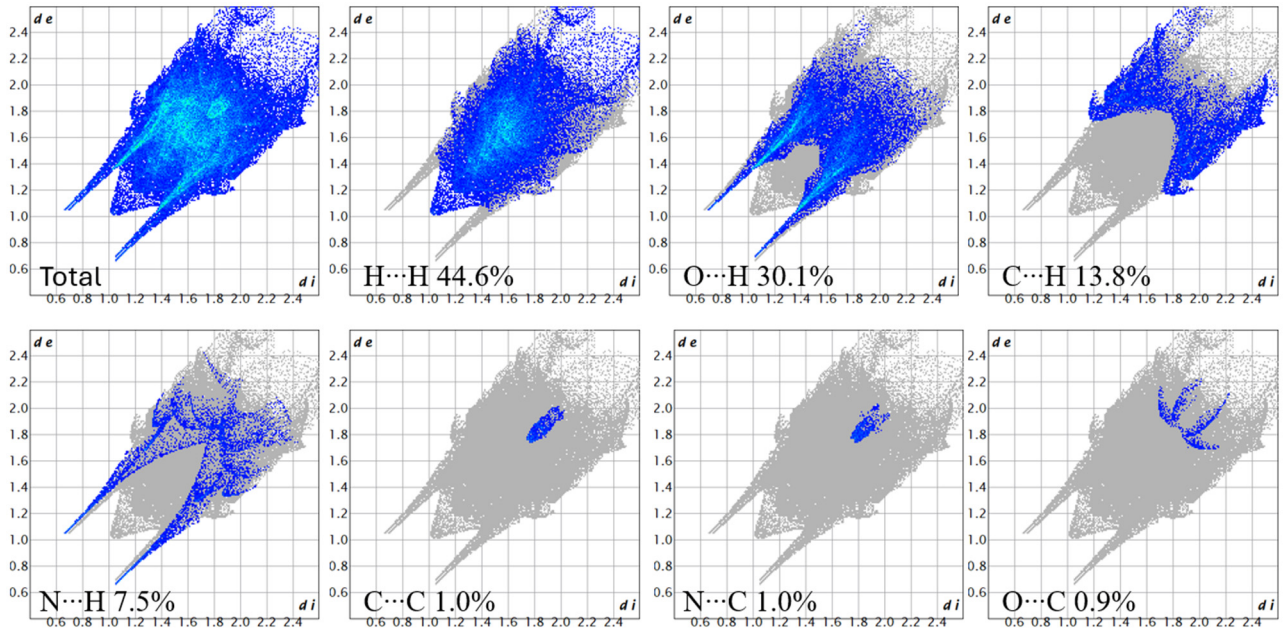

Figure S2: Total fingerprint plots and key complex (1) interactions.

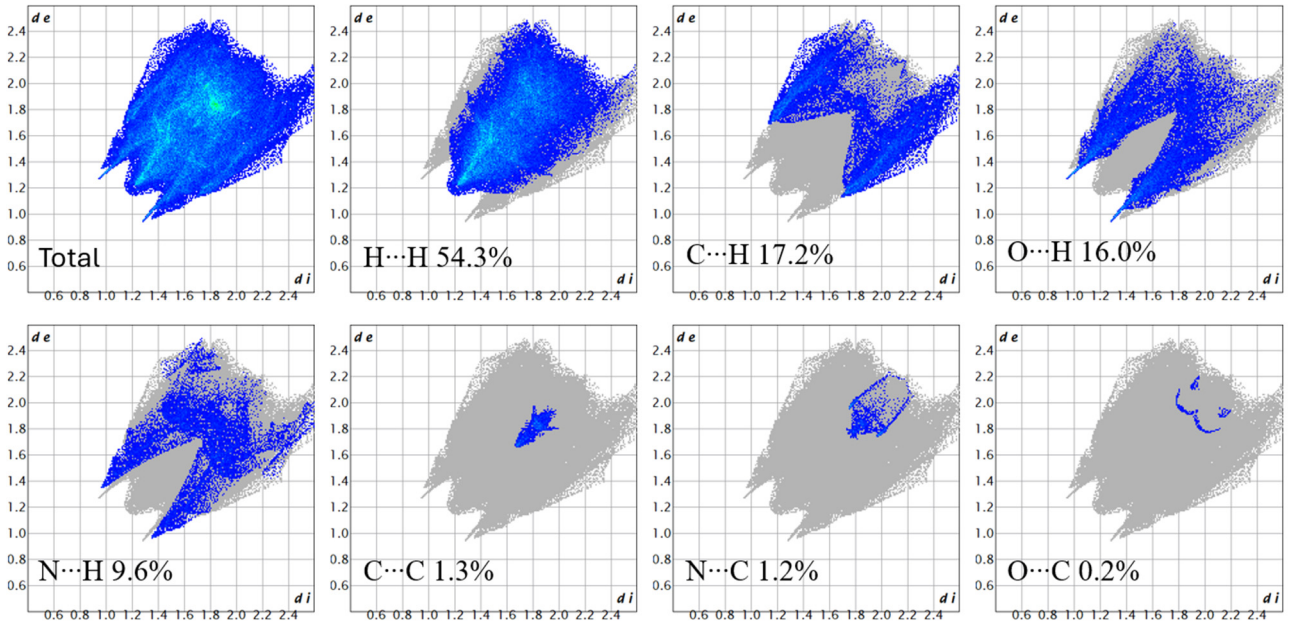

Figure S3: Total fingerprint plots and key complex (2) interactions.

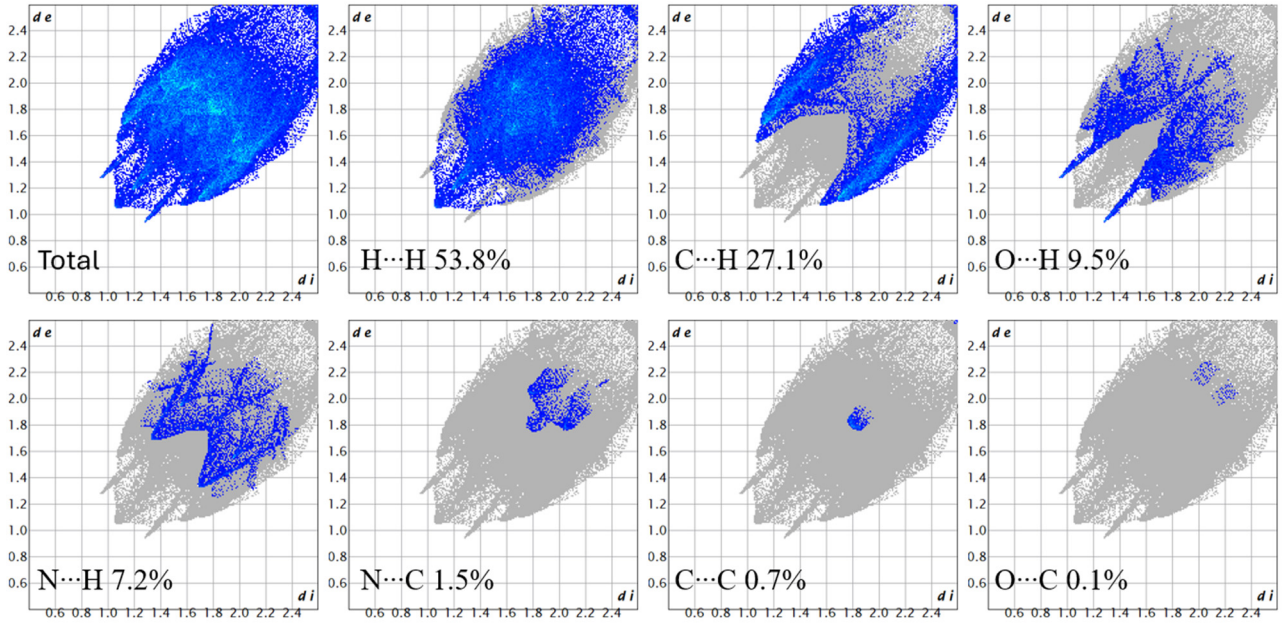

Figure S4: Total fingerprint plots and key complex (3) interactions.

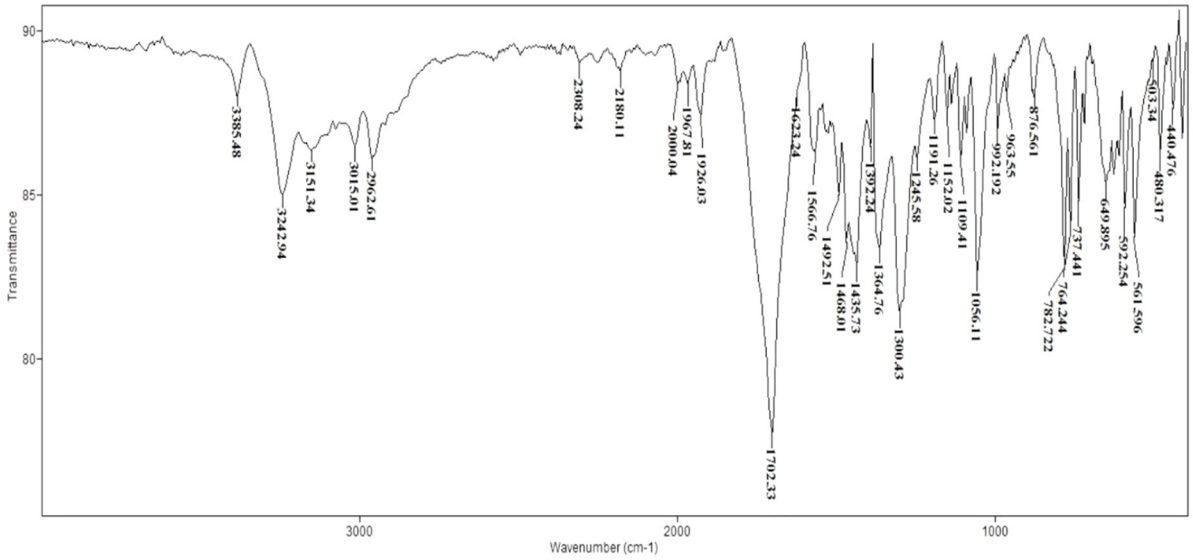

Figure S5: Infrared spectra of HL[1].

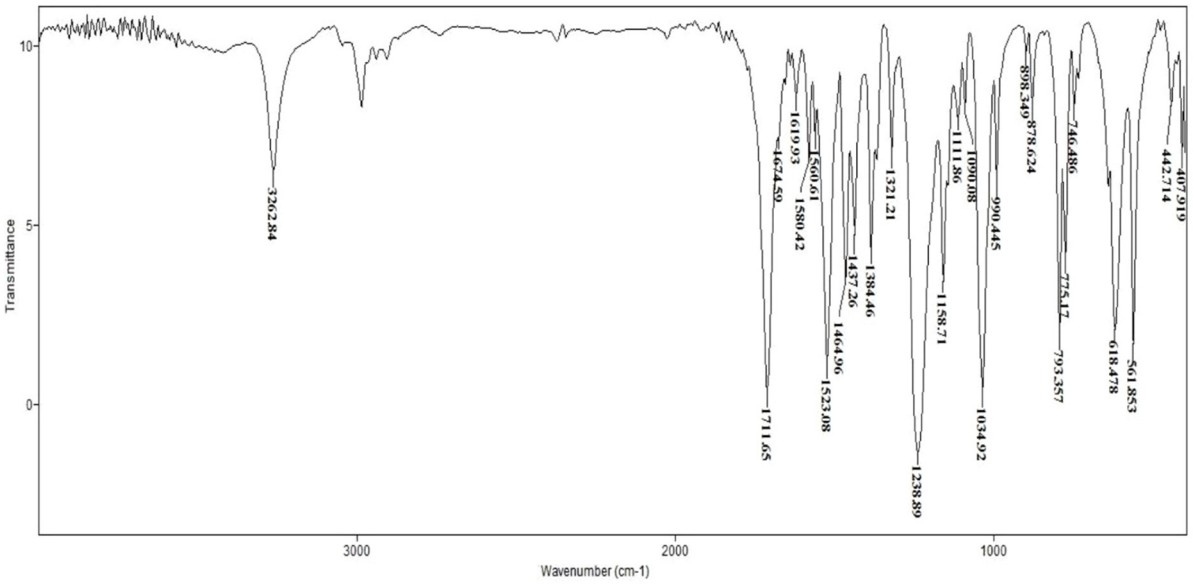

Figure S6: Infrared spectra of HL[2].

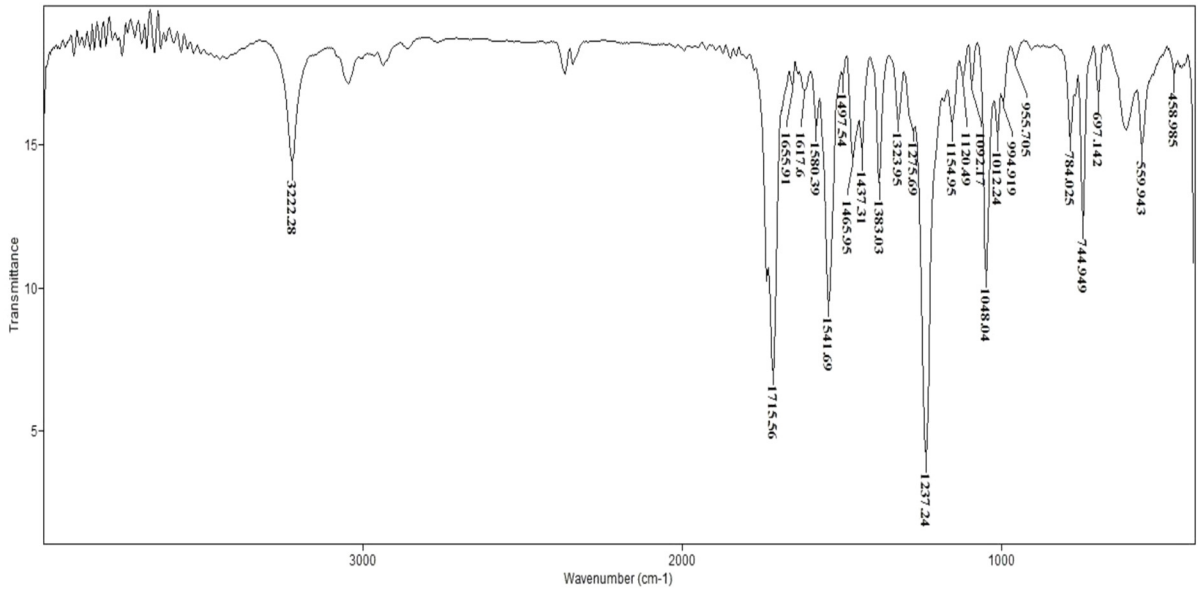

Figure S7: Infrared spectra of HL^3.

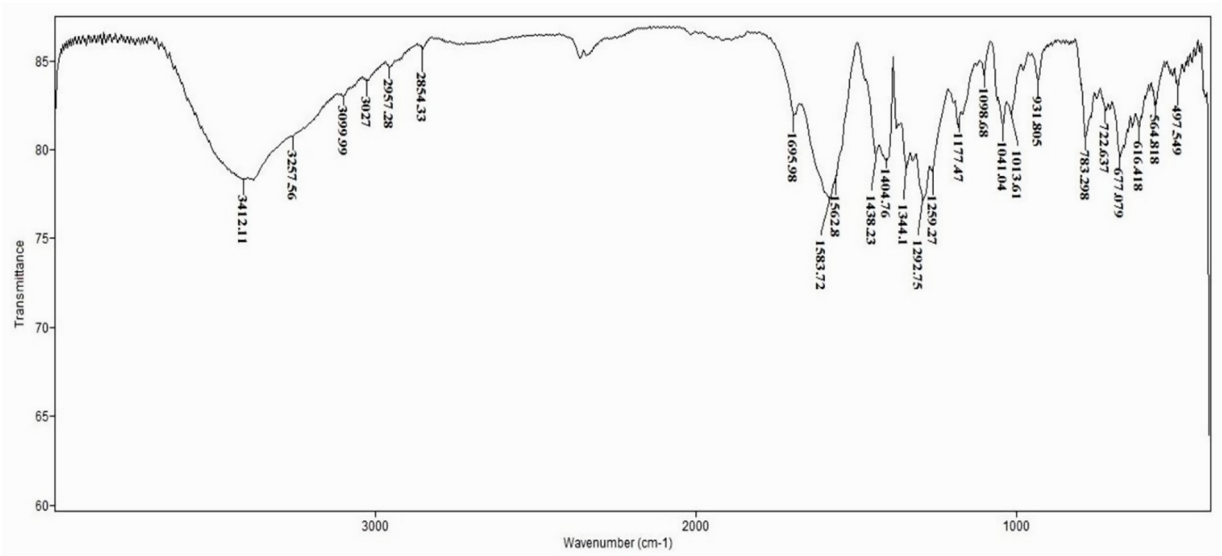

Figure S8: Infrared spectra of complex (1).

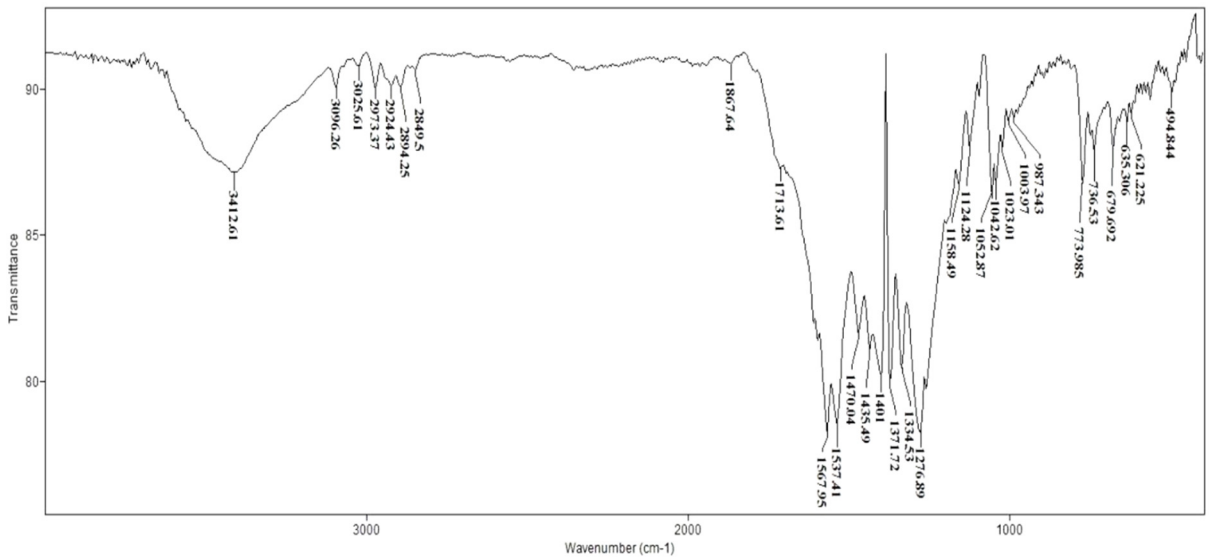

Figure S9: Infrared spectra of complex (2).

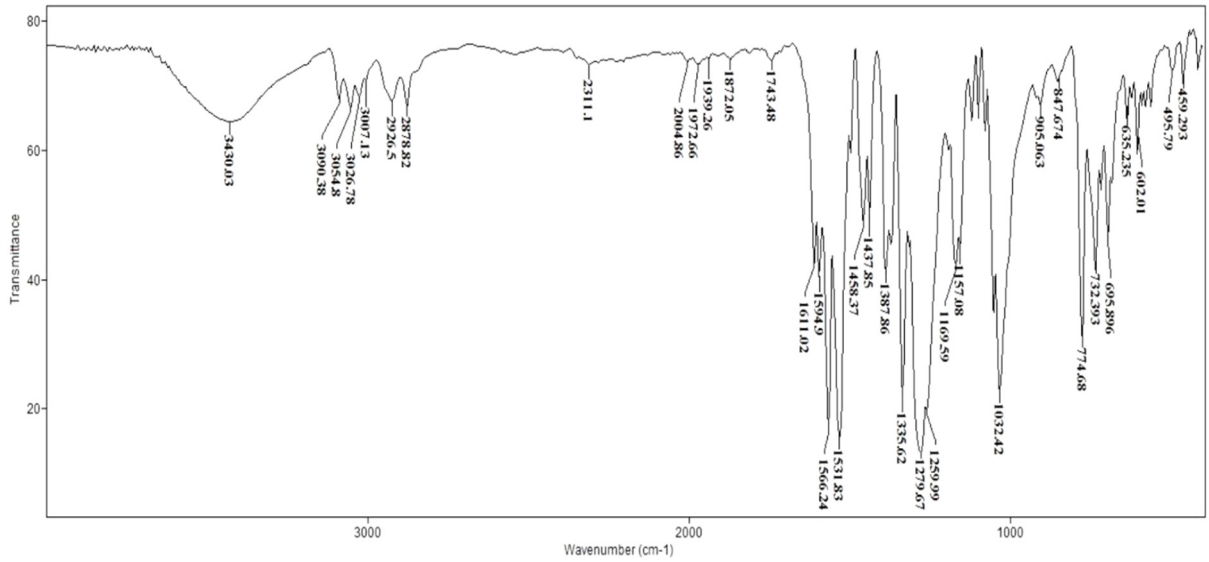

Figure S10: Infrared spectra of complex (3).

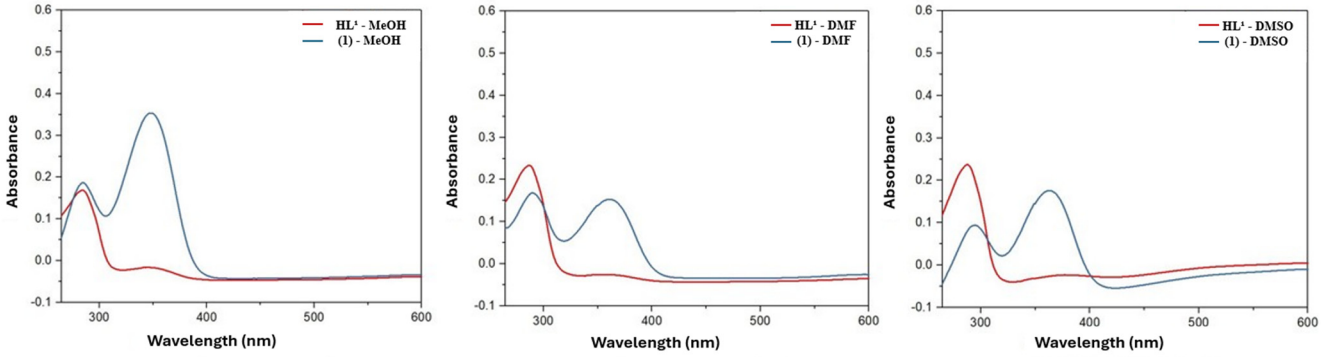

Figure S11: UV-Vis spectra of HL^1 and complex (1) in MeOH, DMF, and DMSO.

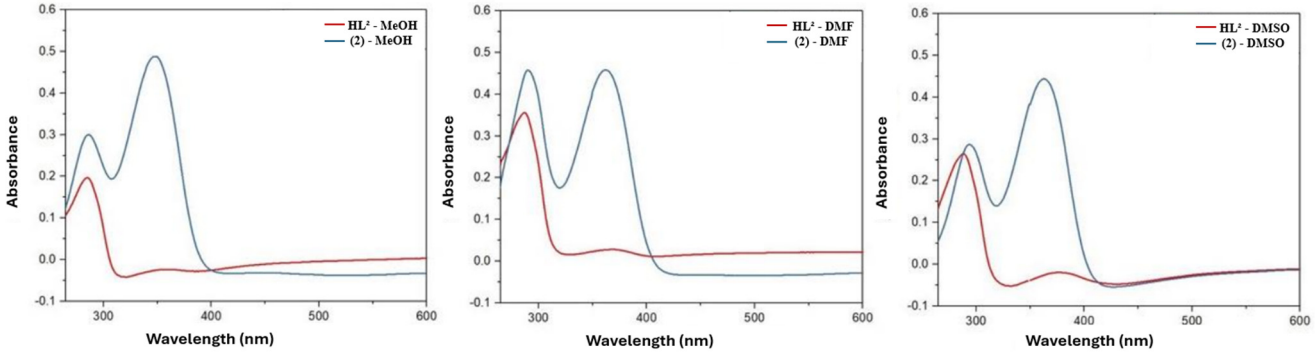

Figure S12: UV-Vis spectra of HL^2 and complex (2) in MeOH, DMF, and DMSO.

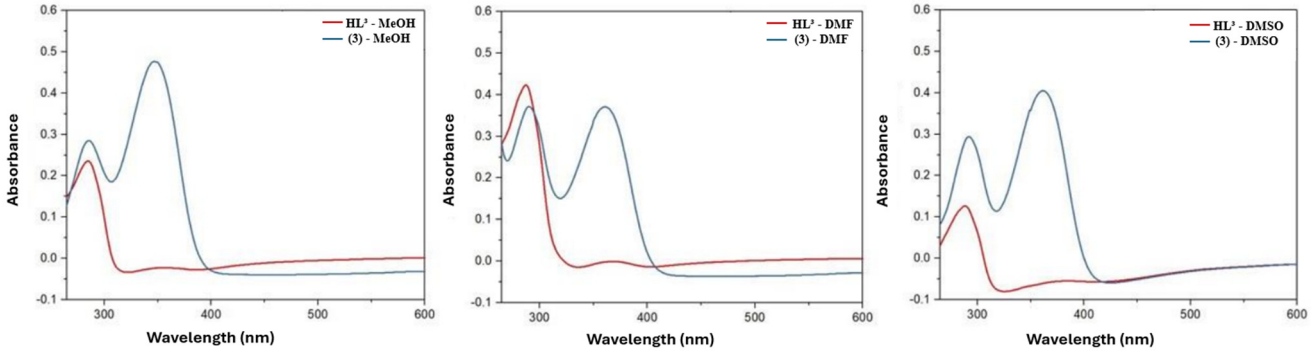

Figure S13: UV-Vis spectra of HL^3 and complex (3) in MeOH, DMF, and DMSO.

Table S1: Absorption values of the bands observed in the electronic spectra of HL^{1-3} and (1-3).

Compound	π→π* Transition (nm)			n→π* Transition (nm)			LMCT Transition (nm)		
	MeOH	DMF	DMSO	MeOH	DMF	DMSO	MeOH	DMF	DMSO
HL^1	284 (3.93)	287 (4.07)	288 (4.06)	347 (2.90)	356 (3.11)	377 (3.06)	-	-	-
HL^2	285 (3.99)	287 (4.25)	288 (4.11)	357 (3.07)	367 (3.15)	377 (2.99)	-	-	-
HL^3	285 (4.07)	288 (4.33)	288 (2.80)	355 (3.05)	368 (1.68)	383 (3.40)	-	-	-
(1)	285 (3.97)	290 (3.92)	295 (3.65)	-	-	-	349 (4.25)	361 (3.88)	363 (3.94)
(2)	286 (4.18)	290 (4.36)	294 (4.15)	-	-	-	348 (4.39)	362 (4.36)	363 (4.35)
(3)	285 (4.15)	290 (4.27)	292 (4.17)	-	-	-	347 (4.38)	361 (4.27)	361 (4.31)

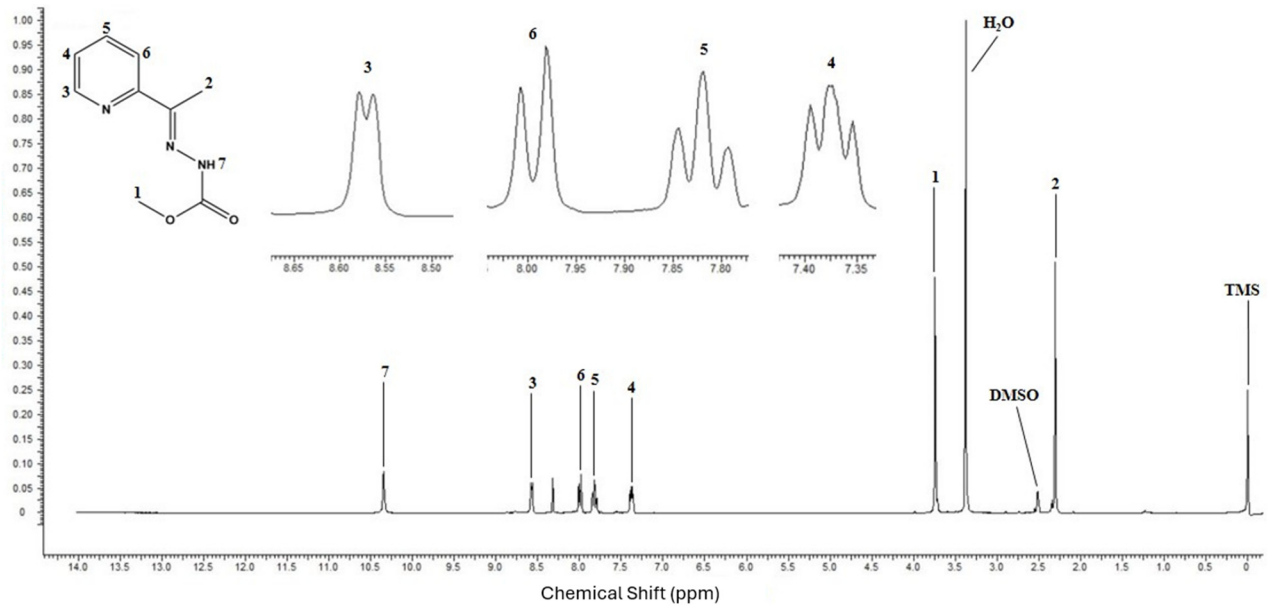

Figure S14: ^{1}H NMR spectra of HL^1 in DMSO-d_6.

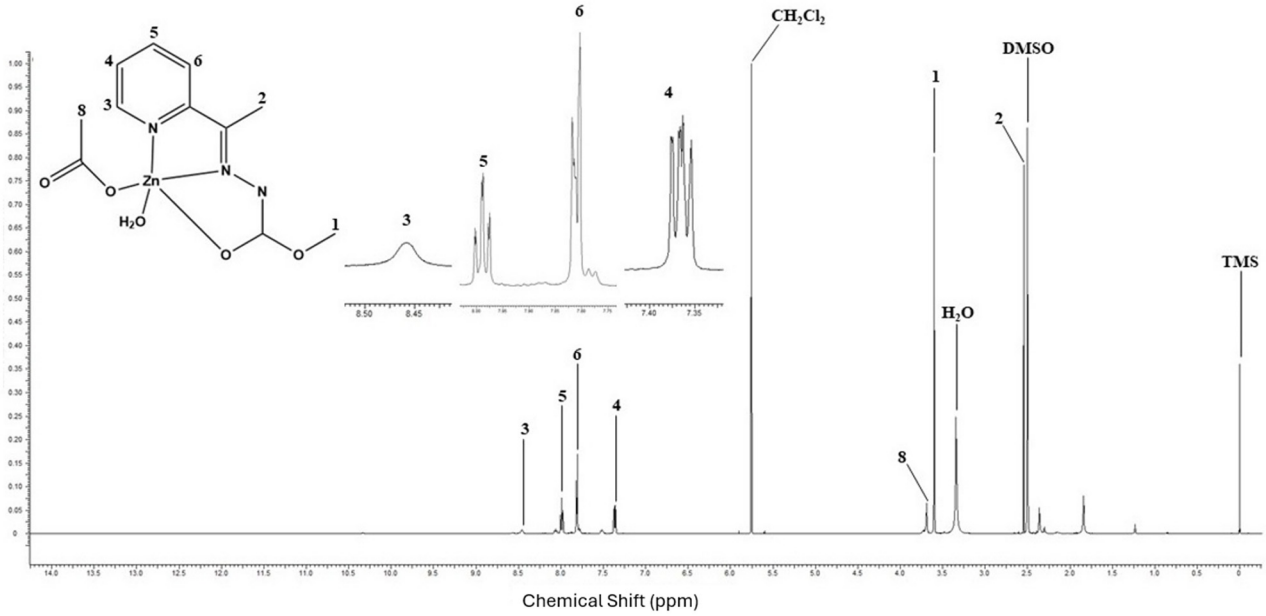

Figure S15: ^{1}H NMR spectra of Complex (1) in DMSO-d$_6$.

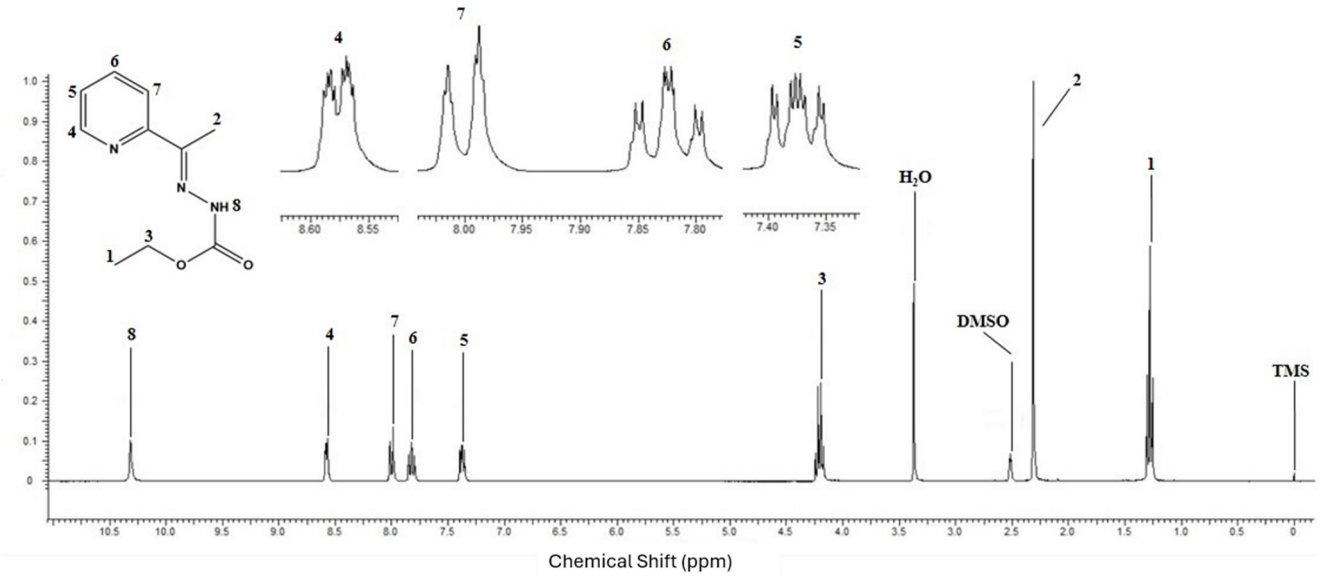

Figure S16: ^{1}H NMR spectra of HL^{2} in DMSO-d$_6$.

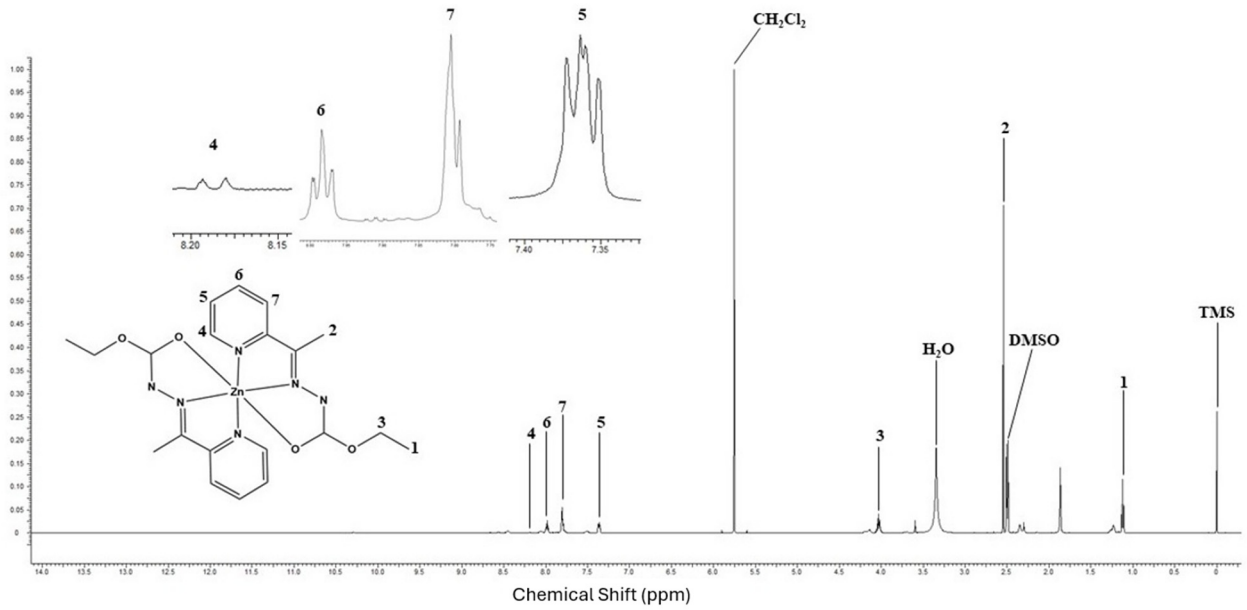

Figure S17: ^{1}H NMR spectra of Complex (2) in DMSO-d$_6$.

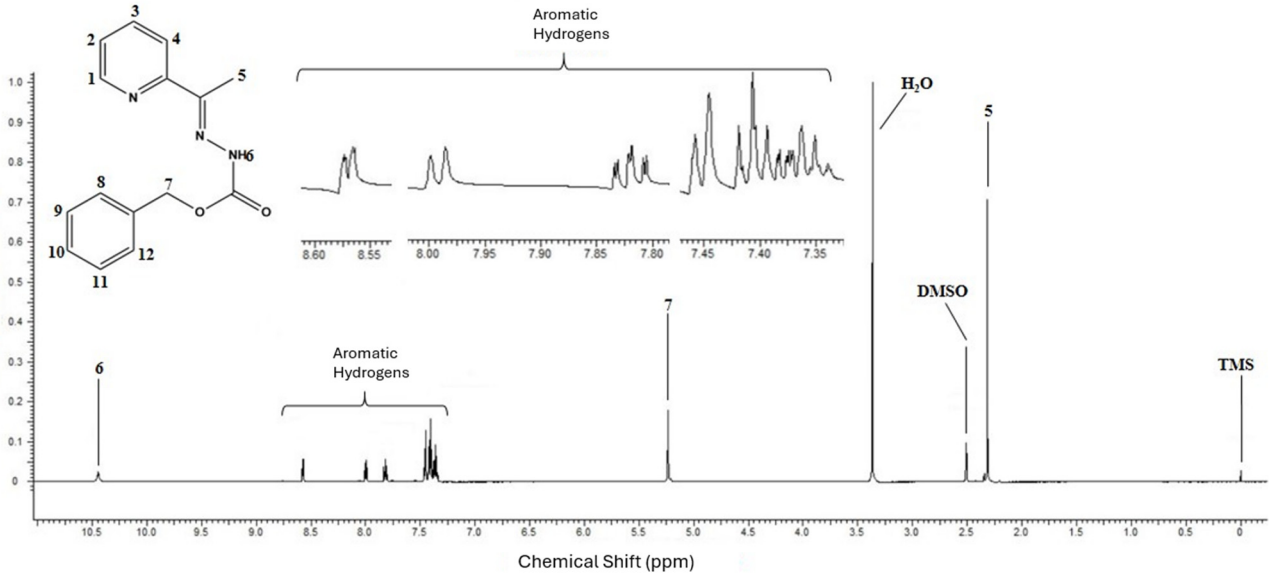

Figure S18: ^{1}H NMR spectra of HL^3 in DMSO-d$_6$.

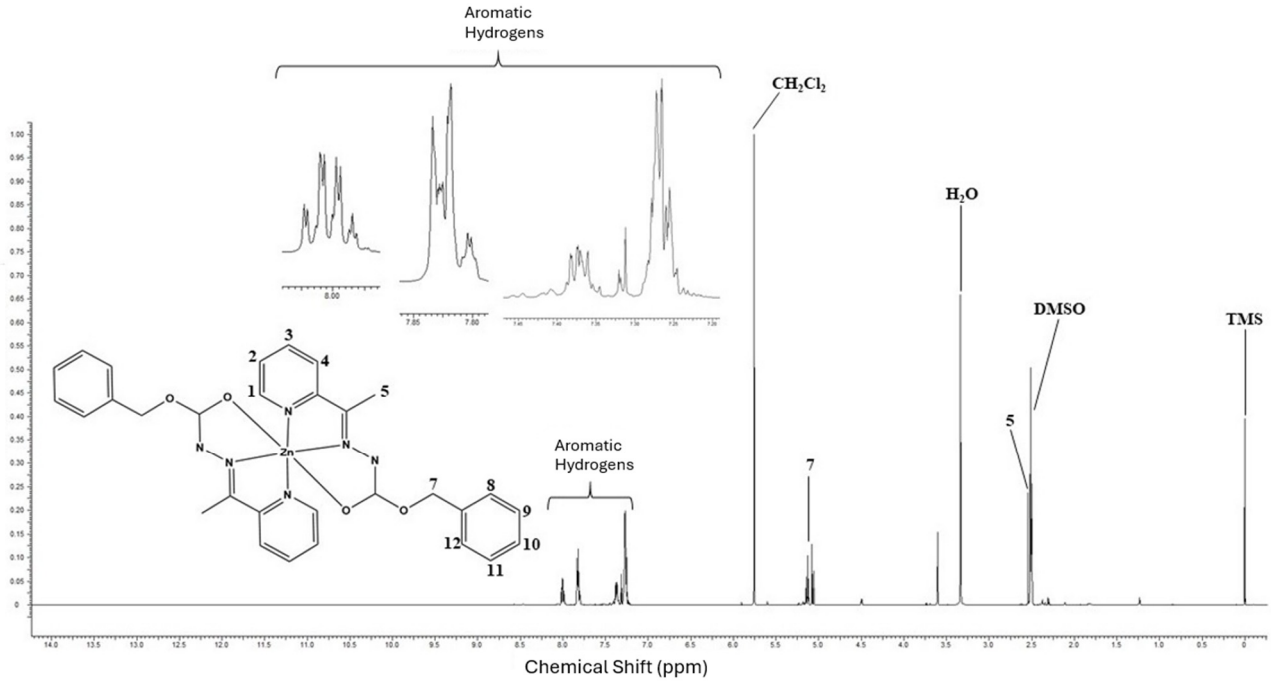

Figure S19: ^{1}H NMR spectra of complex (3) in DMSO-d_6.

Table S2. X-ray diffraction data collection and refinement parameters for the complexes (1–3).

	(1)	**(2)**	**(3)**
Chemical formula	$C_{11}H_{15}N_3O_5Zn$	$C_{20}H_{24}N_6O_4Zn$	$C_{30}H_{28}N_6O_4Zn$
M (g mol^{-1})	334.63	477.82	601.95
Crystal system	Monoclinic	Monoclinic	Orthorhombic
Space group	*P2₁/c*	*P2₁/c*	*Pbcn*
Unit cell			
a (Å)	9.656(12)	10.178(3)	12.084(17)
b (Å)	16.465(2)	21.459(5)	9.809(13)
c (Å)	9.105(11)	10.155(3)	24.457(3)
β (º)	104.823(2)	90.435	90
V ($Å^3$)	1399.3(3)	2217.8(10)	2898.8(7)
Z	4	4	4
Density ($Mg/^{m3}$)	1.588	1.431	1.379
Index ranges	$-10 \le h \le 12$	$-12 \le h \le 12$	$-6 \le h \le 14$
	$-20 \le k \le 20$	$-16 \le k \le 25$	$-11 \le k \le 11$
	$-11 \le l \le 11$	$-9 \le l \le 12$	$-29 \le l \le 27$
Absorption coefficient /mm^{-1}	1.777	1.146	0.893
Absorption correction	multi-scan	multi-scan	multi-scan
Max/min transmission	0.677/0.495	0.836/0.606	0.975/0.994
Measured reflections	14781	14091	13356
Independent reflections / Rint	2878/0.043	3893/0.080	2558/0.054
Refined parameters	192	284	332
R_1 (F)	0.029	0.053	0.047
wR_2 (F^2) ($I > 2\sigma(I)$)	0.069	0.099	0.100
GooF	1.065	1.015	1.020
Largest diff. peak and hole ($eÅ^{-3}$)	0.256 and -0.276	0.298 and -0.508	0.263 and -0.303
CCDC number	2354507	2354508	2354509