

SUPPLEMENTRY INFORMATION

Novel Amide-Based Macrocyclic Co(II) Complexes: Correlating Structural, Computational, and Biological Properties Through DFT and Docking

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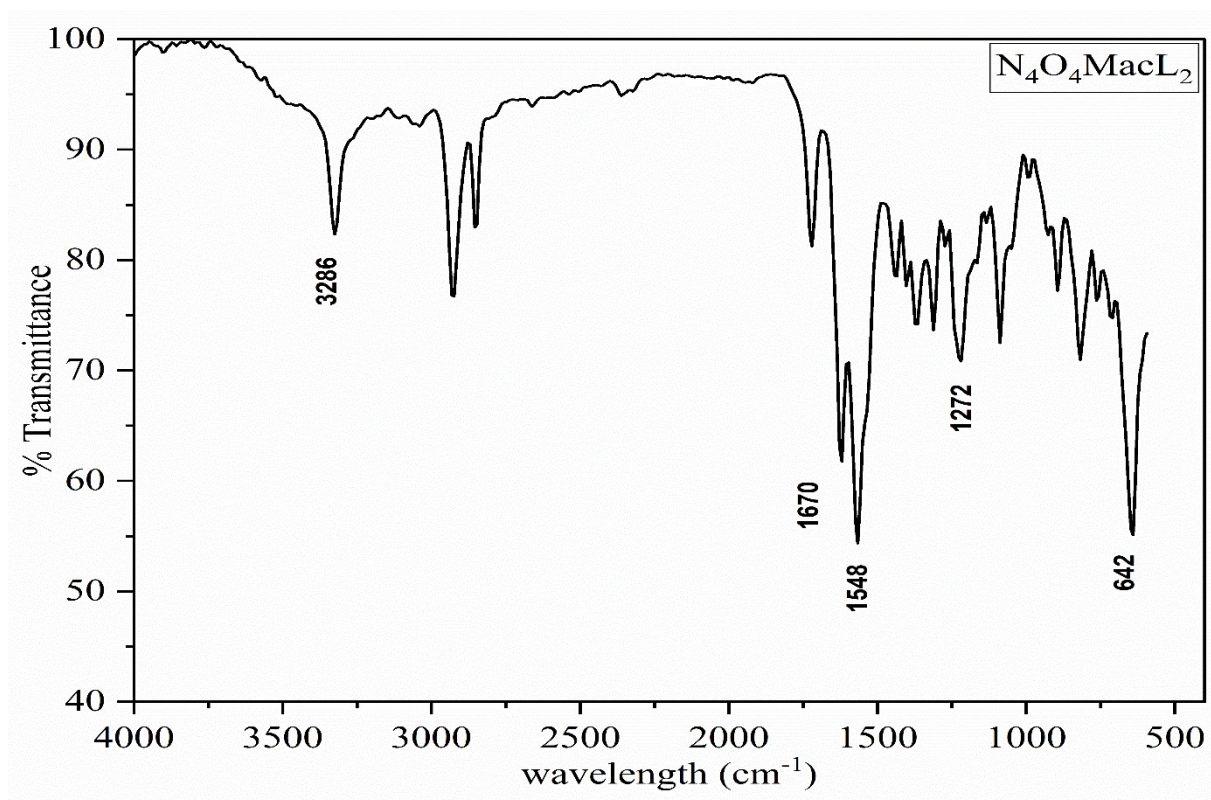


FIGURE S1 FTIR spectra of Macrocyclic ligand $N_4O_4ML_2$

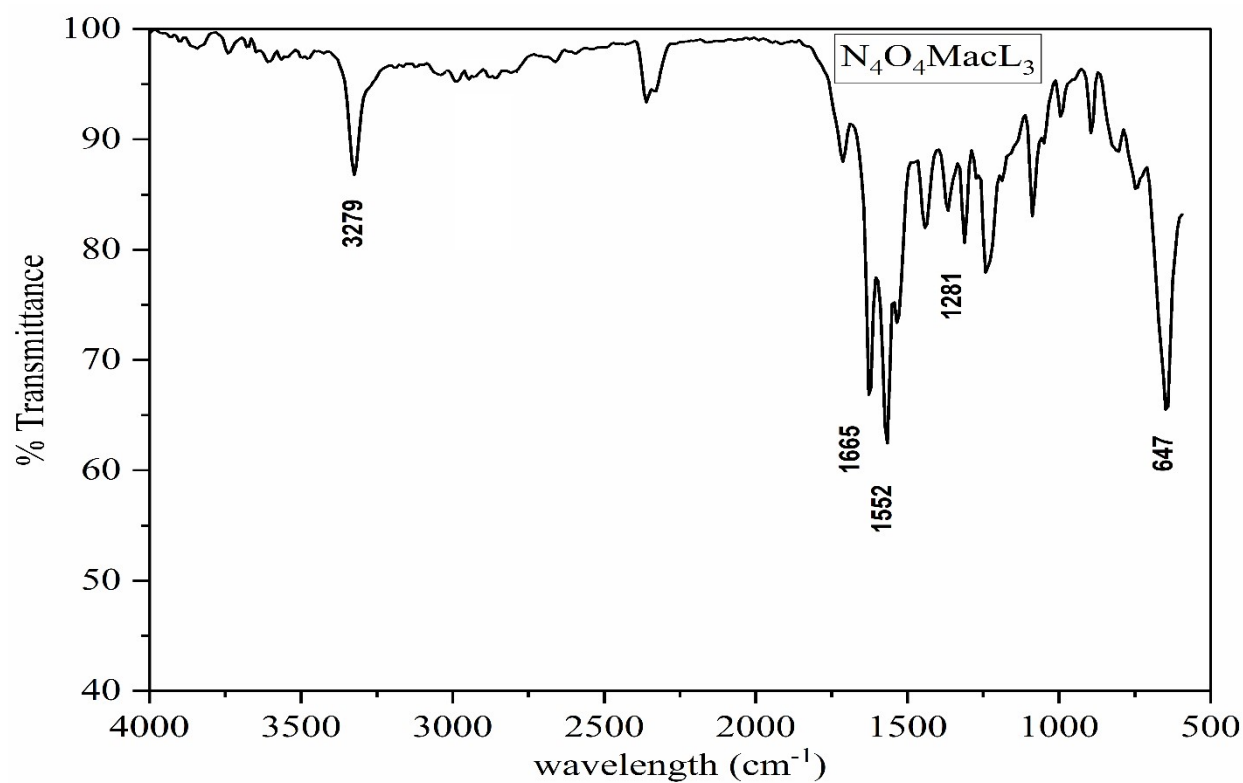


FIGURE S2 FTIR spectra of tetraamide macrocyclic ligand $N_4O_4ML_3$

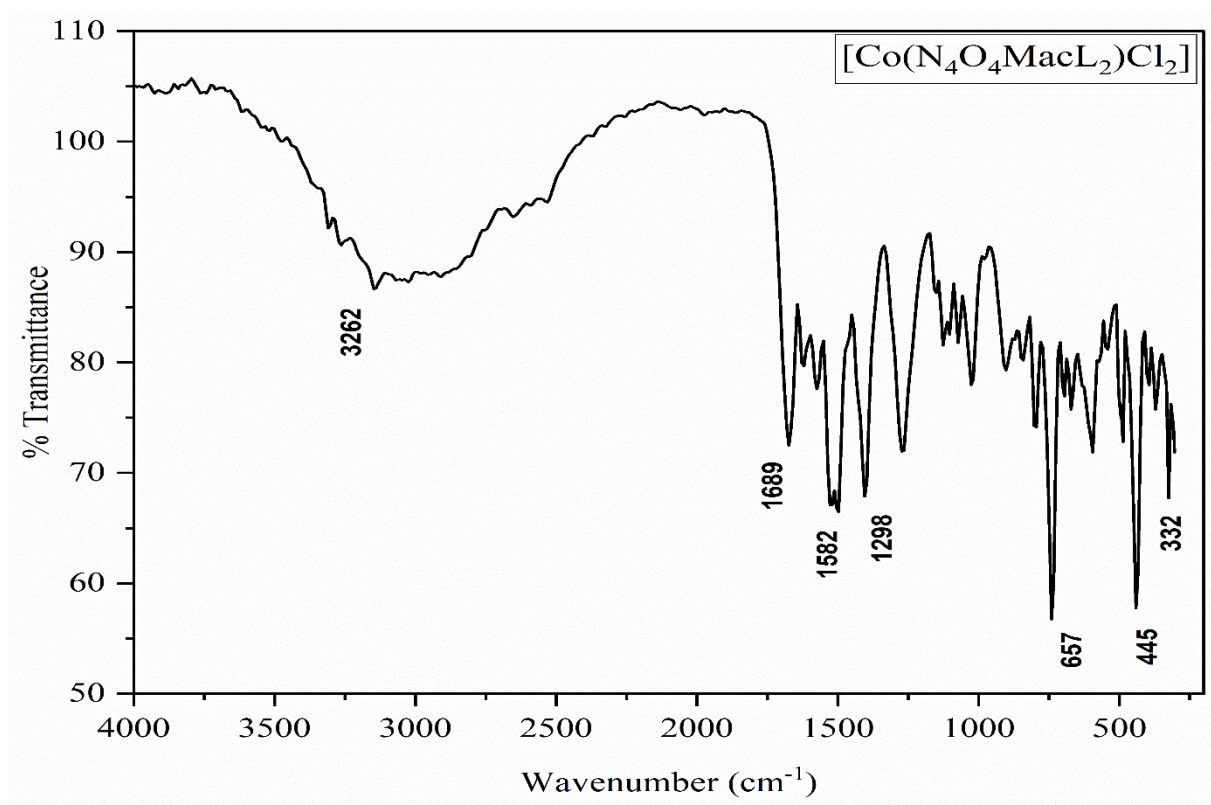


FIGURE S3 FTIR spectra of cobalt(II) Macrocylic Complex $[\text{Co}(\text{N}_4\text{O}_4\text{ML}_2)\text{Cl}_2]$ (8b).

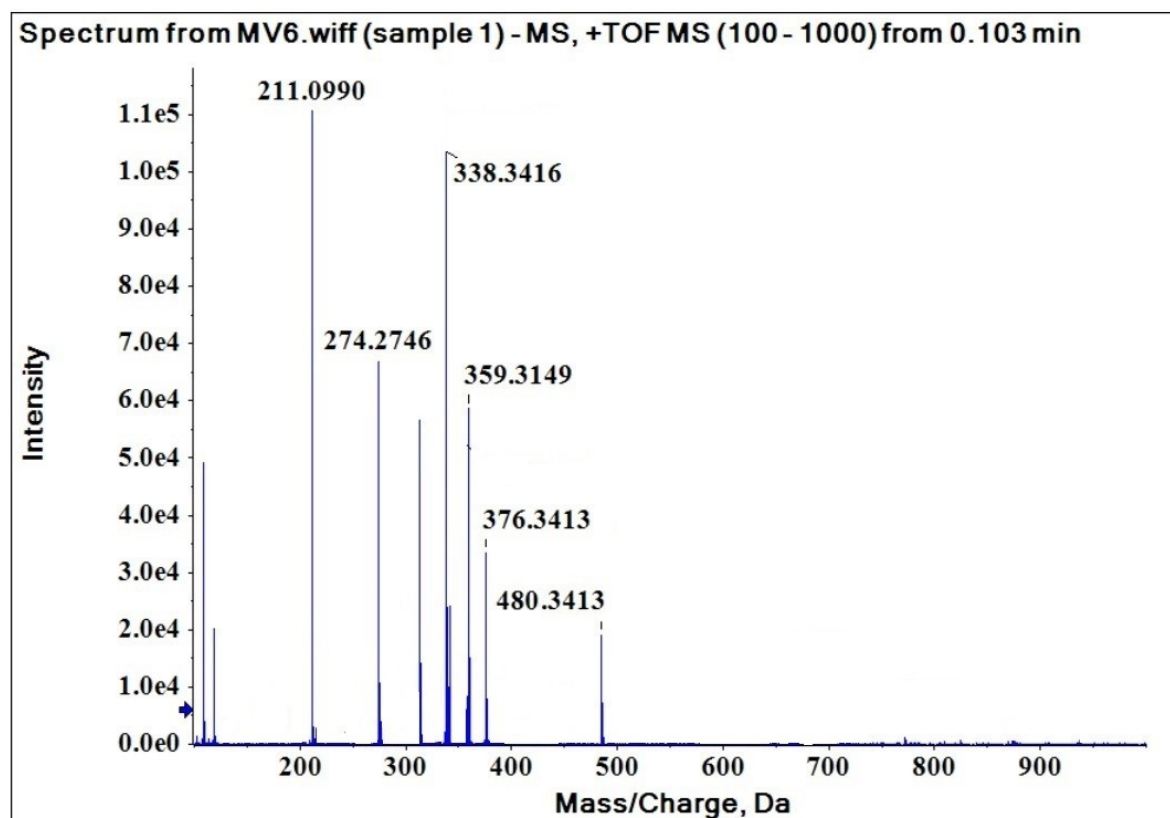


FIGURE S4 Mass spectrum of tetraamide Macrocylic ligand $\text{N}_4\text{O}_4\text{MacL}_1$



FIGURE S5 Mass spectrum of Co (II) Macrocyclic Complex $[\text{Co}(\text{N}_4\text{O}_4\text{ML}_2)\text{Cl}_2]$

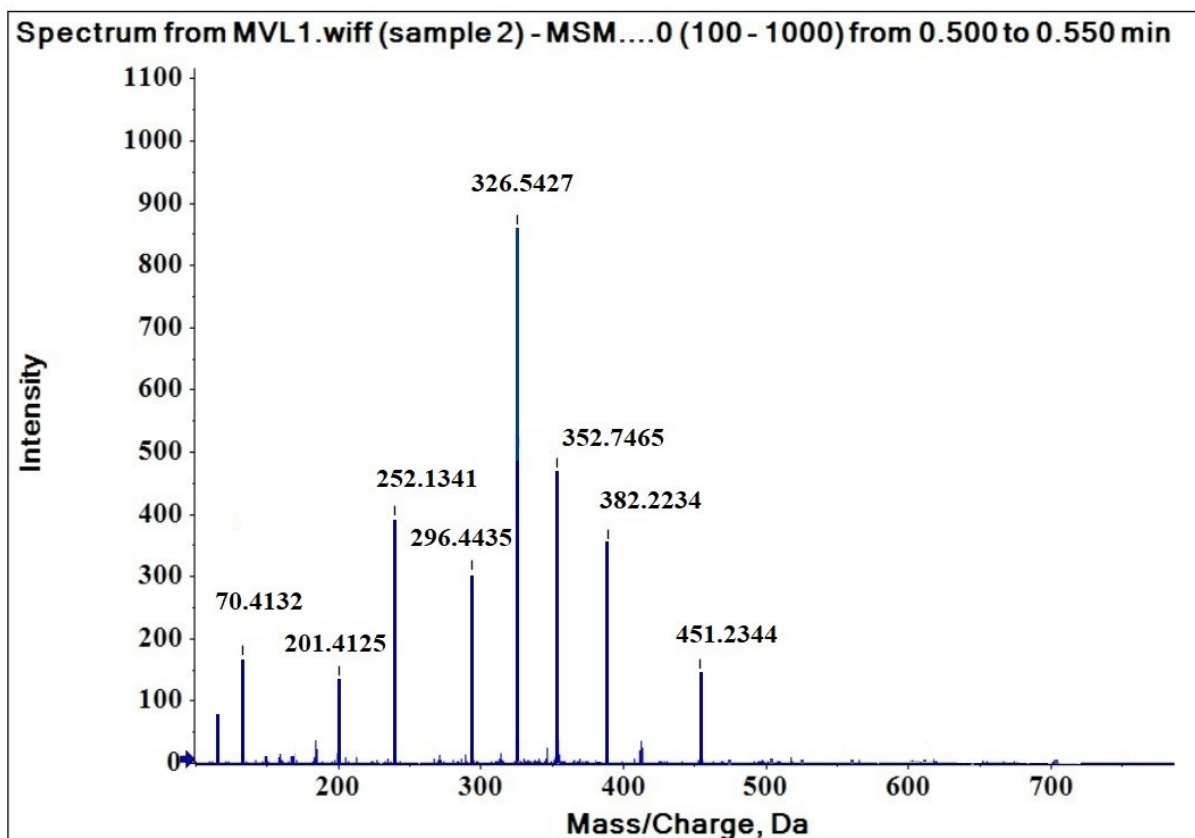


FIGURE S6 Mass spectrum of tetraamide Macrocylic ligand $N_4O_4MacL_1$

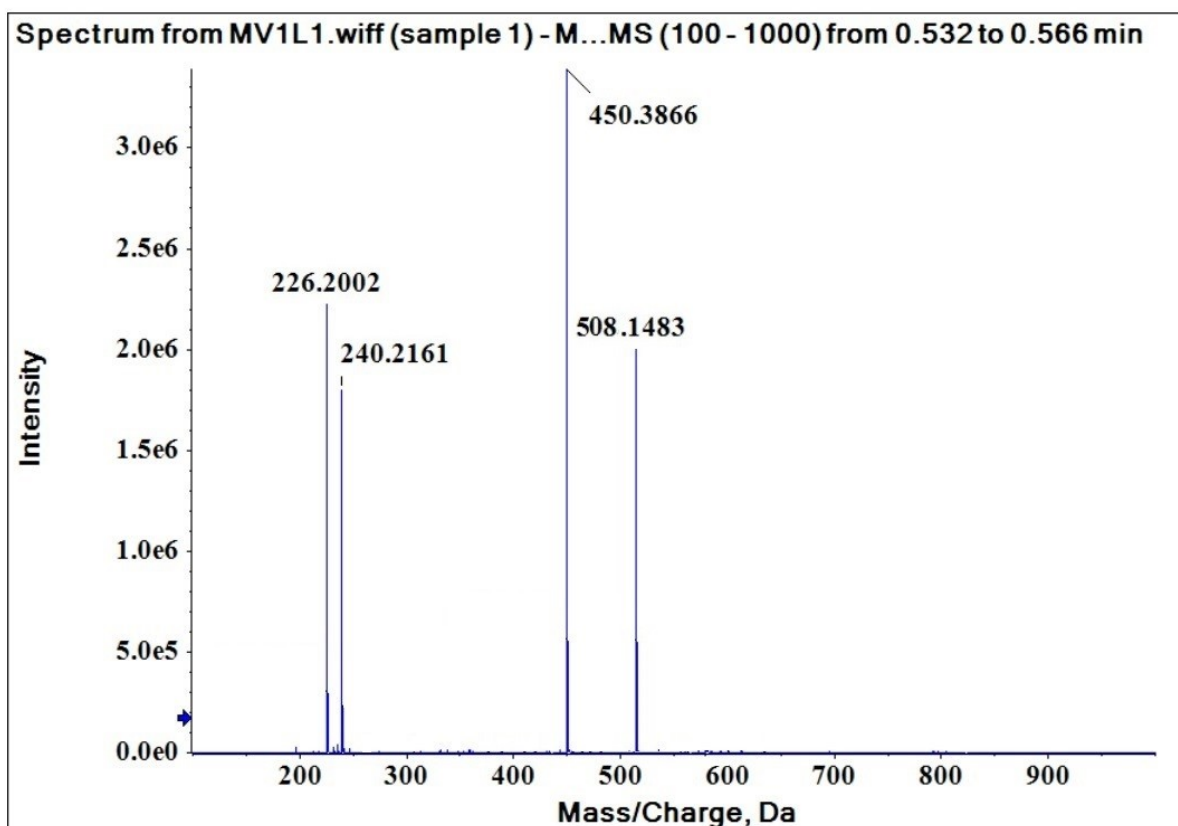


FIGURE S7 Mass spectrum of tetraamide Macrocylic ligand $N_4O_4MacL_3$

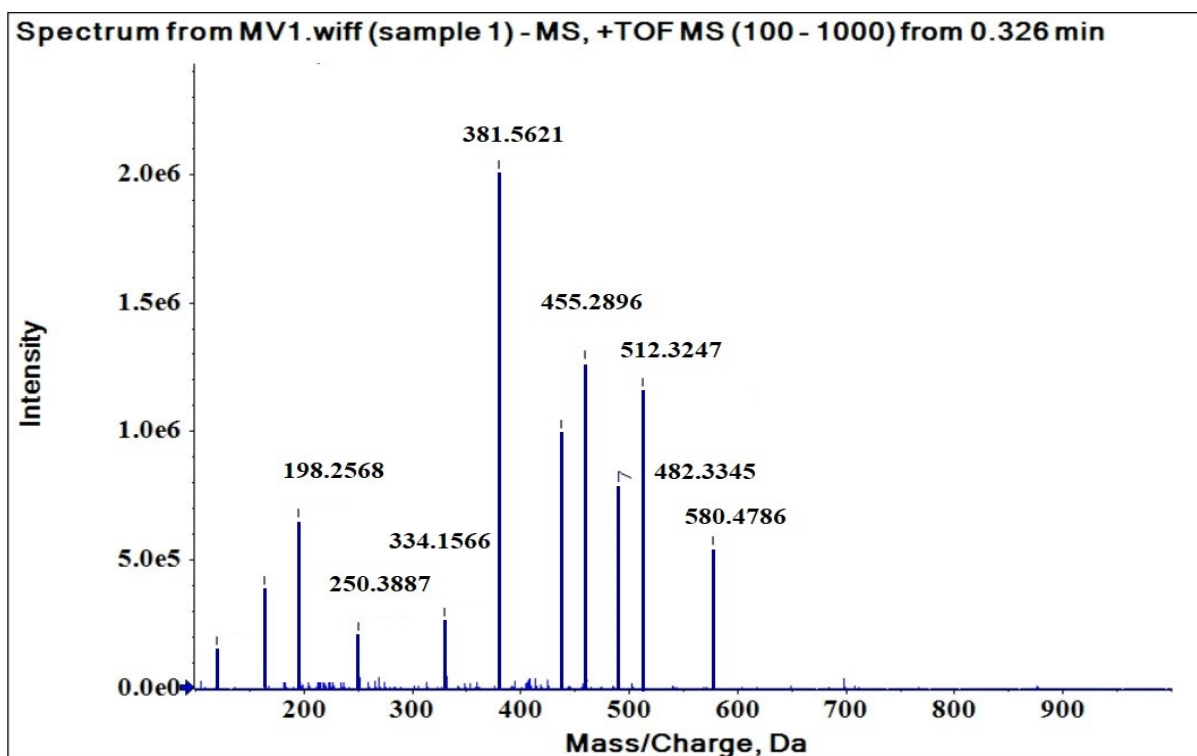


FIGURE S8 Mass spectrum of Co (II) Macrocylic Complex $[\text{Co}(\text{N}_4\text{O}_4\text{ML}_2)\text{Cl}_2]$

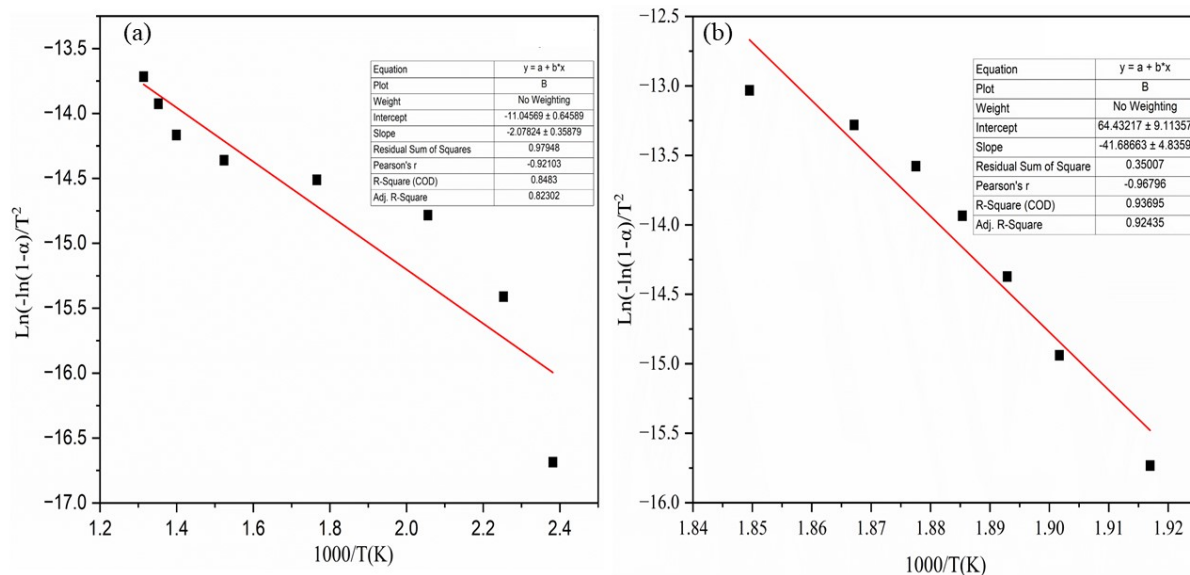


FIGURE S9 Coats-Redfern plots at $10^\circ/\text{min}$ heating rate for macrocyclic ligand $\text{N}_4\text{O}_4\text{MacL}_2$ and complex $[\text{Co}(\text{N}_4\text{O}_4\text{MacL}_2)\text{Cl}_2]$

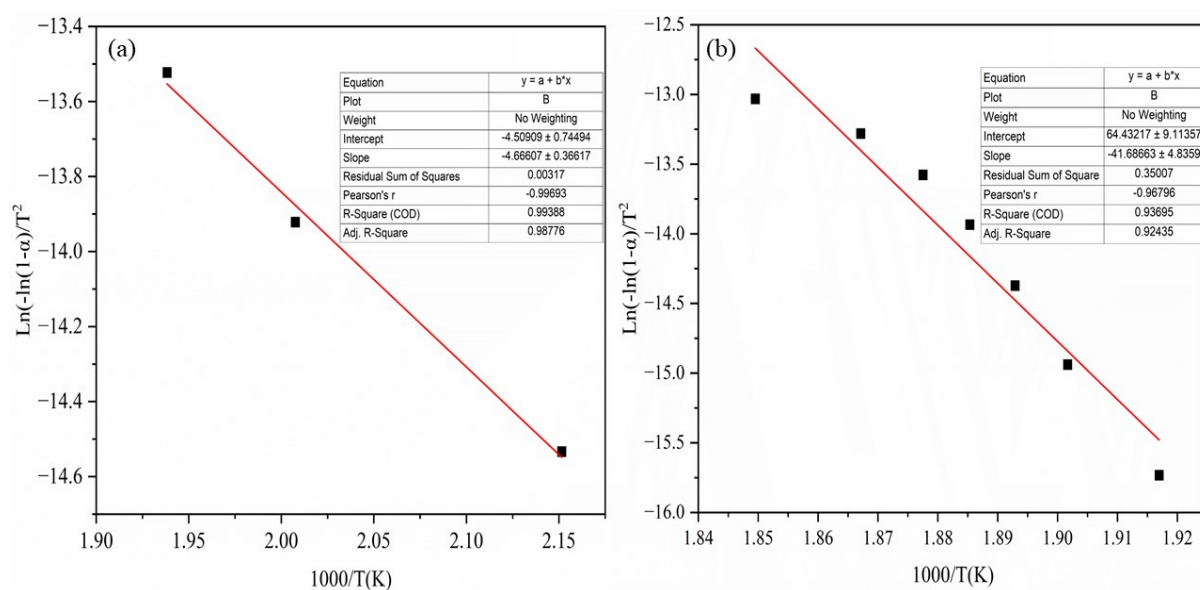


FIGURE S10 Coats-Redfern plots at $10^\circ/\text{min}$ heating rate for macrocyclic ligand $N_4O_4MacL_3$ and complex $[Co(N_4O_4MacL_3)Cl_2]$.

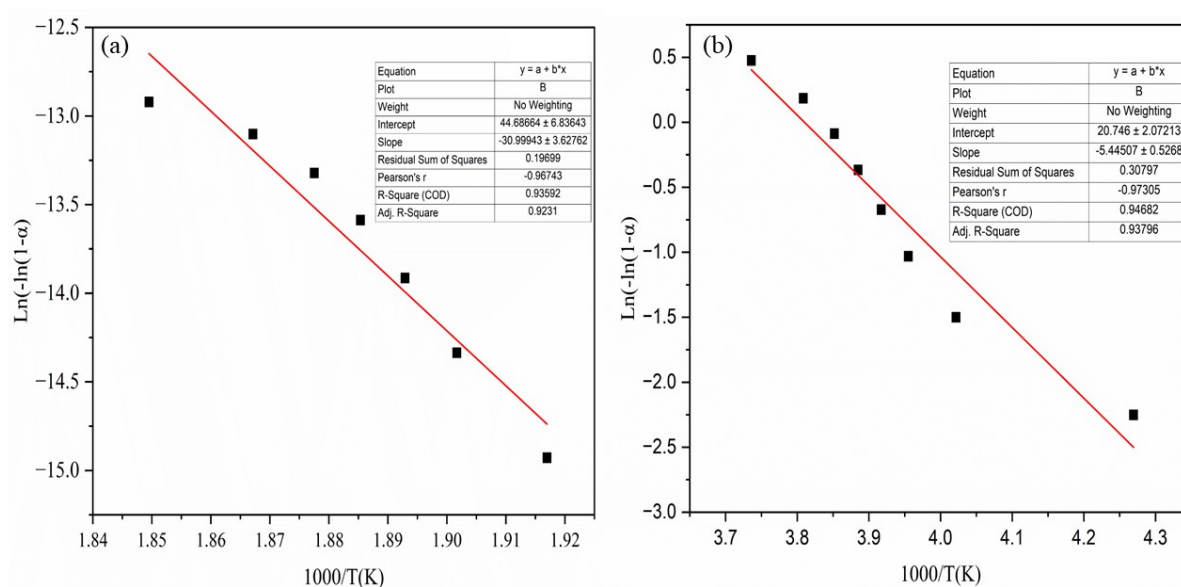


FIGURE S11 The linear fitted curve obtained through FWO method at $10^\circ/\text{min}$ heating rate of macrocyclic ligand $N_4O_4MacL_2$ and Complex $[Co(N_4O_4MacL_2)Cl_2]$

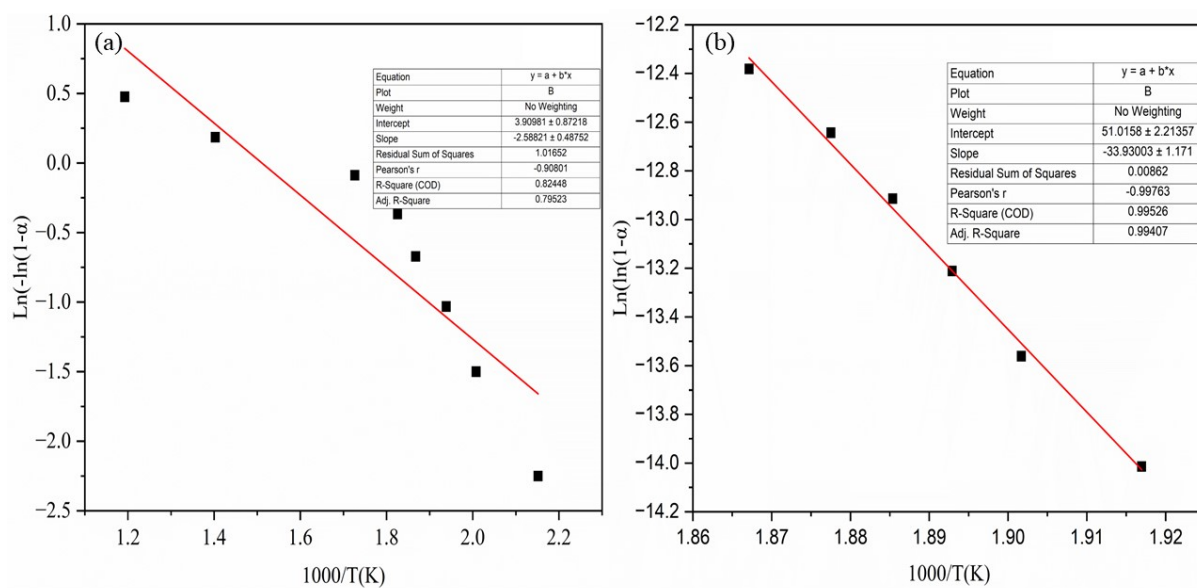


FIGURE S12 The linear fitted curve obtained through FWO method at 10°/min heating rate of macrocyclic ligand $N_4O_4MacL_3$ and Complex $[Co(N_4O_4MacL_3)Cl_2]$

TABLE S1 Physical properties and analytical data of macrocyclic ligands and their Co(II) complexes

Compound	Empirical Formula	% Yield	M.P. ^o C & Colour	Analysis, Found (Calcd.) %					Mol. Wt. Found (Calcd.)
				C	H	N	Cl	Co	
N ₄ O ₄ MacL ₁	C ₂₆ H ₂₀ N ₄ O ₄	75	220-225 Dark Brown	68.45 (69.02)	4.43 (4.46)	12.12 (12.38)	-	-	451.44 (452.47)
N ₄ O ₄ MacL ₂	C ₂₈ H ₂₄ N ₄ O ₄	79	215-221 Brown	68.94 (69.99)	5.08 (5.03)	11.28 (11.66)	-	-	480.3413 (480.52)
N ₄ O ₄ MacL ₃	C ₃₀ H ₂₈ N ₄ O ₄	78	225-232 Brown	70.65 (70.85)	5.37 (5.55)	11.10 (11.02)	-	-	508.14 (508.21)
[Co(N ₄ O ₄ MacL ₁)Cl ₂]	C ₂₆ H ₂₀ Cl ₂ CoN ₄ O ₄	77	245-250 Reddish Pink	53.54 (53.63)	3.38 (3.46)	9.46 (9.62)	12.11 (12.18)	10.02 (10.12)	580.47 (582.32)
[Co(N ₄ O ₄ MacL ₂)Cl ₂]	C ₂₈ H ₂₄ Cl ₂ CoN ₄ O ₄	71	252-257 Brown	55.05 (55.10)	3.79 (3.96)	9.10 (9.18)	11.45 (11.62)	9.59 (9.66)	608.61 (610.36)
[Co(N ₄ O ₄ MacL ₃)Cl ₂]	C ₃₀ H ₂₈ Cl ₂ CoN ₄ O ₄	80	255-259 Brown	56.35 (56.44)	4.32 (4.42)	08.70 (08.78)	11.05 (11.11)	9.18 (9.23)	638.61 (638.41)

Table S2. EPR parameters of Co(II) complexes

Complexes	$g_{\parallel}$	$g_{\perp}$	$ g $	G	$A_{\parallel} \times 10^5 (\text{cm}^{-1})$	$K_{\parallel}^2$	$K_{\perp}^2$	$-\lambda$
[Co(N ₄ O ₄ MacL ₁)Cl ₂]	2.24	2.07	2.12	4.31	605	0.593	0.556	496
[Co(N ₄ O ₄ MacL ₂)Cl ₂]	2.25	2.05	2.12	4.29	605	0.594	0.554	499
[Co(N ₄ O ₄ MacL ₃)Cl ₂]	2.29	2.04	2.12	4.24	604	0.596	0.556	497