

Mixed ligand cobalt(II) picolinate complexes: synthesis, characterization, DNA binding and photocleavage

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Supporting Information:

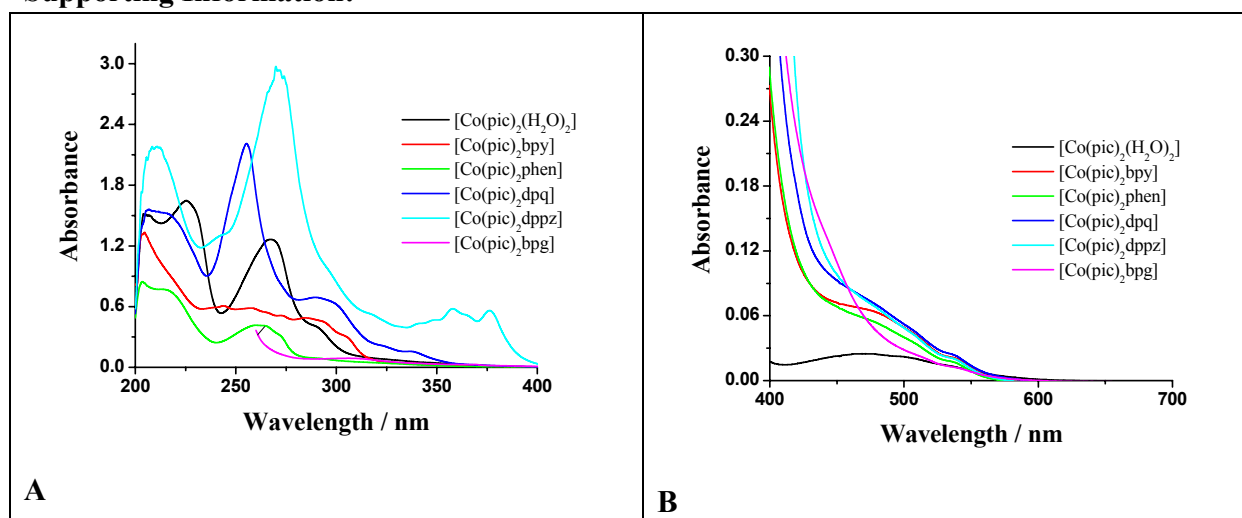
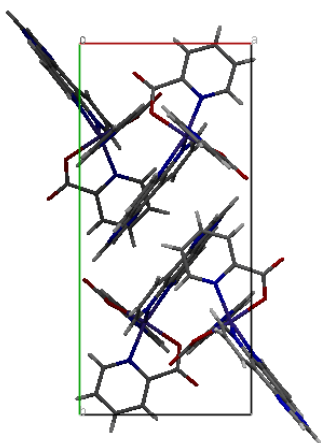


Fig. S1 Absorption spectra of complexes **1–5** in methanol and **6** in DMSO medium **A)** [Complex] = 1.7×10^{-4} M **B)** 1×10^{-3} M.



Fi g. S2 Packing diagram of the complex **4**.

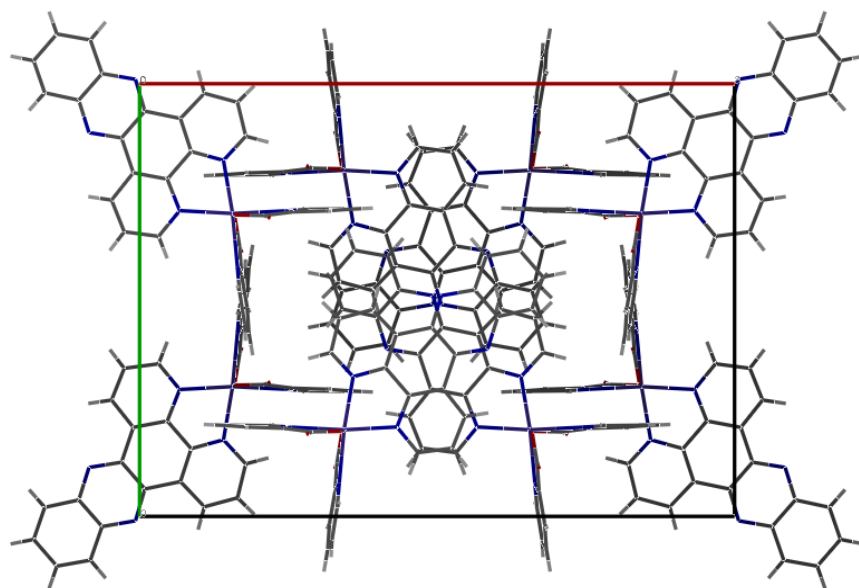


Fig. S3 Packing diagram of the complex 5.

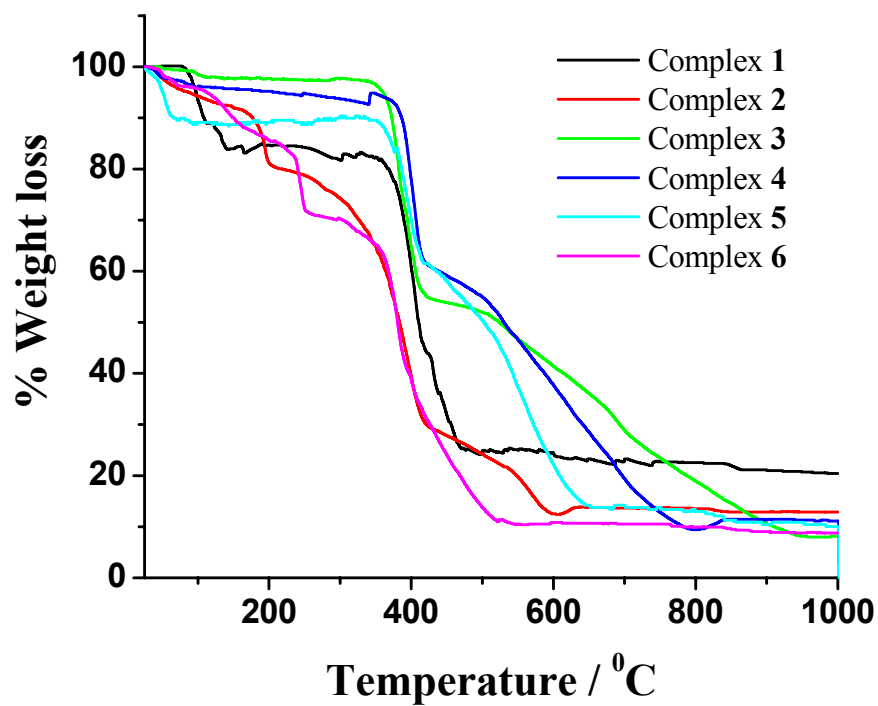


Fig. S4 Thermal analysis curves of the complexes 1–6.

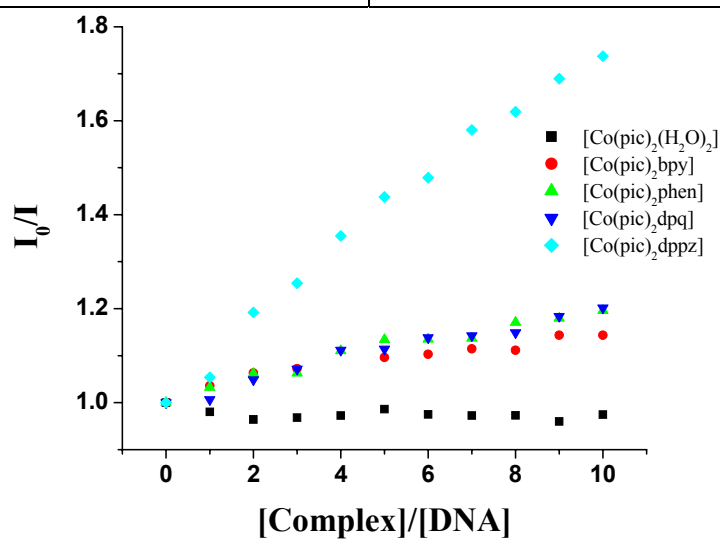
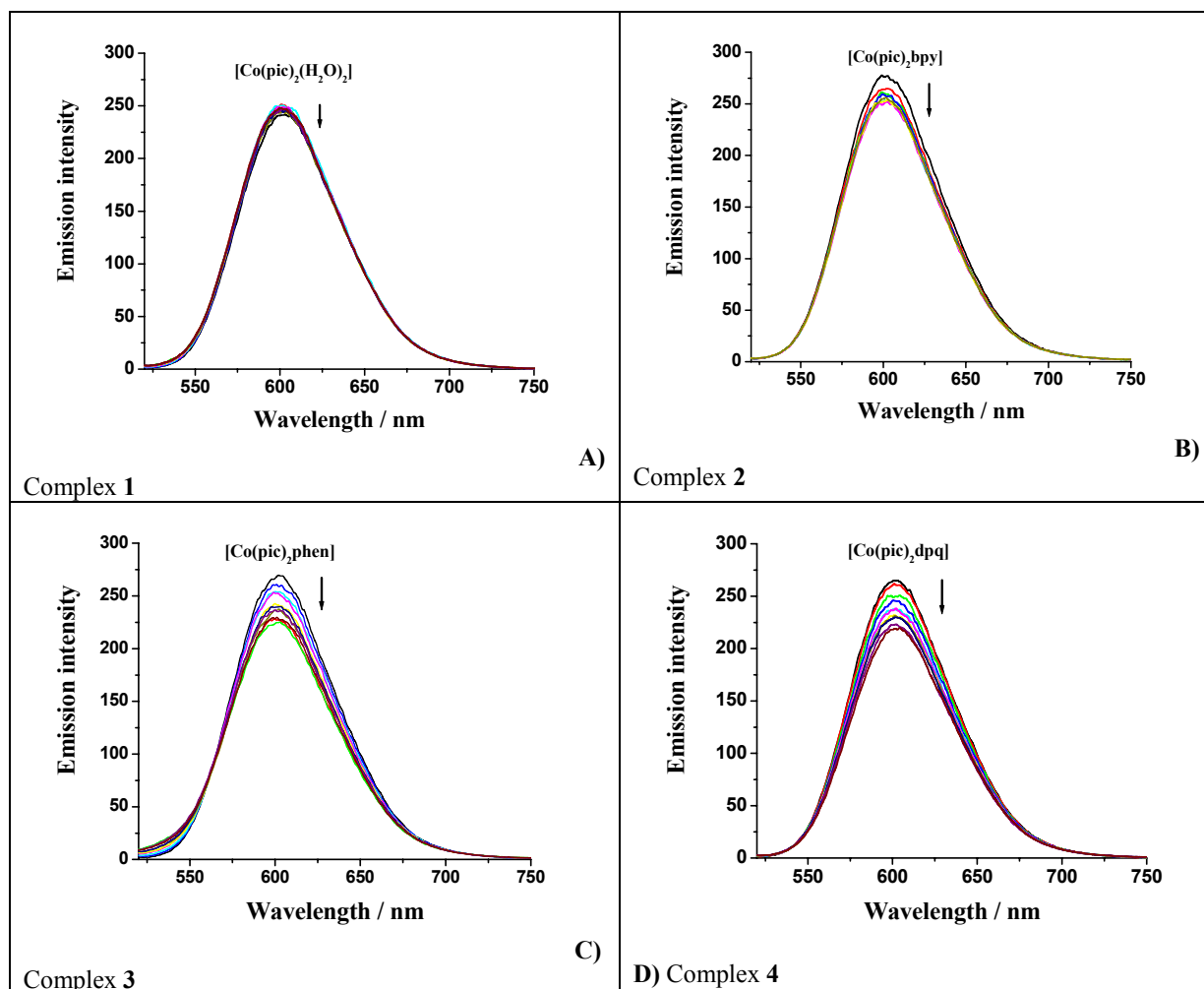


Fig. S5 Fluorescence quenching curves of ethidium bromide bound to DNA by complexes 1–4. $[\text{DNA}] = 20 \mu\text{M}$, $[\text{EB}] = 20 \mu\text{M}$ and $[\text{Complex}] = 0$ to $200 \mu\text{M}$. Effect of increase in concentration of complex 1 (■), 2 (●), 3 (▲), 4 (▼), 5 (◆) on the intensity of EB and the plot of I_0/I vs. $[\text{Complex}]/[\text{DNA}]$. $\lambda_{\text{ex}} = 510 \text{ nm}$.

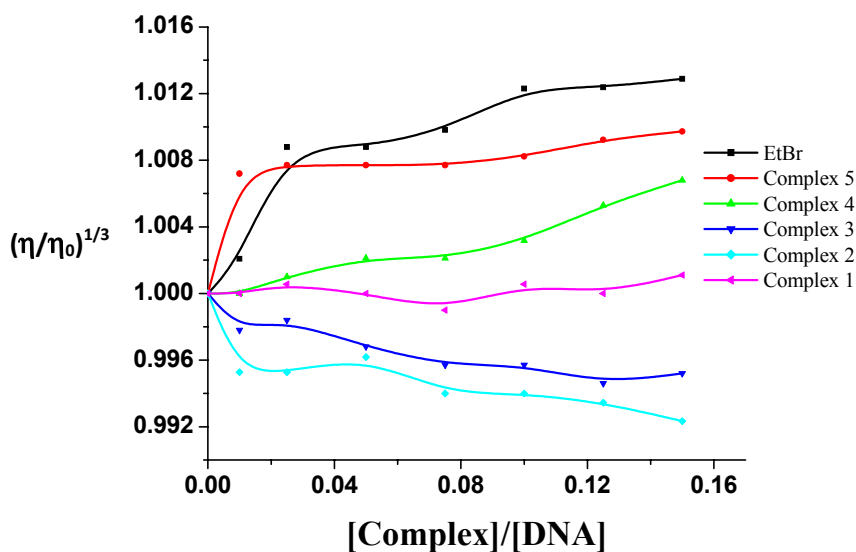


Fig. S6 Change in the viscosity of CT-DNA (200 μM) in the presence of increasing amounts of complexes 1–5.

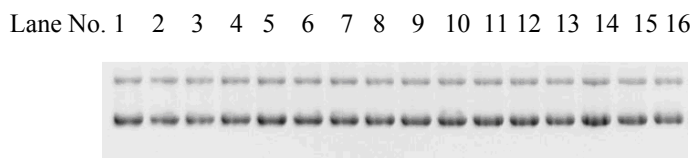


Fig. S7 Gel electrophoresis diagram showing the cleavage of plasmid *pBR322* DNA (300 ng) by Co(II) complexes 1–5 in TBE buffer (pH 8.2). Incubation time 30 min. at 37 °C. [DNA] = 200ng, Lane 1, DNA control; Lane 2, DNA + 1 (20 μM); Lane 3, DNA + 1 (50 μM); Lane 4, DNA + 1 (100 μM); Lane 5, DNA + 2 (20 μM); Lane 6, DNA + 2 (50 μM); Lane 7, DNA + 2 (100 μM); Lane 8, DNA+ 3 (20 μM); Lane 9, DNA + 3 (50 μM); Lane 10, DNA + 3 (100 μM); Lane 11, DNA + 4 (20 μM); Lane 12, DNA + 4 (50 μM); Lane 13, DNA + 4 (100 μM); Lane 14, DNA + 5 (20 μM); Lane 15, DNA + 5 (50 μM); Lane 16, DNA+ 5 (100 μM).

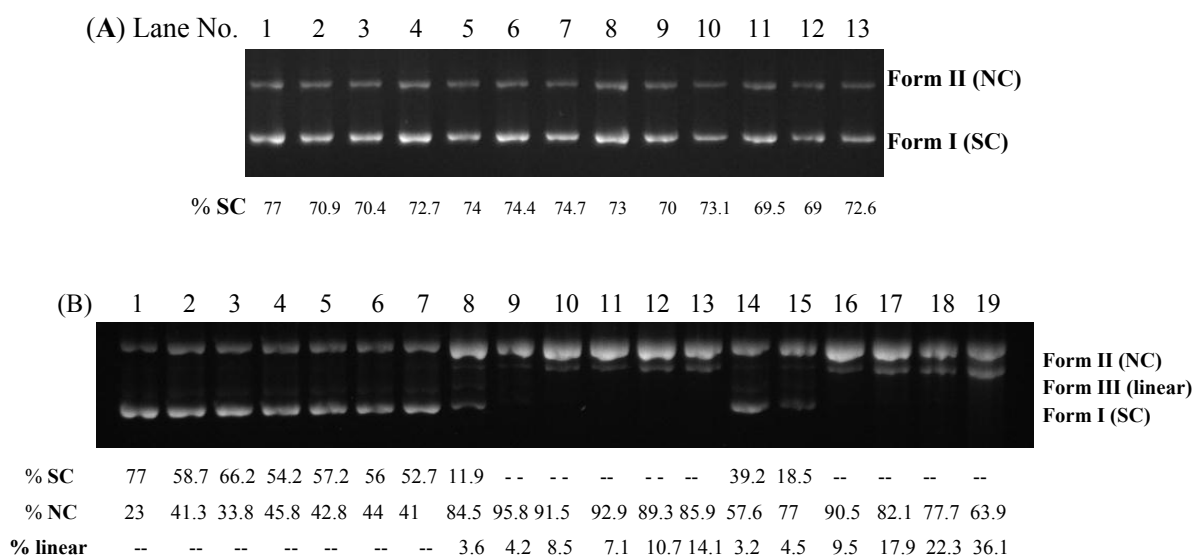


Fig. S8 Gel electrophoresis diagram showing the extent of cleavage of plasmid *pBR322* DNA (300 ng) by complexes **1–5** in TBE buffer (pH 8.2) in presence of H₂O₂. Incubation time 30 min. at 37 °C. [complexes] = 10–100 μM. (A) Lane 1, DNA control; Lane 2, DNA + **1** (10 μM); Lane 3, DNA + **1** (20 μM); Lane 4, DNA + **1** (40 μM); Lane 5, DNA + **1** (60 μM); Lane 6, DNA + **1** (80 μM); Lane 7, DNA + **1** (100 μM); Lane 8, DNA+ **2** (10 μM); Lane 9, DNA + **2** (20 μM); Lane 10, DNA + **2** (40 μM); Lane 11, DNA + **2** (60 μM); Lane 12, DNA + **2** (80 μM); Lane 13, DNA + **2** (100 μM); (B) Lane 1, DNA control; Lane 2, DNA + **3** (10 μM); Lane 3, DNA + **3** (20 μM); Lane 4, DNA + **3** (40 μM); Lane 5, DNA + **3** (60 μM); Lane 6, DNA + **3** (80 μM); Lane 7, DNA + **3** (100 μM); Lane 8, DNA+ **4** (10 μM); Lane 9, DNA + **4** (20 μM); Lane 10, DNA + **4** (40 μM); Lane 11, DNA + **4** (60 μM); Lane 12, DNA + **4** (80 μM); Lane 13, DNA + **4** (100 μM); Lane 14, DNA+ **5** (10 μM); Lane 15, DNA + **5** (20 μM); Lane 16, DNA + **5** (40 μM); Lane 17, DNA + **5** (60 μM); Lane 18, DNA + **5** (80 μM); Lane 19, DNA + **5** (100 μM).

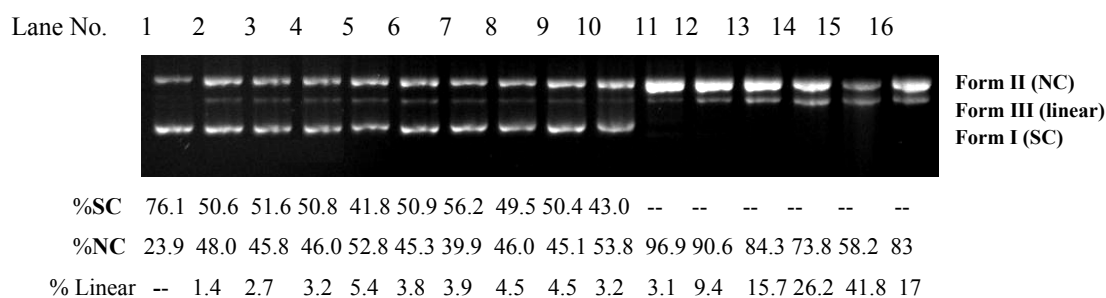


Fig. S9 1 % agarose gel showing the cleavage of *pBR322* plasmid DNA by complexes **1–5**. [DNA] = 200ng, on irradiation for 20 min. at 365 nm after 10 min. incubation at 37 °C, TBE buffer, pH 8.2, (A) Lane 1, DNA control; Lane 2, DNA + **1** (20 μM); Lane 3, DNA + **1** (50 μM); Lane 4, DNA + **1** (100 μM); Lane 5, DNA + **2** (20 μM); Lane 6, DNA + **2** (50 μM); Lane 7, DNA + **2** (100 μM); Lane 8, DNA+ **3** (20 μM); Lane 9, DNA + **3** (50 μM); Lane 10, DNA + **3** (100 μM); Lane 11, DNA + **4** (20 μM); Lane 12, DNA + **4** (50 μM); Lane 13, DNA + **4** (100 μM); Lane 14, DNA + **5** (20 μM); Lane 15, DNA + **5** (50 μM); Lane 16, DNA+ **5** (100 μM).

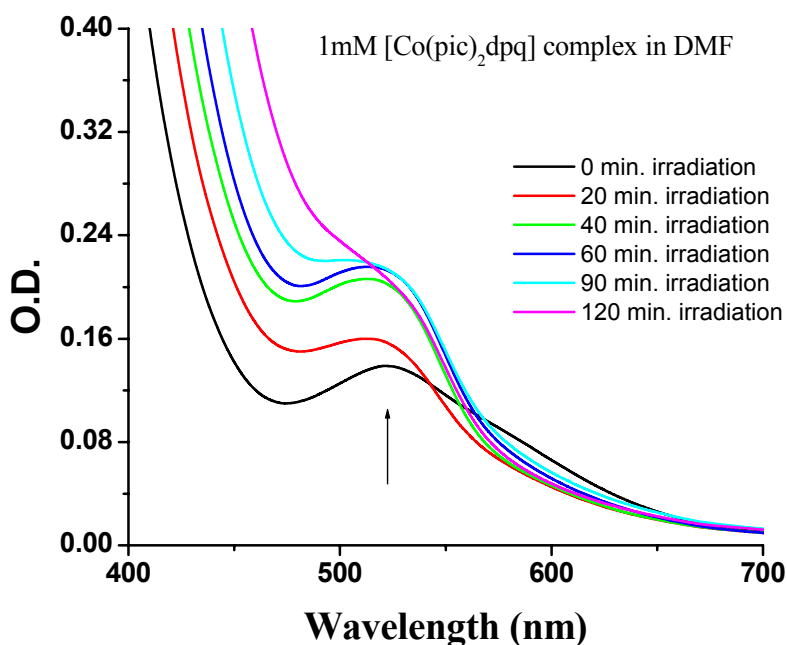


Fig. S10 Absorption spectra of 1mM complex **4** in DMF before and after irradiation.

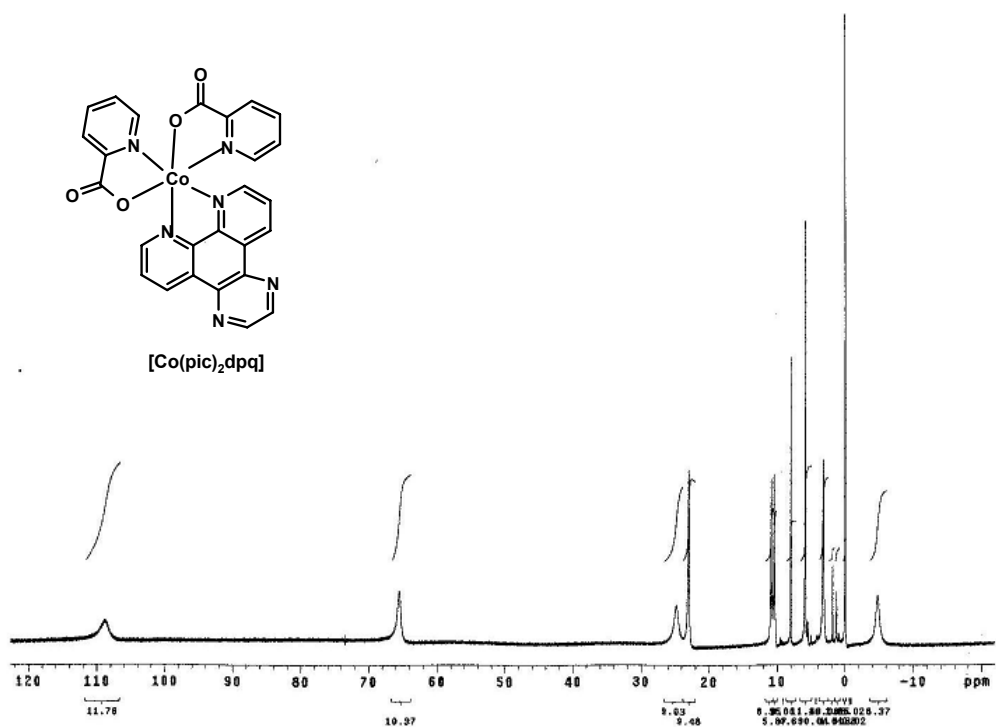


Fig. S11 ¹H NMR of complex 4 in CDCl₃ solvent.

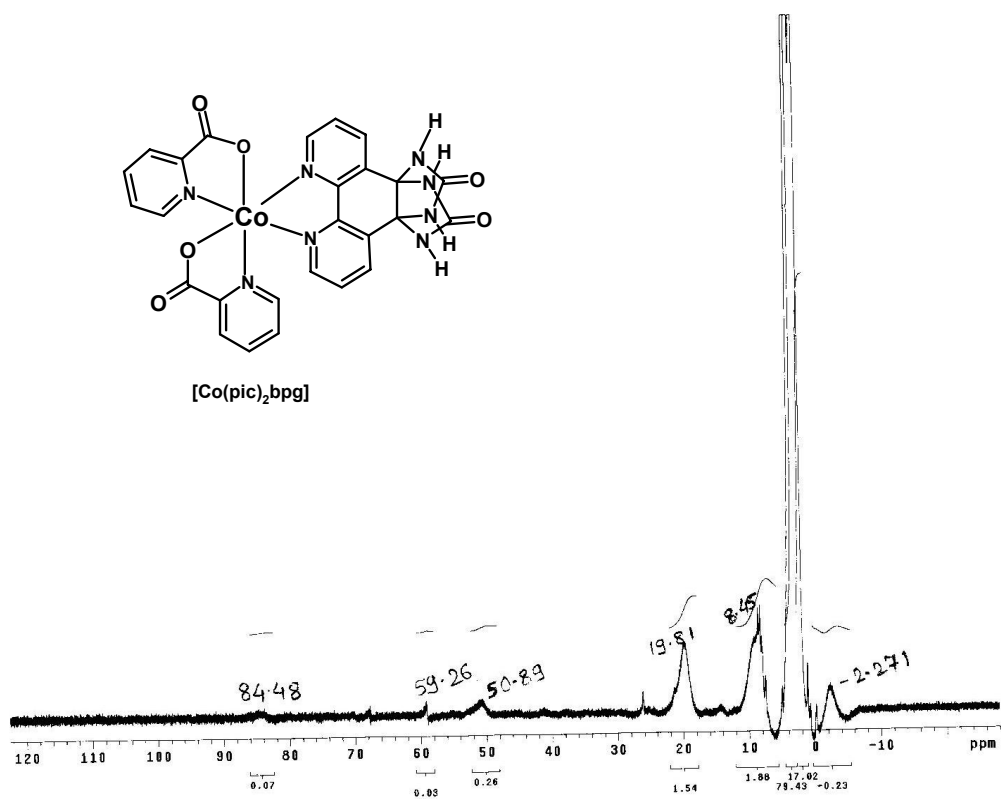


Fig. S12 ¹H-NMR spectra of complex 6 in DMSO-*d*₆.

Table S1. Selected calculated and observed bond lengths [\AA] and angles [$^\circ$] in complexes **2–6**

Complex	2		3		4		5		6	
	Crystal Structure [#]	6-31G (d,p) ^S	Crystal Structure [#]	6-31G (d,p) ^S	Crystal Structure	6-31G (d,p) ^S	Crystal Structure	6-31G (d,p) ^S	Crystal Structure	6-31G (d,p) ^S
Co-N (pic)	2.163(4)	2.203	2.140(3)	2.176	2.122(3)	2.175	2.142(4)	2.176	2.120(6)	2.200
Co-O (pic)	2.047(3)	2.018	2.056(3)	2.031	2.058(2)	2.030	2.045(3)	2.030	2.070(5)	2.012
Co-N (pic)	2.153(4)	2.204	2.135(3)	2.176	2.130(3)	2.175	2.136(4)	2.176	2.120(6)	2.200
Co-O (pic)	2.049(3)	2.018	2.053(3)	2.031	2.061(2)	2.030	2.053(3)	2.030	2.070(5)	2.012
Co-N (NN)	2.137(3)	2.248	2.131(3)	2.232	2.153(3)	2.231	2.158(4)	2.229	2.159(6)	2.265
Co-N (NN)	2.105(16)	2.249	2.135(3)	2.232	2.162(3)	2.231	2.139(4)	2.228	2.159(6)	2.265
N-Co-N (NN)	76.21(11)	71.89	78.59(11)	75.48	77.46(11)	75.19	77.17(14)	75.17	75.41(2)	71.66
N-Co-O (pic)	79.02(14)	78.68	78.64(12)	78.37	78.52(10)	78.40	78.76(14)	78.35	78.50(2)	78.33
N-Co-O (pic)	78.87(13)	78.68	77.89(11)	78.36	78.42(10)	78.40	79.14(14)	78.35	78.50(2)	78.33

pic= picolinate, NN = polypyridyl ligand. [#] Values from Reference No. 20, ^S Basis sets used in geometry calculations.