Evaluation of anticancer potential of a binuclear copper (II) complex with 3-(pyridin-3-yl) coumarin ligand: Synthesis, crystal structure, magnetism, DNA interaction and molecular dynamic simulations

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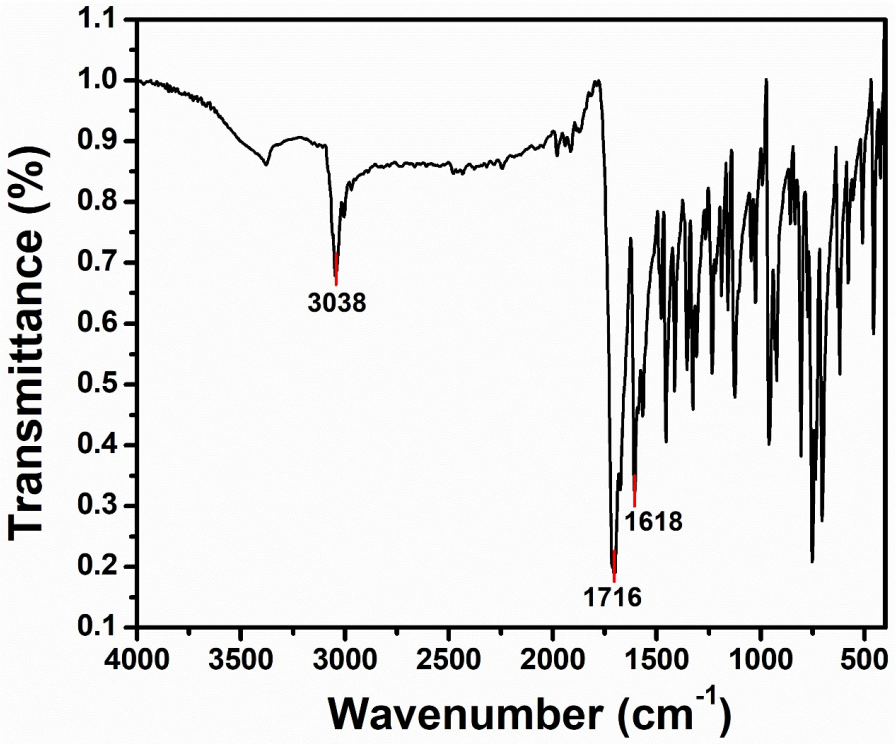

Fig. S1. IR spectrum of 3-(pyridin-3-yl) coumarin (**L**).

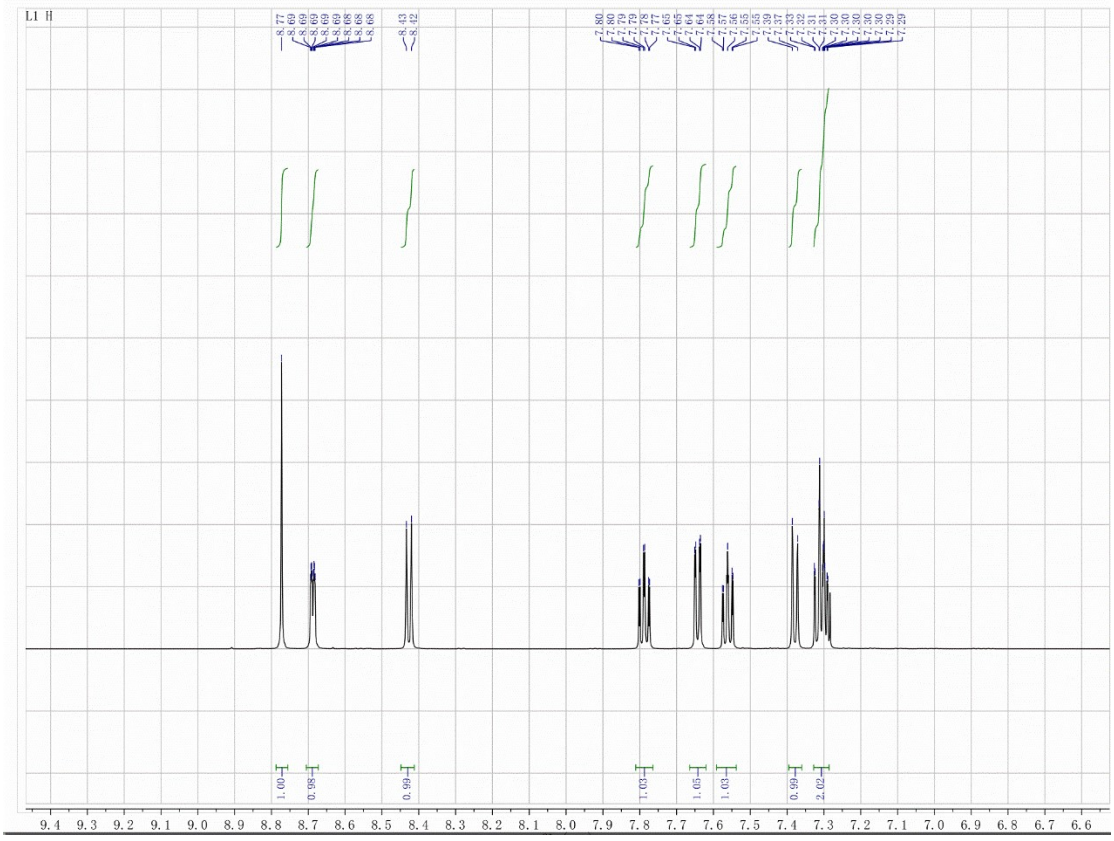

Fig. S2. ^{1}H NMR spectrum of 3-(pyridin-3-yl) coumarin (**L**) in $CDCl_3$.

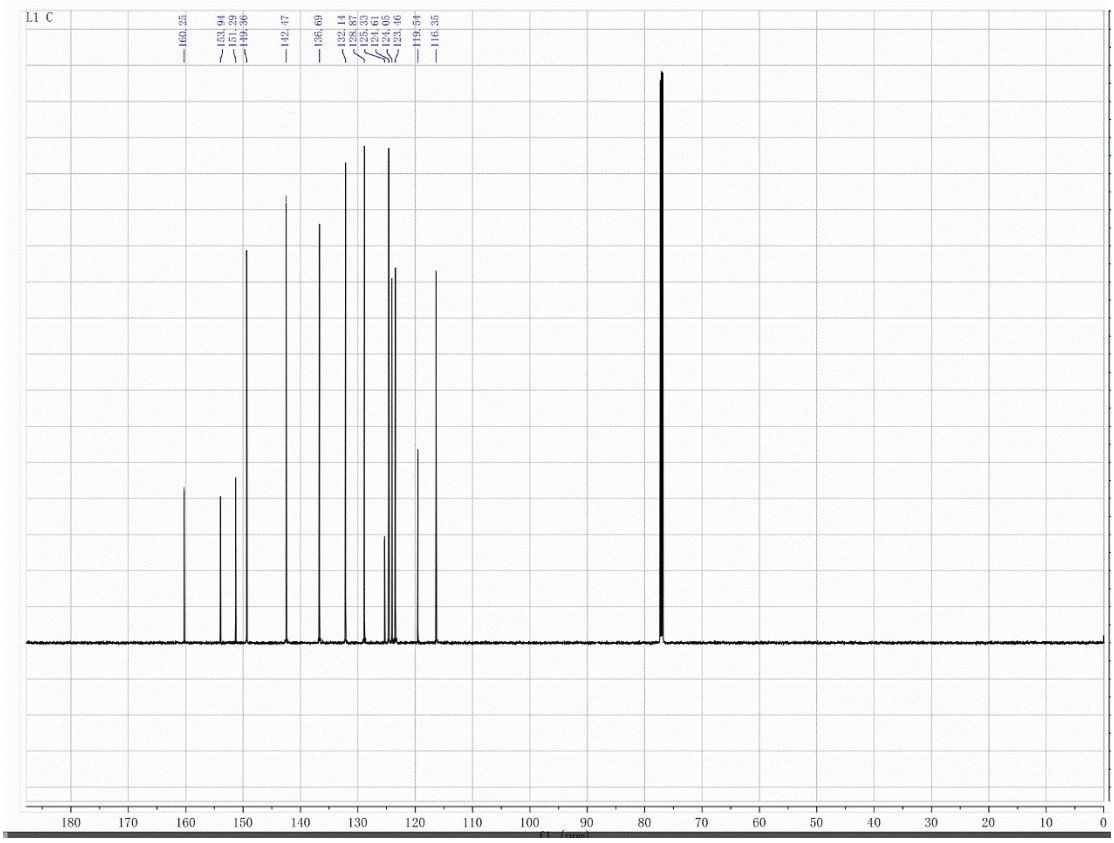

Fig. S3. ^{13}C NMR spectrum of 3-(pyridin-3-yl) coumarin (L) in $CDCl_3$.

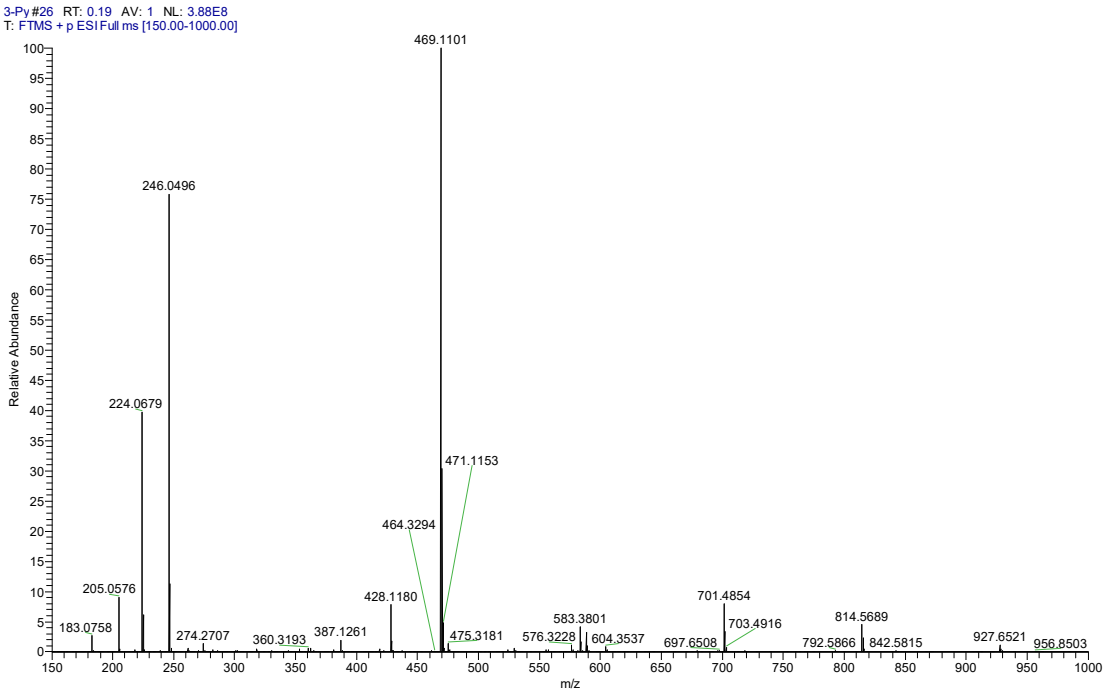

Fig. S4. Mass spectrum of 3-(pyridin-3-yl) coumarin (**L**).

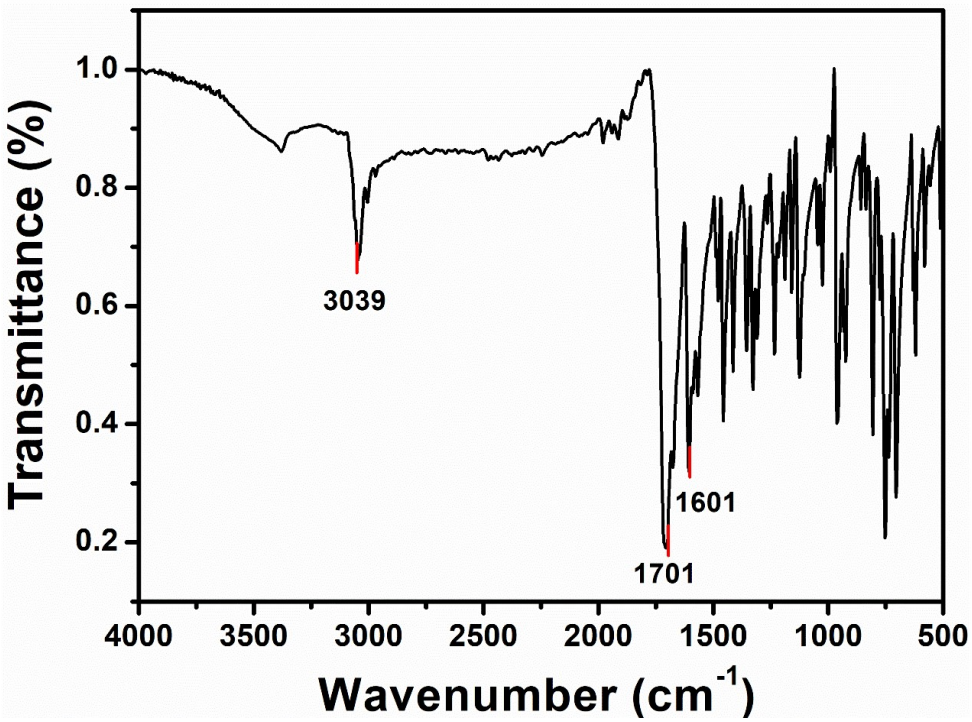

Fig. S5. IR spectrum of complex **Coupy-Cu.**

Table S1. Selected Bond Lengths (Å) and Angles (°) of the complex **Coupy-Cu.**

Bond	Dist.(Å)	**Bond**	Dist.(Å)
Cu1-O8	1.936(12)	Cu2-O7	1.941(14)
Cu1-O1	1.939(14)	Cu2-O4	1.966(11)
Cu1-O3	1.945(13)	Cu2-O2	1.972(18)
Cu1-O6	1.964(15)	Cu2-O5	1.983(15)
Cu1-N1	2.159(17)	Cu2-N2	2.126(16)
Angle	(°)	Angle	(°)
O8-Cu1-O1	88.6(6)	O7-Cu2-O4	170.6(5)
O8-Cu1-O3	165.2(5)	O7-Cu2-O2	90.2(6)
O1-Cu1-O3	89.5(6)	O4-Cu2-O2	89.6(6)
O8-Cu1-O6	87.7(6)	O7-Cu2-O5	88.0(6
O1-Cu1-O6	167.3(7)	O4-Cu2-O5	90.1(6)
O3-Cu1-O6	90.9(6)	O2-Cu2-O5	166.7(7)
O8-Cu1-N1	95.8(5)	O7-Cu2-N2	96.5(6)
O1-Cu1-N1	96.6(6)	O4-Cu2-N2	92.7(6)
O3-Cu1-N1	99.0(6)	O2-Cu2-N2	101.4(6)
O6-Cu1-N1	95.8(6)	O5-Cu2-N2	91.9(7)

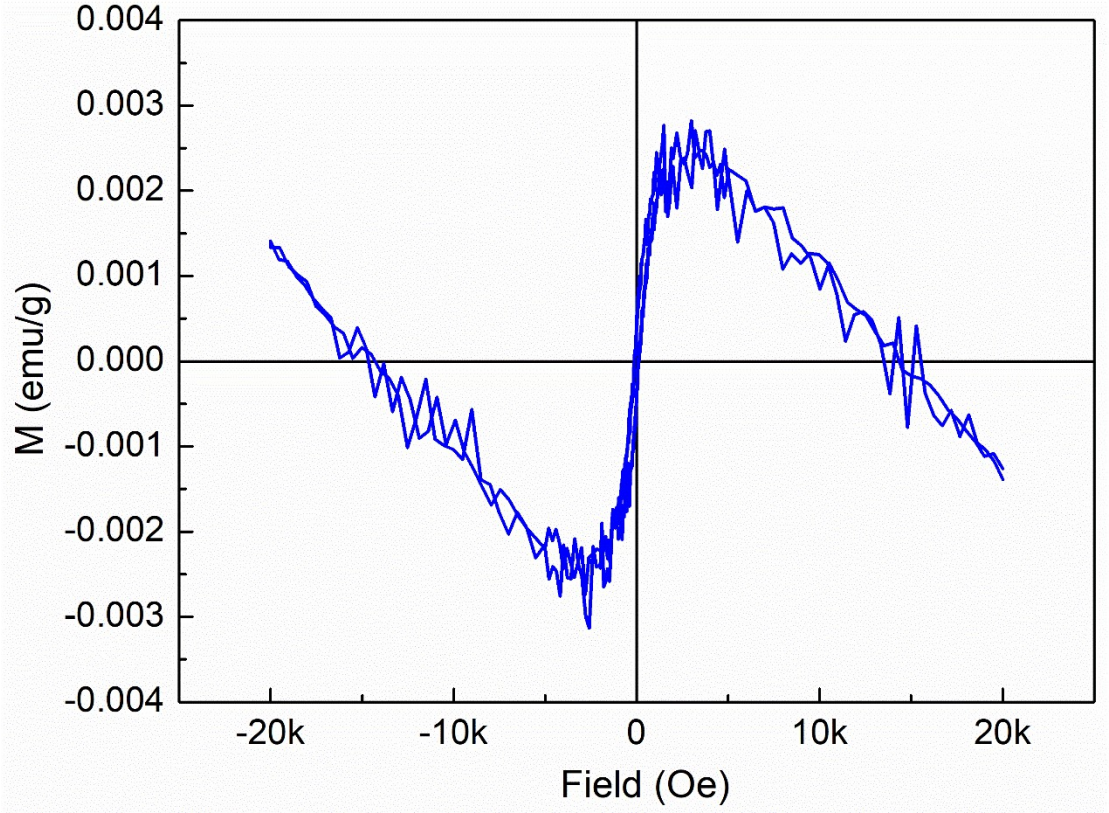

Fig.S6. Magnetization (M, emu/g) as a function of applied magnetic field (Oe) for the complex **Coupy-Cu**, showing the magnetic hysteresis behavior.

Table S2. Summary of simulation parameters for EPR spectra (complex Coupy-Cu).

***g*-value**	**D/cm^{-1}**	***E*/cm^{-1}**	**lw/mT**
2.08 2.41	0.290	0.265	10, 35

* lw is the homogeneous Lorentzian linewidth; the linewidth defines the FWHM (full width at half height, in mT) of the absorption Gaussian (first number) and Lorentzian (second number) broadening of the lines in the spectrum.

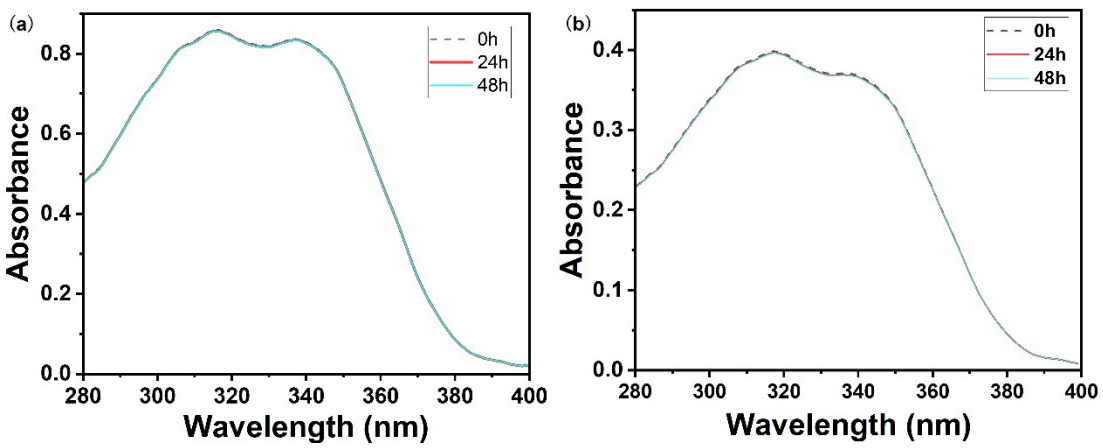

Fig.S7. UV-Vis spectra of ligand **L (a)** and complex **Coupy-Cu (b)** in Tris-HCl/NaCl buffer (pH = 7.2, with DMSO content < 1% v/v).

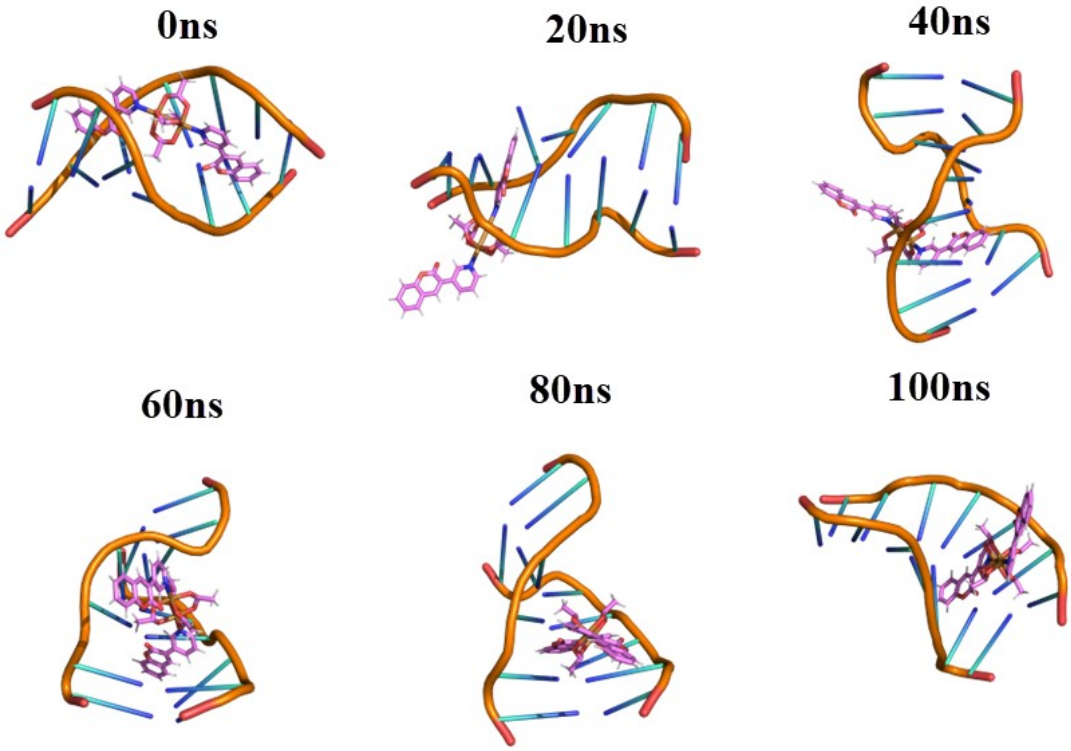

Fig.S8. Snapshot structures during the simulation.