Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2022

Supplementary Material

DNA binding, DNA cleavage, cellular uptake, cytotoxicity, and apoptosis-inducing ability of a binuclear schiff base copper(II)

complex

Dandan Zhao, Yixuan Wu, Wenxin Huang, Silin Gong, Zhanfen Chen*



Figure S1. ¹H NMR spectroscopy of the ligand N-(2-hydroxylbenzylidene)benzo[d]imidazol-2-amine (L) (DMSO-d₆).



Figure S2. ¹³C NMR spectroscopy of the ligand N-(2-hydroxylbenzylidene)-

benzo[d]imidazol-2-amine (L) (DMSO-d₆).



Figure S3. ESI mass spectrometry of the ligand N-(2-hydroxylbenzylidene)benzo[d]imidazol-2-amine (L) in methanol.



Figure S4. IR spectrum of *N*-(2-hydroxylbenzylidene)-benzo[*d*]imidazol-2-amine (L).



Figure S5. High resolution electrospray ionization-mass spectrum (HRMS, ESI) of 1 in methanol solution. The signal at m/z 684.20 should be assigned to $[M - Cl + Na - H]^+$ (M = $[Cu_2(L-H)_2]Cl_2$).



Figure S6. IR spectrum of $[Cu_2(L-H)_2]Cl_2$ (1).



Figure S7. Plot of magnetic moment (μ_{eff}) *versus* temperature (T) for 1 in the solid state with (\blacksquare) representing the experimental data and the line represent the theoretic simulation.



Figure S8. Cyclic voltammogram of complex 1 (2.5×10^{-3} M) in DMF containing 0.1 M TBAP as a supporting electrolyte at room temperature in a potential range of -1.0 to 1.0 V *vs*. Ag/AgCl at 100 mV/s scan rate.



Figure S9. Time-dependent agarose gel electrophoresis patterns for the cleavage of pBR322 plasmid DNA ($0.02 \ \mu g/\mu L$) by complex ($60 \ \mu M$) over a period for 30 min in the presence of Vc (1 mM) in buffer (50 mM Tris-HCl/50 mM NaCl, pH 7.40) at 37 °C. Lane 1, DNA control; Lane 2~7, DNA + complex + Vc. Incubation times of lanes 2~7 equal 5, 10, 15, 20, 25, and 30 min, respectively.



Figure S10. Agarose gel electrophoresis patterns for the cleavage of pBR322 plasmid DNA ($0.02 \mu g/\mu L$) by complex (60 μ M) in the presence of various additives in buffer (50 mM Tris-HCl/50 mM NaCl, pH 7.40) at 37 °C after 30 min of incubation. Lane 1, DNA control; Lane 2, DNA + 1 mM Vc + complex; Lane 3, DNA + 1 mM Vc + complex + 1 M DMSO; Lane 4, DNA + 1 mM Vc + complex + 10 mM KI; Lane 5, DNA + 1 mM Vc + complex + 10 mM NaN₃; Lane 6, DNA + 1 mM Vc + complex + 1 M tert-Butanol.





Figure S11. Plot of cell viability *versus* concentration (μ M) for cisplatin, complex 1, and L against Hela, A549, and MCF-7.