Supplementary information

The effect of gallic acid on copper(II) complex of *N*-(methylpyridin-2-yl)-amidino-*O*-methylurea: Crystal structure, DNA interactions, *in vitro* cytotoxicity and antibacterial activity

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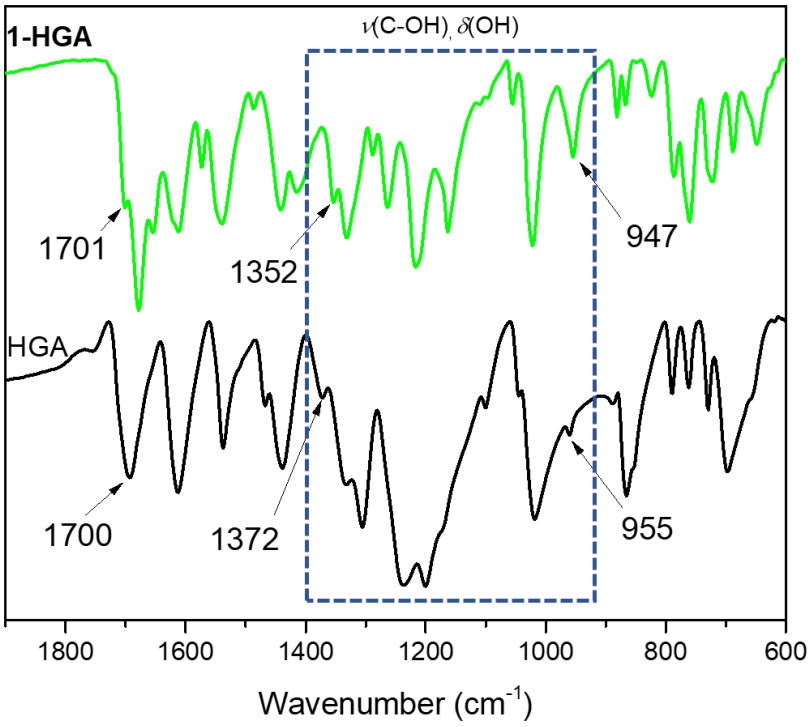

Fig. S1 Overlayered IR spectra of **1-HGA** and gallic acid (HGA) in the region of 2000 – 600 cm^{-1}.

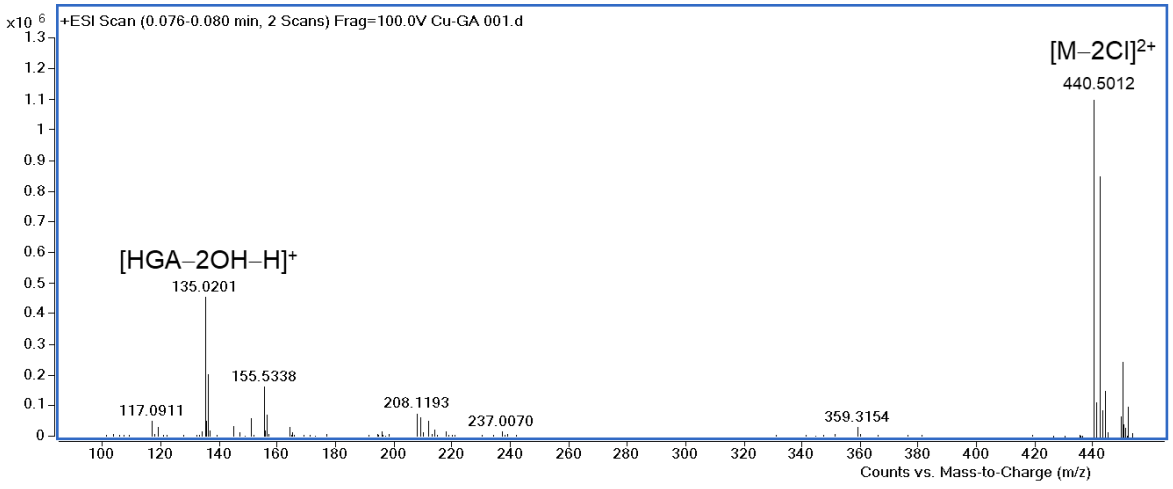

Fig. S2 Mass spectra of **1-HGA** in water : methanol (1 : 3 v/v) solution.

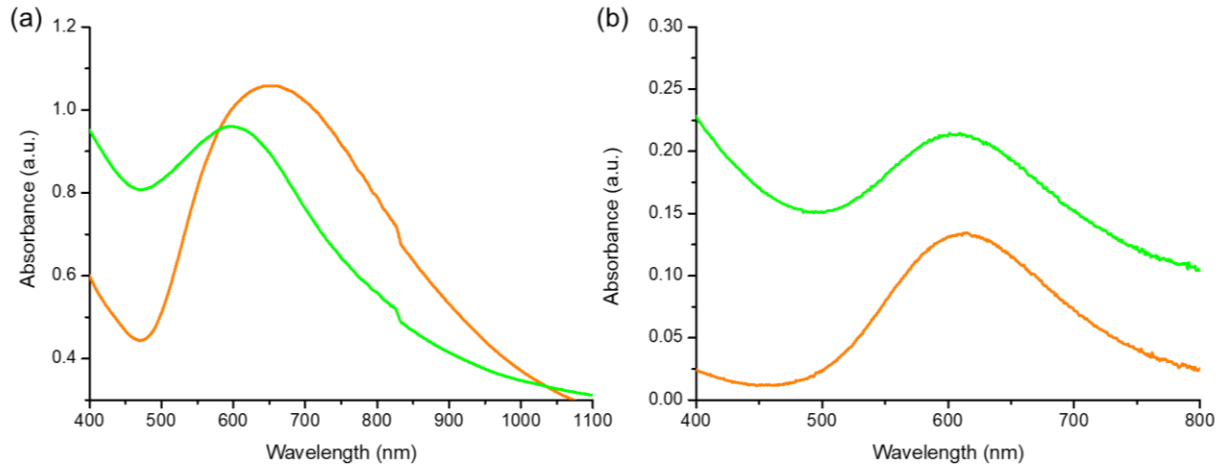

Fig. S3 (a) Diffuse reflectance and (b) UV-Vis spectra of **1** (orange line) and **1-HGA** (green line) in Tris-buffer at pH 7.2.

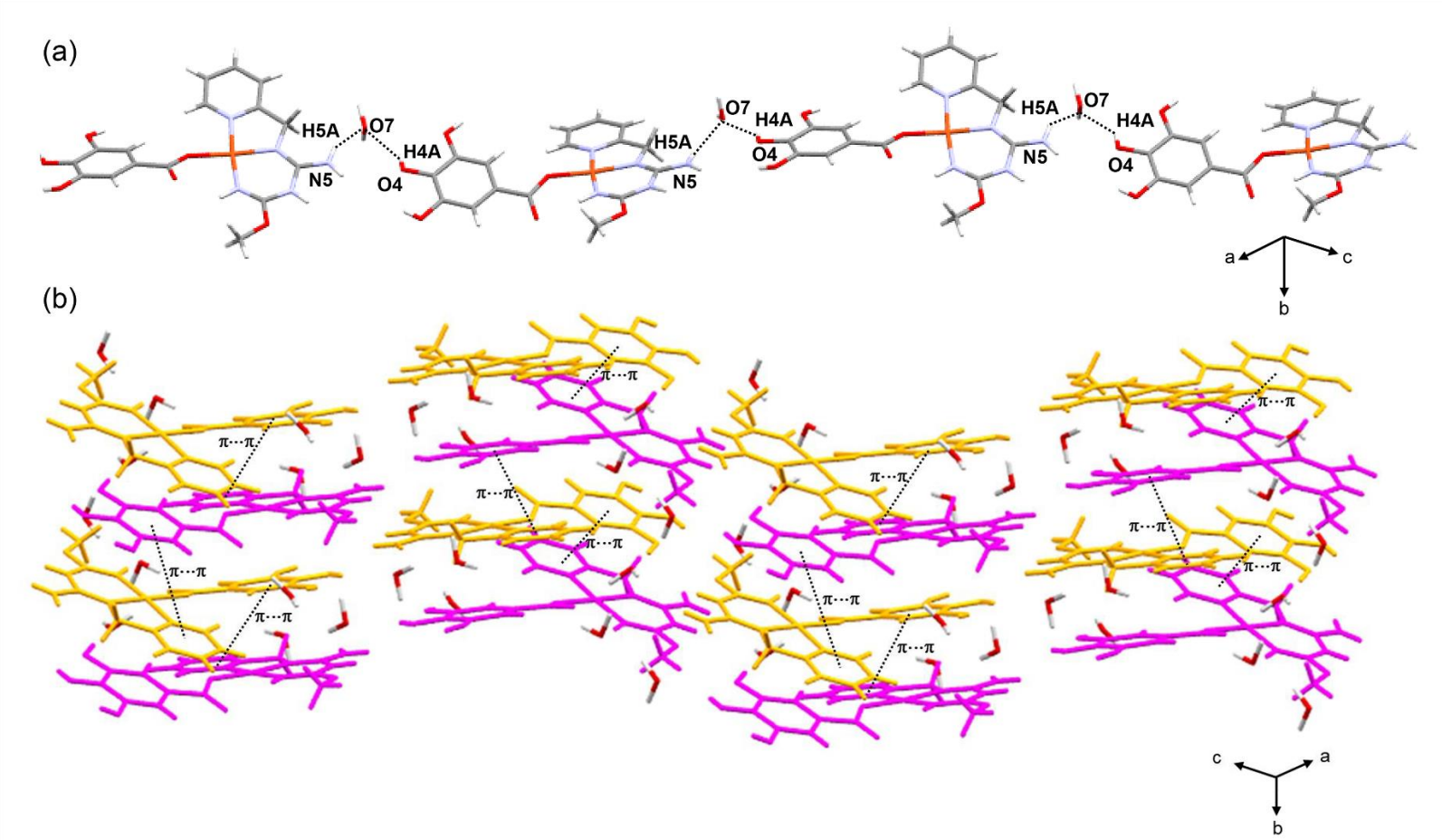

Fig. S4 (a) 1D structure of hydrogen bonds (dashed lines) of lattice water (O7), amide hydrogen atom from L^{3m} (H5A) and phenol hydrogen atom from GA (H4A) and (b) π···π interactions between the central phenol ring of GA and the pyridyl ring of L^{3m}.

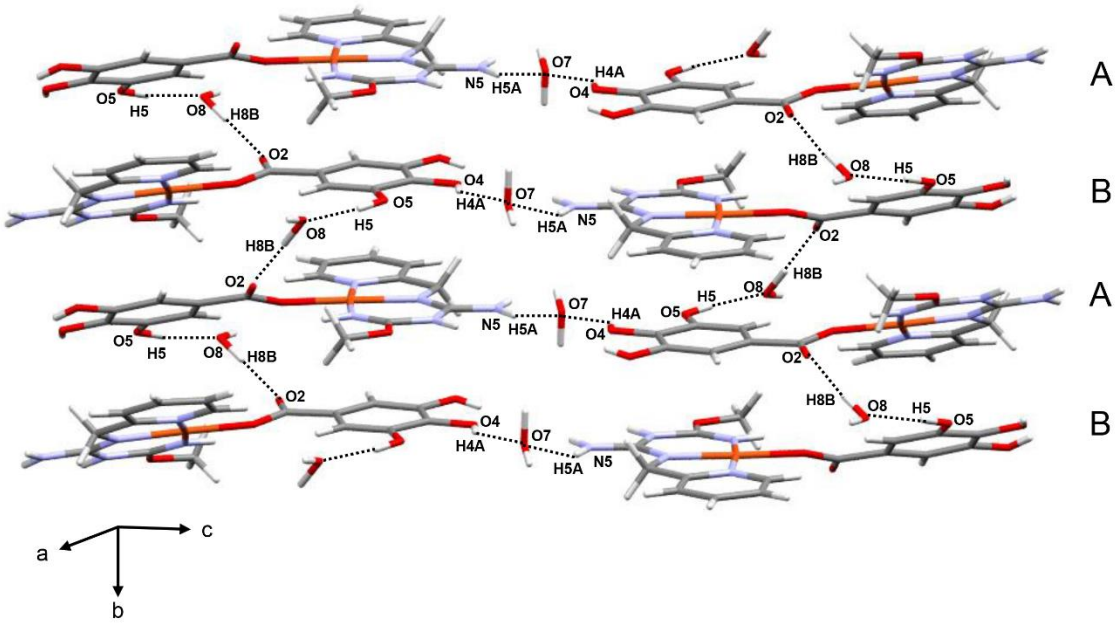

Fig. S5 2D packing diagram of $[CuL^{3m}(GA)]Cl{\cdot}3H_2O$ constructed by intermolecular hydrogen bonded 1D chains in ABAB pattern.

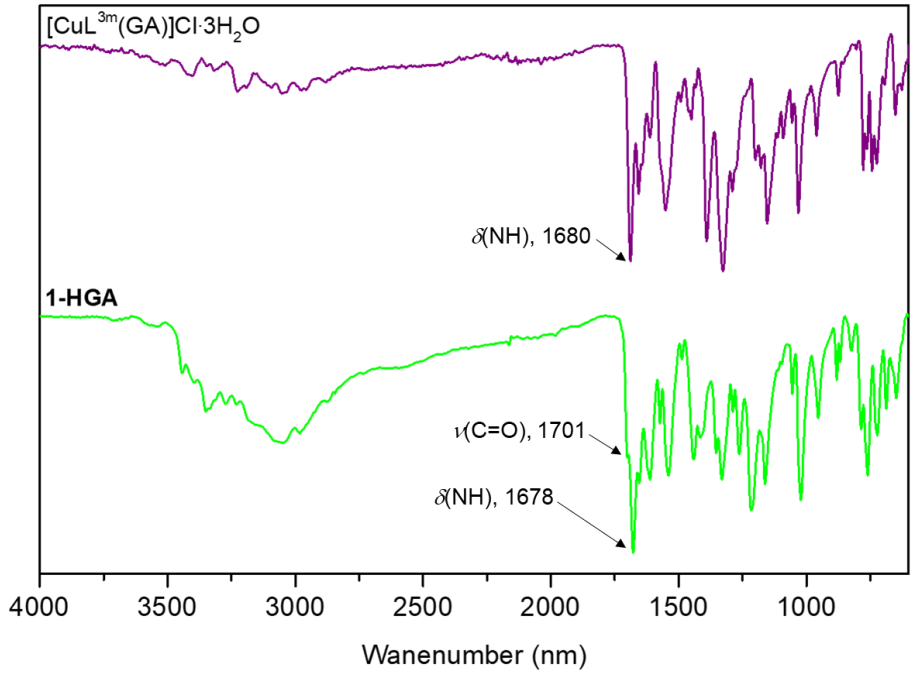

Fig. S6 Overlayered IR spectra of crystal $[CuL^{3m}(GA)]Cl{\cdot}3H_2O$ and **1-HGA**.

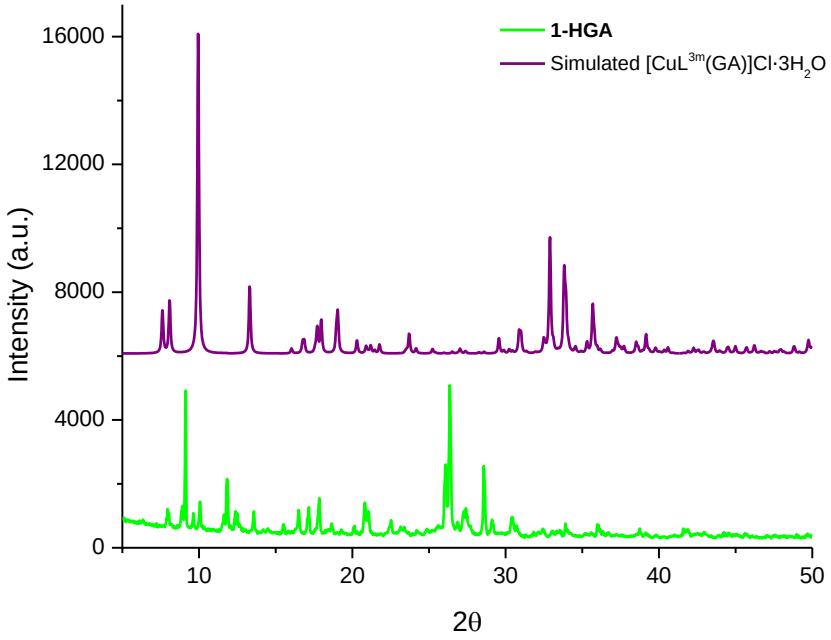

Fig. S7 PXRD patterns of simulated $[CuL^{3m}(GA)]Cl\cdot 3H_2O$ from the single crystal data and **1-HGA**.

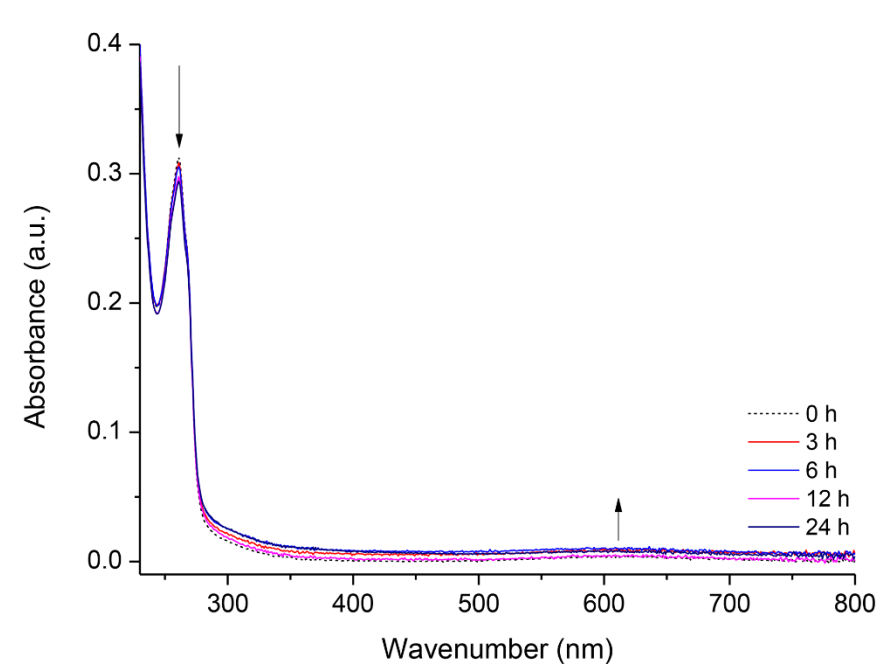

Fig. S8 UV-Vis spectra of **1-HGA** (50 μM) in Tris-buffer at pH 7.2 at 0, 3, 6, 12 and 24 h.

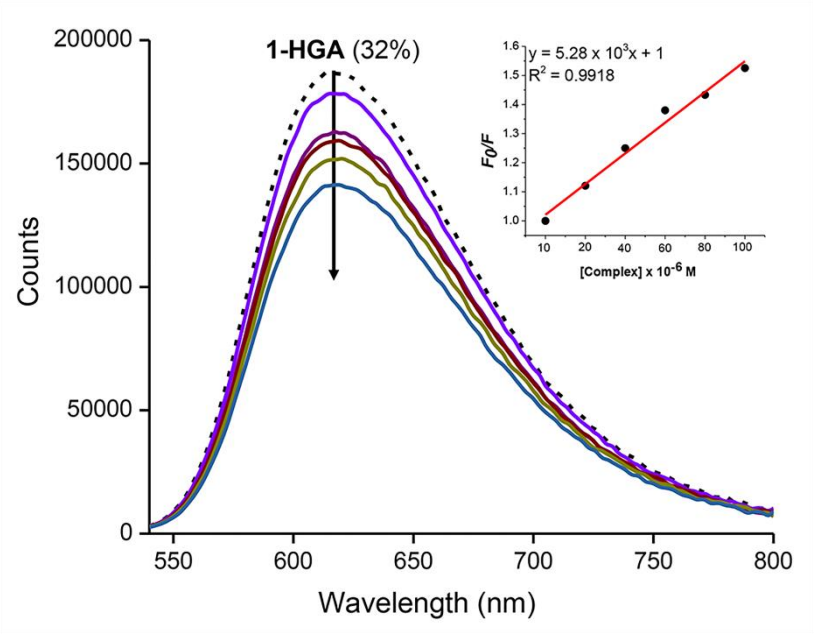

Fig. S9 Emission spectra of EB–DNA (100:50 μM) in the presence of **1-HGA** with the [Complex]/[DNA] ratios of 0.00, 0.20, 0.40, 0.60, 0.80 and 1.00 in Tris-buffer at pH 7.2 for 30 min. Insets: Plots of F_0/F vs. [Complex].

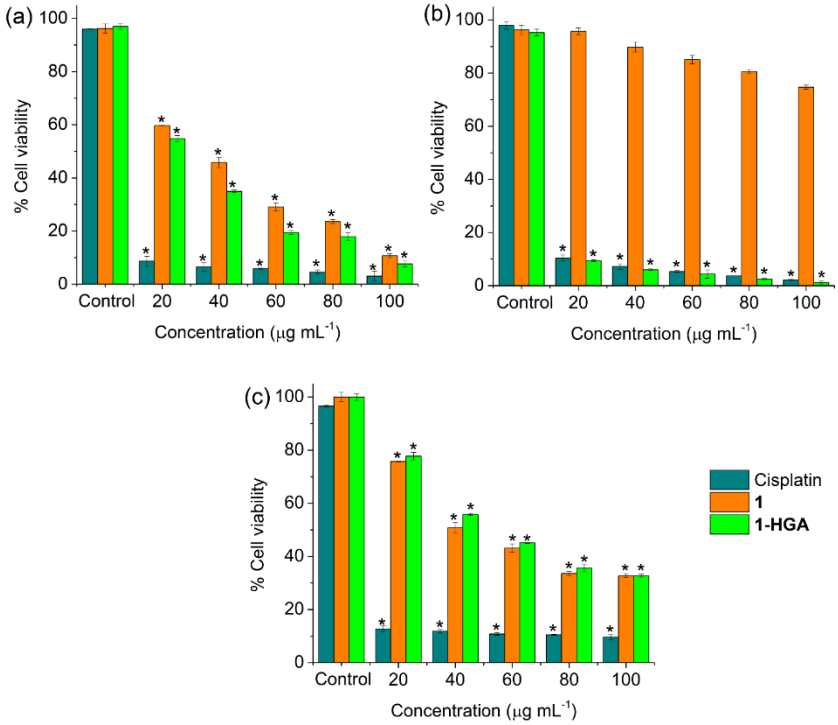

Fig. S10 Cytotoxicity profiles of **1** and **1-HGA** (0 - 100 μM) for (a) HeLa, (b) MCF-7 and (c) Vero cell lines. Data are reported as the mean ± SD for n = 3 and *P<0.01 compared to control.

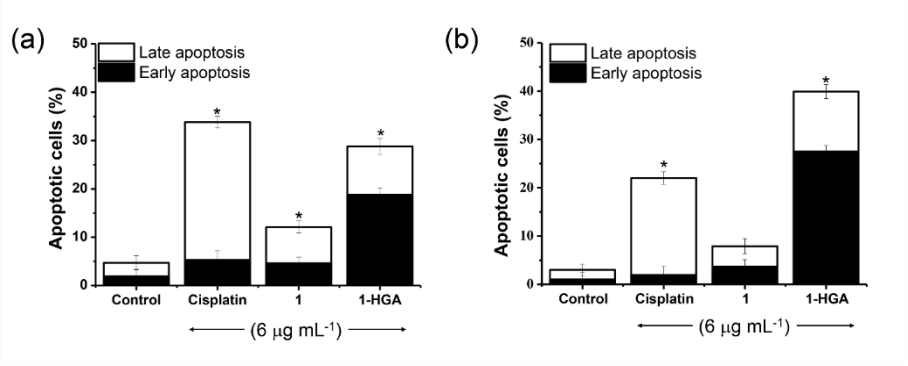

Fig. S11 Percentages of apoptotic cells for (a) HeLa and (b) MCF-7 cell lines. Tris-buffer at pH 7.2 and cisplatin treatment was used as negative and positive controls. Results are the mean ± SD, n = 3. *P<0.01 indicates a significant difference between the treatment and solvent control.

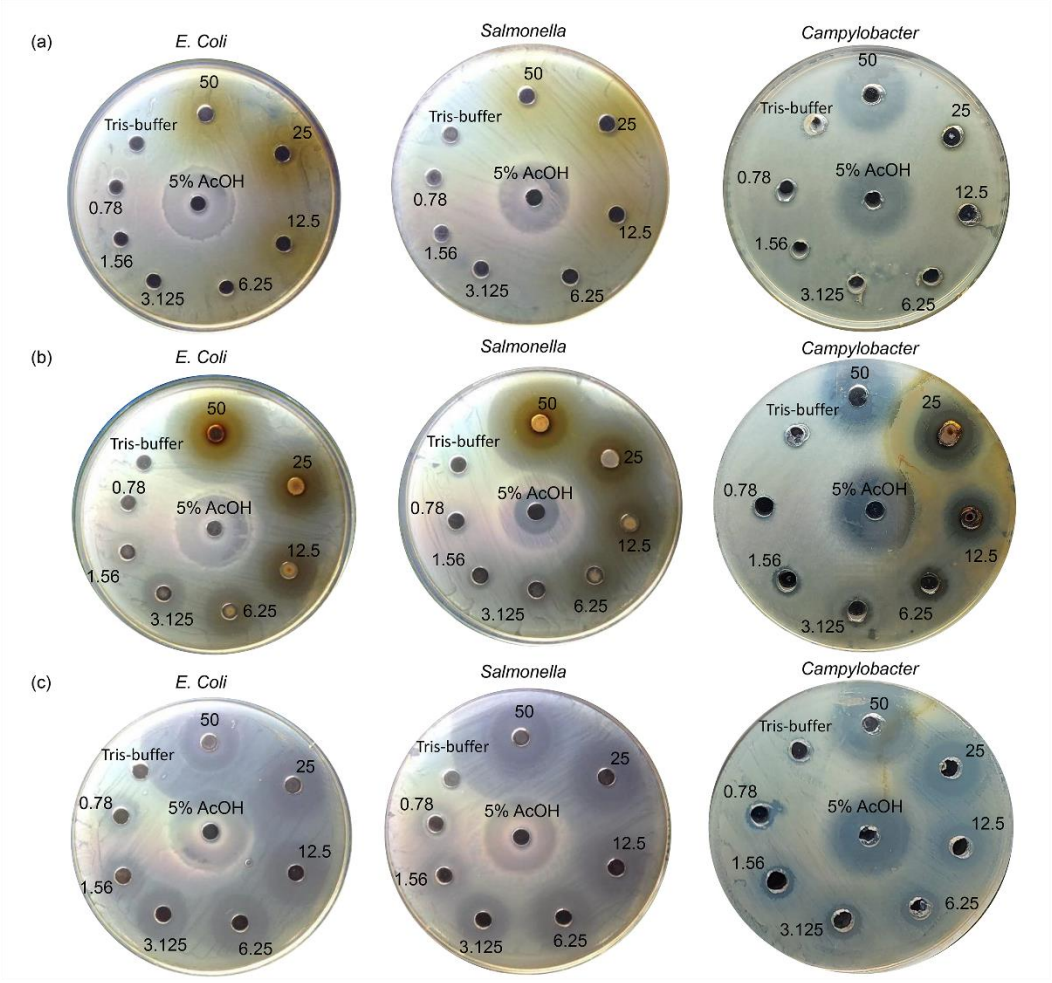

Fig. S12 Antibacterial activity of (a) gallic acid (HGA), (b) $[CuL^{3m}Cl_2]$ (**1**) and (c) $[CuL^{3m}(HGA)Cl_2]$ (**1-HGA**) in the concentration range of 50 - 0.78 μg mL^{-1} against *E. Coli*, *Salmonella* and *Campylobacter* by disc diffusion method.

Table S1. Assignment of infrared vibrational modes for **1**, **1-HGA** and gallic acid (HGA)

Compound	ν(OH), ν(NH)	ν_s(C=O)	ν_{as}(NH), δ(NH)	ν(C=C), ν(C-C)	ν(C-O), ν(C-OH), δ(OH)	δ(OH)	γ(OH)	δ(C=O), γ(CO)
1	3512		1681	1614	1377			
	3360		1642	1573	1341			
	3284			1485				
	3141							
1-HGA	3443	1701	1678	1612	1352	1263	881	688
	3395			1573	1331	1217	867	
	3231			1539		1163	729	
	3076			1487		1022		
	2988			1442		947		
HGA	3485	1700		1613	1372	1237	888	697
	3265			1538	1332	1018	789	
	2646			1438		955	730	

Abbreviation: ν_{as}, *asymmetric* stretching; ν_s, symmetric stretching; δ, bending; γ, out-of-plane bending.

Table S2. Selected bond lengths (Å) and angles (º) for $[CuL^{3m}(GA)]Cl{\cdot}3H_2O$

	Bond lengths (Å)		Bond angles (º)
Cu1–N1	1.973(2)	N1–Cu1–N2	82.89(10)
Cu1–N2	1.947(2)	N1–Cu1–N4	174.04(9)
Cu1–N4	1.920(2)	N2–Cu1–N4	91.18(10)
Cu1–O1	1.931(19)	O1–Cu1–N1	90.62(9)
		O1–Cu1–N2	179.98(9)
		O1–Cu1–N4	95.33(9)

Table S3. Hydrogen bond lengths (Å) and angles (°) for $[CuL^{3m}(GA)]Cl{\cdot}3H_2O$

D—H···A	D—H/Å	H···A/Å	D···A/Å	D—H···A/Å	symmetry
O4—H4A···O7	0.71(3)	2.24(3)	2.848(4)	144(4)	
O5—H5···O8	0.84(4)	1.86(4)	2.895(3)	175(4)	
N5—H5A···O7	0.86	2.22	3.017(5)	153	-1/2+x,1/2-y,1/2+z
O7—H7B···O9	0.96(3)	0.96(3)	3.010(6)	160(2)	-1/2+x,1/2-y,-1/2+z
O8—H8B···O2	0.958(13)	0.96(2)	2.809(3)	174(2)	1/2-x,-1/2+y,3/2-z