Synthesis, X-ray Crystal Structure and Antimicrobial activity of unexpected trinuclear Cu(II) complex from *s*-triazine-Based Di-compartmental Ligand *via* self-assembly

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S1- X-ray Structure Determination

The crystal of $[Cu_3(HL)(Cl)_2(NO_3)(H_2O)_5](NO_3)_2$ (**1**) was immersed in cryo-oil, mounted in a MiTeGen loop and measured at 120 K on a Rigaku Oxford Diffraction Supernova diffractometer using Mo Kα (λ = 0.71073 Å) radiation. The CrysAlisPro [16] program package was used for cell refinement and data reduction. Multi-scan absorption correction (*CrysAlisPro* [16]) was applied to the intensities before structure solution. The structure was solved by intrinsic phasing method using the *SHELXT* [17] software. Structural refinement was carried out using *SHELXL-2017* [17] program and *Olex2* [18] graphical user interface. The NH hydrogen atom was located from the difference Fourier map and refined isotropically. The H_2O hydrogen atoms were also located from the difference Fourier map but constrained to ride on their parent oxygen with U~iso~ = 1.5 U~eq~(parent atom). Other hydrogen atoms were positioned geometrically and constrained to ride on their parent atoms, with C-H = 0.95-0.98 Å and U_{iso} = 1.2-1.5 U_{eq} (parent atom). The crystallographic details are summarized in Table **1**.

Figure S1 Growth inhibition images of target pathogenic microbes with the Cu(II) complex (1) and H_2L (2), negative control DMSO alone (C), positive control, Gentamicin.

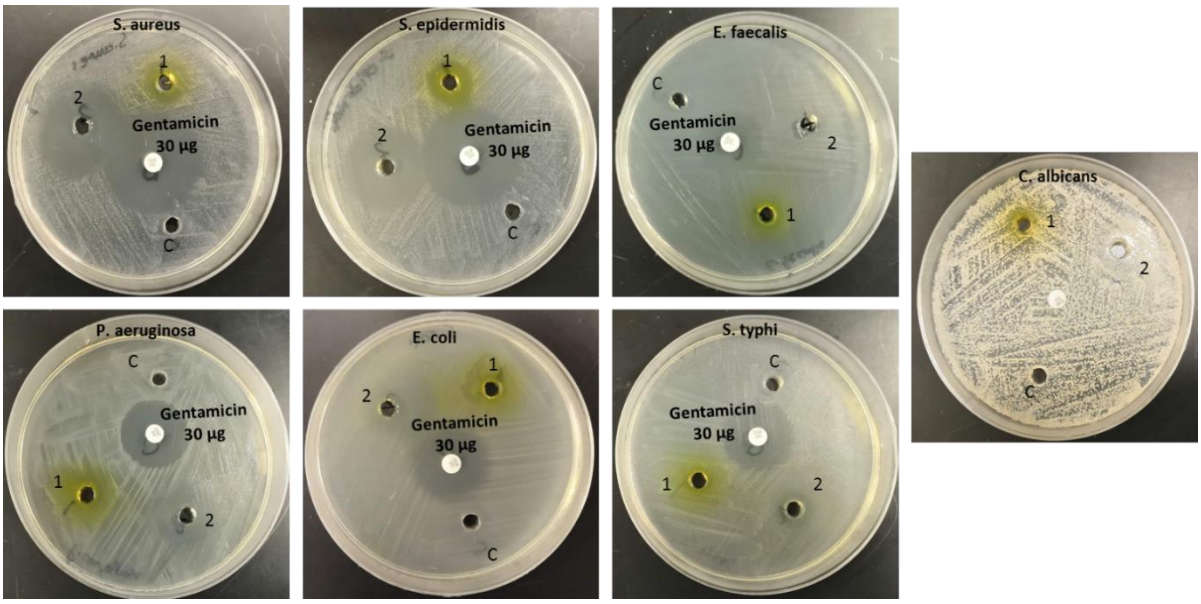

Figure S2 Photography images of inhibition of pathogenic microbe's growth at different concentrations of synthetic compounds to determine their MIC and MBC**;** the Cu(II) complex (1) and H_2L (2).

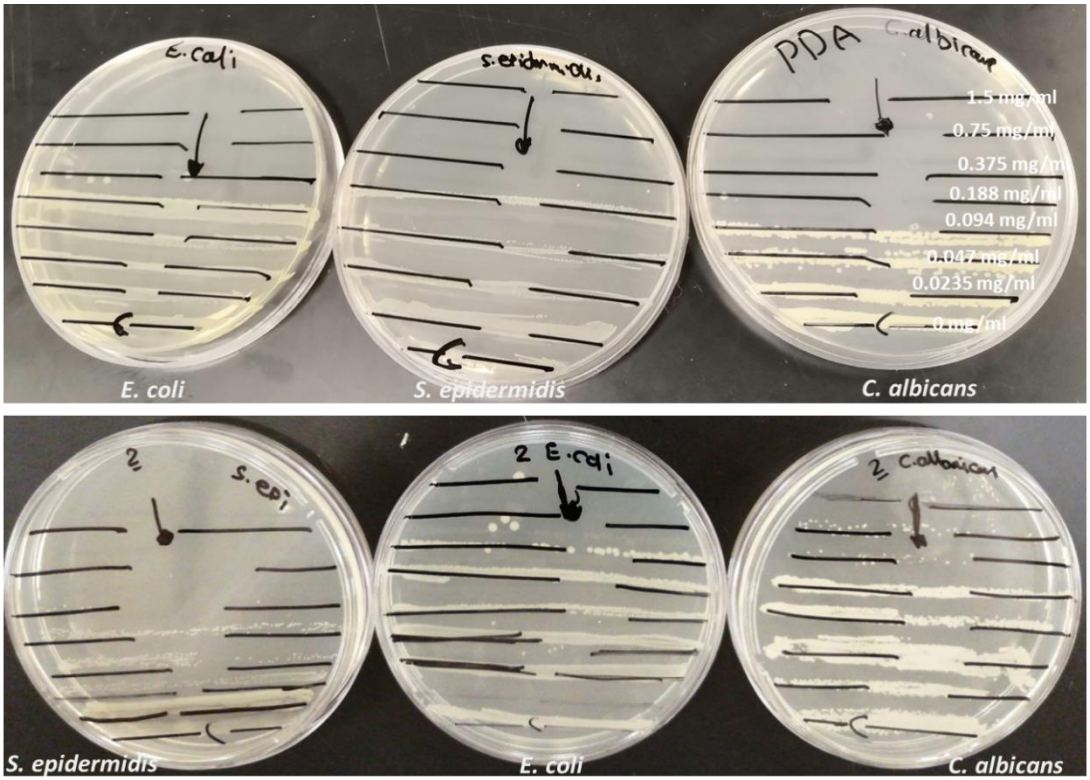

Table S1 AIM Topological parameters (a.u.) of the Cu-N, Cu-Cl and Cu-O interactions.

Bond	ϱ(r)	G(r)	V(r)	H(r)	V(r)/G(r)	E_{int}[a]
Cu1-Cl1	0.0773	0.0745	-0.0979	-0.0234	1.31	30.70
Cu1-O1	0.0373	0.0469	-0.0476	-0.0008	1.02	14.95
Cu1-N1	0.0789	0.0989	-0.1194	-0.0205	1.21	37.46
Cu1-N2	0.0927	0.1310	-0.1582	-0.0272	1.21	49.64
Cu1-N6	0.0739	0.0917	-0.1096	-0.0179	1.20	34.37
Cu2-Cl2	0.0774	0.0822	-0.1058	-0.0236	1.29	33.20
Cu2-O3	0.0317	0.0369	-0.0366	0.0003	0.99	11.49
Cu2-N9	0.0863	0.1087	-0.1333	-0.0246	1.23	41.82
Cu2-N8	0.0954	0.1264	-0.1563	-0.0299	1.24	49.04
Cu2-N4	0.0785	0.1029	-0.1229	-0.0200	1.19	38.56
Cu3-N7	0.0841	0.1106	-0.1337	-0.0231	1.21	41.95
Cu3-O7	0.0398	0.0470	-0.0492	-0.0022	1.05	15.42
Cu3-O6	0.0804	0.1234	-0.1424	-0.0190	1.15	44.67
Cu3-O5	0.0796	0.1302	-0.1478	-0.0176	1.13	46.38
Cu3-O4	0.0858	0.1247	-0.1466	-0.0219	1.18	45.99

[a]kcal/mol