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Electronic supplementary information for:

A new Cu(II) complex derived from the reaction between tris(2-aminoethyl)amine, and Cu(I)-activated acetonitrile; Potent anticancer activity against some cell lines and high affinity for the essential proteins of SARS-CoV-2

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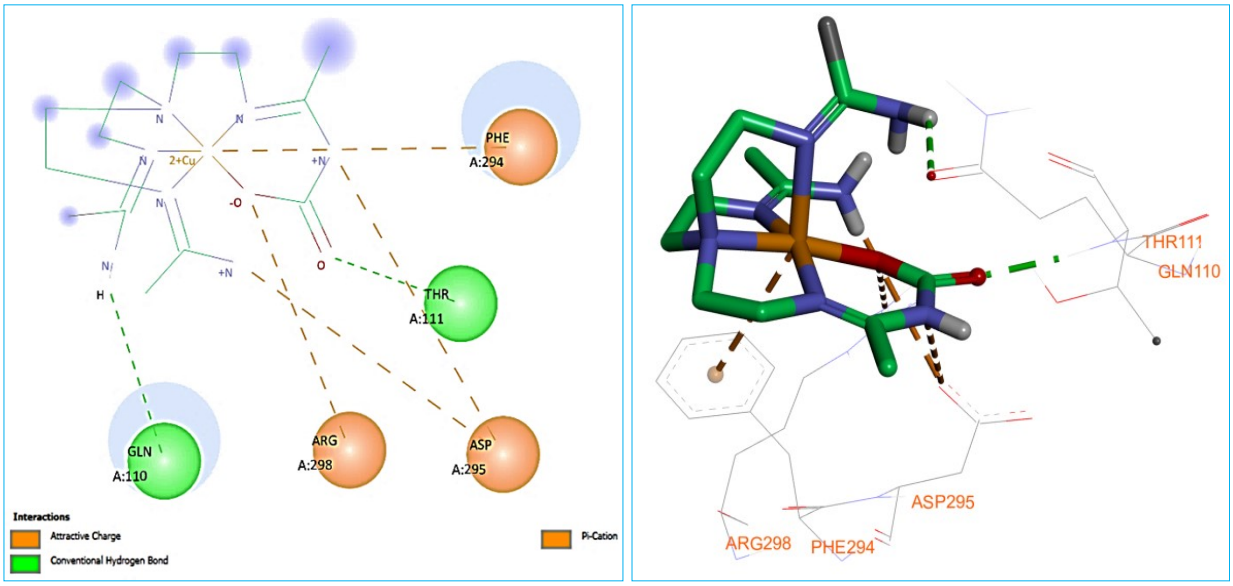
Contains:

Table S1. Crystal data and structure refinement for CuL, CCDC: 2223417

Empirical formula	$C_{13}H_{28}ClCuN_7O_3$
Formula weight	429.41
Temperature/K	100(1)
Crystal system	triclinic
Space group	P-1
a/Å	8.3648(4)
b/Å	11.0439(6)
c/Å	11.5384(8)
α/°	107.679(6)
β/°	103.872(5)
γ/°	106.779(5)
Volume/Å^3	907.55(10)
Z	2
ρ_{calc}g/cm^3	1.571
μ/mm^{-1}	1.379
F(000)	450.0
Crystal size/mm^3	0.335 × 0.226 × 0.038
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.43 to 59.674
Index ranges	$-11 \leq h \leq 11$, $-15 \leq k \leq 11$, $-11 \leq l \leq 15$
Reflections collected	7277
Independent reflections	4481 [Rint = 0.0202, Rsigma = 0.0365]
Data/restraints/parameters	4481/0/233
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R1 = 0.0317, wR2 = 0.0798
Final R indexes [all data]	R1 = 0.0362, wR2 = 0.0826
Largest diff. peak/hole / e Å^{-3}	0.56/-0.50

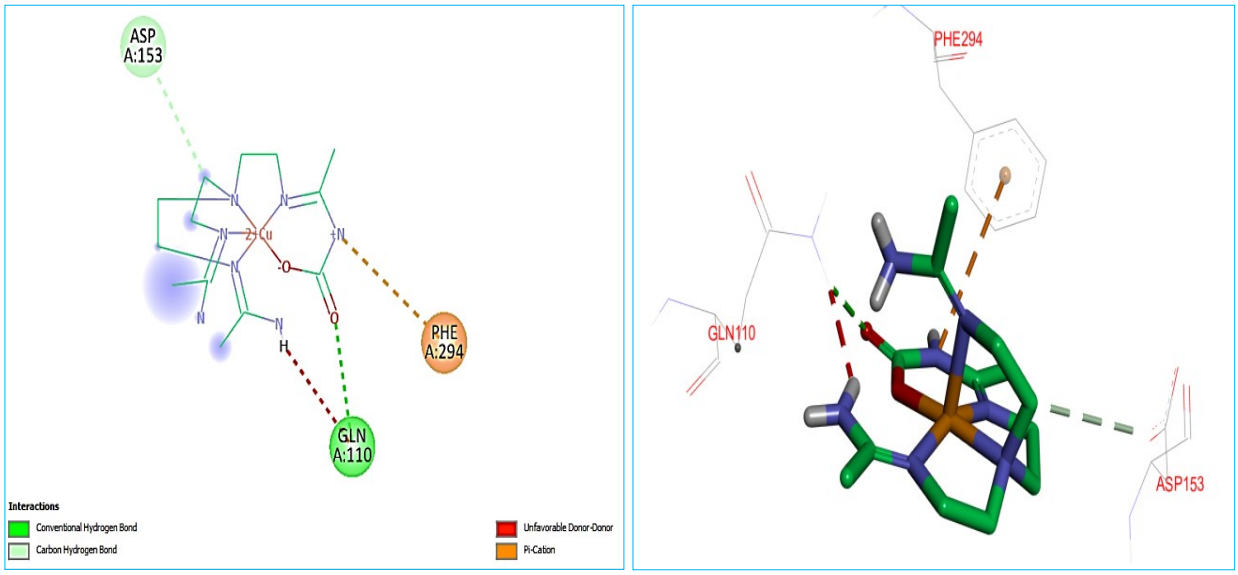
Table S2. Selected bond Angles (°) and bond Lengths (Å) of CuL

Bond angles		**Bond lengths**	
O1─Cu1─N1	172.05(6)	Cu1─O1	1.9525(14)
O1─Cu1─N2	89.69(6)	Cu1─N1	2.0205(16)
O1─Cu1─N3	98.00(6)	Cu1─N2	1.9609(17)
O1─Cu1─N4	103.89(6)	Cu1─N3	2.0033(17)
N1─Cu1─N4	83.44(6)	Cu1─N4	2.2605(17)
N2─Cu1─N1	85.54(7)		
N2─Cu1─N3	161.17(7)		
N2─Cu1─N4	103.75(7)		
N3─Cu1─N1	84.75(7)		
N3─Cu1─N4	91.11(7)		



(a) (b)

Fig. S1. Molecular docking 2D (a) and 3D (b) models of CuL–M^{pro} interaction (PDB ID: 7C8U) which show the binding sites of the CuL with selected amino acids residues of M^{pro}.



(a) (b)

Fig. S2. Molecular docking 2D (a) and 3D (b) models of CuL–M^{pro} interaction (PDB ID: 6LU7) which show the binding sites of the CuL with selected amino acids residues of M^{pro}.