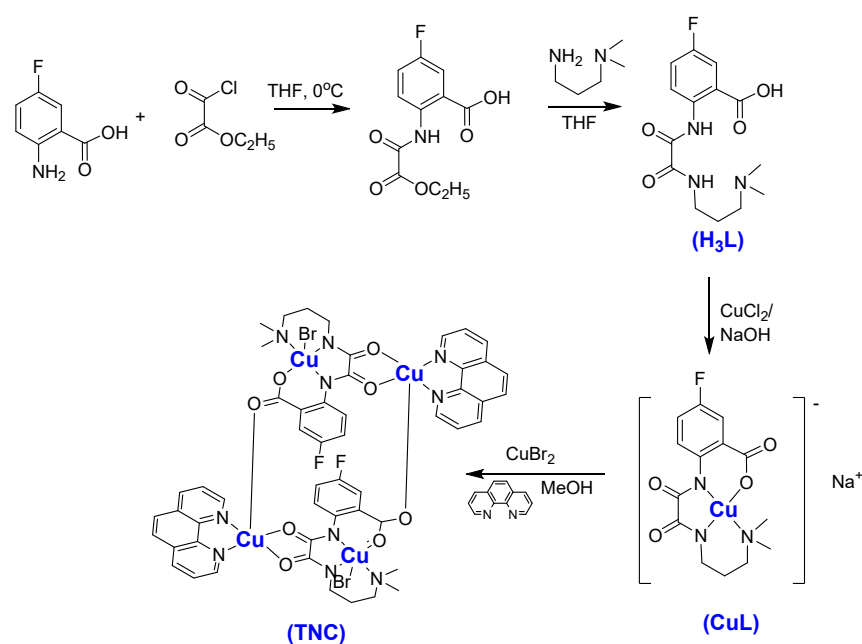


A Novel tetranuclear Cu (II) Complex for DNA-binding and in Vitro Anticancer Activity

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Scheme 1s. The synthetic routes for the mononuclear copper ligand and TNC.

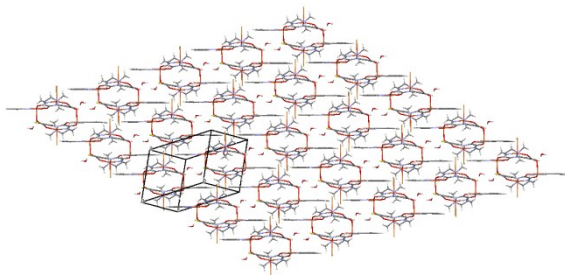


Figure 1S. The 3D supramolecular network for TNC

Table S1 Crystal data and structure refinement for TNC

Identification code	
Empirical formula	$C_{27} H_{29} Br Cu_2 F N_5 O_6$
Formula weight	745.54
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
space group	P-1
Unit cell dimensions	
a	10.8035(8) Å
b	12.1488(11) Å
c	12.9920(12) Å
alpha	67.2590(10)deg.
beta	69.516(2) deg.
gamma	69.334(2) deg.
Volume	1425.7(2) Å ³
Z	2
Calculated density	1.737 Mg/m ³
Absorption coefficient	2.951 mm ⁻¹
F(000)	752
Crystal size	0.37 x 0.23 x 0.02 mm
Theta range for data collection	2.43 to 25.02 deg.
Limiting indices	-12 ≤ h ≤ 9, -14 ≤ k ≤ 14, -15 ≤ l ≤ 12
Reflections collected / unique	7311 / 4958 [R(int) = 0.0686]
Completeness to theta = 25.02	98.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9516 and 0.4082
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4958 / 0 / 383
Goodness-of-fit on F ²	1.072
Final R indices [I > 2σ(I)]	R1 = 0.0656, wR2 = 0.1518
R indices (all data)	R1 = 0.0980, wR2 = 0.1619
Largest diff. peak and hole	0.950 and -0.591 e.Å ⁻³

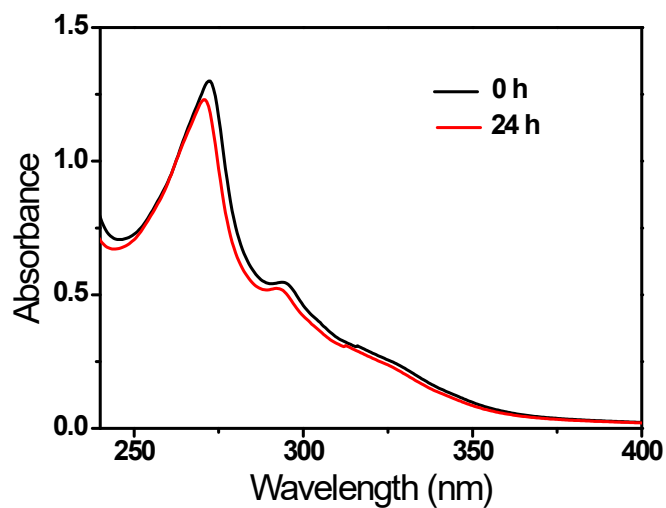


Figure 2S. The stability of TNC in aqueous media.

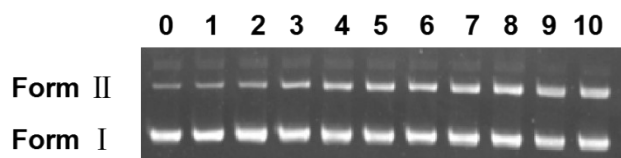


Figure 3S. Cleavage patterns of pUC19 DNA (20 ng/μl) by TNC in the agarose gel electrophoresis. Concentration of TNC: Lane 0: 0; Lane 1: 20 μM; Lane 2: 40 μM; Lane 3: 60 μM; Lane 4: 80 μM; Lane 5: 100 μM; Lane 6: 120 μM; Lane 7: 140 μM; Lane 8: 160 μM; Lane 9: 180 μM; Lane 10: 200 μM.