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Synthesis, characterization, molecular docking and DFT calculation of a copper(II) mixed-ligand complex

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A mixed-ligand complex ([1]) consisting of $[Cu(NO_3)_2].3H_2O$, [2,4,6-trihydrazineyl-1,3,5-triazine] (THT), and Pyridine-2,6-dicarboxylic acid (PDCA) was synthesized and characterized using FT-IR spectroscopy and CHN analysis. The complex [Cu(THT)(PDC)] possesses a unique combination of ligands and has potential applications in coordination chemistry. The complex has a distorted square pyramidal geometry ($\tau = 0.22$) with a CuN_3O_2 environment, where THT acts as a bidentate ligand and PDC acts as a tridentate ligand, binding to the metal atom through one nitrogen atom and two oxygen atoms as shown in Fig(1). The thermodynamic stability of the complex was investigated using DFT([2]). Based on the obtained reaction values, the calculations demonstrate that the reaction products have achieved a higher level of stability, with a difference of (-0.003054) Hartree, compared to the initial substances. This result is presented in Table (1). The biological activity of the complex and its ability to interact with biomacromolecules were investigated through docking calculations ([3]). The results indicate that the complex has a similar activity to doxorubicin in the interaction with B-DNA (Major) and CatB protein, as presented in Table (2).

***Keywords*:** Triazine, Mixed-ligand, Molecular docking, DFT, Coordination chemistry

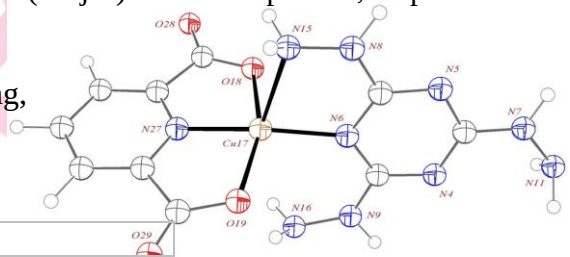


Fig 1. The ortep diagram of the molecular structure of the complex

Table 1. Reaction equation and ΔG calculation

Reaction: THT + PDCA + $Cu(NO_3)_2$ → [Cu(THT)(PDC)]+ $2HNO_3$						
	THT	PDCA	$Cu(NO_3)_2$	Complex	HNO_3	Reaction
ΔG	-612.328308	-625.358664	-756.576616	-1432.500836	-561.765806	-0.003054

Table 2. The calculated fitness values for the ligands and their complexes along with the doxorubicin.values

	B-DNA (Maj)	B-DNA (Min)	BRAF-Kinase	CatB	DNA-Gyrase	HDAC7	rHA	RNR	TrxR	TS	Top II
Complex	26.96	47.68	42.71	21.00	28.45	34.50	33.98	33.20	45.30	37.96	36.29
Doxorubicin	33.47	83.10	54.21	25.95	52.97	50.73	50.10	49.18	66.70	53.34	59.05

References

[1] H. O. Omoregie, O. A. Oloba-Whenu, O. J. Olowu, T. M. Fasina, A. Friedrich and M. Haehnel, *RSC advances*, **2022**, 12, 23513.
[2] S. Y. Ebrahimipour, I. Sheikhshoaie, M. Mohamadi, S. Suarez, R. Baggio, M. Khaleghi, M. T. Mahani and A. Mostafavi, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 142, 410.
[3] K. Paliwal, P. Haldar, P. K. S. Antharjanam and M. Kumar, *ACS Omega*, **2022**, 25, 21961.