

Accepted Manuscript

Research paper

Two Cu(II) complexes containing 2,4-diamino-6-(2-pyridyl)-1,3,5-triazine and amino acids: Synthesis, crystal structures, DNA/HSA binding, molecular docking, and *in vitro* cytotoxicity studies

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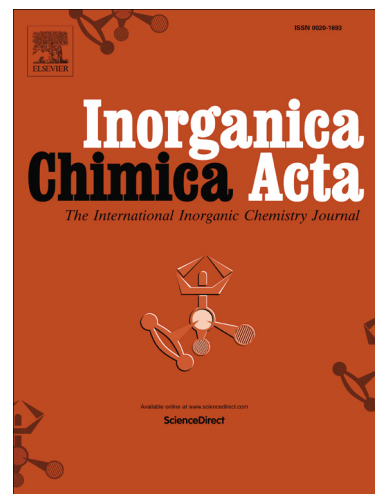
PII: S0020-1693(17)30260-8
DOI: <http://dx.doi.org/10.1016/j.ica.2017.05.030>
Reference: ICA 17599

To appear in: *Inorganica Chimica Acta*

Received Date: 21 February 2017
Revised Date: 23 April 2017
Accepted Date: 11 May 2017

Please cite this article as: F. Shen, Z-B. Ou, Y-J. Liu, W. Liu, B-F. Wang, Z-W. Mao, X-Y. Le, Two Cu(II) complexes containing 2,4-diamino-6-(2-pyridyl)-1,3,5-triazine and amino acids: Synthesis, crystal structures, DNA/HSA binding, molecular docking, and *in vitro* cytotoxicity studies, *Inorganica Chimica Acta* (2017), doi: <http://dx.doi.org/10.1016/j.ica.2017.05.030>

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Two Cu(II) complexes containing 2,4-diamino-6-(2-pyridyl)-1,3,5-triazine and amino acids: Synthesis, crystal structures, DNA/HSA binding, molecular docking, and *in vitro* cytotoxicity studies

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Abstract: Two new copper(II)-amino acid complexes, [Cu(PyTA)(L-Thr)(ClO₄)]₂·1.5H₂O (**1**) and [Cu(PyTA)(L-Arg)(ClO₄)(H₂O)]·ClO₄ (**2**) (PyTA = 2,4-diamino-6-(2-pyridyl)-1,3,5-triazine, L-Thr = L-threonine, L-Arg = L-arginine), were successfully synthesized and characterized. The results determined by single crystal X-ray diffraction showed that the five-coordinated copper of **1** and the six-coordinated copper of **2** were located in the distorted square-pyramidal and distorted octahedral environments, respectively. Spectroscopic titrations, thermal denaturation experiments, viscosity measurements revealed that the complexes bound to DNA *via* a groove binding mode, with the DNA-binding constants of $6.126 \times 10^4 \text{ M}^{-1}$ for **1** and $6.464 \times 10^4 \text{ M}^{-1}$ for **2**. Electrophoresis experiments revealed that the complexes cleaved pBR322 DNA by an oxidative pathway involving in the generation of superoxide free radical (O₂⁻). Multi-spectroscopic analyses showed that the complexes bound to site I of human serum albumin (HSA) with moderate affinities. In particular, *in vitro* cytotoxicities of the complexes against Bel-7402 cell line showed promising anticancer effects (IC₅₀ = 42.1 ± 1.7 μM for **1**; IC₅₀ = 36.3 ± 0.9 μM for **2**). In addition, the binding mechanism and mode of the complexes with DNA/HSA were verified by molecular docking

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