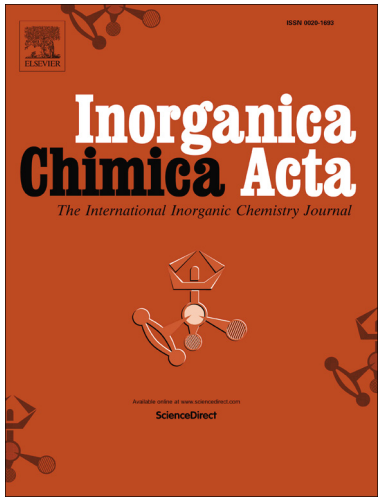

Research paper

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

Fang Shen, Zhi-Bin Ou, Yu-Jia Liu, Wei Liu, Bing-Feng Wang, Zong-Wan Mao, Xue-Yi Le

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

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

Fang Shen[a], Zhi-Bin Ou[a] ,Yu-Jia Liu[a], Wei Liu[b], Bing-Feng Wang[a], Zong-Wan Mao[c], Xue-Yi Le[a,*]

[a] *Department of Applied Chemistry, South China Agricultural University, Guangzhou 510642, PR China*

[b] *College of Materials and Energy, South China Agricultural University, Guangzhou 510642, PR China*

[c] *School of Chemistry, Sun Yat-sen University, Guangzhou 510275, PR China*

Abstract: Two new copper(II)-amino acid complexes, $[Cu(PyTA)(L\text{-Thr})(ClO_4)]_2 \cdot 1.5H_2O$ (**1**) and $[Cu(PyTA)(L\text{-Arg})(ClO_4)(H_2O)] \cdot ClO_4$ (**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 6.126×10^4 M^{-1} for **1** and 6.464×10^4 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 (O_2^-). 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 (IC_{50} = 42.1 ± 1.7 μM for **1**; IC_{50} = 36.3 ± 0.9μM for **2**). In addition, the binding mechanism and mode of the complexes with DNA/HSA were verified by molecular docking

* Corresponding author.

E-mail address: lexyfu@163.com (Xue-Yi Le).