



Solution structure, oxidative DNA damage, biological activity and molecular docking of ternary copper(II) L-argininato complexes

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Continuing our search for metal drugs with markedly higher toxicity to cancer cells than to normal cells, we evaluated the effect of 2,2'-bipyridine (bpy) as a co-ligand in the compounds $[\text{Cu}(\mu\text{-O}, \text{O}'\text{-NO}_3)(\text{L-Arg})(\text{bpy})]\text{NO}_3\}_n$ (**1**) and $[\text{CuCl}(\text{L-Arg})(\text{bpy})]\text{Cl}\cdot 3\text{H}_2\text{O}$ (**2**) (L-Arg = L-arginine), on DNA interaction, cytotoxic and antiproliferative activity, compared to the effects induced by other co-ligands *i.e.* 1,10-phenanthroline (phen) and SCN^- ions, in similar Cu(II) compounds we have studied previously. Potentiometric, X-band EPR and UV-Vis experiments were first used to structurally characterise the complexes formed in solutions **1** and **2** and in model Cu(II)/bpy/L-Arg systems. Gel electrophoresis in the presence of H_2O_2 was used to identify DNA damage by **1** and **2**. In addition, cyclic voltammetry of both compounds was performed to confirm the existence of Cu(II)/Cu(I) redox pairs involved in the free radical mechanism of this DNA damage. The DNA binding constants of **1** and **2** were determined spectrophotometrically. The selectivity of the cytotoxic and antiproliferative activity of compounds **1** and **2** was tested *in vitro* against human lung adenocarcinoma (A549), liver cancer (HepG2) and normal cells in comparison with those previously observed by us for compounds consisting of phen and SCN^- ligands. Molecular docking calculations were performed for $[\text{Cu}(\text{L-Arg})(\text{bpy})]^{2+}$ species (arraised in solutions of **1** and **2**) interacting with B-DNA (aureolin), metalloproteinase (*S. aureus*) and penicillin-binding protein (*E. coli*) to determine the nature of the complex-receptor interaction, potential binding modes and energies.

Słowa kluczowe

L-Arginine, Cu(II) complexes, Potentiometric study, UV-Vis and EPR spectroscopies, Free radicals, Cytotoxic and antiproliferative potential, Molecular docking

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