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ORIGINAL PAPER

Synthesis, characterization, DFT study, DNA/BSA-binding affinity, and cytotoxicity of some dinuclear and trinuclear gold(III) complexes

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Abstract

In this study, we have synthesized a series of dinuclear and trinuclear gold(III) complexes of the general formula $[Au_2(N–N)Cl_6]$ (**1**–**3**) for dinuclear and $[Au_3(N–N)_2Cl_8]^+$ (**4**–**6**) for trinuclear compounds, respectively, in which *N*–*N* is a bidentate ligand (1,4-diaminobutane; 1,6-diaminohexane or 1,8-diaminooctane). These complexes were characterized by elemental analysis, molar conductivity, and spectroscopic techniques (IR, UV–Vis, ^{1}H NMR, ESI–MS). We performed DFT calculations to get insight into the geometry of the studies complexes. DNA-binding studies were performed by UV–Vis spectrophotometry and fluorescence spectroscopy. The results of competitive reactions between gold(III) complexes and ethidium bromide (EB) towards DNA have shown that selected complexes can displace EB from DNA-EB adduct. In addition, these experiments confirm that polynuclear gold(III) complexes interact with DNA covalently or via intercalation. Furthermore, high values of binding constants of gold(III) complexes towards bovine serum albumin (BSA) protein indicate good binding affinity. In addition, redox stability of complexes in the presence of DNA/BSA was confirmed by cyclic voltammetry. Results of the interactions between gold(III) complexes with DNA/BSA were discussed in reference to molecular docking data obtain by Molegro virtual docker. The cytotoxic activity of synthesized gold(III) complexes was evaluated on human breast cancer cell line (MDA-MB-231), human colorectal cancer cell line (HCT-116), and normal human lung fibroblast cell line (MRC-5). All complexes dose-dependently reduced cancer and normal cells viabilities, with significant cytotoxic effects ($IC_{50} < 25$ μM) for trinuclear gold(III) complexes (**4**, **5**) on HCT-116 cells.

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