



Interactions of zinc(II) complexes with 5'-GMP and their cytotoxic activity

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ABSTRACT

The mechanism of substitution from tetrahedral $[\text{ZnCl}_2(\text{en})]$ and square-pyramidal $[\text{ZnCl}_2(\text{terpy})]$ complexes (where en = 1,2-diaminoethane or ethylenediamine and terpy = 2,2':6',2''-terpyridine) by guanosine-5'-monophosphate (5'-GMP) have been investigated by ^1H NMR spectroscopy. The substitution reaction of $[\text{ZnCl}_2(\text{terpy})]$ complex is faster than the reaction of $[\text{ZnCl}_2(\text{en})]$, which was finished after 48 h. Information about the structures of the final products in solution were obtained from the DFT calculations (B3LYP/6-31G(d)) and experimental ^1H NMR data acquired during the course of the reaction. The cytotoxic activity of zinc(II) complexes was tested on human breast cancer cell line MDA-MB-231, human colon cancer cell line HCT-116 and normal human lung fibroblast cell line MRC-5. Both complexes reduced cell viabilities, while $[\text{ZnCl}_2(\text{terpy})]$ was significantly cytotoxic on MDA-MB-231 after 72 h, and HCT-116 after 24 h without dose dependence. The differences in reactivity toward 5'-GMP and cytotoxic activity of Zn(II) complexes may be attributed to the very stable square-pyramidal geometry of $[\text{ZnCl}_2(\text{terpy})]$ in solution, while weak ligand effect of the en compared to the terpy affected slow interaction of tetrahedral $[\text{ZnCl}_2(\text{en})]$ complex with the target biomolecule.

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