

Acid–base characterization, coordination properties towards copper(II) ions and DNA interaction studies of ribavirin, an antiviral drug.

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Streszczenie

We have studied processes of copper(II) ion binding by ribavirin, an antiviral agent used in treating hepatitis C, which is accompanied usually by an increased copper level in the serum and liver tissue. Protonation equilibria and Cu(II) binding were investigated using the UV–visible, EPR and NMR spectroscopic techniques as well as the DFT (density functional theory) calculations. The spectroscopic data suggest that the first complex is formed in the water solution at pH as low as 0.5. In this compound Cu(II) ion is bound to one of the nitrogen atoms from the triazole ring. Above pH 6.0, the metal ion is surrounded by two nitrogen and two oxygen atoms from two ligand molecules. The DFT calculations allowed to determine the exact structure of this complex. We found that in the lowest energy isomer two molecules of the ligand coordinate via O and N4 atoms in *trans* positions. The hypothetical oxidative properties of the investigated system were also examined. It proved not to generate plasmid DNA scission products. However, the calf thymus (CT)-DNA binding studies showed that it reacts with ribavirin and its cupric complex. Moreover, the interaction with the complex is much more efficient.

Słowa kluczowe

Acid–base properties of ribavirin, Complexes with Cu(II), Interaction with plasmid DNA, CT-DNA binding studies, TD DFT calculations

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