
The Cu(II)-fluconazole complex revisited. Part I: structural characteristics of the system.

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Streszczenie

Protonation equilibria and Cu(II) binding processes by an antifungal agent fluconazole, α -(2,4-difluorophenyl)- α -(1H-1,2,4-triazol-1-yl-methyl)-1H-1,2,4-triazole-1-ethanol, were studied using the UV-Vis, EPR and NMR spectroscopic techniques. The protonation constant of fluconazole was determined from NMR titration and attributed to N4' nitrogen atoms using the DFT methods. The spectroscopic data suggest that at pH as low as 0.4 the first complex is formed, in which one or two Cu(II) ions are bound to one of the nitrogen atoms (N4') from triazole rings. Above pH 1.5 each Cu(II) ion is surrounded by two nitrogen atoms (also N4') from two different ligand molecules, forming primary monomeric complexes and above pH=5, both dimeric or oligomeric species occur, which is well registered by the EPR technique. The mixture of Cu(NO₃)₂ with fluconazole in a 1:1 molar ratio in a water (pH=4.5)/ethanol solution gave crystals of [Cu₂(H₂O)₂[(C₆H₃-2,4-F₂)(CH₂N(C₂H₂))₂C-OH][(C₆H₃-2,4-F₂)(CH₂N(C₂H₂))₂C-O}(NO₃)](NO₃)₂·9(H₂O). This complex is the first example of a cupric 3D polymeric structure with a fluconazole ligand coordinated via both N2' and N4' atoms from the same triazole rings. At higher pH values, we obtained a binuclear complex [Cu₂(L)₂(H₂O)₂(NO₃)₂], in which the copper(II) atoms were bridged by the oxygen atoms of the deprotonated OH group of fluconazole. The hypothetical oxidative properties of this system were also examined, however it failed to generate either reactive oxygen species or DNA scission products.

Słowa kluczowe

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