

Copper(II) complexes with *Fusobacterium nucleatum* adhesin FadA : coordination pattern, physicochemical properties and reactivity.

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Streszczenie

Fusobacterium nucleatum is an anaerobic, Gram-negative bacteria linked to colon cancer. It is interesting to determine how metal ions interact with bacterial adhesin proteins. To this end, the coordination of ATDAAS-NH₂ and MKKFL-NH₂ fragments of *Fusobacterium* adhesin A (FadA) to copper(II) ions was studied by potentiometry, spectroscopic techniques (UV-Vis, CD, EPR and NMR) and the density functional theory (DFT) methods. At pH6.8 (colon physiological pH), the metal ion in the first peptide (ATDAAS-NH₂) is coordinated by one oxygen and three nitrogen donors while in the second one (MKKFL-NH₂) - by sulfur and three nitrogen atoms. Both complexes form two five- and one six-membered stable chelate rings. Moreover, reactivity studies confirmed the production of reactive oxygen species such as hydroxyl radical, superoxide anion radical and singlet oxygen. Generation of reactive oxygen species (ROS) was observed during gel electrophoresis and spectroscopic assays with reporting molecules like NDMA (*N,N*-dimethyl-*p*-nitrosoaniline) and NBT (Nitrotetrazolium Blue Chloride). All reactions were conducted in the presence of hydrogen peroxide as endogenous oxidant.

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