

Effect of copper(II) ion binding by porin P1 precursor fragments from *fusobacterium nucleatum* on DNA degradation.

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Streszczenie

Fusobacterium nucleatum is one of the most notorious species involved in colorectal cancer.

It was reported that numerous outer membrane proteins (OMP) are actively involved in carcinogenesis.

In this paper, the structure and stability of certain complexes, as well as DNA cleavage

and ROS generation by fragments of OMP, were investigated using experimental and theoretical

methods. Mass spectrometry, potentiometry, UV-Vis, CD, EPR, gel electrophoresis and calculations

at the density functional theory (DFT) level were applied. Two consecutive model peptides, Ac-

AKGHEHQLE-NH₂ and Ac-FGEHEHGRD-NH₂, were studied.

Both of these were rendered to form

a variety of thermodynamically stable complexes with copper(II) ions. All of the complexes were

stabilized, mainly due to interactions of metal with nitrogen and oxygen donor atoms, as well as rich

hydrogen bond networks. It was also concluded that these complexes in the presence of hydrogen

peroxide or ascorbic acid can effectively produce hydroxyl radicals and have an ability to cleave the

DNA strands. Surprisingly, the second studied ligand at the micromolar concentration range causes

overall DNA degradation.

Słowa kluczowe

porin protein P1, *Fusobacterium nucleatum*, copper(II) binding, DNA degradation, reactive oxygen species generation, NDMA decomposition

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