

Factors affecting nucleolytic efficiency of some ternary metal complexes with DNA binding and recognition domains. Crystal and molecular structure of Zn(phen)(edda)

ABSTRACT

The binding selectivity of the M(phen)(edda) (M = Cu, Co, Ni, Zn; phen = 1,10-phenanthroline, edda = ethylenediaminediacetic acid) complexes towards ds(CG)₆, ds(AT)₆ and ds(CGCGAATTCGCG) B-form oligonucleotide duplexes were studied by CD spectroscopy and molecular modeling. The binding mode is intercalation and there is selectivity towards AT-sequence and stacking preference for A/A parallel or diagonal adjacent base steps in their intercalation. The nucleolytic properties of these complexes were investigated and the factors affecting the extent of cleavage were determined to be: concentration of complex, the nature of metal(II) ion, type of buffer, pH of buffer, incubation time, incubation temperature, and the presence of hydrogen peroxide or ascorbic acid as exogenous reagents. The fluorescence property of these complexes and its origin were also investigated. The crystal structure of the Zn(phen)(edda) complex is reported in which the zinc atom displays a distorted trans-N₄O₂ octahedral geometry; the crystal packing features double layers of complex molecules held together by extensive hydrogen bonding that interdigitate with adjacent double layers via π interactions between 1,10-phenanthroline residues. The structure is compared with that of the recently described copper(II) analogue and, with the latter, included in molecular modeling.

Keyword: Metal(II) ternary complexes; DNA binding; Molecular modeling; Nucleolytic; Intercalation