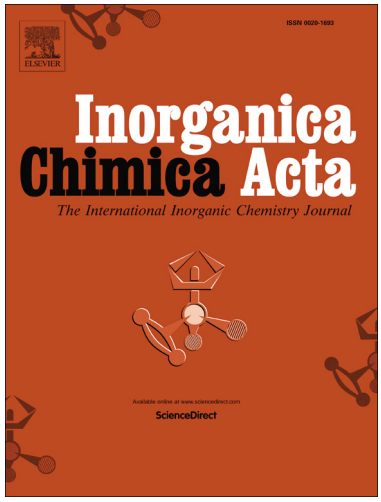

Research paper

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E. Veerashekhar Goud, Akella Sivaramakrishna, Kari Vijayakrishna, C.V.S. Brahmmananda Rao, Vijay M. Khedkar, Prakash C. Jha

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Synthesis, Structure and DNA Interaction Studies of Bisphosphoramides: Theoretical and Experimental Insights

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Abstract

New bisphosphoramides (having phenyl ($EDAPOPh_2$) and ethoxy (EDADEP) substituents attached to phosphoryl groups bridged with ethylenediamine spacer) are synthesized and structurally characterized by spectroscopic techniques as well as elemental analysis. The molecular structure of $EDAPOPh_2$ was determined by single crystal X-ray diffraction technique. The interaction of these bisphosphoramides with calf thymus DNA (*ct*-DNA) is investigated using UV-Visible absorption and fluorescence spectral data as well as the DFT calculations. These studies reveal that $EDAPOPh_2$ and EDADEP interact with DNA in a partial intercalation mode. The intrinsic binding constants K_b of two different bisphosphoramides with *ct*-DNA were determined by fluorescence spectroscopy as 2.08×10^4 and 3.86×10^4 M^{-1} respectively. The results indicated that the two compounds bind to *ct*-DNA with different binding affinities, *i.e.* $EDAPOPh_2$ > EDADEP. The binding mechanism of these bisphosphoramides to *ct*-DNA is also discussed.

Key words: Bisphosphoramides, crystal structure, molecular docking, DNA interaction.