Accepted Manuscript

Research paper

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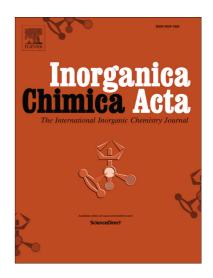
PII: S0020-1693(17)30226-8

DOI: http://dx.doi.org/10.1016/j.ica.2017.02.017

Reference: ICA 17443

To appear in: Inorganica Chimica Acta

Received Date: 4 August 2016 Revised Date: 4 February 2017 Accepted Date: 15 February 2017



Please cite this article as: E. Veerashekhar Goud, A. Sivaramakrishna, K. Vijayakrishna, C.V.S. Brahmmananda Rao, V.M. Khedkar, P.C. Jha, Synthesis, Structure and DNA Interaction Studies of Bisphosphoramides: Theoretical and Experimental Insights, *Inorganica Chimica Acta* (2017), doi: http://dx.doi.org/10.1016/j.ica.2017.02.017

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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 (EDAPOPh₂) 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 EDAPOPh₂ 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 EDAPOPh₂ 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 x 10^4 and 3.86 x 10^4 M⁻¹ respectively. The results indicated that the two compounds bind to ct-DNA with different binding affinities, i.e. EDAPOPh₂ > EDADEP. The binding mechanism of these bisphosphoramides to ct-DNA is also discussed.

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

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