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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

¹E. Veerashekhar Goud, ¹Akella Sivaramakrishna*, ¹Kari Vijayakrishna,
²C.V.S. Brahmmananda Rao, ^{3,4}Vijay M. Khedkar, ⁵Prakash C. Jha

¹Department of Chemistry, School of Advanced Sciences, VIT University, Vellore-632014, Tamil Nadu, India

²Chemistry Group, Indira Gandhi Centre for Atomic Research, Kalpakkam-603102, Tamil Nadu, India

³School of Health Sciences, University of Kwa Zulu Natal, Westville Campus, Durban 4000, South Africa

⁴Combi-Chem Resource Centre, CSIR-National Chemical Laboratory, Pune, 411008 Maharashtra, India

⁵School of Chemical Sciences, Central University of Gujarat, Sector-30, Gandhinagar, Gujarat, India

E-mail: askrishna@vit.ac.in

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 2.08×10^4 and $3.86 \times 10^4 \text{ M}^{-1}$ 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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