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Some pyridyl moiety based metal complexes (*viz.*, Mn^{+2}, Co^{+2} and Zn^{+2}) as potential anticancer agents and DNA nucleobase interaction: A DFT approach

Benzir Ahmed[a], Pratyashee Barukial[a], Basanta Singha[b], Upasana Bora Sinha[b] & Bipul Bezbaruah*[a]

[a] Department of Applied Sciences, Gauhati University, Guwahati 781 014, Assam, India

[b] Department of Chemistry, Nagaland University, Lumami 798 627, Nagaland, India

E-mail: bipulbezbaruah@gmail.com

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Many experimental evidences reveal that a new set of complexes involving transition metals (*viz.*, Mn^{+2}, Co^{+2} and Zn^{+2}) with pyridyl moiety ligands are being investigated as potential anticancer agents due to their intense ability to follow intercalation mechanisms with DNA nucleobases. Although, the interaction mechanism between anticancer agent-DNA nucleobase itself is quite complicated to understand by using conventional techniques; but some computational methods may still be very helpful for analyzing the proper binding mode of interaction. Hence, exploring the favoured interaction sites within an anticancer agent and finding its donor-acceptor ability is really a challenging task. Moreover, for any drug-DNA receptor complex; there must be few changes in their electron charge density, structure of the molecule, chemical reactivity parameters, *etc*. DFT is one of the best known and most affordable methods for investigating such exploration in metal complexed anticancer agents. Herein, we have described an attempt to investigate the interaction mechanism of some pyridyl moiety based Mn^{+2}, Co^{+2} and Zn^{+2} metal complexes as potential intercalating anticancer agents by using computational techniques.

Keywords: Pyridyl moiety, Anticancer agent, DFT, DNA, Metal complex