



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: The Drug Binding Pathways and Conformational Deviations of G-quadruplex DNA under Different Chemical and Thermal Conditions: A Computational Study

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SHORT ABSTRACT

Nucleic acid sequences containing series of guanine can form G-quadruplex structures, which are of special interest because of their high thermal stability, resistance to denaturing conditions, and stiffness. Moreover, due to the diverse and polymeric nature, it draws the attention of the scientific world in significant and diverse fields.

Chapter 1 introduces the formation and stability of the G-quadruplex DNA in different chemical and thermal conditions along with its applications through literature survey. In Chapter 2, we have reported about the conformational changes of the thrombin-binding G-quadruplex aptamer (TBA) under dissimilar SrCl_2 salt concentrations. Chapter 3 deals with the conformational changes of the human telomeric G-quadruplex DNA at varying KCl salt concentrations and temperatures under non-polar and polar confinements. In Chapter 4, we have discussed about the effect of hydrated and non-hydrated choline chloride-urea deep eutectic solvent (namely reline) on TBA G-quadruplex DNA. Chapter 5 describes the role of reline, a natural DES, on temperature induced conformational changes of c-KIT G-quadruplex DNA. In Chapter 6, we have investigated the binding modes and pathway of APTO-253 on c-KIT G-quadruplex DNA. In the last chapter i.e., Chapter 7 we have summarized the overall findings to reflect upon the interpretation about the conformational deviation of the different types of G-quadruplex DNAs under different chemical and thermal conditions and its drug binding pathway.