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## 3D-NuS: A Web Server for Automated Modeling and Visualization of Non-Canonical 3-Dimensional Nucleic Acid Structures

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The inherent conformational flexibility of nucleic acids (DNA, RNA etc.) facilitate the formation of a range of conformations such as duplex, triplex, quadruplex etc., which play crucial roles in biological processes such as mismatch repair, replication, recombination, transcription, translation, gene regulations etc. These unconventional base pairing and structural conformations on DNA/RNA structures at different sequence contexts also induce abruptions in normal cell function which can lead to deformities and diseases (cancer, fragile X syndrome, etc.). To understand the role of these unusual nucleic acid structures in aforementioned biological phenomena and diseases, structural details at atomic level is indispensable. But, experimental methods (such as X-RAY crystallography, NMR etc.) are not always successful in determining structural details and are very expensive. Further, structural insights about nucleic acid triplexes, which are generally not tractable to structure determination by X-ray crystallography or NMR techniques, are essential to establish their biological function(s). A web server,

namely 3D-NuS (<http://iith.ac.in/3dnus/>), has been developed to generate energy minimized models of 80 different types of triplexes, 64 types of G-quadruplexes, left handed ZDNA/RNA duplexes, RNA-DNA hybrid duplex along with inter- and intra-molecular DNA or RNA duplexes comprising a variety of mismatches and their chimeric forms for any user defined sequence and length. It also generates an ensemble of conformations corresponding to the modeled structure. These structures may serve as good starting models for docking proteins & small molecules with nucleic acids, NMR structure determination, cryo-electron microscope modeling, DNA/RNA nanotechnology applications and molecular dynamics simulation studies. The operational milestones that would be accomplished in future include generation of aforementioned structures with modified nucleic acids such as PNA and LNA, intra-molecular triplexes, complex duplexes and models with user defined structural parameters.

The image shows a collage of screenshots from the 3D-NuS web server interface. Key elements include:

- 1'** A section titled "DNA & RNA molecules" with a "Let's build the models of your choice..." button.
- 2'** A section titled "Click on the button to generate DNA models" with options for "Ideal Model", "Sequence specific Model", and "Customized DNA: Input DNA sequence".
- 3'** A section titled "Sequence specific DNA" with input fields for "Insert Sequence 5'---3'", "Insert Sequence 3'---5'", "Length of the DNA", and "Base pair mismatches".
- 4** A section titled "G-Quadruplex" with a "b-type [strand type]" dropdown menu and a "Submit" button.
- Other panels show "user interface of 3D-nus" and "user interface of 3D-NuS" with various dropdown menus and checkboxes for selecting quadruplex classes and strand orientations.