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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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Guide :
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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://iiith.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 screenshot displays the 3D-NuS web server interface with several numbered callouts:

- 1'**: Points to the introductory text and navigation menu.
- 2'**: Points to the "Click on the button to generate DNA models" section, which offers options like "Ideal Model", "Sequence specific Model", and "Customized DNA: Input DNA sequence".
- 3'**: Points to the "Sequence specific DNA" input section, including fields for "Insert Sequence 5'---3'", "Length of the DNA", and "Base pair mismatches".
- 1**: Points to the top navigation bar.
- 2**: Points to the "Select appropriate type of quadruplex from the undergiven options" dropdown menu, showing options like "Monomer all anti-parallel stands (Q1)".
- 3**: Points to the "Select appropriate type of quadruplex from the undergiven options" section, showing a list of quadruplex classes (Q1-Q7) and their strand orientations.
- 4**: Points to the "G-Quadruplex" section, showing input fields for "b-type [strand type]", "Length of the G-quadruplex", and "Quadruplex type".

Central text labels the interface as "user interface of 3D-nus" and "User interface of 3D-NuS". A 3D model of a DNA structure is visible in the bottom right corner.