Prime Scholars Library

Advances in Life Science and Biotechnology

Editorial

Vol. 9 (2), pp.01 – 01 June2021

Available online at
https://primescholarslibrary.org/

3D DNA Model

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DESCRIPTION

Understanding the connection between molecular structure and performance represents a very important goal of undergraduate life sciences. Although evidence suggests that handling physical models supports gains in student understanding of structure–function relationships, such models haven't been widely implemented in biochemistry classrooms. Three-dimensional (3D) printing represents an emerging cost-effective means of manufacturing molecular models to assist students investigate structure–function concepts. We developed three interactive learning modules with dynamic 3D printed models to assist biochemistry students visualize biomolecular structures and address particular misconceptions. These modules targeted specific learning objectives associated with DNA and RNA structure, transcription factor-DNA interactions, and DNA super coiling dynamics. We also designed accompanying assessments to measure student learning.

Students responded favorably to the modules and showed normalized learning gains of 49% with relation to their ability to grasp and relate molecular structures to biochemical functions. By incorporating accurate 3D printed structures, these modules represent a unique advance in instructional design for biomolecular visualization. We offer instructors with the materials necessary to include each module within the classroom, including instructions for acquiring and distributing the models, activities, and assessments. The structures of double-stranded DNA in complex with various ligands often show considerable conformational changes compared to their unbound counterparts. This plasticity originates at a 'local' level within the orientation of 1 base relative to its Watson–Crick partner and of two base pairs relative to 1 another. These 'local' changes accumulate and lead to bending and twisting of the structure at a 'global' level. Only some existing programs, like NAMOT and NAB, offer options to introduce custom bends within the generated DNA conformation and provides control over all local parameters; they however require some expertise from the user and aren't available as web servers.

The 3D-DART web server (3DNA-Driven DNA Analysis and Rebuilding Tool) which we developed to permit for the simple generation of 3D-structural DNA models with an outlined conformation by providing control over both 'global' and 'local' conformational features. The generation of models is accomplished by modification of the well-established rotational and translational parameters that describe the position of 1 base to its Watson–Crick counterpart and of two successive base pairs relative to one another. It's been demonstrated within the past that rebuilding a double-stranded DNA structure using these parameters leads to a near native structure. The sole exceptions are local changes within the sugar and phosphate backbone conformation. The 3D-DART server uses the Roll, Tilt and Twist parameters to introduce bends into the structure. The opposite parameters will be accustomed 'fine-tune' the conformation of the structure. Note that 3D-DART doesn't provide custom control of the sugar-phosphate backbone conformation (in contrast as an example to NAMOT). The 3DNA software is employed to get a 3D-structural model from the modified parameters. The server accepts a nucleotide sequence, a nucleotide (step) parameter file or a DNA-containing PDB coordinate file as input. The server returns 3D-structural models with the required conformation additionally as a set of study and intermediate files. Several additional and convenient functions are available to regulate the markup of the resulting PDB coordinate files, for example to arrange them to be used within the macro-molecular docking program HADDOCK also developed in our group. For the identical purpose the server can automatically generate a DNA restraint file as an extra feature.