Using 3DNA: A Short Introduction

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February 6, 2012

Contents

In the following guide we'll show a step by step introduction to 3DNA from installation of the software to practical examples.

1 Installation

To install 3DNA you will first have to download the software from:

```
http://adna.rutgers.edu
```

The webpage will ask you to register before allowing you to download the program.
Once registered you'll be able to download the file **Linux_X3DNA_v2.0.tar.gz** if you selected the Linux version.
To uncompress issue the following command in a terminal

```
tar -xvzf Linux_X3DNA_v2.0.tar.gz
```

This will create a new folder named **X3DNA** which you will have to include in your environment variables by changing your shell environment configuration file named ".bashrc" in bash, and ".chsrc" in csh and tcsh.
If you are using .bashrc the following lines will need to be added:

```
export X3DNA=/home/yourusername/X3DNA
export PATH=$PATH:$X3DNA/bin
```

A detailed explanation of how to configure X3DNA can be found in the pdf file **x3dna_v1.5.pdf** found in the X3DNA/doc folder.

2 fiber

The fiber program included in the 3DNA package allows you to easily generate protein data bank (pdb) files of fiber models of common nucleic acid conformations, for example A-DNA, B-DNA, and Z-DNA. To get a list of all possible fiber models which you can reconstruct using fiber, type:

```
fiber -l
```

If you type fiber in the terminal you will get a usage message.
Stop and read the usage message carefully.
Now, you know that the crystal structures of A-RNA and B-DNA must have a total of 11 and 10 residues per turn respectively, so, go ahead and use fiber to make an A-RNA with 12 residues and a B-DNA with 11 residues. Using a molecular visualization program such as pymol, vmd, or chimera check the generated structure to corroborate that you have the correct number of residues per turn.

3 find_pair

The find_pair program of 3DNA allows you to find pairs in a given pdb file. To read the usage message open a terminal and type:

```
find_pair
```

Now go to the protein data bank website at `http://www.pdb.org` and download the structure with PDB_ID: 1ehz. This is the structure for yeast phenylalanine tRNA. Run it through find_pair:

```
find_pair 1ehz.pdb 1ehz.inp
```

You will get a file named 1ehz.inp. Go ahead and open the resulting file in a text editor and you will see that the find_pair program has found the canonical Watson-Crick base-pairs G·C and A·U, as well as non-canonical base-pairs such as G·U and A·G.

4 analyze

The analyze program of the 3DNA software package allows you to compute the base-pair and base-pair step parameters associated with a given nucleic acid structure among other analysis features such as computing the overlap areas between stacked nucleic acid bases, sugar conformations, and sugar-phosphate backbone torsion angles.
A requirement of the analyze program is that you have to run the find_pair program beforehand.
Go ahead and read the usage message of the analyze program by typing:

```
analyze --help
```

in your terminal.

Now run the analyze program on the file previously produced using the find_pair program:

```
analyze 1ehz.inp
```

Notice that you can run the find_pair and analyze program in just one line in the terminal by issuing the command:

```
find_pair 1ehz.pdb stdout | analyze
```

This command will produce a wealth of files with structural information, but the main one will just have the name of the input file followed by the .out extension. That is, you should now have a 1ehz.out file in your folder. Go ahead and take a look at the 1ehz.out file in your favorite text editor.

5 rebuild

The very useful 3DNA program called rebuild can do just that, rebuild nucleic acid structures. It uses as input either a set of base step, or base-pair step parameters, or a set of helical parameters to create a pdb file. To test the rebuild program first run find_pair and analyze the A-RNA structure you previously created:

```
find_pair A-RNA.pdb stdout | analyze
```

Issuing the previous command must have created a new file called *bp_step.par*. Open this file in a text editor and change the Twist values from 31.5 degrees to a smaller value, say 25.0 degrees, and save the new file with the name *undertwisted.par*.
Rebuild the undertwisted RNA by typing the following command in your good-ole terminal:

```
rebuild -atomic undertwisted.par undertwisted.pdb
```

This will generate a pdb structure with no sugar-phosphate backbone. To add a sugar-phosphate backbone you will need to issue the cp_std command before you perform the rebuild command, in the following way:

```
cp_std RNA
rebuild -atomic undertwisted.par undertwisted.pdb
```

Now rebuild a pdb file using the unmmodified base-pair step parameters, that is, using the *bp_step.par* file, and open both structures in a molecular visualization program and confirm that one helix is undertwisted with respect to the original.

6 Exercises

1. Run find_pair and analyze on your A-RNA structure and modify the resulting *bp_step.par* file so that the sequence is AAAGGGUUUCCC. Use rebuild to generate such new sequence.
2. Download the file with PBD_ID: 1AOI, that is, chromatins nucleosome core particle. Run it through find_pair