RDCvis Manual

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Abstract

RDCvis (Residual Dipolar Coupling visualizer) is a system for generating visualizations of RDC data in their macromolecular structural context. RDCvis uses specifically formatted NMR data files and PDB structure files in order to calculate and draw RDC representations. It takes advantage of the flexibility of the Kinemage graphics language by outputting results directly to a kinemage file, or directly incorporating the RDC curves into a pre-existing kinemage. The RDCvis package is written in the Java programming language, controlled mainly by a command-line interface, but also includes a KiNG plugin for more interactive control of the software.

1 Getting Started

1.1 What is a kinemage?

A kinemage is a "kinetic image," an interactive, three-dimensional illustration. Because kinemages contain simple geometric objects — points, lines, spheres, *etc.* — they are suited to a great variety of subjects, from simple sketches to sophisticated plots to detailed schematics of 3-D objects. Their strength is in *selective* presentation of information — they were originally intended as an alternative to flat, static illustrations in scientific journals.

In fact, kinemages were first created as a way of visualizing macromolecular structures, particularly x-ray crystal structures of proteins. However, such a kinemage is a *drawing* of a molecule, albeit a 3-D drawing, and not the molecule itself. Thus, the kinemage lacks most of the information in a PDB file, and kinemage display program cannot read PDB files directly. Since their creation, kinemages have been extended to a variety of other fields, from the social sciences to ecology to education.

The kinemage concept is the brainchild of Drs. David and Jane Richardson at Duke University in Durham, North Carolina, USA. Their website is at `http://kinemage.biochem.duke.edu`.

1.2 Download RDCvis

If you don't already have a copy of RDCvis, you can download it from `http://kinemage.biochem.duke.edu/software/rdcvis.php`. Even if you have a copy already, you might check periodically for new version that add features and fix bugs.

1.3 Make sure you have Java

RDCvis is written in the Java programming language, and so requires that the Java libraries (version 1.5 or later) be present on your computer in order for it to run. Newer Apple computers (those running Mac OS X) come with Java. Most PCs do not, though recently several manufacturers have agreed to pre-install Java on their new computers. Look for the coffee-cup icon in your Windows task bar or in the Control Panel.

If you don't have Java, point your web browser to `http://java.sun.com/getjava/index.html`. The software is free and available for Windows, Linux, and Solaris computers. We recommend getting the newest version that is available (1.6.0 as of this writing).

2 Running RDCvis

2.1 Required Files

In order to use RDCvis, you need to have a structure file, in standard PDB format, and an NMR data file, typically a .mr file, that contains RDC data. Currently, RDCvis only recognizes one format of RDC data. In order to use RDCvis, you will need to convert your .mr file so that the RDC data looks like the following example:

```
assign ( resid 500  and name OO  )
       ( resid 500  and name Z   )
       ( resid 500  and name X   )
       ( resid 500  and name Y   )
       ( resid  10  and name N   )
       ( resid  10  and name HN  )  -1.3000  1.000
```

Future releases of RDCvis will hopefully add support for more formats of RDC data.

2.2 From the command line

The RDCvis jar has been built so that the standard "java -jar" command will automatically run the command line functions. An example of a simple command to obtain a kinemage with CA-HA RDC visualizations is the following:

```
java -jar rdcvis.jar file.pdb file.mr CA-HA
```

Running this command will automatically generate a kinemage, named filerdcvis-enstensor.kin which can be viewed in any of our kinemage viewers. Using a -help flag will give more detailed information about the various command line options.

3 Additional Info

3.1 Bug reporting and contact info

RDCvis was created and is being maintained by Vincent Chen, who may be reached via email at vbc3 AT duke.edu. *Please*, do not hesistate to report suggestions, bugs, and problems with RDCvis — your input can only improve the program.

4 Copyright

4.1 Copyright