

SOFTWARE PRESENTATION

PDB2MultiGIF: A Web Tool to Create Animated Images of Molecules

Andreas Bohne

Central Spectroscopy Department, German Research Cancer, D-69120 Heidelberg, Germany.
E-mail: a.bohne@dkfz-heidelberg.de

Received: 30 September 1998 / Accepted: 27 October 1998 / Published: 16 November 1998

Abstract A new web tool, PDB2MultiGIF (<http://www.dkfz-heidelberg.de/spec/pdb2mgif/>), which converts the topological information (atom types, 3D coordinates, molecular connectivity) of molecules (given in PDB format [1]) to a series of animated images (in GIF Format) [2] is described. The molecular visualisation program RASMOL [3] is used to generate the images.

Keywords Molecular visualisation, Electronic publication, Web tool

Introduction

Electronic publishing offers several new features for presenting scientific results in styles and functions that are not possible using traditional printed media. Graphical representations of the shape or conformation of a molecule are widely used to explain its properties, biological functions and reactivity. Molecular visualisation programs such as RASMOL [3] are able to produce many kinds of representations based on topological information (atom types, 3D coordinates, molecular connectivities) of molecules. Until now WWW browsers have not been able to create a molecular representation based on the topological data directly. Common strategies to overcome this problem are to link external applications or to use special Plug-Ins such as Chime [4]. Although these techniques are well established and frequently used, the disadvantages are obvious, especially for novice users and for those who want to take just a quick look at the structures. Additional programs have to be downloaded, installed and correctly linked before one can view the structures. Unfortunately, the installation of the additional programs is not always easy, and some adaptations to the platform in use may also be required. The un-

derlying concept of PDB2MultiGIF is to provide a tool by which animated images of a molecular representation can be generated easily. When included in a web page, this tool allows animated images of molecules to be displayed by all standard web browsers without depending on an extra visualisation program. Thus, any user can view all data of interest.

Input

Figure 1 shows the WWW input form for PDB2MultiGIF. The minimal input requirements are the E-mail address of the user and the molecular topology, which must be provided in the widely used PDB format. This information may be entered using an appropriate copy-paste mechanism on the client computer or a stored PDB file can be selected via the client's file manager and sent directly to the server. All RASMOL-dependent parameters required for generating animated molecular images (image size, rotation axis, rotation step times, etc.) are displayed with default values but can be altered by the user as desired.

Figure 1 Input form for PDB2MultiGIF

E-MAIL	
Your address: <input type="text"/>	
IMAGE SIZE (PIXEL)	
<input type="radio"/>	300 x 300 (very large files!)
<input type="radio"/>	250 x 250 (large files!)
<input type="radio"/>	200 x 200
<input checked="" type="radio"/>	150 x 150
<input type="radio"/>	100 x 100
<input type="radio"/>	75 x 75
<input type="radio"/>	50 x 50
NUMBER OF FRAMES	
<input type="radio"/>	20
<input checked="" type="radio"/>	36
<input type="radio"/>	72
ROTATION AXIS	
On: <input type="radio"/> Off: <input checked="" type="radio"/>	X-Axis
On: <input checked="" type="radio"/> Off: <input type="radio"/>	Y-Axis
On: <input type="radio"/> Off: <input checked="" type="radio"/>	Z-Axis
ROTATION STEP TIME	
<input type="radio"/>	0 sec (very fast)
<input type="radio"/>	0.01 sec
<input checked="" type="radio"/>	0.10 sec
<input type="radio"/>	0.25 sec
<input type="radio"/>	0.50 sec (slow)
RASMOL COMMANDS	
<pre>Centre Wireframe Off # Do not use wireframe! Spacefill Background White #Group Colours</pre>	
PDB INPUT (choose one method)	
File name: <input type="text"/>	<input type="button" value="Browse..."/>
or	
Source:	
<div style="border: 1px solid gray; height: 100px; width: 100%;"></div>	
Use the COPY-PASTE mechanism of your computer to insert the content of the PDB file.	
<input type="button" value="SEND"/>	

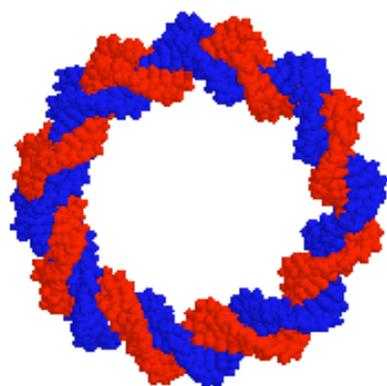


Figure 2 The superhelical structure of DNA becomes clear when the animation is started

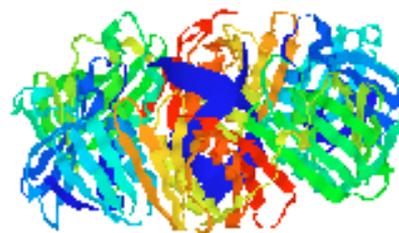


Figure 3 The animation demonstrates nicely how the nucleotidyltransferase surrounds part of a double stranded DNA

Results and output

The animated molecular images in GIF format are calculated using RasMol2 and stored on the server disk. Figure 2 and 3 show typical images which have been generated using PDB2MultiGIF. When the calculation is complete, the user receives by E-mail information explaining how to download the results. This procedure avoids the transmission of large data sets as E-mail attachments which often causes problems. Normally the calculation requires no more than one or two minutes.

Conclusion

PDB2MultiGIF takes a molecular structure representation (PDB inputfile) and creates a series of rotating graphical displays (animation) which can be viewed using standard web browsers without the need for any additional molecular visualisation software.

Supplementary material available statement The HTML version of this paper shows two examples of animated molecules that are generated with the use of the PDB2MultiGIF web tool. The animated images can be displayed with every standard web browser. When the cursor is moved on the figure the animated molecule is displayed. This feature is realised by a JavaScript [5].

References

1. Protein Data Bank <http://www.pdb.bnl.gov/> or German mirror: <http://pdb.gmd.de/>
2. Animated GIF <http://www.kfs.org/~abw/code/multigif.html>
3. RasMol <http://www.umass.edu/microbio/rasmol/>
4. Chime <http://www.umass.edu/microbio/chime/>
5. PDB2MGIF <http://www.dkfz-heidelberg.de/spec/pdb2mgif/clever.html>