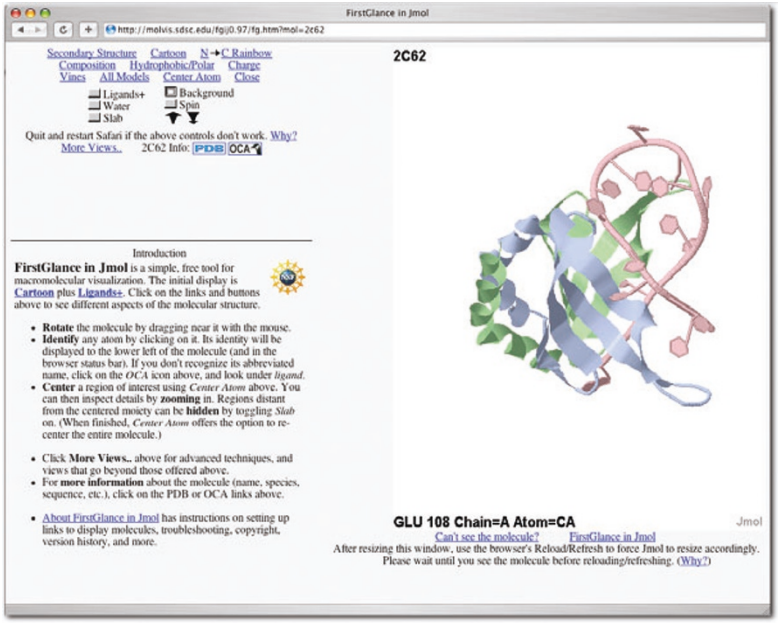
nature structural & molecular biology

We're living in a 3D world

Even a small child can appreciate the vast differences between two- and three-dimensional representations of the same object. While the printed page is still limited in this respect, more and more of our readers are gaining access to our papers through our website. Leaving aside for the moment the argument of whether or not this spells the end of the printed word, it certainly presents a unique opportunity to provide our readers with a way to view and appreciate the structures in three dimensions.

In this issue of *Nature Structural & Molecular Biology* we are excited to be able to introduce a new, simple, tool for three-dimensional molecular visualization called FirstGlance in Jmol.



Here's how it works. You will be able to easily gain access to three-dimensional structures presented in our pages by clicking on the 3D button located on our Table of Contents as well as on the right hand navigation bar of the article page. This will take you directly to a page similar to the one shown here. The molecule(s) first appears as a cartoon. By clicking on the links and buttons from an always visible control panel (upper left-hand corner) you can see different renderings of the molecule(s).

For example, you can view the secondary structure of the molecule (showing α-helices and β-strands). Likewise, molecules can be shown as smoothed backbone traces, with nucleic acids thicker than proteins. One can also view the molecule in spacefilling spheres of van der Waals radii by choosing Composition. The hydrophobic versus polar amino acids can be readily distinguished by selecting Hydrophobic/Polar as can all of the different types of amino acids by clicking Charge. Vines displays all amino acid sidechains and nucleotide bases as sticks colored by atom types, and All Models enables you to see more than one model as in the case of NMR structures. Settings can be turned on or off to show or hide ligands or water molecules, you can zoom in or out, or change the background color. Help about each view or operation, including color keys, appears automatically (lower left-hand corner), and is always in view.

Best of all, these structures can be rotated by you (and your mouse) or be made to spin (by clicking the spin button) right before your very eyes. There is no better way to appreciate the three-dimensional nature of a structure than to be able to rotate it around. In fact, short of building a physical three-dimensional model, it is really the only way.

Of course the structure aficionados may ask what all the hoopla is all about. After all they are computer savvy and know their way around the Protein Data Bank blindfolded. But for our less structurally literate readers we hope this will allow them to quickly and easily take a look at a structure that is of interest to them and, most importantly, zero in on the region(s) that they want to study in greater detail. In this way, they will be able to better interpret existing data and, with any luck, design new experiments based on the structure. One particularly useful feature of FirstGlance is the ability to find your favorite amino acid(s) or base(s) by clicking on it. Its identity and position number will be displayed over the molecule and in the browser status bar.

FirstGlance in Jmol (http://www.bioinformatics.org/firstglance) is free to all and works in most popular browsers and platforms, including Internet Explorer or Firefox on Windows, and Safari and Firefox on Mac OSX. Of course, FirstGlance works best with the newest Mac operating systems and browser updates.

All of the credit for FirstGlance goes to Eric Martz in the Department of Microbiology, University of Massachusetts, Amherst, USA. Since FirstGlance is a user interface to the Jmol java applet, Eric wants to acknowledge the help of the Jmol development team, especially Miguel Howard. He would also like to thank the bioinformatics.org team for providing a home for this project, in particular Jeff Bizzaro; and Phil Bourne, Andy Sanderson, and the San Diego Supercomputer Center for providing a fast server.

We'd like to know what you think about this new feature, so please share your thoughts with us (nsmb@natureny.com). What do you like about it and what could be improved? What other features and settings would you find useful? This is an ongoing project for Eric and his coworkers and for us at Nature Publishing Group. The idea is to make this more and more user friendly over time but we can't do that without input from you, the users, so now the ball (or should I say rotating three-dimensional molecule) is in your court. ■