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COMPUTER SOFTWARE
REVIEWS

BioAdviser 1.0 − High Performance Molecular Rendering and Analysis Software. FQS Poland Sp. z o. o. Palac Pugetow, ul. Starowislna 13-15, 31-038 Krakow, Poland. http://www.fqspl.com.pl/bioadviser/intro.html. See Web site for pricing information.

BioAdviser 1.0 is a versatile 3-D structure graphics viewer, analysis, and animation program for PCs. System requirements are a Windows 98, 2000, or XP operating system, Pentium compatible processor, at least 64 Mb RAM, 50 Mb disk space, and a graphics card with DirectX compatibility. The program comes on a CD, which includes a Help manual. It installed easily on my PC using Windows 2000 with a 1 GHz processor and handled very large protein files without difficulty.

BioAdviser 1.0 features high-speed rendering, allowing large macromolecular structures involving tens of thousands of atoms to be manipulated easily on a moderately powered PC. Although BioAdviser is targeted for use with large protein and nucleic acid structures, it also features tools that are well suited for the analysis of small molecules, including a link that facilitates the initialization and analysis of results using MOPAC 2002 (not included) to compute electronic properties of molecules. Input of molecules is accomplished using a variety of file formats, including the popular pdb, mol, hin, and xyz formats. The molecules can then be viewed in "Wire Frame", "Ball & Stick", "Cylinder", and "Space Filling" styles. Easy menu options allow the side chains of proteins to be turned on or off, and the proteins to be rendered as ribbon wires, ribbon lines, flat ribbons, solid ribbons, "tubby" mode, or as "motifs" where helices are represented as cylinders and β-strands as flattened arrows. In a similar manner, there are options specific to nucleic acids to display "Backbone" or "Rings and Ladder" representations.

The modeling tools allow the user to perform a variety of operations on the displayed molecule using the convenient menus provided. Operations allow for the usual rotations and translations, but also include mutation of amino acid side chains, adjustment of torsion angles, and addition of hydrogens. Many of the operations can be performed on specific residues or on the whole molecule. BioAdviser allows for the convenient "building" of protein chains into a choice of regular secondary structures from a user-defined sequence. This feature does not appear to be available for building nucleic acids, however.

Many of the analytical tools in BioAdviser enable the user to measure distances, etc., but also include features not found in most of the more commonly used molecular graphics programs. This software enables convenient viewing of "Property Plots" of the hydropathic index, Ramachandran plots, or the amino acid sequence of the protein displayed. Multiple files can be open simultaneously, and the user can define "source" and "probe" molecules to calculate the best alignment of two structures to facilitate comparisons between them. Some features for presentation of structures include the ability to annotate and print the image files and to produce animation sequences where the rotations can be defined via a series of adjustable x, y, and z step sequences.

Finally, no review would be complete without pointing out some areas that could be improved in future versions of this software. Most of the operations are fairly intuitive and easily mastered. However, the default background color is black, which makes the wire images hard to see. One can easily select a user-specified background color, but this needs to be done each time rather than allowing one to redefine the default value. Text boxes are readily added to the images, but the control of their location appears limited. The display options allow for stereo viewing. However, the stereo option is not in the first pull-down menu, but found under View/Preferences/Stereo. In the version tested, the stereo angle could be adjusted without difficulty, but the labels for "Straight eyes" versus "Crossed eyes" were mislabeled. The program features excellent rotation speed by turning off the rendering features. Although this allows handling of very large files, it would be desirable to have the option to leave the rendering mode on for small proteins, and especially for small molecules such as the amino acids. Users of RasMol and similar programs will notice that the zoom operation on the mouse works opposite to what they are used to—that is, the size of the object decreases rather than increases as you draw the mouse nearer to you. Finally, this reviewer had some difficulty using the Compare feature in this program. In addition to defining the "source" and "probe" molecules, it is necessary to select the residues to be compared. There are several options for making selections based on the atom, residues, or molecule using different tools such as the pointer or a defined volume; however, it would have been useful to be able to define a range of residues either by residue number or by clicking the start and end points of a given sequence of residues to be included in the alignment.

BioAdviser lists as $200 for academic users and $300 for industrial users. This price is reduced to about half when several (25) licenses are purchased. This places BioAdviser in a competitive price range with many other programs that do not have nearly as many features as this program provides. The casual user will probably prefer to stay with publicly available software like RasMol or Cn3d, but BioAdviser is a good choice for the more serious user who needs the added capabilities this program offers.

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