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MOLMOL: A free biomolecular graphics/analysis package

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Abstract

MOLMOL is a molecular graphics program designed for display and analysis of biological macromolecules, particularly protein or DNA structures determined by nuclear magnetic resonance spectroscopy.

Content

MOLMOL is a molecular graphics program designed for display and analysis of biological macromolecules, particularly protein or DNA structures determined by nuclear magnetic resonance (NMR) spectroscopy, and is freely available from this, its official website. Based on the OpenGL graphics language, MOLMOL was released in 1996 as the result of a collaboration between Bruker/ Spectrospin and the research group of Professor Kurt Wüthrich at ETH in Zurich, Switzerland. The site provides links for downloading the software, as well as a full online version of the manual. Both source code and binary versions of the software are available (Windows, HP and SGI binaries are supported, and i386 Linux binaries have been contributed by users). Also at the site are instructions on how to join the MOLMOL mailing list, an archive of the list dating all the way back to 1996, a short tutorial, a FAQ section and two image galleries which give potential users an idea of the program's graphical capabilities. Some of the most useful capabilities of MOLMOL are its numerous analysis tools that allow one to do things like calculate and display solvent-accessible surfaces, calculate root-mean-square distances, and check structural constraints. One feature that really sets MOLMOL apart from most other packages is that the format in which output can be generated means that MOLMOL can be used as a front end to some of the best ray-tracing software available, allowing one to produce extremely high quality molecular graphics.

Navigation

This site is a straightforward launching point to get new users started with the software and to provide information and support to current users. Navigation is therefore fairly simple. Most of the content is only one link deep, making it easy to find the pages you are looking for. More links interconnecting the various sections of the online manual would make it much easier to use, however.

Reporter's comments

Timeliness

The site is kept up-to-date with respect to the current version of the software, which includes most of the important content. The mailing list archival system is updated whenever there is traffic on the mailing list. The description pages have not been updated in quite some time, but the predominantly historical nature of the information on these pages makes this criticism somewhat insignificant. There were one or two broken links at the time of reporting.

Best feature

The continuously updated archive of the MOLMOL mailing list.

Worst feature

The somewhat inconvenient method of downloading the software from an ftp server.

Wish list

A full-text search engine for the mailing list archive would be a wonderful addition to this site. Even though there is an existing tutorial, more step-by-step examples would be helpful. The online manual could be redesigned to make it easier to navigate, and it would be convenient if it were fully searchable.

Table of links

References

1. MOLMOL: Molecule analysis and molecule display.