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Qmol: A program for molecular visualization on Windows-based PCs

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With the advent of powerful, inexpensive graphics hardware, a variety of molecular modelling tools are now available for personal computers (PCs). While a host of high-quality, free visualization programs exist for Unix-like operating systems, there are relatively few available for Microsoft Windows. Most programs that do run under Windows are designed to interactively visualize experimental data and cannot read binary trajectory data generated by molecular simulations. In addition, many of these programs do not accept command line arguments, limiting their ability to serve as a "helper" application to be run by other applications. To fill this gap in functionality, we present Qmol—a program designed for viewing the output of simulations and theoretical calculations of peptides and small molecules. © *2001 by Elsevier Science Inc.*

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INTRODUCTION

While it is impossible to address all aspects of molecular visualization with a single program, Qmol provides a collection of features not found in existing Windows programs and an intuitive user interface loosely based on the widely used Xmol[1] program. The visualization capabilities of Qmol center on the display of small molecules and peptides, hence ribbon diagrams and other protein secondary structure cartoons are not provided. Table 1 shows a set of features provided by Qmol and other free Windows-based visualization programs.

FEATURES

- Display OpenGL[2] rendered wire frame, stick figure, ball and stick, point and space-filling molecular structures from a PDB file (with depth-cueing, anti-aliased lines, and extended precision)
- Animate molecular trajectories
- Preprocess molecular trajectories (including adjustment of overall rigid body rotation and translation)
- Interactively measure bond lengths, bond angles, and torsion angles
- Dynamically adjust user-selected torsion angles
- Display atom labels
- Display coordinate axis
- Display bounding box
- Dynamic modification of the color scheme by element, atom number, temperature, and occupancy
- Print to any Windows printer and copy images to the Windows clipboard.

A subset of these features is demonstrated in Color Plate 1. The main strength of the program, however, lies in the import and preprocessing of data files.

QPDB File Format

The program reads chemical structures via QPDB files. The QPDB file format is a superset of the PDB[3] file format, supporting extended floating-point precision for atomic coordinates, a bounding box definition and definitions for atom pair monitors. While the three digits of precision for atomic coordinates in a standard PDB file are adequate for experimental structures, higher precision is useful when generating molecular structures on a computer, especially when converting between Cartesian and internal coordinates. The QPDB file format allows three to fifteen places of precision for atomic coordinates, thereby providing both extended precision and the ability to produce a PDB file that can be read by other programs. A bounding box is useful when visualizing periodic systems. The QPDB file format uses bounding box definitions in the form:

REMARK BBOX_R r_x r_y r_z
REMARK BBOX_A a_x a_y a_z
REMARK BBOX_B b_x b_y b_z

Color Plates for this article are on page 609.

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Table 1. Features offered by several free molecular graphics programs for the Microsoft Windows operating systems*

	Display high quality, hardware accelerated 3D graphics	Display and manipulate multiple molecules in the same window	Compute and display molecular surface	Read binary trajectory data	Generate protein structure from sequence	Measure bond lengths, bond angles and torsion angles	Adjust torsion angles	Evaluate electrostatic potential energy	Send output to printers and other programs	Import data specified on the command line	Source code freely available	Program available from
Qmol (v1.2)	●			●		●	●		●	●	●	http://www.mbg.cornell.edu/shalloway/shalloway.html
VMD[6] (v1.6a3)	●	●	●	●		●					●	http://www.ks.uiuc.edu/Research/vmd/vmd-1.6/
ICMlite[7] (v2.8)	●	●			●	●	●					http://www.molsoft.com/icmpages/icmlite.htm
WebLab Viewer Lite[8] (v3.7)	●	●	●			●	●		●	●		http://www.msi.com/life/products/weblab/viewer/register/lite/download_lite.html
Rasmol[9] (v2.6)									●	●	●	http://www.umass.edu/microbio/rasmol/getras.htm#raswin
MolMol[10] (v2K.1)	●				●	●	●	●			●	http://www.mol.biol.ethz.ch/wuthrich/software/molmol/
Swiss-Pdb Viewer[11] (v3.7b1)	●	●	●		●	●	●	●		●	●	http://www.expasy.ch/spdbv/mainpage.htm
gOpenMol[12] (v1.4)	●	●	●	●		●			●	●†	●	http://www.csc.fi/~laaksone/gopenmol/gopenmol.html
Jmol[13] (v0.6.1)						●			●		●	http://www.openscience.org/jmol/index.html

* Free programs listed are those that, in our assessment, offer the best combinations of features and usability. Programs that are under development (e.g., Chimera http://www.cgl.ucsf.edu/chimera/) and web-browser plug-in programs, which have limited file import capabilities, are not included.
† Note that gOpenMol only imports coordinate (not trajectory) files from the command line.

REMARK BBOX_C c_x c_y c_z

where the first vertex of the box is centered at the point (r_x, r_y, r_z) and the edges of the box are given by the vectors a ≡ {a_x, a_y, a_z}, b ≡ {b_x, b_y, b_z}, c ≡ {c_x, c_y, c_z}. A visual linkage, or monitor, between pairs of atoms is a helpful aid for showing the results of theoretical calculations. The QPDB file format allows for an arbitrary number of atomic monitors defined in the form:

REMARK MONITOR ID N_A N_B R G B

where ID is the user defined identification number of the monitor, N_A and N_B are the atom number of the selected atom pair (as defined in the body of the PDB file) and R, G, and B are the integer values (each between 0 and 255) specifying the color of the monitor. Since both the bounding box and monitor definitions are prefaced with the PDB keyword, "REMARK", they are ignored by programs that read standard PDB files. Since the QPDB format is a superset of the PDB file format, Qmol can read standard PDB files without modification.

Molecular Trajectories

Both Monte Carlo and molecular dynamics simulations can generate enormous numbers of structures, and an efficient use of space and fast processing require that they be stored in a binary, not ASCII, file format. The standard format for storing a molecular trajectory (i.e., a set of structures with no relationships) is the CHARMm/Xplor DCD[4] file format. Qmol allows for the preprocessing of trajectory data read from a DCD file, including a rigid body translation of the center mass of each structure to the origin and a rigid body rotation to align each structure with a reference structure.[5] To accommodate DCD files created under a variety of computer architectures, Qmol reads both big- and little-endian data formats.

Command Line Options

To facilitate its use as a "helper" application that is spawned by another program, Qmol accepts the following commands specified as program arguments at run time:

- Reading of both QPDB coordinate files and DCD trajectory files
- Alignment of all trajectory structures with the QPDB structure by rigid body rotation and translation.
- Removal of the center of mass from all input structures
- Suppression of automatic covalent bond determination

All other commands, such as color modification, must be specified interactively. The disabling of automatic covalent bond determination allows Qmol to display general three-dimensional data as a collection of points or spheres, as shown in Color Plate 2. These command line options allow other programs to easily use Qmol as an external viewer.

CONCLUSION

Qmol has been written to provide a set of features not found in existing Microsoft Windows software; special care has been taken to provide a friendly user interface that takes full advantage of the Windows operating system. It is not a replacement for all visualization needs, but instead is a useful tool for viewing the output of theoretical calculations. Qmol is written in C++ using OpenGL and the Microsoft Foundation Classes and runs under Windows 95, 98, NT, and 2000. The executable and source code are freely available from http://www.mbg.cornell.edu/shalloway/shalloway.html.

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