TEQUILA: Displaying molecular distance maps

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It is often difficult to detect large-scale features in the structure of a macromolecule in its three-dimensional representation because important parts are obscured by other atoms or because there is simply too much irrelevant information in the picture. Condensing the information into a two-dimensional representation can in such circumstances help one to grasp the essentials of a structure before studying its interesting details in a three-dimensional display. The comparison of two related structures can be aided also by a two-dimensional representation.

One way of achieving a reduction in dimensionality is to concentrate on the distances between interesting parts of the structure rather than on their absolute positions. In the case of proteins, for example, the distances between α-carbon atoms highlight secondary structure elements of the backbone.

We have implemented a graphics program TEQUILA that displays such distance maps in a color coded representation. In its present incarnation it reads protein atomic coordinates in the Brookhaven Protein Data Bank format. A sample plot is given in Color Plate 1. The colors in this plot represent different numerical values of the distance between two α-carbon atoms, ranging from purple (long distance) to red (short distance). Alternatively, the program may display the shortest distance between any two atoms of different residues (Color Plate 2). This facilitates the detection of favorable or unfavorable close contacts between two amino acid side chains. The program can switch between modes during a session. To examine an interesting spot on the display more closely the user may click the mouse on this spot to learn which residues are involved and where they are located. There is a separate version of the program that takes two configurations as input and displays the differences between corresponding distances in their structures. For more details the reader is referred to the documentation that accompanies the program.

We realize that there may be other programs of similar functionality. However, there is one feature in our implementation that makes TEQUILA particularly attractive: It is implemented with the VOGLE graphics library.[1] VOGLE is available in source code form. It is highly portable, and it already supports many graphics devices, such as PCs with various graphics cards, several workstations (Sun, HP/Apollo and Xwindows) and hardcopy languages like HPGL and Postscript. The use of a portable graphics library makes TEQUILA highly portable and provides an easy route to hardcopy output. We have added a color Postscript driver to the package. For example, the original figures for this article were produced directly on 35-mm slides during a TEQUILA session, at the push of a button.

We are running TEQUILA using the Xwindows driver of VOGLE on a Stardent 1500 (Ardent Titan) graphics workstation. This is not because TEQUILA is particularly demanding on graphics resources but simply because our other molecular graphics software (and hence our data files) reside on that machine. While it should be possible to run TEQUILA on a PC, we have often found it convenient to be able to run several copies of the program concurrently in separate windows, each displaying a different structure. TEQUILA is written in Fortran 77.

TEQUILA has been made available in the CCP5 program library. The distribution contains source code, UNIX makefiles, example files and a short user's manual. For a copy write to the Librarian CCP5 Program Library, SERC, Daresbury Laboratory, Warrington WA4 4AD, UK. For details on how to obtain programs from the library, see a recent copy of the *Information Quarterly in Computer Simulation of Condensed Phases* (the "CCP5 Newsletter"), Daresbury Laboratory. Although we will attempt to fix reported bugs in the code as time permits we will ignore requests for direct support.

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REFERENCES

1 Echidna, E.H. VOGLE: A Very Ordinary Graphics Learning Environment. VOGLE is a portable public-domain graphics library developed at Melbourne University. The source code for VOGLE can be obtained by anonymous ftp from munnari.oz.au

2 Artymiuk, P.J. and Blake, C.C.F. *J. Mol. Biol.* 1981, **152**, 737