Molecular graphics abstracts

The Third International Meeting of the Molecular Graphics Society was held at Royal Holloway College, Egham, UK, 16–18 April 1984. As in previous years there were formal sessions with key papers presented by invited speakers. There was also an exhibition of hardware and software that is currently commercially available. Two new features of this year's meeting were the informal poster sessions and special interest meetings.

The collected abstracts of the meeting are printed here. The abstracts are followed by an author index and an index of keywords. Several papers do not appear as the abstracts were submitted too late to be included.

1

'An interactive interface for protein secondary structural representation' **Burridge, J M and Todd, S J P** IBM UK Scientific Centre, Athelstan House, St Clement Street, Winchester, Hampshire SO23 9DR, UK

Schematic representations of protein secondary structures frequently depict alpha helices as cylinders and strands of beta sheet as arrows. These are extremely useful in demonstrating the overall shapes of protein molecules, relationships between classes and families of proteins, and topological relationships between elements of secondary and super-secondary structure. Originally hand drawn[1], such representations have recently been computer-generated as stereo plots[2] and as combinations of solid primitives on raster display devices[2,3]. Unfortunately none of these techniques readily permit interactive manipulation by the user. This paper describes the generation and display of vector representations of protein secondary structure using the Winchester Graphics System (WGS).

The WGS hardware[4] consists of an IBM 4341 processor, coupled to two IBM Series/1 minicomputers which control a calligraphic display system and a raster display device. IBM 3279 terminals[5] are attached to the 4341 via IBM 3274 control units.

The system software[4] is based upon a relational database[6]. Application programs are written in PL/I and the command executive language REXX. The device independent graphics subsystem holds the mapping transformations to apply to the structure on display. The user modifies the picture in a series of display and interaction operations. The relational database holds a selection of protein structures from the Brookhaven Protein Data Bank[7] which provide the basic data for the program here described.

Alpha helices may be represented either as cylinders or regular helical spirals, the helix endpoints being defined with reference to the first three and last three residues of the helix. The user may select values for the helix radius and drawing parameters.

Beta strands may be represented as striped or single-line arrows. the edges of the arrows are defined by a smoothed set of points derived from the alpha-carbon, carbonyl carbon and amide nitrogen atomic positions of each peptide. These are sufficient to define the orientation of the planar peptide unit.

Sections of randomly coiled polypeptide chain are represented conventionally as virtual Ca—Ca bonds. Atoms or residues of particular interest may be represented as filled circles of colour appropriate to atom type, charge, etc, giving a CPK-like effect.

Computer generation may be controlled by a set of statements supplied by the user, describing the required picture. The simplest case would comprise a list of structure types such as helix, strand, cpk, etc, together with the residue number(s) concerned. Optionally the user may specify details of the drawing process, colour coding for atoms according to type, charge, hydrophobicity, etc, and colour coding for secondary structural elements (to highlight elements of supersecondary structure, for example). If no user control is supplied, the program uses the Brookhaven Data Bank secondary structural information contained within the WGS database, together with default values for drawing parameters.

The resulting vector image may be displayed on the IBM 3279 colour terminal and on the monochrome vector display. The user may then alter the view transform of the display as desired. Colour pictures of selected views may be obtained via the pen plotter, or photographed from the raster device.

The program may also be used as a preliminary to the solid modelling program[3]. A control file describing the solid primitives required to represent the protein secondary structure is written at the time of running. After the user has interactively oriented the displayed picture to his satisfaction, the transformation matrix is written to complete the control file.

REFERENCES

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'TOM' a display program for fitting ligands into protein receptors and performing interactive energy minimization' **Cambillau, C, Horjales, E and Jones T A*** Swedish University of Agricultural Sciences, Department of Chemistry and Molecular Biology, S-750-07 Uppsala, Sweden. * Wallenberg Laboratory, Dag Hammarskjölds v. 21, Box 562, 75122 Uppsala, Sweden

An interactive program written for a VG 3404 driven by a VAX 11/750 allows us to simulate and energy minimize ligand-receptor interaction for a known protein structure. It has been implemented to interface with FRODO[1].

The main differences with DOCKER[2], published recently, are the following:

- TOM allows the use of any type of ligand molecule
- energy minimization is performed interactively
- all the FRODO options are present
- hydrogen atoms are not included

DESCRIPTION OF THE RESIDUE DICTIONARY

The residue description (amino-acids and special groups such as the coenzyme NADH) is partly derived from FRODO's dictionary. Some additional parameters which are used for energy calculation of fitting have been added. They are connectivities, partial charges and Lennard-Jones parameters. The ligand is described in the same way as in the GAUSS *Z*-matrix[3]. Partial atom charges, Lennard-Jones parameters and a special ring parameter to restrict certain dihedral angles have also been added. These data are kept in one file (*Z*-file) for each ligand molecule.

LIGAND COORDINATE FILES

A newly created ligand is automatically inserted in the protein at a chosen position when running TOM. It can then be moved and transformed using the display. Current coordinates are kept in the FRODO file DSN2. The *Z*-file and FRODO's DSN2 file communicate in the following way. The *Z*-file is updated from DSN2 when leaving the display mode. DSN2 is updated when coming into display mode if the *Z*-file has been modified by off display options.

LIGAND FITTING

Ligand fitting can be carried out using (apart from the standard FRODO options FBRT, TOR, MOVE) the BELL option displaying the shortest contacts for the moving atoms, as well as the ENER option which performs energy calculation. It can also be achieved through an automatic procedure FIT which minimizes the energy (Lennard-Jones, torsion and charge potentials) using a conjugate-gradient[4] procedure. The ligand and all the residues within an R1 radius from all the ligand atoms are flexible, all residues within an R2 radius from all the previously chosen moveable atoms form a fixed shell to prevent an 'explosion' of the flexible zone. The conformational space of the ligand and all the flexible residue side chains is explored by FIT. The torsional angles are the minimization parameters. In addition, translation/rotation of the ligand can be included if necessary. During the FIT procedure, a view of the working zone is displayed, and the calculation can be stopped at any time by a command before the convergence criterion is reached.

FIT can also be used for model building of proteins. The *Z*-file is not needed to run TOM, and any amino acid can be treated as the 'ligand' molecule so that a zone of the protein can be energy refined.

The speed of FIT makes it very attractive. For a molecule having 6 torsional angles within a 400 atoms fixed zone, convergence was reached after 20 steps of conjugate gradient, using about one minute of real time and 30 s CPU time.

FUTURE PROJECTS

We plan to speed up the FIT option even more and to include surfacing of both active site and ligand.

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3

'An interactive graphics technique for colouring molecules' **Carlson, C N and Bosshard, H E** European Molecular Biology Laboratory, Postfach 10 2209, 6900 Heidelberg, FRG

Structural colouring serves to orient the viewer of a molecular model. It is an effective way of tagging features of interest so that they are recognizable in a jumble of bonds and electron densities. We have developed a technique of interactive colouring and implemented it as an addition to our version of the crystallographic program Frodo. Our foremost design goal was to offer as wide a range of functionality as possible, while keeping user interaction obvious and intuitive.

We designed a 'paintbrush' technique for colouring molecules which is like an artist dabbing a brush in the palette and painting with it. When the user enters 'colour' mode, a menu of colour options and a colour palette appear on the screen next to the molecular display (Figure 1). The user can at any time 'dip' a digitizing tablet stylus in the palette, picking up a colour whose value is monitored at lower screen right.

Subsequent identification of an atom with the stylus causes a group of atoms to assume the current stylus colour. The atoms belonging to the group are determined by the currently selected menu items. If, for example, the stylus colour is red and the user selects

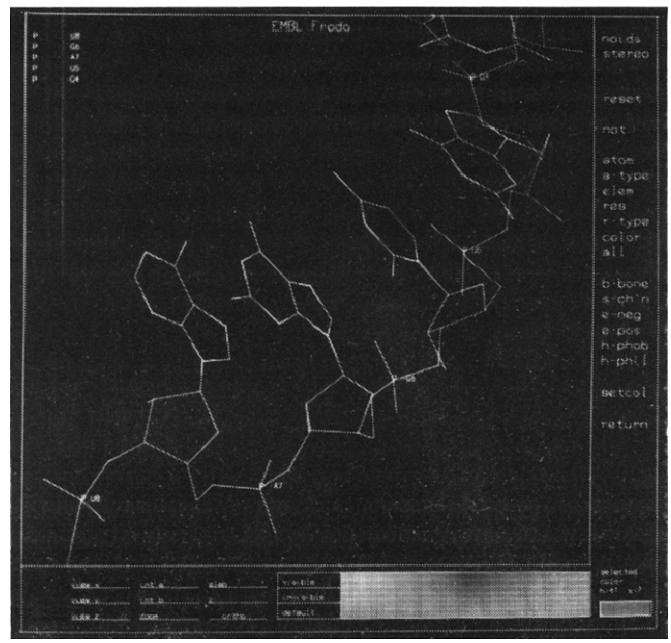

Figure 1. Molecular display in 'colour mode'