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

1 **Dickerson, R E and Geiss, I** *The structure and evolution of proteins* (1969)
2 **Lesk, A M and Hardman, K D** *Science* Vol 216 (1962) p 539
3 **Quarendon, P** *J. Mol. Graphics* Vol 2 No 1 (March 1984) p 4
4 **Heywood, T R et al** *Proc. Eurographics 84 Conf.* in press
5 **Todd, S J P and Morffew, A J** in *Proc. Comnputer Graphics '84 Conf.* in press
6 **Morffew, A J, Todd, S J P and Snelgrove, M J** *Comput. & Chem.* Vol 7 No 1 (1983) p 9
7 **Bernstein, F C et al** *J. Mol. Biol.* Vol 112 (1977) p 535

2

'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: