Molecular graphics abstracts, Part II

The third annual gathering of the Groupe Graphique Moleculaire and the fifth annual meeting of the Molecular Graphics Society were held jointly at Cap d'Agde in France, 11–14 April 1986. The first part of the collected abstracted from the conference (numbers 1–14) was published in the September 1986 issue of this journal. The second and concluding group is presented here, together with an author index.

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Polynomial molecular surfaces

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The projections and clefts inside biological molecules are important to enzymatic function and antigenicity. The goal of this work is to find smooth surfaces which approximate the molecular volume with varying degrees of accuracy, so that clefts and projections can be identified relative to the average surface. These polynomial surfaces generalize the ellipsoidal approximations to protein shape of Thornton *et al.*, presented at last year's International Meeting. The input to the program is a collection of points on the Van der Waals molecular surfaces, or on a solvent accessible surface, as given by Connolly's algorithm. These points are projected onto the unit sphere centred at their centre of gravity, so that the actual point is obtained by multiplying the projected point by a radius-function. Using the 'QR' least squares algorithm, this radius function is fit by the closest degree d polynomial function f of the coordinates x, y, and z on the unit sphere. As the degree d increases, the polynomial more closely approximates the molecular surface. These polynomial surfaces can be represented graphically by computing the radius function at randomly scattered points on the unit sphere, moving the points outward to their appropriate radii, and displaying the resulting dots. In addition, a ray traced raster image may be generated, by eliminating r from the equations

$$r = f(x/r, y/r, z/r), r^2 = x^2 + y^2 + z^2.$$

This gives a polynomial of degree $2d + 2$ in x, y, and z. The intersection of a ray with the surface is then found by solving a polynomial in a single parameter t, representing distance along the ray.

This is joint work with J Tainer and E Getzoff of Scripps Clinic and S Fok and R West of ZeroOne Systems. This work was performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under contract No. W-7045-Eng-48.

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Artificial intelligence for the prevision of protein interactions

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Using learning technics from examples, it is possible to build a set of rules which can be used to detect specific sites in proteins. We have developed these techniques to be able to predict contacts in proteins and probably in some cases to give a starting structure for protein folding. A specific system is necessary to do this work and we will present the architecture that we are using.

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Flexibility and expertise in molecular modelling

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Computer graphical techniques are of great value for:

- molecular structure exploration;
- visualisation of molecular properties;
- modelling of intermolecular interactions;
- reasoning about unknown structures.

A molecular graphics system should be flexible enough in data handling and graphical representation to allow