Molecular graphics abstracts, Part I

Cap d'Agde in the south of France was the setting for a combined international meeting, the third annual gathering of the Groupe Graphique Moléculaire and the fifth annual event of the Molecular Graphics Society. The biggest gathering so far saw a major exhibition of hardware and software in the purpose-built conference centre as well as hearing a wide range of talks, the abstracts of which are reproduced in this issue of the journal with a similar compilation in the December number.

Over three hundred participants attended the meeting, representing over a dozen countries. Almost half the delegates were from universities or public sector research and an equal representation from industry.

During the course of the meeting the creation of a prize for contributors in molecular graphics was announced by Floating Point Systems (France). Other exhibitors were Chemical Design; Digital Equipment Corporation; Evans and Sutherland; Intersys (Silicon Graphics); Masscomp; Metrologie (Megatek, Symbolics, Silicon Graphics); Molecular Design; Polygen; Star Technologies; Sun Microsystems — BIM; Tripos Associates (Sybil) and U-micro.

The meeting underlined the obvious fact that this discipline is still in a phase of rapid growth in every aspect, — hardware, software and in the range of scientific applications — as is evidenced by the abstracts.

W G Richards

1

Structure–activity relationships of methionyl-tRNA synthetase: graphics modelling and genetic engineering

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The high reolution (1.8 Å) crystal structure of methionyl-tRNA synthetase from *E. coli* (tryptic fragment) is under refinement. The zinc ion has been identified and 532 residues of the molecule are now well defined. Using docking and energy minimization, a model describing the interaction of the protein with transfer tRNA's ($tRNA_f^{met}$ and $tRNA^{phe}$) has been built on the graphic system. It incorporates the available chemical information relating to the construction of the synthetase from tRNA. The synthetase gene is currently engineered in order to probe some of the enzyme structure–activity relationships. A series of modified enzymes truncated on the side of the C-terminus have been constructed *in vitro* and assayed for activity. In agreement with the graphics model, the results show that a minimum of 530 intact residues from the N-terminus are necessary to sustain the $tRNA^{met}$ aminoacylation activity. Critical residues for the enzyme activity are searched for using site-directed mutagenesis. The effect on methionyl-tRNA synthetase properties of the mutations will be discussed, in relation with the graphics model.

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Proem: Protein experimental modeller

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Under suitable experimental conditions a protein folds spontaneously to form a unique structure. Numerous theoretical approaches have attempted to emulate this, ranging from energy minimizations to statistical and purely sequence related methods. The former might in principle yield the full 3D structure, but the physicochemical parameters are problematic and the computational difficulties immense. The latter produce indications of the possible secondary structure regions mapped to the sequence, but homologous regions can adopt widely differing structures in unrelated proteins[1]. This may be related to the sequence on either side of the common region, but the final structure might also depend on the developing local 3D environment. During the last few years a relatively small set of principles that govern the structure of proteins have emerged[2,3], and we are developing a rule-based system Proem (protein experimental modeller) using extensions and refinements of these principles, combined with the more conventional methods. Unlike classical program development, which begins with a set of specifications for well-defined tasks, we need tools which allow

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