Collaboration speeds up protein structure research

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A satellite meeting of the 10th International Biophysics Congress was held at Whistler, British Columbia, Canada (July 23–27, 1990), a beautiful International resort centre set amid mountains and lakes. The village atmosphere provided a perfect setting for experts to discuss new horizons in protein structure and dynamics. The meeting was organized by V. Renugopalakrishnan of Harvard Medical School and P. R. Carey of Canada's National Research Council.

A review of NMR in protein research (1985–90) by K. Wüthrich provided the state-of-the-art report on the subject. The use of 2D and 3D FT-NMR techniques, coupled with biosynthetically prepared ^{13}C- and ^{15}N-labelled proteins, has made it possible to assign proton spectra of medium-size proteins (10–15 kDa), and to obtain structural information comparable to that obtained by X-ray diffraction. In at least two proteins, where the initial analysis of X-ray and NMR data were in conflict, the NMR structure was subsequently shown to be correct. R. R. Ernst focused his attention to techniques in NMR for studying peptide dynamics in the time range 30 pico second to 1 second. The main lectures were followed by a number of talks on related subjects, which confirmed that NMR has now matured as a tool complementary to X-ray crystallography for studies in protein stereodynamics.

A critical review of theory and simulation of protein folding by Ray Somarjai provided an insight into the problems associated with the prediction of three-dimensional structure from the primary sequence. A similar message was clear from the talks related to molecular-dynamics studies of proteins. In spite of the optimistic claims, there is no simple solution to the problems associated with the accuracy and validity of empirical potentials, large number of conformational variables, local minima encountered in minimization procedures, solvent environment, etc. Therefore the beautiful colour pictures of protein dynamics generated on graphics workstations should be interpreted with caution.

In a meeting of this kind, it was very surprising to see the absence of protein crystallographers. Tom Blundell, the only representative of this group, talked about comparative studies of topologically similar structures and use of this information for protein modelling and design. Molecular design was the focal theme of a number of other presentations and the emerging principles are being exploited to advantage by a number of pharmaceutical industries.

An important message of the meeting was the importance of multidisciplinary groups and team-work in solving problems related to protein structure, dynamics, design and modelling. The decade of the nineties will be dominated by groups where workers in X-ray crystallography, magnetic resonance, theoretical methods, spectroscopy, organic synthesis, microbiology and biochemistry will work together to predict and synthesize molecules with specific biological activity. Unfortunately, this scenario does not provide a very optimistic future for India, where recognition of work as an individual scientist and personal egos and ambitions frustrate attempts to build strong multidisciplinary teams.

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