

Discussion meeting on macromolecular crystallography—A report

The discussion meeting (held at the Molecular Biophysics Unit (MBU), Indian Institute of Science on May 23–25, 1994) was organized to mark the beginning of phase II of the National Area Detector Facility for X-ray diffraction data collection on single crystals of biological macromolecules. The highlight of the meeting was the participation of M. G. Rossmann, the well-known structural biologist of Purdue University, USA.

Despite the rich tradition of crystallographic research and investigations on biomolecular conformation, serious work on macromolecular crystallography did not begin at the Indian Institute of Science till the early eighties. Around this period, support for equipment required for X-ray instrumentation became available under the thrust area programme of the Department of Science and Technology (DST). Subsequently, with capital investment from MBU and DST, a DST supported national area detector facility was established in the late eighties and significant progress was made in several structural projects. M. Vijayan presented an overview of this development and the key role of MBU in his presidential remarks. G. Padmanaban, remarked in his inaugural address that the mood of research-funding organizations at the present moment is to encourage programmes that promote liaison with industries. He stressed the need to select structural projects that were not only scientifically challenging but also of interest to pharmaceutical industry. Rossmann initiated the discussion meeting with an illuminating talk on viral attachment and cell entry. He described the lessons learnt by him and his team at Purdue University on two key steps in the life cycle of viruses: cell recognition and mechanism of release of genetic material into the cellular matrix.

Rossmann gave two further talks: one was a technical talk on the structure determination of coxsackie virus, which presented tricky problems due to the special orientation and position of virus particles in the unit cell. The other was on obtaining biologically useful structural information on viral surface topography and receptor-binding sites by a combination of electron microscopy and X-ray diffraction.

Rahul Banerjee presented the structure

of peanut lectin tetramer, which unlike most other oligomeric proteins, does not have a closed point group symmetry. The origin and biological role of symmetry in oligomeric proteins were discussed. K. Suguna described crystallographic aspects of the structure determination of a lectin from winged bean seeds. Nagasuma Chandra presented her work on the use of water-mediated transformations of protein crystals to investigate the role of tightly bound water molecules in the stability of proteins and to investigate the rigid and flexible regions of proteins. Sekar presented a progress report on the structure determination of another lectin from jack fruit seeds, jacalin. These talks on plant lectin structures were complemented by Surolia's presentation of his detailed studies on the thermodynamic and structural aspects of lectin-saccharide interactions.

Hosur presented his recent determination of the structure of a ribosome inactivating toxin from jack fruit seeds, gelonin. The structure, currently being refined at high resolution, will help to understand the differences from other well studied toxins of this family such as ricin. The structure will also form the basis for further biochemical investigations in Surolia's laboratory, where the protein was initially purified. U. Sen presented the structure of a Kunitz type inhibitor from winged bean seeds. The structure and molecular modelling studies have revealed the interactions responsible for inhibitor specificity. An interesting analysis of the rotation function calculated using X-ray diffraction data from horse gram inhibitor crystals was presented by Balaji Prakash.

Apart from X-ray diffraction studies, the meeting provided an opportunity to discuss several related biochemical investigations. Balaram and his associates presented seminars describing their investigations on protein modelling and protein stability. They have succeeded in producing thermostable thymidilate synthase by rational design followed by site-directed mutagenesis of the cloned protein. Balaram illustrated various situations where structurally useful information, specifically for protein engineering, could be obtained from an analysis of the protein data bank. Dinakar Salunke presented an information-based approach for modelling

the structures of small peptides. Manju Bansal presented an analysis of the conformational features of interacting helical fragments in protein structures based on the methods developed in her laboratory for the conformational analysis of nucleic acid structures. Lakshmanan Iyer described some of the molecular dynamics studies being carried out in Saraswati Vishweshwara's laboratory. Indira Ghosh of ASTRA Research Centre presented some special applications of molecular dynamics simulations. Jayant Udgaonkar, V. Prakash and Raghavan Varadarajan described interesting projects initiated by them on the protein-folding problem. Jayant Udgaonkar has carried out indepth analysis of the thermodynamics of transition between the native and denatured states of a small protein, barnase. Prakash is investigating the effects on the stability of proteins induced by cosolvent systems that could have industrial applications. Raghavan is developing a novel approach of studying the forces responsible for protein folding in terms of association of protein fragments by a combination of genetic engineering, X-ray crystallography and molecular modelling. Vasantha Patabhi presented data on stabilization of proteins by cross linking. Gautham from Madras University presented his work on the structure of two oligonucleotides.

There was a special session in honour of M. G. Rossmann in which all his former associates made presentations of their work in India. M. R. N. Murthy presented his group's investigations on the structure of a plant virus, sesbania mosaic virus. Pinak Chakrabarti presented his successful use of the protein database to derive biologically significant structural information. Ramkumar described the progress made in the determination of the structure of xylanase. H. S. Savithri described her investigations in structural virology and molecular biology of plant viruses. S. Krishnaswami and R. Usha described their efforts to set up a structural biology laboratory at Madurai Kamaraj University.

A session was dedicated to extensive discussions on the theory and practice of macromolecular crystallography. The indepth discussions on factors that contribute to the accuracy of X-ray diffraction data, refined protein coordinates, methods

for structure determination were clearly an index of the growth of macromolecular science in the country over the past five years spanning the first phase of the national facility at Biophysics Unit. The concluding session was on a discussion on crystallographic research of the present and future in the country. Rossmann was requested to comment on his impressions of the research facilities and activities in the country. Rossmann was very hesitant to make comments as his impressions would inevitably be based on superficial knowledge of the status of work in India. With that understanding he remarked that

the situation in India has always been somewhat strong on the theoretical but weak on experimental work. He appreciated the general atmosphere of enthusiasm in India for scientific research although he felt that it would be necessary to undertake challenging structural problems despite fears of failure for good research to flourish. The willingness to undertake such risks might be related to cultural aspects although it is generally assumed that scientific enterprise transcends cultures. He also felt that the hierarchical structure in India may not be very conducive for healthy scientific

research. Participants were generally happy about the services of the national facility and the progress that has been made at Bangalore and elsewhere. The anticipations for the second phase were very high and it was hoped that the crystallographic community in India will work with solidarity in the coming years to make a qualitative and quantitative improvement of the activity in this exciting area of research.

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CORRESPONDENCE

Enhancing S & T coverage

This has reference to N. C. Jain's proposal to provide several important journals, annual reports, task reports, etc., free to some select science writers and journalists in India (*Current Science*, 1994, 66, 98). I fully endorse his proposal on an experimental basis – in fact, it could become a research project in itself in science popularization, if somebody takes it seriously enough. An experiment of this sort would help us know for instance, whether any media-worthy findings are appearing in our journals or not, whether our science journalists are committed or not, whether science news coverage about Indian work would increase or not, and so on. In fact, the cumulative experiences of the science writers to whom the journals would be provided would give some interesting insights into their minds, the media people and scientists as well. After all, it is only after noticing a scientific finding in an Indian journal that a science writer would contact the concerned scientist or scientists. The interactions that would follow between science writers and scientists would be much more interesting to record and study for our future programmes of science popularization

I only wish somebody takes this 'experiment' seriously enough to monitor its progress and record its findings which would prove useful in working out strategies for future science popularization

programmes. To date, much is talked about Indian media, scientists and science journalists without any proper study. Here is an opportunity which would help clarify our notions about them.

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One of the principle reasons for less coverage of indigenous S & T coverage in our mass media is, to some extent, nonawareness of existence of primary information. Secondly, even if the writers are aware of these sources like learned journals and periodicals containing Indian S & T research reports, reviews, etc., they are beyond direct physical access of majority of science communicators. In support of suggestions made by N. C. Jain, I urge the management of Indian journals to urgently examine these valuable suggestions and undertake steps for their implementation in public interest. The 'scheme', as envisaged by Jain, when implemented, may be run initially for two years and then evaluated with a liberal view. This would perhaps also

help in seeding a temperament among our science communicators to look inward rather than away at foreign source material. Not much expenditure will be incurred on sending a couple of journals to science communicators.

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Apropos N. C. Jain's suggestions on 'Enhancing indigenous science coverage in communication media', the endeavour deserves all praise. Notwithstanding, there is no dearth of science communicators in the country, but because of high priced national/international S & T journals and preoccupations related with the office and home affairs, most of the science writers find themselves unable to afford the same and to spare the time in different libraries on a regular basis; which in turn, results in very poor science coverage in various media in the country. On the other hand, the science communicators from small cities/towns and remote areas have been most unprivileged as far as availability