

## Biomolecular studies using neutrons and X-rays\*

The discussion meeting on biomolecular studies using neutrons and X-rays was one of a series of workshops/seminars, which the Inter-University Consortium for Department of Atomic Energy Facilities (IUC-DAEF), BARC, Mumbai organizes to promote the interaction between scientists from universities and scientists at DAE institutes. The present meeting was the first one where scientists from life sciences departments at various universities were invited to acquaint themselves with major DAE facilities. The facilities, whose role in biological research was discussed at the above meeting, included DHRUVA reactor, synchrotron sources, single crystal X-ray diffractometer, NMR spectrometer and a variety of lasers.

There were 15 invited talks by specialists from various institutions and universities covering different aspects of structures of biological systems. These talks brought out that it is now possible to study very complex biological systems to the same level of sophistication that has been routine with smaller systems. About 30 participants took part in the meeting.

R. Chidambaram, while delivering the keynote address, analysed the status of biological research in the context of technological developments and recent sequencing of genomes, and suggested that structural investigations in India may be focused on two areas; (a) pathogens causing diseases prevalent in India, and (b) radiation-resistant organisms. B. A. Dasannacharya (IUC-DAEF), speaking on X-ray imaging, illustrated how

tumour-diagnosis in a non-invasive fashion has been carried out using X-rays from synchrotrons. M. Ramanadham (BARC) outlined the different types of instruments available at the DHRUVA reactor for neutron beam research. He described in detail, application of single-crystal neutron diffraction technique to accurately characterize hydrogen bond interactions in small molecules such as amino acids and nucleotides. P. S. Goyal (IUC-DAEF) dealt with the technique of small angle neutron scattering (SANS). He presented, using data on various types of surfactant molecules, how variation of H<sub>2</sub>O-D<sub>2</sub>O ratio in the medium can be exploited to locate different chemical components in multi-component systems such as a lipid bi-layer. He pointed out that the SANS instrument available at DHRUVA reactor can be used to study structures of systems ranging in size from 10 to 200 Å. R. V. Nandedkar (CAT, Indore) described the beamlines already commissioned and that are planned to be commissioned on the INDUS-I and INDUS-II synchrotron rings being built by CAT. While INDUS-I generates soft X-rays in the VUV region, INDUS-II will generate hard X-rays suitable for a variety of diffraction experiments.

There were three talks on macromolecular crystallography using hard X-rays. M. V. Hosur (BARC) described the methodology and the contribution that X-ray crystallography has made to biology, especially in the design of drugs against diseases such as AIDS. Dinakar Salunke (NII, Delhi) described the interesting discovery of structural mimicry involving chemically dissimilar molecules, notably peptides and carbohydrates. S. Ramakumar (IISc, Bangalore) presented the structure of the protein xylanase obtained in his laboratory at the very rare 'small-molecule-resolution' of 0.89 Å. In

this context, he pointed out that such high-resolution studies will help in correctly modelling static and dynamic disorders which may have a direct bearing on function.

The talks by B. V. R. Tata (IGCAR, Kalpakkam), A. K. Gupta (SCTIMST, Thiruvananthapuram) and P. K. Gupta (CAT, Indore) dealt with application of lasers in medical imaging. Tata illustrated how confocal microscopy can produce sharp images by eliminating noise. P. K. Gupta dealt with the types of medical applications that have been made using lasers developed at CAT. He also presented data on effects of laser irradiation of biological cells. The talk by A. K. Gupta was about clinical applications of lasers. There were also talks by S. K. Mahajan (BARC) on 'Hot topics for biology research', Chanchal Dasgupta (University of Calcutta) on 'Ribosomal RNA and protein folding' and S. R. Kasturi (TIFR, Mumbai) on 'Frontiers of NMR in biology'.

The participants were taken on a guided tour to DHRUVA reactor and to the National Facility for Macromolecular Crystallography. Scientists of the Solid State Physics Division (SSPD), BARC provided details of the facilities. The participants suggested that a workshop of longer duration be organized, to gain hands-on experience in macromolecular crystallography.

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