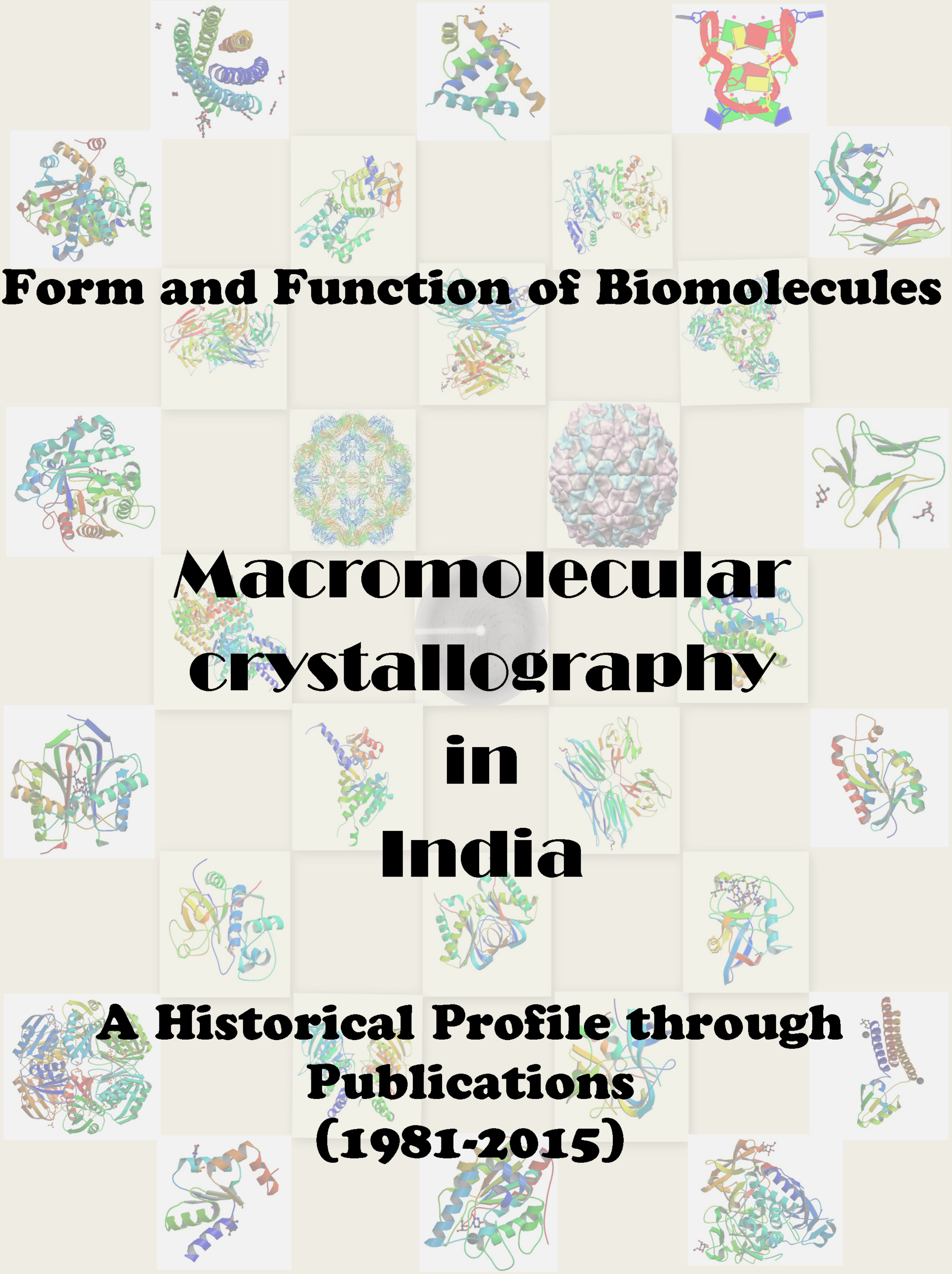

Form and Function of Biomolecules

Macromolecular crystallography in India

A Historical Profile through Publications (1981-2015)

FOREWORD

Structural biology is concerned with the structures of and the structure-function relationship in biomolecules. Macromolecular crystallography is central to structural biology and indeed to modern biology as a whole. Although exploratory efforts in the field were initiated as early as in 1934 by J.D. Bernal and Dorothy Hodgkin (then Crowfoot), substantive results began to appear only by around 1960 with the structure solution of hemoglobin and myoglobin by the groups of Max Perutz and John Kendrew respectively. In an outstanding parallel computational/bioinformatics effort, G.N. Ramachandran and his colleagues at Madras developed what subsequently came to be known as the Ramachandran map which even now remains as the simplest descriptor and tool for validation of protein structures. However, initiation of macromolecular crystallographic studies in India had to wait two more decades.

A few Indians have been involved in the early macromolecular crystallography projects abroad. From among them, I was the first to return to India. When I rejoined the Indian Institute of Science, Bangalore in 1971 after participating in the structure solution of insulin in Dorothy Hodgkin’s laboratory at Oxford, I would have liked nothing more than to straightway start macromolecular crystallography studies in the laboratory, but the resources available then were not even enough to carry out preliminary investigations in the area. I therefore concentrated on studies involving small molecules which are relevant to protein structure, and more so to chemical evolution and origin of life, while at the same time looking for opportunities to initiate macromolecular work. In the meantime, attempts to start macromolecular crystallography were initiated in the late seventies at the Bhabha Atomic Research Centre, Mumbai as well. The efforts truly took off the ground in the country after the Department of Science and Technology (DST) decided in 1983 to handsomely fund the Bangalore Centre under their Thurst Area Programme. The Bangalore laboratory also came to be recognized as a national nucleus for the development of the area in India. Since then, the DST (and now SERB) has continued to support the centres at Bangalore and elsewhere. Over the years, agencies such as the Department of Biotechnology (DBT), the Council of Scientific and Industrial Research (CSIR) and the Department of Atomic Energy (DAE) have also strongly supported the macromolecular crystallography efforts in the country in different ways. In spite of a slow start, work in the area has rapidly expanded in recent years and is being pursued in nearly 40 institutions by about twice as many research groups.

Starting with a single modern in-house facility at Bangalore in the early 1990s for collection of intensity data from macromolecular crystals, dozens of such facilities now exist in different parts of the country. Indian workers now have assured access to the European Synchrotron Facility, thanks to the generous support of the DBT. A dedicated beam line, set up with the support of the DST at Elettra, is expected to be available soon. Happily, the macromolecular crystallography beamline of the second generation synchrotron INDUS-2 at RRCAT, Indore is now fully functional. Thus, although there is a need for setting up a state-of-the art synchrotron facility in India, reasonable arrangements exist for Indian macromolecular crystallographers for collection of diffraction data.

For historical reasons, a majority of macromolecular crystallography groups in the country are led by scientists trained at Bangalore and their descendents. However, over the years, scientists with widely different national and international backgrounds have also established strong groups in different institutions in India. Thus, macromolecular crystallographers in India today constitute a reasonably coherent, vibrant community consisting of a mosaic of backgrounds and expertise, with healthy interactions among themselves and with other concerned biologists. The evolution of the community is perhaps best followed through publications in the area emanating from the country. A historically organized compilation of such publications was first produced in 2005, followed by another in 2011. Much has happened since then and the time is ripe for another compilation. Hence this document which lists relevant papers published till the end of 2015.*

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*The subject matter of the papers in the compilation is meant to be wholly or substantially crystallographic. Efforts have been made to enforce this criterion, probably not with complete success. It is also possible that some publications with substantial crystallographic content, have been eliminated in the process. I apologise to the concerned authors for such omissions, if any.

Macromolecular crystallographic studies in the country now encompass almost all areas of modern biology and also have in some cases medicinal implications. Concerted efforts pertaining to specific systems have also emerged. In some sense, macromolecular crystallography came of age in the country by the turn of the century and was by then equipped to address issues specific to developing countries like India. Even the by the end of 1990s, work had started on proteins from pathogenic microbes which cause infectious diseases. In the early years of this century, we orchestrated a national programme on the structural genomics of microbial pathogens, which provided additional impetus to these efforts. The pathogen that has received maximum attention is *Mycobacterium tuberculosis*, the causative agent of TB which is a major health issue in India. In a loosely coordinated effort, about a dozen laboratories in India are involved in structural studies on TB proteins. Consequently, we now have a robust Indian platform for structure-based inhibitor design which could lead to development of drugs against TB. The other pathogens, the structural biology of which is being pursued in India, include malarial parasites, *Salmonella typhimurium*, *Vibrio cholerae*, *Entamoeba histolytica*, *Staphylococcus aureus*, *Leishmania donovani*, HIV and rotavirus. Thus macromolecular crystallography efforts in India encompass engagement with fundamental biological issues as well as exploration of systems with application potential.

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Bangalore
August, 2016

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