

Nucleic acids in disease and disorder: Understanding the language of life emerging from the ‘ABC’ of DNA

‘Albany 2011: Conversation 17’ was held in June 2011 at SUNY, Albany – a remarkable gathering in a series organized by Prof Ramaswamy Sarma since the first meeting held 39 years ago at SUNY, Albany. As with all Albany gatherings, the 17th Conversation had several elements of excitement in the discussions on biomolecular structure and dynamics (Sarma 2011a). The three of us, along with few other young researchers including doctoral students from various organizations, were representing India.

One of the highlights of the 17th Conversation was the Beveridge celebration – to celebrate the achievements of the living legend Prof David Beveridge, a pioneer in computational biology, DNA structure and dynamics in particular. One of Beveridge’s major contributions has been the monumental effort of setting up of the Ascona B-DNA Consortium (ABC) – a global collection of scientists working with a focus on an identified aspect of computationally understanding DNA structure and dynamics. This concept has been extremely successful in solving large computational problems, overcoming the limited computing capacities available with individual researchers, by dividing the problems into smaller sets that can be solved using local computing resources. It has not only ‘networked’ independent computing environments, but has created a growing global collaborative setup for research (Beveridge *et al.* 2012).

India has had, and continues to have, a rich history of contributions in the field of protein structure and dynamics, from collagen work of Ramachandran with Gopinath Kartha (Ramachandran and Kartha 1954) and subsequently Manju Bansal (Bansal *et al.* 1975; Bansal 1977), to crystallographic works of Vijayan and colleagues (Banerjee *et al.* 1994), to the more recent work of Mittal and Jayaram (Mittal *et al.* 2010; Mittal and Jayaram 2011a, b; Sarma 2011b) – a testament to which are the ongoing and planned Golden Jubilee celebrations for Prof GN Ramachandran’s seminal work on protein conformations (Ramachandran *et al.* 1963). A somewhat lesser appreciated fact in the Indian scientific community, however, is the role of Indian scientists, again initiated by Ramachandran’s group (Sasisekharan *et al.* 1981), in contributing towards developing our current understanding of DNA structure (Jayaram *et al.* 1989; Jayaram and Beveridge 1990; Mohanty and Bansal 1995; Young *et al.* 1997; Madhumalar and Bansal 2003). Somehow this has led to a slower growth in the number of researchers in India being interested in, and contributing towards, understanding the structure and dynamics of nucleic acids compared to the exponential increase in researchers working on protein structure and dynamics. In fact, the DNA community in India is relatively quite small, and has not met in years for a focused discussion – evidenced by the fact that most young researchers in India are not aware that first discoveries of the left-handed DNA structure, while being simultaneously explored by American scientists, happened in India in the late 1970s (Gupta *et al.* 1980; Bansal and Sasisekharan 1986). Further, several early efforts towards exploring structure and dynamics of nucleic acids (Jayaraman and Yathindra 1981; Maiti *et al.* 1983; Malathi and Yathindra 1985; Maiti and Nandi 1986; Santhosh and Mishra 1990; Hosur *et al.* 1990; Kumar *et al.* 1991) have not been followed up. More recently, while contributions such as NuParm (Bansal *et al.* 1995), Chemgenome (Dutta *et al.* 2006), PreDDicta (Shaikh and Jayaram 2007) and PROMBASE (Rangannan and Bansal 2011) have been received well internationally, they are yet to percolate into the Indian scientific community. Essentially there is a requirement to enthuse bright young investigators in India to pursue research in structural and functional aspects of nucleic acids.

Thus, an idea was mooted to host the next ABC meeting at IIT Delhi. The essential goal was to gather Indian scientists working on the structure and dynamics of nucleic acids and to provide a platform to invoke interest in young researchers. A key element was to also try to highlight the importance and imperative requirement of creating a collaborative network inspired by the success of ABC, especially within the

Indian scientific community. A perfect avenue for executing the above plan was provided by the newly established Kusuma School of Biological Sciences at IIT Delhi. Thus evolved an international conference on 'Nucleic acids in disease and disorder', organized by the Kusuma School of Biosciences in association with Supercomputing Facility for Bioinformatics & Computational Biology, from 7 to 9 December 2011 at IIT Delhi. The programme provided an excellent opportunity to the students and the scientific community to discuss the latest developments in the diverse issues pertaining to the structure, dynamics, stability, interaction and function of nucleic acids.

The speakers' list included Prof David Beveridge (ABC of DNA; Beveridge *et al.* 2012); Tom Cheatham (Assessment and validation of MD simulations on nucleic acids); Mihaly Mezei (DNA solvation; Dixit *et al.* 2012); Manju Bansal (Structural and energetic approaches to genomic analyses; Kumar and Bansal 2012); Seyed Hasnain (Genomics of tuberculosis); Garima Khandelwal (Generating physico-chemical finger prints for functional units on genomic DNA based on MD trajectories; Khandelwal *et al.* 2012); Dhananjay Bhattacharyya (Understanding of melting of polymeric DNA using MD simulations; Kundu *et al.* 2012); Prabal Maiti (MD simulations on DNA nanostructures; Nandy *et al.* 2012), Dipak Dasgupta (Interaction of small transcription inhibitors with genomic DNA; Dasgupta *et al.* 2012); D Sundar (DNA recognition by zinc finger proteins; Roy *et al.* 2012); Nirotpal Mrinal (Regulation of gene expression), Nidhi Jain (Sequence effects on conformational heterogeneity of DNA); Sanjay Kumar (Driven DNA); Vibha Tandon (Modulation of PNA-DNA interactions; Singh *et al.* 2012); NR Jena (DNA damage by reactive species; Jena 2012); MR Rajeswari (DNA triplexes in disease; Rajeswari 2012); Pradipta Bandyopadhyay (Monte Carlo simulations on RNA hairpins; Shanker and Bandyopadhyay 2012); G Suresh Kumar (RNA targeting by small molecules; Kumar 2012); Abhijit Mitra (Protonated base pairs in functional RNAs); Suhas Vasikar (Gene networks in neurodegenerative disorders); Khushhali Menaria (Genome to Hit pathway *in silico*); Surat Kumar (NMR in DNA-based drug design; Kumar *et al.* 2012); and K Muniappa (Homologous recombination in mycobacteria). The conference also witnessed 30 poster presentations by students and many lively discussions (Singh and Shah 2012; Mittal and Jayaram 2012). About 150 participants from all over India, in addition to the distinguished speakers from abroad, attended the meeting.

The editors of the *Journal of Biosciences* have kindly consented to bring out the proceedings of the conference as a special issue. This volume is a culmination of these events.

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MANJU BANSAL¹, B JAYARAM^{2,3} and ADITYA MITTAL²

¹*Molecular Biophysics Unit, Indian Institute of Science, Bangalore 560 012, India*

²*Kusuma School of Biological Sciences, ³Department of Chemistry and Supercomputing Facility for Bioinformatics & Computational Biology, Indian Institute of Technology Delhi, New Delhi 110 016, India*

*Corresponding authors (MB – Fax, 91–80–2360 0535; E-mail: mb@mbu.iisc.ernet.in;
BJ – Fax, 91–11–26582037; E-mail: bjayaram@chemistry.iitd.ac.in;
AM – Fax, 91–11–26582037; E-mail: amittal@bioschool.iitd.ac.in)*