

**Workshop
on
'Structure and Dynamics of
Biomolecules 2007'**

December 03 – 08, 2007

*Department of Chemical, Biological &
Macromolecular Sciences,*

**S. N. Bose National Centre for Basic
Sciences, JD Block, Sec III, Salt Lake,
Kolkata 700098**

**Organizers: Ranjit Biswas
Jaydeb Chakrabarti**

Programme Schedule

03 December 2007 (Monday)

09:00 Registration
09:15 – 09:30 Inauguration by the Director, SNBNCBS

Invited Talks: *Chair Person* Professor Samaresh Mitra

09:30 – 10:30 **Invited Talk #1** by Kankan Bhattacharyya on ‘*Study of Organized and Biological Assemblies Using a Femtosecond Laser*’

10:30 – 11:00 **TEA BREAK**

11:00 – 12:00 **Invited Talk #2** by Chaitali Mukhopadhyay on ‘*Structure of Leucine-Enkephalin in GM1 Containing Membrane*’

12:00 – 13:00 **Invited Talk #3** by Raghavan Varadarajan on ‘*Modulating Protein Stability Through Design*’

13:00 – 14:00 **LUNCH BREAK**

14:00 – 15:00 **Invited Talk #4** by B. Jayaram on ‘*Sketching A Physicochemical Pathway from Gene to Drug in Silico*’

15:00 – 15:30 **TEA BREAK**

15:30 – 17:30 **Poster Session**

04 December 2007 (Tuesday)

Invited Talks: *Chair Person* Professor Gautam Basu

09:30 – 10:30 **Invited Talk #5** by Raghavan Varadarajan on ‘*Directed Evolution and Screening of Proteins for Improved Stability and Function*’

10:30 – 11:00 **TEA BREAK**

- 11:00 – 12:00 **Invited Talk #6** by Srabani Taraphder on ‘*Computer Simulation Studies of Enzymatic Catalysis: Investigating the Role of Proteins*’
- 12:00 – 13:00 **Invited Talk #7** by Kankan Bhattacharyya on ‘*Study of Organized and Biological Assemblies Using a Femtosecond Laser*’
- 13:00 – 14:00 **LUNCH BREAK**
- 14:00 – 15:00 **Invited Talk #8** by B. Jayaram on ‘*Sketching A Physicochemical Pathway from Gene to Drug in Silico*’
- 15:00 – 15:30 **TEA BREAK**
- 15:30 – 17:30 **Poster Session**
- 18:00 – 19:00 **Evening Talk** by Indrani Bose on *Microbial Dynamics and Heterogeneity: A Statistical Physics Perspective*
-
-

05 December 2007 (Wednesday)

Invited Talks: *Chair Person* Professor Bimalendu B. Bhattacharyya

- 09:30 – 10:30 **Invited Talk #9** by Amitabha Chattopadhyay on ‘*Dynamics in Biological Membranes: Excitements and Challenges*’
- 10:30 – 11:00 **TEA BREAK**
- 11:00 – 12:00 **Invited Talk #10** by Prabal K. Maiti on ‘*DNA: Self assembled Nanostructures and Ccomplexation with Hyper Branched Polymer*’
- 12:00 – 13:00 **Invited Talk #11** by Srabani Taraphder on ‘*Computer Simulation Studies of Enzymatic Catalysis: Investigating the Role of Proteins*’
- 13:00 – 14:00 **LUNCH BREAK**

14:00 – 15:00 **Invited Talk #12** by Amitabha Chattopadhyay on ‘*Dynamics in Biological Membranes: Excitements and Challenges*’

15:00 – 19:00 **CITY TOUR**

06 December 2007 (Thursday)

Invited Talks: *Chair Person* Professor Dhananjay Bhattacharyya (**Pre-lunch Session**)

09:30 – 10:30 **Invited Talk #13** by Abhijit Chakrabarti on ‘*Organization and Dynamics of Membranes : Fluorescence Probing*’

10:30 – 11:00 **TEA BREAK**

11:00 – 12:00 **Invited Talk #14** by Prabal K. Maiti on ‘*DNA: Self assembled Nanostructures and Complexation with Hyper Branched Polymer*’

12:00 – 13:00 **Invited Talk #15** by Yashwant Singh on ‘*Density-functional theory of a classical system*’

13:00 – 14:00 **LUNCH BREAK**

Invited Talks: *Chair Person* Professor Alok K. Majumdar (**Post-lunch Session**)

14:00 – 15:00 **Invited Talk #16** by Samir K. Pal on ‘*Structure and Dynamics of Biomolecules 2007*’

15:00 – 15:30 **TEA BREAK**

15:30 – 16:30 **Invited Talk #17** by Chaitali Mukhopadhyay on ‘*Structure of Leucine-Enkephalin in GMI Containing Membrane*’

16:30 – 17:30 **Invited Talk #18** by Yashwant Singh on ‘*Density-functional theory of a classical system*’

07 December 2007 (Friday)

Invited Talks: *Chair Person* Professor Abhijit Mookerjee (**Pre-lunch Session**)

09:30 – 10:30 **Invited Talk #19** by Samir K. Pal on ‘Structure and Dynamics of Biomolecules 2007’

10:30 – 11:00 **TEA BREAK**

11:00 – 12:00 **Invited Talk #20** by Sanjoy Bandyopadhyay on ‘Correlated Properties of Water in the Solvation Shell Around Bio-molecules’

12:00 – 13:00 **Invited Talk #21** by Yashwant Singh on ‘Physical Properties of DNA

13:00 – 14:00 **LUNCH BREAK**

Invited Talks: *Chair Person* Professor Bidyendu M. Deb (**Post-lunch Session**)

14:00 – 15:00 **Invited Talk #22** by Abhijit Chakrabarti on ‘Organization and Dynamics of Membranes : Fluorescence Probing’

15:00 – 15:30 **TEA BREAK**

15:30 – 16:30 **Invited Talk #23** by Sanjoy Bandyopadhyay on ‘Correlated Properties of Water in the Solvation Shell Around Bio-molecules’

16:30 – 17:30 **Invited Talk #24** by Yashwant Singh on ‘Physical Properties of DNA

08 December 2007 (Saturday)

Invited Talks: *Chair Person* Professor Surajit Sengupta (**Pre-lunch Session**)

09:30 – 10:00 **Seminar Talk #1** by Gautam Basu on ‘The Colchicine-Binding Site of Tubulin: Origin of Differential Binding Affinities Across Eukaryotic Families and the Biological Role of the Binding Site’

- 10:00 – 10:30 **Seminar Talk #2** by Dhanjay Bhattacharyya on ‘*Non-canonical Base Pairs in RNA: An Algorithmic Approach for Database Analysis*’
- 10:30 – 11:00 **Seminar Talk #3** by Jaydeb Chakrabarti on ‘*A Novel Approach to Solvation Timescale in Nonpolar Solvents via Instability of Solvent Density Modes*’
- 11:00 – 11:30 **TEA BREAK**
- 11:30 – 12:00 **Seminar Talk #4** by Krishnananda Chattopadhyay on ‘*Fluorescence Correlation Spectroscopy and Protein Folding in the Microsecond Time Scale*’
- 12:00 – 12:30 **Seminar Talk #5** by Sanjay Kumar on ‘*Force Induced Stretched State: Effects of Temperature*’
- 12:30 – 13:00 **Seminar Talk #6** by Surajit Sinha on ‘*Conditional Regulation of the Hedgehog (Hh) Signaling Pathway*’
- 13:00 **Vote of Thanks, LUNCH & End of Workshop**

INVITED TALKS

Study of Organized and Biological Assemblies Using a Femtosecond Laser

Kankan Bhattacharyya
Indian Association for the Cultivation of Science
pckb@mahendra.iacs.res.in

The longstanding goal of chemical dynamics is to unravel dynamics in a complex biological system. Significant progress towards this end has been achieved recently, using femtosecond laser spectroscopy. In a biological system, water and the reactive species are often confined in a nanocavity. We will show that nano-confinement affects the dynamics, in particular the ultrafast initial part quite significantly. Firstly, proximity of the reactants in a confined system results in very fast bi-molecular reactions. We will illustrate this with ultrafast fluorescence resonance energy transfer (FRET) and electron transfer (ET) in an organized assembly. Secondly, binding of the water molecules with biological macromolecules greatly restricts its mobility. Solvation dynamics (dielectric response) of so called 'biological water' exhibits an ultraslow component in 100- 1000 ps time scale. This is slower by 2-3 orders of magnitude compared to bulk water. We will discuss several examples of ultraslow solvation dynamics in biological systems and their implications. Finally, we will demonstrate that ultraslow solvation causes dramatic retardation of many polar reactions (e.g. proton transfer).

Correlated Properties of Water in the Solvation Shell Around Bio-molecules

Sanjoy Bandyopadhyay

Molecular Modeling Laboratory, Department of Chemistry,
Indian Institute of Technology, Kharagpur - 721302, India
sanjoy@chem.iitkgp.ernet.in

Water plays important roles in determining the structure, stability, and function of bio-molecules, such as proteins, lipids, nucleic acids and complex carbohydrates. Such roles are played through a dynamical coupling that exists between the bio-molecule and the water around it. A molecular level knowledge of such coupling that arises due to the ability of water to form two-dimensional hydrogen-bonded network spanning the surface of a bio-molecule is necessary to understand the mechanism of the function of the bio-molecule. Considering the importance of the issues involved, this subject has been an area of intense research.

Computer simulations, capable of providing information at an atomistic resolution can play an important role to obtain an understanding of the fundamental issues in this area. Our primary focus has been to study the correlated properties of water present in the solvation shell of proteins in aqueous solutions using molecular dynamics (MD) simulations. Some recent works carried out in our laboratory in this area will be highlighted.

References

1. Chakraborty, S.; Sinha, S. K. and Bandyopadhyay, S. *J. Phys. Chem. B* **2007**, *111* (ASAP Article).
2. Chakraborty, S. and Bandyopadhyay, S. *J. Phys. Chem. B* **2007**, *111*, 7626.
3. Bandyopadhyay, S.; Chakraborty, S. and Bagchi, B. *J. Am. Chem. Soc.* **2005**, *127*, 16660.

Dynamics in Biological Membranes: Excitements and Challenges

Amitabha Chattopadhyay

Centre for Cellular and Molecular Biology, Hyderabad;

amit@ccmb.res.in

Biological membranes are complex assemblies of lipids and proteins that allow cellular compartmentalization and act as the interface, through which cells communicate with each other and with the external milieu (1). The biological membrane therefore constitutes the site of many important cellular functions involving transfer of information from outside to the interior of the cell. In physical terms, membranes can be treated as a complex fluid which is a weakly coupled, non-covalent, and anisotropic assembly of molecules in two-dimensions (and can therefore be treated as soft matter). Membranes are heterogeneous in the context of a wide range of spatiotemporal scales (2,3). A unique aspect of such an assembly is its dynamics spanning a large range of time scales, which supports a wide variety of biological processes, necessary for cellular function. Monitoring membrane dynamics with all its complexities continues to be a challenge in contemporary membrane biology. I will address some of these issues in my lectures with examples taken from literature as well as past and ongoing work in my laboratory (4,5).

References

1. Mouritsen, O.G. (2005) *Life – As A Matter of Fat*, Springer.
2. Jacobson, K., Mouritsen, O.G., and Anderson, R.G.W. (2007) *Nat. Cell Biol.* 9: 7-14.
3. Marguet, D., Lenne, P.-F., Rigneault, H., and He, H.-T. (2006) *EMBO J.* 25: 3446-3457.
4. Pucadyil, T.J., Kalipatnapu, S., Harikumar, K.G., Rangaraj, N., Karnik, S., and Chattopadhyay, A. (2004) *Biochemistry* 43: 15852-15862.
5. Ganguly, S., Pucadyil, T.J., and Chattopadhyay, A., *communicated*.

Organization and Dynamics of Membranes : Fluorescence Probing

Abhijit Chakrabarti

Biophysics Division, Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata 700064; abhijit.chakrabarti@saha.ac.in, abhijit1960@gmail.com

The Fluid Mosaic model of biomembrane was proposed by Singer & Nicholson way back in 1972 where they described the cell membrane as "a two-dimensional oriented solution of integral proteins....in the viscous phospholipid bilayer" (1). Numerous studies, done in the last 35 years, on the organization and dynamics of the membrane proteins and lipids, indicated that the lateral diffusion of many proteins (even lipids, in few cases) are often restricted and non-random in the cell membrane. The model was revisited by Jacobson and coworkers in the year 1995 to incorporate the motional constraints and the lateral heterogeneity in the membrane structure (2) in submicron scale, referred as "domains".

In the first lecture, I would elaborate on the complexity of organization and dynamics of cell surface bilayer membranes focusing on the slower transbilayer movements and the faster lateral diffusion implicated in different membrane mediated biological processes. The second lecture would be devoted to explain the present day domain structure of membranes using experimental data on the lateral diffusion measured by fluorescence recovery after photobleaching (FRAP) technique and proximity measurements by fluorescence resonance energy transfer, FRET (3) between two membrane components. The lipidic GPI-anchored protein, DAF diffused faster in reconstituted phospholipid membranes ($D_{lat} = 8.0 \pm 0.4 \times 10^{-9} \text{ cm}^2/\text{s}$) compared to HLA, a normal membrane protein with a single transmembrane domain ($D_{lat} = 4.6 \pm 0.25 \times 10^{-9} \text{ cm}^2/\text{s}$). However, proximity measurements by FRET indicated both the proteins to form microdomains (4). The lateral diffusion of the GPI-anchored DAF was found to decrease in presence of 10% cholesterol and 5% glycosphingolipids ($D_{lat} = 4.7 \pm 0.3 \times 10^{-9} \text{ cm}^2/\text{s}$) with a concomitant increase in the efficiency of fluorescence resonance energy transfer between donor- and acceptor-labeled DAF in phospholipid membranes. Fluorescence based experiments on lipid mixing involved in membrane fusion will also be discussed.

References

1. Singer, S J. & Nicholson, G L. (1972). *Science*, **175**, 720.
2. Jacobson, K., Sheets, E D. & Simson, R. (1995). **268**, 1441.
3. Chakrabarti, A., Matko, J., Rahman, N A., Barisas, B G. & Edidin, M. (1992). *Biochemistry* **31**, 7182.
4. Chakrabarti, A. & Edidin, M. (unpublished data).
5. B. Alberts, A. Johnson, J. Lewis, M. Raff, K. Roberts, P. Walter, *Molecular Biology of the Cell*, 4th Edition, Garland Science (2002), New York.
6. Gennis, R. B. (1989) *Biomembranes: Molecular Structure and Function*, In: Cantor CR ed. Springer Advanced Texts in Chemistry. New York.
7. J. R. Lakowicz (2006) *Principles of Fluorescence Spectroscopy*. Springer, Singapore.

Sketching A Physicochemical Pathway from Gene to Drug *in Silico*

B. Jayaram

Department of Chemistry, and Supercomputing Facility for Bioinformatics & Computational Biology, Indian Institute of Technology, Hauz Khas, New Delhi-110016, India; bjayaram@chemistry.iitd.ac.in; Website: www.scfbio-iitd.res.in

The world wide genome sequencing efforts and the concurrent developments in scientific software implementations on massively parallel computer architectures grant us the opportunity to dream that drug design could be undertaken against suitable biomolecular targets to develop individualized medicine almost in an automated way. Currently however, without the help of any database, an inspection of a DNA sequence does not tell us whether it is likely to be a gene and if it is a gene for messenger RNA, what the likely three dimensional structure of its protein product is. Also drug design softwares fall short of expectations even if the structures of drug targets are known.

Addressing the above issues from a physico-chemical perspective, we have developed a novel semi-empirical model for whole genome analysis (*ChemGenome*) based on DNA energetics, an all atom energy based computational protocol for narrowing down the search space for locating tertiary structures of small globular proteins (*Bhageerath*) and a binding free energy based methodology for active site directed lead molecule design (*Sanjeevini*). The *ChemGenome* could distinguish genes from non-genes in 331 bacterial genomes and 20 eukaryotic genomes with > 90% accuracy. The start and stop site prediction accuracies of *Chemgenome* are either at par or exceed the current standards. *Bhageerath* could successfully bracket native-like structures to within 3 to 6 Å in the 10 lowest energy structures for 50 small alpha helical globular proteins. The *Sanjeevini* drug design protocol could sort drugs from non-drugs for a few drug targets helping in addressing both affinity and specificity issues in drug design. Progresses recorded in the areas of genome analysis, protein structure prediction and drug design and the software

tools developed and made freely accessible at www.scfbio-iitd.res.in together with challenges and promises there of will be presented.

References

Dutta,S., Singhal,P., Agrawal,P., Tomer,R., Kritee, Khurana,E. and Jayaram.B. *A Physico-Chemical Model for Analyzing DNA sequences*, 2006, *Journal of Chemical Information & Modelling*, 46(1), 78-85.

(a), Narang,P, Bhushan,K., Bose,S. and Jayaram,B. *A computational pathway for bracketing native-like structures for small alpha helical globular proteins*. 2005, *Phys. Chem. Chem. Phys.*, 7, 2364.; (b) Narang,P, Bhushan,K., Bose, S., Jayaram,B. *Protein structure evaluation using an all atom energy based empirical scoring function*, 2006, *J. Biomol. Struct. Dyn.*, 23, 385-4006. (c) Jayaram et al., Bhageerath, 2006, *Nucleic Acid Res.*, 34, 6195-6204.

(a) Latha, N and Jayaram,B. *A Binding Affinity Based Computational Pathway for Active-Site Directed Lead Molecule Design:Some Promises and Perspectives*. 2005, *Drug Design Reviews-Online*, 2(2),145. (b) Jain, T and Jayaram, B. *An all atom energy based computational protocol for predicting binding affinities of protein-ligand complexes*. 2005, *FEBS Letters*, 579, 6659; (c) Jain, T and Jayaram, B. *A computational protocol for predicting the binding affinities of zinc containing metalloprotein-ligand complexes*. 2007, *Proteins: Structure, function & Bioinformatics*, 67, 1167-1178; (d) Shaikh, S., Jayaram. B., *A swift all atom energy based computational protocol to predict DNA-Drug binding affinity and T_m* , 2007, *J. Med. Chem.*, 50, 2240-2244; (e) Shaikh, S., Jain. T., Sandhu, G., Latha, N., Jayaram., B., *A physico-chemical pathway from targets to leads*, 2007, *Current Pharmaceutical Design*, in press.

Structure of Leucine-Enkephalin in GM1 Containing Membrane

Anindita Gayen and Chaitali Mukhopadhyay

Department of Chemistry, University of Calcutta
92, A. P.C. Road, Kolkata - 700 009; chaitalicu@yahoo.com

The structure of the small opiate peptide leucine-enkephalin has been studied in the presence of isotropic phospholipid bicelles. The effect of membrane composition on the peptide conformation was explored using zwitterionic phosphocholine bicelles (DMPC:Chaps 1:4) and negatively charged phosphocholine bicelles doped with ganglioside GM1 (DMPC:Chaps:GM1 1:4:0.3). Structure calculation from torsion angles, chemical shifts and NOE-based distance constraints suggests presence of both the μ - and δ -selective conformers in each bicellar system. Our results suggest that, this small peptide can adopt several conformations in membrane environment with one conformation geometrically favored over the others. GM1, as a component of the membrane, can regulate the conformation of the small peptide.

DNA: Self assembled Nanostructures and Complexation with Hyper Branched Polymer

Prabal K. Maiti

Center for Condensed Matter Theory Unit, Department of Physics,
Indian Institute of Science, Bangalore, 560012; maiti@physics.iisc.ernet.in

In the first part of the talk I will discuss simulation methodologies to study various DNA based nanostructures. I report MD simulations results on cross-over DNA molecules to obtain a comprehensive understanding of relationship between structure, topology, and stability of various Paranemic crossover (PX/JX) DNA molecules. The paranemic crossover (PX) DNA molecules and their topoisomers, recently synthesized by the Seeman group at New York University, are important components for novel nanomechanical devices and for constructing periodic arrays that could be useful in other nanoscale applications. In the second part of the talk

I discuss the structure and dynamics of the complexation between DNA and dendrimer through atomistic molecular dynamics (MD) simulations, accompanied by free energy calculations and inherent structure determination. Complexation shows surprisingly strong sensitivity to the ssDNA sequence which is found to arise from a competition between enthalpic versus entropic rigidity of ssDNA.

Structure and Dynamics of Biomolecules-2007

Samir Kumar Pal

Unit for Nano Science & Technology, and Department of Chemical, Biological & Macromolecular Sciences, S. N. Bose National Centre for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata 700 098; skpal@bose.res.in

Exploration of structure of various biological macromolecules and the dynamics in their close vicinity using steady state and picosecond-resolved spectroscopic techniques will be discussed. Application of semiconductor quantum dots to address various biophysical problems will also be discussed. The talk intends to cover following topics.

1. Ultrafast charge transfer and solvation of DNA minor groove binder: Hoechst 33258 in restricted environments.
2. Simultaneous Binding of Minor Groove Binder and Intercalator to Dodecamer DNA: Importance of Relative Orientation of Donor and Acceptor in FRET.
3. Direct Observation of Essential DNA Dynamics: Melting and Reformation of the DNA Minor Groove.
4. Size and shape-dependent electron-hole relaxation dynamics in CdS nanocrystals.
5. Aggregated CdS Quantum Dots: Host of Biomolecular Ligands.
6. Structural and Functional Characterization of Enzyme-Quantum Dot Conjugates: Covalent Attachment of CdS Nanocrystal to α -Chymotrypsin.
7. Direct Conjugation of Semiconductor Nanocrystals to a Globular Protein to Study Protein-Folding Intermediates.

A. Density-functional theory of a classical system

Y. Sing

Benaras Hindu University (BHU), Varanasi; singhyas_in@yahoo.co.in

A density-functional approach will be developed to describe the properties of an inhomogeneous system. The theory will be applied to describe the freezing transition of a liquid. We will also discuss the free energy of blends of block copolymers expressed as a functional of density distribution of monomers of each block. This expression can be used to calculate the micro- and macro phase separation of the blends of homopolymers and block copolymers.

B. Physical properties of DNA

The lectures will focus on

1. Structure (primary, secondary, tertiary)
2. Interactions, Equilibrium state and Possible motions of bases,
3. Thermal denaturations,
4. Force induced unzipping
5. Bending and cyclization

Computer Simulation Studies of Enzymatic Catalysis: Investigating the Role of Proteins

Srabani Taraphder

Dept. of Chemistry, Indian Institute of Technology, Kharagpur;

srabani@chem.iitkgp.ernet.in

In this series of lectures, we shall discuss at an introductory level how computer simulation studies may help in understanding the role of protein structure and dynamics on the outcome of a chemical reaction that is being catalyzed by an enzyme. We shall first discuss how one may investigate the molecular mechanism of enzyme action by exploring the conformational space of the protein and estimating the free energy changes during conformational transitions. Use of simulation methods to assess the importance of dynamical modes will be discussed next. Application of these methods will be demonstrated in enzymes where the reaction coordinate may or may not be known.

References

1. Dynamics of biochemical and biophysical reactions: insight from computer simulations, A. Warshell and W. W. Parson, Quarterly Reviews of Biophysics (2001) 34, pp. 563-679.
2. QM/MM Methods for Biological Systems, W. Thiel and H. M. Senn, Top Curr Chem (2007) 268, 173-290.
3. Identification of Proton-Transfer Pathways in Human Carbonic Anhydrase II, A. Roy and S. Taraphder, J. Phys. Chem. B (2007) 111, 10563-10576.
4. Reaction coordinate of an enzymatic reaction revealed by transition path sampling, S.L. Quaytman and S.D. Schwartz, Proc. Natl. Acad. Sc. USA (2007), 104, 12253-12258.

Modulating Protein Stability Through Design

R. Varadarajan

Molecular Biophysics Unit, IISc, Bangalore;
varadar@mbu.iisc.ernet.in

Proteins are biopolymers composed of twenty different amino acid building blocks. After synthesis in the cell, proteins fold into complex three dimensional structures which are essential for function. These folded structures are in equilibrium with small amounts of the unfolded polypeptide chain. The thermodynamic stability of a protein is the Gibbs free energy difference between the folded and unfolded states of the protein. Both from a fundamental point of view as well as for various practical applications, it is important to be able to modulate protein stability through mutation. Folded proteins are stabilized by a variety of noncovalent interactions. These include van der Waals, electrostatic and hydrophobic interactions. Disulfide bridges are covalent interactions that are important for protein stability. While these interactions have been understood qualitatively for some time, it remains a challenging task to rationally modulate protein stability by altering specific interactions at the molecular level. A brief description of calorimetric methods to measure protein stability will be provided. Attempts and methodologies to increase or decrease protein stability in a rational manner through site specific mutation will be discussed.

Suggested Reading

1. "Areas, Volumes, Packing and Protein Structure" F. M. Richards, *Ann. Rev. Biophys. Bioeng.* (1977) 6:151-176.
2. "Thermodynamic Problems of Protein Structure" P. L. Privalov, *Ann. Rev. Biophys. Biophys. Chem.* (1989) 18:47-69.
3. Dani, V. S., Ramakrishnan, C., and Varadarajan, R. (2003) MODIP revisited: re-evaluation and refinement of an automated procedure for modeling of disulfide bonds in proteins. *Protein Eng* 16, 187-193.
4. Chakshusmathi, G., Mondal, K., Lakshmi, G. S., Singh, G., Roy, A., Ch, R. B., Madhusudhanan, S., and Varadarajan, R. (2004) Design of temperature-sensitive mutants solely from amino acid sequence. *Proc Natl Acad Sci U S A* 101, 7925-7930.
5. Mondal, K., Dastidar, A. G., Singh, G., Madhusudhanan, S., Gande, S. L., Vijayraghavan, K., and Varadarajan, R. (2007) Design and Isolation of Temperature-sensitive Mutants of Gal4 in Yeast and Drosophila. *J Mol Biol* 370, 939-950.
6. Dantas G, Corrent C, Reichow SL, Havranek JJ, Eletr ZM, Isern NG, Kuhlman B, Varani G, Merritt EA, Baker D. High-resolution structural and thermodynamic analysis of extreme stabilization of human procarboxypeptidase by computational protein design. *J Mol Biol* 366 1209-1221

Directed Evolution and Screening of Proteins for Improved Stability and Function

R. Varadarajan

Molecular Biophysics Unit, IISc, Bangalore

varadar@mbu.iisc.ernet.in

When expressed in *E. coli*, many eukaryotic proteins form insoluble aggregates known as inclusion bodies. Recovery of active proteins from inclusion bodies is technically difficult. Bacterial expression of unstable proteins is also challenging as these often tend to aggregate or be proteolyzed soon after expression. Improving stability, solubility and functional properties of proteins through rational design remains a challenging task. Techniques such as random mutagenesis and DNA shuffling can be used to generate mutant libraries from a parent DNA sequence. While the majority of the sequences in such libraries often have properties inferior to the parent sequence, a small number of sequences may result in proteins with improved stability and solubility. It is therefore important to have efficient screening or selection procedures to fish out clones with these desired properties from the library. Strategies for doing this along with several examples from the literature will be discussed.

Suggested Reading

1. Ignatova, Z. & Gierasch, L. M. (2004). Monitoring protein stability and aggregation in vivo by real-time fluorescent labeling. *Proc Natl Acad Sci U S A* **101**, 523-8.
2. Martin, A., Sieber, V. & Schmid, F. X. (2001). In-vitro selection of highly stabilized protein variants with optimized surface. *J Mol Biol* **309**, 717-26.
3. Mazor, Y., Van Blarcom, T., Mabry, R., Iverson, B. L. & Georgiou, G. (2007). Isolation of engineered, full-length antibodies from libraries expressed in *Escherichia coli*. *Nat Biotechnol* **25**, 563-5.
4. Philipps, B., Hennecke, J. & Glockshuber, R. (2003). FRET-based in vivo screening for protein folding and increased protein stability. *J Mol Biol* **327**, 239-49.
5. Riechmann, L. & Winter, G. (2006). Early protein evolution: building domains from ligand-binding polypeptide segments. *J Mol Biol* **363**, 460-8.
6. Waldo, G. S., Standish, B. M., Berendzen, J. & Terwilliger, T. C. (1999). Rapid protein-folding assay using green fluorescent protein. *Nat Biotechnol* **17**, 691-5.

EVENING TALK; 04 December 2007 at 6:00 PM

Microbial Dynamics and Heterogeneity: A Statistical Physics Perspective

Indrani Bose

Department of Physics, Bose Institute, 93/1, A. P. C. Road Kolkata-700009;
indrani@bosemain.boseinst.ac.in

Recent experiments suggest that microorganisms take advantage of positive feedback and gene expression noise to adapt to unfavourable circumstances including treatment with antibiotic drugs, nutrient depletion, lack of oxygen etc. In a population of bacterial cells with identical genetic makeup, heterogeneities develop in the form of two distinct subpopulations only one of which acquires the ability to adapt. Statistical physics concepts, tools and techniques provide new insight on how the selection of cell fate occurs. I will discuss specific examples which illustrate how an interplay between theory and experiments enriches our understanding of the strategies adopted by microbes to cope with stress. The findings are important not only for developing suitable drug therapies but highlight possible universal mechanisms for the development of “heterogeneity with an advantage” in microbial populations.

SEMINAR TALKS

The Colchicine-Binding Site of Tubulin: Origin of Differential Binding Affinities Across Eukaryotic Families and the Biological Role of the Binding Site

Gautam Basu

Department of Biophysics, Bose Institute, P-1/12 CIT Scheme VIIM, Kolkata 700 054
gautamda@gmail.com

Colchicine-tubulin interaction, responsible for the disruption of microtubule formation, has immense pharmacological importance but is poorly understood in terms of its biological significance. The interaction is characterized by a marked higher affinity of colchicine for animal tubulins compared to tubulins from plants, fungi and protists. From an analysis of tubulin sequences and colchicine-tubulin crystal structure, we propose (Banerjee et al., 2007) that Pro268 β and Ala248 β (270 β and 250 β in the crystal structure 1SA0) in animal tubulin are crucial for the observed differential binding. We also suggest that mediated by the binding of endogenous molecules to the colchicine-binding site, microtubule assembly in eukaryotes is modulated in a family specific manner. Experiments to validate our hypotheses, that Pro268 β and Ala248 β in animal tubulin is responsible for its colchicine-specificity, and that the colchicine-binding site of tubulin binds endogenous molecules, have been initiated. Preliminary results from some of these experiments will be presented.

References

Banerjee et al. (2007) Differential colchicine-binding across eukaryotic families: The role of highly conserved Pro268 β and Ala248 β residues in animal tubulin. *FEBS Lett.* **581**, 5019-23.

Non-canonical Base Pairs in RNA: An Algorithmic Approach for Database Analysis

D. Bhattacharyya^{1,2}, A. Mitra³, B. Sinha³, M. Bansal⁴, J. Das¹, S. Mukherjee¹, P. Majumdar¹, M. Bhattacharyya¹ and A. Roy¹

¹Biophysics Division and ²Center for Applied Mathematics & Computational Science, Saha Institute of Nuclear Physics, Kolkata; ³International Institute of Information Technology, Hyderabad; ⁴Molecular Biophysics Unit, Indian Institute of Science, Bangalore;
[dhananjay.bhattacharyya@saha.ac.in](mailto:ghananjay.bhattacharyya@saha.ac.in)

Prediction of secondary structure of RNA is gaining more attention due to the emergence of therapeutic importance of different forms of micro-RNA. Structure prediction methods never use non-canonical base pairs but several different types of such unusual base pairs are seen quite frequently in the crystal structures of different functional RNA macromolecules. We have developed two new algorithms to detect and analyze structures of canonical or non-canonical base pairs from crystallographic coordinates and have analyzed 209 high-resolution structures of RNA using these methods. We have detected, among others, many short hairpin loops having only two residues in the loop region, several double helical regions with non-canonical base pairs flanked by Watson-Crick base pairs. We calculated three rotational and three translational movements of one base with respect to the other of the pair to define co-planarity of the bases as well as lengths of the H-bonds holding the two bases together. Analysis of structures of the base pairs indicates that most non-canonical base pairs have features quite similar to the canonical Watson-Crick base pairs. They are nearly co-planar, form strong hydrogen bonds and hence can give rise to well-stacked double helical stems in RNA. Some non Watson-Crick base pairs have their characteristic features depending on the edges involving H-bond formation to form a pair. Interaction energy between the paired bases, as obtained from *ab initio* Hartree-Fock calculations, also indicate most of these base pairs having two or more hydrogen bonds are stable. A proper consideration of these various possible base pairing schemes is expected to considerably improve the prediction accuracy of 3-D structures for RNA.

A Novel Approach to Solvation Timescale in Nonpolar Solvents via Instability of Solvent Density Modes

R. Biswas and J. Chakrabarti

Dept. of Chemical, Biological and Macromolecular Sciences, S. N. Bose National Centre for Basic Sciences, JD Block, Salt Lake City, Kolkata 700 098; jaydeb@bose.res.in

We perform linear stability analysis of solvent density modes in the presence of non-polar solute-solvent interaction in a non-polar solvent. The dominant instability given by the maximum positive eigenvalue of the stability matrix, provides the timescale of the solvent rearrangement around a solute. Our theory predicts two long timescales for both in normal non-polar and supercritical fluids (SCF). We discuss the existing experimental results on non-polar solvation dynamics in the light of our prediction¹.

Reference

1. R. Biswas and J. Chakrabarti, **J. Phys. Chem. B.** 2007, **111**; Web Release Date: 14 Nov 2007; DOI: [10.1021/jp075949n](https://doi.org/10.1021/jp075949n)

Fluorescence Correlation Spectroscopy and Protein Folding in the microsecond time scale.

Krishnananda Chattopadhyay

Structural Biology and Bio-informatics, Indian Institute of Chemical Biology, Kolkata

700032; krish@iicb.res.in

Fluorescence correlation spectroscopy is emerging as an important technique in chemistry, biophysics and biochemistry for its applications in measuring diffusional properties and chemical kinetics at nanomolar concentration. The technique involves measuring fluorescence fluctuations resulting from the changes in the number of fluorophore in a small observation volume due to diffusion or chemical reaction under conditions of thermodynamic equilibrium. Applications of FCS in protein biophysics are generally of two kinds. First, the diffusion time and hence the diffusion coefficient of a protein can be measured very accurately. Second, by suitably optimizing the measurement conditions, FCS can be used to study protein dynamics or conformational events in the microsecond time scale. We have recently used combinations of fluorescence quenching and fluorescence correlation spectroscopy to monitor the conformational dynamics of a predominately β -sheet protein in the microsecond time scale. Experiments carried out with unfolded protein at low pH and in presence of high guanidium hydrochloride indicate the presence of residual structure and rapid fluctuation dynamics. The amplitude and the time scale of the unfolded state conformational dynamics depend on the nature of the denaturant and its concentration.

Force Induced Stretched State: Effects of Temperature

Sanjay Kumar

Department of Physics, Banaras Hindu University, Varanasi 221 005;
yashankit@yahoo.com

A model of self-avoiding walks with suitable constraint has been developed to study the effect of temperature on a single stranded DNA (ssDNA) in the constant force ensemble. Our exact calculations for small chains show that the extension (reaction co-ordinate) may increase or decrease with the temperature depending upon the applied force. The simple model developed here, which incorporates semi-microscopic details of base direction provide an explanation of the force-induced transitions in ssDNA as observed in experiments.

References

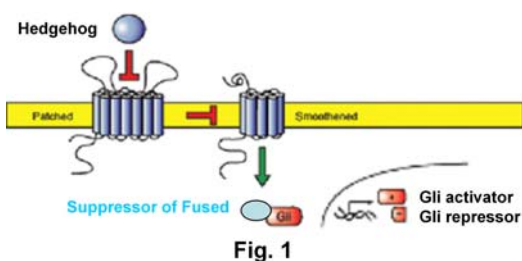
1. Phys. Rev. E ,Vol. 73, 50903(R), (2006)
2. Phys. Rev.Lett. Vol. 98, 128101 (2007)
3. Cond. Matt.: arXiv:0709.0606

Conditional Regulation of the Hedgehog (Hh) Signaling Pathway

Surajit Sinha

Department of Organic Chemistry, Indian Association for the Cultivation of Science,
Jadavpur, Kolkata-700 032; oc55@iacs.res.in

Hedgehog signaling pathway specify embryonic pattern by directing cellular differentiation and proliferationⁱ and it maintains stem cells and regulate repair in adult tissuesⁱⁱ, whereas persistent Hh-pathway activity involves in the formation and growth of several cancers including birth defectsⁱⁱⁱ. This pathway is initiated by the binding of secreted Hh proteins to the twelve-transmembrane protein Patched1 (Ptch1) which normally represses the activity of the seven-transmembrane protein Smoothened (Smo)



and Smo in turn promotes the expression of Hh target genes (**Fig. 1**)¹. Conditional regulation of Hh signaling therefore may have biomedical applications, including the treatment of Hh pathway-dependent stem cell

and cancer diseases.

Light sensitive caged morpholino oligomers has been used to control the regulation of *no tail (ntl)* gene, a source of hedgehog signaling and studied Hh dependent phenotypes in zebrafish model organism^{iv}. The Ntl transcription factor is required in zebrafish for the formation of the tail and notochord, a rod-shaped tissue that provides structural rigidity and secretes proteins to pattern neighbouring tissues. In another study a small molecule called purmorphamine have been used in activation of Hh pathway by targeting smoothened^v, a transmembrane protein.

ⁱ Ingham, P. W. & McMahon, A. P. *Genes Dev.* **15**, 3059-3087 (2001).

ⁱⁱ Beachy, P. A.; Karhadkar, S. S. & Berman, D. M. *Nature* **432**, 324-331 (2004)

ⁱⁱⁱ McMahon, A. P.; Ingham, P. W. & Tabin, C. J. *Curr. Top. Dev. Biol.* **53**, 1-114 (2003)

^{iv} Surajit, S.; Shestopalov, I. A.; Chen, J. K. *Nature Chemical Biology* **3**, 650-651 (2007)

^v Surajit, S.; Chen, J. K. *Nature Chemical Biology* **2**, 29-30 (2006)

POSTER SESSION

Catalysis of Oxidation Reaction by Laccase : A Comparison of *in Silico* and *in Vitro* Approaches

A.Thamarichelvan^a, K. Sathish kumar^b and S. Padmavathy^b

^a Department of Chemistry, Thiagarajar College, Madurai

^b Department of Microbiology, Thiagarajar College, Madurai;
thamaraiselvan2003@gmail.com

Oxidative degradation and removal of environmental pollutants can be carried out by bioremediation. Screening of various xenobiotics for catalytic oxidation by laccase has already been reported. However, *in silico* approaches for predicting the activities of laccase are limited. The present work concerns with evaluating the *in silico* activities of laccase against xenobiotics such as 2,2'-azino-bis(3-ethylbenz-thiazoline-6-sulphonic acid) (ABTS), catechol, pyrogallol, guaiacol, syringaldazine and catechin using docking tools. The results are compared with *in vitro* results obtained by earlier workers.

FRED of OpenEye was employed for docking studies. The scoring function chosen was Chem gauss 3. The results reveal that the catalytic activities of laccase for the oxidation of the compounds are in the order, ABTS ~ catechin > syringaldazine > catechol > guaiacol > pyrogallol as deduced from the scoring functions. The results are in accordance with the *in vitro* results obtained by J.J. Roy et al.(2005). The observations indicate that ABTS and catechin are the best pollutants which could be effectively biodegraded by microorganisms especially fungi that produce laccase. Similar oxidative biodegradation by fungal laccase has already been reported for poly aromatic hydrocarbons in our lab.

Differential Thermal and pH Induced Stability of the Hemoglobin Variants, HbA, HbA₂ and HbE and Oxidative Vulnerability of HbE *in Vitro*.

Dipankar Bhattacharya, and Abhijit Chakrabarti

Structural Genomics Section & Biophysics Division, Saha Institute of Nuclear Physics,
1/AF, Bidhannagar, Kolkata-700064; dipankar.bhattacharya@saha.ac.in

More than 1000 hemoglobin variants are found till date, of which only a handful are associated with hemoglobin disorders. HbA₂, and HbE are two such variants having aberrant expression in the β - and E β -thalassemia. From the structure of these variants, it was observed that these two variants differ significantly in the surface charge density and stability¹. Using the Soret absorption and tryptophan fluorescence measurements we observed that HbA₂, HbE and HbA, all of them follow a two-step pH induced unfolding transition. Using UV-visible absorption and normal and synchronous fluorescence measurements we came to conclude that the three hemoglobin variants have differential thermal stability which falls in the order of HbE < HbA < HbA₂. The thermal aggregation studies using both 90°- and dynamic light scattering techniques also indicated the onset of aggregation at a lower temperature in HbE and HbA₂ was found to be the most thermally stable. HbE also exhibits its vulnerability for self-aggregation in presence of H₂O₂, which could throw light on its role under oxidative stress conditions in hemoglobinopathy².

References

1. [Sen](#) et al., (2004) Crystal structures of HbA₂ and HbE and modeling of hemoglobin delta 4: interpretation of the thermal stability and the antisickling effect of HbA₂ and identification of the ferrocyanide binding site in Hb. *Biochemistry* 43: 12477-88.
2. [Datta](#) et al., (2006) Enhanced oxidative cross-linking of hemoglobin E with spectrin and loss of erythrocyte membrane asymmetry in hemoglobin Ebeta-thalassemia. *Blood Cells Mol Dis.* 37: 77-81

Direct Observation of Essential DNA Dynamics: Melting and Reformation of the DNA Minor Groove

Debapriya Banerjee and Samir K. Pal

Department of Chemical, Biological and Macromolecular Sciences,
S. N. Bose National Centre for Basic Sciences ,Block JD, Sector III
Salt Lake City , Kolkata , PIN 700 098; debapriya@bose.res.in

The dynamics of bound water and ions present in the minor groove of a dodecamer DNA has been decoupled from that of the long-range twisting/bending of the DNA backbone, using the minor groove binder Hoechst 33258 as a fluorescence reporter in the picosecond-resolved time window. The bound water and ions are essential structural components of the minor groove and are destroyed with the destruction of the minor groove when the dodecamer melts at high temperatures and reforms on subsequent cooling of the melted DNA. The melting and rehybridization of the DNA has been monitored by the changes in secondary structure using circular dichroism (CD) spectroscopy. The change in the relaxation dynamics of the DNA has been studied with picosecond resolution at different temperatures, following the temperature-dependent melting and rehybridization profile of the dodecamer, using time-resolved emission spectra (TRES). At room temperature, the relaxation dynamics of DNA is governed by a 40 ps (30%) and a 12.3 ns (70%) component. The dynamics of bound water and ions present in the minor groove is characterized by the 40 ps component in the relaxation dynamics of the probe bound in the minor groove of the dodecamer DNA. Analyses of the TRES taken at different temperatures show that the contribution of this component decreases and ultimately vanishes with the destruction of the minor groove and reappears again with the reformation of the groove. The dynamical behavior of bound water molecules and ions of a genomic DNA (from salmon testes) at different temperatures is also found to be consistent with that of the dodecamer. The longer component of the order of 10 ns in the DNA dynamics is found to be associated with the long-range bending/twisting of the DNA backbone and the associated counterions. The transition from bound water to free water at the DNA surface, indicative of the change in the hydration number associated with each base pair, has also been ascertained in the case of the genomic DNA at different temperatures by employing densimetric and acoustic techniques.

An *in vitro* Study on the Binding of Plasmid pUC19 DNA with the Isolated *E.coli* Lipopolysaccharide Molecules in the Presence of Divalent Cation Ca^{2+}

Subrata Panja and Tarakdas Basu

Department of Biochemistry and Biophysics, University of Kalyani, Kalyani – 741 235,
West Bengal; tarakdb@yahoo.com

With the increasing addition of *E. coli* LPS to the plasmid pUC19 DNA, both dissolved in CaCl_2 , the absorption maxima of DNA at 260nm decreased gradually with the appearance of isosbastic points at both ends of the spectra. Hill plot of the absorbance data showed that the binding interaction was positive cooperative in nature with the binding constant $K_b = 2.95 \times 10^4 \text{ M}^{-1}$. This value of K_b was close to that ($2.76 \times 10^4 \text{ M}^{-1}$) obtained from the isothermal titration calorimetric study. For any fixed concentration of DNA and LPS, the extent of interaction increased as the concentration of CaCl_2 was raised from (0 \rightarrow 1)mM, signifying the electrostatic nature of the interaction, mediated through Ca^{2+} ion. The stepwise addition of EDTA, the chelating agent for divalent cations, to the DNA-LPS bound complex gradually reversed the spectral shift with the increase in absorbance at 260nm, which implied the opening up of the complex or in other words, the reversibility of the interaction. The isothermal titration calorimetric study further showed that the binding was exothermic and enthalpy-driven. The circular dichroism spectral changes of DNA by the addition of LPS indicated partial transition of DNA from B to A-form. The size of the DNA-LPS complex, as measured by the dynamic light scattering instrument, was estimated to be about 5480nm. The formation of DNA-LPS complex was also evident from the retarded mobility of the complex, compared to the mobility of the DNA itself, in agarose gel. The DNA-LPS complex could be visualized using electron and atomic force microscopes. The finer study with the hydrolyzed products of LPS showed that only the core oligosaccharide domain of the LPS was responsible for the interaction with DNA. The biological significance of this *in vitro* interaction was revealed when the LPS-leached *E.coli* cells were found to be transformed more by the DNA-LPS complex than by the DNA only.

Molecular Association of Transcription Activator Proteins, RFXANK and DNA Binding Domain of RFX5

Madhumita Chakraborty and Abhijit Chakrabarti

Biophysics Division and Structural Genomics Section, Saha Institute of Nuclear Physics,
1/AF Bidhannagar, Kolkata-700064; Madhumita.chakrabarti@saha.ac.in

Major Histocompatibility Complex MHC II molecules are essential component of the mammalian adaptive immune response. They present antigenic peptides to CD4+ T cell receptors and help in the process of T cell activation, differentiation and proliferation. There is a direct correlation between the level of expression of MHC II molecules and the ability of the immune system to respond against infection. The expression of MHC II molecules is highly regulated by a number of transcription factors including regulatory factor X (RFX), class II transcriptional activator (CIITA), nuclear factor Y (NFY) and cyclic AMP response element binding protein (CREB). The heterotrimeric RFX complex is the primary DNA binding component of the enhanceosome. It has three subunits RFXANK, RFX5 and RFXAP. A network of protein protein interaction exists in the entire enhanceosome. In this work, recombinant RFXANK and the DNA binding domain (DBD) of RFX5 were expressed in bacterial cells, isolated, purified and characterised by biophysical and biochemical methods. For the first time we have shown the *in vitro* association between RFXANK and the specific DNA binding domain of RFX5 by fluorescence resonance energy transfer (FRET) measurements. We have shown that Rhodamine-labeled RFXANK (R-RFXANK) and Fluorescein labeled RFX5DBD (F-RFX5DBD) interact in 1:1 molar ratio leading to quenching of donor (F-RFX5DBD) fluorescence. The DNA-bound F-RFX5DBD did not alter the efficiency of energy transfer implying that DNA binding is not essential for the association of the two proteins. Such molecular association between the two proteins was estimated by measuring the change in the ratio of the intensities of the first and the third vibronic peaks of Pyrene labeled RFX5DBD (Py-RFX5DBD) in presence of the increasing concentrations of RFXANK. The binding dissociation constant between Py-RFX5DBD and RFXANK was estimated to be ~100 nM at 4°C.

Conformation Microstates of a CH- π Interaction Stabilized cis Pro-Pro Peptide by Molecular Dynamics Simulation

Sarbani Chattopadhyay and Gautam Basu

Department of Biophysics, Bose Institute, P-1/12 CIT Scheme VII M, Kolkata 700 054, India.; sarbani_c84@rediffmail.com

Cis peptide bonds are rarely observed in natively folded proteins and their populations, relative to the trans state, are insignificant in short peptides. However, under certain local sequence compulsions, namely the presence of Xaa-Pro units, the relative importance of the cis conformation of a peptide bond becomes significant. This is especially pronounced when Xaa is an aromatic residue. NMR studies have shown that the extra stability of the cis bond when Xaa is aromatic in Xaa-Pro units arises due to the presence of CH- π interaction in the cis state. A recent study from our laboratory (1) identified yet another local sequence motif that stabilizes cis peptide bonds — the cis Pro-Pro peptide bond in Pro-Pro-Phe sequence motif. The presence of CH- π interaction between the C $^{\alpha}$ -H atom of Pro(i) and the aromatic ring of Phe(i+2) was identified in the cis state of Pro-Pro-Phe by NMR. In addition, detailed thermodynamic analysis of cis-trans energetics was also determined. However, due to the inherent limitations of NMR time scales, the detailed structural characterization the cis state, especially in light of the CH- π interaction was not possible except for average inter-proton distances, chemical shifts and 3J coupling constants that yielded average values for select set of dihedral angles. In this study we report our results on the analysis of ten 100 ns long molecular dynamics simulations for cis Ac-Pro-Pro-Phe-NH $_2$ in water, performed to probe conformational microstates of the cis peptide conformer that could not be probed by NMR study. Each of the ten starting conformations was taken from natively folded proteins that exhibit the Pro-Pro-Phe sequence in the cis state (1SNR, 1JZ8, 1AOC, 1TCA, 1VKY, 1GSA, 1U7P, 1V5V, 1XMB, 1NR0). Analysis of our results not only complement the already published NMR characterization of the cis-state of Ac-Pro-Pro-Phe-NH $_2$, it also sheds light on conformational microstates that the sequence -Pro-Pro-Phe- can access as proteins containing this motif folds.

References

1. Dasgupta B, Chakrabarti P, Basu G. (2007) Enhanced stability of cis Pro-Pro peptide bond in Pro-Pro-Phe sequence motif. FEBS Lett. 581, 4529-32.

Possibility of Making Biphasic Liquid Membranes as a Sensing Device for Artificial Olfaction

A. K. Das

Department of Chemistry, Sikkim Manipal Institute of Technology, Majitar, Rangpo, Sikkim (East), Pin 737132; amlan_snigdha@rediffmail.com

The olfactory system represents one of the oldest sensory modalities in the phylogenetic history of mammals. Olfaction is less developed in humans than in other mammals such as rodents. As a chemical sensor, the olfactory system detects food and influences social and sexual behavior. Olfaction is the most complex of the human senses, relying exclusively on the detection and processing of the chemical information. Despite its proven significance and considerable research in the field, sensing mechanism of olfaction which is one of the most crucial problems in biological science, in spite of the intense attention it has received, is still not as well recognized as the senses of vision and audition.

A novel odour sensing system, which possibly can imitate the process of reception of odorants in biological olfactory system had been developed. Electrical potential oscillations across a biphasic liquid membrane, induced by olfactory agents have been reported. The initial observation indicates that the bipolar liquid membrane system can be established as a good candidate for being an artificial olfaction sensing device.

Mechanism of Ubiquitin Unfolding: Thermal vs Chemical

Atanu Das and Chaitali Mukhopadhyay

Department of Chemistry, University of Calcutta, 92, A.P.C. Road, Kolkata – 700 009;
samrucu@gmail.com

Study of protein folding pathway is a challenging problem to the scientists for many years. Generally three types of perturbations are used to denature a protein molecule – thermal, chemical and mechanical. Behavior of a protein under these perturbing environments is found to be different and the comparison of mechanisms of protein unfolding can reveal important structural information. We have studied unfolding of Ubiquitin – (1) in water at 373K and (2) in 8M aqueous urea solution at 325K; using explicit water model and CHARMM force field. In these two methods, Ubiquitin behaves differently with complete unfolded structure in thermal unfolding simulation and partially unfolded state in chemical unfolding simulation.

Inter-subunit Orientations in Protein-Protein Complexes are Electrostatically Biased

Madhurima Das^{*} and Gautam Basu[‡]

^{*} Bioinformatics Center and [‡] Department of Biophysics, Bose Institute, P-1/12 CIT Scheme VII M, Kolkata 700 054; madhurima.das@gmail.com

Protein-protein interactions are crucial for biological function and in recent years the topic has attracted a lot of attention from both experimental and theoretical perspective. To form the final complex at a reasonably fast rate (k_{on}), the encounter between two protein molecules must have some orientational bias towards the final structure. As a rigid body, the most obvious global property of the protein that may contribute to this bias is the dipole and higher electric moments of a protein. We have analyzed a representative dataset of protein hetero-complexes and proteins with domain-domain interactions, to decipher any underlying electrostatic bias that may be a universal signature of these complexes. Electrostatic calculations were performed both in vacuum and using continuum dielectric models. Our results show that the Coulomb component (vacuum contribution) of the total binding energy is negative for the majority (~83%) of complexes. However when the reaction field component (solvent contribution) is added, the net electrostatic component of the binding energies become positive. This trend is maintained at physiological salt concentrations. The magnitude of this positive energy increases linearly with increasing total buried interface surface area in the complexes. Thus, increasing the interface surface area makes protein association electrostatically more unfavorable, implying that the corresponding non-electrostatic components must scale inversely to finally produce negative free energies. The electrostatic energy between two proteins, modeled here as point charge distributions, can be resolved into interactions between electric mono and multi-poles. Of these, except for the monopole-monopole term, all other terms vary as a function of inter-subunit orientations. Surprisingly, when the monopole-monopole energy term was removed from the total Coulomb energy, 95%

of complexes exhibited negative energy. This indicates that the experimental inter-subunit orientations of protein-protein complexes are biased by electrostatics to avoid unfavorable orientations. This was further probed by analyzing orientations of dipoles and quadrupoles of one subunit in the electric field arising from the other. The angle θ between the dipole moment of one subunit and the vector describing the dipolar potential distribution, at that subunit, arising from the other subunit, were analyzed. Electrostatic energy of placing the dipole in the dipolar potential distribution varies with θ ($E > 0$ for $\theta < 90^\circ$; $E = 0$ for $\theta = 90^\circ$; $E < 0$ for $\theta > 90^\circ$). Both in vacuum and in solvent, distribution of θ clearly indicated that unfavorable ($E > 0$) orientations are avoided in protein-protein complexes. Our results clearly point towards two roles that electrostatics plays in protein-protein complexes: 1) The total electrostatic energy of association is positive which compensates large negative non-electrostatic energies of association, finally yielding small overall negative binding free energies (the overall binding free energies need to be small (1-5 kcal/mol) for the protein-protein complexes to be biologically relevant). 2) Although the total electrostatic energy of association is positive, our result on electrostatic bias of inter-subunit orientation clearly suggest that when proteins associate, the ensemble of orientations that finally lead to the productive complex excludes unfavorable orientations. This explains how electrostatics also makes protein association rates faster than expected from random encounters.

Bimolecular photoinduced electron transfer kinetics in a biomimetic environment

S. Dutta Choudhury, M. Kumbhakar, S. Nath and H. Pal

Radiation & Photochemistry Division, Bhabha Atomic Research Centre, Mumbai 400 085, India;
sharmisthadc@gmail.com

Photoinduced electron transfer (ET) reactions are one of the most fundamental reactions in Chemistry and Biology. The study of such reactions in different types of organized assemblies has attracted much attention because these assemblies have spatially arranged pockets for molecular compartmentalization that can modulate the dynamics and mechanism of ET reactions favorably for various applications. Moreover, organized assemblies also serve as model membrane mimetic systems and so understanding ET in these simple systems can help us in understanding many fundamental aspects of biological ET reactions. Small unilamellar vesicles (SUVs) are especially useful in this respect. We have investigated the photoinduced ET from N,N-dimethylaniline to some coumarin derivatives in SUVs of DL- α -dimyristoyl-phosphatidylcholine, using steady-state and time-resolved fluorescence quenching, both below and above the phase transition temperature of the vesicles. The influence of the topology of SUVs on the photophysical properties of the reactants and consequently on their ET kinetics has also been investigated. Absorption and fluorescence spectral data of the coumarins in SUVs and the variation of their fluorescence decays with temperature indicate that the dyes are localized in the bilayer of the SUVs. Time-resolved anisotropy decays are bi-exponential for all the dyes in SUVs and this has been interpreted in terms of the compound motion model according to which the dye molecules can experience a fast wobbling-in-cone type of motion as well as a slow overall rotating motion of the cone containing the molecule. The expected bimolecular diffusion-controlled rates in SUVs, as estimated by comparing the microviscosities in SUVs (determined from rotational correlation times) and that in acetonitrile solution, are much slower than the observed fluorescence quenching rates, suggesting that reactant diffusion does not play any role in the quenching kinetics in the present systems. Accordingly, clear inversions are observed in the correlation of the fluorescence quenching rate constants, k_q , with the free energy change, ΔG° of the reactions, as predicted by the Marcus ET theory. However, some coumarin dyes show unusually high k_q values and high activation barriers, which are not expected from Marcus theory. This unusual behavior is explained on the basis of participation of the twisted intramolecular charge transfer (TICT) states of these dyes. This modulation of ET kinetics by an intermolecular process of the excited dyes is a unique result in SUVs medium.

Tryptophan Fluorescence in a Designed Peptide with CH- π Interaction

Himal Ganguly¹, Saumya Dasgupta¹, Debapriya Banerjee², Samir K. Pal²,
Gautam Basu¹

¹Department of Biophysics, Bose Institute, P-1/12 CIT Scheme VII M, Kolkata 700 054;

²Department of Chemical, Biological & Macromolecular Sciences, and Unit for Nanoscience & Technology, S. N. Bose National Centre for Basic Sciences, JD Block, Sector III, Salt Lake, Kolkata 700 098; himalganguly@yahoo.com

Tryptophan fluorescence can provide important clues about the nature of Trp environment in proteins. This in turn is used to unravel salient features of folding-unfolding transitions in proteins. However, despite being an important tool, Trp fluorescence is not completely understood, especially the origin of the multiexponential decay of the excited state, and the position of the steady state fluorescence emission maxima. One way to further our understanding of Trp fluorescence is to design short peptides with pre-defined geometries, both backbone and Trp side-chain. Once the structures of these peptides are known, from NMR and / or molecular dynamics simulations, fluorescence data can be correlated with experimental structural features. We have synthesized Trp containing peptides where the Trp side-chain was locked into preferred conformations, due to the presence of designed CH- π interaction with a Pro residue. In addition, the peptides were designed to undergo slow backbone conformational transitions, between cis and trans isomers. Extensive fluorescence experiments, both steady state and time-resolved, were performed on the peptides. The peptides were also characterized by NMR. Analysis of our results will be presented with a focus on: 1) the utility of Trp fluorescence in monitoring cis/trans kinetics where one of the two isomers is associated with a CH- π interaction, 2) correlation of Trp excited states with the known rotamer populations of Trp and with the population of peptides exhibiting CH- π interaction.

Vibrational Analysis of Purine Nucleotides and Nucleobases in Water at pH 2 - 13: ab initio Calculation and UV-Resonance Raman Spectra

Spriha Gogia, Ankur Jain and Mrinalini Puranik*

National Centre for Biological Sciences, Tata Institute for Fundamental Research, UAS-GKVK Campus, Bellary Road, Bangalore; spriha@ncbs.res.in

The DNA synthesis and repair pathways often involve enzymatic intermediates with nucleotides in varying protonation states. The tautomeric structures and ionization states of nucleobases and nucleotides, in complex with enzymes, have been controversial in literature for long. Many techniques have been applied in the past to resolve this but they have met with limited success. In this work, we have obtained reliable spectra of the bases and mononucleotides of 6-oxo-purines in solution at varied pH. We present the UV resonance Raman spectra of various protonation states of nucleotides guanosine 5'-monophosphate (GMP) and inosine 5'-monophosphate (IMP) and the nucleobase Hypoxanthine (Hx). Detailed analysis of the vibrational spectra has been carried out using ab initio quantum mechanical calculations (hybrid DFT-B3LYP/6-31G** and HF/6-31G**). The dominant tautomeric form and protonation states at various pH values in solution has been identified. Comprehensive assignments of the observed bands for the neutral, protonated and deprotonated species have been made and verified by deuterium labeling of labile hydrogen atoms. From these experiments, we predict the normal modes that can be used as markers of protein-DNA interaction.

Dual Fluorescence in (E)-3-(4-Dimethylamino-Naphthalene-1-yl) Acrylic Acid and Its' Novel Application as a Fluorosensor for Some Metal Ions

Shalini Ghosh and Nikhil Guchhait

Department of Chemistry, University of Calcutta, 92, A.P.C. Road, Kolkata-700009;
shalini_chem.2006@yahoo.co.in

From the first observation of dual fluorescence in Dimethylaminobenzonitrile (DMABN) by Lippert et al., molecules with such donor-acceptor moieties and the related photophysics and photochemistry have been studied for many years. Various models have been developed to explain these unusual photophysical properties. In this study, the dual fluorescence from (E)-3-(4-Dimethylamino-naphthalene-1-yl) acrylic acid has been studied in solvents of different polarities and these photophysical properties have been explored using both absorption and emission spectroscopy. An attempt to use this dual fluorescence for fluoro-sensing of metal ions has also been made. In addition, quantum mechanical calculations have been done to explain the excited state processes. Steady state absorption and emission spectra were measured with a Hitachi (UV/Vis) and Perkin–Elmer spectrophotometers respectively. The absorption spectra of our compound in various non-polar and polar solvents show a maxima at ~360 nm. Excitation at 350 nm. leads to a small band.(assigned as Locally Excited or LE band)and a larger, red-shifted band(assigned as Charge Transfer or CT band).The CT band is red-shifted with increasing solvent polarity. According to the TICT (Twisted Intramolecular Charge Transfer) model, this photo-induced Charge Transfer(CT) takes place when the lone pair electron orbital of the N atom of the dimethylamino group is orthogonal to the p-orbitals of the naphthyl ring. The polar nature of this CT state leads to different extents of stabilisation of this species in solvents of different polarities and hence we get the polarity dependant Stokes' shifted emission. Addition of some metal ions such as Ni^{+2} , Fe^{+2} , Cu^{+2} , Hg^+ and Pb^{+2} to solutions of this molecule in acetonitrile show progressive quenching of the CT band and progressive growth of the blue shifted band, making way for it's use as a good fluorosensor for some metal-ions.

References

- 1.E.Lippert, W.Ludder, H.Boos, Advances in Molecular Spectroscopy, ed.A Mangini,Pergamon Press,Oxford,1962p.443
- 2.Z. Grabowski, K. Rotkiewicz, W. Rettig, Chem. Rev. 103 (2003) 3899
- 3.A. Chakraborty, S. Kar, N. Guchhait, Chem. Phys. 320(2006) 75-83
4. A. Chakraborty, S. Kar, N. Guchhait, Chem. Phys. 324(2006) 733-741
5. A. Chakraborty, S. Kar, D.N. Nath,N. Guchhait, J. Phys. Chem,(Article in Press.)

1-(2'-Pyridylazo)-2-naphtholate Complexes of Ruthenium: Synthesis, Characterization, and DNA Binding Properties

Sarmistha Halder, Indrani Pal, Semanti Basu, Saheli Samanta,
Parimal Karmakar and Samaresh Bhattacharya*

Department of Chemistry, Jadavpur University, Kolkata 700 032;
sarmistha77@yahoo.co.in

Reaction of 1-(2'-pyridylazo)-2-naphthol (Hpan) with $[\text{Ru}(\text{dmsO})_4\text{Cl}_2]$ (dmsO = dimethylsulfoxide), $[\text{Ru}(\text{trpy})\text{Cl}_3]$ (trpy = 2,2',2''-terpyridine), $[\text{Ru}(\text{bpy})\text{Cl}_3]$ (bpy = 2,2'-bipyridine) and $[\text{Ru}(\text{PPh}_3)_3\text{Cl}_2]$ afforded different ruthenium complexes of type $[\text{Ru}(\text{pan})_2]$, $[\text{Ru}(\text{trpy})(\text{pan})]^+$ (isolated as perchlorate salt), $[\text{Ru}(\text{bpy})(\text{pan})\text{Cl}]$ and $[\text{Ru}(\text{PPh}_3)_2(\text{pan})\text{Cl}]$. In each of these complexes, the pan ligand is coordinated to the metal center as a monoanionic tridentate N,N,O-donor. Reaction of the $[\text{Ru}(\text{bpy})(\text{pan})\text{Cl}]$ complex with pyridine (py) and 4-picoline (pic) in the presence of silver ion has yielded the $[\text{Ru}(\text{bpy})(\text{pan})(\text{py})]^+$ and $[\text{Ru}(\text{bpy})(\text{pan})(\text{pic})]^+$ complexes (isolated as perchlorate salts) respectively. Chemistry of all the complexes is described in this poster with special reference to structure and, spectral and electrochemical properties. The $[\text{Ru}(\text{trpy})(\text{pan})]\text{ClO}_4$, $[\text{Ru}(\text{bpy})(\text{pan})(\text{py})]\text{ClO}_4$ and $[\text{Ru}(\text{bpy})(\text{pan})(\text{pic})]\text{ClO}_4$ complexes have been observed to interact with DNA, but they have not been able to cleave supercoiled DNA on UV irradiation.

Structure of 8-Oxoguanosine: A Resonance Raman Study

Namrata Jayanth, Srinivas Ramachandran and Mrinalini Puranik*

National Centre for Biological Sciences, TIFR, GKVK Campus, Bellary Road,
Bangalore-560065; namrata@ncbs.res.in

Oxidation of DNA brought about by reactive oxygen species, leads to covalent modification of the bases. These modified bases, known as lesions, are mutagenic in nature and can be lethal to cells. Guanine, due to its low ionization potential is most susceptible to oxidation. A major product of guanine oxidation is 8-oxoguanine. The deleterious effects of lesions such as 8-oxoguanine are combated by the highly efficient glycosylase family of enzymes.

The structure of 8-oxoguanine in solution has been contentious in the past due to the possibility of several keto-enol tautomers. Knowing the solution state structure of the substrate is of prime importance in elucidation of the mechanism of action of these repair enzymes.

In the present work, we show that ultraviolet resonance Raman spectroscopy can be used as a base specific probe to (1) to distinguish between guanine and 8-oxoguanine, and (2) that the predominant tautomer of 8-oxoguanine in solution is the diketo form. Raman spectra obtained with laser excitation at 260 nm of guanine and 8-oxoguanine show remarkably different relative intensities indicative of the difference in the structures of the electronic excited states responsible for the absorption at 260 nm in the two molecules. Experimentally observed spectra are supported by density functional theoretical calculations and normal mode analysis. We further extend these observations to the anionic forms of 8-oxoguanine.

Molecular Level Investigation of Cluster Formation in Ternary Lipid Bilayer: A Computational Approach

Sumita Mondal and Chaitali Mukhopadhyay*

Department of Chemistry, University of Calcutta, 92, A. P. C. Road, Kolkata – 700 009;

smchem_cu@yahoo.co.in

We report here, the clustering of Cholesterol in presence of GM1 and tried to find out the mechanism of clustering from molecular level study during 35 ns simulation run of a ternary lipid system containing POPC, GM1 and Cholesterol and compared it with a binary POPC-Cholesterol and pure POPC bilayer simulations. GM1 present in upper layer and gives two different lipid layers one is ternary and other is binary, which gives comparison of cluster formation between ternary and binary lipid system. The difference in cluster formation in ternary and binary lipid mixture is shown directly from the snapshots at different time point for the upper and lower layer separately. The atom density distribution shows how different lipid component are distributed in unsymmetrical bilayer. The calculation of no. of contact, radial distribution function, rotational reorientation and residence time of sterol can explain the cluster formation. Whereas lateral translational motion, rotational diffusion, order parameter of phospholipids explains the amount of rigidity imparted on the POPC bilayer.

Enhanced Fluorescence of Epicocconone in Surfactant Assemblies and in Protein

Debashis Panda, Soumyakanti Khatua, Anindya Datta

Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai-76
debu82@iitb.ac.in

The extent of fluorescence enhancement of epicocconone which is a cell permeable natural product isolated from the fungus *Epicoccum nigrum*^v, in various micelles is observed to be significantly different.^v The apparently bimodal fluorescence decay of epicocconone in neat solutions is associated with an ultrafast decay, which is missed in the time resolution of our experiments. The ultrafast decay is likely to be due to photoisomerization, as a significant viscosity dependence of the fluorescence quantum yield is observed. The enhancement of the fluorescence intensity in micelles is ascribed to a decrease in the extent of this photoprocess due to a higher depth-dependent microviscosity. The difference in the extent of fluorescence enhancement in TX 100 and SDS is rationalized as an effect of a greater penetration of the fluorescent probe in case of the first micelle, which in turn is due to the difference in the thickness of the hydrophilic palisade/Stern layers of the two micelles.

The N-terminus of protein interacts with epicocconone and forms a stable covalent complex. This is quite evident from the interaction of epicocconone with *n*-butylamine. The enhancement of quantum yield and fluorescence lifetime of epicocconone on addition of SDS to HSA indicates the facilitation of the mode of interaction of fluorophore with protein. It indicates the strong binding of the fluorophore to the human serum albumin and support the contention of a covalent binding.^v

Non Canonical Base Pairs having C-H...O or Sugar Mediated Interactions: DFT Studies

Ashim Roy, Malyasri Bhattacharyya, Swati Panigrahi and Dhananjay Bhattacharyya

Biophysics Division and *Center for Applied Mathematics and Computational Science;
Saha Institute of Nuclear Physics; 1/AF Bidhannagar; Kolkata 700064;
swati.panigrahi@saha.ac.in

Importance of non Watson-Crick base pairs in three-dimensional structure of RNA is now well established. Structure and stability of these non-canonical base pairs are, however, poorly understood. We have attempted to understand structural features of 33 frequently occurring base pairs using density functional theory. These are of three types, namely (i) those stabilized by two or more polar hydrogen bonds between the bases, (ii) those having one polar and another C-H...O/N type interactions and (iii) those having one hydrogen bond between the bases and another involving one of the sugars linked to the bases. We found that the base pairs having two polar H-bonds are very stable as compared to those having one C-H...O/N interaction. Our quantitative analysis of structures of these optimized base pairs indicates that they possess different amount of non-planarity with large propeller or buckle values, as also seen in the crystal structures. We further found that geometry optimization, does not modify the hydrogen-bonding pattern, as values of shear and open angle of the base pairs remain conserved. The structures of initial crystal geometry and final optimized geometry of some base pairs having only one polar H-bond and a C-H...O/N interaction, however, are significantly different, indicating weak nature of the non-polar interaction. The base pair flexibility, as measured from normal mode analysis, in terms of the intrinsic standard deviations of the base pair structural parameters are in conformity with those calculated from RNA crystal structures. We also noticed deformation of a base pair along stretch direction is impossible for all the base pairs and movements of the base pairs along shear and open are also quite restricted. The base pair opening mode through alteration of propeller or buckle are considerably less restricted for most of the base pairs.

Role of Base Pairs in Molecular Recognition in a Protein-DNA Complex

Sudipta Samanta¹, Dhananjay Bhattacharyya and J. Chakrabarti¹
¹S. N. Bose National Centre for Basic Sciences, JD Block, Sector III, Salt Lake, Kolkata 700098; ²Biophysics Division and C.A.M.S., Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata 700064.

We develop a semi-coarse grained approach to estimate the contribution of different base pair (bp) steps in the thermodynamics of a protein-DNA complex using the crystal structure data. We carry out the calculations in particular for the TATA-box binding protein(TBP)-TATA box DNA sequence complex where molecular recognition is exhibited by deforming the DNA structure. We consider an ensemble of configurations from crystallographic data of the TBP-TATA box complex in a given thermodynamic condition and calculate the free energy profiles in terms of the DNA bp step parameters via the binding patterns in the ensemble of the given complex. Similar calculations have been performed for free DNA bp steps as well. The change in the thermodynamic properties upon the complex formation has been estimated from the two sets of free energy profiles. We find the changes in free energy and entropy for each of the bp steps and also the free energy gain of the protein due to binding at each bp step. These results indicate differential role played by different bp steps in the thermodynamic stabilization of the complex.

Participants in the Workshop on Structure and Dynamics of Biomolecules 2007

Name	Affiliation	Participation
Kankan Bhattacharyya	IACS, Kolkata	<i>Invited Speaker</i>
Sanjoy Bandyopadhyay	IIT, Kharagpur	<i>Invited Speaker</i>
Amitabha Chattopadhyay	CCMB, Hyderabad	<i>Invited Speaker</i>
Abhijit Chakrabarti	SINP, Kolkata	<i>Invited Speaker</i>
B. Jayaram	IIT, Delhi	<i>Invited Speaker</i>
Chaitali Mukhopadhyay	Univ. of Calcutta, Kolkata	<i>Invited Speaker</i>
Prabal Maiti	IISc., Bangalore	<i>Invited Speaker</i>
Samir K. Pal	SNBNCBS, Kolkata	<i>Invited Speaker</i>
Yashwant Singh	BHU, Varanasi	<i>Invited Speaker</i>
Srabani Taraphder	IIT, Kharagpur	<i>Invited Speaker</i>
Raghavan Varadarajan	IISc., Bangalore	<i>Invited Speaker</i>
Indrani Bose	Bose Institute, Kolkata	<i>Evening Speaker</i>
Gautam Basu	Bose Institute, Kolkata	<i>Seminar Speaker</i>
Dhananjay Bhattacharyya	SINP, Kolkata	<i>Seminar Speaker</i>
Jaydeb Chakrabarti	SNBNCBS	<i>Seminar Speaker</i>
Krishnananda Chattopadhyay	IICB, Kolkata	<i>Seminar Speaker</i>
Sanjay Kumar	BHU, Varanasi	<i>Seminar Speaker</i>
Surajit Sinha	IACS, Kolkata	<i>Seminar Speaker</i>
A. Thamarichelvan	Thiagarajar College, Madurai, TN	<i>Poster</i>
Dipankar Bhattacharya	SINP	<i>Poster</i>
Debapriya Banerjee	SNBNCBS	<i>Poster</i>
Tarakdas Basu	Kalyani University, Kalyani	<i>Poster</i>
Madhumita Chakrabarti	SINP	<i>Poster</i>
Sarbani Chattopadhyay	Bose Institute	<i>Poster</i>
Amlan K. Das	Sikkim Manipal Institute, Sikkim	<i>Poster</i>
Atanu Das	Univ. of Calcutta, Kolkata	<i>Poster</i>
Madhurima Das	Bose Institute	<i>Poster</i>
Sharmistha Dutta Choudhury	BARC, Mumbai	<i>Poster</i>
Himal Ganguly	Bose Institute	<i>Poster</i>
Spriha Gogia	NCBS, Bangalore	<i>Poster</i>
Shalini Ghosh	Univ. of Calcutta, Kolkata	<i>Poster</i>
Sarmistha Halder	Jadavpur University	<i>Poster</i>
Indrani Pal	Jadavpur University	<i>Poster</i>
Namrata Jayanth	NCBS, Bangalore	<i>Poster</i>
Sumita Mondal	Univ. of Calcutta, Kolkata	<i>Poster</i>
Debashis Panda	IIT, Mumbai	<i>Poster</i>
Swati Panigrahi	SINP, Kolkata	<i>Poster</i>
Sudipta Samanta	SNBNCBS	<i>Poster</i>

Name	Affiliation	Participation
Ajay Shaw	SNBNCBS	Participant
Harun Gazi	SNBNCBS	Participant
Hemant Kashyap	SNBNCBS	Participant
Ranendra Ghosh	IICB	Participant
Sachin Srivastava	SNBNCBS	Participant
Sanchita Mukherjee	SINP	Participant
Shankaraarayanan	SNBNCBS	Participant
Snigdha Chandra	Durgapur Govt. College	Participant
Subrata Panja	Kalyani University	Participant
Sukanya Halder	SINP	Participant
Sunny Sharma	IICB	Participant
Susmita Kar	SNBNCBS	Participant
Swati Nandi		Participant
Tuhin Pradhan	SNBNCBS	Participant
Samaresh Mitra	IICB	Session Chair
Gautam Basu	Bose Inst.	Session Chair
Dhananjay Bhattacharyya	SINP	Session Chair
Bidyendu M. Deb	IISER	Session Chair
Alok K. Majumder	SNBNCBS	Session Chair
Bimalendu B. Bhattacharyya	SNBNCBS	Session Chair
Abhijit Mookerjee	SNBNCBS	Session Chair
Surajit Sengupta	SNBNCBS	Session Chair
Arup K. Raychaudhuri	SNBNCBS	Invited Participant
Asoke P. Chattopadhyay	Kalyani Univ.	Invited Participant
Arindam Banerjee	IICB	Invited Participant
Sushanta Dattagupta	IISER	Invited Participant
Debashis Mukherjee	IACS	Invited Participant
Siddhartha Roy	IICB	Invited Participant
Priya Mahadevan	SNBNCBS	Invited Participant
Tanusri Saha-Dasgupta	SNBNCBS	Invited Participant
Subhrangshu S. Manna	SNBNCBS	Invited Participant
Anita Mehta	SNBNCBS	Invited Participant
Kalyan Mandal	SNBNCBS	Invited Participant
Pratip K. Mukhopadhyay	SNBNCBS	Invited Participant
Subhashis Sinha	SNBNCBS	Invited Participant