# Complete BioData

### **PERSONAL DETAILS**

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DOB: 25/10/1973

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### **PROFESSIONAL HISTORY**

| 7/2019-presen  | Professor, Regional Centre for Biotechnology                            |  |  |  |  |
|----------------|---|--|--|--|--|
| 7/2014-present | Associate Professor, Regional Centre for Biotechnology                  |  |  |  |  |
| 7/2013-6/2014  | Associate Professor, National Centre for Biological Sciences            |  |  |  |  |
| 7/2007- 6/2013 | Reader-F at the National Centre for Biological Science                  |  |  |  |  |
| 7/2004-7/2007  | Instructor at the Mount Sinai School of Medicine                        |  |  |  |  |
| 1/2002-6/2004  | Post-Doctoral Fellow at the Mount Sinai School of Medicine, New         |  |  |  |  |
|                | York (USA) in the laboratory of Professor Aneel K. Aggarwal.            |  |  |  |  |
| 7/1996-12/2001 | Ph.D. in Life Sciences  |  |  |  |  |
|                | National Institute of Immunology, New Delhi.                            |  |  |  |  |
|                | Thesis Supervisor: Dr. Dinakar M. Salunke                               |  |  |  |  |
|                | Thesis Title: Structural rules governing epitope-paratope interactions: |  |  |  |  |
|                | Crystallographic analysis of model peptide antibody complexes.          |  |  |  |  |
| 7/1994-5/1996  | M.Sc in Biotechnology   |  |  |  |  |
|                | Department of Biotechnology, University of Pune, Pune. India.           |  |  |  |  |
| 7/1991-5/1994  | B.Sc in Chemistry   |  |  |  |  |
|                | Fergusson College, University of Pune. Pune. India.                     |  |  |  |  |

# **CURRENT RESEARCH PROGRAM & PREVIOUS RESEARCH CONTRIBUTIONS**

For all cellular processes to function optimally, the integrity of the genome has to be maintained. Conversely, plasticity in the genome may be required to relieve selection pressure imposed by an adverse environment. These two conflicting requirements have led to the presence of molecules and pathways that either prevent or facilitate changes in the genome. We aim to unearth the mechanism utilized by molecules involved in replicative or post-replicative pathways

that serve to either maintain genomic integrity or render genomic plasticity. Our studies will shed light on how organisms evolve and adapt to a dynamic environment. The rise of new variants of SARS-CoV-2, which is responsible for the ongoing COVID19 pandemic, has highlighted the need to understand how pathogens evolve. Our studies on the molecular determinants of genomic integrity and plasticity will help understand how pathogens acquire resistance to drugs and will be exploited to develop novel therapeutic strategies.

The key discoveries made in my laboratory are as follows: (a) Using time resolved crystallography, we have shown that pyrophosphate hydrolysis is an intrinsic and critical step of the DNA synthesis reaction catalyzed by DNA polymerases (NAR, 2018, 46:5875). This study was accorded breakthrough status by the journal Nucleic Acids Research. (b) We have discovered the presence of a polar filter in DNA polymerases that prevents the incorporation of ribonucleotides to prevent genomic instability (NAR, 2019, 47:10693). (c) We have shed light on the mechanism utilize by the primary mismatch sensor in DNA mismatch repair to bind DNA and detect mismatches (NAR, 2018, 46:256). (d) We have used our expertise with DNA polymerases to show that reactive oxygen species contribute to the antimicrobial activity of bactericidal antibiotics and this contribution has resolved a major controversy regarding antibiotic action (Ange. Chemie, 2016, 55:2397). (e) We have shown how GTP binding to the viral RNA-dependent-RNA polymerase ensures accurate initiation of replication of the genome of Japanese-Encephalitis-Virus (NAR, 2014, 42:2758). (f) We have shown how specialized DNA polymerases associated with adaptive mutagenesis ensure that the mutation frequency is calibrated to provide scope for evolution without severely compromising genomic viability (NAR, 2013, 41:5104). (g) We have discovered the mechanism employed by a bacterial DNA polymerase to neutralize genomic damage induced by the nitrofurazone antibiotic and thus reduce sensitivity of bacteria towards this antibiotic (Structure, 2014, 23:56). (h) We have found that the proofreading activity present in DNA polymerases present in Plasmodium falciparum and Staphylococcus aureus can not only process mismatches but also excise out misincorporated oxidized nucleotides and ribonucleotide from the primer to enhance fidelity of DNA synthesis during replication and repair (Sci. Rep. 2020, 10:11157; Sci. Rep. 2021, 168:272). (i) Recently, we have utilized computational methods to identify possible inhibitors of proteins critical for replication of the genome of Sars-CoV-2, which is responsible for the ongoing COVID19 pandemic (IUBMB Life, 2020, 72:2112; Int.J.Biol. Macromol., 2021,168:272). These inhibitors are currently being tested for their ability to inhibit

proteins involved in replication of the virus and to reduce viral titre in cell culture. In summary, my laboratory has shed light on how bacteria and viruses replicate their genome and identified novel intervention points to develop novel therapeutic agents against pathogenic bacteria and viral infections. We have also participated in efforts to develop new methods in macromolecular crystallography to determine and analyze three-dimensional structures (*Nature Methods*, 2014, 12:131; IUBMB Life, 2017, 69:563).

As a post-doctoral fellow (Dec 2001- July 2007) I focused on understanding the structural basis of DNA lesion bypass by eukaryotic Y-family DNA polymerases using X-ray crystallography. Due to the action of a variety of agents, lesions are formed on DNA which interfere with normal replication and may also prove carcinogenic. Eukaryotes possess up to four specialized DNA polymerases that are able to synthesize DNA across these lesions and thus prevent the replication fork from stalling. I determined the crystal structure of the catalytic cores of two such polymerases, human DNA polymerase iota (hPoli) and yeast REV1 (yREV1) -in complex with DNA and incoming nucleotide. The structures of hPoli and yRev1 in complex with undamaged and damaged DNA has shown that these two polymerases prefer altered modes of base-pairing in the active site to facilitate lesion bypass (Nature, 2004, 430:377; Science, 2005, 309:2219; Structure, 2005, 13:1569; Structure, 2006, 14:749; Nat. Struct. Mol. Biol., 2006, 13:619; Structure, 2008, 16:239; Structure, 2009, 17:530). Both hPoli and yREV1 have unique active sites that facilitate the formation of non-Watson-Crick base pairs to achieve lesion bypass and rescue stalled replication. Overall, the mode of action employed by hPoli and yREV1 represents a significant paradigm shift. I have also played a role in the determination of the structure of a third Y-family polymerase human DNA Polymerase kappa in its functional state (Mol. Cell, 2007, 25:601). In addition, I played secondary roles in projects aimed at understanding the nature of interactions between the translational regulator Pumilio and non-cognate RNA targets (Structure, 2008, 16:549) and discerning the preference of hPoli for incorporating dGTP when the base of the templating nucleotide is thymine (Structure, 2009, 17:974).

My doctoral thesis (July 1996- Dec 2001) describes the crystallographic analysis of a panel of three murine monoclonal antibodies raised against the same promiscuous peptide antigen PS1 (HQLDPAFGANSTNPD). (*J Immunol, 2000, 165:6949; J. Immunol, 2002, 168:2371*). The comparison of the structure of the antibodies in their bound and unbound state suggests there could be a convergence of both epitope and paratope conformations in an antibody response against a

flexible immunodominant epitope (*J. Immunol, 2002, 168:2371*). I also carried out a computational analysis of the conformational propensities of native and retro-inverso versions of B-cell and T-cell epitopes (*J. Immunol, 2003, 170:1362*). This study showed that conformational and functional mimicry can be achieved through retro-inversion only if the native peptide is present in a linear extended conformation in its functional state. I was also involved in the structure determination of an antibacterial protein from tasar silkworm *Antheraea mylitta (J. Biol. Chem., 2001, 276:41377*). In addition, I modelled the complex of the ribonuclease restrictocin and its rRNA substrate (*Biochemistry, 2001, 40:9115*).

# **PUBLICATIONS**

- Bhatia, S., Narayanan, N., Nagpal, S., and Nair, D. T. (2021) Antiviral therapeutics directed against RNA dependent RNA polymerases from positive-sense viruses. *Mol. Aspects. Med.* (in press) (Impact Factor: 14.235)
- 2. Nagpal, S., and Nair, D. T. (2021) The PHP domain of PolX from Staphylococcus aureus aids high fidelity DNA synthesis through the removal of misincorporated deoxyribo-, ribo- and oxidized nucleotides. *Sci Rep.* 11:4178. (Impact Factor: 4.379)
- 3. Narayanan, N. and **Nair, D. T.** (2021) Ritonavir may inhibit exoribonuclease activity of nsp14 from the SARS-CoV-2 virus and potentiate the activity of chain terminating drugs. *Int. J. Biol Macromol*. 168:272-278. (Impact Factor: 6.953)
- 4. Narayanan, N. and **Nair, D. T.** (2020) Vitamin B12 May Inhibit RNA-Dependent-RNA Polymerase Activity of nsp12 from the SARS-CoV-2 Virus. *IUBMB Life* 72:2112-2120. (Impact Factor: 3.885)
- 5. Sharma, M., Narayanan, N. and **Nair, D. T.** (2020) The proofreading activity of Pfprex from *Plasmodium falciparum* can prevent mutagenesis of the apicoplast genome by oxidized nucleotides. *Sci. Rep.* 10:11157. (Impact Factor: 4.379)
- 6. Jain, A., Kumar, A., Shikhi, M., Kumar, A., Nair, D. T. and Salunke, D. M. (2020) The structure of MP-4 from *Mucuna pruriens* at 2.22 Å resolution. *Acta Crystallogr F Struct Biol Commun*. 76:47-57. (Impact Factor: 1.056)
- Narayanan, N., Banerjee, A., Jain, D., Kulkarni, D. S., Sharma, R., Nirwal, S., Rao, D. N. and Nair, D. T. (2020) Tetramerization at low pH licenses DNA methylation activity of M.HpyAXI in the presence of acid stress. *J. Mol. Biol.* 432:324-342. (Impact Factor: 5.469)

- 8. Johnson, M. K., Kottur, J., and **Nair, D. T.** (2019) A polar filter in DNA polymerases prevents ribonucleotide incorporation. *Nucleic Acids Res.* 47:10693-10705. (Impact Factor: 16.907)
- 9. Ghodke, P. P., Bommisetti, P., **Nair, D. T.**, and Pradeepkumar, P. I. (2019) Synthesis of N(2)-Deoxyguanosine Modified DNAs and the Studies on Their Translesion Synthesis by the *E. coli* DNA Polymerase IV. *J Org Chem.* 84:1734-1747. (Impact Factor: 4.354)
- Shikhi, M., Nair, D. T., and Salunke, D. M. Structure-guided identification of function: role of *Capsicum annuum* vicilin during oxidative stress. (2018) *Biochem J.* 475:3057-3071. (Impact Factor: 3.857)
- 11. Kottur, J., and Nair, D. T. (2018) Pyrophosphate hydrolysis is an intrinsic and critical step of the DNA synthesis reaction. *Nucleic Acids Res.* 46:5875-5885. (Impact Factor: 16.971)
  This article was accorded Breakthrough status by the journal.
- 12. Sharma, R., Nirwal, S., Narayanan, N., and **Nair, D. T.** (2018) Dimerization through the RING-Finger Domain Attenuates Excision Activity of the piggyBac Transposase. *Biochemistry.* 57:2913-2922. (Impact Factor: 3.162)
- 13. Kumar, A., Kaur, H., Jain, A., **Nair, D. T.**, and Salunke, D. M. (2018) Docking, thermodynamics and molecular dynamics (MD) studies of a non-canonical protease inhibitor, MP-4, from *Mucuna pruriens*. *Sci Rep.* 8:689. (Impact Factor: 4.379)
- Nirwal, S., Kulkarni, D. S., Sharma, A., Rao, D. N. and Nair, D. T. (2018) Mechanism of formation of a toroid around DNA by the Mismatch Sensor protein. *Nucleic Acids Res.* 46:256-266. (Impact Factor: 16.971)
- 15. Salunke, D. M., Nair, D. T. (2017) Macromolecular structures: Quality assessment and biological interpretation. *IUBMB Life*. 69:563-571. (Impact Factor: 3.885)
- 16. Kumar, A., Gupta, C., **Nair, D. T.** §, Salunke, D. M. § (2016) MP-4 Contributes to Snake Venom Neutralization by *Mucuna pruriens* Seeds through an Indirect Antibody-mediated Mechanism. *J Biol Chem.* 291:11373-84. (Impact Factor: 5.157)
- 17. Kottur, J. and **Nair, D. T.**§ (2016) Reactive Oxygen Species Play an Important Role in the Bactericidal Activity of Quinolone Antibiotics. *Angew Chem Int Ed Engl.* 55:2397-2400. (Impact Factor: 15.336)
- 18. Ghodke, P. P., Gore, K. R., Harikrishna, S., Samanta, B., Kottur, J., Nair, D. T. and Pradeepkumar, P. I. (2016) The N(2)-Furfuryl-deoxyguanosine Adduct does not alter the structure of B-DNA. *J. Org. Chem.* 81:502-511. (Impact Factor: 4.354)

- 19. Jain, D., Narayanan, N. and Nair, D. T. (2016) Plasticity in repressor-DNA interactions neutralizes loss of symmetry in bipartite operators. *J. Biol. Chem.* 291:1235-1242. (Impact Factor: 5.157).
- 20. Nair, D. T., Kottur, J. and Sharma, R. (2015) A rescue act: Translesion DNA synthesis past N(2)-deoxyguanosine adducts. *IUBMB Life*. 67:564-574. (Impact Factor: 3.141)
- 21. Kottur, J., Sharma, A., Gore, K. R., Narayanan, N., Samanta, B., Pradeepkumar, P. I. and Nair, D. T.§ (2014) Unique Structural Features in DNA Polymerase IV enable efficient bypass of the N²-Adduct induced by the Nitrofurazone antibiotic. *Structure* 23:56-67. (Impact Factor: 5.006)
- 22. Weinert, T., Olieric, V., Waltersperger, S., Panepucci, E., Chen, L., Zhang, H., Zhou, D., Rose, J., Ebihara, A., Kuramitsu, S., Li, D., Howe, N., Schnapp, G., Pautsch, A., Bargsten, K., Prota, A. E., Surana, P., Kottur, J., Nair, D. T., Basilico, F., Cecatiello, V., Pasqualato, S., Boland, A., Weichenrieder, O., Wang, B. C., Steinmetz, M. O., Caffrey, M. and Wang, M. (2014) <u>Fast native-SAD phasing for routine macromolecular structure determination.</u> *Nat Methods*. 12:131-133. (Impact Factor: 28.547).
- 23. Surana, P., Vijaya, S. and **Nair, D. T.**§ (2014) RNA-dependent RNA polymerase of Japanese Encephalitis Virus binds the initiator nucleotide GTP to form a mechanistically important preinitiation state. *Nucleic Acids Res.* 42:2758-2773. (Impact Factor: 16.971).
- 24. Sharma A., Kottur, J., Narayanan, N. and **Nair, D. T.**§ (2013) A strategically located serine residue is critical for the mutator activity of DNA Polymerase IV from *Escherichia coli*. *Nucleic Acids Res.* 41:5104-5114. (Impact Factor: 16.971).
- 25. Jain, D. and **Nair, D. T**<sup>§</sup> (2013) Spacing between core recognition motifs determines relative orientation of AraR monomers on bipartite operators. *Nucleic Acids Research*. 41:639-647. (Impact Factor: 16.971).
- 26. Sharma, A., Subramanian, V. and Nair, D. T. § (2012) The PAD region in the mycobacterial dinB homolog MsPolIV exhibits positional heterogeneity. *Acta Crystallogr D Biol Crystallogr*. 68:960-967. (Impact Factor: 7.652)
- 27. Sharma, A. and Nair, D. T.§ (2012) MsDpo4—a DinB Homolog from *Mycobacterium smegmatis*—is an Error-Prone DNA Polymerase that can Promote G:T and T:G Mismatches. *Journal of Nucleic Acids*, vol. 2012, Article ID 285481.

- 28. Sharma A. and Nair, D. T.§ (2011) Cloning, expression, purification, crystallization and preliminary crystallographic analysis of MsDpo4: a Y-family DNA polymerase from *Mycobacterium smegmatis*. *Acta Crystallogr Sect F Struct Biol Cryst Commun*. 67:812-816. (Impact Factor: 1.056)
- 29. Namadurai, S., Jain, D., Kulkarni, D. S., Tabib, C. R., Friedhoff, P., Rao, D. N. and **Nair, D. T.**§. (2010) The C-terminal domain of the MutL homolog from *Neisseria gonorrhoeae* forms an inverted homodimer. *PLoS One*. 5:e13726. (Impact Factor: 3.240)
- 30. **Nair, D. T.**, Johnson, R. E., Prakash, L., Prakash, S. and Aggarwal, A. K. (2011) DNA Synthesis across an Abasic Lesion by Yeast Rev1 DNA Polymerase. *J Mol Biol.* 406:18-28. (Impact Factor: 5.469)
- 31. Jain, R., **Nair, D.T.**, Johnson, R. E., Prakash, S., Prakash, L. and Aggarwal, A. K. (2009) Replication across template T/U by human DNA polymerase-iota. *Structure*. 17:974-980. (Impact Factor: 5.006)
- 32. **Nair, D.T.**, Johnson, R. E., Prakash, S., Prakash, L. and Aggarwal, A. K. (2009) DNA synthesis across an abasic lesion by human DNA polymerase iota. *Structure*. 17:530-537. (Impact Factor: 5.006)
- 33. Gupta, Y.K., **Nair, D.T.**, Wharton, R. P., and Aggarwal, A. K. (2008). Structures of Human Pumilio with Noncognate RNAs Reveal Molecular Mechanisms for Binding Promiscuity. *Structure*. 16:549-557. (Impact Factor: 5.006)
- 34. **Nair, D.T.\***, Johnson, R. E.\*, Prakash, S., Prakash, L. and Aggarwal, A. K. (2008) Protein-template directed synthesis across an acrolein-derived DNA adduct by yeast Rev1 DNA Polymerase. *Structure*. 16:239-245. (Impact Factor: 5.006)
- 35. Lone, S.\*, Townson, S. A.\*, Uljon, S. N.\*, Johnson, R. E., Brahma, A., **Nair, D.T.**, Prakash, S., Prakash, L. and Aggarwal, A. K. (2007) Human DNA Polymerase kappa encircles DNA: implications for mismatch extension and lesion bypass. *Mol. Cell.* 25:601-614. (Impact Factor: 17.97)
- 36. **Nair, D.T.\***, Johnson, R. E.\*, Prakash, S., Prakash, L. and Aggarwal, A. K. (2006) Hoogsteen base pair formation promotes synthesis opposite the 1,N6-ethenodeoxyadenosine lesion by human DNA Polymerase iota. *Nat. Struct. Mol. Biol.* 13:619-625. (Impact Factor: 15.369)

- 37. **Nair, D.T.**, Johnson, R. E., Prakash, S., Prakash, L. and Aggarwal, A. K. (2006) Incoming nucleotide imposes a syn conformation on templating purine in the human DNA polymerase 1 active site. *Structure (Camb)*. 14:749-755. (Impact Factor: 5.006)
- 38. **Nair, D.T.**, Johnson, R. E., Prakash, S., Prakash, L. and Aggarwal, A. K. (2005) Human DNA Polymerase iota incorporates dCTP opposite template G via a G.C<sup>+</sup> Hoogsteen base pair. *Structure (Camb)*. 13:1569-1577. (Impact Factor: 5.006)
- 39. **Nair, D.T.**, Johnson, R. E., Prakash, S., Prakash, L. and Aggarwal, A. K. (2005) Rev1 employs a novel mechanism of DNA synthesis using a protein template. *Science*. 309:2219-2222. (Impact Factor: 47.728)
- 40. **Nair, D.T.**, Johnson, R. E., Prakash, S., Prakash, L. and Aggarwal, A. K. (2004) Replication by human DNA polymerase-iota occurs by Hoogsteen base-pairing. *Nature*. 430:377-380. (Impact Factor: 49.962)
- 41. **Nair, D.T.**, Kaur, K. J., Singh, K., Mukherjee, P., Rajagopal, D., George, A., Bal, V., Rath, S., Rao, K. V. and Salunke, D. M. (2003) Mimicry of native peptide antigens by the corresponding retro-inverso analogs is dependent on their intrinsic structure and interaction propensities. *J. Immunol.* 170:1362-1373. (Impact Factor: 5.422)
- 42. Nair, D.T., Singh, K., Siddiqui, Z., Nayak, B. P., Rao, K. V. S. and Salunke, D. M. (2002) Epitope recognition by diverse antibodies suggests conformational convergence in an antibody response. *J. Immunol.* 168:2371-2382. (Impact Factor: 5.422)
- 43. Nayak, S.K., Bagga, S., Gaur, D., **Nair, D.T.**, Salunke, D.M. and Batra, J.K. Mechanism of specific target recognition and RNA hydrolysis by ribonucleolytictoxin restrictocin. (2001) *Biochemistry*. **40**:9115-9124. (Impact Factor: 3.162)
- 44. \*Jain, D., \*Nair, D.T., Swaminathan, G. J., Abraham, E.G., Nagaraju, J. and Salunke, D.M. (2001) Structure of the Induced Antibacterial Protein from Tasar Silkworm, *Antherea mylitta:* Implications to molecular evolution. *J. Biol. Chem.* 276:41377-41382. (Impact Factor: 4.379)
- 45. **Nair, D.T.**, Singh, K., Shahu, N., Rao, K. V. S. and Salunke, D. M. (2000). Crystal structure of an antibody bound to an immunodominant peptide epitope: novel features in peptide-antibody recognition. *J. Immunol*. **165**:6949-6955. (Impact Factor: 5.422)
- (\*Equal contribution, §= corresponding author)

### **PATENT**

"Synthesis of N2-Furfuryl Deoxyguanosine Phosphoramidite and modified Oligonucleotides" by Gore, Kiran R.; Nair, Deepak T. and Pradeepkumar, P. I. granted on 30/3/2018 (Patent No. 295309)

### **PDB DEPOSITIONS**

76: 6JUS, 6JUR, 6JUQ, 6JUP, 6JUO, 6JUN, 6JUM, 6JUL, 6JBP, 6K0W, 5YUU, 5YUX, 6IG1, 5YV0, 5YUZ, 5ZLV, 5YV3, 5YUW, 5YUS, 5YUY, 5YJS, 5YUV, 5YYE, 5YYD, 5YV2, 5YV1, 5YUT, 5YUR, 5YK4, 5X9W, 5C5J, 5DSS, 5D4S, 5D4R, 4Q45, 4Q44, 4Q43, 4R8U, 4R8T, 4MTP, 4HDH, 4HDG, 4IRK, 4IR9, 4IRD, 4IRC, 4IR1, 4H0E, 4EGZ, 4EGY, 2FLL, 4DEZ, 3OSP, 3G6Y, 3G6X, 3G6V, 3H4D, 3H4B, 3H40, 3NCV, 3BSB, 3BJY, 3BSX, 2DPJ, 2DPI, 2ALZ, 2FLP, 2FLN, 2AQ4, 1T3N, 1KC5, 1KCV, 1KCU, 1KCS, 1KCR, & 1IIZ.

### **ACTIVE GRANTS\***

| No. | Title  | Amount<br>Sanctioned | Status | Funding<br>Agency | Date              |
|-----|--|----------------------|--------|-------------------|-------------------|
| 1.  | Does variation occur in the <i>dinB</i> gene during stress adaptation?         | Rs. 60 lakhs         | PI     | DBT               | 2018-<br>2021     |
| 2.  | Renewal of Access to<br>Structural Biology Facilities<br>at ESRF, France       | Rs. 2639.84<br>lakhs | PI     | DBT               | 2021-<br>2024     |
| 3.  | Development of small molecule antivirals against CHIKV and JEV                 | Rs. 633.5<br>lakhs   | Co-PI  | DBT               | 2020-<br>2023     |
| 4.  | Setting up of the Indian<br>Biological Data Centre-Phase<br>I                  | Rs. 7578.8<br>lakhs  | Co-PI  | DBT               | 2020-<br>2022     |
| 5.  | Bioinformatics Centre for<br>Computational Drug<br>Discovery at RCB, Faridabad | Rs. 197.31 lakhs     | PI     | DBT               | 3/2021-<br>3/2026 |

<sup>\*</sup>Since I am part of the SERB PAC on Interdisciplinary research in Biology, I cannot apply to SERB for grants for the period 2020-2023.

### **AWARDS, FELLOWSHIPS AND HONOURS**

- Shanti Swarup Bhatnagar Prize for Biological Sciences 2017, from Council of Scientific & Industrial Research (Govt. of India)
- 2. National Bioscience Award for Career Development 2014, from Department of Biotechnology (Govt. of India)
- 3. Ramanujan Fellowship (Department of Science & Technology) 2008-2013
- 4. Member, Guha Research Conference 2013 onwards

# **CONTRIBUTIONS TO ADMINISTRATION IN SCIENCE RESEARCH**

# **BM14 PROJECT (2009-2016)**

The BM14 project is a collaboration between the Department of Biotechnology, European Synchrotron Radiation Facility (ESRF) and European Molecular Biology Organization (EMBO). This program allows dedicated access to the BM14 beam line in ESRF to structural biologists in India for the collection of X-ray diffraction data (http://process.mbu.iisc.ernet.in/BM14/). Since its inception in 2009, I helped standardize logistical and scientific procedures and liaised with numerous subscribers of this program from all over India to help them carry out their experiments successfully

### ESRF ACCESS PROGRAM (2017-present)

This program of the RCB provides access to seven beamlines at the ESRF for macromolecular crystallography and small angle X-ray scattering experiments (http://esrf.rcb.res.in). An agreement between RCB and ESRF was signed by Prof. Sudhanshu Vrati and Dr. Francesco Sette to start this program. The program is supported by a generous grant from DBT. I am the local coordinator of this program at the RCB, PI of the grant from DBT that supports this proposal and the main proposer of the India Beatime-Allocation-Group in ESRF.

The above two programs have helped multiple researchers from different parts of India to conduct experiments at ESRF and has resulted in more than 350 publications in the last twelve years.

### **ADVANCED TECHNOLOGY PLATFORM CENTER (2016-2020)**

ATPC houses cutting-edge technologies to fuel innovation in the NCR-Biotech Science Cluster. For a period of four years from 2016 to 2020, I was part of the team involved in the development

of the ATPC. I was involved in procurement of equipment that populate the following facilities: Electron Microscopy, Optical Microscopy, Mass Spectrometry, Molecular Interactions and Genetics/Genomics.

# MEMBERSHIPS OF PROFESSIONAL /ACADEMIC BODIES/EDITORIAL BOARDS/REVIEW BOARDS

## Professional Body

- 1. Member, Guha Research Conference (2013-present)
- 2. Member, Indian Crystallographic Association
- 3. Executive Council Member, Indian Crystallography Association (2020-2021)
- 4. Member, Society of Biological Chemists
- 5. Member, Indian Biophysical Society

## Academic Body

- 1. Member, Academic Committee, Regional Centre for Biotechnology
- 2. Member, Board of Studies, Regional Centre for Biotechnology (2018-2020)

#### Review Board

- 1. Co-Opted Member of the Program Advisory Committee on Interdisciplinary Biological Sciences of the Science & Engineering Research Board.
- 2. Member, Committee to review NCP and FBR Projects under Healthcare Theme of the Council of Scientific and Industrial Research
- 3. Member, Screening Committee to shortlist proposals submitted under the SAHAJ scheme of the Department of Biotechnology.
- 4. Member, Screening Committee to shortlist proposals submitted under the BUILDER scheme of the Department of Biotechnology
- 5. Member, Technical Committee to review proposals submitted to the European Synchrotron Radiation Facility Access Program of the Regional Centre for Biotechnology which is supported by the Department of Biotechnology, Government of India.
- 6. Member, Technical Review Committee of the Indian Biological Data Centre (IBDC)

### RCB COMMITTEES

- 1. Vigilance Officer, Regional Centre for Biotechnology
- 2. Member, IT Committee

### ORGANIZATION OF CONFERENCES, WORKSHOPS & MEETINGS

- 1. Online Workshop titled "Cloud based Hands on Workshop: Computational Structure based Screening and Explicit Molecular Dynamics" to be held on 5<sup>th</sup>-6<sup>th</sup> October, 2021.
- 2. Panel Discussion on Antimicrobial Resistance on October 17, 2020 as part of the Vaishwik Bharatiya Vaigyanik Summit.
- 3. International Symposium titled "Multidisciplinary research at ESRF: An opportunity for Indian Science" held at the Regional Centre for Biotechnology on June 14, 2019.
- 4. International Symposium & Workshop titled "Structure Assisted Development of Novel Therapeutics" held at the Regional Centre for Biotechnology from February 12-16, 2019.
- 5. Workshop titled "RCB Mass Spectrometry and Proteomics Workshop" held at the Regional Centre for Biotechnology from December 17-20, 2018.
- 6. Student Symposium titled "Applications of Structural Bioinformatics: A student symposium of the National Capital Region- Structural Biology Group" on November 18, 2017 at AIIMS, New Delhi.
- Inauguration of the "ESRF Access Program" of RCB & DBT on 19/6/2017 by the Honorable Minister for Science & Technology, Dr. Harsh Vardhan followed by Seminar Symposium.
- 8. Symposium titled "Form & Function in Biology" on February 20, 2016 at RCB, Faridabad.
- 9. International Workshop titled "Computational Biotechnology at the Nanoscale: CCP4 Workshop 2016" during 15-19 February, 2016 at RCB, Faridabad.
- 10. International Symposium & Workshop titled "Frontiers of Structural Biology: New Advances in X-ray Diffraction and Cryo-electron Microscopy" during December 15-17, 2014 at INSA, New Delhi.

## **SELECTED SEMINARS**

- Delivered an invited talk online titled "DNA Replication: New answers to old questions" at Sukshjeev Society, Dept. of Microbiology, Bhaskaracharya College of Applied Sciences, University of Delhi on 19<sup>th</sup> March, 2021.
- 2. Delivered an invited talk online titled "New answers to old questions regarding DNA synthesis by DNA polymerases" at IISER-Trivandrum on 16<sup>th</sup> October, 2020.
- 3. Delivered an invited talk titled "DNA synthesis by DNA polymerases: Old questions and new answers" as part of the webinar series titled Progress and Prospects in Biology on 2<sup>nd</sup> August, 2020.
- 4. Delivered an invited talk titled "An overview of the COVID19 pandemic" at the Colloquium on 19<sup>th</sup> May, 2020 organized by the IUCAA Centre for Astronomy Research and Development, Delhi University.
- 5. Delivered an invited talk titled "Computational drug discovery and a potential antiviral for SARS-CoV-2" at the Global Online Conference on "Combating COVID-19: Through Biobased Technologies" on 16<sup>th</sup> April, 2020 organized by Bennet University.
- 6. Seminar titled "Chemistry & Biology of a DNA polymerase" at the Department of Bioinformatics, Savitribai Phule Pune University on October 9, 2019.
- 7. Seminar titled "Structural Biology: Imaging at the Molecular Level" at the DST Sponsored Fourth Lecture Workshop on Trans-disciplinary Areas of Research and Teaching by Shanti Swarup Bhatnagar Awardees September 27-28, 2019.
- 8. Seminar titled "New insight regarding long-standing questions about DNA synthesis by DNA polymerases" at International Conference on Molecular Medicine held at CHARUSAT, Gujarat from September 25-27, 2019.
- 9. Seminar titled "New insights regarding old questions about DNA synthesis by DNA polymerases" at inStem on May 15, 2019
- 10. Seminar titled "New answers to old questions regarding DNA synthesis by DNA polymerases" at IIT-Roorkee on March 22, 2019.
- 11. Seminar titled "Chemistry and Biology of a DNA polymerase" at NCR Bio-cluster meeting held at ICGEB, New Delhi on January 25, 2019.
- 12. Seminar titled "Pyrophosphate hydrolysis is an intrinsic and critical step of the DNA synthesis reaction catalysed by DNA polymerases" at the 5<sup>th</sup> DNA polymerase meeting

- held at Leiden, the Netherlands from September 23-26, 2018. (International)
- 13. Seminar titled "Time-resolved crystallography provides snapshots of the DNA synthesis reaction catalyzed by DNA polymerase IV" at Genome Biology 2018: Mechanisms in Health and Disease held at NIMHANS, Bangalore from July 13-14, 2018.
- 14. Seminar titled "Time-resolved crystallography illuminates steps of the DNA synthesis reaction catalyzed by DNA polymerase IV" at 46<sup>th</sup> National Seminar on Crystallography held at NIMHANS, Bangalore from June 27-29, 2018.
- 15. Seminar titled "Time-resolved crystallography provides snapshots of the birth of a phosphodiester bond." at the Department of Biological Sciences of the Tata Institute of Fundamental Research, Mumbai on June 1, 2018.
- 16. Seminar titled "Structural Biology of DNA polymerases" at DST Science Camp organized by NIST, Behrampur, March 20-24, 2018.
- 17. Seminar titled "Time-resolved crystallography reveals snapshots of the DNA synthesis reaction" at the Indian Biophysical Society Meeting held at IISER-Pune, from March 9-11, 2018.
- 18. Seminar titled "Structural Studies on Molecular Determinants of Genomic Integrity" at Indo-US Conference on Transcription, Chromatin Structure, DNA Repair and Genomic Stability at IISc, Bangalore held from March 6-10, 2018. (International Conference)
- 19. Seminar titled "Mechanism of formation of a toroid around DNA by the Mismatch Sensor Protein" at the National Conference on Protein Structure and Dynamics in Health and Agriculture held at Jamia Milia Islamia from November 3-4, 2017.
- 20. Seminar titled "Birth of the Phosphodiester bond" at the conference titled "Structure across Scales" held at NCBS, Bangalore from October 7-8, 2017. (International Symposium)
- 21. Seminar titled "DNA polymerase IV, reactive oxygen species and antibiotics: A lethal combination." delivered at the Indraprastha Institute of Information Technology, New Delhi, September 5, 2017.
- 22. Seminar titled "Mechanism of formation of a toroid around DNA by the Mismatch Sensor Protein" delivered at the 5<sup>th</sup> Annual Science Festival titled "BioSparks" organized at School of Life Sciences, Jawaharlal Nehru University, and Delhi on March 30, 2017.

- 23. Seminar titled "The role of GTP in initiation of replication of the JEV genome" delivered at the 5<sup>th</sup> Molecular Virology Meeting held at the NCR-Biotech Science Cluster from February 11-13, 2017.
- 24. Seminar titled "Reactive oxygen species play an important role in the bactericidal activity of quinolone antibiotics" delivered at the "19<sup>th</sup> International Conference on Emerging Infectious Diseases" organized by the United States-Japan Cooperative Medical program of the National Institutes of Health, USA and held in Seoul (South Korea) from February 7-10, 2017. (International Conference)
- 25. Seminar titled "Yin and Yang: The conflicting roles of DNA polymerase IV in oxidative stress" delivered at the meeting "Structural Proteomics of Macromolecular complexes using X-ray crystallography & Proteomics" organized at Regional Centre for Biotechnology, Faridabad held from December 18-20, 2016. (International Conference)
- 26. Seminar titled "Mechanistic insights into the role of DNA polymerase IV in evolution and replication illuminate a novel strategy to combat multidrug resistance" at the 16<sup>th</sup> Conference of the Science Council held at Colombo, Sri Lanka. (International Conference)
- 27. Seminar titled "Reactive Oxygen Species, Antibiotics and a DNA polymerase." At the NII Alumni Meeting held at NII, New Delhi from December 23-24, 2016.
- 28. Seminar titled "License to Methylate: Mechanism of low-pH induced activation of a Type III DNA methyltransferase from *H. pylori*" at the conference titled "Bacterial Expressions II" held at NCBS, Bangalore from December 1-5, 2016. (International Conference)
- 29. Seminar titled "Mutagenic and translesion DNA synthesis by DNA Polymerase IV from *Escherichia coli*: twin routes to drug resistance." at the International Congress on Friedreich's Ataxia and DNA structures in Health and Disease held at the All India Institute of Medical Sciences, New Delhi during 11-13<sup>th</sup> April 2015.
- 30. Seminar titled "DNA Polymerase IV and Antibiotic Induced Oxidative Stress" at the Bio-Epoch 2015 held at the School of Biotechnology, Jawaharlal Nehru University during10-11 April 2015.
- 31. Seminar titled "DNA Polymerase IV and Oxidative Stress" at the 39th Annual Meeting of the Indian Biophysical Society: "Biophysics in 21st Century" held at Jamia Millia Islamia, New Delhi, India during 14-17<sup>th</sup> February 2015.

- 32. Mentor Seminar titled "Mechanistic Insights into Bacterial and Viral Replication" at the Ramalingaswami Fellows Conclave held at Bhubaneshwar, Orissa during 30 January-1 February 2015.
- 33. Seminar titled "Structural basis of mutagenic and translesion DNA synthesis by DNA polymerase IV from *Escherichia coli*" at the 43rd National Seminars in Crystallography held at Central Drug Research Institute, Lucknow during 12<sup>th</sup>-14<sup>th</sup> November 2014.
- 34. Seminar titled "A close look at translesion DNA synthesis by DNA polymerase IV from *Escherichia coli*" at the International Symposium cum workshop titled "Frontiers in Structural Biology: New Methods in X-ray Diffraction and Cryo-Electron Microscopy." held at the Indian National Science Academy, New Delhi during 15<sup>th</sup> -17<sup>th</sup> December, 2014 (International Conference)
- 35. Seminar titled "Structural basis of mutagenic and translesion DNA synthesis by DNA polymerase IV from *Escherichia coli*" at the 43<sup>rd</sup> National Seminars in Crystallography held at Central Drug Research Institute, Lucknow from 12<sup>th</sup> -14<sup>th</sup> November, 2014.
- 36. Seminar titled "Replication of the flaviviral genome: Structure of a pre-initiation state and mechanism of initiation" at the Indo-US conference meeting on "Recent advances in Structural Biology and Drug Discovery (RASBDD-IIT-2014)" during 9<sup>th</sup>-11<sup>th</sup> October, 2014 at Indian Institute of Technology Roorkee.
- 37. Seminar titled "Mutagenic and Translesion DNA synthesis by DNA Polymerase IV from *Escherichia coli*: Structure and Mechanism" at the Zing Conference on DNA polymerases in Replication, Disease and Biomedical Applications held at Robinson College (Cambridge, UK) from 31<sup>st</sup> August- 4<sup>th</sup> September, 2014.

### **TEACHING**

- Molecular Biology & Genetic Engineering (RCB303) for M.Sc-Ph.D students, 19 Lectures in academic year 2020-2021.
- 2. Methods in Genetic Engineering (RCB306) for M.Sc-Ph.D, 5 practical sessions in academic year 2020-2021.
- 3. Molecular Biology & Genetic Engineering (RCB303) for M.Sc-Ph.D students, 16 Lectures in academic year 2019-2020.

- 4. Methods in Genetic Engineering (RCB306) for M.Sc-Ph.D, 4 practical sessions in academic year 2019-2020.
- 5. Molecular Biology & Genetic Engineering (RCB303) for M.Sc-Ph.D students, 19 Lectures in academic year 2018-2019.
- Methods in Genetic Engineering (RCB306) for M.Sc-Ph.D, 5 practical sessions in academic year 2018-2019.

## **TRAINING & MENTORING**

### Ph.D. Students

- 1. Amit Sharma (2008-2012)
- 2. Parag Surana (2008-2013)
- 3. Rahul Sharma (2011-2018)
- 4. Jithesh Kottur (2011-2017)
- 5. Shivlee Nirwal (2012-2018)
- 6. Naveen Narayanan (2013-2020)
- 7. Mary K. Joseph (2013-2020)
- 8. Shilpi Nagpal (2013-present: Thesis submitted)
- 9. Minakshi Sharma (2014-present: Thesis submitted)
- 10. Patterson Clement (2016-present)
- 11. Dalchand (2019-present)
- 12. V. Thangaraj (2020-present)
- 13. Bhawna Mawri (2020-present)
- 14. AbhayDeep Pandey (2019-present)
- 15. Ritika (2021-present)

### **Post-Doctoral Fellows**

- 1. Dr. Vaibhav K. Pandya (2014-2019)
- 2. Dr. Jithesh Kottur (2017-2018)
- 3. Dr. Nishant K. Varshney (2017-2019)
- 4. Dr. Sonam Bhatia (2020-present)
- 5. Dr. Naveen Narayanan (2020-present)

# **Masters Students**

- 1. Rashmi Joshi (2019-2020)
- 2. Vaibhav Joshi (2020-present)