

Manoj Munde, Ph.D.

Assistant Professor
School of Physical Sciences,
Jawaharlal Nehru University,
New Delhi, 110067
<http://biophysicalchemistrylabsps.in>

Email: mundemanoj@gmail.com
mmunde@mail.jnu.ac.in
Phone: (+91) 9910052147

Areas of Specialization: *Biophysical chemistry*

Current Areas of Research: *Protein-DNA and Drug-DNA interactions, modulators of biomolecular complexes, thermodynamic and kinetics studies*

Publications: 44 (Peer reviewed)

Total Impact Factor: 206; **Citations:** 1008; **h-Index:** 21.0; **i10 Index:** 31.0

No. of Book Chapters: 1

No. of Conference Abstract Published: 5

International conference presentations: 12

Employment Details

Aug, 2014-present

Assistant Professor (Chemistry)
School of Physical Sciences,
JNU, New Delhi

Sept, 2013-Aug, 2014

Assistant Professor
Department of Chemistry,
Central University of Rajasthan,
Bandarsindri, Rajasthan (India)

Aug, 2005-July 2013

Postdoctoral Associate
Georgia State University,
Atlanta, USA

PhD Details:

Indian Institute of Technology Bombay, India (*July 2001-Jan 2006*)
(Advisor: Prof. Nand Kishore)

Dissertation Title: "*Calorimetric and spectroscopic approach to understand protein folding and protein solvent interaction*".

Publications (Refereed/Peer-reviewed)

1. Tiwari N., Mishra R, Gupta S, Srivastava R, Aggarwal S, Bandopadhyay P, **Munde M.**, Synthetic Tunability and Biophysical Basis for Fabricating Highly Fluorescent and Stable DNA Copper Nanoclusters *Langmuir*, 37, 9385-9395, **2021 (IF: 3.9)**
2. Hooda P, Ishtikhar M, Saraswat S, Bhatia P, Mishra D, Trivedi A, Kulandaisamy R, Aggarwal S, **Munde M**, Ali N, AlAsmari AF, Rauf MA, Inampudi KK, Sehgal D. Biochemical and Biophysical Characterization of the Hepatitis E Virus Guanine-7-Methyltransferase, *Molecules*. **2022**, 27, 1505.
3. Gupta S, Tiwari N, Verma J, Waseem M, Subbarao N, **Munde M**. Estimation of Stronger Heparin Binding Locus in Fibronectin Domain III14 using Thermodynamic and Molecular Dynamic Study. *RSC Adv*, 10, 20288-20301, **2020 (IF: 3.05)**
4. Jain R, Dey P, Gupta S, Pati S, Bhattacharjee A, **Munde M**, Singh S "Molecular dynamics simulations and biochemical characterization of Pf14-3-3 and PfCDPK1 interaction towards its role in growth of human malaria parasite" *Biochem J*, **2020**, 477 (12): 2153–2177. (IF: 4.3)
5. Kandari D, Joshi H, Tanwar N, **Munde M**, Bhatnagar R, Delineation of the Residues of Bacillus anthracis Zinc Uptake Regulator Protein Directly Involved in Its Interaction with Cognate DNA. *Biol Trace Elem Res*. 199, 3147-3158, **2021. (IF: 3.78)**
6. Jain R, Gupta S, **Munde M**, Pati S, Singh S, Development of Novel Anti-Malarial From Structurally Diverse Library of Molecules, Targeting Plant-Like CDPK1, a Multistage Growth Regulator of P. Falciparum, *Biochem J*, 477, 1951-1970, **2020. (IF: 4.3)**
7. Anam Z, Joshi N, Gupta S, Yadav P, Chaurasiya A, Kaur A, Kaushik S., **Munde M**, Ranganathan A, Singh S, denovo peptide from a high throughput peptide library blocks Myosin A -MTIP complex formation in Plasmodium falciparum. *International Journal Molecular Sciences*, 21, 6158, **2020. (IF:4.55)**
8. Tandon S, Manhas R, Tiwari N, **Munde M**, Vijayan R, Gourinath S, Muthuswami R, Madhubala R, Deciphering the interaction of benzoxaborole inhibitor AN2690 with connective polypeptide 1 (CP1) editing domain of Leishmaniadonovani leucyl-tRNA synthetase, *Journal of Biosciences*, **2020**, 45, 63. (IF: 1.64)
9. Gogoi H, Mani R. Soumya A. Malik A., **Munde M**, Bhatnagar R. Crystalline and Amorphous Preparation of Aluminum Hydroxide Nanoparticles Enhances Protective Antigen Domain 4 Specific Immunogenicity and Provides Protection Against Anthrax *International Journal of Nanomedicine*, **2020** 15 239–252. (IF: 4.47)
10. Gupta S, Tiwari N, **Munde M**. A Comprehensive Biophysical Analysis of the Effect of DNA binding Drugs on Protamine-induced DNA Condensation *Scientific Reports*, **2019**, 9, 5891. (IF: 4.6)
11. Joshi H, Malik A, Aggarwal S, **Munde M**, Maitra SS, Adlakha N, Bhatnagar R. In-vitro Detection of Phytopathogenic Fungal Cell Wall by Polyclonal Sera Raised Against Trimethyl Chitosan Nanoparticles. *International Journal of Nanomedicine*. **2019**,14, 10023-10033. (IF: 4.47)

12. Chadha S, Vijayan R, Gupta S, **Munde M**, Gourinath S, Madhubala R, Genetic Manipulation of Leishmania donovani Threonyl tRNA Synthetase Facilitates its Exploration as a Potential Therapeutic Target" *PLOS Neglected Tropical Diseases* **2018**, 12, e0006575 (IF: 3.83)
13. Reetika Manhas, Smriti Tandon, Shib Sen, Neha Tiwari, **Manoj Munde**, Rentala Madhubala "Leishmania parasites are inhibited by the benzoxaborole AN2690 targeting leucyl-tRNA synthetase" *Antimicrobial Agents and Chemotherapy* **2018**, 2, e00079-18 (IF: 4.6)
14. Tiwari N, Tanwar N, **Munde M**. Molecular insights into trypanothione reductase-inhibitor interaction: A structure-based review. *Arch Pharm.* **2018**, 351 (6), 1700373 (IF: 2.29)
15. Tanwar N, **Munde M**. Thermodynamic and conformational analysis of the interaction between antibody binding proteins and IgG. *Int J Biol Macromol.* **2018**, 112:1084-1092. (IF: 3.9)
16. Tiwari N, Srivastava A, Kundu B, **Munde M**. Biophysical insight into the heparin-peptide interaction and its modulation by a small molecule. *J Mol Recognit.* **2018**, 31, e2674 (IF: 1.9)
17. Pasari N, Adlakha N, Gupta M, Bashir Z, Rajacharya GH, Verma G, **Munde M**, Bhatnagar R, Yazdani SS. Impact of Module-X2 and Carbohydrate Binding Module-3 on the catalytic activity of associated glycoside hydrolases towards plant biomass. *Sci Rep.* **2017**, 7, 3700. (IF: 4.6)
18. Mechanistic Heterogeneity in Site Recognition by the Structurally Homologous DNA-Binding Domains of the ETS-Family Transcription Factors Ets-1 and PU.1 Sang S, Linde MH, Carvalho V, Munde M, Wilson WD, Poon G, *Journal of Biological Chemistry* (2014), 289, 21605-16 (IF: 4.13)
19. An Unusual Monomer Recognition of Guanine Containing Mixed Sequence DNA by a Dithiophene Heterocyclic Diamidine. Munde M, Kumar A, Peixoto P, Depauw S, Ismail MA, Farahat AA, Paul A, Say MV, David-Cordonnier MH, Boykin DW, Wilson WD. *Biochemistry* (2014) 53, 1218-27 (IF 3.0)
20. Structure-dependent inhibition of the ETS-family transcription factor PU.1 by novel heterocyclic diamidines. Munde M, Wang S, Kumar A, Stephens CE, Abdelbasset A. Farahat, Boykin DW, Wilson WD, Poon GM. *Nucleic Acid Research* (2014) 42, 1379-90 (IF 11.56)
21. Green fluorescent diamidines as diagnostic probes for trypanosomes. Giordani F, **Munde M**, Wilson WD, Ismail MA, Kumar A, Boykin DW, Barrett MP. *Antimicrob Agents Chemother.* (2013) 58,1793-6. (IF 4.6)
22. Structure dependent binding of Arylimidamides to the DNA Minor Groove. Chai Y., Munde M., Kumar A., Mickelson L., Lin S., Campbell NH, Banerjee M., Akay S., Liu Z., Farahat AA, Nhili R., Depauw S., David-Cordonnier MH, Neidle S, Boykin DW, Wilson WD *ChemBioChem.* (2013) 15, 68-79 (IF 3.74)
23. Probing the electrostatics and pharmacologic modulation of sequence-specific binding by the DNA-binding domain of the ETS-family transcription factor PU.1: a binding affinity and kinetics investigation. Munde M, Poon GM, Wilson WD. *J Mol Biol.* 425, 1455-59 (2013). (IF 4.63)
24. On and off-target effects of telomere uncapping G-quadruplex selective ligands based on pentacyclic acridinium salts. Iachettini S., Malcolm FG Stevens, Frigerio M., Hummersone M. G., Hutchinson I., Garner T. P., Searle M. S., Wilson D. W., Munde M., Nanjunda R., D'Angelo C., Zizza P., Rizzo A., Cingolani C., Cicco F. D., Porru M., D'Incalci M., Leonetti C., Biroccio A., Salvati E. *Journal of Experimental & Clinical Cancer Research* (2013), 32:68 (IF 3.07)

25. Synthesis and antiprotozoal activity of dicationic 2,6-diphenylpyrazines and aza analogues. Hu L, Patel A, Bondada L, Yang S, Wang MZ, Munde M, Wilson WD, Wenzler T, Brun R, Boykin DW. **Bioorg Med Chem.** (2013) 21, 6732-41 (IF 3.1)
26. Targeting the DNA binding activity of the human ERG transcription factor using new heterocyclic dithiophene diamidines. Nhili R, Peixoto P, Depauw S, Flajollet S, Dezitter X, Munde M, Ismail MA, Kumar A, Farahat AA, Stephens CE, Duterque-Coquillaud M, Wilson, WD, Boykin DW, David-Cordonnier MH **Nucleic Acid Research** 41, 125-38 (2012). (IF 11.56)
27. 8,8-Dialkyldihydroberberines with Potent Antiprotozoal Activity. Endeshaw M, Zhu X, He S, Pandharkar T, Cason E, Mahasenani KV, Agarwal H, Li C, Munde M, Wilson WD, Bahar M, Doskotch RW, Kinghorn AD, Kaiser M, Brun R, Drew ME, Werbovetz KA. **J Nat Prod.** 76, 311-5 (2012) (IF 3.28)
28. Synthesis, DNA binding and antileishmanial activity of low molecular weight bis-arylimidamides. Banerjee, M., Farahat, A. A., Kumar, A., Wenzler, T., Burn, R., Munde, M., Wilson, W. D., Zu, X., Werbovetz, K.A., Boykin, D. W. **Eur J Med Chem.** 55, 449-54 (2012) (IF 3.2)
29. Microscopic Rearrangement of Bound Minor Groove Binders Detected by NMR. Rettig, M; Germann, M; Ismail, M; Batista-Parra, A; Munde, M; Boykin, D; Wilson, W. **J. Phy. Chem.** 116, 5620–5627. (2012) (IF 3.18)
30. Evaluation of arylimidamides DB1955 and DB1960 as candidates against visceral leishmaniasis and Chagas' disease: in vivo efficacy, acute toxicity, pharmacokinetics, and toxicology studies. Zhu, X., Liu, Q., Yang, S., Parman, T., Green, C. E., Mirsalis, J.C., Soeiro, M.D., Souza, E.M., Silva CF, Batista DD, Stephens CE, Banerjee, M., Farahat, A.A., Munde, M., Wilson, W.D, Boykin, D.W., Wang, M.Z., Werbovetz, K.A., **Antimicrob Agents Chemother.** 56, 3690-9. (2012) (IF 4.6)
31. Complexity in the binding of minor groove agents: netropsin has two thermodynamically different DNA binding modes at a single site. Lewis, E. A., Munde, M., Wang, S., Rettig, M., Le, V., Machha, V., and Wilson, W. D., **Nucleic Acids Res** 39, 9649-58. (2011) (IF 11.56)
32. The trypanocidal activity of amidine compounds does not correlate with their binding affinity to *Trypanosoma cruzi* kinetoplast DNA. Daliry, A., Pires, M. Q., Silva, C. F., Pacheco, R. S., Munde, M., Stephens, C. E., Kumar, A., Ismail, M. A., Liu, Z., Farahat, A. A., Akay, S., Som, P., Hu, Q., Boykin, D. W., Wilson, W. D., De Castro, S. L., and Soeiro, M. N. **Antimicrob Agents Chemother** 55, 4765-4773 (2011). (IF 4.6)
33. Wang, S., Munde, M., and Wilson, W. D. Minor groove to major groove, an unusual DNA sequence-dependent change in bend directionality by a distamycin dimer, **Biochemistry** 50, 7674-7683 (2011). (IF 2.98)
34. Induced topological changes in DNA complexes: influence of DNA sequences and small molecule structures. Hunt, R. A., Munde, M., Kumar, A., Ismail, M. A., Farahat, A. A., Arafa, R. K., Say, M., Batista-Parra, A., Tevis, D., Boykin, D. W., and Wilson, W. D. **Nucleic Acids Res** 39, 4265-4274 (2011). (IF 11.56)
35. DNA minor groove induced dimerization of heterocyclic cations: compound structure, binding affinity, and specificity for a TTAA site. Munde, M., Kumar, A., Nhili, R., Depauw, S., David-Cordonnier, M. H., Ismail, M. A., Stephens, C. E., Farahat, A. A., Batista-Parra, A., Boykin, D. W., and Wilson, W. D., **J Mol Biol** 402, 847-864 (2010). (IF 4.63)

36. DNA recognition: design, synthesis and biophysical characteristics of pyrrole(H) based polyamides. Chavda, S., Mulder, K., Brown, T., Mackay, H., Babu, B., Westrate, L., Ferguson, A., Lin, S., Kiakos, K., Ramos, J. P., Munde, M., Wilson, W. D., Hartley, J. A., and Lee, M., **Med Chem** 6, 150-158 (2010). (IF 1.6).
37. Targeting the ICB2 site of the topoisomerase IIalpha promoter with a formamido-pyrrole-imidazole-pyrrole H-pin polyamide. Franks, A., Tronrud, C., Kiakos, K., Kluza, J., Munde, M., Brown, T., Mackay, H., Wilson, W. D., Hochhauser, D., Hartley, J. A., and Lee, M., **Bioorg Med Chem** 18, 5553-5561 (2010). (IF 2.93)
38. Novel arylimidamides for treatment of visceral leishmaniasis. Wang, M. Z., Zhu, X., Srivastava, A., Liu, Q., Sweat, J. M., Pandharkar, T., Stephens, C. E., Riccio, E., Parman, T., Munde, M., Mandal, S., Madhubala, R., Tidwell, R. R., Wilson, W. D., Boykin, D. W., Hall, J. E., Kyle, D. E., and Werbovetz, K. A. **Antimicrob Agents Chemother** 54, 2507-2516 (2010) (IF 4.6).
39. Synthesis and activity of azaterphenyl diamidines against Trypanosoma brucei rhodesiense and Plasmodium falciparum. Hu, L., Arafa, R. K., Ismail, M. A., Patel, A., Munde, M., Wilson, W. D., Wenzler, T., Brun, R., and Boykin, D. W., **Bioorg Med Chem** 17, 6651-6658 (2009). (IF 2.93)
40. Azaterphenyl diamidines as antileishmanial agents. Hu, L., Arafa, R. K., Ismail, M. A., Wenzler, T., Brun, R., Munde, M., Wilson, W. D., Nzimiro, S., Samyesudhas, S., Werbovetz, K. A., and Boykin, D. W., **Bioorg Med Chem Lett** 18, 247-251 (2008). (IF 2.54)
41. Novel linear triaryl guanidines, N-substituted guanidines and potential prodrugs as antiprotozoal agents. Arafa, R. K., Ismail, M. A., Munde, M., Wilson, W. D., Wenzler, T., Brun, R., and Boykin, D. W., **Eur J Med Chem** 43, 2901-2908 (2008). (IF 3.2).
42. Induced fit conformational changes of a reversed amidine heterocycle: optimized interactions in a DNA minor groove complex. Munde, M., Lee, M., Neidle, S., Arafa, R., Boykin, D. W., Liu, Y., Bailly, C., and Wilson, W. D., **J Am Chem Soc** 129, 5688-5698 (2007). (IF 14.3)
43. Design of DNA minor groove binding diamidines that recognize GC base pair sequences: a dimeric-hinge interaction motif. Munde, M., Ismail, M. A., Arafa, R., Peixoto, P., Collar, C. J., Liu, Y., Hu, L., David-Cordonnier, M. H., Lansiaux, A., Bailly, C., Boykin, D. W., and Wilson, W. D., **J Am Chem Soc** 129, 13732-13743 (2007). (IF 14.3)
44. Volumetric Properties of Aqueous 2 chloroethanol solutions and volume of transfer of some amino acids and peptides from Water to Aqueous 2-chloroethanol solutions. Munde M. M., Kishore, N. **Journal of Solution Chemistry**, 32, 791-802. (2003). (IF 1.34)

Book Chapter

45. Nanjunda, R., **Munde, M.**, Liu, Y., and Wilson, W. D. (2011) Real-time monitoring of nucleic acid interactions with Biosensor Plasmon Resonance in the book, **Methods for Studying DNA/Drug Interactions** published on December 20, 2011 by CRC Press - 392 Pages (ISBN 9781439839744)

Technical Report

46. S Wang, **MM Munde**, WD Wilson, Critical Performance Characteristics of the Nano ITC SV When Used in the Study of Complex Binding Reactions, (2013)

Conference Abstract:

-
47. Expanding DNA Sequence Recognition with Minor Groove Binders. **Munde, M.**, A Kumar, R Nhili, S Depauw, MH David-Cordonnier, D Boykin, D Wilson, ***Biophysical Journal***, 100, 234, (2011).
 48. Sequence selective binding of the DNA helix by heterocyclic diamidines: From 5'-AATT to a 5'-TTAA selectivity R Nhili, S Depauw, **M Munde**, A Kumar, DW Boykin, WD Wilson, Marie-Helene David-Cordonnier, ***International Journal Of Molecular Medicine*** 28, S9-S9, 2011.
 49. Towards Pharmacological Modulation of ETS-Dependent Transcription. **Munde, M.** Miles H. Linde, Gregory M.K. Poon, W. David Wilson, ***Biophysical Journal***, Volume 104, Issue 2, 254a-255a, (2013).
 50. Hydrational Control of ETS-Family Transcription Factors: A Possible Resolution of the “Specificity Conundrum” Miles H. Linde, **Munde, M.**, W. David Wilson, Gregory M.K. Poon ***Biophysical Journal***, Volume 104, Issue 2, Page 420a (2013).
 51. Mechanistic Diversity in DNA Site Discrimination by Structurally Homologous ETS-Family Transcription Factors MH Linde, A Tolic, **MM Munde**, WD Wilson, GMK Poon, ***Biophysical Journal*** 106 (2), 497a, (2014)

Research funding:

-
- “A multi-targeted approach encompassing fundamental and applied studies towards drug discovery for Leishmaniasis.”
Funding Agency: Science and Engineering Research Board (SERB), DST (IRHPA)
Period: 2020-2025
Level of Funding: 293 lacs
Role: Co-PI
 - “National Centre For Screening Of Natural Products For Parasitic Diseases” .
Funding Agency: DST under ‘Drugs and Pharmaceuticals Research Programme’ (DPRP)
Period: 2019-2022
Level of Funding: 500 lacs
Role: Co-PI
 - “Exploiting Thermodynamic, Spectroscopic and Microscopic Studies to Understand Mechanism of GAG-peptide interaction”.
Funding Agency: DST-SERB
Period: 2016-2019
Level of Funding: 48.79 lacs
Role: PI
 - “Molecular Basis of Trypanothione Reductase Recognition by Small Molecules for Antiparasitic Rational Drug Design”
Funding Agency: Start up Grant by BSR-UGC
Period: 2015-2016
Level of Funding: 6.0 lacs
Role: PI
 - “Biophysical Basis of Interaction of Drugs with Trypanothione Reductase”,
Funding Agency: UPE, Jawaharlal Nehru University

Period: 2014-2019
 Level of Funding: 11.0 lacs
 Role: PI

Professional recognition, Awards and Achievements

- Early carrier research award, DST SERB, 2016
- Basic Scientific Research Faculty Fellowship, UGC, 2015
- Recipient of UGC Faculty Recharge Program Fellowship, (UGC-FRP), 2014
- Editorial Board member of *Scientific Reports* since 2019
- NIH postdoctoral fellowship to work on *Antiparasitic Drug Discovery* project, Jan2006-July2013 at Georgia State University, Atlanta, USA

Education

Degree	Specialization Discipline	University/Institute	Year of passing
PhD	Biophysical chemistry	Indian Institute of Technology Bombay, India	2006
MSc	Chemistry	Vidya Bharati Mahavidyalaya, Amravati University, Amravati, MH, India	1999
BSc	Chemistry, Biology	S.S.S.K.R. Innani Mahavidyalaya, Karanja, Amravati University, Amravati, MH, India	1997
HSC(10+2)	Chemistry, Physics, Biology	Vidyabharati college, Karanja, Amravati Board, Amravati, MH, India	1993

Other Academic Activities:

- Member of IQAC committee for processing of CARE journal task given to JNU as the Nodal University of the North India.
- Co-coordinated 1st Refresher Course in Chemistry at the UGC-HRDC, JNU, New Delhi, January 2-24, 2017
- Member of a University-level committee at JNU to prepare a 'Digital Tracking System' for Research Dissertation, Submissions etc
- Member of the committee for University Placement Cell, JNU.
- Drafted Departmental Proposal under 'Special Assistance Programme' (SAP) initiated by UGC at Central University of Rajasthan.
- Drafted Departmental Proposal under "Fund for Improvement of S&T infrastructure in universities & higher educational institutions (FIST)" initiated by DST at Central University of Rajasthan.
- Participated in Orientation Workshop on "Best Teaching Practices" at Central University of Rajasthan.

Industrial Collaboration: I had following collaboration/interaction experience with industry during my postdoctoral research at Georgia State University.

Sl. No.	Organization	Nature of Work	Period
1	Pharminox Ltd, oncology R&D company, UK	Biophysical studies of anticancer compounds against telomere DNA sequences	2009-2011

Research Work/Experience (Past and Present)

Assistant Professor: (Aug, 2014-present)

School of Physical Sciences, JNU, New Delhi

- Studying biophysical aspects of antibody binding protein
- Understanding mechanism of DNA condensation.
- Biophysical basis of DNA templated nanocluster formation
- Mentoring PhD, MSc and undergraduate students

Assistant Professor: (September 2013-August 2014)

Department of Chemistry, Central University of Rajasthan, NH-8, Bandar Sindri

- To apply principles of physical chemistry to study biomolecular interactions.
- Study USP1-drug interaction for anticancer drug design.
- Mentoring PhD, MSc and undergraduate students

Postdoctoral Research (Jan 2006-Aug 2013) Georgia State University, Atlanta, USA

- Investigated thermodynamics and kinetics of DNA-drug complex formation using biophysical tools.
- Studied the binding thermodynamics of analogues of clinically useful compound with DNA sequences (**Collaboration: Professor Stephen Neidle, Director of Cancer Research UK, Biomolecular Structure Group, Director of the Centre for Cancer Medicines**).
- Performed biophysical analysis of drugs with potential anticancer activity that inhibits human telomerase activity by targeting G-quadruplex DNA.
- Investigated conformational changes in DNA as a possible mode of action for antiparasitic compounds.
- Collaborated with the UK based Company 'Pharminox Ltd' to analyze drugs to develop anticancer therapeutics.
- Employed multidisciplinary approach using state of the art biophysical tools to elucidate the molecular basis of protein-DNA, DNA-drug interactions.
- Demonstrated thermodynamics of DNA binding mechanism of ETS family of proteins (known to be important transcription factors in human cancers) (**Collaboration: Prof. Gregory M.K.Poon, Washington State University, College of Pharmacy, Pullman, WA**).
- Discovered a new compound structure that inhibits the activity of transcriptional activity of ERG protein. (**Collaborations: Dr. David Boykin, Georgia State University, Atlanta, USA And Dr. Marie-Hélène David-Cordonnier INSERM U-837, Jean-Pierre Aubert Research Center, Institut de Recherches sur le Cancer de Lille, Place de Verdun, F-59045Lille, France**)
- Designed biophysical assays for studying small molecule inhibitors of protein-DNA complexes, a method to control gene expression.

Doctoral Research, (July 2001-Jan 2006) Indian Institute of Technology Bombay, India (Advisor: Prof. Nand Kishore)

Dissertation Title: "Calorimetric and spectroscopic approach to understand protein folding and protein solvent interaction".

- Studied the energetics of heme proteins with significant physiological functions to understand folding/unfolding pathways.
- Characterized intermediate folded states of protein using spectroscopy techniques.
- Characterized thermodynamically the structural transition of myoglobin in the presence of denaturants to understand its folding pathway.

Junior Research Fellow (Dec 2000-June2001) Indian Institute of Technology Bombay, India

- Investigated an important role played by ion-hydrophilic and hydrophilic-hydrophilic forces in amino acids and cosolvent interactions.

Academic talks

1. Invited Talk on "Biomolecular Targets and Drug Design: Approaches and Opportunities" at the 19th Science Setu open day lecture, 19th Aug, 2021 at National Agri-Food Biotechnology Institute (NABI), Mohali, Punjab.
2. Invited Talk on 'Synthetic Tunability and Biophysical Basis for Fabricating Highly Fluorescent and Stable DNA Copper Nanoclusters' at International Online Conference on Nano Materials (ICN 2021) 9-11 April 2021 at Mahatma Gandhi University, Kottayam, Kerala, India
3. Invited Talk on 'DNA Packaging and Effect of DNA Binding Drugs' at "National Seminar On Biophysics Biophysika" 4th October, 2019 at Jamia Milia Islamia, New Delhi.
4. Invited Lecture on "Biophysical tools in Drug Design" in 17th Refresher Course in Physical Sciences & Nano Sciences, November 22nd, 2019 at the UGC-HRDC, JNU, New Delhi.
5. Delivered a Talk on 'Implications of Isothermal Titration Calorimetry (ITC) in Drug Discovery' at "30th National Congress of Parasitology & Global Summit on Malaria Elimination" September 26-28, 2019, JNU, New Delhi, India.
6. Invited talk on, "Unfolding the role of protamine in insulin formulation" at SPS Soft Matter Meeting-2019, School of Physical Sciences, Jawaharlal Nehru University, New Delhi.
7. Invited Lecture on "Biophysical Interaction for Drug Design" in 1st Refresher Course in Chemistry at the UGC-HRDC, JNU, New Delhi, January 24, 2017.
8. Delivered a Talk in Workshop: "Surface Plasmon Resonance and Galvanostat and Potentiostat" at AIRF, JNU, New Delhi, May 6, 2015.
9. Delivered a Talk on Science Day, "Implications of Molecular Driving Forces in Drug Design" in JNU, New Delhi, Feb 26, 2016.
10. Invited talk on 'DNA as Therapeutic Target for Antiparasitic Drug Design' at the Central University of Gujarat, Gandhinagar, Gujarat, India on April 5, 2013.

11. Delivered Lecture in “13th Refresher Course in Physics” at Academic Science College, JNU, New Delhi, Oct 17, 2014
12. Delivered a talk on, “DNA Packaging and Its Accessibility by DNA Binding Drugs”, March Meeting, School of Physical Science, JNU, 16-17th March, 2018
13. Delivered a talk on “Understanding the Thermodynamic Basis of the Biomolecular Interactions” at ‘In-House Colloquium 2015’ at School of Physical Sciences, JNU March 27-28, 2015.

Conference presentations

1. Synthetic Tunability and Biophysical Basis for Fabricating Highly Fluorescent and Stable DNA Copper Nanoclusters International OnlineConference on **Nano Materials (ICN 2021) 9-11 April 2021** at Mahatma Gandhi University, Kottayam, Kerala, India
2. 30th National Congress of Parasitology & Global Summit on Malaria Elimination” September 26-28, **2019**, JNU, New Delhi, India.
3. 42nd Annual Meeting of the Indian Biophysical Society (IBS-2018) on “Emerging Trends in Biophysics”, IISER Pune, India, **9-11 March, 2018**.
4. “Expanding DNA sequence recognition with minor groove binders”. 55th Biophysical Annual Meeting, Baltimore, Maryland, United States, **March 5-9. (2011)**.
5. “Strong and selective molecular recognition of the DNA minor groove: Compound and DNA chemistry and unusual conformational matching” 240th ACS National Meeting, Boston, MA, United States, **August 22-26,(2010)**.
6. “DNA molecular recognition and compound design to specifically target the DNA minor groove”. 237th ACS National Meeting, Salt Lake City, UT, United States, **March 22-26, (2009)**.
7. “Design and Synthesis of An f-PIP H-Pin Polyamide That Targets the ICB2 Topoisomerase II Promoter”. 60th Southeast Regional Meeting of the American Chemical Society, Nashville, TN, United States, **November 12-15 (2008)**.
8. “Effect of Base Mutations in GC Rich Binding Site on Recognition by Minor Groove Binding Dications”. 59th Southeast Regional Meeting of the American Chemical Society, Greenville, SC, United States, **October 24-27 (2007)**.
9. “GC base pair recognition by minor groove binding diamidines: an important role for nitrogen heterocycles”. 58th Southeast Regional Meeting of the American Chemical Society, Augusta, GA, United States, **November 1-4 (2006)**.
10. “Analysis of reverse amidine - DNA minor groove complexes”. 231st ACS National Meeting, Atlanta, GA, United States, **March 26-30, (2006)**.
11. National Conference on Recent Advances in Thermodynamics of Chemical and Biological Systems, Guru Nanak Dev University, Amritsar, India, **May 7-9 (2001)**.

Teaching and course development

Courses Taught

- (PS459C) Concepts in Physical Chemistry
- (CHT105) Thermodynamics and Statistical Thermodynamics
- (CHT104) Electrochemistry and Kinetics
- (CHT206) Solid State, Surface and Material Chemistry
- (PS612C) Analytical Methods In Chemistry
- (PS455C) Mathematical Methods for chemist
- (PCHT102) Topics in Chemistry

Courses designed:

Biophysical Chemistry (PS469C; 03 credits)

Course description: This course has been designed to apply principles of physical chemistry in the study of biological macromolecules for students of chemistry at the master's level. The course is designed to review important concepts of physical chemistry in the context of understanding the biological systems. As per requirement, relevant examples from recent scientific literature have been used to illustrate various principles.

Concepts in Physical Chemistry (PS459C; 03 credits)

Course description: This course has been designed to study fundamental topics in physical chemistry, including classical and statistical thermodynamics, and kinetics and electrochemistry for students of chemistry at the master's level. The course will deliver higher-level concepts with the aim of generating significant amount of curiosity and interest in students in the field of physical chemistry. The course will also involve challenging tutorials.

Undergraduate (B. Tech) Chemistry Lab (Partial contribution):

Course description: This course is designed to review and improve the basic knowledge of experimental chemistry in undergraduate B.Tech students. The aim is to provide exposure to the students coming from vastly different backgrounds and create analytical thinking in them.

Mentoring and advising

Doctoral Students

Soumya Agarwal (2016-current)

Pooja Negi (2020-current)

Laxmi Kashyap (2020-current)

Pooja Dahiya (2021-current)

Former Students:

PhD

Neha Tiwari (2014-2020)

Sakshi Gupta (2015-2021)

Neetu Tanwar (2015-2022)

MSc/Project

Aditi Dahiya (Project): Joined PhD at Washington State University

Vipin Choubisa

Sarita

Pinky Kardam