CURRICULUM VITAE

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Citation	313
h-index	11
i10-index	12

**Citation, h-index and i10-index as on 22 Sept,2023 according to Google Scholar*

Professional experience

- 2 years 9 months and 14 days of Postdoctoral research experience at the Department of Biochemistry and Biophysics, **Texas A&M University, Texas, USA. (29 Feb 2016 to 14 Dec 2018)**
- 3 years of Postdoctoral research experience at the Department of Biochemistry, University of Allahabad, Allahabad. **India. (17 Dec 2018 to 16 Dec 2021)**
- 11 months of research experience as **Project Scientist-II**, at **Translational Health Science and Technology Institute,** Faridabad, **India. (26 July, 2022 to till 23 June, 2023)**

Educational Qualification

Ph.D. (2009-2015): Thesis title: 'Molecular and Biochemical studies on Thymidylate kinase of Filarial parasite' under the supervision of Dr. J.K. Saxena (Chief Scientist, Biochemistry Division, **CSIR-Central Drug Research Institute, Lucknow, India**) and Prof. (Mrs.) Sushma Rathaur (Department of Biochemistry, Faculty of Science, **Banaras Hindu University, Varanasi, India**).

M.S. (2006-2008): ** Master of Science in **Biochemistry, Department of Biochemistry, Faculty of Science, **Banaras Hindu University**, Varanasi, India.

Honor/Award/Fellowship (In India)

- Awarded **CSIR-Junior Research Fellowship** (June 2008); Conducted by Council of Scientific and Industrial Research *and* University Grants Commission (CSIR-UGC), New Delhi, India
- Awarded **ICMR-Junior Research Fellowship** (July 2008); Conducted by Indian Council of Medical Research, New Delhi, India
- Awarded **NET-LS (National Eligibility Test for Lectureship)** (December 2007); Conducted by Council of Scientific and Industrial Research *and* University Grants Commission (CSIR-UGC), New Delhi, India

Publications:

Research articles: 20

1. Molecular cloning and characterization of *Brugia malayi* thymidylate kinase. **Doharey PK**, Suthar MK, Verma A, Kumar V, Yadav S, Balaramnavar VM, Rathaur S, Saxena AK, Siddiqi MI, Saxena JK. **Acta Trop. 2014** May; 133:83-92. doi: 10.1016/j.actatropica.2014.02.003. Epub 2014 Feb 17. PMID: 24556140. **[I.F. 3.222]**
2. Insights into the structure-function relationship of *Brugia malayi* thymidylate kinase (BmTMK). **Doharey PK,** Singh SK, Verma P, Verma A, Rathaur S, Saxena JK. **Int J Biol Macromol. 2016** Jul; 88:565-71. doi: 10.1016/j.ijbiomac.2016.04.004. Epub 2016 Apr 1. PMID: 27044348. **[I.F. 8.025]**
3. Protein features for assembly of the RNA editing helicase 2 subcomplex (REH2C) in *Trypanosome* holo-editosomes. **Kumar V*, Doharey PK*,** Gulati S, Meehan J, Martinez MG, Hughes K, Mooers BHM, **Cruz-Reyes J. PLoS One. 2019** Apr 29;14(4): e0211525. doi: 10.1371/journal.pone.0211525. PMID: 31034523; PMCID: PMC6488192. **[I.F. 3.752]**
4. Site-specific and substrate-specific control of accurate mRNA editing by a helicase complex in *trypanosomes.* Kumar V, Ivens A, Goodall Z, Meehan J, **Doharey PK,** Hillhouse A, Hurtado DO, Cai JJ, Zhang X, Schnaufer A, **Cruz-Reyes J. RNA. 2020** Dec;26(12):1862-1881. doi: 10.1261/rna.076513.120. Epub 2020 Sep 1. PMID: 32873716; PMCID: PMC7668249. **[I.F. 4.942]**
5. *In silico* study indicates antimalarials as direct inhibitors of SARS-CoV-2-RNA dependent RNA polymerase. **Doharey PK,** Singh V, Gedda MR, Sahoo AK, Varadwaj PK, Sharma B**. J Biomol Struct Dyn. 2021** Jan 21:1-18. doi: 10.1080/07391102.2021.1871956. Epub ahead of print. PMID: 33475021; PMCID: PMC7842134. **[I.F. 5.235]**
6. Repurposing of gastric cancer drugs against COVID-19. **Sonkar C*, Doharey PK*,** Rathore AS, Singh V, Kashyap D, Sahoo AK, Mittal N, Sharma B, Jha HC. **Comput Biol Med. 2021** Oct; 137:104826. doi: 10.1016/j.compbiomed.2021.104826. Epub 2021 Sep 6. PMID: 34537409; PMCID: PMC8420180. **[I.F. 6.698]**
7. Synthesis, molecular docking and *Brugia malayi* thymidylate kinase (BmTMK) enzyme inhibition study of novel derivatives of [6]-shogaol. Singh VK, **Doharey PK,** Kumar V, Saxena JK, Siddiqi MI, Rathaur S, Narender T. **Eur J Med Chem. 2015** Mar 26;93:74-82. doi: 10.1016/j.ejmech.2015.01.035. Epub 2015 Jan 20. PMID: 25659753. **[I.F. 7.1]**
8. Designing, synthesis of selective and high-affinity chalcone-benzothiazole hybrids as *Brugia malayi* thymidylate kinase inhibitors: In vitro validation and docking studies. Sashidhara KV, Avula SR, **Doharey PK,** Singh LR, Balaramnavar VM, Gupta J, Misra-Bhattacharya S, Rathaur S, Saxena AK, Saxena JK. **Eur J Med Chem. 2015** Oct 20; 103:418-28. doi: 10.1016/j.ejmech.2015.09.004. Epub 2015 Sep 8. PMID: 2638312**[I.F. 7.1]**
9. Modulating catalytic activity of human topoisomerase II α enzyme by fluorescent gold nanoclusters. Dubey A, Singh V*, **Doharey PK*,** Sk MP, Samanta SK, Nema V, Sharma B, Varadwaj PK, Sahoo AK. **Int J Biol Macromol. 2021** Feb 15; 170:523-531. doi: 10.1016/j.ijbiomac.2020.12.129. Epub 2020 Dec 30. PMID: 33387542. **[I.F. 8.025]**

10. Behavior of *Plasmodium falciparum* purine nucleoside phosphorylase in macromolecular crowded environment. Suthar MK, **Doharey PK,** Verma A, Saxena JK**. Int J Biol Macromol. 2013** Nov; 62:657-62. doi: 10.1016/j.ijbiomac.2013.09.036. Epub 2013 Oct 1. PMID: 24095713. **[I.F. 8.025]**
11. Single tryptophan of disordered loop from *Plasmodium falciparum* purine nucleoside phosphorylase: involvement in catalysis and microenvironment. Suthar MK, Verma A, **Doharey PK**, Singh SV, Saxena JK. **Appl Biochem Biotechnol. 2013** Jun;170(4):868-79. doi: 10.1007/s12010-013-0228-9. Epub 2013 Apr 25. PMID: 23615735. **[I.F. 2.431]**
12. Molecular cloning and characterization of glucose-6-phosphate dehydrogenase from *Brugia malayi*. Verma A, Suthar MK, **Doharey PK,** Gupta S, Yadav S, Chauhan PM, Saxena JK. **Parasitology. 2013** Jun;140(7):897-906. doi: 10.1017/S0031182013000115. Epub 2013 Mar 18. PMID: 23506961. **[I.F. 2.783]**
13. *In silico* and *in vitro* studies on the protein-protein interactions between *Brugia malayi* immunomodulatory protein calreticulin and human C1q. Yadav S, Gupta S, Selvaraj C, **Doharey PK,** Verma A, Singh SK, Saxena JK. **PLoS One. 2014** Sep 3;9(9): e106413. doi: 10.1371/journal.pone.0106413. PMID: 25184227; PMCID: PMC4153637. **[I.F. 3.752]**
14. Identification of novel PTP1B inhibitors by pharmacophore-based virtual screening, scaffold hopping and docking. Balaramnavar VM, Srivastava R, Rahuja N, Gupta S, Rawat AK, Varshney S, Chandasana H, Chhonker YS, **Doharey PK,** Kumar S, Gautam S, Srivastava SP, Bhatta RS, Saxena JK, Gaikwad AN, Srivastava AK, Saxena AK. **Eur J Med Chem. 2014** Nov 24; 87:578-94. doi: 10.1016/j.ejmech.2014.09.097. Epub 2014 Oct 2. PMID: 25299681. **[I.F. 7.1]**
15. $NADP^+$ binding effects tryptophan accessibility, folding and stability of recombinant *B. malayi* G6PD. Verma A, Chandra S, Suthar MK, **Doharey PK,** Siddiqi MI, Saxena JK. **Int J Biol Macromol. 2016** Apr; 85:645-54. doi: 10.1016/j.ijbiomac.2015.12.087. Epub 2016 Jan 4. PMID: 26763177. **[I.F. 8.025]**
16. Molecular cloning and characterization of protein disulfide isomerase of *Brugia malayi,* a human lymphatic filarial parasite. Verma P, **Doharey PK,** Yadav S, Omer A, Singh P, Saxena JK. **EXCLI J. 2017** Jun 1; 16:824-839. doi: 10.17179/excli2017-214. PMID: 28827998; PMCID: PMC5547380. **[I.F. 4.022]**
17. Molecular cloning, purification and characterization of *Brugia malayi* phosphoglycerate kinase. Kumar R, **Doharey PK,** Saxena JK, Rathaur S. **Protein Expr Purif. 2017** Apr; 132:152-163. doi: 10.1016/j.pep.2017.02.005. Epub 2017 Feb 10. PMID: 28192198. **[I.F. 1.695]**
18. Operative conversions of 3-carboxy-4-quinolones into 3-nitro-4-quinolones via ipso-nitration: potential antifilarial agents as inhibitors of *Brugia malayi* thymidylate kinase. CS Azad, VM Balaramnavar, IA Khan, **Doharey PK**, JK Saxena, A K Saxena. **RSC Advances** 2015, 5 (100), 82208-82214. **doi.org/10.1039/C5RA18036H. [I.F. 4.036]**
19. Biochemical Characterization of Different Chemical Components of *Parthenium hysterophorus* and Their Therapeutic Potential against HIV-1 RT and Microbial Growth. Jaiswal J, **Doharey PK,** Singh R, Tiwari P, Singh N, Kumar A, Gupta VK, Siddiqui AJ, Sharma B. **Biomed Res Int. 2022** Apr 28;2022:3892352. doi: 10.1155/2022/3892352. PMID: 35528165; PMCID: PMC9071890. **[I.F. 2.583]**

20. **Doharey PK,** Verma P, Dubey A, Singh SK, Kumar M, Tripathi T, Alonazi M, Siddiqi NJ, Sharma B. Biophysical and *in-silico* studies on the structure-function relationship of *Brugia malayi* protein disulfide isomerase. **J Biomol Struct Dyn.** 2023 Apr 20:1-11. doi: 10.1080/07391102.2023.2201849. **[I.F. 5.235]**

Review Article: 2

1. Cruz-Reyes J, Mooers BHM, **Doharey PK**, Meehan J, Gulati S. Dynamic RNA holo-editosomes with subcomplex variants: Insights into the control of trypanosome editing. **Wiley Interdiscip Rev RNA. 2018** Nov;9(6): e1502. doi: 10.1002/wrna.1502. Epub 2018 Aug 12. PMID: 30101566; PMCID: PMC6185801. **[I.F. 9.957]**
2. Jaiswal J, Singh N, Gupta VK, **Doharey PK,** Siddiqi NJ, Sharma B. Pharmacological Chemistry and Biomedical Implications of Chemical Ingredients from Parthenium hysterophorus. **Curr Top Med Chem. 2022** Mar 7. doi: 10.2174/1568026622666220307145027. Epub ahead of print. PMID: 35255797. **[I.F. 3.295]**

Book chapter published in International Book: 2

1. Filariasis: Biochemistry and Chemotherapeutic Targets. Jitendra Kumar Saxena, Anita, Manish Kumar Suthar, **Pawan K. Doharey**, Alok R. Singh. In Nematodes: Morphology, Functions and Management Strategies. Publisher: **Nova Publisher USA**. ISBN 978-1-61470-784-4. 83-107, **2013.**
2. Control Mechanisms of the Holo-Editosome in Trypanosomes in RNA Metabolism in Mitochondria. Jorge Cruz-Reyes, Blaine H.M. Mooers, Vikas Kumar, **Pawan K. Doharey**, Joshua Meehan, Luenn Chhapro. **Springer, Cham**, 978-3-319- 78189-1. 125-144, **2018.**

Conferences: Attended/Participated/Talk

1. National Congress of Parasitology (NCP-2009). Held at Department of Zoology, Centre for advance studies (UGC), Panjab University, Chandigarh. Punjab, India. November 14-16, 2009 **(Attended)**
2. Cloning and expression of *Brugia malayi* thymidylate kinase. **Pawan K. Doharey,** Anita Verma, Manish K. Suthar, Shiv V. Singh and Jitendra K. Saxena. 22nd National Congress of Parasitology (NCP-2010). Held at Department of Zoology, University of Kalyani, Kalyani. West Bengal, India. October 30-November 1, 2010
3. Characterization of *Brugia malayi* thymidylate kinase a putative drug target. **Pawan K. Doharey,** Anita Verma, Manish K. Suthar, Shiv V. Singh and Jitendra K. Saxena. Indian society of chemist and biologist (ISCBC-2011). Held at Department of Chemistry, Saurashtra University, Rajkot. Gujrat, India. February 4-7, 2011
4. Biochemical characterization of *Brugia malayi* thymidylate kinase; a putative drug target. **Pawan K. Doharey,** Manish K. Suthar, Sunita Yadav, Smita Gupta, Sushma Rathaur and Jitendra K. Saxena. 24th National Congress of Parasitology (NCP-2013). Held at Regional medical research centre for tribals (ICMR), Jabalpur. Madhya Pradesh, India. April 27-29, 2013

5. Characterization of *Brugia malayi* thymidylate kinase a putative drug target: Biochemical and in-silico analysis. **Pawan K. Doharey,** Manish K. Suthar, Anita Verma, Sunita Yadav, Smita Gupta, Sushma Rathaur and Jitendra K. Saxena. Current trends in drug development and research (CTDDR-2013). Held at CSIR- Central drug research institute, Lucknow. Uttar Pradesh, India. February 26-28, 2013
6. Effect of Nucleoside analogues on *Brugia malayi* thymidylate kinase (BmTMK). **Pawan K. Doharey,** Sunita Yadav, Smita Gupta, Pravesh Verma, Sushma Rathaur and Jitendra K. Saxena.25th National Congress of Parasitology (NCP-2014). Held at CSIR- Central drug research institute, Lucknow. Uttar Pradesh, India. October 16-18, 2014
7. A holo-editosome catalytic RNA helicase subcomplex in the trypanosome. **Pawan K. Doharey.** Kinetoplastid Cell Molecular Biology Meeting. Held at Marine Biological Laboratory, **Woods Hole, MA, USA**. April 22-26, 2017 **(Talk)**

Research Summary

Research Summary (Ph. D)

In my Ph.D. work, Thymidylate kinase of *Brugia* malayi (Human lymphatic filarial parasite) was selected as the chemotherapeutic target; ***Bmtmk* gene was successfully cloned and expressed in *E. coli*.** The expressed protein was purified by affinity chromatography and characterized using different biochemical and biophysical techniques. The native molecular weight of rBmTMK was determined by FPLC and glutaraldehyde crosslinking The equilibrium unfolding and refolding studies of rBmTMK using urea and guanidine hydrochloride were performed to determine the different intermediate during the unfolding and refolding of the rBmTMK protein. Many nucleoside analogues were tested against rBmTMK and good inhibition was observed by a few of these compounds. [6]-shogaol and its derivatives were synthesized in our chemistry collaboration and the significant inhibitory effect of these compounds was observed. Similarly, chalcone-benzothiazone hybrids showed significant inhibition against rBmTMK activity. A homology model of BmTMK was constructed and the refined model was used for the docking studies with its substrates and different inhibitors to support our *in-vitro* results. *Ex-vivo* studies were also performed to check the effect of some selected chalcone-benzothiazone hybrids on the *Brugia malayi* parasites.

Research Summary (Postdoctoral Research Associate, USA)

During my Postdoc work at **Texas A&M University, College Station, TX, USA**, I worked on a very interesting genetic process known as "**RNA editing"** in pathogenic kinetoplastid parasites. My project was to identify the residues involved in the binding of the different proteins (mainly RNA Editing Helicase-2 & Zinc finger containing F1protein) involved in the RNA editing mechanism of trypanosomes. I established many very important different types of wild-type and mutant clone constructs. Specifically, these constructs were expression constructs that allowed us to express recombinant proteins in bacteria and trypanosomes, these proteins are essential for RNA editing mechanism. I worked on the activity and physical interaction between these proteins by performing molecular biology and

biochemical techniques like cloning, expression, protein purification, immuno-precipitations, western blot, qPCR, radioactivity assays, and different type of cross-linking etc. I have also prepared several samples for Illumina **N**ext-**G**eneration **S**equencing for another project running in the lab.

Research Summary (UGC-Dr. D.S. Kothari Postdoc fellow, India)

During my Postdoc work at **University of Allahabad, India** I worked on to find out the inhibitors against *Leishmania donovani* Tryparedoxin peroxidase enzyme. To fulfill these first in-silico studies were performed. Several important small molecule libraries were screened against the *Leishmania donovani* Tryparedoxin peroxidase enzyme. Cloning of the Tryparedoxin peroxidase gene was done and transformed in the E. coli cells for the recombinant protein expression. The selected compounds were purchased and tested in-vitro on *Leishmania donovani* culture as well as on recombinant purified Tryparedoxin peroxidase enzyme.

Besides this, I have worked to find out the inhibitors against SARS-CoV-2-RNA-dependent RNA polymerase. In silico work was performed to find out the inhibitors. Mainly repurposing of the antimalarial drugs were tested and good results were observed. In another project, Gastric cancer inhibitors were also tested against SARS-CoV-2-RNA dependent RNA polymerase-NiRAN domain and good results were obtained.

Scientific Expertise

- **Molecular biology techniques:** DNA/RNA/isolation and purification, transformation, transfection, PCR, Real-time/qPCR, cloning, **Site-directed mutagenesis** (SDM) etc.
- **RNA:** *In-vitro* transcription, radioactive labeling of RNA, Radioactive RNA probe synthesis.
- **Protein purification:** Purification of recombinant protein by different chromatography techniques *viz.* Affinity, Gel Filtration (FPLC) etc.
- **Culture techniques:** Mammalian cell culture, Single-cell parasite culture.
- **Electrophoretic techniques:** PAGE (Native, SDS, Urea etc.)**,** EMSA (Electrophoretic mobility shift assay) to check protein-nucleic interaction.
- **Crosslinking:** Glutaraldehyde crosslinking, BS3 crosslinking (Protein-protein), UV crosslinking (protein-nucleic acid).
- **Enzyme Kinetics:** Determination of K_m, V_{max}, $IC_{50,}$ and K_i values, type of inhibition, etc (**Spectrophotometric**), RNA unwinding assay (**Radioactive**).
- **Immunoprecipitation/pulldown assay:** To determine the assembly of proteins, responsible for a specific mechanism in the cell/parasite.
- **Next-generation sequencing (Illumina library preparation):** Sample preparation **(**RNA isolation, cDNA synthesis, Gene-specific PCR, Adaptor PCR, Index PCR, TAPE station to check quality of library).
- **Fluorometric Techniques:** Quenching of protein with substrates and different types of quenchers, BSA binding experiment in support of pharmacokinetics.
- **Immunology Technique:** Western blotting, Immunization, ELISA, etc.

- **Animal handling:** Swiss mice and Rabbits for immunization.
- **Bioinformatics exposure:** Homology modeling and its validation. Internet Applications including Homology search/analysis on BLAST/FASTA, SWISS PROT, Expasy, hydrophobicity analysis, etc. Primer designing for PCR/qPCR. Docking on Autodock and Schrodinger platforms. MD simulation on Schrodinger.
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Computer proficiency

- Windows operating systems and application software like Microsoft Office package (MS Word, Excel, PowerPoint, Publisher).
- Scientific data retrieval from various internet portals like Science Direct, PubMed, SciFinder, and Google Scholar etc.
- Technical software (Scientific software) Reference Management Software (Endnote, Zotero), Graph pad Prism software etc.

Area of interest

- Drug target discovery and development
- Structural Biology
- Vaccine development
- Gene editing
- RNA editing

Strengths and Qualities

- The capability of designing and executing the experiments independently.
- Good team spirit
- Quick learning, problem-solving, and capable to work independently as well as in a team.
- My confidence, positive attitude, and leadership skill.

Personal Profile

Male
Married
Nationality: Indian
Languages Known: English and Hindi

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References

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(Relationship: Ph.D. Supervisor)
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Department of Biochemistry,
University of Allahabad,
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