# Dr. Manish Kumar Tripathi

Research Associate Department of Biophysics All India Institute of Medical Sciences Ansari Nagar, New Delhi-110029

E-mail: manishtripathi41@gmail.com

Mobile No.: +91-9575620437, +91-9452604477



## **Professional Experience**

February 2020-Continue Research Associate, AIIMS, New Delhi
July-2017- February 2020 Post-Doctoral Fellow, IIT BHU, Varanasi, Uttar Pradesh
May-2016 – January 2017 Project Associate, Maulana Azad National Institute of

Technology, Bhopal, Madhya Pradesh

#### **Academic Background**

**Ph.D.** in *Bioinformatics* from *Maulana Azad National Institute of Technology*, *Bhopal* (2016) with course work SGPA 7.91.

**Title:** "Computational study to investigate the role of industrial pollutants on immune proteins against tuberculosis"

Thesis Supervisor: Prof. Rahul M Shrivastava

**Master of Science (M.Sc.)** in *Bioinformatics* from *University of Allahabad* (2009) with 68.68 %.

**Bachelor of Science (B.Sc.)** in *Botany and Chemistry* from *University of Allahabad* (2007) with 70.96 %.

#### **Bioinformatics Skills:**

- Sequence Analysis & Phylogenetics- BLAST, PSI-BLAST, Clustal W, MEGA, PAUP & PHYLIP.
- Molecular Modelling- Protein modelling, structure based drug design, virtual screening, pharmacophore modelling, free energy calculation, quantum calculation and docking studies using Schrödinger, Discovery studio and Autodock.
- Molecular Dynamics simulation- Gromacs and Desmond
- > Operating System- Unix, Windows/DOS etc.
- Scripting- Unix shell scripting, knowledge of Python and MATLAB
- > Statistical analysis- R

<u>Technical Skills:</u> UV Spectroscopy, Elisa, Gel Electrophoresis, SDS PAGE, *In vitro* Enzyme assay methods, Enzyme Inhibition kinetics, Kinetic characterization of enzyme drug targets (IC50, kinetic constants).

# Academic Scholarship/Awards/Achievements

- Received CSIR-Foreign Travel Grant in 2019 for visiting Basel, Switzerland to attend Basel Life Congress-2019
- Received Institutional Post-Doctoral fellowship in 2017 from IIT-BHU.

- Received Best poster award in National seminar on Science for shaping the future of India organized by Indian Science Congress Association Bhopal Chapter & MPCST Bhopal (30-31Oct 2012).
- Received MHRD Institute fellowship in 2012 for completion of Ph.D.
- Qualified in GATE (Graduate Aptitude test in Engineering-2011, 2012).
- Secured 1<sup>st</sup> rank in Degree College during graduation.

## **List of Publications**

- 1. Chaubey PK, Tripathi A, **Tripathi MK**, Seth A, Shrivastava SK (2021) Design, Synthesis, and Evaluation of N-Benzylpyrrolidine and 1,3,4-Oxadiazole as Multitargeted Hybrids for the Treatment of Alzheimers Disease. *Bioorganic Chemistry* 111, 104922 (I.F.-4.8).
- 2. Singh P, **Tripathi MK** #, Shrivastava R (2021) *In silico* identification of linear B-cell epitope in coronavirus 2019 (SARS-CoV-2) surface glycoprotein: A prospective towards peptide vaccine. *Minerva Biotecnology and Biomolecular Research*. (I.F.-1.1) (#Equal contribution)
- **3. Tripathi MK,** Singh P, Sharma S, Singh TP, Ethayathulla AS, Kaur P (2020) Identification of Bioactive Molecule from *Withania somnifera* (Ashwagandha) as SARS-CoV-2 Main Protease Inhibitor. *Journal of Bimolecular Structure and Dynamics* 8;1–14 (I.F.-3.3)
- **4. Tripathi MK**, Sharma P, Srivastava P, Tripathi A, Tripathi PN, Seth A, Shrivastava SK (2020) Computational exploration and experimental validation to identify a dual inhibitor of cholinesterase and amyloid-beta for the treatment of Alzheimer's disease. *Journal of Computer-Aided Molecular Design* 34:983-1002. (I.F.-3.2)
- **5. Tripathi MK**, Yasir M, Singh P, Shrivastava.R (2020) A comparative study to explore the effect of different compounds in immune proteins of human beings against tuberculosis: An *In silico* Approach. *Current Bioinformatics* 15:155-164. (I.F.-2.0)
- 6. Singh P, **Tripathi MK** #, Shrivastava R, Yasir M, Khare R, Tripathi MK, Shrivastava.R (2020) Potential Inhibitors for SARS-CoV-2 and Functional Food Components as Nutritional Supplement for COVID-19: A Review. *Plant Food for Human* Nutrition 75,458–466. (I.F.-2.9) (#Equal contribution).
- 7. Singh P, Yasir M, Khare R, Tripathi MK, Shrivastava R (2020) Snake Venom Phospholipase A2 and its Natural Inhibitors. Natural Product Sciences. 26(3): 259-267
- **8.** Tripathi A, Chaubey PK, Seth A, Sharma P, **Tripathi MK**, Shrivastava SK (2020) Design and Development of Multifunctional Hybrids of Ferulic Acid and 1,3,4-Oxadiazoles for the Treatment of Alzheimer's Disease. *Current Trends in Biotechnology and Pharmacy* 14(1):81-96.
- 9. Shrivastava SK, Sinha SK, Srivastava P, Tripathi PN, Sharma P, **Tripathi MK**, Tripathi A, Choubey PK, Waiker DK, Aggarwal LM, Dixit M, Kheruka SC, Gambhir S, Shankar S, Srivastava RK (2019) Design and Development of Novel p-Aminobenzoic Acid Derivatives as Potential Cholinesterase Inhibitors for the Treatment of Alzheimer's disease. *Bioorganic Chemistry* 82: 211-223. (I.F.-4.8)

- **10.** Tripathi PN, Srivastava P, Sharma P, **Tripathi MK**, Seth A, Tripathi A, Rai SN, Singh S, Shrivastava SK (2019) Biphenyl-3-oxo-1,2,4-triazine linked piperazine derivatives as potential cholinesterase inhibitors with anti-oxidant property to improve the learning and memory. *Bioorganic Chemistry* 85:82-96. (I.F.-4.8)
- 11. Sharma P, Tripathi A, Tripathi PN, Prajapati SK, Seth A, **Tripathi MK**, Srivastava P, Tiwari V, Krishnamurthy S, Shrivastava SK. (2019) Design and Development of Multitarget-Directed N-Benzylpiperidine Analogs as Potential Candidates for the Treatment of Alzheimer's Disease. *European Journal of Medicinal Chemistry* 167:510-524. (I.F.-5.5)
- **12.** Tripathi A, Choubey PK, Sharma P, Seth A, Tripathi PN, **Tripathi MK**, Prajapati SK, Krishnamurthy S, Shrivastava SK. (2019) Design and Development of Molecular Hybrids of 2-Pyridylpiperazine and 5-Phenyl-1,3,4-oxadiazoles as Potential Multifunctional Agents to Treat Alzheimer's Disease. *European Journal of Medicinal Chemistry* 183:111707 (I.F.-5.5)
- **13.** Yasir M, **Tripathi MK**, Singh P, Shrivastava R (2019) The genus *Glycosmis* (*Rutaceae*): A comprehensive review on its Phytochemical and pharmacological perspectives. *The Natural Products Journal* 9:98-124.
- **14.** Singh M, **Tripathi MK**, Singh AK, Shekhar C, Gambhir IS, Kumar B, Purohit S (2018) A therapeutic approach to target mitochondrial dysfunction using molecular docking studies: Screening of natural drugs for Oral Carcinoma. *Pharmacognosy Magazine* 14(55):192-196. (I.F.-1.5)
- **15.** Shrivastava SK, Patel BK, Tripathi PN, Srivastava P, Sharma P, Tripathi A, Seth A, **Tripathi MK** (2018) Synthesis, evaluation and docking studies of some 1,3,4-thiazolinone derivatives as effective lipoxygenase inhibitors. *Chemical Papers* 72(11):2769-2783. (I.F.-1.6)
- **16.** Yasir M, Singh J, **Tripathi MK**, Singh P, Shrivastava R (2017) Green Synthesis of Silver Nanoparticles Using Leaf Extract of Common Arrowhead Houseplant and Its Anticandidal Activity. *Pharmacognosy Magazine* 13(52):840-844. (I.F.-1.5)
- **17. Tripathi MK**, Yasir M, Singh P, Tayubi IA, Gupta R, Shrivastava R (2016) Toxic effect of chemicals dumped in premises of UCIL, Bhopal leading to environmental pollution: An *In-Silico* Approach. *Asian Pacific Journal of Tropical Diseases* 6(4): 284-290. (I.F.-0.7)
- **18.** Shrivastava R, Yasir M, **Tripathi MK**, Singh P (2016) *In silico* interaction of methyl isocyanate with immune protein responsible for *Mycobacterium tuberculosis* infection using molecular docking. *Journal of Toxicology & Industrial health* 32(1): 162-167. (I.F.-1.7)
- **19.** Singh P, Yasir M, **Tripathi MK**, Shrivastava R (2016) A review on in vitro screening assay for inhibitory effect against venom enzymes using medicinal plants. *Toxicology International* 23(3):207-211.
- **20. Tripathi MK**, Yasir M, Gurjar VS, Bose P, Dubey A, Shrivastava R (2015) Insights from the molecular docking of hydrolytic products of Methyle Isocyanate (MIC) to inhibition of human immune proteins. *Interdisciplinary Sciences: Computational Life Sciences* 7(3): 287-294. (I.F.-1.5)

- 21. Yasir M, Tripathi MK, Singh P, Prakash V, Sarkar R, Shrivastava R (2015) Efficacy of natural inhibitors from *Glycosmis pentaphylla* against protein kinase C: An *In silico* approach to combact skin cancer. *Oxidation Communications* 38(1):114-121. (I.F.-0.5)
- **22.** Yasir M, Singh P, **Tripathi MK**, Tayubi IA, Shrivastava R (2015) Antioxidant and antifungal activity of *Glycosmis pentaphylla* roots against dermatophytes and yeast-like fungi responsible for various skin ailments. *Oxidation Communications* 38(4):1622-1631. (I.F.-0.5)

## **Book Chapters:**

- **1. Tripathi MK**, Sharma S, Singh TP, Ethayathulla AS, Kaur P (2021) Computational Intelligence in Drug Repurposing for COVID-19. Computational Intelligence Methods in COVID-19: Surveillance, Prevention, Prediction and Diagnosis. 273-294 (DOI:10.1007/978-981-15-8534-0\_14)
- 2. Sharma P, **Tripathi MK**, Shrivastava SK. (2020) Cholinesterase as a drug target for drug development in Alzheimer's disease. Methods in Molecular Biology. 257-256 (ISBN No:978-1-0716-0162-4)
- **3. Tripathi MK**, Sinha J, Shrivastava SK, Kumar D. (2019) Bioinformatics in skin cancer: A system biology approach to understanding the molecular mechanisms and it's regulation. Skin Ageing and Cancer.101-11. (ISBN No.: 978-981- 13-2540-3).

#### **Patent Filed:**

1. Asthana RK, Singh U, Shrivastava SK, **Tripathi MK**. (2020) A chemical fingerprinting of a potent fraction from a cyanobacterium Arthrospira platensis through HR-LC/MS and in silico molecular docking: Identification of an antifungal (arachidonoyl dopamine) and anti-HIV as well as antibacterial (fluocinolone) biomolecules (BT/BPFC/04/209/2020-PID).

## **Conference Proceedings:**

- 1. Singh P, Yasir M, **Tripathi MK**, Shrivastava R (2016) Review: Anticancer perspectives of green silver nanoparticles: In proceedings of futuristic scope in Biotechnological advancement and allied instrumentation organised by Amity University, Raipur, Chhattisgarh (28-29 July 2016). 111-115 (ISBN: 9789352670888).
- 2. Shrivastava R, Singh P, Yasir M, **Tripathi MK**, (2016) Lipase-Catalyzed transesterification for biodiesel production from vegetable oil: A Review. In proceedings of World congress on applied science engineering & technology (WCASET16) organised by IFERP (02-03 January 2016): 59-61. (ISBN: 9788192958002).
- 3. Shrivastava R, **Tripathi MK**, Yasir M, Singh P, Tiwari A (2015) Molecular docking study to investigate role of toxic chemicals dumped in the UCIL, Bhopal in degradation of human immune protein. In proceedings of International Conference on Pharmaceutical, Medical & Environmental Health Sciences organised by ICPhaeME-PUNE (29 March 2015): 39-42. (ISBN: 9789382702849).
- **4.** Singh P, Yasir M, **Tripathi MK**, Shrivastava R (2014) A Review: Biomarkers for Glioblastoma using proteomics studies. In proceedings of the All India Seminar on Recent Advances in Biotechnology and Human Health Care organized by The Institution of Engineers Bhopal (29-30 March 2014): 47-51. (ISBN: 9783330041233)

#### **Conference and Scientific Presentations:**

- **1.** Presented a poster entitled "Identification of potential inhibitors targeting cholinesterase: an in silico and in vitro approach" in International conference Basel Life-2019 organized by EMBO-Basel Life, at Basel, Switzerland (09-12 September 2019).
- 2. Presented a paper entitled "Computational study for identification of potential inhibitors targeting achetylcholinesterase (AChE)" in International conference on Innovations and Translational Dimensions: Food, Health and Environmental Biotechnology (Biosangam 2018) organized by Department of Biotechnology, Motilal Nehru National Institute of Technology Allahabad (09-11 March 2018).
- **3.** Presented a paper entitled "Lipase-Catalyzed transesterification for biodiesel production from vegetable oil: A Review" in World congress on applied science engineering & technology (WCASET-16)" organised by IFERP (02-03 January 2016).
- **4.** Presented a paper entitled "Molecular docking study to investigate role of toxic chemicals dumped in the UCIL, Bhopal in degradation of human immune protein" in 23<sup>rd</sup> IRF International conference on pharmaceutical, medical& Environmental health sciences" organised by ICPhaeME-PUNE (29 March 2015).
- 5. Presented a paper entitled "Inhibition of human immunoproteins against pulmonary tuberculosis by Methyl Isocyanate using computational biology approach" in All India Seminar on Recent Advances in Biotechnology and Human Health Care organized by The Institution of Engineers Bhopal (29-30 March 2014).
- **6.** A poster entitled "Molecular modelling of methyl isocyanate, its hydrolytic products and residues dumped in (UCIL) Bhopal with human immune proteins" in International conference on Health, Environment & Industrial Biotechnology (Biosangam 2013) organized by Department of Biotechnology, Motilal Nehru National Institute of Technology Allahabad (21-23 Nov 2013).
- 7. A poster entitled "In-silico toxicity analysis of MIC against pulmonary tuberculosis" in National seminar on Science for shaping the future of India organized by Indian Science Congress Association Bhopal Chapter & MPCST Bhopal (30-31 Oct 2012).

## **Workshop and Training Attended:**

- **1.** Participated in EMBL-EBI Workshop on "Analysis of Genome Scale Data from Bulk and Single Cell Sequencing" organized by EMBL-EBI and National Institute of Biomedical Genomics, Kalyani, Kolkata (19-23 November 2018).
- **2.** Participated in Workshop on "Emerging Trends in Drug Design and Molecular Modelling" organized by IIT-BHU, Varanasi (19-21 July 2017).
- **3.** Participated in Short Term Training Programme on "*Frontiers of material science and technology*" organized by Maulana Azad National Institute of Technology, Bhopal (02-06 May 2016).
- **4.** Participated in International Workshop on "Softcomputing and Applications (ISCA-15)" organized by Indian Statistical Institute Kolkata and South Asian University New Delhi (25-27 March 2015).

- **5.** Participated in Short Term Training Programme on "Synthesis Characterization and Application of Biomaterial" organized by Maulana Azad National Institute of Technology, Bhopal (25-29 June 2014).
- **6.** Participated in interdisciplinary workshop on "Advanced Tools for Materials Characterizations" organized by Department of Chemical Engineering & Biotechnology & MSME, Maulana Azad National Institute of Technology, Bhopal (1-5 April 2013).
- **7.** Participated in Short Term Training Programme on "*Bioinformatics for Biologists*" organized by Department of Chemical Engineering & Biotechnology, Maulana Azad National Institute of Technology, Bhopal (18-22 March 2013).
- **8.** Participated in National seminar on "*Deployment and Collaboration of SPSS Reports and Models*" organized by Department of Management studies, Maulana Azad National Institute of Technology, Bhopal (15 Dec 2012).
- **9.** Participated in 2 Week Workshop on "*Introduction to Research Methodologies*" organized by IIT Bombay in Association with Maulana Azad National Institute of Technology, Bhopal (25 June-4 July 2012).
- **10.** Participated in the National seminar and workshop on "*Metabolic Networks and Drug Designing*" organized by MMV, Banaras Hindu University, Varanasi (28-30 Nov 2008).
- **11.** Participated in National Seminar on "*Intellectual Property Right Plant Varieties and Genome Conservation*" Organized by Dr. S.P.M. Govt Degree College Phaphamau Allahabad (14-15 Oct 2006).

## **Extra-Curricular Activities**

- **1.** Worked as Repertoire in 6th International Conference of International Academy of Physical Sciences on (Advances in Chemistry and Chemical Technology) organized by IIT (BHU) Varanasi (18-20 December 2020).
- **2.** Worked as Technical Committee Member in Short Term Training Programme on "Frontiers of material science and technology" organized by Maulana Azad National Institute of Technology, Bhopal (02-06 May 2016).
- **3.** Worked as Technical Committee Member in All India seminar on "Recent trends of Nanotechnology in Environmental and Biological Applications" organized by The Institution of Engineers Bhopal (22-23 Nov 2014).
- **4.** Worked as Committee Member in Short Term Training Programme on "Synthesis Characterization and Application of Biomaterial" organized by Maulana Azad National Institute of Technology, Bhopal (25-29 June 2014).
- **5.** Worked as Committee Member in All India Seminar on "Recent Advances in Biotechnology and Human Health Care" organized by The Institution of Engineers, Bhopal (29-30 March 2014).

## **Areas of Research Interest:**

- Chemoinformatics & Drug designing.
- ➤ Molecular dynamics simulation studies.
- ➤ Protein modelling and structure function relationship.
- > Structural Bioinformatics.
- Network & System biology for protein-protein interaction networks.
- > NGS data analysis.

## **References:**

#### 1. Prof. Rahul M Shrivastava

Department of Biological Science & Engineering Maulana Azad National Institute of Technology,

Bhopal, Madhya Pradesh, Pin-462003

Mobile No: +91-9981753702

Email: shrivastavarm1972@gmail.com, shrivastavarm@manit.ac.in

## 2. Prof. Sushant Kumar Shrivastava

Department of Pharmaceutical Engg & Technology

Indian Institute of Technology

Banaras Hindu University

Varanasi, Uttar Pradesh, Pin-221005

Mobile No: +91-9452156527

Email: skshrivastava.phe@iitbhu.ac.in

#### 3. Prof. Punit Kaur

Department of Biophysics

All India Institute of Medical Sciences

New Delhi, Pin-110029

Mobile No: +91-99100 26423

Email: punitkaur1@hotmail.com

# 4. Dr. Abhigyan Nath

Medical Biotechnology Division,

Department of Biochemistry,

Pt. Jawahar Lal Nehru Memorial Medical College

Raipur, CG-492001

Mobile No: +91-9956015187

Email: abhigyannath01@gmail.com

#### **Declaration:**

I hereby declare that all information furnished above is true to the best of my knowledge and the document in support of the information will be forwarded whenever it required.

(Manish Kumar Tripathi)