

Dr Navaneet Chaturvedi

Current Position: Assistant Professor-II, Amity Institute of Biotechnology, Amity University, Noida, India (Joined: Sept 25, 2023).

E-mail: 14.navneet@gmail.com ; **ORCID** : 0000-0002-4265-9255, **LinkedIn:** <https://www.linkedin.com/in/navaneet-chaturvedi-04b3414a/> **Gender:** Male; **Date of Birth:** January 14, 1984; **Nationality:** INDIA; **Passport:** INDIA, **Marital Status:** Married, **Mobile/WhatsApp:** +91-9451067728; **Skype:** navneetonskype1

#BACKGROUNDS / RESEARCH AREAS

Structural bioinformatician	Computational biophysics	Computational chemistry	Structural Research
Protein-Protein interactions	Bio-molecular interactions	Molecular Dynamics Simulations	Computational Modelling
AI/ML	QM/MM	Protein Folding	Molecular Docking
Molecular Modelling	Free Energy Perturbation	Structure prediction	Sequence & Phylogenetic Analysis
Python	MATLAB	Microbiology	Molecular Biology techniques

#TOOLS/SOFTWARE Gromacs, Python, AMBER, PyMOL, VMD, Avogadro, Coot,

#PROFESSIONAL PROFILE

Structural bioinformatician and computational (bio)chemist with over **7 years of post-PhD experience**, specializing in **structural Bioinformatics/Biology**, disease-focused research, and rational drug discovery. Expertise spans **computational protein biochemistry**, protein structure-function analysis, and biomolecular interactions, including protein-protein, protein-DNA/Metals, and protein-ligand systems. Actively integrates **machine learning with physics-based simulations** to achieve high-confidence predictions of molecular recognition and dynamics. Proficient in advanced MD and free-energy methods, including **GROMACS, AMBER, FEP, umbrella sampling, QM/MM, replica-exchange MD**, and structure-based and ensemble docking workflows.

#EDUCATION:

Course	Institution	Award Date		Publications/ Remark
PhD (Bioinformatics) Title: “ <i>In silico</i> analysis and characterization of metal binding proteins of microbial system with reference to heavy metal tolerance”	Center of Bioinformatics, IIDS, University of Allahabad, India Supervisor: Prof P N Pandey	Start	Awarded	05 / Awarded
		November 05, 2009	October 27, 2014	
Master of Science (Bioinformatics) Project: Prediction of Transmembrane proteins prediction using machine learning	Center of Bioinformatics, IIDS, University of Allahabad, India	July 2006	July 2008	01 / Passed (First Div)

#TEACHING EXPERIENCE

- Assistant Professor : Univ. of Information Science and Technology, Ohrid, **Macedonia. (10 Months)**
- Visiting Lecturer : Ashoka Institute of Management and Science, Varanasi, **India (06 Months)**
- Teaching (As a PhD Student) : University of Allahabad, Prayagraj, **India. (04 Years)**

#RESEARCH EXPERIENCE & ACCOMPLISHMENTS (07.5 Years)

	Organization	Country	Position & Tenure	Duties	Accomplishments
0	Amity University, Noida, Delhi NCR (Current)	India	Assistant Professor-II (Current position) Sept 2023 to continuing	Teaching, Research, research activities, organizing conferences/ seminars, Drug discovery projects	□ Published research articles/reviews/chapters. □ Books proposals □ Taught Master and bachelor students
1.	PharmCADD	South Korea (Remote)	Senior Scientist 2022 - 23 (13 Months)	Molecular Dynamics simulation, Free energy calculation, QM/MM, AI & Contribution to ongoing projects	• First Industry Experience • Studied basic ML & AI

2.	University of Leicester	<i>The United Kingdom</i>	Research Associate 2020 - 21 (15 Months)	Replica Exchange Molecular Dynamics simulation, Ensemble docking, Seminar, Discussion and Academic writing	- Promotion of NMR exchange format to scientific community - Published 04 articles in collaboration
3.	University of Information Science and Technology, St Paul the Apostle, Ohrid	<i>North Macedonia</i>	Assistant Professor 2019 – 20 (10 Months)	Taught 5 lectures in a week, Writing research proposal, Molecular Dynamics simulation, Seminar, Discussion and Academic writing, Interim-Dean	- Designed and published research work - Established collaboration with South Korea
4.	School of Biochemical Engineering, IIT(BHU), Varanasi	<i>India</i>	Research Associate 2018 – 19 (13 Months)	<i>In-silico</i> experiments set-up, Research, Suggestions to PhD students, Discussion/seminar, Research writing	- Teaching/Advice/Discussion to PhD students - Published Articles 2, 6, 9 & 11
5.	Tel-Aviv University, Tel-Aviv	<i>Israel</i>	Postdoc researcher 2013 – 17 (46 Months)	Research, Set-up wet lab (<i>In-vitro</i>) experiments, Set-up <i>in-silico</i> experiments and Seminar	- Published 02 research articles. - Completed three projects on structural biology/bioinformatics. - Established collaboration with pharma company.

#OTHER COLLABORATIVE PROJECTS

Completed 08 projects by establishing collaboration with the lab of *India, Israel, Korea, Saudi Arabia*.

#AWARDS & FELLOWSHIPS

Award	Agency	Year
Project JRF	Department of Biotechnology (DBT), New Delhi, <i>India</i>	2009
Young Scientist Award	International Academy of Physical Sciences at SVNIT, Surat, <i>India</i>	2011
3 rd Best Poster Presentation	Tel Aviv University, <i>Israel</i>	2016
Award of Appreciation for Online Training on Advanced Bioinformatics	Bansal Institute of Engineering and Technology, Lucknow, <i>India</i>	2020

Fellowships	Agency	Institution	Duration (Months)
Post-Doctorate (2014-17)	PBC (Planning and Budgeting Committee), <i>Israel</i>	Tel Aviv University, <i>Israel</i>	36
Post-Doctorate (2013-14)	Ministry of Foreign Affairs, <i>Israel</i>	Tel Aviv University, <i>Israel</i>	08
DPhil (2009-13)	University Grant Commission, New Delhi, <i>India</i>	University of Allahabad, <i>India</i>	48
Project JRF (2009)	Department of Biotechnology, New Delhi, <i>India</i>	GB Pant University of Agriculture & Technology, <i>India</i>	04

#INVITED LECTURE / TALK / ORGANIZE CONFERENCES

- Delivered *lecture* : Ashoka Institute of Science and Management, Varanasi, *India* (2015).
- Organize a workshop : Event of “2nd workshop on Bioinformatics 2015” at Ashoka Institute of Science and Management, Varanasi, *India* (2015).
- *Invited lecture* : 05 invited lectures have been delivered in International conferences.
- Delivered lectures : Bansal Institute of Sciences and Technology, Lucknow, *India* (2020).
- Organized a workshop : **3 days** at Bansal Institute of Sciences and Technology, Lucknow, *India* (2020).
- Presented 18 Papers/posters in National/International conferences.
- Delivered a *talk* entitled “*Insights into System Biology mediated Structural Bioinformatics & Modelling Algorithms for Advanced Research*” at Manipal Academic of Higher Education (Private University in Manipal), Karnataka, India

#LIST OF PUBLICATIONS

#PATENTS

02 patents have been granted and additional 02 patents have been filed and are currently under examination. (detail will be furnished as per the call)

#EDITED BOOK

1. Vuister, G. W., Kumar, A., **Chaturvedi, N.**, & Santoyo, G. (Eds.). **2026. *Emerging Omics Technologies for Sustainable Agriculture***. Academic Press (Elsevier). ISBN: 978-0443403163. DOI: 10.1016/C2024-0-02023-1 (Published)
2. Chaturvedi, N., Kumar V., (2026) Structural Biology of Ubiquitination, Academic Press (Elsevier). ISBN: 9780443449741 (To be published on October 2026)
3. Jasleen G, Chaturvedi N., Kumar V, Nachliel, E (2026), COMPUTATIONAL MODELING AND INTELLIGENT SYSTEMS IN HEALTHCARE: EXPLAINABLE AI, NETWORKS, AND TRANSLATIONAL APPLICATIONS (To be published in April 2027)

#BOOK CHAPTERS

1. Lalwani H., Arora Y., Narula S. S., Rawal K, **Chaturvedi N***. (2026), Study of Deep Learning and Bioprospecting for Black Fungus Identification and Treatment, *ed: Integrative Approach to Fungal Infections and Bioprospecting for Drug Discovery*, 1, 19.
2. Sharma, K., Tushita, Rawal, K., Yashi, & **Chaturvedi, N***. (2026). Machine learning models for crop yield prediction. In *Emerging Omics Technologies for Sustainable Agriculture* (pp. 201–225). doi:10.1016/b978-0-443-40316-3.00009-6
3. **Chaturvedi, N.**, Zaidi, A., Dhiman, I., Jigyasa, Kumar, D., Pandey, R., ... Sinha, D. (2026). Machine learning innovations for accurate crop yield forecasting. In *Emerging Omics Technologies for Sustainable Agriculture* (pp. 401–424). doi:10.1016/b978-0-443-40316-3.00017-5
4. Malhotra, Y., Yadav, D., **Chaturvedi, N.**, Gujar, A., John, R., & Ahmad, K. (2025). AI in infectious disease diagnosis and vaccine development. *Methods in Microbiology*. Academic Press. <https://doi.org/10.1016/bs.mim.2024.12.005> .
5. Arora Y., Lalwani H., Kumar A, Mathur P., **Chaturvedi N.**, Mishra V. (2025), AI-Driven antimicrobial peptides for drug development. In *Methods in Microbiology*. Elsevier. <https://doi.org/10.1016/bs.mim.2024.08.003> (In press)
6. Yadav, M. K., Tripathi, M. K., **Chaturvedi, N.**, Nath, A., & Kumar, U. (2025). Chapter 12 - Deep learning in predictive medicine: Current state of the art. In K. Raza (Ed.), *Deep Learning in Genetics and Genomics* (pp. 261–291). Elsevier, <https://doi.org/10.1016/B978-0-443-27574-6.00008-4>
7. Sinha, S., Goyal, A., Singh, R., & **Chaturvedi, N***. (2024). Sustainable nanomaterials for chromium removal from wastewater. *Advances in Chemical Pollution, Environmental Management and Protection*. Elsevier. <https://doi.org/10.1016/bs.apmp.2024.10.003> .
8. Shahid, R., Shahid, S., Gund, J., & **Chaturvedi, N***. (2024). AI-based advances in crop disease detection and health improvement. In *Methods in Microbiology*. Elsevier. <https://doi.org/10.1016/bs.mim.2024.08.001>
9. Mishra, V., Mishra, S. K., Srivastava, A., Dubey, C. K., Dharmani, K., & **Chaturvedi, N.** (2024). Leveraging artificial intelligence (AI) and machine learning (ML) for enhanced drug discovery and development from microbes. In *Methods in Microbiology* (pp. 125–140). Elsevier. <https://doi.org/10.1016/bs.mim.2024.05.005> .
10. **Chaturvedi, N.**, Yadav, M. K., & Sharma, M. (2024). Applications of artificial intelligence and machine learning in microbial diagnostics and identification. In *Methods in Microbiology* (pp. 213–230). Elsevier. <https://doi.org/10.1016/bs.mim.2024.05.013>
11. Dharmani, K., Sinha, A., & **Chaturvedi, N***. (2024). AI-driven microbial medicine development. In *Methods in Microbiology* (pp. 101–124). Elsevier. <https://doi.org/10.1016/bs.mim.2024.05.008>
12. Vivek Kumar Soni,, **Navaneet Chaturvedi**, Dhananjay Shukla and Naveen Kumar Vishvakarma (2023) Mushrooms Against Malignancies: from Chemosensitization to Immunopotentiality, *Mushrooms: A Wealth of Nutraceuticals and An Agent of Bioremediation*, 9-34 (26). Springer, DOI: 10.2174/9789815080568123010005 .
13. Soni, V. K., Shukla, D.,....**Chaturvedi N.**....., Vishvakarma, N. K. (2022). Antineoplastic effects of curcumin against colorectal cancer: Application and mechanisms. In D. Shukla, N. K. Vishvakarma, & G. P. Nagaraju (Eds.), *Colon cancer diagnosis and therapy* (Vol. 3). Springer, Cham. https://doi.org/10.1007/978-3-030-72702-4_18
14. Mehta A.....**Chaturvedi N.** (2021) Short-Chain Fatty Acids as Therapeutic Agents in Colon Malignancies. In: Nagaraju G.P., Shukla D., Vishvakarma N.K. (eds) *Colon Cancer Diagnosis and Therapy*. Springer, Cham. https://doi.org/10.1007/978-3-030-63369-1_10.

#RESEARCH ARTICLES

15. **Chaturvedi, N***, Mishra, V, Haque, S., Khatoon, S. Rawal, Kamal; Kumar, V., (2026) Leveraging Advanced AI Frameworks for Dual PPAR α/γ Agonist Discovery in Alzheimer's Disease, *ACS Chemical Neuroscience* (Accepted, June 25, 2026). [IF: 4.5]
16. Aggarwal, H., Chaudhary, D., Kumari, T., Pradhan, N., Mishra, V., Kumar, A., ...**Chaturvedi, N.**, Joshi, N. C. (2026). Chlorpyrifos degradation by *Zhihengliuella* sp. ISTPL4: An esterase-driven actinobacterial platform for organophosphorus bioremediation. *Journal of Hazardous Materials Advances*, 22(101239), 101239. doi:10.1016/j.hazadv.2026.101239 [IF: 9.1]
17. Bantun, F., **Chaturvedi, N***, Jalal, N. A., Faidah, H., Babalghith, A. O., Aldairi, A. F., ... Kumar, V. (2026). Molecular dynamics-driven optimization of triterpenoid, amidinium, and flavonoid inhibitors targeting dengue NS2B-NS3 protease. *Computational Biology and Chemistry*, 109013. doi:10.1016/j.compbiolchem.2026.109013 [IF: 3.4]
18. Singh, K., Negi, C., Kumar, A., **Chaturvedi, N***, & Vyas, P. (2025). Heavy Metal Toxicity in Cereals: Uptake Mechanisms, Physiological Impacts, and Mitigation Strategies. *Toxics*, 13(12), 1074. [IF: 4.9]
19. Malhotra, Y., John, J., Yadav, D., Sharma, D., Vanshika, Rawal, K., ... **Chaturvedi, N.*** (2025). Advancements in protein structure prediction: A comparative overview of AlphaFold and its derivatives. *Computers in Biology and Medicine*, 188, 109842. <https://doi.org/10.1016/j.compbiomed.2025.109842> [IF: 7.0]

20. Dudeja, C., Masroor, S., Mishra, V.,.... **Chaturvedi N** et al. (2025) Cyanobacteria-based bioremediation of environmental contaminants: advances and computational insights. *Discov Agric* 3, 42. <https://doi.org/10.1007/s44279-025-00193-9>
21. Yadav, M. K., Dahiya, V., Tripathi, M. K., **Chaturvedi, N.**, Rashmi, M., Ghosh, A., & Raj, V. S. (2024). Unleashing the future: The revolutionary role of machine learning and artificial intelligence in drug discovery. In *European Journal of Pharmacology* (Vol. 985, p. 177103). Elsevier BV. <https://doi.org/10.1016/j.ejphar.2024.177103> [IF: 5.7]
22. Karthic, A.; Kesarwani, V.; Singh, R.K.; Yadav, P.K.; **Chaturvedi, N.**; Chauhan, P.; Yadav, B.S.; Kushwaha, S.K. (2022) Computational study reveals monomethylated triazolopyrimidine as a novel inhibitor of SARS-CoV-2 RNA-dependent RNA polymerase (RdRp), *Molecule*, 27, 801. [IF: 5.1].
23. Choudhary, D. K., **Chaturvedi, N.**, Singh, A., & Mishra, A. (2022). Catechin isolated from faba beans (*Vicia faba* L.): insights from oxidative stress and hypoglycemic effect in yeast cells through confocal microscopy, flow cytometry, and in silico strategy. *Journal of biomolecular structure & dynamics*, 40(20), 10470–10480. [IF: 2.4]
24. Mutaib MM, **Chaturvedi N.**, et al (2021) Biocomputational Prediction Approach Targeting FimH by Natural SGLT2 Inhibitors: A Possible Way to Overcome the Uropathogenic Effect of SGLT2 Inhibitor Drugs, *Molecules*, 26(3), 582 (Equally contributed with first author). [IF: 5.1].
25. V. K. Soni, A. Mehta, Y. K Ratre, A. K. Tiwari, A. Amit, R. P. Singh, S. C. Sonkar, **N. Chaturvedi**, D. Shukla, N. K. Viswakarma (2020) Curcumin, a traditional spice component, can hold the promise against COVID-19?, *European Journal of Pharmacology*, 886, 173551. [IF: 5.7].
26. Singh, S., **Chaturvedi, N.**, & Rai, G. (2020). De novo modeling and structural characterization of IL9-IL9 receptor complex: A potential drug target for hematopoietic stem cell therapy. *Netw Model Anal Health Inform Bioinforma*, 9, 29. [IF: 2.4].
27. **Chaturvedi, N.**, Nachliel, E., & Gutman, M. (2020). Characterization of Pre-Dissociative Structures of the E6AP Trimer by All-atom Unbiased Molecular Dynamics. In *Israel Journal of Chemistry* (Vol. 60, Issue 7, pp. 744–753). [IF: 2.1].
28. Choudhary, D. K., **Chaturvedi, N.**, Singh, A., & Mishra, A. (2020). Investigation of hypoglycemic effects, oxidative stress potential and xanthineoxidase activity of polyphenols (gallic acid, catechin) derived from faba bean on 3T3-L1 cell line: Insights into molecular docking and simulation study. *Toxicology Research*, 9(3), 308-322. [IF: 2.9].
29. **N Chaturvedi***, K Ahmad, BS Yadav, EJ Lee, SC Sonkar, N Marina, I Choi (2020), Understanding Calcium-Dependent Conformational Changes in S100A1 Protein: A Combination of Molecular Dynamics and Gene Expression Study in Skeletal Muscle, *Cells* 9 (1), 181. [IF: 6.0]
30. BS Yadav, **N Chaturvedi**, N Marina (2019) Recent Advances in System Based Study for Anti-Malarial Drug Development Process, *Current pharmaceutical design* 25 (31), 3367-3377. [IF: 3.2]
31. D K Choudhary, **N Chaturvedi**, A Singh, A Mishra (2019), Characterization, inhibitory activity and mechanism of polyphenols from faba bean (gallic-acid and catechin) on α -glucosidase: insights from molecular docking and simulation study, *Preparative Biochemistry & Biotechnology* 50 (2), 123-132. [IF: 1.9]
32. Khurshid Ahmad, Vishal M. Balaramnavar, **Chaturvedi N.**, Inho Choi (2019), Targeting Caspase 8: Using structural and ligand-based approaches to identify potential leads for the treatment of multi-neurodegenerative diseases, *Molecules* 24 (9), 1827. [IF: 5.1]
33. **Chaturvedi N***, Mishra Abha, Rawat Varun (2019), Synthesis and Characterization of Oxygen Depleted Tert-Amine Calix[4]Arene Ligands and Study the Effect on Sigma Non-Opioid Intracellular Protein Receptor, *Struct Chem* 30, 1899–1910. [IF: 2.3]
34. Yadav BS, **Chaturvedi N**, Yadav P, Marina N, Ganash M, Barreto GE, Ashraf GM, Baig MH(2019) Protein modelling, molecular network and molecular dynamics study of newly sequenced interleukin-18 (IL-18) gene in *Mus musculus*, *Journal of cellular physiology* 234 (8), 14285-14295. (equally contributed) [IF: 4.0].
35. **Chaturvedi N***, Brijesh Singh Yadav , Paras Nath Pandey, Vijay Tripathi (2017) The effect of the β -glucan and its Potential Analog on the Structure of Dectin-1 Receptor, *Journal of Molecular Graphics and Modelling*, Vol74 315–325. [IF: 3.1].
36. Yadav PK, Yadav BS, Panigrahi PN, Tripathi V, **Chaturvedi N**, Kataria M., (2017) Molecular characterization and insilico analysis of the tissue inhibitor of metalloproteinases-3 (TIMP-3) gene of canine mammary tumor, *Comb Chem High*, Vol-20 1-12. [IF: 1.7].
37. HariKrishna Pillai, Yadav BS, **Chaturvedi N** et al. (2017), Protein modelling and molecular dynamics simulation of cloned Regucalcin (RGN) gene from *Bubalus bubalis*, *Comb Chem High*. Vol- 20, 186-192. [IF: 1.7]
38. Amber-Vitos O, **Chaturvedi N**, Nachliel E, Gutman M, Tsfadia Y. (2016), The effect of regulating molecules on the structure of the PPAR-RXR complex, *Biochim Biophys Acta*. 2016 Nov; 1861(11):1852-1863. [IF: 3.8].
39. **Chaturvedi N***, Micheal Kaszik, Stephen Forsythe, Paras Nath Pandey (2015), Protein Sequences Insight into Heavy Metal Tolerance in *Cronobacter sakazakii* BAA-894 encoded by Plasmid pESA3, *Archives of Microbiology*, 197, 11411149. [IF: 3.4].
40. **Chaturvedi N*** Paras Nath Pandey (2014), Phylogenetic analysis of Gammaproteobacterial arsenate reductase proteins specific to Enterobacteriaceae family, signifying arsenic toxicity suggests importance of Enterobacter species in arsenic toxicity, *Interdiscip Sci.*, 6(1): 57-62. [IF: 5.2]
41. **Chaturvedi N***, Vinay Kumar Singh, Paras Nath Pandey (2013), Computational identification and analysis of arsenate reductase protein in *Cronobacter sakazakii* ATCC BAA-894 suggests potential microorganism for reducing arsenate, *J Struct Funct Genomics.*, 14(2):37-45.
42. **Chaturvedi N*** et al. (2011) Hidden Markov Model for the Prediction of Transmembrane proteins using MATLAB, *Bioinformation* 7(8): 418- 421.
43. Raksha Singh, **Chaturvedi N** and Vinay Kumar Singh (2012), *In-silico* study of novel herbal compounds (Baicalin, Curcumin and Dronabinol) as MAO inhibitors for Parkinson's disease treatment, *International journal of Life science & Pharma Research*, 2(3) 81-98.
44. A. Rahman, **Chaturvedi N** et al (2013), Computational protein modeling and Analysis of UV-stress protein in *Synechocystis sp.* PCC 6803, *Bioinformation*, 9(12): 639-644.
45. **Chaturvedi N*** and Pandey PN (2011) *In Silico* Genome Analysis of Gammaproteobacteria with Reference to Metal Binding Sites, *Proceedings of International Acad. of Physical Sciences*, vol. 15, (special issue) pp. 501-50
46. S C Sonkar, A Mishra, **N Chaturvedi*** (2019), A Road-map to Tackle the Challenges of Antimicrobial Resistance: Act Today for Better Tomorrow, *EC Microbiology* 15 (10), 1154-1156.
47. **Chaturvedi N*** and Pandey PN (2020) Molecular Dynamical Investigation of a YodA Protein Signifies Zinc IonResidues Interactions, *International Acad. of Physical Sciences* 24(1) 105-114.
48. Soni VK, Mehta A, Sharma K, Ratre YK, Dwivedi M, **Chaturvedi N**, et al. (2022) Immunity boosters in COVID-19: Reality or myth? *Med India*, 1:3. doi:10.25259/MEDINDIA_1_2021.