


NAME	Dr Navaneet Chaturvedi	
DESIGNATION	Assistant Professor-II	
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CONTACT NUMBER	9451067728	
RESEARCH INTERESTS	Structural Bioinformatics, Computational Drug Design, Computational (Bio)chemistry, Biomolecular Interactions study, ML, AI	

EDUCATIONAL QUALIFICATIONS:

Name of College / University	Degree	Year
Center of Bioinformatics, University of Allahabad	Master of Science (Bioinformatics)	2008
Center of Bioinformatics, University of Allahabad	DPhil (Bioinformatics)	2014

Title of Ph.D. thesis:

EXPERIENCE (in chronological order): Total 20 Years Research & Teaching

Designation	Type of post held (teaching/ research)	Name of the Institute	Year (From – To)
PostDoc	Research	Tel Aviv University, Israel	2013-2017
Research Associate	Research	School of Biochemical Engineering, IIT(BHU), India	2018-2019
Assistant Professor	Teaching and Research	University of Information Science and Technology, St Paul the Apostle, Ohrid, North Macedonia	2019-2020
Research Associate	Research	University of Leicester, UK	2020-2021
Scientist	Research	PharmCADD India Pvt Ltd, Hyderabad	2022-2023

No. of Ph.D. students supervised

No. of Post-Doc

No. of M.Tech. Students supervised:

No. of B.Tech. Students supervised:

PUBLICATIONS

(mention total no. here)

Details:

1. 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 <https://doi.org/10.3390/molecules27030801>.

2. D K Chaodhary, **N Chaturvedi**, A Singh, A Mishra (2021) 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 and Dynamics* <https://doi.org/10.1080/07391102.2021.1945953>.
3. 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, <https://doi.org/10.3390/molecules26030582> (*Equally contributed with first author*).
4. 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 <https://doi.org/10.1016/j.ejphar.2020.173551>.
5. **N Chaturvedi**, E Nachliel, M. Gutman (2020) Characterization of Pre-Dissociative Structures of the E6AP Trimer by All-atom Unbiased Molecular Dynamics, *Israel Journal of Chemistry*, doi.org/10.1002/ijch.202000016.
6. D K Chaodhary, **N Chaturvedi**, A Singh, A Mishra (2020) Investigation of hypoglycaemic effects, oxidative stress potential and xanthine-oxidase activity of polyphenols (gallic-acid, catechin) derived from faba bean on 3 T3-L1 Cell line: insights through molecular docking and simulation study, *Toxicology Research*, doi.org/10.1093/toxres/tfaa025.
7. **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.
8. 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.
9. 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.
10. Khurshid Ahmad, Vishal M. Balaramnavar, **Chaturvedi N.**, Saif Khan, Shafiul Haque, Yong-Ho Lee, 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.

11. **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 DOI: 10.1007/s11224-019-01324-x.
12. 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 with first author*).
13. **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.
14. 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.
15. 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.
16. 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.
17. **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.
18. **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.
19. **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.
20. **Chaturvedi N*** et al. (2011) Hidden Markov Model for the Prediction of Transmembrane proteins using MATLAB, *Bioinformatics* 7(8): 418- 421.
21. 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*

	<p><i>Life science & Pharma Research</i>, 2(3) 81-98.</p> <p>22. A. Rahman, Chaturvedi N <i>et al</i> (2013), Computational protein modeling and Analysis of UV-stress protein in <i>Synechocystis sp. PCC 6803</i>, <i>Bioinformatics</i>, 9(12): 639-644.</p> <p>23. Chaturvedi N* and Pandey PN (2011) <i>In Silico</i> Genome Analysis of Gammaproteobacteria with Reference to Metal Binding Sites, <i>Proceedings of International Acad. of Physical Sciences</i>, vol. 15, (special issue) pp. 501-50</p> <p>24. S C Sonkar, A Mishra, N Chaturvedi* (2019), A Roadmap to Tackle the Challenges of Antimicrobial Resistance: Act Today for Better Tomorrow, <i>EC Microbiology</i> 15 (10), 1154-1156.</p> <p>25. S Singh, N Chaturvedi, G Rai (2020) <i>De novo</i> modeling and structural characterization of IL9-IL9 receptor complex: A potential drug target for hematopoietic stem cell therapy, <i>Network Modeling Analysis in Health Informatics and Bioinformatics</i>. doi.org/10.1007/s13721-020-00236-9.</p> <p>26. Chaturvedi N* and Pandey PN (2020) Molecular Dynamical Investigation of a YodA Protein Signifies Zinc IonResidues Interactions, <i>International Acad. of Physical Sciences</i> 24(1) 105-114.</p> <p>27. Soni VK, Mehta A, Sharma K, Ratre YK, Dwivedi M, Chaturvedi N, et al. (2022) Immunity boosters in COVID-19: Reality or myth? <i>Med India</i>, 1:3. doi:10.25259/MEDINDIA_1_2021</p> <p>28. 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) <i>Colon Cancer Diagnosis and Therapy</i>. Springer, Cham. https://doi.org/10.1007/978-3-030-63369-1_10.</p> <p>29. Soni V.K. et al. (2022) Antineoplastic Effects of Curcumin Against Colorectal Cancer: Application and Mechanisms. In: Shukla D., Vishvakarma N.K., Nagaraju G.P. (eds) <i>Colon Cancer Diagnosis and Therapy Vol. 3</i>. Springer, Cham. https://doi.org/10.1007/978-3-030- 72702-4_18.</p>
PATENTS (<i>total no.</i>)	<i>Details: 01 Processed (Israel)</i>
RESEARCH PROJECTS Completed: (<i>total no.</i>) Ongoing: (<i>total no.</i>)	<i>Details:</i>
AWARDS & HONOURS/ DISTINCTIONS	<p><i>Details: 1. Project JRF (from DBT) at GB Pant University of Agriculture & Technology, Pantnagar, Uttarakhand</i></p> <p><i>2. Best Poster Award at Tel Aviv University, Israel</i></p> <p><i>3. Young Scientist Award at SVNIT, Surat, Gujrat</i></p> <p><i>4. Postdoc Fellowship from Ministry of foreign affairs, Israel</i></p> <p><i>5. PBC fellowship from Government of Israel</i></p> <p><i>6. MRC Fellowship, UK</i></p>
MEMBERSHIP with Professional/ Academic bodies	<p><i>Details: 1. Indian Biophysical Society, India</i></p> <p><i>2. Bioclues Organization, India</i></p> <p><i>3. International Academy of Physical Sciences, India</i></p>

