

Dr Navaneet Chaturvedi

(Research Associate)

Prof Geerten Vuister's Lab: 018,

Henry Wellcome Building,

University of Leicester, LE2 7RH, UK

E-mail : 14.navaneet@gmail.com, ORCID : [0000-0002-4265-9255](https://orcid.org/0000-0002-4265-9255)

Sex: Male, Date of Birth : January 14, 1984 (India)

Whats-app: +91-9451067728, Mobile: +44-7717678825

#Present work Aims to develop methodology for generating ensembles that better reflect the dynamical properties of the biomolecule from readily available NMR data.

#Research Interest Protein-Protein interaction, Protein-Small-compound interaction, Molecular Dynamics Simulation, Molecular Modeling, Protein Engineering, Protein Folding, Structure-Function relationship, Structure prediction.

#Research Experience**Post-Doctoral Experience**

Mentors : Prof. Gali Prag, Dr. Yossi Tsfadia & Prof (Emeritus) Menachem Gutman
 Institution : Department of Biochemistry and Molecular Biology,
Tel Aviv University, Israel.
 Duration : From December 01, 2013 to Sept 30, 2017 (**45 months**)

Researcher (Collaboration with Tel Aviv University, Israel)

Mentor : Prof Dr. Abha Mishra, School of Biochemical Engineering, **IIT(BHU), India**
 Duration : From February, 2018 to February 2019

Research Associate (University of Leicester, the United Kingdom)

Mentor : Prof Geerten Vuister, Department of Molecular and Cell Biology, Henry
 Wellcome Building, **University of Leicester, UK**
 Duration : From March 03, 2020 to October 20, 2021

Note: Project was terminated due to COVID19 in October 2021.

#Teaching Experience

- Worked around a year as an **Assistant Professor** and **interim-Dean** at University of Information Science and Technology, St Paul, The Apostle, **Ohrid, North Macedonia**.
- Around 4-years **teaching** experience (during DPhil) to Bachelor and Master Students from June 2009 to May 2013 at University of Allahabad, Allahabad, **India**.

#Educational Qualification**DPhil (Bioinformatics)**

Thesis Title : "In silico analysis and characterization of metal binding proteins of microbial system with reference to heavy metal tolerance"
 Institution : Center of Bioinformatics, IIDS, University of Allahabad, Prayagraj, **India**
 Awarded : October 27, 2014

Master of Science (MSc) in Bioinformatics from center of Bioinformatics, IIDS, University of Allahabad, Prayagraj, **India** [Aug 2006 to July 2008].

Post Graduate Diploma in Bioinformatics from Dev Sanskriti Vishwavidyalaya, Gayatrikunj, Haridwar, Uttarakhand, **India** [July 2004 to June 2005].

Bachelor of Science (BSc) Botany and Chemistry from VBS Purvanchal University, **India** [2000-2003].

#Achievements**Award / Honor Received**

- **Award of Junior Research Fellowship** from Department of Biotechnology (DBT), New Delhi, India in 2009
- **Young Scientist Award** in 14th International Conference of International Academy of Physical Sciences at SVNIT, Surat, **India** on December 22-24, 2011.
- **3rd best poster and presentation** in departmental retreat program at Tel Aviv University, **Israel**, Feb 15, 2016.
- **Certificate of Appreciation for Online Training on Advanced Bioinformatics** from Department of Biotechnology, Bansal Institute of Engineering and Technology, Lucknow, **India** on July 13 – August 07, 2020.

Fellowship Received

- Post-doc Fellowship from PBC (Planning and Budgeting Committee), **Israel** (in 2014) : **3-years**
- Post-doc Fellowship from MFA (Ministry of Foreign Affairs-**Israel**) (in 2013) : **8-months**

- Award of University Grant Commission (UGC) research fellowship, since Nov, 2009 to Oct, 2013 for doing research at University of Allahabad, **India**.
- Received fellowship of Department of Biotechnology (DBT), New Delhi for the position of Project JRF at G. B. Pant University of Agriculture of Technology, Pantnagar, (Uttarakhand) **India** (in 2009).

Invited Lecture/Talk

- Delivered **lecture** and worked as **main resource person** of an event “2nd workshop on Bioinformatics 2015” at Ashoka Institute of Science and Management, Varanasi, India on 06, 07 Nov 2015. Covered protein modeling and molecular dynamics simulation.
- Delivered **lecture** in International conference of International Academy of Physical Sciences (CONIAPS-XXI) on 28-30 October, 2017 at Hisar, Haryana, India.
- Main resource person and delivered lectures for three days at Bansal Institute of Sciences and Technology, Lucknow in July 23-25, 2020.

Conferences

Presented 15 Papers/posters in National/International conferences (certificates will be furnished as per ask).

#List of Publications

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>. [IF: 4.412]
2. D K Chaudhary, **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>. (IF: 2.99).
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 contribution**). [IF: 4.412]
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>. (IF: 4.432)
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 . (IF: 3.33)
6. D K Chaudhary, **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/taaa025. (IF: 3.524)
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. (IF: 6.60)
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. (IF: 3.116)
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. (IF: 2.162)
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. [IF: 4.412]
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. (IF: 1.887)
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 (**Equal Contribution**). (IF: 6.384)
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. (IF: 2.518)

14. Yadav PK, Yadav BS, Panigrahi PN, Tripathi V, **Chaturvedi N**, Kataria M., (2017) Molecular characterization and in-silico analysis of the tissue inhibitor of metalloproteinases-3 (TIMP-3) gene of canine mammary tumor, *Comb Chem High*, Vol-20 1-12. (IF: 1.339)
15. Harikrishna Pillai, Yadav BS, **Chaturvedi N** et al. (2017), Protein modeling and molecular dynamics simulation of cloned Regucalcin (RGN) gene from Bubalus bubalis, *Comb Chem High*. Vol- 20, 186-192. (IF: 1.339)
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. (IF: 4.698)
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, 1141-1149. (IF: 2.552)
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. (IF: 2.233)
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, *Bioinformation* 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 Life science & Pharma Research*, 2(3) 81-98.
22. 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.
23. **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
24. 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.
25. S Singh, **N Chaturvedi**, G Rai (2020) De novo modeling and structural characterization of IL9-IL9 receptor complex: A potential drug target for hematopoietic stem cell therapy, *Network Modeling Analysis in Health Informatics and Bioinformatics*. doi.org/10.1007/s13721-020-00236-9.
26. **Chaturvedi N*** and Pandey PN (2020) Molecular Dynamical Investigation of a YodA Protein Signifies Zinc Ion-Residues Interactions, *International Acad. of Physical Sciences* 24(1) 105-114.
27. 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

Book Chapter

1. 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.
2. 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) *Colon Cancer Diagnosis and Therapy* Vol. 3. Springer, Cham. https://doi.org/10.1007/978-3-030-72702-4_18.

References

| <u>DPhil Supervisor</u> | <u>Post-Doc Mentor</u> | <u>Post-Doc Mentor</u> | <u>Post-Doc Mentor</u> | <u>Post-Doc Mentor</u> |
|---|--|--|--|---|
| Prof P N Pandey (Ex-Head) Department of Mathematics University of Allahabad, India Mobile: +91-9450609696 Email pnpiaps@gmail.com | Prof Dr Gali Prag (Scientist, Lecturer) Dept of Biochemistry & Molecular Biology, George wise faculty of Life Science, Tel Aviv University, Israel Phone: +972-03-6409828 Email: prag@tauex.tau.ac.il | Dr Yossi Tsfadia (Scientist, Lecturer) George wise faculty of Life Science, Sherman Building Tel Aviv University, Israel Telephone +972-03-6405766 Email yossit@tauex.tau.ac.il | Prof Dr Menachem Gutman (Emeritus Scientist) George wise faculty of Life Science, Tel Aviv University, Israel Telephone 972 36409875 Fax +972-03-6409875 Email me@hemi.tau.ac.il | Prof Dr Geerten Vuister Department of Molecular and Cell Biology, Leicester Institute of Structural and Chemical Biology, University of Leicester Henry Wellcome Building, Lancaster Road, Leicester, LE1 9HN, The United Kingdom Phone: +44 116 229 7076 Email: gv29@leicester.ac.uk |

Date: March 13, 2022

(Navaneet Chaturvedi)