

Dr. Nagendra Singh



Department of Biotechnology

University School of Biotechnology

Gautam Buddha University

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SUMMARY SHEET

1.	Total Research Experience: 25 years	2.	Teaching Experience: 15 years
3.	No. of research publications: 80	4.	No. of citations: 1600
5.	H-index: 25	6.	I10 index: 40
7.	Research Gate (RG) Score: 33	8.	Avg. impact factor/paper: ~3.0
9.	No. of Protein Data Bank entries: 225	10.	No. of extramural research projects: 07
11.	No. of invited lectures: 10	12.	No. of Awards/Honors: 20
13.	International Conferences participation: 14	14.	National Conferences participation: 14
15.	Masters Thesis Supervision: 35	16.	PhD Students supervision: 06
17.	International Conference organized: 01	18.	National Workshops Organized: 03
19.	Administrative Responsibilities: > 50	20.	UGC-API Score: >1500

Career Profile

Position	University/Institute	Duration	Experience
Assistant Professor (PB3-AGP8000)	GBU, Greater Noida	March 2010- present	15 Years
Senior Research Associate	AIIMS, New Delhi	September 2009-March 2010	6 months
Senior Research Officer	AIIMS, New Delhi	October 2005-August 2009	3 years, 11 months
Young scientist Fellow	AIIMS, New Delhi	Jan 2005-September 2005	9 months
Senior Research Fellow	AIIMS, New Delhi	Jan 2002- Dec. 2004	3 Years
Junior Research Fellow	AIIMS, New Delhi	Jan 2000- Dec. 2001	2 Years
Research Assistant	AIIMS, New Delhi	July 1999- Dec. 1999	6 months
Post PhD experience			16 years
Total Experience			24 years, 6 months

Education Profile

Degree	Specialization/ Subjects	Duration Years	University/Institute	Division
PhD	Structural Biology	2000-2004	All India Institute of Medical Sciences, New Delhi	Successful with best PhD thesis Award
MSc	Biochemistry	1997-1999	Jamia Hamdard, New Delhi	I st
BSc	Zoology, Botany, Chemistry	1994-1997	J.V.College, Baraut (CCS University, Meerut)	I st
UGC-NET CSIR-JRF	Life Sciences	1999	UGC & CSIR	Qualified for Lectureship and CSIR-JRF
GATE	Life Sciences	1999	IIT Delhi	All India Rank-80

Research Profile

Research Interest:

- Elucidating roles of human splicing factors in cancers.
- Structure-Function studies on Enzymes involved in RNA metabolism from microbial origin
- Structure based drug development of novel antimicrobial agents.

Research Specialization:

- Molecular Structural Biology
- X-ray crystallography
- Drug Design

Supervisory Experience

- PhD-06
- JRF-05
- SRF-02
- MTech-25
- MSc-10

International Visits

Germany, South Africa, United Kingdom, Trieste, Hong Kong, Malaysia, Taiwan etc.

Academic Profile

Teaching Interest

Biophysical Chemistry, Structure Biology, Biochemistry, Proteomics, Protein Engineering, Biomolecules, Metabolism, Bioanalytical Techniques etc to UG and PG levels

Administrative Responsibilities

University Level

- 1) Chairperson, Sports Council (2019-till date)
- 2) Incharge-Horticulture (2024- till date)
- 3) National Service Scheme (NSS)-Program officer, (2018- 2022)
- 4) Warden, Tulsidas Boys Hostel (2017 - 2022)
- 5) Member, GBU Sports council (2017-2019)
- 6) Member GBU-RUSA Committee-2020
- 7) Member, organizing team of Swachh Pakhwada Week at GBU, October 2017-18
- 8) Member Stage decoration committee, GBU convocation 2016
- 9) Member Dias management committee, GBU convocation 2016
- 10) Convener and member of GBU Research Advisory committee (2013-14).
- 11) Member of Central Purchasing Committee, GBU.(2011-12)
- 12) Dy. Coordinator of Sponsored Research & Consultancy Committee (2010-11).
- 13) Member of Institutional Bio Safety Committee (2010-11).
- 14) *Participated in organizing Abhivyanjana (2010-25)*
- 15) *Participated in organizing Shauroyatsav (2010-25)*

Department Level

- 1) HOD, Department of Biotechnology (2021-2024)
- 2) Timetable coordinator (2017- present)
- 3) Dissertation coordinator (2015- 2021)
- 4) Faculty coordinator, CIF (2015- present)
- 5) Faculty in-charge Proteomics lab (2015- 2021)
- 6) Member of Board of Studies of School of Biotechnology (2013-14).
- 7) Coordinator, Time table and Course allocation committee (2014-2016).
- 8) Member of Examination Committee (2014-15).
- 9) *Convener Exam paper moderation committee (2013-14)*
- 10) Member of Aesthetic committee (2011-12)
- 11) Member of consumables organizing committee (2010-11).
- 12) Member of equipments organizing committee (2010-11).
- 13) Member of Placement Coordination Committee (2013-14).
- 14) *Member, unfair means committee (2011-12)*

Awards and Recognitions

- 1) Best Research paper publication appreciation 2021 from Vice chancellor, GBU
- 2) Invited lecture at the annual "Conference on Translational (Engineering) and Regenerative Medicine" (CoTERM 2020), 21-23 Jan 2020, Noida International University, Greater Noida
- 3) Invited speaker at Faculty Development Program "**approaches of insilico drug designing: 3-7 July 2018**", College of engineering & Technology, IILM Academy, Greater Noida.
- 4) Invited Speaker at 2nd National conference on "**Advances in Biotechnology: an Interdisciplinary approach**", November 2-3, 2018, Sharda University, Greater Noida.
- 5) Venus International Foundation **Young Scientist Award-2016**
- 6) National Academy of Sciences of India (NASI **young scientist PLATINUM JUBILEE award-2009**)
- 7) Invited speaker in DBT Sponsored national workshop on "**Protein structure prediction and function analysis**" at Banasthali University, March 2-4, 2017
- 8) Invited speaker in **Current Trends in Structural Biology**, AIIMS, New Delhi-2013
- 9) DST young scientist fellowships-2005

- 10) Awarded “**Meeting of Noble Laureates and Students**” in the field of medicine, Lindau, Germany by DST, June-July 2003.
- 11) **Talekar Medal for the best PhD thesis-2004** in department of Biophysics, AIIMS
- 12) **Best paper of the year award for 2006**, by Society of young Scientist, AIIMS
- 13) **CSIR-Senior Research fellowship** (2002-2004)
- 14) **CSIR-Junior Research fellowship and NET-UGC** (1999)
- 15) **Graduate Aptitude Test in Engineering (GATE-IIT)-1999**, AIR-80
- 16) **Best Poster award in 5th Biotech Research Society of India (BRSI) conference 2008**, Hyderabad
- 17) **Best Poster award in Indian Biophysical Symposium (IBS-2004)**, Bangalore
- 18) **Best Poster award in International Biophysics Congress-2005** Montpellier, France
- 19) Travel awards from **DST, DBT, CSIR and INSA**
- 20) **CCP4 UK WeekEnd travel award-02**
- 21) Member of **Indian Biophysical Society**
- 22) Member of **Indian Crystallographic Association**

Research Projects (07)

1. “*Structure based ligand design of anti-inflammatory drugs using phospholipase A₂ and cyclooxygenase-2 enzymes as target molecules*”. Department of Science and Technology (DST), India (2005-2008, **12 lakhs**)
2. “*Cloning, over expression, purification and structure determination of tRNA modifying enzymes from P. aeruginosa*”. Indian Council of Medical research (ICMR), India (2015-2018, **46 lakhs**)
3. Structural and functional characterization of SRp508, Council of scientific and Industrial Research (CSIR), **26 lakhs**, ongoing (2016-2020)
4. Structure basis of nickel transport in *Klebsiella pneumoniae* Indian Council of Medical research (ICMR), India (2017-2020, **25 lakhs**)
5. Structure based drug design of anticancer agents using SF2/ASF as target molecule. (2017-2020, **42. Lakhs**, ICMR as CO-PI)
6. Structural studies of TadA enzyme from *Pseudomonas aeruginosa* (2023-2026), 54 lakhs. (ICMR)
7. DBT-National Networking Project (NNP), 2023-26, 15 Lakhs (DBT)

Best Research Publications

- 1) Gurjar V, Iqara S, Chandra A, Qamar I, **Singh N.** (2023). COVID19: Drugs swapping in coronavirus strains: a structural biology view. **J Biomol Struct Dyn.** 2023 Feb 6:1-8. doi: 10.1080/07391102.2023.2175037. ISSN: 0739-1102 Online ISSN: 1538-0254 (IF=5.2)
- 2) Chandra A, Gurjar V, Qamar I, **Singh N.** (2022) Exploring inhibitor of SARS-CoV2 replicase from FDA approved drugs using insilico drug discovery methods. **J Biomol Struct Dyn. J Biomol Struct Dyn.** 2022 Aug;40(12):5507-5514. doi: 10.1080/07391102.2020.1871416. Print ISSN: 0739-1102 Online ISSN: 1538-0254 (IF=5.2)
- 3) Chandra A, Ananda H., Qamar I, **Singh N.** (2021) Identification of a novel and potent small molecule inhibitor of SRPK1: mechanism of dual inhibition of SRPK1 for the inhibition of cancer progression. *Aging (Albany NY).* Jan 15; 13(1): 163–180. (In press) (IF=6.0) **ONLINE ISSN: 1945-4589**
- 4) Chandra A, Gurjar V, Qamar I, **Singh N.** (2020) Identification of potential inhibitors of SARS-COV-2 endoribonuclease (EndoU) from FDA approved drugs: a drug repurposing approach to find therapeutics for COVID-19. **J Biomol Struct Dyn.** Aug;39(12):4201-4211. doi: 10.1080/07391102.2020.1775127. Print ISSN: 0739-1102 Online ISSN: 1538-0254 (IF=5.2)

- 5) Goyal N, Chandra A, Qamar I, **Singh N.** (2019) Structural studies on dihydrouridine synthase A (DusA) from *Pseudomonas aeruginosa*. **Int J Biol Macromol.** 2019 Mar 28;132:254-264. doi: 10.1016/j.ijbiomac.2019.03.209. (IF: 8.1) ISSN: 0141-8130 (print); 1879-0003 (web)
- 6) AK. Dwivedi, V. Gurjar, S. Kumar, **N. Singh.** (2015) Molecular basis for nonspecificity of nonsteroidal anti-inflammatory drugs (NSAIDs). **Drug Discovery Today**; 20(7):863-73. (IF= 8.4) Online ISSN: 1878-5832, Print ISSN: 1359-6446
- 7) P. Sharma, D. Dube, A. Singh, B. Mishra, **N. Singh,** M. Sinha, S. Dey, P. Kaur, D. K. Mitra, S. Sharma, T. P. Singh (2011): Structural Basis of Recognition of Pathogen-associated Molecular Patterns and Inhibition of Proinflammatory Cytokines by Camel Peptidoglycan Recognition Protein. **J. Biol. Chem.** 286(18):16208-16217. (IF=5.5) ISSN 0021-9258
- 8) **N. Singh,** A. K. Singh, M. Sinha, A. Bhushan, P. Kaur, A. Srinivasan, S. Sharma, T. P. Singh (2009): Binding modes of aromatic ligands to mammalian heme peroxidases with associated functional implications: crystal structures of lactoperoxidase complexes with acetylsalicylic acid, salicylhydroxamic acid, and benzylhydroxamic acid. **J. Biol. Chem.**; 284(30):20311-8. DOI:10.1074/jbc.M109.010280 (IF=5.5)
- 9) A.K. Singh, R. P. Kumar, N. Pandey, **N. Singh,** M. Sinha, A. Bhushan, P. Kaur, S. Sharma, T. P. Singh (2009): Mode of binding of the tuberculosis prodrug isoniazid to heme peroxidases: binding studies and crystal structure of bovine lactoperoxidase with isoniazid at 2.7 Å resolution. **J. Biol. Chem.** 11/2009; 285(2):1569-76. DOI:10.1074/jbc.M109.060327 (IF=5.5)
- 10) A. Sheikh, A. K. Singh, **N. Singh,** M. Sinha, S. B. Singh, A. Bhushan, P. Kaur, A. Srinivasan, S. Sharma, T. P. Singh (2009): Structural evidence of substrate specificity in mammalian peroxidases: structure of the thiocyanate complex with lactoperoxidase and its interactions at 2.4 Å resolution. **J. Biol. Chem.** 284(22):14849-56. DOI:10.1074/jbc.M807644200 (IF=5.5)
- 11) M. I. Hassan, S. Bilgrami, V. Kumar, **N. Singh,** S. Yadav, P. Kaur, T. P. Singh (2008): Crystal Structure of the Novel Complex Formed between Zinc α 2-Glycoprotein (ZAG) and Prolactin-Inducible Protein (PIP) from Human Seminal Plasma. **J. Mol. Biol.** ; 384(3):663-72. DOI:10.1016/j.jmb.2008.09.072 IF:6.1 Online ISSN: 1089-8638, Print ISSN: 0022-2836
- 12) P. Sharma, **N. Singh,** M. Sinha, S. Sharma, M. Perbandt, C. Betzel, P. Kaur, A. Srinivasan, T. P. Singh (2008): Crystal structure of the peptidoglycan recognition protein at 1.8 Å resolution reveals dual strategy to combat infection through two independent functional homodimers. **J. Mol. Biol.**; 378(4):923-32. DOI:10.1016/j.jmb.2008.03.018 (IF=6.1)
- 13) A. K. Singh, **N. Singh,** S. Sharma, S. Baskar Singh, P. Kaur, A. Bhushan, A. Srinivasan, T. P. Singh (2008): Crystal structure of lactoperoxidase at 2.4 Å resolution. **J. Mol. Biol.**; 376(4):1060-75. DOI:10.1016/j.jmb.2007.12.012 (IF=6.1)
- 14) **N. Singh,** Rishi K Somvanshi, S. Sharma, S. Dey, P. Kaur, T. P. Singh (2007): Structural elements of ligand recognition site in secretory phospholipase A₂ and structure-based design of specific inhibitors. **Current Topics in Medicinal Chemistry**; 7(8):757-64. DOI:10.2174/156802607780487669 (IF=3.6)
- 15) **N. Singh,** T. Jabeen, R. K Somvanshi, S. Sharma, S. Dey, T. P. Singh (2004): Phospholipase A₂ as a target protein for nonsteroidal anti-inflammatory drugs (NSAIDs): crystal structure of the complex formed between phospholipase A₂ and oxyphenbutazone at 1.6 Å resolution. **Biochemistry**; 43(46):14577-83. DOI:10.1021/bi0483561 (IF=3.3)

Research Publications (80)

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Avg Impact Factor = 3.1

- 1) Mishra SK, Chandra A, Mitra N, Krishna N, **Singh N**, Akash S, Jordan YAB, Bourhia M, George JJ. Exploring the Dynamics of Asparagus racemosus Phytochemicals as Dual Target Inhibitors of Monkeypox Virus. **Curr Med Chem.** 2025 Feb 7. doi: 10.2174/0109298673361923250101072831. Epub ahead of print. PMID: 39931982. (IF 4.1)
- 2) Padhy I, Banerjee B, Sharma T, Achary PGR, **Singh N**, Chandra A. (2025), Antilipase and antioxidant activities of topiramate-phenolic acid conjugates: Computational modelling, synthesis, and in-vitro investigations. **Biochem Biophys Res Commun.** 2025 Jan;745:151200. doi: 10.1016/j.bbrc.2024.151200. Epub 2024 Dec 18. PMID: 39729676. (IF 2.5)
- 3) Rajkumari Urmi, Pallabi Banerjee, Manisha Singh, Risha Singh, Sonam Chhillar, Neha Sharma, Anshuman Chandra, **Nagendra Singh**, Imteyaz Qamar. (2024). Revolutionizing biomedicine: Aptamer-based nanomaterials and nanodevices for therapeutic applications. **Biotechnology Reports.** Volume 42, June 2024, e00843. <https://doi.org/10.1016/j.btre.2024.e00843>. ISSN 2215-017X (IF 4.6)
- 4) Ibrahim MT, Ja'afaru SC, Uzairu A, Chandra A, Sallau MS, **Singh N** (2024) Computational design of novel therapeutics targeting Schistosomiasis, a neglected tropical disease, **Scientific African**, Volume 25, e02326, ISSN 2468-2276, <https://doi.org/10.1016/j.sciaf.2024.e02326> (IF=2.7)
- 5) Aminu KS, Uzairu A, Chandra A, Singh N, Abechi SE, Shallangwa GA, Umar AB. Exploring the potential of 2-arylbenzimidazole scaffolds as novel α -amylase inhibitors: QSAR, molecular docking, simulation and pharmacokinetic studies. **In Silico Pharmacol.** 2024 Apr 11;12(1):29. doi: 10.1007/s40203-024-00205-4. PMID: 38617707; ISSN 2193-9616
- 6) Mustapha Abdullahi, Adamu Uzairu, Gideon Adamu Shallangwa a, Paul Andrew Mamza a, Muhammad Tukur Ibrahim a, Anshuman Chandra c, **Nagendra Singh**. (2023). In-silico design of novel 2-((4-chloro-6-methoxy-1H-indol-3-yl)thio)-N-(2-ethoxyphenyl)acetamide derivatives as potential inhibitors of influenza neuraminidase protein receptor. **Intelligent Pharmacy**, In Press, <https://doi.org/10.1016/j.ipha.2023.12.002>
- 7) Choudhury A, Chandra A, Dawoud TM, Nafidi HA, **Singh N**, Bourhia M. Immunoinformatics and reverse vaccinology approach in designing a novel highly immunogenic multivalent peptide-based vaccine against the human monkeypox virus. **Front Mol Biosci.** 2023 Nov 22;10:1295817. doi: 10.3389/fmolb.2023.1295817. PMID: 38074091; PMCID: PMC10703375. ISSN 2296-889X (IF-3.9)
- 8) Shukla R, Chandra A, Kumar A, Kandpal P, Avashthi H, Goel VK, Qamar I, **Singh N**, David J. Kelvin DJ & Singh TR. (2023) Repurposing of drugs against methyltransferase as potential Zika virus therapies. **Scientific Reports** 2023, 13: 7870, doi: 10.1038/s41598-023-33341-6. ISSN No: 2045-2322 (IF=3.8)
- 9) Chaudhary, J., **Singh, N.**, Srivastava, V.K. et al. Exploring the significance of diaminopimelate epimerase as a drug target in multidrug resistant Enterococcus faecalis. **Vegetos** 36, 1–9 (2023). <https://doi.org/10.1007/s42535-022-00485-1>
- 10) Banerjee P, Chandra A, Mohammad T, **Singh N**, Hassan MI, Qamar I (2023). Identification of high-affinity pyridoxal kinase inhibitors targeting cancer therapy: an integrated docking and molecular dynamics simulation approach. **J Biomol Struct Dyn.** 2023 Aug 14:1-18. doi: 10.1080/07391102.2023.2246580. (IF=2.7)
- 11) Gurjar V, Iqara S, Chandra A, Qamar I, **Singh N**. (2023). Drugs swapping in coronavirus strains: a structural biology view. **J Biomol Struct Dyn.** 2023 Feb 6:1-8. doi: 10.1080/07391102.2023.2175037. Print ISSN: 0739-1102 Online ISSN: 1538-0254 (IF=5.2)

- 12) Singh T, Banerjee P, Udit, Kumari S, Chopra A, **Singh N**, Qamar I. (2022). Expression of Regucalcin, a calcium-binding protein is regulated by hypoxia-inducible factor-1 α . **Life Sci.** 2022 Jan 15;120278. doi: 10.1016/j.lfs.2021.120278. ISSN-0024-3205. (IF=5.2)
- 13) Chandra A, Gurjar V, Qamar I, **Singh N**. (2022) Exploring inhibitor of SARS-CoV2 replicase from FDA approved drugs using insilico drug discovery methods. **J Biomol Struct Dyn.** 2022 Aug;40(12):5507-5514. doi: 10.1080/07391102.2020.1871416. Print ISSN: 0739-1102 Online ISSN: 1538-0254 (IF=2.7)
- 14) Chandra A, Ananda H., Qamar I, **Singh N**. (2021) Identification of a novel and potent small molecule inhibitor of SRPK1: mechanism of dual inhibition of SRPK1 for the inhibition of cancer progression. **Aging (Albany NY).** Jan 15; 13(1): 163-180. doi: 10.18632/aging.202301. ONLINE ISSN: 1945-4589 (IF=5.9)
- 15) Chandra A, Chaudhary M, Qamar I, **Singh N**, Nain V. (2022) In silico identification and validation of natural antiviral compounds as potential inhibitors of SARS-CoV-2 methyltransferase. **J Biomol Struct Dyn.** 2022 Sep;40(14):6534-6544. doi: 10.1080/07391102.2021.1886174. Print ISSN: 0739-1102 Online ISSN: 1538-0254 (IF=2.7)
- 16) Singh A, Banerjee P, Anas M, **Singh N**, Qamar I. (2020). Traditional Nutritional and Health Practices Targeting Lifestyle Behavioral Changes in Humans. **J Lifestyle Med.** Jul 31;10(2):67-73. doi: 10.15280/jlm.2020.10.2.67. (IF=1.9) 2288-1557
- 17) Chandra A, Gurjar V, Qamar I, **Singh N**. (2020) Identification of potential inhibitors of SARS-COV-2 endoribonuclease (EndoU) from FDA approved drugs: a drug repurposing approach to find therapeutics for COVID-19. **J Biomol Struct Dyn.** Aug;39(12):4201-4211. doi: 10.1080/07391102.2020.1775127. Print ISSN: 0739-1102 Online ISSN: 1538-0254 (IF=2.7)
- 18) Mannully ST, Rekha VPB, **Singh N**, Shanthi C, Pulicherla KK.(2020) Purification and in vivo stability and half-life of recombinant lipid modified staphylokinase. **Biologicals.** 2020 Mar; 64:15-22. doi: 10.1016/j.biologicals.2020.01.009, 1045-1056 (IF=1.8)
- 19) Anshuman Chandra, Nainee Goyal, Imteyaz Qamar, **Nagendra Singh**(2020)Identification of Hot Spot Residues on Serine-Arginine Protein Kinase-1 by Molecular Dynamic Simulation Studies. **J. Biomolecular Structure & Dynamics** 2020 Mar;39(5):1579-1587. doi: 10.1080/07391102.2020.1734487. Epub 2020, Print ISSN: 0739-1102 Online ISSN: 1538-0254 (IF=2.7)
- 20) Das S, Batra S, Gupta PP, Kumar M, Srivastava VK, Jyoti A, **Singh N**, Kaushik S. (2019) Identification and evaluation of quercetin as a potential inhibitor of naphthoate synthase from *Enterococcus faecalis*. **J Mol Recognit.** Jul 28:e2802. doi: 10.1002/jmr.2802. [Epub ahead of print] (IF: 2.2) 0952-3499
- 21) Goyal N, Chandra A, Qamar I, **Singh N**. (2019)Structural studies on dihydrouridine synthase A (DusA) from *Pseudomonas aeruginosa*. **Int J Biol Macromol.** 2019 Mar 28;132:254-264. doi: 10.1016/j.ijbiomac.2019.03.209. (IF: 7.7) 0141-8130
- 22) Sanjit Kumar, Ravindra Singh Rawat, Sudhir Kumar PalS, **Nagendra Singh**. (2018) Molecular Mechanism of anti-inflammatory effects nb flavonoids. **Ind. J. Inflammation Research.** DOI: 10.15305/ijir/v2i1/278
- 23) Lavania S, Das R, Dhiman A, Myneedu VP, Verma A, **Singh N**, Sharma TK, Tyagi JS. (2018) Aptamer-Based TB Antigen Tests for the Rapid Diagnosis of Pulmonary Tuberculosis: Potential Utility in Screening for Tuberculosis. **ACS Infect. Dis.** 2018,4,(12),1718-1726, doi: 10.1021/acscinfdis.8b00201. [Epub ahead of print] (IF: 4.1) 2373-8227
- 24) Kaushik, N. Iqbal, N. **Singh**, J. S. Sikarwar, P. K. Singh, P.Sharma1, P. Kaur, S. Sharma, M. Owais and T. P. Singh (2018). Search of Multiple Hot Spots on the Surface of Peptidyl-tRNA Hydrolase: Structural,Binding and Antibacterial Studies. **Biochem J.** 2018 Feb 9;475(3):547-560. doi: 10.1042/BCJ20170666. (IF=4.4) 0264-6021
- 25) Lavania S, Anthwal D, Bhalla M, **Singh N**, Halder S, Tyagi JS (2017) Direct detection of Mycobacterium tuberculosis rifampin resistance in bio-safe stained sputum smears. **PLoS ONE** 12(12): e0189149.S. <https://doi.org/10.1371/journal.pone.0189149> IF: 2.8) 1932-6203

- 26) Chaudhary B, **Singh N**, Pandey DK. (2017). Bioengineering of crop plants for improved tetrahydrofolate production. **Bioengineered** Jan 1;9(1):152-158. doi: 10.1080/21655979.2017.1373537m . (IF=2.2) 21655979
- 27) S. Kumar, Qamar I., **Singh N** (2017). Non steroidal Anti-inflammatory drugs (NSAIDs). ELS, Willey Sciences Published Online: 20 MAR 2017, DOI: 10.1002/9780470015902.a0024221
- 28) DK Pandey, A Kumar, JS Rathore, N Singh, B Chaudhary. (2017) Recombinant over expression of dihydroneopterin aldolase catalyst potentially regulates folate-biofortification. **Journal of Basic Microbiology** 57 (6), 517-524 doi: 10.1002/jobm.201600721. (IF=2.65) 0233-111X
- 29) Qamar I, **Singh N.**, Waseem S., Prakash P., Nagoria VS, Ahmad MF (2016). 'Cloning and expression of novel LINGO-1 gene from Bubalus bubalis. **World J Pharmacy & Pharmaceutical Sciences**. 5 (6), 2013-2024. (IF=8.1) 2278-4357
- 30) AK. Dwivedi, V. Gurjar, S. Kumar, **N. Singh**. (2015) Molecular basis for nonspecificity of nonsteroidal anti-inflammatory drugs (NSAIDs). **Drug Discovery Today**; 20(7):863-73. doi: 10.1016/j.drudis.2015.03.004. (IF= 6.5) 1359-6446
- 31) Bhardwaj R, Qamar I and **Singh N** (2015). Persister Formation in Klebsiella pneumoniae: Recombinant Expression and Purification of hipA and hipB proteins from K. pneumoniae. **Int. J. Applied & pure Science & Agriculture**, 1(11), 1-7. (IF= 3.76) 2394-5532
- 32) N. Arora, S. Sahi and **N. Singh** (2013). Structural mapping of ligand binding sites on P-glycoproteins: Mechanism of inhibition of P-glycoprotein by herbal isoflavones. **Int. J. Biochem. Res. And Reviews**, 3(4), 421-435. 2231-086X
- 33) S. Kaushik, **N. Singh**, S. Yamini, A. Singh, M. Sinha, A. Arora, P. Kaur, S. Sharma, T. P. Singh (2013). The Mode of Inhibitor Binding to Peptidyl-tRNA Hydrolase: Binding Studies and Structure Determination of Unbound and Bound Peptidyl-tRNA Hydrolase from Acinetobacter baumannii. **PLoS ONE** 8(7):e67547. DOI:10.1371/journal.pone.0067547 (IF=2.9) 1932-6203
- 34) A. Kumar, **N. Singh**, R. Yadav, R.P. Kumar, S. Sharma, A. Arora, T. P. Singh(2012). Crystal structure of peptidyl-tRNA hydrolase from mycobacterium smegmatis reveals novel features related to enzyme dynamics. **Int. J. Biochem. Mol. Biol.**3(1):58-69. (IF=5.1) 0141-8130
- 35) P. Sharma, D. Dube, A. Singh, B. Mishra, **N. Singh**, M. Sinha, S. Dey, P. Kaur, D. K. Mitra, S. Sharma, T. P. Singh(2011): Structural Basis of Recognition of Pathogen-associated Molecular Patterns and Inhibition of Proinflammatory Cytokines by Camel Peptidoglycan Recognition Protein. **J. Biol. Chem.** 286(18):16208-16217. doi: 10.1074/jbc.M111.228163 (IF=4.0) 0021-9258
- 36) N. Kaur, A. Gautam, S. Kumar, A. Singh, **N. Singh**, S. Sharma, R. Sharma, R. Tewari, T. P. Singh (2011). Biochemical studies and crystal structure determination of dihydrodipicolinate synthase from Pseudomonas aeruginosa. **International J. Biol. macromolecules**; 48(5):779-87. DOI:10.1016/j.ijbiomac.2011.03.002 (IF= 7.7) 0141-8130
- 37) D. N. Chandra, G. K. Prasanth, **N. Singh**, S. Kumar, O. Jithesh, C. Sadasivan, S. Sharma, T. P. Singh, M. Haridas (2011). Identification of a novel and potent inhibitor of phospholipase A2 in a medicinal plant: Crystal structure at 1.93Å and Surface Plasmon Resonance analysis of phospholipase A2 complexed with berberine. **Biochimica et Biophysica Acta**; 1814(5):657-63. DOI:10.1016/j.bbapap.2011.03.002 (IF=4.38) 0006-3002
- 38) S. Kumar, **N. Singh**, B. Mishra, D. Dube, M. Sinha, S. B. Singh, S. Dey, P. Kaur, S. Sharma, T. P. Singh (2010): Modulation of inhibitory activity of xylanase - α -amylase inhibitor protein (XAIP): binding studies and crystal structure determination of XAIP- II from Scadoxus multiflorus at 1.2 Å resolution. **BMC Struct. Biol.**; 10:41. DOI:10.1186/1472-6807-10-41 (IF=2.2) 1472-6807
- 39) R. Mir, **N. Singh**, G. Vikram, M. Sinha, A. Bhushan, P. Kaur, A. Srinivasan, S. Sharma, T. P. Singh (2010): Structural and binding studies of C-terminal half (C-lobe) of lactoferrin protein with COX-2-specific non-steroidal anti-inflammatory drugs (NSAIDs). **Arch. of Biochem. Biophysics** 500(2):196-202. DOI:10.1016/j.abb.2010.05.026 (IF=3.4) 0003-9861

- 40) S. Kumar, N. Singh, M. Sinha, D. Dube, S. B. Singh, A. Bhushan, P. Kaur, A. Srinivasan, S. Sharma, T. P. Singh (2010): Crystal structure determination and inhibition studies of a novel xylanase and alpha-amylase inhibitor protein (XAIP) from *Scadoxus multiflorus*. **FEBS Journal** 277(13):2868-82. DOI:10.1111/j.1742-4658.2010.07703.x (IF=5.5) 1742-464X
- 41) A.K Singh, N. Singh, A.Tiwari, M. Sinha, G. S. Kushwaha, P. Kaur, A. Srinivasan, S. Sharma, T. P. Singh (2010): First structural evidence for the mode of diffusion of aromatic ligands and ligand-induced closure of the hydrophobic channel in heme peroxidases. **J. Biol. Inorg. Chem;** 15(7):1099-107. DOI:10.1007/s00775-010-0669-3 (IF=2.8) 0949-8257
- 42) R. Mir, R. P. Kumar, N. Singh, G. Vikram, M. Sinha, A. Bhushan, P. Kaur, A. Srinivasan, S. Sharma, T. P. Singh (2010): Specific interactions of C-terminal half (C-lobe) of lactoferrin protein with edible sugars: Binding and structural studies with implications on diabetes. **International J. Biological Macromolecules;** 47(1):50-9. DOI:10.1016/j.ijbiomac.2010.03.021 (IF=8.0) 0141-8130
- 43) R. Mir, N. Singh, G. Vikram, R. P.Kumar, M. Sinha, A. Bhushan, P. Kaur, A. Srinivasan, S. Sharma, T. P. Singh (2009): The Structural Basis for the Prevention of Nonsteroidal Antiinflammatory Drug-Induced Gastrointestinal Tract Damage by the C-Lobe of Bovine Colostrum Lactoferrin. **Biophysical J.;** 97(12):3178-86. DOI:10.1016/j.bpj.2009.09.030 (IF=4.0) 0006-3495
- 44) N. Singh, R. P. Kumar, S. Kumar, S. Sharma, R. Mir, P. Kaur, A. Srinivasan, T. P. Singh (2009): Simultaneous inhibition of anti-coagulation and inflammation: crystal structure of phospholipase A₂ complexed with indomethacin at 1.4 Å resolution reveals the presence of the new common ligand-binding site. **J. Mol. Recognition;** 22(6):437-45. DOI:10.1002/jmr.960 (IF=2.9) 1099-1352
- 45) A.K. Singh, R. P. Kumar, N. Pandey, N. Singh, M. Sinha, A. Bhushan, P. Kaur, S. Sharma, T. P. Singh (2009): Mode of binding of the tuberculosis prodrug isoniazid to heme peroxidases: binding studies and crystal structure of bovine lactoperoxidase with isoniazid at 2.7 Å resolution. **J. Biol. Chem.** 285(2):1569-76. DOI:10.1074/jbc.M109.060327(IF=5.5) 0021-9258
- 46) S. Kumar, N. Singh, M. Sinha, P. Kaur, A. Srinivasan, S. Sharma, T. P. Singh (2009): Isolation, purification, crystallization and preliminary crystallographic studies of amaryllin, a plant pathogenesis-related protein from *Amaryllis belladonna*. **Acta Crystallogr. Sect. F Structural Biology and Crystallization Communications;** 65(Pt 6):635-7. DOI:10.1107/S174430910901745X (IF=0.98) 2053-230X
- 47) N. Singh, A. K. Singh, M. Sinha, A. Bhushan, P. Kaur, A. Srinivasan, S. Sharma, T. P. Singh (2009): Binding modes of aromatic ligands to mammalian heme peroxidases with associated functional implications: crystal structures of lactoperoxidase complexes with acetylsalicylic acid, salicylhydroxamic acid, and benzylhydroxamic acid. **J. Biol. Chem.;** 284(30):20311-8. DOI:10.1074/jbc.M109.010280 (IF=5.57) 0021-9258
- 48) V. Kumar, Y. Roske, N. Singh, U. Heinemann, T. P. Singh, S. Yadav (2009): Purification and preliminary X-ray crystallographic studies of beta-microseminoprotein from human seminal plasma. **Acta Crystallogr. Sect. F Structural Biology and Crystallization Communications;** 65(Pt 5):518-21. DOI:10.1107/S1744309109013670(IF=1.07) 2053-230X
- 49) P. Mishra, R. P. Kumar, A. S. Ethayathulla, N. Singh, S. Sharma, M. Perbandt, C. Betzel, P. Kaur, A. Srinivasan, V. Bhakuni, T. P. Singh (2009): Polysaccharide binding sites in hyaluronate lyase-crystal structures of native phage-encoded hyaluronate lyase and its complexes with ascorbic acid and lactose. **FEBS Journal;** 276(12):3392-402. DOI:10.1111/j.1742-4658.2009.07065.x (IF=5.5) 1742-464X
- 50) P. Sharma, N. Singh, M. Sinha, S. Sharma, M. Perbandt, C. Betzel, P. Kaur, A. Srinivasan, T. P. Singh (2009): Tryptophan as a three-way switch in regulating the function of the secretory signalling glycoprotein (SPS-40) from mammary glands: structure of SPS-40 complexed with 2-methylpentane-2,4-diol at 1.6 Å resolution. **Acta Crystallogr. Sect. D Biological Crystallography;** 65(Pt 4):375-8. DOI:10.1107/S0907444909002327 (IF=5.3) 2053-230X

- 51) A. Sheikh, A. K. Singh, **N. Singh**, M. Sinha, S. B. Singh, A. Bhushan, P. Kaur, A. Srinivasan, S. Sharma, T. P. Singh (2009): Structural evidence of substrate specificity in mammalian peroxidases: structure of the thiocyanate complex with lactoperoxidase and its interactions at 2.4 Å resolution. **J. Biol. Chem.** 284(22):14849-56. DOI:10.1074/jbc.M807644200(IF=4.57) 0021-9258
- 52) A.K. Singh, **N. Singh**, S. Sharma, K. Shin, M. Takase, P. Kaur, A Srinivasan, T P Singh (2009): Inhibition of Lactoperoxidase by Its Own Catalytic Product: Crystal Structure of the Hypothiocyanate-Inhibited Bovine Lactoperoxidase at 2.3-Å Resolution. **Biophysical Journal**; 96(2):646-54. DOI:10.1016/j.bpj.2008.09.019 (IF=4.037) 0006-3495
- 53) M. I. Hassan, S. Bilgrami, V. Kumar, **N. Singh**, S. Yadav, P. Kaur, T. P. Singh (2008): Crystal Structure of the Novel Complex Formed between Zinc α 2-Glycoprotein (ZAG) and Prolactin-Inducible Protein (PIP) from Human Seminal Plasma. **J. Mol. Biol.** ; 384(3):663-72. DOI:10.1016/j.jmb.2008.09.072 (IF=5.5) 0022-2836
- 54) R. Mir, M. Sinha, S. Sharma, **N. Singh**, P. Kaur, A Srinivasan, T. P. Singh (2008): Isolation, purification, crystallization and preliminary crystallographic studies of sagitoxin, an oligomeric cardiotoxin from the venom of *Naja naja saggitifera*. **Acta Crystallogr. Sect. F Structural Biology and Crystallization Communications**; 64(Pt 6):545-7. DOI:10.1107/S1744309108014334 (IF=1.058) 2053-230X
- 55) P. Sharma, **N. Singh**, M. Sinha, S. Sharma, M. Perbandt, C. Betzel, P. Kaur, A. Srinivasan, T. P. Singh (2008): Crystal structure of the peptidoglycan recognition protein at 1.8 Å resolution reveals dual strategy to combat infection through two independent functional homodimers. **J. Mol. Biol.**; 378(4):923-32. DOI:10.1016/j.jmb.2008.03.018 (IF=5.5) 0022-2836
- 56) A. K. Singh, **N. Singh**, S. Sharma, S. Baskar Singh, P. Kaur, A. Bhushan, A. Srinivasan, T. P. Singh (2008): Crystal structure of lactoperoxidase at 2.4 Å resolution. **J. Mol. Biol.**; 376(4):1060-75. DOI:10.1016/j.jmb.2007.12.012 (IF=5.5) 0022-2836
- 57) Sharma, P., **Singh, N.**, Sinha, M., Sharma, S., Perbandt, M., Betzel, Ch., Kaur, P., Srinivasan, A. and Singh, T.P. (2008). Crystal Structure of Peptidoglycan Recognition Protein at 1.8Å Resolution. **Acta Cryst. Sect. A**64, C314. (IF=1.96) 2056-9890
- 58) Jain, R., Sharma, P., **Singh, N.**, Sharma, S., Kaur, P. and Singh, T.P. (2008). Crystal Structure of the Complex of Camelina Peptidoglycan Recognition Protein with Disaccharide at 3.2Å Resolution. **Biophysical Journal** 94: 3256 (IF=3.97) 0006-3495
- 59) Kumar, R.P., **Singh N.**, Sharma S., Kaur, P., Srinivasan A., and Singh T.P. (2007) Crystal structures of complexes of phospholipase A₂ with natural and synthetic inhibitors. **The FASEB Journal**. 2007;21:649.6 (IF=5.0)
- 60) J. Kumar, A. S. Ethayathulla, D. B. Srivastava, **N. Singh**, S. Sharma, P. Kaur, A. Srinivasan, T. P. Singh (2007): Carbohydrate-binding properties of goat secretory glycoprotein (SPG-40) and its functional implications: structures of the native glycoprotein and its four complexes with chitin-like oligosaccharides. **Acta Crystallogr. Sect. D Biological Crystallography** 05/2007; 63(Pt 4):437-46. DOI:10.1107/S0907444907001631(IF=5.7) 2059-7983
- 61) **N. Singh**, Rishi K Somvanshi, S. Sharma, S. Dey, P. Kaur, T. P. Singh (2007): Structural elements of ligand recognition site in secretory phospholipase A₂ and structure-based design of specific inhibitors. **Current Topics in Medicinal Chemistry**; 7(8):757-64. DOI:10.2174/156802607780487669 (IF=3.6) 1568-0266
- 62) D. B Srivastava, A. S. Ethayathulla, J. Kumar, **N. Singh**, S. Sharma, U. Das, A. Srinivasan, T. P. Singh (2007): Crystal structure of a secretory signalling glycoprotein from sheep at 2.0Å resolution. **J. Struct. Biol.**; 156(3):505-16. DOI:10.1016/j.jsb.2006.05.008 (IF=3.2) 1047-8477
- 63) R. K. Somvanshi, A. S. Ethayathulla, **N. Singh**, R. Gopal, A. K. Singh, S. Sharma, P. Kaur, S. Dey, T. P. Singh: Design of specific anti-inflammatory agents using structure-based approach: Crystal structure of complex formed between phospholipase A₂ and tetrapeptide inhibitor dehydro Val-Ala-Arg-Ser (Delta V-A-R-S). **Inflammation Research**; 55:S124-S124 (IF=3.1)
- 64) M. Sharma, A. S. Ethayathulla, T. Jabeen, **N. Singh**, K. Sarvanan, S. Yadav, S. Sharma, A. Srinivasan, T. P. Singh (2006): Crystal structure of a highly acidic neurotoxin from scorpion

- Buthus tamulus at 2.2 Å resolution reveals novel structural features. *J. Struct. Biol.*; 155(1):52-62. DOI:10.1016/j.jsb.2005.12.005 (IF=3.23) 1047-8477
- 65) N. Singh, T. Jabeen, A. Pal, S. Sharma, M. Perbandt, C. Betzel, T. P. Singh (2006): Crystal structures of the complexes of a group IIA phospholipase A2 with two natural anti-inflammatory agents, anisic acid, and atropine reveal a similar mode of binding. *Proteins Structure Function and Bioinformatics*; 64(1):89-100. DOI:10.1002/prot.20970 (IF=3.8) (1097-0134)
 - 66) S. Dey, R. K. Somvanshi, A. Kumar, R. Gopal, A. K. Singh, D. Gupta, N. Singh, A. S. Ethayathulla, S. Sharma, T. P. Singh (2006) Structure-based rational drug - design against inflammation, rheumatism and arthritis. *Inflammation Research*; 55:S106-S106. (IF=3.1)
 - 67) N. Singh, T. Jabeen, S. Sharma, R. K. Somvanshi, S. Dey, A. Srinivasan, T. P. Singh (2006): Specific binding of non-steroidal anti-inflammatory drugs (NSAIDs) to phospholipase A2: structure of the complex formed between phospholipase A2 and diclofenac at 2.7 Å resolution. *Acta Crystallogr. Sect. D Biological Crystallography*; 62(Pt 4):410-6. DOI:10.1107/S0907444906003660 (IF=5.7) 2059-7983
 - 68) T. Jabeen, N. Singh, R. K. Singh, A. S. Ethayathulla, S. Sharma, A. Srinivasan, T. P. Singh (2006): Crystal structure of a novel phospholipase A2 from Naja naja sagittifera with a strong anticoagulant activity. *Toxicon*; 46(8):865-75. DOI:10.1016/j.toxicon.2005.08.008 IF:2.2 0041-0101(IF=3.0) ISSN 0041-0101
 - 69) T. Jabeen, N. Singh, R. K. Singh, J. Jasti, S. Sharma, P. Kaur, A. Srinivasan, T. P. Singh (2006): Crystal structure of a heterodimer of phospholipase A2 from Naja naja sagittifera at 2.3 Å resolution reveals the presence of a new PLA2-like protein with a novel cys 32-Cys 49 disulphide bridge with a bound sugar at the substrate-binding site. *Proteins Structure Function and Bioinformatics* 62(2):329-37. DOI:10.1002/prot.20708 (IF=3.8) (1097-0134)
 - 70) Jain R., Kumar S., Singh N., Sharma S. and Singh T.P. (2005). Characterization of proteins from human pleural fluid. *Eur. Biophys. J.* 34, 825. (2.1)
 - 71) T. Jabeen, N. Singh, R. K Singh, S. Sharma, R. K. Somvanshi, S. Dey, T. P. Singh (2005): Non-steroidal anti-inflammatory drugs as potent inhibitors of phospholipase A2: structure of the complex of phospholipase A2 with niflumic acid at 2.5 Angstroms resolution. *Acta Crystallogr. Sect. D Biological Crystallography*; 61(Pt 12):1579-86. DOI:10.1107/S0907444905029604(IF=5.7) 2059-7983
 - 72) Srivastava D.B., Kumar J., Srivastava P., Mandal A., Jain R., Jabeen T., Singh N., Sharma S., Srinivasan A. and Singh T.P. (2005). Clinical Proteomics: characterization and structural studies of new proteins from human body fluids and tissues. *Eur. Biophys. J.* 34, 773. (IF=2.1) 0175-7571(
 - 73) T. Jabeen, S. Sharma, N. Singh, A. Bhushan, T. P. Singh (2005): Structure of the zinc-saturated C-terminal lobe of bovine lactoferrin at 2.0 Å resolution. *Acta Crystallogr. Sect. D Biological Crystallography*; 61(Pt 8):1107-15. DOI:10.1107/S0907444905016069 (IF=5.7) 2059-7983
 - 74) R. K. Singh, N. Singh, T. Jabeen, S. Sharma, S. Dey, T. P. Singh (2005): Crystal structure of the complex of group I PLA2 with a group II-specific peptide Leu-Ala-Ile-Tyr-Ser (LAIYS) at 2.6 Å resolution. *J. Drug Target.*; 13(6):367-74. DOI:10.1080/10611860500254450 (IF=3.4) 1061-186X
 - 75) T. Jabeen, S. Sharma, N Singh, R. K. Singh, P. Kaur, M. Perbandt, C. Betzel, A. Srinivasan, T. P. Singh (2005): Crystal structure of a calcium-induced dimer of two isoforms of cobra phospholipase A2 at 1.6 Å resolution. *Proteins Structure Function and Bioinformatics*; 59(4):856-63. DOI:10.1002/prot.20464 (IF=3.8) (1097-0134)
 - 76) Singh, N., Sarvanan, K., Paramasivam, M., Sharma, S., Srinivasan, A. and Singh T. P. (2005). Purification and partial characterization of neurotoxins from Indian red scorpion venom and cloning of toxin cDNAs. *Ind. J. Phys.* 6, 77-86. (IF=1.37) 973-1458 ISSN-0973-1458
 - 77) T. Jabeen, S. Sharma, N. Singh, R. K Singh, A. K. Verma, M. Paramasivam, A. Srinivasan, T. P. Singh (2005): Structure of the zinc-induced heterodimer of two calcium-free isoforms of phospholipase A(2) from Naja naja sagittifera at 2.7 angstrom resolution. *Acta Crystallogr. Sect.*

- D Biological Crystallography**; 61(Pt 3):302-8. DOI:10.1107/S0907444904033165 (IF=5.7) 2059-7983
- 78) N. Singh, T. Jabeen, S. Sharma, I. Roy, M. N. Gupta, S. Bilgrami, R. K Somvanshi, S. Dey, M. Perbandt, C. Betzel, A. Srinivasan, T. P. Singh (2005): Detection of native peptides as potent inhibitors of enzymes. Crystal structure of the complex formed between treated bovine alpha-chymotrypsin and an autocatalytically produced fragment, Ile-Val-Asn-Gly-Glu-Glu-Ala-Val-Pro-Gly-Ser-Trp-Pro-Trp, at 2.2Å resolution. **FEBS Journal**; 272(2):562-72. (IF=5.54) 1742-464X (IF=5.62) doi: 10.1111/j.1742-4658.2004.04499.x.
- 79) N. Singh, T. Jabeen, R. K Somvanshi, S. Sharma, S. Dey, T. P. Singh (2004): Phospholipase A₂ as a target protein for nonsteroidal anti-inflammatory drugs (NSAIDs): crystal structure of the complex formed between phospholipase A₂ and oxyphenbutazone at 1.6Å resolution. **Biochemistry**; 43(46):14577-83. DOI:10.1021/bi0483561 (IF=3.1) 0006-2960
- 80) K. Sharma, S. Kumar, V. Sharma, A. Nagpal, N. Singh, I. Tamboli, I. Mani, G. Raman, T. P. Singh (2001): Lactoferrin-melanin interaction and its possible implications in melanin polymerization: Crystal structure of the complex formed between mare lactoferrin and melanin monomers at 2.7Å resolution. **Proteins Structure Function and Bioinformatics**; 45(3):229-36. DOI:10.1002/prot.1143 (IF=3.76) (1097-0134)

International Conferences

1. Singh N. (2016). Molecular basis for nonspecificity of nonsteroidal anti-inflammatory drugs (NSAIDs). International Conference on Metals in Genetics (ICMG-2016), Feb 17-19, 2016, IISc, Bangalore, India
2. Singh N.(2016). Crystal Structure of AbPTH in unbound and bound states from *Acinetobacter baumannii*. **International conference on Emerging Trends in Biomedical Sciences (ICETBS-2016)**. March 7-9, 2016, AMU, Aligarh, India
3. Singh N., Kaushik S., Chaudhary A., Sharma S. and Singh, T.P. (2014). Crystal Structure of chorismate synthase at 2.6 Å resolution from *Acinetobacter baumannii*. **Recent advances in Structural Biology and Drug Discovery (RASBDD-IIT-2014)**. October 9-11, 2014, IIT Roorkee, India.
4. Singh N., Chaudhary A., Sharma S. and Singh, T.P. (2014). Crystal Structure of chorismate synthase at 2.6 Å resolution from *Acinetobacter baumannii*. **Current Trends in Structural Biology**, February 27-28, 2014, AIIMS, New Delhi, India.
5. Kaur, P., Sharma, P., Singh, N., Sharma, S. and Singh, T.P. (2008) Crystal Structure of Peptidoglycan Recognition Protein, a molecule involved in innate immunity in **Second International Symposium on Recent Trends in Macromolecular Structure and Function** on January 22-24, 2008 in Chennai, India.
6. Singh, N., Mishra, P., Sharma, S, Kaur, P., Bhakuni, V. and Singh, T.P. (2008) Mapping of substrate-binding site of a phage encoded bacteriophage: crystal structures of the complexes of HylP2 with lactose and ascorbic acid. **8th conference of the Asian Crystallographic Association** on Nov 4-7, 2007 in Taipei, Taiwan.
7. Singh, N., Singh, A.K., Sharma, S., Bhushan, A., Kaur, P., and Singh, T.P. (2007). Crystal structure of goat lactoperoxidase at 2.4 Å resolution in **8th conference of the Asian Crystallographic Association** on Nov 4-7, 2007 in Taipei, Taiwan.
8. Singh, N., Mishra, P., Sharma, S, Kaur, P., Bhakuni, V. and Singh, T.P. (2007). Crystal structure of hyaluronate lyase (HylP2) and its complexes. **4th Biotech Research Society of India (BRSI) conference**, NHBT 26-29, November 2007, Trivandrum.
9. Singh, N., Jabeen, T., Sharma, S., Bhushan, A., Kaur, P., and Singh, T.P. (2006) Crystal structure of phospholipase A₂ with diclofenac at 2.7Å resolution. **Drug Development Conference for the Third World**, Jun 2006, ICTP, Trieste, Italy.
10. Singh, N., Kumar, R.P., Sharma, S., Bhushan, A., Kaur, P., and Singh, T.P. (2006) Non-competitive inhibition of phospholipase A₂ by indomethacin: Crstal structure of PLA₂ with

indomethacin at 1.4Å resolution Oral presentation in **International Symposium on Recent Trends in Macromolecular Structure and Function**, Jan 18-20,2006, Chennai, India.

11. **Singh, N.**, Jabeen, T., Roy, I., Sharma, S., Kaur, P., Gupta, M.N. and Singh, T.P. (2004) Crystal structure of a complex of chymotrypsin with a peptide fragment at 2.2Å resolution. VI meeting of **Asian Crystallographic Association** (AsCA-2004), June 27-30, Hong Kong.
12. **Singh, N.**, Sharma, A.K, Kumar, S., Sharma, S, Kaur, P., and Singh, T.P. (2001) Regulation of melanin polymerization under influence of lactoferrin. **IV meeting of Asian Crystallographic Association** (AsCA-2001) Nov 18-21, Bangalore.

National Conferences

1. **Singh, N.**, Mishra, P., Sharma, S, Kaur, P., Bhakuni, V. and Singh, T.P. (2008) Mapping of substrate-binding site of a phage encoded bacteriophage: crystal structures of the complexes of HyIP2 with lactose and ascorbic acid. **5th BRSI conference**, November 2008, Hyderabad
2. Mirza, Z., Vikram, G., **Singh, N.**, Sinha, M., Sharma, S., Kaur, P., Srinivasan, A. and Singh, T.P. (2009) Crystal structure of the complex of Phospholipase A2 with a C-terminal fragment of A-beta polypeptide at 2.1 Å resolution in **38th National Seminar on Crystallography (NSC38)** on Feb 11-13, 2009 in Mysore.
3. Sharma, P., **Singh, N.**, Sinha, M., Sharma, S., Kaur, P. and Singh, T.P. (2009) Trp78 as the Ligand-Induced two-way switch for the binding and inhibition of the secretory signalling glycoprotein in **38th National Seminar on Crystallography (NSC38)** on Feb 11-13, 2009 in Mysore.
4. Kaur, P., Sharma, P., **Singh, N.**, Sinha, M., Sharma, S., and Singh, T.P. (2007). Crystal Structure of Peptidoglycan Recognition Protein and its complexes with ligands in **XXXVIIth National Seminar on Crystallography (NSC37)** on February 6-8, 2008, Kolkata.
5. Kaur, P., **Singh, N.**, Sharma, S., Yadav, S., Srinivasan, A. and Singh, T.P (2007) Protein Structural Studies at AIIMS, New Delhi in **INSA-CAS Workshop on Structural Biology** on December 21-23, 2007, Bangalore.
6. Kumar, R.P., Mishra, P., Bhakuni, V., **Singh, N.**, Sharma, S., Kaur, P. & Singh, T.P. (2007) Crystal structure of a bacteriophage-associated hyaluronate lyase in **National Symposium on Biophysics : Trends in Biomedical Research (IBS 2007)** on Feb 13-17, 2007 in New Delhi, India.
7. Singh, A. K., **Singh, N.**, Sharma, S., Bhushan, A. & Singh, T.P. (2007) Crystal structure of the complex of bovine lactoperoxidase with hypothiocyanate at 2.3 Å resolution in **National Symposium on Biophysics : Trends in Biomedical Research (IBS 2007)** on Feb 13-17, 2007 in New Delhi, India.
8. **Singh, N.**, Jabeen, T., Roy, I., Sharma, S., Kaur, P., Gupta, M.N. and Singh, T.P. (2002) Inhibition of bovine alpha-chymotrypsin by catalytically generated its own peptide fragment. **National Seminar on Crystallography (NSC-2002)** Oct 24-26, Jammu.
9. **Basis of Melanin polymerization by lactoferrin. XXXI National Seminar on Crystallography (NSC)** June 19-22, 2001, BARC, Mumbai

INVITED TALKS

1. Invited lecture in **International Conference BIOTRENDZ**, 13-14 November 2024, NIET, Greater Noida
2. Invited lecture in **Interdisciplinary exploration of Science: From Basic to Advanced Research and Innovation.**, 13-14 November 2024, RK(PG) College, Shamli, U.P.
3. Resource person in **“High end workshop on recombinant protein production, structural and functional studies”** sponsored by SERB, 11-17 March 2024, Amity Rajasthan.
4. Participated as resource person in the AICTE Training And Learning (ATAL) Academy Online Elementary FDP on "Computer Science and Biology : Impact of Bioinformatics and Molecular

- Biology on Drug Discovery" from 04/10/2021 to 08/10/2021 at COLLEGE OF ENGINEERING & TECHNOLOGY, IILM ACADEMY OF HIGHER LEARNING
5. Singh N (2020). **"COVID19 Disease control: Opportunities and challenges for drug discovery and development: Drug repurposing and Alternative medicine"** Organized by VIT Vellore July 24, 2020.
 6. Singh N (2020). **"Impact of COVID19 on Research & Education"** organized by IILM College of Engineering, July 4, 2020, Greater Noida.
 7. Singh N (2020) "Conference on Translational (Engineering) and Regenerative Medicine" (CoTERM 2020), 21-23 Jan 2020, Noida International University, Greater Noida
 8. Singh N (2018). "Protein structure and its applications in drug design". **2nd National conference on "Advances in Biotechnology: an Interdisciplinary approach"**, November 2-3, 2018, Sharda University, Greater Noida.
 9. Structure and functional analysis of proteins" DBT sponsored National Workshop on "Protein structure prediction and functional analysis", Center for Bioinformatics, Banasthali University, March 2-4, 2017.
 10. Crystal structure of peptidyltRNA hydrolase from acenetobacter baumannii. Current trends in structural biology. April 2, 2012

WORKSHOPS Participated (9)

1. Participated in 15 days workshop on "Swacchta Pakhwada" sept 1-15, 2017, GBU
2. **Advanced School on Synchrotron Radiation Techniques and Nanotechnology: A synergic approach to Life science and Medicine.** November 11-22, 2013, Cape Town Campus, Stellenbosch, South Africa
3. **From Genes to Structures**, April 23-27 2012, ICTP, Trieste, Italy
4. **Workshop on Open educational resources & Wiki educator**, 9-11 June 2010.
5. **CCP4 workshop on macromolecular crystallography**, Feb 18-22, 2008, Bangalore, India.
6. **CCP4 WEEKEND**, Jan 2007, Reading, UK.
7. **CCP4 WEEKEND**, Jan 2006, Leeds, UK.
8. **Drug Development Conference and workshop for the Third World**, June 2006, ICTP, Trieste, Italy
9. **CCP4 Workshop on Macromolecular crystallography**, April 2005, Bangalore, India

Faculty Development Programs Attended(10)

1. Participated in the AICTE Training And Learning (ATAL) Academy Online Elementary FDP on "Drug Discovery & Designing 21st Century" from 2021-7-5 to 2021-7-9 at Netaji Subhas University of Technology.
2. Participated in the online faculty development programme on **'SARS-CoV-2 Research: Insights from Computational Biology'** organized by the Department of Life Sciences, Kristu Jayanti College (Autonomous), Bengaluru from 11. 05. 2020 to 15. 05. 2020
3. Participated in **"Outcome based Education and Accreditation"** Organized by IILM college of Engineering, May 25-29, 2020.
4. Participated in two weeks FDP on **"Online Teaching Pedagogies"** Organized by GBU July 20-August 2 2020.
5. FDP on **"Research Methodologies: Tools and Techniques"** organized by IILM College of Engineering, May 18-22, 2020.
6. FDP on **"Emerging Trends on Biotechnological Advancements: Challenges and prospectus in tackling human diseases"** Organized by NIT Warangal, July 13-17, 2020.

7. Participated in FDP workshop on "Teaching and Learning of Molecular Biology and Enzymology through hands-on experience" organized by NIT, Warangal, September 18-23, 2018.
8. Participated in faculty development program on "approaches for in silico drug designing", July 3-7, 2018, IILM Academy of higher learning, Greater Noida.
9. Participated in 15 days workshop on "Swacchta Pakhwada" sept 1-15, 2017, GBU
10. **Advanced School on Synchrotron Radiation Techniques and Nanotechnology: A synergic approach to Life science and Medicine.** November 11-22, 2013, Cape Town Campus, Stellenbosch, South Africa.

Guest Lectures

1. "Approaches for drug discovery" Organize by IFTM University, Lodhipur Rajput, Jan 9, 2021
2. "Proteins Structure and its applications" Organized by Amity University, Noida October 31, 2020
3. "From Amino acids to Proteins" Organized by VIT University, Vellore November 2, 2020.

Books

- 1) **"CURRENT DEVELOPMENTS IN THE DETECTION AND CONTROL OF MULTI DRUG RESISTANCE"**, Bentham Science Publishers Ltd. ISBN: 978-981-5049-88-6 (Print) ISBN: 978-981-5049-87-9 (Online) Year of Publication: 2022, DOI:10.2174/97898150498791220101

Book Chapters (06)

- 1) Goyal, N., Chandra, A., Vashistha, M., Singh, A.P., Goel, V.K., **Singh, N.** (2024). Natural Product-Based Treatment for Food Poisoning. In: Sharma, T., Sahoo, C.R., Bhattacharya, D., Pati, S. (eds) Natural Products for Antibacterial Drug Development: Recent Advancement of Computational Approach. Springer, Singapore. https://doi.org/10.1007/978-981-97-9634-2_9.
- 2) Singh, K.S., Mohanty, D., Meena, A., **Singh, N.**, Sharma, G.S. (2024). Effect of Organic Osmolytes on Protein Folding Intermediates. In: Singh, L.R., Dar, T.A., Kumari, K. (eds) Cellular Osmolytes. Springer, Singapore. https://doi.org/10.1007/978-981-97-6001-5_2.
- 3) Chandra A., Goel N, **Singh N.** Goel V, Agarwal S., Arya A., **Stem cell based informatics development and approaches**, January 2024, DOI: 10.1016/B978-0-443-13222-3.00026-5, In book: Computational Biology for Stem Cell Research, Editors: Pawan Raghav, Rajesh Kumar, Anjali Lathwal, Navneet Sharma, ISBN: 9780443132223 eBook ISBN: 9780443132216 , ELSEVIER
- 4) Singh N. **"Principle and applications of Biomolecular Crystallography"**, Cutting Edge Techniques in Biophysics, Biochemistry and Cell Biology: From Principle to Applications. Pages 88-101. ISBN (Online): 978-981-14-2285-0, (Print): 978-981-14-2286-7 © 2019, Bentham eBooks imprint. Published by Bentham Science Publishers Pte. Ltd. Singapore.
- 5) S. Kumar, Qamar I., **Singh N** (2017). **Non steroidal Anti-inflammatory drugs (NSAIDs)**. ELS, Wiley Online Library, eLS, 2017, p. 1-7, Publisher: John Wiley & Sons, Ltd. Online ISBN: 9780470015902 | Copyright © 2001 John Wiley & Sons, Ltd. All rights reserved. DOI: 10.1002/9780470015902.a0024221,
- 6) **Singh, N.**, Sarvanan, K., Paramasivam, M., Sharma, S., Srinivasan, A. and Singh T. P. (2005). Purification and partial characterization of neurotoxins from Indian red scorpion venom and cloning of toxin cDNAs. **Frontiers in Biophysics**, Vol. 6, Allied Publishers, 2005, ISBN 8177648551/9788177648553

Conferences/workshops organized (08)

1. Organized “3 Day workshop on Gel to Gene: Mastering PCR, Primer Designing and Electrophoresis”, 19-21 November 2024
2. Organized “2nd National Workshop on Molecular Biology Techniques” April 23-27, 2024
3. Organized “International Conference on Structural Biology & Drug Discovery” (ICSBDD-2023), October 11-12, 2023
4. Organized National Workshop on Molecular Biology Techniques” April 25-29, 2023
5. Organized :National Science Day-2023”
6. Organized Blood/Organ/Eye donation camp on September 7, 2022 at GBU
7. “Organized Webinar on Orientation Program of GBU-2020”
8. Organized Industry-Academia workshop, Feb 2016

Lectures organized

1. Organized Interaction meeting on NBA Accreditation of Engineering and Management Programs by Prof Rashmi Mishra,” Feb 27, 2023
2. Organized Guest lecture by Prof. D. Velmurgan” November 18, 2022

Journal Reviewer (Selected)

1. J. Drug Targeting, Bentham Science
2. Int J Biol.Macromol., Elsevier
3. Molecular Biology Reports, Springer Nature
4. Future Virology
5. Chemical Biology & Drug Design
6. J. Biomol Struct. Dynamics

The above mentioned information is true to the best of my knowledge and belief.

(Dr. Nagendra Singh)