

Curriculum Vitae

Dr. Shankar Prasad Kanaujia
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Educational details

Degree	Subject of specialization	University/Institution	Year	Percentage marks & (Class/Grade)
B.Sc. (Hons.)	Statistics	Banaras Hindu University Varanasi	1996-1999	71.6 & First
M.Sc.	Applied Statistics & Informatics	Indian Institute of Technology Bombay	2000-2002	7.0/10 & First
M.Tech.	Bioinformatics	Indian Institute of Information Technology Allahabad	2003-2005	9.9/10 & First
Ph.D.	Structural Biology and Bioinformatics	Indian Institute of Science Bangalore	2005-2011*	8.3/10 & First
* PhD thesis submission date: October 11, 2010				
Thesis Title: Structural studies on bovine pancreatic phospholipase A ₂ and proteins involved in molybdenum cofactor biosynthesis				

Research Interests

Scientific Interests: To understand the structure-function relationships of Protein Translation Initiation Factors, Ribosome Biogenesis, ABC Transporters and Multidrug Resistance.

Protein Translation Initiation: The translation initiation in archaea is suggested to be similar to eukarya than to bacteria. We are trying to identify and understand the structure-function relationship of putative initiation factors in archaea.

Ribosome Biogenesis and Antibiotic Resistance: About 200 factors are hypothesized to be involved in ribosome biogenesis. Among these, rRNA methyltransferases play a key role in ribosome biogenesis by modifying rRNA molecules and are also known to be associated with antibiotic resistance. Our interest is to understand the structure-function relationship and design inhibitors against them.

ABC Importers: ABC importers are identified only in prokaryotes, though in few plants too. Due to this, bacterial ABC importers are considered to be potential drug targets and are also being used as drug delivery systems, biosensors, and biomarkers. They are also known to be involved in drug resistance. In this context, we have been trying to elucidate the structures of few ABC importers such as sugar, metal, lipid, and antimicrobial peptides.

Experimental Techniques: Structural Biology using Macromolecular Protein X-ray Crystallography, Small-angle X-ray scattering (SAXS), Cryo-Electrom Microscopy (Cryo-EM), Molecular Biology and Biochemistry.

Computational Methods: Bioinformatics, Molecular Dynamics Simulations, Structure-based Drug Design.

Research and Work Experience

Sep 2021 – Till date	Professor , Department of Biosciences and Bioengineering, Indian Institute of Technology Guwahati
Nov 2016 – Sep 2021	Associate Professor , Department of Biosciences and Bioengineering, Indian Institute of Technology Guwahati
Apr 2012 – Nov 2016	Assistant Professor , Department of Biosciences and Bioengineering, Indian Institute of Technology Guwahati
Jan 2011 – Apr 2012	Research Associate , Supercomputer Education Research Centre, Indian Institute of Science Bangalore
Oct 2010 – Jan 2011	Research Assistant , Supercomputer Education Research Centre, Indian Institute of Science Bangalore
Apr 2003 – Jun 2003	Research Assistant , Department of Mathematics, Indian Institute of Technology Bombay
Jan 2001 – Dec 2001	System Administrator , Department of Mathematics, Indian Institute of Technology Bombay

Teaching

S. No.	Name of the course	Credit details	UG/ PG	Class strength	Single/ Shared	No. of times taught
1.	Bioinformatics and Computational Biology (BT301)	2-0-0-4	UG	40-55	Shared	4
2.	Bioinformatics and Computational Biology Laboratory (BT 310)	0-0-6-6	UG	40-55	Shared	4
3.	Bioinformatics (BT302)	2-0-2-6	UG	70-80	Shared	4
4.	Biological Data Analysis (BT307)	2-0-2-6	UG	80-90	Shared	1
5.	Drug Design and Discovery (BT420)	3-0-0-6	UG	10	Shared	1
6.	Quantitative Biology (BT502)	3-0-2-8	PG	30-60	Shared	13
7.	M.Tech. Seminar (BT 600)	0-0-2-2	PG	50-60	Single + Shared	3
8.	Protein Structure and Function (BT 631)	3-0-0-6	UG + PG	30-70	Single	2
9.	Frontiers in Biomolecular Simulation (BT610)	3-0-0-6	UG + PG	30	Single	2

Awards/Fellowships and Recognitions

- **Unit of Excellence 2017**, Department of Biotechnology (DBT), Government of India.
- **Early Career Research (ECR) Award 2019**, Science and Engineering Research Board (SERB), Department of Science and Technology, Govt. of India.
- **Reviewer Certificate, 2019** from **Journal of Cellular Biochemistry**.
- **DST Young Investigator Award 2013**, Department of Science and Technology, Ministry of Science and Technology, Government of India.
- Recipient of **IUCr Travel Support Award** to present a poster in AsCA'07 meeting at Taipei, Taiwan (2007).
- **Institute Scholarship** by Indian Institute of Science, Bangalore (2005-2010).
- **Institute Silver Medal** at Indian Institute of Information Technology, Allahabad (2005).
- **MHRD Scholarship**, Ministry of Human Resource and Development, Govt. of India (2003-2005).
- Qualified **Graduate Aptitude Test Examination (GATE)** in Computer Science and Engineering (2003).
- **National Merit Scholarship**, Academic Board Uttar Pradesh (1995-1996).

Member of Professional Societies

- [Member of The Society for Integrative Biosciences](#)
- [Member of World Crystallographers Directory](#)
- [Life Member of Indian Crystallographic Association](#)

Research Publications

Total number of publications: 59

Total number of book chapters: 1

Total cumulative journal impact factor: 200.7

Total number of citations: 669

1. Ghosh K and Kanaujia SP (2025). [Illicit uptake of peptide-based antibiotics through bacterial peptide transporters: an approach towards overcoming drug resistance.](#) *Computers in Biology and Medicine*, 193, 110444. (Journal Impact Factor: 6.3).
2. Bora K, Kanaujia SP, Dubey VK (2025). [Targeting Antioxidant Defense System Enzymes for Leishmaniasis Treatment.](#) *International Journal of Biological Macromolecules*, 316(1), 144650. (Journal Impact Factor: 8.5).
3. Dutta A, Patel S and Kanaujia SP (2025). [Coordinated subdomain movements of MlaC regulate ligand binding and transport.](#) *Computational and Structural Biotechnology Journal*, 27, 2074-2097. (Journal Impact Factor: 4.5).
4. Dasgupta P and Kanaujia SP (2025). [Biophysical characterization of a putative antimicrobial peptide-binding protein of Escherichia coli highlights its dual functionality.](#) *FEBS Letters*, Accepted. (Journal Impact Factor: 3.864).
5. Bora K, Kumar S, Kanaujia SP, and Dubey VK (2025). [Development and evaluation of novel dual-target drugs encapsulated in liposome against visceral leishmaniasis.](#) *Journal of Drug Delivery Science and Technology*, 107, 106883. (Journal Impact Factor: 4.5).
6. Tripathi R, Ayekpam D and Kanaujia SP (2025). [Unveiling multiple copies of MlaC highlights its multifaceted nature.](#) *Archives of Microbiology*, 207(5), 107. (Journal Impact Factor: 2.3).
7. Saha S and Kanaujia SP (2025). [Structural analysis of the ribosome assembly factor Nep1, an N1-specific pseudouridine methyltransferase, reveals mechanistic insights.](#) *The FEBS Journal*, 292(9), 2338-2358. (Journal Impact Factor: 5.4).
8. Dasgupta P and Kanaujia SP (2025). [Enlightening the multifarious attributes of the Escherichia coli Sap transport system: A computational perspective.](#) *Journal of Biomolecular Structure and Dynamics*, 1-17. (Journal Impact Factor: 4.4).
9. Bora K, Sarma M, Kanaujia SP, and Dubey VK (2024). [Development of novel dual-target drugs against visceral leishmaniasis and combinational study with miltefosine.](#) *Free Radical Biology and Medicine*, 225, 275-285. (Journal Impact Factor: 7.1).
10. Saha S and Kanaujia SP (2024). [Decoding substrate selectivity of an archaeal RlmCD-like methyltransferase through its salient traits.](#) *ACS Biochemistry*, 63(19), 2477-2492. (Journal Impact Factor: 2.9).
11. Saha S and Kanaujia SP (2024). [Structural and functional characterization of archaeal DMT1 unveils distinct protein dynamics essential for efficient catalysis.](#) *Structure*, 32(10), 1760-1775.e7. (Journal Impact Factor: 4.4).
12. Dasgupta P, Vinil K, and Kanaujia, S.P. (2024). [Evolutionary trends indicate a coherent organization of sap operons.](#) *Research in Microbiology*, 104228. (Journal Impact Factor: 2.5).
13. Saha S, Mandal SK, and Kanaujia SP (2024). [Distinct characteristics of putative archaeal 5-methylcytosine RNA methyltransferases unveil their substrate specificities and evolutionary ancestries.](#) *Journal of Biomolecular Structure and Dynamics*, 1-18. (Journal Impact Factor: 4.4).
14. Dutta A, and Kanaujia SP (2024). [The structural features of MlaD illuminate its unique ligand-transporting mechanism and ancestry.](#) *The Protein Journal*, 43, 298-315. (Journal Impact Factor: 3.0).
15. Bora K, Sarma M, Kanaujia SP and Dubey VK (2023). [Dual-target drugs against Leishmania donovani for potential novel therapeutics.](#) *Scientific Reports*, 13, 18363. (Journal Impact Factor: 4.996).
16. Tomar TS, Dasgupta P and Kanaujia SP (2023). [Operon Finder: a deep learning-based web server for accurate prediction of prokaryotic operons.](#) *Journal of Molecular Biology*, 435(14), 167921. (Journal Impact Factor: 5.6)
17. Dutta A and Kanaujia SP (2022). [MlaC belongs to a unique class of non-canonical substrate-binding proteins and follows a novel phospholipid-binding mechanism.](#) *Journal of Structural Biology*, 214, 107896. (Journal Impact Factor: 3.0).
18. Anand V, Prabhakaran HS, Gogoi P, Kanaujia SP and Kumar M (2022). [Structural and functional characterization of Cas2 of CRISPR-Cas subtype I-C lacking the CRISPR](#)

- [component](#). *Frontiers in Molecular Biosciences*, 9, 988569. (Journal Impact Factor: 5.0).
19. Mandal SK and Kanaujia SP (2022). [Role of an orphan substrate-binding protein MhuP in transient heme transfer in *Mycobacterium tuberculosis*](#). *International Journal of Biological Macromolecules*, 211, 342-356. (Journal Impact Factor: 8.2).
 20. Mandal SK and Kanaujia SP (2021). [Structural and thermodynamic insights into a novel Mg²⁺-citrate-binding protein from the ABC transporter superfamily](#). *Acta Crystallographica Section D: Structural Biology*, 77(12), 1516-1534. (Journal Impact Factor: 2.2).
 21. Chandravanshi M, Tripathi SK and Kanaujia SP (2021). [An updated classification and mechanistic insights into ligand binding of the substrate-binding proteins](#). *FEBS Letters*, 595(18), 2395-2409. (Journal Impact Factor: 3.864).
 22. Dutta A, Chandravanshi M and Kanaujia SP (2021). [Conserved features of the MlaD domain aid the trafficking of hydrophobic molecules](#). *Proteins: Structure, Function, and Bioinformatics*, 89(11), 1473-1488. (Journal Impact Factor: 2.9).
 23. Mandal SK, Nayak SG and Kanaujia SP (2021). [Identification and characterization of metal uptake ABC transporters in *Mycobacterium tuberculosis* unveil their ligand specificity](#). *International Journal of Biological Macromolecules*, 185, 324-337. (Journal Impact Factor: 8.2).
 24. Hemant K, Mandal SK, Gogoi P and Kanaujia SP (2021). [Structural and functional role of invariant water molecules in matrix metalloproteinases: a data-mining approach](#). *Journal of Biomolecular Structure and Dynamics*, 1-12. (Journal Impact Factor: 4.4).
 25. Chandravanshi M, Samanta R and Kanaujia SP (2021). [Structural and thermodynamic insights into the novel dinucleotide-binding protein of ABC transporter unveils its moonlighting function](#). *The FEBS Journal*, 288(15), 4614-4636. (Journal Impact Factor: 5.622).
 26. Sharma A, Gogoi P, Chandravanshi M and Kanaujia SP (2021). [Water-mediated structural rearrangement establishes active conformation of caspases for apoptosis and inflammation](#). *Journal of Biomolecular Structure and Dynamics*, 1-14. (Journal Impact Factor: 4.4).
 27. Dhara A, Hussain S, Kanaujia SP and Kumar M (2021). [Acyldepsipeptide activated ClpP1P2 macromolecule of *Leptospira*, an ideal Achilles' heel to hamper the cell survival and deregulate ClpP proteolytic activity](#). *Research in Microbiology*, 172(2), 103797. (Journal Impact Factor: 2.6).
 28. Chandravanshi M, Samanta R and Kanaujia SP (2020). [Conformational trapping of a \$\beta\$ -glucosides-binding protein unveils the selective two-step ligand-binding mechanism of ABC importers](#). *Journal of Molecular Biology*, 432, 5711-5734. (Journal Impact Factor: 5.6).
 29. Gogoi P, Mordina P and Kanaujia SP (2020). [Exploiting the rationale behind substrate recognition by promiscuous thermophilic NDP-sugar pyrophosphorylase for expanding glycorandomization: an *in-silico* study](#). *Journal of Biomolecular Structure and Dynamics*, 1-13. (Journal Impact Factor: 4.4).
 30. Chandravanshi M, Gogoi P and Kanaujia SP (2020). [Structural and thermodynamic correlation illuminates the selective transport mechanism of disaccharide \$\alpha\$ -glycosides through ABC transporter](#). *The FEBS Journal*, 287, 1576-1597. (Journal Impact Factor: 5.622).
 31. Gogoi P and Kanaujia SP (2019). [Role of structural features in oligomerization, active-site integrity and ligand binding of ribose-1,5-bisphosphate isomerase](#). *Computational and Structural Biotechnology Journal*, 17, 333-344. (Journal Impact Factor: 6.0).
 32. Chandravanshi M, Sharma A, Dasgupta P, Mandal SK and Kanaujia SP (2019). [Identification and characterization of ABC transporters for carbohydrate uptake in *Thermus thermophilus* HB8](#). *Gene*, 696, 135-148. (Journal Impact Factor: 3.5).
 33. Sinha AK, Dutta A, Chandravanshi M and Kanaujia SP (2019). [An insight into bacterial phospholipase C classification and their translocation through Tat and Sec pathways: A data mining study](#). *Meta Gene*, 20, 100547. (Journal Impact Factor: 0.7).
 34. Mandal SK, Adhikari R, Sharma A, Chandravanshi M, Gogoi P and Kanaujia SP (2019). [Designating ligand specificities to metal uptake ABC transporters in *Thermus thermophilus* HB8](#). *Metallomics*, 11, 597-612. (Journal Impact Factor: 3.4).
 35. Gogoi P, Mordina P and Kanaujia SP (2019). [Structural insights into the catalytic mechanism of methylthioribose-1-phosphate isomerase](#). *Journal of Structural Biology*,

- 205(1), 67-77. (**Journal Impact Factor: 3.0**).
36. Gogoi P and Kanaujia SP (2018). [Archaeal and eukaryal translation initiation factor 1 differ in their RNA interacting loops](#). *FEBS Letters*, 592, 1602-1610. (**Journal Impact Factor: 3.864**).
 37. Gogoi P and Kanaujia SP (2018). [A presumed homologue of the regulatory subunits of eIF2B functions as ribose-1,5-bisphosphate isomerase in *Pyrococcus horikoshii* OT3](#). *Scientific Reports*, 8:1891. (**Journal Impact Factor: 4.996**).
 38. Adhikari R, Singh D, Chandravanshi M, Dutta A and Kanaujia SP (2017). [UgpB, a periplasmic component of the UgpABCE ATP-binding cassette transporter, predominantly follows the sec translocation pathway](#). *Meta Gene*, 13, 129-139. (**Journal Impact Factor: 0.7**).
 39. Mandal SK, Chandravanshi M, Gogoi P and Kanaujia SP (2017). [In silico characterization of TTHA0596: A potential Zn²⁺ binding protein of ATP-binding cassette transporter](#). *Gene Reports*, 6, 132-141. (**Journal Impact Factor: 1.3**).
 40. Jha S, Kanaujia SP and Limaye AM (2016). [Direct inhibition of matrix metalloproteinase-2 \(MMP-2\) by \(-\)-epigallocatechin-3-gallate: a possible role for the fibronectin type II repeats](#). *Gene*, 593, 126-130. (**Journal Impact Factor: 3.5**).
 41. Chandravanshi M, Gogoi P and Kanaujia SP (2016). [Computational characterization of TTHA0379: a potential glycerophosphocholine binding protein of Ugp ATP-binding cassette transporter](#). *Gene*, 592, 260-268. (**Journal Impact Factor: 3.5**).
 42. Srivastava A, Gogoi P, Deka B, Goswami S and Kanaujia SP (2016). [In silico analysis of 5'-UTRs highlights the prevalence of Shine-Dalgarno and leaderless-dependent mechanisms of translation initiation in bacteria and archaea, respectively](#). *Journal of Theoretical Biology*, 402, 54-61. (**Journal Impact Factor: 2.0**).
 43. Gogoi P, Srivastava A, Jayaprakash P, Jeyakanthan J and Kanaujia SP (2015). [In silico analysis suggests that PH702 and PH0208 encode for methylthioribose-1-phosphate isomerase and ribose-1,5-bisphosphate isomerase, respectively, rather than aIF2B \$\beta\$ and aIF2B \$\delta\$](#) . *Gene*, 575, 118-126. (**Journal Impact Factor: 3.5**).
 44. Gogoi P, Chandravanshi M, Mandal SK, Srivastava A and Kanaujia SP (2015). [Heterogeneous behavior of metalloproteins towards metal ion binding and selectivity: insights from molecular dynamics studies](#). *Journal of Biomolecular Structure and Dynamics*, 1-16. (**Journal Impact Factor: 4.4**).
 45. Nayak SK, Mallik SB, Kanaujia SP, Sekar K, Ranganathan KR, Ananthalakshmi V, Jeyaraman G, Saralaya SS, Nagarajan K and Guru Row TN (2013). [Crystal structures and binding studies of atovaquone and its derivatives with cytochrome bc₁-complex: a molecular basis for drug design](#). *CrystEngComm*, 15, 4871-4884. (**Journal Impact Factor: 3.1**).
 46. Manjunath K, Kanaujia SP, Surekha K, Jeyakanthan J and Sekar K (2013). [Structure of SAICAR synthetase from *Pyrococcus horikoshii* OT3: Insights into Thermal Stability](#). *International Journal of Biological Macromolecules*, 53, 7-19. (**Journal Impact Factor: 8.2**).
 47. Vaishnavi K, Saxena N, Shah N, Singh R, Manjunath K, Uthayakumar M, Kanaujia SP, Kaul SC, Sekar K and Wadhwa R (2012). [Differential Activities of the Two Closely Related Withanolides, Withaferin A and Withanone: Bioinformatics and Experimental Evidences](#). *PLoS ONE*, 7(9), e44419. (**Journal Impact Factor: 3.725**).
 48. Dhanasekaran V, Velmurugan V, Kanaujia SP and Sekar K (2011). [Role of invariant water molecules and water-mediated ionic interactions in D-xylose isomerase from *Streptomyces rubiginosus*](#). *Journal of Biomolecular Structure and Dynamics*, 1-9. (**Journal Impact Factor: 4.4**).
 49. Kanaujia SP, Jeyakanthan J, Shinkai A, Kuramitsu S, Yokoyama S and Sekar K (2011). [Crystal structures, dynamics and functional implications of molybdenum cofactor biosynthesis protein MogA from two thermophilic organisms](#). *Acta Cryst.* F67, 2-16. (**Journal Impact Factor: 0.9**).
 50. Kanaujia SP, Jeyakanthan J, Nakagawa N, Sathyaramya B, Shinkai A, Kuramitsu S, Yokoyama S and Sekar K (2010). [Structures of apo and GTP-bound molybdenum cofactor biosynthesis protein MoaC from *Thermus thermophilus* HB8](#). *Acta Cryst.* D66, 821-833. (**Journal Impact Factor: 2.2**).
 51. Jeyakanthan J, Kanaujia SP, Nishida Y, Nakagawa N, Praveen S, Shinkai A, Kuramitsu S, Yokoyama S and Sekar K (2010). [Free and ATP-bound structures of Ap₄A hydrolase from *Aquifex aeolicus* V5](#). *Acta Cryst.* D66, 116-124. (**Journal Impact Factor: 2.2**).

52. **Kanaujia SP** and Sekar K (2009). [Structural and Functional Role of Water Molecules in Bovine Pancreatic Phospholipase A₂: A Data-Mining approach](#). *Acta Cryst.* D65, 74-84. (**Journal Impact Factor: 2.2**)
53. Jeyakanthan J, Rangarajan S, Mridula P, **Kanaujia SP**, Shiro Y, Kuramitsu S, Yokoyama S and Sekar K (2008). [Observation of a calcium-binding site in the gamma-class carbonic anhydrase from *Pyrococcus horikoshii*](#). *Acta Cryst.* D64, 1012-1019. (**Journal Impact Factor: 2.2**)
54. **Kanaujia SP** and Sekar K (2008). [Structures and molecular dynamics studies of three active site mutants of bovine pancreatic phospholipase A₂](#). *Acta Cryst.* D64, 1003-1011. (**Journal Impact Factor: 2.2**)
55. **Kanaujia SP**, Ranjani CV, Jeyakanthan J, Ohmori M, Agari K, Kitamura Y, Baba S, Ebihara A, Shinkai A, Kuramitsu S, Shiro Y, Sekar K and Yokoyama S (2007). [Cloning, expression, purification, crystallization and preliminary X-ray crystallographic study of molybdopterin synthase from *Thermus thermophilus* HB8](#). *Acta Cryst.* F63, 324-326. (**Journal Impact Factor: 0.9**)
56. **Kanaujia SP**, Ranjani CV, Jeyakanthan J, Baba S, Kuroishi C, Ebihara A, Shinkai A, Kuramitsu S, Shiro Y, Sekar K and Yokoyama S (2007). [Cloning, expression, purification, crystallization and preliminary X-ray crystallographic study of DHNA synthetase from *Geobacillus kaustophilus*](#). *Acta Cryst.* F63, 103-105. (**Journal Impact Factor: 0.9**)
57. **Kanaujia SP**, Ranjani CV, Jeyakanthan J, Baba S, Chen L, Liu Z-J, Wang B-C, Nishida M, Ebihara A, Shinkai A, Kuramitsu S, Shiro Y, Sekar K and Yokoyama S (2007). [Crystallization and preliminary crystallographic analysis of molybdenum cofactor biosynthesis protein C from *Thermus thermophilus*](#). *Acta Cryst.* F63, 27-29. (**Journal Impact Factor: 0.9**)
58. **Kanaujia SP**, Ranjani CV, Jeyakanthan J, Nishida M, Kitamura Y, Baba S, Ebihara A, Shimizu N, Nakagawa N, Shinkai A, Yamamoto M, Kuramitsu S, Shiro Y, Sekar K and Yokoyama S (2007). [Preliminary X-ray crystallographic study of glucose dehydrogenase from *Thermus thermophilus* HB8](#). *Acta Cryst.* F63, 446-448. (**Journal Impact Factor: 0.9**)
59. Sekar K, Yogavel M, **Kanaujia SP**, Sharma A, Velmurugan D, Poi M-J, Dauter J and Tsai M-D (2006). [Suggestive evidence for the involvement of the second calcium and surface loop in interfacial binding: Monoclinic and trigonal crystal structures of a quadruple mutant of phospholipase A₂](#). *Acta Cryst.* D62, 717-724. (**Journal Impact Factor: 2.2**)

Book Chapters

1. **Kanaujia SP** (2017). [Understanding the toxic metal binding proteins and peptides](#). In "Handbook of Metal-Microbe Interactions and Bioremediation", edited by Surajit Das and Hirak Ranjan Dash, **CRC Press (Taylor & Francis Group) (ISBN 9781498762427)**.

Conferences

Total number of confereces: 80 (National: 65, International: 15)

1. Kushal Bora, Manash Sarma, **Shankar Prasad Kanaujia**, and Vikash Kumar Dubey. Development of novel dual-target drugs against visceral leishmaniasis and combinational study with miltefosine. Drug Discovery 2025: Emerging Trends and Future Prospects. February 24-26, 2025, Centre for Interdisciplinary Research in Basic sciences, Jamia Millia Islamia, New Delhi, India. [**Best poster presentation award**]
2. Kushal Bora, Manash Sarma, **Shankar Prasad Kanaujia**, and Vikash Kumar Dubey. Development of novel dual-target drugs against visceral leishmaniasis and combinational study with miltefosine. 9th international conference on Current Trends in Drug Discovery Research. February 19-22, 2025, CSIR-Central Drug Research Institute, Lucknow, India. [**Oral and Poster presentation**]
3. Kalyan Ghosh and **Shankar Prasad Kanaujia**. Bacterial peptide transporters as gateways for illicit transport of peptide-based antibiotics. 51st National Seminar on Crystallography (NSC-51). November 27-29, 2024, VNIT Nagpur, Maharashtra, India. [**Oral Presentation**].
4. Ritu Tripathi and **Shankar Prasad Kanaujia**. Unveiling multiple copies of phospholipid-binding protein (PTC): A study of its multifaceted nature. 51st National Seminar on Crystallography (NSC-51). November 27-29, 2024, VNIT Nagpur, Maharastra, India. [**Best**

Oral Presentation Award].

5. Arpana Gupta and **Shankar Prasad Kanaujia**. A proposed hypothetical model of archaeal aIF2B involved in protein translation initiation. 51st National Seminar on Crystallography (NSC-51). November 27-29, 2024, VNIT Nagpur, Maharashtra, India. [**Oral Presentation**].
6. Kalyan Ghosh and **Shankar Prasad Kanaujia**. Advancement and applications of analytical instruments (AAAI-24). November 9, 2024. [**Workshop**].
7. Ritu Tripathi and **Shankar Prasad Kanaujia**. Advancement and Applications of Analytical Instruments (AAAI-24). November 9, 2024. [**Workshop**].
8. Arpana Gupta and **Shankar Prasad Kanaujia**. Advancement and Applications of Analytical Instruments (AAAI) 2024. November 9, 2024. [**Workshop**].
9. Sayan Saha and **Shankar Prasad Kanaujia**. Structural and evolutionary insights into an archaeal rRNA methyltransferase involved in the modification of 5-methyluridine. Research and Industrial Conclave - Integration'2024. August 09-11, 2024, IIT Guwahati, Assam, India. [**Oral Presentation**].
10. Pratik Dasgupta and **Shankar Prasad Kanaujia**. Evolutionary insights into the conservation of a class of antimicrobial peptide transporter operons. Research and Industrial Conclave - Integration'2024. August 09-11, 2024, IIT Guwahati, Assam, India. [**Oral Presentation**].
11. Kalyan Ghosh and **Shankar Prasad Kanaujia**. Unveiling illicit transport of peptide-based antibiotics by bacterial peptide transporters. Research and Industrial Conclave - Integration'2024. August 09-11, 2024, IIT Guwahati, Assam, India. [**Poster Presentation**].
12. Ritu Tripathi and **Shankar Prasad Kanaujia**. Revealing the multifaceted nature of phospholipid-binding protein in Gram-negative bacteria: a data mining study. Research and Industrial Conclave - Integration'2024. August 09-11, 2024, IIT Guwahati, Assam, India. [**Oral Presentation**].
13. Kushal Bora, Manash Sarma, **Shankar Prasad Kanaujia**, and Vikash Kumar Dubey. Dual-target drugs against Leishmania donovani for potential novel therapeutics. Young scientist conference (9th India International Science Festival 2023). January 17-20, 2024, DBT THSTI-RCB, Faridabad, Haryana, India. [**Poster presentation**].
14. Sayan Saha and **Shankar Prasad Kanaujia**. Unveiling the protein dynamics of archaeal DMT1 rRNA methyltransferase for efficient catalysis. 50th National Seminar on Crystallography (NSC-50). November 22-24, 2023, CSIR-Institute of Microbial Technology Chandigarh, India. [**Oral Presentation**].
15. Pratik Dasgupta and **Shankar Prasad Kanaujia**. Unravelling the multifarious behaviour of a putative antimicrobial peptide-binding protein via computational strategies. 50th National Seminar on Crystallography (NSC-50). November 22-24, 2023, CSIR-Institute of Microbial Technology Chandigarh, India. [**Poster Presentation**].
16. Kushal Bora, **Shankar Prasad Kanaujia**, and Vikash Kumar Dubey. Basics Cell Culture Technology. November 6-9, 2023, DST-National Centre for Cell Science, Pune University, Pune, India. [**Workshop**].
17. Kushal Bora, Manash Sarma, **Shankar Prasad Kanaujia**, and Vikash Kumar Dubey. Dual-target drugs against Leishmania donovani for potential novel therapeutics. 4th world drug congress on drug discovery & development-2023. October 28-29, 2023, Indian Institute of Science, Bengaluru, India. [**Poster presentation**].
18. Kushal Bora, Manash Sarma, **Shankar Prasad Kanaujia**, and Vikash Kumar Dubey. Dual-target drugs against Leishmania donovani for potential novel therapeutics. International Conference on Structural Biology and Drug Discovery (ICSBDD-2023). October 11-12, 2023, Gautam Buddha University, Uttar Pradesh, India. [**Poster presentation**].
19. Kushal Bora, **Shankar Prasad Kanaujia**, and Vikash Kumar Dubey. 4th Online International Flow Cytometry Course "Flow Cytometry and its Applications in Basic and Advanced Research". September 22-24, 2023, Trust for Education and Training in Cytometry (TETC). [**Workshop**].
20. Angshu Dutta and **Shankar Prasad Kanaujia**. MlaD is a non-canonical substrate-binding protein that follows a novel phospholipid-binding mechanism. Research and Industrial Conclave 2023 (RIC 2023). May 14-16, 2023, IIT Guwahati, Guwahati, Assam, India. [**Best Oral Presentation Award**].
21. Angshu Dutta and **Shankar Prasad Kanaujia**. Exploring the structural and mechanistic intricacies of non-canonical substrate-binding proteins. Research and Industrial Conclave

- 2023 (RIC 2023). May 14-16, 2023, IIT Guwahati, Guwahati, Assam, India. **[Three Minutes Thesis Presentation]**.
22. Sayan Saha and **Shankar Prasad Kanaujia**. Unveiling the substrate specificities and evolutionary ancestries of putative archaeal 5-methylcytosine RNA methyltransferases. Research & Industrial Conclave – Integration (RIC 2023). May 14-16, 2023, IIT Guwahati, Assam, India. **[Best Poster Award]**.
 23. Ritu Tripathi and **Shankar Prasad Kanaujia**. The structural and functional diversity of the Mla system calls for a new classification scheme. Research and Industrial Conclave 2023 (RIC 2023). May 14-16, 2023, IIT Guwahati, Guwahati, Assam, India. **[Poster Presentation]**
 24. Arpana Gupta and **Shankar Prasad Kanaujia**. Identification, structural and functional characterization of archaeal translation initiation factor. Research and Industrial Conclave 2023 (RIC 2023). May 14-16, 2023, IIT Guwahati, Guwahati, Assam, India. **[Poster Presentation]**
 25. Angshu Dutta and **Shankar Prasad Kanaujia**. MlaC belongs to a unique class of non-canonical substrate-binding proteins and follows a novel phospholipid-binding mechanism. National Seminar on Crystallography (NSC-49). November 28-30, 2022, University of Jammu, Jammu, India. **[Professor Kailasam Venkatesan Award for Best Oral Presentation Award]**.
 26. Sayan Saha and **Shankar Prasad Kanaujia**. Unveiling the substrate specificities and evolutionary ancestries of putative archaeal 5-methylcytosine RNA methyltransferases. National Seminar on Crystallography (NSC-49). November 28-30, 2022, University of Jammu, Jammu, India. **[Oral Presentation]**
 27. Pratik Dasgupta and **Shankar Prasad Kanaujia**. In silico analysis reveals the evolutionary conservation of a class of antimicrobial peptide (AMP) transporter operons. National Seminar on Crystallography (NSC-49). November 28-30, 2022, University of Jammu, Jammu, India. **[Oral Presentation]**
 28. Suraj Kumar Mandal and **Shankar Prasad Kanaujia**. Deciphering the mechanism of transient heme transfer by an orphan substrate-binding protein MhuP in *Mycobacterium tuberculosis*. National Seminar on Crystallography (NSC-48). November 25-27, 2021, IIT Roorkee, Uttarakhand, India. **[Best Oral Presentation Award]**.
 29. Angshu Dutta and **Shankar Prasad Kanaujia**. Unveiling the mechanistic aspects of a novel substrate-binding protein in Gram-negative bacteria. National Seminar on Crystallography (NSC-48). November 25-27, 2021, IIT Roorkee, Uttarakhand, India. **[Best Oral Presentation Award]**.
 30. Sayan Saha and **Shankar Prasad Kanaujia**. In silico studies enlighten the salient features of putative archaeal 5-methylcytosine methyltransferases. National Seminar on Crystallography (NSC-48). November 25-27, 2021, IIT Roorkee, Uttarakhand, India. **[Poster Presentation]**.
 31. Pratik Dasgupta and **Shankar Prasad Kanaujia**. In silico analysis of a putative antimicrobial peptide-binding protein highlights its promiscuous nature. National Seminar on Crystallography (NSC-48). November 25-27, 2021, IIT Roorkee, Uttarakhand, India. **[Poster Presentation]**.
 32. Kalyan Ghosh and **Shankar Prasad Kanaujia**. 48th National Seminar on Crystallography (NSC-48). November 25-27, 2021, IIT Roorkee, Uttarakhand, India.
 33. Suraj Kumar Mandal and **Shankar Prasad Kanaujia**. Structural and functional characterization of an Mg²⁺-citrate-binding protein from a thermophilic bacteria. PDB 50th Anniversary Symposium in Asia. November 24, 2021, PDBj and Institute for Protein Research, Osaka University, Japan. **[Poster Presentation]**.
 34. Angshu Dutta and **Shankar Prasad Kanaujia**. Exploring the structural aspects of a novel phospholipid-binding protein. PDB 50th Anniversary Symposium in Asia. November 24, 2021, PDBj and Institute for Protein Research, Osaka University, Japan. **[Best Poster Award]**.
 35. Sayan Saha and **Shankar Prasad Kanaujia**. In silico characterization of putative 5-methylcytosine methyltransferases from *Pyrococcus horikoshii*. PDB 50th Anniversary Symposium in Asia. November 24, 2021, PDBj and Institute for Protein Research, Osaka University, Japan. **[Poster Presentation]**.
 36. Pratik Dasgupta and **Shankar Prasad Kanaujia**. In silico studies enlighten the salient features of a putative antimicrobial peptide-binding protein. In silico studies enlighten the salient features of a putative antimicrobial peptide-binding protein. PDB 50th Anniversary

- Symposium in Asia. November 24, 2021, PDBj and Institute for Protein Research, Osaka University, Japan. **[Poster Presentation]**.
37. Kalyan Ghosh and **Shankar Prasad Kanaujia**. PDB 50th Anniversary Symposium in Asia. November 24, 2021, PDBj and Institute for Protein Research, Osaka University, Japan.
 38. Suraj Kumar Mandal and **Shankar Prasad Kanaujia**. A transient mechanism of heme transfer by an orphan substrate-binding protein MhuP in *Mycobacterium tuberculosis*. Bringing Molecular Structure to Life: 50 Years of the PDB. October 20-22, 2021, European Molecular Biology Laboratory (EMBL), Heidelberg, Germany. **[Poster Presentation]**
 39. Angshu Dutta and **Shankar Prasad Kanaujia**. Deciphering the structural aspects of a novel substrate-binding protein. Bringing Molecular Structure to Life: 50 Years of the PDB. October 20-22, 2021, European Molecular Biology Laboratory (EMBL), Heidelberg, Germany. **[Poster Presentation]**
 40. Sayan Saha and **Shankar Prasad Kanaujia**. Characterization of putative archaeal 5-methylcytosine methyltransferases: An *in silico* approach. Bringing Molecular Structure to Life: 50 Years of the PDB. October 20-22, 2021, European Molecular Biology Laboratory (EMBL), Heidelberg, Germany. **[Poster Presentation]**
 41. Pratik Dasgupta and **Shankar Prasad Kanaujia**. Insights into a putative antimicrobial peptide binding protein: An *in silico* approach. Bringing Molecular Structure to Life: 50 Years of the PDB. October 20-22, 2021, European Molecular Biology Laboratory (EMBL), Heidelberg, Germany. **[Poster Presentation]**
 42. Kalyan Ghosh and **Shankar Prasad Kanaujia**. Bringing Molecular Structure to Life: 50 Years of the PDB. October 20-22, 2021, European Molecular Biology Laboratory (EMBL), Heidelberg, Germany.
 43. Sayan Saha and **Shankar Prasad Kanaujia**. Associazione Italiana Cristallografia School 2021 (AICS2021). August 31 – September 4, 2021. **[Workshop]**
 44. Suraj Kumar Mandal and **Shankar Prasad Kanaujia**. Understanding the structural and functional aspects of a novel Mg²⁺-citrate-binding protein. 25th Congress of the International Union of Crystallography (IUCr)-2021. August 14-22, 2021, Prague, Czech Republic. **[Poster Presentation]**
 45. Angshu Dutta and **Shankar Prasad Kanaujia**. MlaC represents a unique class of solute-binding proteins. 25th Congress of the International Union of Crystallography (IUCr)-2021. August 14-22, 2021, Prague, Czech Republic. **[Poster Presentation]**
 46. Monika Chandravanshi and **Shankar Prasad Kanaujia**. Structural insights into the selective transport mechanism of α -glycoside ABC transporter and its thermodynamic correlation. 16th Conference of the Asian Crystallographic Association (AsCA2019). December 17-20, 2019, National University of Singapore (NUS), Singapore. **[Oral Presentation and IUCr Young Scientist Award]**
 47. **Shankar Prasad Kanaujia**. Structure-based functional characterization of protein translation initiation factors and their homologs in archaea. National Seminar on Crystallography (NSC-47). June 19-22, 2019, Bhabha Atomic Research Centre (BARC) Mumbai, India. **[Oral & Poster Presentation]**
 48. Prerana Gogoi and **Shankar Prasad Kanaujia**. Understanding the rationale of substrate promiscuity of thermophilic NDP-sugar pyrophosphorylases. National Seminar on Crystallography (NSC-47). June 19-22, 2019, Bhabha Atomic Research Centre (BARC) Mumbai, India. **[Poster Presentation]**
 49. Monika Chandravanshi and **Shankar Prasad Kanaujia**. Structural insights into the selective transport mechanism of disaccharide α -glycosides through ABC transporter. National Seminar on Crystallography (NSC-47). June 19-22, 2019, Bhabha Atomic Research Centre (BARC) Mumbai, India. **[Poster Presentation]**
 50. Suraj Kumar Mandal and **Shankar Prasad Kanaujia**. Metal binding spectrum of a putative metal-specific substrate-binding protein from *Thermus thermophilus* HB8. National Seminar on Crystallography (NSC-47). June 19-22, 2019, Bhabha Atomic Research Centre (BARC) Mumbai, India. **[Poster Presentation]**
 51. Suraj Kumar Mandal and **Shankar Prasad Kanaujia**. Functional annotation of metal sequestering ABC transporters in *Thermus thermophilus* HB8. Emerging Trends in Disease Model Systems. March 25-27, 2019, The National Centre for Cell Science (NCCS) Pune, India. **[Poster Presentation]**
 52. Prerana Gogoi and **Shankar Prasad Kanaujia**. Structure-based functional characterization of archaeal translation initiation factors. National Seminar on Crystallography (NSC-46). June 27-29, 2018, The National Institute of Mental Health and

- Neuro-Sciences (NIMHANS) Bangalore, India. **[Poster Presentation]**
53. Monika Chandravanshi and **Shankar Prasad Kanaujia**. Structural and functional characterization of Trehalose/maltose-binding protein from *Thermus thermophilus* HB8. National Seminar on Crystallography (NSC-46). June 27-29, 2018, The National Institute of Mental Health and Neuro-Sciences (NIMHANS) Bangalore, India. **[Best Poster Merit Award]**
 54. Suraj Kumar Mandal and **Shankar Prasad Kanaujia**. Structural and functional characterization of a putative metal-specific substrate-binding protein from *Thermus thermophilus* HB8. National Seminar on Crystallography (NSC-46). June 27-29, 2018, The National Institute of Mental Health and Neuro-Sciences (NIMHANS) Bangalore, India. **[Best Oral Presentation Award]**
 55. Angshu Dutta and **Shankar Prasad Kanaujia**. Functional annotation, classification and assignment of translocation pathway of phospholipases C. Research Conclave 2018. March 08-11, 2018, Indian Institute of Technology (IIT) Guwahati, India. **[Best Poster Presentation Award]**
 56. Prerana Gogoi and **Shankar Prasad Kanaujia**. Structural and functional characterization of a presumed homologue of the regulatory subunits of eIF2B. Research Conclave 2018. March 08-11, 2018, Indian Institute of Technology (IIT) Guwahati, India. **[Oral Presentation]**
 57. Prerana Gogoi and **Shankar Prasad Kanaujia**. Structural and functional characterization of ribose-1,5-bisphosphate isomerase in archaea. 24th Congress and General Assembly of International Union of Crystallography (IUCr 2017). August 21-28, 2017, Hyderabad, India. **[Poster Presentation]**
 58. Monika Chandravanshi and **Shankar Prasad Kanaujia**. Structural insight into the glycerophosphocholine binding protein of ABC transporter. 24th Congress and General Assembly of International Union of Crystallography (IUCr 2017). August 21-28, 2017, Hyderabad, India. **[Poster Presentation]**
 59. Suraj Kumar Mandal and **Shankar Prasad Kanaujia**. *In silico* characterization of a potential Zn²⁺ ABC transporter. 24th Congress and General Assembly of International Union of Crystallography (IUCr 2017). August 21-28, 2017, Hyderabad, India. **[Poster Presentation]**
 60. Angshu Dutta and **Shankar Prasad Kanaujia**. UgpB protein dominantly follows Sec translocation pathway. 24th Congress and General Assembly of International Union of Crystallography (IUCr 2017). August 21-28, 2017, Hyderabad, India. **[Poster Presentation]**
 61. Prerana Gogoi and **Shankar Prasad Kanaujia**. Architecture of ribose-1,5-bisphosphate isomerase, an enzyme unique to archaea. National Seminar on Crystallography (NSC-45). July 9-12, 2017, Indian Institute of Technology (BHU) Varanasi, India. **[Best Poster Presentation Award]**
 62. Angshu Dutta and **Shankar Prasad Kanaujia**. Deciphering the structural aspects of an antimicrobial peptide importer in Gram-negative bacteria for developing drugs. National Seminar on Crystallography (NSC-45). July 9-12, 2017, Indian Institute of Technology (BHU) Varanasi, India. **[Poster Presentation]**
 63. Monika Chandravanshi and **Shankar Prasad Kanaujia**. Heterogeneous behavior of metalloproteins toward metal ion binding and selectivity: insights from molecular dynamics studies. National Seminar on Crystallography (NSC-44). July 10-13, 2016, Indian Institute of Science Education and Research (IISER) Pune, India. **[Poster Presentation]**
 64. Prerana Gogoi and **Shankar Prasad Kanaujia**. *In silico* analysis suggests that PH0702 and PH0208 encode for methylthioribose-1-phosphate isomerase and ribose-1, 5-bisphosphate isomerase, respectively, rather than aIF2B β and aIF2B δ . National Seminar on Crystallography (NSC-44). July 10-13, 2016, Indian Institute of Science Education and Research (IISER) Pune, India. **[Poster Presentation]**
 65. Monika Chandravanshi and **Shankar Prasad Kanaujia**. Heterogeneous behaviour of metalloproteins toward metal ion binding and selectivity: insights from molecular dynamics studies. Recent Developments in Medical Biotechnology and Structure-Based Drug Designing (RDMBSBDD-2015). December 6-7, 2015, Indian Institute of Technology (IIT) Guwahati, India. **[Poster Presentation]**
 66. Prerana Gogoi and **Shankar Prasad Kanaujia**. *In silico* analysis suggests that PH0702 and PH0208 encode for methylthioribose-1-phosphate isomerase and ribose-1,5-bisphosphate isomerase, respectively, rather than aIF2B β and aIF2B δ . Recent

Developments in Medical Biotechnology and Structure-Based Drug Designing (RDMBSBDD-2015). December 6-7, 2015, Indian Institute of Technology (IIT) Guwahati, India. **[Poster Presentation]**

67. Gauri Deb, Shaline Jha, Sahil Batra, **Shankar Prasad Kanaujia** and Anil M Limaye. Inhibition of matrix metalloproteinase-2 (MMP-2) by the green tea polyphenol Epigallocatechin-3-gallate (EGCG): mechanistic insights from biochemical and *in silico* studies. 34th Annual Convention of Indian Association for Cancer Research on "Cancer research: from bench to bedside". February 19-21, 2015, Jaipur, India.
68. Ambuj Srivastava and **Shankar Prasad Kanaujia**. Interfacial analysis of oligomeric proteins in improving molecular docking algorithms. INDO-US CONFERENCE and WORKSHOP on Recent advances on Structural Biology & Drug Discovery (RASBDD-IIT-2014). October 9-11, 2014, Indian Institute of Technology (IIT) Roorkee, India. **[Poster Presentation]**
69. **Shankar Prasad Kanaujia**. Eighth Asia-Pacific Bioinformatics Conference (APBC 2010). January 18-21, 2010, Bangalore, India.
70. **Shankar Prasad Kanaujia** and K. Sekar. Structural and functional role of water molecules in bovine pancreatic phospholipase A₂: A data-mining approach. 38th National Seminar on Crystallography (NSC-38). February 11-13, 2009, University of Mysore, India. **[Poster Presentation]**
71. **Shankar Prasad Kanaujia**. IISc Centenary Conference. December 13-16, 2008, Indian Institute of Science (IISc) Bangalore, India.
72. **Shankar Prasad Kanaujia** and K. Sekar. Structures and molecular-dynamics studies of three active-site mutants of bovine pancreatic phospholipase A₂. Eighth Conference of the Asian Crystallographic Association (AsCA-2007). November 4-7, 2007, Taipei, Taiwan. **[Poster Presentation]**
73. **Shankar Prasad Kanaujia**. Understanding Molecular Simulations. January 22-27, 2007, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) Bangalore, India.
74. **Shankar Prasad Kanaujia**. Drug Design Workshop. July 30 - Aug 3, 2007, Indian Institute of Science (IISc) Bangalore, India.
75. **Shankar Prasad Kanaujia**. 11th ADNAT International Conference on Advances in Structural Biology and Structure Prediction. February 23-25, 2007, Centre for Cellular & Molecular Biology (CCMB) Hyderabad, India.
76. **Shankar Prasad Kanaujia**. 36th National Seminar on Crystallography (NSC-36). January 22-24, 2007, University of Madras, Tamil Nadu, India.
77. **Shankar Prasad Kanaujia**. Computational Insights into Biological Systems: InCoB 2006 Satellite Meeting. December 26-28, 2006, Indian Institute of Science (IISc) Bangalore, India.
78. **Shankar Prasad Kanaujia**. Fifth International Conference on Bioinformatics (InCoB 2006). December 18-20, 2006, New Delhi, India.
79. **Shankar Prasad Kanaujia**. Third Indo-French Bioinformatics Meeting (IFBM 2006). June 12-14, 2006, National Centre for Biological Sciences (NCBS) Bangalore, India.
80. **Shankar Prasad Kanaujia**. National Seminar-cum-Workshop on Bioinformatics. March 1-2, 2006, Indian Institute of Science (IISc) Bangalore, India.

Invited Lectures

1. **Structural and functional characterization of archaeal DDMT1**. 51st National Seminar on Crystallography (NSC-51). Visvesvaraya National Institute of Technology (VNIT), Nagpur, India (November 27-29, 2024).
2. **Distinct structural features of MlaC and MlaD reveal their unique phospholipid binding and transport mechanisms**. 50th National Seminar on Crystallography (NSC-50). CSIR-Institute of Microbial Technology Chandigarh, India (November 22-24, 2023).
3. **Identification and characterization of translation initiation factors in archaea**. National Conference on Emerging trends in Bioinformatics for Agriculture, Food and Health, Jacob Institute of Biotechnology and Bioengineering, Sam Higginbottom University of Agriculture, Technology and Sciences (March 15-16, 2023).
4. **Sugar ABC importers in bacteria: potential drug targets and delivery systems**. Refresher course in Biotechnology, Centre of Biotechnology, University of Allahabad (January 10-24, 2022).
5. **Molecular Medicine**. National Conference on Computational and Biochemical Drug Discovery [NCCBDD-2021]. I-DAPT HUB FOUNDATION IIT (BHU), VARANASI and

Bioinformatics and Drug Discovery Society, India (September 11-12, 2021). **[Session Chair]**

6. **Sugar ABC importers as potential drug targets and delivery systems.** National Conference on Computational and Biochemical Drug Discovery [NCCBDD-2021]. I-DAPT HUB FOUNDATION IIT (BHU), VARANASI and Bioinformatics and Drug Discovery Society, India (September 11-12, 2021).
7. **Protein sequence alignment, phylogeny, structure prediction, and visualization.** Computer-aided drug design and protein analysis. School of Biochemical Engineering, Indian Institute of Technology (BHU) Varanasi, Uttar Pradesh, India (February 22-26, 2021).
8. **Structural bioinformatics: tips and tools.** Principles of drug designing. Department of Molecular Biology and Biotechnology, Tezpur University, Assam, India (March 5-6, 2016).
9. **Computational methods for functional annotation of membrane proteins.** Advances in Computational Biology and Computer-Aided Drug Design. Department of Biosciences and Bioengineering, Indian Institute of Technology Guwahati, Assam, India (June 24-25, 2015).
10. **Peptide Drugs: from Modeling to Practice.** Department of Biotechnology, Indian Institute of Technology Guwahati, Assam, India (November 7-8, 2014).
11. **ab initio Protein Structure Prediction using I-TASSER.** Molecular Tools in Medical Biotechnology Investigations. Department of Biosciences and Bioengineering, Indian Institute of Technology Guwahati, Assam, India (December 2-6, 2013).
12. **Protein Structure Prediction: ab initio to homology.** Bioinformatics Center, Faculty of Veterinary Science, Assam Agricultural University, Khanapara, Guwahati, Assam, India (November 7-9, 2012).
13. **X-ray Crystallography: principles and applications.** Biophysics and Computational Biology Week. Department of Biotechnology, Indian Institute of Technology Guwahati, Assam, India (October 16, 2012).

Journal's Reviewer

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- [Journal of Cellular Biochemistry](#)
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Sponsored Projects

List of Ongoing Projects:

S. No.	Title	Funding Agency	Budget (INR)	Period		Co-Investigators	PI or Co-PI; PI name if not PI
				From	To		
1.	Elucidation of structural and evolutionary insights into ribosomal RNA methyltransferases involved in ribosome biogenesis and antibiotic resistance	DBT	73,42,560	29.04.2025	28.04.2028	MK	PI
2.	Elucidating structural aspects of antimicrobial peptide transporter in <i>Escherichia coli</i> : a study for structure-based drug designing	DBT	70,95,240	12.08.2022	11.08.2025	MK	PI
3.	Structural And Functional Studies Of A Putative Membrane Protein Complex Of Mycobacterium Tuberculosis Involved In Invasion And Cholesterol Transport	SERB	48,95,264	11.03.2022	10.03.2025	-	PI
4.	An investigation of self-assembled nanostructured protein-based therapeutic approaches in Breast cancer	TARE-SERB	18,30,000	30.01.2023	29.01.2026	Prof. Shailendra Kumar Mahanta (Kaziranga University)	Co-PI

List of Completed Projects:

S. No.	Title	Funding Agency	Budget (INR)	Period		Co-Investigators	PI or Co-PI; PI name if not PI
				From	To		
1.	Role of Trigger factor in caseinolytic protease system of <i>Leptospira</i>	SERB	56,24,000	31.12.2020	30.12.2022	Dr. Shankar Prasad Kanaujia	Dr. Manish Kumar

2.	Study of in-depth genetic heterogeneity with respect to resistome and compensatory adaption of MDR Mtb clinical strains inside BM-Mesenchymal stem cells circulating in the North-East Region for therapeutic implications	DBT	68,41,000	13.09.2019	12.09.2022	Dr. Shankar Prasad Kanaujia	Prof. Sanjukta Patra
3.	Structural and functional characterization of an ABC transporter involved in the maintenance of lipid asymmetry in <i>Escherichia coli</i> and <i>Shigella flexneri</i> : structure-based drug-designing	SERB	27,50,000	16.03.2019	15.03.2022	-	PI
4.	Repurposing endogenous CRISPR-Cas type_I machinery for efficient markerless genome editing tool in <i>Leptospira interrogans</i>	DBT	23,75,000	31.08.2020	28.02.2022	Dr. Shankar Prasad Kanaujia	Dr. Manish Kumar
5.	Elucidating the role of Cas6, Cas7, and Cas8 in spirochetes CRISPR adaptive immunity against alien genetic elements	DBT	68,75,000	28.06.2018	27.12.2021	Dr. Shankar Prasad Kanaujia	Dr. Manish Kumar
6.	Structural and functional investigation of mammalian cell entry (MCE) proteins from human pathogens: development of structure-based lead molecules	SERB	42,51,000	19.03.2018	18.06.2021	-	PI
7.	Structural investigation of sugar ABC transporters in <i>Mycobacterium</i>	DBT	126,38,400	31.03.2017	30.03.2020	-	PI

	tuberculosis and thermophiles: application to the development of drug carriers and biosensors						
8.	Understanding the mechanism of ABC-type metal sequestering proteins: structure-based novel drug development against human pathogens	DBT	73,55,000	20.01.2017	19.07.2020	Prof. Vikash Kumar Dubey	PI
9.	Elucidation of the substrate delivery and specificity mechanism of solute binding proteins cognate to the ABC transporters	SERB	24,00,000	30.10.2013	29.10.2016	-	PI
10.	Understanding the mechanism of substrate delivery through solute binding proteins related to ABC transporters	SERB	47,19,000	17.07.2013	18.08.2017	-	PI
11.	Structural and Functional Studies of Translation Initiation Factors from <i>Pyrococcus horikoshii</i> OT3	DBT	77,00,000	07.01.2013	30.06.2016	Prof. Vikash Kumar Dubey	PI
12.	Structural determinants and protein engineering of metal-binding of Phospholipase A2	IITG	5,00,000	11.12.2012	10.12.2014	-	PI
13.	Biochemical and biophysical studies of rRNA methyltransferase from <i>Helicobacter pylori</i>	DBT-RA	4,82,000	26.07.2017	25.07.2019	Dr. Ankita Gupta	Dr. Shankar Prasad Kanaujia
14.	Unraveling the rationale behind solvent stability of proteins	DBT	45,00,000	02.05.2014	01.05.2017	Dr. Shankar Prasad Kanaujia	Prof. Sanjukta Patra
15.	To investigate how apoptosis and splicing - associated protein (ASAP) complex interface with	SERB	43,38,000	04.06.2016	03.06.2019	Dr. Shankar Prasad Kanaujia	Dr. Kusum Kumari Singh

	splicing and connects Exon Junction Complex (EJC)						
16.	Identification of novel drug targets of <i>Leishmania donovani</i> : Studies on CAAX prenyl protease I and II of the pathogens	DBT	73,69,000	15.09.2014	14.09.2017	Dr. Shankar Prasad Kanaujia	Prof. Vikash Kumar Dubey
17.	Study on the Caseinolytic proteases of <i>Leptospira interrogans</i> , a promising target for treating bacterial infection	SERB	70,00,000	27.09.2016	26.03.2019	Dr. Shankar Prasad Kanaujia	Dr. Manish Kumar
18.	Deciphering the role and architecture of CRISPR/Cas defense system in <i>Leptospira interrogans</i>	DBT	50,70,000	04.10.2013	04.04.2017	Dr. Shankar Prasad Kanaujia	Dr. Manish Kumar

Protein Structures Deposited to PDB

Total Number of Protein Crystal Structures deposited to PDB: 143

PDB Ids: **9JGB, 9JGC, 9JGD** (PhNep1); **8Z62** (PhRmlCD); **8X3W, 8X41, 8X44, 8X45, 8X46, 8X47, 8X4G, 8X4I, 8X4L, 8X4O, 8X4P** (PhDlMT1); **8HPZ, 8HQ9, 8HQA** (EcMlaD); **7VR6** (EcMlaC); **7F84** (LinCas2c); **7FHM** and **7FHP** (MtMhuP); **7F6E, 7F6F, 7F6K, 7F6N, 7F6O, 7F6P, 7F6Q, 7F6R, 7F6S, 7F6T, 7F6U** (metal-citrate-binding protein, MctA); **7C0F, 7C0K, 7C0L, 7C0O, 7C0R, 7C0S, 7C0T, 7C0U, 7C0V, 7C0W, 7C0X, 7C0Y, 7C0Z, 7C14, 7C15, 7C16, 7C19** and **7C1B** (ABC transporter dinucleotide-binding protein, U3GBP); **7C63, 7C64, 7C66, 7C67, 7C68, 7C69, 7C6F, 7C6G, 7C6H, 7C6I, 7C6J, 7C6K, 7C6L, 7C6M, 7C6N, 7C6R, 7C6T, 7C6V, 7C6W, 7C6X, 7C6Y, 7C6Z, 7C70** and **7C71** (ABC transporter β -glycoside-binding protein, β GlyBP); **6J9W, 6J9Y, 6JAD, 6JAG, 6JAH, 6JAI, 6JAL, 6JAM, 6JAN, 6JAO, 6JAP, 6JAQ, 6JAR, 6JAZ, 6JB0, 6JB4, 6JBA, 6JBB** and **6JBE** (ABC transporter α -glycoside-binding protein, α GlyBP); **6A34** and **6A35** (5-methylthioribose 1-phosphate isomerase, M1Pi); **5ZCY** (Archaeal initiation factor 1, aIF1); **5YFJ, 5YFS, 5YFT, 5YFU, 5YFV, 5YFW, 5YFX, 5YG5, 5YG6, 5YG7, 5YG8, 5YG9** and **5YGA** (Ribose-1,5-bisphosphate isomerase, R15Pi); **3MCH, 3MCI** and **3MCJ** (Molybdenum cofactor biosynthesis protein MoaB); **3JQJ, 3JQK** and **3JQM** (Molybdenum cofactor biosynthesis protein MoaC); **3I7U** and **3I7V** (Ap₄A hydrolase); **2ZP3, 2ZP4**, and **2ZP5** (Bovine Pancreatic Phospholipase A₂); **3U54** and **3U55** (SAICAR Synthetase); **3CQ2** and **3CQ3** (DTDP-4-Keto-L-Rhamnose Reductase); **2PQO** (Hypothetical protein, GK_1056); **2PBP** and **2QQ3** (ENOYL-CoA hydrates subunit I, GK_2039); **2PPY** (Enoyl-CoA hydrates, GK_1992); **2QQ4** (Iron-sulfur cluster biosynthesis protein IscU); **2PBR** and **2PLR** (Thymidylate kinase); **2PCJ** and **2PCL** (Lipoprotein-releasing ATP-binding protein LolD); **2PCN** (SAM: 2-demethylmenaquinone methyltransferase); **2PCQ** (Dihydrodipicolinate synthase); **2PD2** (Conserved hypothetical protein, ST_0148); **2PE3** (Frv operon protein FRVX, PH1821); **2IEX** (Dihydroxynaphthoic acid synthetase); **2III** (S-adenosylmethionine decarboxylase); **2OMD** (Molybdopterin converting factor subunit 2); **2ISM** (Glucose dehydrogenase); **2QYH** (Hypothetical protein GK1056).

Students Supervised

Post-doctoral Fellows			
1.	Dr. Ankita Gupta	July 2017 – December 2018	Completed
Ph.D. Students			
S. No.	Name	Period	Status
1.	Ms. Monisha Dhar	July 2024 – till date	Ongoing
2.	Ms. Aditi Dey	July 2023 – till date	Ongoing
3.	Ms. Shimpy Nigam	December 2022 – till date	Ongoing
4.	Ms. Ritu Tripathi	July 2021 – till date	Ongoing
5.	Ms. Arpana Gupta	July 2021 – till date	Ongoing
6.	Mr. Kushal Bora	July 2021 – till date	Ongoing
7.	Mr. Kalyan Ghosh	July 2020 – till date	Ongoing
8.	Mr. Pratik Das Gupta	July 2017 – October 2024	Completed
9.	Mr. Sayan Saha	December 2016 – August 2024	Completed
10.	Mr. Angshu Dutta	July 2016 – July 2023	Completed
11.	Mr. Suraj Kumar Mandal	July 2014 – September 2021	Completed
12.	Ms. Monika Chandravanshi	December 2013 – April 2021	Completed
13.	Ms. Prerana Gogoi	December 2012 – April 2019	Completed
Project Assistants			
1.	Mr. Harsh Vardhan Baid	April 2025 – till date	Ongoing
2.	Ms. Ankita Mallick	September 2024 – till date	Ongoing
3.	Ms. Reshama Samanta	June 2018 – March 2020	Completed
4.	Ms. Smriti Tapan Dolai	June 2018 – May 2019	Completed
5.	Mr. Rahi Adhikari	July 2017 – February 2018	Completed
6.	Ms. Prerana Mordina	June 2017 – June 2018	Completed
7.	Mr. Akash Deep Biswas	July 2015 – January 2016	Completed
8.	Mr. Arunabh Sharma	February 2015 – May 2015	Completed
9.	Mr. Suraj Kumar Mandal	September 2013 – July 2014	Completed
10.	Ms. Preeti Sarkar	March 2013 – March 2014	Completed
M.Tech. Students			
1.	Mr. Mrityunjay Nigam	July 2025 – till date	Ongoing
2.	Ms. Aarthi Murali	July 2024 – May 2025	Completed
3.	Mr. Ankit	July 2023 – June 2024	Completed
4.	Mr. Smit Patel	July 2022 – June 2023	Completed
5.	Mr. Jeancolar Thoudam	July 2022 – till date	Ongoing
6.	Ms. Ankita Jingar	July 2021 – May 2022	Completed
7.	Ms. Sakshi Chauhan	July 2020 – May 2021	Completed
8.	Ms. Pratiksha P. Bhat	July 2020 – May 2021	Completed
9.	Ms. Shreya LB	July 2019 – May 2020	Completed
10.	Mr. Pratap Narayan Roy	July 2018 – May 2019	Completed
11.	Ms. Harishini P.	July 2018 – May 2019	Completed
12.	Ms. Arpita Sachan	July 2017 – May 2018	Completed
13.	Ms. Tarini Devi Sahu	July 2016 – May 2017	Completed
14.	Ms. Kanchan Chauhan	July 2015 – May 2016	Completed
15.	Mr. Ambuj Srivastava	July 2014 – May 2015	Completed
16.	Ms. Shalineer Jha	July 2013 – May 2014	Completed
B.Tech. Students			
1.	Jayesh Muralidhar Sonawane	July 2024 – May 2025	Completed
2.	Mangroliya Dhruv Ghanshyambhai	July 2024 – May 2025	Completed
3.	Mr. Deepak	July 2023 – May 2024	Completed
4.	Ms. Shreya Sajal	June 2022 – May 2023	Completed
5.	Mr. Kabilan M	June 2022 – May 2023	Completed

6.	Mr. Tejasvi Singh Tomar	July 2021 – May 2022	Completed
7.	Mr. Krishan Kant	July 2020 – May 2021	Completed
8.	Mr. Rahul Saroha	July 2020 – May 2021	Completed
9.	Ms. Namrata Gupta	July 2019 – May 2020	Completed
10.	Mr. Prashant Kumar	July 2019 – May 2020	Completed
11.	Mr. Hemant Kumar	July 2018 – May 2019	Completed
12.	Mr. Anjaney Sharma	July 2018 – May 2019	Completed
13.	Mr. Ajeet Kumar	July 2017 – May 2018	Completed
14.	Mr. Ankit Kumar Sinha	July 2016 – May 2017	Completed
15.	Mr. Sandesh Arya	July 2015 – May 2016	Completed
16.	Mr. Alakesh	July 2015 – May 2016	Completed
17.	Mr. Gaurav Jumde	July 2015 – May 2016	Completed
18.	Mr. Adarsh Sharma	July 2015 – May 2016	Completed
19.	Mr. Ayush Singhal	July 2014 – May 2015	Completed
20.	Mr. Shivam Chandak	July 2014 – May 2015	Completed
21.	Mr. Swapnil Chauhan	July 2014 – May 2015	Completed
22.	Mr. Mehul Garg	July 2013 – May 2014	Completed
23.	Mr. Vatshank Chaturvedi	July 2013 – May 2014	Completed
24.	Mr. Ujjwal Nandan	July 2012 – May 2014	Completed

Trainees

1.	Mr. Rishi Chaubey	May 2025 – till date	Ongoing
2.	Mr. Harsh Rander	May 2025 – till date	Ongoing
3.	Mr. Ahammed Siyad	May 2025 – till date	Ongoing
4.	Mr. Soumyaditya Roy	June 2025 – till date	Ongoing
5.	Mr. Shubhankar Roy	June 2025 – till date	Ongoing
6.	Ms. Manalisha Deka	June 2025 – till date	Ongoing
7.	Ms. Aastha Baruah	June 2025 – till date	Ongoing
8.	Mr. Harsh Vardhan Baid	October 2024 – March 2025	Completed
9.	Mr. Adrish Chakraborty	May 2024 – July 2024	Completed
10.	Mr. Dipankar Das	Dec 2023 – December 2023	Completed
11.	Mr. Dylan Ayekpam	July 2023 – August 2023	Completed
12.	Ms. Jahnabi Goswami	June 2023 – July 2023	Completed
13.	Mr. Jaya Simha Varma	May 2023 – July 2023	Completed
14.	Mr. Bharat Sharma	May 2023 – July 2023	Completed
15.	Mr. Arnab Choudhary	October 2022 – May 2023	Completed
16.	Mr. Gautam Kumar	October 2022 – May 2023	Completed
17.	Mr. Aman Singh	February 2023 – May 2023	Completed
18.	Mr. Sanjay Chhaba	February 2023 – May 2023	Completed
19.	Ms. Kavya Vinil	June 2022 - July 2022	Completed
20.	Ms. Sujanaa Shaaradaa Sai	Sept 2021 – November 2021	Completed
21.	Mr. Satya Gopal Nayak	January 2020 – June 2020	Completed
22.	Mr. Sisir Kant Tripathi	January 2020 – June 2020	Completed
23.	Mr. Jayesh Damani	Sept 2019 – December 2020	Completed
24.	Mr. Vikas Parshuram Patel	May 2019 – June 2019	Completed
25.	Ms. Prema Mondal	May 2018 – July 2018	Completed
26.	Mr. Ajeet Singh Chauhan	February 2018 – March 2018	Completed
27.	Mr. Hemant Kumar	July 2017 – April 2018	Completed
28.	Ms. Prerna Kothari	June 2017 – July 2017	Completed
29.	Mr. Anjaney Sharma	May 2017 – April 2018	Completed
30.	Mr. Aniket Bhattacharyya	June 2016 – July 2016	Completed
31.	Mr. Arbin Basak	May 2016 – July 2016	Completed
32.	Mr. Rahi Adhikari	May 2016 – July 2016	Completed
33.	Mr. Deepak Singh	May 2016 – July 2016	Completed
34.	Ms. Srija Gupta	Dec 06 – December 30, 2015	Completed
35.	Mr. Anand Kumar	Dec 06 – December 30, 2015	Completed
36.	Mr. Angshu Dutta	July 2015 – September 2015	Completed
37.	Ms. Aashiyana A Hussain	June 2015 – July 2015	Completed

38.	Mr. Tushar Dubey	July 2014 – December 2015	Completed
39.	Mr. Amartya Mandal	July 2014 – June 2015	Completed
40.	Mr. Ankit Kumar Sinha	July 2014 – December 2015	Completed
41.	Mr. Manjunath	July 2014 – January 2015	Completed
42.	Mr. Akshay Kumar	July 2014 – January 2015	Completed
43.	Mr. Sandesh Arya	July 2014 – June 2015	Completed
44.	Ms. Bhagyashree Deka	June 2014 – July 2014	Completed
45.	Ms. Shrayanti Goswami	May 2014 – June 2014	Completed
46.	Mr. Akeshwar Jha	June 2014 – July 2014	Completed
47.	Mr. Abhay Sharma	January 2014 – July 2014	Completed
48.	Mr. Gaurav Jumde	April 2014 – June 2015	Completed
49.	Mr. Ayush Khare	January 2014 – May 2014	Completed
50.	Mr. Adarsh Sharma	January 2014 – June 2015	Completed