

# CENTER FOR ADVANCED RESEARCH AND INNOVATION IN STRUCTURAL BIOLOGY OF DISEASES (CARISBD)

**Prof. (Dr.) BURRA V L S PRASAD**

PDF (BIMR, UCSD), Ph. D. (IISc), M.Sc (UOHYD), B.Tech (Ag. Engg, ANGRAU)

Head - Center for Advanced Research and Innovation in Structural  
Biology of Diseases

Professor, Dept of Biotechnology,

K L (Deemed to be University)

Vaddeswaram, 522502,

Ph: 0863-2399999 Ext 1023

Mob: 09810655546, 07350263747

Email: dr.prasad.bvls@gmail.com



**Teaching: 20yrs (2003) Industry: 5yrs (2003) Research: 21 yrs (2002) Total: 26 yrs**

**Publications: 42** PNAS(USA), PLoSOne, JMB, ACTA D, Proteins, Viruses, JIB, 3  
Biotech, Bioorganic Chemistry, JBSD.

**Project Grants: 6** : Agencies: **DST-CRG, ICMR, DST-NSM (HPC\_Applications),  
MSME - ~1Cr**

**Senior Editor:** IMCRJournal, **Review Editor:** Frontiers in Microbiology, Bioengineering  
& Systems Biology, International Journal of Peptide Research and Therapeutics (IJPR)

**Patents (to file):**

1. **Multi-Epitope Vaccine Candidates, Drug Candidates & Methodology yet to file as Patent**
2. **Design Development of Healthy-Healers Smart Foot wearables (Healthy Healers)**
3. **Design and development of Inhibitors as a therapeutic strategy for tuberculosis**

**Past patents (filed):**

1. **US:10/873,923 (BioBhasha - OO Biological Application Framework)**
2. **US:10/579,171 (MACS - Macromolecular Architecture Component System)**

**Extramural Grants:**

**Current Ongoing Sponsored Project Grants Total Budget Rs. 11,459,600.00  
(1.1Cr)**

	Grant Title	Funding Agency	Budget	Duration(Yrs)
1	Design and Development a statistical scoring system against a library of Multi-Epitope based Peptide (MEBP) vaccine constructs to identify best vaccine candidates	DST/NSM/R&D_HP C_Applications/Sa nction/2021/16	Rs. 10 Lakhs	1 (On-Going)
2	Structure determination and analysis of native-, hybrid-,	SERB, CRG/2018/003276	Rs. ~32 Lakhs	3 (Completed)

	mutant- RecA and cy-di-AMP, complexes to develop novel allosteric inhibitors against Tuberculosis			
3	Design and Development a statistical scoring system against a library of Multi-Epitope based Peptide (MEBP) vaccine constructs to identify best vaccine candidates	DST/NSM/R&D_HP C_Applications/Sa nction/2021/16	Rs. 20,59,600/-	2 (Completed)
4	<i>in silico</i> drug designing against Tuberculosis targeting a novel protein from M.Tuberculosis - N2G966 16S rRNA methyltransferase (RsmD)	ICMR, ISRM/12(07)/2019	Rs. ~19 Lakhs	3 (Completed)

### Commercial & Entrepreneurial Grants Funded by MSME Total Budget:

1	Technology development for faster, cheaper and more diverse single domain antibodies for disease prognostics, diagnostics and therognostics	Technology platform	Rs. 18 L
2	Design Development of Healthy-Healers Smart Foot wearables	Smart Foot Wearables	Rs. 15 L

### Active Collaborations:

1	Collaboration: Drug Docking, Designing and Modeling and Simulation Studies with Dr. Aniket Sarkate's Lab, Dr. B A M University, Aurangabad
2	Collaboration: Drug Docking, Designing and Modeling and Simulation Studies with Prof. Ramakrishna Kancha Lab, Osmania University, Hyderabad
3	Collaboration: Designing novel modulators to increase the fecundity in Fishes, Prof. Jahageerdar, Central Institute of Fisheries Education (CIFE), Mumbai
4	Collaboration: Designing novel drug molecules to inhibit PolyPhenol Oxidase(PPO) to stop melanin formation, Dr. Sanath Kumar, Central Institute of Fisheries Education (CIFE), Mumbai
5	NE Collaboration: Genomics Technologies: Evaluation of Genetic Diversity and Core germplasm collection of Indigenous Rice in Arunachal Pradesh, Eastern Himalaya.
6	NE Collaboration: NGS Technologies: Understanding the sexual and olfactory dysfunction in Parkinson's Disease subjects through Drosophila model and therapeutic intervention

### a) LAB MEMBERS

1. Partha Sarathi Sahoo - PhD Scholar
2. Mangal Sugrao Kadam - PhD Scholar
3. Andoju Vijay Bhargav - Intern
4. Bomma Sharath Chandra - Intern
5. Maram Vignaya (2100010046)
6. Manogna Vuppalapati (2100010047)

7. **B Akshay Tanishq (2100080012)**
8. **P Akash Kumar (2100080050)**
9. **M Nikshit (2100080051)**
10. **P K K V V M Pratap (2100080052)**
11. **M Rupa (2100080053)**
12. **P Shyamraj (2100080054)**
13. **Akhil Chowdary (2200099009)**

**b) Publications:**

1. Jayanth Jeevanandam, V L S Prasad Burra, N T Saraswathi. Conformational variation of site specific glycated albumin: A Molecular dynamics approach Computers in Biology and Medicine, 2023 July 17;164:107276. doi: 10.1016/j.combiomed.2023.107276.
2. Mangal S Kadam, \*Burra V L S Prasad, S-adenosyl-l-methionine interaction signatures in methyltransferases, Journal of Biomolecular Structure and Dynamics, Page No. 1-11, 2023 Doi: 10.1080/07391102.2023.2217679
3. Burra V L S Prasad, Sahoo Partha Sarathi, Dhankhar, Amit, Jhaji Jatinder, Kasamuthu Prasanna Sudharson, K, S. S. V. Kiran, Macha Samuel Krupa Rakshan, Understanding the structural basis of the binding specificity of c-di-AMP to M. smegmatis RecA using computational biology approach, Journal of Biomolecular Structure and Dynamics, Year 2023 Doi:10.1080/07391102.2023.2227709
4. Srinivasa R. Vulichi, Ashish Runthala, Siva K. Rachamreddy, Radhika S. P. Yaramanedi, Partha Sarathi Sahoo, Prasad V. L. S. Burra, Nameet Kaur, Sudheer Akkiraju, Somasekhar Reddy Kanala, Appa Rao Chippada, and Sistla Durga Srinivasa Murthy Appraisal of Pancreatic Lipase Inhibitory Potential of Ziziphos oenoplia (L.)Mill. Leaves by In Vitro and in silico Approaches, ACS Omega 2023, 8, 19, 16630-16646 DOI: 10.1021/acsomega.2c07361
5. Sanjay Madala, S S V Kiran K1, Burra V L S Prasad *in silico* Design Of Natural Compound-Derived Novel Inhibitors Against Rdrp Of Sars-Cov-2, 10.1039/9781837671090-00142, 15 Dec 2023, Proceedings of CTD4-2022, RSC.
6. Mangal S Kadam and Burra V L S Prasad, *in silico* Screening, Analysis And Design Of Potential Inhibitors Against RsmD For Treating Tuberculosis, 10.1039/9781837671090-00155, 15 Dec 2023, Proceedings of CTD4-2022, RSC.
7. Mullaguri SC, Akula S, Sahoo PS, Ashireddygari VR, Mupparapu V, Silveri R, Prasad Burra VLS, Kancha RK. Molecular docking analysis reveals differential binding affinities of multiple classes of selective inhibitors towards cancer-associated KRAS mutants.3 Biotech. 2022 Dec;12(12):343. Epub 2022 Nov 6. PMID: 36353445
8. Burra V L S Prasad, Cofactor-Receptor interactions based pharmacophore design for development of novel inhibitors: A case study against Tuberculosis, Drugs from bench to bedside: A methodological compendium 2022
9. MuthuRaj S., Burra V L S Prasad, in silico design of novel SAM analogs as potential inhibitors against N2G966 16s rRNA methyltransferase Letters in Drug Design & Discovery Doi: 10.2174/1570180819666220616105517
10. Mullaguri SC, Akula S, Ashireddygari VR, Sahoo PS, Burra VLSP, Silveri R, et al. Estimated sensitivity profiles of lung cancer specific uncommon BRAF mutants towards experimental and clinically approved kinase inhibitors. Toxicol Appl Pharmacol. 2022; 116213 Doi: 10.1016/j.taap.2022.116213

11. MuthuRaj S, Prasanna K S, S Aathmanathan Burra V L S Prasad, An *in silico* approach to study the role of epitope order in multi-epitope-based peptide (MEBP) vaccine against Spike protein of SARS-CoV-2, Nature Scientific Reports (10.1038/s41598-022-16445-3)
12. MuthuRaj, Veena B, Burra V L S Prasad, 2022, 16S rRNA Methyltransferases as novel drug targets against Tuberculosis, PROTEINS Feb;41(1):97-130. doi: 10.1007/s10930-021-10029-2
13. Sultan M. Faheem<sup>1</sup>, Jancie D'Mello, Sultan M. Kaleem, Burra V. L. S. Prasad, Khalid Siddiqui, Rapid Serological Testing for Managing the COVID-19 Pandemic: A Review, The Open Biomarkers Journal 11(1):99-107
14. Ratnadeep Saha, Pratik Ghosh, Burra V L S Prasad, Designing a Next Generation Multi-Epitope Based Peptide Vaccine candidate against SARS-CoV-2 using Computational Approaches, 3Biotech, Springer doi: 10.1007/s13205-020-02574-x
15. Sarkate AP, Dofe VS, Tiwari SV, Lokwani DK, Karnik KS, Kamble DD, H S H Ansari M, Dodamani S, Jalalpure SS, Sangshetti JN, Azad R, V L S Burra P, Bhandari SV. One pot synthesis, in silico study and evaluation of some novel flavonoids as potent topoisomerase II inhibitors. Bioorg Med Chem Lett. 2021 Mar 6:127916. doi: 10.1016/j.bmcl.2021.127916.
16. P.S. Payal, Shrinivas Jahageerda\*, Sanath H. Kumar and Burra V.L.S Prasad, "Homology modeling and virtual screening of 3-deoxy-D-manno-octulosonic acid transferase of *Aeromonas hydrophila* as a potential target for novel natural inhibitory compounds", Letters in Drug Design & Discovery (2021) 18: 1.
17. Karnik KS, Sarkate AP, Tiwari SV, Azad R, Burra PVLS, Wakte PS. Computational and Synthetic approach with Biological Evaluation of Substituted Quinoline derivatives as small molecule L858R/T790M/C797S triple mutant EGFR inhibitors targeting resistance in Non-Small Cell Lung Cancer (NSCLC). Bioorg Chem. 2021 Jan 5;107:104612 doi: 10.1016/j.bioorg.2020.104612.
18. Dofe VS, Sarkate AP, Tiwari SV, Lokwani DK, Karnik KS, Kale IA, Dodamani S, Jalalpure SS, Burra PVLS. Ultrasound assisted synthesis of tetrazole based pyrazolines and isoxazolines as potent anticancer agents via inhibition of tubulin polymerization. Bioorg Med Chem Lett. 2020 Sep 30;30(22):127592
19. Karnik KS, Sarkate AP, Lokwani DK, Narula IS, Burra PVLS, Wakte PS. Development of triple mutant T790M/C797S allosteric EGFR inhibitors: a computational approach. J Biomol Struct Dyn. 2020 Jul 1:1-23
20. MuthuRaj S, Prasanna K S, Burra V L S Prasad, 2021. Epitope order matters in multi-epitope based peptide vaccine design: an in silico study, Bioinformatics. bioRxiv
21. Saha, Ratnadeep, and Burra V. L. S. Prasad\*. 2020. "in silico Approach for Designing of a Multi-Epitope Based Vaccine against Novel Coronavirus (SARS-CoV-2)." Bioinformatics. bioRxiv
22. Burra V L S Prasad\*, Biological Object based Software (BOS): An integrative biological programming environment, Vivechan International Journal of Research, 2019, 10(1), 56-69, ISSN No. 0976-8211
23. Venkataraman S, Dhankar A, Sinha KM, Bandopadhyay K, Iqbal N, Singh TP, et al. Crystal structure of a new form of RsmD-like RNA methyltransferase from *Mycobacterium tuberculosis* determined at 1.74 Å resolution. TO BE PUBLISHED [Internet]. [cited 2018 Dec 19]; Available from: <http://dx.doi.org/10.2210/pdb6aie/pdb>
24. Sangita Venkataraman, Burra V L S Prasad\*, Ramasamy Selvarajan, RNA dependent RNA Polymerases: Insights from structure, function, and evolution, Viruses (2018), 10(2),76;

25. Burra V L S Prasad\*, Biological Object based Software (BOS): An integrative biological programming environment, Proceedings of National Innovation Conclave-2015, October 5-6th 2015, Allied Publishers, P:63-70, Amity University, Gurgaon.
26. Sanket Desai and Prasad Burra\*, "BioInt: An integrative biological object-oriented application framework and interpreter" - IJBRA (2014), 11(3), 247-256.
27. Anand MT, Prasad BV. The computational analysis of human testis transcriptome reveals closer ties to pluripotency. *J Hum Reprod Sci* (2012), 5, 266-273.
28. Burra PV, Kalmar L, Tompa P. Reduction in structural disorder and functional complexity in the thermal adaptation of prokaryotes. *PLoS One*. 2010 Aug 11;5(8):e12069
29. Burra PV, Zhang Y, Godzik A, Stec B. Global distribution of conformational states derived from redundant models in the PDB points to non-uniqueness of the protein structure. *Proc Natl Acad Sci U S A*. 2009 Jun 30;106(26):10505-10. Epub 2009 Jun 24. Erratum in: *Proc Natl Acad Sci U S A*. 2009 Jul 28;106(30):12560.
30. Boguslaw Stec, B.V.L.S. Prasad, Ying Zhang, Adam Godzik., Defining a protein: Mining the protein structure Database *Acta Cryst.* (2008). A64, C627-628
31. B.V.L.S. Prasad and K.Suguna, "Effect of pH on the structure of rhizopuspepsin", *Acta Cryst.* (2003), D59, 1755 -61.
32. B.V.L.S. Prasad and K.Suguna, "Role of water molecules in the structure and function of Aspartic Proteinases", *Acta Cryst.* (2002), D58, 250 -259.
33. D. Ashok Reddy, B.V.L.S. Prasad, Chanchal K. Mitra, "Functional classification of transcription factor binding sites: Information content as a metric", *Journal of Integrative Bioinformatics.*(2006):3(1),32-44
34. D. Ashok Reddy, B.V.L.S. Prasad, Chanchal K. Mitra, "Comparative analysis of core promoter region: Information content from mono and dinucleotide substitution matrices", *Computational Biology and Chemistry.*(2006),30, 58-62.
35. B.V.L.S.Prasad and Mohan C. Vemuri, "Genome Analysis for nucleotide interactions in fully sequenced genomes of selective prokaryotes", *J.Biosci.* (1998), 23:255 -263.
36. Mohan R.K. Nimmagadda and B.V.L.S. Prasad, Strategic Management of Bio-Pharmaceutical Knowledge for Improved R&D Productivity, *Global Business Review* August 2003 4: 257-269.
37. Das D, Moiani D, Axelrod HL, Miller MD, McMullan D, Jin KK, Abdubek P, Astakhova T, Burra P, et. al. Crystal structure of the first eubacterial Mre11 nuclease reveals novel features that may discriminate substrates during DNA repair. *J Mol Biol.* 2010 Apr 2;397(3):647-63.
38. Xu Q, Carlton D, Miller MD, Elsliger MA, Krishna SS, Abdubek P, Astakhova T, Burra P, Chiu HJ, et. al. Crystal structure of histidine phosphotransfer protein ShpA, an essential regulator of stalk biogenesis in *Caulobacter crescentus*. *J Mol Biol.* 2009 Jul 24;390(4):686-98.
39. Das D, Kozbial P, Axelrod HL, Miller MD, McMullan D, Krishna SS, Abdubek P, Acosta C, Astakhova T, Burra P, Carlton D, et. al. Crystal structure of a novel Sm-like protein of putative cyanophage origin at 2.60 Å resolution. *Proteins.* 2009 May 1;75(2):296-307.
40. Das D, Krishna SS, McMullan D, Miller MD, Xu Q, Abdubek P, Acosta C, Astakhova T, Axelrod HL, Burra P, Carlton D, et. al. Crystal structure of the Fic (Filamentation induced by cAMP) family protein SO4266(gil24375750) from *Shewanella oneidensis* MR-1 at 1.6 Å resolution. *Proteins.* 2009 Apr;75(1):264-71.

41. Bakolitsa C, Bateman A, Jin KK, McMullan D, Krishna SS, Miller MD, Abdubek P, Acosta C, Astakhova T, Axelrod HL, Burra P, Carlton D, et. al. The structure of Jann\_2411 (DUF1470) from Jannaschia sp. at 1.45 Å resolution reveals a new fold (the ABATE domain) and suggests its possible role as a transcription regulator. Acta Crystallogr Sect F Struct Biol Cryst Commun. 2010 Oct 1;66(Pt 10):1198-204.
42. Bakolitsa C, Kumar A, Jin KK, McMullan D, Krishna SS, Miller MD, Abdubek P, Acosta C, Astakhova T, Axelrod HL, Burra P, Carlton D, et. al. Structures of the first representatives of Pfam family PF06684 (DUF1185) reveal a novel variant of the Bacillus chorismate mutase fold and suggest a role in amino-acid metabolism. Acta Crystallogr Sect F Struct Biol Cryst Commun. 2010 Oct 1;66(Pt 10):1182-9.
43. Das D, Grishin NV, Kumar A, Carlton D, Bakolitsa C, Miller MD, Abdubek P, Astakhova T, Axelrod HL, Burra P, Chen C, et. al. The structure of the first representative of the Pfam family PF09836 reveals a two-domain organization and suggests involvement in transcriptional regulation. Acta Crystallogr Sect F Struct Biol Cryst Commun. 2010 Oct 1;66(Pt 10):1174- 81.

### c) PhD Student Details:

1)

Name: Partha Sarathi Sahoo  
 Name of the Supervisor: Dr. Burra V. L. S Prasad  
 Ph.D Registration Number: 2102010005  
 Ph.D Admission Date: 15th March 2022



### Project Enrollment Details:

Name of the Project: Design and Development a statistical scoring system against a library of Multi-Epitope based Peptide (MEBP) vaccine constructs to identify best vaccine candidates

Reference No: DST/NSM/R&D\_HPC\_Applications/2021/03.23 dated March 23, 2021

Duration: 6th January 2022 - 31st March 2023

Position : Project Associate-I

Name of the Project: "Optimization of the component parameters of MEBPVCs to further improve the vaccine potency"

Reference No: DST/NSM/R&D\_HPC\_Applications/ Extension Grant/2023/30

Duration: 1st April 2023 - Continuing

Position : Senior Research Fellow (SRF)

### Achievements:

#### **Publications:**

- Mullaguri, Sai Charitha, Sravani Akula, Vigneshwar Reddy Ashireddygari, **Partha Sarathi Sahoo**, V. L. S. Prasad Burra, Ravalika Silveri, Vyshnavika

Mupparapu, et al. 2022. "Estimated Sensitivity Profiles of Lung Cancer Specific Uncommon BRAF Mutants towards Experimental and Clinically Approved Kinase Inhibitors", *Toxicology and Applied Pharmacology* 453 (October): 116213.

- Mullaguri, Sai Charitha, Sravani Akula, **Partha Sarathi Sahoo**, Vigneshwar Reddy Ashireddygari, Vyshnavika Mupparapu, Ravalika Silveri, V. L. S. Prasad Burra, and Rama Krishna Kancha. 2022. "Molecular Docking Analysis Reveals Differential Binding Affinities of Multiple Classes of Selective Inhibitors towards Cancer-Associated KRAS Mutants." *3 Biotech* 12 (12): 343.
- Srinivasa R Vulichi , Ashish Runthala , Siva K Rachamreddy , Radhika S P Yaramanedi, **Partha Sarathi Sahoo** , Prasad V L S Burra , Nameet Kaur , Sudheer Akkiraju , Somasekhar Reddy Kanala , Appa Rao Chippada, Sistla Durga Srinivasa Murthy. 2023. "Appraisal of Pancreatic Lipase Inhibitory Potential of *Ziziphus oenopia* (L.)Mill. Leaves by In Vitro and *in silico* Approaches". *ACS Omega*. 8(11):16630.
- V. L. S. Prasad Burra, **Partha Sarathi Sahoo** ,Amit Dhankhar,Jatinder Jhaggi,Prasanna Sudharson Kasamuthu,S. S. V. Kiran K & Samuel Krupa Rakshan Macha.2023."Understanding the structural basis of the binding specificity of c-di-AMP to *M. smegmatis* RecA using computational biology approach ". *Journal of Biomolecular structure and dynamics*.1(15):0739

### **Conferences:**

- Certificate of Participation in the International Conference on "Current Sustainable Agricultural, Biotechnology, Nutritional and Pharmaceutical Interventions to Combat Global Challenges (SABINP-2023)", Vijayawada, Andhra Pradesh, India. Poster Title - "Advancing Multi-Epitope Based Peptide Vaccines: Enhancing Immunogenicity through *in silico* Optimization Strategies".
- Certificate of Participation in the International Conclave on AMR and Future of Antibiotics (ICAFA - 2023), Andhra Pradesh, India.
- Certificate of Participation in the International Conference on Recent Innovations in Science and Technology (RIST-2023), Hyderabad, India. Poster Title - "Efforts Towards Optimising the Multi-Epitope Based Peptide Vaccines: An *in silico* Approach for Enhanced Immunogenicity".
- Certificate of Participation in the International Conference On Drug Discovery (ICDD-2022), GOA, India. Poster Title - "Comparative inhibiting potencies of flavonoids from *Scutellaria baicalensis* against the mutants of SARS-CoV-2 main protease (Mpro)".
- Certificate of Participation in the International conference on Current Trends in Drug Discovery and Delivery (CTD4-2022),Guntur, AP, India. Poster Title - "A novel *in silico* methodology to design multi-epitope-based peptide (MEBP) vaccine candidates against SARS-CoV-2 S Protein".

### **Awards and Recognition:**

- Felicitated with the **Young Scientist Award** in the 17th Annual Convention of Association of Biotechnology and Pharmacy on 19-21st Dec 2023. The Presentation title was - “Advancing Multi-Epitope Based Peptide Vaccine: Enhancing Immunogenicity through *in silico* Optimization Strategies”.
- Felicitated as a **Resource Person** in the “Workshop/Hands-on training on Bioinformatics Essentials: navigating Integrative Omics Data” on 11-15th Sep 2023 at ICAR-Central Institute of Fisheries Education, Mumbai.

### **Volunteering:**

- Organizing Committee at the Global Workshop on Implementation of State Action Plans for Containment of Antimicrobial Resistance, Vijayawada, AP, On November 2022
- Organizing Committee and training instructor at the Symposium-cum Hands-on Workshop on *in silico* MEBP Vaccine Design, Organised by the Center of Advanced Research and Innovation in Structural Biology and Diseases (CARISBD), Department of Biotechnology, KLEF.

2)

Name: Mangal S Kadam  
Name of the Supervisor: Dr. Burra V. L. S Prasad  
Ph.D Registration Number: 2102010004  
Ph.D Admission Date: 15th March 2022



### **Project Enrollment Details:**

Name of the Project: *in silico* drug designing against Tuberculosis targeting a novel protein from M. Tuberculosis - N2G966 16S rRNA methyltransferase (RsmD)  
Reference No: ICMR, ISRM/12(07)/2019 dated March - 2019  
Duration: 6th January 2022 - 28th May 2023  
Position : Project Assistant

Name of the Project: *in silico* drug designing against Tuberculosis targeting a novel protein from M. Tuberculosis - N2G966 16S rRNA methyltransferase (RsmD)  
Reference No: ICMR, ISRM/12(07)/2019 dated March - 2019  
Duration: 28th May 2023 - 15th March 2025  
Position : PhD Student

### **Achievements:**



### **Publications:**

- Mangal S Kadam, Burra V L S Prasad, "S-adenosyl-I-methionine interaction signatures in methyltransferases" Doi: 10.1080/07391102.2023.2217679, Journal of Biomolecular structure and dynamics, 2023 Jun 1:1-11.
- Mangal S Kadam, Burra V L S Prasad, "*In silico* Screening, Analysis and Design of Potential Inhibitors Against RsmD for Treating Tuberculosis", Doi: <https://doi.org/10.1039/9781837671090-00155>, 15 Dec 2023, Royal Society of Chemistry (Conference Proceedings).

### **Conferences:**

- International Conference on Current Trends in Drug Discovery, Development & Delivery (CTD4-2022), K L University, Title: *In silico* Screening, Analysis and Design of Potential Inhibitors Against RsmD for Treating Tuberculosis -21-10-2022.
- International Conference On Drug Discovery (ICDD-2022), BITS Pilani Campus, Goa, Title: *In silico* screening of natural compounds as potent inhibitors against RsmD - a methyltransferase as a novel target against Tuberculosis 10-11-2022 & 11-11-2022.
- 1st International Conference on "RECENT INNOVATIONS IN SCIENCE AND TECHNOLOGY" (RIST-2023), Hyderabad, Title: Preliminary Structural Insights into 16S rRNA Methyltransferase, 30-09-2023.
- International Conclave on AMR and Future of Antibiotics, SRM University, Amaravati, Title: From Structure to Resistance: 16S rRNA Methyltransferases in Tuberculosis and the Challenge of AMR, 08-11-2023 to 09-11-2023.
- International Conference on Current Sustainable Agricultural, Biotechnological, Nutritional and Pharmaceutical Interventions to Combat Global Challenges (SABINP-2023), 19th - 21st December, 2023, Received Junior Scientist Award.

### **Awards and Recognition:**

- Felicitated with the **Junior Scientist Award** in the 17th Annual Convention of Association of Biotechnology and Pharmacy on 19-21st Dec 2023. The Presentation title was "16S rRNA Methyltransferases and Strategic Approaches Against AMR and TB".
- International Conference on Current Sustainable Agricultural, Biotechnological, Nutritional and Pharmaceutical Interventions to Combat Global Challenges (SABINP-2023), 19th - 21st December, 2023, Received Junior Scientist Award, **First Prize in Poster Presentation.**
- 1st International Conference on "RECENT INNOVATIONS IN SCIENCE AND TECHNOLOGY" (RIST-2023), Hyderabad, Title: Preliminary Structural Insights into 16S rRNA Methyltransferase, 30-09-2023, Received **First Prize in Poster Presentation.**

- International Conference on Current Trends in Drug Discovery, Development & Delivery (CTD4-2022), K L University, Title: *in silico* Screening, Analysis and Design of Potential Inhibitors Against RsmD for Treating Tuberculosis -21-10-2022, Received **Certificate of Appreciation**.

#### **Volunteering:**

- Organizing Committee at the Global Workshop on Implementation of State Action Plans for Containment of Antimicrobial Resistance, Vijayawada, AP, 25-11-2022 & 26-11-2022.
- Organizing Committee and training instructor at the Symposium-cum Hands-on Workshop on *in silico* MEBP Vaccine Design, Organised by the Center of Advanced Research and Innovation in Structural Biology and Diseases (CARISBD), Department of Biotechnology, KLEF, 10-05-2023 to 12-05-2023.

#### **Project Enrollment Details:**

Name of the Project: Design Development of Healthy-Healers Smart Foot wearables  
 Reference No: Commercial & Entrepreneurial Grants Funded by MSME Nov-2022  
 Duration: Nov 2022 - April 2024  
 Position : Project Interns  
 Total Budget: 15 Lakhs

- **Maram Vignaya (2100010046)**
- **Manogna Vuppalapati (2100010047)**
- **B Akshay Tanishq (2100080012)**
- **P Akash Kumar (2100080050)**
- **M Nikshit (2100080051)**
- **P K K V V M Pratap (2100080052)**
- **M Rupa (2100080053)**
- **P Shyamraj (2100080054)**
- **Akhil Chowdary (2200099009)**

## **Research Disciplines in Our Lab**

Driven by a relentless quest to advance healthcare and technology, our lab delves into diverse research avenues characterised by rigorous scientific exploration and collaborative pursuit of groundbreaking solutions.

### **1. Vaccine Development: Immunoproteomic Spearheading**

- **Computational Design:** We've forged a novel methodology for crafting multi-epitope peptide vaccine candidates (MEBPVCs), wielding a published

paper in Scientific Reports as our shield. This methodology, a testament to our computational prowess, empowers us to rapidly design and evaluate vaccine constructs with enhanced potency and targeted immunogenicity.

- **Biophysical Characterization:** Beyond computational realms, we delve into the physical world through meticulous biophysical characterization experiments. From cloning and expression to purification and intricate structural elucidation, these endeavours validate our *in silico* predictions and shed light on the biomolecular mechanisms underlying vaccine efficacy.
- **Immunological Orchestration:** Ultimately, our vaccine development efforts culminate in the realm of immunology, where we aim to orchestrate targeted immune responses against a multitude of diseases. By understanding the intricate dance between antigens, immune cells, and immunological pathways, we strive to unlock the full potential of MEBPVCs for disease prevention and therapeutic intervention.

## 2. Drug Discovery: Molecular Warfare Against Pathogens

- **Computational Drug Design:** Our drug discovery arsenal boasts potent *in silico* weapons, honed through meticulous computational design strategies. Against the formidable foe of Mycobacterium tuberculosis RsmD, we've deployed these weapons to identify promising lead compounds, each a potential bullet aimed at the heart of this pathogenic target.
- **Medicinal Chemistry:** The journey from computational predictions to tangible solutions necessitates the expertise of medicinal chemistry. In our lab, we wield the tools of synthesis and characterization to forge these lead compounds into potent pharmacological blades, ready for evaluation in the fight against disease.
- **Microbiological Battlefield:** Our focus on Mycobacterium tuberculosis stems from its relentless assault on human health. Through a deep understanding of its microbiological intricacies, we strategically target critical pathways like RsmD, aiming to disarm this formidable foe and alleviate the suffering it inflicts.

## 3. Bioinformatics: Decoding the Language of Life

- **Protein Structure Prediction:** We employ the art of protein structure prediction to unlock the secrets of complex biomolecules like RsmD and potential vaccine epitopes. By deciphering their intricate folds and functionalities, we gain invaluable insights into their mechanisms of action and vulnerabilities.
- **Molecular Modeling and Simulation:** Our arsenal extends to molecular modelling and simulation, allowing us to envision the dynamic battles between drug candidates and their targets. These computational experiments guide our optimization efforts and accelerate the discovery of potent therapeutic agents.

- **Web Service Development:** Recognizing the transformative potential of our MEBPVC design methodology, we've embarked on the development of MEVaxiDO, a cloud-based web service. This democratisation effort aims to empower researchers worldwide to leverage our computational tools for accelerated vaccine development.

#### 4. Structural Biology: Delving into the Fabric of Life

- **Protein Dynamics and Biotensegrity:** Beyond static structures, we venture into the fascinating realm of protein dynamics and biotensegrity. By understanding the intricate dance of atoms and the underlying energetic principles, we strive to unveil the hidden orchestrations that govern protein function and guide the design of novel biomolecules.
- **Synthetic Protein Design:** Inspired by nature's ingenuity, we embark on the ambitious journey of synthetic protein design. By harnessing our understanding of functionally important structural components (FISCs), we aim to engineer novel proteins with tailor-made functionalities, opening doors to unprecedented therapeutic and technological possibilities.

#### 5. Biomedical Engineering: Blending Technology and Health

- **Wearable Technology:** Our interest extends beyond traditional scientific boundaries, embracing the fusion of technology and health with "Smart Foot wearables." Inspired by the ancient wisdom of Marma Chikitsa from Ayurveda, we aim to create cutting-edge wearables that seamlessly integrate traditional knowledge with modern technological advancements to enhance well-being.
- **Noninvasive Diagnostics:** We envision a future where disease detection is swift, painless, and accessible. The exploration of nanobody-based diagnostics represents our cavalry against a wide range of diseases, offering the potential for early detection and personalised treatment interventions.

#### 6. Precision Medicine: Harnessing Individuality for Optimal Health (Continued)

- **Personalised Nutrition:** Recognizing the unique nutritional needs of each individual, we've embarked on a bold mission to create an individualised dietary roadmap through a "Personal Digital Fitness Assistant App and Wearables." Inspired by the holistic principles of Ayurveda, this mobile application leverages cutting-edge data analysis and NGS technologies to curate customised dietary recommendations. By incorporating factors like lipid profiles, climatic conditions, and individual body type (Vata, Pitta, Kapha), we strive to empower individuals to make informed dietary choices and optimise their well-being.

### Conclusion: A Collaborative Odyssey Towards a Healthier Tomorrow

Our lab's diverse research endeavours, encompassing various scientific disciplines, paint a vibrant picture of collaborative exploration and unwavering commitment to improving human health and well-being. Through a potent blend of computational prowess, rigorous experimentation, and innovative design, we strive to translate scientific discoveries into tangible solutions that address pressing medical and technological challenges. We believe that by fostering interdisciplinary collaborations and embracing cutting-edge technologies, we can pave the way for a healthier and brighter tomorrow.

**Active Collaborators:**

1	<b>Collaboration:</b> Dr. Aniket Sarkate's Lab, Dr. B A M University, Aurangabad
2	<b>Collaboration:</b> Prof. Ramakrishna Kancha, CPMB, Osmania University, Hyderabad
3	<b>Collaboration:</b> Prof. Jahagirdar, Central Institute of Fisheries Education (CIFE), Mumbai
4	<b>Collaboration:</b> Dr. Sanath Kumar, Central Institute of Fisheries Education (CIFE), Mumbai
5	<b>NE Collaboration: Genomics Technologies:</b> Evaluation of Genetic Diversity and Core germplasm collection of Indigenous Rice in Arunachal Pradesh, Eastern Himalaya.
6	<b>NE Collaboration: NGS Technologies:</b> Understanding the sexual and olfactory dysfunction in Parkinson's Disease subjects through <i>Drosophila</i> model and therapeutic intervention