

2 Days Workshop and Hands-on-Training on Structural Bioinformatics and Computer-Aided Drug Designing

Organized By: **Medical Biotechnology and Computational Drug Designing Laboratory, Pushpagiri Research Centre, Tiruvalla, Kerala**

Date : **15th – 16th November, 2024**

Venue : **PRC Conference Hall**

The workshop aimed to equip participants with the foundational and advanced techniques in structural bioinformatics and computer-aided drug design (CADD), emphasizing practical hands-on training

Dr. Aniket Naha, Scientist in charge of Bioinformatics Centre, PRC served as the resource person delivering insightful lectures and facilitated all six hands-on sessions.

Ph.D. scholars, postgraduate and undergraduates from various reputed institutes like CSIR NIIST, Trivandrum, Karunya Institute of Technology and Sciences, Coimbatore, MG University, MACFAST (Tiruvalla), PIMSRC (Tiruvalla), and Believers Church Medical College (Tiruvalla).

Topics Covered:

The workshop was divided into lectures and practical sessions on the following topics:

- Protein Modeling and Structure Prediction: Techniques for modeling protein structures and their validation
- Mutational Analysis and Thermodynamics: Understanding the impact of mutations on protein stability and function
- Introduction to Small Compound Databases: Navigating databases to source potential drug-like molecules
- Molecular Docking and Analysis: Exploring receptor-ligand interactions using docking tools
- Molecular Dynamics Simulation: Simulating biomolecular movements to evaluate drug-target interactions

Hands-on Training

- Six practical sessions provided participants with direct exposure to advanced bioinformatics tools and methodologies
- The sessions focused on translating theoretical knowledge into practice, enhancing skills in computational drug design

Feedback

- Participants expressed their appreciation for the interactive sessions and expert guidance
- Suggestions for follow-up workshops on advanced topics like QSAR modeling and AI applications in drug discovery were noted
- The event concluded with a vote of thanks and distribution of participation certificates

Action Items

- Dissemination of workshop materials, software and tutorials to all participants
- Planning of future workshops with a focus on advanced computational techniques and data integration

The 2 days workshop ended with the closing statement from DrSoumya RS and certificate dissemination to all participants



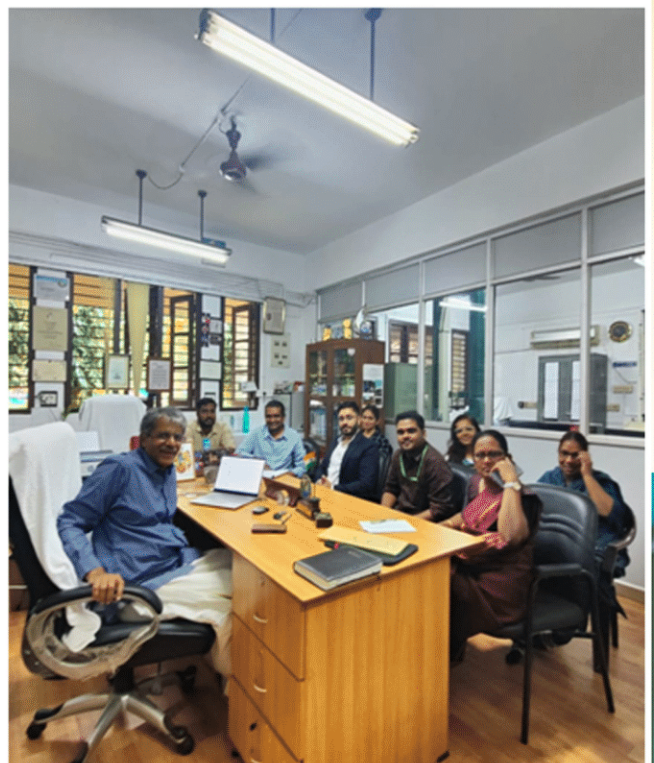
LEADS CLINICAL RESEARCH AND BIO SERVICES



A meeting took place on November 1, 2024, between Pushpagiri Research Centre (PRC) and LEADS Clinical Research and Bio Services Pvt. Ltd. to discuss potential collaborations, especially in clinical trials. During the meeting, LEADS, a Bangalore-based company specializing in clinical trials, presented their experience, expertise, and operational structure. LEADS highlighted their extensive network of collaborations with medical institutions across India and their successful track record in conducting over 150 clinical studies, resulting in multiple publications. PRC faculty actively engaged in the discussions, seeking clarification on various aspects of the collaboration, including study subject recruitment, principal investigator selection, trial responsibilities, and site coordination. PRC expressed interest in collaborating on both clinical trials and animal studies, leveraging their well-equipped animal research facility. Both PRC and LEADS expressed a positive outlook on the potential partnership and agreed to move forward with developing a Memorandum of Understanding to facilitate future cooperation.

"Pioneering Tissue Engineering Research: MGU, PIMS & RC, and Charite University Germany Ready to Form Strategic Alliance"

The meeting was held at Mahatma Gandhi University (MGU), Kottayam, on November 5, 2024 marking a significant milestone in the collaborative research efforts between MGU, PIMS & RC and Charite University (Germany). The meeting, attended by faculty members from MGU including Prof. Sabu Thomas, Dr. Aneesh (Charite University Germany), Dr. Nebu George Thomas, and Dr. Ampadi A N (PIMS & RC) focused on exploring new avenues for research collaboration, funding opportunities, and student exchange programs. The meeting also highlighted plans to organize a conference on tissue engineering in 2025 at PRC in association with MG University and Charite Germany. Prof. Sabu Thomas graciously offered to assist in extending animal works from international universities to perform at PRC. The meeting concluded with a special thanks to Dr. Nandakumar for his invaluable support in organizing the session. This collaborative effort marks a significant step forward in promoting cutting-edge research and academic excellence in the region.





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ORIGINAL ARTICLE

Pharmacology and Articular Cartilage Regeneration: A New Strategy for Osteoarthritis

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Title : Designing Novel Serine Protease Inhibitors against Potential Biomarkers Specific to Lung Adenocarcinoma through Systems Biology and Structural Bioinformatics Approaches

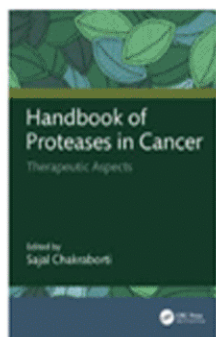
Authors : Anamika Mishra, Soundharya H., Aniket Naha, SoumitraNath, Nibu Varghese, R. S. Soumya

Book : Handbook of Proteases in Cancer

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Chapter

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Book [Handbook of Proteases in Cancer](#)

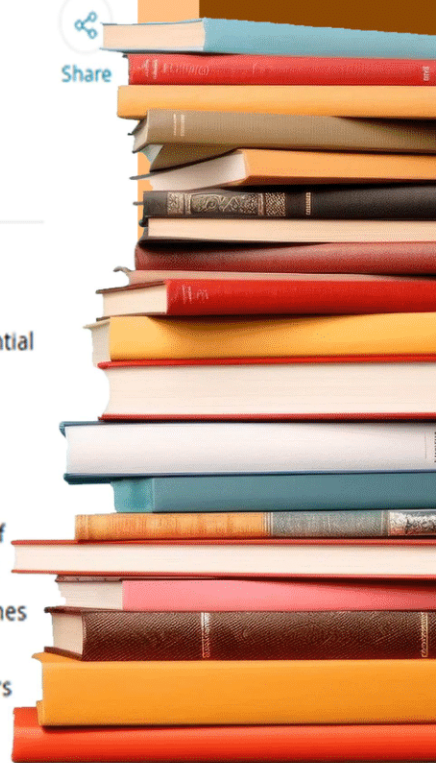
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ABSTRACT

Lung Adenocarcinoma (LUAD), a prevalent subtype of non-small-cell lung cancer (NSCLC), poses a substantial challenge in designing sustainable therapeutic strategies. This study seeks to address the multifaceted complexity of LUAD by concentrating on the identification of biomarkers enabling precise diagnosis, prognosis and personalized treatment. This review underscores the therapeutic potential of protease inhibitors and their roles in cancer progression, as curtailing the activity of proteases has demonstrated promise in obstructing tumour growth, invasion and metastasis. The process entails a structured series of stages encompassing target identification, drug design, screening and the development of peptide-based inhibitors. The review presented special attention to systems biology and structural bioinformatics pipelines to facilitate inhibitor design through the optimization of lead compounds and molecular modelling approaches. Overall, this study presents a comprehensive outlook for designing potent protease inhibitors for the treatment of LUAD.



Research Updates from Medical Biotechnology and Computational Drug Designing Lab and Microbial Technology Research and Infectious Disease Laboratory, Pushpagiri Research Centre

Dr. Aniket Naha, Scientist and Student Coordinator has successfully isolated and characterized 3 novel probiotic strains from indigenous foods. The research endeavour was achieved by the research students (Ms. Elizabeth Annie George, Ms. Adithi-Aneesh and Ms. Joby Rose Jacob) working under the guidance of by DrAniket.

The strains were sequenced and submitted to National Centre for Biotechnology Information (NCBI; <https://www.ncbi.nlm.nih.gov/>) and accession numbers received are as follows:

Pediococcus pentosaceus(PRCAAJA1) : <https://www.ncbi.nlm.nih.gov/nuccore/PP938697.1/>

Lactiplantibacillus plantarum(PRCAAJA2) : <https://www.ncbi.nlm.nih.gov/nuccore/PP938712>

Weissella confusa (PRCAAJA3) : <https://www.ncbi.nlm.nih.gov/nuccore/PP938715>

Weissella confusa (PRCAAJA4) : <https://www.ncbi.nlm.nih.gov/nuccore/PP938716>

GenBank - Send to -

Pediococcus pentosaceus strain PRCAAJA1 16S ribosomal RNA gene, partial sequence

GenBank PP938697.1
[FASTA](#) [Graphics](#)

GenInfo

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 REFERENCE 1 (bases 1 to 1285)
 AUTHORS Naha,A., Adithi,A., Joby,R.J., George,E.A. and Varghese,N.
 TITLE Prcaja1
 JOURNAL Unpublished
 REFERENCE 2 (bases 1 to 1285)
 AUTHORS Naha,A., Adithi,A., Joby,R.J., George,E.A. and Varghese,N.
 TITLE Direct Submission
 JOURNAL Submitted (22-JUN-2024) Medical Biotechnology and Computational Drug Designing Laboratory, Pushpagiri Institute of Medical Sciences and Research Centre, Pathanamthitta, Tiruvalla, Kerala 689581, India

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Lactiplantibacillus plantarum strain PRCAAJA2 16S ribosomal RNA gene, partial sequence

GenBank PP938712.1
[FASTA](#) [Graphics](#)

GenInfo

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 AUTHORS Naha,A., Adithi,A., Joby,R.J., George,E.A. and Varghese,N.
 TITLE Prcaja2
 JOURNAL Unpublished
 REFERENCE 2 (bases 1 to 1246)
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Weissella confusa strain PRCAAJA3 16S ribosomal RNA gene, partial sequence

GenBank PP938715.1
[FASTA](#) [Graphics](#)

GenInfo

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 REFERENCE 1 (bases 1 to 1389)
 AUTHORS Naha,A., Adithi,A., Joby,R.J., George,E.A. and Varghese,N.
 TITLE Prcaja3
 JOURNAL Unpublished
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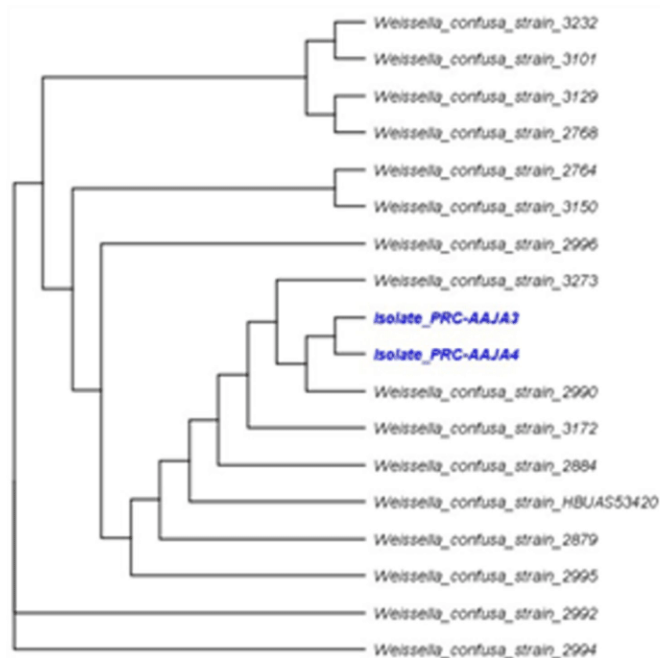
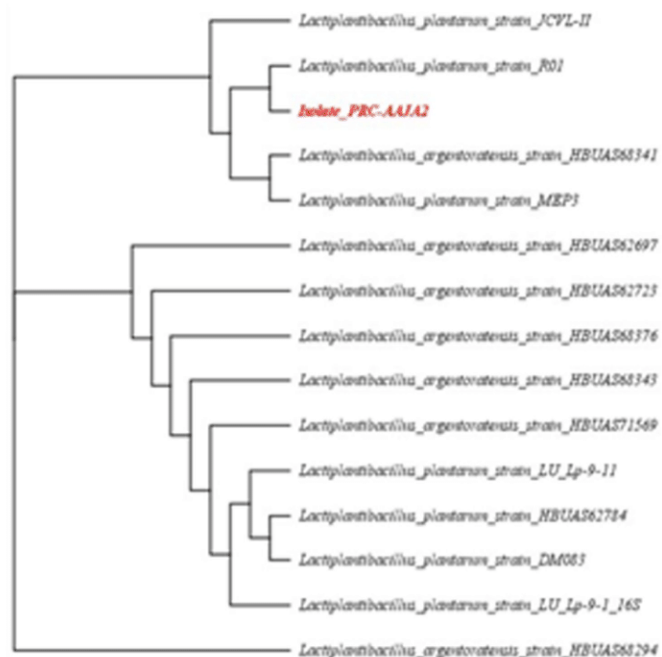
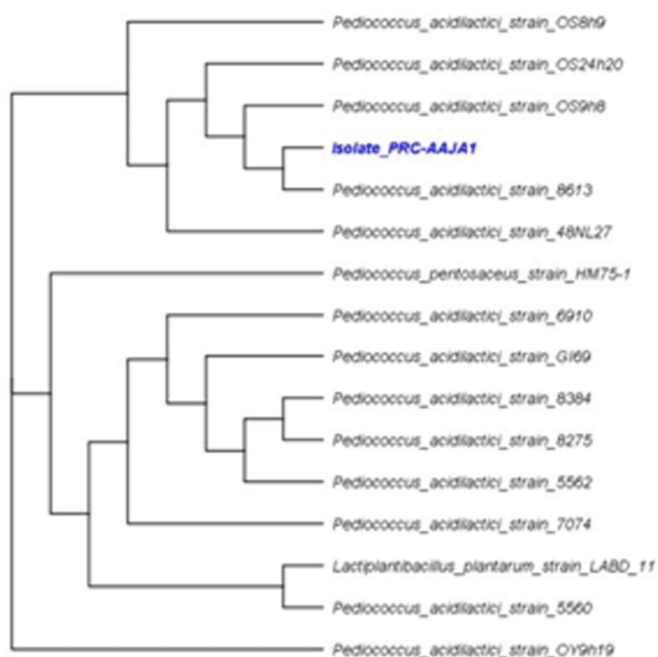
GenBank - Send to -

Weissella confusa strain PRCAAJA4 16S ribosomal RNA gene, partial sequence

GenBank PP938716.1
[FASTA](#) [Graphics](#)

GenInfo

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 REFERENCE 1 (bases 1 to 1291)
 AUTHORS Naha,A., Adithi,A., Joby,R.J., George,E.A. and Varghese,N.
 TITLE Prcaja4
 JOURNAL Unpublished
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The phylogenetic tree of the 4 novel probiotic strains PRC-AAJA1, PRC-AAJA2, PRC-AAJA3 and PRC-AAJA4