

**Conference Presenter List – 3<sup>rd</sup> International Conference cum Workshop**  
**on Recent Trends in Structural Bioinformatics and Computer Aided Drug**  
**Design (ICSBCADD'25) – Oral Presentations**

S. No	Name	Title of Presentation
OP-1	Aditi Roy Research Scholar	Identification of Berberine Analogues as Promising <i>Escherichia coli</i> FtsZ Inhibitors Through Machine Learning, Molecular Docking, and Molecular Dynamics Approaches
OP-2	Avani Panickar Research Scholar	Machine learning and DFT-based discovery of natural inhibitors against $\beta$ -lactam-resistant PBP2x mutants in <i>Streptococcus pneumoniae</i>
OP-3	Elizabeth Annie George Research Scholar	Novel HFIAP-1 Mutant Antimicrobial Peptide Identified as a Potential Inhibitor of Extended-Spectrum $\beta$ -Lactamases in <i>Escherichia coli</i> : An In-silico Study
OP-4	Srujal Kacha Research Scholar	Computational Identification of Novel Therapeutics for the PBP3 F533L Mutant of <i>Pseudomonas aeruginosa</i> Using Machine Learning Techniques
OP-5	Rhitam Biswas Research Scholar	Structure-Based Identification of Novel Zinc-Binding Inhibitors Against the Essential Metalloprotein DapE in <i>Klebsiella pneumoniae</i>
OP-6	Sara Pearl Research Scholar	Unraveling the Genomic Complexity of Resistome, Virulome, and Mobilome in Nosocomial <i>Acinetobacter baumannii</i>
OP-7	Ambiga Chinnathambi Research Scholar	In-silico study of 1-methyl-3-phenylindole from <i>Terminalia bellirica</i> as an estrogen receptor modulator for breast cancer treatment
OP-8	Muthulakshmi Muthumanickam Research Scholar	Targeting Bcl-2 anti-apoptotic receptor with gossypetin from <i>Moringa oleifera</i> : An in silico study for colorectal cancer prevention
OP-9	Ramprakash Yadav Research Scholar	AI-Driven Drug Design and Screening of Aryl Benzoyl Hydrazide Analogues as Potential Inhibitors of ZIKV NS2B-NS3 Protease
OP-10	Rupali Daheriya Research Scholar	Structure and Stability of Different Tautomers of Some Antibiotics
OP-11	Selvaraj Anupriya Research Scholar	Integrated Computational Identification and Evaluation of Novel c-Src Inhibitors as Potential Therapeutics for Colorectal Cancer
OP-12	Shankari Gopalakrishnan Research Scholar	Small molecules targeting ARID1A in the MDA-MB-231 cell line revealed by hub gene analysis of SWI/SNF chromatin remodeling complex along with structure-based virtual screening and in vitro confirmation
OP-13	Dr. A. Bharathi Associate Professor	Docking and Molecular Dynamics Simulations of Anti-Hypertensive Peptides from Seaweeds

OP-14	M. Nithish PG (M. Sc. Student)	NLP-Driven screening and Computational Identification of Bioactive Peptides from Fermented Foods for Therapeutic Intervention in PCOS Management
OP-15	Dr. A. Anand Senior Lecturer	Synergistic Application of Metabolic Glycan Labelling and Click Chemistry to create a Novel Exosome-Based Therapeutic Against AZT Toxicity

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S. No	Name	Title of Presentation
OP-16	Muralidharan Jothimani Research Scholar	Pharmaco-Informatics Profiling of Small Molecules Targeting c-Kit Protein
OP-17	Gowri Sundaraganesan Research Scholar	Computational Evaluation of GC-MS Derived Phytocompounds from Two Medicinal Plants as Potential RAC1 Inhibitors for Breast Cancer Therapy
OP-18	Rajesh Sivamoorthy Research Scholar	Computational Exploration of <i>Amomum subulatum</i> Phytocompounds Through Network Pharmacology to Identify Hub Genes and Potential Therapeutics for Breast Cancer
OP-19	R. Narmatha Research Scholar	Computational and Experimental Investigation of phytocompounds from <i>Andrographis echiooides</i> plant and synthesis of Metal Oxide nanoparticles by green method
OP-20	Saravanan Priyadarshini Research Scholar	Systematic Analysis to Identify Prognostic Biomarkers, Potential Target, and Natural Inhibitors for Cervical Cancer
OP-21	Muthuraja Arun Pravin Research Scholar	Integrative ML-Guided Multi-Omics and Structure-Based Drug Design to Unveil Diagnostic Biomarkers and Host-Directed Therapeutics Against Dengue Virus
OP-22	Rajaram Abhirami Research Scholar	Disrupting TasA-Induced NF-κB Activation in <i>Bacillus cereus</i> Biofilms: A Novel Strategy for Gastric Cancer Prevention
OP-23	Dr. Manikandan Jayaraman Project Scientist – I	Computational Insights into Potential Marine Natural Products as Selective Inhibitors of <i>Mycobacterium tuberculosis</i> InhA: A Structure-Based Virtual Screening Study
OP-24	Pradeep Kumar Sriram Research Scholar	Investigating Marine Natural Products as Prospective Anti-AgrA Drug Candidates Against <i>Enterococcus faecium</i> : A Subtractive Proteomics Facilitated Multi-Tier Screening Study for Addressing Antimicrobial Resistance
OP-25	Maharaja Muthuvairam Subbulakshmi Research Scholar	A Multi-Tiered Computational Framework for Functional and Structural Characterization of Hypothetical Proteins in <i>Nocardia asteroides</i> FDAARGOS1485: An Integrated Structure-Based Virtual Screening and Molecular Dynamics Validation of Marine-Derived Inhibitors
OP-26	Heyram Krishnakumar Research Scholar	Multi-Targeted Computational Evaluation of Phytochemical Modulators Targeting Metabolic Enzymes SIK2 and GCK in Type 2 Diabetes
OP-27	M. Manikandan Research Scholar	Computational Design of a Novel Disulfide-Bond Based Prodrug IMQ-S-S-IMQ for Breast Cancer Therapy
OP-28	Rubhashri Gurunathan Research Scholar	Molecular Modeling and Dynamics-Based Structural Characterization of the HTLV-1 SU Protein (gp46)

OP-29	Sappanimuthu Priyanka Research Scholar	Structural and Mechanistic Analysis of WaaQ in Coordinating LPS Core Assembly in Multidrug-Resistant <i>Klebsiella pneumoniae</i> through Computational Approaches
OP-30	Veena Radhakrishnan Research Scholar	Genomic Insights into the Resistome and Virulence of <i>Nocardia pneumoniae</i> from a Post operative Ocular Infection
OP-31	Sethu Meenal Research Scholar	Green Synthesis of Cerium Oxide Nanoparticles Supported by Molecular Docking Driven Identification of Bioactive Phytocompounds from <i>Cymodocea serrulata</i>
OP-32	Rohit Karn Project Scientist – I	In Silico Identification of selective CDK9 Inhibitors disrupting P-TEFb complex against Triple-Negative Breast Cancer
OP-33	Nalina Viswanath Research Scholar	In-silico Approach of Antifungal Properties of Natural Plant Compounds Against <i>Candida Albicans</i>