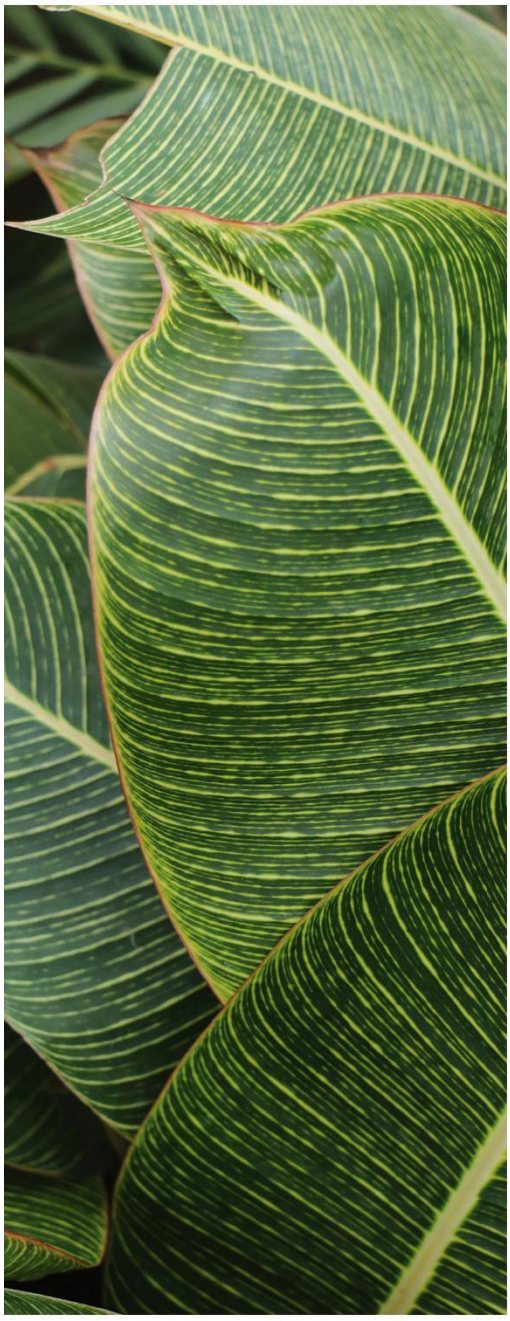
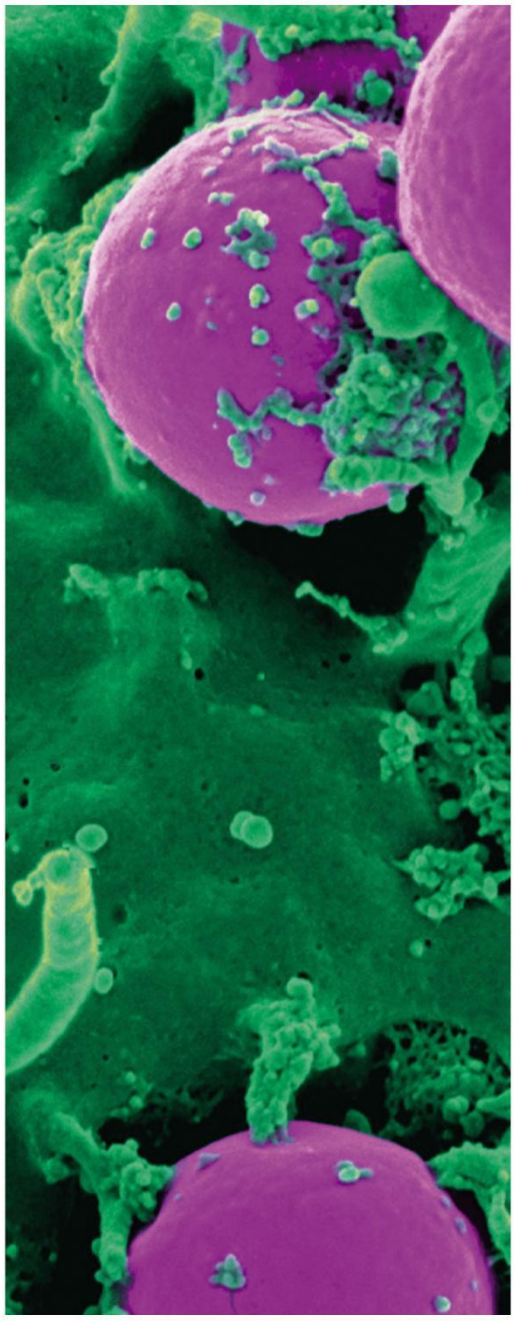
PROCEEDINGS OF 43RD ANNUAL SESSIONS 2023

The Institute of Biology
Sri Lanka





BIOLOGICAL WEALTH FOR ECONOMIC PROSPERITY

INSTITUTE OF BIOLOGY

SRI LANKA

PROCEEDINGS OF THE 43RD ANNUAL SESSIONS

Theme

Biological Wealth for Economic Prosperity

Institute of Biology, Sri Lanka

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Predicting the structure and active site of a putative xylanase in *Mycobacterium tuberculosis*.

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Tuberculosis is one of the most common diseases that causes many deaths around the world. As a result of the continuous evolution of *Mycobacterium tuberculosis*, some novel strains show high resistance to most anti-TB drug therapies. Antibiotic resistance associated with *Mycobacterium tuberculosis* can be resolved by the development of anti-virulence drug targets. The MarR gene family is one of the major transcriptional regulation families in *Mycobacterium tuberculosis*, and this family mainly contributes to controlling several bacterial responses, such as bacterial virulence. The regulator Rv 3095 which was identified as a virulence gene regulator, mainly regulates the expression of Rv 3096 gene that codes for a putative xylanase enzyme. The main objective of this study is to determine the structure and active site of the putative xylanase enzyme. Molecular docking was conducted to identify possible antibiotic ligands that can block the active site of putative xylanase enzyme. The FASTA sequence of Rv 3096 was downloaded from the NCBI database, and the structure of the protein was predicted by using alpha fold and Robetta fold protein prediction servers. The active site of the Rv 3096 protein was determined by using CoachD active site prediction server. The molecular docking was done by using PyRx software, and ligand libraries were downloaded from the Zinc 15 database. The structure of the N-terminal end of the protein was predicted by both protein prediction servers with high confidence levels. However, both protein prediction servers were unable to predict the structure of the C-terminal end of the protein with high confidence levels. The pocket which has the highest C score is considered an active site of the predicted protein. In the virtual screening, the highest binding affinities to the active site of the xylanase enzyme were recorded by drug ligands that belong to the penicillin and doxycycline drug groups.

Keywords: *Mycobacterium tuberculosis*, Rv 3096 protein, MarR gene family, Bacterial virulence, Virtual drug screening

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