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# Investigation of Potential Targets and Their Inhibitors in Mycobacterium Tuberculosis

by Ankit Verma

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# List of abbreviations

MTB	: Mycobacterium tuberculosis
mAGP	: Mycolyl-arabinogalactan- peptidoglycan
MmpLs	: Mycobacterial membrane protein large
TMM	: Trehalose monomycolate
THPPs	: Tetrahydro-pyrazolopyrimidine carboxamide
PMF	: Proton motive force
ТМН	: Transmembrane helices
<i>GlfT1</i> and <i>GlfT2</i>	: Galactofuranosyltransferases
MurB	: UDP-N-Acetylenolpyruvoylglucosamine reductase
β	: Beta
PAINS	: Pan assay interference compounds
PG	: Peptidoglycan
NADPH	: Nicotinamide adenine dinucleotide phosphate
ТВ	: Tuberculosis
UI	: Unit interval
HIV	: Human immunodeficiency virus
ADMET	: Absorption distribution metabolism excretion toxicity
PDB	: Protein data bank
PDBQT	: Protein Data Bank, Partial charge (Q) & Atom type (T) format
3D	: Three dimensional
SDF	: Structure data file
Kcal/mol	: Kilocalorie per mole
RMSD	: Root mean square deviation
KI	: Inhibition constant
PLIP	: Protein-ligand interaction profiler

MD	: Molecular simulation
MDS	: Molecular simulation study
TIP4P	: Transferable intermolecular potential 4 points
NPT	: Isothermal isobaric
ATCC	: American-type culture collection
MTCC	: Microbial Type Culture Collection
OADC	: Oleic albumin dextrose catalase
PBS	: Phosphate buffered saline
NaCl	: Sodium chloride
SEM	: Standard error of the mean
OD	: Optical density
RPMI	: Roswell Park Memorial Institute medium
FBS	: Fetal bovine serum
DMEM	: Dulbecco's modified essential medium
DMSO	: Dimethyl sulfoxide
MTT	:(3-(4,5-dimethyl thiazolyl-2)-2,5-diphenyltetrazolium bromide assay
π	: Pi
A	: Alpha
Å	: Angstrom
H-bond	: Hydrogen bond
DNA	: Deoxyribonucleic acid
2-D	: Two dimensional
G-score	: Binding affinity
nM	: Nanomoles
Pm	: Picomoles
LogP	: Aqueous solubility
CSID	: ChemSpider ID
DBID	: Drug Bank ID

NS	: Nanoseconds
RMSF	: Root mean square fluctuations
HTS	: High throughput screening
CADD	: Computer-aided drug discovery
UGM	: UDP-galactopyranose mutase
QSAR	: Quantitative structure-activity relationship
UN	: United Nations
GC	: Guanine or Cytosine
AIDS	: Acquired Immunodeficiency Syndrome
LTBI	: Latent TB infection
WHO	: World Health Organization
MTBC	: Mycobacterium complex
NGOs	: National Government Organization
BCG	: Bacillus Calmette Guerin
DOTS	: Directly observed treatment short-course
RIFR-TB	: Rifampicin-resistant tuberculosis
MDR-TB	: Multidrug-resistant tuberculosis
XDR-TB	: Extensively drug-resistant tuberculosis
DR-TB	: Drug-resistant tuberculosis
IRIS	: Immune reconstitution inflammatory syndrome
EMB	: Ethambutol
RIF	: Rifampicin
PZA	: Pyrazinamide
INH	: Isoniazid
TDR-TB	: Total drug-resistant
DNA	: Deoxyribonucleic acid
PAS	: Para-aminosalicylic acid
NADH	: Nicotinamide adenine dinucleotide
ICL	: Iso-citrate lyase

NCE	: Novel chemical substances
PS	: Pantothenate synthetase
LPS	: Lipopolysaccharides
NADPH	: Nicotinamide adenine dinucleotide phosphate
AG	: Arabinogalactan
MIC	: Minimum inhibitory concentration
SAR	: Structure-activity relationship
BTZ	: Nitrobenzothiazoinone
FAS	: Fatty acid synthase
RND	: Resistance-nodulation-division
ROS	: Reactive oxygen species
QTcF	: Corrected QT interval using Fridericia's formula
OBR	: Optimized background regimen
RNAP	: RNA polymerase
TCA	: Tricarboxylic acid
ETC	: Electron transport chain
BDQ	: Bedaquiline
FDA	: Food and Drug Administration
CFZ	: Clofazimine
HTS	: High-throughput screening
LPZ	: Lansoprazole
CFU	: Colony forming units
LJ	: Lowenstein-Jensen
DGI	: Difference in growth
NMR	: Nuclear magnetic resonance
IZD	: Inhibition zone diameter
SRHU	: Swami Rama Himalayan University
GI	: Growth index