Process of Developing MccJ25 as Universal Antimicrobial Drug

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Antimicrobial Peptide(AMP) MicrocinJ25 (MccJ25) is naturally secreted by E.coli & is efficient anti-bacterial. MccJ25 reduces intestinal inflammation & promotes healthy gut-bacteria. Unlike most synthetic drugs MccJ25 is less toxic , has low immunogenicity & do not increase drug resistance. Current research investigates the role of MccJ25 as preventive & universal antimicrobial drug. Molecular interaction of the MccJ25 is studied with following microorganisms and molecules, Sars-Cov2 protein & enzyme, human- Angiotensin converting enzyme-2 receptor ,Sars-CoV2 Omicron variants ,RSV,influenza,HIV; bacteria Streptococcus & Enterococcus; fungus Candida auris & Rhizopus ; parasites Leishmania & Necator. Molecular structures were downloaded from PDB, followed by use of FTMap to identify the active residues. Molecular interaction were performed using HADDOCK2.4,PRODIGY & Discovery Studio Visualizer. Results show MccJ25 binds efficiently with all tested molecules based on HADDOCK Score,BSA,Z score & binding energy and hence has potential to be effective universal antimicrobial drug. Software ADMET & Molinspiration were used to test pharmacokinetics & drug likeness property using Lipinski rule. MccJ25 did not pass Lipinski rule. Historically, other AMP like Insulin & Nisin have not passed Lipinski rule in their native forms. They have to be bioengineered to make them suitable for drug development. Based on research, amino acid(AA) at position 9 &18 of MccJ25 are most active site & 9 is essential for inhibition of bacterial RNA polymerase. Rational bioengineering of MccJ25 from E.coli to increase pharmacokinetics while preserving AA at position 9 & 18 is required. This will make MccJ25 suitable for in-vitro & in vivo trials to be developed as a Universal Antimicrobial drug.