Preface

The discovery of antibiotics revolutionized modern healthcare and increased the lifespan of humans by more than twenty years, but their unregulated use has resulted in antimicrobial resistance (AMR). AMR kills at least 7 lakh people in poor and middle-income countries each year, and the WHO ranks it as one of the top ten public health hazards. To counteract this condition, novel antimicrobial compounds are required, and antimicrobial peptides (AMPs) show promise in this regard. AMPs are proteins produced by diverse organisms naturally and can be classified into multiple groups, such as antiviral (AVPs), antifungal (AFPs), and antibacterial peptides (ABPs).

To avoid the high costs and time associated with identifying novel AMPs in the lab, researchers use *in-silico* tools for preliminary screening of natural sources. However, the existing tools available for this purpose have poor performance, which limits their applicability for wet-lab researchers. Thus, we have proposed AI-based frameworks for identifying AFPs, AVPs, and ABPs from natural sources in different studies.

All amino acids are not equally important in classifying a peptide. Existing AI-based tools do not provide information about the essential amino acids responsible for classifying a peptide. Therefore, we developed an explainable framework that not only classifies the peptides but also provides information about the essential amino acids responsible for classifying a peptide.

The WHO categorizes bacteria into three categories (critical, high, and medium), and the ESKAPEE pathogens are a major threat as they range from high to critical

WHO-priority pathogens. Earlier studies can identify ABPs from natural resources but do not provide minimum inhibitory concentration (MIC) values against the ESKAPEE pathogens. Thus, for identifying optimal ABPs (which work at low MIC), wet-lab researchers have to test the identified ABPs against ESKAPEE pathogens at different concentrations, leading to a loss of time and money. To address this issue, we proposed a framework that predicts the MIC values for ABPs against ESKAPEE pathogens. The proposed framework can help identify optimal ABPs that can work at low MICs against the entire ESKAPEE group of bacteria.

Peptide toxicity is a major hurdle in the development of therapeutic peptides. Hemolytic activity against red blood cells is one of the key factors to consider when evaluating peptide toxicity. High hemolytic activity can lead to anemia and other blood disorders, making highly hemolytic peptides unsuitable for pharmaceutical use. However, discovering low hemolytic peptides is a labor-intensive and time-consuming process that involves testing on mammalian red blood cells. To address this, we proposed a framework to identify low hemolytic therapeutic peptides.

All the frameworks we developed as part of different studies have also been made available as web applications. The wet-lab researchers can use these tools to narrow the search space while discovering low hemolytic AMPs active against different pathogens.