

## Article

# Antimicrobial Peptide Databases as the Guiding Resource in New Antimicrobial Agent Identification via Computational Methods

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**Abstract:** In light of the growing interest in antimicrobial peptides (AMPs) as potential alternatives to traditional antibiotics, proteomic research has increasingly focused on this area. Addressing this significant scientific need, we undertook an initiative to review and analyze the available databases containing information on AMPs. These databases play a pivotal role as a foundation for most AMP-related studies, enabling not only the identification of new compounds, but also a deeper understanding of their properties and therapeutic potential. As part of this study, we evaluated the quality of information within selected AMP databases, considering their accessibility, content, and research potential. The initial step of the analysis involved a comparison of the per-database and cross-database peptide sequences. A *diamond*, high-throughput protein alignment program was used to compare the degree of sequence similarity among peptides across the individual databases. The redundancy of the data was also evaluated. Collected information was used for an *in silico* evaluation of the selected species' venom proteomes in order to identify putative antimicrobial peptide candidates. An example candidate was further evaluated via a combination of structural analysis based on the computed homology based structural model, the *in silico* digestion of the source protein, and the antimicrobial potential.

**Keywords:** AMP; AMP databases; *diamond* alignment; homology modeling

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## 1. Introduction

### 1.1. Antimicrobial Peptides (AMPs)—Natural Defenders with Therapeutic Applications

Antimicrobial peptides constitute a crucial component of innate immunity, and are present in the majority of living organisms. They possess the ability to induce immune responses and exhibit activity against a wide range of microorganisms, including bacteria, fungi, and viruses. Moreover, AMPs can target cancer cells, making them potential therapeutic agents for cancer treatment [1,2].

AMPs are peptide compounds composed of amino acids, typically containing 6 to 100 residues, although peptides with longer sequences also exist. They occur in four main structural forms:  $\alpha$ -helices,  $\beta$ -sheets, extended conformations, and loops. Under natural conditions,  $\alpha$ -helical and  $\beta$ -sheet structures predominate. Linear peptides lose their structure in solution, whereas cyclic peptides form stable  $\beta$ -sheets maintained by disulfide bonds. Antimicrobial peptides are characterized by a cationic charge and a high content

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