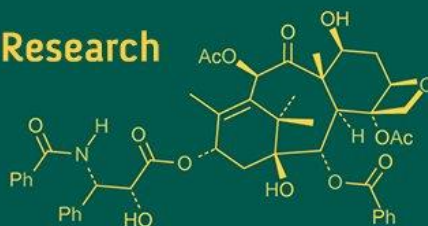


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Assessment studies over the identification of antimicrobial peptides (AMPs) from almond

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Abstract

Antimicrobial peptides (AMPs) are naturally occurring molecules with broad-spectrum antimicrobial activity, offering a promising alternative to traditional antibiotics. In this in-silico study, we aimed to identify and characterize AMPs from almond (*Prunus dulcis*) using BLAST and Macrel prediction tools.

A total of 438 and 345 potential AMPs were identified from almond through BLAST and Macrel prediction, respectively. Comparative analysis of the predicted AMPs revealed that the majority possessed moderate net positive charge (0 to +4.9), low hydrophobicity (<1), low amphiphilicity (<1), and isoelectric point values of ≥ 5 , indicating their potential antimicrobial nature. Among the predicted AMPs, 33 and 39 peptides exhibited high hydrophobicity (≥ 1) under BLAST and Macrel predictions, respectively, while 108 and 110 peptides showed high amphiphilicity (≥ 1). The study also highlighted the importance of physicochemical properties such as net charge, hydrophobicity, amphiphilicity, isoelectric point, and sequence length in determining the antimicrobial potential of the predicted peptides. The average sequence length of the predicted AMPs was 29 amino acids in BLAST prediction and 20 amino acids in Macrel prediction, indicating that most of the identified peptides were short antimicrobial peptides.

Our findings suggest that almond is a promising source of antimicrobial peptides, possessing a diverse repertoire of potential AMPs with desirable physicochemical characteristics associated with antimicrobial activity. This study demonstrates the potential of in-silico approaches in identifying novel AMPs from plant sources and provides a valuable resource for further experimental validation and application.

Keywords: Antimicrobial peptides, almond, Chinese chestnut, In-Silico analysis, blast, Macrel

1. Introduction

India's nut crop production, despite its varied agro-climatic conditions, faces significant challenges due to microbial diseases. The reliance on chemical control methods has led to compromised quality, microbial resistance, and failure to meet international market standards. However, plants offer a promising alternative as they contain numerous bioactive compounds with antimicrobial properties (Harris *et al.*, 2009; Lee and Lee, 2015; Dutta and Das, 2016) [2, 3, 4]. Antimicrobial peptides (AMPs), in particular, have shown potential in treating human infectious diseases, cancer, viral, and parasitic infections (De Lucca, 2000; Tanaka, 2001; Wong *et al.*, 2010; Mansour *et al.*, 2014) [1, 5, 6, 7]. This study aims to identify and analyze potential AMPs in whole-genome sequenced nut crops, such as almond and Chinese chestnut, to develop novel antimicrobial agents.

2. Materials and Methods

The study entitled "Assessment Studies over the Identification of Antimicrobial Peptides (AMPs) from Almond and Chinese Chestnut" was performed during the year 2020-2021 in Department of Horticulture, Central University of Tamil Nadu, Tiruvavur. This chapter outlines the materials used and the methods employed in conducting the experiments presented in this study.

2.1. Identification and Retrieval of reference genome

It has been executed with the identification of whole genome sequenced nut crops based on their high economic value viz., Almond and Chinese chestnut for the *insilico* identification of

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AMP sequences from reference genome. Through the literature survey, reference genome assembly for these crops were identified and retrieved from their respective repositories (Table 2.1).

Table 1: Data availability of whole genome sequence of selected nut crops

Crop	Genome size (Mb)	Data availability
Almond	236.937	https://www.ncbi.nlm.nih.gov/genome/?term=txid3755[orgn]

2.2 Collection of AMP database

DRAMP database was an open-access, manually compiled database that includes sequences, structures, operations, physicochemical, patent, clinical, and reference information for AMPs. All the general AMP datasets from this database were downloaded for the purpose of present research.

2.3 AMP prediction and screening

There are numerous softwares available for AMP prediction and screening now days. Prediction of AMP activity requires different techniques than the homology-based methods that are applicable for longer proteins. Macrel (Santos-Júnior *et al.*, 2020) [8] is a novel end-to-end pipeline for the identification of high-quality AMP candidates by the use of both computational and Machine learning capabilities.

The amino acid FASTA files of predicted ORF's by the Trans Decoder is used as the input. The output file consists of predicted AMPs and general gene prediction information. The predicted AMPs were annotated to the retrieved AMP

datasets. The physicochemical properties of predicted AMPs were analysed. Database of Antimicrobial Activity and Structure of Peptides (DBAASP) (Pirtskhalava *et al.*, 2021) [9] were used to manually curate the crucial physicochemical parameters.

2.4 Comparative analysis

The predicted AMPs from MACREL and the peptides identified through homology search were taken for further analysis.

3. Experimental results & discussion

3.1. AMP prediction and screening

In case of Macrel retrieval of potential AMPs from almond, a total of 3944 predicted AMPs were obtained. After applying the filtration criteria of E-value < 1 and sequence identity $\geq 50\%$, 345 AMPs were retained as filtered AMPs, representing approximately 8.7% of the predicted AMPs.

While discussing the BLAST-based retrieval of potential AMPs, 3782 annotated AMPs were identified from the almond dataset. Following filtration using the same criteria (E-value < 1 and identity $\geq 50\%$), 438 AMPs were retained, accounting for approximately 11.6% of the annotated AMPs.

These results indicate that although both approaches retrieved a large number of potential AMPs, the BLAST-based method retained a higher number and proportion of filtered AMPs (438; 11.6%) compared to the Macrel approach (345; 8.7%) under the applied filtration parameters. (Figure 3.1.1)

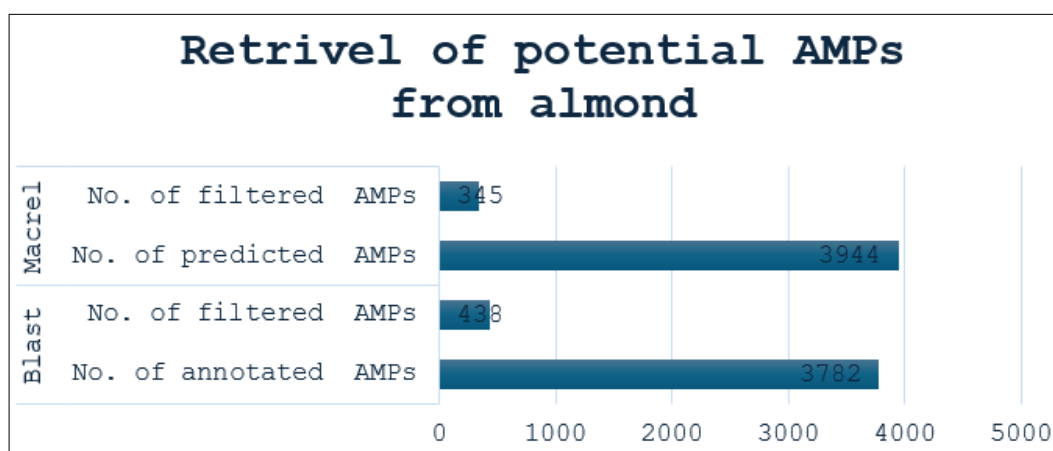


Fig 1: Potential AMPs from almond

3.2. Physicochemical properties study

The anticipated AMPs' physicochemical properties were studied. The important physicochemical parameters were manually curated using the Database of Antimicrobial Activity and Structure of Peptides (DBAASP). In this study five major physicochemical properties namely, net charge, hydrophobicity, isoelectric point, amphiphilicity and sequence length were analyzed.

3.2.1. Net charge

Net charge of all the AMPs varied greatly from negative to positive. Net charges of both normal blast predicted as well

as Macrel predicted AMPs categorized into AMPs net charge value of $\geq +5$, $0 \leq x \leq +4.9$ and < 0 . In case of Macrel predicted AMPs from almond, 74% of the predicted AMPs were lying between 0 and +4.9, and 20% of them were lying under the below zero (< 0) category. Only 6% of the Macrel predicted AMPs had a net charge of $\geq +5$.

While discussing blast predicted AMPs, 59% of the AMPs had a net charge between 0 and +4.9. About 18% and 23% of the predicted AMPs were having net charge values of < 0 and $\geq +5$, respectively. (Figure 3.2.1.a. & 3.2.1.b)

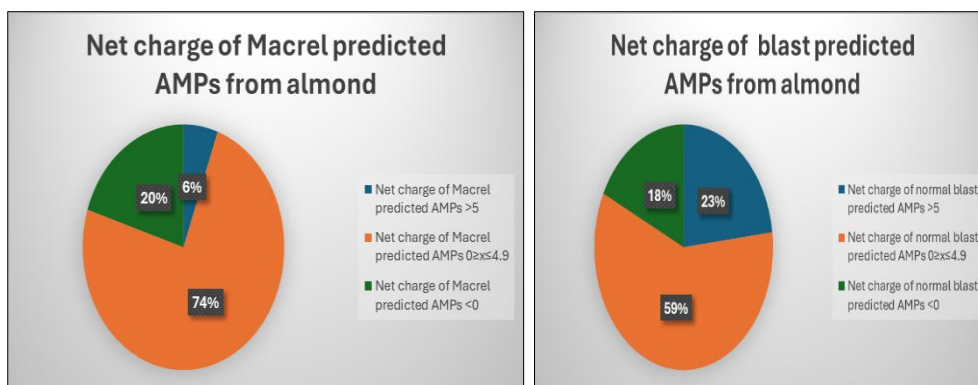


Fig 2a & 2b: Net charges of AMPs retrieved from Almond

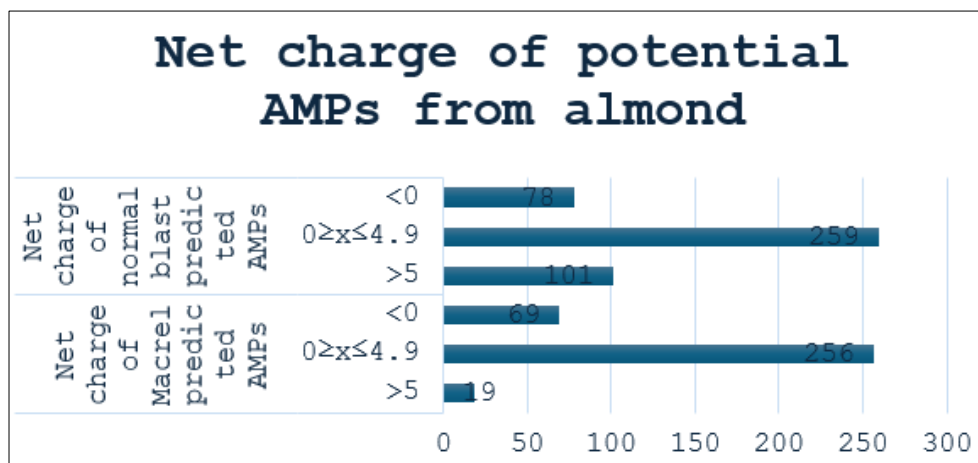


Fig 2c: No. of AMPs having different range of Net charges retrieved from Almond

3.2.2. Hydrophobicity

Hydrophobicity value of all the predicted AMPs were categorized into <1 and ≥ 1 . In case of Macrel predicted AMPs from almond, 89% of the predicted AMPs had hydrophobicity values of <1, while only 11% of them were

found under the ≥ 1 hydrophobicity category. While discussing BLAST predicted AMPs, 92% of the predicted AMPs exhibited hydrophobicity values of <1. Only about 8% of the predicted AMPs were having hydrophobicity values of ≥ 1 .

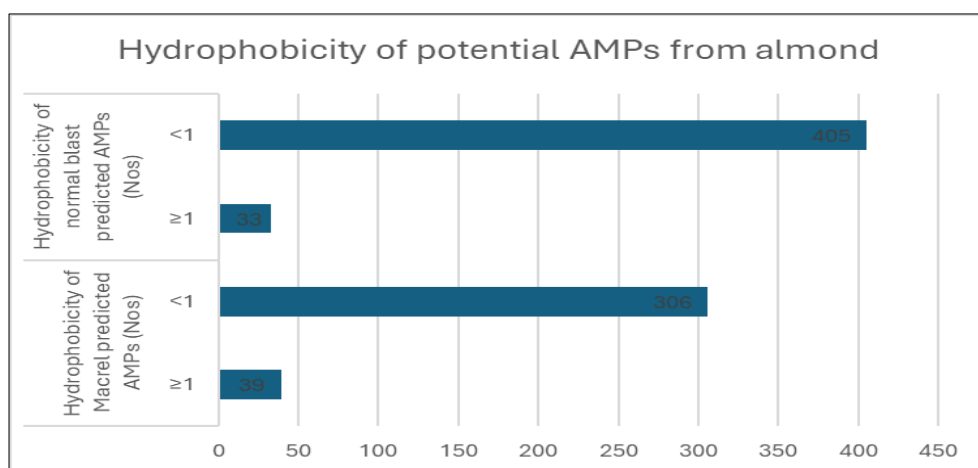


Fig 3: Hydrophobicity of potential AMPs from almond

3.2.3. Isoelectric point

The isoelectric point value of all the predicted AMPs were grouped into <5 and ≥ 5 categories. In both Macrel and normal BLAST predicted AMPs, about 80-85% of the predicted AMPs were having an isoelectric point value of

≥ 5 , whereas only 15-20% of the predicted AMPs were found under the <5 category. In Macrel predicted as well as normal BLAST predicted AMPs, almond exhibited a high proportion of AMPs under the ≥ 5 isoelectric point category. (Figure 3.2.3)

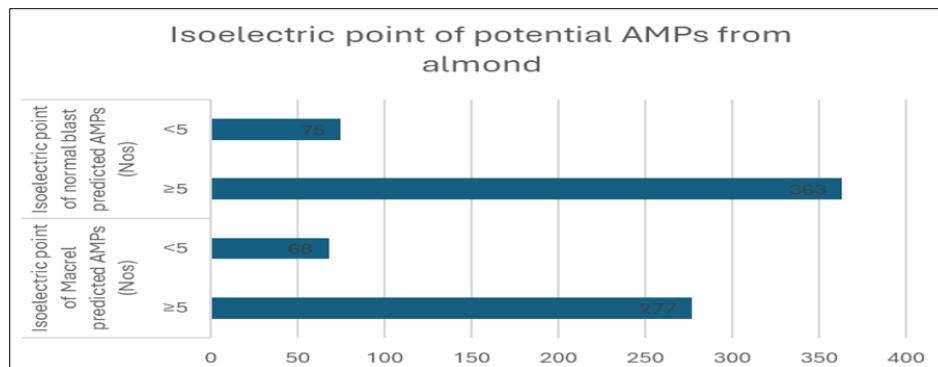


Fig 4: Isoelectric point of AMPs retrieved from selected nut crops

3.2.4. Amphiphilicity

The amphiphilicity value of all the predicted AMPs were classified into <1 and ≥ 1 . In both the methods of AMP

prediction, about 25-32% and 68-75% of the predicted AMPs were having amphiphilicity values of ≥ 1 and <1 , respectively. (Figure 3.2.4)

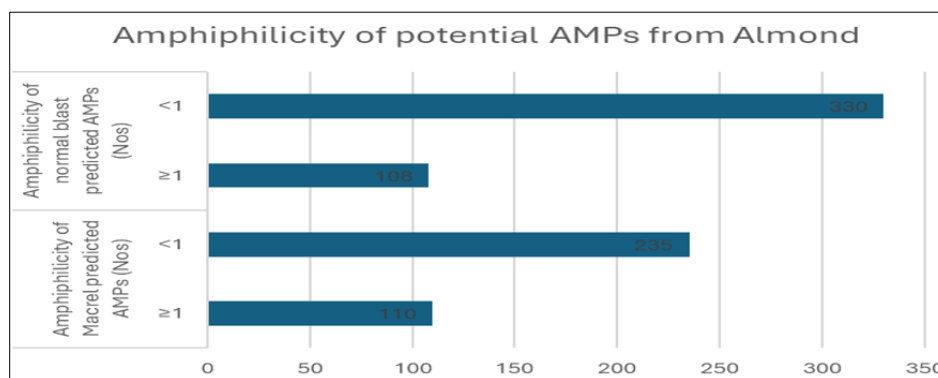


Fig 4: Amphiphilicity of AMPs retrieved from selected nut crops

For Almond, the majority of the predicted AMPs exhibited an amphiphilicity index of <1 , indicating that peptides with relatively low amphiphilic characteristics predominate. Under the BLAST prediction, 330 AMPs had an amphiphilicity index of <1 , whereas 108 AMPs showed an amphiphilicity index of ≥ 1 . Similarly, the Macrel prediction identified 235 AMPs with an amphiphilicity index of <1 and 110 AMPs with an amphiphilicity index of ≥ 1 . In both prediction methods, approximately 68-75% of the predicted AMPs belonged to the <1 amphiphilicity category, while only 25-32% exhibited an amphiphilicity index of ≥ 1 . Overall, the results indicate that the predicted AMP repertoire of almond is dominated by peptides with low amphiphilicity, whereas a smaller proportion of peptides possess higher amphiphilic properties that may contribute to enhanced antimicrobial activity.

3.2.5. Predicted AMP sequence length

The sequence length of the predicted AMPs from almond varied considerably, ranging from a minimum of 8 amino acids to a maximum of 139 amino acids. Apart from the minimum and maximum sequence lengths, the average sequence length provides a clearer understanding of the AMP population. In the case of Macrel predicted AMPs, the average sequence length was 20.25 amino acids, indicating that most of the predicted AMPs were short peptides. The maximum sequence length attained was 74 amino acids. While considering BLAST predicted AMPs, the average sequence length was 29.60 amino acids, with the maximum sequence length reaching 139 amino acids. These results indicate that the BLAST prediction retrieved comparatively longer AMPs with a broader sequence length distribution than the Macrel predicted AMPs, whereas Macrel predominantly identified shorter peptide sequences. (Figure 3.2.5)

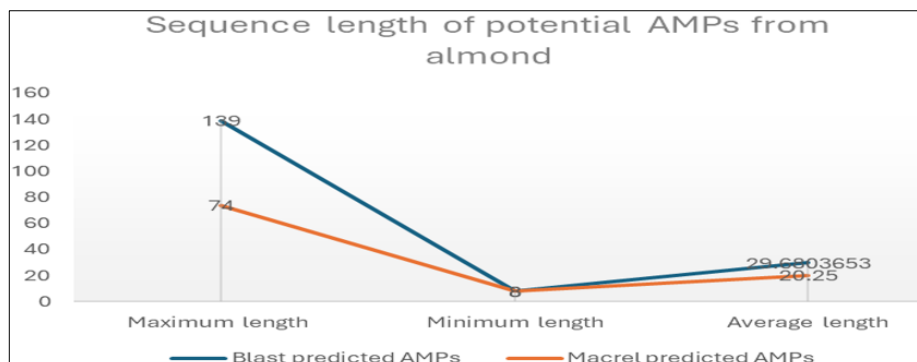


Fig 5: Sequence length of AMPs retrieved from selected nut crops

4. Conclusion

The total number of BLAST predicted potential AMPs from almond was 438. And the total number of Macrel predicted potential AMPs from almond was 345.

From the above research findings, it was concluded that the diversity of physicochemical properties among the predicted potential AMPs from almond would provide a broad spectrum of diversified AMPs that can be utilized for a wide range of applications. The predicted AMPs from almond were characterized by:

- **Moderate to high net positive charge**, which is highly desirable for antimicrobial activity.
- **Appropriate hydrophobicity**, which is important for interaction with and specificity towards target pathogens.
- **Favourable amphiphilicity**, which contributes to membrane interaction, α -helical structure formation, and antimicrobial efficacy.

Thus, almond can be considered a promising source of antimicrobial peptides with potential commercial applications in pharmaceutical, agricultural, food preservation, and biotechnology sectors.

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