

Prediction and Selection of anti-*Propionibacterium acnes* peptide from *Cannabis sativa* Seed peptidome with bioinformatics

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Introduction

Acne is a disease that is generally found in teenagers. It was reported that 75.5% of students get acne (Tayel et al., 2020). *Propionibacterium acnes* was a significant cause of acne. The inhibition of *P. acnes* is mainly executed by using antibiotics, but if it is not used properly, it has a side effect that bacteria will create a drug-resistant ability within the genes. Using natural substances is a choice of acne treatment. *Cannabis sativa* seed contends Albumin and Edestin (Aluko, 2017) which are capable of being antimicrobial substances. But the examination of peptides from *Cannabis sativa* seeds may require a large number of resources. Therefore, the researcher chooses bioinformatics techniques for the selection and prediction of the antibacterial efficacy of *Cannabis sativa* seed peptides. As a benefit of this study, using an antibacterial peptide from *Cannabis sativa* seeds to inhibit *P. acnes* will be a possible choice in the treatment of acne to avoid the creation of drug resistance in bacteria.

Result

- Albumin and Edestin from *Cannabis sativa* seeds contain 90 peptides after simulating the cut of the peptide bonds from the protein sequence by Trypsin, and 9 peptides had more than 60% antibacterial probability from a prediction by the iAMPpred server. The sequences, and their properties are shown in Table 1, all of which also had non-toxicity to normal human cells.
- According to the peptide mode of action prediction servers, 3 antibacterial peptides were cell-penetrating, and 1 antibacterial peptide was an antibiofilm peptide. Only a certain antibacterial peptide with the amino acid sequence 'FHLAGNPHR' is effective on both biofilm inhibition and cell penetration, resulting in the most effective peptide.

No.	Sequences	Hydrophobicity	Charge	Structure
1	TCQFHSR	-0.38	1.5	
2	AQVNQLAGK	-0.15	1	
3	ASAQGFEWIAVK	0.04	0	
4	NIPSMCGMQPR	-0.19	1	
5	FHLAGNPHR	-0.19	2	
6	MMESAR	-0.31	0	
7	QEQQEMR	-0.68	-2	
8	WQSQCQFQR	-0.42	1	
9	QQNQCQIDR	-0.57	0	

Table 1 Sequences of Antibacterial Peptides and their Properties

Methodology

The procedure for antibacterial prediction and selection of peptides using various programs are shown in this flowchart.

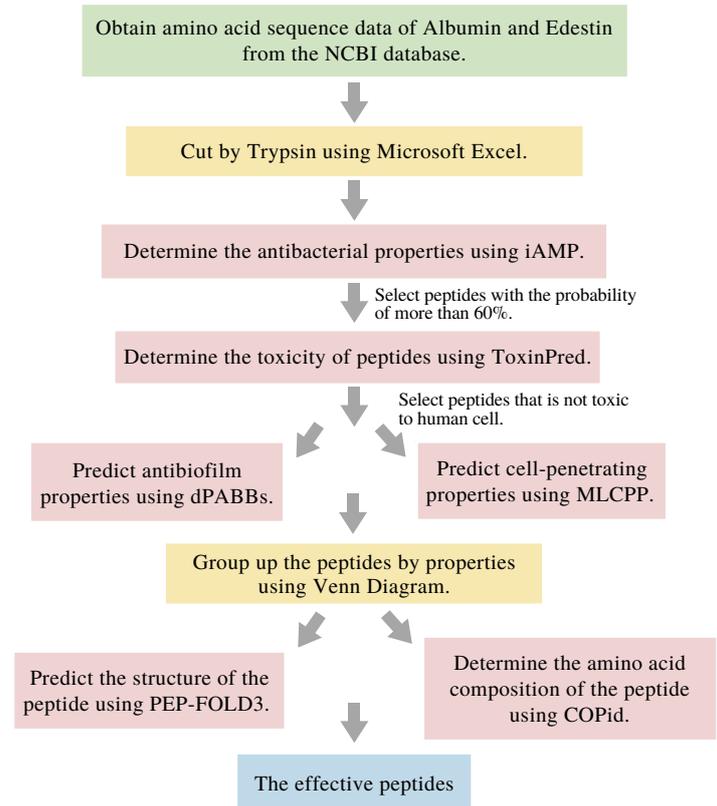


Fig 1 Flowchart of methodology

Conclusion

From this research, the antibacterial peptides are likely to be 6-12 amino acids in length. And the most found structure is the random coiled and single helix with positive charges and the property of being hydrophilic. It is discovered that the most efficient peptide from *Cannabis sativa* seeds is FHLAGNPH and is expected to be further researched with in vitro methods to determine the effects against *P. acnes* to be synthesized as acne treatment products.

References

- Aluko, R. (2017). Hemp seed (*Cannabis sativa* L.) proteins: composition, structure, enzymatic modification, and functional or bioactive properties. *Sustainable ProteinSources*, 121–132.
- Tayel, K., Attia, M., Agamia, N., & Fadl, N. (2020). Acne vulgaris: prevalence, severity, and impact on quality of life and self-esteem among Egyptian adolescents. *Journal of the Egyptian Public Health Association*, 95(1), 1-7.