UNIVERSITI TEKNOLOGI MARA

POTENTIAL MECHANISM OF ACTION OF ANTIMICROBIAL PEPTIDES THROUGH COMPUTER-ASSISTED METHOD

JAMALIAH BINTI MD YUSOF

BACHELOR OF ENGINEERING (HONS.)
CHEMICAL AND BIOPROCESS

July 2018

ABSTRACT

For many centuries, the first antibiotics that have been found as natural compounds used by one class of microorganisms which is fungi. It is the main medical weapon that is used to eliminate bacterial attack or competition. Since they are very specific to target molecular cells, it commonly inhibit enzymes that are unique and essential for bacteria. At the same time, this specificity characteristics of the antibiotics made it easier for bacteria to develop resistance. It leads for the bacteria to share it with other bacterial strains and even to develop multiple resistance against several conventional antibiotics. This research have been carried out to study the mechanism of actions of antimicrobial peptides using bioinformatics technique. The aim of this research is to find out the amino acid sequences for antimicrobial peptides in all groups of organisms, to determine and visualize the 3-dimensional structure of the secondary structure of the antimicrobial peptide, to classify and compare the antimicrobial peptides based on the secondary structure: α-helical, β-strand, α+β structure and non-α+β structure and to determine the effect of net charge of the antimicrobial peptides on their mechanism of action. The mechanism of action of antimicrobial peptides has studied by bioinformatics techniques, using any related databases such as APD, PDB, UniProt and DBAASP. The results shows that most of antimicrobial peptides are α-helical and α+β secondary structure. The peptides are also cationic which makes them interact with negative-charges of bacterial cell membranes.

ACKNOWLEDGEMENT

Firstly, I wish to thank God for giving me the opportunity to embark on my degree and for completing this long and challenging journey successfully. My gratitude and thanks go to my supervisor Dr Tan Huey Ling. Without her assistance and dedicated involvement in every step throughout the process, this paper would have never been accomplished. I would like to thank you very much for your support and understanding over these past few years.

I take this opportunity to express gratitude to all of the Department faculty members for their help and support. Finally, this thesis is dedicated to the loving memory of my very dear late father and mother for the vision and determination to educate me. This piece of victory is dedicated to both of you. Alhamdulillah.

TABLE OF CONTENTS

CHAPTER 1

INTRODUCTION

1..1 Research Background

Bioinformatics has been defined in many different ways. Basically, bioinformatics has been commonly considered as a combination of both biological and computer sciences, along with other contributing disciplines. The words of 'bio' from bio-informatics is referring to the biology in the terms of molecules (in the sense of physical chemistry). Whereas, the 'informatics' is applying to the "informatics techniques" in order to understand and organize the information associated with these molecules (Greenbaum, Luscombe, & Gerstein, 2001). It is derived from disciplines such as applied maths, computer science and statistics. In short, bioinformatics is a management information system for molecular biology for processing any biologically-derived information, whether DNA sequences or breast X-rays (Arunkumar, et al., 2008).

Generally, bioinformatics is widely used in finding information for research that is related in biology field. It involves the integration of computers, software tools and databases in an effort to address any biological questions that is popped out. This bioinformatics approaches are often used for major initiatives that usually generate large data sets.

In this research, bioinformatics approaches is used that involves biological information for anti-microbial peptide. Peptide is a short protein that is approximately contains of 12-50 amino acids long (Ping Wang, et al., 2011). In other words, antimicrobial peptide is the protein that may be a part of an evolutionarily ancient system for immune defense that produced as a first line of defense by all multicellular organisms that have broad activity to directly kill bacteria, yeasts, fungi, viruses and even cancer cells (Zhang & Gallo, 2016). These antimicrobial peptides can be found in various different organisms including mammalians, amphibians, birds, insects, as well as plants.

In this new era, the bacterial resistance and emerging infectious diseases has become potential threats to human. This scenario has leads to ribosomally synthesized antimicrobial peptides to become a promising focus area in antibiotic research. This antimicrobial peptides can be classified as either non-ribosomally synthesized peptides