7th International Conference on

PHARMACEUTICS & ADVANCED DRUG DELIVERY SYSTEMS

March 27-28, 2023 | London, UK

Received date: 15-07-2022 | Accepted date: 17-07-2022 | Published date: 03-04-2023

Identification of marine fish peptides as a treatment option against the multidrug resistant Acinetobacter baumannii

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Acinetobacter baumannii is one of the most dangerous multidrug resistant (MDR) pathogens with an immense ability to acquire or upregulate antibiotic drug resistance determinants. For MDR pathogens, antimicrobial peptides (AMPs) may be the last hope that they do not develop resistance easily. Fish peptides are essential to the survival of the fish as well as having critical functions in human physiology and pathophysiology. The identification of viable peptides from marine fish is a significant objective in drug research. It is necessary to study the interactions of specific peptides with the target protein to identify targeted therapeutics for antibiotic-resistant bacteria. The shortchain dehydrogenase/reductase (SDR) enzyme can play a role in the type II fatty acid synthesis (FASII) pathway, which is vital for a Gram-negative bacterium and inhibition of the protein can block the replication activity of the bacteria. Therefore, we intend to apply an in-silico technique to examine the new peptides as therapeutic candidates against A. baumannii by targeting the SDR protein. Initially, 34 peptides have been retrieved from marine fishes and docked against the SDR protein. Three peptides, namely Histone H2A (DRAMP18698), Piscidin-1 (DRAMP02330), and HKPLP (AP02038), have been selected based on their docking scores of -258.4, -250.4, and -250.1 kcal/mol, respectively. Subsequently, the peptides were evaluated based on allergenicity and toxicity properties. The allergenicity and toxicity analyses revealed the efficacy and non-toxic properties of the peptides. Computational analysis revealed the virtuous value of the selected three peptides against the targeted protein that can be effective and promising antimicrobial resistance (AMR) drug candidates against the pathogen in a significant and worthwhile manner. Although *in vitro* and *in vivo* studies are required for further evaluation of the peptide against the targeted protein. Recent

Recent Publications

1. Application of Mathematical Modeling and Computational Tools in the Modern Drug Design and Development Process (2022). Molecules, 27(13):4169.

2. Epigenetics and Probiotics Application toward the Modulation of Fish Reproductive Performance (2022). Fishes, 7(4):189.

3. Exploring the therapeutic potential of marine-derived bioactive compounds efficiency against tilapia lake virus by targeting CRM1 receptor: A drug design approach (2022). Marine drugs (under review)

Biography

Afsar Ahmed Sumon is a PhD fellow in the marine biology department of the Faculty of Marine Sciences at King Abdul-Aziz University (KAU), Saudi Arabia. His scientific interests include marine fish and shellfish biology, marine natural products, drug design, molecular biology, microbiology, and fish Immunology. His current Ph.D. study focuses on the isolation of novel natural products from marine organisms and the development of anti-infective drugs for both aquatic and human infectious diseases. Additionally, he has published peer reviewed articles and is engaged in several collaborative research activities.

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