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In-silico antibacterial activity of active phytocompounds from the ethanolic leaves extract of *Eichhornia crassipes* (Mart) Solms. against selected target pathogen *Pseudomonas fluorescens*

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Abstract
The computational drug designing is the principal streamline to evaluate the affinity of small molecules toward specific targets that unveils a potential to disparage the consumption of time in industries with the combination of computational, biological and chemical knowledge. *In-silico* approaches in drug development play a key role to reconnoitre molecular aspects of targeting specific proteins through various tools and softwares, and analyzing the bioactivities and inhibitory effects across mechanisms underlying for treatment of several chronic diseases. The main aim of the study is to identify the phytocompounds with antibacterial properties from the ethanolic leaves extract of *Eichhornia crassipes* and also to find the inhibitors of AprX enzyme through molecular docking. GC-MS was performed for the ethanolic leaves extract of *Eichhornia crassipes*. Various phytochemical compounds were identified through GCMS. The identified compounds are 17-Pentatriacontene, Dibutyl phthalate, Octasiloxane, Stigmasterol and 1-Monolinoleoylglycerol trimethylsilyl ether. These compounds were *in silico* screened against AprX enzyme as a target protein for the antibacterial activity through docking studies. The binding energy is evaluated through docking studies of the ligand with the target protein. The interactions of the phytocompound with the amino acid residues of the AprX enzyme showed high affinity with in the active site binding pocket. These Phytochemical compounds have a high docking score and glide energy. Results of our study suggested that these phytochemical compounds can be considered as strong inhibitors for AprX enzyme and possess potential medicinal values with anti-microbial properties.

Keywords: *Eichhornia crassipes*, GC-MS, AprX enzyme, molecular docking

Introduction
Molecular docking plays an important role in the rational design of drugs. In the field of molecular modeling, docking is a method which predicts the preferred orientation of one molecule to a second when bound to each other to form a stable complex. Molecular docking can be defined as an optimization problem, which would describe the "best-fit" orientation of a ligand that binds to a particular protein of interest [1]. In recent years the use of plants in the management and treatment of diseases has gained considerable importance. Plants and fruits are considered one of the main sources of biologically active compounds an estimate of the world health organization (WHO) states that around 85-90% of the world's population consumes traditional herbal medicines [2]. Plants are rich source of the traditional medicine in several countries and produce a diverse array of bioactive molecules, the source of potential and powerful drugs. The medicinal plants are useful for healing as well as for curing of human diseases because of the presence of phytochemical constituents. Phytochemicals are naturally occurring in the medicinal plants, leaves, vegetables and roots that have defense mechanism and protect from various diseases [3].

Human being identified bioactive compounds and chemicals to cure infectious diseases before the discover of microbes. These attempts made them to use organic compounds from plants and their extracts, many of these herbal remedies proved successful [4]. Many works have been done and being conducted with a goal to know the different antimicrobial and phytochemical properties of plants, and using them against microbial infections as an alternative to conventional synthetic drugs. Like drop in an ocean still medicinal properties of many plants are yet to be investigated for therapeutic uses and there is an urgent need to identify unique bioactive compound that act against resistant pathogens [5].

Pseudomonas fluorescens is an aquaculture pathogen that can infect many fish species, including Indian major carps, black carp and common carp. Infection of fish by *P. fluorescens* leads to the development of the so-called Red Skin Disease, which can occur at any time in a year and especially in fish injured due to improper handling and transportation.

When the normal environmental conditions change, the disease often leads to mortality, thus causing heavy economic losses [6]. *Pseudomonas* considers one of the most pathogenic bacteria affecting fish farms especially the Indian major carps. *Eichhornia crassipes* is an important medicinal plant belongs to family Pontederiaceae commonly name as water hyacinth. The plants have been traditionally used to heal wounds, antioxidant activity, antitumor activity, antimicrobial activity and Larvicidal activity. The plant is also considered to be a adsorbate efficiently removes a vast range of pollutants, from suspended materials, nutrients and organic matter to heavy metals [7]. Hence the present study focused on *In- silico* antibacterial activity of active phytocompounds from the ethanolic leaves extract of *Eichhornia crassipes* (Mart) Solms. against selected target pathogen *Pseudomonas fluorescens.*

Materials and Methods

Collection of plant materials

The leaves of *Eichhornia crassipes* were collected from Saliyamangalam area of than javur region and authenticated by professionals in the Department of Botany, St. Joseph's College, Tiruchirappalli, Tamil Nadu, India. The herbarium number of the plant is GD001.

Processing of plant material

After authentication, the defoliated leaves was washed with running tap water and later dried at room temperature. Thus obtained leaves dried and powdered using a electric blender. The powder obtained was sieved and stored in a air tight container at room temperature for further analysis [8].

Preparation of leaves extract

The dried and powdered leaves of *E. crassipes* (500 g) were extracted using Soxhlet extractor by evaporating with 75% ethanol. The Soxhlet extraction was carried out for 3 days, and the extract was collected. The excess ethanol was evaporated using vacuum evaporator. The sample is evaporated to dryness under boiling water bath at 55 °C.

GC-MS analysis

Clarus 500 Perkin-Elmer (Auto System XL) was used to carry out GC-MS analysis.

Structure elucidation

The 2D structures of phytochemical compounds were obtained from Chemspider database (http:// www.chemspider.com/). Then 2D structures are converted to 3D structures using swiss pdb viewer (http:// www.spdbv.vital-it.ch/). They act as a ligand. Sequence and 3-D structure of particular protein are provided by the UniProt KB/Swiss-Prot database. AprX is retrieved from UniProt KB / Swiss-Prot database (http:// www.uniprot.org/). Hex docking program (hex.loria.fr/ dist50/) is used to dock AprX with these bioactive compounds.

Docking studies

The Protein-Ligand interaction plays a significant role in structural based drug designing. In the present study, AprX is selected as receptor and the bioactive compounds from leaves of *E.crassipes* are selected as ligands. The receptor was docked against ligands and the energy values were obtained using the docking software.

Results

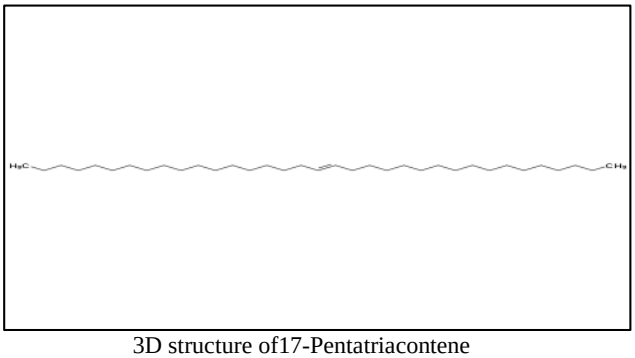
Molecular docking

In order to find out the best effective drug, Hex docking was carried out. In this docking Dibutyl phthalate, Octasiloxane, 1-Monolinoleoylglycerol trimethylsilyl ether, 17-Pentatriacontene and Stigmasterol compounds were taken into consideration for docking as ligand molecules. These ligands have been used to target AprX which bound to the receptor to inhibit its function. The nature of the complex between the drug and the receptor molecule was identified via docking and the inhibition nature of the ligands and their binding affinities were calculated using free energy simulations.

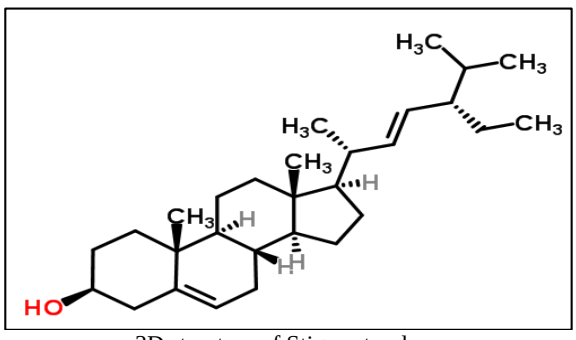
Docking results between AprX receptor and phytochemical drugs were tabulated (Table. 1). *E. crassipes* produced bioactive compound 17-Pentatriacontene showed a maximum e-value (-267.35) followed by Stigmasterol (-252.65), Dibutyl phthalate (-188.27), Octasiloxane (-195.37) and 1-Monolinoleoylglycerol trimethylsilyl ether (-77.41).

Table 1: Docking of ligands with AprX

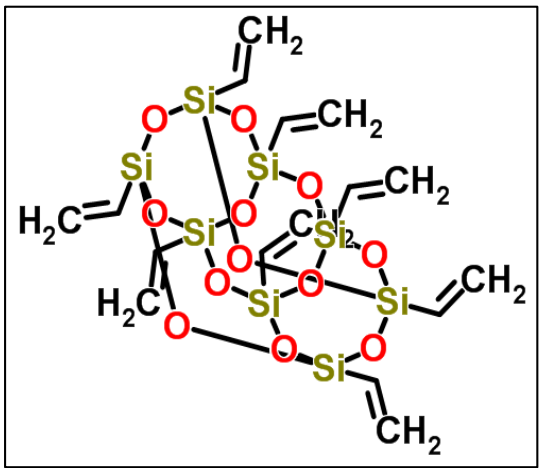
S. No	Name of Bioactive Compounds	e-values
	Eichornia crassipes	
1	17-Pentatriacontene	-267.35
2	Stigmasterol	-252.65-
3	Octasiloxane	195.37-
4	Dibutyl phthalate	-188.27
5	1-Monolinoleoylglycerol trimethylsilylethel	-77.41



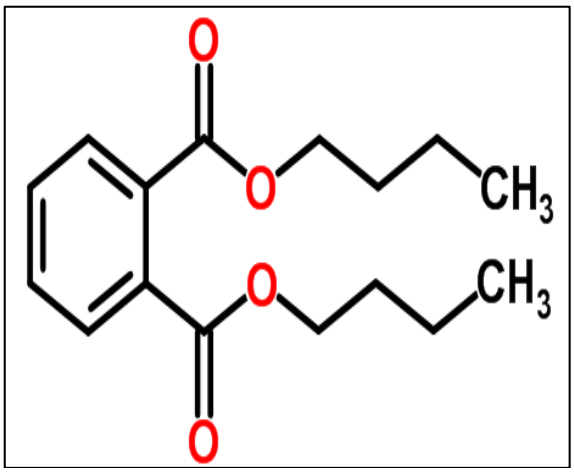
3D structure of17-Pentatriacontene



3D structure of Stigmasterol



3D structure of Octasiloxane



3D structure of Dibutyl phthalate

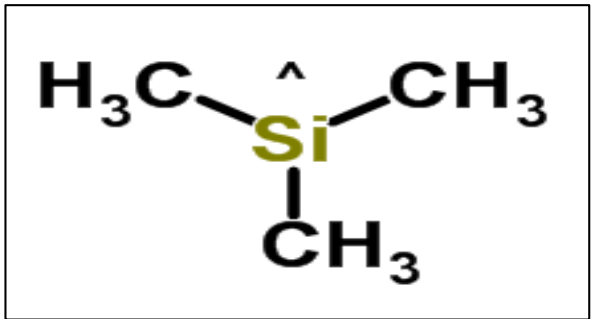


Fig 1: 3D structure of1-Monolinoleoylglycerol trimethylsilyl ether

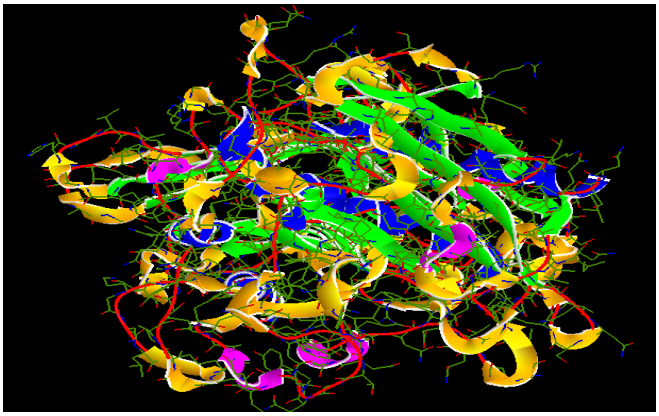


Fig 2: 3D structure of AprX

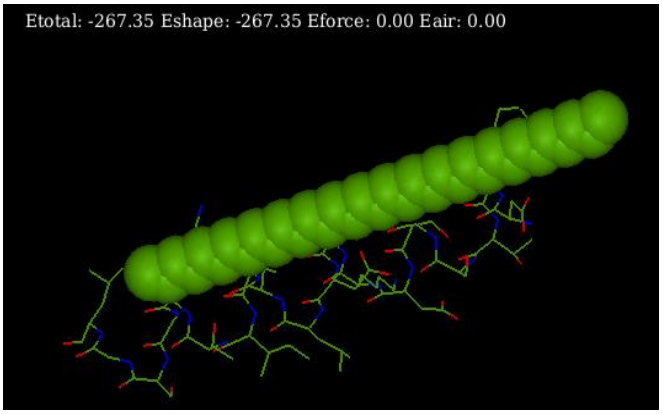


Fig 3: Docking of 17-Pentatriacontene with AprX (*E. crassipes*)

Discussion

The occurrence of antibiotic resistant bacteria associated with fish diseases is a worldwide problem in aquaculture, which has received considerable attention in the last years and this issue continues to increase due to the absence of a more effective and safer use of antibiotics [9]. Resistance to antibiotics and chemical treatments subject to increasing restriction because of their potential harmful impact on the environment and eradication of an infected fish group because by the time disease is diagnosed, most of the fish are infected. The occurrence of bacterial strains associated with fish diseases that show resistance to commonly used antibiotics is a worldwide problem in aquaculture. This phenomenon has received considerable attention in the recent years and its importance continues to increase due to the absence of a methodology for more effective and safer use of antibiotics [10].

Chemotherapy has progressed internationally for treating the most diversified infectious disease of fish [11]. However, there are problems associated with the use of such chemicals. It was the demand of the time to look for alternative means of commercial synthetic drugs. Medicinal plants are vital source of drugs from the ancient time holding the scenario of the Indian system of medicine [12]. The medicinal plants are rich sources of bioactive compounds and thus serve as important raw materials for drug production. Antibiotics used in medicines have been tried experimentally to treat bacterial infections of fish. Problems including solubility, palatability, toxicity, cost, delivery and governmental restrictions have limited the available antibiotics to a select few, especially in ornamental fish culture [13]. Increasing failures in antibiotic resistance exhibited by microbial pathogens has led to screening of several medicinal plants for their potential antimicrobial activity [14].

Plant synthesizes natural products as its chemical weapon that arrests the growth of environmental microbes and some plants inhibit the growth of potential human pathogens too [15]. The present study showed that the phytochemicals such as Dibutyl phthalate, Octasiloxane, 1-Monolinoleoylglycerol trimethylsilylethe, 17-Pentatriacontene and Stigmasterol compounds possess potential medicinal values with antibacterial properties. These phytocompounds could be the potential inhibitory source against microbial protein. The phytocompounds of *E. crassipes* showed a better docking simulation and interaction analysis. No studies reported *in silico* antibacterial activity of *E. crassipes* Our *in silico* docking studies strongly recommend *E. crassipes* was found to be more effective against aquaculture microbes.

Conclusion

The molecular docking of AprX enzyme with the phytocompounds of *E. crassipes* revealed that these identified

phytocompounds would be used for antibacterial agent. The results obtained from this study were useful for understanding the inhibitory mode of *E. crassipes* phytochemicals as well as accurately predicting the activities of phytochemical inhibitors on the basis of docking scores and Glide energy. The results of our study not only give a base for further research but also useful for drug development. Hence our study should therefore play a guiding role in the experimental design and development of antibacterial drug in the present and future to treat aquaculture pathogens and many ailments. Also our study provides us hope to overcome failures of drug resistance profiles. This study also means a natural alternative to antibiotics, which is an exhilarating and potentially extreme area of research.

Conflict of interest statement

We declare that we have no conflict of interest.

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