IJEP 39 (9) : 787-792 (2019)

Physico-Chemical, Microbial, Heavy Metals And Pharmaceutical Analysis Of Water Samples From Bengaluru Lakes

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In spite of Bengaluru not being blessed with any river source for its water needs, it has sustained itself so far on the bedrock of a thriving man-made lake system. This study aims to evaluate the quality of potable drinking water from 12 lakes in and around Bengaluru. The physical properties of samples were assessed using standard methods for the examination of water and wastewater by the American Water Work Association. The heavy metals concentration and evaluation of antibiotic resistance were carried out using standard methods. Total hardness in Hennur lake (791 mg/L) has exceeded the recommended range as specified by the Bureau of Indian Standards (BIS). The ammonium (662.2 mg/L) and phosphate concentration (169.4 mg/L) were high in Vartur lake and chloride concentration (366.886 mg/L) in Hennur lake has exceeded the permissible range. Microbial analysis showed the presence of seven dominant bacterial strains. Toxicity screening for heavy metals showed all the lakes were within the recommended BIS range for cadmium (<0.01) but has exceeded the permissible limit for lead (<0.05) and nickel (<0.02). Antibiotic profiling of Hennur and Rachennahalli lake samples clearly highlighted the presence of diclofenac (1.0 μg/L and 0.38 μg/L) in both the samples, respectively. Proper water management practices and constant monitoring of water bodies should take place to sustain the ecosystem and aquatic life in the lake.

KEYWORDS

Bengaluru lakes, Heavy metal poisoning, Water quality, Urbanization, Pollution

1. INTRODUCTION

In the absence of any river close by, lakes in Bengaluru have been a major source of water for the expanding city for many years. The creation of these lakes can be traced back to as early as the 16th century with the aim of enabling the city with an ample amount of drinking water, irrigation, fishing, etc. It was evident that there were 262 water bodies until 1960 in Bangalore and it has declined to about 81 of which 34 are recognized as live lakes as of 2016 [1]. Not only the number of lakes in the city has been steadily declining, the quality of water and the flora, fauna have also suffered irreparable damage [2]. The rapidly growing urban populations, coupled with increasing demand for freshwater resources and the extensive growth of industrial activities have given rise to environmental problems [3].

Water is the most essential component of an ecosystem as it helps to sustain life on earth. Especially lakes in Bangalore contribute to the chain of hydrological connection as there is no perennial river in Bangalore. These lakes help to recharge groundwater and to trap rainwater. However, due to various human intervention, like entry of domestic sewage, industrial wastes, untreated effluents from industry and homes near and around lakes keeps on pouring in, this coupled with illegal large scale waste disposal disturbs not only the aquatic ecosystem but also creates hazardous environmental situation, like lake foaming, uncontrollable growth of weeds tantamounting complete breakdown of eco-balance in the city [4]. Apart from this, the consumption of aquatic animals from contaminated water bodies shown to cause reproductive disorders and impaired health in European and North American population [5]. The cause for these incidents was identified as the presence of organochlorines and organic heavy metals which had been assimilated by the animals via their skin and respiratory systems or through food chains with associated concentration. Aquatic organisms require a healthy environment to live, adequate nutrients for their growth and optimal physico-chemical characteristics for maximum productivity [6,7]. Therefore, the present study was conceived with the aim of evaluating the level of physico-chemical characteristics, microbial contamination, heavy metal and detection of antibiotic residues in 12 lakes in and around Bengaluru. Antibiotics profiling by liquid chromatography-mass spectrometry (LC-MS) was also performed to determine the presence of antibiotic residues, if any.

Assembly of Ni-Based Metal-Organic Framework through Interconnected Adamantane like Cages

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Abstract

Metal-Organic Frameworks (MOFs) are promising class of crystalline materials that have attracted great research interest due to their extraordinary properties such as intriguing architecture and topology, unrivalled degree of tunability and exceptionally large surface area. A Nickel based micro scale Metal Organic Framework (MOF) [Ni(BPE)(BPDC)].4DMF where BPE is 1,2-Di(4-pyridyl) ethylene and BPDC is Biphenyl-4,4'-dicarboxylic acid, was synthesized through solvothermal synthesis method.

Structural characterization using X-ray diffraction techniques revealed the crystal to follow "dia" topology with repeating adamantane molecule like units. Another interesting feature observed in the structure was the four-fold interpenetration leading to a compact cage like assembly. The structure was made even more rigid by the presence of solvent molecules in the cage and it imparts stability to the structure.

Keywords: Metal Organic Framework, Nickel, Dia topology, 4-fold interpenetration.

Introduction

Metal-Organic Frameworks (MOFs) or Porous Coordination Polymers (PCPs) represent the class of micro/mesoporous crystalline materials which consist of metal ions or metal clusters linked to multifunctional organic ligands and result in large number of crystals with topologically diverse open network type structures through self-assembly at molecular level.[1-4] The organic linkers are generally multidentate ligands such as carboxylates, azoles and nitriles. They offer enormous variety of chemical composition allowing both their structure and functionality to be tuned by the choice of building blocks.[5]

MOFs exhibit extraordinary properties like fascinating topology, large surface area and tunable porosity. Due to their intriguing properties, they have been widely applied for different applications such as gas storage, catalysis, sensors, separation, magnetism, super-capacitors and drug-delivery.[6-8] Therefore these materials are considered as the best platform where the properties can be controlled for targeted applications.

Among them, especially the nickel based MOFs are important as they have plenty of applications by exploiting the property of Ni^{2+} ion. The square-planar geometry of Ni^{2+} might make the metal ion an ideal candidate for the formation of 2D structures.[9] A work on the synthesis of layered two-dimensional (2D) Ni-MOF and its application as high performance cathode catalyst for rechargeable Li-O2 batteries has been reported.[7] Also the redox behaviour of the metal ions in MOF can provide a transport pathway for the electrons.[8] Therefore, the synthesis of Ni-based MOF opens up a myriad of possibilities to work upon.

Material and Methods

Ligands employed in the synthesis also play a vital role in the structure determination and functionality of MOFs. Highly porous crystalline frameworks capable of undergoing structural reorganization under the application of external stimuli such as light, heat, changes in pH can extend the practical applications to include sensors.[10-12] Light sensitive MOFs with permanent porosities have been reported where the photosensitivity is based exclusively upon the cis-trans isomerization of ligands.[10] Hence, understanding the influential factors of the coordinated structures is very important as it regulates and controls the characteristics of MOFs.

We have synthesised a nickel based three dimensional (3D) MOF [Ni(BPE)(BPDC)].4DMF using 1,2-Di(4-pyridyl)ethylene and Biphenyl-4,4'-dicarboxylic acid as the organic ligands.

Synthesis of [Ni(BPE)(BPDC)].4DMF: 0.5 mmol of $Ni(NO_3)_2$, 0.75 mmol of 1,2-Di(4-pyridyl)ethylene and 0.75 mmol of Biphenyl-4-4'-dicarboxylic acid were dissolved in 10 mL dimethylformamide (DMF) as solvent in a Teflon lined autoclave. The mixture was then sonicated for 5 minutes and placed in oven at 100 ^{0}C for 72 hrs. Green colour crystals were formed. The crystals were then washed with DMF three times and used as such for further characterizations. The synthesis was done by varying the experimental conditions like temperature, solvent, and metal to ligand mol ratio (Table 1). We could obtain only the same structure for all conditions and it shows the stability of the structure formed.

Results and Discussion

The compound structure was analysed using single crystal X-ray diffraction (SCXRD) method. The compound was crystallised in monoclinic crystal system with a space group $P21/n$. The metal is found to be six coordinated with distorted octahedral geometry (Figure 1a). The metal is coordinated to both the ligand molecules through oxygen

Chemistry - A European Journal

10.1002/chem.202100610

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REVIEW

Conductive Metal-Organic Frameworks: Electronic Structure and Electrochemical Applications

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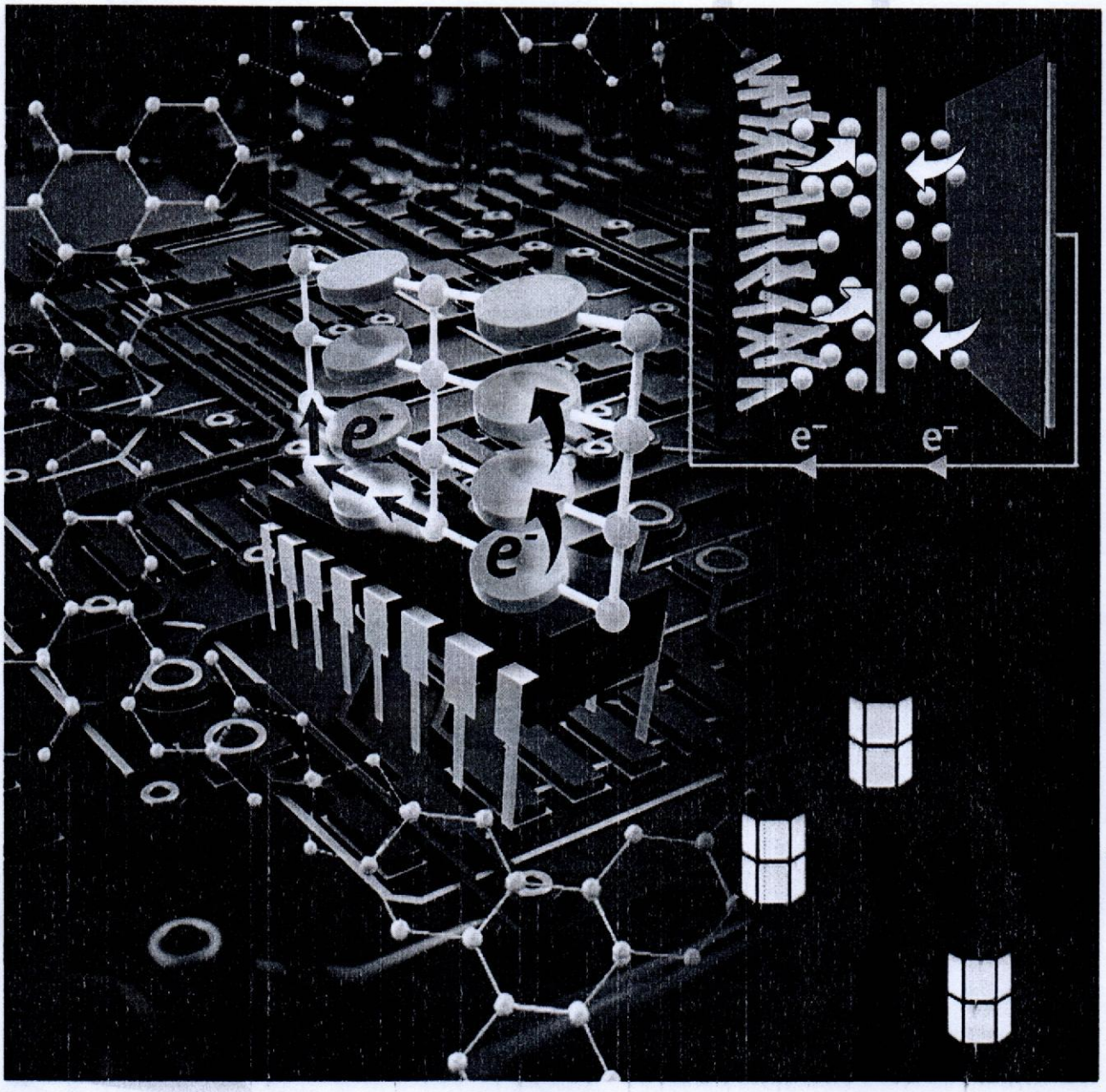

10.1002/chem.202100610

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Abstract: Smarter and minimization of devices are consistently substantial to shape the energy landscape. Significant amounts of endeavours have come forward as promising steps to surmount this formidable challenge. It is undeniable that material scientists were contemplating smarter material beyond purely inorganic or organic materials. To our delight, metal-organic frameworks (MOFs), an inorganic-organic hybrid scaffold with unprecedented tunability and smart functionalities, have recently started their journey as an alternative. In this review, we focus on such propitious potential of MOFs that was untapped over a long time. We cover the synthetic strategies and (or) post-synthetic modifications towards the formation of conductive MOFs and their underlying concepts of charge transfer with structural aspects. We addressed theoretical calculations with the experimental outcomes and spectroelectrochemistry, which will trigger vigorous impetus about intrinsic electronic behaviour of the conductive frameworks. Finally, we discussed electrocatalysts and energy storage devices stemming from conductive MOFs to meet energy demand in the near future.

1. Introduction

Metal-organic frameworks (MOFs) were not conductive hitherto. By birth, gas storage, gas separation, catalysis was the initial propensity to synthesis MOFs attributed to their high porosity and structural integrity. [1] In fact, MOFs are serving unequivocally at their best for the last two decades. Right now, electronics are shaping the world, which warrants miniaturization of the devices as well as low-cost production.[2] Thanks to metal-oxide-semiconductors to make the fabricated devices cost-effectively at initial days. However, some pitfalls were evinced due to scarcity of usable inorganic anions and limited tailoring of the structural design. An updated roadmap was suggested on the verge of this situation where material scientists were directed to move beyond the conventional inorganic materials.[2] Once again, MOFs have come up with a vast number of feasibilities to draw the next-level energy landscape in the electronics world in the near future.

MOFs are crystallized out with an infinite combination of metal and linker molecules to generate an extended integrated structure with permanent porosity. Beyond the utilization of inside porosity (which was the initial surge to synthesize MOFs), the scaffold of these tailor-made materials has evinced a fundamental role for electronic applications. The incorporation of redox-active moiety into the insulating frameworks engender an exquisite level of charge transfer of divergent extent in conductive MOFs. The charge transfer in the conductive MOFs can be achieved either by redox hopping of neighbouring redox-active centres or band transport of extended delocalized π-conjugated systems. From our synthetic perspective, conductive MOFs can be constructed either by the 'through-bond' approach attributed to high orbital overlap or 'through-space' approach stemming from non-covalent π-π interaction. Furthermore, guest incorporation and chemical engineering set out to devise another promising strategy toward facile charge-transport avenue in the framework materials. The potential of this class of materials has recently begun to be realized from its infancy state. Scientists have put much effort into this field from the last decades, albeit the significant advancement in the last five years.

This review highlights the recent progress of conductive MOFs from their dawn with the emphasis of design strategy, measurement technique, practical limitation, and vast of applicabilities centering around its electronic properties. Many reviews have covered the potential applications and fabrication of these materials towards functional nanodevices.[2-3] However, to our best knowledge, no reported review has covered the fundamental of charge transport in detail. We centre on the underlying concept of charge transfer in a solid material, the development of different models to interrogate the conductivity, and how these will be validated to mitigate the rudimentary electronic properties in the framework model. Moving from the physical point of view, we discuss the practical design strategies from our chemical intuition. Here, we account for the conductive framework materials having convincing permanent porosity. We also consider some related condense MOFs and conductive MOFs with no porosity after post-synthetic modification, when appropriate. Furthermore, we exemplify the solid-state spectroelectrochemistry to evaluate the extent of inter-valance charge transfer and spectroscopically detect the active species during transformation. Lastly, we conclude that how the electronic properties of conductive MOFs direct the potentiality towards electrochemical applications, like supercapacitors, batteries, oxygen reduction reactions (ORRs), oxygen evolution reactions (OERs), hydrogen evolution reaction (HERs), electrochemical sensors etc. with some reported knowledge. The review is aimed to delineate enormous literature describing the structure-property relation of conductive MOFs and the careful investigation of their electronic properties, which open up the prospect of future applications.

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2020

ADVANCES IN APPLIED CERAMICS
https://doi.org/10.1080/17436753.2020.1865094

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RESEARCH ARTICLE

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Zirconia: as a biocompatible biomaterial used in dental implants

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ABSTRACT

Zirconia is a bioinert ceramic biomaterial. Zirconia having composition of 97% Zirconia oxide and 3% Yttria oxide finds its vital application in the field of dental ceramics as an implant material for having good inert characteristics like minimum interaction with the adjacent tissues and exhibits good aesthetic property. This paper presents the *in-vitro* tests conducted to evaluation toxicity by cell culturing on zirconia biomaterial used in the dental implant by both direct contact and extraction method. In the present study, *in-vitro* assessment of tissue biocompatibility was conducted on L929 cell line (mouse fibroblast). *In-vitro* test, the toxicity of Zirconia specimen was done by computing percentage of viability in a cell-cultured medium. An MTT system was used to measure the active cell activities with mitochondrial dehydrogenases, which is an easy method which gives accurate and precision results. The results of biocompatibility *in-vitro* test by both Direct and Extraction methods confirmed that Zirconia exhibits the highest cell growth of 93.17% and resulted with zero-grade cytotoxicity. Zirconia having good aesthetic characteristics, i.e. colour of the implant matches with the tooth colour. Hence Zirconia is a candidate implant material than other metal implants.

ARTICLE HISTORY
Received 26 June 2020
Revised 1 December 2020
Accepted 14 December 2020

KEYWORDS
Zirconia; biomaterial; cytotoxicity; *In-vitro*; dental implant; MTT

Introduction

Zirconia or zirconium oxide is the oxide of zirconium metal, which occurs as a natural mineral found in igneous rocks such as granites and syenites. Zirconia is used as an important bi-inert material in the field of dental implantation. Zirconium material has good strength as similar to metals and matches with the colour of the tooth [1,2]. Pure Zirconia is extracted from baddeleyite by hydrothermal concentration process and it contains small amounts of silica and iron as impurities. Baddeleyite contains Zirconia levels ranging from 96.5% to 98.5%. At room temperature, zirconia is monoclinic structure. Zirconia naturally occurs in oxide form that undergoes purification process and synthesised to form cubic structure at high temperatures known as cubic crystal structure. Hence, it is also known as 'ceramic steel,' which poses good biomechanical properties as a single piece implant. Zirconia has been used in dentistry since 1989 and fist used as fixed dental prostheses in 1998 [3].

Phases of Zirconia

Zirconia usually occurs in three phases: (M) Monoclinic, (T) Tetragonal and (C) Cubic. Purest Zirconia at room temperature will be monoclinic and this stable phase exists up to 1170°C. Heating above, it will transform from (M) Monoclinic to (T) Tetragonal at 2370° C. Further, continued heating above 2370°C, it will transform to (C) Cubic as shown in Figure 1.

a. Unstabilised Zirconia

Unstabilized Zirconia is known as pure Zirconia. Pure Zirconia is monoclinic (m) at room temperature below 1170°C; hence, it has low thermal shock resistivity. Pure Zirconia as a bulk refractory is not feasible due to the large volume change of tetragonal to monoclinic phase transformation. The problem has been alleviated by the use of alloys of Zirconia with other oxides, preventing the transformation.

b. Partially stabilised Zirconia (PSZ)

A partially stabilised Zirconia will be formed when stabiliser concentration in the material is such that it consists of tetragonal, cubic (and monoclinic) mixture at a temperature between 1170°C and 2370°C. The higher temperature phases may thus be stabilised by the addition into a solid solution of specific cubic oxides.

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Ozone exposure promoting growth of *Oryzae sativa* (Rice) seedlings and inhibiting its pathogen *Xanthomonas oryzae*

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Abstract

A laboratory study was undertaken to find the effect of ozone on the growth of rice seeds (Oryzae sativa Linn.) and also on the viability of its pathogen Xanthomonas oryzae that causes bacterial blight disease. We used a commercial ozone generator to produce ozone and tested its effects in our laboratory studies. Our results showed that ozone at a concentration of 0.2 ppm inhibited the rice pathogen X. oryzae and promoted growth of rice seedlings. We observed that inhibition of bacterial cells by ozone is attributed to altered membrane permeability leading to leakage of cellular constituents and resulting in possible cell death.

Furthermore, reduced Oxygen Uptake Rate (OUR) was also observed in ozone-treated bacterial cells indicating the inhibition of respiratory enzymes. Interestingly, ozone exposure increased both the root length and shoot length in rice seedlings that appeared healthier compared to untreated seeds. Thus, our study demonstrated that ozone at low concentrations could be used in agriculture both as a growth enhancer and for pathogen control.

Keywords: Ozone, Rice seeds, *Oryzae sativa*, *Xanthomonas oryzae*, Cell permeability, Oxygen uptake rate.

Introduction

Atmospheric ozone is formed by the interaction of oxygen with electrical discharges and by the action of ultraviolet (UV) radiation. On the other hand, anthropogenic ozone occurs due to inefficient internal combustion of millions of automobiles which release pollutants in the form of hydrocarbons and nitrogen dioxide[1]. Ozone (O_3) is an allotrope of oxygen (O_2) and is a trioxygen molecule containing 3 oxygen atoms instead of 2. It is well known that O_3 if used under controlled conditions has a variety of industrial and medical applications such as water disinfection, air purification, bleaching of textile dyes, pollutant treatment, vegetable cleaning[2], cleaning of seafood[3] and as disinfectant[4].

In the industrial perspective, disinfectant action of ozone does not release any toxic by-products or potential health hazards when compared to the commonly used disinfectant chlorine which is used for sanitizing agricultural food commodities[5]. In addition, ozone can effectively kill bacteria through antimicrobial action and 4–5 times more effective than chlorine[6,7]. Unlike the chemicals that leave residual compounds with carcinogenic properties, ozone quickly decomposes into oxygen without any traces[8]. For this reason, ozone has received 'Generally Recognized as Safe (GRAS)' status in the United States and was also approved by US-FDA (2001) for use in the food industry.

In the medical perspective, inhibitory effect of ozone on bacteria and fungi has already been reported[9-11]. Several studies have been conducted to analyse the effect of ozone on human pathogenic bacteria such as *Escherichia coli*, *Pseudomonas fluorescens*, *Salmonella typhi* and *Klebsiella pneumoniae* and of them, *E. coli* showed high sensitivity[12].

The mode of action of ozone on inactivation of bacteria and fungi is more complex owing to the unsaturated lipids of cell membrane and cytoplasmic components of the microbes[13]. Majority of the microbial components are cell membrane constituents (proteins, respiratory enzymes and unsaturated fatty acid), cell envelopes (peptidoglycans), cytoplasm (enzymes, nucleic acids), spore coats and virus capsids (proteins and peptidoglycan)[14-16]. Restino et al[17] have also reported ozone as an abiotic control to arrest the growth of several food-related microorganisms. In addition, the rate of synthesis of various enzymes would be curtailed by ozone leading to a decline in metabolism and subsequent death of cells[2].

Further, ozone has a very high oxidation and reduction potential, it acts as an oxidant of constituent elements of cell walls of bacteria. Thus, continuous exposure of ozone causes destruction of large number of membrane barriers in bacteria causing cell lysis and eventually cell death. According to Kim et al[18] cellular leakage occurs due to the degradation of unsaturated lipids present in the membrane. Heavy damage in the nucleic acids also leads to cell death. Among nucleobases, rather than cytosine or uracil, thymine is found to be more ozone sensitive[14].

In the agriculture perspective, ozone is considered as both phytotoxic and growth stimulant. Ozone acts as a phytotoxic air pollutant and causes extensive damage to crops like soybean, cotton, peanut, sorghum, corn, winter wheat and also detrimental to forest trees at higher concentration[19]. Interestingly, it has been shown that at low concentrations and controlled environments, ozone acts as a fumigant[20]. In tomatoes, low ozone exposure for 2 min/day for 10 days showed a positive effect on the growth parameters of the

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Biosc.Biotech.Res.Comm. Vol 13 No (4) Oct-Nov-Dec 2020 Pp 2118-2124

Biological Control of Fusarium Wilt of *Cajanus cajan*

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ABSTRACT

Cajanus cajan (L.) Millsp. commonly called Pigeon Pea a leguminous plant grown extensively for food, feed, fodder, fuel also grown as an intercrop and in crop rotation to improve the fertility of the soil in sustainable organic farming. This plant gets infected by the pathogen *Fusarium udum* causing wilt disease which is one of the major constraints in the production and productivity of pigeon pea. This pathogen is reported throughout the world infecting *C. cajan*. The extensive use of chemical fungicides results in environmental pollution, the resistance of pathogens towards fungicides, hazardous to humans and animals. This necessitated the need to adopt eco-friendly and sustainable management of diseases, like using antagonistic fungi against the pathogen. In our present study, 15 different fungal isolates were isolated from different rhizosphere soil and used for Our present study involved the in vitro - dual culture assay as well as in vivo - greenhouse bioassay was performed to analyze the antifungal efficacy of antagonistic fungi against *F. udum*. The *in vitro* and *in vivo* investigations showed that *Cephalosporium acremonium, Lasiodiplodia pseudotheobromae, Penicillium frequentans* and *Epicoccum sorghinum* equally inhibited *F. udum* when compared to various *Trichoderma* spp. Also, under greenhouse conditions, the root length, shoot length, and the number of leaves of plants was found to be increased significantly ($p \leq 0.05$) in treatments with the talc-based biopesticide formulations of the antagonistic fungi. Hence these fungal isolates can also be used as a potential biocontrol agent for sustainable wilt diseases management caused by *Fusarium udum* and the extensive usage of chemical fungicides can be avoided to control the wilt disease of *Cajanus cajan*.

KEY WORDS: BIOCONTROL, EPICOCCUM SORGHINUM. FUSARIUM SP,, LASIODIPLODIA PSEUDOTHEOBROMAE, WILT DISEASE.

INTRODUCTION

Cajanus cajan is an important constituent in the category of pulses among all Indians due to the availability of 20-21% protein providing an energy-rich cereal diet. According to FAO statistics, this crop is cultivated in an area covering 4.6 million hectares globally and India accounted for about 73% of the global production in the year 2007. It is also an important crop of Karnataka contributing about 18% and 12% to total area and production respectively (GOI, Agricultural statistics, 2013). This protein-rich legume is prone to a multitude of diseases of which fungal diseases lead to a productivity loss of approximately 22 - 25 % each year amounting to a loss of up to Rs. 50,000 crores annually. Among the fungal diseases, *Fusarium* wilt disease caused by a soil-borne pathogen *Fusarium udum* (Fu) Butler is associated with extensive yield losses of pigeon pea in India. *Fusarium*

ARTICLE INFORMATION

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Received 24th Oct 2020 Accepted after revision 10th Dec 2020
Print ISSN: 0974-6455 Online ISSN: 2321-4007 CODEN: BBRCBA

Thomson Reuters ISI Web of Science Clarivate Analytics USA and Crossref Indexed Journal

Clarivate Analytics Crossref

NAAS Journal Score 2020 (4.31) SJIF: 2020 (7.728)

Online Contents Available at: http//www.bbrc.in/
DOI: http://dx.doi.org/10.21786/bbrc/13.4/73

Int. J. Pharm. Investigation, 2020;10(3):273-278

Original Article

Homology Modelling and *in silico* Characterization of Laccase from *Lentinula edodes*

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ABSTRACT

Introduction: Laccases are phenol oxidases which belong to the superfamily of multicopper oxidases. Laccases are found in almost all wood-rotting fungi. There is evidence that laccases can play an important role in lignin degradation, fruiting body formation, pigment formation during asexual development, competitor interactions and pathogenesis. Laccase from *Lentinula edodes* is used in variety of applications like to reduce toxicity, partial decolourization of effluent water and decolourization of chemically different dyes like Remazole brilliant blue R, bromophenol blue, methyl red and naphtol blue black. The objectives of this study include prediction of three-dimensional (3D) structure of laccase from *Lentinula edodes* using homology modelling, *in silico* characterization and analysis of laccase from this organism using computational methods. **Methods:** The sequence of laccase from *Lentinula edodes* was retrieved from UniProt database and sequence analysis was carried out using BLAST for the selection of template. The protein 3D structure was modelled using ModWeb server. The obtained 3D model of the laccase from *Lentinula edodes* was visualized and analyzed using RasMol. The quality of the 3D structure of protein was verified by its energy and stereochemical properties. The erred regions were remodelled by loop modelling using SWISS PDB viewer. Further, the *in sillico* characterization of the laccase from *Lentinula edodes* was computed. **Results:** The 3KW7 A of Trametes Sp AH28-2 is used as template for model building of laccase from *L. edodes*. The atom model obtained in PDB format showed unstable region in the model. These unstable regions were selected and remodelled by loop modelling. The remodelled structure was further evaluated by its stereochemical quality and energy. The quality of the remodelled structure was found to be improved. **Conclusion:** Evaluated 3D structure of laccase from *L. edodes* shows that predicted model was of good quality because maximum residues are present in favoured region which indicates that stereochemical quality of predicted 3D structure was reasonably good. It suggests that this model can be used to understand molecular interaction of this laccase with the other proteins.

Key words: Laccase, *Lentinula edodes*, Homology modelling, *In silico*, BLAST, MODWEB, Swiss PDB Viewer.

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DOI: 10.5330/ijpi.2020.3.50

INTRODUCTION

Laccases are copper containing oxidase enzymes found in many plants, fungi and micro-organisms. Laccases were also found in various basidiomycetous and ascomycetous fungi.[1] The first report of a bacterial laccase was from the Gram-negative soil bacterium *Azospirillum lipoferum*[2] and the enzyme was believed to be involved in melanisation.[3] These enzymes can be used for textile finishing or textile dyeing, teeth whitening and also it has industrial, environmental, diagnostic and synthetic uses.[4] Laccases can also be used in bioremediation.[5] *Lentinula edodes* (shiitake) is one of the world's second largest cultivated medicinal and edible mushrooms used as functional foods. It is used in the treatment of tumors, flu, heart diseases, high blood pressure, obesity, problems related to sexual dysfunction and ageing, diabetes, liver ailments, respiratory diseases, exhaustion and weakness.[6] *L. edodes* is considered to be one of the most valuable medicinal mushrooms.[7,8] The experimental methods to determine the protein 3D structure like X-ray crystallography, nuclear magnetic resonance spectroscopy are technically demanding, time consuming and may not keep with which new protein sequences are being discovered by genomics research. Although a large number of genes are being discovered, the number of protein structures being solved by experimental methods is limited.

Alternative strategies for structure prediction and modelling of proteins are computational methods. The major computational methods for predicting the structure of proteins are *ab initio* methods and homology modelling. Homology modelling remains the most accurate prediction method.[9] It helps to bridge the gap between the available sequences and structural information by providing reliable and accurate protein models. Homology modelling is a technique for predicting or generating detailed 3D structures of proteins based on coordinates of known homologues.

The main steps to create a Homology model are as follows: 1) Identification of structural homologues. 2) Selection of structural homologues used as templates for modeling. 3) Alignment of templates with the protein sequence to be modelled. 4) Model building. 5) Evaluation and refinement of the model.

The objectives of this present study are to predict the three-dimensional (3D) structure of laccase from *Lentinula edodes* using homology modelling, *in silico* characterization and analysis of laccase from this organism using computational methods.

MATERIALS AND METHODS

Retrieval of laccase sequence of *Lentinula edodes* from UniProt database

The sequence details of the laccase from *Lentinula edodes* was retrieved from UniProt database. The UniProt Knowledgebase (UniProtKB) is the central hub for the collection of functional information on proteins, with accurate, consistent and rich annotation.[10]

Isolation of Fungal Endophytes and Growth Hormones From Santalum *album* and its Effect of Plant Growth in Bacopa *monnieri* and Alternanthera *sessilis.*

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Abstract:

Soil is a media with macro nutrients and micro nutrients for the growth of micro-organisms which is supported by the root exudates of plants. The study of endophytes in the rhizosphere and rhizoplane of plant roots play an important role in understanding the symbiotic associations, growth and production of metabolites. The present study of fungal endophytes for growth promoters were isolated from medicinal plants of *Santalum album,* reported dominant fungal species *Chalaropsis*sp., *Phoma glomerata, Collectotrichum* sp. and *Fusarium solani.* The endophytic fungus*Fusarium solani* was reported to produce auxins, growth hormone.The study of growth promoters of *Fusarium solani* on *Alternanthera sessilis* and *Bacopa monnieri* showed a significant increase in plant growth. The fungal metabolites of *Fusarium solani* quantified *by* HPLCshowed aRetention Time of 3.03with corresponding area is 117 giving the concentration of IAA= 4.48 µg / ml

Introduction:

Endophytes are commonly referred as a group of microbes that reside in different parts of the plant root or the shoot. Fungal Endophytes are ubiquitous in the plant kingdom, with a few millions of species. Endophytic fungi are one of the most important groups of study with their secondary metabolites representing a rich biodiversity. Now a days, much attention and importance is given to study endophytic biodiversity, biochemical activities of endophytic metabolites and the relationships between endophytes and host plants (Tan and Zou, 2001; Schulz *etal.*, 2002). Tryptophan has been identified as a main precursor for IAA biosynthesis pathway (Karthikeyan and Suryanarayanan *et al.*, 2010).

Rational of the study:

The study of fungal endophyte and their metabolites in roots was selected to understand the logical concept of growth hormones. The plant produces various growth hormones like auxins and gibberellins constitutively but the rational study is to analyze the endophytic fungus in roots to produce similar growth hormones supporting plant growth.

Objectives:

1. To isolate and screen for the endophytic fungi from roots of medicinal plant *Santalum album.*
2. To investigate the effect of growth promoters by selective endophytic fungi on plant growth.
3. Quantification of the growth promoters.

Hypothesis: The study of growth promoters produced by endophytic fungi was mainly to understand the role of fungus in relation to plant growth. To correlate the research hypothesis the endophyte was isolated from the host plant *Santalum album* and the fungus was cultured

Fluorescence studies of Lanthanum (III) complexes of N, N′ bis-(alkyl/aryl)-substituted oxamides and phenanthroline bases

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Abstract

The photoluminescent properties of the Lanthanum complexes greatly depend on the nature and geometry of the coordinated ligands. The fluorescence ability is induced to the non-luminescent lanthanum metal complex by coordinating chromophoric ligands such as substituted oxamides. These oxamides containing auxochromic groups such as O, N through amide bonds sufficiently induce fluorescence to the La(III) metal ion through ligand to metal charge transfer. Of all the synthesized complexes, La(oxae)(phen)](NO$_3$)$_3$ was found to be highly luminescent complex with quantum efficiency reaching almost to unity.

Among all the tested La(III) complexes, mononuclear La(III) complexes show good fluorescence efficiency than hetero-binuclear La(III) complexes. Also, fluorescence efficiency of the complexes was found better in solid state rather than in DMF.

Keywords: Lanthanum(III) complex, alkyl/aryl substituted oxamides, quantum efficiency.

Introduction

Luminescence is a physical phenomenon in which light emits by stimulation of the absorbed energy. This can be of any kind: photoluminescence, thermoluminescence, bioluminescence, chemiluminescence or electroluminescence. Photoluminescence is the emission of energy in the form of photons due to the absorption of light. Photoluminescence is basically of two types: fluorescence and phosphorescence. "Fluorescence" is spin allowed emission which occurs without change in spin, typically $S_1 \rightarrow S_0$ and for "phosphorescence" transitions implying a change in spin, typically $T_1 \rightarrow S_0$.

The electronic configuration of the lanthanide (Ln) atoms and their derived ions in aqueous solutions is their trivalent state Ln^{III} ([Xe]4f^n, n = 0 – 14) due to various degrees of stabilization experienced by the 4*f*, 5*d*, and 6*s* orbitals upon ionization. The shielding of the 4*f* orbitals by the filled $5p^6 6s^2$ sub-shells results in parity-forbidden 4*f* – 4*f* absorptions having very low molar absorption coefficients (typically < 3 M^{-1} s^{-1}) and characteristic narrow-line emission, mostly in the visible and near infrared ranges.[1,2] Since Ln based metal ions are weak emitters as the *f*-electrons are shielded by $5p^6 6s^2$ subshells, they require a linker or chromophoric organic molecules to enhance the emission by transferring their energy. These linkers are generally organic molecules with conjugated aromatic system. When chromophores such as *N,N*-heterocyclic bases coordinate to Ln(III) ion, they function as UV-light collectors. These ligands absorb light in the UV-region, can sufficiently transfer their energy into the excited energy levels of lanthanide ions by a process called "antenna effect" through coordination. For the efficient transfer of energy, the ligand triplet energy states must closely match or slightly above the metal ion's resonance energy levels.[3,4]

The unique physical properties of Ln(III) ions are greatly dependent on geometrical and molecular structures of their complexes. The overall quantum yields depend on the sensitivity of the *4f*- excited states to the coordinating chromophoric groups bearing N, O and C–H oscillators which suppress non-radiative deactivation and also enhance efficient energy transfer between the antenna and the coordinating Ln(III) ions.[5-8]

The sensitization of the Ln(III) ions using ligands containing O, N atoms has resulted in high quantum efficiencies that can be employed in the field of various immunoassays and hybridization technology by probing the former with various antibodies. The luminescent materials have long lifetime (millisecond) and narrow width emission bands. They are hypersensitive to the change in coordination environment[9].

The luminescent Ln(III) complexes are of considerable interest in current research as they find their potential applications in the field of chemo and bio sensing technology, labeling probes in cellular and bioimaging, contrast agents in MRI technology and organic light emitting diodes (OLEDs).[10,11] The luminescent Ln(III) complexes are also utilized in labeling nucleic acids/ proteins and thus are proved to be efficient diagnostic tools in biological field.[1,9,12,13] Among rare earth complexes, La(III) complexes are less employed in the field of luminescent technology because of the absence of *f* – *f* electronic transitions.

Only very few reports on luminescent properties of La(III) complexes are available. La(III) complexes containing salen moiety[14], 2,2′-bipyridine-3,3′-dicarboxylic acid[15], bis(oxazolinylphenyl)amide[16], Schiff bases[5] etc. have shown significant fluorescence properties. La(III) ions when doped with other cations such as Eu(III), Tb(III) and Cd(II) have enhanced their luminescence properties.[17,18]

JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS
https://doi.org/10.1080/07391102.2020.1861982

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Molecular docking and dynamic simulation to identify potential phytocompound inhibitors for EGFR and HER2 as anti-breast cancer agents

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Communicated by Ramaswamy H. Sarma

ABSTRACT

Breast cancer is the most prevalent cancer in women worldwide. To treat human breast cancer by inhibiting EGFR and HER2 targets is an important therapeutic option. Phytochemicals are found to have beneficial health effects in treating various diseases. An effort has been made to virtually screen phytochemical inhibitor by molecular docking and dynamic simulation in the current studies. The docking scores analysis resulted in a common hit Panaxadiol ligand with a low dock score for EGFR and HER2 targets. The inhibitory action of the phytocompounds was also validated by comparing it with the reference compounds Erlotinib for EGFR and Neratinib for HER2. Molecular dynamic simulation of EGFR and HER2 lead complexes ensure the ligand's appropriate refinement in the dynamic system. The target and ligand complex interaction motif established a high affinity of lead candidates in a dynamic system similar to molecular docking results. This study reveals that Panaxadiol hit molecule can be developed as a novel multi-target EGFR and HER2 target inhibitor with greater potential and low toxicity.

ARTICLE HISTORY
Received 27 August 2020
Accepted 5 December 2020

KEYWORDS
Breast cancer; EGFR; HER2; molecular docking; molecular dynamic simulation

1. Introduction

Breast cancer is one of the widespread types of cancer in women and accountable for the high number of cancer mortality cases worldwide. Every year ~1.7 million people are identified with breast cancer, and >0.5 million women die from breast cancer worldwide (Ren et al., 2020). Breast cancer is a diversified disease mainly of three types, the first being hormone receptor-positive breast cancer includes 60% in the presence of Estrogen receptor (ER) and Progesterone receptor (PR). The second type consists of 15–20% of cases in the presence of Human Epidermal growth factor Receptors 2 (HER2), belongs to HER family such as HER-1, HER-2, HER-3, and HER-4 and the third type is triple-negative breast cancer (TNBC) which lacks ER, PR, and HER2 receptors (Tripathi et al., 2018). Highly significant HER protein families are most widely considered protein-tyrosine kinase due to their role in cell proliferation, differentiation, and migration, leading to several downstream signaling pathways. Breast cancer is caused by overexpression, aberration, mutation, and abnormal signal transduction in HER protein.

The widely discussed first member of HER family protein is the epidermal growth factor receptor (EGFR/HER1) because of its role in cell signaling and oncogenesis (James & Ramanathan, 2018). It is 170 kDa glycoprotein and plays a significant role in signal transduction involving apoptosis and cell proliferation. EGFR gene amplification results in the overexpression and deregulation of signaling pathways. Cell growth, development, cell migration, and metastasis were influenced by overexpression and genetic mutation on EGFR (Singh & Bast, 2014). In the natural progression of breast cancer development, HER2-overexpression tumors also play an important role. The HER2-HER3 heterodimer triggers an oncogenic signaling pathway and is extensively activated in different human cancers. Downstream signaling pathways that mediate HER2 and its tumorigenic functions are complex. As a result, HER2 was considered a major target for anti-cancer drug development (Iqbal & Iqbal, 2014).

HER-2 positive breast cancer treatment is more effective with the use of both EGFR and HER-2 targets inhibitors. The limitations of the single target treatments are overcome by multi-target therapeutics. Multi-target drug therapy is more effective and less susceptible to resistance (Tripathi et al., 2018). Gefitinib, Erlotinib, Afatinib, and Osimertinib are Tyrosine kinase inhibitors that specifically target EGFR and are currently approved by the FDA. These four drugs are associated with adverse effects that can effectively impact

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Supplemental data for this article can be accessed online at https://doi.org/10.1080/07391102.2020.1861982.

JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS
https://doi.org/10.1080/07391102.2020.1790424

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Exploration and evaluation of bioactive phytocompounds against BRCA proteins by *in silico* approach

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Communicated by Ramaswamy H. Sarma

ABSTRACT

The proteins encoded by the two major breast cancer genes (BRCA1 and BRCA2), ensure the stability of DNA and prevent uncontrolled cell growth; mutation of these genes is linked to the development of hereditary breast cancers. Exploration of human breast cancer inhibitors plays a vital role in the drug discovery process. In the current work, *in silico* studies were performed which involves a computational approach for the identification of active phytocompounds from the diverse set of medicinal plant products against the BRCA receptor. The *in silico* study through pharmacokinetics and pharmacodynamics properties shown promising outcomes for these phytocompounds data set as breast cancer inhibitors. It was observed that the compounds conformed to the Lipinski's rule of five and had good bioavailability. The drug-likeness model score and ADMET profile of the designed ligands also established their potential as a drug candidate. The docking study provided useful insights on potential target-lead interactions and indicated that the newly designed leads had a good binding affinity for BRCA targets. A pharmacophore model was built to explore the scaffolds for BRCA inhibitory activity. An effort is made to screen an inhibitor against BRCA targets by combining the use of ADMET, docking score, and pharmacophore model.

ARTICLE HISTORY
Received 23 May 2020
Accepted 25 June 2020

KEYWORDS
Phytocompounds; docking; drug-likeness; in silico; BRCA; anti-breast cancer; ADMET

1. Introduction

Cancer is projected as the leading cause of death worldwide. There were an estimated 18.1 million new cancer cases and 9.6 million deaths due to cancer as reported in 2018. Among females, breast cancer is the most commonly diagnosed cancer and it is the primary cause of cancer mortality, followed by colorectal and lung cancer (Bray et al., 2018). Most of the new cases are frequently found to be female breast cancer in the majority of countries and cervical cancer is the primary cause in remaining countries. In developed and developing countries, the mortality profile of women is heterogeneous with respect to breast and cervical cancer (Bray et al., 2018). The incidence of breast cancer in India is expected to be more than 90,000 in the coming years and over 50,000 women die each year (Suganya et al., 2014). There is a significant increase in the incidence and cancer-associated illness and mortality in the Indian subcontinent as pronounced in global and Indian studies. Earlier cervical cancer was the most commonly found cancer in Indian women but now the incidence of breast cancer has surpassed cervical cancer and is the leading cause of cancer deaths (Malvia et al., 2017).

Breast cancer is characterized by the uninhibited growth of malignant abnormal cells. Epithelial tissues are the most affected part of the breast due to cancer. Identification and early detection of breast cancer through signs or symptoms had helped in the reduction of the mortality rate of the disease. In the case of women carrying breast cancer susceptibility gene type 1 (BRCA1) mutations, the risk of having breast cancer in their lifetime was found to be at 80%, on the other hand in the case of breast cancer susceptibility gene type 2 (BRCA2) variant the breast cancer risk stands at about 6% (Ikhuoria & Bach, 2018). BRCA1 and BRCA2 play a crucial role in maintaining genome integrity by repairing double-strand DNA breaks, through homologous recombination repair (HRR) pathway. Mutations in BRCA1 and BRCA2 genes cause functional disruption of BRCA proteins, which play a crucial role at a higher risk of developing breast and ovarian cancer in women (Godet & Gilkes, 2017, Sukanya et al., 2018).

There are various treatments available to cure cancer such as chemotherapy, radiotherapy, and chemically derived drugs. The U.S. Food and Drug Administration (FDA) has approved the use of Lynparza (Olaparib) for the treatment of metastatic and tumour in breast cancer patients, that have specifically inherited BRCA gene mutations. Treatments such as chemotherapy can put patients under a lot of strain and further damage their health (Greenwell & Rahman, 2015). Regardless of their initial efficacy, the majority of the patients develop acquired resistance to the therapy, along with major

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Supplemental data for this article can be accessed online at https://doi.org/10.1080/07391102.2020.1790424.

International Journal of Botany Studies
ISSN: 2455-541X; Impact Factor: RJIF 5.12
Received: 19-11-2020; Accepted: 04-12-2020: Published: 16-12-2020
www.botanyjournals.com
Volume 5; Issue 6; 2020; Page No. 508-515

In silico screening of phytochemicals to explore potent anti-breast cancer inhibitors against estrogen receptors

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Abstract

Breast cancer is the second most common cancer across the globe, there is a need for the development of effective therapeutic agents. Current computational studies play a significant role in identifying new leads for disease treatment. This study was performed to screen the effective bioactive molecules against estrogen receptors. A dataset of plant-based natural anti-breast cancer compounds was selected. Molecular docking was performed to estimate the spatial affinity of target compounds for the active sites of the estrogen receptor. The *In silico* ADMET studies were performed for the lead molecules. Results showed that Genistein, Daidzein and Panaxadiol are having the best docking score and good binding affinity than other ligands. Hence, Genistein, Daidzein and Panaxadiol can be considered as a better drug candidate for anti-breast cancer inhibitors against estrogen receptors which can be explored further.

Keywords: ADMET, breast cancer, estrogen receptor, molecular docking, phytocompounds

1. Introduction

Breast cancer is strangely common among the population across the globe. An estimated 2.1 million cancer cases accounted for in 2018, found to be a fifth leading cause among cancer mortality worldwide. A ratio of persons suffering from breast cancer to healthy population was found to be 1 out of every nine women among the developed nations and 1 in every 20 persons in less developed nations as reported in 2018 (Dolatkhah, *et al.*, 2020) [9]. Different types of breast cancers exist, few may have hormone receptors like estrogen or progesterone (others may have both) and are called ER+ or PR+ breast cancer, respectively. The main driver among, the majority of breast cancer cases is the estrogen receptor ER since it is found to exist among 75% of overall breast cancer cases (Masoud and Pagès, 2017) [17].

For the normal female physiology, reproduction and behavior, the steroid hormone estrogen is essential, because of its effects on cellular processes together with cell proliferation and cell survival. The nuclear estrogen receptors (ERα and ERβ) facilitate these effects. The ERα and ERβ estrogen receptors are encrypted by separate genes, positioned on different chromosomes. ERα-positive cells make a vital involvement in mammary development. On the contrary, normal development happens for the mammary glands of ERβ mice. When the two receptors are co-expressed in breast cancer cell lines, ERβ functions as an adversary of ERα, harming the ability of estrogen to arouse proliferation. Minimum 70% of the breast cancers are categorized as ER-positive breast cancers and meddling with estrogen action has been a linchpin of breast cancer therapeutics for over a century (Musgrove and Sutherland, 2009) [18].

Herbal medicine has turned out to be a very safe, non-toxic, and easily accessible source of compounds used in cancer treatment. Phytocompounds are thought to counteract the effects of diseases in a body due to the possession of various biomolecular characteristics (Khan, *et al.*, 2020) [12]. Exploration of human breast cancer inhibitors executes a vital part in the drug discovery method. Based on previous *in silico* studies, a review shows that 131 phytocompounds were selected from 51 plant families (Prabhavathi, *et al.*, 2020) [23]. These plant families comprises Apocynaceae (Richard, *et al.*, 2015; Omogbadegun, 2013) [25, 19]. And Euphorbiaceae family (Dasaroju and Gottumukkala, 2014) [7]. Has got 4.58% of plant compounds from each family respectively, followed by Lamiaceae has got 6.10% phytocompounds (Akhtar and Swamy, 2018; Kim, *et al.*, 2016; Preethi and Padma, 2016; Woźniak, *et al.*, 2015; Wang, *et al.*, 2012) [1, 13, 24, 28, 27]. From Asteraceae family, 9.92% of plants compounds (Omogbadegun, 2013; Csupor-Löffler, *et al.*, 2011) [19, 5]. And rest of the compounds are grouped as other plant families (Lee, *et al.*, 2017; Levitsky and Dembitsky, 2015; Pierpaoli, *et al.*, 2015; Gladys, *et al.*, 2013; Bhoopat, *et al.*, 2011) [14, 15, 20, 10, 3]. From these plants, the active phytocompounds were identified from a varied set of medicinal plants as anti-breast cancer agents.

Virtual screening thousands of compounds is made possible using the *in silico* approaches, in a very reasonable time. This drastically reduces the costs involved in the identification of hits and further increasing the probabilities of finding the anticipated drug candidates. One of the widely popular and systematic structure-based *in silico* methodology is molecular docking studies. Molecular docking is among one of the most popular and successful structure-based *in silico* methods, which help predict the interactions occurring between molecules and biological targets. It helps to find the interactions happening among the molecules and biological targets. This methodology is normally achieved by first predicting the molecular orientation of a ligand within a receptor, and then assessing their complementarity through the use of a scoring function (Pinzi and Rastelli, 2019) [22]. This study aims at screening a set of phytocompounds which could inhibit ER. The study