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IN-SILICO TARGETING OF WASTEWATER POLLUTANTS WITH LACCASE ENZYME USING MOLECULAR DOCKING

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CANDIDATE'S DECLARATION

I Aalia Qaiser, Roll No. 2K21/MSCBIO/01 student of M.Sc. Biotechnology, hereby declare that the project Dissertation titled "**In-silico targeting of wastewater pollutant with laccase enzyme using Molecular docking**" which is submitted by me to the Department of Biotechnology, Delhi Technological University, Delhi in partial fulfillment of the requirement for the award of the degree of Master of Science, is original and not copied from any source without proper citation. This work has not previously formed the basis for the award of any Degree, Diploma Associateship, Fellowship or other similar title or recognition.

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CERTIFICATE

I hereby certify that the Project Dissertation titled "**In-silico targeting of wastewater pollutant with laccase enzyme using Molecular docking** "which is submitted by Aalia Qaiser, Roll No. 2K21/MSCBIO/01, Department of Biotechnology, Delhi Technological University, Delhi in partial fulfilment of the requirement for the award of the degree of Master of Science, is a record of the project work carried out by the students under my supervision. To the best of my knowledge this work has not been submitted in part or full for any Degree or Diploma to this University or elsewhere.

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ABSTRACT

Water resource preservation, environmental preservation, and public health protection all depend on effective wastewater treatment. It aids in preventing water body contamination, upholds ecological harmony, and assures a sustainable water supply for a variety of uses. It is important to remove toxins, pollutants, and other undesirable elements from wastewater as part of the wastewater treatment process. Its objective is to safely transform wastewater such that it can either be released into the environment or recycled for a variety of uses. In recent years, molecular docking has been successfully applied to the research of the biodegradation mechanism for environmental remediation. Although molecular docking has mostly been used in the fields of biology and medicine, it has shown to be a practical and economical way to accurately comprehend how proteins or enzymes interact with their ligands. This article seeks to provide an overview of how molecular docking has been used to investigate how organic contaminants and enzymes interact. The basic understanding of molecular docking, including its theory, available software tools, and key databases, is summarised in the paper's opening paragraphs. For successful docking research, it is essential to comprehend these factors. Following that, the review concentrates on five different categories of pollutants: phenols, BTEX (benzene, toluene, ethylbenzene, and xylenes), nitrile, polycyclic aromatic hydrocarbons (PAHs), and high polymers like lignin and cellulose. Through docking studies, the molecular interactions of these contaminants with enzymes are examined. The report also provides a detailed explanation of several removal procedures employing docking technology. The docking investigations shed light on how contaminants interact with enzymes and travel through the degradation process. Researchers can create better environmental remediation solutions by comprehending these mechanisms. Although molecular docking has some interesting uses in the study of biodegradation, the publication notes that more research is still required to apply the findings to actual environmental settings. It is crucial to verify the findings of docking studies using experimental data and to take into account the numerous environmental variables that could have an impact on the biodegradation process. In conclusion, this research discusses the use of molecular docking to investigate the interaction between organic contaminants and biodegradation enzymes. The fundamentals of molecular docking are covered, as well as the molecular features of various contaminants and removal strategies. Although molecular docking has potential, further study is required to close the gap between theoretical discoveries and practical implementations.

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LIST OF SYMBOLS, ABBREVIATIONS AND NOMENCLATURE

EPA	Environmental Protection agency
BTEX	Benzene, Toulene, Ethylbenzene, Xylene
PCB	Polychlorinated Biphenyl
PAH	Polycyclic Aromatic Hydrocarbon
OH	Hydroxyl
HRP	Horeseradish Peroxidase
Fe	Iron
VOC	Volatile Organic Comounds
PDB	Protein Data Bank
EM	Electron Microscopy
GO	Gene Ontology
SMD	Small Molecule Database
NCBI	National Center for Biotechnology Information
NLM	National Library of Medicine
ADME	Absorption, Distribution, Metabolism, Excretion
Qsar	Quantitative structure-activity relationship
SIB	Swiss Institute of Bioinformatics
FFT	Fast Fourier Transform
UCSF	University of California, San Francisco
PLIP	Protein-Ligand Interaction profiler
HB	Hydrogen Bond
VdW	VanderWaal
TRP	Tryptophan
HSD	Histidine
TYR	Tyrosine

CHAPTER 1

INTRODUCTION

Polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs), and hydrocarbon derivatives are only a few examples of the organic pollutants that have grown to be a major problem for environmental pollution. Due to their persistence, toxicity, and ability to have a negative impact on ecosystems and human health, these pollutants are regarded as being dangerous. The Environmental Protection Agency (EPA) has designated **phenols, PAHs, nitriles, and BTEX (benzene, toluene, ethylbenzene, and the three xylene isomers)** as priority control pollutants in environmental samples. [1][2]

Given the volatility and persistence of these contaminants, addressing the environmental risks they cause is difficult. However, biodegradation holds promise among the chemical, physical, and biological approaches for pollution treatment because of a number of benefits [3]-[6].

1. Complete breakdown: By using microorganisms, biodegradation has the ability to totally transform organic contaminants into less harmful, simpler chemicals. Through this process, the pollutants are transformed into safe byproducts while serving as a source of energy and carbon [7].

2. Lower cost: Biodegradation typically offers lower operational and maintenance expenses than alternative techniques like chemical or physical treatments. It doesn't require expensive chemical reagents or energy-intensive processes because it relies on the action of naturally occurring microbes[8].

3. Minimal secondary pollution: Comparing biodegradation to other remediation techniques, secondary contamination is often produced at a low level. Physical and chemical processes could leave behind byproducts or residues that need to be properly disposed of, raising further environmental issues. Contrarily, biodegradation primarily results in the production of innocuous byproducts like carbon dioxide and water[9].

The efficiency of biodegradation can, however, vary depending on the specific contaminants, environmental factors, and the presence of compatible microbial populations, so it's crucial to keep this in mind. The biodegradation process can be influenced by variables like pH, temperature, oxygen availability, and the presence of co-contaminants.

Understanding the properties of the pollutant, site-specific conditions, and the appropriate selection of microbial cultures or tactics to boost microbial activity are essential for implementing biodegradation as a successful remediation strategy. For the biodegradation

process to be efficient and effective in reducing organic pollutants, monitoring and optimisation are also necessary.

In conclusion, although biodegradation shows promise as a potentially efficient and environmentally friendly method for addressing organic pollutant contamination, careful consideration and evaluation of site-specific factors are required to determine its suitability and success in a specific remediation scenario.

In fact, in recent years, the study of the biodegradation mechanism for environmental remediation has successfully used molecular docking. Although molecular docking's primary applications have historically been in biology and medical science, it can also be used in a variety of other industries due to its adaptability.

A computational technique called molecular docking is used to forecast the interactions that will occur when a tiny molecule (or ligand) binds to a target protein or enzyme. It can shed light on the ligand's molecular recognition and binding mechanisms in the protein's active site by mimicking the docking procedure.

CHAPTER 2

LITERATURE REVIEW

The interaction between pollutants or other environmental contaminants and the enzymes or proteins involved in their biodegradation can be studied using molecular docking in the context of environmental restoration. Researchers can improve the biodegradation process and create more effective bioremediation techniques by better understanding the binding processes and interactions between the pollutants and the degrading enzymes.

When compared to experimental techniques, molecular docking has the convenience and relative low cost of being convenient. A wide spectrum of researchers can run docking simulations thanks to the availability of software tools and computer power. Additionally, thanks to improvements in computational methods and algorithms, molecular docking accuracy has considerably increased, making predictions of ligand-protein interactions more trustworthy.

Overall, molecular docking has shown to be a useful method for accurately and affordably studying the interactions between proteins, enzymes, and ligands in the investigation of biodegradation pathways for environmental remediation.

Enzymatic catalysis is frequently used to biodegrade organic pollutants. Specialised proteins called enzymes function as biological catalysts, accelerating chemical reactions without being eaten. They are essential for dissolving intricate chemical compounds into more manageable components.

Enzymes bind to organic contaminants at their active sites during biodegradation. The portion of the enzyme's surface known as the active site is designed precisely to accommodate the pollutant molecule, enabling precise and selective binding. The building blocks of proteins, called amino acids, are normally arranged in a particular way to create the active site.

The enzyme's active site attracts the organic contaminant, which then undergoes a number of chemical processes that break it down into smaller molecules. These reactions may involve enzymatic processes like hydrolysis, oxidation, reduction, or other mechanisms. The organic pollutant eventually decomposes into less toxic or dangerous for the environment simpler components like carbon dioxide and water.

Exploring biodegradation pathways at the molecular level has revealed details on the specific enzymes involved, their active sites, and the chemical reactions they promote. The creation of enzymes with improved organic pollutant degrading capabilities and the development of more effective bioremediation procedures can both benefit from an understanding of these processes.

2.1PHENOLS

A hydroxyl (-OH) group is joined to an aromatic ring in phenols, a category of organic molecules. Based on the number of phenol units, they can be divided into two primary categories: polyphenols, which have several phenol units, and simple phenols, which have a single phenol unit.

Phenols are synthesised naturally by plants and microorganisms in addition to through industrial methods [10][11]. Phenols can build up in soil, groundwater, and surface water after being introduced into the environment, providing potential dangers to ecosystems.[12]

Microorganisms can be crucial in the context of water treatment for phenol pollution.

Pseudomonas spp. and Acinetobacter spp. are two bacterial species that have been used for their capacity to break down phenols and remove them from polluted water sources.[13]

The chemical phenol itself is a significant raw material with several industrial uses.

The manufacture of bakelite, oils, cokes, textiles, dyes, insecticides, and pharmaceuticals all heavily rely on it. As a result, it is among the main contaminants in industrial effluent.

It's vital to remember that phenol and its vapours have the potential to be toxic and damaging to people's health. They may irritate and harm the eyes, skin, and respiratory system. The strong chemical characteristics of phenol produce denaturation of proteins, which is what causes the corrosive effects on mucosal membranes and skin. As a result, when handling phenol and working with chemicals that include phenol, the required safety precautions and safeguards should be implemented.[14]

According to the results of the molecular docking, phenol and laccase interact through hydrogen bonds and hydrophobic interactions [14]. This phenol-laccase binding on microbe surfaces may prevent the microorganism from effectively interacting with hydrophobic organic pollutants present in the aqueous phase [15]. To put it another way, the presence of phenol might make it more difficult for the microbe to break down hydrophobic organic contaminants.

However, it is feasible to lessen phenol's toxicity to cells and speed up phenol elimination by using certain surfactants. Surfactants, such as water and a hydrophobic material, are substances that can lessen the surface tension between two phases [16]. When Candida tropicalis is used as the degrading bacteria, the inclusion of surfactants can improve the interaction between the microbe and phenol, increasing the effectiveness of the degradation.[17]-[19],[15]

Surfactants can improve the dispersion of hydrophobic organic pollutants in the aqueous phase and increase their accessibility to the microbe by lowering surface tension. This enables

Candida tropicalis to efficiently breakdown phenol and other organic contaminants that are hydrophobic.[15] [17]

It's important to note that the compatibility of a certain surfactant with the microorganism and pollutants present in the system should be taken into consideration. The toxicity of phenol and Candida tropicalis' ability to degrade it may be affected differently by various surfactants. Therefore, to find the best surfactant for a particular situation, significant thought and trial are required.

An enzyme called horseradish peroxidase (HRP) has been employed in a number of processes, including the purification of phenol-containing wastewater. Phenols are organic substances that are frequently present in industrial wastewater and can be hazardous to the environment.

phenols can be oxidised by HRP, which produces less hazardous chemicals as a result. This is accomplished by catalysing a process with hydrogen peroxide that converts phenols into less dangerous, simpler compounds. Wastewater polluted with phenol can be effectively treated using this enzymatic oxidation method.

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It's crucial to remember that applying HRP for the remediation of persistent pollutants and the treatment of wastewater may call for unique circumstances and optimisation for each situation. The pH, temperature, substrate content, and presence of other substances in the wastewater can all affect how efficient and effective the enzyme is in these processes. Therefore, to ensure that HRP-based remediation procedures are implemented successfully, extensive research and experimentation are required.

2.2Nitriles

The interactions between nitriles and many degrading enzymes, particularly amidase, nitrile hydratase, and nitrilase, were explicitly shown using visual models.[23]

A hydroxide ion may be adsorbed into acrylonitrile due to nucleophilicity and activation, according to a comparison of the relative locations of crystal water and the chemical compound.

In this context, it is said that the metal atom in the enzyme plays a crucial part as a Lewis acid in the electrical receptor.[24]

There are specific instructions for the Co-type nitrile hydratase-mediated biodegradation of acrylonitrile. Three phases make up the process:

1. Water molecules give the cobalt ion at the active site an OH group, forming the Co2+-OH complex.

2. A carbon-nitrogen double bond and a C-OH bond are formed when an oxygen atom from these complex attacks a carbon atom of the carbon-nitrogen triple bond in acrylonitrile.

3. A serine residue takes away the hydrogen atom from the C-OH bond. Acrylonitrile is transformed into acrylamide through this process.[25]

According to the statement, Fe-type nitrile hydratase degrades differently from Co-type nitrile hydratase. Molecular docking and analysis revealed that the oxygen atom of the carbonyl group from the glutamine residue can activate a water molecule and take part in a chemical reaction in the case of Fe-type nitrile hydratase.[26]

2.3BTEX

The acronym BTEX stands for the isomers of benzene, toluene, ethylbenzene, and xylene, which are all aromatic hydrocarbons. These substances are frequently present in oil and are created as byproducts of various refining techniques, such as the catalytic reforming of naphtha.[27]

The petrochemical industry relies heavily on the catalytic reforming process to transform low-octane hydrocarbons into higher-octane compounds that can be utilised to make petrol. The typical feedstock for catalytic reforming is naphtha, a light component of crude oil. The naphtha is heated and passed over a catalyst during this process, causing chemical reactions that result in the synthesis of aromatic hydrocarbons.

BTEX, also known as benzene, toluene, ethylbenzene, and xylene, are useful chemical intermediates with several industrial uses. They are sometimes referred to as volatile organic compounds (VOCs), and because of their toxicity and propensity for contaminating groundwater, they are linked to issues with the environment and human health [28]. As a result, petrochemical businesses have put policies in place to cut back on BTEX compound emissions and lessen their negative effects on the environment.

Findings suggest that an in-silico approach based on molecular docking and molecular similarity search can be used to identify and screen proteins with toluene. Additionally, toluene's considerable binding to six proteins, including DNA polymerase, haemoglobin, serum albumin, and cytochrome P450 2E1, was successfully demonstrated by the docking data [29]. Catechol-2,3-dioxygenase (EC 1.13.11.2), a typically multimeric enzyme, splits the

benzene rings of a variety of environmental pollutants, such as naphthalene, xylene, toluene, and derivatives of the biphenyl ring, and its catalytic action is dependent on Fe [30].

It's an intriguing idea to use docking technology in the realm of materials to investigate adsorption capacity. Studying the interactions between molecules and materials can be done using docking, which is frequently employed in molecular biology and drug discovery.

It is a good idea to study the zeolite's ability to bind benzene using supercagep-based molecular docking. The porous nature of zeolites allows for the selective adsorption of particular molecules based on their size, shape, and polarity [31]. By using molecular docking, one may forecast and examine interactions between benzene molecules and the zeolite surface, revealing information about the adsorption procedure and capacity.

In order to explore other pollutants' adsorption, benzene could potentially be replaced with them. The effectiveness of materials for environmental clean-up can be evaluated using this application. Researchers can assess the potential for adsorption of various pollutants and create more potent adsorbents for eliminating toxins from water or the air by virtually docking them with various materials.

In terms of the interactions between materials and benzene, - stacking and Van der Waals interactions are the main causes of benzene breakdown by oxygenase. It is true that these interactions play important parts in how aromatic chemicals, like benzene, bond to materials. The attractive forces between aromatic rings are referred to as "- stacking," and "Van der Waals interactions" refer to a variety of weak intermolecular forces, such as London dispersion forces.

Additionally, the presence of a hydroxyl group (OH) can change the way organic pollutants reacts. Involvement in hydrogen bonding by hydroxyl groups can change a molecule's overall chemistry. The presence or absence of hydroxyl groups can change the reactivity, solubility, and adsorption characteristics of organic compounds in the context of organic pollution, affecting their fate and behaviour in the environment.

In conclusion, the use of docking technology to materials opens up possibilities for investigating adsorption capacities and creating more effective adsorbents. Understanding the interactions between materials and organic pollutants requires taking into account factors like the function of "-" stacking, Van der Waals contacts, and the impact of hydroxyl groups.

2.4Polycyclic Aromatic Hydrocarbon

In fact, PAHs (polycyclic aromatic hydrocarbons) are made of hydrogen and carbon atoms and are made up of two or more fused benzene rings. They are organic substances that are created when carbon-containing substances like oil, coal, petrol, and tobacco are burned partially.

PAHs include anthracene, phenanthrene, pyrene, and benzo[a]pyrene. These substances are recognised by their distinctive ring structures and are frequently present in a variety of environmental sources, such as industrial processes, exhaust emissions, and some forms of fossil fuels.

PAHs are classified as neutral and non-polar molecules since they are primarily composed of hydrocarbons. They don't have any polar functional groups or substantial charges, which makes them somewhat insoluble in water but soluble in organic solvents. Their fondness for oil and coal, where they can amass, is also a result of their non-polar nature.

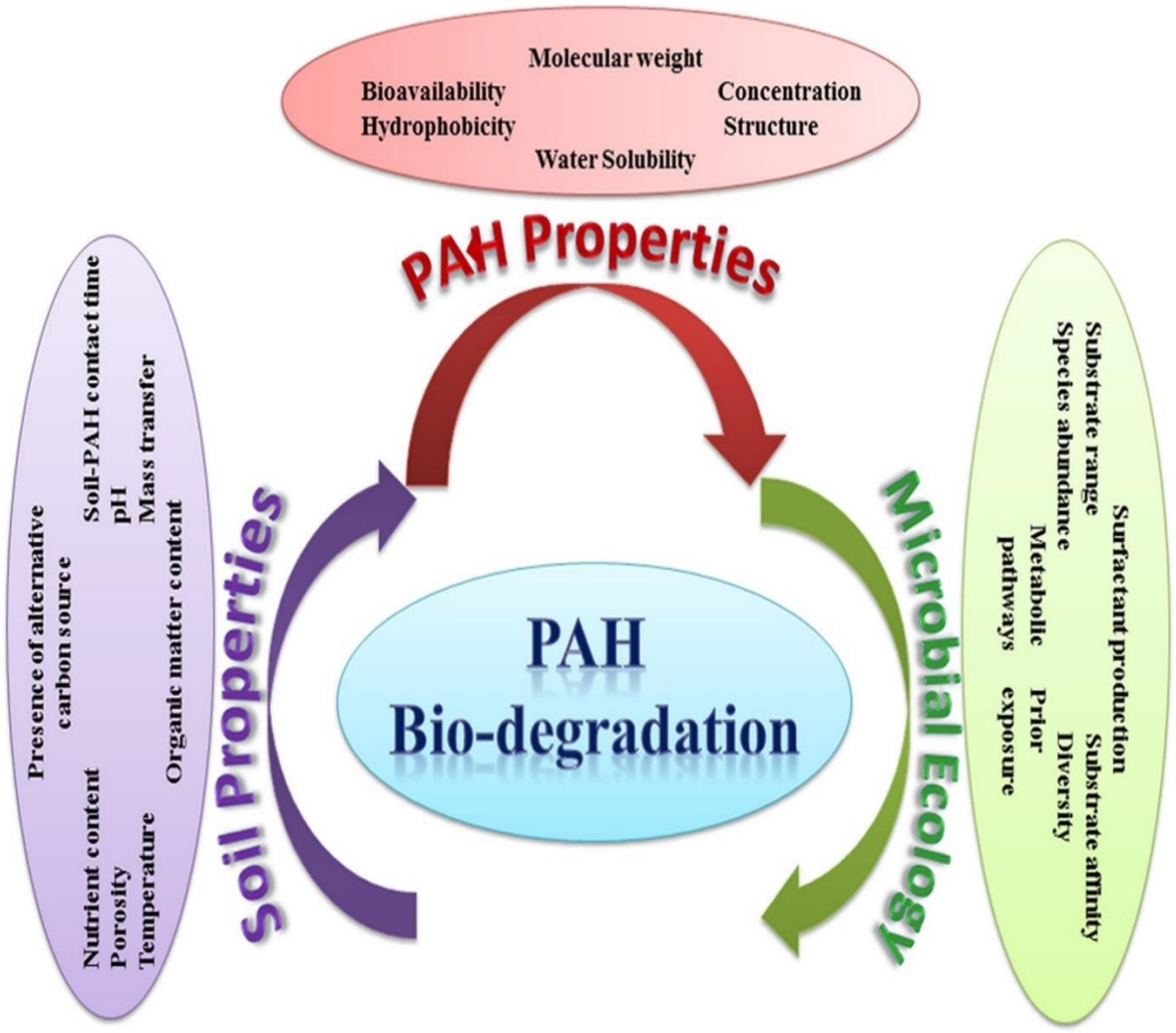

Figure 1: Abiotic abd Biotic factor influencing the breakdown of PAHs in soil

It's crucial to remember that PAHs have raised significant environmental and health concerns because of their potential for toxicity and carcinogenicity. Exposure to PAHs, especially by ingestion, absorption, or skin contact, has been linked to negative health impacts in people and can be dangerous for both ecological and social systems. In order to reduce potential risks, efforts are conducted to monitor and control PAH levels in a variety of sectors and environmental contexts.[32],[33]

Polycyclic aromatic hydrocarbons, or PAHs, are created when organic materials like wood, tobacco, and fossil fuels are pyrolyzed or burned insufficiently. Because of their poor reactivity and resilience to deterioration, PAHs are recognised as persistent pollutants in the environment.

The particular PAH chemical, environmental circumstances (such as temperature, pH, oxygen availability), existing microbial populations, and the presence of co-contaminants are some of the factors that affect the biodegradability of PAHs. Due to variations in their chemical characteristics and structures, certain PAHs biodegrade more quickly than others.[34]

Through a variety of methods, PAH biodegradation can be accelerated in environmental remediation schemes. Introduce specialised microorganisms or microbial groups that can break down PAHs into contaminated areas as part of bioremediation. Enhancing environmental factors, such as offering oxygen and nutrients, can be used in conjunction with this strategy to encourage microbial activity and growth.

It's vital to remember that the individual conditions and complexity of the PAH-contaminated site can affect how efficient biodegradation is as a remediation strategy. To get satisfactory results, it could be essential to combine various remediation techniques, such as biodegradation and physical or chemical treatments.

Overall, biodegradation has tremendous potential to convert PAHs into harmless byproducts while being effective and environmentally acceptable, making it a key area of attention in the field of environmental rehabilitation.

2.4.1Environmental and Chemico-physical Parameters Affecting Degradation

Polycyclic aromatic hydrocarbons (PAHs) can be degraded by enzymes in response to a variety of chemico-physical parameters as well as other factors[35]. The effectiveness, reaction kinetics, and selectivity of PAH breakdown by enzymes are significantly influenced by these variables. The following are some of the crucial factors and variables that can influence enzymatic PAH degradation:

1. Substrate properties: The molecular size, hydrophobicity, solubility, and volatility of PAHs, together with other physical and chemical characteristics, can have a big impact on

how quickly they are degraded by enzymes. Based on these characteristics, enzymes might favour certain PAHs over others.

2. Enzyme specificity: The degree of selectivity that various enzymes have towards PAHs varies. Due to variations in their active site structures and binding affinities, some enzymes may be more effective at destroying particular PAHs than others.

3. Enzyme concentration: The quantity of enzymes in the reaction mixture can have an impact on how quickly and effectively PAHs are degraded. If other parameters are not limiting, higher enzyme concentrations may improve the rate of breakdown.

4. Temperature and pH: The stability and activity of enzymes are influenced by temperature and pH levels. To ensure the highest level of enzyme activity for PAH breakdown, ideal temperature and pH ranges should be maintained.

5. Co-factors and co-substrates: Co-factors or co-substrates are frequently needed for enzymatic reactions in order to speed up the degrading process. The effectiveness and selectivity of PAH degradation may be impacted by the concentration and availability of these compounds.

6. Presence of inhibitors: Enzymatic PAH breakdown may be inhibited by specific substances or environmental elements. Inhibitors may directly interfere with the enzymatic reaction or compete with PAHs for enzyme binding sites, decreasing the efficiency or selectivity of breakdown.

7. Enzyme-inducing agents: Specific enzymes involved in the breakdown of PAHs can be produced in response to certain chemicals or substances. These inducers can increase enzyme activity and boost PAH breakdown processes' effectiveness.

8. Environmental conditions: Enzymatic PAH breakdown may be impacted by environmental conditions such as oxygen availability, moisture content, and the presence of additional microbes or organic materials. The overall effectiveness and selectivity of the degradation process may be affected by the competitive or inhibitory effects created by these circumstances.

Understanding and improving these chemico-physical characteristics, along with other variables, can help with the development of methods to improve the efficiency, kinetics, and selectivity of enzymatic PAH degradation.

While anaerobic conditions refer to the lack of oxygen, aerobic conditions refer to the presence of oxygen in the surrounding environment or reaction system. The aerobic condition significantly affects the effectiveness, reaction kinetics, and selectivity of the degradation process when it comes to the enzymatic breakdown of polycyclic aromatic hydrocarbons (PAHs).

Microorganisms, such as bacteria or fungi, that have the enzymes necessary to degrade these sophisticated chemical molecules frequently perform PAH breakdown.

CHAPTER - 3

MATERIALS AND METHODS

3.1. Material Used

The software and databases used for in-silico molecular docking are briefly described here.

3.1.1.PDB

The PDB (Protein Data Bank) is a well-known and often used resource in the field of structural biology. It is a database that users can visit to view three-dimensional experimentally determined models of biological macromolecules like proteins, nucleic acids, and complex assemblies. The PDB is managed by the Worldwide Protein Data Bank (wwPDB) organisation, a collaboration of various institutions from around the world.

Important PDB features include:

1. The PDB acts as a central repository for experimentally confirmed structural information on biological macromolecules. The structures of proteins, nucleic acids, and complexes are fully described, along with extensive atomic coordinates and other significant information. The PDB ID is a unique identifying number that is assigned to each entry in the PDB, each of which represents a different structure.
2. **Protein Structures and Macromolecular Complexes:** A substantial collection of protein structures, including those of enzymes, receptors, antibodies, and other relevant proteins, can be found in the Protein Data Bank (PDB). It also encompasses the structures of nucleic acids like DNA and RNA as well as complexes formed by interactions between proteins, nucleic acids, and ligands. A vast range of species, including bacteria, viruses, plants, and animals, are included in the database.
3. **Experimental Techniques**: The experimental methods used to create the structures are described in full in the PDB. Cryo-eletron microscopy (cryo-EM), NMR spectroscopy, X-ray crystallography, and hybrid methods are all covered in this. Thanks to the availability of the specifics of the experimental setup and data collection methods, researchers may assess the accuracy and dependability of the structures.
4. **Structural Annotations and Metadata:** Each entry in the PDB has a wealth of structural annotations and metadata. This includes information on the biological function, ligand-binding sites, post-translational modifications, and other relevant properties. It also includes information on the sequence of the protein or nucleic acid.

Additional annotations could include details on biological assembly, crystal packing details, and experimental conditions.

5. The PDB's tools and resources enable the analysis and visualisation of protein structures. Users can examine structures in a variety of representational types, such as ribbon, space-filling, and cartoon models. With the use of interactive viewers and molecular visualisation software, detailed investigation and analysis of structural properties, such as ligand interactions, active sites, and conformational variations, is also available.
6. **Cross-referencing and Data Integration:** The PDB interfaces with other databases and resources in order to provide more details and enhance data analysis. Cross-references to other databases, including as UniProt, Gene Ontology (GO), and Small Molecule Database (SMD), enable researchers to obtain additional information about proteins, functional annotations, and ligands associated with the structures.
7. **Data Deposition & Community Contribution:** At the PDB, researchers from all around the world can deposit data. It encourages academics to share the structures they have empirically uncovered, expanding the corpus of knowledge and enhancing academic research. It is made feasible for other researchers to build on the discoveries and carry out further study by placing the data in the PDB.

3.1.2. PubChem

The expansive database PubChem is maintained by the National Centre for Biotechnology Information (NCBI), a section of the National Library of Medicine (NLM) of the United States. It is a helpful tool for researchers in the fields of biology, bioinformatics, and chemistry. PubChem covers the biological activities, chemical structures, and properties of minute organic molecules.

Substances, compounds, and bioassays are the three primary categories of the database. The substances section contains information about unusual chemical substances, including chemical structures, synonyms, and links to related resources. The compounds section provides comprehensive information on specific chemical compounds, including citations to scholarly works, details on their physical and chemical properties, and experimental and anticipated features. The bioassays section contains details on how chemicals affect biological processes. Descriptions of the assays, their outcomes, and bioactivity rankings are all included here.

PubChem offers a range of search and analytical tools to make it easier to retrieve and examine data. Users can search the database using chemical names, IDs, molecular formulas, and chemical structures. Additionally, PubChem provides resources for searching chemical structure similarity, substructure searching, and compound grouping.

Researchers can use PubChem data for a variety of applications. Finding potential therapeutic targets, searching the chemical universe for novel medications, and predicting the biological activities and toxicological profiles of molecules are all made feasible by it.

Additionally, it is simpler to create structure-activity relationship (SAR) models and assess chemical and biological data for research and development purposes.

Users get access to further information on the biological and medical implications of the chemicals and compounds of interest because to PubChem's links to other well-known databases, like PubMed. For scientists conducting work in the areas of chemical biology, small molecule study, and drug discovery, it is a helpful tool.

3.1.3. BIOVIA Discovery Studio Visualizer

Bioinformatics is a vital component of contemporary drug development and research because it allows for the analysis and interpretation of vast amounts of biological data. For the purpose of facilitating bioinformatics activities, Dassault Systèmes developed the comprehensive toolbox known as BIOVIA Discovery. It provides a range of functions for data management, analysis, visualisation, and predictive modelling.

Researchers working in bioinformatics have access to tools for data administration, analysis, visualisation, and predictive modelling through a comprehensive software package called BIOVIA Discovery. Thanks to its extensive set of tools and capabilities, researchers may prioritise drug candidates, speed up the drug development process, and gain valuable knowledge about biological systems. By integrating various data formats, supporting cutting-edge analysis techniques, and encouraging collaboration, BIOVIA Discovery makes it easier to find new medicines and progress bioinformatics research.
In this presentation, I will discuss the primary features and applications of BIOVIA Discovery in the field of bioinformatics research.

Data Management and Integration: Strong data management capabilities in BIOVIA Discovery enable researchers to efficiently organise, store, and retrieve biological data. Different forms of data, including genomes, proteomics, chemical structures, and experimental results, are easier to combine as a result.

a. **Data Integration:** Data from many sources, such as internal data repositories, external databases, and internally generated experimental data, can be integrated using BIOVIA Discovery. This link makes data more accessible and facilitates cross-domain analysis and interpretation.

b. **Data Visualisation:** The programme equips researchers with powerful visual analysis tools for exploring and analysing complex biological datasets. It provides interactive visualisations that help scholars understand the relationships, patterns, and trends in the data.

c. **Data Mining:** Innovative data mining techniques like association rule mining, clustering, and classification are used by BIOVIA Discovery. These techniques make it possible to meaningfully extract data from large databases, find hidden patterns, and generate research hypotheses.

Analysis Tools and Algorithms for Bioinformatics Research: An extensive selection of analysis tools and algorithms are offered by BIOVIA Discovery. These tools aid in the understanding of biological processes, the search for biomarkers, and the prediction of the consequences of genetic variations.

a. **Sequence Analysis:** Sequence alignment, motif detection, and the identification of conserved regions are all features of the programme. When comparing and annotating DNA and protein sequences, these characteristics make it simpler to spot functional elements and evolutionary relationships.

b. **Structure Analysis:** Protein structures may be examined and visualised with the help of BIOVIA Discovery, making it simpler to understand how proteins fold, remain stable, and interact with one another. In order to support efforts in structure-based drug discovery and protein engineering, it offers tools for molecular dynamics simulations, protein-ligand docking, and protein structure prediction.

c. **Network Analysis:** The programme includes tools for network analysis of biological pathways, protein-protein interactions, and gene regulatory networks. These technologies can be used by researchers to identify key players, appreciate network dynamics, and identify fresh medicinal targets.

Predictive modelling and virtual screening tools integrated into BIOVIA Discovery enable the prioritisation and evaluation of potential drug candidates.

a. **QSAR and ADME Models:** The programme simplifies the development and application of quantitative structure-activity relationship (QSAR) and absorption, distribution, metabolism, and excretion (ADME) models. These models predict the biological activity, toxicity, and pharmacokinetic properties of pharmaceuticals, which aid in lead optimisation and compound selection.

b. **Virtual Screening:** Finding potential drug candidates from vast compound libraries is made simpler by the virtual screening techniques in BIOVIA Discovery. It makes use of docking algorithms, pharmacophore modelling, and machine learning approaches to rank compounds according to their anticipated binding affinities and drug-like features.

Cooperation and Workflow Management: The data sharing, project management, and version control features provided by BIOVIA Discovery promote collaboration and speed up bioinformatics workflows.

a. The software enables collaboration by making it simpler to share data, organise projects, and communicate with your team. It enables many researchers to work together, share discoveries, and exchange ideas in a centralised space.
b. **Workflow Management:** The workflow management features of BIOVIA Discovery can be used by researchers to build and utilise bioinformatics pipelines. Its support for automation, repeatability, and the integration of various analysis tools simplifies complex analytical procedures.

3.1.4. SwissDock

One of the main objectives of the field of bioinformatics is to comprehend the interactions between small chemicals (ligands) and target proteins. It supports the study of drug binding mechanisms, the forecasting of protein-ligand complexes, and the creation of new pharmaceuticals. SwissDock, a powerful molecular docking system developed by the Swiss Institute of Bioinformatics (SIB), has received high praise for its accuracy, efficacy, and user-friendly layout. In this post, we'll look at SwissDock's primary attributes and applications within the context of bioinformatics research.

The computational technique known as molecular docking is used to anticipate the ideal orientation and binding affinity of a ligand molecule to a target protein. It involves taking samples of different ligand conformations and orientations within the protein's binding site and scoring them. The goal is to identify the most energetically beneficial docking location, which can provide insight into the interactions between ligands and proteins and guide drug discovery efforts.

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Features and Capabilities of SwissDock: Several tools and algorithms are combined in the web-based molecular docking platform SwissDock to provide accurate and efficient simulations of protein-ligand docking. It is a popular choice for bioinformatics researchers due to a variety of features and skills, including:

a. **User-Friendly Interface:** SwissDock's user-friendly interface makes it simple for researchers to enter their protein and ligand structures, choose docking settings, and view the docking results. The platform is accessible to both seasoned professionals and newcomers to the field.
b. **Ligand and Target Preparation:** Users can carry out tasks including adding missing atoms, improving hydrogen bonds, and charging their ligand and target protein

structures using SwissDock. These pre-processing methods enable the input structures to be optimised for accurate docking simulations.

c. **Docking techniques:** The docking methods used by SwissDock include those based on the fast Fourier transform (FFT), molecular dynamics, and others. These algorithms examine several ligand conformations and orientations inside the protein's binding area in order to establish the ideal docking posture.
d. **Scoring and Ranking:** In order to evaluate the ligand and protein's capacity to bind to one another, SwissDock employs a number of scoring techniques. Hydrogen bonding, electrostatic interactions, van der Waals forces, and shape complementarity are among the factors that these scoring formulas consider. The software ranks the docking poses according to the anticipated binding energies or scores.
e. **Visualisation and Analysis:** SwissDock provides visualisation tools to help researchers analyse the docking data. Users can examine the interactions between ligands and proteins, hydrogen bonding patterns, and residues on binding sites that are crucial for complex formation through interactive exploration of docked complexes.

3.1.5. Chimera

UCSF Chimaera is a versatile piece of software that offers many features for molecular imaging, analysis, and modelling in the field of bioinformatics. Researchers may discover a lot about complicated biomolecular structures and activities thanks to its user-friendly interface and advanced capabilities. UCSF Chimaera enables tasks including protein engineering, molecular dynamics simulations, and structure-based drug design, enhancing bioinformatics research and contributing in the development of fresh medicinal strategies.

In the discipline of bioinformatics, it is crucial to be able to view and interpret complex molecular structures in order to comprehend biological processes and create new therapeutic strategies. UCSF Chimaera, a powerful programme developed by the University of California, San Francisco (UCSF), is well-known for its broad range of molecular imaging, analysis, and modelling features. In this study, we will analyse the key features and applications of UCSF Chimaera within the context of bioinformatics research.

a. Using the broad variety of capabilities provided by UCSF Chimaera, proteins, nucleic acids, and other molecular structures, as well as small molecules, can all be visualised and examined. Using its user-friendly interface, researchers may examine and interact with intricate biomolecular systems, learning crucial information about their structures and functions.
b. UCSF Chimaera is a highly interactive and flexible 3D visualisation environment that enables users to rotate, zoom, and study molecular structures. Support for a wide variety of representational techniques, such as surface representations, ribbon diagrams, and molecular surfaces, facilitates the exploration and analysis of complex macromolecular assemblies.

c. Researchers can see and analyse molecular dynamics simulations, which mimic how biomolecules behave and migrate over time. It provides tools for trajectory analysis, computation of key dynamics parameters, and visualisation of dynamic aspects in order to help researchers better understand protein movements and conformational changes.
d. The sequence and structure analysis tools included in UCSF Chimaera enable researchers to perform tasks including sequence alignment, structure superposition, and structural motif identification. Comparing protein structures, identifying conserved regions, and learning about functional domains are all aided by these traits.
e. **Molecular Modelling and Simulation:** Researchers can build and enhance 3D models of biomolecules based on experimental findings or computational predictions utilising UCSF Chimera's potent molecular modelling and simulation capabilities.

A. Chimaera can be used to generate **homology models**, which forecast the three-dimensional structure of a protein based on its sequence similarity to experimentally identified structures. It provides insightful information about how proteins' structure and function interact to one another and develops precise models using state-of-the-art algorithms.
B. UCSF Chimaera incorporates **molecular docking**, a computer technique that predicts the binding mechanisms and affinities of tiny molecules to target proteins. Researchers may study binding interactions, dock ligands into protein binding sites, and assess the stability of the resulting complexes using Chimaera.
C. **Calculations of electrostatic potentials on molecular surfaces:** Chimaera gives users the ability to compute and visualise electrostatic potentials on molecular surfaces, which makes it easier to understand protein-ligand interactions and identify proteins. This characteristic has significant potential for use in the study of protein binding sites, the identification of key residues involved in ligand binding, and the creation of novel therapeutic compounds.
D. **Integration & Extensibility:** Because UCSF Chimaera supports a wide number of file formats, researchers can import and export data from numerous sources. It efficiently connects to other applications and databases, facilitating the data transmission and expediting complex bioinformatics research workflows.
E. Researchers can expand Chimera's functionality by developing new plugins or by utilising those that have already been developed by the UCSF Chimaera community thanks to the plugin architecture of the software. Because of its extensibility, Chimaera can be tailored to fit specific research goals and integrated into current bioinformatics procedures.
F. **Database Connectivity:** With the help of UCSF Chimera's ability to connect to external databases like the Protein Data Bank (PDB), users can retrieve and view experimental structures right away. The ability to obtain current structural data and conduct comparative research is facilitated by this relationship.

3.1.6. PLIP

An understanding of the interactions between proteins and small molecules is essential in many fields of bioinformatics, including drug discovery, protein engineering, and structural biology. PLIP (Protein-Ligand Interaction Profiler) is a powerful bioinformatics tool for investigating and visualising protein-ligand interactions. The binding processes, significant residues, and non-covalent interactions found in protein-ligand complexes are all usefully revealed. In this study, we will look at the primary features and applications of PLIP in the context of bioinformatics research.

1. **Protein-Ligand Interaction Analysis:** PLIP allows for in-depth analysis of protein-ligand interactions using a wide range of computational approaches. It examines three-dimensional protein-ligand complex structures and generates in-depth analyses and visualisations that highlight crucial interactions and highlight how they influence ligand binding.
2. A critical step in the investigation of ligand recognition and protein function is the automatic identification of binding sites within protein structures by PLIP. Since it identifies cavities, pockets, and active areas, it enables researchers to concentrate on certain areas of interest.
3. **Interaction Profiling:** The non-covalent interactions between proteins and their ligands, such as hydrogen bonds, hydrophobic contacts, salt bridges, and interactions involving the - stacking group, are examined by PLIP. The intensity and frequency of these interactions are quantified, highlighting relevant information about the stability of the protein-ligand complex as well as their frequency and strength.
4. **Residue Analysis:** The contributions made by the main residues involved in ligand binding are described by PLIP. By providing information on the type and degree of interactions for each residue, it helps with understanding the chemical basis of ligand recognition and binding specificity.

In order to analyse protein-ligand interactions and gain a greater understanding of the complex structure-function relationships, PLIP offers visualising tools.

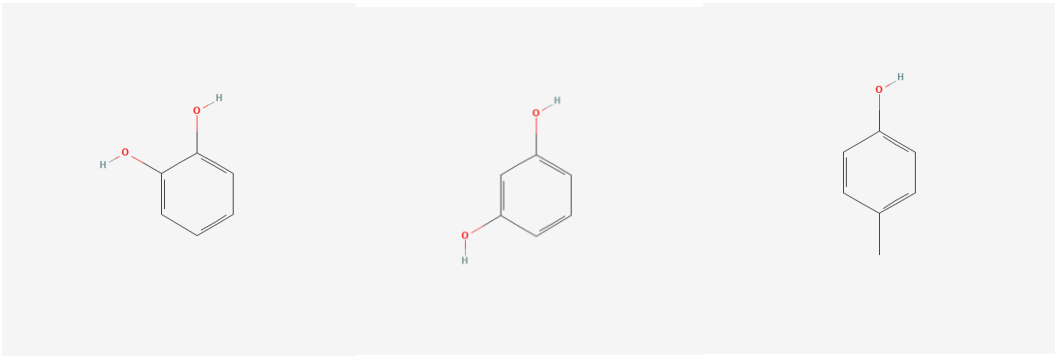
a. PLIP creates **interactive 3D visualisations of protein-ligand complexes** that allow scientists to explore the structure and interactions of the complex. It provides a clear view of the ligand-binding site and identifies key residues implicated in ligand binding.
b. **Interaction Diagrams:** Diagrams of the non-covalent interactions between a protein and a ligand are produced using PLIP. These illustrations provide a concise description of the binding modes and make it simple to identify important interactions that affect ligand binding.
c. **Binding Affinity Estimation:** PLIP connects to other resources such as databases in order to determine the binding affinity between a protein and its

ligand. By employing molecular docking or scoring techniques to gain understanding of the strength of the protein-ligand interaction, scientists can choose prospective treatment possibilities.

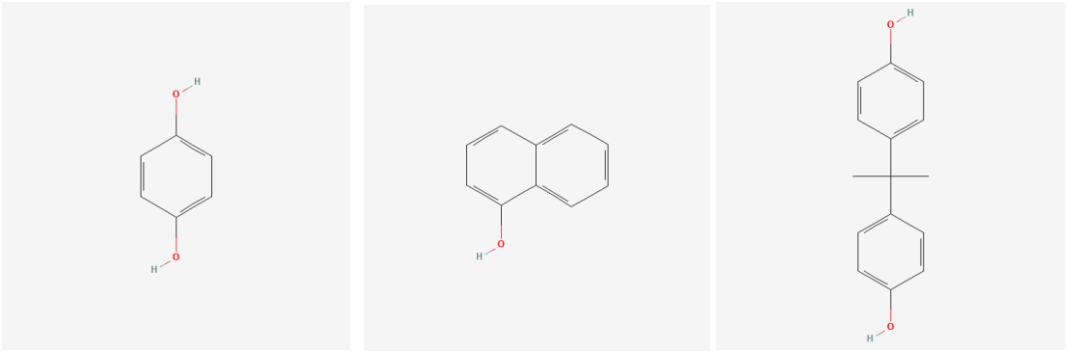
3.2. Workflow

2.2.1. Receptor (enzyme) Ligand (Organic Pollutant) Interaction:

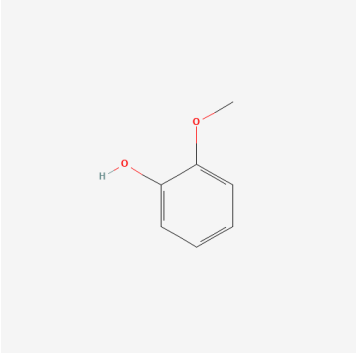
The in-silico ligand (organic pollutant) structure data was obtained from PubChem, while the receptor (enzyme) studies were obtained from Protein Data Bank (PDB) (https://www.rcsb.org/). The docking of the target enzyme laccase, 2H5U, and 10 ligands (organic pollutants) including catechol, resorcinol, cresol, hydroquinone, naphthol, bisphenol, and guaiacol was produced using Biovia Discovery Studio Visualizer (https://discover.3ds.com/discovery-studio-visualizer-download). To create the ligand and receptor, hetero atoms must be taken out of substances like water, non-amino acid groups, and other ligand molecules.



3. Catechol 2. Resorcinol 1. Cresol



5. Hydroquinone 4. Naphthol 6. Bisphenol



7. Guaiacol

Figure. The 2D structure of organic pollutants used for docking analysis. 1. Catechol, 2. Resorcinol, 3. Cresol, 4. Hydroquinone, 5. Naphthol, 6. Bisphenol and 7. Guaiacol

Figure 3: 3D structure of Laccase enzyme

3.2.2. Molecular Docking

In-silico molecular docking typically starts with the design of ligands and receptors. The target enzyme was docked using the SwissDock internet server (http://www.swissdock.ch/docking#) against a few chosen organic pollutants.

3.2.3. Docking Interaction Analysis

Affinity binding (G) values were measured and evaluated. UCSF Chimaera investigated the relationships between organic pollutants and the selected target laccase enzyme. (https://www.cgl.ucsf.edu/chimera/). UCSF Chimaera offers dynamic molecular structure visualisation and analysis through the study of amino acids and associated data, including as density maps and sequence alignments. After comparing the binding energies of organic pollutants and the control, high binding energy organic pollutants were selected.

3.2.4. PLIP Analysis

The amino acid via which the organic contaminants bind to the enzyme was determined using PLIP analysis of the SwissDock outputs that had been downloaded. After comparing the binding energies of the ligands and standards, high binding energy organic pollutants were chosen.The PLIP analysis identified the individual amino acids in the enzyme that interact with the organic pollutants. Only a handful of the interactions described by PLIP include hydrogen bonds, VanderWaals interactions, hydrophobic contacts, and electrostatic interactions. By looking at the output, the amino acids involved in the organic contaminants' binding to the enzyme were found.

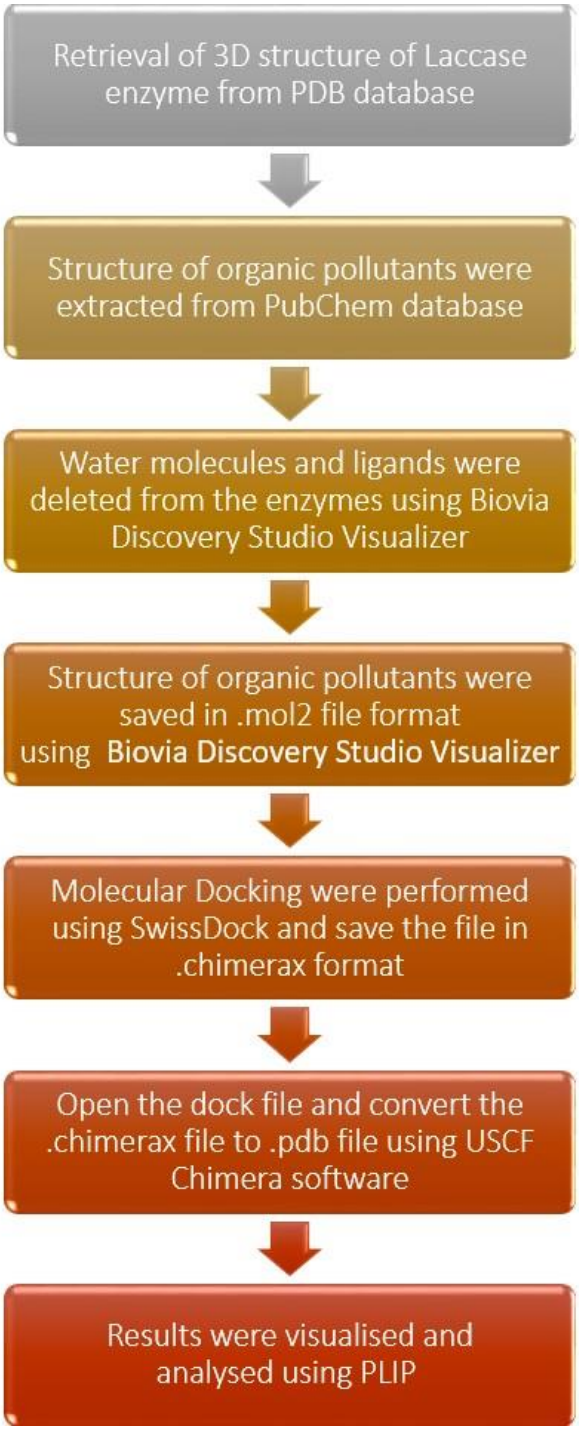


Figure 4: Flowchart of protocol followed

CHAPTER - 4

RESULT AND DISCUSSION

According to the docking results, the laccase enzyme residues of TRP107A, HSD109Z, and TYR116A can form hydrogen bonds (HB), Vander Wall interactions, hydroquinone, cresol, bisphenol, and guaiacol, with respective free energy binding values of -6.32, -6.59, -6.30, -6.36, and -7.

It has been found that the laccase enzyme residues and organic pollutants interact via hydrogen bonds and Vander Waals interactions, indicating a high level of compatibility and affinity. According to the favourable free energy of binding, the organic pollutants may be able to bind to the laccase enzyme's active site. These results have important implications because they show that the laccase enzyme can catalyse and breakdown the organic contaminants. For the contaminants to be effectively degraded, there needs to be a strong Vander Waals contact between them and the enzyme that results in a long-lasting binding in the active site. The identified residues TRP107A, HSD109Z, and TYR116A are crucial for the catalytic activity of the laccase enzyme as well as its ability to bind and degrade these organic pollutants. Further investigation into the precise mechanisms and enzymatic processes that break down these contaminants may shed light on laccase's potential applications in pollution control and environmental remediation. These findings contribute to our understanding of the molecular interactions between organic pollutants and the enzyme laccase and the ability of laccase to degrade organic pollutants. They establish the foundation for future studies that aim to enhance the enzymatic breakdown of organic pollutants and look into laccase's potential as a biotechnological tool for wastewater treatment and environmental remediation.

Table 1: Binding energy (in kcal/mol) of selected organic pollutants

S.No.	Organic Pollutants	ΔG
1.	Hydroquinone	-6.36
2.	Catechol	-6.32
3.	Bisphenol	-7.34
4.	Cresol	-6.30
5.	Resorcinol	-6.59

6.	Guaiacol	-6.25
7.	Naphthol	-6.24

Resorcinol

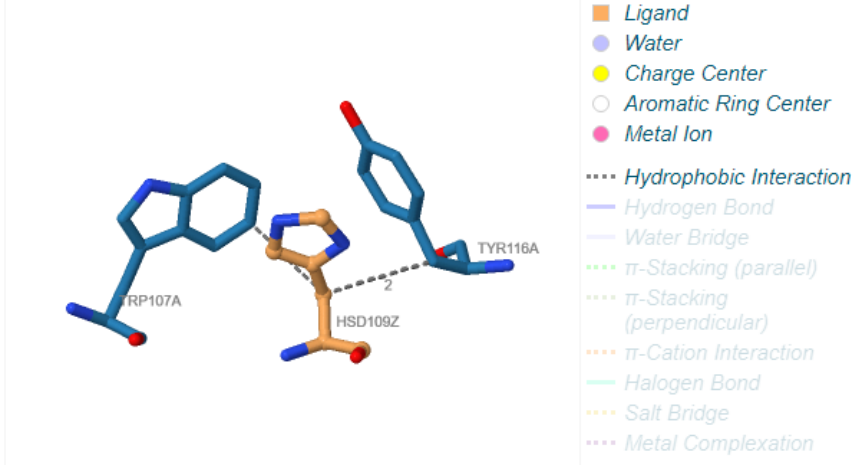
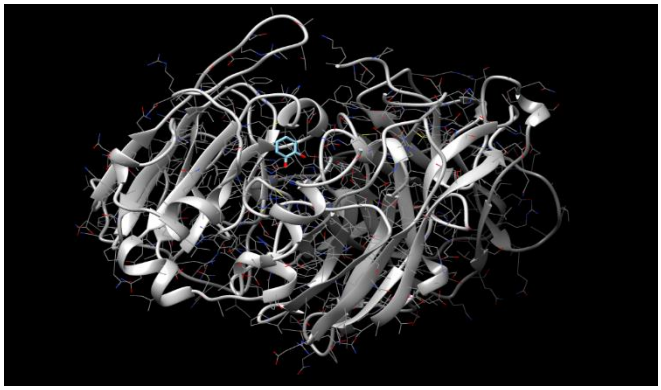


Figure 5: 1. Docking of Resorcinol with Laccase enzyme, 2. PLIP analysis

Catechol



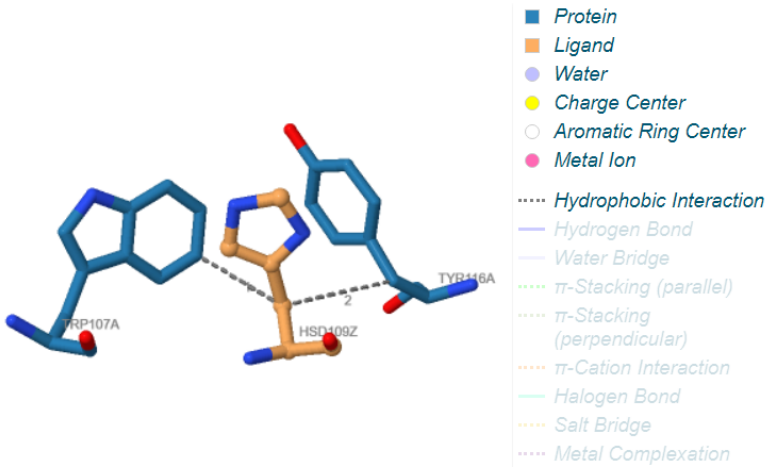
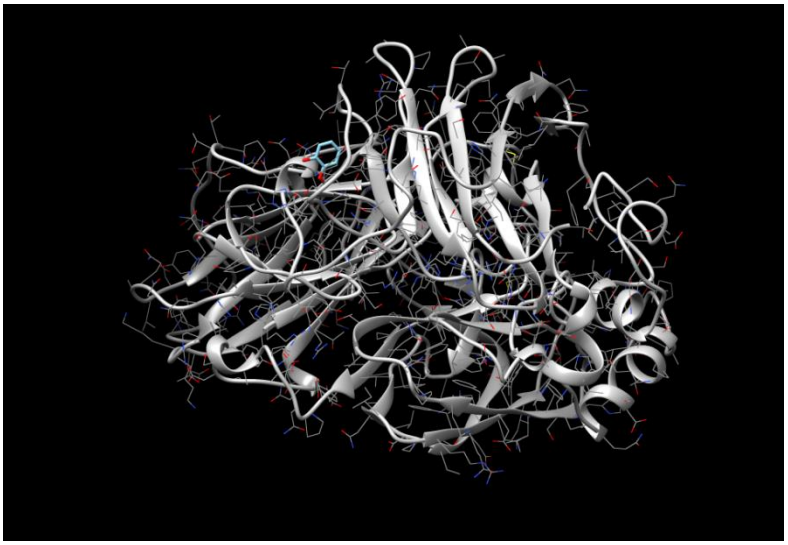


Figure 5: 1. Docking of Catechol with Laccase enzyme, 2. PLIP analysis

Guaiacol



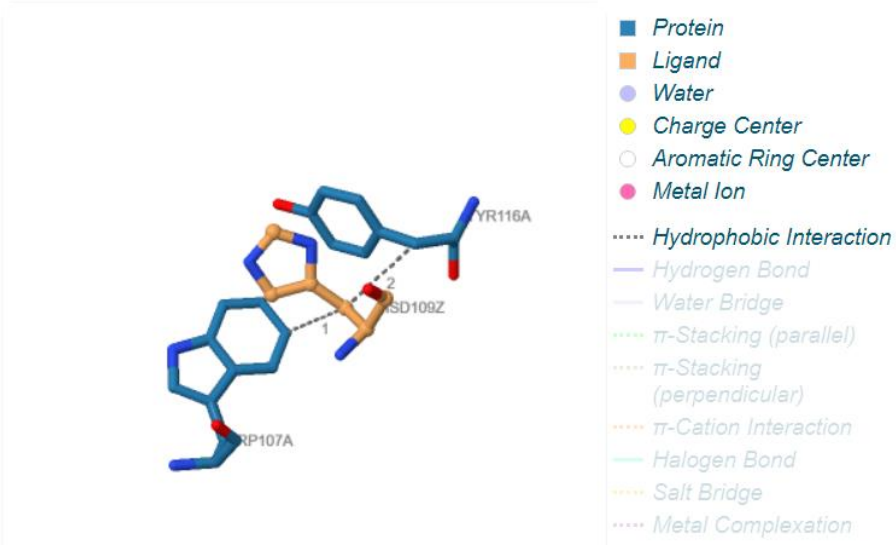
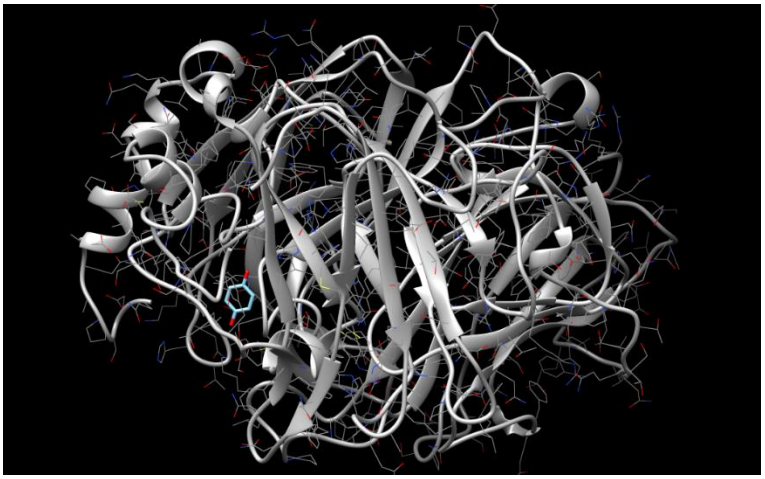


Figure 6: 1. Docking of Guaiacol with Laccase enzyme, 2. PLIP analysis

Hydroquinone



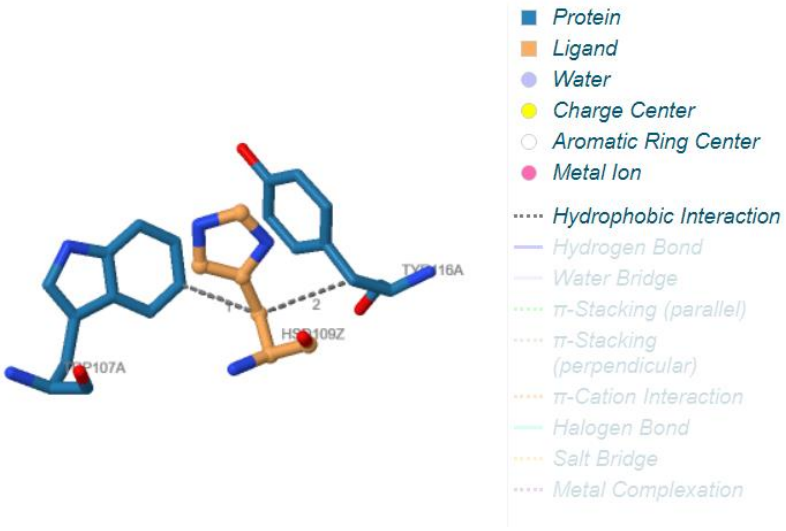


Figure 7: 1. Docking of Hydroquinone with Laccase enzyme, 2. PLIP analysis

Bisphenol

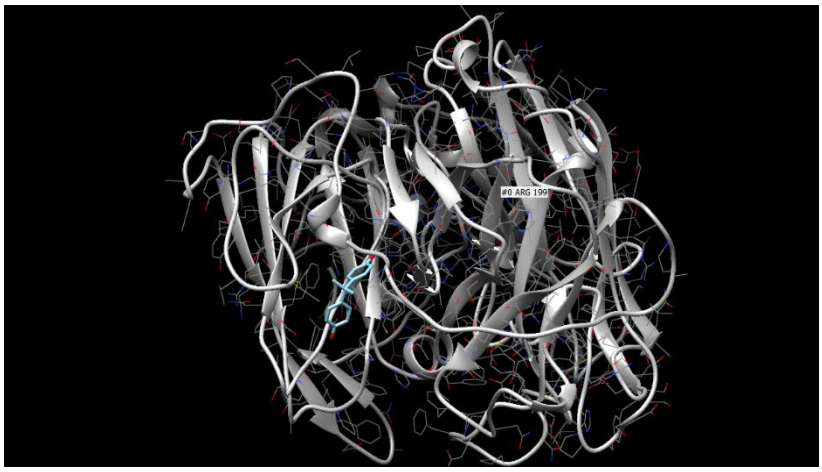


Figure 8: 1. Docking of Bisphenol with Laccase enzyme

Cresol

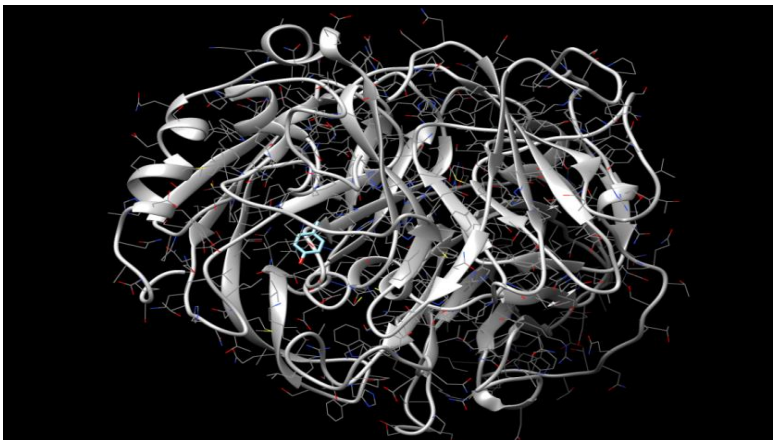


Figure 9: 1. Docking of Cresol with Laccase enzyme

CHAPTER - 5

CONCLUSION AND FUTURE PERSPECTIVE

The effectiveness of contaminant removal by controlling and altering reaction circumstances has received more attention in recent years, but underlying factors including the transformation of enzymes have received less focus. However, enzymes are essential to biodegradation. Studies on how an enzyme and a substrate interact and change can help guide other research projects. Examples of interactions include electrostatic interactions, hydrogen bonds, and hydrophobic interactions. The main lesson to be learned from this review is how promising molecular docking is. The ease of usage and low cost of molecular docking made it popular across many scientific fields. The mechanism of the biological process can be predicted and explained through molecular docking. Humanity won't always profit from advances in science and technology, and some new toxins must be removed. In conclusion, studying reaction pathways utilising this technique will be encouraging for environmental clean-up. However, there are several challenges in melding theory and reality because of diverse circumstances and attention. Molecular docking is a technique used to investigate the physical properties of a substance at the molecular level. The mechanics of electron transfer and enzymatic reactions are complex at the atomic level. The mechanism of the biological process can be predicted and explained, in particular, through molecular docking. Humanity won't always profit from advances in science and technology, and some new toxins must be removed. In conclusion, studying reaction pathways utilising this technique will be encouraging for environmental clean-up. However, there are several challenges in melding theory and reality because of diverse circumstances and attention. Molecular docking is a technique used to investigate the physical properties of a substance at the molecular level. The mechanics of electron transfer and enzymatic reactions are complex at the atomic level.

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