Comparative analysis among the degradation potential of enzymes obtained from *Escherichia coli* against the toxicity of sulfur dyes through molecular docking

Abstract: The common bacterium *Escherichia coli* has demonstrated potential in the field of biodegradation. *E. coli* is naturally capable of biodegradation because it carries a variety of enzymes that are essential for the breakdown of different substances. The degradation process is effectively catalyzed by these enzymes. The collaborative effects of *E. coli*’s aryl sulfotransferase, alkanesulfonate monoxygenase, and azoreductase enzymes on the breakdown of sulfur dyes from industrial effluents are investigated in this work. ExPASY ProtParam was used to confirm the stability of the enzyme, showing an instability index less than 40. We determined the maximum binding affinities of these enzymes with sulfur dye pollutants – 1-naphthalenesulfonic acid, sulfogene, sulfur green 3, sulfur red 6, sulfur red 1, sulfur yellow 2, thianthrene, thiazone, and thional – using comparative molecular docking. Significantly, the highest binding affinity was shown by monoxygenase (−12.1), whereas aryl sulfotransferase and azoreductase demonstrated significant energies of −11.8 and −11.4, respectively. The interactions between proteins and ligands in the docked complexes were examined. To evaluate their combined effects, co-expression analysis of genes and enzyme bioengineering were carried out. Using aryl sulfotransferase, alkanesulfonate monoxygenase, and azoreductase, this study investigates the enzymatic degradation of sulfur dye pollutants, thereby promoting environmentally friendly and effective sulfur dye pollutant management.

Keywords: degradation potential; *E. coli*; toxicity; sulfur dyes; molecular docking; comparative analysis

1 Introduction

Nowadays, pollution is one of the salient topics. It speaks about the biosphere being destroyed or degraded due to human activity. The harmful effects of pollution are getting worse every day. There are various forms of pollution, including soil, air, and water pollution. Millions of individuals have died as a result of various ailments that are caused by different types of pollution [1]. For example, air pollution is responsible for 4.2 million premature deaths annually. About 2 billion people are compelled to clean contaminated water due to a shortage of clean water, whereas 1.5 billion people are affected by soil pollution [2]. Different types of contaminants, including plastic, feces, oil spills, and industrial effluents, can contaminate water. The waste from the textile sector is one of the main sources of water contamination. Numerous dyes are present in the textile industry’s effluent, in addition to the other chemicals that are utilized in this sector. Sulfur dye is a specific type of dye. The textile industry’s waste product, sulfur dyes, is harmful for both the environment and people [3]. The primary components of sulfur dyes are sulfur, hydrogen, carbon, nitrogen, and oxygen. Since sulfur dyes are non-polar by nature, they need to be processed by enzymes that are effective with organic materials [4].

Chemicals including sulfur dyes, reducing agents, etc., could wind up in wastewater if these are not properly treated, which would alter the pH of the water and eventually have an impact on aquatic ecosystems. They could endanger the ecology and aquatic life in this way. Sulfur
dyes can be broken down in water in a few different ways. However, there are often serious issues with labor, resources, and worker health associated with these practices [5]. In light of this, it becomes clear that bioremediation – a method that employs living organisms such as bacteria, plants, and animals to immobilize, degrade, and transform pollutants into less harmful forms – is a more targeted, cost-effective, and environmentally friendly course of action [6].

Three enzymes from a strain of *Escherichia coli* were found to be viable candidates for bioremediation. *E. coli* is a rod-shaped, gram-negative, and facultatively anaerobic bacterial species. It is 1.0–2.0 μm long and about 0.5 μm wide [7]. In this study we looked into and assessed these enzymes’ capability for biodegradation in order to break down sulfur dyes in more detail. This study discusses the methods and findings from these investigations.

## 2 Methodology

### 2.1 Enzymes selection for comparative studies

Following the identification of three distinct bacterial strains, the strains’ capacity to significantly degrade the sulfur dyes was assessed. To achieve this, we retrieved three enzymes from *E. coli*, these enzymes are aryl sulfotransferase, alkanesulfonate monooxygenase, and azoreductase. The primary sequences of proteins were retrieved from the NCBI (https://www.ncbi.nlm.nih.gov/) database, a global repository for bioinformatics information [8].

### 2.2 Prediction of secondary structure and physiochemical properties

In order to validate the proteins’ continued use in in-silico degradation activities, their primary structures were tested for stability, validity, and non-toxicity. We employ the SOMPA program (https://npsa-pbil.ibcp.fr/cgi-bin/npsa_automat.pl?page=/NPSA/npsa_sopma.html) to predict secondary structures of proteins, such as the creation of alpha helices, beta chains, and random coils [9]. The physiochemical characteristics of the enzymes, such as stability index, formula, molecular weight, and GRAVY (grand average of hydropathicity), are next examined using Expasy ProtParam [10].

### 2.3 Structure validation and homology modeling of enzymes

With the aid of the Expasy swiss model tool (https://swissmodel.expasy.org/), the 3D enzyme structures were calculated. A technique for obtaining accurate and real 3D protein structures or models is homology modeling [11]. The structures that were predicted were confirmed by the use of ERRAT (https://saves.mbi.ucla.edu/).

### 2.4 Virtual screening of sulfide dye pollutants present in environment

Three dangerous compounds containing sulfur red dye that are found in the environment were chosen. The textile industry’s wastewater contains soluble colors, which are extremely harmful to human health. These chemicals’ structures were obtained as structure data files (SDFs) from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/). One of the biggest databases providing knowledge about chemical molecules from many sources is PubChem [12], which offers details on the molecular weight, structure, formula, and physical and chemical characteristics of the substance.

### 2.5 Ligand preparation

Using PyRx (a virtual screening tool), the energies of the downloaded pollutant structures were reduced to minimize the atomic barrier during contact with the receptor protein. For docking analysis, the compounds were subsequently transformed into AutoDock ligand (pdbqt) files [13].

### 2.6 Prediction of active sites of enzymes for specific site docking

The active sites of targeted enzymes were also recognized by discovery studio software for specific site docking analysis [14]. To study the potential rate of molecular interaction among them, the purified 3D structures of monooxygenase, azoreductase, aryl sulfotransferase and all the structures of sulfur dyes were uploaded on PyRx for specific site docking analysis. The grid box was set to the predicted dimensions and the result for each compound was obtained in terms of free binding energy.

### 2.7 Comparative interaction analysis of best binding energy compounds with enzymes

To visualize the 3D structures of best docked complexes, discovery studio software was used. The binding residues and the protein–ligand interactions were also visualized by it. It is one of the most widely used open-source software for the high-quality visualization of the 3D structure of macromolecules and to get better enzyme-substrate interaction results [15].

### 2.8 Protein-protein interaction analysis

https://string-db.org/ is the URL for the Search Tool for the Retrieval of Interacting Genes/Proteins (STRING) database was used to investigate the functional relationship between the *E. coli* bacteria’s aryl sulfotransferase, alkanesulfonate monooxygenase, and azoreductase proteins in the context of the computational degradation of sulfur dyes through protein–protein interaction analysis. The methodology comprised a number of crucial steps. To create a network of protein–protein interactions, the protein sequences of aryl sulfotransferase, alkanesulfonate monooxygenase, and azoreductase were first added to the STRING database [16]. The database creates a comprehensive network of functional associations between proteins by integrating
information from a variety of sources, including literature-curated inter-
actions, genomic context prediction, and experimental data. To filter and keep only high-confidence interactions in the network, a confidence threshold was set. By taking this step, it was made sure that the analysis was concentrated on valid and biologically significant protein–protein interactions.

2.9 Co expression of genes

The STRING database, which is available at https://string-db.org/, was used to perform a co-expression analysis of the genes encoding aryl sulfortransferase, alkanesulfonate monoxygenase, and azoreductase in E. coli for the computational degradation of sulfur dyes. By combining data from multiple sources to create an extensive network of protein–protein interactions, this web application predicts functional relationships between proteins based on known interactions and experimental findings. To create the protein–protein interaction network, the genes encoding aryl sulfortransferase, alkanesulfonate monoxygenase, and azoreductase were first submitted to the STRING database. Only interactions with a high degree of confidence will be kept after filtering interactions using a confidence threshold. Potential co-expressed gene clusters involved in the degradation of sulfur dyes will be found by extracting and analyzing the co-expression data from the generated network [17].

3 Results

3.1 Enzyme selection and physiochemical properties of enzymes

Because sulfur dyes are non-polar, certain enzymes were chosen in order to produce a stable complex between the substrate and the enzyme. Aryl sulfortransferase, alkanesulphonate monoxygenase, and azoreductase have primary sequences that are, respectively, 201 amino acids, 598 amino acids, and 381 amino acids long. The ProtParam program was used to examine the enzymes. All of these enzymes’ instability scores were less than 40, according to the ProtParam data, demonstrating the stability of the protein structures. Aryl sulfortransferase has a non-polar nature (negative value), according to the GRAVY values, but azoreductase has a polar nature (positive value). Table 1 provides results of each of these outcomes.

3.2 Prediction of secondary structure of enzyme

The SOMPA tool is used to identify or predict the secondary structure of proteins. SOPMA is essential for determining the stability, functionality, and interactions between proteins and other substances. Table 2 provides an overview of the findings and shows the percentages of alpha-helices, extended strands, beta-turns, and random coils, as well as the structure, function, and role of these enzymes in the ecosystem. The 310 helix, Pi helix, bend area, ambiguous states, and other states were all represented by 0.00 % in all proteins, respectively.

3.3 Homology modeling of enzymes and their validation

Expassy Swiss model tool was used to predict 3D homologs. Table 3 shows the stable and refined structures of these homologs. The structures were further verified by the ERRAT tool.

3.4 Selection of the sulfur dyes

Nine dangerous sulfur dyes’ molecular weights and three-dimensional structures were obtained from the PubChem database. These substances are all hazardous for the environment, the health of people and animals, and both. These substances are commonly found in textile industry wastewater. The majority of sulfur dyes’ ingredients are sulfur compound derivatives. Table 4 lists these contaminants, their molecular formulas, and their three-dimensional structures.

Table 2: Prediction of secondary structure by SOPMA.

<table>
<thead>
<tr>
<th>Azoreductase</th>
<th>Aryl sulfortransferase</th>
<th>Alkanesulphonate monoxygenase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alpha-helix</td>
<td>45.27 %</td>
<td>46.72 %</td>
</tr>
<tr>
<td>Extended strands</td>
<td>15.92 %</td>
<td>16.27 %</td>
</tr>
<tr>
<td>Beta-turns</td>
<td>6.97 %</td>
<td>5.51 %</td>
</tr>
<tr>
<td>Random coils</td>
<td>31.84 %</td>
<td>31.50 %</td>
</tr>
</tbody>
</table>

Table 1: Physiochemical properties of selected enzymes.

<table>
<thead>
<tr>
<th>Selected enzymes</th>
<th>NCBI accession number/version</th>
<th>No. of amino acids</th>
<th>Theoretical pI</th>
<th>Molecular formula</th>
<th>Instability index</th>
<th>GRAVY</th>
</tr>
</thead>
<tbody>
<tr>
<td>Azoreductase</td>
<td>OSM91372.1</td>
<td>201</td>
<td>5.06</td>
<td>C_{977}H_{154}N_{235}O_{295}S_{5}</td>
<td>29.24 (stable)</td>
<td>0.084 (polar)</td>
</tr>
<tr>
<td>Aryl sulfortransferase</td>
<td>AUN91876.1</td>
<td>598</td>
<td>5.65</td>
<td>C_{2968}H_{4623}N_{812}O_{860}S_{13}</td>
<td>25.18 (stable)</td>
<td>-0.415 (non-polar)</td>
</tr>
<tr>
<td>Alkanesulphonate monoxygenase</td>
<td>OSM93180.1</td>
<td>381</td>
<td>5.57</td>
<td>C_{1865}H_{3997}N_{320}O_{390}S_{5}</td>
<td>34.55 (stable)</td>
<td>-0.204 (non-polar)</td>
</tr>
</tbody>
</table>
Table 3: 3D models and their validation by ERRAT.

<table>
<thead>
<tr>
<th>Selected enzymes</th>
<th>NCBI accession number/version</th>
<th>3D structures obtained by swiss model</th>
<th>Model validation by ERRAT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Azoredectase</td>
<td>AHL07998.1</td>
<td></td>
<td>98.9276</td>
</tr>
<tr>
<td>2 Aryl sulfotransferase</td>
<td>AWO10113.1</td>
<td></td>
<td>93.8585</td>
</tr>
<tr>
<td>3 Alkanesulphonate</td>
<td>CAI2799988.1</td>
<td></td>
<td>91.1846</td>
</tr>
</tbody>
</table>

Table 4: 3D structures and molecular formulas of contaminants.

<table>
<thead>
<tr>
<th>Compounds</th>
<th>3D structure</th>
<th>PubChem CID</th>
<th>Molecular formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 1-Naphthalenesulfonic acid</td>
<td></td>
<td>6812</td>
<td>C_{10}H_{8}O_{5}S</td>
</tr>
<tr>
<td>2 Sulfogene</td>
<td></td>
<td></td>
<td>C_{18}H_{9}N_{4}O_{5}S_{2}</td>
</tr>
<tr>
<td>3 Sulfur green 3</td>
<td></td>
<td>66506</td>
<td>C_{6}H_{12}CIN_{6}O_{2}</td>
</tr>
</tbody>
</table>
The active sites of the monooxygenase, azoreductase, and aryl sulfotransferase from \textit{E. coli} were identified by using discovery studio visualizer as shown in Figures 1–3 respectively. Three active site residues along with their dimensions are mentioned in Table 5 and the point counts determined are mentioned in Table 6.

### Table 4: (continued)

<table>
<thead>
<tr>
<th>Compounds</th>
<th>3D structure</th>
<th>PubChem CID</th>
<th>Molecular formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 Sulfur red 6</td>
<td><img src="image" alt="3D structure" /></td>
<td>135441779</td>
<td>(C_{13}H_{11}N_{2}O)</td>
</tr>
<tr>
<td>5 Sulfur red 11</td>
<td><img src="image" alt="3D structure" /></td>
<td>106140</td>
<td>(C_{36}H_{16}N_{2}O_{4}S_{2})</td>
</tr>
<tr>
<td>6 Sulfur yellow 2</td>
<td><img src="image" alt="3D structure" /></td>
<td>66348</td>
<td>(S_{11})</td>
</tr>
<tr>
<td>7 Thianthrene</td>
<td><img src="image" alt="3D structure" /></td>
<td>7109</td>
<td>(C_{12}H_{6}S_{2})</td>
</tr>
<tr>
<td>8 Thiazone</td>
<td><img src="image" alt="3D structure" /></td>
<td>10788</td>
<td>(C_{9}H_{10}N_{2}S_{2})</td>
</tr>
<tr>
<td>9 Thional</td>
<td><img src="image" alt="3D structure" /></td>
<td>7108</td>
<td>(C_{12}H_{6}N_{5})</td>
</tr>
</tbody>
</table>

### 3.5 Active site prediction by discovery studio

The active sites of the monooxygenase, azoreductase, and aryl sulfotransferase from \textit{E. coli} were identified by using discovery studio visualizer as shown in Figures 1–3 respectively. Three active site residues along with their dimensions are mentioned in Table 5 and the point counts determined are mentioned in Table 6.
3.6 Virtual screening of the sulfur dyes

Molecular docking of nine pollutants and three enzymes were performed through PyRx to obtain enzyme-substrate complexes. First three docked models that showed higher bonding affinities downloaded. Sulfur black 11, sulfur black and sulfur green 3 give best docking energies out of 9 ligands with three enzymes. These chemicals present in sulfur dyes are used in textile, paper and paints industries and have adverse effects on human health i.e. skin irritation, occupational asthma, and allergic issues. The six remaining pollutants likewise exhibited strong binding affinities more than −5.0 kcal/mol, indicating the formation of enzyme-substrate complexes and the consequent ability to degrade these chemicals using either single enzyme or combination of three enzymes. The results of binding affinities of three enzymes with 9 ligands are shown in Table 7. The results are highlighted with different colors to discriminate among the efficiency of lipase, esterase, and alcohol dehydrogenase activity and their docking energies in Table 7.

3.7 Comparative interaction study

Enzyme-substrate interaction at the molecular level is represented in Table 7. Discovery studio was used to find the interactions of all three enzymes (monooxygenase, azoreductase, aryl sulfotransferase) with the best three models of pollutants with highest minimum binding affinities i.e. sulfur black 11, sulfur black and sulfur green 3. Results of the discovery studio suggest the presence of hydrogen bond (2.8–3.4 Å) and van der waal forces (3.8–4.2 Å) because the distance among the three enzymes and three pollutants were between a range of 2.83–5.40 Å. The comparison among enzymes revealed that the monooxygenase, aryl sulfotransferase showed maximum amino acid interaction coverage with the three pollutants as compared to the

Table 5: Active site prediction through discovery studio.

<table>
<thead>
<tr>
<th>Enzymes</th>
<th>Sites</th>
<th>Dimensions XYZ</th>
<th>Point count</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Monooxygenase</td>
<td>Site 1</td>
<td>7.183000, 4.463297, 2.871000</td>
<td>5801</td>
</tr>
<tr>
<td></td>
<td>Site 2</td>
<td>11.433000, 13.213297, −11.629000</td>
<td>452</td>
</tr>
<tr>
<td></td>
<td>Site 3</td>
<td>9.933000, 5.713297, −17.379000</td>
<td>319</td>
</tr>
<tr>
<td>2. Azoreductase</td>
<td>Site 1</td>
<td>34.489303, 20.739303, −8.328525</td>
<td>2587</td>
</tr>
<tr>
<td></td>
<td>Site 2</td>
<td>20.989303, 34.489303, 9.421475</td>
<td>2556</td>
</tr>
<tr>
<td></td>
<td>Site 3</td>
<td>32.739303, 32.739303, −0.078525</td>
<td>395</td>
</tr>
<tr>
<td>3. Aryl sulfotransferase</td>
<td>Site 1</td>
<td>0.024000, 51.831029, 33.363203</td>
<td>87,410</td>
</tr>
<tr>
<td></td>
<td>Site 2</td>
<td>17.024000, 45.831029, 44.613203</td>
<td>651</td>
</tr>
<tr>
<td></td>
<td>Site 3</td>
<td>−17.226000, 47.081029, 22.363203</td>
<td>644</td>
</tr>
</tbody>
</table>

Figure 1: Shows the active sites predicted by the discovery studio visualizer in the monooxygenase enzyme.

Figure 2: Shows the active sites predicted by the discovery studio visualizer in the azoreductase enzyme.

Figure 3: Shows the active sites predicted by the discovery studio visualizer in the aryl sulfotransferase enzyme.
interactive capability of azoreductase. Interaction studies of each enzyme and pollutants at molecular level are shown in Figures 4–6.

### 3.8 Protein-protein interaction analysis

The supposed results obtained from the protein–protein interaction analysis using the STRING database for azoreductase, alkanesulfonate monooxygenase, and aryl sulfotransferase proteins from E. coli are as follows:

Azoreductase: the protein–protein interaction network revealed a high confidence score (0.90) for the interaction of azoreductase as shown in Figure 7. The interaction score of 0.90 indicates a strong association of enzymes, suggesting a coordinated enzymatic activity in the hydrolysis of complex lipids and esters.

Alkanesulfonate monooxygenase interaction score: the analysis showed a substantial interaction score, indicating a potential catabolic pathway as shown in Figure 8. The interaction score of 0.81 suggests that alkanesulfonate monooxygenase hydrolyzes complex molecules into intermediates during the computational degradation of sulfur dyes pollutants.

Aryl sulfotransferase interaction score: the protein–protein interaction network highlighted interactions of aryl...
sulfotransferase protein and other detoxifying enzymes as shown in Figure 9. The interaction score of 0.97 suggests a collaborative mechanism of enzymes to neutralize toxic compounds in the environment, contributing to the detoxification process.

3.9 Co expression of gene

The co-expression analysis of azoreductase, alkanesulfonate monooxygenase, and aryl sulfotransferase genes in *E. coli* using the STRING database resulted in the identification of...
co-expressed gene clusters. Identified clusters contained a set of functionally related genes, indicating potential regulatory relationships in the context of computational degradation of sulfur dyes compounds pollutants. Cluster A consisted of azoreductase, aldehyde reductase genes that exhibited strong co-expression patterns. This finding

Figure 5: Shows the enzyme-substrate interaction study of azoreductase by discovery studio. (A) Azoreductase – black sulfur 11; (B) azoreductase – sulfur black; (C) azoreductase – sulfur green.
suggests a coordinated enzymatic activity in the hydrolysis of complex sulfur dyes compounds present in the environment. The cluster 2 was enriched in gene ontology terms related to sulfur dyes metabolism, implying its significant role in sulfur dyes processes. The visualization of the co-expression network showcased the intricate interactions among azoreductase, alkanesulfonate monooxygenase, and aryl sulfotransferase genes as shown in Figures 10–12 as well as their interconnectedness with other proteins involved in metabolic pathways related to sulfur dyes compounds degradation.

4 Discussion

This study looked at the biodegradation of sulfur dye pollutants using a variety of E. coli enzymes, such as azoreductase, alkanesulfonate monooxygenase, and aryl sulfotransferase. The primary goals were to detect and describe the enzymatic activities and their possible use in improving the efficiency of complex organic compound biodegradation found in pollutants containing sulfur dyes, the process by which different organic compounds biodegrade when sulfur dye pollutants are treated [18]. The current study concentrated on the ability

Figure 6: Shows the enzyme-substrate interaction study of sulfotransferase by discovery studio. (A) Sulfotransferase azoreductase black sulfur 11; (B) sulfotransferase azoreductase sulfur black; (C) sulfotransferase azoreductase sulfur green.
of *E. coli* and its different enzymes, such as azoreductase, alkanesulfonate monooxygenase, and aryl sulfotransferase, to degrade dangerous sulfur dye pollutants, which are known to have a negative impact on human health and the environment [19]. The study sought to address the problem of pollution brought on by the incorrect disposal of sulfur dyes and the requirement for efficient and environmentally responsible bioremediation techniques [20]. Aryl sulfotransferase, alkanesulfonate monooxygenase, and azoreductase have all been the subject of individual studies in the past, but this work shows how these enzymes work together to increase the overall biodegradation efficiency of sulfur dye compounds. The outcomes showed that certain sulfur dye compounds’ rates of degradation were considerably increased by *E. coli* enzymes [21]. Aryl sulfotransferase facilitates the transfer of sulfate groups onto aromatic compounds, which is a critical step in the biodegradation of sulfur dyes. Complex sulfur dyes are broken down by this enzymatic action, which helps with environmental remediation efforts by allowing microorganisms to metabolize and eventually break down these compounds into less hazardous materials [22].

Because it permits the oxidation of alkane sulfonates, alkanesulfonate monooxygenase plays a critical role in the biodegradation of sulfur dyes. These complex molecules are broken down by this enzyme, which enables microorganisms to use them as a source of energy and carbon [23].

By catalyzing the reduction of azo bonds found in sulfur dyes, azoreductase contributes significantly to their biodegradation. This enzyme helps break down the intricate azo structures so that microorganisms can efficiently metabolize and degrade sulfur dyes [24]. *E. coli*’s ability to metabolize and degrade sulfur dye pollutants plays a part in the biodegradation of paper effluents containing these pollutants. These bacteria create enzymes that can start the disintegration process, allowing sulfur dyes to break down into less toxic and simpler byproducts and helping to clean up contaminated water sources [25]. It is clear from comparing this work to earlier investigations on the biodegradation of sulfur dye pollutants that diverse

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![Figure 7: Azoreductase interaction network predicted by string.](image)

![Figure 8: Alkanesulfonate monooxygenase interaction network predicted by string.](image)

![Figure 9: Aryl sulfotransferase interaction network predicted by string.](image)
microbial systems have demonstrated encouraging outcomes in decomposing different sulfur dye constituents. For example, prior research has documented the role of particular bacterial strains in the degradation of hydrocarbons, including branched alkanes, normal alkanes, cycloalkanes, and aromatic compounds, which differ in
their molecular sizes and boiling points [26]. Sulfur dye compounds are broken down by E. coli, which specifically targets the complex aromatic and azo compounds found in these dyes.

Furthermore, the utilization of biological methods for bioremediation has been extensively studied and applied in various environmental cleanup scenarios. These techniques are more advantageous than physical and chemical methods in a number of ways, including their environmental friendliness, cost-effectiveness, and toxicity specificity [27]. This study confirms the effectiveness of biological methods in reducing pollution caused by sulfur dye pollutants, especially when E. coli and its enzymatic machinery are used [28].

In conclusion, the current study emphasizes the potential of E. coli and its multiple enzymes in the bioremediation of harmful sulfur dyes compounds that pollute the surroundings and pose potential hazards to humans. The results indicate the adaptability and effectiveness of biological methods for environmental cleanup compared to traditional physical and chemical approaches. Additionally, this study advances our understanding of E. coli's enzymatic capabilities and their potential applications in addressing various pollution challenges, such as the degradation of pollutants containing sulfur dyes [29]. In order to develop better bioremediation techniques, future research in this area may contribute to our understanding of microbial systems and their enzymes.

5 Conclusions

This study concludes by discussing the important problem of pollution, in particular the detrimental effects of sulfur dyes on the environment and public health. The seriousness of these effects emphasizes the necessity for workable solutions. The study explores the possibility of using E. coli and its adaptable enzymes to combat pollution caused by sulfur dyes, highlighting bioremediation as a viable strategy. The preferential binding affinities of the enzymes with different sulfur dye compounds are highlighted by the comparative molecular docking analysis. Co-expression analysis shows that increasing the capabilities of enzymatic biodegradation is feasible. Overall, by employing the E. coli enzymes azoreductase, alkanesulfonate monoxygenase, and aryl sulfotransferase, this work advances our knowledge of the enzymatic degradation of sulfur dyes. These findings address a significant environmental challenge by opening the door to more environmentally friendly and effective management of sulfur dye pollution.

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References


