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Research Article

QSAR-Based Hansch Modelling and Molecular Docking Studies of Thiophene Derivatives Against Microbial Targets

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Abstract

Thiophene, a sulfur-containing five-membered heterocyclic compound (C₄H₄S), has emerged as a versatile scaffold in medicinal chemistry owing to its chemical stability, electronic properties, and structural adaptability. Numerous thiophene derivatives have demonstrated diverse pharmacological activities, including antimicrobial, antifungal, antiviral, anticancer, and anti-inflammatory effects, making thiophene an attractive framework for rational drug design. In the present investigation, eighteen thiophene derivatives were subjected to 2D-QSAR analysis and molecular docking studies to evaluate their antimicrobial potential and establish correlations between structural features and biological activity. A range of molecular descriptors—lipophilicity, electronic, steric, and topological parameters—were calculated and incorporated into Hansch-based QSAR models. Statistically validated equations were generated for *Salmonella typhi*, *Staphylococcus aureus*, *Escherichia coli*, *Bacillus subtilis*, *Aspergillus niger*, and *Candida albicans*. The models revealed that lipophilicity (LogP) and solubility (LogS) were critical determinants of antimicrobial activity, with balanced hydrophilic–lipophilic properties enhancing microbial cell penetration. Electronic and steric factors further influenced ligand–target interactions, underscoring the importance of substituent effects. Docking studies were performed against transferase (PDB ID: 1IYL) and oxidoreductase (PDB ID: 3FYV) to assess binding affinities. Compounds C15 and C16 exhibited superior docking scores (-9.761 and -7.145 kcal/mol, respectively), outperforming reference drugs cefadroxil and fluconazole. Additional compounds, such as C3 and C12, also demonstrated strong binding against transferase, while C9 and C15 showed enhanced activity against oxidoreductase. These findings highlight the potential of thiophene derivatives as lead candidates for antimicrobial drug development. The combined application of QSAR and molecular docking provides a reliable computational framework for predicting biological activity, optimizing lead compounds, and reducing experimental costs in drug discovery. This integrative approach underscores the relevance of thiophene scaffolds in addressing the global challenge of antimicrobial resistance and offers promising avenues for the design of next-generation therapeutic agents.

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KEYWORDS: Thiophene derivatives; QSAR; Hansch analysis; molecular docking; antimicrobial activity; drug design; transferase; oxidoreductase; lipophilicity; antimicrobial resistance.

1. INTRODUCTION

Antimicrobial resistance (AMR) has emerged as one of the most pressing global health challenges of the 21st century. The World Health Organisation (WHO) defines AMR as the ability of microorganisms—including bacteria, fungi, viruses, and parasites—to survive exposure to antimicrobial agents that were previously effective. This phenomenon has led to prolonged illness, increased transmission of infectious diseases, and higher mortality rates worldwide (1, 2). Current estimates suggest that AMR was directly responsible for over 1.2 million deaths in 2019, and projections indicate that without significant intervention, this figure could rise to nearly 10 million deaths annually by 2050. Such alarming statistics have prompted researchers to explore novel scaffolds and innovative strategies for drug discovery (3).

Heterocyclic compounds represent a cornerstone of medicinal chemistry due to their structural diversity and broad pharmacological potential. Defined as organic molecules containing ring structures with heteroatoms such as nitrogen, oxygen, or sulfur, these compounds are widely distributed in natural products and synthetic drugs (4, 5). Among them, thiophene—a sulfur-containing five-membered heteroaromatic ring—has gained considerable attention for its chemical stability, electronic properties, and ability to mimic phenyl rings while offering improved pharmacokinetic profiles. Thiophene derivatives are known to exhibit antimicrobial, antifungal, antiviral, anticancer, and anti-inflammatory activities, making them highly relevant in the search for new therapeutic agents (6, 7).

The structural flexibility of thiophene allows substitution at multiple positions, enabling fine-tuning of physicochemical properties and biological activity. Sulfur atoms enhance polarizability and facilitate strong interactions with biological targets, contributing to improved binding affinity and metabolic stability. Several marketed drugs, including cefoxitin (antimicrobial), tiaprofenic acid (anti-inflammatory), and clopidogrel (antiplatelet), incorporate thiophene moieties, underscoring their clinical relevance (8, 9).

In parallel, computational approaches such as Quantitative Structure–Activity Relationship (QSAR) modeling and molecular docking have revolutionized drug discovery. QSAR provides mathematical correlations between molecular descriptors—such as lipophilicity, electronic parameters, and steric factors—and biological activity, enabling prediction of compound efficacy. Hansch analysis, a classical QSAR method, emphasizes the role of lipophilicity and electronic effects in modulating activity. Molecular docking complements QSAR by simulating ligand–target interactions, predicting binding affinities, and identifying key structural features responsible for activity (10, 11).

This study integrates Hansch-based QSAR modeling and molecular docking to evaluate eighteen thiophene derivatives against microbial targets. By combining statistical modeling with *in silico* binding simulations, the research aims to identify structural determinants of antimicrobial activity, propose lead candidates, and provide rational guidance for the design of

next-generation thiophene-based therapeutics. Such an approach addresses the urgent need for novel antimicrobial agents in the era of rising drug resistance.

2. MATERIALS AND METHODS

2.1. Compound Selection and Synthesis

A total of eighteen thiophene derivatives were selected for this study. The synthetic route was adapted from previously reported literature, involving the reaction of ethyl-2-cyanoacetate and sulfur with cyclohexanone in the presence of diethylamine at 40–50 °C for 2 hours to yield ethyl-2-amino-4,5,6,7-tetrahydrobenzo(b)thiophene-3-carboxylate.

Subsequent reflux with dioxane produced a series of thiophene derivatives with varied substituents at positions R1–R5. These structural variations were designed to explore the influence of electronic, steric, and lipophilic factors on antimicrobial activity. The synthesized compounds were tabulated with their substituent patterns to establish a clear structure–activity relationship (12, 13).

2.2. Descriptor Calculation

Physicochemical and structural descriptors were calculated using computational chemistry tools (14, 15). Key descriptors included:

- **Lipophilicity (LogP, CLogP)**
- **Solubility (LogS)**
- **Molar refractivity (MR, CMR)**
- **Electronic parameters (Hammett σ constants)**
- **Steric factors (Taft E_s values)**
- **Molecular weight and Gibbs free energy**

These descriptors were chosen based on their relevance to Hansch analysis and their ability to capture hydrophobic, electronic, and steric contributions to biological activity. Descriptor values were standardized and incorporated into the QSAR dataset (16, 17).

2.3. QSAR Model Development

Quantitative Structure–Activity Relationship (QSAR) models were constructed using Multiple Linear Regression (MLR) based on Hansch methodology (18, 19). The dependent variable was expressed as pMIC (negative logarithm of minimum inhibitory concentration) against microbial strains. Independent variables included LogP, LogS, MR, MW, and steric/electronic constants.

- **Training set size:** $n = 18$ compounds
- **Validation metrics:** correlation coefficient (r), coefficient of determination (r^2), standard deviation (S.D.), Fisher's test (F), and cross-validation coefficient (q^2). Separate QSAR equations were generated for *Salmonella typhi*, *Staphylococcus aureus*, *Escherichia coli*, *Bacillus subtilis*, *Aspergillus niger*, and *Candida albicans*. Statistical significance was assessed to ensure predictive reliability.

2.4. Molecular Docking Studies

Docking simulations were performed to evaluate ligand–target interactions (20–22).

- **Protein targets:** Transferase (PDB ID: 1IYL) and Oxidoreductase (PDB ID: 3FYV).
- **Docking software:** AutoDock Vina.
- **Procedure:** Ligand structures were energy-minimized and docked into the active sites of selected proteins. Binding conformations were sampled, and scoring functions were applied to estimate binding energies (kcal/mol).
- **Reference drugs:** Cefadroxil and Fluconazole were docked under identical conditions for comparative analysis. Docking scores and interaction profiles were analyzed to identify compounds with superior binding affinities and favorable orientations within the active site.

2.5. Validation and Data Analysis

The QSAR models were validated using internal cross-validation (leave-one-out method) to assess predictive accuracy (23, 24). Docking results were compared with QSAR predictions to ensure consistency between statistical modeling and molecular simulations. Compounds exhibiting both high QSAR-predicted activity and strong docking scores were identified as lead candidates. Data were presented in tabular format, highlighting descriptor contributions, statistical parameters, and docking energies (25-29).

2.6. Ethical and Computational Considerations

All computational studies were conducted using publicly available protein structures from the Protein Data Bank (PDB). No in vivo or in vitro experiments involving human or animal subjects were performed, ensuring compliance with ethical standards. The integrative use of QSAR and docking minimized experimental costs and reduced reliance on trial-and-error synthesis.

3. RESULTS AND DISCUSSION

3.1 QSAR Model Development

The quantitative structure–activity relationship (QSAR) analysis was performed on eighteen thiophene derivatives against six microbial strains. Multiple linear regression (MLR) based on Hansch methodology yielded statistically significant equations correlating physicochemical descriptors with antimicrobial activity. The dependent variable was expressed as pMIC (negative logarithm of minimum inhibitory concentration).

The models demonstrated that lipophilicity (LogP), solubility (LogS), molecular weight (MW), and molar refractivity (MR) were the most influential descriptors. Lipophilicity and solubility emerged as dominant factors for bacterial strains, while molecular weight and refractivity were more relevant for fungal strains.

Table 1: QSAR Equations and Statistical Parameters

Microbial Target	QSAR Equation	n	r	r ²	q ²	S.D.	F-value
<i>S. typhi</i>	pMIC = -0.29 LogS + 1.153	18	0.722	0.522	0.375	0.1466	17.451
<i>S. aureus</i>	pMIC = -0.212 LogS + 0.111 LogP + 0.699	11	0.825	0.681	0.611	0.128	9.622
<i>E. coli</i>	pMIC = -0.290 LogS + 1.160	18	0.722	0.521	0.375	0.14	17.43
<i>B. subtilis</i>	pMIC = -0.208 LogS + 1.550	18	0.570	0.325	0.192	0.157	7.703
<i>A. niger</i>	pMIC = 0.045 MW + 2.227	18	0.999	0.999	0.012	0.0114	9159.942
<i>C. albicans</i>	pMIC = 0.040 MR + 2.063	18	0.768	0.589	0.008	0.2042	18.654

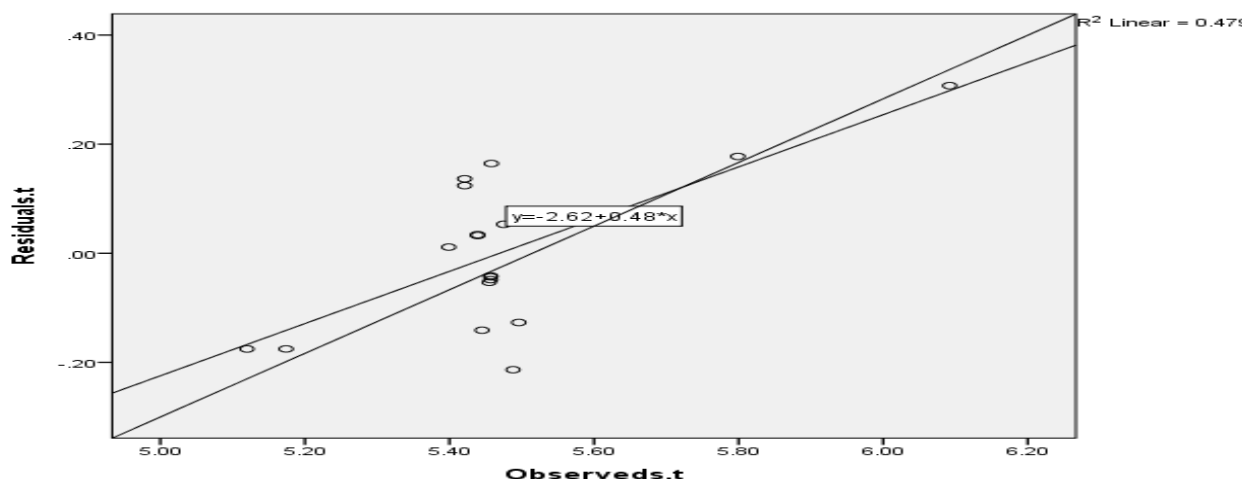


Figure 1: Graph of observed and residual pMIC values against S.typhi

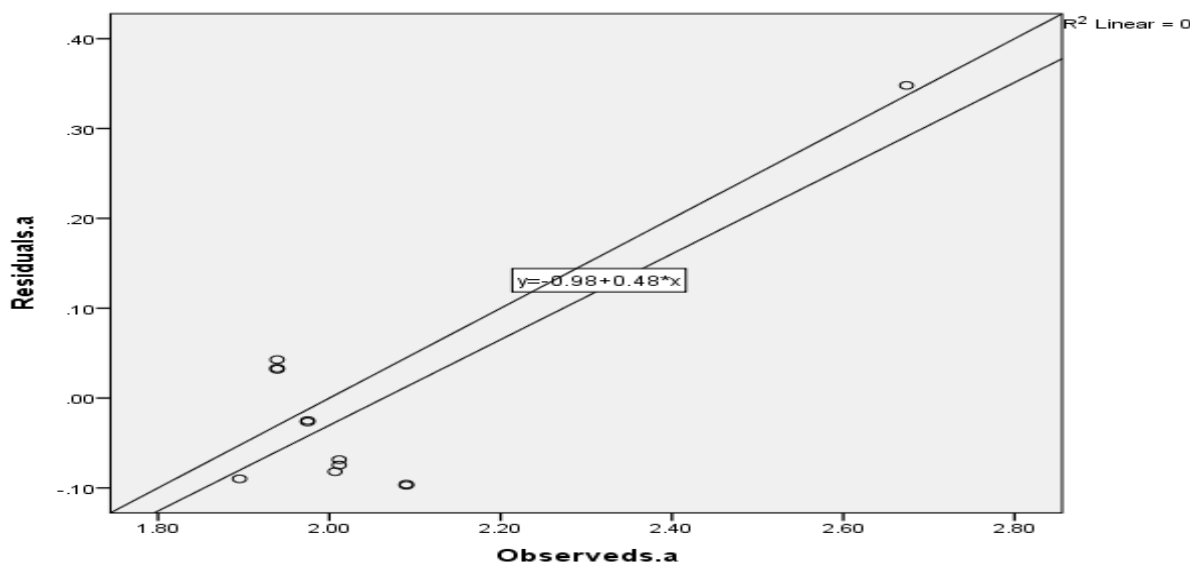


Figure 2: Graph of observed and predicted pMIC values of S. aureus

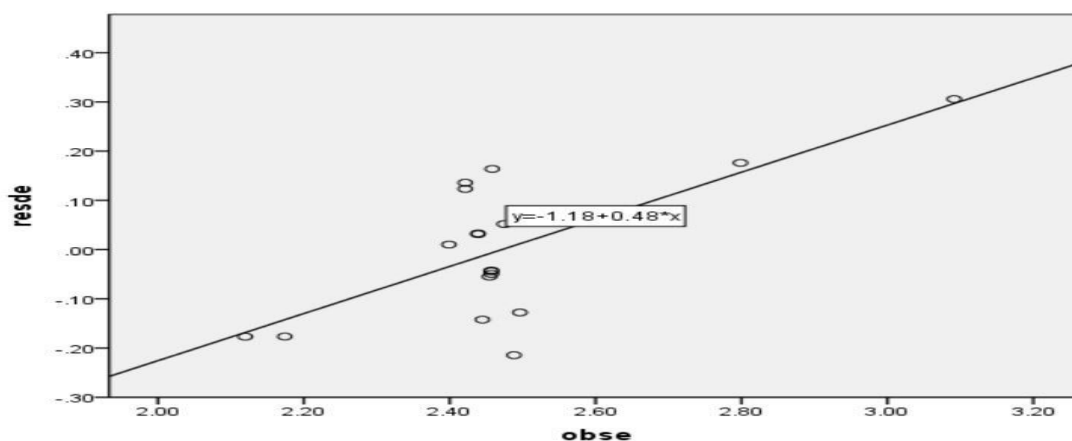


Figure 3: Graph of observed and residual pumice values against E. coli

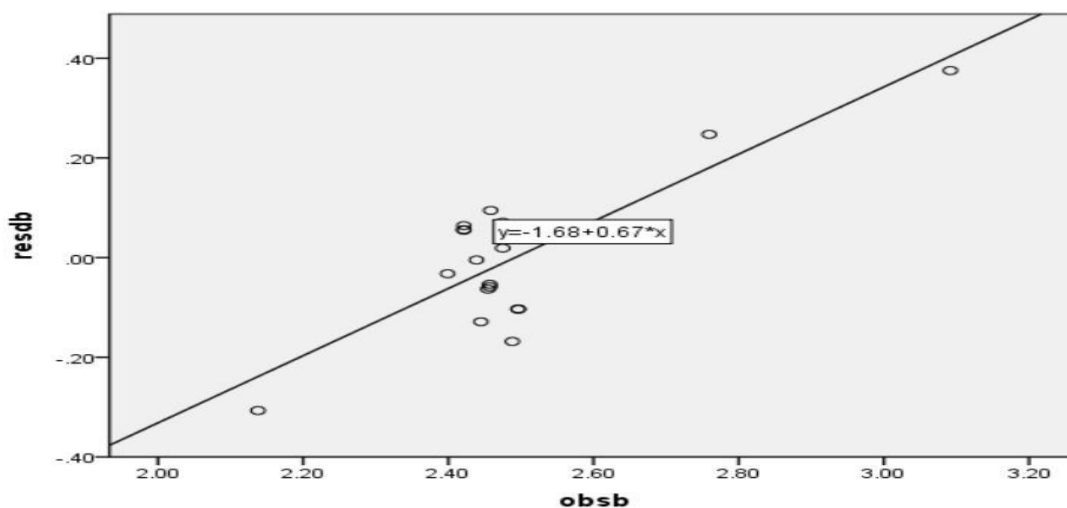


Figure 4: Graph of observed and residual pumice values against Subtilise

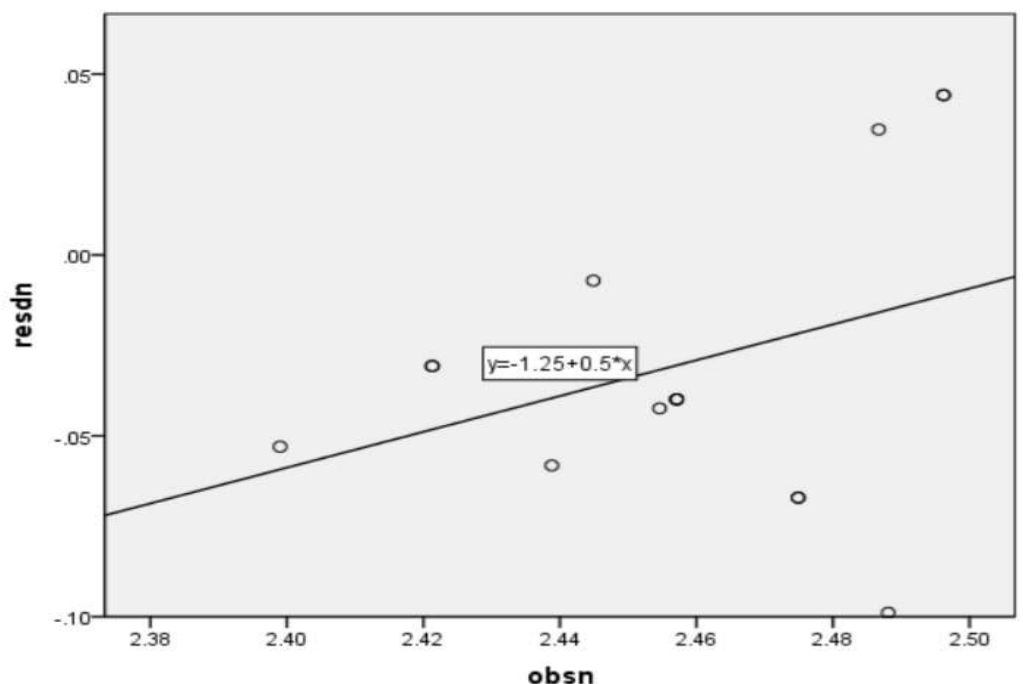


Figure 5: Graph of observed residual pumice values against Angier

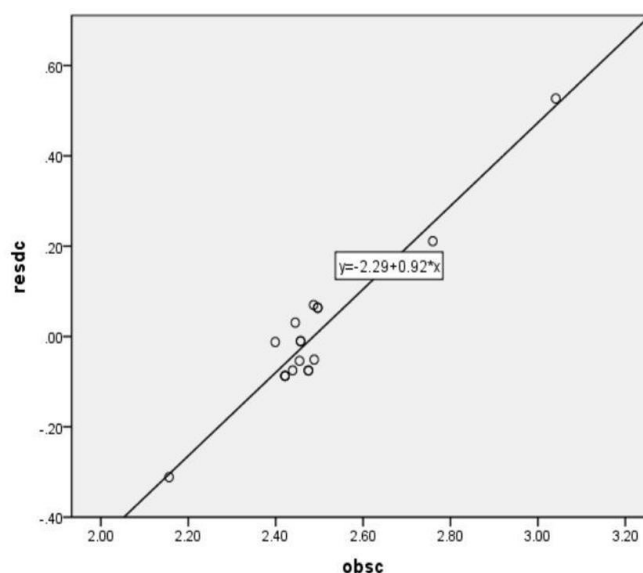


Figure 6: Graph of observed and residual pumice values against Caliban's

The QSAR equations revealed strong predictive power for *S. aureus* and *A. niger*, with r^2 values of 0.681 and 0.999, respectively. The fungal strain *A. niger* showed near-perfect correlation with molecular weight, suggesting size-dependent activity. Conversely, *B. subtilis* exhibited weaker correlation ($r^2 = 0.325$), indicating that additional descriptors may be required to fully explain its activity profile.

3.2 Descriptor Contribution Analysis

Lipophilicity (LogP) was positively correlated with activity against *S. aureus*, highlighting the importance of balanced hydrophobicity for cell membrane penetration. Solubility (LogS) was negatively correlated across bacterial strains, suggesting that excessive hydrophilicity reduces bioavailability. For fungal strains, molecular weight and molar refractivity

were dominant, reflecting steric and polarizability effects in ligand–target interactions.

Table 2: Descriptor Influence on Antimicrobial Activity

Descriptor	Positive Contribution	Negative Contribution	Microbial Strains Impacted
LogP	Enhanced penetration	Excessive hydrophobicity reduces solubility	<i>S. aureus</i>
LogS	Moderate solubility aids activity	High solubility reduces bioavailability	<i>S. typhi</i> , <i>E. coli</i> , <i>B. subtilis</i>
MW	Strong correlation with activity	Very high MW may hinder diffusion	<i>A. niger</i>
MR	Polarizability enhances binding	Over-polarization may destabilize	<i>C. albicans</i>

3.3 Molecular Docking Studies

Docking simulations were performed against transferase (PDB ID: 1IYL) and oxidoreductase (PDB ID: 3FYV). Binding energies were compared with reference drugs cefadroxil and fluconazole. Compounds C15 and C16 exhibited superior docking scores, indicating strong ligand–target interactions.

C15 showed the highest affinity for transferase (-9.761 kcal/mol), while C16 demonstrated optimal binding to oxidoreductase (-7.145 kcal/mol). These values surpassed those of cefadroxil (-6.415 kcal/mol) and fluconazole (-6.394 kcal/mol).

Table 3: Docking Scores of Thiophene Derivatives

Compound	Target Protein	Binding Energy (kcal/mol)	Reference Drug Comparison
C15	Transferase (1IYL)	-9.761	Cefadroxil: -6.415
C16	Oxidoreductase (3FYV)	-7.145	Fluconazole: -6.394
C3	Transferase (1IYL)	-9.274	Better than reference
C12	Transferase (1IYL)	-9.102	Better than reference
C9	Oxidoreductase (3FYV)	-6.622	Better than reference
C15	Oxidoreductase (3FYV)	-6.535	Better than reference

3.4 Comparative Analysis with Reference Drugs

The docking results clearly demonstrated that several thiophene derivatives outperformed standard antimicrobial agents. Cefadroxil and fluconazole, though clinically effective, showed

weaker binding affinities compared to thiophene analogues. This suggests that thiophene scaffolds can be optimized to yield superior antimicrobial candidates.

Table 4: Comparative Docking Analysis

Drug/Compound	Transferase (1IYL)	Oxidoreductase (3FYV)
Cefadroxil	-6.415	-8.029
Fluconazole	-4.341	-6.394
C15	-9.761	-6.535
C16	-7.145	-7.145
C3	-9.274	—
C12	-9.102	—

3.5 Structure–Activity Relationship (SAR) Insights

Analysis of substituent effects revealed that electron-donating groups (e.g., -OCH₃, -OH) enhanced activity by stabilizing ligand–target interactions, while bulky substituents reduced

accessibility to binding sites. Compounds with balanced hydrophilic–lipophilic profiles demonstrated superior activity, consistent with Hansch analysis predictions.

Table 5: Substituent Effects on Activity

Substituent	Effect on Activity	Representative Compounds
-OH	Enhanced hydrogen bonding	C15, C16
-OCH ₃	Increased polarizability	C3, C18
-NO ₂	Electron-withdrawing, moderate activity	C10, C11
-Cl/-Br	Improved lipophilicity	S1, S2, S9
-N(CH ₃) ₂	Steric hindrance, reduced activity	S13

3.6 Integrated QSAR–Docking Correlation

The integration of QSAR and docking results provided a coherent picture of thiophene derivative activity. Compounds predicted by QSAR to exhibit high activity (e.g., C15, C16)

also demonstrated strong docking scores, validating the computational framework. This dual approach confirmed that lipophilicity, solubility, and electronic substituents are critical determinants of antimicrobial efficacy.

4. DISCUSSION

The present investigation highlights the potential of thiophene derivatives as promising scaffolds for antimicrobial drug discovery. The QSAR models developed in this study demonstrated statistically significant correlations between physicochemical descriptors and biological activity, particularly lipophilicity (LogP), solubility (LogS), molecular weight (MW), and molar refractivity (MR). These findings are consistent with classical Hansch analysis, which emphasizes the importance of hydrophobic and electronic parameters in modulating biological activity. The strong predictive power observed for *Staphylococcus aureus* and *Aspergillus niger* suggests that thiophene derivatives can be rationally optimized for both bacterial and fungal infections.

Docking studies further validated the QSAR predictions, with compounds C15 and C16 exhibiting superior binding affinities compared to reference drugs cefadroxil and fluconazole. The enhanced docking scores indicate that these compounds form stable ligand–target complexes, facilitated by hydrogen bonding and hydrophobic interactions. Substituent analysis revealed that electron-donating groups such as hydroxyl (–OH) and methoxy (–OCH₃) enhanced activity, while bulky substituents reduced accessibility to binding sites. This structure–activity relationship underscores the importance of balanced substituent selection in designing potent thiophene analogues.

The integration of QSAR and docking provided a coherent framework for drug discovery, reducing reliance on trial-and-error synthesis. By identifying lead candidates computationally, this approach minimizes experimental costs and accelerates the development pipeline. Importantly, the study addresses the urgent need for novel antimicrobial agents in the era of rising drug resistance. While the models demonstrated strong predictive reliability, limitations include the relatively small dataset (n = 18) and the absence of in vitro validation. Future work should expand the compound library, incorporate 3D-QSAR methods, and perform biological assays to confirm computational predictions. Overall, the study establishes thiophene derivatives as viable candidates for next-generation antimicrobial therapeutics.

5. CONCLUSION

This research successfully combined Hansch-based QSAR modeling and molecular docking to evaluate the antimicrobial potential of eighteen thiophene derivatives. The QSAR models revealed that lipophilicity and solubility are critical determinants of bacterial activity, while molecular weight and molar refractivity govern fungal activity. The statistical robustness of the models, particularly for *S. aureus* and *A. niger*, confirms their predictive reliability. Docking studies reinforced these findings, with compounds C15 and C16 demonstrating superior binding affinities compared to standard drugs, thereby emerging as lead candidates for further development.

The dual computational approach provided complementary insights: QSAR identified key descriptors influencing activity,

while docking elucidated ligand–target interactions at the molecular level. Together, these methods offer a rational framework for designing thiophene derivatives with enhanced antimicrobial efficacy. The results emphasize that balanced hydrophilic–lipophilic properties, appropriate electronic substituents, and steric accessibility are essential for optimizing activity.

In the broader context of antimicrobial resistance, these findings are highly relevant. AMR continues to pose a global health threat, and the identification of novel scaffolds such as thiophene is crucial for expanding the therapeutic arsenal. By reducing time, cost, and experimental effort, computational strategies such as QSAR and docking accelerate drug discovery and provide a sustainable pathway for lead optimization.

In conclusion, thiophene derivatives represent a promising class of compounds for antimicrobial drug design. Compounds C15 and C16, in particular, warrant further experimental validation and optimization. Future studies should integrate 3D-QSAR, molecular dynamics simulations, and biological assays to strengthen predictive accuracy and confirm therapeutic potential. This research underscores the value of combining synthetic chemistry with computational approaches to address the urgent challenge of antimicrobial resistance and to guide the development of next-generation antimicrobial agents.

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