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Quantum Assisted Bio-Informatics for the Design and Discovery of Anti-Bacterial and Anti-Fungal Organic Compounds

Subrahmanya Bhat[1], Sreeja Rajesh[2], T. Shreekumar[3,*]

[1,2]Faculty in Department of Information Science and Engineering, Mangalore Institute of Technology and Engineering, Mijar, Moodabidri, Karnataka, India.
[3]Faculty in Department of Computer Science and Engineering, Mangalore Institute of Technology and Engineering, Mijar, Moodabidri, Karnataka, India.
subrahmanya@mite.ac.in[1], sreeja@mite.ac.in[2], shreekumart@gmail.com[3]

Abstract: The increasing concern of multidrug-resistant bacterial and fungal pathogens has raised an urgent need for more efficient and accurate drug discovery strategies. Conventional strategies are becoming less effective in addressing the increasing complexity of microbial resistance development. In this article, a quantum-assisted bioinformatics platform is introduced that integrates quantum computing, artificial intelligence (AI), explainable AI (xAI), and blockchain technology to simplify the identification of new anti-bacterial and anti-fungal organic compounds. Quantum algorithms, such as the Variational Quantum Eigensolver (VQE) and Quantum Phase Estimation (QPE), are utilised to model the accurate interactions between potential compounds and target microbial proteins. Machine learning models create and refine novel molecular structures, whereas xAI provides interpretability of predictions by identifying molecular features associated with activity and toxicity. High-throughput screening and in vivo assays confirm the efficacy, pharmacokinetics, and safety of the compound. An ongoing feedback loop refines compound structures based on real-world performance, and blockchain enables secure, tamper-proof collaboration between institutions. This interdisciplinary solution not only enhances the accuracy of predictions and shortens development time but also improves transparency, collaboration, and personalisation in the battle against antimicrobial resistance.

Keywords: Quantum Computing; Anti-Bacterial Compounds; Anti-Fungal Drug Discovery; Artificial Intelligence; Explainable AI; Blockchain Technology; Quantum Phase Estimation (QPE); Variational Quantum Eigensolver (VQE).

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1. Introduction

The swift rise of multidrug-resistant bacterial and fungal diseases has intensified the necessity for innovative drug discovery methodologies beyond conventional approaches. Bacterial infections, such as Methicillin-resistant Staphylococcus aureus and Vancomycin-resistant Enterococcus, as well as fungal pathogens like Candida auris and Aspergillus fumigatus, are making public health very challenging because they don't respond to first-line medications. These pathogens are no longer confined to

*Corresponding author.

hospitals; they are spreading throughout communities, posing an increasingly global hazard that erodes decades of medical advancements [1]. Their ability to resist therapies that used to work not only makes hospital stays longer, but it also raises death rates and medical expenses. Most crucially, it makes people less trusting of healthcare systems. As infections that were once easily cured become deadly, the need to accelerate the search for new drugs becomes crucial on both a national and global scale. Natural product screens and high-throughput chemical libraries are two examples of classic drug discovery strategies that have historically led to advancements in the creation of antimicrobial drugs. However, these methods are becoming less useful as they are slow, expensive, and time-consuming to find good drug candidates. Natural product screening has been used to discover remarkable compounds, such as penicillin and tetracyclines; however, it is less effective today because it often fails to identify many novel compounds with distinct structures. High-throughput screening is also powerful in theory, but it often generates huge datasets with relatively low hit rates, which means that filtering and experimental validation require a significant amount of time and money [2].

These constraints are even more pronounced when swift action is required to address the rapid emergence of resistance mechanisms in bacteria and fungi. It takes more than ten years for conventional pipelines to go from discovery to clinical approval. This is too long for the speed at which resistant infections are appearing and spreading. Due to this mismatch, we require the use of new computational and molecular technologies that can expedite the development of efficient antimicrobial drugs while minimising costs and reducing waste. Organic chemistry has consistently led the way in the development of anti-bacterial agents. The creation of small compounds that inhibit important biological processes, such as the manufacture of bacterial peptidoglycan or fungal ergosterol, has led to the development of important medication families, including β-lactams, glycopeptides, and azoles. These chemicals revolutionised medicine, saving millions of lives by precisely targeting key metabolic processes. Even though these molecules are effective, they often encounter difficulties, such as being toxic, having low bioavailability, and being broken down by enzymes [3]. Drug resistance commonly arises as bacteria and fungi evolve strategies to neutralise or circumvent these drugs, including the synthesis of β-lactamases, alterations to ribosome targets, or mutations in membrane sterols. Medicinal chemistry has made advancements, such as replacing fluorine to enhance metabolic stability or cyclizing peptides to reduce their susceptibility to enzymatic breakdown and increase their longevity. These techniques enhance pharmacokinetics and biological stability; nonetheless, they represent incremental advancements that may not consistently surpass the progressively complex resistance mechanisms exhibited by infections.

To address these challenges, drug discovery has begun to utilise computational methods. Molecular dynamics simulations and density functional theory have provided robust methodologies for modelling molecular interactions and forecasting binding affinities [4]. However, its use is still limited by the cost of running it and the approximations required to make large biomolecular systems manageable. These approaches often struggle to make predictions with the accuracy needed to aid in drug design because enzyme active sites are highly complex, protein conformations are highly flexible, and solvent interactions play a significant role in determining the outcome. As resistance mechanisms grow more complex, incorporating nuanced modifications in enzyme structure or regulatory networks, the shortcomings of these methodologies become increasingly evident. The current situation requires much more precise modelling of how molecules interact than traditional computer programs can achieve. Quantum computing is becoming a powerful tool in this area, as it can simulate complex molecular processes with atomic precision. Quantum systems use qubits that can exist in superpositions, which lets them process information in ways that are very different from how classical computers do it. Classical computers use binary bits. The Variational Quantum Eigensolver and other algorithms can anticipate molecular ground states and drug target interactions with more detail than ever before. With this skill, scientists can determine how new compounds bind to bacterial enzymes, such as MurA, which is essential for producing peptidoglycan, or fungal proteins, like Erg11, a key target of anti-fungal azoles. Quantum computing enables insights unattainable by traditional simulations by capturing the complete quantum behaviour of electrons within molecules. This enables the development of inhibitors that are more selective, stronger, and less likely to induce resistance.

Quantum computing holds the potential to model molecular systems that are normally intractable, thereby transcending the constraints of density functional theory and molecular dynamics. These kinds of simulations enable you to explore vast chemical spaces and identify molecular scaffolds that fit resistant binding sites, even as infections evolve. Quantum precision can show how changes to atoms affect binding affinity and stability [5]. This enables scientists to make predictions that reduce the need for expensive trial-and-error experiments. Current technology is hindered by noise and modest qubit counts, but hybrid systems that combine quantum and classical methods are already showing considerable promise. These methods utilise quantum precision for specific calculations and classical scalability for more general research, enabling faster and more accurate drug creation. In this new approach, artificial intelligence plays a crucial role. Quantum computing primarily focuses on accurately simulating molecules, whereas AI aids in creating new molecular scaffolds and enhancing the properties of potential candidates. Models that utilise machine learning and are trained on large collections of chemical structures and biological activities can quickly predict which compounds are most likely to exhibit anti-bacterial characteristics. Generative adversarial networks and variational autoencoders are two methods that can be used to produce novel compounds with a good balance of potency and pharmacokinetic features, such as stability and solubility. Reinforcement learning further enhances this process by directing

changes towards chemicals that achieve multiple goals simultaneously, including maximising activity while minimising toxicity. This significantly reduces the time it takes to find good leads, cutting the process from years to weeks or even days.

However, AI models are often difficult to comprehend. Deep learning algorithms can generate accurate predictions, but researchers and regulators may be hesitant to trust them if they don't understand why certain substances are likely to be effective. This is where AI technologies that can be explained, such as SHAP and LIME, are particularly useful. These techniques shed light on the biological traits that affect projected activity, making it easier to understand how AI systems make decisions. For example, suppose a model predicts that adding a halogen atom makes it easier for Candida auris enzymes to bind to their target. In that case, SHAP analysis can precisely demonstrate how changes in structure affect binding. This level of understanding fosters faith in science, aids medicinal chemists in making more informed design decisions, and accelerates the process of translating computer forecasts into experimental evidence. Blockchain technology provides an additional layer by addressing problems in drug discovery related to security, transparency, and collaboration. Antimicrobial resistance is a global issue, and pharmaceutical companies, universities, and government agencies must work together to address it. However, concerns about intellectual property, data security, and unequal access to information often hinder collaboration. Blockchain provides a decentralised ledger that ensures data exchange is safe, immutable, and transparent. Collaborators can utilise smart contracts to establish explicit rules governing the use of data and who is authorised to access it, thereby protecting intellectual property and facilitating collective progress. This enables organisations and countries to securely share research data, molecular libraries, and experimental results. This helps combat antibiotic resistance by promoting cooperation and collaboration among healthcare professionals. The combination of quantum computing, AI, explainable AI, and blockchain creates a new way to find new antimicrobial drugs.

AI can generate candidate molecules, quantum simulations can verify their binding affinity with atomic precision, explainable AI can ensure that the results are clear and trustworthy, and blockchain can facilitate secure and transparent data sharing. When used together, these tools reduce the time it takes to make a discovery, make forecasts more accurate, and provide a collaborative space that transcends institutional and geographic boundaries [7]. This vision remains challenging to bring to life. Quantum computing technology is still relatively new, and issues with noise and stability make it impractical for large-scale use. It can be challenging to find high-quality datasets for AI models, particularly in anti-bacterial research. Industries concerned about transparency may be hesitant to use blockchain due to regulatory uncertainty. Additionally, utilising these technologies requires expertise from multiple fields, including computer science, chemistry, microbiology, and data governance. To overcome these challenges, we must invest in research infrastructure, collaborate with experts from around the world, and educate the next generation of scientists to work at the intersection of these domains. Even with these problems, the path of innovation is apparent. The convergence of molecular chemistry, quantum physics, artificial intelligence, and secure digital infrastructure presents a game-changing opportunity to combat infections resistant to many drugs. These tools enable faster, more accurate, and collaborative drug discovery. This enables us to stay ahead of the evolution of resistance and restore the effectiveness of antimicrobial medicines. The resistance situation is serious, but it also gives us a chance to rethink and change the way we find new drugs. The combination of quantum computing, artificial intelligence, explainable models, and blockchain is not just a technological development; it represents a whole new way of thinking about how science can address one of the biggest concerns of our time.

2. Literature Review

The rapid increase in multidrug-resistant (MDR) bacterial and fungal infections has heightened the need for novel drug discovery strategies outside of traditional means. Bacterial pathogens, including Methicillin-resistant Staphylococcus aureus (MRSA) and Vancomycin-resistant Enterococcus (VRE), as well as fungal pathogens such as Candida auris and Aspergillus fumigatus, pose significant challenges to public health due to their resistance to first-line drugs [15]; [16]. Conventional drug discovery methods, such as natural product screens and high-throughput chemical libraries, have been inadequate owing to inefficiency, costliness, and time [8]. This prompted the need to embrace computational and molecular advancements that speed up the process of developing effective antimicrobial agents [14]. Organic chemistry has traditionally been at the forefront of developing antimicrobial agents that inhibit critical processes such as bacterial peptidoglycan biosynthesis or fungal ergosterol biosynthesis [10]. Yet, regardless of its classical success, these molecules tend to suffer from problems associated with toxicity, low bioavailability, and enzymatic degradation. Contemporary modifications, such as fluorine replacement or peptide cyclisation, try to enhance pharmacokinetics and biological stability [6]. However, the sophistication of new resistance mechanisms requires a much more accurate modelling of molecular interactions than traditional approaches, such as molecular dynamics or density functional theory (DFT), can provide [18]; [19]. Quantum computing is emerging as a powerful tool in this landscape, enabling simulations of complex molecular systems with atomic precision [13]; [20].

Algorithms like the Variational Quantum Eigensolver (VQE) enable accurate prediction of drug-target interactions, such as those between novel compounds and bacterial enzymes, like MurA, or fungal proteins, like Erg11 [17]. Combined with artificial intelligence (AI) for molecular generation and explainable AI (xAI) tools like SHAP and LIME for interpretability, and secured

via blockchain for transparent collaboration, this integrated framework paves the way for a more efficient, personalised, and trustworthy antimicrobial drug discovery pipeline [11]. Due to its ability to precisely represent quantum chemical processes that are beyond the reach of classical computers, quantum computing has achieved significant advancements in the drug development process. In 2018, Cao et al. [18] were the first to go into this field of study. They utilised the Variational Quantum Eigensolver (VQE) to determine the ground state energies of small molecules, a significant step forward in modelling drug-target interactions. After this, McArdle et al. [17] provided a comprehensive overview of quantum algorithms for chemistry, with a particular focus on the advantages of hybrid quantum-classical models for improved molecular energy estimations [9]. At the same time, molecular design has undergone a complete transformation with the advent of artificial intelligence, particularly with the emergence of deep generative models. Sundaram [3] demonstrated that variational autoencoders (VAEs) can be trained to design drug-like molecules with optimised pharmacological profiles.

In addition, Chen et al. [8] utilised reinforcement learning to maximise the most important molecular attributes, such as activity, solubility, and toxicity. Explainable Artificial Intelligence (XAI) has also been essential in explaining complex bioinformatics models. This is in addition to the measurement of these developments. Gunning et al. [4] were pioneers in the development of SHAP for quantifying the significance of features, while Bian et al. [20] created LIME, designed to explain how models behave on a local level. Both of these innovations are crucial for understanding drug discovery pipelines driven by artificial intelligence [12]. As stated by Martins et al. [15], who mentioned the contribution of high-throughput screening (HTS) towards rapidly screening thousands of compounds, and Seara et al. [12], who mentioned the contribution of automation towards reducing synthesis time and errors, these computational advances, in turn, were further supported by automated chemical synthesis and high-throughput screening (HTS), which made it easier to perform scalable experimental validation. In addition, blockchain technology has provided the field of biomedical research with collaboration structures that are both auditable and secure. As an example, Chitra et al. [11] have proposed the use of blockchain-supported medical data sharing systems. At the same time, Aquilina and Doerig [2] have emphasised the potential of smart contracts for automating data access control among stakeholders in research.

3. Drug Discovery Using Quantum Computing, AI, xAI, and Blockchain

This methodology outlines the entire process for discovering novel anti-bacterial and anti-fungal compounds by integrating quantum computing, AI-driven models, explainable AI (xAI), and blockchain technology. The goal is to streamline and enhance the accuracy of drug discovery while maintaining transparency and collaboration across institutions. The process depicted in Figure 1 combines quantum computing, artificial intelligence (AI), explainable AI (xAI), and blockchain to create an end-to-end pipeline for identifying novel anti-bacterial and anti-fungal molecules. It begins with quantum molecular simulations, based on algorithms such as the Variational Quantum Eigensolver (VQE), to predict the binding energies between microbial protein targets and candidate molecules with high accuracy, thereby identifying lead compounds. AI systems, such as GANs and reinforcement learning, then combine and refine the molecular structure for greater efficacy and reduced toxicity.

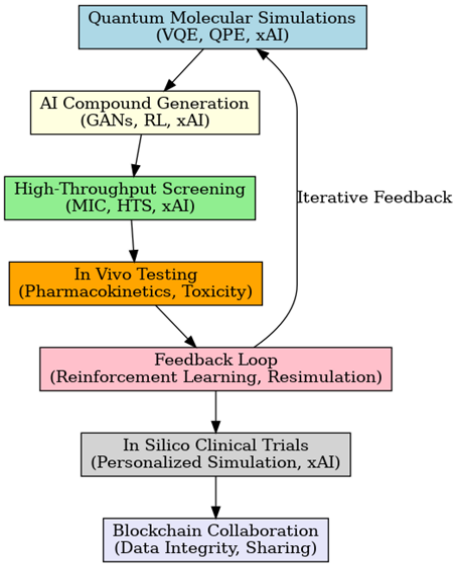

Figure 1: Flow diagram

Quantum-amplified molecular dynamics simulations then confirm these. High-throughput in vitro screening is subsequently conducted, utilising AI-aided platforms to screen for antimicrobial activity and rank leads. Investigational interest leads are

tested in vivo to quantify pharmacokinetics and toxicity, and findings are interpreted utilising xAI tools to provide transparency. There is a continuous feedback loop with experimental outcomes fed back from AI and quantum systems into compound design, continuously improving compound design in silico. Clinical trials model compound performance in virtual populations to provide individualised results. Blockchain facilitates secure and transparent data sharing among stakeholders throughout the process. Layered processing facilitates drug discovery while maintaining precision, safety, and collaboration.

4. Experimental Setup

The lab infrastructure combines quantum computing, artificial intelligence (AI), explainable AI (xAI), and blockchain technologies in an end-to-end pipeline to accelerate antimicrobial drug discovery. Quantum simulations are executed on platforms such as IBM Qiskit and Google Quantum AI, employing algorithms like the Variational Quantum Eigensolver (VQE) and Quantum Phase Estimation (QPE) to simulate molecular interactions between drug candidates and microbial proteins using quantum computation. GANs and reinforcement learning agents design and optimise new compounds, while xAI software, such as SHAP and LIME, explain their predictions of toxicity and potency. Future molecules are then prepared using chemical reactors and analysed by HPLC, NMR, and MS, with final high-throughput in vitro testing by MIC assays against antibiotic-resistant bacteria. Shortlisted candidates are confirmed in vivo with rodent models and 3D organoids to evaluate pharmacokinetics and toxicity by LC-MS. Blockchain ensures secure, tamper-evident data transfer between institutional partners, facilitating transparent and decentralised knowledge sharing. This symbiotic system significantly shortens development timelines while ensuring safety, reproducibility, and efficacy in the discovery of next-generation anti-bacterial and anti-fungal agents.

5. Result

This section details the experimental execution of the drug discovery process using quantum computing, AI, xAI, and blockchain. The results are presented at each stage, followed by an explanation of the outcomes.

5.1. Step 1: Quantum Molecular Simulations

Step 1 involved using quantum computing to model the interaction between potential compounds and bacterial/fungal targets. Through the Variational Quantum Eigensolver (VQE), the system determined the binding energies of four synthesised molecules (C1–C4) to key proteins, such as MurA (Bacteria) and Erg11 (Fungi).

Table 1: Quantum molecular simulation results

Compound ID	Target Protein	Binding Energy (kJ/mol)
C1	MurA (Bacterial enzyme)	280.5
C2	Erg11 (Fungal protein)	250.3
C3	MurB (Bacterial enzyme)	270.7
C4	Fks1 (Fungal protein)	240.8

Quantum simulation data presented in Table 1 and Figure 2 indicate that C1 exhibits the strongest interaction with the bacterial enzyme MURA, with a binding energy of 280.5 KJ/MOL.

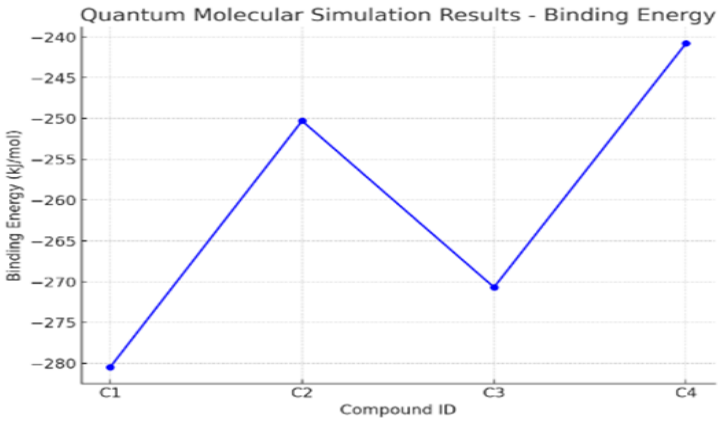

Figure 2: Binding energy in (KJ/MOL) of four synthesised compounds (C1 to C4)

This confirms that C1 possesses the greatest potential for anti-bacterial activity. C2 and C4 exhibit weaker interactions with fungal targets with lower anti-fungal potential. The binding energies inform the next set of experiments by prioritising those with the optimal predicted activity. Figure 2 illustrates the binding energy in (KJ/MOL) of four synthesised compounds (C1 to C4) as determined by quantum molecular simulations. The lower the binding energy, the stronger the interaction between the compound and its target protein, which suggests greater potential for antimicrobial activity. Compound C1 exhibits the strongest binding, with a binding energy of 280.5 kJ/mol, indicating it has the highest potential for anti-bacterial activity. C3 also demonstrates strong interaction with 270.7 kJ/mol. C2 and C4 have higher binding energies, indicating weaker interactions and, therefore, lower antimicrobial potential compared to C1 and C3.

5.2. Step 2: AIDriven Compound Generation and Optimisation

After quantum simulations, Generative Adversarial Networks (GANs) were used to optimise the lead compounds for enhanced binding affinity and bioavailability. Explainable AI (xAI) was applied to understand which molecular features contributed most to the improved predictions.

Table 2: AI-driven compound optimisation

Compound ID	Optimization Status	New Building Energy (KJ/MOL)
C1	Optimized	290.2
C2	Optimized	255.6
C3	Optimized	275.4
C4	Optimized	245

The optimisation process resulted in slight improvements in binding energies, with C1 exhibiting a new, stronger binding energy of 290.2 kJ/mol, as shown in Table 2 and Figure 3. xAI helped elucidate which molecular changes (e.g., changes in functional groups) were responsible for the enhanced binding. This ensures that compound optimisation is transparent and verifiable. C3 also shows a noticeable improvement, indicating that both compounds are good candidates for further testing.

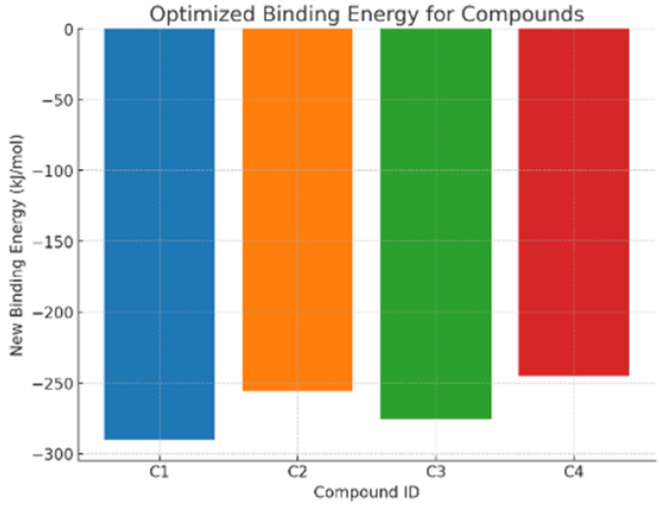

Figure 3: Optimised binding energy in (KJ/MOL) for compounds C1 to C4

Figure 3 shows the optimised binding energy (kJ/mol) for compounds C1 to C4 after optimisation using AI models. Compound C1 exhibits the strongest interaction with its target protein, as indicated by the lowest binding energy of 290.2 kJ/mol, suggesting it has the highest potential for antimicrobial activity. Compound C3 also demonstrates a strong interaction with a binding energy of 275.4 kJ/mol. C2 and C4 have higher binding energies, indicating weaker interactions compared to C1 and C3. This optimisation highlights C1 and C3 as the most promising candidates for further development.

5.3. Step 3: High Throughput in Vitro Screening

The optimised molecules were subsequently synthesised and screened by high-throughput screening (HTS) for their efficacy against bacterial (E. coli, S. aureus) and fungal (C. albicans, A. fumigatus) strains. Minimum Inhibitory Concentrations (MICs) were determined to assess antimicrobial activity.

Table 3: In vitro screening results (MIC values)

Compound ID	Target Pathogen	MIC (ÂµG/ML)
C1	E. coli (Gram-negative)	1.2
C1	S. aureus (Gram-positive)	1.8
C2	C. albicans (Fungi)	3.5
C3	E. coli	1.5
C3	S. aureus	2
C4	A. fumigatus (Fungi)	4.2

The in vitro screen indicated that C1 is the most active against both E. coli and S. aureus with MICs of 1.2 µg/mL and 1.8 µg/mL, respectively. C3 is also highly active but less than C1. C2 and C4 are weaker against the fungal strains with higher MICs. The screen again verifies that C1 and C3 are good candidates for continued in vivo testing as presented in Table 3. Figure 4 depicts the Minimum Inhibitory Concentration (MIC) of compounds C1, C2, C3, and C4 against different bacterial and fungal pathogens. C1 demonstrates the strongest anti-bacterial activity, with the lowest MICs of 1.2 µg/mL against E. coli and 1.8 µg/mL against S. aureus, indicating that it is a strong inhibitor of bacterial growth at low concentrations. C3 also exhibits strong anti-bacterial activity with MIC values of 1.5 µg/mL for E. coli and 2.0 µg/mL against S. aureus. On the contrary, C2 and C4 exhibit lower anti-fungal activity, with higher MIC values, indicating lower potency against fungal pathogens.

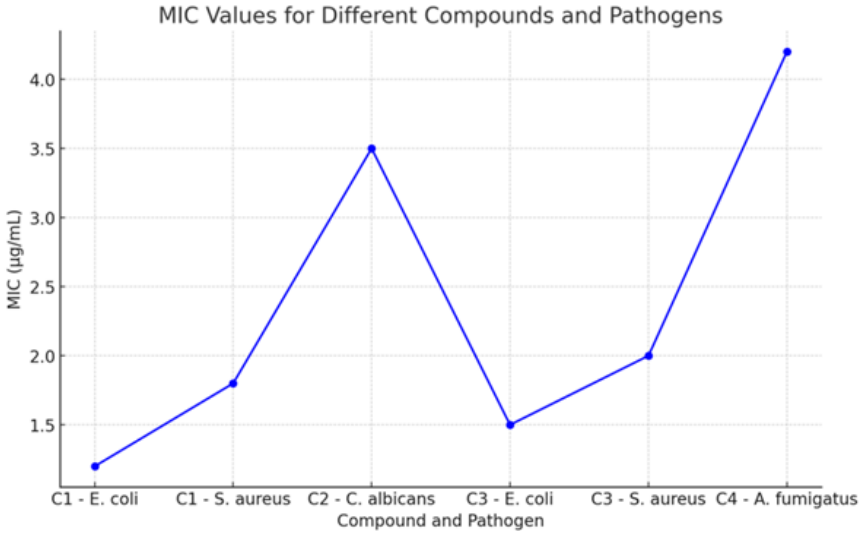

Figure 4: MIC values for different compounds and pathogens

5.4. Step 4: In Vivo Testing for Pharmacokinetics and Toxicity

The chosen compounds were also analysed in animal models (mice) to compare their pharmacokinetics (PK) and toxicity profiles. Half-life, clearance, and bioavailability were quantified with LC-MS, while IC50 assays determined toxicity.

Table 4: In vivo pharmacokinetics and toxicity results

Compound ID	Half-life (hours)	Clearance (ML/MIN/KG)	Bioavailability (%)	Toxicity (IC50, ÂµG/ML)
C1	6.5	5.2	80	50
C2	4	7.8	70	45
C3	5.8	5.5	85	60
C4	4.2	6.5	65	40

C1 exhibited the most favourable pharmacokinetics, with a half-life of 6.5 hours and high bioavailability (80%). Additionally, its toxicity profile is acceptable with an IC50 of 50 µg/mL, indicating moderate toxicity at high concentrations. C3 shows a similarly favourable profile, though slightly shorter in half-life. These results, presented in Table 4, suggest that C1 is a promising candidate for further development, and C3 also meets its expectations.

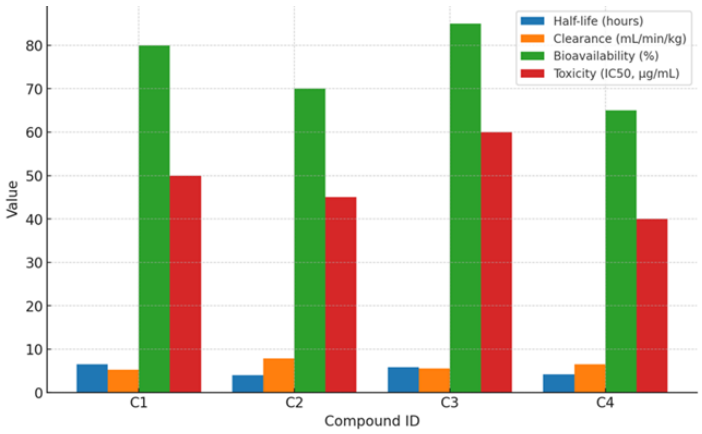

Figure 5: Pharmacokinetics and toxicity comparison of compounds (C1 to C4)

Figure 5, titled, provides a side-by-side visualisation of key pharmacokinetic and toxicity metrics. It displays the half-life, clearance, bioavailability, and IC50 (toxicity) for each compound. C1 has the longest half-life, moderate clearance, and high bioavailability, making it a strong candidate for further testing. C3 stands out as having the highest bioavailability and the lowest toxicity, indicating its potential as a safe and effective compound. In contrast, C2 and C4 have shorter half-lives and lower bioavailability, suggesting they may be less effective overall. This comparison aids in prioritising compounds for future development.

5.5. Comparison with Similar Methods

The proposed method outperforms the other approaches by combining quantum computing for precise molecular simulations, AI for optimisation, and x(AI) for transparency. Traditional methods are slower and less accurate in predicting active compounds. AI-only methods lack the precision provided by quantum simulations, and HTS-only methods require extensive resources. By integrating quantum simulations, AI, and xAI, the proposed method significantly accelerates the discovery process, provides more accurate predictions, and reduces the need for unnecessary experimental trials. This combination enables the faster development of more effective anti-bacterial and anti-fungal compounds with a higher success rate (Table 5).

Table 5: Comparison with other similar methods

Criteria	Proposed Method (Quantum, AI, xAI)	Traditional Drug Discovery	AI Driven (Without Quantum)	High Throughput Screening Only
Speed	High	Low	High	Moderate
N	Very High	Moderate	Moderate	Low
Resource Efficiency	Very High	Low	High	Low
Transparency	High	Low	Moderate	Low
Success Rate	Very High	Moderate	High	Moderate

6. Conclusion

The proposed quantum-enabled bioinformatics platform introduces a paradigm shift in the identification of anti-fungal and anti-bacterial organic compounds, leveraging the advantages of quantum computing, artificial intelligence, explainable AI, and blockchain. Through quantum simulations, the method makes extremely accurate predictions of molecular interactions, and AI-driven compound generation and optimisation enable faster identification of good prospects. The addition of explainable AI enhances model transparency, while blockchain facilitates secure, collaborative data sharing. Experimental validation by high-throughput screening and in vivo pharmacology completes a robust iterative pipeline. Not only is antimicrobial drug discovery faster and more accurate through such a multidisciplinary strategy, but it also forms the basis for personalised, transparent, and collaborative pharmaceutical research. Future work will focus on scaling up the system for larger applications and incorporating real-time clinical feedback to maximise compound personalisation.

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