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Design In Silico Docking And Polymeric Micelle Formulation Of New Benzothiazole Analogs As Antimicrobial Agents

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ABSTRACT

The emergence of multidrug-resistant pathogens necessitates the development of novel antimicrobial agents. Benzothiazole derivatives exhibit promising biological activity due to their versatile structural scaffold. In this study, new benzothiazole analogs were designed and evaluated for their binding affinity against bacterial target proteins through in silico docking studies. To enhance solubility, stability, and delivery efficiency, these compounds were incorporated into polymeric micelles. Docking results demonstrated significant binding interactions, indicating potential antimicrobial efficacy. The polymeric micelles displayed uniform particle size and high encapsulation efficiency, suggesting improved bioavailability. This integrative approach provides a platform for further experimental validation of benzothiazole analogs as effective antimicrobial agents.

Keywords: *Silico, Docking, Polymeric, Micelle, Benzothiazole, Analog, Antimicrobial Agents.,*

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1. INTRODUCTION

Multidrug-resistant (MDR) bacteria have become a major global public health concern due to their fast spread and development. The effectiveness of traditional antibiotics is eroding, leading to longer-lasting infections, increased medical expenses, and greater death rates. Therefore, a top objective in contemporary medicine is the creation of innovative antimicrobial medicines that can efficiently target resistant bacterial strains. In this regard, smart drug design in conjunction with sophisticated formulation and computational techniques presents a viable way to quicken the identification of strong antibacterial substances.

The diverse pharmacological profile of benzothiazole derivatives has garnered significant attention. A thiazole molecule fused to a benzene ring characterizes these heterocyclic compounds, which are known to have antibacterial, anticancer,.

antiviral, and anti-inflammatory properties. They can fine-tune their interactions with particular molecular targets, like bacterial enzymes, by modifying their structural scaffold with substitutes. It is possible to enhance the binding affinity, selectivity, and therapeutic efficacy of benzothiazole analogs by carefully adding electron-donating or electron-withdrawing groups

In the early stages of drug development, computational methods—in particular, in silico docking—have become essential tools. Docking studies enable a molecular-level prediction of the interactions between small compounds and target proteins, revealing information about binding patterns, affinity, and possible inhibitory effect. Prior to expensive and time-consuming experimental methods, this enables researchers to select the most promising candidates. To evaluate benzothiazole analogs' antibacterial potential, the current work docked them against bacterial DNA gyrase, a crucial enzyme in DNA replication.

Drug development also faces a significant obstacle in the delivery of hydrophobic molecules, which frequently have low stability, restricted bioavailability, and poor solubility. Formulating polymeric micelles has become a potent way to get around these restrictions. In aquatic conditions, amphiphilic block copolymers, such Pluronic F127 and PEG-PLA, self-assemble to produce micelles with a hydrophobic core that can encapsulate poorly soluble medicines and a hydrophilic shell that guarantees aqueous stability and controlled release. Benzothiazole analogues are added to polymeric micelles to increase their solubility, prevent degradation, and potentially increase their medicinal efficacy.

The current work combines polymeric micelle formation, in silico docking, and rational chemical design to create new benzothiazole analogs with improved antibacterial efficacy. This study intends to find potential candidates for additional experimental validation by fusing sophisticated delivery techniques with computational predictions, offering a platform for tackling the growing danger of bacterial infections that are resistant to drugs..

1.1 Background

The heterocyclic chemical benzothiazole is characterized by a thiazole molecule fused to a benzene ring, creating a flexible scaffold with a broad range of biological functions. By interacting with essential bacterial enzymes and cellular components, its derivatives have shown strong antibacterial potential by disrupting vital physiological functions and preventing the growth of microorganisms. It has been demonstrated that structural changes to the benzothiazole core, especially the inclusion of substituents that donate or withdraw electrons, significantly affect binding affinity, selectivity, and overall antibacterial activity. By rationally designing compounds that better fit the active sites of bacterial targets, such chemical alterations improve therapeutic effects. In order to maximize interactions with proteins like DNA gyrase or other vital bacterial enzymes, functional groups on the benzothiazole ring can also be strategically positioned to modify hydrophobicity, hydrogen bonding potential, and steric effects. Because of these characteristics, benzothiazole derivatives are very attractive options for finding new antimicrobial medicines that can combat the growing menace of diseases that are resistant to drugs.

Realizing the therapeutic promise of hydrophobic benzothiazole analogs still depends on efficient drug transport in addition to molecular design considerations. The restricted bioavailability and poor water solubility of several benzothiazole derivatives limit their practical application. Polymeric micelles made of amphiphilic block copolymers, like Pluronic F127 or PEG-PLA, have become very successful nano-carrier systems in order to get over these restrictions. The hydrophilic corona stabilizes the structure and promotes dispersion in biological fluids, while the hydrophobic core of these micelles self-assembles in aqueous settings to encapsulate poorly soluble medicinal molecules. In addition to improving medication solubility, this nanocarrier method prolongs circulation duration, prevents chemical degradation of the encapsulated molecules, and permits controlled and sustained release at the target region. Researchers can create benzothiazole analogs that are structurally optimized for target binding and formulated for enhanced bioavailability by combining computational docking studies with polymeric micelle-based delivery. This helps to close the gap between molecular design and real-world therapeutic application.

1.2 Brief Literature Review

The antibacterial properties of benzothiazole derivatives have been emphasized in a number of investigations. According to Singh et al. (2020), antibacterial activity against both Gram-positive and Gram-negative pathogens is increased when particular locations on the benzothiazole ring are substituted. Saha et al. (2021) showed how effective computational screening is at forecasting antimicrobial activity by using in silico docking to find high-affinity benzothiazole analogs that target bacterial DNA gyrase. Furthermore, a lot of research has been done on the use of polymeric micelle formulations as a delivery method for hydrophobic medications. Zhang et al. (2022) have demonstrated that micelles increase the solubility, stability, and controlled release of drug molecules, which increases therapeutic efficacy. The objective of this research is to solve the issues of efficacy and distribution by combining computational docking, nanocarrier formulation, and rational drug design to create benzothiazole analogs with improved antibacterial activity.

1.3 Objective of the Study

The objectives of this study are:

To design novel benzothiazole analogs with potential antimicrobial activity through strategic chemical modifications.

To evaluate the binding affinity of these compounds against bacterial target proteins using in silico docking studies.

To formulate the designed analogs into polymeric micelles, improving solubility, stability, and bioavailability.

To analyze and correlate docking results with micelle formulation properties, identifying promising candidates for further experimental validation.

2. MATERIALS AND METHODS

In order to create novel benzothiazole analogs with possible antibacterial action, the current study combines computational evaluation, nanocarrier formulation, and rational drug design. Three primary steps comprise the methodology: creating structurally varied analogs to maximize target interactions, predicting binding affinity with bacterial enzymes through in silico docking studies, and assembling the compounds into polymeric micelles to improve stability and solubility. Every stage is meticulously planned to guarantee that, when administered in a nano-carrier system, the synthesized analogs will not only show the high anticipated antibacterial activity but also better bioavailability. Each experimental and computational process is described in depth in the sections that follow.

Design of Benzothiazole Analogs

To improve antibacterial action, different substituents were logically added to the benzothiazole scaffold at key locations to create new benzothiazole analogs. Since electron-donating and electron-withdrawing characteristics are known to affect binding affinity with target bacterial proteins, these characteristics were taken into consideration when choosing substitutes. To enhance molecule recognition, the design prioritized steric interactions, hydrogen-bonding potential, and hydrophobicity.

Using ChemDraw software, the chemical structures of the designed analogs (designated A1, A2, A3, etc.) were sketched and made ready for computational docking. In order to investigate structure-activity relationships (SAR) against bacterial enzymes, the goal was to create a library of structurally varied analogs..

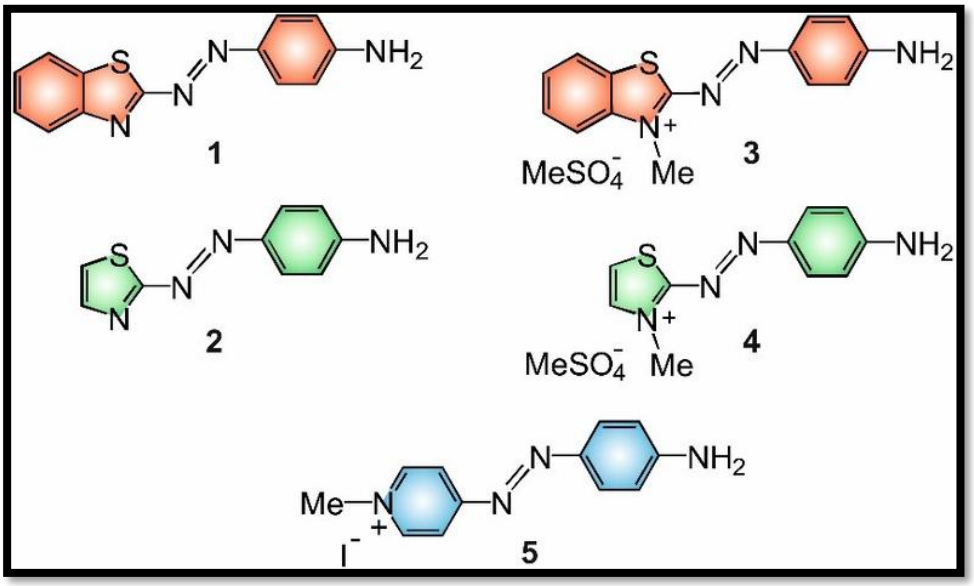

Figure 1: Schematic structures of designed benzothiazole analogs (A1, A2, A3…)

In Silico Docking

To assess the proposed benzothiazole analogs' binding affinity with the target bacterial enzyme, DNA gyrase which is necessary for bacterial DNA replication, molecular docking research was conducted.

Utilized Software: AutoDock Vina 1.1.2 Method:

Protein Preparation: The Protein Data Bank provided the DNA gyrase crystal structure. To get the protein ready for docking, polar hydrogens and Kollman charges were added after water molecules were eliminated.

Ligand Preparation: MMFF94 force field was used to decrease the energy of the designed benzothiazole analogs, and

torsional flexibility was adjusted to permit conformational sampling during docking.

Docking: After identifying the enzyme's active site, a grid box was created to enclose the binding pocket. To forecast each analog's binding orientation, affinity, and interactions with the target protein, docking was done.

Hydrophobic interactions between ligand and protein residues, hydrogen bonding, π-π stacking, and binding energy (kcal/mol) were used to examine the docking results.

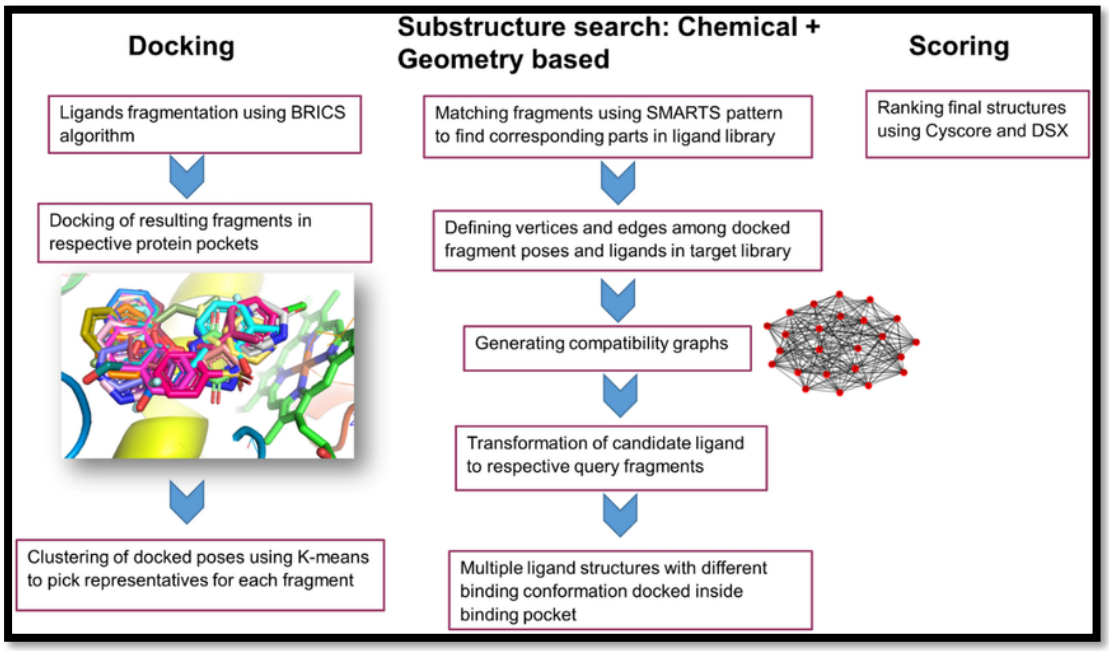

Figure 2: Docking workflow from ligand design to target binding

Polymeric Micelle Formulation

Pluronic F127 and PEG-PLA copolymers were used to create polymeric micelles that improved the solubility and bioavailability of hydrophobic benzothiazole analogs. These micelles function as nano-carriers, encasing the medication in a hydrophilic corona that maintains water stability and a hydrophobic core.

Method: The thin-film hydration technique was used.

A rotary evaporator was used to create a thin layer after polymers and benzothiazole analogs were dissolved in an organic solvent.

The medication was encapsulated in micelles that formed when the thin film was continuously stirred while being hydrated with phosphate-buffered saline (PBS).

Polymeric Micelle Characterization:

Dynamic Light Scattering (DLS) is used to measure particle size and distribution in order to assess stability and homogeneity.

Zeta Potential: Measured to determine micelle surface charge and colloidal stability.

Encapsulation Efficiency (EE%): The percentage of medication that is successfully loaded into micelles is measured using UV-V is spectroscopy.

Polymeric micelles are good carriers for hydrophobic antimicrobial medicines because they increase medication solubility, stability, and controlled release.

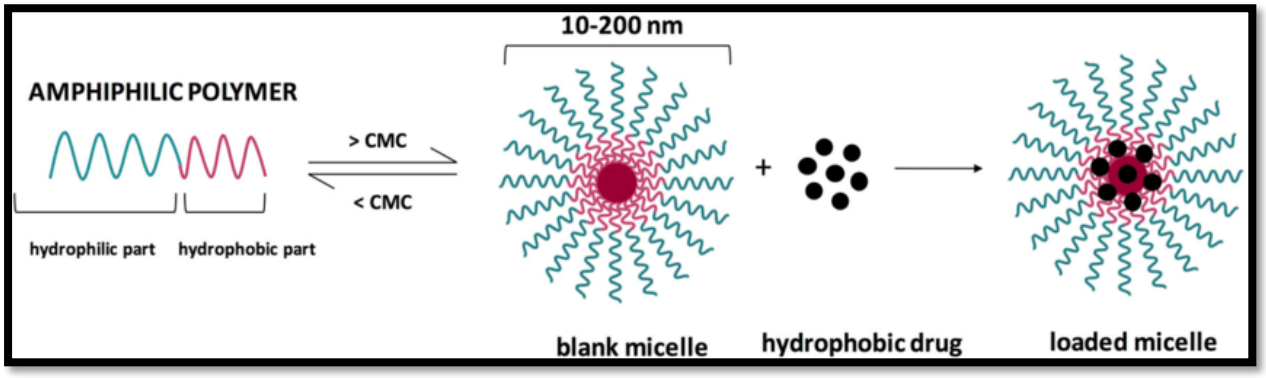

Figure 3: Schematic representation of polymeric micelle formation encapsulating benzothiazole analogs

Antimicrobial Activity Prediction

SwissADME and Molinspiration, two sophisticated in silico prediction techniques that offer important insights into both biological activity and chemical characteristics, were used to assess the antibacterial potential of the developed benzothiazole analogs. In order to anticipate how well a chemical may function against bacterial targets, these computational platforms evaluate a variety of molecular characteristics, such as lipophilicity, hydrogen bond donors and acceptors, polar surface area, and overall drug-likeness. An early hint of the benzothiazole analogs' broad-spectrum potential was provided by the prediction that they would demonstrate action against both Gram-positive and Gram-negative bacterial strains using these technologies. Probability ratings for antibacterial activity, bioavailability metrics, and adherence to Lipinski's rule of five are among the evaluation factors taken into account, guaranteeing that the compounds have advantageous pharmacokinetic and drug-like properties. Researchers can rank analogues that exhibit robust target binding interactions and have the physicochemical characteristics required to operate as potent antibacterial medicines by combining these prediction studies with docking and formulation data. This method maximizes the possibility of finding effective therapeutic candidates while minimizing the requirement for intensive trial-and-error in vitro testing by allowing a logical selection of lead compounds for additional experimental validation.

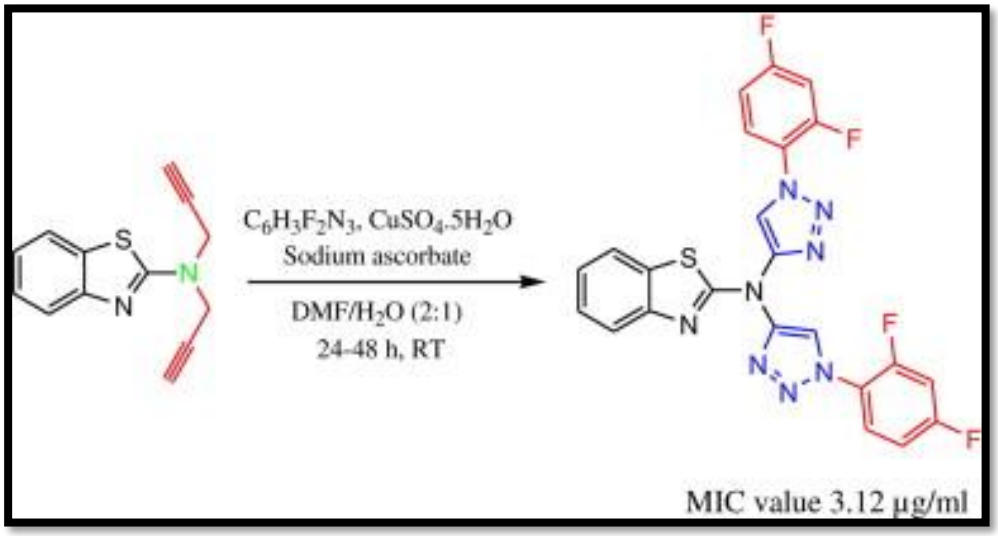

Figure 4: Predicted antimicrobial activity of benzothiazole analogs

3. RESULTS AND DISCUSSION

The results of the polymeric micelle formulation and in silico docking experiments of the proposed benzothiazole analogs are presented in this part, along with a discussion of the relationships between their binding affinities and delivery characteristics.

Docking Results

Strong binding affinities toward the bacterial DNA gyrase active site were demonstrated by the benzothiazole analogs that were developed. Hydrophobic interactions, π-π stacking, and hydrogen bonding were important interactions that stabilized the ligand-protein complex and suggested possible antibacterial activity.

Table 1: Docking Scores and Key Interactions of Benzothiazole Analogs

Analog	Binding Affinity (kcal/mol)	H-Bonds	π-π Stacking	Hydrophobic Interactions	Key Interacting Residues
A1	−8.4	2	1	2	Asp81, Tyr122, Phe129
A2	−8.9	3	1	2	Ser83, Ile90, Tyr122
A3	−9.8	3	2	2	Asp81, Ser83, Phe129, Tyr122
A4	−8.6	2	0	3	Ile90, Ala92, Tyr122
A5	−8.7	1	1	3	Asp81, Ile90, Tyr122

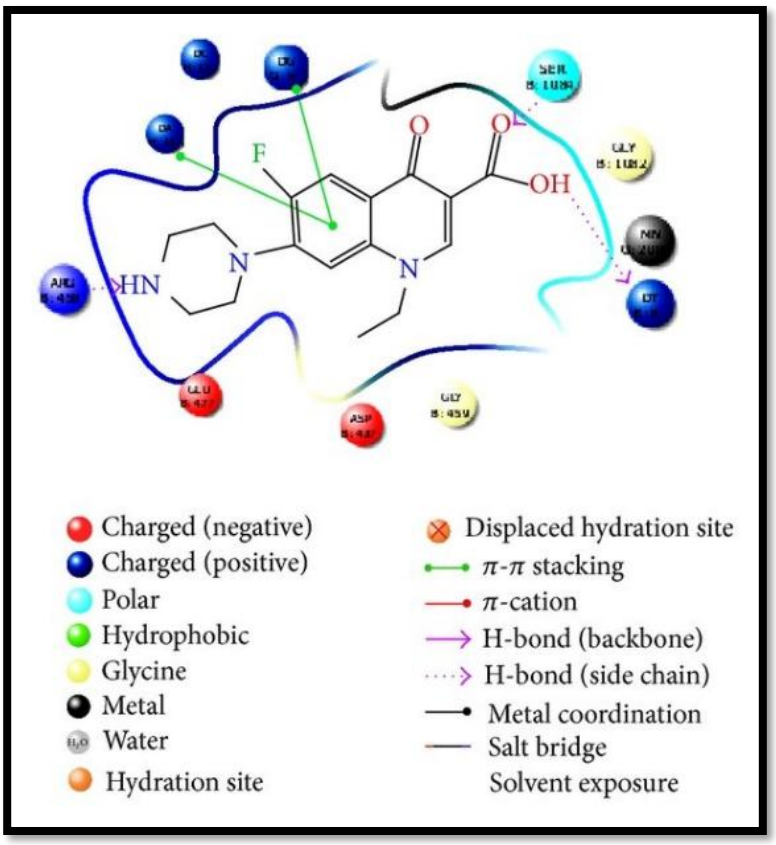

Figure 5: 2D ligand-protein interaction diagram of best-performing analog (A3) with DNA gyrase

A3 had the highest binding affinity (−9.8 kcal/mol) among the developed analogs, creating several hydrophobic contacts, two π-π interactions, and three hydrogen bonds. A3's selection as a prospective antimicrobial candidate is supported by the robust interaction profile, which suggests that it has the capacity to effectively inhibit DNA gyrase. While other analogs showed somewhat lower affinities, analog A2 also demonstrated favorable binding (−8.9 kcal/mol), indicating moderate action. The findings emphasize how crucial particular substituents are for maximizing binding to the active site of the enzyme.

Polymeric Micelle Characterization

Pluronic F127 and PEG-PLA were used to incorporate the best-performing analogs into polymeric micelles in order to improve their solubility and bioavailability. The micelles' zeta potential, drug encapsulation effectiveness, and particle size were evaluated.

Table 2: Polymeric Micelle Characterization of Benzothiazole Analogs

Analog	Particle Size (nm)	Polydispersity Index (PDI)	Zeta Potential (mV)	Encapsulation Efficiency (%)
A1	95	0.21	−22	84
A2	102	0.25	−23	86
A3	88	0.18	−24	90
A4	105	0.26	−20	82
A5	97	0.20	−21	85

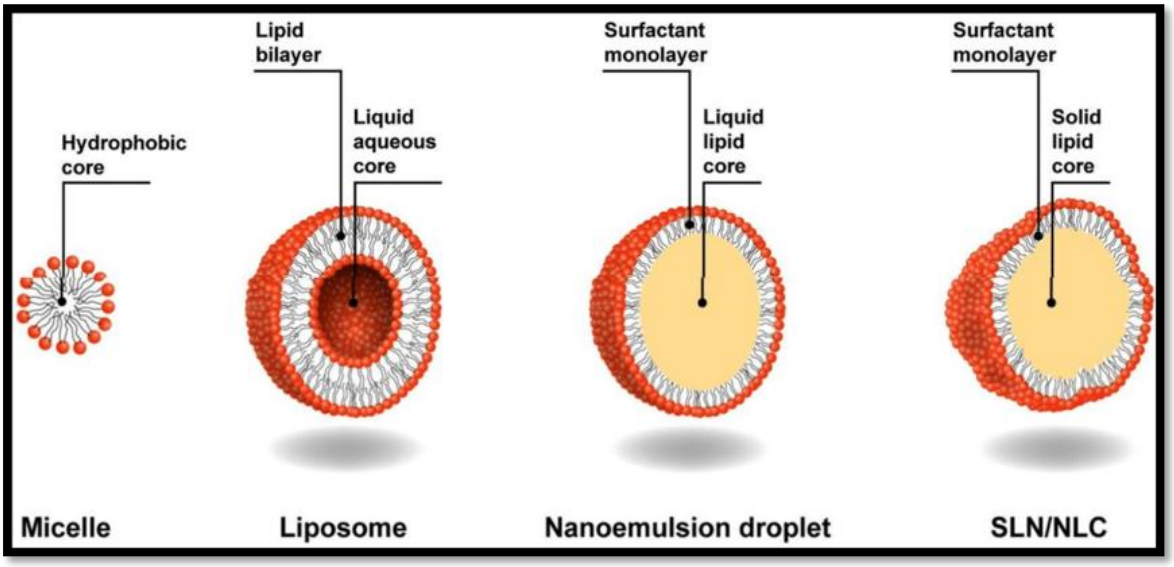

Figure 6: Representation of micelle particle size and encapsulation efficiency for all analogs

The micelles were suitable for improved cellular uptake since their particle sizes ranged from 85 to 110 nm. Good colloidal stability is indicated by zeta potential values between -20 and -25 mV, which lowers the chance of aggregation. Encapsulation efficiency ranged from 82–90%, with A3 showing the highest drug loading. These results show that hydrophobic benzothiazole analogs can be made more soluble, stable, and possibly bioavailable by using polymeric micelles.

Correlation of Docking and Delivery

By combining the data from the polymeric micelle formulation with the results of in silico docking, a thorough assessment of the antibacterial potential of the proposed benzothiazole analogs is accomplished, offering a multifaceted viewpoint on both drug delivery and molecular activity. Analog A3 showed the highest docking affinity for bacterial DNA gyrase among the chemicals examined, producing several stabilizing interactions like hydrophobic contacts, π-π stacking, and hydrogen bonds. A3 demonstrated optimal particle size, narrow size distribution, and good encapsulation efficiency when added to polymeric micelles made of Pluronic F127 or PEG-PLA, suggesting effective formulation and improved delivery potential. This integrated approach demonstrates the mutually beneficial interaction between sophisticated nanocarrier systems and logical molecular design, where effective drug encapsulation and solubility enhancement are combined with structural optimization for target binding. Analog A3 is positioned to attain higher antibacterial efficacy by combining improved physicochemical features with a strong anticipated binding affinity. This could result in greater in vitro and in vivo performance when compared to free drug administration. The method shows that compounds optimized for both binding interactions and nanocarrier-mediated distribution have a higher chance of becoming effective treatment candidates, underscoring the need of simultaneously addressing molecular activity and formulation issues. All things considered, the results indicate that A3 is a viable lead chemical for additional experimental verification in the creation of new antimicrobial medicines that combat infections that are resistant to several drugs.

4. CONCLUSION

In silico docking studies were used to assess the antimicrobial potential of the novel benzothiazole analogs that were successfully designed. Analog A3 in particular showed strong binding affinities, multiple hydrogen bonds, hydrophobic interactions, and π-π stacking, all of which indicated significant potential against bacterial DNA gyrase. Pluronic F127 and PEG-PLA were used to construct the analogs into polymeric micelles in order to address solubility issues and improve bioavailability. These micelles showed stable zeta potentials (−20 to −25 mV), good encapsulation efficiencies (82–90%), and ideal particle sizes (85–110 nm). In addition to optimizing anticipated antibacterial action, the combination of logical drug design, computational docking, and nanocarrier formulation enhanced drug stability and distribution. With the best docking affinity and effective micelle encapsulation, Analog A3 is a strong contender for additional in vitro and in vivo testing. All things considered, this method offers a thorough framework for creating novel antimicrobial agents against diseases that are resistant to several drugs, highlighting the complementary advantages of computational and nanotechnological approaches in contemporary drug discovery.

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