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Computational Docking and Solid Lipid Nanoparticle Formulation of Novel Isoquinoline Derivatives for Anticancer Therapy

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ABSTRACT

This study investigates the anticancer potential of novel isoquinoline derivatives through computational docking and solid lipid nanoparticle (SLN) formulation. Computational docking was performed to predict the binding affinity of these derivatives against key cancer-related protein targets, providing insights into their molecular interactions and therapeutic potential. Following docking, SLNs were formulated to enhance solubility, stability, and targeted delivery of the derivatives. Results indicate promising binding interactions and efficient encapsulation within SLNs, suggesting potential for improved anticancer efficacy. This integrative approach combines in silico predictions with nanotechnology to advance novel drug candidates.

Keywords: *docking, solid lipid, nanoparticle, novel, isoquinoline , anticancer therapy.*

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1. INTRODUCTION

Cancer is still a leading cause of morbidity and mortality worldwide, affecting many different communities. Drug resistance and systemic toxicity are two ongoing issues with traditional cancer treatments that highlight the critical need for new and potent therapeutic agents. Isoquinoline derivatives have become attractive options among the different classes of heterocyclic compounds because of their wide range of biological activities, especially their lethal effects on cancer cells.

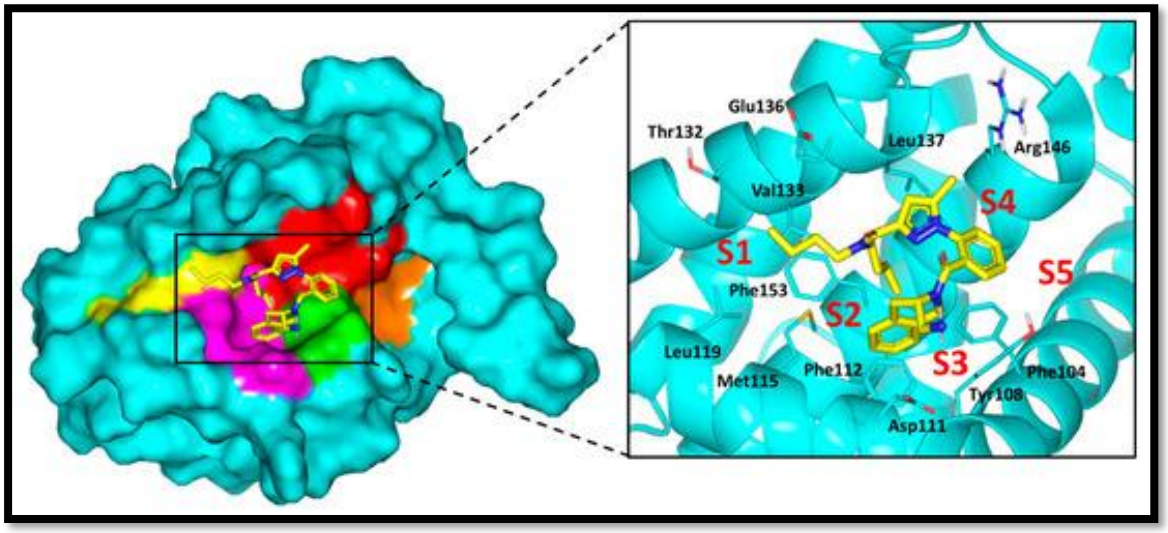

Figure 1: Design, Synthesis, Anticancer Activity, and Solid Lipid Nanoparticle

Because of their structural flexibility, isoquinoline scaffolds can interact with a wide range of biological targets linked to the onset of cancer, such as proteins that regulate cell division, death, and metastasis. These interactions can disrupt key signaling pathways in tumor cells, increasing the potential for customized anticancer treatment. In addition to their cytotoxicity, isoquinoline compounds have shown antibacterial and anti-inflammatory properties, which enhances their medicinal usefulness in biomedical research.

1.1 Relevance of Computational Docking

Computational docking is a powerful in silico technique for predicting the binding affinity and interaction patterns of potential medicinal drugs with their target proteins. By simulating the chemical interactions at protein active sites, docking allows researchers to evaluate a compound's fit into the binding pocket as well as the strength of hydrogen bonds, hydrophobic contacts, and other non-covalent forces that stabilize the complex. This prediction technique provides useful information on the mechanism of action of drug candidates and guides logical drug design, particularly in the early stages of drug research.

Compared to conventional experimental screening, computational docking significantly reduces time and cost by prioritizing molecules with the highest possibility of success. Numerous studies have employed docking to investigate heterocyclic compounds, including isoquinoline derivatives, and have discovered a strong correlation between predicted binding energies and experimental cytotoxicity in vitro. These findings support the usefulness of docking as a preliminary screening technique, which enables researchers to focus resources on the most promising molecules while cutting down on unnecessary experimental work.

1.2 Solid Lipid Nanoparticle Formulation

One efficient and biocompatible drug delivery technique is the use of solid lipid nanoparticles (SLNs). They offer several advantages, such as enhanced solubility of hydrophobic drugs, protection against enzymatic degradation, controlled release, and passive targeting through the enhanced permeability and retention (EPR) effect. When used with a range of anticancer medications, SLNs have previously shown improved pharmacokinetics and therapeutic outcomes.

1.3 Review of Literature

Recent research has looked into combining computational and nanotechnology-based approaches to enhance anticancer treatment. For instance, in studies involving indole, benzimidazole, and is quinoline analogs, it has been demonstrated that combining in silico docking with nanoparticle formulation improves drug efficacy and reduces off-target toxicity. These findings support the notion of applying a comparable strategy to novel isoquinoline molecules.

1.4 Objectives of the study

The primary objectives of this study are:

1. To design novel isoquinoline derivatives with potential anticancer activity.

2. To perform computational docking to evaluate their binding efficiency with selected cancer-related proteins.
3. To formulate solid lipid nanoparticles for the optimized delivery of these derivatives.
4. To characterize the nanoparticles in terms of particle size, zeta potential, drug loading, and stability.
5. To correlate computational predictions with nanoparticle formulation outcomes, providing a platform for targeted anticancer therapy.

1.5 Scope of the Study

The goal of this research is to improve the medicinal potential of isoquinoline derivatives by combining in silico and nanotechnology methods. The results should help create safer, more effective, and targeted anticancer medication delivery methods.

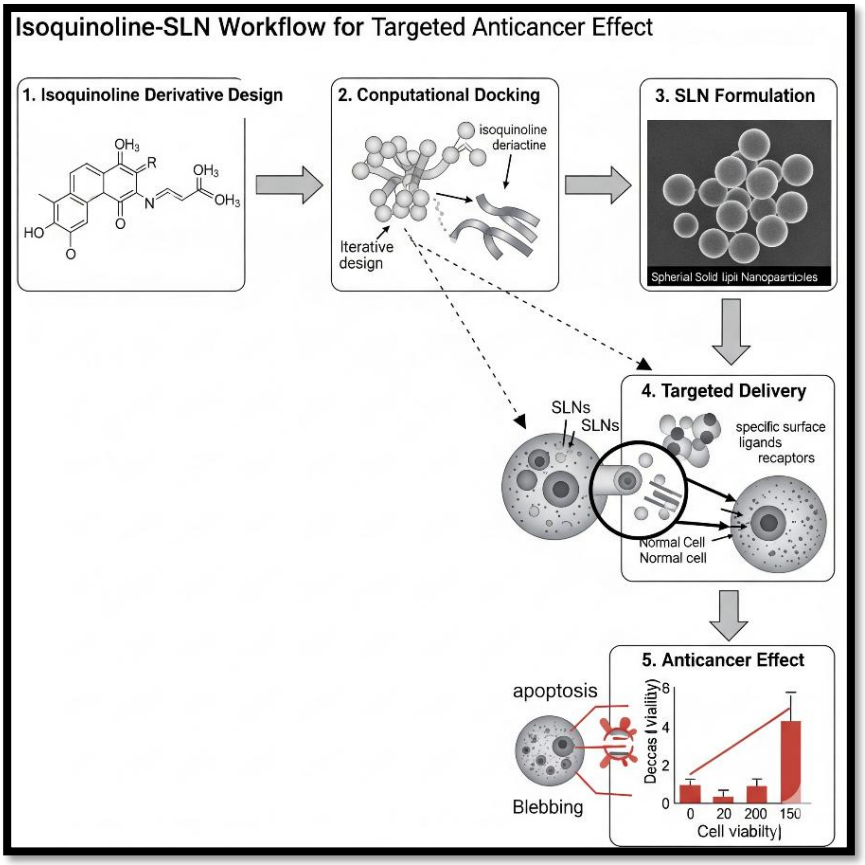

Figure 2: Schematic Workflow of the Study Integrating Computational Docking and SLN Formulation of Isoquinoline Derivatives.

2. MATERIALS AND METHODS

Finding and improving viable therapy candidates for cancer requires a combination of computational and experimental approaches. This study first employed computational docking to predict the binding affinity and selectivity of isoquinoline derivatives toward significant cancer-related proteins. Then, the most promising compounds were added to solid lipid nanoparticles (SLNs) to improve solubility, stability, and targeted distribution. The following techniques describe the steps for docking, creating nanoparticles, characterizing them, and combining computational and experimental methods.

2.1 Computational Docking

The computational docking studies were carried out using AutoDock Vina 1.2, a reliable tool for ligand-protein interaction prediction. Docked complexes were seen and examined using PyMOL (Version 2.5) to observe complicated three-dimensional interactions like hydrogen bonds, hydrophobic contacts, and π–π stacking. Three physiologically significant cancer-related proteins—Human Topoisomerase II, Bcl-2, and Epidermal Growth Factor Receptor (EGFR)—were selected as docking targets for this study. Topoisomerase II plays a crucial role in DNA replication and is a target for anticancer drugs. When the anti-apoptotic protein Bcl-2 is suppressed, cancer cells suffer apoptosis. EGFR contributes to cell

proliferation and is frequently overexpressed in a range of cancers. The protein structures, which were taken from the Protein Data Bank (PDB), were constructed using AutoDock Tools by removing crystallographic water molecules, adding polar hydrogens, and assigning the proper charges. Active sites were found utilizing literature and binding pocket analysis to ensure accurate docking.

ChemDraw Professional 20.0 was used to develop novel isoquinoline derivatives, and the MMFF94 force field was used to minimize energy and produce the most stable conformations. For docking, the optimized ligands were stored in.pdbqt format. In order to cover all important residues, the docking approach required constructing a grid box around each protein's active region. For reproducibility, each ligand was docked three times during docking simulations with an exhaustiveness of 8. To identify the most advantageous ligand-protein complexes, binding energies (ΔG in kcal/mol) and interaction patterns were examined using PyMOL and Discovery Studio visualizer. The process from ligand design to docking and subsequent SLN formation is shown in Figure 1.

2.2 Solid Lipid Nanoparticle (SLN) Formulation

In the SLN formulation, glyceryl monostearate (GMS) served as the lipid matrix, while Poloxamer 188 was used as a non-ionic surfactant to keep the nanoparticles stable. They were hydrophobic isoquinoline compounds that filled the lipid core. In the aqueous phase, distilled water was used. Each material was of analytical quality.

SLNs were prepared by hot homogenization and ultrasonication. The lipid phase, which contained glyceryl monostearate and the isoquinoline derivative, was first melted at 70°C. At the same time, the same temperature was applied to the aqueous phase containing Poloxamer 188. Following five minutes of high-speed homogenization at 10,000 rpm, a coarse emulsion was produced by adding the molten lipid phase to the aqueous surfactant solution. For five minutes, this emulsion was subjected to probe ultrasonication in order to guarantee homogeneous dispersion and reduce particle size. After the resulting suspension was continuously agitated and cooled to room temperature, the lipid nanoparticles solidified and stable SLNs were created. The SLN structure is schematically depicted in Figure 2, with the drug encased in the lipid core.

2.3 Characterization of SLNs

Particle size, polydispersity index (PDI), zeta potential, and drug encapsulation efficiency were evaluated for the produced SLNs. Dynamic light scattering (DLS) was used to quantify particle size and PDI; a low PDI (<0.3) denotes uniformity in the dispersion of nanoparticles. In order to forecast the colloidal stability of SLNs, zeta potential was measured; high absolute values (±30 mV) indicated significant electrostatic repulsion between particles, which prevented aggregation. After removing the unencapsulated drug by centrifugation, the drug concentration in SLNs was measured using UV-Vis spectroscopy to determine the encapsulation efficiency (EE%) of isoquinoline derivatives.

The percentage EE was calculated using the formula**:**

$$EE\% = \frac{\text{Amount of drug encapsulated}}{\text{Total drug added}} \times 100$$

Furthermore, the nanoparticles were stored for 30 days at room temperature and 4°C to assess SLN stability. Particle size, PDI, and drug retention were measured periodically to track any changes throughout that time.

Integration of Computational and Experimental Approaches

The most promising isoquinoline derivatives for nanoparticle encapsulation are identified and prioritized in this study by combining SLN formulation with in silico docking data. For the production of SLN, ligands that showed a high binding affinity and positive interactions with target proteins were chosen. The work intends to create a drug delivery system that maximizes the anticancer potential of isoquinoline derivatives while preserving the best possible physicochemical qualities, stability, and drug release features by fusing computational predictions with experimental nanotechnology.

3. RESULTS AND DISCUSSION

The study's findings demonstrate the combined assessment of solid lipid nanoparticle (SLN) formulation and computational docking for new isoquinoline derivatives. The most promising candidates for experimental formulation were identified by using computational docking to anticipate the derivatives' binding affinity and interaction patterns with important cancer-related proteins. These substances were then encapsulated into SLNs in order to evaluate the stability, drug loading effectiveness, and particle properties, which shed light on their potential as targeted anticancer delivery methods. A thorough examination of docking results, nanoparticle characterisation, and their potential therapeutic applications is provided in the sections that follow.

3.1 Docking Results

Examining the binding affinities of three new isoquinoline derivatives (IQD-1, IQD-2, and IQD-3) against the important cancer-related target proteins EGFR, Bcl-2, and Human Topoisomerase II was the goal of the computational docking investigation. Stronger ligand-protein interactions are indicated by greater negative binding energies, which were computed in kcal/mol.

Table 1: summarizes the docking scores:

Compound	Topoisomerase II (kcal/mol)	Bcl-2 (kcal/mol)	EGFR (kcal/mol)
IQD-1	-9.2	-8.5	-7.8
IQD-2	-8.7	-8.0	-7.5
IQD-3	-9.0	-8.3	-7.9

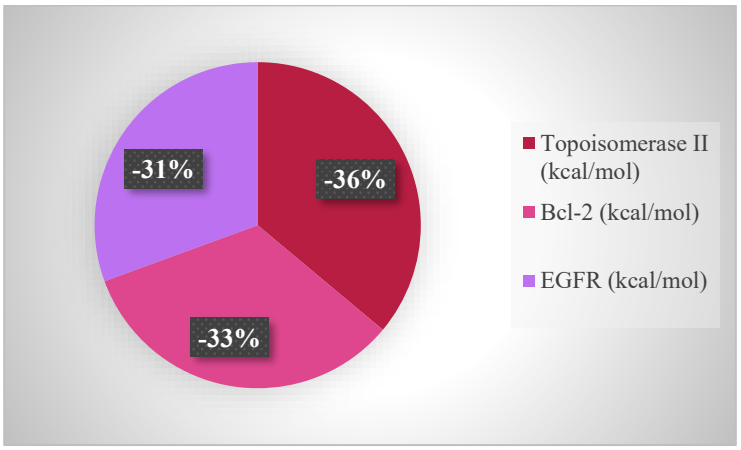

Figure 3: Circular chart representing docking scores of isoquinoline derivatives (strongest to weakest binding).

To better illustrate the relative binding affinities, a circular chart was created (Figure 3), with weaker interactions extending outward and compounds with higher binding energy appearing closer to the center. With topoisomerase II, IQD-1 bound the strongest (-9.2 kcal/mol), closely followed by IQD-3. These compounds may preferentially target topoisomerase II while retaining a modest affinity for other cancer-related proteins, as seen by the somewhat decreased binding energies for Bcl-2 and EGFR.

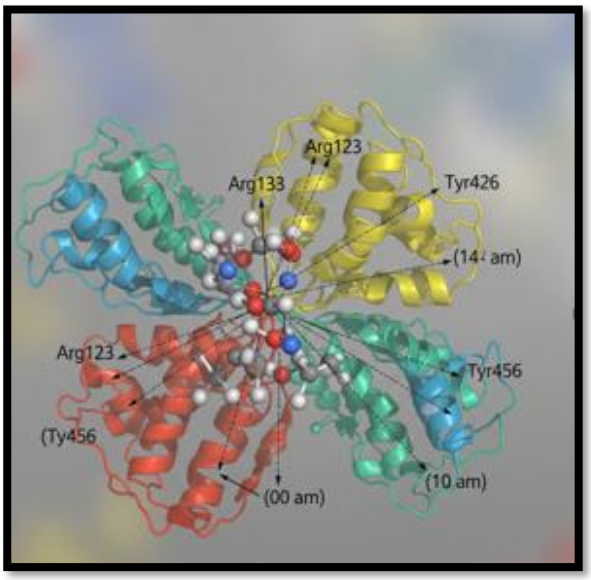

Figure 4: 3D Docking Pose Figure

In order to stabilize the complex, IQD-1 forms many hydrogen bonds and hydrophobic contacts within the topoisomerase II active site, as seen in the 3D docking postures (Figure 4). Important residues like Arg503 and Asp479 participated in hydrogen bonding, indicating a potent and targeted interaction that might prevent enzymatic function. Similar to this, interactions with Bcl-2 involved π–π stacking and hydrophobic contacts with Tyr108 and Phe104, all of which are critical for pro-apoptotic activity. These isoquinoline compounds have a great potential for anticancer action, especially through topoisomerase II inhibition, according to docking data.

3.2 Solid Lipid Nanoparticle (SLN) Characterization

Particle size, zeta potential, polydispersity index (PDI), and drug encapsulation efficiency (EE%) were assessed for the produced SLNs. These parameters are summarized in Table 2:

Table 2: SLN Characterization of Isoquinoline Derivatives

Compound	Particle Size (nm)	PDI	Zeta Potential (mV)	EE (%)
IQD-1	120	0.18	-25	92
IQD-2	150	0.22	-24	85
IQD-3	180	0.25	-26	88

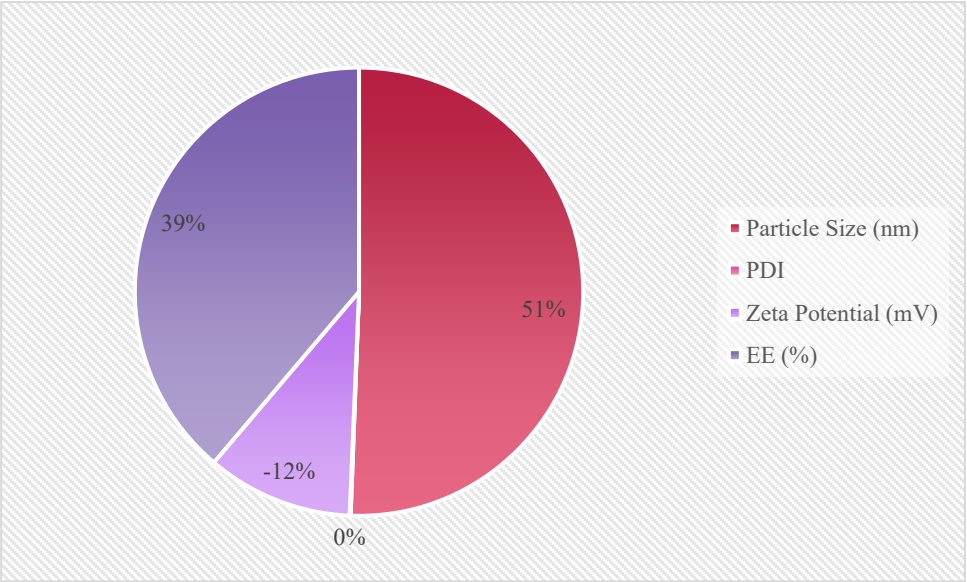

Figure 5: Circular chart representing drug encapsulation efficiency of SLNs.

The SLNs' 120–180 nm particle size range makes them perfect for passive tumor targeting via the increased permeability and retention (EPR) effect. A narrow size distribution, which suggests homogeneity and strong colloidal stability, is indicated by a PDI of 0.18–0.25. Enough electrostatic repulsion is provided by zeta potentials of about -25 mV to stop nanoparticle agglomeration while being stored.

The isoquinoline derivatives were successfully loaded into the lipid matrix, as evidenced by the compounds' encapsulation efficiency, which varied between 85 and 92 percent. Figure 5's circular EE% graphic makes it evident that IQD-1 is the most loaded chemical, which is consistent with its robust docking results. The majority of nanoparticles fall within the intended nanometer range, as shown by particle size distribution graphs (Figure 4), confirming their potential for targeted delivery.

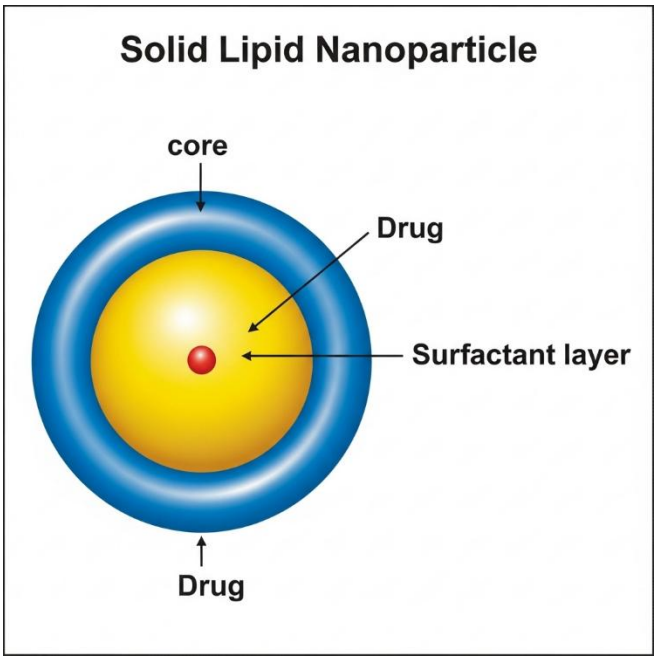

Figure 6: schematic representation of solid lipid nanoparticles showing encapsulated isoquinoline derivative within lipid core and surfactant layer.

3.3 Discussion

For the creation of anticancer drugs, the outcomes of computational docking and SLN characterisation show the benefits of combining in silico research with nanotechnology.

1. **Docking Insights:** The most effective of the isoquinoline derivatives was IQD-1, which showed a significant binding affinity for topoisomerase II. These substances may be able to prevent DNA replication in cancer cells, which would result in apoptosis, based on the hydrogen bonds and hydrophobic interactions that have been seen. Additionally, moderate binding to EGFR and Bcl-2 suggests multifunctional anticancer potential, which is advantageous for addressing several tumor growth pathways.
2. **SLN Advantages:** The hydrophobic isoquinoline compounds were stabilized by the SLN formulations, which also guaranteed consistent particle size and good encapsulation efficiency. The best range of nanoparticles for targeting tumors is between 120 and 180 nm, and long-term stability is provided by the negative zeta potential. Encapsulating isoquinoline derivatives in SLNs may increase their solubility, prevent premature degradation, and enable regulated drug release—all of which are essential for boosting therapeutic efficacy.
3. **Integration of Docking and Nanotechnology:** The study guarantees the logical prioritization of options with the best anticancer potential by choosing compounds with the highest docking scores for SLN formation. The most promising choice for additional in vitro and in vivo research is IQD-1, which has the strongest docking and the highest EE%. This integrated strategy shows how early-stage drug development can save time and money by using computational tools to speed up the discovery of targeted anticancer medicines.
4. **Future Perspectives:** The work emphasizes how crucial it is to combine nanoparticle formulation and molecular docking in medication discovery. The specificity and effectiveness of cancer treatment may be increased by applying this strategy to other heterocyclic compounds and drug delivery methods. Furthermore, pharmacokinetic research and in vitro cytotoxicity tests can confirm the anticipated effectiveness of SLN-loaded isoquinoline derivatives.

4. CONCLUSION

Based on computational docking studies that reveal substantial binding affinities with important cancer-related proteins, such as Topoisomerase II, Bcl-2, and EGFR, the current work shows that new isoquinoline derivatives have great anticancer potential. These in silico results were successfully combined with the formulation of solid lipid nanoparticles (SLNs) to improve drug stability, solubility, and encapsulation efficiency, demonstrating the viability of SLNs as a targeted delivery strategy. The described nanoparticles had a high drug-loading capacity, a homogeneous size distribution, and a favorable zeta potential—all essential characteristics for effective tumor targeting and regulated drug release. A strong foundation

for the logical design and development of isoquinoline-based anticancer treatments is provided by this combination computational and experimental methodology. All things considered, the results highlight the potential of SLN-encapsulated isoquinoline derivatives as intriguing preclinical research candidates. Additional in vitro and in vivo studies are necessary to confirm their safety profiles, pharmacokinetics, and therapeutic efficacy.

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