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Comparative Study of Anticancer and Antibacterial Effects of Synthetic Drug Molecules and Natural Extracts from *Simarouba glauca, Zingiber officinale,* and *Azadirachta indica*

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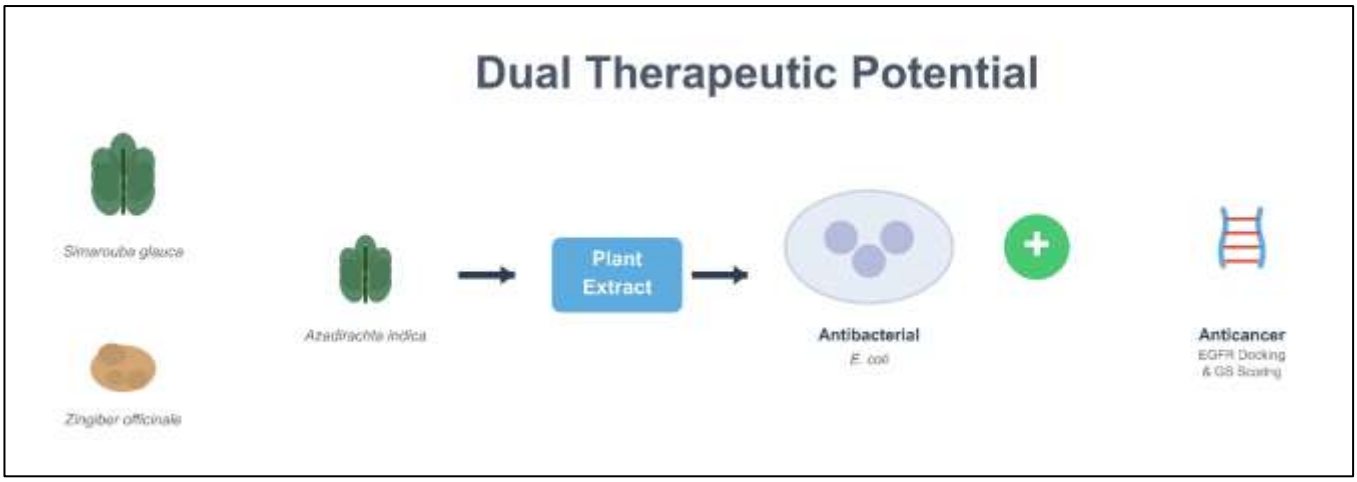
Abstract

Natural plant-derived bioactives have emerged as promising candidates for addressing two major global health concerns - cancer and antimicrobial resistance - through their diverse biochemical mechanisms and low cytotoxicity. This study explored the dual therapeutic potential of *Simarouba glauca*, *Zingiber officinale*, and *Azadirachta indica* extracts, focusing on their antibacterial activity against *Escherichia coli* and their molecular interaction with the Epidermal Growth Factor Receptor (EGFR), a critical target in cancer therapy. Ethanolic extracts of each plant were evaluated using agar well diffusion and spectrophotometric assays, revealing that *Simarouba glauca* and *Zingiber officinale* exhibited significant bacterial growth inhibition at 2500 µg/mL, achieving 93.9% and 87.8% inhibition respectively, while neem showed moderate activity. Complementary molecular docking studies using AutoDock 4 demonstrated that the neem compound exhibited the most favorable binding affinity with EGFR (−8.05 kcal/mol), followed by *Simarouba glauca* and *Zingiber officinale*, suggesting strong anticancer potential at the molecular level. Together, these findings highlight that naturally derived phytocompounds can simultaneously suppress microbial growth and interact effectively with cancer-associated targets, underscoring their potential as multifunctional therapeutic leads in the development of safer, plant-based biomedical agents.

Keywords: *Simarouba glauca*, *Zingiber officinale*, *Azadirachta indica*, EGFR docking, antibacterial assay, dual bioactivity



Graphical Abstract of the Study.

1. Introduction

Cancer remains one of the leading causes of morbidity and mortality worldwide, with an estimated 19.3 million new cases and nearly 10 million deaths in 2020 alone (Sung et al., 2021). Despite significant advancements in chemotherapy, radiotherapy, and immunotherapy, the limitations of conventional cancer treatments - including systemic toxicity, drug

resistance, and non-specific targeting - continue to necessitate the search for alternative therapeutic strategies (Chakraborty et al., 2022). Natural products and plant-derived phytochemicals have long been considered valuable sources of anticancer agents, owing to their structural diversity, bioactivity, and lower toxicity compared to synthetic drugs (Cragg & Pezzuto, 2016).

Among medicinal plants, *Simarouba glauca* (commonly known as paradise tree), *Zingiber officinale* (ginger), and *Azadirachta indica* (neem) have attracted attention for their broad spectrum of pharmacological properties. Extracts of Simarouba glauca contain bioactive compounds such as quassinoids, triterpenoids, and alkaloids. Studies have reported that quassinoids like glaucarubinone and tricaproin exhibit cytotoxic and pro-apoptotic activity against cancer cell lines, in part through inhibition of histone deacetylase and disruption of cell cycle progression (Puranik et al., 2017). Ginger, widely used in traditional medicine, contains bioactive molecules such as [6]-gingerol, [10]-gingerol, and shogaol. These compounds are known to induce apoptosis, suppress angiogenesis, and modulate signaling pathways, making them promising candidates for chemoprevention and therapy of prostate and breast cancers (Shukla & Singh, 2007; Zhu et al., 2019). Neem has been extensively studied

for its immunomodulatory and anticancer potential, with limonoids such as azadirachtin and nimbolide showing inhibitory effects on cancer proliferation, angiogenesis, and metastasis (Kumar et al., 2018).

Figure 1: *Simarouba glauca, Zingiber officinale,* and *Azadirachta indica* provide bioactive compounds with dual anticancer and antimicrobial therapeutic potential for integrated treatment approaches.

Modern research tools such as molecular docking have made it easier to study these natural compounds in detail. Docking allows scientists to virtually "fit" plant molecules into cancer-related proteins and predict how strongly they might bind. This in silico approach can save both time and resources, while helping to identify the most promising drug candidates before moving to laboratory or animal studies (Morris & Lim-Wilby, 2008).

Another important aspect is that cancer patients are often highly vulnerable to infections, particularly from bacteria such as *Escherichia coli*. The growing problem of antibiotic resistance makes this an even greater concern (Geller et al., 2018).

Interestingly, extracts from ginger, neem, and simarouba are also known for their antimicrobial activity, meaning they could serve a dual role - fighting both cancer cells and harmful bacteria (Kharwar et al., 2020; Park et al., 2008).

This study set out to explore the potential of *Simarouba glauca*, ginger, and neem as sources of bioactive compounds with dual therapeutic effects. Specifically, we investigated their anticancer potential through molecular docking with cancer- associated proteins, and assessed their antibacterial activity against *E. coli*. By combining computational analysis with experimental validation, this research aims to shed light on how traditional medicinal plants might contribute to future cancer therapy while also offering protection against bacterial infections.

2. Materials and Methods

2.1. Microbiological Assay for Antibacterial Evaluation

2.1.1. Bacterial Strain and Culture Maintenance

A reference strain of *Escherichia coli* was employed as the model Gram-negative organism. Cultures were maintained on nutrient agar slants at 4 °C and sub-cultured bi-weekly to preserve viability and genetic stability (Jorgensen & Ferraro, 2009). Prior to each assay, a fresh overnight culture was prepared in nutrient broth at 37 °C under aerobic conditions.

2.1.2. Preparation of Plant Extracts

Dried, authenticated plant material of Neem (*Azadirachta indica*), Garlic (*Allium sativum*), and Simarouba (*Simarouba glauca*) was procured. Each sample was pulverized to fine powder, and then dissolved in ethanol to prepare the solution. Extracts were stored at −20 °C in amber vials to minimize degradation.

2.1.3. Agar Well Diffusion Assay

Antibacterial activity was quantified via the inhibition-zone method. Sterile Nutrient agar plates were seeded with 100 µL of standardized *E. coli* suspension (≈10^6

CFU/mL). Wells (6 mm diameter) were aseptically bored and filled with 50 µL of each extract (test), 50 µL of gentamicin (10 µg/mL; positive control), and 50 µL of solvent (negative control)(Balouiri et al., 2016; Valgas et al., 2007). Plates were incubated at 37 °C for 18–24 h. Zone diameters were measured in millimeters using a calibrated scale.

2.1.4. Spectrophotometric Analysis of Antibacterial Activity

2.1.4.1. Bacterial Preparation

The E. coli strain was grown overnight in LB broth at 37°C in the presence of plant-based antibacterial extracts. The different concentrations used are summarized in Table 3.

Table 3: Plant Extract Stock Solutions

Plant Extract	Code	Concentration (µg/mL)
	S1	5000
Simarouba glauca	S1.5	2500
	S0.5	1250
	G1	5000
Zingiber officinale (Ginger)	G1.5	2500
	G2	1250
	N1	5000
Azadirachta indica (Neem)	N1.5	2500
	N2	1250

2.1.4.2. Spectrophotometric Assay

After incubation, bacterial growth was measured at 600 nm wavelength using a spectrophotometer. Each test was done in triplicate.

Growth inhibition was calculated as:

$$\% \text{ Inhibition} = \frac{(\text{Control OD} - \text{Treatment OD})}{\text{Control OD}} \times 100$$

2.2. In-silico studies on screening of pharmacoactive compounds against Human Epidermal Growth Factor (EGFR) for anticancerous properties

2.2.1. Retrieval and preparation of EGFR protein in UCSF Chimera

The respective target protein Epidermal Growth factor Receptor (EGFR) of Homo sapiens has been retrieved from PDB database with given PDB ID: 6Z4B with a high resolution of 2.5Å which has been detected by X-ray diffraction method (Sussman, 1998). Thereafter, the target protein has been prepared in UCSF Chimera by eliminating the water molecule and other heteroatoms which might possibly play a part in hindering the running of an effective molecular docking process.

2.2.2. ADMET screening of anticancer compounds

The following compounds, *Simarouba glauca, Zingiber officinale* (ginger) and *Azadarachta indica* (neem) were taken and screened for their anticancerous properties against EGFR protein. The ADMET properties of each pharmacologically active compound has been screened using ADMET lab 3.0 (Fu, 2024) and then taken for respective docking process. Once the ADMET evaluation is done, the compounds are good to be taken further for molecular docking process.

2.2.3. Screening of pharmacoactive compounds for their anticancerous properties against EGFR by Molecular Docking and Visualisation

Once the ADMET evaluation of each compound has been done, the in silico analysis of each is performed. The target protein EGFR is made to be tested with three pharmacoactive compounds as stated above for their respective anticancerous properties against EGFR. The interaction is studied with the help of molecular docking method, using Autodock 4 and Autodock MGL tools (Meng, 2011). Post docking, the respective binding energies of each compound is checked where the most negative binding energy of a compound signifies its best interaction with protein and may be called the one with the maximum anticancerous property amongst all.

Thereafter, the respective protein-ligand interactions between the protein and each target compound have been checked on LIGPLOT.

3. Results and Discussion

The antibacterial activity of ethanolic extracts from *Simarouba glauca*, *Zingiber officinale*, and *Azadirachta indica* was evaluated against *Escherichia coli* using spectrophotometric analysis of bacterial growth at 600 nm. The optical density (OD_{600}) readings are summarized in Table 4. Among the tested concentrations, notable growth inhibition was observed at 2500 µg/mL for all three extracts. *Simarouba glauca* exhibited the highest antibacterial activity, achieving 93.9% inhibition of *E. coli* growth, followed by *Zingiber officinale* with 87.8% inhibition and *Azadirachta indica* with 75.5% inhibition. In contrast, some samples at higher or lower concentrations showed OD values greater than the control, suggesting no inhibitory or possibly stimulatory effects on bacterial proliferation at those levels. These findings indicate a concentration-dependent antibacterial response, with optimal efficacy achieved at intermediate extract concentrations.

Table 4: Bacterial Growth Inhibition Results

Sample Code	Average OD_{600}	Growth Inhibition (%)
C– (Control)	0.049	–
G1–	0.041	16.3%
G1.5–	0.008	83.7%
G2–	0.007	85.7%
N1–	0.100	No inhibition*
N1.5–	0.012	75.5%
N2–	0.111	No inhibition*
S0.5–	0.095	No inhibition*
S1–	0.031	36.7%
S1.5–	0.003	93.9%

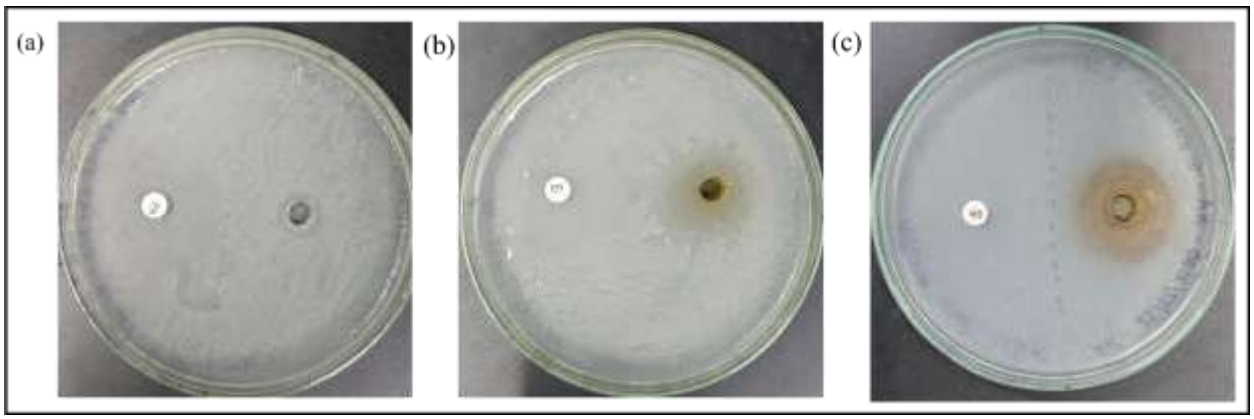


Figure 2: Zone of Inhibition observed after 24 hours of incubation with (a) *Zingiber officinale* (b) *Azadarachta indica* (c) *Simarouba glauca*

The three-dimensional structure of EGFR protein has been visualised in RasMol (Figure 1). The screening of respective compounds *Simarouba glauca, Zingiber officinale* (ginger), and *Azadarachta indica* (neem) (Figure 2) has been performed for their ADMET properties using ADMET lab 3.0 and verified (Table 1). The properties verified the absorption, distribution, metabolism, excretion, and toxicity levels of each compound to be within their normalised ranges, each being classified as non-

Figure 3: PDB structure of EGFR visualised in RasMol

carcinogenic and having no such side effect on the system. This is due to the fact that each of them being natural compounds, are available in nature and thus seem to pose no side effect on the human system.

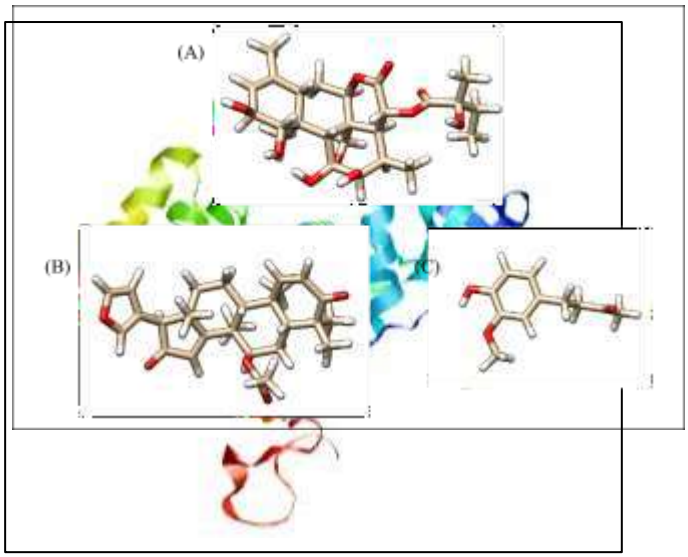


Figure 4: Structures of each compound : (A) *Simarouba glauca*, (B) *Azadarachta indica* (C) *Zingiber officinale*

Table 5: ADMET properties of each pharmacoactive compound

Name of Compound	Caco-2 Permeability	PPB (Plasma Protein Binding)	CYP1A2 Inhibitor	CLplasma	Carcinogenicity
Simarouba glauca	–5.687	57.9%	Inhibitor	2.318	0.132
Zingiber officinale (*Ginger*)	–4.827	96.6%	Inhibitor	7.694	0.521
Azadirachta indica (*Neem*)	–4.995	88.5%	Inhibitor	9.228	0.897

Thereafter, upon running molecular docking the binding energies of the compounds are evaluated, where the binding energy of *Azadarachta indica* (neem) was found to be the least, which possibly lead to deduce that it has the highest anticancerous property amongst the other two compounds, followed by *Simarouba glauca* (Table 2) and then *Zingiber officinale*. Previous studies performed on such compounds had too verified the potential anticancerous property of neem components against malignant cells which included inhibition of cell proliferation, induction of cell death and suppression of cancer angiogenesis and enhancement of host immune responses against cancer cells. Moreover, the action of neem leaf glycoprotein as a natural immunomodulator has been shown which plays an important role in modification of tumor cells rather than directly attacking than directly attacking immune cells. Thus, neem has been identified as a potential anticancer agent due to its reduced toxicity and side effect (Meng, 2011, Agu, 2023).

Table 6: Respective binding energies of each compound and the interacting amino acid residues with each other

Name of protein	Target	Name of Compound	Free energy of binding (kcal/mol)	Estimated Inhibition constant (Ki, µM)	Interacting amino acid residues of protein
Epidermal Growth		*Simarouba glauca*	-4.61	416.42	Glu762, Phe723, Lys745, Leu747, Ile749, Glu758, Ala722, Leu858, Gly857, Asp855

Factor (EGFR)	Receptor	*Zingiber officinale* (ginger)	-4.15	905.73	Thr790, Ala743, Leu844, Lys745, Val726, Leu792, Met793, Gln791
		Azadarachta indica (neem)	-8.05	1.27	Arg841, Asn842, Phe723, Thr854, Asp800,Leu718, Gly719, Leu798, Leu844, Gln791, Met793

The interacting residues of EGFR revealed a lot of hydrophobic residues which show interaction with each compounds (Table 2), therefore revealing that hydrophobic residues are responsible for taking part in protein-ligand or protein-protein interactions (Figure 3,4). Previous studies had highlighted the interaction of EGFR ligands and adnectin 1 which interact with more commonly present hydrophobic residues. The predominant residues leucine, phenylalanine and valine form stabilising interactions which are crucial for the receptor's activation and inactivation. They create hydrophobic cores and pockets which is a key for ligand binding and regulating conformational changes (Hao et al., 2014, Moga et al., 2018).

Study of anticancerous properties of pharmacologically active compound s has been common till date (Batra et al., 2022, Paul et al., 2011). Further extensive research to determine the anticancerous or medicinal properties of other natural compounds is being performed for the betterment of mankind.

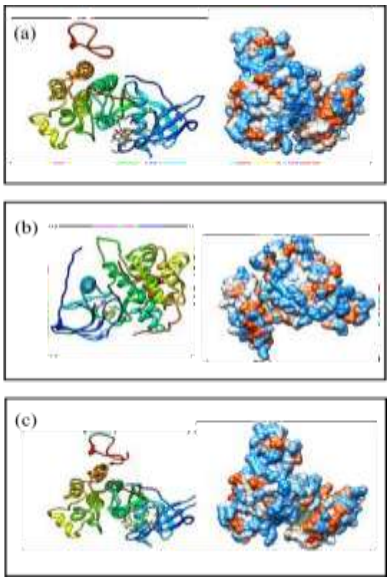


Figure 5: The docked models visualised both in i. ribbon and ii. hydrophobic surface
(a) EGFR- *Simarouba* complex (b) EGFR- *Zingiber* complex (c) EGFR- *Azadarachta* docked complex

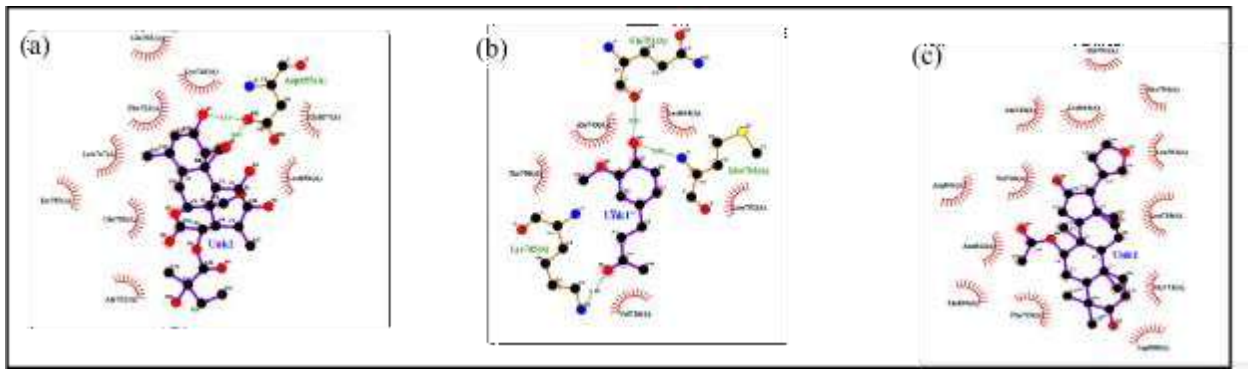


Fig 6: The interacting amino acid residues of EGFR with its respective target ligand compounds visualised in LIGPLOT. (a). EGFR- *Simarouba glauca* (b). EGFR-*Zingiber officinale* (c). EGFR-*Azadarachta indica*

The integration of *in vitro* antibacterial evaluation with *in silico* docking analysis provides a comprehensive understanding of the dual bioactivity of these plant extracts. The inhibition assays revealed that extracts of *Simarouba glauca* and *Zingiber officinale* demonstrated substantial bacteriostatic effects against *E. coli*, which may be attributed to the presence of secondary metabolites such as quassinoids and gingerols known to disrupt microbial cell membranes. In parallel, molecular docking against the EGFR protein revealed high binding affinities for neem-derived compounds, particularly azadirachtin, indicating a potential for anticancer activity through inhibition of receptor signaling pathways. The alignment between strong docking affinity and previously reported cytotoxic or antiproliferative mechanisms (Hao et al., 2014; Moga et al., 2018) reinforces the hypothesis that these bioactives may serve as dual- action therapeutic agents. While *Simarouba glauca* exhibited the most potent antibacterial effect experimentally, neem demonstrated superior molecular interactions with the cancer-associated target, collectively suggesting that different plant bioactives may contribute complementary therapeutic advantages. Such integrated results validate the conceptual link between antimicrobial efficacy and anticancer potential within natural extracts, providing a mechanistic foundation for future translational research.

4. Conclusion

This dual-model investigation demonstrates that selected medicinal plants - *Simarouba glauca*, *Zingiber officinale*, and *Azadirachta indica* - possess significant potential for multifunctional therapeutic use. The antibacterial assays confirmed strong inhibitory effects, particularly from *Simarouba glauca*, while molecular docking revealed that neem-derived bioactives form stable complexes with the EGFR protein, suggesting a possible role in modulating cancer-associated pathways. Collectively, these results underscore the therapeutic versatility of phytochemicals, capable of targeting both microbial infections and oncogenic signaling mechanisms. Importantly, this approach aligns with the growing emphasis on sustainable, plant-based alternatives to synthetic pharmaceuticals, which often face issues of toxicity and resistance.

Looking forward, future studies should aim to isolate and purify the key bioactive molecules responsible for the observed activities, followed by cytotoxicity screening against established cancer cell lines to validate the *in silico* predictions. Integration of spectroscopic and chromatographic techniques (GC–MS, LC–MS, NMR) can aid in compound characterization and structure–activity relationship analysis. Moreover, nanoformulation or polymeric encapsulation strategies may enhance the bioavailability and stability of these extracts. By extending this dual- evaluation model to additional pathogens and cancer targets, the research paves the way for developing eco-friendly, plant-derived therapeutic agents that bridge the domains of microbiology, oncology, and green drug design.

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