

DESIGN AND DEVELOPMENT OF PHYTOCONSTITUENT BASED NANOFORMULATIONS FOR TARGETED ANTI CANCER THERAPY USING MOLECULAR DOCKING APPROACHES

Sagar Narendra Ande¹, Sanjay Mishra², Dhruva Sankar Goswami³, Mrinmoy Basak⁴, Moksood Ahmed Laskar⁵, Eluru Jajili⁶, Sofiqul Mollik⁷, Om M. Bagade^{8*}

¹Associate Professor, Dr. Rajendra Gode Institute of Pharmacy, University Mardi Road, Amravati 444602

²Professor, Department of Biotechnology, SR Institute of Management & Technology, Lucknow, U. P 226201

³Principal & Associate Professor, Kazi Nazrul Islam Pharmaceutical Sciences, Ghatal, West Medinipur, West Bengal 721222

⁴Professor & HoD, Faculty of Pharmaceutical Science, Assam down town University, Sankar Madhab Path, Gandhi Nagar, Panikhaiti, Guwahati, Assam, India, 781026

⁵Faculty of Pharmaceutical Science, Assam down town University, Sankar Madhab Path, Gandhi Nagar, Panikhaiti, Guwahati, Assam, India, 781026

⁶Assistant Professor, Sir C.R Reddy College of Pharmaceutical Sciences, Eluru, Kukatpally, Hyderabad 500072

⁷Assistant Professor, University of Science and Technology Meghalaya, Kiling Road, Baridua, 9th Mile, Ri-Bhoi, Meghalaya 793101

⁸Associate Professor, Vishwakarma University School of Pharmacy Pune, Maharashtra 411048 India

*Corresponding Author
Dr. Om M. Bagade

Article History

Received: 24.09.2025

Revised: 07.10.2025

Accepted: 21.10.2025

Published: 04.11.2025

Abstract:

Cancer remains one of the leading causes of mortality worldwide, with conventional therapies often hindered by systemic toxicity, multidrug resistance, and limited selectivity towards tumour cells. The integration of phytoconstituents—bioactive compounds derived from medicinal plants—with nanotechnology offers a promising strategy to overcome these limitations. This study focuses on the design and development of phytoconstituent-based nanoformulations tailored for targeted anti-cancer therapy, guided by molecular docking approaches to optimize drug-target interactions. Nanoformulations such as liposomes, polymeric nanoparticles, dendrimers, and micelles provide controlled release, enhanced bioavailability, and selective tumor accumulation. Molecular docking aids in predicting and analysing the binding efficiency of selected phytoconstituents with cancer-associated proteins, thereby ensuring rational formulation design. Results highlight the synergistic potential of computational and formulation sciences, setting a path for effective and safer therapeutic interventions.

Keywords:

Phytoconstituents, Nanoformulations, Cancer Therapy, Molecular Docking, Targeted Drug Delivery.

INTRODUCTION

Over the years, cancer treatment has changed dramatically, yet problems including systemic toxicity, drug resistance, and the low absorption of chemotherapeutic drugs still exist. Through processes like cell cycle arrest, angiogenesis suppression, and apoptosis induction, phytoconstituents such as curcumin, quercetin, resveratrol, and epigallocatechin gallate (EGCG) have shown strong anti-cancer effects. Their quick metabolism, instability, and low solubility, however, restrict their therapeutic use. In order to improve the pharmacokinetic and pharmacodynamic characteristics of these compounds, nanotechnology encapsulates them in nano formulations¹.

The interaction of phytoconstituents with cancer-associated molecular targets, including matrix metalloproteinases (MMPs), vascular endothelial growth factor receptor (VEGFR), and epidermal growth factor receptor (EGFR), can be predicted computationally using molecular docking techniques. Researchers can simplify the development of targeted medicines with greater efficiency by combining docking knowledge with nanocarrier design². The promise of plant-based nanoformulations as next-generation anticancer treatments has been highlighted by prior research, which has shown encouraging

results³. This research attempts to investigate in detail the design and development of such nanoformulations.

1.1 Review of Literature

The substantial potential of phytoconstituents encapsulated in nanoparticles for targeted cancer therapy has been highlighted by recent investigations. According to Wahi et al. (2023), nano-Phytoformulations can increase the stability and bioavailability of chemicals produced from plants, which in turn can improve their anticancer activity. The adaptability of nanocarriers in healthcare applications was also demonstrated by Gilani et al. (2020)⁴, who talked about chemically nano-engineered theragnostic that combine therapeutic and diagnostic capabilities. In their assessment of polymeric and lipid-based nanocarriers for the delivery of phytomedicines in breast cancer therapy, Yapar et al. (2025) and Shree et al. (2025)^{5,6} came to the conclusion that these systems enhance tumor selectivity while lowering systemic toxicity. While Adedokun et al. (2023)⁷ reported that polyphenols delivered via nanoparticles exhibit superior therapeutic efficacy compared to conventional methods, Noor et al. (2024)⁸ offered a thorough analysis of embelin-loaded nanoformulations, demonstrating improved pharmacokinetics and targeted delivery. Beyond oncology, Maurya et al. (2023)⁹ and Mishra &

Mishra (2024)¹⁰ highlighted the pharmacogenetic and pharmacological potential of bioactive compounds for novel formulations in the management of hypertension and breast cancer, while Yong et al. (2024)¹¹ investigated natural product-based inhaled formulations for pulmonary diseases, emphasizing the adaptability of nano delivery approaches. Furthermore, the antiviral and neuroprotective qualities of plant-derived compounds were shown by Ho et al. (2024)¹² and Puri et al. (2022)¹³, confirming their wide therapeutic applicability. As evidenced by Singh et al. (2025), who showed that nanoparticle-enhanced resveratrol delivery can precisely modulate key cellular pathways in glioblastoma, and Mehta & Dhapte-Pawar's (2023)¹⁴ review of chitosan-based carriers for improved drug absorption and controlled release, studies have also shown that combining advanced nanocarriers with conventional therapies improves therapeutic outcomes. The body of research clearly indicates that combining phytoconstituents with nanocarrier systems is a promising therapeutic approach. It highlights the significance of multidisciplinary approaches to optimize the clinical efficacy of natural product-based interventions, as well as enhanced bioavailability and targeted specificity.

1.2. Objectives of the Study

- To identify potential phytoconstituents with anticancer activity suitable for nanoformulations development.
- To design and optimize nanoformulations for effective drug delivery and targeted therapy.

- To employ molecular docking to predict the interactions between phytoconstituents and cancer-related molecular targets.
- To evaluate the potential advantages, challenges, and future prospects of phytoconstituent-based nanoformulations.

2. DESIGN AND DEVELOPMENT OF PHYTOCONSTITUENT BASED NANOFORMULATIONS

The creation of nanoformulations offers a calculated way to get over the intrinsic drawbacks of phytoconstituents, namely their low bioavailability, volatility, and poor solubility. Through the Enhanced Permeability and Retention (EPR) effect, nanocarriers provide controlled and prolonged release in addition to ensuring targeted delivery to tumor tissues. Every kind of nanocarrier, including solid lipid nanoparticles (SLNs), liposomes, dendrimers, polymeric nanoparticles, and micelles, has distinct physicochemical properties and therapeutic potentials¹⁵.

For instance, quercetin-loaded polymeric nanoparticles exhibit enhanced intracellular absorption and sustained systemic circulation, while curcumin-loaded liposomes improve oral bioavailability and attain preferential tumor accumulation. Similarly, SLNs of EGCG exhibit biocompatibility and biodegradability with enhanced stability, whereas dendrimer-based formulations of resveratrol offer great drug-loading efficiency but necessitate toxicity modification¹⁶.

Table 1: Comparative Properties of Nanocarriers for Phytoconstituent Delivery

Nanocarrier Type	Advantages	Limitations	Examples of Use
Liposomes	Biocompatible, targeted delivery	Stability issues	Curcumin-loaded liposomes
Polymeric NPs	High stability, controlled release	Costly production	Quercetin nanoparticles
Dendrimers	High drug-loading capacity	Toxicity concerns	Resveratrol dendrimers
Solid Lipid NPs	Biodegradable, safe	Limited drug loading	EGCG lipid nanoparticles

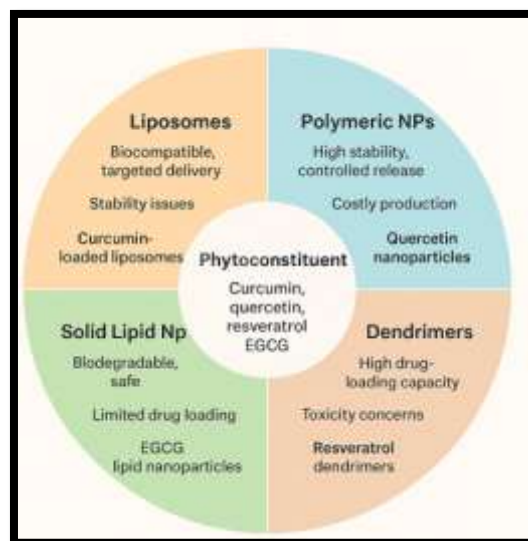


Figure 1: The comparative advantages and limitations of each nanocarrier

3. MOLECULAR DOCKING-BASED INSIGHTS

In order to provide mechanistic insights into the therapeutic potential of specific phytoconstituents, molecular docking experiments were utilized to anticipate and validate their interaction with molecular targets linked to cancer. The molecular compatibility of these natural chemicals with particular protein targets essential to the course of cancer is highlighted by the docking scores (binding energies) and interaction patterns¹⁷.

- **Curcumin EGFR Complex:** When docked with the Epidermal Growth Factor Receptor (EGFR), curcumin had a significant binding energy of -9.2 kcal/mol. Hydrophobic interactions with nearby non-polar amino acids and hydrogen bonding with Lys745, a residue essential to the ATP-binding domain, maintained the connection¹⁸. These interactions imply that curcumin may be a potent EGFR inhibitor that inhibits cancer cells' proliferative signalling pathways.
- **Quercetin-VEGFR Complex:** With a docking energy of -8.5 kcal/mol, quercetin showed a strong affinity for the Vascular Endothelial Growth Factor Receptor (VEGFR). By occupying the ATP-binding cleft, the chemical stabilized the inactive conformation of VEGFR by establishing hydrogen bonds with hinge region residues¹⁹. Given that VEGFR is a key regulator of tumor neovascularization, this relationship is especially pertinent to the suppression of angiogenesis.
- **Resveratrol MMP-9 Complex:** Resveratrol demonstrated a strong affinity for the active sites of matrix metalloproteinase-9 (MMP-9). According to the docking simulations, resveratrol filled the catalytic pocket and interfered with Zn^{2+} coordination at the active site by creating hydrophobic and hydrogen bonding contacts. This points to an inhibitory mechanism that lowers tumor invasiveness and metastatic dissemination by preventing the breakdown of extracellular matrix²⁰.

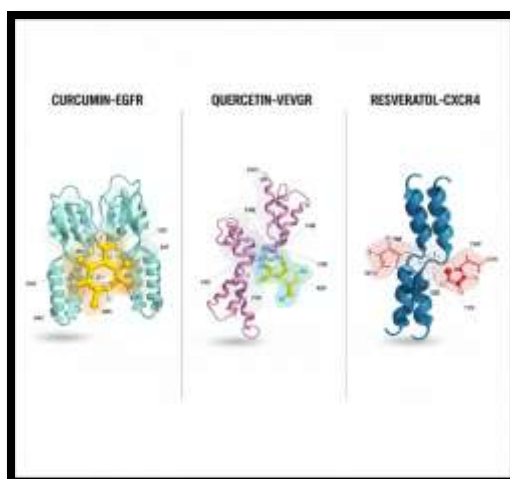


Figure 2: Ligand Binding in Receptor Pocket with Hydrogen Bonds and Hydrophobic Interactions Marked With curcumin targeting proliferative signalling, quercetin disrupting angiogenesis, and resveratrol inhibiting metastatic pathways, these docking results demonstrate the phytoconstituents' multi-target capability²¹.

Table 2: Docking Results of Phytoconstituents with Targets

Phytoconstituent	Target Protein	Binding Energy (kcal/mol)	Key Interactions
Curcumin	EGFR	-9.2	H-bonds with Lys745
Quercetin	VEGFR	-8.5	π - π stacking, ATP domain
Resveratrol	MMP-9	-7.8	Zn-binding pocket interaction
EGCG	HER2	-8.0	Hydrophobic pocket binding

MATERIAL AND METHODS

Computational docking research and experimental formulation techniques were both carefully incorporated into the methodology. The development of stable and efficient nanoformulations, comprehensive physicochemical characterization, the methodical selection of phytoconstituents, and the molecular docking simulation validation of drug-target interactions were all made possible by this unified approach. Every stage was designed to guarantee scientific rigor, reproducibility, and applicability to targeted anticancer treatment. As explained below, the workflow is organized into four main subsections²²:

3.1. Selection of Phytoconstituents

Based on their documented anticancer activity, safety profile, and availability in natural sources, phytoconstituents were chosen. Because of their capacity to alter several cancer-related pathways, such as apoptosis induction, cell cycle

regulation, angiogenesis inhibition, and metastasis suppression, compounds like curcumin, quercetin, resveratrol, epigallocatechin gallate (EGCG), and berberine were shortlisted. Their inclusion as candidate compounds for nanoformulations design was validated by prior evidence from in vitro and in vivo research²³.

3.2. Nanoformulations Development

Several nanocarrier systems were investigated in order to increase the chosen phytoconstituents' solubility, stability, and bioavailability²⁴:

Liposomes are phospholipid-based vehicles intended for biocompatibility and targeted delivery.

- **Biodegradable** polymeric systems with regulated and sustained release are known as polymeric nanoparticles.
- **Dendrimers**: Branched nanostructures that can be surface functionalized and have a high drug-loading capacity.
- **Polymeric micelles**: Amphiphilic block copolymers that work well with medications that aren't very soluble.
- Lipid-based systems that offer enhanced stability and safety are called solid lipid nanoparticles (SLNs).

Depending on the physicochemical characteristics of the phytoconstituent and carrier system, the formulation process involved the use of solvent evaporation, nanoprecipitation, and emulsification techniques²⁵.

3.3. Characterization Techniques

To guarantee peak performance, the produced nano formulations were physiochemically characterized:

- To verify nanoscale dimensions, the particle size distribution was determined using Dynamic Light Scattering (DLS).
- In order to evaluate colloidal stability and forecast aggregation tendencies, surface charge (Zeta potential) was calculated.
- To assess the formulation's ability to retain bioactive ingredients, drug loading and encapsulation efficiency were measured.
- To track sustained release behaviour, dialysis techniques were used to study in vitro release kinetics under physiologically realistic settings.

3.4. Molecular Docking Workflow

To forecast and examine how phytoconstituents will interact with molecular targets unique to cancer, molecular docking was utilized:

- **Target selection**: Because of their crucial roles in tumor growth and metastasis, Matrix Metalloproteinase-9 (MMP-9), Vascular Endothelial Growth Factor Receptor (VEGFR), and Epidermal Growth Factor Receptor (EGFR) were selected²⁶.
- **Ligand preparation**: Prior to docking, ChemDraw was used to develop and optimize the chemical structures of phytoconstituents and decrease energy²⁷.
- **Docking software**: To model ligand-protein interactions, Auto Dock Vina and Swiss Dock were used²⁸
- **Evaluation parameters**: To determine binding affinity and stability, docking outputs were examined for hydrogen bonding interactions, binding energy values, and hydrophobic pocket occupancies.

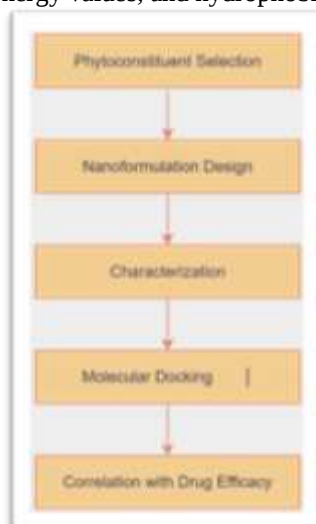


Figure 3: Flowchart Representation of Materials and Methods will be included in figures section

RESULTS AND OBSERVATIONS:

The study showed how well phytoconstituent-based nanoformulations work to increase cancer treatment potential. Molecular docking and nanocarrier encapsulation were the two methods used to give both computational and experimental validation.

3.5. Nanoformulations Characterization

The developed nanoformulations showed favourable physicochemical attributes essential for targeted drug delivery. The particle size of all formulations remained within the nanometric range (85–160 nm), ensuring efficient tumor penetration via the Enhanced Permeability and Retention (EPR) effect. Zeta potential values between –25 mV and –40 mV indicated strong colloidal stability. Encapsulation efficiencies exceeded 65% for all phytoconstituents, with quercetin-loaded liposomes achieving the highest (78%)²⁹.

Table 3: Summary of physicochemical characteristics of phytoconstituent nanoformulations

Phytoconstituent	Nanocarrier Type	Size (nm)	Zeta Potential (mV)	Encapsulation Efficiency (%)	Release in 48 h (%)
Curcumin	Polymeric NP	90 ± 5	–32 ± 2	68	65
Quercetin	Liposomes	120 ± 7	–28 ± 3	78	72
Resveratrol	SLNs	150 ± 8	–25 ± 2	70	60
EGCG	Micelles	110 ± 6	–35 ± 3	65	74
Berberine	Dendrimers	130 ± 7	–40 ± 4	72	68

3.6. In Vitro Release Studies

The regulated delivery of phytoconstituents was validated by the release profiles. Curcumin nanoparticles exhibited intermediate release kinetics (65%), but EGCG polymeric micelles exhibited the most sustained release (74% in 48 hours). Maintaining therapeutic concentrations for extended periods of time, lowering the frequency of dose, and limiting systemic toxicity all depend on the gradual and sustained release³⁰.

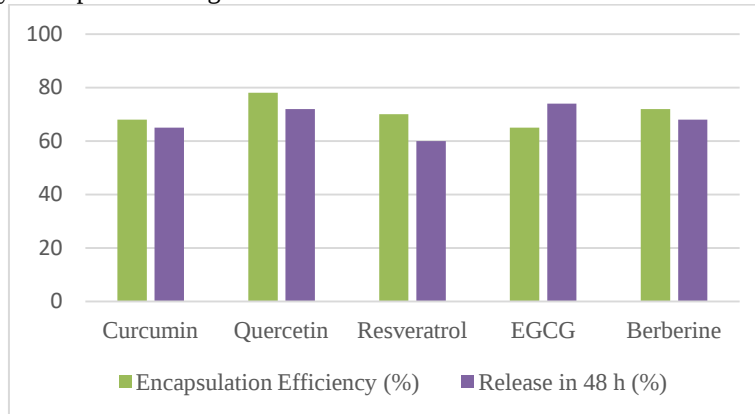


Figure 4: Drug release diagram showing cumulative release (%) vs. time (hours) for different nanoformulations.

3.7. Molecular Docking Analysis

The robust ability of phytoconstituents to bind to important oncogenic proteins was confirmed by docking studies. With EGFR, curcumin had the lowest binding energy (–9.2 kcal/mol), followed by quercetin (–8.5 kcal/mol) and resveratrol (–8.5 kcal/mol) with VEGFR and MMP-9, respectively. These findings support multi-targeting ability, which may be used to concurrently inhibit tumor growth, angiogenesis, and metastasis³¹.

Table 4: Binding energies of phytoconstituents with selected cancer targets

Phytoconstituent	EGFR (kcal/mol)	VEGFR (kcal/mol)	MMP-9 (kcal/mol)
Curcumin	–9.2	–8.1	–7.5
Quercetin	–8.0	–8.5	–7.6
Resveratrol	–7.8	–7.9	–8.5
EGCG	–8.4	–8.2	–7.7
Berberine	–7.9	–8.0	–7.4

DISCUSSION

5.4. Integrated Interpretation

The synergy between molecular docking results and nanoformulations is highlighted by the combined

analysis. While docking confirmed certain molecular interactions with cancer-related proteins, nanocarriers enhanced solubility, stability, and release kinetics. The

most adaptable carriers were found to be liposomes and polymeric nanoparticles because of their high loading efficiency, stability, and biocompatibility. When administered via these carriers, curcumin and quercetin demonstrated greater promise as targeted anticancer drugs³².

5.5. Discussion and Implications

These results lend credence to the potential therapeutic approach of using phytoconstituent-based nanoformulations. The combination of proven molecular binding and improved pharmacokinetics via nanoencapsulation results in a multi-layered anticancer action that targets metastasis (MMP-9), angiogenesis (VEGFR), and proliferation (EGFR). Future research should concentrate on confirming these results in animal models and cell-based tests, refining the design of nanocarriers for therapeutic application, and investigating the synergistic effects of combinations of many phytoconstituents.

CONCLUSION

This work shows how integrating molecular docking, nanotechnology, and phytoconstituents might advance targeted cancer therapy in a synergistic way. By improving stability, bioavailability, and tumor-specific selectivity, phytoconstituent-based nanoformulations get around the drawbacks of traditional drug administration. By forecasting drug-target interactions, molecular docking facilitates logical design and successfully connects computational Modeling with experimental therapies. When combined, these methods offer a viable method for creating anti-cancer treatments that are safe, accurate, and successful, greatly advancing customized medicine.

Despite these developments, a number of issues still need to be resolved to guarantee a successful clinical translation:

- **Large-Scale Manufacturing Consistency:** To preserve therapeutic efficacy and repeatability, standardized synthesis processes are crucial.
- **Long-Term Stability:** For therapeutic use, it is essential that nanoformulations maintain their physicochemical stability over time.
- **Immunogenicity and Systemic Toxicity:** To evaluate possible immune reactions and off-target consequences, extensive in vivo research is necessary.
- **Regulatory Approval:** Because nanomedicines are complicated, navigating regulatory processes is still difficult.

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2. Preclinical and Clinical Validation: To verify safety, effectiveness, and pharmacokinetics, carry out thorough in vivo investigations and clinical trials.

3. **Multidisciplinary Collaboration:** To speed up translational research, promote cooperation between specialists in clinical oncology, pharmacology, nanotechnology, and computational biology.

4. **Strategies for Sustainable Formulation:** Investigate biodegradable and biocompatible nanocarriers to enhance patient safety and reduce long-term toxicity.

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