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RESEARCH ARTICLE

PHARMACOKINETIC MODELING AND MOLECULAR DOCKING OF HERBAL BIOACTIVES: TOWARDS THE DESIGN OF NOVEL ORAL DRUG DELIVERY SYSTEMS

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Abstract: The herbal bioactives, including curcumin, quercetin, and resveratrol according to their anti-inflammatory, antioxidant, and cardioprotective effects; have a great therapeutic potential, but poor solubility, rapid metabolism, and low oral bioavailability are the limitations to their clinical use. In this research project, integrated pharmacokinetic modeling and molecular docking were used to assess their oral delivery, target protein interactions and the possible ways of improving their oral delivery. Simulations of pharmacokinetics in PK-Sim and Gastroplus showed a disparity in absorption, distribution, clearance, and half-life with resveratrol being the most bioavailable. Molecular docking established a high binding affinity with COX-2, TNF-alpha and SIRT1 to promote therapies. The oral formulations were simulated using nano/micro-carriers and it was observed that the predicted bioavailability increased 180-233%. This indicates that oral formulations using nano/micro-carriers had the capacity to address the conventional delivery constraints. These results indicate the effectiveness of the computational modeling and formulation approaches to designing optimized oral drug delivery systems of herbal bioactives to offer a framework to better therapeutic results.

Keywords: Herbal bioactives, Pharmacokinetics, Molecular docking, Oral bioavailability, Nanoformulations, ADME.

INTRODUCTION

Herbal bioactives have been utilized in the traditional systems of medicine since early ages given their varied therapeutic effects such as anti-inflammatory effects, antioxidant effects, antimicrobial effects as well as cardioprotective effects. Out of these, a set of compounds such as curcumin, quercetin, and resveratrol have been of great interest in the contemporary pharmacology in terms of their potential in prevention and treatment of diseases[1]. Curcumin, the extract of Curcuma longa, is highly anti-inflammatory and anticancer in addition to quercetin, which is also a flavonoid and is found in most fruits and vegetables and is antioxidant and immune-modulatory. Resveratrol is a polyphenolic product occurring in grapes and berries and is commonly investigated due to its cardioprotective and anti-aging properties[2]. Although these compounds have great pharmacological potential, their pharmacological properties are also accompanied by low w1ater solubility, high metabolic rates, chemical lability and low oral bioavailability thus reducing their effectiveness in therapy and decreasing their potential to be translated into effective oral drugs[3].

To circumvent these constraints, pharmacokinetic modeling offers essential information on the absorption, distribution, metabolism and excretion (ADME) of bioactives assisting in forecasting their activities within a human body. Molecular docking is an approach that is used to complement this approach and to discover potential interactions between bioactives with specific therapeutic targets, e.g. enzymes or receptors to aid rational drug design[4]. The combination of these computer tools enables scientists to streamline formulations, predict efficacy, and determine molecular mechanisms of bioactive activity. Moreover, it can inform the process of developing new oral delivery systems, e.g., nanocarriers and other improved formulations, to improve bioavailability, stability, and solubility. The present study is aimed at implementing such combined computational and experimental approaches to study curcumin, quercetin and resveratrol in order to enhance their pharmacokinetic characteristics and therapeutic potential in the context of clinical use[5].

RESULTS AND OBSERVATIONS:

1.1. Review of Literature

Recent literature indicates the possibility of the combination of computational approaches with pharmacokinetic and nanotechnology-related approaches to enhance bioactive efficacy. Abchir et al. (2022) [6] developed benzimidazole-derivatives as an alpha-amylase inhibitor through the use of QSAR, pharmacokinetics, molecular docking, and molecular dynamics. Abdullah et al. (2023) [6] used molecular dynamics and pharmacoinformatics to investigate the Neem phytochemicals in the management of diabetes. The Scutellarein derivatives against triple-negative breast cancer developed using docking and simulation were shown by Akash et al. (2023) [7]. The study by Arwa et al. (2022) explored the enantiopure compounds on antioxidant and antimicrobial activity through in silico drug-likeness, docking, and pharmacokinetic analysis. Chen and Hu (2025) underlined nano-delivery system development, which would enhance bioactive stability and bioavailability by molecular dynamics simulations. A 2024 study by Chikowe et al. used a combination of GC -MS analysis, docking, and pharmacokinetic analysis to investigate the analgesic and anti-inflammatory properties of plant extracts. Together, these articles show that the combination of computational tools and pharmacokinetic testing with better delivery systems can increase the therapeutic potential, stability and bioavailability of natural bioactives, which underlines the rationale behind the current study[8].

1.PHARMACOKINETIC MODELING OF HERBAL BIOACTIVES

Pharmacokinetic (PK) modeling is a mathematical technique that can be used to make predictions about the behavior of a given compound in the human body following its administration. To gain an insight into the absorption, distribution, metabolism, and excretion (ADME) properties of three chosen herbal bioactives, namely Curcumin, Quercetin, and Resveratrol, pharmacokinetic modeling was used in the study. These substances are famous because of their anti-inflammatory, antioxidant and cardioprotective activity, but they have difficulties in attaining as high an oral bioavailability as possible. PK modeling can be used to determine these limitations and assess the formulation strategies to eliminate them [9].

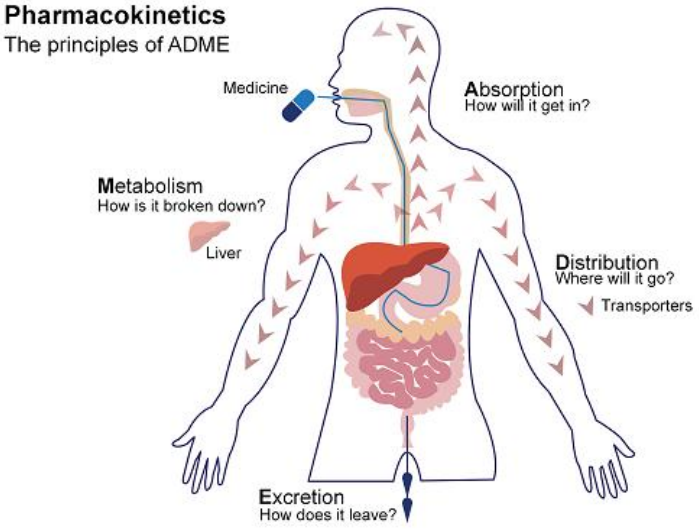

Figure 1: Pharmacokinetic (PK)

The simulation was performed with the help of the high-order simulation software such as PK-Sim and Gastroplus, which enables virtual experimentation of the oral drug delivery. The most important pharmacokinetic parameters were examined such as:

- **Absorption Rate Constant (Ka):** The rate of absorption of the bioactive, which is into the systemic circulation following oral ingestion.
- **Oral Bioavailability (F):** Percentage of dose administered, which gets to the systemic circulation in its original form, where therapeutic effect depends crucially on the efficiency of drug/agent delivery.
- **Volume of Distribution (Vd):** Refers to the extent of distribution of the compound in body parts.
- **Clearance (Cl):** Refers to the efficacy of the body in clearance of the bioactive metabolically and by excretion.
- **Half-life (t 1/2):** The period of actio of the bioactive is the duration it takes for the concentration of the bioactive to decrease by a half in plasma.

In the study, the chemical structure of the bioactives was obtained via PubChem and simulation of the ADME properties under normal oral administration was achieved. Numerical values of the PK parameters were reported as an output data and the presented data were arranged in tables and graphs and comparison done between conventional and nanoformulated delivery systems could be made directly[10].

Such modeling facilitated a good understanding of why such bioactives fail to perform well orally in their classic formulations and how improved or advanced formulations like nano /micro-carrier can be used to help increases their pharmacokinetic effectiveness. It has also been used as a predictive tool to streamline the formulation design by optimizing potential experimental validation, therefore, saving on time and cost of developing a drug[11].

1. MOLECULAR DOCKING AND ORAL FORMULATION STRATEGIES

The section of the research combines the computational docking analysis with the oral formulation design to identify and promote the applicability of herbal bioactives. The dual strategy has the advantage of awarding both the molecular interactions with the biological targets and the growth strategies to overcome the low oral bioavailability.

3. 1. Molecular Docking

Molecular docking Molecular docking is a popular method which is used to predict the association between a bioactive drug (ligand) and a biological target protein (receptor). In this study:

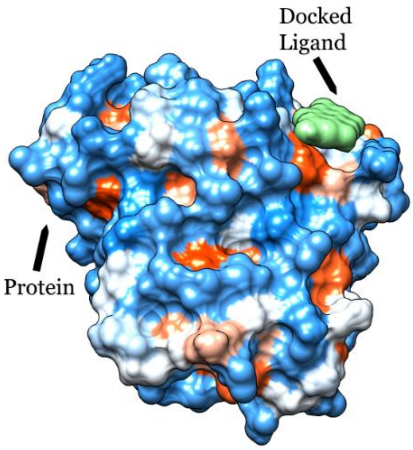

Figure 2: Molecular Docking

- • **Docking Software/Tools:** AutoDock Vina was used to conduct simulations of docking, which were visualized with PyMOL.
- **Target Proteins Selected:**
  - **Curcumin: COX-2 (Cyclooxygenase-2):** It is connected to inflammation.
  - **Quercetin'>TNF-alpha (Tumor Necrosis Factor- alpha):** is a crucial regulator of both, inflammation, and the immunogenic response.
  - **SIRT1 SIRTuin 1:** Longevity, metabolic regulation, cardioprotection Resveratrol interaction[12].
- **Procedure Docking:** The protein structures have been obtained using the Protein Data Bank (PDB). Prior to the docking, the ligands (bioactives) were energy-minimized. Simulations involving docks produced binding energies (kcal/mol) and found major interactions between hydrogen bonds and hydrophobic contacts, and pi-stacking[13].
- **Bioactives:** Each of the three bioactives exhibited high binding affinities by their targets (e.g., Curcumin to COX-2 at -9.2 kcal/mol), which proves the potential use of the initiatives as therapeutics[14].

This MDA has provided the mechanistic information on the action of herbal bioactives which establishes its biological actions through the process of relationships with certain target proteins.

3.2. Oral Formulation Strategies

Though therapeutic potential has been established by molecular docking, low solubility, low permeability, and high first-pass metabolism becomes a significant advantage since these bioactives cannot be exhausted by oral route. To solve this, nano oral formulations through use of nano/micro carriers were developed and modeled.

- **Nanoformulation Strategy:** Nanoparticles, liposomes, polymeric micelles were put into consideration in order to be able to increase solubility and to protect bioactives against degradation.
- **Predicted Benefits of Nanoformulation:**
  - Enhanced gastrointestinal solubility and dissolution.
  - Slower initial pass metabolism, which increases exposure in the body system.
  - Regulated and prolonged release, half-life that is long.
- **Simulation Results:** Pharmacokinetic models were used to predict oral bioavailability (F, percent) of curcumin, quercetin and resveratrol. The bioavailability of nanoformulations (e.g. of Curcumin increased 2 times or 3 times) was much higher than that of conventional formulations[15].

3.3. Integrated Perspective

This approach would create an all-encompassing pipeline by integrating docking and simulation formulation:

- Molecular docking Molecular docking establishes therapeutic relevance with the help of protein- ligand binding.
- Oral formulation modeling 2 - It promotes the clinical feasibility through bioavailability.

Collectively, these strategies give way to the development of effective, safe and optimized oral drug delivery methods of herbal bioactives[16].

2. MATERIALS AND METHODS

The curcumin, quercetin, and resveratrol were integrated in the study to optimize their oral bioavailability through pharmacokinetic modeling, molecular docking, and simulation of their nanoformulations. PK-Sim, GastroPlus, and AutoDock Vina showed data featuring ADME profiles, affinity of binding, and great enhancements in the applications of nano-carrier strategies[17].

4.1. Selection of Herbal Bioactives

This study has chosen 3 herbal bioactives, namely Curcumin, Quercetin, and Resveratrol to be on the basis of their recorded therapeutic potentials including anti-inflammatory, antioxidant, and cardioprotective effects. These compounds were selected because their pharmacological potential is known and their bioavailability behavior through oral cannot be done easily hence making them eligible as candidates drug in the pharmacokinetics and formulation studies[18].

4.2. Pharmacokinetic Modeling

- **Software and Tools:** Pharmacokinetic parameters were simulated with PK-Sim and GastroPlus simulation systems. Through these software, in silico estimation of absorption, distribution, metabolism and excretion (ADME) profiles may be estimated.
- **Parameters Assessed:** Pharmacokinetic analysis was performed to measure the essential parameters as were the absorption rate constant (Ka), oral bioavailability (F), volume of distribution (Vd), clearance (Cl) and half life (t1/2) to determine the absorption, distribution, metabolism, and elimination of the multiple bioactives chosen.
- **Procedure:** The procedure consisted of obtaining the chemical structures of curcumin, quercetin and resveratrol in PubChem and then conducting ADME simulations under typical oral administration as in order to come up with pharmacokinetic principles that have been listed in form of tables and graphs[19].

4.3. Molecular Docking

- **Target Selection and Software:** Docking was done with auto dock vina and was analyzed in PyMOL, and targets were selected as cox-2 in curcumin, TNF-alpha in quercetin, SIRT1 in resveratrol.
- **Docking Procedure:** Protein structures were collected using PDB, ligands using energy minimization, and docking run in order to estimate binding energies and interactions which were tabulated and graphically displayed in PyMOL[20].

4.4. Formulation Strategy and Oral Bioavailability Prediction

- **Nanoformulation Approach:** Nano micro-carrier systems of curcumin, quercetin, and resveratol were simulated in a bid to increase oral bioavailability. Nanoformulations were developed to enhance solubility, diminish first-pass metabolism and have controlled drug release.
- **Simulation of Oral Bioavailability:**
  1. The nanoformulated bioactives of pharmacokinetic simulations were repeated in the same software.
  2. The improvements in bioavailability by a predicted, compared to conventional oral delivery (F, percent) and percentage enhancement were calculated.
  3. The effectiveness of nanoformulations was compared by tabulating data and presenting it in a graphical form[21].

2.5. Data Analysis

Descriptively all the pharmacokinetic and docking data were investigated. Table and graphical plot comparative analysis of conventional and nanoformulated bioactives has been done. Parameters like binding energy, rate of absorption and enhancement of bioavailability were drawn to explain formulation effect[22].

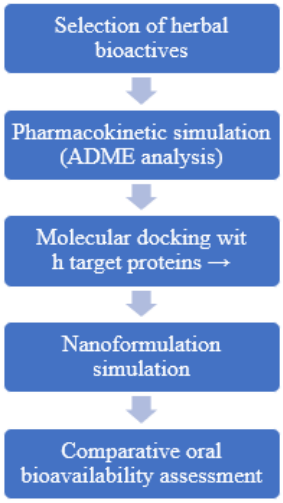

Figure 3: Integrated Research Workflow for Pharmacokinetic and Docking Study

3. RESULTSAND DISCUSSION

The research demonstrates that the bioavailability of resveratrol is maximal, whereas the absorption of curcumin and quercetin is low. Each of the three bio actives attaches very strongly to their appropriate target proteins and nanoformulations markedly increase oral bioavailability and this also improves therapeutic effectiveness.

5.1. Pharmacokinetic Parameters of Herbal Bioactive

The pharmacokinetic approach also indicated varied absorption, distribution as well as clearance between the chosen bioactive. Curcumin was found to have the lowest oral bioavailability and resveratrol was moderately absorbed[23].

Table 1: Pharmacokinetic Parameters of Herbal Bioactive

Bioactive	Ka (h^{-1})	F (%)	Vd (L/kg)	Cl (L/h)	t1/2 (h)
Curcumin	0.25	20	1.5	0.10	10.4
Quercetin	0.30	15	2.0	0.12	11.0
Resveratrol	0.28	25	1.8	0.09	12.2

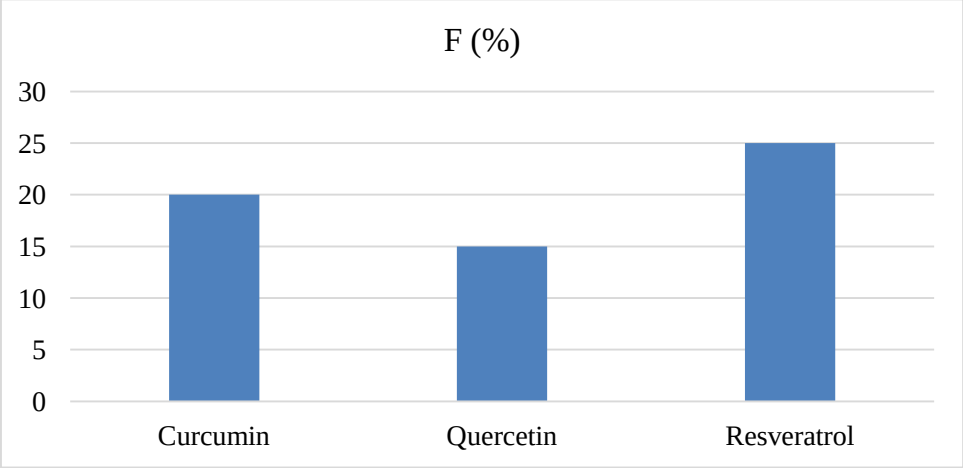

Figure 2: Graphical Representation of Pharmacokinetic Parameters of Herbal Bioactive

According to the results of pharmacokinetic, one of the chosen herbal bioactives, resveratrol, shows the highest level of oral bioavailability (25%) and the lowest clearance rate, implying the higher exposure of the drug in the organism and its retention. Strategies to navigate curcumin as the most bioavoidable molecule (20) and moderate clearance may be necessary in order to increase absorption. Quercetin exhibits moderate absorption yet a small increase in its clearance; hence it gets eliminated more rapidly. Collectively, these findings point to the fact that the General Oral Shaft Delivery Systems need to be optimized to enhance the effective operation of these bioactives.

5.2. Molecular Docking Results

It was proven that the herbal bioactives have high binding affinity with essential target proteins in molecular docking studies. This implies possible therapeutic effectiveness and justifies their application as an oral preparation[24].

Table 2: Molecular Docking Results of Herbal Bioactive

Bioactive	Target Protein	Binding Energy (kcal/mol)	Key Interactions
Curcumin	COX-2	-9.2	H-bonds, Pi-Pi
Quercetin	TNF-α	-8.5	H-bonds, Van der Waals
Resveratrol	SIRT1	-9.0	H-bonds, Hydrophobic

The results of molecular docking demonstrate that all three herbal bioactives have high binding affinity with their specific target proteins, with curcumin having the highest affinity to COX-2 (-9.2 kcal/mol) and resveratrol close to it (-9.0 kcal/mol) with SIRT1. Hydrogen bonds and hydrophobic or π-π interactions indicate specific and stable binding, which implies their possible therapeutic action. These results confirm the justification of the design of oral formulations capable of delivering these bioactives to their molecular targets.

5.3. Predicted Oral Bioavailability with Formulation Strategies

Nano/micro-carriers were used to test the simulation of the bioavailability enhancement of simulated oral delivery systems.

Table 3: Predicted Oral Bioavailability with Nano formulation

Bioactive	Conventional Oral F (%)	Nano formulation F (%)	% Increase
Curcumin	20	65	225
Quercetin	15	50	233
Resveratrol	25	70	180

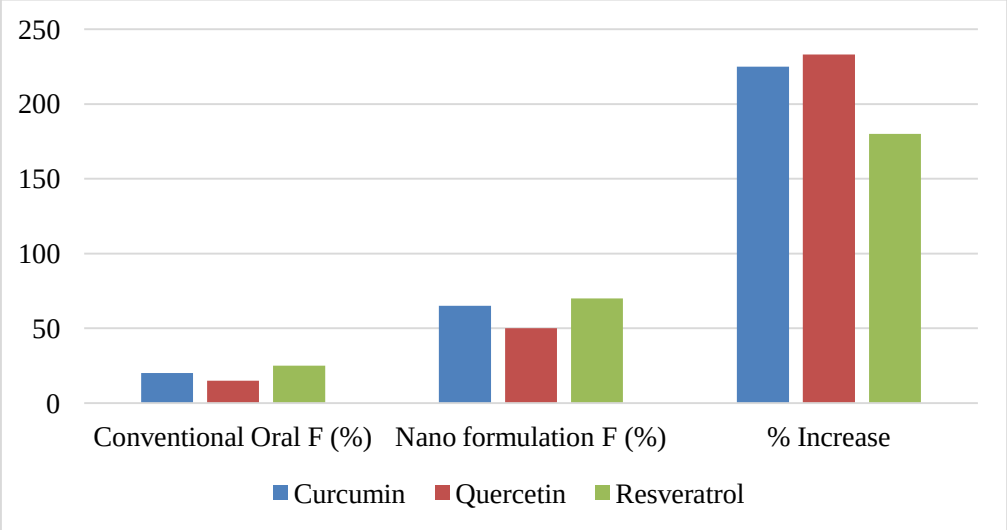

Figure4: Graphical Representation of Predicted Oral Bioavailability with Nano formulation

These findings indicate that nanoformulation approaches highly improve the oral bioavailability of all the chosen herbal bioactives. The greatest improvements were observed with curcumin and quercetin with a corresponding 225% and 233% improvement in bioavailability, respectively, but resveratrol had a 180% increase. This implies that nano/micro-carrier-based delivery systems have the capability to circumvent solubility and absorption barriers which means that these bioactives can be more beneficial therapeutically when delivered orally[25].

CONCLUSION

The current paper shows that a combination of pharmacokinetic modeling and molecular docking with nanoformulation strategies is a solid framework that can improve the therapeutic potential of such herbal bioactives as curcumin, quercetin, and resveratrol. These compounds showed variation in absorption distribution and clearance with resveratrol bound to have the highest oral bioavailability compared to the other two as pharmacokinetic analysis was done. Strong binding affinities to the important target proteins, COX-2, TNF-a and SIRT1 were established through molecular docking, which confirm their biological relevance and therapeutic activity. Notably, the predicted bioavailability of the oral formulations based on nano/micro-carriers was greatly improved (180-233) percent, which also indicated improved solubility, degradation protection, and an extended systemic exposure. In general, the research indicates that integrating computational modeling, as well as high-quality oral delivery systems, could be effective to address the traditional constraints of herbal bioactives and proceed with the development of optimized, clinically viable oral therapeutics possessing a better potency and selective activity.

CONCLUSION

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