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MOLECULAR DOCKING OF HERBAL COMPOUND (CURCUMIN)

Sainath Vijaysing Gadekar*[1], Dr. Rahul Prakash Lokhande[2], Parth Dnyaneshwar Dathkhil[1], Shrutika Pralhad Gadge[1], Aditya Sampat Dere[1], Sakshi Rajesh Gaikwad[1], Tanvi Sopan Dongare[1]

[1]Student, Samarth Institute of Pharmacy, Belhe, Pune, Maharashtra, India.

[2]Associate Professor, Department of Pharmaceutical Chemistry, Samarth Institute of Pharmacy, Belhe, Maharashtra, India.

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***Corresponding Author: Sainath Vijaysing Gadekar**
Student, Samarth Institute of Pharmacy, Belhe, Pune, Maharashtra, India
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ABSTRACT

Curcumin is an important thing in pharmaceutical sciences. This is because it can affect different things that happen inside our cells. There is a big problem when it comes to using curcumin in medicine. It does not get absorbed by our bodies well. This review looks at some studies that used computers to see how curcumin interacts with certain targets in our body like NF-κB, CDK2 and the PI3K/Akt pathway. We want to understand how curcumin works and how it can affect different things at the same time. We also want to look at the bad things about using computers to design new drugs. The big problem with curcumin is that it does not get absorbed by our bodies well. We can use computers to help us find ways to make it work better. For example, we can use computers to find the combinations of ingredients to mix with curcumin. This paper state that what various studies not defines. It suggests some new ways that we can use curcumin to make new drugs. In the future we can use computers to make better predictions, about how curcumin will work. We can use something called dynamics and artificial intelligence to make our predictions more accurate. This will help us make drugs that use curcumin and that will really work well. We can make tiny formulations of curcumin that will get absorbed by our bodies and will be very effective.

KEYWORDS: Curcumin, Pharmacokinetics, NF-κB signaling, PI3K/Akt pathway, Molecular docking, Nanoformulations.

INTRODUCTION

Background

Molecular docking is a part of computer-aided drug design. It helps us figure out how a drug candidate will interact with a target protein. Molecular docking tries to find the way a drug candidate will fit into a protein. This is like a lock and key. The drug molecule has adrees into the protein.

Molecular docking uses computer programs to try different ways a drug candidate can fit into a protein. Then it uses math to see which way is the best. This math is called scoring functions. It helps us see which drug candidates are the likely to work. We want the ones that have an energy score. This means they will interact with the protein in a way. Molecular docking is very important in making drugs. It helps us find the drug candidates and make them even better. It also helps us see how the drug candidates will interact with the protein. This includes things like hydrogen bonding and hydrophobic forces. These things are important for making sure the drug works right.

Molecular docking is not perfect. It has some problems. Thus if the protein stucture is not good then the results will varyWe also have to consider that proteins can change shape. The math we use to score the drug candidates is not always right. Some computer programs do not take into account the way things really work in the body. They do not consider the solvent and the way proteins really move. Molecular docking is still an useful tool, for making new drugs. We use docking to find the best drug candidates. Molecular docking helps us make sure the drug candidates will work with the protein. We use docking to make new and better drugs.

The way we discover drugs has changed a lot. We do not just look for one drug that targets one thing anymore. This is especially true when we look at things like curcumin. Curcumin is a type of polyphenol. It is a special molecule that can do a lot of things. It can talk to different molecules inside our body like the ones that cause inflammation the ones that help our cells survive and the ones that send signals.

Curcumin is very good at doing what it does. It has some problems. It does not mix well with water it breaks down quickly in our body. It is hard for our body to use it. These problems make it hard for us to use curcumin as a drug. So, we need to use computer tools to understand how it works and to make it better. One way we do this is by using something call docking. This is a way to figure out how small molecules fit into the spots on proteins where they can bind. It is like a puzzle. We use computers to simulate how the atoms in the molecule and the protein interact with each other. This helps us see what makes the molecule stick to the protein.

We want to understand how curcumin works and how we can make it a better drug. Curcumin is a special compound. It can do things because it affects many different parts of our body. It does not just target one thing it targets things. This is because of its chemical structure. It has a group called a beta-diketone group and two rings that have oxygen atoms. These things allow curcumin to work in different ways.

- It has different mechanisms
- It can affect different things in our body
- It is a useful compound

The general way that curcumin works is by affecting many different things. It is, like a key that can open different doors. This is called a framework. It means that curcumin can do things because it can affect many different parts of our body.

1. Regulation of the NF-κB Signaling

Pathway Curcumin effectively inhibits the Nuclear Factor kappa B (NF-κB) pathway, which is a key regulator of inflammation and cell death.

2. Multi-Kinase Inhibition and Cell Cycle Arrest

Curcumin directly targets several oncogenic kinases, including:

- **Cyclin-Dependent Kinases (e.g., CDK2):** It binds within the ATP-binding cleft, mimicking traditional inhibitors and inducing G1/S phase arrest.
- **PI3K/Akt/mTOR Axis:** Curcumn inhibits the phosphorylation of Akt and mTOR, which are hyperactivated in numerous malignancies, thereby promoting apoptosis.
- **MAPK and STAT Pathways:** It disrupts signaling through Mitogen-Activated Protein Kinases and Janus Kinases, which govern cell proliferation and survival.

Advantages, Disadvantages, and Limitations of Molecular Docking

Feature	Advantage in Pharmaceutics	Disadvantage / Limitation
Virtual Screening (VS)	Low cost; high speed; ability to screen millions of compounds (e.g., lipid libraries).	High rate of false positives; limited by the accuracy of the scoring function.
Rigid Docking	Computational efficiency, suitable for screening large protein datasets.	Fails to account for "induced fit" where the protein changes shape upon binding.
Flexible Docking	High accuracy, closest to real biological situations; accounts for rotatable bonds.	Extremely intensive computationally; requires high hardware resources.
Scoring Functions	Provides a quantitative value (ΔG) to rank compounds.	Often fails to correlate with actual experimental binding affinities (IC_{50}).
Solvent Modeling	Simplifies the docking process by removing water molecules.	Ignores the critical role of water in mediating ligand-receptor interactions.

Plant profile

Curcuma long

- *Curcuma longa* (turmeric) is a perennial herb belonging to the family **Zingiberaceae**, mainly cultivated for its medicinal rhizomes.
- The **official drug part is the dried rhizome**, which is branched, yellow-orange in color, and has a characteristic aromatic odor.

- Its major active constituents are **curcuminoids**, mainly curcumin, along with demethoxycurcumin and bisdemethoxycurcumin.
- It also contains **volatile oils** such as turmerone and zingiberene, which contribute to its aroma and biological effects.
- Pharmacologically, it shows **anti-inflammatory, antioxidant, antimicrobial, hepatoprotective, and anti-ulcer activities**.
- These effects are mainly due to curcumin's action on inflammatory mediators and oxidative stress pathways.
- It is used in liver disorders, digestive problems, skin infections, and inflammatory conditions like arthritis.
- Adulteration may occur with starch or harmful coloring agents such as lead chromate.
- Overall, turmeric is an important and widely used herbal drug in pharmacognosy and traditional medicine.

MATERIALS AND METHODS

CATEGORY	DETAILS
HARDWARE	High-performance workstations (e.g., Intel Core i7, 16 GB RAM, dedicated GPU)
SOFTWARE	AutoDock 4.2.6, AutoDock Vin, PyRx (0.8) for simulation; PyMOL and BIOVIA Discovery Studio for visualization

MATERIAL	CATEGORY	ROLE IN PHARMACEUTICAL RESEARCH / DOCKING
CURCUMIN (API)	Diarylheptanoid	Primary ligand for docking against multi-disease targets
GMS (GLYCERYL MONOSTEARATE)	Solid Lipid	Preferred matrix for NLCs due to high affinity (-8.6 kcal/mol)
OLEIC ACID	Liquid Lipid	Used to optimize drug loading in nano-lipid carriers
L-PROLINE	Co-former	Employed for co-crystallization to enhance solubility (71% CDR)
PIPERINE	Bioavailability Enhancer	Used as a co-former and metabolic inhibitor (CYP3A4)
POLOXAMER 188	Surfactant	Stabilizer for polymeric and lipid nanoparticles

Method of Preparation

1. The molecular docking procedure starts by choosing the receptor protein, downloading its 3D structure from the Protein Data Bank (PDB) (e.g., 1KE6 for CDK2), and eliminating extraneous molecules such as water and co-crystallized ligands.
2. The receptor is subsequently prepared by incorporating absent hydrogen atoms, applying Kollman charges, and conducting energy minimization to achieve a stable structure.
3. The ligand is then generated by transforming its 2D representation into a 3D structure, followed by geometry optimization using the MM2 method and assigning Gasteiger charges.
4. Following the preparation of the ligand, the active site is identified and grid box parameters are configured by detailing coordinates (x, y, z) and grid spacing (typically 0.375 Å).
5. The docking simulation utilizes software like AutoDock or AutoDock Vina, employing algorithms such as the Lamarckian Genetic Algorithm or the Vina scoring function.
6. The approach is confirmed by redocking the ligand and computing the RMSD value; if it is below 2.0 Å, the docking outcomes are deemed trustworthy.
7. Ultimately, the bound complex is examined, and interactions like hydrogen bonds and hydrophobic interactions are assessed to comprehend ligand–protein binding.

RESULT

The review artical studies show that Curcumin works well because it can affect important biological targets at the same time.

These targets include

- NF-kB,
- PI3K/Akt,
- CDKs.

This is why Curcumin is effective.Curcumin targets NF-kB thus,Curcumin also targets PI3K/Akt and Curcumin targets CDKs too.

CONCLUSION

Curcumin is a model of multi-targeted medicinal treatment. This review confirms that its pleiotropic effects spanning from NF-κB suppression to kinase inhibition result from its tautomeric flexibility and phenolic interactions. Although molecular docking offers an efficient framework for discovering new targets and enhancing formulation excipients, its dependence on static models and estimated scoring functions is a significant drawback. Combining semi-flexible docking with molecular dynamics and strategic SAR alterations presents the most effective strategy for tackling the biopharmaceutical challenges associated with curcumin. Ultimately, the shift from in silico prediction to standardized clinical formulations will determine curcumin's place in contemporary evidence-based medicine.

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