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Molecular Docking of Bioactive Compounds against Leukemia Protein Targets

Kanimozhi. B.[1], Keerthana N.[2], Kiruba Shiny S.[3], Sr. Dr. S. Kulandai Therese[4]
[1, 2, 3]*Bachelor of Science In Chemistry, Nirmala College for Women (Autonomous), Coimbatore, Bharathiar University, Coimbatore*
[4]*M.Sc., M. Phil., Ph.D, Assistant Professor, Department Of Chemistry, Nirmala College For Women (Autonomous), Bharathiar University, Coimbatore*

Abstract: ***Cancer is one of the leading causes of death worldwide and is characterized by uncontrolled cell growth and the ability of abnormal cells to spread to other parts of the body. Among different types of cancer, leukemia is a serious blood cancer that affects the bone marrow and blood-forming tissues. Targeting specific proteins involved in cancer progression has become an important strategy in modern drug discovery. Molecular docking is a computational technique widely used to predict the interaction between small molecules and target proteins, helping researchers identify potential therapeutic compounds.***
The present study focuses on the molecular docking analysis of selected natural bioactive compounds against the FLT3 (FMS-like tyrosine kinase 3) receptor, which plays a significant role in the development and progression of acute myeloid leukemia. The compounds selected for this study include Curcumin, Resveratrol, Quercetin, Camptothecin, and Vincristine. Venetoclax was used as the standard drug for comparison. The three-dimensional structures of ligands were obtained from chemical databases and prepared using computational tools, while the receptor structure was retrieved from the Protein Data Bank. Docking simulations were carried out using Auto Dock software to evaluate binding affinity, ligand efficiency, inhibitory constant, and hydrogen bond interactions. The docking results indicated that Venetoclax exhibited the highest binding affinity with a binding energy of –8.83 kcal/mol. Among the tested compounds, Vincristine and Camptothecin showed comparatively stronger interactions with the FLT3 receptor, while Curcumin, Quercetin, and Resveratrol demonstrated moderate binding affinity. Hydrogen bond interactions with key amino acid residues further confirmed stable ligand–protein complexes. Overall, the study suggests that these natural compounds possess potential inhibitory activity against FLT3 and may serve as promising candidates for further experimental validation and drug development in leukemia treatment.

I. INTRODUCTION

Cancer is a group of diseases characterized by uncontrolled growth and division of abnormal cells in the body. Normally, cells grow and divide in a regulated manner, but in cancer this control mechanism fails, leading to formation of tumors and possible metastasis to other organs. Cancer is one of the leading causes of death worldwide, but early detection and treatment can improve survival rates [1]. Cancer develops due to genetic mutations caused by several factors including radiation, chemical exposure, viral infections, smoking, alcohol consumption and environmental pollutants. These factors damage DNA and lead to abnormal cellular behavior. Tumors formed due to uncontrolled cell division can be either benign or malignant. [1-5]

II. REVIEW OF LITERATURE

The review of literature presented in this paper synthesizes key studies and findings from a wide range of academic sources, primarily gathered from Google Scholar. It highlights the evolution of research in the relevant field, identifying major trends, gaps, and emerging themes. By analyzing both classic and recent contributions, the review aims to provide a comprehensive understanding of the topic. The selected studies offer valuable insights into the methodologies, results, and theoretical frameworks employed. Ultimately, this review sets the foundation for further research and contributes to the ongoing scholarly discourse in the field. [6-30]

III. MATERIALS AND METHOD

A. Compounds

Curcumin – derived from turmeric with anti-inflammatory and anticancer activity.
Resveratrol – polyphenol found in grapes with antioxidant and anticancer activity.
Quercetin – flavonoid present in fruits and vegetables.
Vincristine – alkaloid derived from Catharanthus roseus used in chemotherapy.
Camptothecin – natural compound inhibiting topoisomerase I enzyme.

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B. Target Protein

FLT3 (FMS-like Tyrosine Kinase 3) is a receptor tyrosine kinase expressed in hematopoietic stem cells. Mutations in FLT3 are frequently associated with acute myeloid leukemia and therefore it is an important therapeutic target.

C. Software Used

PubChem – used to obtain ligand structures.
My Corina – used to obtain ligand 3D structure.
Protein Data Bank – used to obtain 3D structure of FLT3.
AutoDock – used to perform molecular docking.
PyMOL – used for visualization of ligand–protein interactions.

D. Docking Procedure

The receptor structure was prepared by removing water molecules and adding polar hydrogens. Ligands were prepared by adding Gasteiger charges and defining rotatable bonds. Grid parameters were set around the active site and docking simulations were performed using the Auto Dock genetic algorithm. Binding energy, inhibition constant and hydrogen bond interactions were analyzed from docking results.

IV. RESULT AND DISCUSSION

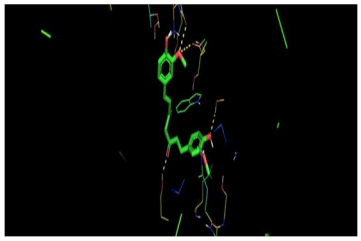
1) Docking result of standard drug: The docking analysis of Venetoclax showed strong binding affinity toward FLT3 with a binding energy of –8.83 kcal/mol. Several hydrogen bond interactions were observed with residues such as SER3, SER240 and HIS181.
2) Docking Results of Natural Compounds: Camptothecin showed a binding energy of –6.43 kcal/mol forming hydrogen bonds with ALA1, THR247 and TYR196. Curcumin demonstrated moderate binding affinity (–5.68 kcal/mol) with multiple hydrogen bonds. Resveratrol and Quercetin showed moderate inhibitory potential, while Vincristine exhibited comparatively strong interaction among the natural compounds with binding energy of – 6.65 kcal/mol.

Compounds	Binding energy (kcal /mol)	Ligand efficiency (kcal/mol)	Inhibitory constant	Inhibitory constant unit	No.of hydrogen bonds	Binding interactions
Camptothecin	-6.43	-0.25	19.32	µM	3	f:ALA1:HNI::O9 f:THR247:HN::O9 f:TYR196:HH:011
Curcumin	-5.68	-0.21	68.97	µM	5	Curcumin:H43::ASP69:OD2 flt3:HISI81:HDI::O25 flt3: ALA1: HN1 :: O27 flt3 : SER240 : HG1 :: O15 flt3 : SER67 : HG :: O24
Reservatrol	5.13	-0.30	172.22	µM	3	R:H27::THR242:OG1 R:H28::ASP69:OD1 R:H29::SER240:OG
Vincristine	-6.65	-0.11	13.25	µM	1	f:SER3:HG::O46
Quercetin	-5.25	-0.24	142.27	µM	2	Q:H28::SER183::OG f:SER67:HG::O19

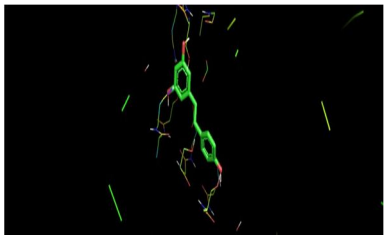
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In this table, the docked molecules, docking scores are represented. In this Vincristine shows the comparatively high binding energy.

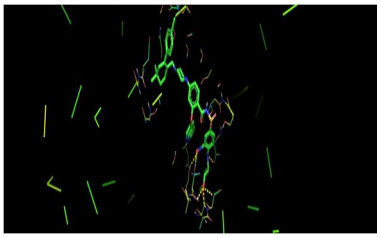
1) Camptothecin: Camptothecin showed a binding energy of −6.43 kcal/mol with the FLT3 receptor. The compound formed three hydrogen bonds, indicating a stable interaction and potential inhibitory activity.
2) Curcumin: Molecular docking analysis revealed a binding energy of −5.68 kcal/mol against the FLT3 protein. It formed five hydrogen bonds, suggesting moderate binding stability with the target protein.
3) Resveratrol: Resveratrol exhibited a binding energy of −5.13 kcal/mol with the FLT3 receptor. The compound formed three hydrogen bonds, indicating a relatively weaker interaction compared to other ligands.
4) Vincristine: Docking results showed that vincristine had the binding energy of −6.65 kcal/mol, indicating the strongest interaction among the tested compounds. It formed one hydrogen bond with the FLT3 protein.
5) Quercetin: The docking analysis showed a binding energy of −5.25 kcal/mol with the FLT3 receptor. It formed two hydrogen bonds, demonstrating moderate binding affinity with the target protein.



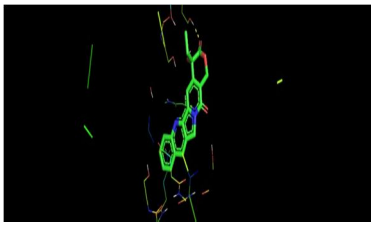
Interaction between Venetoclax and FLT3



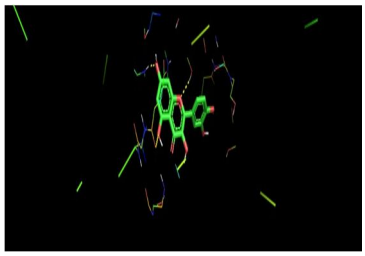
Interaction between Camptothecin and FLT3



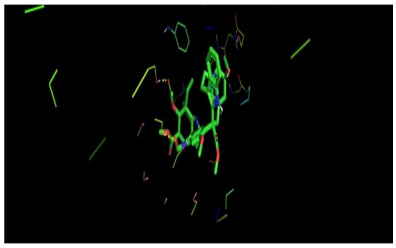
Interaction between Curcumin and FLT3



Interaction between Resveratrol and FLT3



Interaction between Vincristine and FLT3



Interaction between Quercetin and FLT3

V. CONCLUSION

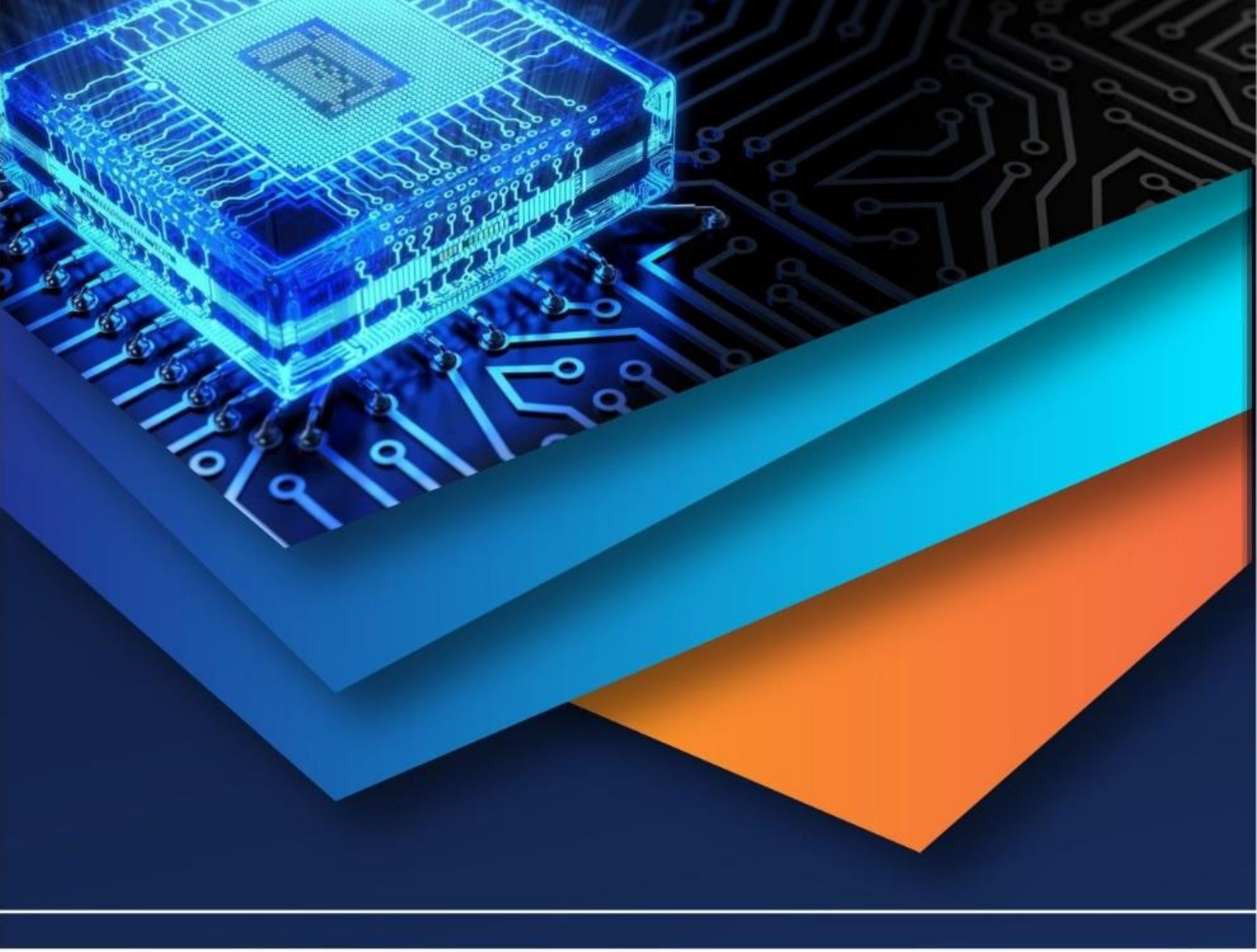
The docking study compared the interaction of natural compounds with the FLT3 protein against the standard drug Venetoclax. Venetoclax showed the strongest binding affinity (–8.83 kcal/mol). Among the tested natural compounds, Vincristine displayed relatively strong interaction followed by Camptothecin. Curcumin, Resveratrol and Quercetin showed moderate inhibitory potential. These compounds may serve as potential leads for further experimental and structural optimization in leukemia treatment.

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