e-ISSN: 2249 – 7781
Print ISSN: 2249 – 779X

International Journal of Pharmaceutical Research & Analysis
www.ijpra.com

Review Article

MOLECULAR DOCKING AND ADMET ANALYSIS OF OPHIORRHIZA RECURVIPETALA PLANT CONSTITUENT WITH MULTIPLE PHARMACOLOGICAL ACTIVITIES

Saravanan C, Vaishnavi G*

Aadhibhagawan college of pharmacy, Rantham, Thiruvannamalai, Tamil Nadu, India

ABSTRACT

Ophiorrhizarecurvipetala is a medicinal plant known for its diverse therapeutic potential attributed to its rich phytochemical profile. In the present study,major phytochemicals—camptothecin, gallic acid, betulinic acid, ursolic acid, β-sitosterol, kaempferol,quercetin and someother phytochemicals—were evaluated through in-silico molecular docking using the CB-Dock2 and ADMET analysis platform to predict their binding affinity, pharmacokinetic parameters and interaction potential against key protein targets associated with various biological activities. The selected biological activities and their corresponding protein targets included antioxidant (SOD-1), anticancer (Bcl-2), anti-inflammatory (COX-2), antibacterial (Human tetrameric LL-37), antifungal (Lanosterol-14-α-D-methylase CYP51), antiviral (Zinc finger antiviral protein), antidiabetic (Human lysosomal acid- Alpha glycosidase), and hepatoprotective pathways. Ligands and protein structures were prepared and docked to identify binding cavities and estimate interaction energies. Docking analyses revealed that several phytochemicals exhibited strong affinity toward multiple targets, suggesting multi-functional therapeutic potential. Notably, compounds such as camptothecin, betulinic acid, kaempferol, and quercetin demonstrated significant binding interactions correlating with their known pharmacological properties. The study highlights the potential of O. recurvipetala phytochemicals as promising leads for drug development and ADMET analysis supports further experimental validation through in-vitro and in-vivo investigations.

Keywords: Ophiorrhizarecurvipetala, Docking, Phytochemicals, Binding Energy, Pharmacokinetic parameters.

INTRODUCTION

Plant resources provide not only essential dietary nutrients but also biologically active compounds that play a crucial role in human health and disease management. These plants contain diverse phytochemicals, including alkaloids, flavonoids, glycosides, and lipids, which have applications in dietary, pharmaceutical, and cosmetic industries. In countries like India, traditional medicines derived from plants often serve as a primary healthcare resource due to the therapeutic properties of these compounds. Medicinal formulations in traditional systems are usually prepared from crude plant extracts, which contain a complex mixture of metabolites. While many plant species produce a wide variety of secondary metabolites, only a few have been systematically studied and identified as significant bioactive compounds. These compounds demonstrate potential therapeutic effects, including anti-inflammatory, antioxidant, anticancer, and antimicrobial activities, which have attracted increasing scientific interest [1].

Ophiorrhizarecurvipetala, a novel plant species from the family Rubiaceae, was recently described in Assam, India. Belonging to the genus Ophiorrhiza, this plant is distributed across tropical and subtropical regions of Asia, Australia, and the moist forests of the Pacific Islands. Species of the Ophiorrhiza genus are well-known for their diverse medicinal applications. Previous phytochemical studies have identified bioactive compounds such as

Corresponding Author
Vaishnavi G

Email: gvaishnavi2304@gmail.com

alkaloids, terpenoids, flavonoids, and phytosterols in various parts of these plants, which are recognized for their potent therapeutic and antioxidant properties. Despite these findings, the precise mechanisms through which these phytochemicals exert their effects remain largely unexplored [2].

Molecular Docking Study

Molecular docking, an in-silico approach, allows the prediction of interactions between bioactive ligands and target proteins of known three-dimensional structure. This technique can identify potential therapeutic candidates by evaluating binding affinities and specific interaction patterns [3].

The present study mainly Aim to investigate the in-silico properties of bioactive compounds extracted from Ophiorrhizarecurvipetala leaves and assess their interactions with selected target proteins associated with diverse biological activities, providing insights into their therapeutic potential [4].

MATERIALS AND METHODS

Selection of Plant and Phytochemicals:

Ophiorrhizarecurvipetala was selected for this study owing to its reported biological activities and the presence of diverse secondary metabolites. Thirteen phytochemicals previously documented in Ophiorrhiza species were shortlisted for virtual screening. These included Camptothecin (ID: 24360), Gallic acid (ID: 370), Ferulic acid (ID: 445858), Quercetin (ID: 5280343), β-Sitosterol (ID: 222284), Betulinic acid (ID: 64971), Stigmasterol (ID: 5280794), Stearic acid (ID: 5281), Palmitoleic acid (ID: 445638), Nonadecanoic acid (ID: 12591), Linalool (ID: 6549), Kaempferol (ID: 5280863) and ursolic acid (ID: 64945). Selection of these compounds was based on their known antioxidant, anti-inflammatory and therapeutic potential.

Ligand Preparation:

SMILES structures of the selected phytochemicals were generated using the PubChem tool. These SMILES strings were subsequently converted into 3D conformations using the CACTUS (NCI/CADD) SMILES Translator platform, and the resulting ligand files were downloaded in PDB format. Further optimization, including structural refinement and removal of unwanted fragments, was performed using Discovery Studio Visualizer (BIOVIA) to ensure proper geometry and suitability for molecular docking analyses[5].

Target Selection and Preparation:

The above mentioned ligands were subjected for the bioactive properties such as Antioxidant (Human SOD 1 complexed with Isoproterenol ID: 5YTU), Anti-cancerous (Bcl-2 complex with Beclin ID: 5VAX), Anti-inflammatory/Anti-Asthmatic (Aspirin acetylated human cyclooxygenase-2 ID: 5F19), Antimicrobial (Human Tetrameric LL-37 peptide ID: 7PDC), Antiviral (Zinc Finger Anti viral protein ID: 7KZH), Antifungal (Human lanosterol 14 alpha-demethylase complex with ketoconazole ID: 3LD6), Hepatoprotective (Human cytochrome P450 2E1 with inhibitor indazole ID: 3E6I), Anti-diabetic (Human lysosomal acid - alpha glucosidase complex with N- acetyl cysteine ID: 5NN4)

The target protein structure used for docking was retrieved from the RCSB Protein Data Bank (https://www.rcsb.org/). The corresponding PDB file was downloaded and prepared for docking analysis. Protein preprocessing—including the removal of water molecules, heteroatoms, and bound ligands—was performed using Discovery Studio Visualizer (BIOVIA). The cleaned and optimized protein structure was then saved inpdb format for subsequent molecular docking analyses [6].

Molecular Docking Using CB-Dock2:

Structure-based molecular docking was carried out using the CB-Dock2 platform, which integrates automated binding-cavity detection with the AutoDock Vina docking engine. CB-Dock2 preprocesses the uploaded protein structure by removing crystallographic water molecules, cofactors, and previously bound ligands prior to docking [7]. The prepared protein was uploaded first, followed by the refined ligand structures. For each phytochemical, CB-Dock2 generated predicted binding cavities, optimal docking poses, Vina binding affinity scores, and the interacting amino-acid residues within the active site. Docking outputs were further visualized and analyzed using Discovery Studio Visualizer (BIOVIA) to examine hydrogen bonding, hydrophobic interactions, and other molecular interaction features [8].

RESULTS:

Anti-oxidant

Control drug – N-Acetylcystine

Target Protien ID – 5ytu

Structure-based blind docking results, the standard antioxidant drug N-acetylcysteine exhibited a relatively weaker binding affinity (−4.8 kcal/mol), whereas several phytochemicals—such as Camptothecin (−9.9 kcal/mol), Kaempferol (−9.2 kcal/mol), and Quercetin (−9.1 kcal/mol)—showed significantly stronger binding affinities, indicating more stable and favorable interactions compared to the standard. Additionally, compounds including β-Sitosterol, Ursolic Acid, Stigmasterol, and Betulinic Acid demonstrated moderate binding affinity within the large C1 cavity. In contrast, weaker binders such as Gallic Acid, Ferulic Acid, Palmitoleic Acid, and Linalool exhibited lower affinities relative to the majority of the phytochemicals. Overall, these results suggest that most of the plant-derived phytochemicals may serve as promising leads for further biological or therapeutic evaluation [9, 10]

Anti Inflammatory
Control Drug – Indomethacin
Target Protien ID – 5F19

Based on blind docking analysis, indomethacin, with a binding affinity of –8.9 kcal/mol at the C1 pocket, served as the control ligand. A significant number of phytochemicals exhibited stronger binding affinities than the standard. These include stigmasterol (–10.7 kcal/mol), betulinic acid (–10.2 kcal/mol), ursolic acid (–10.0 kcal/mol), beta-sitosterol (–9.7 kcal/mol), quercetin (–9.7 kcal/mol), camptothecin (–9.8 kcal/mol), and kaempferol (–9.3 kcal/mol). In contrast, gallic acid, ferulic acid, palmitoleic acid, stearic acid, linalool, and nonadecanoic acid showed weaker affinities than the standard. Overall, these results indicate that several phytochemicals, particularly those belonging to the sterol and triterpenoid classes, possess stronger binding potential than indomethacin [11,12]

Anti-Microbial
Control Drug – Amoxcillin
Target Protien ID – 7PDC

In the antimicrobial blind docking study, amoxicillin, with a binding affinity of –6.0 kcal/mol at the C1 pocket, was used as the standard drug. Multiple phytochemicals demonstrated superior binding affinities compared to the standard, including beta-sitosterol (–7.3 kcal/mol), betulinic acid (–7.6 kcal/mol), ursolic acid (–7.6 kcal/mol), stigmasterol (–7.2 kcal/mol), and camptothecin (–7.0 kcal/mol). Additionally, kaempferol (–6.6 kcal/mol) and quercetin (–6.2 kcal/mol) exhibited slightly higher affinities than amoxicillin. In contrast, compounds such as gallic acid, ferulic acid, palmitoleic acid, linalool, stearic acid, and nonadecanoic acid showed comparatively weaker binding [13,14] Overall, these findings highlight that phytochemicals belonging to sterols and pentacyclic triterpenoids exhibit stronger binding affinities and possess promising antimicrobial potential.

Anti-Fungal
Control Drug – Fluconazole
Target Protien ID – 3LD6

In the antifungal docking analysis, fluconazole, with a binding affinity of –7.6 kcal/mol at the C2 pocket, served as the standard drug. Several phytochemicals from the plant demonstrated stronger predicted binding affinities than the standard. Notably, betulinic acid (–11.4 kcal/mol), ursolic acid (–11.3 kcal/mol), stigmasterol (–10.3 kcal/mol), beta-sitosterol (–10.0 kcal/mol), and camptothecin (–9.6 kcal/mol) exhibited substantially higher affinities. Additionally, certain phytochemicals showed moderately strong binding, such as kaempferol (–8.4 kcal/mol) and quercetin (–8.3 kcal/mol), both exceeding the affinity of fluconazole. In contrast, compounds including gallic acid, ferulic acid, palmitoleic acid, linalool, and stearic acid displayed comparatively weaker binding affinities. Some phytochemicalshowa responsible antifungal activity [15,16]

Antiviral
Control Drug – Zidovudine
Target Protien ID – 7KZH

In this docking analysis, zidovudine, with a binding affinity of –7.4 kcal/mol at the C1 pocket, served as the control ligand. Several phytochemicals demonstrated stronger binding affinities than the standard, including stigmasterol (–8.4 kcal/mol), ursolic acid (–8.7 kcal/mol), beta-sitosterol (–8.1 kcal/mol), betulinic acid (–8.4 kcal/mol), and camptothecin (–7.7 kcal/mol). These compounds showed enhanced binding potential compared with zidovudine. In contrast, kaempferol (–6.9 kcal/mol), quercetin (–7.0 kcal/mol), palmitoleic acid (–5.9 kcal/mol), gallic acid (–6.1 kcal/mol), ferulic acid (–6.7 kcal/mol), stearic acid (–6.0 kcal/mol), linalool (–5.4 kcal/mol), and nonadecanoic acid (–5.0 kcal/mol) exhibited comparatively weaker binding affinities. Overall, the findings indicate that several phytochemicals—particularly sterols and pentacyclic triterpenoids—possess stronger binding interactions than zidovudine. [17,18]

Hepatoprotective Activity
Control Drug – Silibinin
Target Protien ID – 3E6I

Based on the results of Structure Based Blind Docking silibinin, with a binding affinity of –10.2 kcal/mol at the C3 pocket, served as the standard ligand. Only a few phytochemicals approached or matched its strong binding profile. Among themquercetin (–9.7 kcal/mol), beta-sitosterol (–8.6 kcal/mol), camptothecin (–8.2 kcal/mol), ursolic acid (–9.3 kcal/mol), kaempferol (–9.3 kcal/mol), and stigmasterol (–9.4 kcal/mol) exhibited relatively high binding affinities, although all remained lower than silibinin. Other compounds, including gallic acid (–6.2 kcal/mol), ferulic acid (–6.9 kcal/mol), palmitoleic acid (–6.3 kcal/mol), nonadecanoic acid (–6.8 kcal/mol), stearic acid (–6.9 kcal/mol), and linalool (–5.7 kcal/mol), showed moderate to weak binding interactions. These findings provide that although silibinin remains the strongest binder, several flavonoids and sterols exhibit substantial binding potential [19,20].

Anti Diabetic
Control Drug – Acarbose
Target Protien ID – 5NN4

Drug Acarbose, with a binding affinity of –7.1 kcal/mol at the C2 pocket, served as the standard compound. Several phytochemicals demonstrated stronger binding affinities than the control, including ursolic acid (–8.3 kcal/mol), camptothecin (–8.1 kcal/mol), stigmasterol (–7.7 kcal/mol), and beta-sitosterol (–7.0

kcal/mol). Compounds such as betulinic acid (–7.4 kcal/mol), kaempferol (–6.8 kcal/mol), and quercetin (–6.7 kcal/mol) exhibited moderately strong binding values, comparable to the standard. In contrast, gallic acid (–6.0 kcal/mol), ferulic acid (–5.8 kcal/mol), palmitoleic acid (–5.0 kcal/mol), stearic acid (–5.2 kcal/mol), linalool (–5.1 kcal/mol), and nonadecanoic acid (–5.0 kcal/mol) displayed weaker interactions. Overall, these results indicate that sterol- and triterpenoid-based phytochemicals possess superior binding potential compared with acarbose [21,22].

Anti-Cancer

Drug Used – Venetoclax

Target Protien ID – 5VAX

According to blind molecular docking carried out using the target protein 5-VAX, with Venetoclax as the reference drug, Venetoclax showed the highest binding affinity of −11.2 kcal/mol. Among the phytochemicals, camptothecin, kaempferol, quercetin, and betulinic acid exhibited strong binding affinities ranging approximately from −8.0 to −8.9 kcal/mol, indicating stable interactions with the target protein, and they predominantly occupied the C3 and C4 binding pockets, which possess the largest cavity volumes. Moderate binding affinities were observed for β-sitosteritol, stigmasterol, ursolic acid, nonadecanoic acid, ferulic acid, stearic acid, and palmitoleic acid, showing comparatively lower binding energies and weaker interactions with the target protein[23,24].

Admet Analysis of Ophiorrhiza Recurvipetala:

In silico ADMET assessment to investigate the pharmacokinetic parameters and safety profile of the bioactive compounds of the plant Ophiorrhizarecurvipetala. For this purpose, SwissADME is used to predict physicochemical properties, drug-likeness, absorption including gastrointestinal absorption, Lipinski's rule, bioavailability scores, and distribution parameters such as blood–brain barrier permeability and P-gp. Metabolism-related parameters, particularly CYP450-associated factors, are also evaluated. In addition, the pkCSM tool is employed to assess a result of toxicity. Briefly, SMILES notation is required to predict ADMET properties and obtain the results. The SMILES structures are retrieved from the PubChem database and submitted to the SwissADME and pkCSM tools to identify and analyze the results [25,26].

Overall, the ADMET analysis of Ophiorrhizarecurvipetala revealed favorable pharmacokinetic properties. Most compounds exhibited high gastrointestinal absorption and complied with Lipinski's rule, indicating good drug-likeness. The predicted bioavailability ranged from 0.55 to 0.85, suggesting good oral bioavailability. Blood–brain barrier permeability was limited to a few compounds, while most were non-BBB permeant. Metabolic predictions indicated that some phytochemicals may inhibit cytochrome P450 enzymes, particularly CYP3A4 and CYP2C9, whereas none were substrates of the renal OCT2 transporter [27]. Total clearance values varied among the compounds, with fatty acids showing comparatively higher clearance rates. Toxicity analysis showed that most compounds were non-mutagenic and non-hepatotoxic; however, camptothecin, betulinic acid, and ursolic acid exhibited potential hepatotoxicity, and a few compounds showed AMES toxicity. Acute oral toxicity (LD_{50}) values indicated moderate to low toxicity for the majority of the compounds [28].

Table 1: Results of Anti-Oxidant

Phytochemicals	Curpockets	Binding affinity	Cavity volume
N- Acetylcysteine*	C1	-4.8	14218
Camptothecin	C3	-9.9	2831
Gallic ACID	C1	-6.3	14218
Ferulic ACID	C5	-6.7	2106
Beta-Sitosterol	C1	-8.3	14218
Betulunic ACID	C1	-7.4	14218
Kaempferol	C4	-9.2	2453
Palmitoleic ACID	C1	-5.2	14218
Quercetin	C4	-9.1	2453
Stearic ACID	C1	-5.8	14218
Linalool	C1	-5.2	14218
Stigmasterol	C1	-7.6	14218
NONADECANOIC ACID	C1	-5.4	14218
URSOLIC ACID	C1	-8.0	14218

Table 2: Results of Anti-Inflammatory

Phytochemicals	Curpocket	Binding affinity	Cavity volume
Indomethacin*	C1	-8.9	26246
Camptothecin	C1	-9.8	26146
Gallic acid	C1	-6.8	26146
Ferulic acid	C4	-7.3	1233
Beta-sitosterol	C5	-9.7	1167
Betulunic acid	C5	-10.2	1167
Kaempferol	C2	-9.3	4431
Palmitoleic acid	C2	-6.7	4431
Quercetin	C2	-9.7	4431
Stearic acid	C2	-7.0	4431
Linalool	C2	-6.1	4431
Stigmasterol	C5	-10.7	1167
Nonadecanoic acid	C2	-7.4	4431
Ursolic acid	C5	-10.0	1167

Table 3: Results of Anti-Microbial

Phytochemicals	**Curpacket id**	**Binding affinity**	**Cavity volume**
Fluconazole*	C2	-7.6	2131
Camptothecin	C1	-9.6	2539
Gallic acid	C1	-5.6	2539
Ferulic acid	C1	-6.6	2539
Beta-sitosterol	C3	-10.0	1827
Betulunic acid	C4	-11.4	1582
Kaempferol	C2	-8.4	2131
Palmitoleic acid	C1	-6.7	2539
Quercetin	C2	-8.3	2131
Stearic acid	C1	-6.4	2539
Linalool	C1	-5.6	2539
Stigmasterol	C2	-10.3	2131
Nonadecanoic acid	C3	-6.6	1827
Ursolic acid	C1	-11.3	2539

Table 4: Results of Anti-Fungal

Phytochemicals	**Curpacket ID**	**Binding Affinity**	**Cavity Volume**
Zidovudine*	C1	-7.4	245
Camptothecin	C1	-7.7	245
Gallic acid	C1	-6.1	245
Ferulic acid	C1	-6.7	245
Beta-sitosterol	C4	-8.1	129
Betulunic acid	C4	-8.4	129
Kaempferol	C1	-6.9	245
Palmitoleic acid	C1	-5.9	245
Quercetin	C2	-7.0	221
Stearic acid	C1	-6.0	245
Linalool	C1	-5.4	245
Stigmasterol	C1	-8.4	245
Nonadecanoic acid	C3	-5.0	203
Ursolic acid	C4	-8.7	129

Table 5: Results of Anti-viral

Phytochemicals	CURPACKET ID	BINDING AFFINITY	CAVITY VOLUME
Zidovudine*	C1	-7.4	245

Camptothecin	C1	-7.7	245
Gallic acid	C1	-6.1	245
Ferulic acid	C1	-6.7	245
Beta-sitosterol	C4	-8.1	129
Betulunic acid	C4	-8.4	129
Kaempferol	C1	-6.9	245
Palmitoleic acid	C1	-5.9	245
Quercetin	C2	-7.0	221
Stearic acid	C1	-6.0	245
Linalool	C1	-5.4	245
Stigmasterol	C1	-8.4	245
Nonadecanoic acid	C3	-5.0	203
Ursolic acid	C4	-8.7	129

Table: 6 Results of Hepatoprotective activity

Phytochemicals	Curpacket ID	Binding Affinity	Cavity Volume
Silibinin*	C3	-10.2	1881
Camptothecin	C5	-8.2	1572
Gallic acid	C1	-6.2	1925
Ferulic acid	C3	-6.9	1881
Beta-sitosterol	C3	-8.6	1881
Betulunic acid	C5	-8.2	1572
Kaempferol	C1	-9.3	1925
Palmitoleic acid	C1	-6.3	1925
Quercetin	C1	-9.7	1925
Stearic acid	C1	-6.9	1925
Linalool	C4	-5.7	1710
Stigmasterol	C1	-9.4	1925
Nonadecanoic acid	C3	-6.8	1881
Ursolic acid	C5	-9.3	1572

Table 7: Results of Anti-Diabetic

Phytochemicals	Curpocket ID	Binding affinity	Cavity volume
Acarbose*	C2	-7.1	963
Camptothecin	C1	-8.1	1236
Gallic acid	C3	-6.0	853
Ferulic acid	C3	-5.8	853
Beta-sitosterol	C5	-7.0	451
Betulunic acid	C3	-7.4	853
Kaempferol	C3	-6.8	853
Palmitoleic acid	C1	-5.0	1236
Quercetin	C4	-6.7	771
Stearic acid	C3	-5.2	853
Linalool	C3	-5.1	853
Stigmasterol	C5	-7.7	451
Nonadecanoic acid	C3	-5.0	853
Ursolic acid	C5	-8.3	451

TABLE: 8 Results of Anti-Cancer

Phytochemicals	Curpocket	Binding Affinity	Cavity Volume
Venetoclax*	C1	-11.2	2787
Camptothecin	C1	-8.7	2787
Gallic acid	C1	-5.8	2787
Ferulic acid	C1	-6.2	2787

Beta-sitosterol	C4	-7.9	771
Betulunic acid	C1	-8.5	2787
Kaempferol	C4	-8.1	771
Palmitoleic acid	C1	-5.3	2787
Quercetin	C4	-8.9	771
Stearic acid	C1	-5.3	2787
Linalool	C1	-5.3	2787
Stigmasterol	C1	-9.2	2787
Nonadecanoic acid	C2	-5.3	1028
Ursolic acid	C1	-9.5	2787

TABLE: 9 Results of Absorption, Distribution, Metabolism Parameter

Phytochemicals	GI-Absorption	Lipinski	Bio Availability Score	BBB Permeant	P-Gp	CYP3A4	CYP2C9
Camptothecin	High	YES	0.55	NO	YES	YES	YES
Gallic Acid	High	YES	0.56	NO	NO	YES	NO
Ferulic Acid	High	YES	0.85	YES	NO	NO	NO
Beta-Sitosterol	Low	YES	0.55	NO	NO	NO	NO
Betulunic Acid	Low	YES	0.85	NO	NO	NO	YES
Kaempferol	High	YES	0.55	NO	NO	YES	NO
Palmitoleic Acid	High	YES	0.85	YES	NO	NO	YES
Quercetin	High	YES	0.55	NO	NO	YES	NO
Stearic Acid	High	YES	0.85	NO	NO	NO	NO
Linalool	High	YES	0.55	YES	NO	NO	NO
Stigmasterol	Low	YES	0.55	NO	NO	NO	YES
Nonadecanoic Acid	High	YES	0.85	NO	NO	NO	NO
Ursolic Acid	Low	YES	0.85	NO	NO	NO	NO

Table 10: Results of Excretion and Toxicity Parameters

Phytochemicals	Total Clearance	Renal OCT2 Substrate	AMES Toxicity	LD50 Oral Rat Acute Toxicity
Camptothecin	0.629ml/min	YES	YES	2.656mol/kg
Gallic Acid	0.625ml/min	NO	NO	2.03mol/kg
Ferulic Acid	0.619ml/min	NO	NO	2.322mol/kg
Beta-Sitosterol	0.628ml/min	NO	NO	2.445mol/kg
Betulunic Acid	0.113ml/min	NO	NO	4.594mol/kg
Kaempferol	0.591ml/min	NO	YES	2.35mol/kg
Palmitoleic Acid	1.813ml/min	NO	NO	2.365mol/kg
Quercetin	0.486ml/min	NO	YES	2.773mol/kg
Stearic Acid	1.832ml/min	NO	NO	1.406mol/kg
Linalool	0.446ml/min	NO	NO	1.929mol/kg
Stigmasterol	0.618ml/min	NO	NO	2.54mol/kg
Nonadecanoic Acid	1.862ml/min	NO	NO	2.669mol/kg
Ursolic Acid	0.079ml/min	NO	NO	4.351mol/kg

Figure 1: Ophiorrhiza Recurvipetala Plant.

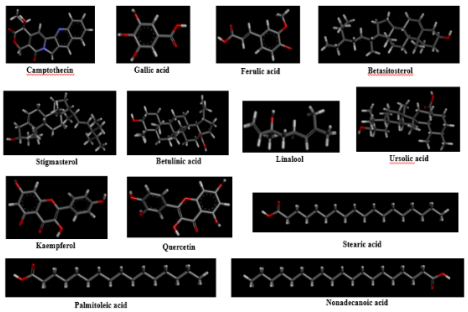

Figure 2: Phytochemicals of Ophiorrhiza Recurvipetala.

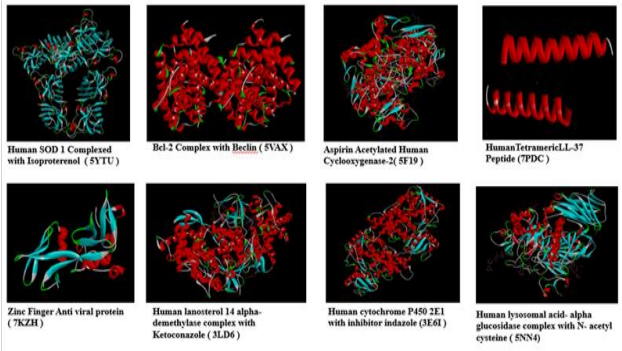

Figure 3: Protein Used for This Molecular Docking.

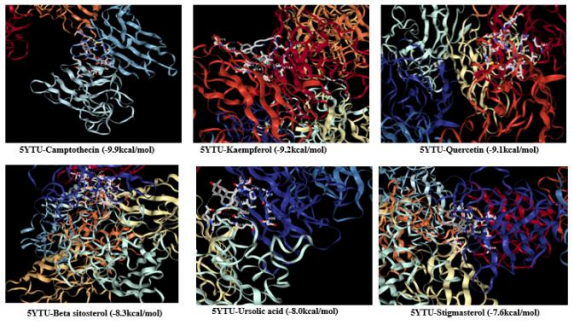

Figure 4: Compounds Show Stronger Binding Affinitiy As Anti-Oxidants

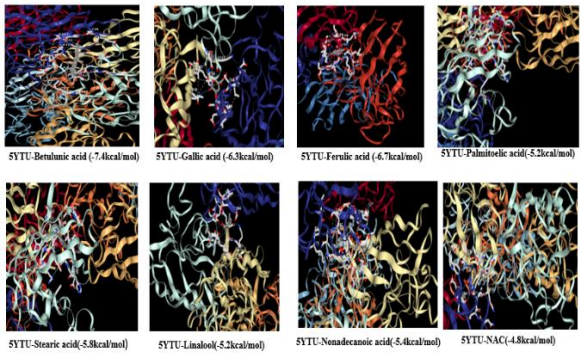

Figure 5: Compounds Show Weaker Binding Affinity as Anti-Oxidants

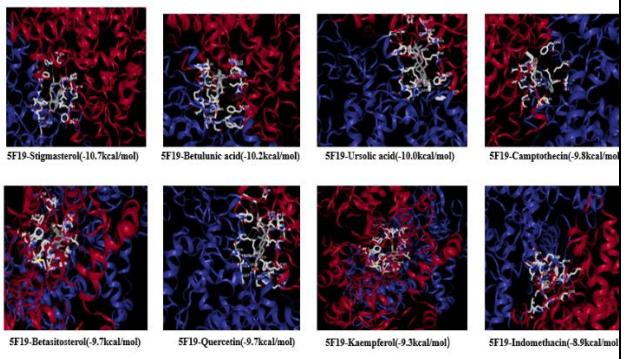

Figure 6: Compounds Show Stronger Binding Affinity for Anti-Inflammatory.

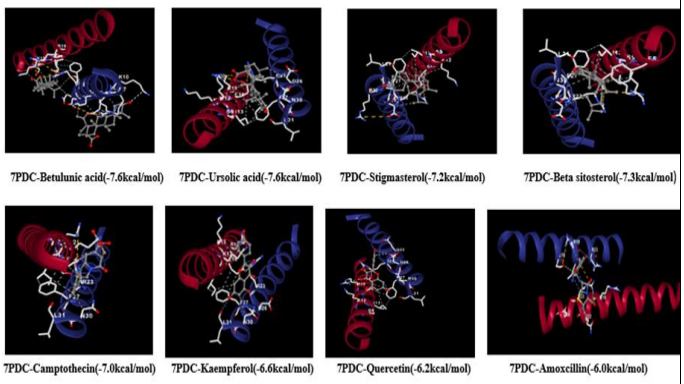

Figure 7: Compounds Show Weaker Binding Affinity for Anti-Inflammatory.

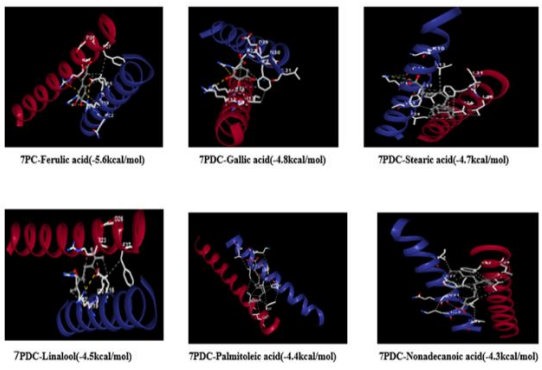

Figure 8: Compounds Show Stronger Binding Affinity for Anti-Microbial.

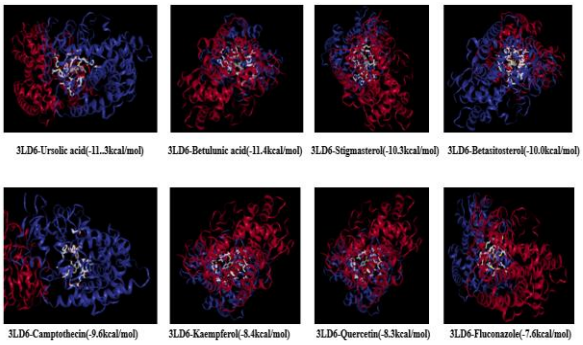

Figure 9: Compounds Show Weaker Binding Affinity for Anti-Microbial.

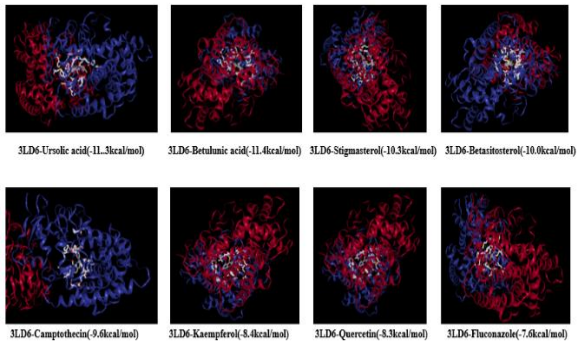

Figure 10: Compounds Show Stronger Binding Affinity for Anti-Fungal.

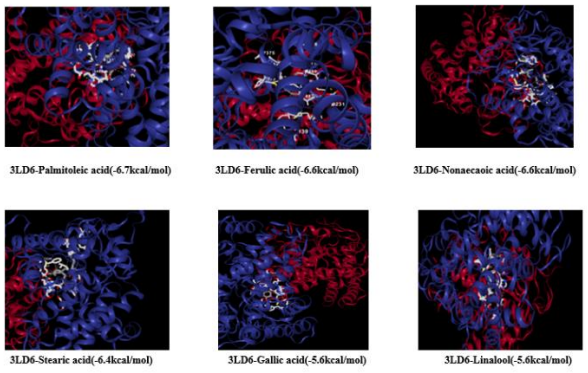

Figure 11: Compounds Show Weaker Binding Affinity for Anti-Fungal.

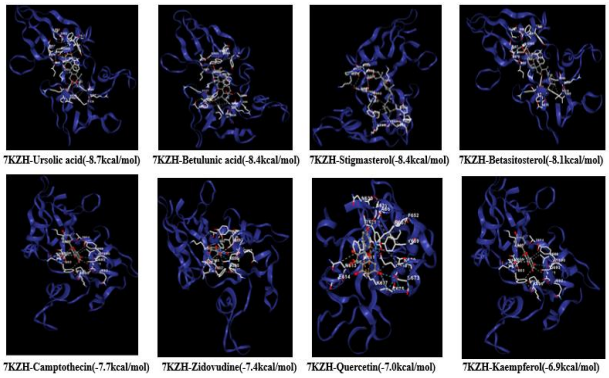

Figure 12: Compounds Show Stronger Binding Affinity for Anti-Viral.

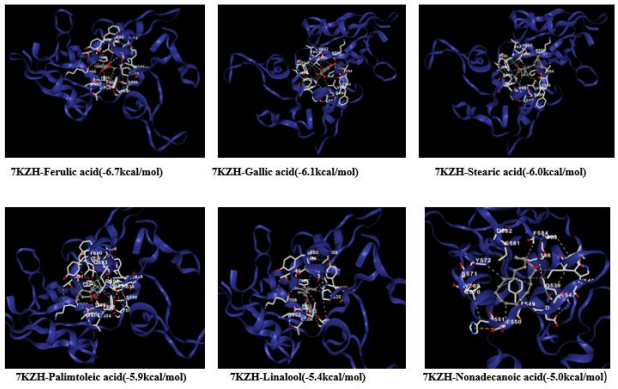

Figure 13: Compounds Show Weaker Binding Affinity for Anti-Viral.

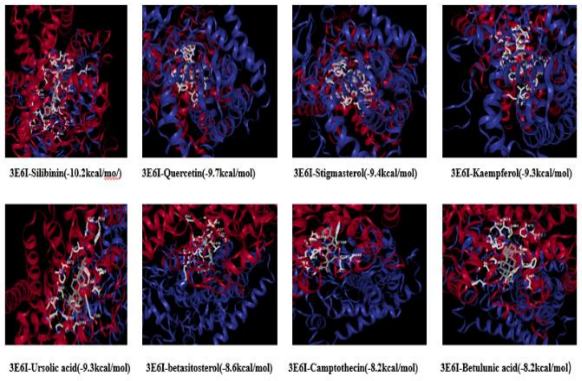

Figure 14: Compounds Show Stronger Binding Affinity for Hepatoprotective Activity.

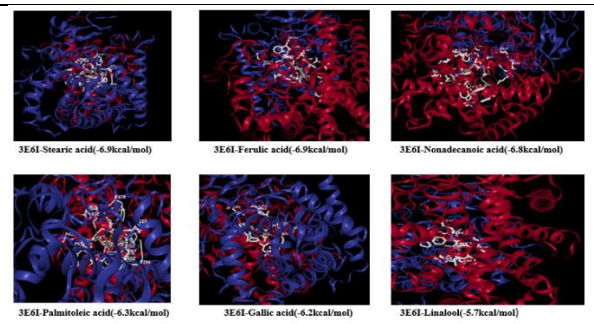

Figure 15: Compounds Show Weaker Binding Affinity for Hepatoprotective Activity

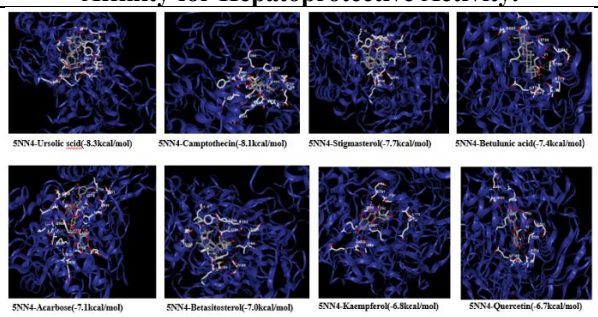

Figure 16: Compounds Show Stronger Binding Affinity for Anti-Diabetic.

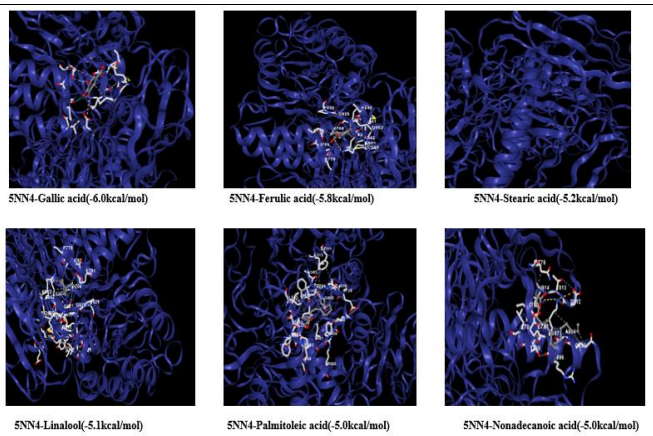

Figure 17: Compounds Show Weaker Binding Affinity For Anti-Diabetic.

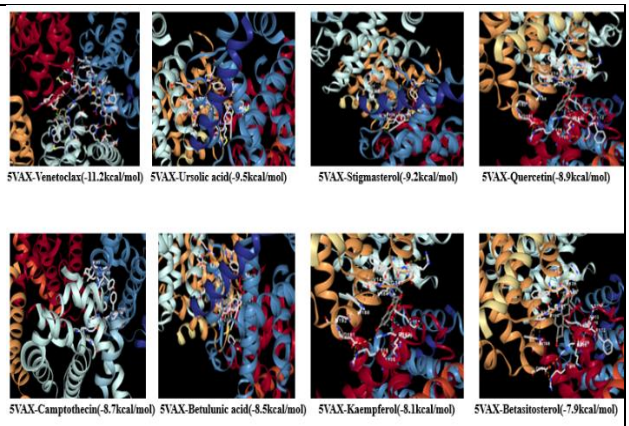

Figure 18: Compounds Show Stronger Binding Affinity For Anti-Cancer.

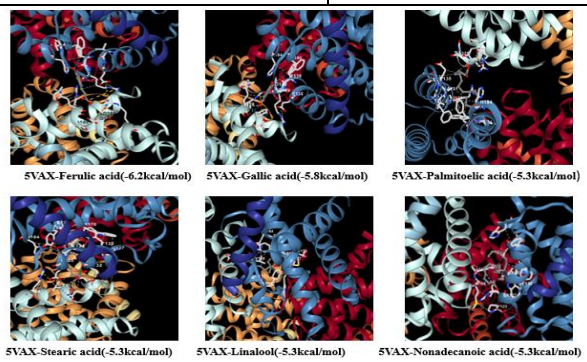

Figure 19: Compounds Show Weaker Binding Affinity for Anti-Cancer.

DISCUSSION

This study employed structure-based blind molecular docking and ADMET analysis to evaluate the binding potential of plant-derived phytochemicals against a selected therapeutic target using an appropriate control drug and their pharmacokinetic parameters. The study indicates that compounds with well-defined structures, such as rigid polycyclic scaffolds and larger hydrophobic surface areas exhibited more favorable interaction with the protein cavities.

This suggests that molecular size, conformational stability, and lipophilicity play an important role in binding efficiency. In contrast, smaller and more flexible molecules showed reduced interaction stability. Phyto chemicals in ophiorrhizarecurvipetala capable of effectively occupying these binding pockets appeared to form stronger non-covalent interactions, including hydrophobic contact and pie-based interactions, which likely contributed to enhanced binding stability. When compared with the control drug, the natural compounds demonstrated notable therapeutic potential due to their structural diversity and biological activity. Unlike many conventional drugs that are designed to act on a single specific target, phytochemicals often interact with multiple targets, which may be advantageous in complex disease conditions. These categories may be beneficial in treatment of complex diseases such as inflammation, infection, metabolic disorder, and cancer. Their ability to act on multiple targets also supports their long-standing use in traditional medicine and their potential application in drug discovery and development.

The strong interactions observed for sterol and triterpenoid-based compounds indicate that these molecular frameworks are well-suited for binding to proteins with large hydrophobic regions. Flavonoids and alkaloids also exhibit a notable interaction with the target protein.Although docking stimulation provides valuable view into binding feasibility and interaction trend, they do not consider dynamic biological factors such as bioavailability, metabolism, solubility, or off target effect.

The ADMET analysis indicates that the investigated bioactive compounds possess favorable drug-like properties suitable for oral administration. The limited blood–brain barrier permeability observed for most compounds may minimize potential central nervous system–related adverse effects, while the predicted inhibition of cytochrome P450 enzymes suggests a possible risk of drug–drug interactions. Although the overall safety profile is acceptable, the toxicity concerns identified for a limited number of compounds**.**

CONCULSION

The present molecular docking study evaluated the binding interaction of selected plant phytochemical with the target protein by comparing their binding behavior against a suitable control drug. The control ligand consistently occupied by binding pocket of the protein and provide a benchmark for assessing the phytochemical in the docking results. Among the different class of phytochemicals such as sterol and pentacyclic triterpenoids exhibited the strongest binding affinity across the docking analysis. Flavonoids and alkaloids showed moderate to strong binding affinity due to affinity of forming hydrogen bonds and aromatic interaction with target protein. On the opposite, phenolic acid, fatty acid, and monoterpenes are smaller and more flexible or shows weaker binding affinity within the binding pockets. Overall, the docking study indicates that the phytochemical class and structural features play a crucial role in determining binding efficiency while docking provide a ligand-protein interaction experimental validation for biological relevance and therapeutic potential of these compounds. The ADMET analysis of Ophiorrhizarecurvipetala showed favourable pharmacokinetic and drug like properties and have a ability to support the therapeutic potential of the plant. This is computational foundation for future drug discovery effects based on phytochemical of ophiorrhizarecurvipetala through in vitro and in vivo studies.

REFERENCES

1. Gopalakrishnan, K.; Krishnan, S.; Narayanan, K.P. *et al*. Tissue culture studies and estimation of camptothecin from Ophiorrhizaprostrata D. Don. *Indian J. Plant Physiol*. 23, 2018, 582–592.
2. Hareesh, V.S. & Sabu, M. The genus Ophiorrhiza (Rubiaceae) in Andaman and Nicobar Islands, India with a new species. *Phytotaxa*, 383, 2018, 259–272.
3. Hamzah, & A.S. Isolation, Characterization and Biological Activities of Chemical Constituents of Ophiorrhiza and Hedyotis Species. Master's Thesis, University Putra Malaysia, Serdang, *Malaysia*, 1994.
4. Supriya, B. & Nutan, M. Secondary metabolites as DNA topoisomerase inhibitors: A new era towards designing of anticancer drugs. Pharmacogn. *Rev*. 4, 2010, 12–26.
5. Prabha, G. & Karuppusamy, S. Phytochemical profile and radical scavenging activity of alcoholic extract of Ophiorrhiza radicans Gardner (Rubiaceae)—A rare plant of Southern Western Ghats of India. *Trends Biosci*. 11, 2018, 1572–1576.
6. Grinde, B., & Patil, G. G. Biophilia: does visual contact with nature impact on health and well-being? *International journal of Environmental research and public health*, 6(9), 2009, 2332-2343.
7. Niazi, P., Alimyar, O., Azizi, A., Monib, A. W., & Ozturk, H. *et al*. People-plant Interaction: Plant Impact on Humans and Environment. *Journal of Environmental and Agricultural Studies*, 4(2), 2023, 01–07.
8. Schanzer IA. Three new species of Ophiorrhiza (Rubiaceae-Ophiorrhizeae) from Thailand. Thai For Bull.33, 2005, 161-70.
9. Deb DB, & Mondal DC. Taxonomic revision of the genus Ophiorrhiza L. (Rubiaceae) in Indian subcontinent. Bull Bot *Surv India*. 39, 1997, 1-148.
10. Martins D, & Nunez CV. Secondary metabolites from Rubiaceae species. *Molecules*. 20(7), 2015, 13422-95.
11. Prabha G, & Karuppusamy S. Phytochemical profile and radical scavenging activity of alcoholic extract of Ophiorrhiza radicans Gardner (Rubiaceae)-A rare plant of southern western ghats of India. *Trends Biosci*. 11, 2018, 1572-6.
12. Arnao MB, Cano A, Acosta M. *et al.* The hydrophilic and lipophilic contribution to total antioxidant activity. *Food Chem.* 73(2), 2001,239-44.
13. Munro B, Vuong QV, Chalmers AC, Goldsmith CD, Bowyer MC, Scarlett CJ. *et al.* Phytochemical, antioxidant and anti-cancer properties of euphorbia tirucallicmethanolic and aqueous extracts. Antioxidants (*Basel*). 4(4), 2015, 647-61.
14. Coppin JP, Xu Y, Chen H, Pan MH, Ho CT, Juliani R, Simon JE, Wu Q. *et al.* Determination of flavonoids by LC/MS and anti-inflammatory activity in *Moringa oleifera of Functional Foods*. 5(4), 2013, 1892-9.
15. Uma B, Prabhakar K, Rajendran S, Sarayu LY. *et al.* Studies on GC/MS spectroscopic analysis of some bioactive antimicrobial compounds from Cinnamomum zeylanicum. *J MedPlants*. 8(31), 2009, 125-31.
16. Dong JW, Cai L, Xiong J, Chen XH, Wang WY, Shen N, *et al.* Improving the antioxidant and antibacterial activities of fermented Bletilla striata with Fusarium avenaceum and Fusarium oxysporum. *Process Biochem*.; 50, 2015, 8-13.
17. Mosmann T. Rapid colorimetric assay for cellular growth and survival: application to proliferation and cytotoxicity assays. *Journal of immunological methods.* 65(1-2), 1983, 55-63
18. Li F, Jiang T, Li Q, Ling X. *et al.* Camptothecin (CPT) and its derivatives are known to target topoisomerase I (Top1) as their mechanism of action: did we miss something in CPT analogue molecular targets for treating human disease such as cancer?. *American journal of cancer research*.7(12), 2017, 2350.
19. Thaning, C., Welch, C.J., Borowicz, J.J., Hedman, R., Gerhardson, B. *et al.* Suppression of Sclerotinia sclerotiorum apothecial formation by the soil bacterium Serratia plymuthica: identification of a chlorinated macrolide as one of the causal agents. *Soil Biology and Biochemistry* 33, 2001, 1817–1826.

20. Teichler, G. The anthelminthic action of the root cortex of Vangueria edulis. *Archiv fur Schiffs- und Tropen-Hygiene* 39, 1935, 211–213.
21. Barcelona.Gonzalez, M. E., Alarc ´on, B., and Carrasco, L. *et al*. Polysaccharides as antiviral agents: antiviral activity of carrageenan. Antimicrob. *Agents Chemother*. 31, 1987, 1388–1393.
22. Gonzalez, M. E., Mart´ınez-Abarca, F., and Carrasco, L. *et al*. Flavonoids: potent inhibitor of poliovirus RNA synthesis. *Antiviral Chem. Chemother*. 1, 1990, 203–209
23. Berraaouan, A.; Abid, S.; Bnouham, M. *et al.* Antidiabetic oils. Curr. *Diabetes Rev*. 9, 2013, 499–505.
24. Ping, H.; Zhang, G.; Ren, G. *et al.* Antidiabetic effects of cinnamon oil in diabetic KK-Ay mice. Food Chem. *Toxicol.* 48, 2010, 2344–2349.
25. Oums F. Molecular modeling and computer aided drug design, examples of their applications in medicinal chemistry. *Curr Med Chem* 7, 2000, 141–158.
26. Daina, A., Michielin, O., & Zoete, V. *et al.* SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and *medicinal chemistry friendliness of small molecules*. 2017.
27. Ahmed, S. F., Ahmed, M. R., Hemal, M. F. P., *et al*. In silico evaluation of Ocimum sanctum phytochemicals for diabetic foot ulcer therapy. 2025.
28. Lipinski CA, Franco L, Dominy BW, *et al.* Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings. *Adv Drug Deliv Rev*.23, 1997, 3–25.

Cite this article:
Saravanan C, Vaishnavi G. Molecular Docking and Admet Analysis of Ophiorrhiza Recurvipetala Plant Constituent with Multiple Pharmacological Activities. *International Journal of Pharmaceutical Research & Analysis,* 16(1), 2026, 32-43.