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Research Article

Computational assessment of bioactives from *Phyllanthus emblica* leaves as potential anti-obesity agents

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Obesity is a chronic metabolic disorder associated with serious health complications, including cardiovascular diseases, type 2 diabetes mellitus, and dyslipidemia. The increasing prevalence of obesity has created a need for safer and more sustainable therapeutic alternatives. Plant-derived waste materials are rich sources of bioactive compounds and offer significant potential for drug discovery. The present study investigated the anti-obesity potential of phytoconstituents obtained from amla leaves (*Phyllanthus emblica*) using an in-silico approach. Obesity-related target proteins (PDB IDs: 9MIZ and 9VG4) involved in lipid metabolism and adipogenesis were selected for molecular docking studies. Ligand structures were retrieved from the PubChem database and docked using AutoDock Vina. Protein–ligand interactions were analyzed using Discovery Studio Visualizer. Drug-likeness and pharmacokinetic properties were evaluated through ADME analysis, while toxicity prediction was performed to assess safety profiles. The results demonstrated that several phytoconstituents exhibited favourable binding affinities toward both target proteins and formed stable interactions with key amino acid residues. Furthermore, selected compounds satisfied Lipinski's Rule of Five and Ghose filter criteria, showed acceptable ADME characteristics, and exhibited low predicted toxicity. These findings suggest that phytoconstituents derived from plant waste materials possess promising anti-obesity potential and may serve as lead candidates for further development. However, experimental validation through in vitro and in vivo studies is required to confirm their efficacy and safety.

Keywords: obesity, molecular docking, plant waste*, Phyllanthus emblica*, ADME, toxicity prediction, anti-obesity activity

Introduction

Obesity is a long-term metabolic condition marked by the abnormal or excessive accumulation of adipose tissue due to a persistent imbalance between caloric consumption and energy utilization. It has become a significant global public health challenge because it increases the risk of developing several chronic diseases, including type 2 diabetes, cardiovascular disorders, hypertension, non-alcoholic fatty liver disease, and various forms of cancer (Blüher, 2020; Bray et al., 2017). According to the World Health Organization (WHO), obesity affects millions of individuals worldwide, with prevalence continuing to rise across both developed and developing countries (World Health Organization (WHO, 2026). Beyond its impact on physical health, obesity also contributes to reduced quality of life, increased healthcare expenditure, and premature mortality. The pathophysiology of obesity involves complex interactions among genetic, environmental, hormonal, and behavioral factors. Excess adipose tissue functions as an endocrine organ and secretes various adipokines and inflammatory mediators that contribute to insulin resistance, chronic low-grade inflammation, and metabolic

dysfunction (Saltiel & Olefsky, 2017). Key molecular pathways involved in obesity include adipogenesis, lipogenesis, lipid absorption, and appetite regulation. Transcription factors such as peroxisome proliferator-activated receptor gamma (PPAR-γ) and enzymes involved in lipid metabolism have therefore become attractive targets for anti-obesity drug development(Lu et al., 2018). Current treatment strategies include dietary modifications, physical activity, behavioral interventions, pharmacotherapy, and bariatric surgery. Although approved drugs such as Orlistat, Semaglutide, and Liraglutide have shown significant efficacy in weight management, their long-term use may be associated with adverse effects, high cost, and limited accessibility (Apovian et al., 2023; Wilding et al., 2021). These limitations have stimulated interest in identifying safer and naturally derived therapeutic alternatives. Medicinal plants have historically served as valuable sources of bioactive compounds with diverse pharmacological activities. Among them, *Emblica officinalis* Gaertn. (Amla), belonging to the family Euphorbiaceae, is widely used in traditional medicine and is recognized for its antioxidant, anti-inflammatory, hypolipidemic, antidiabetic, and hepatoprotective properties (Baliga et al., 2011). While the fruits of amla have been extensively investigated, the leaves generated during cultivation and processing are often discarded despite containing significant amounts of biologically active phytochemicals. Previous phytochemical studies have reported the presence of gallic acid, ellagic acid, quercetin, kaempferol, rutin, and other phenolic compounds in amla leaves, which exhibit strong antioxidant and metabolic regulatory activities (Chang et al., 2024; Nazish & Ansari, 2018; Prananda et al., 2023; Ankalikar, A.,2025).

Recent evidence suggests that polyphenols and flavonoids can influence obesity-related pathways by suppressing adipocyte differentiation, regulating lipid metabolism, enhancing energy expenditure, and reducing oxidative stress and inflammation(Hasani-Ranjbar et al., 2009; Pan et al., 2016). Therefore, phytoconstituents present in amla leaves may possess promising anti-obesity potential. Furthermore, the utilization of amla leaves as an agro-waste resource supports sustainable waste management and promotes the valorization of underutilized plant materials into value-added therapeutic products (Sagar et al., 2018). Advances in computer-aided drug discovery have enabled the rapid screening of phytochemicals against disease-associated molecular targets. Molecular docking, coupled with ADME and toxicity prediction, provides valuable insights into ligand–protein interactions, pharmacokinetic behavior, and safety profiles before experimental validation. Therefore, the present study aimed to evaluate the anti-obesity potential of phytoconstituents identified from *Emblica officinalis* leaves through molecular docking, drug-likeness assessment, ADME analysis, and toxicity prediction to identify promising lead compounds for further development.



Figure 1. *Emblica officinalis* plant

Methods

Molecular Docking

Computer-aided drug discovery has become an indispensable tool for identifying bioactive molecules with therapeutic potential. Among these approaches, molecular docking is extensively utilized to investigate the binding behavior of small molecules toward specific biological targets. The technique predicts the most energetically favourable orientation of a ligand within the active site of a receptor and estimates the strength of interaction through docking scores and binding energy calculations. By simulating molecular recognition events, docking studies provide valuable information regarding ligand–protein interactions, binding stability, and potential biological activity. Consequently, molecular docking serves as

a rapid and cost-effective strategy for the preliminary screening of compounds before experimental validation (Butt et al., 2020; Sakshi Ubale et al., 2026; Shedame et al., 2026).

Selection and Preparation of Receptor

The selection of suitable protein targets is a crucial step in the identification of novel anti-obesity agents. Obesity is associated with multiple metabolic abnormalities involving lipid metabolism, adipogenesis, and energy regulation pathways. Therefore, proteins participating in these pathways were considered appropriate targets for the present investigation (Loos & Yeo, 2022). Based on an extensive literature review, protein structures with PDB IDs 9MIZ and 9VG4 were selected due to their reported relevance in obesity-associated metabolic processes. The crystallographic structures of these proteins were downloaded from the RCSB Protein Data Bank in PDB format. Prior to docking analysis, the receptor molecules were processed using UCSF Chimera software to obtain structurally optimized proteins suitable for computational studies. Co-crystallized ligands, solvent molecules, and other non-essential heteroatoms were removed from the structures. Missing hydrogen atoms were subsequently added, and appropriate protonation states were assigned to ensure structural accuracy. Any incomplete residues or side-chain irregularities were corrected wherever required. To improve structural stability and eliminate unfavourable atomic contacts, the protein models were subjected to energy minimization procedures (Pettersen et al., 2004). The optimized receptor structures were exported in PDB format and further prepared using AutoDock Tools. Kollman charges were incorporated, non-polar hydrogens were merged, and the final receptor files were generated in PDBQT format. These prepared structures were subsequently employed for molecular docking experiments (Berman, 2000; Trott & Olson, 2010).

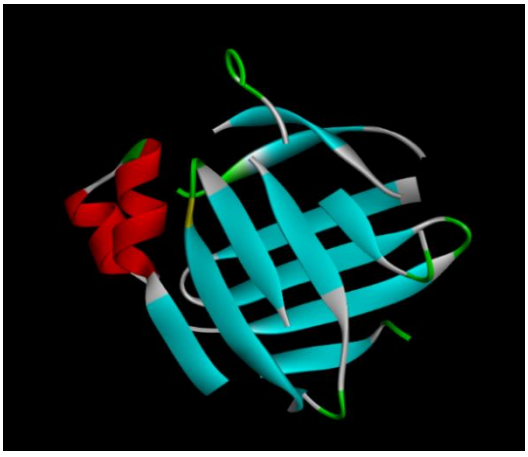


Figure 2. Three-dimensional structure of protein 9MIZ

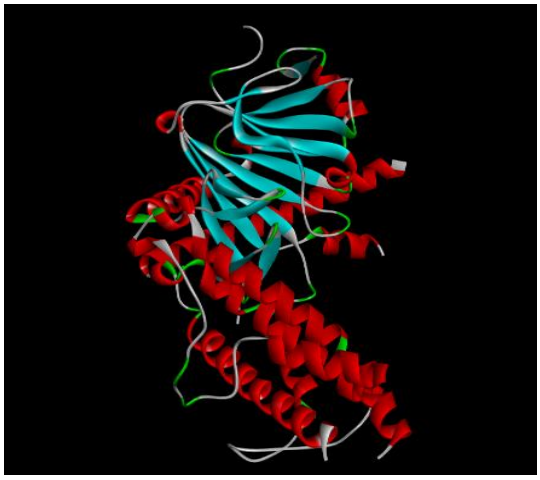


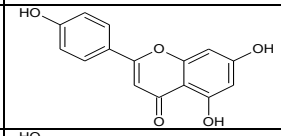
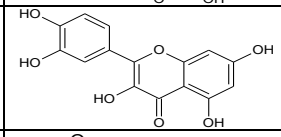
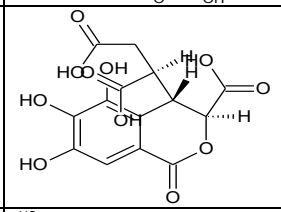
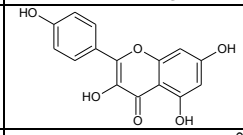
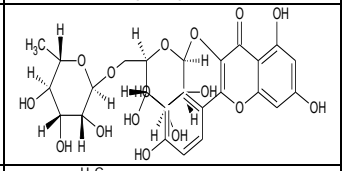
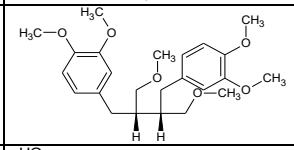
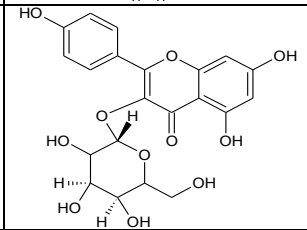
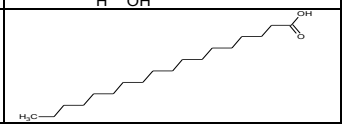
Figure 3. Three-dimensional structure of protein 9VG4

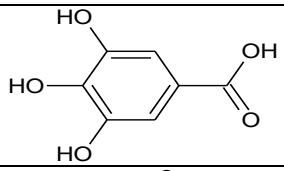
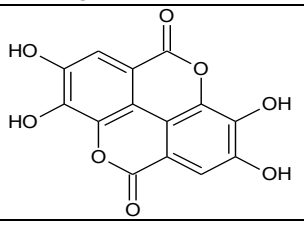
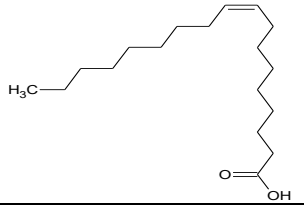
Selection and Preparation of Ligands

Emblica officinalis Gaertn. (Amla) leaves represent an underexploited agricultural by-product generated during cultivation and harvesting practices. Although frequently discarded, the leaves are a rich reservoir of biologically active phytochemicals including gallic acid, ellagic acid, quercetin, kaempferol, rutin, emblicanin A, and emblicanin B. These

compounds have been reported to exhibit antioxidant, anti-inflammatory, hypolipidemic, and metabolic regulatory activities, suggesting their possible role in obesity management (Baliga et al., 2011; Chang et al., 2024; Prananda et al., 2023). The phytoconstituents selected for the present study were identified through an extensive survey of published literature. Their three-dimensional chemical structures were retrieved from the PubChem database and subjected to geometry optimization to obtain stable molecular conformations. The optimized ligand structures were converted into PDBQT format and utilized for docking studies against the selected protein targets(Kim et al., 2021). Following docking analysis, compounds displaying strong binding affinities and favorable interaction profiles were shortlisted for further evaluation. Drug-likeness assessment was carried out using Lipinski's Rule of Five and Ghose filter parameters, while pharmacokinetic properties were investigated through ADME prediction studies. In addition, computational toxicity assessment was performed to evaluate the safety of the selected phytoconstituents. The integrated analysis enabled the identification of potential lead molecules from *Emblica officinalis* leaves possessing favorable receptor binding, acceptable pharmacokinetic characteristics, and low predicted toxicity, thereby highlighting their potential application as anti-obesity agents.(Banerjee et al., 2018; Ghose et al., 1999; Kar et al., 2024; Lipinski et al., 2001; Ononamadu & Ibrahim, 2021).

Table 1. Chemical constituents of *Phyllanthus emblica leaves.*(Mirunalini & Krishnaveni, 2010; Sharma et al., 2020; Singh et al., 2011)

sr.no.	Chemical Constituent	Structure
1.	Apigenin	
2.	Quercetin	
3.	Chebulic acid	
4.	Kaempferol	
5.	Rutin	
6.	Phyllanthin	
7.	Kaempferol-3-o-gluco-side	
8.	Stearic acid	

9.	Gallic acid	
10.	Ellagic acid,	
11.	Oleic acid	

Evaluation of Ligands on the Basis of Drug-Likeness, ADME and Toxicity Studies

The pharmacokinetic properties and drug-likeness characteristics of the selected phytoconstituents from *Emblica officinalis* leaves were assessed using the SwissADME web server, developed by the Swiss Institute of Bioinformatics and available at SwissADME. Compounds exhibiting promising docking performance were subjected to further screening to evaluate their suitability as potential drug candidates. Various physicochemical parameters, including molecular weight (MW) ≤ 500 Da, lipophilicity (Log P) ≤ 5, topological polar surface area (TPSA) ≤ 140 Å², molar refractivity (MR), hydrogen bond donor ≤ 5 and acceptor counts ≤ 10, and the number of rotatable bonds ≤ 10, were calculated.(Daina et al., 2017; Lipinski et al., 2001; Ononamadu & Ibrahim, 2021). Drug-likeness assessment was performed according to Lipinski's Rule of Five, which predicts the oral bioavailability of compounds. In addition to Lipinski's criteria, the Ghose filter was employed to further evaluate drug-likeness. According to the Ghose model, compounds are considered drug-like when they possess molecular weight between 160 – 480 Da, Log P values between − 0.4 and 5.6, molar refractivity ranging from 40 – 130, and total atom counts between 20 and 70 (Ghose et al., 1999). The toxicity profile of the selected phytoconstituents was predicted using the ProTox-3.0 online platform. This computational tool estimates various toxicity endpoints, including hepatotoxicity, carcinogenicity, mutagenicity, immunotoxicity, cytotoxicity, and predicted LD_{50} values. Compounds demonstrating favourable pharmacokinetic characteristics along with low predicted toxicity were considered suitable candidates for further molecular docking investigations.(Banerjee et al., 2018; Kar et al., 2024).

Preparation of Ligands

The phytoconstituents selected from *Emblica officinalis* leaves were chosen based on extensive literature reports describing their biological and pharmacological activities. Major compounds such as gallic acid, ellagic acid, quercetin, kaempferol, rutin, emblicanin A, and emblicanin B were included in the study.(Singh et al., n.d.-b) Orlistat was used as reference compounds for comparative analysis.(Ballinger & Peikin, 2002). The chemical structures of the selected compounds were retrieved from the PubChem database in the form of SMILES (Simplified Molecular Input Line Entry System) notation. These SMILES strings were imported into Avogadro software to generate three-dimensional molecular structures.(Bingul et al., 2025; Kim et al., 2021) Following structure generation, hydrogen atoms were added automatically, and molecular geometries were examined to ensure structural correctness. The generated ligand structures were subjected to geometry optimization using the MMFF94 force field to obtain energetically stable conformations and minimize steric strain. The optimized molecules were saved in PDB format and subsequently imported into AutoDock Tools. During ligand preparation, Gasteiger charges were assigned, non-polar hydrogen atoms were merged, and rotatable bonds were defined to provide conformational flexibility during docking simulations. Finally, all ligand structures were converted into PDBQT format and utilized for molecular docking studies.(Hanwell et al., 2012; Morris et al., 2009).

Molecular Docking

Molecular docking studies were carried out to investigate the interaction patterns and binding affinities of selected *Emblica officinalis* phytoconstituents against obesity-associated target proteins. The prepared receptor structures and optimized ligands in PDBQT format were imported into the PyRx virtual screening environment, which incorporates the

AutoDock Vina docking engine (Dallakyan & Olson, 2015; Trott & Olson, 2010). Initially, the receptor proteins were loaded as macromolecules, while the ligand structures were imported into the ligand workspace. The stability of the ligand molecules was verified prior to docking. A grid box was defined around the active site region of each target protein to ensure adequate coverage of amino acid residues involved in ligand recognition and binding. Grid dimensions were adjusted appropriately to allow efficient exploration of the binding pocket.(Eberhardt et al., 2021; Kitchen et al., 2004; Meng et al., 2011). Docking simulations were performed using the AutoDock Vina algorithm with optimized search parameters. Multiple binding poses were generated for each ligand, and the conformation exhibiting the lowest binding energy was selected as the most favorable binding mode. Binding affinity values were expressed in kcal/mol, where more negative values indicated stronger ligand–protein interactions(Pagadala et al., 2017). Following docking, the resulting complexes were analyzed using Discovery Studio Visualizer and UCSF Chimera. Various intermolecular interactions, including hydrogen bonding, hydrophobic interactions, electrostatic interactions, π–π stacking, and van der Waals contacts, were examined in detail. Compounds exhibiting strong binding affinity together with favourable interaction profiles were identified as promising anti-obesity candidates and selected for further evaluation (Eberhardt et al., 2021; Pettersen et al., 2004).

Results and Discussion

The docking of the constituents was done and the findings are reported in the table 2. The Drug Likeness of various phytoconstituents of *Emblica officinalis leaves* specifying the details of each component such as Rotatable Bonds, H Bond Acceptor, H Bond donar, Log P, Follows Lipinsk, No Of Violations and Ghose has been reported.

Table 2. Drug Likeness of various phytoconstituents of *Emblica officinalis*

Sr no.	Constituent Name	Molecular Weight (G/Mol)	Rotatable Bonds	H Bond Acceptor	H Bond donar	Log P	Follows Lipinsk	No Of Violations	Ghose
1.	Apigenin	270.24	1	5	3	1.89	Yes	0	Yes
2.	Quercetin	302.24	1	7	5	1.63	Yes	0	Yes
3.	Chebulic acid	356.24	5	11	6	-0.67	No	2	Yes
4.	Kaempferol	286.24	1	6	4	1.70	Yes	0	Yes
5.	Rutin	610.52	16	6	10	0.46	No	3	No
6.	Phyllanthin	418.52	13	6	0	4.24	Yes	0	Yes
7.	Kaempferol-3-o-glucoside	448.38	4	11	17	1.29	No	2	Yes
8.	Stearic acid	284.48	16	2	1	4.30	Yes	0	No
9.	Gallic acid	170.12	1	5	4	0.21	Yes	0	No
10.	Ellagic acid,	302.19	0	8	4	0.79	Yes	0	Yes
11.	Oleic acid	282.46	15	2	1	4.01	Yes	0	No

Table 3. Evaluation of *Emblica officinalis* on the basis of ADME parameter

Sr.no.	Constituents Name	GI absorption	BBB permeant	CYP1A2 inhibitor	Bioavailability Score
1.	Apigenin	High	No	Yes	0.55
2.	Quercetin	High	No	Yes	0.55
3.	Chebulic acid	Low	No	No	0.11
4.	Kaempferol	High	No	Yes	0.55
5.	Rutin	Low	No	No	0.17
6.	Phyllanthin	High	Yes	No	0.55
7.	Kaempferol-3-o-glucoside	Low	No	No	0.17
8.	Stearic acid	High	No	Yes	0.85
9.	Gallic acid	High	No	No	0.56
10.	Ellagic acid	High	No	Yes	0.55
11.	Oleic acid	High	No	Yes	0.85

The drug-likeness evaluation revealed that most of the phytoconstituents from *Emblica officinalis* leaves possessed favorable physicochemical properties. Apigenin, quercetin, kaempferol, phyllanthin, gallic acid, and ellagic acid complied with Lipinski's Rule of Five without any violations, indicating good oral bioavailability potential. Among these, apigenin,

quercetin, kaempferol, phyllanthin, and ellagic acid also satisfied the Ghose criteria, suggesting strong drug-like characteristics. In contrast, chebulic acid, rutin, and kaempferol-3-O-glucoside exhibited multiple violations, which may affect their pharmacokinetic behavior. Overall, apigenin, quercetin, kaempferol, phyllanthin, and ellagic acid emerged as the most promising candidates for further anti-obesity studies.

The ADME analysis demonstrated that most of the selected phytoconstituents exhibited favorable pharmacokinetic characteristics. Apigenin, quercetin, kaempferol, phyllanthin, gallic acid, ellagic acid, stearic acid, and oleic acid showed high gastrointestinal absorption, indicating good potential for oral administration. In contrast, chebulic acid, rutin, and kaempferol-3-O-glucoside exhibited low GI absorption, which may limit their bioavailability. None of the compounds, except phyllanthin, were predicted to cross the blood–brain barrier, suggesting a lower likelihood of central nervous system-related effects. Several compounds, including apigenin, quercetin, kaempferol, ellagic acid, stearic acid, and oleic acid, were identified as CYP1A2 inhibitors, indicating possible interactions with drug-metabolizing enzymes. Overall, phyllanthin, apigenin, quercetin, kaempferol, gallic acid, and ellagic acid demonstrated favorable ADME profiles and may be considered promising candidates for further anti-obesity investigations.

Table 4. Evaluation on the basis of toxicity study

Sr.no.	Constituents Name	Predicted Toxicity Score	Predicted LD50 (mg/kg)
1.	Apigenin	5	2500mg/kg
2.	Quercetin	3	159mg/kg
3.	Chebulic acid	4	1000mg/kg
4.	Kaempferol	5	3919mg/kg
5.	Rutin	5	5000mg/kg
6.	Phyllanthin	4	1300mg/kg
7.	Kaempferol-3-o-glucoside	5	5000mg/kg
8.	Stearic acid	4	900mg/kg
9.	Gallic acid	4	2000mg/kg
10.	Ellagic acid	4	2991mg/kg
11.	Oleic acid	2	48mg/kg

The toxicity prediction results indicated varying safety profiles among the selected phytoconstituents from *Emblica officinalis* leaves. Rutin and kaempferol-3-O-glucoside exhibited the highest predicted safety with a toxicity class of 5 and LD_{50} values of 5000 mg/kg, suggesting low acute toxicity. Apigenin and kaempferol also demonstrated favorable safety profiles with high LD_{50} values of 2500 mg/kg and 3919 mg/kg, respectively. In contrast, quercetin and oleic acid showed comparatively lower LD_{50} values (159 mg/kg and 48 mg/kg), indicating relatively higher toxicity risks. Overall, most of the evaluated phytoconstituents exhibited moderate to low toxicity, supporting their potential suitability for further anti-obesity drug development studies.

Table 5. Docking score of all phytochemicals of *Emblica officinalis*

Sr. no.	Plant	Constituent Name	9MIZ	9VG4
1.	Standard	Orlistat	-4.6	-5.9
2.	*Phyllanthus emblica* (leaves)	Apigenin	-7.9	**-9.3**
3.		Quercetin	-8.1	-9.2
4.		Chebulic acid	-7.2	-6.6
5.		Kaempferol	-7.9	-8.6
6.		Rutin	**-9.9**	-9.2
7.		Phyllanthin	-7	-7.1
8.		Kaempferol-3-o-glucoside	-9.6	-8.9
9.		Stearic acid	-5.6	-6.7
10.		Gallic acid	-5.1	-6.7
11.		Ellagic acid,	-8.1	**-9.3**
12.		Oleic acid	-5.8	-6.4

The molecular docking study revealed that all selected phytoconstituents from *Phyllanthus emblica* leaves exhibited stronger binding affinities toward both obesity-associated targets (9MIZ and 9VG4) compared to the standard drug Orlistat. Among the tested compounds, rutin showed the highest binding affinity against 9MIZ with a docking score of −9.9 kcal/mol, followed by kaempferol-3-O-glucoside (−9.6 kcal/mol). Against 9VG4, apigenin and ellagic acid demonstrated the strongest interactions with docking scores of −9.3 kcal/mol, while quercetin and rutin exhibited scores of −9.2 kcal/mol. Kaempferol also showed significant binding affinity toward both targets, indicating stable ligand–protein

interactions. Overall, rutin, kaempferol-3-O-glucoside, apigenin, quercetin, and ellagic acid emerged as the most promising phytoconstituents, exhibiting superior docking performance compared to Orlistat and suggesting their potential role as anti-obesity agents.

Visualization Study

The active pocket was considered to be the site where selected model complexes with active chemical constituents of *Phyllanthus emblica.* The 2d-interaction is generally based on the binding and bonds between ligand and macromolecule.

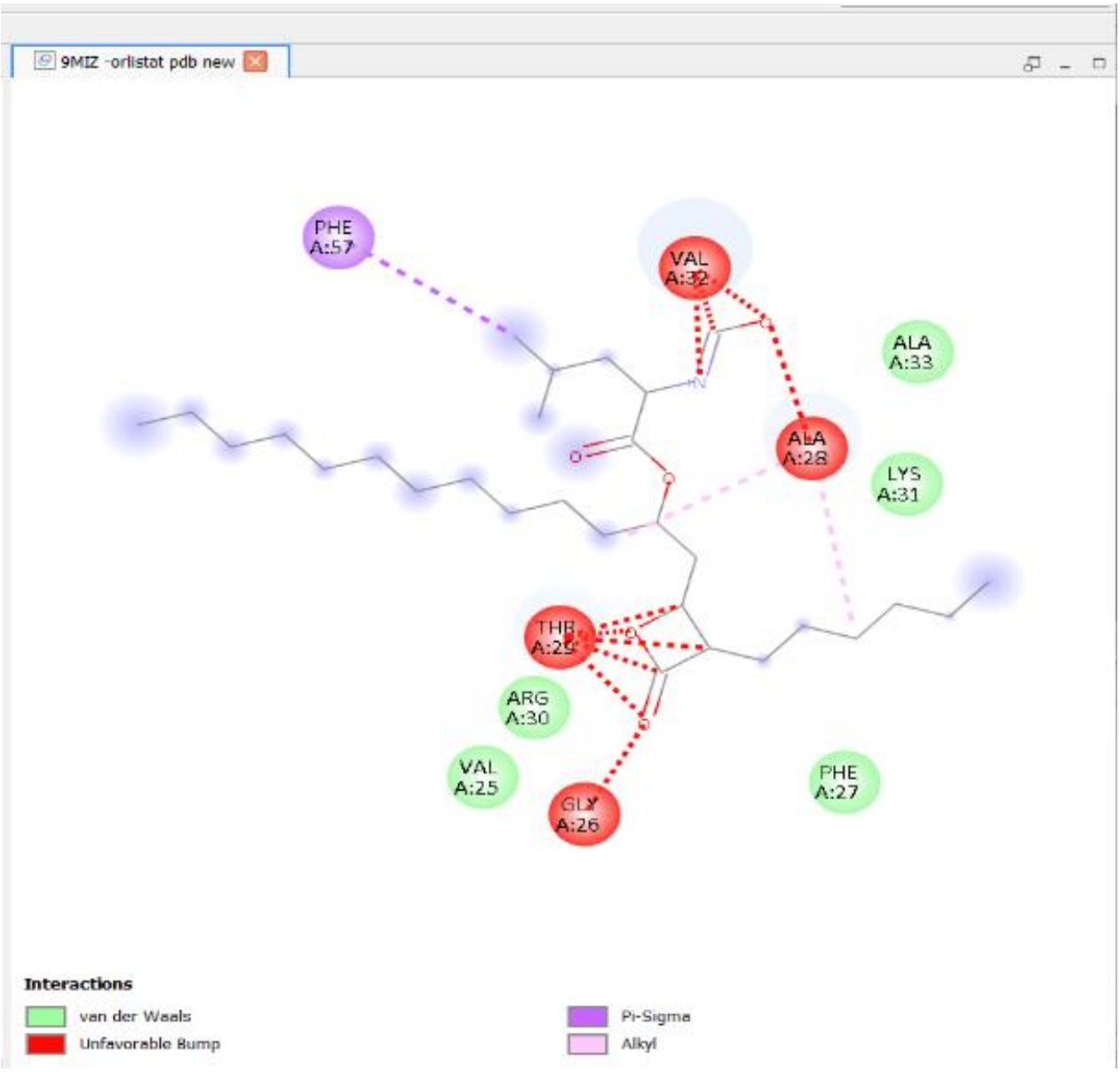


Figure 4. 2D-interation between 9MIZ – Orlistat

The active pocket model (9MIZ- Orlistat) consist of 10 amino acid residues as PHE A:57, VAL A: 32, ALA A:28, ALA A:33, LYS A:31, THR A:29, ARG A:30, VAL A:25, GLY A:26, PHE A:27. Whereas the amino acids are attached to ligand molecules using Van der Waals force, Pi- Sigma, Alkyl. As shown in above Figure 4.

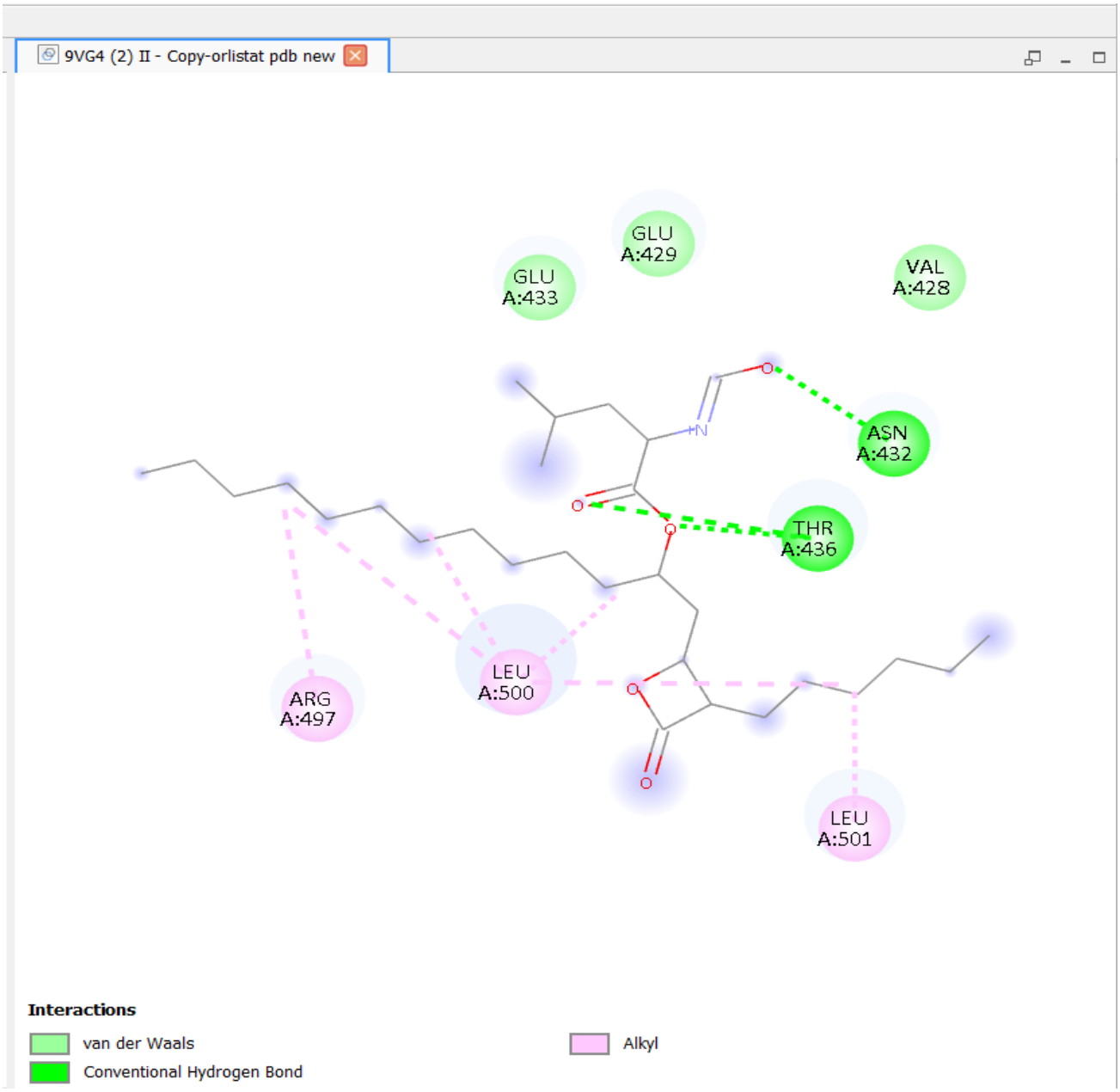


Figure 5. 2D-interation between 9VG4- Orlistat.

The active pocket model (9VG4- Orlistat) consist of 8 amino acid residues as, GLU A:433, GLU A:429, VAL A:428, ASN A:432, THR A:436, ARG A:497, LEU A:500, LEU A:501. Whereas the amino acids are attached to ligand molecule using Van der Waals force, Alkyl, Conventional Hydrogen Bond. As shown in above Figure 5.

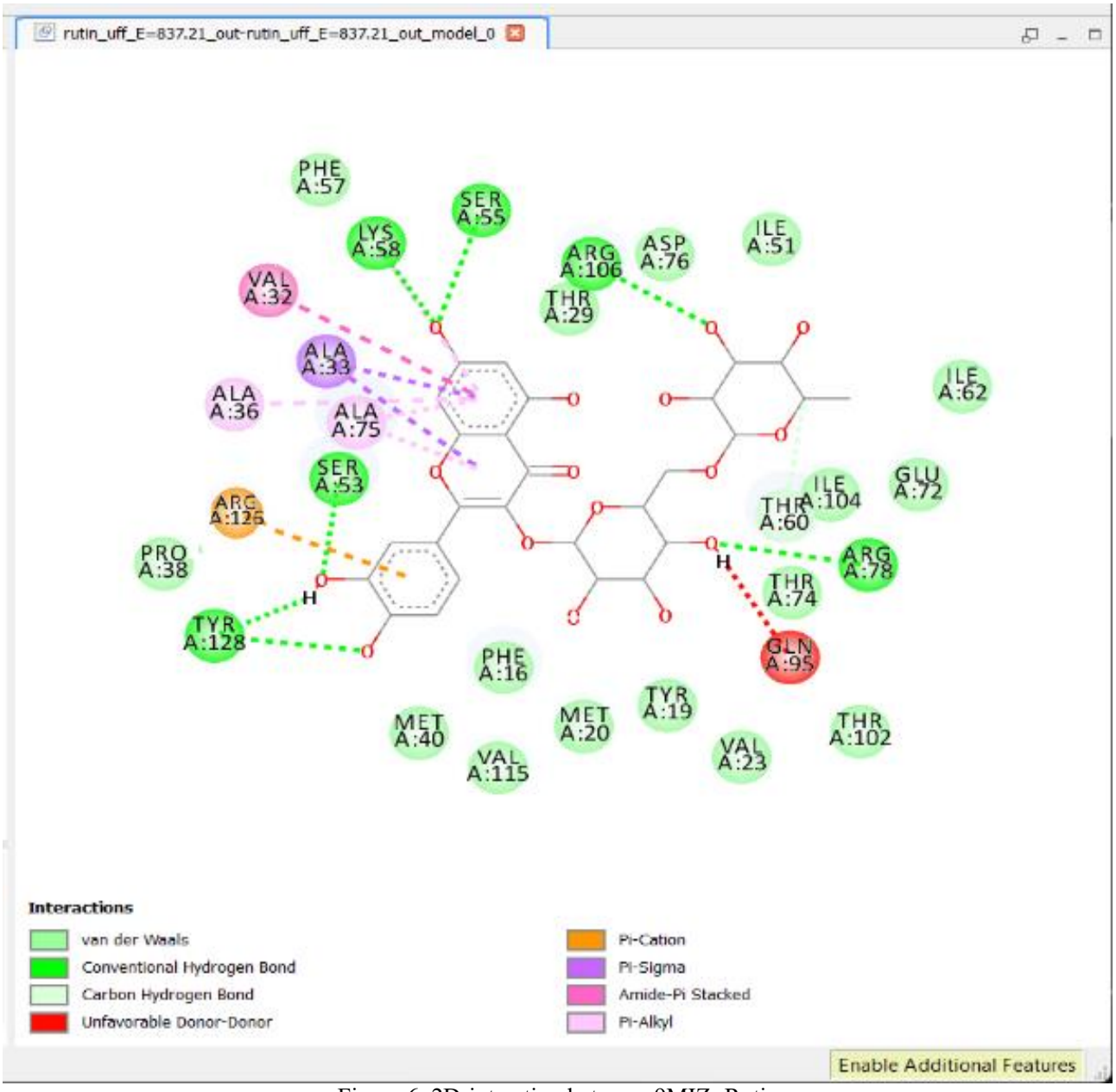


Figure 6. 2D-interation between 9MIZ- Rutin

The active pocket model (9MIZ- Rutin) consist of 29 amino acid residues as, PHE A:57, LYS A:58, SER A:55, VAL A:32, ALA A:33, ALA A:36, ALA A:75, SER A:53, ARG A:126, PRO A:38, TYR A:128, PHE A:16, MET A:40, VAL A:115, MET A:20, TYR A:19, VAL A:23, THR A:102, GLN A:95, THR A:102, THR A:74, ARG A:78, THR A:60, ILE A:104, GLU A:72, ILE A :62, ILE A:62, ILE A :51, ASP A:76, ARG A:106, THR A:29. Whereas, the amino acid are attached to ligand molecule using Van der Waals, Conventional Hydrogen Bond, Carbon Hydrogen Bond, Pi-Cation, Pi-Sigma, Amide-Pi Stacked, Pi-Alkyl. As shown in Figure 6.

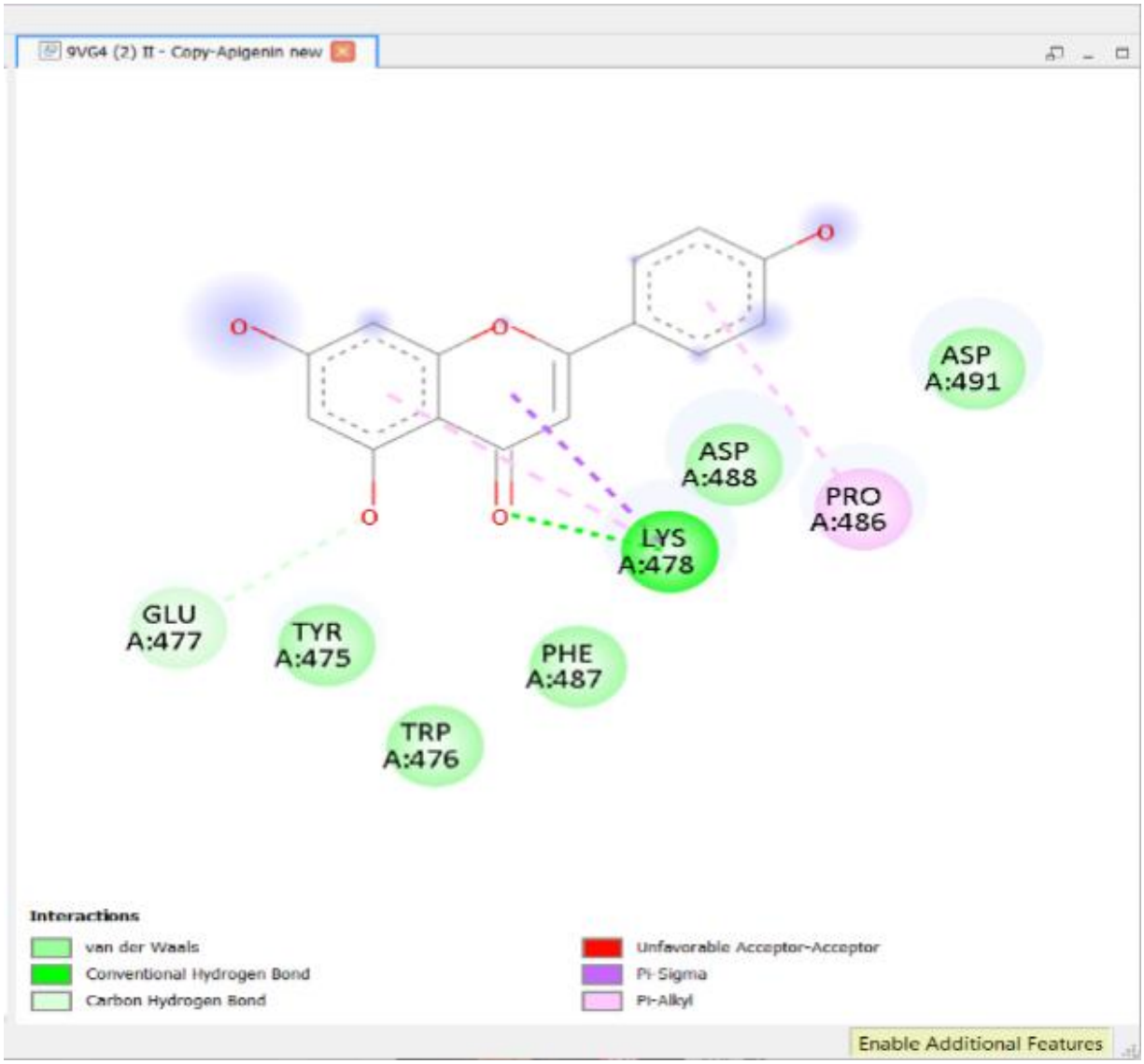


Figure 7. - 2D-interation between 9VG4- Apigenin

The active pocket model (9VG4- Apigenin) consist of 8 amino acid residues as, ASP A:491, GLU A:477, TYR A:475, TRP A:476, PHE A:487, LYS A:478, ASP A:488, PRO A:486. Where as the amino acid are attached to ligand molecule using Van der Waals, Conventional Hydrogen Bond, Carbon Hydrogen Bond, Pi-Sigma, Pi-Alkyl. As shown in Figure 7.

Conclusion

The present in- silico study demonstrated the potential of phytoconstituents derived from *Phyllanthus emblica* leaves as promising anti-obesity agents against the target proteins 9MIZ and 9VG4. Molecular docking results revealed that several compounds, particularly rutin, kaempferol-3-O-glucoside, apigenin, quercetin, and ellagic acid, exhibited strong binding affinities and favorable interactions with the selected targets, surpassing the standard drug Orlistat. Drug-likeness and ADME evaluation indicated that most phytoconstituents possessed acceptable pharmacokinetic properties, while toxicity prediction suggested a favorable safety profile for the majority of compounds. These findings suggest that *Phyllanthus emblica* leaves, an underutilized agro-waste resource, are a valuable source of bioactive molecules with potential anti-obesity activity. However, further *in-vitro*, *in-vivo*, and clinical investigations are required to validate the biological efficacy, safety, and therapeutic applicability of these phytoconstituents for obesity management.

Author contributions

Concept and study design: Sakshi Ubale, Shailju Gurunani.
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