International Journal of Scientific Research in Science and Technology
Available online at : www.ijsrst.com
Peer Reviewed and Refereed International Scientific Research Journal
Print ISSN: 2395-6011 | Online ISSN: 2395-602X
doi : https://doi.org/10.32628/IJSRST26133185

Insilico Evaluation of *Arachis Hypogaea (Linn)* for its Potential Antiobesity Activity

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ARTICLEINFO

Article History:
Accepted : 15 May 2026
Published: 01 June 2026

Publication Issue :
Volume 13, Issue 3
May-June -2026

Page Number :
648-660

ABSTRACT

Obesity is a complex metabolic disorder associated with serious health complications, including cardiovascular diseases, diabetes, and dyslipidemia. The growing demand for safer and sustainable anti-obesity therapeutics has encouraged the exploration of bioactive compounds from plant-derived waste materials. In the present study, an insilico approach was employed to evaluate the anti-obesity potential of phytoconstituents obtained from the hulls of Arachis hypogaea. Obesity-related target proteins with PDB IDs 9MIZ and 9VG4, involved in lipid metabolism and adipogenesis, were retrieved from the PDB. Optimized Ligand structures were taken from PubChem Molecular docking was carried out using AutoDock Vina to predict binding affinities and interaction profiles. Post-docking analysis of ligand–protein interactions, was conducted using Discovery Studio. To evaluate the drug-likeness and pharmacokinetic suitability of the docked compounds, ADME and toxicity profiling was performed using computational prediction tools. Compounds were screened based on Lipinski's Rule of Five and Ghose filter criteria, and additionally, toxicity parameters overall safety profiles were predicted to identify suitable lead candidates. The results demonstrated that several phytoconstituents, from Arachis hypogaea exhibited strong binding affinities toward both targets and successfully satisfied drug-likeness, ADME, and toxicity criteria. This study highlights the potential of plant waste materials as promising, eco-friendly sources of anti-obesity agents.

Keywords: Obesity, Agrowaste, Arachis hypogaea, Docking, Lipinski's Rule of Five and Ghose filter criteria, Swiss ADME, Protox 3.0.

I. INTRODUCTION

Obesity has become a major global health challenge and continues to increase at an alarming rate. It is characterized by excessive accumulation of adipose tissue that negatively affects health and increases the risk of several chronic diseases. In recent decades, the frequency of obesity has increased dramatically due to

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changes in lifestyle, dietary habits, and reduced physical activity[1], [2].Obesity is defined by a body mass index (BMI) which is determined by dividing weight in kg by height in m2 (kg/m2). Persons are classified in three categories on basis of BMI. Underweight or normal weight is 25 kg/m2, followed by overweight (25 to 30 kg/m2), moderate obesity (30 to 35 kg/m2), and severe obesity (BMI 35 kg/m2)[3], [4].

The World Health Organization (WHO) defines obesity as a chronic relapsing disease that is the product of the complex interaction between genetics, neurobiology, eating behaviours, access to a healthy diet, market forces and the wider environment. Over the past few decades, obesity has spread around the world as countries have improved food security, socioeconomic development and changes in diet, physical activity and societal and individual behaviour, associated with globalisation and industrialised food systems[5]. Obesity is related to lower life expectancy, reduced quality of life and disabilities, mostly in those individuals that develop cardiovascular diseases, type 2 diabetes, osteoarthritis and cancer [1], [6], [7].

Generally, the prevalence of obesity is greater in older persons and women[2] although rates have increased in all ages and both sexes regardless of geographical locality, ethnicity or socioeconomic status. Furthermore, the increasing prevalence of overweight and obesity in children and adolescents has become a burden of this disease on global health systems[8], [9]. In 2022, 1 in 8 people worldwide lived with obesity. Adult obesity worldwide has more than doubled since 1990, and adolescent obesity has quadrupled. In 2022, 2.5 billion adults (aged 18 years or older) were overweight. Of these, 890 million were living with obesity. In 2022, 43% of adults aged 18 years and over were overweight and 16% were living with obesity. 35million of children under 5 years of age were overweight in 2024 [5].

The pathophysiology of obesity is complex and involves interactions between genetic, environmental, and physiological factors. The underlying mechanism is the imbalance between energy intake and energy expenditure, leading to excess fat accumulation in adipose tissue[10]. Adipose tissue acts as an endocrine organ and releases a number of molecules referred to as adipokines, including leptin and adiponectin. These molecules are involved in appetite regulation, lipid metabolism and inflammatory responses [11], [12]. Dysregulation of adipokine pathways is involved in the metabolic disturbances and the development of obesity diseases.

Adipogenesis, the differentiation of preadipocytes into mature adipocytes, also plays a critical role in obesity process is regulated by transcription factors such as peroxisome proliferator-activated receptor gamma (PPAR-γ) and CCAAT/enhancer-binding proteins (C/EBPs), which promote lipid accumulation within the adipose tissue [13], [14]. In addition, digestive enzymes such as pancreatic lipase are needed for the digestion and absorption of dietary lipids. Obesity treatment includes several therapeutic approaches, such as lifestyle modification, pharmacotherapy and bariatric surgery. Lifestyle interventions including calorie restriction, increased physical activity and behavioural therapy remain the first line strategies for weight management [15], [16]. Lifestyle changes such as eating a more balanced diet activity and behavioural therapy as the primary strategies for weight management [10].

Many synthetic drugs have been developed for the treatment of obesity including drugs that target appetite regulation, fat absorption and metabolic pathways. Orlistat inhibits gastric and pancreatic lipase and prevent hydrolysis of fat and thus reduces fat absorption in the gastrointestinal tract [17] .

The peptide-1 receptor agonists (e.g. Liraglutide and Semaglutide) have shown to be highly effective in inducing satiety, delaying gastric emptying and decreasing food intake and thus may help weight loss by suppressing appetite and delaying gastric emptying [18], [19]. Another drug, Phentermine is a weight loss drug that works by stimulating the hypothalamus to release norepinephrine which suppresses appetite and

decreases caloric intake [20]. Additionally, the combination therapy Naltrexone/Bupropion acts on pro-opiomelanocortin neurons in the hypothalamus to reduce appetite and control food cravings, providing an effective pharmacological approach for obesity management [21]. Although these drugs have demonstrated promising outcomes, their long-term use may be limited by adverse effects, high cost, and accessibility issues.

In recent years, increasing attention has been directed toward the use of natural products and plant-derived bioactive compounds for obesity management. Phytochemicals such as polyphenols, flavonoids, tannins, and alkaloids have demonstrated potential anti-obesity effects through multiple mechanisms, including inhibition of adipogenesis, stimulation of lipid metabolism, and reduction of oxidative stress [13], [22], [23]. Consequently, medicinal plants have become an important focus in the search for safer and more effective therapeutic agents for obesity. The valorization of agro-waste materials not only provides an economical source of bioactive compounds but also contributes to environmental sustainability and waste management[24], [25], [26].



Fig 1: - shell of *Arachis hypogaea.*

The plant-derived agricultural residues hulls of *Arachis hypogaea*, which are typically discarded during peanut processing, have been reported to contain polyphenols and tannins with potential lipid-lowering effects [27], [28]. Considering the increasing prevalence of obesity and the limitations associated with currently available pharmacological therapies, the exploration of plant-derived agro-waste materials as potential sources of anti-obesity agents represents a promising area of research. Therefore, the present study aims to investigate the anti-obesity potential of selected agro-waste materials through computational approaches, which may contribute to the development of sustainable and cost-effective therapeutic strategies for obesity management.

II. METHODS AND MATERIAL

Molecular docking is a widely used computational approach in modern drug design and development, which helps to predict the interaction between small molecules and biological targets. It explores the possible conformations of ligands within the binding site of a macromolecular receptor and estimates the binding free energy of different ligand–receptor complexes. In this process, small molecular compounds are positioned into the active site of the target protein, and their binding affinity is evaluated to identify potential therapeutic candidates. This technique plays a crucial role in structure-based drug design, as it enables the analysis of binding interactions and geometries using efficient and accurate computational protocols [29], [30].

2.1 Selection and preparation of Receptor: -

The identification of appropriate molecular targets is essential for understanding obesity mechanisms and developing effective therapeutic strategies [30]. Two different target protein structures were selected to represent different pathways associated with various dysfunctions in obesity. Protein structures such as 9MIZ and 9VG4 were chosen due to their involvement in lipid metabolism pathways based on literature survey. The selected target proteins are retrieved from RCSB protein data bank (PDB) in PDB format [31]. The selected protein structures were carefully examined, and unnecessary molecules such as co-crystallized ligands, water molecules, and ions were removed and adding missing hydrogen atoms to

the structure to ensure correct protonation states, particularly for polar residues. The structure was then subjected to energy minimization to relieve steric clashes and optimize geometry the cleaned and optimized protein structure was saved in PDB format and further converted into PDBQT format using AutoDock Tools [32], [33].

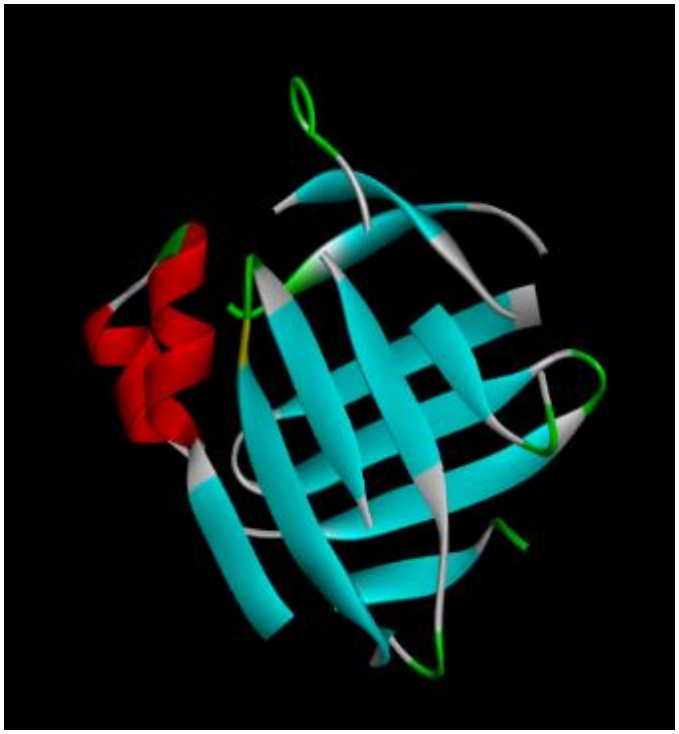


Fig.2: -2D structure of 9MIZ

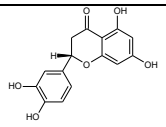
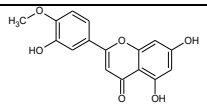
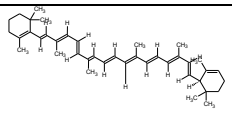
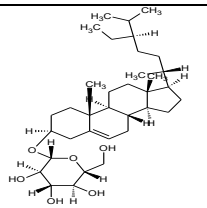
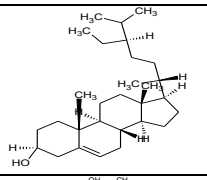
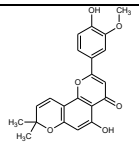
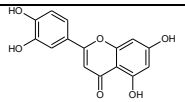
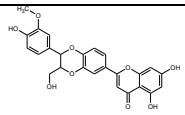
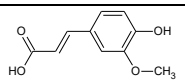
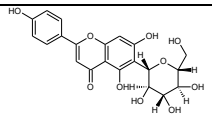
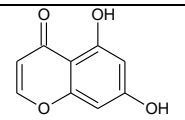
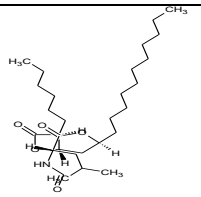


Fig.3: -2D structure of 9VG4

2.2 Selection and preparation of Ligands: -

Agro-industrial plant wastes like hull of *Arachis hypogaea* is rich in bioactive phytochemicals with antioxidant and metabolic regulatory properties, offering both therapeutic potential and environmental sustainability. All the chemical constituent of plant are selected on the basis of the literature survey the ligands with highest negative docking score were evaluated for the druglikeness, and pharmacokinetic suitability of the docked compounds, ADME Lipinski's Rule of Five and Ghose filter criteria, and toxicity profiling revels that selected one are non-toxic, no harm and can be best candidate from agrowaste against obesity associated target. The three-dimensional structure of ligands was downloaded from PubChem database; the chemical structures of selected ligands were obtained in the form of SMILES (Simplified Molecular Input Line Entry System) notation from the PubChem [34]. The SMILES strings were then imported into Avogadro (https://avogadro.cc/, n.d.) to generate three-dimensional (3D) structures of the ligands [35], [36], [37]. Upon import, Avogadro automatically converted the SMILES notation into a 2D/3D molecular structure. Hydrogen atoms were added to satisfy valency, and the molecular geometry was checked and corrected where necessary. The generated structures were then subjected to energy minimization. The optimized ligand structures were saved in PDB format the ligands were converted into PDBQT format and used for molecular docking studies.

Table 1: - Chemical constituents of *Arachis hypogaea.[38], [39], [40]*

	Chemical Constituent	Smile notation	Structure
Arachis hypogaea. (hull)	Eriodictyol	C1[C@H](OC2=CC(=CC(=C2C1=O)O)O)C3=CC(=C(C=C3)O)O	
	Diosmetin	COC1=C(C=C(C=C1)C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O	
	Carotene	CC1=C(C(CCC1)(C)C)/C=C/C(=C/C=C/C(=C/C=C/C=C(\\C)/C=C/C=C(\\C)/C=C/[C@H]2C(=CCCC2(C)C)C)/C)/C	
	Daucosterol	CC[C@H](CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O[C@H]5[C@@H]([C@H]([C@@H]([C@H](O5)CO)O)O)O)C)C)C(C)C	
	β-sitosterol	CC[C@H](CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)C(C)C	
	Racemoflavone	CC1(C=CC2=C(O1)C=C(C3=C2OC(=CC3=O)C4=CC(=C(C=C4)O)OC)O)C	
	Luteolin	C1=CC(=C(C=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O)O	
	Hydnocarpin	COC1=C(C=CC(=C1)C2C(OC3=C(O2)C=CC(=C3)C4=CC(=O)C5=C(C=C(C=C5O4)O)O)CO)O	
	Ferulic acid	COC1=C(C=CC(=C1)/C=C/C(=O)O)O	
	Isosaponaretin	C1=CC(=CC=C1C2=CC(=O)C3=C(O2)C=C(C(=C3O)[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)O)O	
	5,7-Dihydroxychromone	C1=COC2=CC(=CC(=C2C1=O)O)O	
Standard	Orlistat	CCCCCCCCCCC[C@@H](C[C@H]1[C@@H](C(=O)O1)CCCCCC)OC(=O)[C@H](CC(C)C)NC=O	

2.3 Molecular docking:

Molecular docking analysis was performed to evaluate the binding affinity between the prepared ligands and

the target protein. The prepared protein structure (in PDBQT format) and optimized ligands were imported into PyRx, which integrates the AutoDock Vina algorithm for docking studies [41], [42], [43]Initially, the protein was loaded as a macromolecule, and ligands were imported into the ligand workspace. Energy minimization of ligands was reconfirmed within PyRx using the universal force field (UFF) to ensure stability before docking[44] The grid box was then defined around the active binding site of the protein, covering key amino acid residues involved in ligand interaction. The grid dimensions were adjusted to encompass the entire active site region[45], [46]. Docking simulations were performed using the AutoDock Vina algorithm with default parameters, Multiple binding poses were generated for each ligand, and the best conformation was selected based on the lowest binding energy (kcal/mol) [42], [47], [48]. The docking results were analyzed by visualizing protein–ligand interactions using Discovery Studio Visualizer and UCSF Chimera. Key interactions such as hydrogen bonds, hydrophobic interactions, and van der Waals forces were identified. The ligand exhibiting the lowest binding energy and maximum favourable interactions was considered the most potent candidate [44,79]

2.4 Evaluation of Ligand on the basis of Drug Likeness, ADME and Toxicity study

The in-silico ADME screening and drug-likeness evaluation were performed using the free web tool SwissADME, which is developed by the Swiss Institute of Bioinformatics and freely available at www.swissadme.ch and Drug likeness test of phytochemicals based on the Lipinski rule using SwissADME software [56]. The compounds with high-ranking binding energy scores were subjected to this part of the screening process [57]. Simple physicochemical properties such as molecular weight (MW), molecular refractivity (MR), atom counts, and polar surface area (PSA) were computed. Drug-likeness candidature was executed by Lipinski, Ghose rule of 5. [57,58] they are as follow; Molecular weight less than equal to 500, Log p should be less than 5, H bond donor and acceptor should be less than equal to 5, TPSA should be less than 140 angstroms, No. of rotatable bonds should be less than 10.[59] The Ghose filter is used to evaluate drug-likeness of molecules based on physicochemical properties. According to this rule, a compound is more likely to be drug-like if it has: molecular weight (160–480), log P (–0.4 to 5.6), molar refractivity (40–130), and total number of atoms (20–70) [49]. Toxicity studies can be perform using Protox 3.0. [61] this software is used to screen various compound on the basic of various toxicities such as organ toxicity, carcinogenicity, immunotoxicity, mutagenicity, cytotoxicity etc, it also helps us to give predicted toxicity score and predicted lethal dose [62,63].

III.RESULTS AND DISCUSSION

3.1 Molecular Docking: - Results of molecular docking are stated below

Table 2: - Docking score of phytoconstituent of *Arachis hypogaea (hull).*

Compound	Constituent Name	9MIZ	9VG4
Arachis hypogaea. (hull)	Eriodictyol	-8.1	-6.4
	Diosmetin	-7.9	-6.3
	Daucosterol	-7.6	-6.8
	β-sitosterol	-8.7	-6.1
	Racemoflavone	**-9.3**	-6.8
	Luteolin	-8.2	**-8.8**
	Hydnocarpin	-7.5	-8
	Ferulic acid	-6	-6.5
	Isosaponaretin	-6.6	-5.8
	5,7-Dihydroxychromone	-5.8	-5.5
Standard	Orlistat	-4.6	-5.9

Discussion based on docking score: -The docking of the macromolecule 9MIZ and 9VG4 with phytoconstituent of agrowaste such as *Arachis hypogaea* has been done. The table 2 shows the Binding Energy of 10 compounds including the

standard. In-silico studies revealed that all the molecules show good binding affinity toward the target protein ranging from -9.9 to -5.5.

3.2 Evaluation of Ligand on the basis of Drug Likeness

Table 3: - Evaluation of ligand on the basic of druglikeness.

Compound	Constituent Name	Molecular Weight (G/Mol)	Rotatable Bonds	H Bond Acceptor	H Bond donar	Log P	Follows Lipinski	No Of Violations	Ghose
Arachis hypogaea. (hull)	Eriodictyol	288.25	1	6	4	1.62	Yes	0	Yes
	Diosmetin	300.26	2	6	3	2.47	Yes	0	Yes
	Daucosterol	576.85	9	6	4	5.17	Yes	1	No
	β-sitosterol	414.71	6	1	1	5.05	Yes	1	No
	Racemoflavone	366.36	2	6	2	3.54	Yes	0	Yes
	Luteolin	286.24	1	6	4	1.86	Yes	0	Yes
	Hydnocarpin	464.42	4	9	4	2.31	Yes	0	Yes
	Ferulic acid	194.18	3	4	2	1.62	Yes	0	Yes
	Isosaponaretin	432.38	3	10	7	1.60	Yes	1	Yes
	5,7-Dihydroxy chromone	178.14	0	4	2	0.72	Yes	0	Yes
Standard	Orlistat	495.73	24	5	1	8.31	Yes	1	No

Discussion based on Drug Likeness

The drug-likeness study of phytoconstituents from Arachis hypogaea hull showed that most compounds satisfied Lipinski's Rule of Five, indicating good oral bioavailability and drug-like properties. Eriodictyol, diosmetin, luteolin, hydnocarpin, ferulic acid, and racemoflavone showed no violations and good physicochemical characteristics. Daucosterol, β-sitosterol, and isosaponaretin exhibited one violation due to higher molecular weight or lipophilicity. Daucosterol and β-sitosterol also failed the Ghose filter because of their larger molecular size. The standard drug Orlistat also showed one violation, indicating that some effective drugs may not fully satisfy all drug-likeness criteria. Overall, the results suggest promising pharmacological and anti-obesity potential of peanut hull phytoconstituents.

3.3 Evaluation on the basis of ADME parameter: -

Table 4: - Evaluation of ligand on the basic of ADME parameter.

Constituent Name	GI absorption	BBB permeant	CYP1A2 inhibitor	Bioavailability Score
Eriodictyol	High	No	No	0.55
Diosmetin	High	No	Yes	0.55
Daucosterol	Low	No	No	0.55
β-sitosterol	Low	No	No	0.55
Racemoflavone	High	No	Yes	0.55
Luteolin	High	No	Yes	0.55
Hydnocarpin	Low	No	No	0.55
Isosaponaretin	Low	No	No	0.55
5,7-Dihydroxy chromone	High	No	No	0.55

Discussion based on ADME Parameter.

The ADME analysis of phytoconstituents from Arachis hypogaea hull revealed that most compounds exhibited favorable pharmacokinetic properties. Eriodictyol, diosmetin, racemoflavone, luteolin, and 5,7-dihydroxychromone showed high gastrointestinal absorption, suggesting good oral bioavailability. None of the compounds were found to be BBB permeant, indicating lower chances of central nervous system side effects. Diosmetin, racemoflavone, and luteolin showed CYP1A2 inhibitory activity, which may influence drug metabolism and potential drug–drug interactions. Compounds such as daucosterol, β-sitosterol, hydnocarpin, and isosaponaretin exhibited low GI absorption, possibly due to higher molecular weight and polarity. All compounds showed a bioavailability score of 0.55, indicating moderate potential for systemic availability and therapeutic application.

3.4 Evaluation on the basis of toxicity study: -

Table 5: - Evaluation of ligand on the basic toxicity study.

Constituent Name	Predicted Toxicity Score	Predicted LD50 (mg/kg)
Eriodictyol	4	2000mg/kg
Diosmetin	5	3919mg/kg
Daucosterol	6	8000mg/kg
β-sitosterol	4	890mg/kg
Racemoflavone	5	5000mg/kg
Luteolin	5	3919mg/kg
Hydnocarpin	5	5000mg/kg
Isosaponaretin	3	159mg/kg
5,7-Dihydroxy chromone	5	3200mg/kg

Discussion based on toxicity study: -

The toxicity prediction study of phytoconstituents from Arachis hypogaea hull indicated that most compounds possess relatively low toxicity and acceptable safety profiles. Diosmetin, racemoflavone, luteolin, hydnocarpin, and 5,7-dihydroxychromone showed high LD_{50} values ranging from 3200–5000 mg/kg, suggesting lower acute toxicity. Daucosterol exhibited the highest predicted LD_{50} value of 8000 mg/kg, indicating comparatively safer characteristics. In contrast, isosaponaretin showed a lower LD_{50} value of 159 mg/kg with toxicity class 3, indicating relatively higher toxicity compared to other compounds. Overall, the toxicity analysis suggests that most phytoconstituents possess moderate to low toxic potential and may be considered suitable for further pharmacological and anti-obesity investigations.

3.5 Visualization Study: -

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

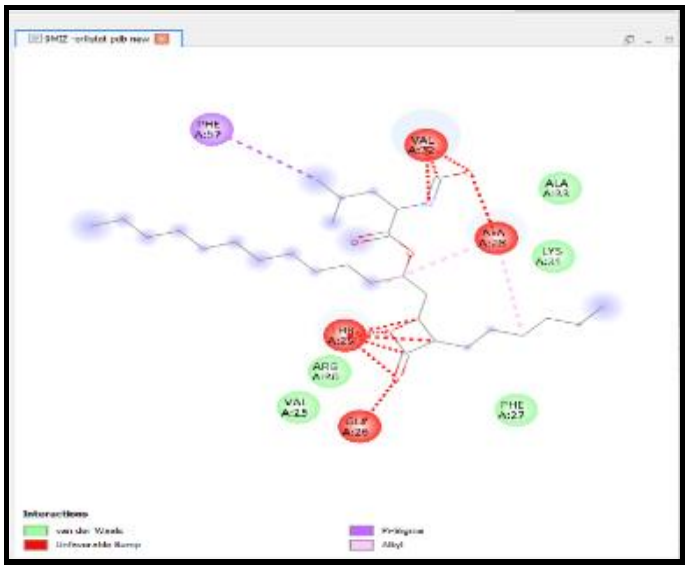


Fig.4- 2D-interation between 9MIZ – Orlistat.

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 Fig.4.

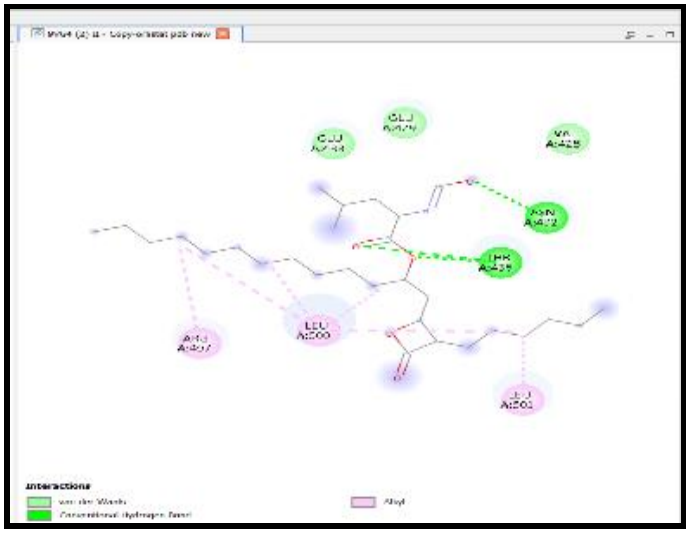


Fig 5: - 2D-interation between 9VG4- Orlistat.

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 Fig.5.

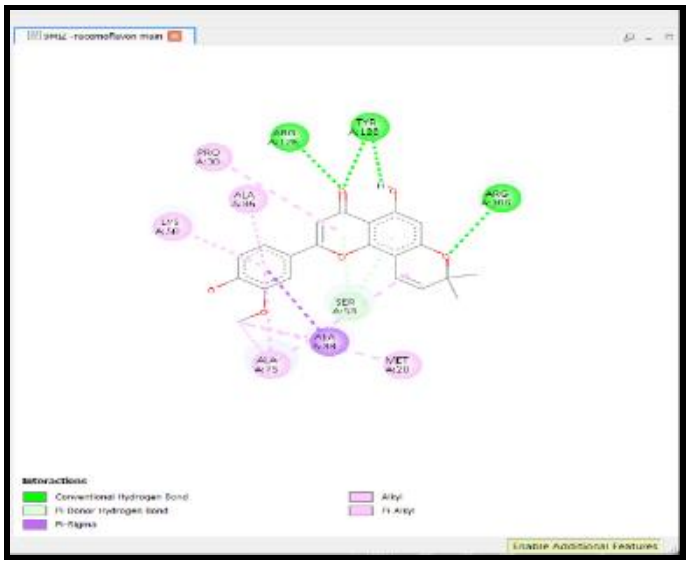


Fig 6: -2D-interation between 9MIZ-Racemoflavon.

The active pocket model (9MIZ-Rracemoflavon) consist of 10 amino acid residues as, PRO A:38, ALA A:36, LYS A:58, ARG A:126, TYR A:128, ARG A:106, SER A:53, ALA A:33, MET A:20, ALA A:75. Whereas the amino acids are attached to ligand molecule using Conventional Hydrogen Bond, Pi-Donar Hydrogen Bond, Pi-sigma, Alkyl, Pi- alkyl. As shown in Fig 6.

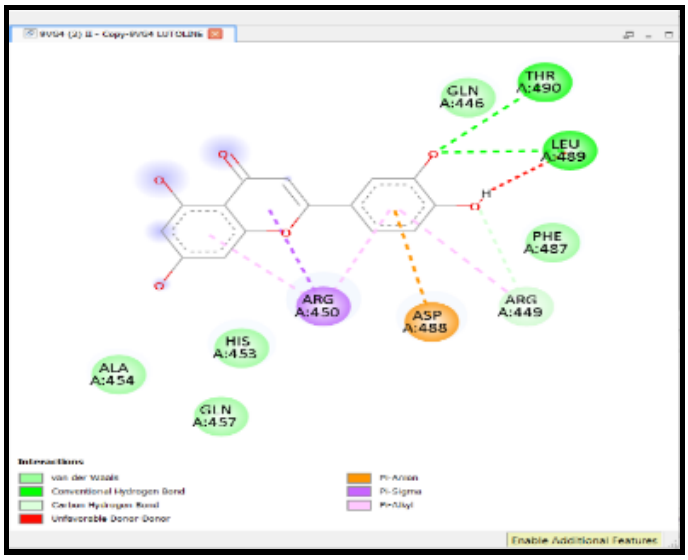


Fig 7: -2D-interation between 9VG4-Lutoline

The active pocket model (9MIZ-Racemoflavon) consists of 10 amino acid residues as, GLN A:446, THR A:490, LEU A:489, PHE A:487, ARG A:449, ASP A:488, ARG A:450, HIS A:453, GLN A:457, ALA A:454. Whereas the amino acids are attached to ligand molecule using Van der Waals, Conventional Hydrogen Bond, Carbon Hydrogen Bond, Pi-Anion, Pi-sigma, Pi- Alkyl. As shown in Fig 7.

IV. CONCLUSION

The present molecular docking study highlights the potential of phytoconstituents derived from agricultural waste materials, *Arachis hypogaea* hulls as promising inhibitors of obesity-associated protein targets 9MIZ and 9VG4. Compounds with higher negative docking scores formed stable interactions within the active site, suggesting potential inhibitory activity. Drug-likeness, ADME, and toxicity profiling confirmed favorable pharmacokinetic properties and non-toxic behavior. The integration of docking, pharmacokinetic, and toxicity analysis highlights their suitability as safe lead candidates. Agro-waste materials therefore represent a valuable and sustainable source for drug discovery. Further

experimental validation through invitro and in vivo study is necessary to confirm their therapeutic effectiveness.

REFERENCES

[1]. G. A. Bray, K. K. Kim, and J. P. H. Wilding, "Obesity: a chronic relapsing progressive disease process. A position statement of the World Obesity Federation," Obesity Reviews, vol. 18, no. 7, pp. 715–723, Jul. 2017, doi: 10.1111/obr.12551.

[2]. Y. C. Chooi, C. Ding, and F. Magkos, "The epidemiology of obesity," Metabolism, vol. 92, pp. 6–10, Mar. 2019, doi: 10.1016/j.metabol.2018.09.005.

[3]. Z. J. Ward et al., "Projected U.S. State-Level Prevalence of Adult Obesity and Severe Obesity," New England Journal of Medicine, vol. 381, no. 25, pp. 2440–2450, Dec. 2019, doi: 10.1056/NEJMsa1909301.

[4]. R. Ghai et al., "An Investigative Study of Medicinal Herbs for Anti-obesity Potential: (A-Review)," Oriental Journal Of Chemistry, vol. 39, no. 6, pp. 1437–1460, Dec. 2023, doi: 10.13005/ojc/390605.

[5]. WHO, "overweight and obesity," 2026.

[6]. M. Blüher, "Metabolically Healthy Obesity," Endocr. Rev., vol. 41, no. 3, Jun. 2020, doi: 10.1210/endrev/bnaa004.

[7]. A. H. Faghfouri et al., "The effects of N-acetylcysteine on inflammatory and oxidative stress biomarkers: A systematic review and meta-analysis of controlled clinical trials," Eur. J. Pharmacol., vol. 884, p. 173368, Oct. 2020, doi: 10.1016/j.ejphar.2020.173368.

[8]. N. H. Phelps et al., "Worldwide trends in underweight and obesity from 1990 to 2022: a pooled analysis of 3663 population-representative studies with 222 million children, adolescents, and adults," The Lancet, vol. 403, no. 10431, pp. 1027–1050, Mar. 2024, doi: 10.1016/S0140-6736(23)02750-2.

[9]. X. Zhang et al., "Global Prevalence of Overweight and Obesity in Children and Adolescents," JAMA Pediatr., vol. 178, no. 8, p. 800, Aug. 2024, doi: 10.1001/jamapediatrics.2024.1576.

[10]. K. D. Hall and S. Kahan, "Maintenance of Lost Weight and Long-Term Management of Obesity," Jan. 01, 2018, W.B. Saunders. doi: 10.1016/j.mcna.2017.08.012.

[11]. A. R. Saltiel and J. M. Olefsky, "Inflammatory mechanisms linking obesity and metabolic disease," Jan. 03, 2017, American Society for Clinical Investigation. doi: 10.1172/JCI92035.

[12]. M. Blüher, "Obesity: global epidemiology and pathogenesis," Nat. Rev. Endocrinol., vol. 15, no. 5, pp. 288–298, May 2019, doi: 10.1038/s41574-019-0176-8.

[13]. M.-H. Pan, Y.-C. Tung, G. Yang, S. Li, and C.-T. Ho, "Molecular mechanisms of the anti-obesity effect of bioactive compounds in tea and coffee," Food Funct., vol. 7, no. 11, pp. 4481–4491, 2016, doi: 10.1039/C6FO01168C.

[14]. M. Lu, Y. Cao, J. Xiao, M. Song, and C.-T. Ho, "Molecular mechanisms of the anti-obesity effect of bioactive ingredients in common spices: a review," Food Funct., vol. 9, no. 9, pp. 4569–4581, 2018, doi: 10.1039/C8FO01349G.

[15]. P. M. Mollerup, T. R. H. Nielsen, C. Bøjsøe, J. T. Kloppenborg, J. L. Baker, and J.-C. Holm, "Quality of life improves in children and adolescents during a community-based overweight and obesity treatment," Quality of Life Research, vol. 26, no. 6, pp. 1597–1608, Jun. 2017, doi: 10.1007/s11136-017-1504-x.

[16]. A. Galler et al., "Clinical characteristics and outcomes of children, adolescents and young adults with overweight or obesity and mental health disorders," Int. J. Obes., vol. 48, no. 3, pp. 423–432, Mar. 2024, doi: 10.1038/s41366-023-01449-4.

[17]. J. S. Torgerson, J. Hauptman, M. N. Boldrin, and L. Sjöström, "XENical in the Prevention of Diabetes in Obese Subjects (XENDOS) Study," Diabetes Care, vol. 27, no. 1, pp. 155–161, Jan. 2004, doi: 10.2337/diacare.27.1.155.

[18]. H. C. Q. Tan, O. A. Dampil, and M. M. Marquez, "Efficacy and Safety of Semaglutide for Weight Loss in Obesity Without Diabetes: A Systematic Review and Meta-Analysis," Nov. 01, 2022, ASEAN Federation of Endocrine Societies. doi: 10.15605/jafes.037.02.14.

[19]. J. P. H. Wilding et al., "Once-Weekly Semaglutide in Adults with Overweight or Obesity," New England Journal of Medicine, vol. 384, no. 11, pp. 989–1002, Mar. 2021, doi: 10.1056/NEJMoa2032183.

[20]. G. A. Bray and D. H. Ryan, "Medical Therapy for the Patient With Obesity," Circulation, vol. 125, no. 13, pp. 1695–1703, Apr. 2012, doi: 10.1161/CIRCULATIONAHA.111.026567.

[21]. F. L. Greenway et al., "Effect of naltrexone plus bupropion on weight loss in overweight and obese adults (COR-I): a multicentre, randomised, double-blind, placebo-controlled, phase 3 trial," The Lancet, vol. 376, no. 9741, pp. 595–605, Aug. 2010, doi: 10.1016/S0140-6736(10)60888-4.

[22]. S. Hasani-Ranjbar, N. Nayebi, B. Larijani, and M. Abdollahi, "A systematic review of the efficacy and safety of herbal medicines used in the treatment of obesity," Jul. 07, 2009, Baishideng Publishing Group Co. doi: 10.3748/wjg.15.3073.

[23]. U. F. Shaik Mohamed Sayed et al., "Natural products as novel anti-obesity agents: insights into mechanisms of action and potential for therapeutic management," Front. Pharmacol., vol. 14, Jun. 2023, doi: 10.3389/fphar.2023.1182937.

[24]. S. Yadav et al., "Valorisation of Agri-Food Waste for Bioactive Compounds: Recent Trends and Future Sustainable Challenges," Molecules, vol. 29, no. 9, p. 2055, Apr. 2024, doi: 10.3390/molecules29092055.

[25]. N. A. Sagar, S. Pareek, S. Sharma, E. M. Yahia, and M. G. Lobo, "Fruit and Vegetable Waste: Bioactive Compounds, Their Extraction, and Possible Utilization," Compr. Rev. Food Sci. Food Saf., vol. 17, no. 3, pp. 512–531, May 2018, doi: 10.1111/1541-4337.12330.

[26]. J. de D. M. Ufitikirezi et al., "Agricultural Waste Valorization: Exploring Environmentally Friendly Approaches to Bioenergy Conversion," Sustainability, vol. 16, no. 9, p. 3617, Apr. 2024, doi: 10.3390/su16093617.

[27]. J. Yu, M. Ahmedna, and I. Goktepe, "Effects of processing methods and extraction solvents on concentration and antioxidant activity of peanut skin phenolics," Food Chem., vol. 90, no. 1–2, pp. 199–206, Mar. 2005, doi: 10.1016/j.foodchem.2004.03.048.

[28]. R. Singh, S. Mishra, and Dr. S. Ahmad, "A comprehensive review on the therapeutic applications and recent trends of Arachis hypogaea Leaves: An Exploration," J. Pharmacogn. Phytochem., vol. 13, no. 3, pp. 406–414, Jan. 2024, doi: 10.22271/phyto.2024.v13.i3e.14982.

[29]. S. S. Butt, Y. Badshah, M. Shabbir, and M. Rafiq, "Molecular Docking Using Chimera and Autodock Vina Software for Nonbioinformaticians," JMIR Bioinform. Biotech., vol. 1, no. 1, p. e14232, Jun. 2020, doi: 10.2196/14232.

[30]. S. P. Shedame, Y. N. Gholse, R. H. Kasliwal, and D. R. Chaple, "IN-SILICO STUDY OF PASSIFLORA EDULIS FOR ITS ANTI-DIABETIC ACTIVITY," Certified Journal | 684 WORLD JOURNAL OF PHARMACY AND PHARMACEUTICAL SCIENCES SJIF Impact Factor, vol. 13, no. 5, p. 685, 2024, doi: 10.20959/wjpps20245-27197.

[31]. https://www.rcsb.org, "https://www.rcsb.org."

[32]. E. F. Pettersen et al., "UCSF Chimera—A visualization system for exploratory research and analysis," J. Comput. Chem., vol. 25, no. 13, pp. 1605–1612, Oct. 2004, doi: 10.1002/jcc.20084.

[33]. H. M. Berman, "The Protein Data Bank," Nucleic Acids Res., vol. 28, no. 1, pp. 235–242, Jan. 2000, doi: 10.1093/nar/28.1.235.

[34]. S. Kim et al., "PubChem in 2021: new data content and improved web interfaces," Nucleic Acids Res., vol. 49, no. D1, pp. D1388–D1395, Jan. 2021, doi: 10.1093/nar/gkaa971.

[35]. A. Hernndez-Santoyo, A. Yair, V. Altuzar, H. Vivanco-Cid, and C. Mendoza-Barrer, "Protein-Protein and Protein-Ligand Docking," in Protein Engineering - Technology and Application, InTech, 2013. doi: 10.5772/56376.

[36]. A. A. Bingul, S. Ercan, and N. Pirinccioglu, "Development of new inhibitor candidates for Sars-Cov-2 3CLpro (Main Protease): A molecular docking and molecular dynamics simulation study," J. Mol. Graph. Model., vol. 140, p. 109133, Nov. 2025, doi: 10.1016/j.jmgm.2025.109133.

[37]. D. Weininger, "SMILES, a chemical language and information system. 1. Introduction to methodology and encoding rules," J. Chem. Inf. Comput. Sci., vol. 28, no. 1, pp. 31–36, Feb. 1988, doi: 10.1021/ci00057a005.

[38]. M. Zhang et al., "Resource Utilization of Peanut Shells: Nutritional Characteristics, Regulation of Antinutritional Factors, and Application Potential in Livestock and Poultry Production.," Food Sci. Nutr., vol. 13, no. 12, p. e70994, Dec. 2025, doi: 10.1002/fsn3.70994.

[39]. A. Zuo, Y. Sun, S. Qian, and G. Rao, "[Study on Chemical Constituents of Peanut Hull].," Zhong Yao Cai, vol. 38, no. 2, pp. 302–4, Feb. 2015.

[40]. B. Adhikari, S. K. Dhungana, M. W. Ali, A. Adhikari, I.-D. Kim, and D.-H. Shin, "Resveratrol, total phenolic and flavonoid contents, and antioxidant potential of seeds and sprouts of Korean peanuts," Food Sci. Biotechnol., vol. 27, no. 5, pp. 1275–1284, Oct. 2018, doi: 10.1007/s10068-018-0364-7.

[41]. S. Dallakyan and A. J. Olson, "Small-Molecule Library Screening by Docking with PyRx," 2015, pp. 243–250. doi: 10.1007/978-1-4939-2269-7_19.

[42]. O. Trott and A. J. Olson, "AutoDock Vina: Improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading," J. Comput. Chem., vol. 31, no. 2, pp. 455–461, Jan. 2010, doi: 10.1002/jcc.21334.

[43]. S. Forli, R. Huey, M. E. Pique, M. F. Sanner, D. S. Goodsell, and A. J. Olson, "Computational protein–ligand docking and virtual drug screening with the AutoDock suite," Nat. Protoc., vol. 11, no. 5, pp. 905–919, May 2016, doi: 10.1038/nprot.2016.051.

[44]. A. K. Rappe, C. J. Casewit, K. S. Colwell, W. A. Goddard, and W. M. Skiff, "UFF, a full periodic table force field for molecular mechanics and molecular dynamics simulations," J. Am. Chem. Soc., vol. 114, no. 25, pp. 10024–10035, Dec. 1992, doi: 10.1021/ja00051a040.

[45]. X.-Y. Meng, H.-X. Zhang, M. Mezei, and M. Cui, "Molecular Docking: A Powerful Approach for Structure-Based Drug Discovery," Current Computer Aided-Drug Design, vol. 7, no. 2, pp. 146–157, Jun. 2011, doi: 10.2174/157340911795677602.

[46]. D. B. Kitchen, H. Decornez, J. R. Furr, and J. Bajorath, "Docking and scoring in virtual screening for drug discovery: methods and applications," Nat. Rev. Drug Discov., vol. 3, no. 11, pp. 935–949, Nov. 2004, doi: 10.1038/nrd1549.

[47]. J. Eberhardt, D. Santos-Martins, A. F. Tillack, and S. Forli, "AutoDock Vina 1.2.0: New Docking Methods, Expanded Force Field, and Python Bindings," J. Chem. Inf. Model., vol. 61,

no. 8, pp. 3891–3898, Aug. 2021, doi: 10.1021/acs.jcim.1c00203.

[48]. N. S. Pagadala, K. Syed, and J. Tuszynski, "Software for molecular docking: a review," Biophys. Rev., vol. 9, no. 2, pp. 91–102, Apr. 2017, doi: 10.1007/s12551-016-0247-1.

[49]. A. K. Ghose, V. N. Viswanadhan, and J. J. Wendoloski, "A Knowledge-Based Approach in Designing Combinatorial or Medicinal Chemistry Libraries for Drug Discovery. 1. A Qualitative and Quantitative Characterization of Known Drug Databases," J. Comb. Chem., vol. 1, no. 1, pp. 55–68, Jan. 1999, doi: 10.1021/cc9800071.