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Exploring molecular mechanism of *Gymnosporia montana* leaf bioactive as potent *anti-diabetic* agent: Ethnomedicine for drug discovery

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ABSTRACT

Background: *Diabetes mellitus* is a primary contributor to morbidity and death globally. The principal signs of this illness are hyperglycemia, or elevated blood sugar levels, succeeded by polydipsia and polyuria. Retinal degeneration, renal impairment, and neuropathy are instances of future repercussions. Furthermore, diabetes mellitus will expedite the progression of cardiovascular disease. *Gymnosporia montana* (GM), a species of the Celastraceae family, is commonly known as Bharatti and Vikalo. It is a shrub or tree that naturally occurs in dry locations and is common in Maharashtra, Gujarat, and other areas of India. It is widely employed for the management of pain, ulcers, gastrointestinal disorders, dental pain, and dysentery.

Purpose: This study aimed to assess the antidiabetic activity of GM leaf bioactive through in-silico molecular docking.

Method: α -glucosidase was chosen as the target proteins in the current investigation. The bond was found using the Auto Dock software using a grid-based docking method. Compounds' 2D structures were generated, converted to 3D, and subsequently energetically lowered up to an arms gradient of 0.01 using the Merck Molecular Force Field (MMFF).

Result: The synergetic effect of flavonoid, terpenoid and resin found to be effective *anti-diabetic* component and effectively binds to be target protein α -glucosidase with binding energy -7.75, -8.27 & -6.61 kcal mol⁻¹ for α -amyrin, betulin & kaempferol respectively.

Conclusion: The finding of the *in-silico* molecular docking showed that both lead compound is effective binds & inhibitory action on target protein. The molecular docking of ligands like α -amyrin, betulin & kaempferol with α -glucosidase receptor revealed that it has exhibited the chemical interaction with the amino acids in the active pockets.

Keywords: *G. montana*, Molecular docking, *A-glucosidase* enzyme, A-amyrin, Betulin, Kaempferol

Introduction

Diabetes is a metabolic disorder that impacts proteins, lipids, and glucose, caused by diminished insulin production or the emergence of insulin resistance. Chronic hyperglycemia due to diabetes results in the glycation of bodily proteins, leading to secondary problems that negatively impact the kidneys, eyes, nerves, and arteries (Kameswara Rao *et al.*, 1999) [1]. Diabetes is linked to hyperglycemia, dyslipidaemia, and both microvascular and macrovascular problems, which are the primary contributors to morbidity and death in diabetic persons (Virella-Lopes *et al.*, 2003) [2]. Management can be accomplished by pharmacological medicines, dietary alterations, and physical exercise; but, these methods may entail substantial expenses, have adverse consequences, or impose additional constraints (Nagappa *et al.*, 2003; Krishna *et al.*, 2004) [3, 4]. The quest for hypoglycemic agents that are safer and more effective. A range of conditions is collectively referred to as diabetes mellitus. The unique aetiology and/or pathogenesis can define specific diabetes symptoms; nevertheless, overlapping phenotypes in many individuals hinder etiological and pathogenetic categorisation (Leslie, 1997) [5]. *Gymnosporia montana*, belonging to the family Celastraceae, is often known as Baikal in Hindi. It is allegedly advantageous for jaundice, inflammation, rheumatic pain, corneal opacity, ulcers, gastrointestinal disorders, diarrhoea, toothache, and as a vermifuge. It is employed in the management of jaundice, inflammation, and haematological disorders. The use of mature fruit has been recognised for its blood-purifying and anti-inflammatory characteristics. Leaf extract is employed in the therapy of pandu (anaemia) and applied as eye drops to address corneal opacity. Bark is employed to eradicate lice and treat other scalp problems. The application of leaf extract in ocular ailments, namely for corneal opacity, irritation, and burning sensations (Dhru Bhavita *et al.*, 2017) [6].

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***G. montana***

In-silico molecular docking study

Molecular docking is a crucial technique in the development of novel pharmaceuticals. The docking technique allows for the characterisation of a test molecule's behaviour inside the binding site of the target receptor. A docking approach must accurately anticipate the binding

affinity between the ligand and the receptor complex. In computational chemistry, in silico analysis has facilitated the identification of novel active pharmaceuticals with reduced adverse effects. Molecular docking analysis has been utilised to estimate the binding affinities of various bioactive chemicals and to elucidate unique interaction sites between these compounds and target proteins (Mooers, 2020; Paul *et al.*, 2018; Jitender k Malik *et al.*, 2013) [7, 8, 9].

Conceptual work flow of *in-silico* molecular docking

Experimental works

Scientific Validation of Bioactive of

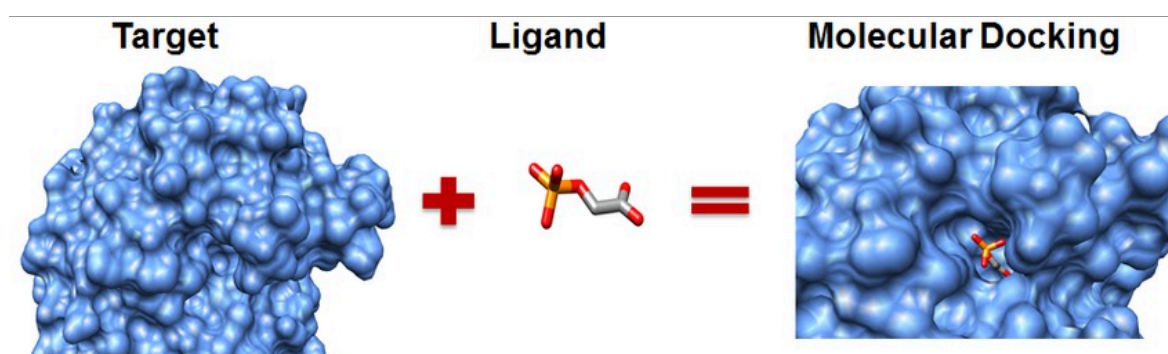
G. montana leaf against Diabetic by Molecular docking

Selection of lead molecule

According to the literature review, several bioactive such as tingenone, 3-*O*-acetyloleanolic acid, hexacosane, hexacosanol, *n*-triactanol, betulin, α -amyrone, α -amyrin, β -sitosterol, celacinnine, and kaempferol have been extracted from the leaves of *Gymnosporia montana* (Kochar *et al.*, 2020) [10]. Betulin is a natural triterpene that has preventive properties against cardiovascular and hepatic disorders, cancer, diabetes, oxidative stress, and inflammation (Adepoju *et*

al., 2023) [11]. Kaempferol is recognised for its antioxidant, anti-cancer, antibacterial, neuroprotective, and hepatoprotective properties (Yu *et al.*, 2013) [12]. Previous investigations have partially validated the analgesic, *anti*-inflammatory, anticonvulsant, antidepressant, gastroprotective, hepatoprotective, antipancreatic, anticholinergic, anti-hyperglycemic, and hypolipidemic properties of α -amyrin (Amaurilio *et al.*, 2018) [13].

Literature indicates that the leaf of *G. montana* is a rich source of phytoconstituents and has been utilised in ethnopharmacological treatment in the past. "The plant comprised a combination of triterpene, flavonoid, and resin, which may exhibit significant anti-diabetic effectiveness; hence, betulin, kaempferol, and α -amyrin were chosen as lead compounds for this study."



Description of lead molecule [14-19]

Selection of target receptors

α -glucosidase

α -glucosidase inhibitors are the most effective medication for managing postprandial hyperglycemia and its adverse physiological consequences, particularly in type 2 diabetes. The enzyme α -glucosidase, which hydrolyses carbohydrates, is often blocked competitively by α -glucosidase inhibitors, leading to delayed glucose absorption in the small intestine and eventually regulating postprandial hyperglycemia

(Hossain *et al.*, 2020) [20]. In current studies, α -glucosidase was chosen as a target molecule involved in the hyperglycaemia.

Molecular docking studies

Ligand Preparation:

2D Structure of amyrin, betulin and kaempferol were drawn using ChemSketch [21], the two-dimensional structure of the prepared ligand and was converted into their 3-D structures optimized with 3D geometry. The optimized structure was saved in PDB format for AutoDock compatibility. The basic structures of the prepared ligand were given below:

Description	<i>Betulin</i>	<i>kaempferol</i>	<i>α-Amyrin</i>
Molecular formula	C ₃₀ H ₅₀ O ₂	C ₁₅ H ₁₀ O ₆	C ₃₀ H ₅₀ O
Synonym	Betulinol	Robigenin	Viminalol
Molecular weight	442.7 g/mol	286.24 g/mol	426.7 g/mol
Pharmacology	Protective against Cardiovascular, liver diseases, cancer, diabetes, oxidative stress and hyperglycemia .	cardioprotective, neuroprotective, hepatoprotective, and <i>anti</i> -diabetic.	antitumor, <i>anti</i> -inflammatory, anxiolytic, and hepatoprotective.

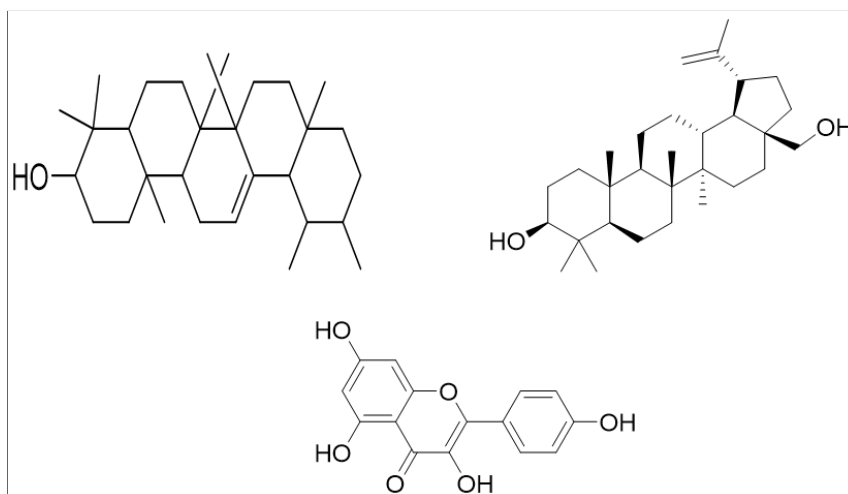


Figure 1. 2D structure of amyrin, betulin and kaempferol

Preparation of the grid file

The regions of interest used by Autodock were defined by considering grid area by making a grid box around the active sites. Grid box plays a central role in process of docking as it is made to cover all the amino acids present in active sites necessary for binding other than

those present in receptor. Grid box has 3 thumbwheel widgets which let us change the number of points in the x, y and z dimensions. The spacing and grid points for all the considered receptors in the current study are given in table 1 (Morris *et al.*, 2009; Soni *et al.*, 2024; Soni *et al.*, 2025) [22, 23, 24].

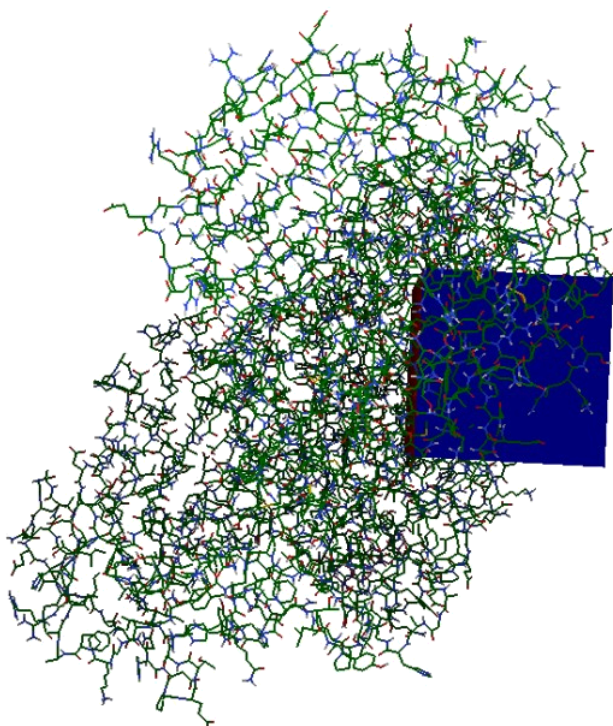


Figure 2. Grid box covering all active sites in α -glucosidase receptor

Preparation of the docking file

All the calculations were carried out by using Autodock 4.2 as docking tool. The visualization and other programs necessary for docking studies were performed out by means of Pymol, Chimera, DS visualizer, MMP Plus (Soni *et al.*, 2024; Soni *et al.*, 2022; Soni *et al.*, 2020) [25, 26, 27].

Docking study

Crystal structure

The crystal structure of the protein consisting of α -glucosidase receptors were downloaded from the Protein Data Bank portal. All the primary information regarding all the receptor's structure was registered in the Protein data bank (Soni *et al.*, 2020; Soni *et al.*, 2019; Soni *et*

al., 2014; Soni *et al.*, 2025) [28, 29, 30, 31]. The complex ligand was separated by using Chimera software for all the target receptors.

Table 1. Grid parameters used in current docking analysis of α -glucosidase

S. No.	Receptor	x-axis	y-axis	z-axis	Spacing	x center	y center	z center
1	α -glucosidase	50	50	50	0.458	15.255	26.418	12.753

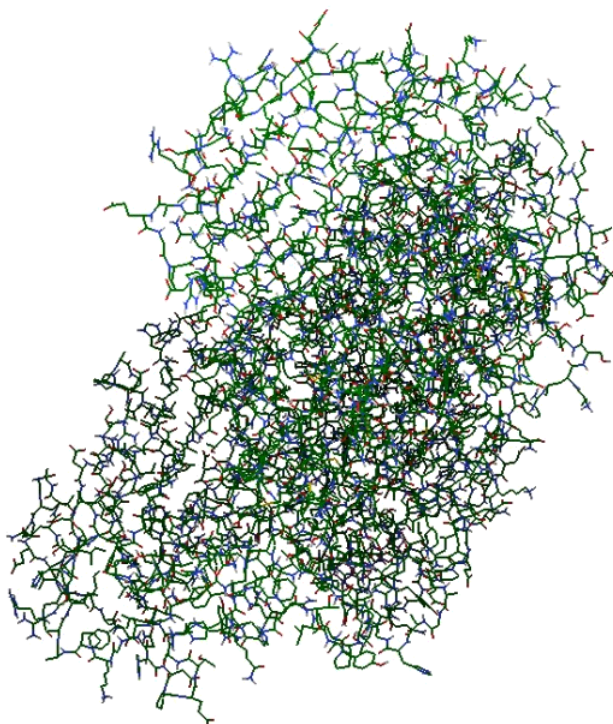


Figure 3. Crystal structure of α -glucosidase receptor (PDB ID-7kb6)

Processing of Protein

All the downloaded receptor proteins are having only one chains, i.e. chain A, which has been selected for experimental purpose and complex ligand was removed from it. The bound ligand was separated from the macromolecular complex by using software Chimera (Soni *et al.*, 2011; Kciuk *et al.*, 2022) [32, 33].

Molecular docking simulation studies

Docking of ligands like amylin, betulin and kaempferol against α -glucosidase receptor was performed by Autodock. All the bonds of each ligand were kept flexible, while no residues in receptor were made flexible (Kciuk *et al.*, 2022; Soni *et al.*, 2025) [34, 35].

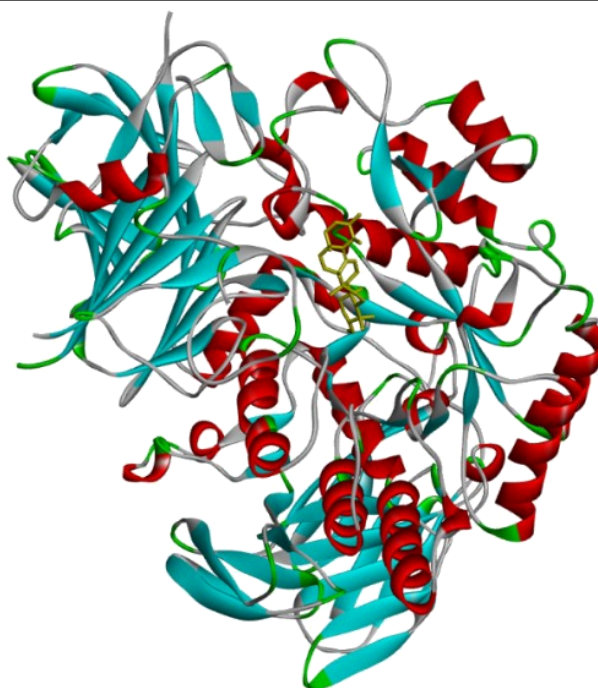


Figure 4. Binding mode of amylin within the active site of α -glucosidase receptor

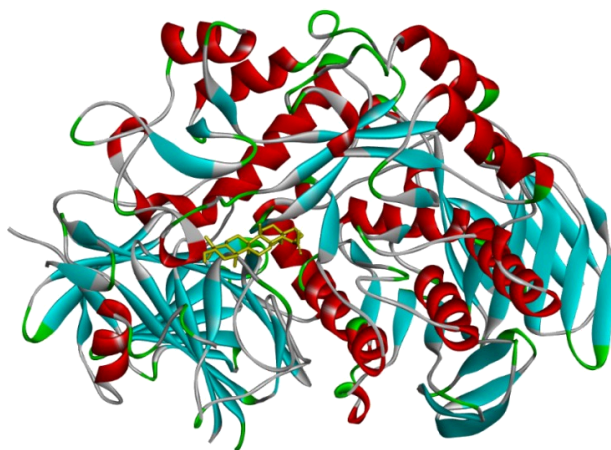


Figure 5. Binding mode of betulin within the active site of α -glucosidase receptor



Figure 6. Binding mode of kaempferol within the active site of α -glucosidase receptor

Toxicity & ADME-T studies

The ligand molecules viz. amylin, betulin and kaempferol were studied by online program OSIRIS, for prediction of presence of any toxic group as well as presence of any toxic group and ADME-T properties [36].

Result and Discussion

Diabetes mellitus (DM) is a chronic metabolic condition of carbohydrates characterised by disrupted glucose homeostasis and elevated blood glucose levels. *Diabetes mellitus* (DM) is recognised as one of the most hazardous diseases of the twenty-first century globally. A range of oral hypoglycemic medications has been utilised in clinical practice to address this disease. These pharmaceuticals, classified into many categories, include α -glucosidase inhibitors, biguanides, sulfonylureas, thiazolidinediones (TZD), meglitinides, and dipeptidyl peptidase (IV) inhibitors. Each class concentrates on a certain organ type and operates uniquely. In practice, several combinations of *anti*-diabetic drugs are commonly utilised to improve treatment efficacy. Although these medicines offer various advantages, extended use may also result in long-term adverse consequences, such as cardiovascular disease, lactic acidosis, hypoglycemia, gastrointestinal issues, among others. Molecular docking tests have been performed to evaluate these natural chemicals as potential innovative *anti*-diabetic drugs with low long-term side effects, comparing their efficacy to that of current commercial *anti*-diabetic medications. Molecular docking is

an essential computational technique for forecasting possible drug-protein interactions, which entails the selection of a ligand representing a bioactive chemical sourced from medicinal plants. Regulating postprandial plasma glucose concentrations is essential for the early treatment of diabetes mellitus. An effective medication for mitigating postprandial hyperglycemia involves the inhibition of enzymes responsible for carbohydrate metabolism. Natural compounds provide a more reliable means of inhibition than synthetic medications. The principal enzymes that catalyse the hydrolysis of carbohydrates and promote glucose absorption into the circulation are α -amylase and α -glucosidase. Synthetic drugs that obstruct α -amylase and α -glucosidase comprise acarbose, miglitol, and voglibose. These medications have special drawbacks, since they are nonspecific and may cause considerable adverse effects, including gastrointestinal discomfort and worsening of diabetic problems. Herbal products have recently gained prominence as supplementary and alternative therapies for the treatment of diabetes mellitus. *Gymnosporia montana* (GM), a member of the Celastraceae family, is often referred to as Bharatti and Baikal. It is a shrub or tree that grows naturally in arid regions and is prevalent in Maharashtra, Gujarat, and other parts of India. It is extensively utilised for the treatment of soreness, ulcers, gastrointestinal ailments, toothache, and dysentery. “The current investigation focused on the plant’s abundant bioactive compounds, noting that less research has been conducted on it previously. The current work aims to clarify the suggested antidiabetic mechanism of *G. montana* leaf bioactive using *in-silico* molecular docking targeting the α -glucosi

dase enzymes". The literature analysis indicates that *G. montana leaf* is a rich source of flavonoid, terpene and resin. As a result, kaempferol (flavonoid), betulin (triterpenoid), betulin (triterpenoid) and α -amyrin (resin) were chosen as lead compounds against α -glucosidase enzymes. The results of the current investigation indicated that the selected lead molecules serve as effective in treating and preventing hyperglycemia, binding to the target protein of α -glucosidase with binding energies of -7.75, -8.27 & -6.61 kcal/mol for α -amyrin, be-

tulin and kaempferol respectively. The outcome was recorded in Table 2. The binding mode of lead molecules against α -glucosidase showed in fig 4-6 The two-dimensional and three-dimensional interactions of the selected chemical are illustrated in Figures 7-12. The affinity of lead compounds for the receptor was determined to be relatively comparable. The interaction of lead molecules with the active site of α -glucosidase was illustrated as follows:

Compound	Binding against α -glucosidase							
	Conventional Hydrogen bonding	π -alkyl	Alkyl	Week Vander's interaction	π -Anoin	π - σ	Sulfur-X	π - π stacked
<i>α-amyrin</i>	Asp640	Phe571 Phe674 Trp523 Trp525 Trp423 His700	-----	ASN572 Met565 Phe673	-----	Phe307	----	----
<i>betulin</i>	Asp305	Val576 Phe307 His700 Phe674 Trp423	Trp525	Ser569 Met565 Tyr318 Asp640 Phe673	-----	Phe525	----	-----
<i>kaempferol</i>	Asp305 His700 Asp451	-----	-----	Phe571 Ser569 ILE452 ILE488 Trp562 His698 Trp423	Asp564 Asp640	----	Met565	Phe673 Phe307

The interaction results indicated that lead molecules attach at comparable positions by typical hydrogen, alkyl, π -alkyl, π - σ and van der waal's interactions, demonstrating a synergistic effect of both compounds from *G. montana leaf* in exerting protective action on diabetic.

The pharmacokinetic profile indicates a favourable pharmacokinetic profile; however, it also presents significant hazardous consequences, including mutagenicity, tumorigenicity, and reproductive toxicity. The pharmacokinetic and toxicity profiling data of ligands such as α -amyrin, betulin and kaempferol are presented in Figures 13-15 and Tables 3-5. All ligand compounds have demonstrated promising docking scores theoretically.

Finding of investigation

The aforementioned finding demonstrated the antidiabetic efficacy of *G. montana leaf*. The scientific confirmation of the antidiabetic effect of leaf bioactive was conducted using *in-silico* molecular docking. The chosen lead compounds, α -amyrin, betulin, and kaempferol, were directed towards the α -glucosidase enzymes to clarify their antidiabetic mechanisms of action. The results indicated that -amyrin, betulin and kaempferol had significant inhibitory effects on chosen targets. The findings of the present investigation revealed that the *G. montana leaf* had antidiabetic effects, particularly in type 2 diabetes. The present investigation proven the folklore uses of GM leaf led to discovery antihyperglycemic potential of bioactive.

Divulgence of Investigation

The proposed mechanism of action of *G. montana leaf* bioactive displayed in following manner:

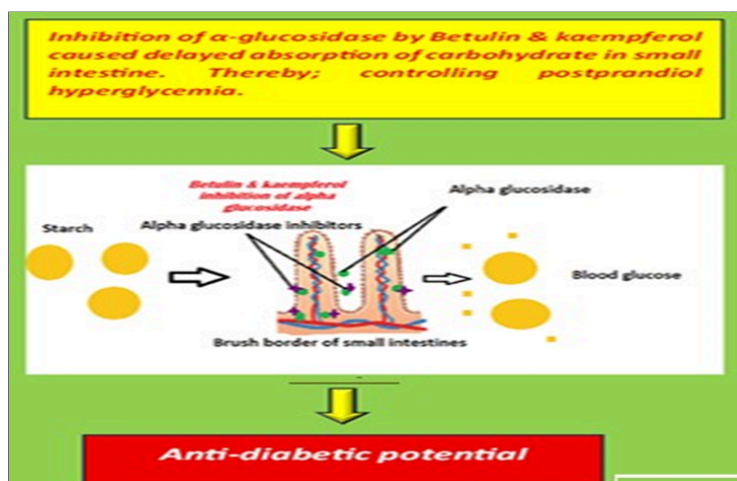
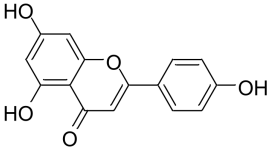
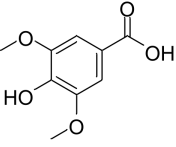
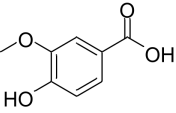
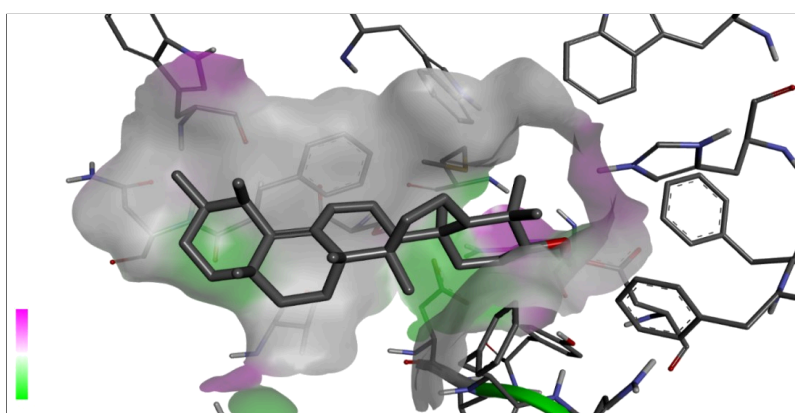
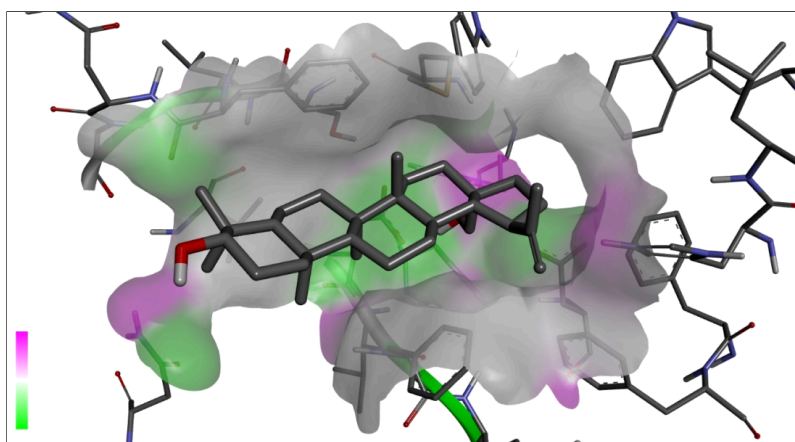


Table 2. Results of docking of ligands like amyirin, betulin and kaempferol against α -glucosidase receptor

S. No.	Compound Name	Structure	α -glucosidase
1	α -Amyrin		-7.75
2	Betulin		-8.27
3	Kaempferol		-6.61

**Figure 7.** Three-dimensional binding mode of amyirin within the active site of α -glucosidase receptor**Figure 8.** Three-dimensional binding mode of betulin within the active site of α -glucosidase receptor

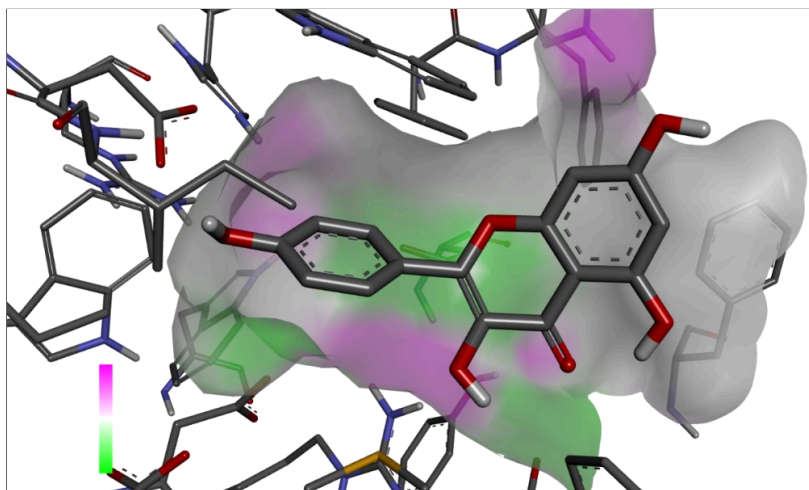


Figure 9. Three-dimensional binding mode of kaempferol within the active site of α -glucosidase receptor

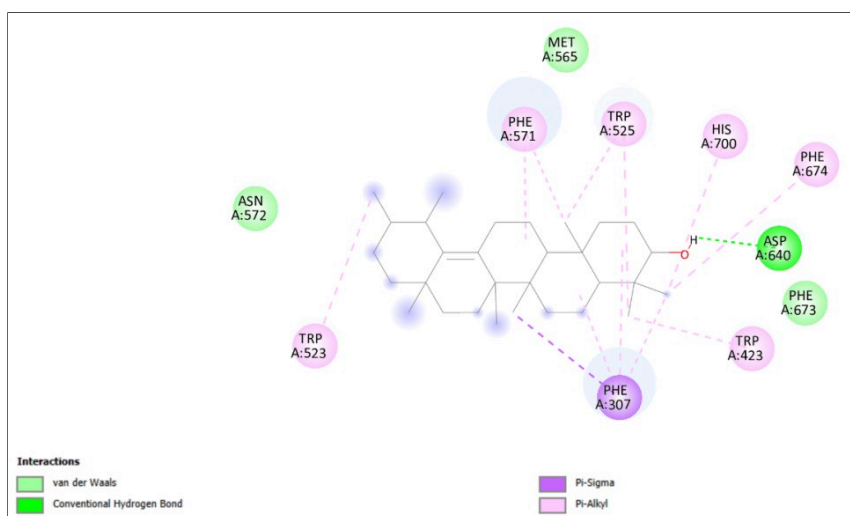


Figure 10. Two-dimensional binding mode of amylin within the active site of α -glucosidase receptor

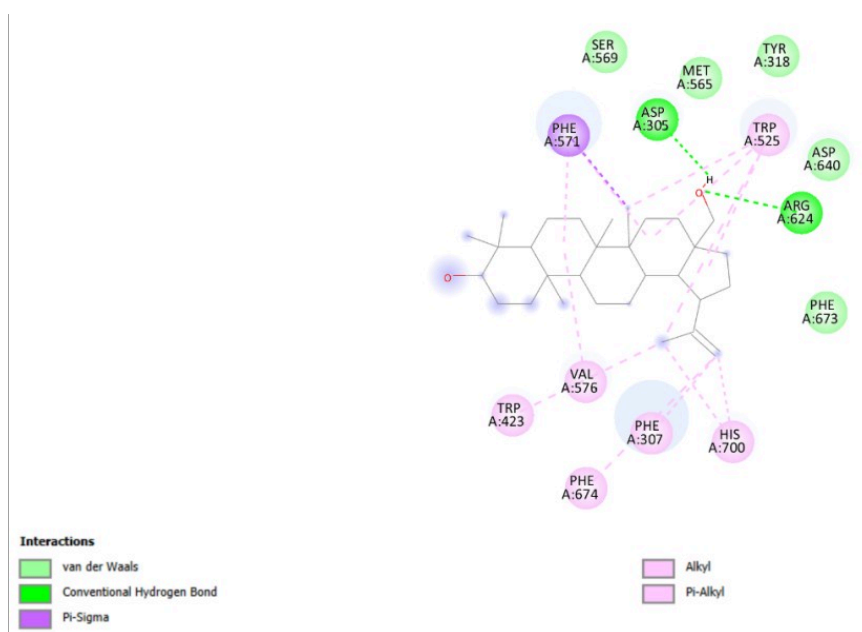


Figure 11. Two-dimensional binding mode of betulin within the active site of α -glucosidase receptor

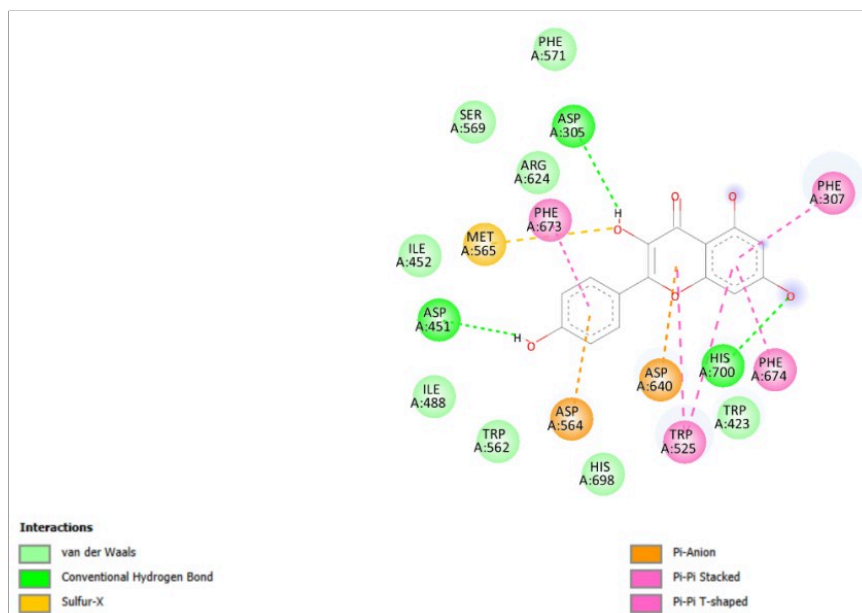


Figure 12. Two-dimensional binding mode of kaempferol within the active site of α -glucosidase receptor

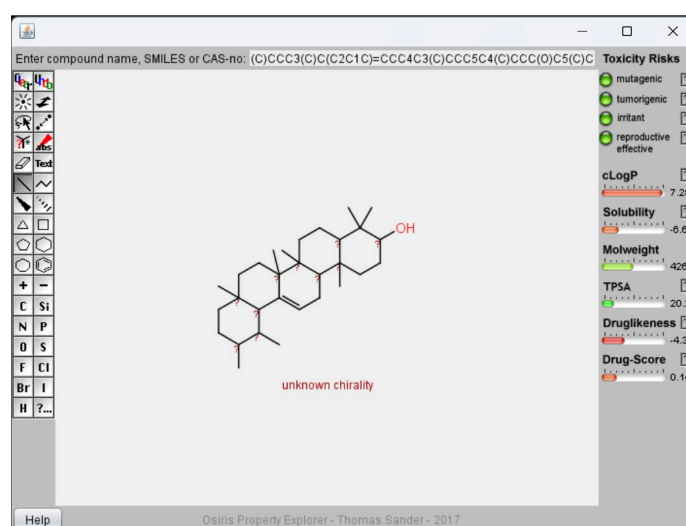


Figure 13. Pharmacokinetic and toxicity profiling of α -amyrin

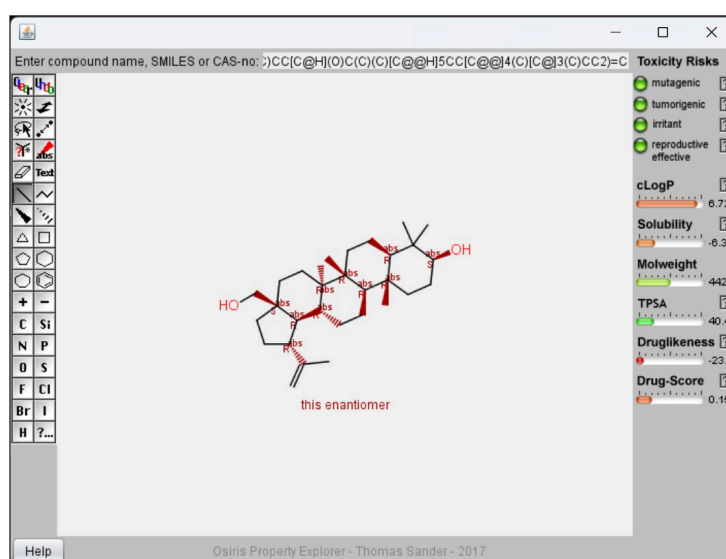


Figure 14. Pharmacokinetic and toxicity profiling of betulin

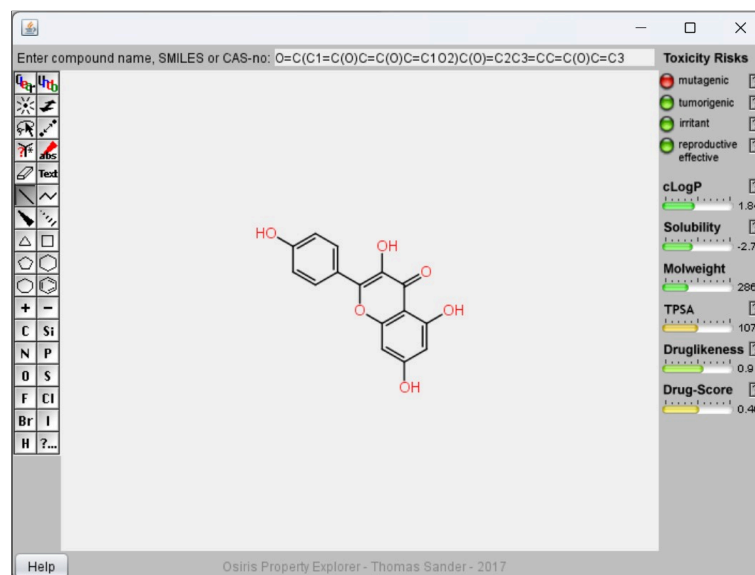


Figure 15. Pharmacokinetic and toxicity profiling of kaempferol

Table 3. Pharmacokinetic Profiling of lead molecules

Compound	ADMET			
	Mutagenic	Tumorigenic	Irritant	Reproductive effectivity
Betulin	NO	NO	NO	NO
Kaempferol	NO	NO	NO	NO
A-amyrin	NO	NO	NO	NO

Table 4. Lipinski Properties of lead molecules

Compound	cLogP	Solubility	Mol.wt.	TPSA	Drug likeness	Drug score
α -amyrin	7.28	-6.64	426	20.23	-4.37	0.14
Betulin	6.72	-6.3	442	40.46	-23.95	0.15
Kaempferol	1.84	-2.79	286	107.2	0.9	0.46

Table 5. Drug likeness of lead molecules

Compound	Lipinski rule of five	H bond donar (< 5)	H bond acceptor (< 10)
Betulin	Yes	2	2
Kaempferol	Yes	4	6
α -amyrin	Yes	1	1

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