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Original Research Article

Probing the Potential of Flavonoids of *Stigma maydis* as an Inhibitor for Lifestyle Diseases: Molecular Docking-Based Approach

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Abstract

Background: *Stigma maydis* are becoming more popular as a healthy substitute for people with lifestyle disorders. They offer dietary fiber, polyphenols, minerals, vitamins, protein, and antioxidants. The evidence that is now available indicates that the leading causes of sickness, disability, and death in India are chronic obstructive and mental disorders, hypertension, cardiovascular illnesses, cancer, diabetes, lung disease, chronic renal disease, trauma, and stroke. When it comes to treating the illness and its repercussions, allopathic medications are not very effective. However, how the *Stigma maydis*-derived chemical compounds work in treating diabetes remains unclarified. Herein, we integrate molecular docking and network pharmacology to elucidate the active constituents and potential mechanisms of *Stigma maydis* against diabetes. ***Purpose:*** This study aimed to validate the antidiabetic effect of *Stigma maydis* silk lead molecule through *in-silico* molecular docking. ***Method:*** α-amylase was chosen as the target proteins in the current investigation of antidiabetic effect respectively. 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:*** Maysin and isoorientin found to be effective component for anti-diabetic potential and effectively binds to be target protein α-amylase with binding energy-8.11 & -5.96 kcal/mol respectively and showed potent inhibitory action on target proteins. ***Conclusion:*** The results of the current investigation demonstrated that the chosen lead molecule (Maysin and isoorientin) had significant inhibitory effects on the selected target proteins, consequently showed potent antidiabetic efficacy. The molecular docking analysis demonstrated significant binding energy.

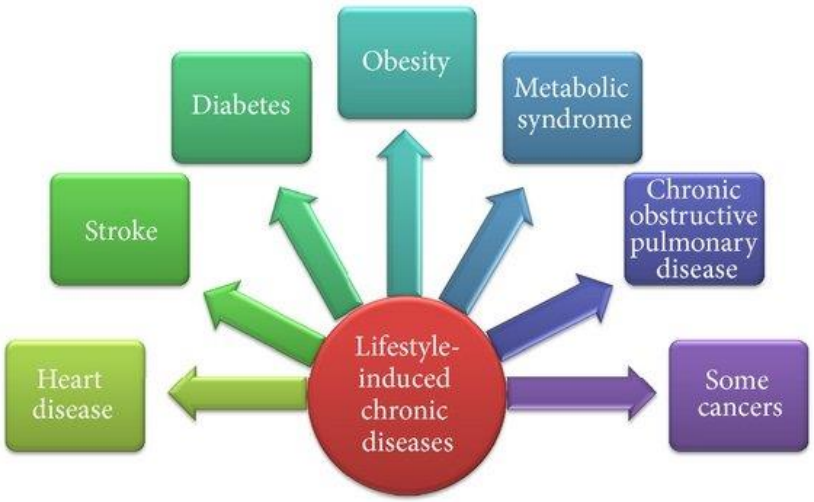
Keywords: *Stigma maydis* silk (corn silk) α-amylase, Maysin isoorientin & molecular docking.

INTRODUCTION

About 40 million people die from non-communicable diseases (NCDs) annually, accounting for about 70% of all fatalities worldwide1. The chronic nature of NCDs makes them unable to spread from one individual to another. They are caused by a confluence of environmental, behavioral, physiological, and genetic variables. In addition to cancer, the two primary categories of NCDs include chronic respiratory and cardiovascular conditions. Because of their strong correlation with lifestyle choices, NCDs include cardiovascular diseases (CVD), stroke, diabetes, and some types of cancer are sometimes referred to as lifestyle diseases [1].

Diabetes mellitus (DM)

The most prevalent endocrine condition, diabetes mellitus (DM), affects over 100 million people globally, or 6% of the population. It is brought on by insufficient or inefficient insulin production by the pancreas, which causes blood glucose levels to rise or fall. Numerous bodily systems, including the blood vessels, eyes, kidney, heart, and nerves, are shown to be harmed by it. [2]. Insulin-dependent diabetes mellitus (IDDM, Type I) and non-insulin-dependent diabetes mellitus (NIDDM, Type II) are the two categories of diabetes mellitus. In contrast to Type II diabetes, which is defined by peripheral insulin resistance and decreased insulin production, Type I diabetes is an autoimmune illness that is characterized by a local inflammatory response in and around islets, followed by the selective death of cells that secrete insulin. [3]. The presence of DM shows increased risk of many complications such as cardiovascular diseases, peripheral vascular diseases, stroke, neuropathy, renal failure, retinopathy, blindness, amputations etc. [4].



Various Lifestyle induced chronic diseases

Epidemiology

In 2011, it was predicted that 366 million individuals had diabetes mellitus; by 2030, this number is projected to increase to 552 million. The prevalence of type 2 diabetes mellitus is rising globally, with 80% of affected individuals residing in low- and middle-income nations. Diabetes mellitus resulted in 4.6 million fatalities in 2018. It is projected that 439 million individuals would have type 2 diabetes mellitus by the year 2030.The prevalence of type 2 diabetes mellitus significantly differs among geographical regions due to environmental and behavioural risk factors [5]. The incidence of type 2 diabetes mellitus (DM) among adults is anticipated to rise during the next two decades, predominantly in emerging nations, where most patients are aged between 45 and 64 years [6]. NCDs include cardiovascular diseases (CVD), stroke, diabetes, and some types of cancer are sometimes referred to as lifestyle diseases. Corn, or Maize, is among the most prevalent cereal grains globally. Members of the Poaceae family, often known as grasses, have several advantages as a carbohydrate source.

Stigma maydis

The chemical makeup of maize silk is notably varied. The substances extracted and classified from maize silk may primarily be categorised into six types: flavonoids, polyphenols, sterols, terpenoids, amino acids, and organic acids [7-9]. Flavonoids constitute the primary chemical constituents of maize silk, comprising flavonoid glycosides, flavonols, and isoflavones. Apigenin, luteolin, robinin, and chrysoeriol possess similar mother nucleus structures. Recent phytochemical research on maize silk indicates the identification of 80 flavonoid components, including luteolin, apigenin, maysin, and other O-glycosides and C-glucosides of flavonoids [10]. Corn silk is commonly utilised in everyday life for the enhancement of cardiovascular disorders, diabetes, Alzheimer's disease, hyperuricemia, chronic nephritis, and several other ailments [11-15].

Experimental work

Selection of lead molecule from Corn silk

A multitude of investigations has demonstrated that flavonoids can proficiently impede obesity and associated metabolic diseases. The anti-obesity actions of flavonoids arise from their regulation of proteins, genes, and transcription factors that reduce lipogenesis, enhance lipolysis, increase energy expenditure, stimulate β-oxidation of fatty acids, and facilitate the digestion and metabolism of carbohydrates. Furthermore, it alleviates inflammatory reactions and diminishes oxidative stress [16]. According to the literature review, flavonoids are the primary chemical constituents of maize silk, comprising flavonoid glycosides, flavonols, and isoflavones. Apigenin, luteolin, robinin, and chrysoeriol possess similar mother nucleus structures. In recent years, 80 flavonoid compounds have been documented, including luteolin, apigenin, maysin, isoorientin, and other O-glycosides and C-glucosides of flavonoids [17-18]. Prior studies have demonstrated that maysin suppresses the expression of genes associated with adipocyte differentiation, fat deposition, and fat

synthesis, while promoting the expression of genes related to lipolysis and fat oxidation, hence further decreasing body fat formation and weight gain [19]. Numerous studies have demonstrated that isoorientin enhances obesity-related insulin resistance *in-vitro* by improving glucose absorption, metabolic activity, mitochondrial energetics, and inhibiting lipid accumulation [20]. Maysin and isoorientin were chosen as lead molecules for the evaluation of their anti-diabetic and anti-obesity potential in the current study.

Selection of Target ligands

The alpha (α)-amylase is a calcium metalloenzyme that aids digestion by breaking down polysaccharide molecules into smaller ones such as glucose and maltose. In addition, the enzyme causes postprandial hyperglycaemia and blood glucose levels to rise. α-Amylase is a well-known therapeutic target for the treatment and maintenance of postprandial blood glucose elevations. Various enzymatic inhibitors, such as acarbose, miglitol and voglibose, have been found to be effective in targeting this enzyme, prompting researchers to express an interest in developing potent alpha-amylase inhibitor molecules [21].

Molecular docking studies

Ligand Preparation:

2D Structure of maysin and isoorientin were drawn using ChemSketch [22], the two-dimensional structure of the prepared ligand 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:

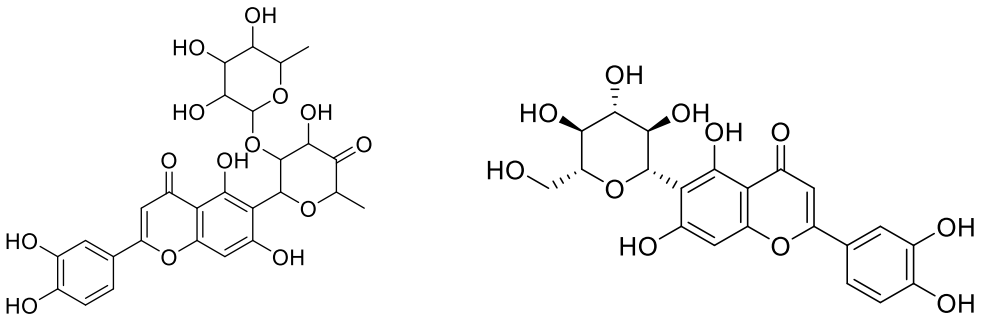


Figure 1: 2D structure of maysin and isoorientin

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 [23-24].

Table 1: Grid parameters used in current docking analysis of GSK3β, Alpha amylase, α-amylase and α-glucosidase

S. No.	Receptor	x-axis	y-axis	z-axis	Spacing	x center	y center	z center
1	alpha amylase	40	40	40	0.431	62.103	15.687	18.204

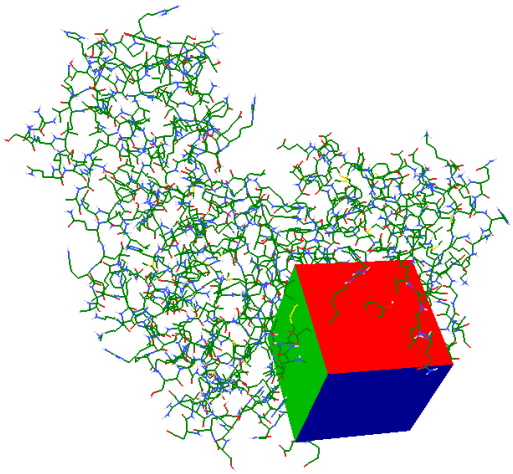


Figure 2: Grid box covering all active sites in alpha amylase receptor

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 [25-27].

Docking Study

Crystal structure

The crystal structure of the protein consisting of alpha amylase receptor is downloaded from the Protein Data Bank portal. All the primary information regarding all the receptor's structure was registered in the Protein data bank [28-30]. The complex ligand was separated by using Chimera software for all the target receptors.

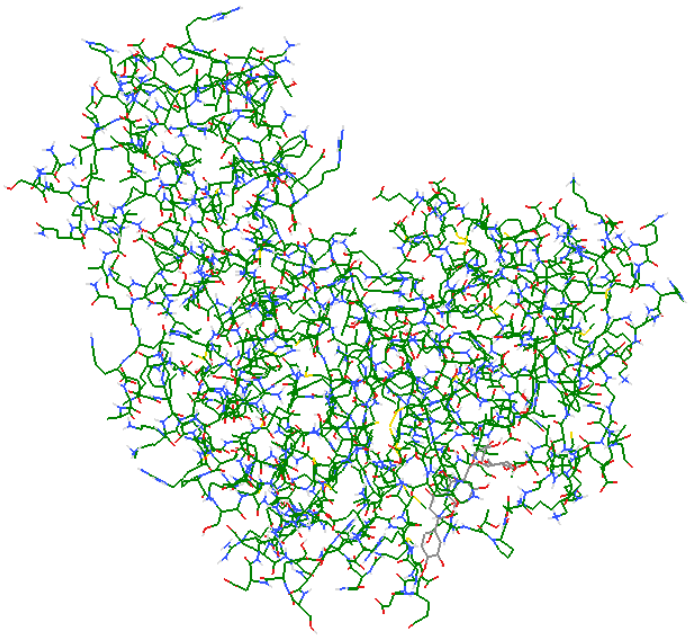


Figure 3: Crystal structure of alpha amylase receptor (PDB ID-4ixc)

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 [31-32].

Molecular Docking Simulation Studies

Docking of ligands like maysin and isoorientin against alpha amylase receptor was performed by Autodock. All the bonds of each ligand were kept flexible, while no residues in receptor were made flexible [33-37].

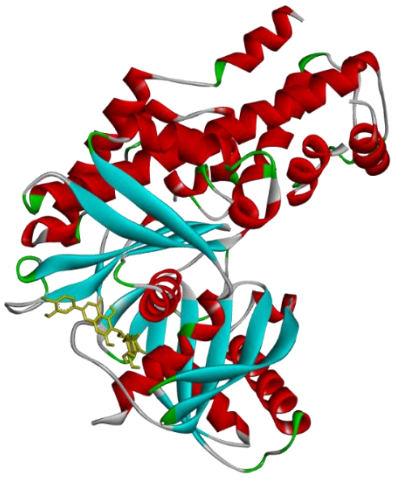


Figure 4: Binding mode of maysin within the active site of alpha amylase receptor

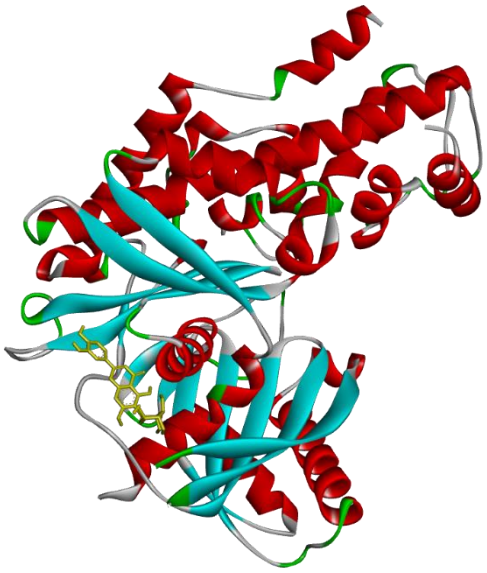


Figure 5: Binding mode of isoorientin within the active site of alpha amylase receptor

Toxicity & ADME-T Studies

The ligand molecules viz. maysin and isoorientin 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 [38].

RESULT AND DISCUSSION

Lifestyle illnesses are ailments predominantly attributable to an individual's everyday habits. Habits that inhibit physical exercise and promote a sedentary lifestyle can lead to several health issues, including potentially fatal chronic non-communicable illnesses. They cannot be transmitted from one individual to another. Our susceptibility to several diseases is influenced by our lifestyle, genetics, and environment. Non-communicable illnesses and injuries constitute 52% of fatalities in India. It is expected that without significant government intervention to prevent and manage non-communicable diseases (NCDs) and their risk factors, the prevalence of NCDs and subsequent mortality would increase. Current data reveals that the primary causes of morbidity, disability, and mortality in India are chronic obstructive pulmonary disease, mental disorders, hypertension, cardiovascular diseases, cancer, diabetes, pulmonary disease, chronic renal disease, trauma, and stroke. Allopathic drugs are largely ineffective in treating the condition and its consequences. Consequently, focus has switched to the traditional medical system. The increasing prevalence of lifestyle illnesses in India and the examination of herbal-based nutraceuticals as adjunct or alternative therapeutic strategies. It underscores the necessity of a comprehensive strategy for addressing chronic diseases, recognising the efficacy of ancient medicines in conjunction with contemporary therapy. The essay specifically discusses numerous critical points. It elucidates the increasing incidence of lifestyle disorders in India, offering a comprehensive overview of the present health scenario. Furthermore, it presents the notion of herbal-based nutraceuticals and their prospective advantages in the management of certain disorders, providing alternative remedies. Flavonoids function as antioxidants that regulate oxidative stress in the body by neutralising the effects of nitrogen and oxygen species, hence avoiding illness. The antidiabetic properties of flavonoids facilitate the modulation of carbohydrate metabolism, insulin signalling, insulin release, glucose absorption, and adipose tissue accumulation. They aim at several molecules that regulate many pathways, such as enhancing β-cell proliferation, stimulating insulin secretion, decreasing apoptosis, and ameliorating hyperglycemia *via* modulating glucose metabolism in the liver. The possible antioxidant and therapeutic applications of *Stigma maydis* include its use as a diuretic agent, in the reduction of hyperglycemia, and as an antidepressant and anti-fatigue agent, as reported in many studies. Corn silk is also utilised in teas and supplements for the treatment of urinary issues. The prospective use is closely associated with the characteristics and mechanisms of action of the plant's bioactive ingredients, including flavonoids and terpenoids. Considering the pharmacological potential and the plethora of phytochemicals in Stigma maydis, this study aims to clarify the mechanism of flavonoids discovered in Stigma maydis in relation to lifestyle illnesses, particularly diabetes. According to the literature review, flavonoids are the primary chemical constituents of maize silk, comprising flavonoid glycosides, flavonols, and isoflavones. Maysin and isoorientin were chosen as lead molecules for the *in-silico* validation against *α-amylase* of their anti-diabetic and anti-obesity potential in the current study. α-Amylase is a well-known therapeutic target for the treatment and maintenance of postprandial blood glucose

elevations. Expression of the pancreas and saliva α-amylases is responsible for converting polysaccharides such as starch. The molecular docking results are presented in Table 2, indicating binding energies of maysin and isoorientin -8.11 and -5.96 kcal/mol for α-amylase respectively. The binding mode is illustrated in figures 4-5. The 3D and 2D binding interactions displayed in fig 6-9. The chosen lead compounds had favorable interactions with the selected ligand. The binding interactions of lead molecules are as follows:

Lead molecule	Vander waal's intraction	Conventional Hydrogen bonding	CH bonding	Pi-donar H bond	π-π stacked	π-Alkyl	π-Sulfur
Maysin	Glu221 Pro66 Tyr215 Met210 Met235	Gly68 Glu67 Leu451	Thr65 Typ99	Tyr214	-----	Val62 ILE211 Val452 Val455 His218	------
Isoorientin	Met210 ILE 24 Ala454 Tyr215	Gly68 Glu67 Glu221 Leu451	His218 Arg250 Ser64	-----	Tyr214	Val 455	Met235

The pharmacokinetic analysis of the lead molecule indicates a favorable pharmacokinetic profile, devoid of significant adverse consequences such as reproductive toxicity, irritating characteristics, tumorigenicity, and mutagenicity. The pharmacokinetic and toxicity profiling data of the lead compound are presented in Figures 10-11 and Tables 3-5.

Summary and Conclusion

The incidence of lifestyle illnesses, such as type II diabetes, malignancies, obesity, cardiovascular ailments, and liver cirrhosis, is rising tremendously. The primary causes of these illnesses encompass an unhealthy lifestyle characterised by several variables, including smoking, alcohol use, tobacco use, a sedentary lifestyle, and stress. The contemporary shift towards the use of herbal medicines in various healthcare domains necessitates the substitution of synthetic compounds with phytoconstituents due to their biocompatibility, biodegradability, cost-effective extraction methods, and accessibility from natural sources. *Corn silk* (CS) is the component of corn shown to possess medicinal and therapeutic properties. It contains secondary metabolites such as flavonoids, proteins, vitamin K, calcium, magnesium, volatile oils, and tannins. The results of the current inquiry indicated that scientific validation of chosen flavonoids from corn silk shown substantial inhibitory potential against α-amylase using *in-silico* molecular docking.

Divulgence of Current Investigation

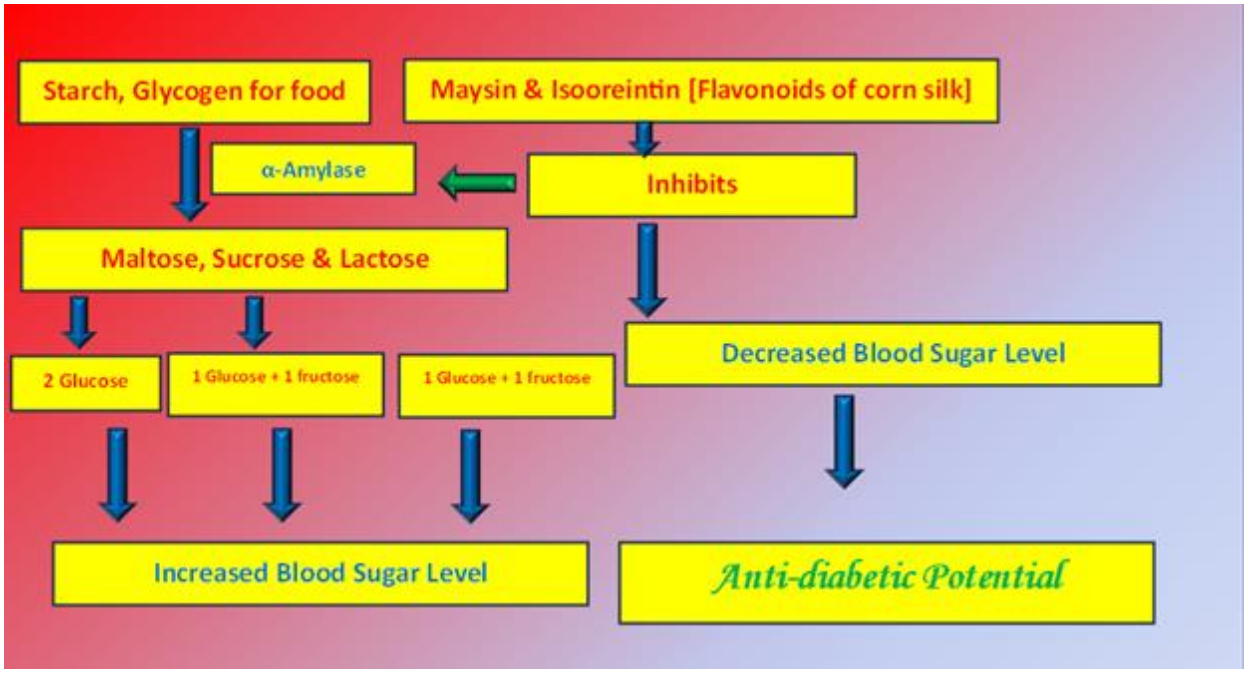
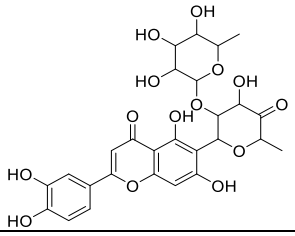
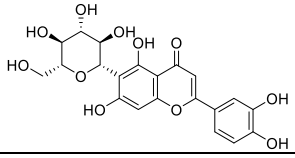


Table 2: Results of docking of ligands like maysin and isoorientin against alpha amylase receptor

S. No.	Compound Name	Structure	alpha amylase
1	Maysin		-8.11
2	Isoorientin		-5.96

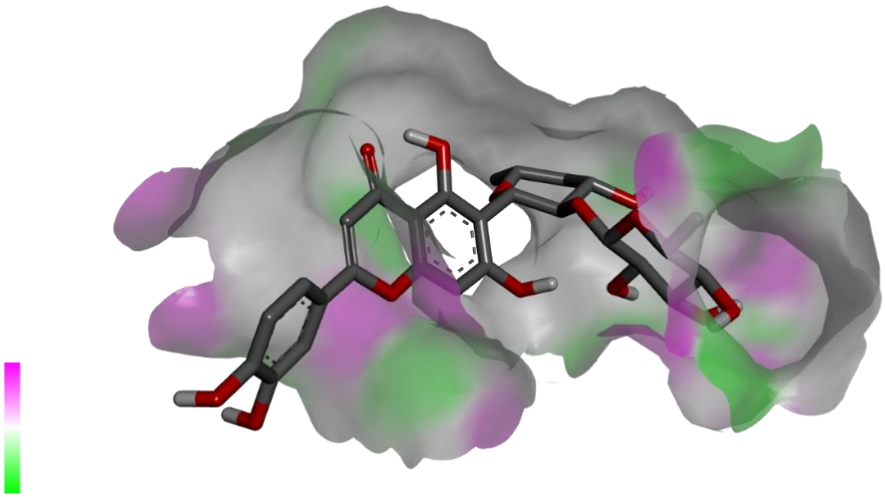


Figure 6: Three-dimensional binding mode of maysin within the active site of alpha amylase receptor

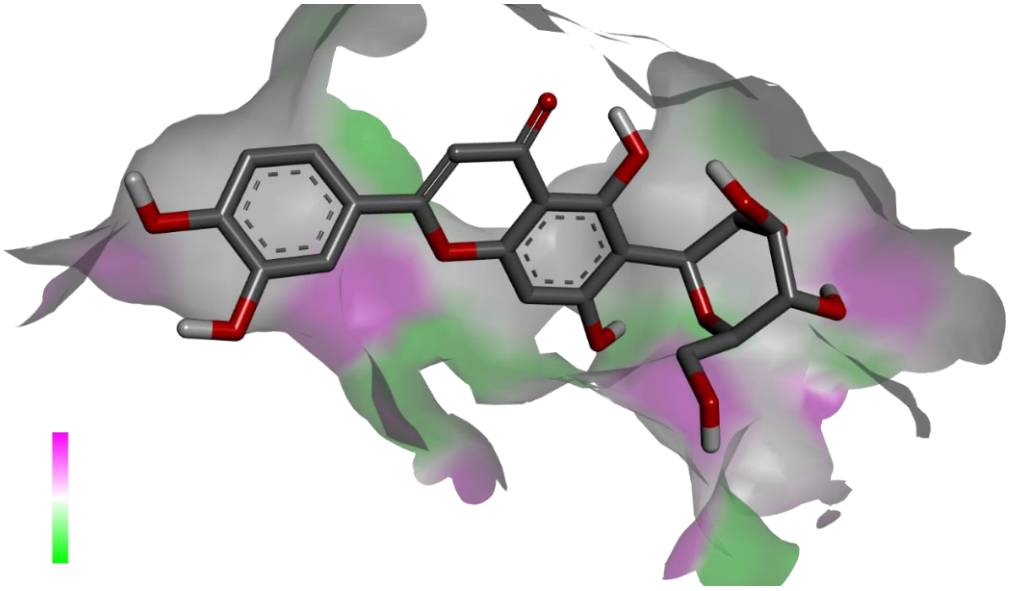


Figure 7: Three-dimensional binding mode of isoorientin within the active site of alpha amylase receptor

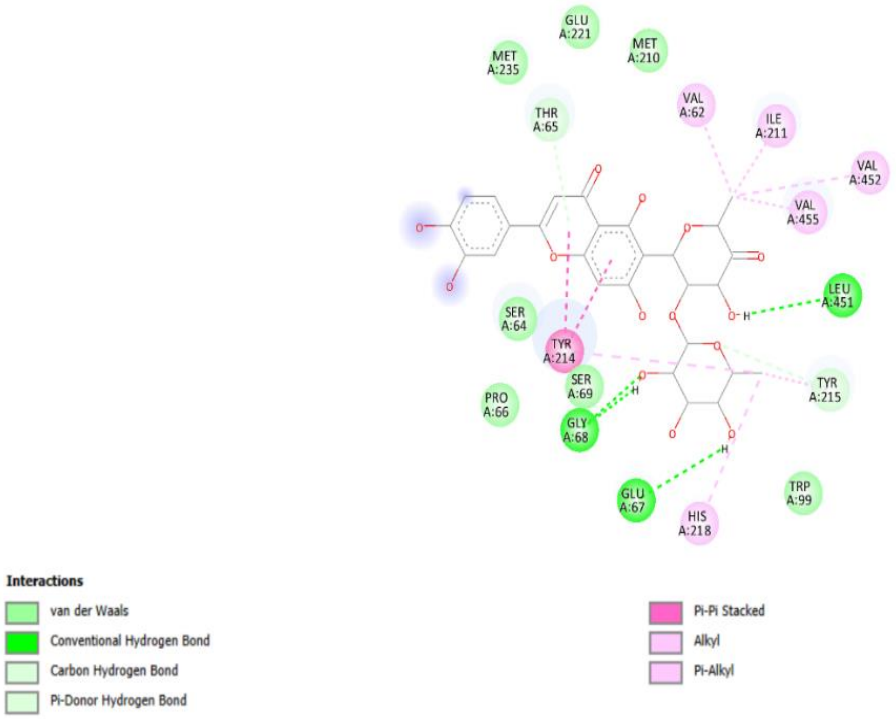


Figure 8: Two-dimensional binding mode of maysin within the active site of alpha amylase receptor

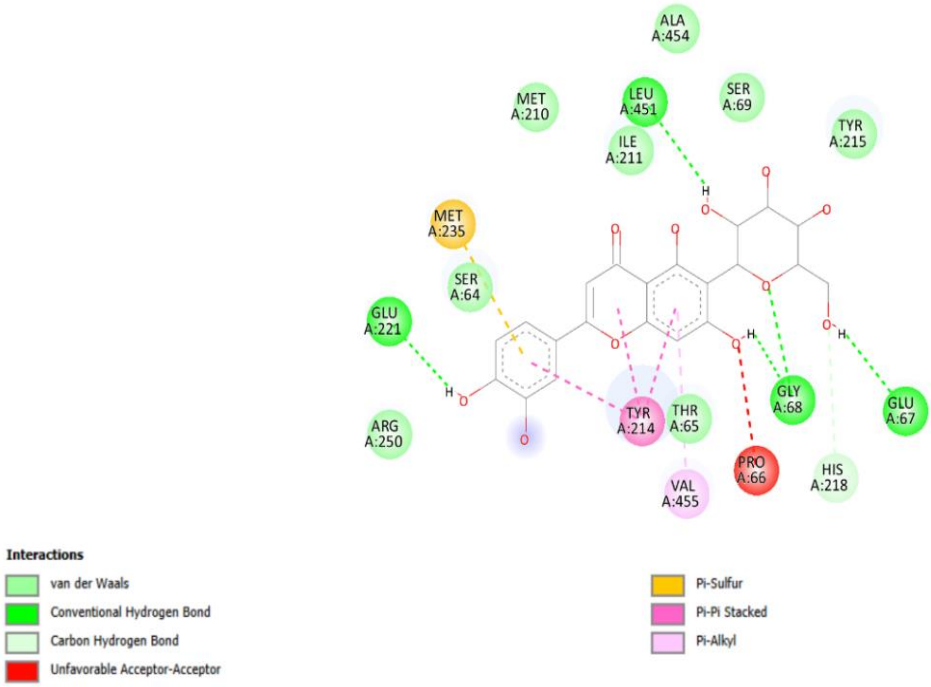


Figure 9: Two-dimensional binding mode of isoorientin within the active site of alpha amylase receptor

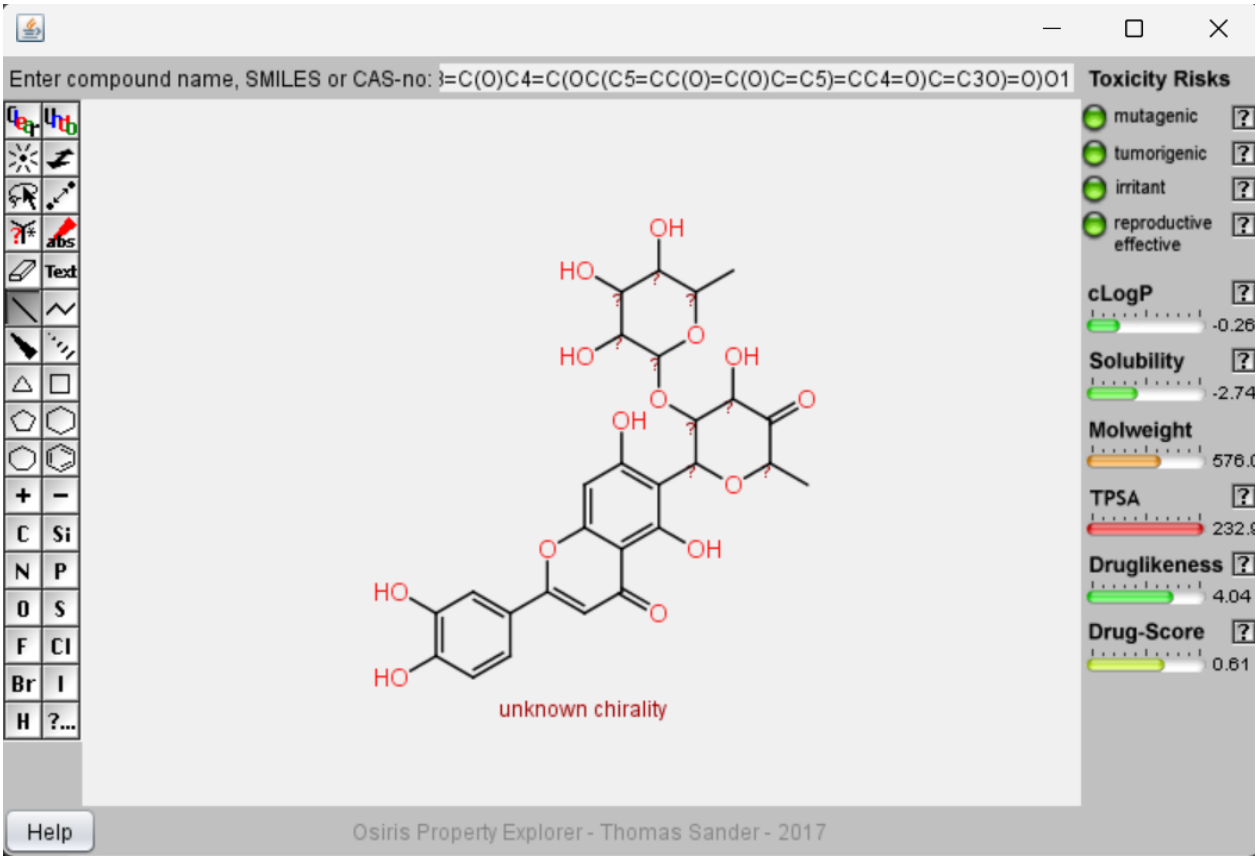


Figure 10: Pharmacokinetic and toxicity profiling of maysin

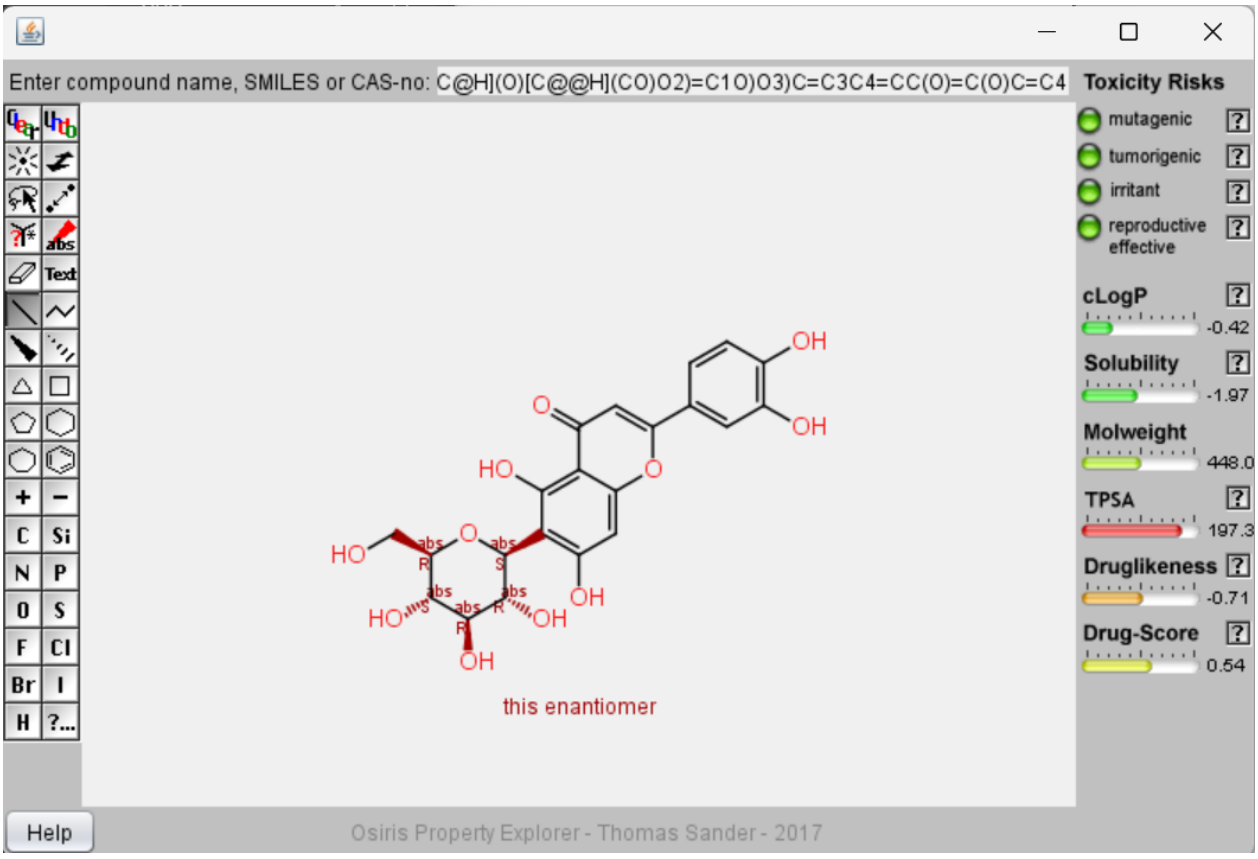


Figure 11: Pharmacokinetic and toxicity profiling of isoorentin

Table 3: Pharmacokinetic Profiling of lead molecules

Compound	ADMET			
	Mutagenic	Tumorigenic	Irritant	Reproductive effectivity
Maysin	NO	NO	Yes	NO
Isoorientin	NO	NO	NO	No

Table 4: Lipinski Properties of lead molecules

Compound	*cLogP*	Solubility	Mol.wt.	TPSA	Drug likeness	Drug score
Maysin	-0.26	-2.74	576	232	4.04	0.61
Isoorentin	-0.42	-1.97	448	197.3	-0.71	0.54

Table 5: Drug likeness of lead molecules

Compound	Lipinski rule of five	H bond donar	H bond acceptor
Maysin	Yes	8	8
Isoorientin	Yes	14	10

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