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Characterization and Computational Validation of Morin as an Antidiabetic Flavonoid: A Combined Experimental and Docking Study

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KEYWORDS

Diabetes mellitus, Morin, FT-IR, *in silico* docking and Aldose reductase

ABSTRACT:

Among the non-communicable diseases, diabetes mellitus (DM) stands next to cardiovascular diseases and cancer in terms of mortality. The commonness of T2DM is increasing alarmingly worldwide and its incidence is closely linked to genetic and environmental factors. T2DM accounts for more than 90% of the diabetic population. Though, several drugs are commercially available to maintain normoglycemia in diabetic individuals through different mechanisms of action. However, most of them prompt undesirable chronic side effects and attenuation after prolonged use. The traditional medicinal plants serve as a potential source for the identification of lead molecules for the development of successful drugs. Morin, a pentahydroxyflavone, is an important phytochemical in many plants belonging to the *Moraceae* family (*M. alba*) and this flavonol is found in several medicinal plants including *Psidium guajava (Myrtaceae), Maclura pomifera and Maclura tinctoria (Moraceae)*. In the present study, an attempt has been made to isolate and identify the phytochemicals from Morin, the traditionally known medicinal plant Guava leaves, extract using suitable solvent extraction followed by HPLC separation. The individual phytochemicals isolated were characterized by spectral studies such as FT-IR, ^{13}C NMR, ^{1}H NMR and Mass spectral studies. Since the above plants have been traditionally used for the treatment of diabetes and its related complications, the present study was designed to evaluate their antidiabetic properties using *in silico* docking studies by choosing important targets such as Aldose reductase, Glycogen phosphorylase, Glycogen synthase, Phosphoenolpyruvate kinase and Glucokinase.

INTRODUCTION

At the dawn of the third millennium, non-communicable diseases such as cardiovascular diseases, diabetes, cancer and mental disorders appeared to be sweeping the entire globe, with an increasing trend in developing countries [1]. Globally, the proportion of the burden of diseases is shifting from communicable diseases to non-communicable diseases. The major risk factors associated with non-communicable diseases include overweight, obesity, chronic hyperglycemia and hyperlipidemia which considered modifiable through changes in behaviors or medications [2]. Among the non-communicable diseases, diabetes mellitus is the most prevalent and pervasive metabolic disorder next to cancer and its burden is exacerbated by micro and macro vascular complications leading to blindness, amputations, kidney failure and heart diseases [3].

Diabetes is a group of metabolic diseases characterized by hyperglycemia resulting from defects in insulin secretion, insulin action, or both. The chronic hyperglycemia in diabetes is associated with long-term damage, dysfunction, and failure of different organs, especially the eyes, kidneys, nerves, heart, and blood vessels. Several pathogenic processes are implicated in the development of diabetes [4]. These range from autoimmune destruction of the β-cells of the pancreas with consequent insulin deficiency to abnormalities that result in resistance to insulin action. The basis of the abnormalities in carbohydrate, fat, and protein metabolism in diabetes is the deficient action of insulin on target tissues [5].

Type 2 diabetes is an epidemic currently, is increasing worldwide predominantly due to poor diet, sedentary

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lifestyle and the fact that we are living longer. The greatest number of people with diabetes worldwide is between the ages of 40 and 59. Every six seconds someone, dies from diabetes. Diabetes imposes unacceptably high human, social and economic costs on countries at all income levels [6].

Ayurveda, the Indian traditional system of medicine, is one of the world's oldest systems to have documented the diagnosis and treatment of diabetes. The medicinal value of the plants lies in some active chemical substances called phytochemicals that produce a definite physiological action on the human body [7]. Primary phytochemical constituents comprise common sugars, amino acids, proteins and chlorophyll, while secondary phytochemical constituents consist of alkaloids, terpenoids, flavonoids, tannins, phenolic compounds [8]. Morin (3,2′,4′,5,7-pentahydroxyflavone) is a flavone that belongs to the *Moraceae* plant family. It is a phytochemical of the class flavonol found in several medicinal plants, including *Psidium guajava (Myrtaceae), Maclura pomifera and Maclura tinctoria (Moraceae)* and is recognized for its anti-carcinogenic and anti-inflammatory roles in different pathologies, including cancer [9].

In silico experiments have been conducted using the above phytochemicals as ligands and the major targets responsible for the onset of secondary complications, such as retinopathy and other metabolic pathways as receptors.

Aldose reductase (AR) is a cytosolic, monomeric oxidase that converts glucose to sorbitol in the polyol pathway of carbohydrate metabolism. This enzyme plays a crucial role in diminishing glucose levels in diabetic individuals. The human AR gene has been mapped to chromosome 7 region q35 [10]. Sorbitol is formed more rapidly than it is converted to fructose, resulting in a net accumulation of sorbitol.

Glycogen degradation and synthesis during the diurnal cycle are facilitated by changes in the actions of phosphorylase and glycogen synthase. Phosphorylase is controlled by phosphorylation of serine-14. Only the phosphorylated form of liver phosphorylase (GPa) is catalytically active. GPa to GPb conversion is a major arduous event in the regulation of glycogen synthesis by glucose, its downstream metabolites and extracellular signals such as insulin and neurotransmitters [11].

Hexokinase is the broadly scattered isoform. Its low Km allows glucose to enter cells, especially brain cells and RBCs, under fasting conditions. Excess removal of glucose from the blood into tissues is prohibited by the allosteric inhibition of hexokinase by its product, G6P. The β-cells in the pancreatic islets of Langerhans contain glucokinase to prevent the inappropriate secretion of insulin, which would lead to persistent hypoglycemia [12]. Since the elevated glucose 6-phosphate serves as the insulin release signal, insulin is released only when the blood glucose rises above the normal fasting levels.

Phosphoenol pyruvate carboxykinase (PEPCK) is essentially a critical enzyme in the regulation of gluconeogenesis because of its part in the hepatic glucose output, which plays an energetic role in the onset of diabetes and its secondary complications. It is a well-known fact that the PEPCK gene expression in the liver is persuaded by fasting or by a diet devoid of carbohydrates due to a decrease in insulin levels and an increase in glucagon levels, the typical features of the fasted state [13]. The powerful negative effect of insulin on PEPCK- C gene transcription has been well conventional.

In view of the above factual reports, in the present study, an attempt has been made to isolate and identify the phytochemical Morin from the traditionally known medicinal plant Guava leaves extract using suitable solvent extraction followed by HPLC separation. The individual phytochemicals isolated were characterized by spectral studies such as FT-IR, ^{13}C NMR, ^{1}H NMR and Mass spectral studies. Since the above plant have been traditionally used for the treatment of diabetes and its related complications, the present study was designed to evaluate their antidiabetic properties using *in silico* docking studies by choosing important targets such as Aldose reductase, Glycogen phosphorylase, Glycogen synthase, Phosphoenolpyruvate kinase and Glucokinase.

MATERIALS AND METHODS

The leaves of *Psidium guajava* were collected from a fruit vendor in the Koyambedu Market, Chennai. The material was washed, dried in a hot air oven at 40°C and subsequently ground into powder in an electrical grinder, which was stored in an airtight brown container at 5°C

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until further use. The grounded plant material was delipidated with petroleum ether (60 - 80° C) overnight. It was then filtered and soxhalation was performed with 95% Ethanol. Ethanol was evaporated in a rotary evaporator at 40 – 50° C under reduced pressure.

Spectral studies

Infrared (IR) spectral studies were carried out in the solid state as pressed KBr pellets using a Perkin Elmer Fourier transform (FT)-IR spectrophotometer in the range of 400-4000/cm. The mass spectrum of the complex was obtained using Jeol Gcmate. The ^{1}H nuclear magnetic resonance (NMR) and ^{13}C NMR at 500.13 and 125.758 MHz were carried out, respectively [14]. The spectra were recorded without any correction for instrumental characteristics.

***In silico* analysis**

Preparation of receptors

Crystal structures of aldose reductase, glycogen phosphorylase, glycogen synthase, hexokinase and PEPCK were obtained from the RSCB protein data bank. Preparation of aldose reductase, glycogen phosphorylase, glycogen synthase, hexokinase and PEPCK with the Auto Dock Tools involved in the addition of hydrogen atoms to the target enzyme, which is a necessary step for the computation of partial atomic charges [15]. Kollman united atom charges, salvation parameters and polar hydrogens were added into the receptor PDB file for the preparation of protein docking simulation.

Preparation of ligand

The phytochemical was considered as a ligand molecule. The ligand was constructed using Chemsketch and then converted into a PDB file format by adding the hydrogen bonds.

Auto Dock

The Graphical User Interface program "Auto-Dock Tools" was used to prepare, run and analyze the docking simulations. Auto Dock 4.2 is used to study the molecular interactions between the phytochemicals and the enzyme receptors such as aldose reductase, glycogen phosphorylase, glycogen synthase, hexokinase and PEPCK [16].

Auto Dock requires pre-calculated grid maps, one for each type of atom present in the flexible molecules being docked and its stores the potential energy arising from the interaction with rigid macromolecules. This grid must surround the region of interest in the rigid macromolecule. The grid box size was set at the active site of the enzymes to include all the amino acid residues that are present in rigid macromolecules. Auto Grid 4.2, Program, supplied with Auto Dock 4.2 was used to produce grid maps. The spacing between grid points was 0.375 angstroms.

Auto Dock results were analyzed to study the interactions and the binding energy of the docked structure. It was run several times to get various docked conformations and to analyze predicted docking energy. The best ligand-receptor structure from the docked structures was chosen based on the lowest energy and minimal solvent accessibility of the ligand. The docking results were visualized using the Acceryls Visualizer discovery studio tool.

RESULTS AND DISCUSSION

Natural harvests from therapeutic plants, either as pure complexes or as consistent extracts, provide boundless chances for new drug leads because of the unparalleled accessibility of chemical diversity. Due to an increasing demand for chemical diversity in screening programs, looking for beneficial drugs from natural products, interest particularly in palatable plants has grown throughout the world. Botanicals and herbal preparations for therapeutic usage contain various types of bioactive compounds. This study aims to perform diagnostic practices, which include the extraction, isolation and characterization of active elements in botanicals and herbal preparations. The analysis of bioactive compounds presents in the plant extract, involving the applications of common analytical techniques such as HPLC, Fourier Transform Infra-Red (FT-IR) and NMR studies is discussed.

Isolation and characterization of Morin from Guava leaves extract

HPLC analysis: Figure 1 and 2 depicts the HPLC analysis of Morin from Guava leaves extract. The retention time for Morin was 53mins.

Figure 1 HPLC Chromatogram of Morin from *Psidium guajava* leaves extract

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Figure 2 HPLC Chromatogram of Morin (With Standard)

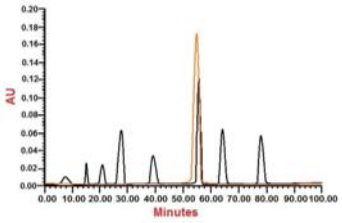


Figure 6 ^{13}C NMR SPECTRUM OF MORIN

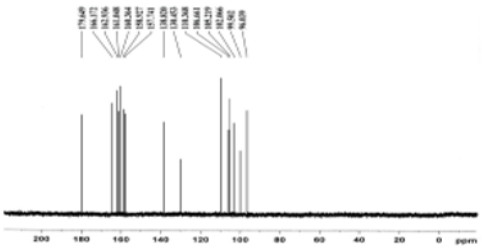


Figure 3 FTIR Spectrum of Morin

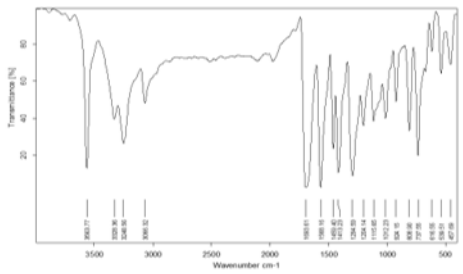
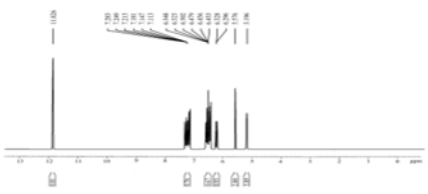


Figure 5 ^{1}H NMR SPECTRUM OF MORIN



FT-IR: The IR spectral data of Morin is shown in Figure 3 [IR (KBr, vcm−1) 3563 [–OH], 1693 (C=O)].

Mass spectra: Figure 4 represents the EI mass spectrum of the morin (m/z): 302.2355 g/mol.

NMR Studies: ^{1}H-NMR and ^{13}C-NMR of Morin

Figure 4 - Mass Spectrum of Morin

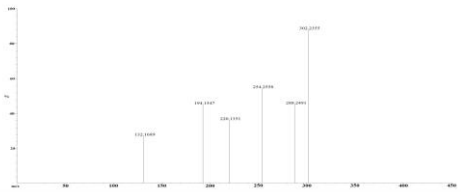


Figure 5 &Figure 6 represents ^{1}H-NMR and ^{13}C-NMR of Morin. Proton NMR studies carried out on a Bruker AM500 instrument using DMSO as solvent showed ten proton peaks for the Morin. The ^{13}C NMR of the flavonol was recorded in Bruker AM500 NMR spectrophotometer at 125.75 MHz, using DMSO as the solvent. The peak at δ 178.72 indicates the carbonyl group.

MOLECULAR DOCKING THROUGH *IN SILICO* ANALYSIS

The observations recorded and the results obtained in the study molecular docking and validation of medicinal effects of Morin are targeted to the five active important key enzymes which cause severe effect of diabetes, such enzymes are Aldose Reductase, Glucokinase, Glycogen Synthase Kinase-3β, Glycogen Phosphorylase and PEPCK are represented.

Protein target selection and preparation

Through extensive literature survey we chosen the five different target proteins involved in the metabolic pathway of diabetes were identified as a target receptor molecule such as Aldose Reductase (PDB ID - 1ef3), PEPCK (PDB ID - 1khb), Glucokinase (PDB ID - 3id8), Glycogen Phosphorylase (PDB ID - 1fc0) and Glycogen synthase kinase 3β (PDB ID - 4pte) [17]. These enzymes play a vital role in type 2 diabetes and also these enzymes are the primary key enzymes for the target and damage several organs and causing many diseases like diabetic nephropathy, diabetic neuropathy etc., and also these enzymes stimulate the metabolic pathways like gluconeogenesis, glucogenolysis etc.,

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Molecular docking

Morin was allowed to bind at the active site of the enzyme, aldose reductase, and docking was performed at 50 different conformations. The docking conformation of Morin shows a low binding energy of -10.87 Kcal/Mol with aldose reductase at conformation 7 (Figure 7). The docking of Morin into the active site of the aldose reductase is visualized in Pymol (Figure 8). The hydroxyl group of Morin forms a hydrogen bond with the amino acid TYR48, HIS110, HIS110, TRP111, ALA299 & LEU301 at the active site of the enzyme & the length of the hydrogen bond is measured. Docking Energy and hydrogen bond interaction are shown in Table 1.

Figure 7: 3D Docking Model Showing The Binding Sites Of Aldose Reductase With Morin

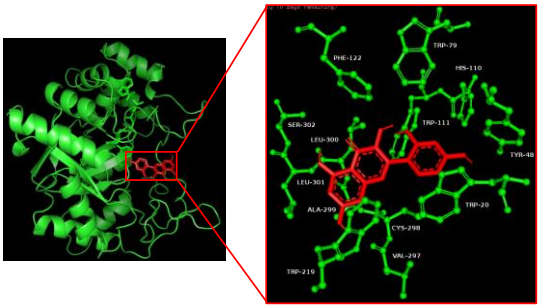


Figure 8: Visualizing Hydrogen Bond Interaction Between Aldose Reductase And Morin Using Pymol

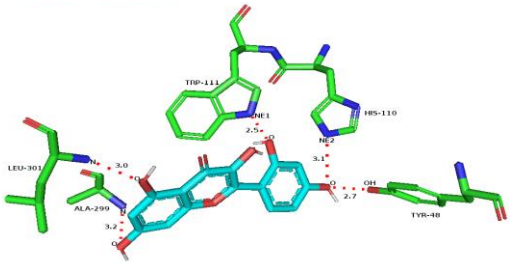
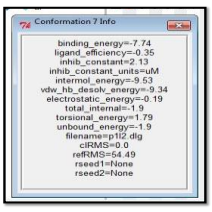


Table 1. Docking Energy for Morin with Aldose Reductase

ALDOSE REDUCTASE		MORIN	DISTANCE (Å)	DOCKING ENERGY (Kcal/Mol)
Residue	Atom			
TYR48	OH	O	2.7	-7.74
HIS110	NE2	O	3.1	
TRP111	NE1	O	2.5	
ALA299	N	O	3.2	
LEU301	N	O	3.0	



Morin was allowed to bind at the active site of the enzyme, PEPCK, and docking was performed at 50 different conformations. The docking conformation of Morin shows a low binding energy of – 6.78 Kcal/Mol with PEPCK at conformation 50(Figure 9). The docking of Morin into the active site of the PEPCK is visualized in Pymol (Figure 10).

Figure 9. 3D Model Showing The Binding Sites Of PEPCK With Morin

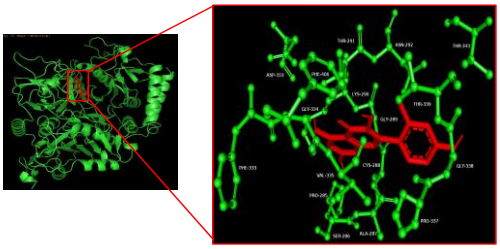
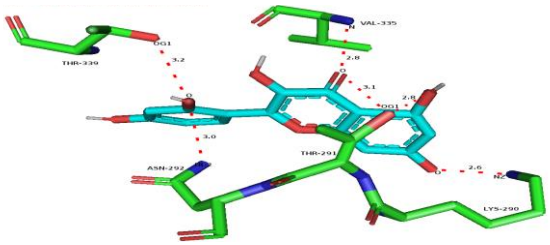


Figure 10: Visualizing Hydrogen Bond Interaction Between PEPCK And Morin Using Pymol



The hydroxyl group of Morin forms a hydrogen bond with the amino acid LYS290, THR291ASN292, VAL335 & THR339 at the active site of the enzyme & the length of the hydrogen bond is measured. Docking Energy and hydrogen bond interaction are shown in Table 2.

Table 2. Docking Energy For Morin With PEPCK

PHOSPHOENOL PYRUVATE CARBOXYKINASE		MORIN	DISTANCE (Å)	DOCKING ENERGY (Kcal/Mol)
Residue	Atom			
LYS290	NZ	O	2.6	- 6.75
THR291	OG1	O	2.8	
THR291	OG1	O	3.1	
ASN292	ND2	O	3.0	
VAL335	N	O	2.8	
THR339	OG1	O	3.2	

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Morin was allowed to bind at the allosteric site of the enzyme, Glucokinase, and docking was performed at 50 different conformations. The docking conformation of Morin shows a low binding energy of - 10.18 Kcal/Mol with Glucokinase at conformation 10 (Figure 11). The docking of Morin into the allosteric site of the Glucokinase is visualized in Pymol (Figure 12). The hydroxyl group of Morin forms a hydrogen bond with the amino acid ARG63 & TRY215 at the allosteric site of the enzyme & the length of the hydrogen bond is measured. Docking Energy and hydrogen bond interaction are shown in Table 3.

Figure 11: 3D Docking Interactions Showing the Binding Sites of Glucokinase With Morin

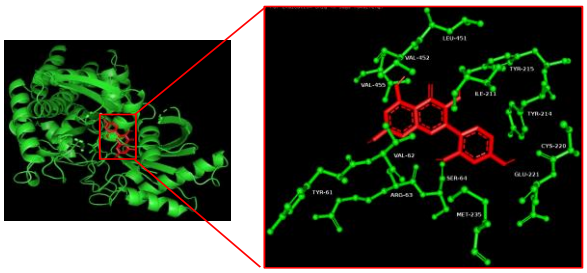


Figure 12: Visualizing Hydrogen Bond interaction Between Glucokinase and Morin Using Pymol

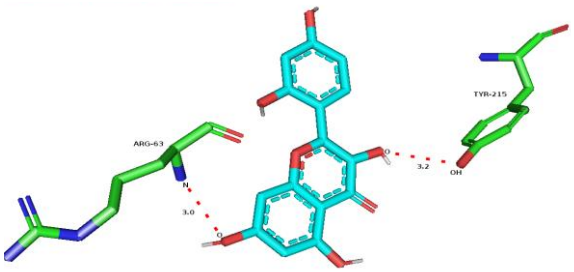


Table 3. Docking Energy For Morin With Glucokinase

GLUCOKINASE		MORIN	DISTANCE (Å)	DOCKING ENERGY (Kcal/Mol)
Residue	Atom			
ARG63	N	O	3.0	- 8.29
TYR215	OH	O	3.2	

Morin was allowed to bind at the active site of the enzyme, Glycogen Phosphorylase, and docking was performed at 50 different conformations. The docking conformation of Morin exhibits a binding energy of 21.77 Kcal/Mol with Glycogen Phosphorylase at conformation 42(Figure13). The docking of Morin into the active site of the Glycogen Phosphorylase is visualized in Pymol (Figure 14). The hydroxyl group of Morin forms a hydrogen bond with the amino acid LEU136, ASN284, HIS341, SER674 & GLY675 at the active site of the enzyme & the length of the hydrogen bond is measured. Docking Energy and a hydrogen bond interaction are shown in Table-4.

Figure13: 3D Docking Model Showing The Binding Sites Of Glycogen Phosphorylase With Morin

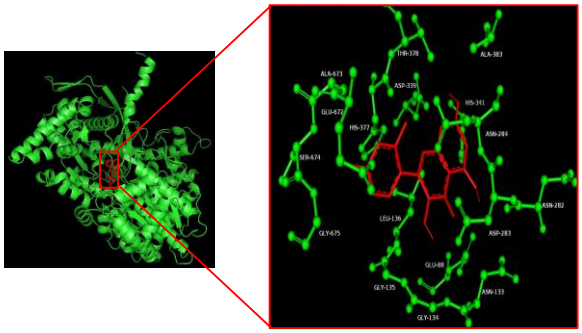


Figure 14: Visualizing Hydrogen Bond Interaction Between Glycogen Phosphorylase and Morin Using Pymol

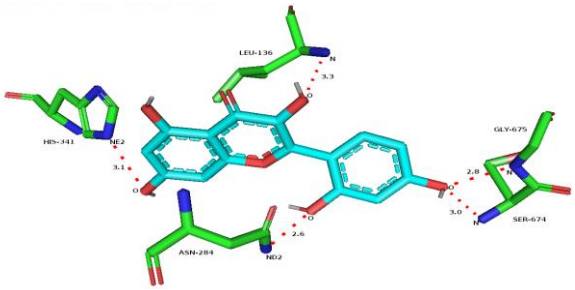
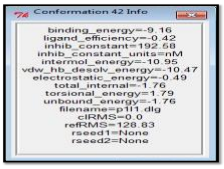


Table 4. Docking Energy For Morin With Glycogen Phosphorylase

GLYCOGEN PHOSPHORYLASE		MORIN	DISTANCE (Å)	DOCKING ENERGY (Kcal/Mol)
Residue	Atom			
LEU136	N	O	3.3	- 9.16
ASN284	ND2	O	2.6	
HIS341	NE2	O	3.1	
SER674	N	O	3.0	
GLY675	N	O	2.8	



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Morin was allowed to bind at the active site of the enzyme, glycogen synthase kinase-3β, and docking was performed at 50 different conformations. The docking conformation of Morin shows a low binding energy of –8.82 Kcal/Mol with glycogen synthase kinase-3β at conformation (Figure 15). The docking of Morin into the active site of the glycogen synthase kinase-3β is visualized in Pymol (Figure 16). The hydroxyl group of Morin forms a hydrogen bond with the amino acid VAL135 at the active site of the enzyme & the length of the hydrogen bond is measured. Docking Energy and hydrogen bond interaction are shown in Table-5.

Figure15: 3D Docking Model Showing The Binding Sites Of Glycogen Synthase Kinase-3β With Morin

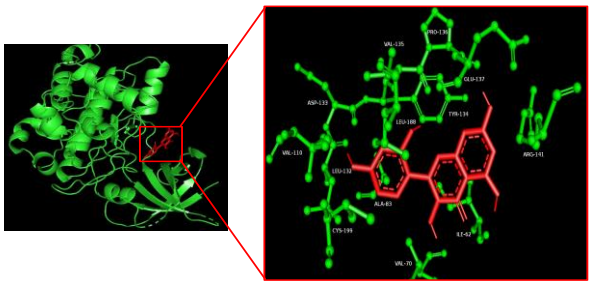


Figure 16: Visualizing Hydrogen Bond Interaction Between Glycogen Synthase Kinase-3β and Morin Using Pymol

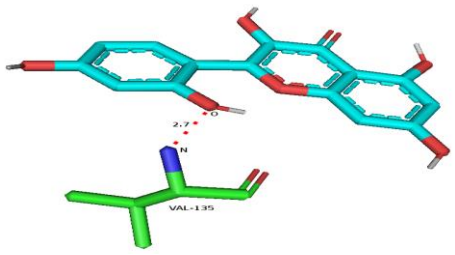
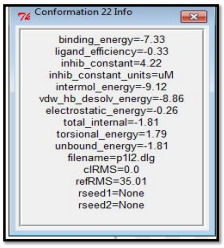


Table 5 Docking Energy For Morin With Glycogen Synthase Kinase-3β

GLYCOGEN SYNTHASE KINASE 3β		MORIN	DISTANC E (Å)	DOCKING ENERGY (Kcal/Mol)
Residue	Atom			
VAL135	N	O	2.7	-7.33



CONCLUSION:

Diabetes mellitus (DM) is a chronic metabolic disorder characterized by persistent increased glucose levels resulting from flaws in insulin secretion, insulin action, or both. It is the most predominant ailment worldwide, with a high risk of morbidity and mortality from primary as well as secondary complications. There are presently several oral antidiabetic medications available on the market with varying mechanisms of action, such as stimulation of insulin secretion from β-cells in the pancreas (sulfonylureas), the reduction of hepatic glucose production (biguanides), increasing the sensitivity of tissues to insulin (thiazolidinediones), and/or delaying the digestion and absorption of carbohydrates (acarbose). However, all these drugs provoke detrimental side effects with prolonged use. Hence, the search continues for plant derived products for the treatment of diabetes as they are devoid of side effects, are relatively low-priced and claimed to be effective.

The results of the spectral studies evidenced that Morin, is the major secondary metabolite present in the medicinally important plant guava. The *in-silico* studies established the efficacy of the phytochemicals in controlling the major secondary complications of type 2 diabetes.

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