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ANTI-HYPERGLYCEMIC ACTIVITY OF *ABUTILON INDICUM* LINN. THROUGH MOLECULAR DOCKING METHOD

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ABSTRACT

Background: Diabetes mellitus is a multifactorial disorder characterized by a chronic elevation in blood sugar levels. Currently, antidiabetic drugs are available in order to counteract the associated pathologies. Their connected effects are necessitated to the investigation for a good and safe drug aimed to diminish blood sugar levels with fewer side effects. **Method:** The present study was undertaken to review the role of natural products using in silico interaction studies. Molecular docking studies were carried out with3 target proteins to evaluate its antidiabetic potential Luteolin is a compound present in *Abutilon indicum* was found as a potential anti- diabetic agent. **Result:** The study showed the highest interactions with **3W37** (-8.8 kcal/mol). Molecular docking analysisresulted in favourable binding energy of interaction ranging low as - 5.1 to - 8.8 kcal/mol for luteolin, *in silico* pharmacokinetics and toxicity profile of luteolin were studied using SwissADMET, PKCSM online software's. It was predicted that luteolin as non-carcinogenic and non-mutagenic. The drug-likeliness was calculated using PYRx respecting Lipinski's rule of 5. The compound was found to adjust to Lipinksi rules. **Conclusion** The study suggested that luteolin can be a possible anti-diabetic agent. As it showed prominentresults

Keywords: Diabetes mellitus, molecular Docking, luteolin, Insilco analysis, PYRx, SwissADMET, PKCSM

1. INTRODUCTION

Diabetes Mellitus (DM) is most prevalence metabolic disorder which affects the worldwide. Diabetes generously elevates other complications in people such as cardiac arrhythmia, neuropathy and hypertension etc. DM is related with

inappropriate elevation of blood glucose level it is derived in two main categories i.e., Type 1 and Type 2 Insulin is a peptide hormone produced by beta cells of the pancreatic islets encoded in humans. It is considered to be the main anabolic hormone of the body. The major purpose of insulin is to regulate the body's energy supply by balancing micronutrients levels during the fed state. Insulin is useful in transporting intracellular glucose to insulin dependent cells/tissue such as liver, adipose tissue and muscles. T1DM has caused by the destruction of βcells of pancreas that enables to secrete quantities insulin.The prevalence of type 1has largely increase locally and globally, there is insufficient of β-cells which leadto insufficiency of insulin. T2DM is an insulin resistant disorder where β-cells of pancreas produce insulinbut body does not respond to it. Currently 6.2% of global population is affected by T2DM. Globally the targetachieved by DM about 422 million people at 2025. The majority people living in below poverty line and each year death of 1.5 million people is because of diabetes. In India death of every 1 in 11 people occurs due to diabetes andalso in US as per global data it is 7th leading cause of death **[1-3]**. Hypoglycaemia is regularly described via way of means of a plasma glucose attention below 70 mg/dL; however, symptoms and signs might not arise till plasma glucose concentrations drop beneath 55 mg/dL **[1]**. Glucose is the number one metabolic fuel for the mind below physiologic conditions. Unlike different tissues of the body,the mind may be very restricted in providing its glucose. Expectedly, the mind calls for a constant deliver of arterial glucose for good enough metabolicfunction **[4-5]**. Abutilon Indicum, usually known as "Thuthi" or "Kanghi" in hindi, is a local plant of South Asia. Abutilon Indicum (Linn.) sweet (Malvaceae) usually known as 'Country Mallow' is a perennial plant up to a few meters in height. Easily grown from seeds. Prefers fertile & well- drained soils. Propagated by seeds or by taking tip cuttings. The genus name is derived from Arabic awbutilun abutilon It performs a crucial function to maintain our health. India is one ofthe maximum medico-culturally stable country. Here, the primary conventional structures of medication consist of Ayurveda, Unani and Siddha in India specific components of medicinal flowers had been used for curing diverse illnesses from historical times. In this regard, one such plant is Abutilon Indicum. The Abutilon L. genus of the Malvaceae own circle of relatives contains approximately a hundred and fifty annual or perennialherbs, shrubs or maybe small timber broadly dispensed withinside the tropical and subtropical international locations of America, Africa, Asia and Australia. Some of the flowers belonging to the species are

among lots are claimed Ayurvedic herbs and withinside the current progress there is a renewed clinicalhobby in exploring the species **[2]**. Roots are prescribed in fever, chest affection and urethritis. Abutilon Indicum (Linn.) is 3 meter in height. Traditionally, Root andbark are used as aphrodisiac, antidiabetic, nervine tonic,and diuretic. Seeds are utilized in urinary disorders. The seeds are used as a laxative in piles and withinside the remedy of cough. The Phyto chemical investigation of A. indicum leaves confirmed the presence of aminoacids, glucose, fructose and galactose. From the roots, non–drying oil which include numerous fatty acids viz. linoleic, oleic, stearic, palmitic, lauric, myristic, caprylic, capric and uncommon fatty acid having 6 carbon skeleton structures sitosterol, and amyrin from unsaponifiable be counted had been yielded in the extract **[1-8]**. It is an online software that aims to predict the structure of ligand within binding site along with the correct estimation of binding sit along with the correct estimation of binding strength. It predicts theinteraction between ligand and receptor complex. In the structure-based drug design (SBDD) estimation ofbinding affinity is an important goal fulfilled by molecular dynamic (MD). MD is simulated to forecasting a specific interaction of receptor and ligand. This affinity of binding- based on the binding energy and hydrogen and hydrophobic interaction. The Ramachandran plots for the proteins had been additionally plotted for the understanding ofthe bounded residues **[9, 11]**.

2. MATERIALS AND METHODS

2.1 Platform for Molecular docking:

Molecular docking between the ligand and the receptors was carried out using PYRX 0.8 autodock vina tool. Docked poses were visualized using DS Visualizer and the interactions were ranked according to their docked energy. Docking scores were calculated and compared with two standard drugs.

2.2 Selection and preparation of receptor:

Three-dimensional crystal structure of α-glycosidase (PDB ID: 3W37) involve in type II diabetes were downloaded in pdb format from the RCSB protein data bank (www.rcsb.org). Structure of the protein targetwere prepared and refined using digital studio visualizer 2021. The proteins with PDB id are 7DCH, 7D9B,7DCG, 3W37 and 1XSK were used as targeted hypoglycaemic proteins for molecular docking experiments. In DS visualizer the necessary hydrogen atoms were added and unwanted amino acids, het atoms and water molecules were removed.

2.3. Preparation of receptor and ligand:

A total of 7 ligands of abutilon indicum were selected by literature survey and used

forpresent study. They include luteolin, chrysoeriol (5280666), phytol (5280435), hinesol (289964), cubenol (519857), palmiticacid (985), pinellic acid (9858729) respectively. The 3D sdf format were downloaded from PubChem database. Energy minimization, geometrical confirmation and hydrogen bond is supplemented by PYRx- virtual screening tool.

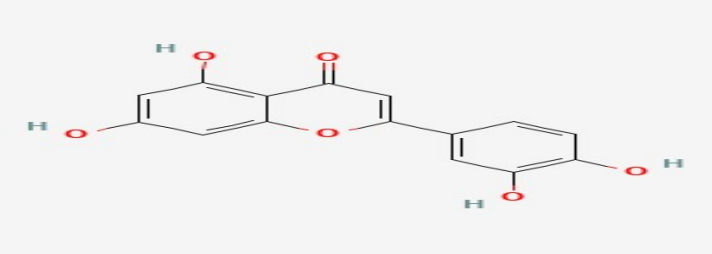
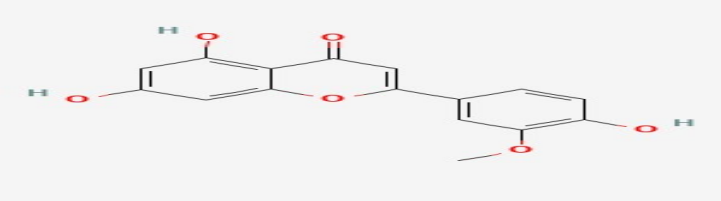
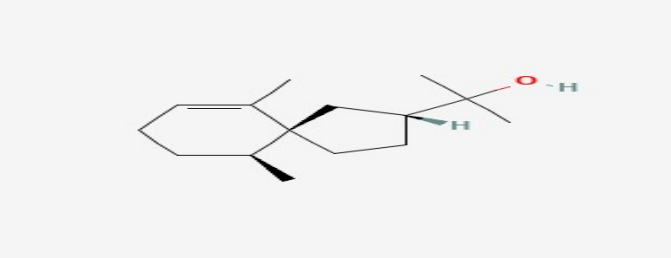
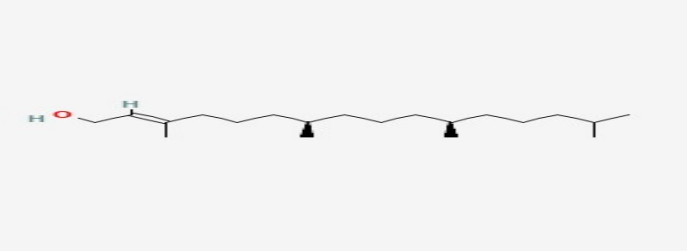
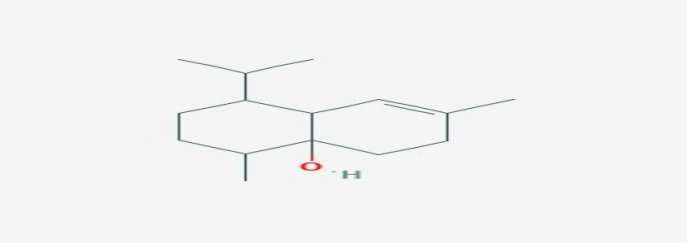
Molecular Properties and ADMET Study

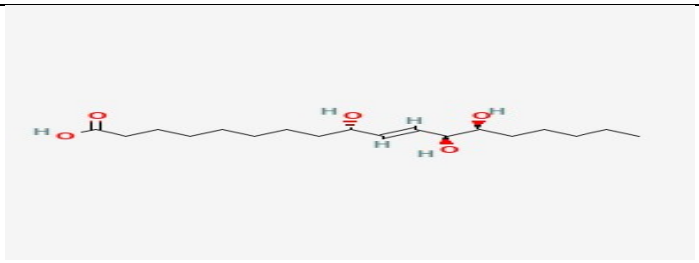
ADME covers the pharmacokinetic problems figuring out whether or not a drug molecule gets to the goal protein withinside the body, and the way lengthy it'll live withinside the bloodstream. SWISS ADME and PkCSM, an online server was used to predict the toxicity upon consumption of compounds and asserts whether the drug follows the Lipinski Rule. Human intestinal absorption (hia), blood–brain barrier (bbb) penetration, caco-2 permeability, carcinogens toxicity and other factors were predicted.The SMILES of the ligands was submitted to the SWISS ADME and PkCSM program for their pharmacokinetics and toxicity properties. The phytoconstituents of plant were selected by studying their Lipinski rules factor that includes hepatotoxicity, water solubility, polar surface area, molecular weight, HB acceptor, HB donor, oral acute toxicity, AMES toxicity, BBB, with also log p value. Swiss ADME and PKCSm are the internet tool which are freely used to predict the chemical science properties, absorption, distribution, metabolism, elimination and pharmacokinetic properties of molecules that play key factors to further selection for the clinical trials.

Table 1: Proteins with their description

Sr. no.	Proteins	Description
1	7D9B	Crystal structure of alpha-glucosidase
2	7D9c	Alpha-glucosidase from Weissella cibaria BBK-1 bound withmaltose
3	7DCH	Alpha-glucosidase from Weissella cibaria BBK-1 bound withacarbose
4	3W37	Sugar b*eet al*pha-glucosidase with acarbose

Table 2: phytoconstituents(ligands) structure and IUPAC names

Sr. No.	Ligands	Structure/IUPAC
1	Luteolin	 2-(3,4-dihydroxyphenyl)-5,7-dihydroxychromen-4-one
2	Chrysoeriol	 5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl) chromen-4-one
3	Hinesol	 2-[(3*R*,5*S*,6*S*)-6,10-dimethylspiro[4.5]dec-9-en-3-yl]propan-2-ol
4	Phytol	 (E,7R,11R)-3,7,11,15-tetramethylhexadec-2-en-1-ol
5	Cubenol	 4,7-dimethyl-1-propan-2-yl-2,3,4,5,6,8a-hexahydro-1H-naphthalen-4a-ol

6	Palmitic acid	 hexadecenoic acid
7	Pinellic acid	 (*E*,9*S*,12*S*,13*S*)-9,12,13-trihydroxyoctadec-10-enoic acid

2.4. RESULT AND DISCUSSION

We docked 7 ligands Luteolin (5280445), chrysoeriol (5280666), hinesol (1087861), phytol (5280435), cubenol (519857), palmitic acid (985), pinellic acid (9858729) with α-glycosidase in order to study the interactions with four proteins separately by docking software's. Study of standard drugs interaction with proteins was carried out by PYRxsoftware. Selected ligands that showed best results were further evaluated for ADMETproperties using SwissADME and pkCSM online tools.

The docking score and binding energy of all targeted protein and ligands are shown in **Tables 3 and 4** respectively.

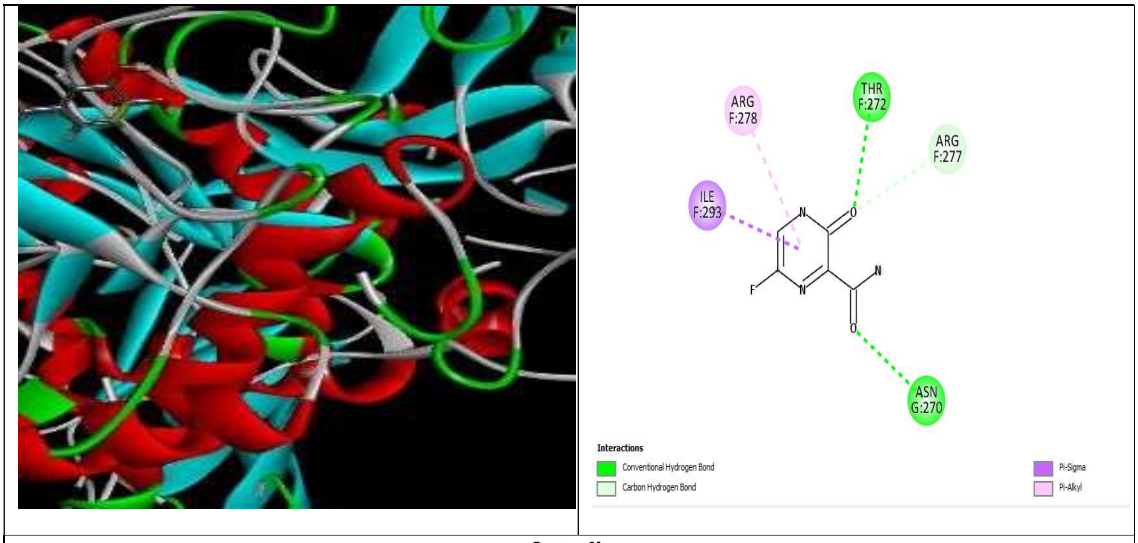
Analysis of binding affinity of selected ligands were in the ranges of -8.8 to -4.6 kcal/mol. From docked result, it is observed that luteolin possess highest binding affinity (-8.8kcal/mol) with selected protein, considering standard drugs docking results protein 3W37 showed prominent activity of -9.0 kcal/mol.

Table 3: Binding Energy (kcal/mol) Of Selected proteins and ligands

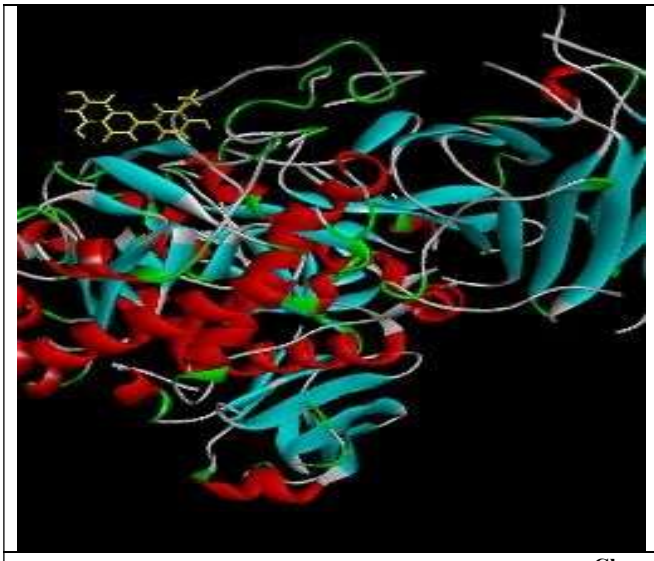
Ligands/Proteins	7D9B	7D9C	7DCH	3W37
Chrysoeriol	-7	-8	-8.1	-8.5
Hinesol	-6.8	-7.4	-7.1	-8.1
Phytol	-7.6	-8	-8.2	-4.6
Luteolin	-5.1	-5	-5.1	-8.8
Cubenol	-5.7	-7.4	-6.7	-7.9
Palmitic acid	-3.9	-5.3	-4.7	-5.6
Pinellic acid	-5.3	-6.1	-6.2	-6.6

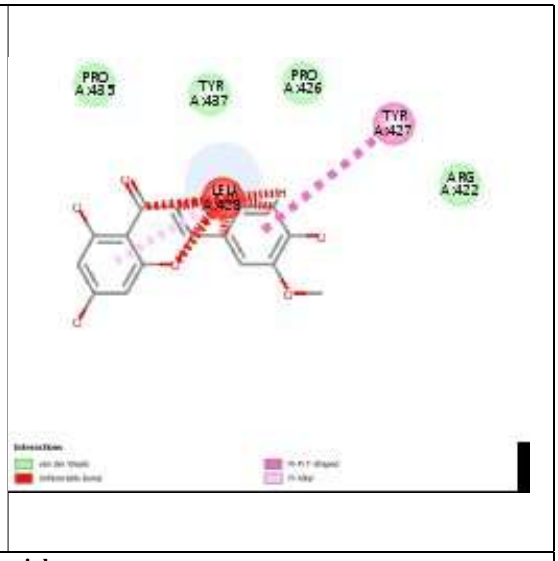
Table 4: Binding Energy (kcal/mol) Standard drugs with protein

Standard drugs/Proteins	7DCH	3W37
Metformin	-5.2	-5.2
Sitagliptin	-8.6	-9.0

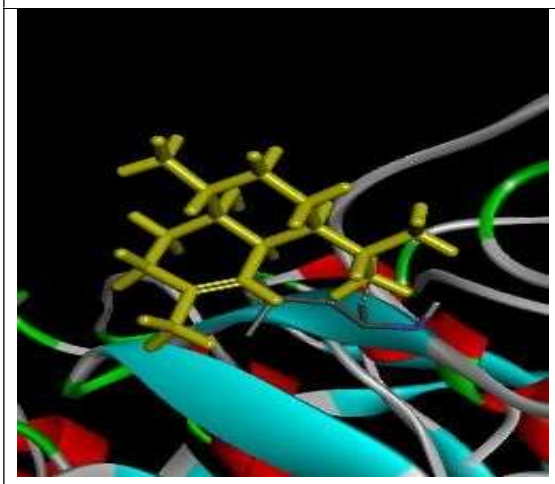


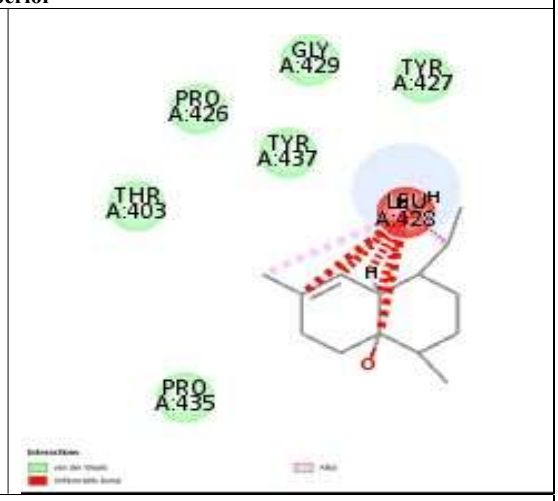
Luteolin



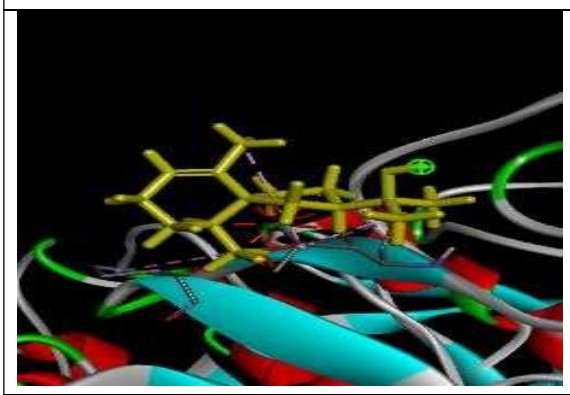


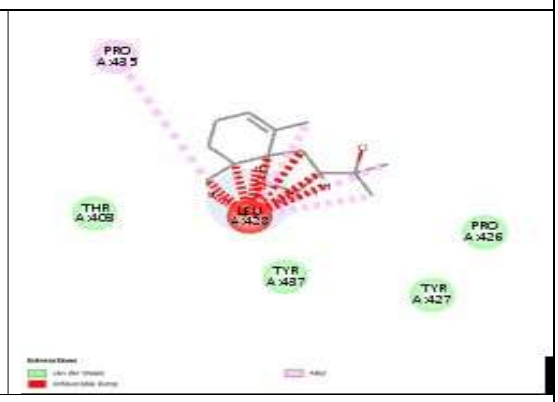
Chrysoeriol



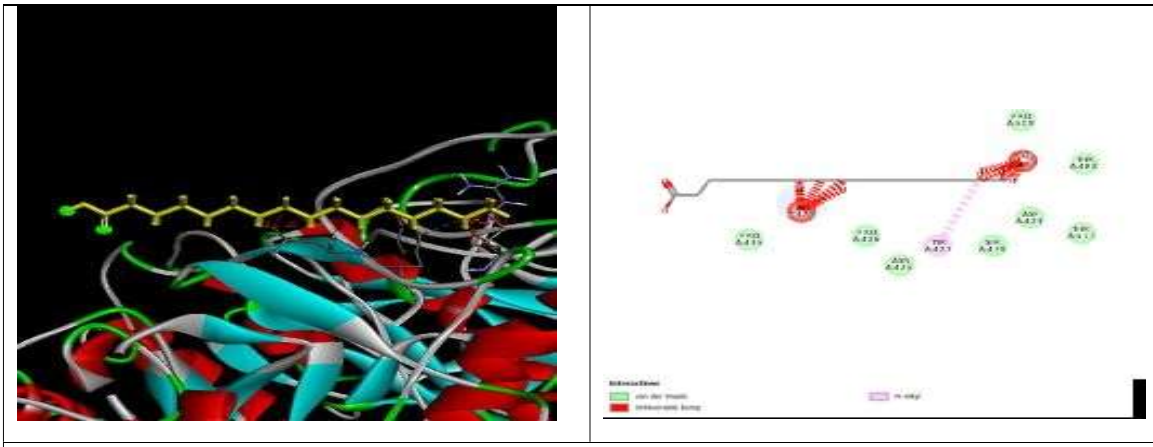


Cubenol

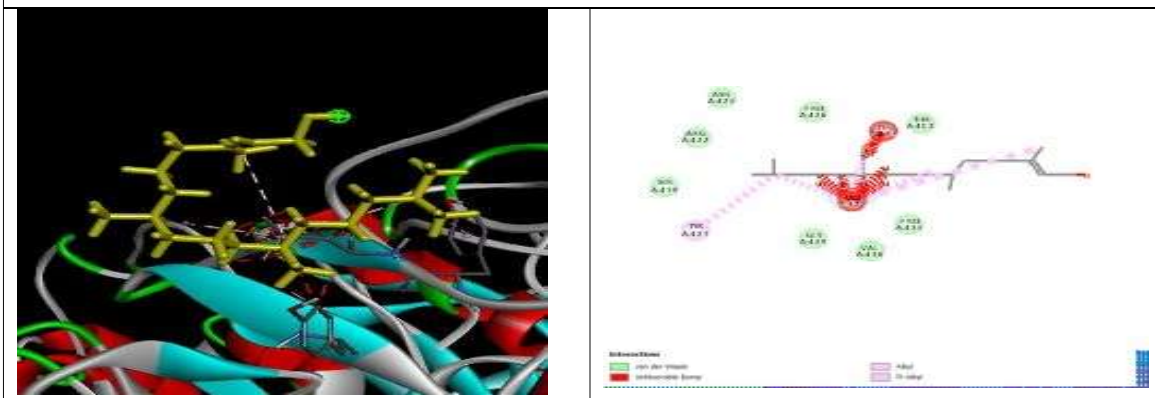




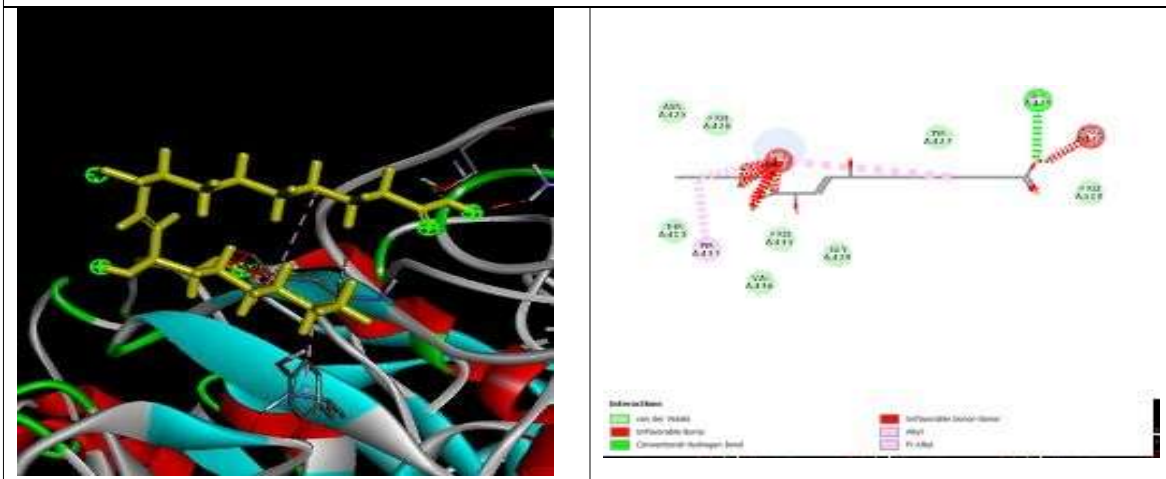
Hinesol



Palmitic acid



Phytol



Pinellic acid

Figure 1: Interaction of phytoconstituents of plants to protein target 3W37

Luteolin showed binding affinity of -8.8 kcal/mol with 3W37 protein it showed van der wall bonding with Pro:426, TYR A:427, AGR A:422, TYR A:437, THR A:403 **(Figure 1)**. Chrysoeriol showed binding affinity of -8.5 kcal/mol with protein 3W37 with Pi-Alkyl bond TYR A:427 along with the distance of 5.85. It also shows van der wall bonding with PRO A: 426, TYR A:437, PRO A:436, ARG A:422 it also shows unfavourable bump of LEU A:428 **(Figure 2)**. Cubenol showed binding affinityof -7.9 Kcal/mol with 3W37 protein. It shows unfavourable bump with LEU A:428 with binding distance of 3.79. It also shows TYRA: 427, TYR A: 437, PRO A: 426, GLY A:429, THR A:403, PRO A:435 **(Figure 3)**. Hinesol showed binding affinity of -8.1 with 3W37. It shows Alkyl bond with PRO A:435 along with the distance of 5.00. It also shows van der wall bond of THR A:403, TYR A:437, TYR A: 437, PRO A:426. It also shows unfavourable bump with LEU A: 426 **(Figure 4)**. Palmitic acid shows binding affinity of -5.6 Kcal/mol. It shows Pi-Alkyl bond with TYR A:427 along with the distance of 5.1. It also shows van der wall bonding with PRO A:435, PRO A:426, ASN A:425, SER A: 479, PRO A:509, ASP A:423, THR A:482. It also showed unfavourable bump with LEU A:428, ARG A:428 **(Figure 5)**. Phytol shows binding affinity of -4.6 with protein 3W37. It also shows van der wall bond with ASN A:425, ARG A:422, SER A:479, PRO A:426, THR A: 403, GLY A:429, PRO A:435, VAL A: 436. It also shows unfavourable bump with LEU A:428, TYR A:437 **(Figure 6)**. Pinellic acid shows binding affinity of -6.6 Kcal/mol with protein 3W37. It shows Pi-Alkyl bond and van der wall bond with TYR A:437, SER A:479 along with the distance of 4.06 and 3.09. It shows van der wall bondwith ASN A;425, PRO A:426, TYR A:427, PRO A:509, PRO A:435, THR A:403, VAL A:436. It also shows unfavourable bump of LEU A:428, ARG A:428 **(Figure 7)**.

ADME and toxicity studies

ADME covers the pharmacokinetic problems figuring out whether or not a drug molecule gets to the goal protein withinside the body, and the way lengthy it'll live withinside the bloodstream. In this study, we perform ADMET studies using SwissADME and pkCSM tools. Compound need to meet Lipinski's rule of 5 which includes MW < 500 kDa, donor HB < 5, accept HB < 10, and logP w/o < 5 to own drug-like characteristics and additionally it needs to meet percentage human oral absorption values. To study whether the drug follows the Lipinski Rule.Human intestinal absorption (hia), blood–brain barrier (bbb) penetration, caco-2 permeability, carcinogens toxicity and other factors were predicted with SwissADMET and pkCSM servers.

Table 5: ADMET Analysis

Phytoconstituents	Hepatotoxicity	Log po/w	Blood brain barrier	Water solublity	Polar surfac earea	Lipinski rule violation	AMES toxicity
Chrysoeriol	No	2.44	No	2.83	96.2	0	No
Hinesol	No	3.24	Yes	4.429	20.2	0	Yes
Luteolin	NO	1.86	No	2.829	107	0	No
Phytol	No	4.85	No	2.991	20.2	1	No
Cubenol	No	3.24	Yes	1.049	20.2	0	No
Palmitic acid	No	3.85	Yes	5.62	37.3	1	No
Pinellic acid	No	3.61	No	3.628	98	0	No

CONCLUSION

Docking research of photoactive compounds in *Abutilon indicum* Linn towards diabetes mellitus confirmed conductive end result with prominent hypoglycemic activity was found with phytoconstituents, Luteolin, chrysoeriol, hinesol, phytol, cubenol, palmitic acid, pinellic acid with α-glycosidase. For the phytoconstituents selection their Lipinski rule was studied that influences their metabolism, cell permeation and bioavailability. It was done using Swiss ADMET, PKCSM servers. By studying the protein-ligand interaction through PYRx software. Receptor 3W37 showed highest binding affinity with Luteolin (-8.8) and standard drug Sitagliptin (-9.0) whichmakes it most favourable confirmation. Thus, plant formulation proved significant hypoglycemic activity in diabetics by protein (3W37) and ligand (luteolin) interaction, thus the referred plant may be used in order to grow into an amazing antidiabetic drug.

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