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ORIGINAL ARTICLE **OPEN ACCESS**

In-Silico elucidation of *Abrus precatorius* phytochemical against *Diabetes mellitus*

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ABSTRACT

For certain medicinal applications, Abrus precatorius is used. It is commonly cultivated around the world due to dietary and pharmacological principles. Abru sprecatorius leaves are high in minerals, vitamins, and several other health-efficient secondary metabolites and have great diabetic potential. The Insilco research may also be worth mentioning in order to extend this plant into successful antidiabetic drugs. The goal of this analysis was to identify the best bioactive compounds. A. precatorius by In-silico process as a possible treatment agent for diabetes mellitus. Phytochemicals structures have been isolated from PubChem for this purpose, and are bound to mutant PBD protein. Then, datasets for ligand-based drugs have been prepared and their pharmacophoric characteristics have been provided by molinspiration. There were selected two phytochemicals, Abruquinone B, Abruquinone C, which showed successful binding inside the targeted protein active binding pocket. The Pharmacophore model centered in Ligand had the main characteristics, i.e. HBD, HBA, ring, hydrophobic, ionizing surface necessary to bind the receptor. Results indicate that A.precatorius screened phytochemicals could be used as possible therapeutic candidates for the treatment of diabetes mellitus

Key word: *Abrus precatorius, Abruquinone B, Abruquinone C, Diabetes mellitus, 5HHW*

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INTRODUCTION

About 90 percent of all diabetes cases are due to type 2 diabetes mellitus (T2DM). In T2DM, the insulin response is reduced and is defined as resistance to insulin. In this condition, insulin is ineffectual. The insulin production has been initially balanced by an increase in glucose homeostasis, but insulin production has declined over time leading to T2DM. In people above the age of 45, T2DM is most frequently observed. Rising amounts of obesity, physical inactivity, and energy-dense diets also exist in teenagers, teens, and younger adults.

Abrus precatorius is commonly known by some different names i.e. "Rosary pea, Crab's eye, Jequirity, Precatory bean, Saga, Gunchi, Rati Gedi." Twins with a distinct toxic red seed at the base *Abrusrecatorius* is a woody plant with a black circle [1]. Scientifically rosary pea is called as *Abrus precatorius* belongs to the *Fabaceae* family and higher classification of*A. precatorius*, Kingdom of*Plantae*. This plant is a well-known plant genus and is the most distributed, they are substitute and globous and have two pairs of paripinnate leaflets. Flowers in the races, shorter than the branches, obsessed with swollen nodes, pink and pink-white, small, hairy calyx-lobes. pods 1,5-5.0 x 0,8-1,5 cm, turgid, oblong, rugged, and strongly deflexed beak, silky, 3-5 pod. The seeds are elliptic, and the diameter is 0.5 cm., flat, glittery, red bright, and black-blocked. *Abrus precatorius* is an important plant for its many medicines that have diabetes, nephronectins, neuroprotectants, analgesics and more. *A. precatorius* is abundant in numerous chemical

elements, including root, seed, leaves. There are a variety of important amino acids rich in this plant including Serine, Alanine, Valine, Choline, and Methyl ester. It is well established that secondary metabolites make a major contribution to the medicinal application of plant species to the conventional healing method. Numerous bioactive compounds from various parts of the *A. precatorius* have been identified. In the same way, the different parts of *A. precatorius* have highly contained medicinal values, described in table 1 [2]. Various parts of *A. precatorius* are the high value of aboral, abrasine, precol, precasin, Abrine, Abraline, abrasine, Abruquinones B, C. The mentioned phytochemicals make an important contribution to the prevention of various health conditions, such as metabolic disorder (Anti-diabetic activity), neuron disorder (Anti-convulsant activity), renal Protectivity (Diuretic activity), antimicrobial activity, anticancer activity properties for various sections of *Abrusprecatorius*.

Table 1: Medicinal use of A. precatorius(Tamilselvan *et al.*, 2014)

Plant Parts	Medicinal Use
Seed	Dry powdered seeds of *A. precatorius* is taken for two days for warm infection and used for tuberculosis and malaria.
Root	Treat jaundice and haemoglobin uric bile. Root paste is used to relieve stomach pain, cancers, and abortion as well. Melt root are taken three times a day for four days to treat cough with pure clarified butter.
Leaf	The herb leaves are used to treat flu, cough and cold. They have antifouled features. They are made of lime which are added to acne surfaces, boils which abscesses. Decoction of the leaves for cough and influenza is taken orally.

International Diabetes Federation (IDF) latest results display that more than 353 million diabetes mellitus (DM) is impaired worldwide population are projected to rise to 555 million or even more in 2040, more. Mellitus type 2 diabetes (DMT2) is an irregular glucose tolerance clinical syndrome; universal, deficient insulin, neuropathy, microangiopathy Secrecy. The effect of weak Insulin plays a significant role in the underlying metabolic disorders Hyperglycaemia with type 2 diabetes (T2DM) public health issue that is rising [3]. T2DM people have a high danger with all complications high macro-vascular and complications that contribute to hyperglycemia, *i.e.* cardiovascular comorbidities and the (metabolic) condition of insulin resistance. In the case of DMT2, the whole-cell complement is curable. The zygote cell affects the insulin receptor. The present prevalence of type 2 DM in India as 12.35per cent, with males accounting for 10.20per cent and females accounting for 9.19 percent. In comparison, DM accounts for 13.78% in urban areas and 11.24% in rural areas of India most of everything.
In-silico analysis of the different metabolites of *Abrus precatorius* anti-diabetic drug. As a result, we analysed some of the main compounds from *Abrus precatorius* and docked them with the mutant diabetes mellitus receptor protein [4-8].

Figure 1: Plant leaf and seeds of *Abrusprecatorius*

MATERIAL AND METHODS

Selection of Disease

Diabetes mellitus has been chosen for an anti-diabetic impact with *Abrus precatorius* as a target disorder. DM is a chronic metabolic condition that is rising increasingly both internationally and worldwide. To date, this condition has not been treated adequately and successfully. In diabetic patients, one popular problem is the disruption of insulin production [9]. Type 2 is a complex disease that comprises disabled pancreatic beta-cell insulin discharge.

Gene Identification

The INSR gene is a member of protein receptor tyrosine kinase and has been identified by Gene Card (www.genecard.org). The hereditary syndromes with extreme insulin resistance are caused by variations in the gene. As well as the synthesis or accumulation of sugars, lipids, and protein insulin and other compounds bound to its receptor, the insulin signaling route that regulates the intake and release of glycolysis is activated. Gene Card presented comprehensive genome, proteome, transcriptome, and characteristic statistics for both known and predicted human genes [10] Gene Card is an important source of knowledge for study in bioinformatics.

Selection of Protein

The insulin receptor is a transmembrane receptor activated by insulin aid,5HHW belongs to the tyrosine kinase domain of the human insulin receptor. Metabolism of the insulin receptor plays a crucial function in decreasing glucose homeostasis and can induce significant diseases such as diabetes and cancer. Homeostasis can cause problems.The composition of the insulin receptor protein has been derived from the RCSB PDB (https:/www.rcsb.org) [11]. The X-ray crystal structure of the tyrosine kinase domain of the human insulin receptor has been increasingly determined by multi-wavelength anomaly diffraction and optimized to 1.8 A resolution [12]. Insulin-Receptor-Kinase complex arrangement Insulin-receiver domain crystal structure with cyclobutyl-(3-(azetidin-1-ylmethyl)-5-(3-(2H-pyran-2-yl)methoxy)phenyl-7H-pyrelo [2,3-d]pyrrimidine-4-amine (5HHW) has been retrievedFigure 3.

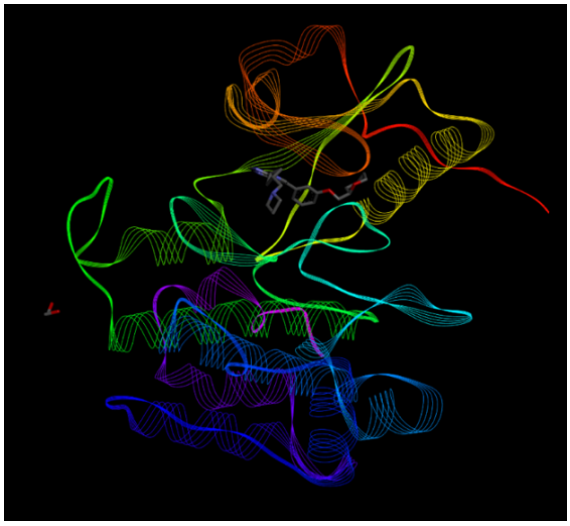


Figure 2: Structure of insulin kinase (5HHW)

Protein Structure Validation

The refined protein structure of 5HHW was evaluated individually using Ramachandran plot from the PROCHECKER web server and observed the allowed regions for the backbone dihedral angles ψ against φ od amino acid residues. The Ramachandran plot of initial validation of the proteins showed less than 90% of residues in the allowed region but after the refinement of the proteins showed more than 90% of residues in the allowed region and thus making the proteins stable to carry out with further molecular docking studies [13]. The percentage of residues in favored, allowed, and outlier regions of all the three proteins are shown in (Table 2).

Table2: Analysis of Ramachandran Plot

Protein Name	Number of Residues in the Favoured Region (%)	Number of Residues in the Allowed Region (%)	Number of Residues in the Outliner Region (%)
1TRK	93.6	5.6	0.4

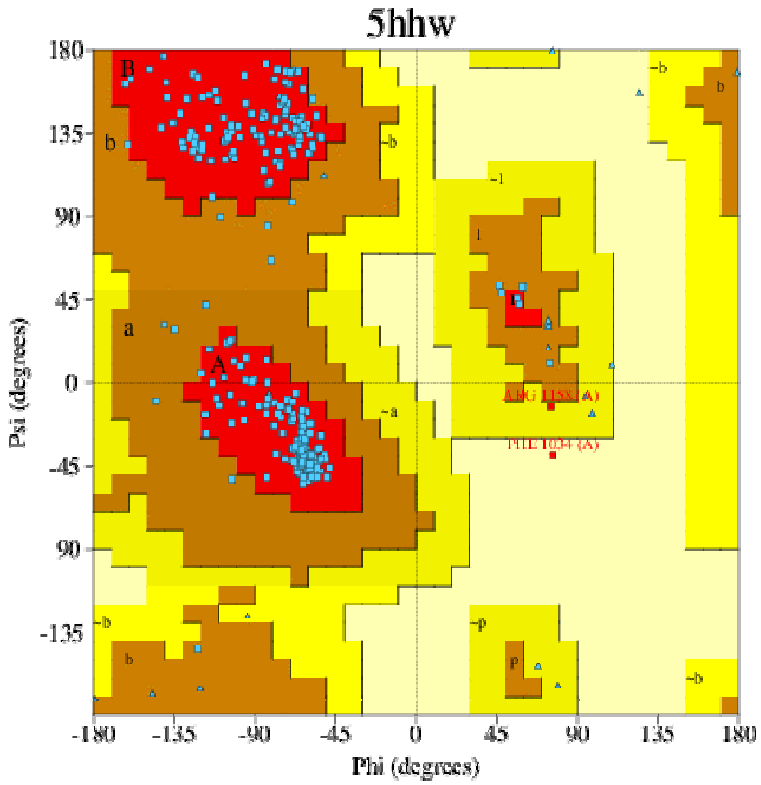


Figure 3: Structure Validation of Protein 5HHW

Selection of Plant

Traditional tetanus is used for the management and prevention of rabies in *Abrusprecatorius*. For medicinal purposes, leaves, roots, or seeds are used. In certain conventional remedies, the herb is used to treat cuts and sores and wounds of dogs, cats and mouse and is also used for the prevention of leukoderma with other ingredients. *Abrusprecatorius*plant is rich in various valuable amino acids such as serine, alanine, valine, choline, and methyl ester. Seeds are toxic and are compounded with Abrine as a concept [14].*Abrus precatorius* plant have some pharmacological activities such as anti-cancers, anti-diabetic, anti-depressant activity, diuretic activity. Well matured roots and leaves are used for antidiabetic treatments.

Structure of Phytochemicals

The structure of various phytochemical presents in *Abrus precatorius* like AbruquinoneB**,**Abruquinone C, Abrine, Gallic-acid, Abruslacton, Abricin, Abrussic-acid, choline, Picatorine,and Precasine using Pub Chem,(http://pubchem.ncbi.nlm.nih.gov) have been isolated and processed PubChem shall have free access to information on chemical compounds and their biological activities [15]. The commodity database includes chemical information generated by specific PubChem data providers and stores defining chemical structures obtained from the PubChem data base [16].

Identification of Toxicity

Toxic properties of isolated phytochemicals of *Abrus precatorius* is calculated by swiss ADME (http:/swiffadme.ebi) out of 10 phytochemicals, two compounds i.e.,Abruquinone C and Abruquinone B have been selected for further analysis. The scope was focused on the level of toxicity and bioactive compounds with 5 or 6 were picked [17]. The Swiss ADME database server has a basic interface based on the 3D configuration of the atoms in which the danger is predicted.

Table3: Represents the pharmacokinetic and drug likeness level of those compound from swissADME tool.

Compound	Pharmacokinetics						Drug Likeness			
	BBB Permeant	GI Absorption	CYP1A2 Inhibitor	P-gp Substrate	CYP2D6 Inhibitor	Log Kp(cm/s)	Ghose	Lipinski	Bioavailability Score	Veber
B	No	High	Yes	No	No	-7.21	Yes	Yes 0 violation	0.56	Yes
C	No	High	Yes	No	No	-7.6	Yes	Yes 0 violation	0.56	Yes

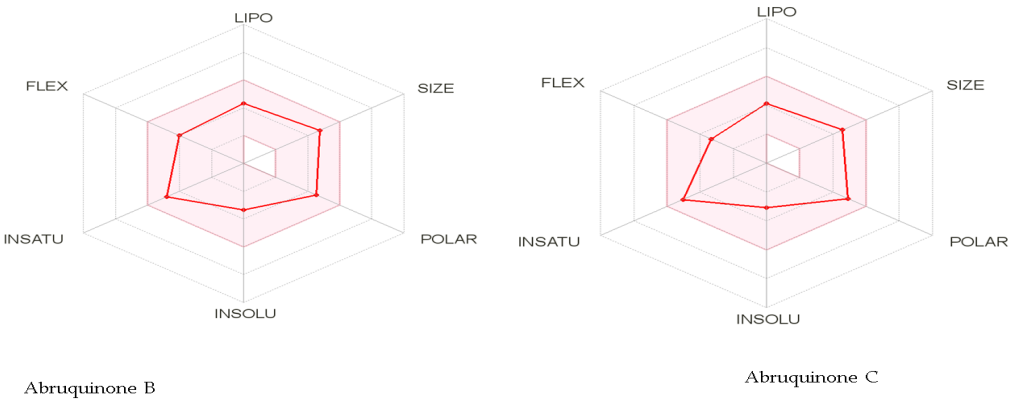
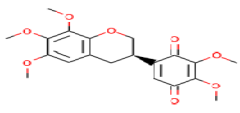
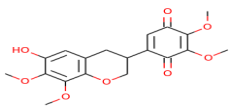


Figure 4: Bioavailability radar selected compounds a) Abruquinone B b) Abruquinone C

Selected phytochemicals docking complex with marker protein

The potential phytochemical was selected using Pyrx toolset by considering the Lipinski principle and the mutant target protein in DM. Pyrx is a server based on a molecular docking virtual based on geometry and the docking outcomes were analysed by using Discovery Studio. It is designed to detect docking changes that establish a good molecular shape.

Table 4:Scientific name, compound name, molecular formula and 2D structure of selected plant

Sl. No.	Plant Name	Scientific Name	Compound Name	Molecular Formula	2D Structure of Compound
1	Rosary pea	*Abrus precatorius*	Abruquinone B	$C_{20}H_2O_8$	
2	Rosary pea	*Abrus precatorius*	Abruquinone C	$C_{19}H_{20}O_8$	

Pharmacophore Training Preparation Datasets

The 3D structure of two phytochemicals of *Abrus precatorius* was Abruquinone B, Abruquinone C were chosen to demonstrate an efficient bind inside the desired protein's active binding pocket. The pharmacophores model based on Ligand demonstrated the main characteristics *i.e.* Aromatic HBD, HBA, hydrophobic, ionizing positive surface invaluable for binding the receptor. To make sure that each of them has all-atom arrangements, followed by energy minimization, specific hydrogen atoms have been added to each inhibitor [18]. Since the maximal ligands are bendy, considering a few different conformations with each molecule is a crucial prerequisite for the creation of a pharmacophore such that it can get a shape identical to real orientations of the experiment.

Generation of Pharmacophore Model

Abrus precatorius is an effective drug therapy target for DM. The study conducted molecular docking based on a ligand, the method for defining novel structural elements and scaffolds. Each ligand's pharmacophoric function was tested. Imports of phytochemical compounds (ligands) have been made in the Molinspiration ligand-based view of producing pharmacophores [19].The molinspiration software was used Protein-ligand activity for recognition and visualization of the sites and generation of the pharmacophore model. It retrieves ligands PDB files and assigns bonds to their protein setting and tiny molecule features (compounds) in automated Path or circulated. The software also generates and visualizes pharmacophore models that represent interactions, a universal mixture of protein and ligand.

RESULTS

Various part of *A. precatorius* plant is use for several medicinal activities like anti- cancer, anti- diabetic. This plant consists toxic and non-toxic phytochemicals such as Abruquinone B, Abruquinone C, Abrine, Gallic-acid, Trigonelline, Abricin, choline, Picatorine, Palmitic, Octadecanoate present in *Abrus precatorius* were extracted and analysed using PubChem [20].Just two of the ten phytochemical A. precatoriuscomponents met the law of Lipinski 5 and were chosen for pharmacophoric models. The selected compounds and their chemical characteristics are discussed in table 5.

The structural weight of the mutant insulin receptor protein kinase is 35448.66, atom count is 2480, residue count is 307, and one protein strand (Figure 2) is having crystal structure of the cis-(R)-7-(3-(azetidine-1yl-methyl) cyclobutyl)-5-(3- (tetrahydro-2H-pyran-2-yl) methoxy)-7H-pyrrolo [2,3-d] pyrimidine 4- amine insulin receptor kinase complex [21]. Two mutations, *i.e.* the 5HHW protein showed C5S, D156N. The removal of non-standard residues has optimized the protein structure, the PyRx docking file for the study of ligand-protein interactions and the structure of the targeted protein with the compound was sent to the docking Pyrx server [22].

The molecular docking of the Pyrx program to concentrate on important binding interactions was performed to verify the proposed model [23]. The molecular pattern of association between mutated proteins and any phytochemical site to which the ligand is bound has been explored. The effects of docking were analysed and contrasted to the discovery studio. Two compounds were found to successfully bind into the desired protein's active binding pocket (figure7a-b). The interactions with protein ligands indicate both the protein and the efficient van der Waals residues interacting. The 2D diagrams display both interactive protein residues and heavy Vanderwaals force as shown in figure 7 [24].Results of the docking of two compounds with targeted protein in the binding area of the INSR shown. The interactions between protein ligands reveal all the residues of the Proteins and Vander Waals's solid intensity.

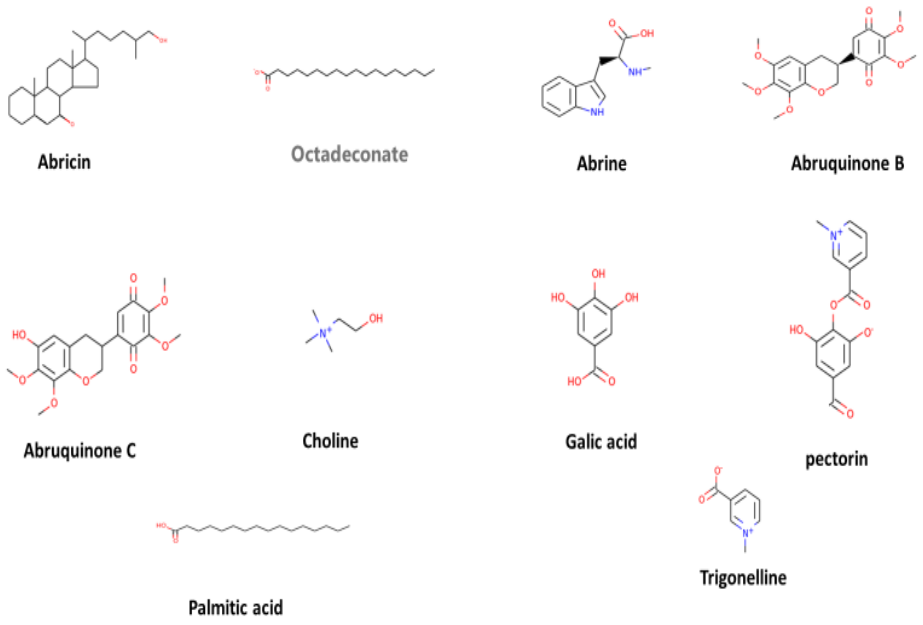
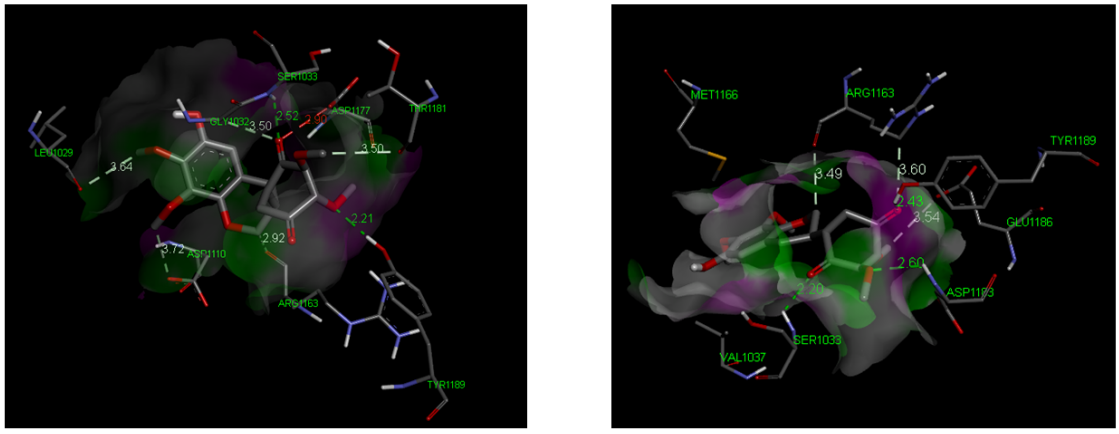


Figure 5: 2d structure of phytochemical of *Abrusprecatorius*

Table5: Phytochemical of A. precatorius following Lipinski rule of 5 and toxicity class

Phytochemical	HBD (hydrogen bond donor)	HBA (hydrogen bond acceptor)	MW(g/Mol) (molecular weight)	RB (rotatable bonds)	CP (complexity)	TC (toxicity class)
AbruquinoneB	0	8	390.39	6	682	5
AbruquinoneC	1	8	376.9	5	667	5



Abruquinone B Abruquinone C

Figure 6: 3D Protein ligand structure interactions in the active binding pocket of diabetes mellitus mutated protein

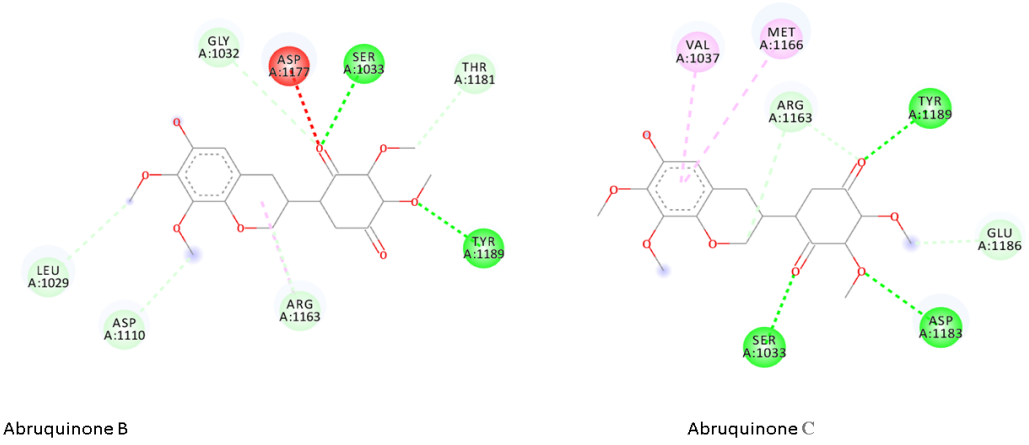
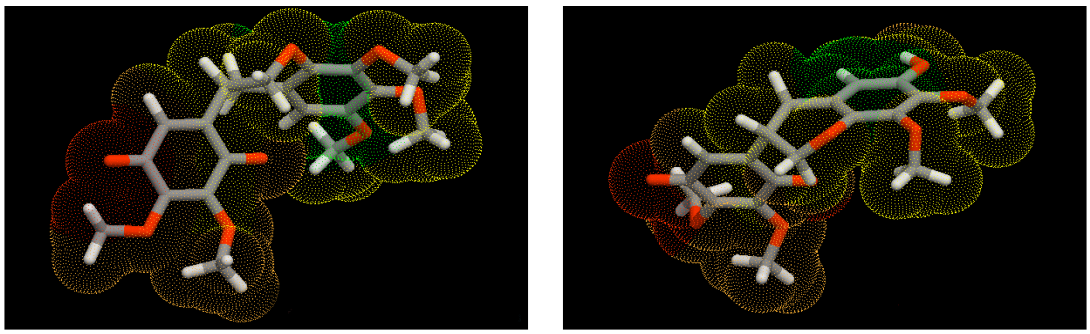


Figure 7: 2D Structure of Docking Result

Table6: Docking result selected ligands with 5HHW receptor protein(binding score, interaction residue)

Compound	Abruquinone B		Abruquinone C	
	Docking score (ΔG, Kcal/mol)	H- bonds	Docking score (ΔG,Kcal/mol)	H- bonds
1	-7	_	-7.4	_
2	-6.8	SER1003, ASP1177, THR1181	-.72	ARG1163, TYR1183
3	-6.8	ASP1110, GLY1032	-7.2	GLYU1186, ASP1183
4	-6.6	LEU1029, ASP1183	-6.8	SER1033
5	-6.5	LEU 1029	-6.7	MET116
6	-6.3	PHE1033	-6.4	VAL1037
7	6.3	MET1167	-6.4	SER1033

2D protein interactions diagrams showed all Protein and the forceful van der Waal communicating residues as figure 7. [(11)] shown. The result of docking of 2 phytochemical constitutes of *A. precatorioua* with binding region of INSR targeted protein figure 8. shows that *Abruquinone B* was interacting with SER1003, ASP1177, THR1181, ASP1110, GLY1032, LEU1029. Likewise, Abruquinone C ARG1163, TYR1183, GLU1186, ASP1183, SER1033. The study of pharmacophores was calculated as an integral component of the layout for drugs.The pharmacophore was developed with the assistance of, Molinspiration confirmed a number of the chosen chemical components Properties like the acceptor of hydrogen bonds (HBA), hydrogen bonds Donor (HBD), Hydrophobic (H), aromatic and positive ionizable (I) (AR) rings. The selected chemicals each pharmacophore model for constituents. The red color reflects the acceptor of hydrogen bonds. The colour green reflects the donor of hydrogen bonds and the yellow spheres Hydrophobic, blue rings represent an aromatic shell. Positive ionizable spheres and blue spheres, as seen in Figure 9. Besides, several excluded quantities have been developed within the Models to exhibit distance balance. The models consisted of aromatic rings, which were hydrophobic as a typical characteristic also hydrogen-bond acceptors, hydrogen bond donors. Like the 3D Structure of Abruquinone B, Abruquinone C Includes aromatic ring,(Funatsu *et al.*, 1988)strong ionizable and hydrophobic, hydrogen bond acceptors, hydrogen bond donors. Comparative review of the kinase domain of insulin receptors in the complex Cis-(R)-7-(3-(azetidine-1-ylmethyl) cyclobutyl)-5-(3-((tett)) cis-(R)-7-(3-(azetidine-1-ylmethyl) cyclobutyl) Methoxy) phenyl)-7H-pyrrolo [2,3-d] hydro-2H-pyran-2-yl) Pyrimidine-4-amine and two other plant chemicals are included in Figure. 8. This study is the validation stage for all phytochemicals screened. Likewise, its initial ligand docked inside the protein active binding pocket, as seen in Figure10.



a b

Figure 9: Ligand-based pharmacophore a) Abruquinone B, b) Abruquinone C

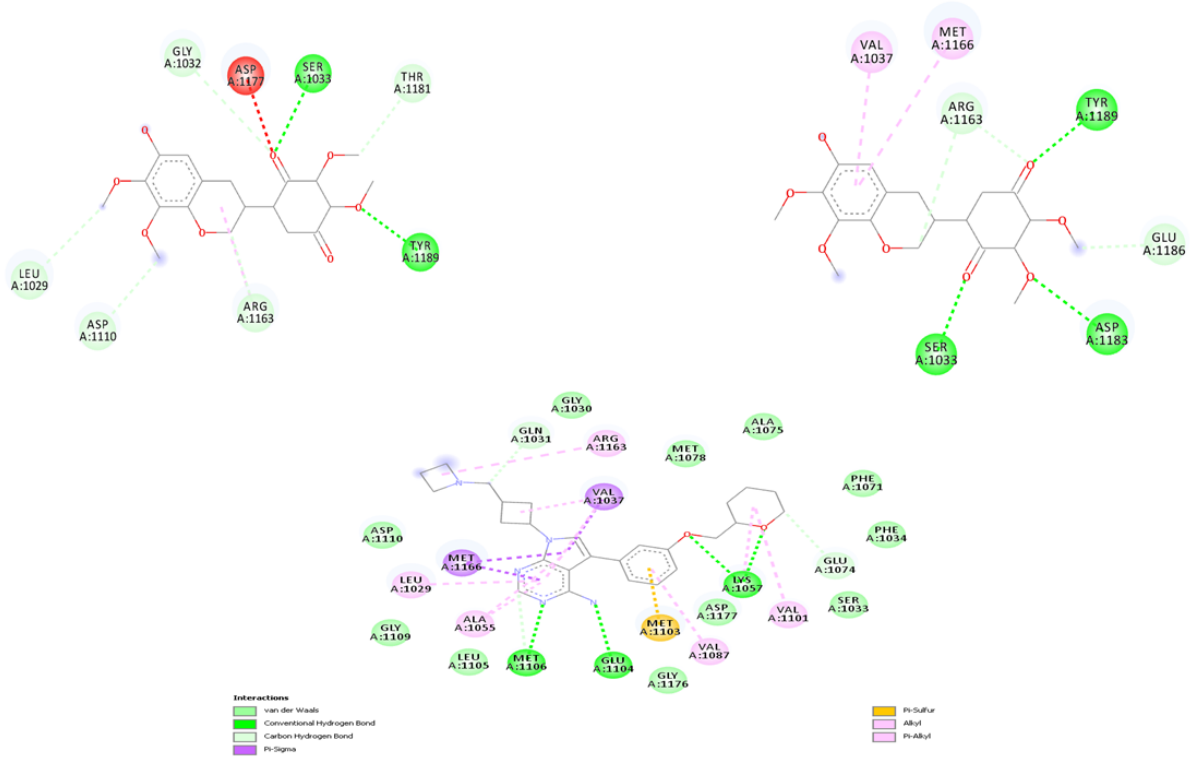


Figure 10: 2D Contrast of Proteins and Two Phytochemicals

DISCUSSION

As a healing agent, various medicinal plants have been used *A. precatorius* is a very popular medicinal plant or different illnesses. As is typically utilized for the treatment of different health problems, including Diabetes Type 2 Non-insulin-induced DM (type II), is typically caused by elevated levels of postprandial glucose, is the most prevalent form of diabetes. Glucosidases, a family of enzymes (a-amylase and a-glucosidase) in which complex carbohydrates (starches and oligosaccharides) are broken down into basic sugars such as maltose and glucose. In a randomized trial with untreated T2DM patients, anti-hyperglycaemic shows activity *A. precatorius* leaves have been identified. In T2DM patients, their dietary intake substantially decreased the level of glucose in the bloodstream. *A. precatorius* leaves and seeds have been reported as having comparatively high antioxidant activity. In vivo experiments indicate that aqueous abrasion extract decreases blood glucose levels in healthy rats and normalizes high blood glucose levels in a sub-, moderate, and substantially diabetic rats, besides, it increases glucose tolerance in normal, sub-and severe diabetic animals. It is important to note that the sample was more successful than the reference drug. The presence of phytochemicals Abruquinone B, Abruquinone C, may be attributed to this substantial decrease in blood glucose content. The aqueous extract has previously been reported to exhibit higher anthraquinone concentrations, a category of naturally occurring phenolic compounds found in *A. precatorius* leaves. Apart from its antimicrobial impact, it is also likely that it has

potential as a diabetes therapeutic agent. The activity of the phytochemicals examined was evaluated on a statistical basis in this report. *In-silico* molecular docking suggests that they were highly selective and screened for phytochemicals. Significant associations with mutant diabetes protein have been shown. The production of *A. precatorius* was demonstrated by the phytochemical examination of bioflavonoids that can promote glucose absorption in peripheral tissues and control the function of enzymes involved in the metabolism of carbohydrates. Flavonoids aid to secrete insulin, likely by affecting pleiotropic pathways to reduce DM complications. In the present research, and *In-silico* analysis was performed to examine the anti-diabetic activity of *A. precatorius*phytochemicals. The structure of flavonoids was derived from PubChem and its toxicity class was regulated. Docking analysis of flavonoid with mutated protein shows that it binds within the pocket, but unfavourable bumps have been found which expose weak binding between interactive amino acids and drug atoms. This study shows that ligands have been highly selective in their target protein. Abruquinone B, Abruquinone C, is closely related to the modified diabetic antigen. A 3D structure of the ligand-based pharmacophore model, showing the key features, i.e. HBD, HBA, Scent Ring, Hydrophobic, positive ionizable, essential to bind to the receptor in the potential, these pharmacophoric properties in phytochemicals will enable the development of new anti-diabetic medicines. Also, in-silicon elucidation has shown that such experiments make a substantial contribution to the design and development of effective chemical compounds for various health conditions such as cancer, coronary disorders, neuro-generative complications, pathogenic pathogens, respiratory diseases, and genetic anomalies. In contrast, the efficacy of these ligands with a serious risk of diabetes can be confirmed by *in-vivo* and *in-vitro* trials.

CONCLUSIONS

Many drugs have been pursuing ethno-pharmaceuticals and the conventional therapies into the world market. While herbal medicinal products have been used for millennia. Molecular docking and pharmacophoric tests of Potential bio-molecular targets have been shown by *Abrus precatorius*. It has been determined that Abruquinone A, Abruquinone C, phytochemical groups, and structural manifolds are likely to target mutated diabetes mellitus proteins. These findings will include a model for the synthesis of bioactive phytochemicals, de novo structural motive synthesis and further phytochemical investigations. The active binding bucket of the mutated proteins, the simulated complexes showed equilibrium, and ligands persisted. In this analysis, these screened phytochemicals may be used as a possible treatment candidate for diabetes mellitus prevention.

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