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Molecular Docking and TLC Analysis of Candidate Compounds from Lesser used Medicinal Plants Against Diabetes Mellitus Targets

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Abstract

The present work intends to investigate the potential of phytochemicals from less commonly used medicinal plants as possible candidates for Type 2 Diabetes (T2D) treatment using an *in silico* method. Plant ligands with T2D targets were studied using molecular docking techniques. The total binding energies of the targets and commonly used allopathic drugs were assessed and compared. The docking studies demonstrated very high binding energies between phytochemicals and diabetes targets as compared to the allopathic drugs. The presence of pharmacologically active components of the genus in the selected raw material of the plant species was also established. The study suggests that phytochemicals from the three species, *Silybum marianum*, *Eriobotrya japonica, and Withania coagulans,* can be effective therapeutic products for the treatment of T2D, calling for focused research on pharmacological investigations and product formulation.

Keywords: Diabetes mellitus, Silybum marianum, Eriobotrya japonica, Withania coagulans Molecular Docking

1. Introduction

Diabetes mellitus is a metabolic disorder where either the pancreas is unable to produce enough insulin (Type 1 diabetes) or is unable to utilize the insulin produced (Type 2 diabetes or NIDMM-Non-insulin dependent diabetes mellitus), or both. It can also occur during pregnancy (Gestational diabetes). Type 2 diabetes (T2D) is the most common of the three types (American Diabetes Association, 2009). Diabetes aggravates the chances of cardiovascular, neurological, and immunological failures and is known to affect around 463 million people worldwide (Saeedi *et al*., 2019). Different treatments for diabetes have been prescribed in Ayurveda, Unani, Allopathy, Homeopathy, etc. Sulfonylureas, GLP-1 agonists, DPP4 inhibitors, PPAR-gamma agonists, GPR119 agonists, bariatric surgeries, and therapies like SGLT2 are all common medications available in today's allopathic medicine and surgery system (Kaladhar et al., 2012). They do, however, have drawbacks, such as limited efficacy with hyperglycemic individuals and potential adverse effects such as low blood sugar, liver, kidney, and other organ damage (Feingold, 2020). Plant-based medications are highly suggested for diabetes therapy in this scenario (**Al Jamal, 2009**). The use of many plants for the treatment of diabetes is mentioned in Ayurveda (one of the oldest therapeutic sciences) (Pandey et al., 2013). Despite the fact that more than 400 plants have been found to have anti-hyperglycemic properties, only a few are consistently used in the production of herbal drugs (Verma et al., 2018). As a result, there is a need to investigate different medicinal plants for the production of herbal drugs.

In bioinformatics, molecular docking has been useful in predicting the orientation of targets and ligands to create a stable complex, which is then used for drug discovery and drug designing (Ahmad et al., 2016). The efficacy of a therapeutic molecule is anticipated in these studies based on the interaction and 'best-fit' between a ligand and the target (Abuhamdah *et al*.**,** 2020**).** The aim of this study was to apply these methodologies to forecast the anti-diabetic potential of less widely used medicinal plants for the treatment of T2D and to compare their efficacy to that of commonly used allopathic diabetes medicines.

2. Materials and Methods

2.1. Survey of Literature

An extensive literature survey was done to identify plants with anti-diabetic properties but rarely used in diabetes treatment. Following that, a list of potential plants was compiled by studying the ingredients of commercially available ayurvedic formulations. Simultaneously, a study was conducted on the various types of allopathic drugs used to treat diabetes (Gandhi *et al*., 2017; Narhe *et al*., 2018).

2.2. Ligand and Target Preparation

For docking experiments, the active components of chosen plants with anti-diabetic potential were employed as ligands. Commonly used allopathic drugs served as a control ligands. Docking was performed on 20 probable T2D targets. The Protein Data Bank (PDB) file format of

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selected ligands and targets was acquired from the Research Collaboratory for Structural Bioinformatics PDB (https://www.rcsb.org/) (Natarajan *et al*., 2015) and canonical or isomeric smiles from Pubchem database (https://pubchem.ncbi.nlm.nih.gov/) (Ahmad *et al*., 2016) (later converted into PDB format) (https://cactus.nci.nih.gov/translate/) (Renuka and Berla 2013).

2.3. Molecular Docking

For molecular docking, the iGemdock software was employed. All of the targets were docked with each ligand. Default settings such as population size of 200, generation size of 70, and number of solutions 2 were used to predict docking locations. The interaction of ligands and targets was investigated.

2.4. Thin layer chromatography (TLC) analysis

To identify the active components in the plant extracts, TLC was used with a variety of aqueous media and solvent solutions.

2.4.1. Sample and Solvent preparation

2.4.1.1. Silymarin from Silybum marianum (S. marianum)

The starting material was defatted *S. marianum* seeds obtained from Sorich Organics (New Delhi, India) (Figure 1a), from which two samples were made. Seeds were weighed, macerated, and dissolved in 70 % ethanol (v/v) in a 1:3 (w/v) ratio for the first sample, which was stored at room temperature for 24 hours. 70 % ethanol (v/v) was added to this extract (1:10 v/v). After repeating the process four times, 1 ml of the extract was collected and kept for future use (Natarajan *et al*., 2015). For the second sample, the crushed seeds were treated in 100% methanol. The solution was incubated at room temperature for 24 hours before being processed in the same way as sample 1.

The solvent systems used were chloroform: acetone: formic acid (75:16.5:8.5), ethyl acetate: n-hexane (40:60), benzene: ethyl acetate (70:30), methanol: water (9:1) and 100% methanol (Suha and Khadeem, 2007; Abouzid, 2012).

2.4.1.2. Ursolic Acid from Eriobotrya japonica (E. japonica)

E. japonica leaves were collected from the mother plant growing at Laxman Chowk (Dehradun, Uttarakhand, India) (Figure 1b), oven-dried (40°C for 24 hours), crushed and used as an extracting material for two samples. The first sample was prepared by dissolving extracted material in 100% methanol (1:1 ratio w/v) and incubating it at room temperature for 24 hours with intermittent shaking (Khatik *et al*., 2019). Crushed leaves were dissolved in 100% ethanol (1:5 w/v) and kept at room temperature for 24 hours with intermittent shaking for the second sample (Delfanian et al., 2016). The samples were evaporated in a water bath at 64°C for methanol and 78°C for ethanol until thick concentrated samples were obtained. Toluene: ethyl acetate: formic acid (8:2:0.1), acetonitrile: water (3:2) and butanol: acetic acid: water (4:1:5) were utilized as mobile phases (Gupta *et al*., 2011).

2.4.1.3. Withanolide A and Withaniferin A from Withania coagulans (W. coagulans)

Seeds of *W. coagulans* were procured from a local Ayurvedic medicinal store in Dehradun, Uttarakhand, India (Figure 1c). Seeds were dried, crushed, dissolved in 100% methanol (1:4 ratio w/v) and kept at room temperature for 24 hours with intermittent shaking for sample preparation (Peerzade et al., 2018). The solution was evaporated at 64°C in a water bath until a concentrated solution was obtained. For the second sample, 15-20 seeds of *W. coagulans* were soaked in 50 ml water. The solution was incubated at room temperature for 24 hours before being evaporated in a water bath at 100°C until a concentrated solution of 1ml was produced.

The solvent systems used were butanol: water: acetic acid (7:1:2), toluene: ethyl acetate: formic acid (5:5:1), chloroform: methanol (9:1) and benzene: ethyl acetate (2:1) (Sudhanshu *et al*., 2012, Preethi and Senthil, 2014; Poorani, 2014;).

2.4.2. Solvent application, development of chromatogram and visualization

The chromatographic analysis was performed on a heat activated aluminium, precoated silica gel 60 F_{254} TLC plate (E. Merck) of uniform thickness (0.2mm). A 100 µl syringe was used and a 10 µl sample was loaded. The component separation was carried out at room temperature in a twin trough glass chamber (20 x 10 cm) filled with 20 ml of the solvent system. The TLC plates were then visualized at 256 nm and 366 nm and the R_f value was evaluated.

Figure 1 Plant material for sample preparation for chromatographic analysis 1a: Seeds of *Silyburn marianum* 1b: Leaves of *Eriobotrya japonica* 1c:Seeds of *Withania coagulans*

3. Results

The aim of this research was to find medicinal herbs that have excellent anti-diabetic properties but are underutilized in commercial pharmaceutical compositions. Besides the existing literature, the Ayurvedic medicines available in Indian marketplaces for diabetes management were investigated. Diabecon Tablets 60, Diabecon (DS) Tablets 60, Dabur Madhu Rakshak Tablets, and Dabur Vasant Kusumakar Ras Tablets, Dia-beta plus 60 veggi capsules, are a few examples. Based on above findings, eight plants were identified with strong anti-diabetic properties. Chemically active ingredients of these plants were also identified to be used as ligands for docking studies (Table 1). The 20 powerful targets were chosen based on their functions in the human body (Table 2). A total of 400 ligand-target combinations were examined. The efficiency of medicinal plant ligands for diabetes treatment was also compared to commercially accessible

and commonly used allopathic drugs. Control ligands Metformin, Glimepiride, Pioglitazone, and Gliclazide were used docked with 20 potential targets, making a total of 80 combinations of control treatments.

Table 1. Medicinal plants with antidiabetic potential and their active components.

S.N	Scientific name	Active component
1.	*Commiphora wightii* (Sarup *et al*., 2015)	E-guggulsterone Guggulsterol2 Guggulsterol3 Guggulsterol4 Guggulsterone Z- guggulsterone
2.	*Swertia chirayita* (Kumar and Staden, 2016)	Mangiferin Swerchirin Amarogentin
3.	*Withania coagulans* (Maurya, 2010)	Coagulin C Coagulin L Withanferin A 17 β Withanolide K
4.	*Eriobotrya japonica* (Liu *et al*., 2016; Zhou *et al*., 2007)	Ursolic Acid Triterpenoid
5.	*Berberis vulgaris* (Rahimi-Madiseh *et al*., 2017)	Berberine
6.	*Silybum marianum* (Kazazis *et al*., 2014)	Silymarin
7.	*Myrica esculenta* (Sood and Shri *et al*., 2018)	Myricetin Quercetin
8.	*Tinospora cordifolia* (Saha and Ghosh. 2012)	Tinosporin Quercetin Berberine

Table 2. Protein targets and their role in Type 2 Diabetes (T2D) regulation.

S.N.	Target name	Role
1.	T-cell protein tyrosine phosphatase (TCPTP) (Dodd *et al.,* 2019)	Regulates insulin receptor signalling and gluconeogenesis in the liver.
2.	PTP1B (Kumar and Staden, 2016; Dodd *et al.,* 2019; Thareja *et al.,* 2012)	Dephosphorylates the insulin receptor in liver and muscle to regulate glucose homeostasis.
3.	α amylase (Kumar *et al*., 2016)	Responsible for postprandial glucose levels
4.	α galactosidase	Increases blood glucose levels.
5.	11β-Hydroxysteroid-dehydrogenase type 1(Kumar and Staden, 2016)	Inhibition of this helps in reducing tissue-specific gluconeogenesis and fatty acid metabolism.
6.	Aldose Reductase (Natarajan *et al*., 2015; Oates, 2008)	Catalyzes the reduction of glucose to sorbitol in the polyol pathway.
7.	Fructose 1 6 biphosphatase (Poelje *et al*., 2006)	Fructose 1,6-bisphosphatase (FBPase) is a key enzyme in gluconeogenesis. It is a potential drug target in the treatment of type II diabetes
8.	AMPK subunit beta-1 (Zhang *et al.,* 2009)	Maintains glucose homeostasis
9.	α 2 subunit	Helps in proper β-cell Ca^{2+} influx through multiple HVCC isoforms. Its absence lowers insulin secretion and results in impaired glucose tolerance.
10.	Sodium glucose cotransporter inhibitor (Kumar and Staden, 2016)	Helps kidneys in lowering blood glucose levels.
11.	Glycogen synthase kinase 3 (Natarajan *et al*., 2015; Ring *et al*., 2003)	Regulates glycogen synthesis
12.	Gpr40 (Kumar and Staden, 2016)	It is highly expressed in pancreatic β cells and is involved in insulin secretion.
13.	Sulfonyl ureas (Del Prato and Pulizzi, 2006)	Stimulates insulin secretion from pancreatic β cells
14.	Glucokinase (Natarajan *et al*., 2015; Ferre *et al*., 2003)	Functions as a glucose sensor in the β cells by controlling the rate of glucose entry into the glycolytic pathway
15.	PPAR-γ (Natarajan *et al*., 2015; Kumar and Staden, 2016)	Regulates insulin sensitivity.
16.	Glucagon-like peptide 1 (Glp 1) (Kumar and Staden, 2016)	Stimulates insulin secretion and inhibits glucagon secretion.
17.	Cytochrome P450 (Eid *et al*., 2009)	Increases the drug response in different disease
18.	DGAT0 1 (Kumar and Staden, 2016)	Catalyzes triglycerides synthesis
19.	Pyruvate dehydrogenase kinase isoform 2 (Lee, 2014)	Helps in glucose disposal
20.	17β-Hydroxysteroid-dehydrogenase type 1 (Kumar and Staden, 2016)	Activates functionally inert glucocorticoid precursors (cortisone) to active glucocorticoids (cortisol) within insulin target tissues, such as adipose tissue, thereby regulating local glucocorticoid action.

3.1. Docking results

The aim of molecular docking is to achieve an optimal orientation and conformation of the ligand-receptor binding complex, demonstrated by less free energy of the binding. The energy levels obtained from the plant ligand-target combinations and allopathic medicine ligand-target combinations showed better docking results between plants' active ingredients and the targets as compared to the docking combination of allopathic medicines with their specific targets. Out of the different combinations, good energy levels were obtained with chemical constituents of *S. marianum*, *E. japonica*, and *W. coagulans* with targets Ptp1b and 11 Beta HSD1 (Table 3, Figure 2).

Table 3. Docking results of active components of *Silybum marianum*, *Eriobotrya japonica* and *Withania coagulans* with various targets of Type 2 Diabetes.

S.N.	Target- ligand	Plant used for extraction	Total energy of binding (kcal/mol)
1	ptp1b-silymarin	*S.marianum*	-323.716
2	ptp1b-coagulinL	*W.coagulans*	-301.848
3	ptp1b-triterpenoid	*E.japonica*	-285.77
4	ptp1b-coagulinC	*W.coagulans*	-284.116
5	ptp1b-ursolicacid	*E.japonica*	-262.094
6	ptp1b-withanolide A	*W.coagulans*	-251.823
7	DGAT1-triterpenoid	*E.japonica*	-151.823
8	11 beta HSD1-silymarin	*S.marianum*	-150.736
9	17beta HSD1-silymarin	*S.marianum*	-139.748

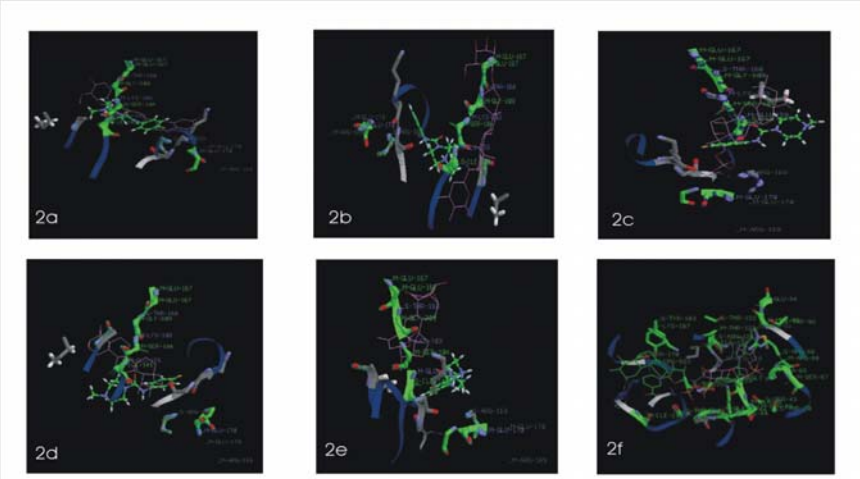

Fig 2: Docking interactions from iGemdock software (2a) Silymarin with Ptp1b (2b) CoagulinL with Ptp1b (2c) Triterpenoid with Ptp1b (2d) Ursolic acid with Ptp1b (2e) Withanolide A with Ptp1b and (2f) Silymarin and 11 Beta HSD1

For target PPARγ, the best results were obtained with Coagulin L from *W. coagulans*. The total binding energy was observed at-115.16 kcal/mol, which is comparatively higher than the energy observed with other plant ligands, Silymarin (-103.886 kcal/mol), Ursolic acid (-106.6196 kcal/mol), all of which were much higher than the binding energy of Pioglitazone (-93.79 kcal/mol) with the target (Figure 3). For Cytochrome P450, the best docking results were observed with withanolide A (active component of *W. coagulans*) showing binding energy of-120.897 kcal/mol, which was higher than that obtained with allopathic medicines, gliclazide and glimepiride (-97.93 kcal/mol and-100.9 kcal/mol, respectively) (Figure 4). For target AMPK subunit beta-1, the best results were obtained with silymarin (*S. marianum), the* total binding energy being-113.586 kcal/mol, higher than the energy observed with commonly used metformin (-52.7833 kcal/mol) (Figure 5).

Docking studies revealed that *S. marianum* (common name: Milk Thistle), *E. japonica* (common name: Loquat), and *W. coagulans* (common name: Indian rennet) have chemical components with substantially strong anti-diabetic potential.

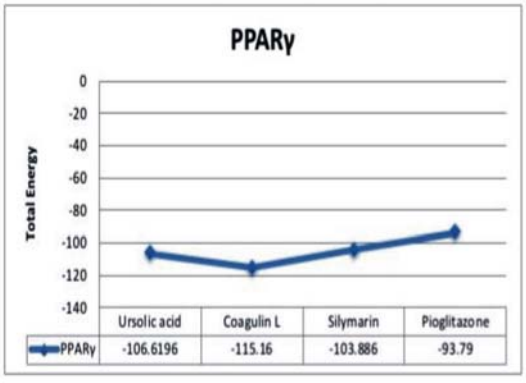

Figure 3: Comparison of total binding energies of Pioglitazone (an allopathic medicine) and other plant ligands with PPARγ

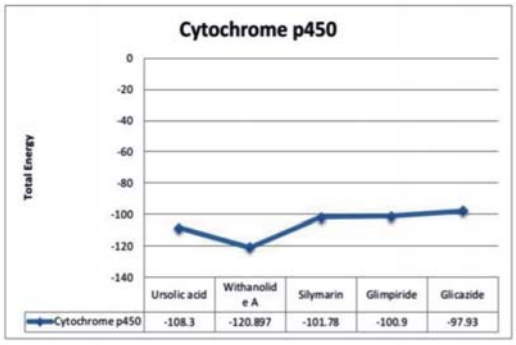

Figure 4: Comparison of total binding energies of allopathic medicines Glimpiride and Glicazide and other plant ligands with Cytochrome p450

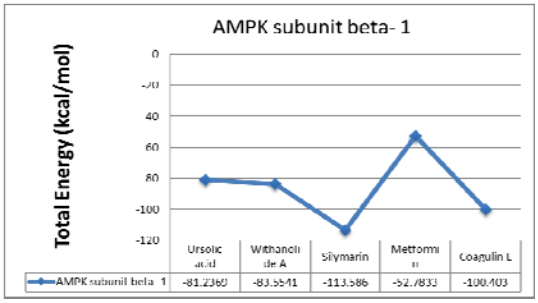

Figure 5. Comparison of binding total energies of allopathic medicine Metformin and other plant ligands with AMPK subunit beta-1.

3.2. Thin layer chromatography (TLC analysis)

Silymarin from *S. marianum*, ursolic acid from *E. japonica*, withaniferin A and withanolide A from W. *coagulans* were the four active components identified based on their binding energies. TLC in different solvent systems was used to confirm their existence in the readily accessible plant source material.

3.2.1. Silymarin

Identification was done on the basis of the standard R_f value, 0.57 in the various solvent systems (Suha and Khadeem, 2007). Of the different combinations tried, the best results were obtained in the ethanolic and 100% methanolic extracts in the benzene: ethyl acetate (70:30) solvent system (Table 4). The ethanolic extract had a dark wide band while a narrow band was observed in the 100% methanolic extract with an R_f value of silymarin, confirming that the seeds contain silymarin (Figure 6).

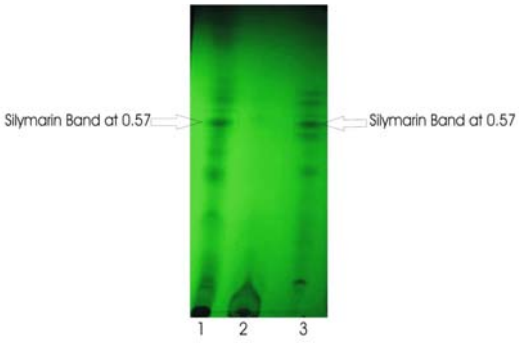

Figure 6: TLC plate developed in benzene:ethyl acetate (70:30) solvent system (Lane 1-Ethanol, lane 2- Ethyl acetate, Lane 3- 100%

Table 4: TLC observations of Silymarin in benzene: ethyl acetate (70:30) solvent system.

100% Methanol		Ethanol		Ethyl acetate	
Distance moved (cms)	R_f	Distance moved (cms)	R_f	Distance moved (cms)	R_f
6.3	0.41	3.5	0.23	5.7	0.37
6.8	0.45	5.8	0.38	7.0	0.46
7.2	0.47	6.8	0.45	7.3	0.48
8.7	0.57	7.2	0.47	7.5	0.49
10	0.66	8.7	0.57		
		11.8	0.78		

3.2.2. Ursolic Acid

On the basis of a standard R_f value of 0.42, the presence of ursolic acid in the leaf extract of *E. japonica* was confirmed (Naumoska et al., 2013). The best results were obtained using the solvent system toluene: ethyl acetate: formic acid (8:2:0.1) (Table 5). At the standard R_f value, a green colour band was detected in the 100% methanolic extract (Figure 7).

Table 5: TLC observation of Ursolic Acid in toluene: ethyl acetate: 0.1% formic acid (8:2:0.1) solvent system.

100% Methanol		Ethanol		Ethyl acetate		Chloroform	
Distance moved (cms)	R_f	Distance moved (cms)	R_f	Distance moved (cms)	R_f	Distance moved (cms)	R_f
4.3	0.29	5.4	0.36	4.6	0.31	4.6	0.61
5.1	0.34	6	0.4	7.9	0.53		
5.8	0.39	6.7	0.45	8.1	0.54		
6	0.40	12.1	0.80	12.1	0.80		
6.3	0.42						

Figure 7: TLC plate developed in toluene: ethyl acetate:0.1% formic acid (8:2:0.1) solvent system (E-Ethanol extract, M-100% Methanol extract, CM-Chloroform methanol extract, EA-Ethyl acetate extract).Methanol)

3.2.3. Withanolide A and Withaniferin A

Standard R_f values of 0.932 and 0.81 in different solvent systems were used to determine the presence of withanolide A and withaniferin A in the seed extract (Peerzade et al., 2018). Of the different combinations tried, the best results were obtained in the Butanol: Water: Acetic acid (7:1:2) solvent system (Table 6). As per the R_f value of withanolide A and withaniferin A, bands were observed in the 100% methanolic extract (Figure 8).

Table 6. TLC observations of Withanolide A and Withaniferin A in butanol: water: acetic (7:1:2) solvent system.

100% Methanol		Acetone	
Distance moved (cms)	R_f	Distance moved (cms)	R_f
3.6	0.24	2.5	0.16
4.5	0.25	3.7	0.24
6.4	0.42	4.6	0.30
7.7	0.50	6.4	0.42
9.2	0.60	7.8	0.51
12.4	0.81	9.2	0.60
14.3	0.93	11.3	0.74
		14	0.91

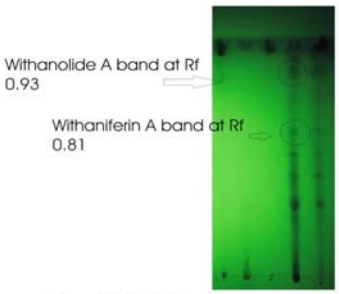

Figure 8: TLC plate developed in butanol: water: acetic (7:1:2) solvent system (C-Chloroform, W- water, P- Pteroleum ether, M-100% Methanol, A-Acetone)

4. Discussion

In our study, molecular docking studies were performed on plants that have been reported to be known in the traditional systems of medicine for diabetes treatment (Modak *et al*., 2007; Mondal *et al*., 2012). iGemdock is a graphical-automatic drug design system for docking, virtual screening, and identifying pharmacological interactions between ligand molecules and receptors (Kaladhar *et al*., 2012; Dar and Mir, 2017). In this study on molecular docking, three plants *S. marianum*, *E. japonica*, and *W. coagulans* outperformed other plants and commonly used allopathic drugs such as metformin, glimepiride, pioglitazone, and gliclazide. Metformin is reported to have a strong affinity for AMPK receptors (Leclerc *et al*., 2004; Leverve *et al*., 2003). Out of the different ligands tested, including metformin, the best docking results were observed between the AMPK subunit beta1 receptor and the silymarin ligand. The contributing bonds between target and ligand were hydrogen bonds with a -25.1233 kcal/mol and vander waals bonds with a –88.66 kcal/mol contribution to the total binding energy level. The major amino acids involved in this binding were arginine at 63, 138 and 171, serine at 173, leucine at 170, methionine at 163 and asparagine at 162. In the present investigation, Withanolide A was found to be a better ligand than allopathic drugs gliclazide and glimepiride, since it had the highest total binding energy with cytochrome P450. Hydrogen bonds (contribution-21.117 kcal/mol) and vander waals bonds (contribution-99.78 kcal/mol) were the most prominent bonds during this binding. The amino acids lysine (391), phenylalanine (393), glycine (396), and asparagine (395) contributed to this binding.

Similarly, thiazolidinediones are reported to be highly effective ligands for PPARγ receptors (Wilson *et al*., 1996). According to this study, Coagulin L from *W. coagulans* is more successful as a ligand in binding to the target than Pioglitazone, a thiazolidinedione. The major contributors to binding between Coagulin L and the PPARγ receptor were hydrogen bonds and vander waals bonds. Hydrogen bonds contributed- 104.77 kcal/mol energy whereas vander waals bonds contributed-10.39 kcal/mol energy to the total binding energy level, which is-115.16 kcal/mol. The amino acids that took part in the binding were serine at 370, phenylalanine at 315, isoleucine at 369, arginine at 316 and glutamic acid at 371.

Our results are in consonance with prior research that found active compounds in the selected plants to be promising candidates for diabetic treatment. Silymarin (from *S. marianum)* has been reported to be a complex of 7 active molecules that can be utilized for various therapeutic targets of T2D (Gupta *et al*., 2011; Ahmad *et al*., 2019). Wu *et al*., 2015 reported that ursolic acid and its triterpene analogues could be a potential ligand for treating T2D because of its high binding energy levels with the targets. Likewise, anti-diabetic properties have been reported for *W. coagulans* constituents (Guzman *et al*., 2018; Subburaya *et al*., 2020).

A chromatographic analysis of readily accessible raw materials of target plants was also performed as part of our research to establish the presence of active compounds. Solvents such as chloroform: acetone: formic acid (75:16.5:8.5) (Abouzid et al., 2012), ethyl acetate: n-hexane (40:60), benzene: ethyl acetate (70:30) (Suha and Khadeem, 2007), methanol: water (9:1), and 100% methanol were previously used to detect silymarin in *S. marianum*. Ursolic acid in *E. japonica* leaves has been determined using toluene: ethyl acetate: formic acid (8:2:0.1) (Gupta *et al*., 2011), acetonitrile: water (3:2) and butanol: acetic acid: water (4:1:5) (Khatik *et al*., 2019). For withanolide A and withaniferin A in *W.coagulans,* different reports have suggested the use of solvent systems including benzene: ethyl acetate (2:1) (Sudhanshu *et al*., 2012), toluene: ethyl acetate: formic acid (5:5:1) (Preethi *et al*., 2014), chloroform: methanol (9:1) (Poorani, 2014) and butanol: acetic acid (7:1:2) (Peerzade *et al*., 2018).

Our results confirm prior research that identified silymarin, ursolic acid, withanolide A and withaniferin A in the plant raw material.

5. Conclusion

Diabetes mellitus is a rapidly spreading threat to public health, healthcare, and the economy. Long-term use of allopathic drugs has been linked to debilitating side effects as well as potentially significant metabolic diseases. As a result, there is a growing demand for herbal remedies for diabetes therapy, which has resulted in overexploitation of several medicinal plants. There is a need to explore different phytochemical–target protein interactions to facilitate judicious drug development. Docking is a simple and effective method for predicting a phytochemical's efficiency by modelling plant ligand and protein receptor interaction. According to the findings of this study, Silymarin, Ursolic acid, Withanolide A, and Withaniferin A are prospective medication candidates that might be employed to build a successful therapeutic product.

Furthermore, TLC research has revealed that these compounds are present in commonly available plant materials. More concentrated efforts on these plants should be made for extensive phytochemical characterization, genotype-based active ingredient analysis, and subsequent herbal medicine development.

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