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Research Article

IN SILICO EVALUATION OF *ALOE VERA* PHYTOCONSTITUENTS FOR DIABETES MANAGEMENT

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ABSTRACT

Background:
Diabetes mellitus is a chronic metabolic disorder marked by elevated blood glucose due to insulin dysfunction. The rising global prevalence necessitates safer and more effective antidiabetic treatments. The disease through the ayurvedic to review the phytochemical constituents of *Aloe vera* that contribute to its antidiabetic properties.
Material and Methods:
Aloe vera, traditionally recognized for wound healing and anti-inflammatory effects, contains numerous phytochemicals with antidiabetic potential[(2)]. Key constituents like acemannan, emodin, and glycine are of particular interest .An *in silico* approach was employed to evaluate Aloe vera's compounds through molecular docking. Four diabetic target proteins—4WQ6, 1V4S, 5KZX, and 1VNF—were selected, and docking was performed using AutoDock Vina[(4).] Drug-likeness was assessed via Lipinski's rule, and target predictions were evaluated using bioinformatics tools like SwissADME and SwissTargetPrediction[(5)].
Results:
Molecular docking showed that glycine (-8.0 kcal/mol), acemannan (-7.7), and chrysophanol (-7.9) had strong binding affinities. All compounds complied with Lipinski's rules. Target prediction indicated interactions with GLUT4, DPP-4, and PPAR-α, key players in glucose metabolism.
Conclusion:
Aloe vera demonstrates significant potential in diabetes management via inhibition of diabetic targets. This computational evidence supports further pharmacological and clinical exploration of its constituents.

KEYWORDS
Aloe vera, Diabetes, Docking, *In silico*, Phytochemicals

INTRODUCTION

Diabetes mellitus (DM) is a chronic metabolic disorder marked by elevated blood glucose levels resulting from either insufficient insulin production, impaired insulin action, or both[(1).] It is one of the most pressing global health challenges,

affecting millions worldwide. The long-term complications of unmanaged diabetes include cardiovascular disease, nephropathy, neuropathy, retinopathy, and impaired wound healing. Despite the availability of various synthetic antidiabetic drugs such as insulin analogs, sulfonylureas, and DPP-4 inhibitors, their prolonged use often results in side effects, decreased patient compliance, and drug resistance. This has prompted increased interest in plant-derived compounds as safer, more sustainable alternatives for diabetes management.[2]

In traditional systems of medicine, numerous plants have been documented for their role in glycemic control. Among these, *Aloe vera* (*Aloe barbadensis* Miller), a well-known medicinal plant, holds significant promise[2]. Used for centuries in Ayurveda and other folk remedies, *Aloe vera* is widely recognized for its healing, anti-inflammatory, and immune-modulating properties. The plant contains a rich profile of bioactive compounds, including anthraquinones (e.g., aloin, aloe-emodin), polysaccharides (e.g., acemannan), vitamins, minerals, enzymes, and amino acids. Recent pharmacological studies have highlighted the plant's potential in lowering bloodglucose levels, enhancing insulin sensitivity, and reducing oxidative stress[2]. These findings underscore the relevance of *Aloe vera* as a natural candidate in the search for novel antidiabetic agents. The primary aim of this study is to explore the antidiabetic potential of *Aloe vera* using in silico computational techniques. By integrating molecular docking, ADME (Absorption, Distribution, Metabolism, and Excretion) analysis, and target prediction tools, this study seeks to assess the therapeutic viability of *Aloe vera*-derived phytochemicals against key diabetic protein targets.

The specific objectives of this study are to identify and select key bioactive compounds from *Aloe vera* with reported antidiabetic activity, to perform molecular docking of these compounds with major diabetic protein targets such as GLUT4, DPP-4, IRS, and PPAR-α[3,4], to predict the drug-likeness and pharmacokinetic properties of the selected phytochemicals using computational tools[5]. To analyze molecular interactions and pathways involved in glucose metabolism using target prediction databases.

MATERIALS AND METHODS

- Software Used:

The computational tools employed in this study include AutoDock Vina for molecular docking[4] , PyRx for ligand and receptor preparation and 3D visualization[5] , and SwissADME for pharmacokinetic and ADME (Absorption, Distribution, Metabolism, and Excretion) analysis[5] . AutoDock Vina for molecular docking, PyRx for 3D visualization, SwissADME for ADME (Absorption, Distribution, Metabolism, and Excretion) analysis.

- Ligands:

Phytochemical compounds present in Aloe vera were retrieved from the PubChem database. These compounds were screened based on Lipinski's Rule of Five to evaluate their drug-likeness and oral bioavailability[5] . Phytochemicals of *Aloe vera* were sourced from PubChem and screened for Lipinski's Rule of Five.

- Targets:
  Diabetic targets including 4WQ6 (GLUT4), 1V4S (DPP-4), 5KZX (IRS), and 1VNF (PPAR-α) were downloaded from the RCSB PDB.
- Preparation:

All selected protein structures were prepared by removing water molecules, adding polar hydrogen atoms, and optimizing the structures. Grid box parameters were defined based on the active site residues to ensure accurate docking. Ligands were energy-minimized and converted into PDBQT format using PyRx[3] . Water molecules were removed, hydrogens added, and docking grids were defined.

- Docking Parameters:

Molecular docking was performed using AutoDock Vina[4]. The output included binding energy (B.E.), Root Mean Square Deviation (RMSD) values, and hydrogen bonding interactions to evaluate ligand-receptor affinity and stability. Binding energy (B.E.), RMSD values, and hydrogen bond interactions were analyzed.

- Target Prediction:

Pharmacological pathways and potential protein targets were predicted using SwissTargetPrediction. ADME(Absorption, Distribution, Metabolism, and Excretion) profiles, including gastrointestinal absorption, BBB permeability, and cytochrome inhibition, were assessed via SwissADME [5] .To evaluate the pharmacokinetic potential of the selected phytochemicals. Binding interactions and pharmacological pathways were predicted using online databases like SwissTargetPrediction.

OBSERVATION AND RESULTS

TABLE 1 : *In silico* study of *Aleo vera*

Sr. No.	Phytochemical constituent	Molecular docking				ADME					Target prediction
		1st Protein 4WQ6	2nd Protein 1V4S	3rd Protein 5KZX	4th Protein 1VNF	MW	#H-bond	#H-bond	I LOGP	Lipinski #violations	

		B.E*	RMSD value	B.E*	RMSD value	B.E*	RMSD value	B.E*	RMSD value		acceptors	donors			
1	Acemannan	-7.7	5.22	-7	4.542	-7.3	4.54	-7.4	2.212	222.19	7	4	0.87	0	Pancreatic β-cells, GLUT4
2	Rhamnose	-5.4	2.921	-5.4	8.052	-4.8	32.377	-5.4	29.067	178.18	5	4	0.94	0	Dipeptidyl peptidase IV DPP4
3	Carboxypeptidase	-4.1	35.738	-5.1	3.309	-5	2.361	-5.5	31.454	247.33	5	5	1.85	0	Glutamate receptor ionotropic, AMPA 2
4	Glutamic Acid	-4.8	23.538	-5.1	16.873	-5.2	51.751	-5.2	4.454	147.13	5	3	0.4	0	Dipeptidyl peptidase IV DPP4 Peroxisome proliferator activated receptor alphaPPARA
5	Glutamin	-4.8	2.055	-4.6	19.964	-4.6	15.402	-5.2	2.324	146.14	4	3	0.38	0	Insulin secretion
6	Glycine	-8	3.221	-7	6.068	-7.5	50.061	-3.6	15.098	75.07	3	2	0.37	0	Antioxidant
7	Soleucine	-4.5	4.514	-4.7	28.423	-5.2	3.692	-5	2.543	147.17	4	3	0.47	0	Peroxisome proliferator-activated receptor alpha PPARA
8	Leucine	-4.6	2.733	-4.8	35.284	-4.7	29.61	-5.1	29.284	131.17	3	2	1.15	0	Peroxisome proliferator activated receptor alpha PPARA
9	Lysine	-4.8	3.519	-5.9	36.706	-5.7	50.217	-4.8	27.875	146.19	4	3	0.97	0	Peroxisome proliferator activated receptor alpha PPARA
10	Methionine	-4.5	35.216	-4.7	1.993	-5	30.626	-5.2	4.211	149.21	3	2	1.12	0	Dipeptidyl peptidase IV DPP4
11	Proline	-4.2	4.842	-4.5	36.047	-4.4	2.832	-4.8	28.563	115.13	3	2	0.84	0	Dipeptidyl peptidase IV DPP4
12	Threonine	-4.7	23.834	-4.5	34.45	-4.4	51.308	-7.9	2.333	115.13	4	3	0.33	0	Peroxisome proliferator

															activated receptor alpha PPARA
13	Valine	-4.8	2.063	-4.8	2.694	-4.6	3.376	-4.9	2.302	117.15	3	2	1.03	0	Glucose metabolism
14	Chrysophanol	-7.2	2.157	-7.2	21.337	-6.6	48.009	-7.9	7.413	254.24	4	2	2.22	0	Insulin receptor substrate (IRS), PI3K
15	Emodin	-6.4	18.894	-7.7	6.266	-6.3	36.664	-7.7	20.06	270.24	5	3	1.8	0	PPAR-γ, Akt
16	Caprylic acid	-4.5	2.341	-4.7	21.003	-4.6	12.454	-5	29.175	144.21	2	1	1.95	0	Peroxisome proliferator activated receptor alphaPPARA
17	Myristic acid	-3.6	2.529	-3.9	3.133	-3.5	22.615	-5.5	43.475	228.37	2	1	3.32	0	Peroxisome proliferatoractivated receptor alpha PPARA

*B.E.= Binding Energy / Affinity

DISCUSSION

The molecular docking study of *Aloe vera* compounds reveals promising interactions with key diabetic targets. Glycine displayed the strongest binding affinity (-8.0 kcal/mol) with GLUT4 (4WQ6), while emodin and chrysophanol also showed strong binding across multiple targets such as DPP-4 and IRS. These interactions suggest potential modulation of glucose uptake, insulin signaling, and lipid metabolism[4] .

All selected compounds followed Lipinski's Rule of Five, ensuring oral bioavailability and drug-likeness[5] . Most compounds interacted with more than one target, implying a multitarget mechanism—a desirable feature in chronic conditions like diabetes. For instance, acemannan, a known polysaccharide, showed strong interactions with GLUT4, supporting its known role in enhancing glucose uptake[2] .

PPAR-α, a key regulator of lipid metabolism and insulin sensitivity, was a common target for several compounds such as leucine, valine, and lysine. This suggests *Aloe vera* may have both hypoglycemic and hypolipidemic actions.

In silico reduce the time and cost of initial screening. The docking scores and predicted targets are promising, these findings are theoretical and require biological validation. In vitro and in vivo studies are necessary to confirm these results and evaluate pharmacodynamics and toxicity profiles.

CONCLUSION

The present *in silico* investigation confirms that *Aloe vera* contains multiple bioactive compounds with potential antidiabetic properties. Key compounds such as glycine, emodin, chrysophanol, and acemannan showed high binding affinity toward diabetic targets like GLUT4, DPP-4, and PPAR-α. These proteins play pivotal roles in insulin action, glucose metabolism, and lipid regulation.

The all compounds followed drug-likeness criteria suggests that they are viable for further pharmacological development. The multitarget profile observed for several phytochemicals supports the use of *Aloe vera* in holistic diabetes management strategies.

These provide a strong foundation for future experimental research. Clinical validation, dosage optimization, and formulation development are crucial next steps. The *Aloe vera* as a candidate for natural, plant-based diabetes treatment.

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REFERENCES

1. American Diabetes Association. Diagnosis and classification of diabetes mellitus. Diabetes Care. 2010;33(Suppl 1):S62–S69.

2. Eshun K, He Q. Aloe vera: a valuable ingredient for the food, pharmaceutical and cosmetic industries—a review. Crit Rev Food Sci Nutr. 2004;44(2):91-6.
3. Morris GM, Huey R, Olson AJ. Using AutoDock for ligand-receptor docking. Curr Protoc Bioinformatics. 2008;24(1):8-14.
4. Trott O, Olson AJ. AutoDock Vina: improving the speed and accuracy of docking with a new scoring function. J Comput Chem. 2010;31(2):455-461.
5. Daina A, Michielin O, Zoete V. SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Sci Rep.2017;7:42717.