RESEARCH PAPER

Identification of Therapeutic Active Compounds from Solanum torvum by Using Computational Methodology

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ABSTRACT

This study's area was to use a computational approach model to find pharmacologically active chemical elements in fruit extracts from Solanum torvum. Following de-replication and ADMET screening, a subset of compounds was prioritized for molecular docking against the primary metabolic targets, the PPARγ receptor and HMG-CoA reductase, in order to screen for antidiabetic and antihyperlipidemic treatment efficacy, which are targeted to the management of diabetes and hypercholesterolemia. LC-MS analysis of hexane and ethanolic extracts revealed the presence of 12,250 and 9,963 constituents, respectively. Numerous ligands, including quercetin, maritimetin, chrysin 5-xyloside, and sigmoidin G, showed strong binding charms and stable interaction patterns in docking simulations, suggesting their potential as dual inhibitors. Strong ligand–receptor docking was demonstrated by contacts that were primarily stabilized by hydrophobic and hydrogen bonding interactions. This study offers a pharmacological explanation for the conventional use of Solanum torvum in the treatment of metabolic disorders and validates the efficacy of combining LC-MS profiling with In Silico screening to characterize bioactive molecules from complex plant constituents, providing opportunities for additional drug development.

Keywords: Solanum torvum, LCMS, Computational methodology, Docking studies, Soxhlet extraction

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1.Introduction:

The perennial plant *Solanum torvum*, commonly known as the turkey berry, fits to the Solanaceae family. In humid and subtropical areas, it is extensively dispersed. These comprise the South as well as parts of the Caribbean, Africa, and Southeast Asia [1]. However, the plant grows well in a variety of environments, including deteriorated soils and the borders of forests. And this shows how adaptable and resilient it is. Prickly stems, wide leaves, and clusters of tiny green berries are characteristics of S. torvum. When mature, these berries turn red. The berries, leaves, roots, and stems all contain bioactive compounds. From the standpoint of traditional medicine, *Solanum torvum* has been utilized in numerous indigenous medical systems. Folk medicine and Ayurveda also played a role in this. The fruits are eaten like vegetables, and their nutritional and medicinal qualities are becoming more and more well-known. Its usage with anemia, inflammation, infections, and metabolic diseases is indicated by ethnomedical traditions. This extensive use suggests the presence of numerous pharmacologically active substances, including phenolic compounds, alkaloids, flavonoids, and saponins.[2] However, in order to prove efficacy, safety, and modes of action, conventional claims need to be systematically validated by science.[3] In addition to its therapeutic uses, S. torvum is employed as a rootstock for grafting in solanaceous crops, particularly eggplant. Because of its resilience to nematodes and soil-borne diseases, it is preferred. This application in agriculture demonstrates the plant's plasticity and metabolic resilience. Despite its numerous applications, it is still difficult to pinpoint the precise chemicals that provide therapeutic benefits [4].

Numerous secondary metabolites have been found via traditional phytochemical research. However, little is known about the relationships between these substances and molecular targets [5]. A calculated approach to closing this gap is to use computational techniques, particularly molecular docking. The molecular interactions between phytoconstituents and biological targets are predicted by *In Silico* methods [6]. This aids in locating possible lead compounds. The method lowers the expense and duration of experimental screening. Additionally, it improves drug discovery accuracy. Our knowledge of plant bioactives is advanced when computational techniques are used in conjunction with methodical extraction and characterization. Thus, the goal of this research is to apply computational techniques to identify therapeutically useful chemicals from *Solanum torvum*. The research attempts to provide the plant's traditional usage a logical foundation by combining *In Silico* analysis with phytochemical expertise. It also aims to aid in the creation of drugs. This interdisciplinary approach draws attention to a recent development in the study of natural products. Here, traditional knowledge is combined with contemporary computational technologies to provide results that have been verified by science [6].

2. Materials and methods:

2.1 Collection of the crude drugs:

Fresh *Solanum torvum* fruits were collected from the vicinity of Gwalior Jhansi Road and authenticated by a botanist. A voucher specimen was deposited in the Pharmacognosy Laboratory, ITM University, Gwalior (specimen number R/21-26-001).

2.2 Drying of the crude drug:

Collected *S. torvum* fruits were thoroughly washed to eliminate debris, then cut into small pieces and dried in the shade for 7 to 10 days. Dried fruits were pulverized and passed through sieve #22 to ensure uniform particle size.

2.3 Extraction of crude drugs:

Hexane and ethanol were the two solvents used in a Soxhlet system to extract the resulting powder. In order to fully separate the phytoconstituents into the menstruum, each extraction was conducted for 72 hours. After being dried in a rotary evaporator, the extracts were kept in glass containers until they were needed again.

2.4 LC-MS testing:

After preliminary phytochemical screening identified the main compounds in the extracts, the extracts were tested with LC-MS[7]. The Thermoscientific Orbitrap Exploris 240 model was used, as shown in Figure 1.

2.4.1 Methodology for LC–MS Analysis of *Solanum torvum* Fruit Extracts

The phytoconstituents in ethanolic and hexane extracts of *Solanum torvum* fruits were analyzed using liquid chromatography–mass spectrometry (LC–MS). Each extract was dried by evaporation, then redissolved in methanol to a working concentration of about 1 mg/mL. The samples were filtered through 0.22 µm PTFE syringe filters and placed in LC–MS vials for analysis[8].

A C18 column (2.1 × 100 mm, 1.7 µm) was used for the analysis. The column temperature stayed at 40°C. The flow rate was set to 0.30 mL/min, and the injection volume was 2 µL. Water with 0.1% formic acid was mobile phase A; acetonitrile with 0.1% formic acid was mobile phase B. A 40-minute gradient was used. The base peak appeared in both positive and negative ion modes, as shown in Figures 1 and 2.

LC–MS analysis was performed with a Thermo Scientific Orbitrap Exploris 240 in positive H-ESI mode. The spray voltage was 3200 V. The ion transfer tube was set to 300°C, and the vaporizer to 320°C. Using EASY-IC internal calibration, comprehensive scan mass spectrometry data were collected at a resolution of 120,000 in the m/z range of 100 to 4000[9].

2.4.4 Data Processing: We used Xcalibur/Compound Discoverer to look at the raw data.

We identified phytoconstituents using precise mass measurement (≤5 ppm), isotopic distribution analysis, adduct production, and, when possible, MS/MS spectral comparison [10].

Seven compounds were finalized and docked to the enzymes **PPARγ** (2PRG) and HMG-CoA (1HW9). Docking was performed to determine **binding scores and the compounds' ability to inhibit diabetes and hyperlipidemia.**

2.5 Docking software:

We used PyRx, based on AutoDock Vina, for molecular docking studies. These studies estimated the binding affinity of phytochemicals to the active sites of target proteins[11].

2.5.1 Getting ready for target proteins:
We obtained the 3D structures of PPAR gamma and HMG CoA from the Protein Data Bank, with PDB IDs 2PRG and 1HW9, respectively. With Biovia Discovery Studio Visualizer, we removed non-essential water molecules, heteroatoms, and co-crystallized ligands from the targets. This was done to avoid interference with docking. Using AutoDock tools, we added polar hydrogens, assigned charges, and converted the refined protein to PDBQT format in PyRx [12,13].

2.5.2 Getting Ligands Ready
We obtained all phytochemical structures in SDF format from PubChem. DS software converted the ligands into PDB format. Open Babel was then used to import the compounds into PyRx. UFF minimized them, and they were then converted to PDBQT format.
We loaded the target protein and ligands into the Auto Dock Vina wizard. Then, we set up a docking grid box to cover the active site and ensured the dimensions were correct so the binding pocket was fully covered. Using default exhaustiveness, docking was performed, and the software generated several binding poses for each ligand, ranked by predicted binding affinity (kcal/mol) [14]. The pose with the lowest binding energy, the right orientation, and hydrophobic interactions was chosen as the best one [15]. The best poses were saved as PDB files. Discovery Studio Visualizer was used to show how proteins and ligands interact with each other. We made a table of the binding energies for all the ligands we tested and compared them.

3.Results and discussion:
3.1 Extractive value: The extractive value of the hexane extract was found to be 7% w/v, and the ethanolic extract was found to be 14%.

3.2 Analyzing and Characterizing Phytochemicals
We used either Thermo Scientific Xcalibur/Compound Discoverer or the available software to analyze the raw files we received. High-resolution profile spectra were used to identify features. The computer did peak identification, deisotoping, and predicting the chemical formula on its own. We figured out what the phytoconstituents in the both the extracts were by using Accurate mass measurement (≤ 5 ppm mass deviation) by using Matching of the distribution of isotopes, finding adducts like $[M+H]^+$, $[M+Na]^+$, and so on, features of retention time on the C18 column, A comparison of MS/MS spectra to library spectra (if MS/MS data was obtained), The measured m/z, retention time, suggested molecular formula, ppm error, and identification level (putative or confirmed) were all recorded for each compound.

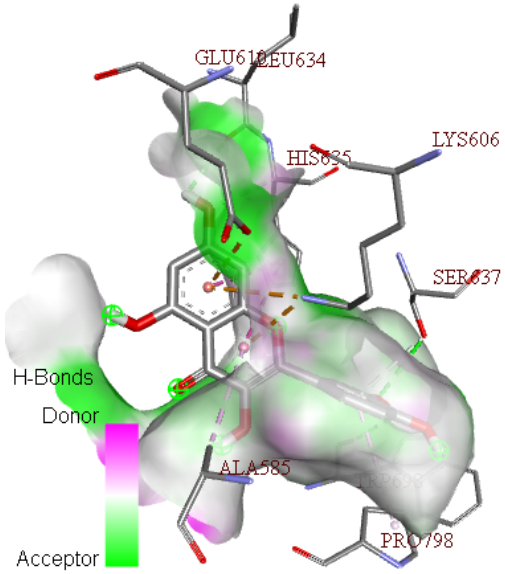
3.3. Process of finalisation of compound from the LCMS STUDY:
The LC-MS analysis of the hexane extract of *Solanum torvum* fruits found a total of 12,250 compounds. After the data was cleaned up, duplicate entries were removed, and the remaining compounds were tested for molecular docking and ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity). Seven compounds were chosen as possible bioactive candidates based on how well they bind and how well they work in the body. The LC–MS analysis of the ethanolic extract also showed that it had 9,963 different compounds. Following the elimination of superfluous molecules and their assessment by molecular docking and ADMET analyses, three compounds emerged as interesting candidates exhibiting drug-like characteristics. The reduction in the quantity of compounds from initial detection to final selection highlights the stringency of the screening process and emphasizes the importance of integrating computational filtering with experimental identification to prioritize biologically relevant phytoconstituents. Seven compounds were completed and docked with the enzymes PPARγ (2PRG) and HMG-CoA (1HW9). The results are presented in Table 1.

Table 1 Docking ability score of the identified compounds toward PPAR and HMG CoA enzymes

S.No	**Ligand**	PPAR γ(2PRG) Score (kcal/mol)	HMG CoA **(1HW9)** Score (kcal/mol)
1	Maritimetin	-8.8	-8.4
2	Castillene C	-8.5	-7.8
3	2'-Hydroxy-5',6'-dimethoxy-3,4-methylenedioxyfurano [	-7.8	-6.4

	2",3":4',3' dihydrochalcone]		
4	Chrysin 5-xyloside	-8.9	-8.4
5	Glabrachromene I	-8.4	-8.2
6	Sigmoidin G	-8.1	-8.3
7	2',4'-Dihydroxydihydrochalcone	-7.8	-7.0
8	(3S)-6-hydroxy-8-methoxy-3-methyl-3,4-dihydroisocoumarin	-7.1	-6.5
9	5-hydroxymethylfurfural	-5.1	-4.9
10	Quercetin	-9.2	-8.5

The pictures of docking for the best shown compound were represented in the figure 1, 2,



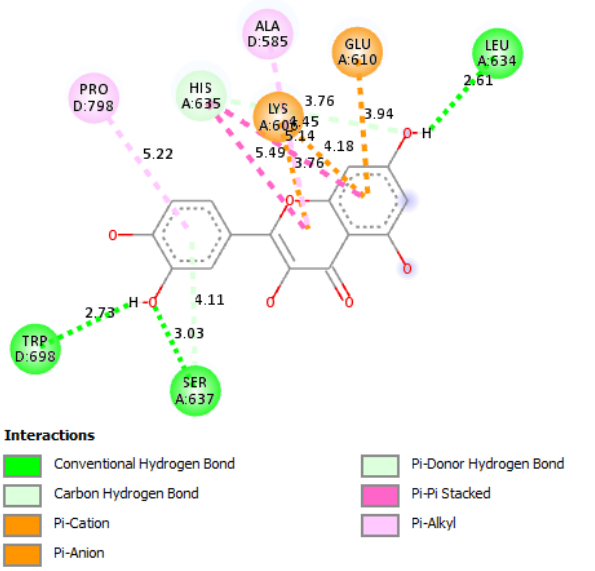


Figure:1; 3D & 2Dinteractions of Quercetin with HMG Co A

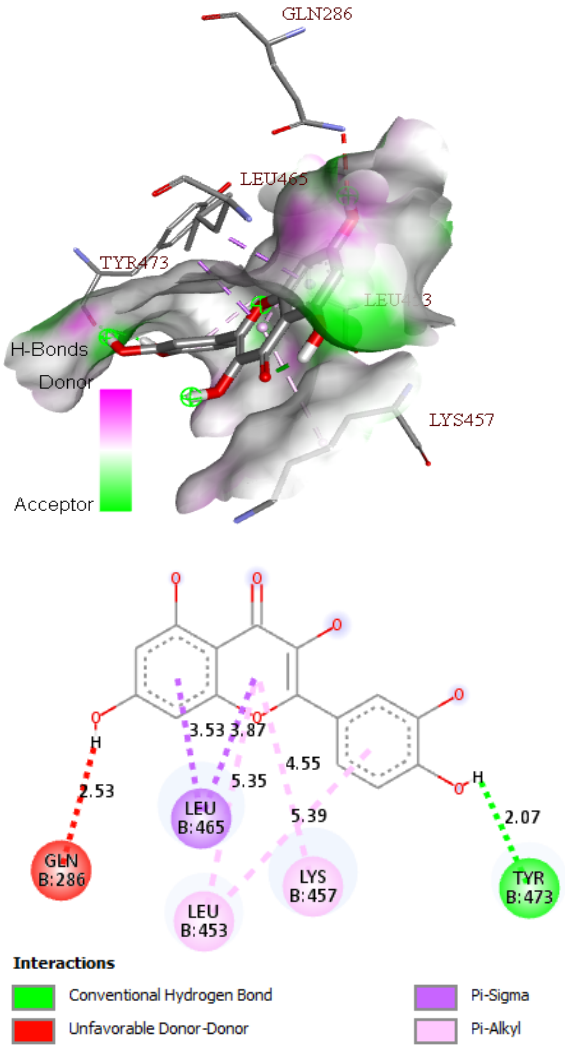


Figure-2; 3D & 2Dinteractions of Quercetin With PPAR gamma

The chosen phytoconstituents from *Solanum torvum* extracts were subjected to molecular docking investigations targeting two primary therapeutic proteins: the PPAR gamma receptor and HMG-CoA reductase, which are crucial in the management of diabetes and hyperlipidemia, respectively. The docking outcomes were evaluated based on binding affinity (kcal/mol) and interaction patterns. Quercetin exhibited the highest binding affinity for PPARγ among the evaluated ligands, with a docking score of −9.2 kcal/mol. Chrysin 5-xyloside (−8.9 kcal/mol) and maritimetin (−8.8 kcal/mol) were close behind. These compounds demonstrated persistent contacts inside the active site, notably through traditional hydrogen bonding with essential amino acid residues such as TYR473, GLU272, and ARG280, along with hydrophobic interactions, including π–alkyl and π–sigma interactions. The existence of many contact types implies significant ligand stability inside the receptor binding site, suggesting possible agonistic activity pertinent to glucose metabolism. Docking studies on HMG-CoA reductase revealed that quercetin (−8.5 kcal/mol) and maritimetin (−8.4 kcal/mol) had the highest binding energies, followed by chrysin 5-xyloside (−8.4 kcal/mol) and sigmoidin G (−8.3 kcal/mol). These ligands established significant hydrogen bonds with residues including GLU610, LYS606, and SER637, which are recognized as critical for enzyme activity. Additionally, π–cation, π–anion, and hydrophobic interactions enhanced the total binding stability. This indicates that they may inhibit cholesterol synthesis. Additional compounds such as castillene C, glabrachromene I, and 2',4'-dihydroxydihydrochalcone exhibited moderate binding affinities (ranging from −7.0 to −8.5 kcal/mol) with consistent interaction profiles. This indicates they may assist, but are less proficient in preventing an occurrence. 5-hydroxymethylfurfural had the lowest binding affinity for both targets, with values of −5.1 kcal/mol for PPARγ and −4.9 kcal/mol for HMG-CoA. This indicates that it does not significantly contribute to treatment efficacy. An extensive analysis of interaction patterns revealed that the majority of high-affinity ligands established many conventional hydrogen bonds alongside hydrophobic contacts, such as π–alkyl and π–sigma interactions, which are essential for maintaining ligand–receptor stability[19]. However, the presence of occasional adverse interactions (e.g., donor–donor or acceptor–acceptor clashes) in specific compounds indicated possible steric or electronic limitations that hinder optimum binding. The docking results indicated that quercetin, maritimetin, chrysin 5-xyloside, and sigmoidin G emerged as the most promising candidates due to their ability to inhibit both PPARγ and HMG-CoA reductase. The results endorse the potential relevance of *Solanum torvum* phytoconstituents in managing diabetes and hyperlipidemia, hence confirming their therapeutic value.

4.Conclusion:

The study coupled LC–MS phytochemical profiling with computational screening to recognize medicinal agents from *Solanum torvum* fruit extracts. Following the filtration of chemicals from hexane and ethanolic extracts, multiple candidates were discerned by molecular docking studies targeting the PPAR gamma receptor and HMG-CoA reductase, with quercetin, maritimetin, chrysin 5-xyloside, and sigmoidin G demonstrating notable binding affinities. These chemicals exhibited the ability to simultaneously influence two targets, indicating their potential involvement in both glucose metabolism and cholesterol production via stabilizing interactions. The research emphasizes the necessity of combining experimental methods with computational validation to select bioactive chemicals, which offers a scientific basis for the traditional application of *Solanum torvum* in the treatment of metabolic diseases. Nonetheless, further in vitro and in vivo tests are required to confirm the biological functions and safety of these drugs. This study develops a paradigm for drug discovery from natural products and illustrates that *Solanum torvum* may be a source of multi-target bioactive compounds.

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6. Conflicts of interest: No conflicts of interest

7. References:

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