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Original Article

Exploring the Therapeutic Potential of *Plectranthus amboinicus*: LC-MS Profiling and Molecular Docking Insights

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ABSTRACT

Introduction: *Plectranthus amboinicus* is noted for its diverse phytochemical profile, which includes various semi-polar compounds and significant secondary metabolites. These compounds may offer therapeutic benefits for diabetes management. **Objectives:** This study investigates the anti-diabetic potential of phytoconstituents from *Plectranthus amboinicus* by utilizing both Liquid Chromatography-Mass Spectrometry (LC-MS) and molecular docking techniques. **Materials and Methods:** The study employed LC-MS to identify and analyze the phytoconstituents in *Plectranthus amboinicus*, providing detailed separation and detection of its bioactive compounds. Molecular docking simulations were conducted to evaluate how these phytoconstituents interact with diabetes-related target proteins, specifically alpha-amylase and alpha-glucosidase. The docking process involved 2 main steps: pose prediction to determine the ligand's conformation and positioning and scoring to assess binding affinity. **Results:** LC-MS analysis identified several key bioactive compounds in *Plectranthus amboinicus*. Molecular docking studies showed that these compounds interact specifically with alpha-amylase and alpha-glucosidase, indicating potential effectiveness in inhibiting these enzymes. **Conclusion:** The integration of LC-MS and molecular docking provides a robust methodology for discovering and characterizing potential anti-diabetic agents in *Plectranthus amboinicus*. The present investigation involves the LC-MS analysis and *in silico* study that aims to investigate the interaction between alpha-amylase, alpha-glucosidase, and the compounds (ligands) derived from *Coleus amboinicus*. This study underscores the therapeutic potential of its phytoconstituents and highlights the importance of combining analytical and computational approaches in the development of new diabetes treatments.

Keywords: Alpha-amylase, Alpha-glucosidase, Diabetes, Drug Discovery, LC-MS, Molecular Docking, Phytoconstituents, *Plectranthus amboinicus*.

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INTRODUCTION

Plectranthus amboinicus (Lour.) *Spreng.*, also known as *Coleus amboinicus* or *Lamiaceae*, is a perennial plant native to Indonesia and widely grown in tropical regions across Asia, Australia, and Africa. It is valued for its uses in traditional medicine and its role as a culinary spice and ornamental plant.[1] In particular, the leaves of *Plectranthus amboinicus* are often consumed raw or used as a flavoring. In India, they are commonly added to buttermilk, yogurt and other foods to help manage diarrhea related to infections.[2] *Coleus aromaticus* plays a significant role in managing diabetes. This plant is effective in lowering blood sugar levels and acts as a hypoglycemic agent. It may also alleviate other complications associated with high blood sugar, such as neuropathy and other related conditions. Its benefits extend to improving overall metabolic control and managing symptoms linked to elevated glucose levels.[3-5] Phytochemicals identified in *Coleus amboinicus* include various phenolic compounds, such as several methoxylated flavonoids and hydroxycinnamic acids like rosmarinic acid, salvianolic acids A and L and shimobashiric acid C, along with numerous minor constituents. Additionally, the plant contains significant amounts of isoprenoids, including phytosterols, as well as a range of volatile mono- and sesquiterpenoids found in its essential oils.[6-9]

Liquid Chromatography-Mass Spectrometry (LC-MS) is a crucial analytical method that combines the separation power of liquid chromatography with the precise detection capabilities of mass spectrometry. This technique is particularly effective for analyzing complex plant biochemical profiles, which include various semi-polar compounds and secondary metabolites. LC-MS provides detailed separation and identification of these

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compounds, making it invaluable for their study and potential applications in various fields. In addition to LC-MS, molecular docking is an essential computational method used to simulate the interactions between small molecules and proteins at the atomic level. This technique offers insights into how these molecules bind to target proteins, including those involved in diseases such as diabetes. Molecular docking involves two primary steps: pose prediction, which determines the optimal conformation and positioning of the ligand within the protein's binding site, and scoring, which evaluates the binding affinity.

Molecular docking has emerged as a crucial component of *in silico* drug development in recent years. This technique involves modeling the interaction between a small molecule and a protein at the atomic level.[10] Combining LC-MS with molecular docking offers a comprehensive approach to identifying and characterizing bioactive compounds, thereby advancing the development of new and effective therapeutic agents. The present investigation involves the LC-MS analysis and *in silico* study that aims to investigate the interaction between alpha-amylase, alpha-glucosidase, and the compounds (ligands) derived from *Coleus amboinicus*.

MATERIALS AND METHODS

The mixture used for mobile phase consisted of 2 parts: an Aqueous phase (A) with 0.1% formic acid and an organic phase (B) made of acetonitrile. The flow rate was set at 0.4 mL/min and a gradient method was used. This method started with 10% B, increased to 95% over the initial 4 min, remained at 95% for 3 min, decreased from 90% to 10% over 2 min and then stayed at 10% for 1 min. A 5 µL sample was inserted and the column temperature was maintained at 22°C throughout the process. Positive polarity Electrospray Ionization (ESI) was used for mass spectrometric detection. Important instrument parameters included a cone gas flow rate of 50 L/hr, a desolvation gas flow rate of 750 L/hr, and probe and source temperatures of 450°C and 150°C, respectively. The sampling cone voltage was adjusted to 30 V, with a source offset voltage of 80 V. Argon was used as the collision gas, with a collision energy ramp starting at 6 eV. The mass range was set between 50 and 1500 m/z and the sample infusion rate were 5 µL/min. Mass Lynx software (V4.1, Waters Corporation, Milford, MA, USA) was employed for data acquisition and analysis as described in (Tables 1 and 2).

Molecular Docking

The 3D structure of human Pancreatic α-amylase (PDB ID: 4GQR) was retrieved from the Protein Data Bank (PDB). Water molecules and other non-protein components were removed. The structure was then prepared for docking using Auto Dock Tools, which involved adding polar hydrogen atoms and assigning Kollman united atom charges. The active site of α-amylase (4GQR) was used for docking the prepared ligands using Auto Dock Vina. The grid box was strategically positioned to target the active site residues responsible for facilitating ligand binding. Default parameters were used for the docking simulations to produce multiple binding poses for each ligand. The most favorable binding pose for each ligand was determined based on the lowest binding energy. An in-depth analysis was conducted on the binding affinities (in kcal/mol) and the crucial amino acid residues involved in ligand-protein interactions. The predicted binding affinities and interactions of Syringic acid, Eugenol, Rosmanol and Vicenin were compared with those of Acarbose, a well-established α-glucosidase inhibitor. This comparative analysis aimed to reveal the potential of the tested ligands as alternative inhibitors of α-amylase.

The hyphenated LC-MS/MS technique is an advanced method that merges the separating the power of liquid chromatography with the exceptionally sensitive and selective mass analysis offered by three-dimensional quadrupole mass spectrometry. LC-MS/MS data can be employed to ascertain the molecular weight, structure, identity and certain distinct constituents of the sample. A total of twenty-two phytoconstituents were found represented in Table 3.

Summarizes the 22 phytoconstituents identified in the sample. Each compound is listed with its retention time in minutes, name, molecular formula, and the molecular ion $[MH]^-$ with the corresponding m/z value. These compounds are indicative of various bioactive phytochemicals, potentially contributing to the therapeutic properties of the samples.

Table 1: Liquid Chromatography (LC) Parameters.

Sl. No.	Parameters	Conditions
1	Instrument Model	Acquity H-class UPLC.
2	Column	Accucore C-18 Column (50×4.6 mM, 2.6 µM).
3	Mobile phase	0.1% Formic acid: Acetonitrile buffer.
4	Run time	10 min
5	Flow rate	0.4 mL/min
6	Elution type	Gradient: initial to 4 min (10 to 95%) mobile phase B, held for 3 min, 7 to 9 min (90 to 10%) and held at 10% for 1 min.
7	Injection volume	5 µL
8	Column oven temperature	22°C
9	Detector	Photodiode Array Detector (DAD).

Table 2: MS parameter.

Sl. No.	Parameters	Conditions
1	Ionisation source	Electrospray ionisation
2	Desolvation gas	Nitrogen
3	Cone gas	Nitrogen
4	Probe temperature	450°C
5	Source temperature	450°C
6	Sampling cone voltage	30 V
7	Source offset voltage	80 V
8	Collision gas	Argon
9	Collision ramp energy	6E v
10	Mass range	50-1500 m/z

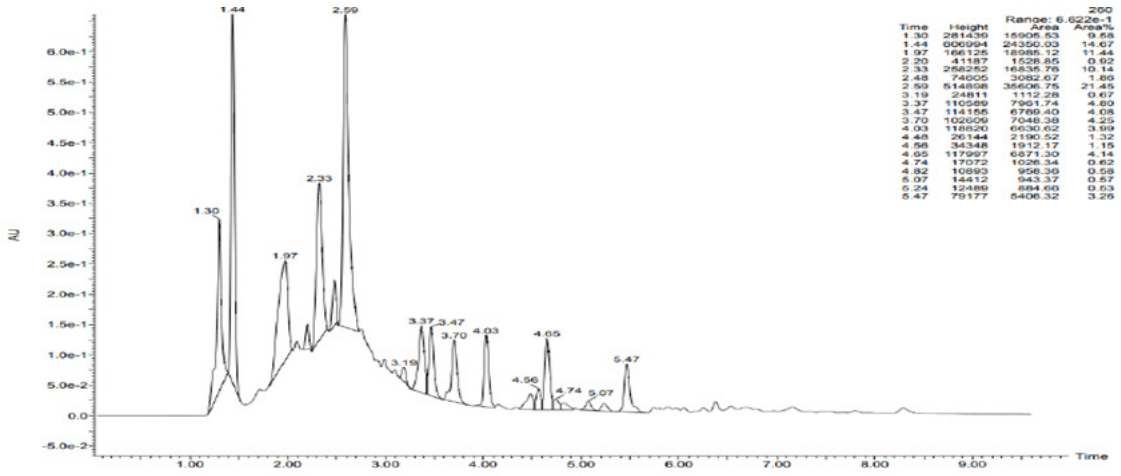


Figure 1: The LC-MS/MS chromatogram of PA.

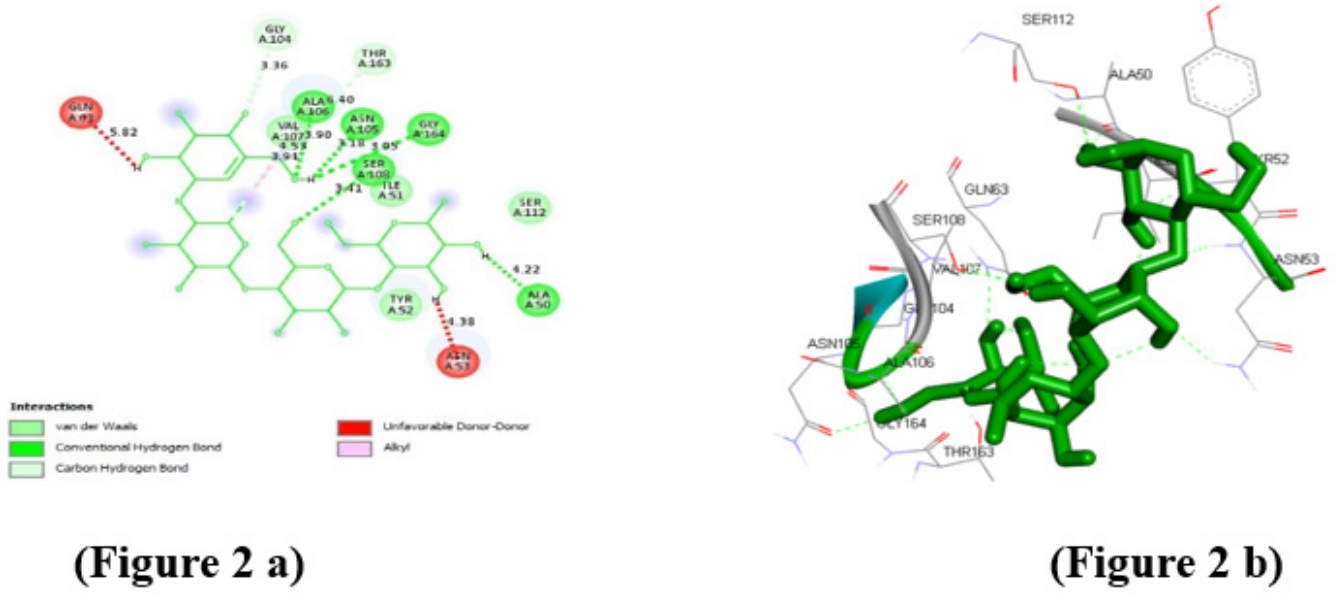
RESULTS

The chemical profiles of *Plectranthus amboinicus* were investigated using LC-MS/MS, leading to the identification of several bioactive compounds, as summarized in (Table 3) and illustrated in (Figure 1). Among the key compounds identified were caffeic acid, rosmarinic acid, eugenol, Kaempferide 7-glucuronide, Apigenin 7-glucuronide, α -linolenic acid, Rutin, Salviaflaside, Quinic acid, Vicenin and Syringic acid. These compounds have been previously reported to possess anti-diabetic activity. The activity of α-galactosidases,[11] α -amylase and α-glucosidases,[12] breaks down complex carbohydrates into monosaccharides through enzymatic degradation. Therefore, compounds that inhibit intestinal α-glucosidase enzymes affect the digestion rate of complex carbohydrates and disaccharides by competitively and reversibly inhibiting α-glucosidases found in the brush border membrane of enterocytes lining the intestinal villi.[12,13] Carbohydrate digestion and monosaccharide absorption in the proximal jejunum are reduced or incomplete in the distal jejunum and ileum. This leads to a decrease and/or delay in the rise of postprandial plasma glucose levels. By inhibiting α-glucosidase, these inhibitors give the pancreatic β-cell more time to increase insulin secretion in response to the rise in plasma glucose level.[2] Specifically, the compounds interact with key enzymes involved in carbohydrate digestion, including α-galactosidases, α-amylase and α-glucosidases, by inhibiting their enzymatic breakdown of complex carbohydrates (e.g., starches) into monosaccharides. Inhibition of α-glucosidase reduces the absorption of monosaccharides in the small intestine, delaying the rise in postprandial glucose levels, thus contributing to better blood sugar management. Moreover, these compounds are thought to offer a potential therapeutic approach for managing diabetes, as they can delay glucose absorption and enhance insulin secretion in response to postprandial glucose spikes. The plant extract exhibited over 22 phytochemicals, with four flavonoids chosen for further investigation due to their prominent role in modulating diabetic effects *in vitro*. These flavonoids were subjected to *in silico* molecular docking studies to predict their binding affinity to α-amylase and α-glucosidase, key targets for anti-diabetic drugs. The binding energies of the ligands ranged from -8.3 to -7.1 kcal/mol, suggesting a stronger binding affinity than the standard anti-diabetic drug, acarbose (binding energies of -7.1 kcal/mol

for α-amylase and -7 kcal/mol for α-glucosidase). Molecular interactions involving Acarbose, as illustrated in (Figure 2a, b), attach to the active site of α-amylase through multiple stabilizing connections. A series of conventional hydrogen bonds form with ASN (A105), SER (A112), ALA (A164) and TYR (A52), while van der Waals forces engage ALA (A50), ALA (A51), VAL (A103) and ALA (A104). The relationship between ALA (A50) and ASN (A53) aids in establishing the hydrophobic environment essential for the stability of acarbose. Although a donor-donor interaction exists between GLN (A93) and acarbose, it does not notably affect binding because of the overall stability afforded by the other interactions. These interactions play a key role in acarbose's inhibitory effect, which lowers carbohydrate breakdown and supports blood glucose management in diabetes. The images in (Figure 3a, b) depict Eugenol's engagement with α-amylase through conventional hydrogen bonds with ASN (position 362) at 3.12 Å and carbon-hydrogen bonds with PRO (positions 360, 361). Alkyl interactions with VAL (position 358) further secure the ligand within the binding pocket. The stability of the ligand is also enhanced by van der Waals interactions with TRP (357), PHE (55), ARG (56), ARG (343), GLY (359) and LYS (368), which contribute to the ligand's binding and inhibitory capabilities. (Figure 4a, b) illustrates Rosmanol's attachment to α-amylase through a blend of van der Waals interactions with ASP (197), ASP (300) and HIS (101), alongside conventional hydrogen bonds with THR (163) and GLN (63). Additionally, pi-sigma interactions with TRP (59) and alkyl interactions with TRP (58), LEU (300) and TYR (62) enhance the stabilization of the ligand. These interactions support the stability and specificity of Rosmanol's binding. In (Figure 5a, b), Syringic acid establishes conventional hydrogen bonds with SER (108), ASN (53), TYR (52) and SER (112). Other types of interactions include carbon-hydrogen bonds with ALA (106), ILE (51) and VAL (107). Alkyl interactions with ALA (50) and PHE (119), along with hydrophobic contacts with ALA (50) and VAL (49), maintain stability in the binding. Such molecular interactions improve the ligand's binding affinity and specificity. Vicenin binds to α-amylase using conventional hydrogen bonds with TYR (A52), SER (A112) and ASN (A31) at distinct distances, in addition to van der Waals interactions with ALA (A50), ALA (A52) and ILE (A51). A noted adverse donor-donor interaction

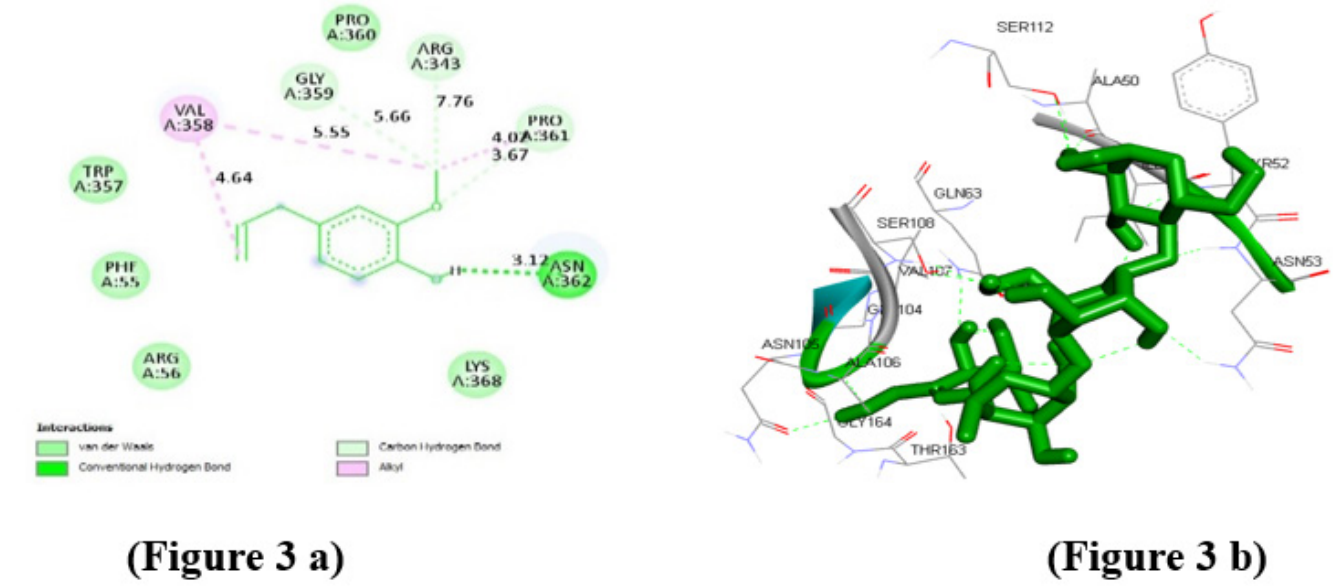
Table 3: Phytoconstituents identified in the sample by their retention time, compound name, molecular formula, and molecular ion (m/z [M-H]$^-$).

Sl. No.	Retention time (min)	Name of the compound	Molecular formula	Molecular Ion (m/z [M-H]$^-$)
1	1.252	Syringic acid	$C_9H_{10}O_5$	135.0435
2	1.252	Apigenin derivative	$C_{15}H_{10}O_5$	269.0462
3	1.252	Eugenol	$C_{10}H_{12}O_2$	447.0929
4	1.895	Salvianolic acid C	$C_{26}H_{20}O_{10}$	491.0979
5	1.895	Diterpene derivative	$C_{20}H_{26}O_4$	343.1559
6	2.301	Rosmanol	$C_{20}H_{26}O_5$	345.1713
7	2.673	Nagilactone E	$C_{20}H_{28}O_5$	347.1868
8	2.673	Epirosmanol	$C_{20}H_{26}O_5$	345.1719
9	2.673	Vicenin	$C_{26}H_{28}O14$	343.1559
10	2.673	Rosmarinic acid	$C_{18}H_{16}O_8$	345.1550
11	2.673	5,7-Dihydroxy-40,6-dimethoxyflavone	$C_{17}H_{14}O_6$	313.0721
12	2.876	Quinic acid	$C_7H_{12}O_6$	389.1985
13	3.045	Apigenin-O-acetyl glucuronide	$C_{24}H_{24}O_{11}$	487.0882
14	3.248	Isosalvianolic acid	$C_{26}H_{20}O_{10}$	491.0982
15	3.248	Protocatechuic acid	$C_7H_60_4$	623.1981
16	3.587	Salicylic acid glucoside	$C_{13}H_{16}O_8$	521.1298
17	3.587	Rutin	$C_{27}H_{30}O_{16}$	537.1032
18	3.724	Madasiatic acid derivative	$C_{30}H_{48}O_5$	487.3424
19	3.772	Caffeic acid	$C_9H_8O_4$	179.0345
20	3.772	Apigenin 7-glucuronide	$C_{21}H_{18}O_{11}$	445.0773
21	4.669	Salviaflaside	$C_{24}H_{26}O_{13}$	521.1302
22	4.838	Kaempferide 7-glucuronide	$C_{22}H_{20}O_{12}$	475.0887



(Figure 2 a) (Figure 2 b)

Figure 2: (a, b) Molecular interactions of Acarbose-α-amylase.



(Figure 3 a) (Figure 3 b)

Figure 3: (a, b) Molecular interactions of Eugenol-α-amylase.

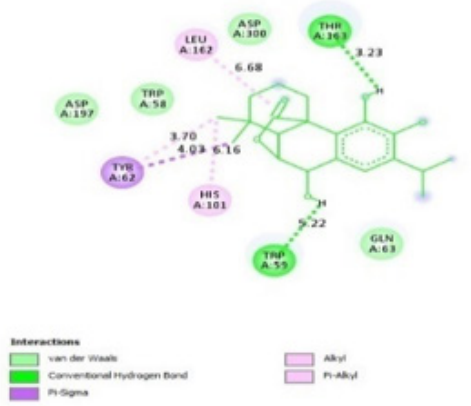
with TYR (A52) and vicenin, displayed in (Figure 6a, b), does not compromise the overall binding strength. These interactions are essential in maintaining the ligand's stability within the active site.

Acarbose binds α-glucosidase through hydrogen bonds as shown in (Figure 7a, b) with ASN (356), ASP (356) and other residues like ALA (327), ASN (290) and HIS (237). Van der Waals interactions with ILE (324), LEU (354) and aromatic residues such as TRP (690) and PHE (680) further stabilize the ligand. Hydrophobic contacts with VAL (512) ensure proper positioning within the active site, contributing to acarbose's inhibitory effect on α-glucosidase. The images shown in (Figure 8a, b) are Eugenol's interactions with α-glucosidase including van der Waals forces with ALA (A237), PRO (A130, A131, A238) and VAL (A236), which stabilize the ligand. Hydrogen bonds with SER (A85) and carbon-hydrogen bonds with ARG (A89) and VAL (A484) contribute to strong binding. Pi-alkyl interactions with PHE (A90, A129) further enhance the ligand's binding and stability. (Figure 9a, b) shows Rosmanol interacting with α-glucosidase

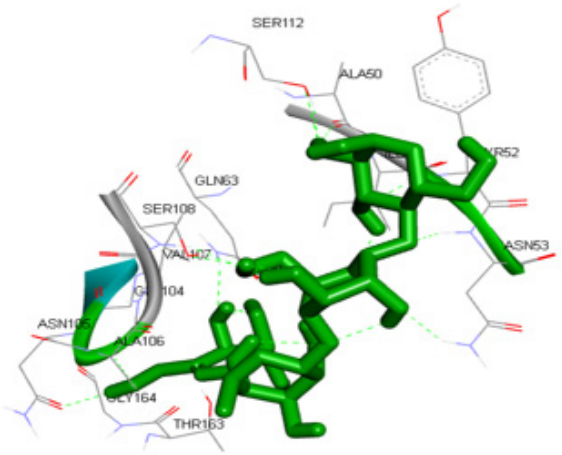
via hydrogen bonds with THR (235), VAL (236) and SER (88). Van der Waals forces involving VAL (236), PHE (90), ALA (237) and TYR (133) help stabilize the ligand. Additional pi-alkyl interactions with PHE (90, 131) and alkyl interactions with PRO (130) further contribute to the binding stability, ensuring the ligand's effective positioning in the active site. Syringic acid binds α-glucosidase through hydrogen bonds with SER (A88) and VAL (A84) and van der Waals interactions with VAL (A236) and PHE (A90, A129). Alkyl interactions with ALA (A237) stabilize the ligand within the binding pocket, while pi-alkyl interactions with PHE (A90) and PHE (A129) provide additional binding stability shown in (Figure 10a, b). Vicenin interacts with α-glucosidase shown in (Figure 11a, b) through hydrogen bonds with ASP (95), GLY (550) and VAL (544). Carbon-hydrogen bonds with ARG (275) and ARG (106) further stabilize the ligand. Additionally, van der Waals forces with PHE (159, 160, 161) and interactions with PRO (541, 542) ensure the ligand's stable positioning within the binding site.

DISCUSSION

The LC-MS/MS profiling of *Plectranthus amboinicus* revealed the presence of several bioactive compounds, many of which have documented anti-diabetic activities. Among the identified compounds, eugenol, rosmanol, syringic acid and vicenin

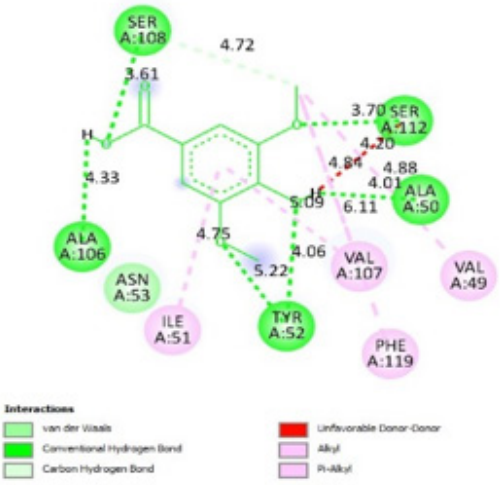


(Figure 4 a)

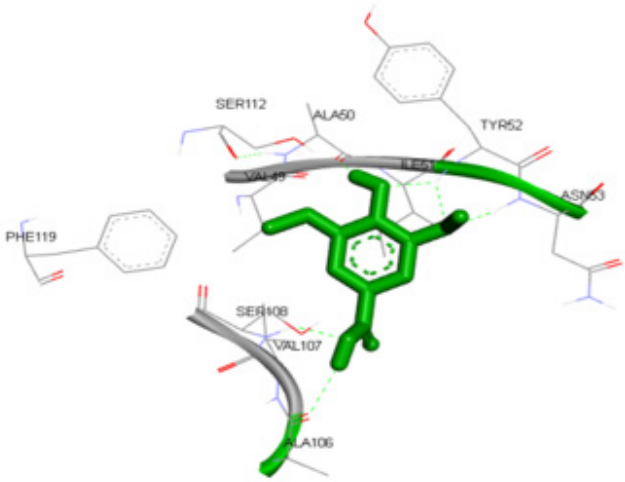


(Figure 4 b)

Figure 4: (a, b) Molecular interactions of Rosmanol-α-amylase.

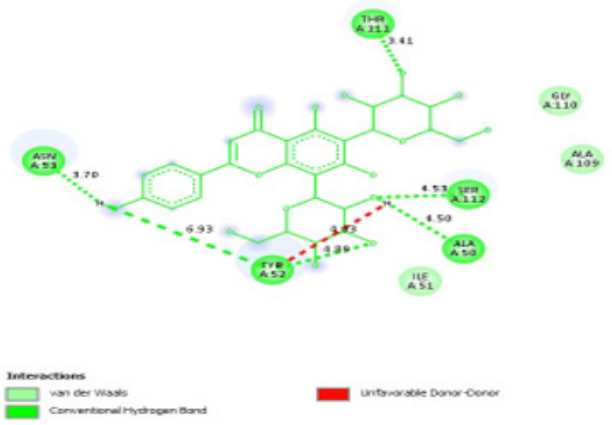


(Figure 5 a)

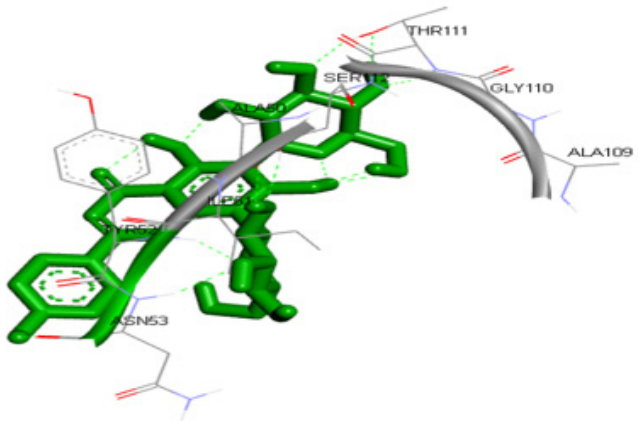


(Figure 5 b)

Figure 5: (a, b) Molecular interactions of Syringic acid-α-amylase. image6

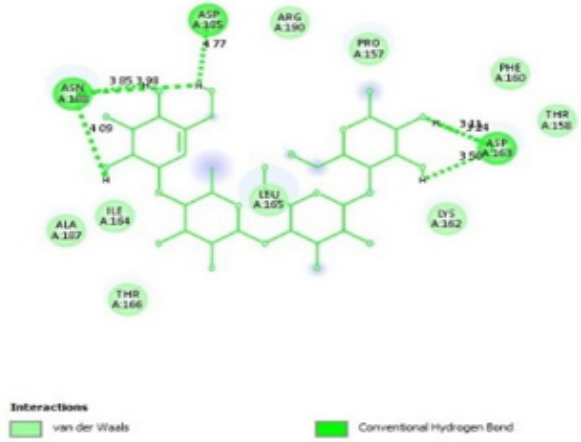


(Figure 6 a)

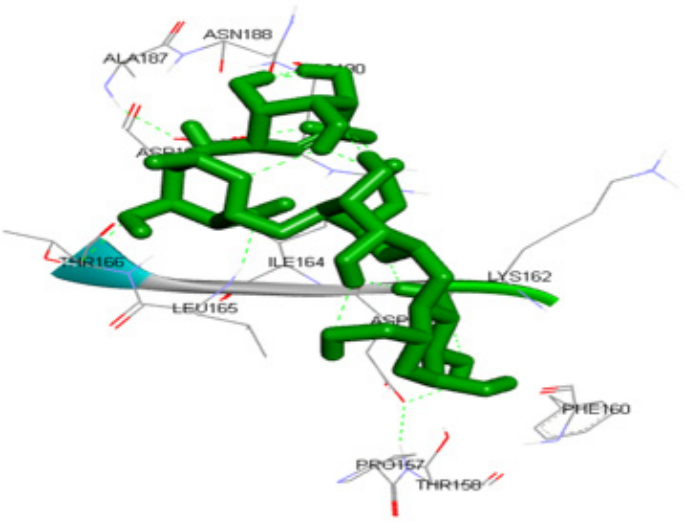


(Figure 6 b)

Figure 6: (a, b) Molecular interactions of Vicenin-α-amylase.



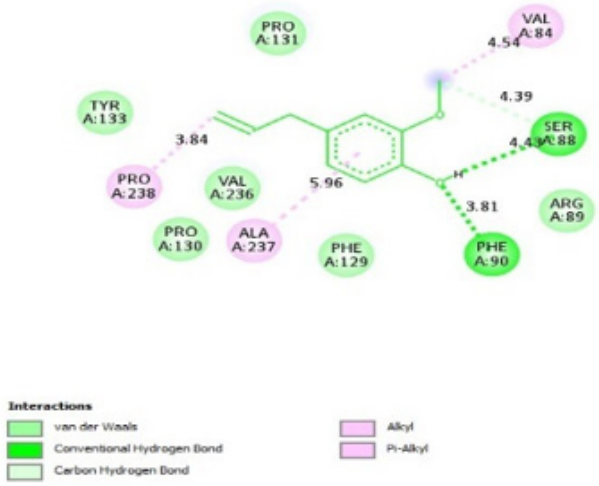
(Figure 7 a)

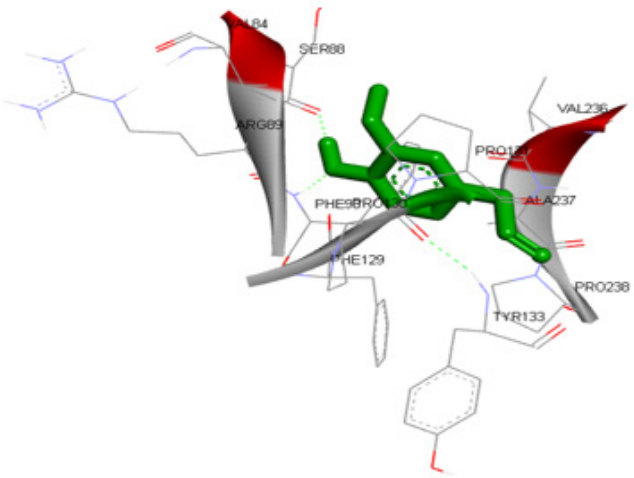


(Figure 7 b)

Figure 7: (a, b) Molecular interactions of acarbose-α-glucosidase.

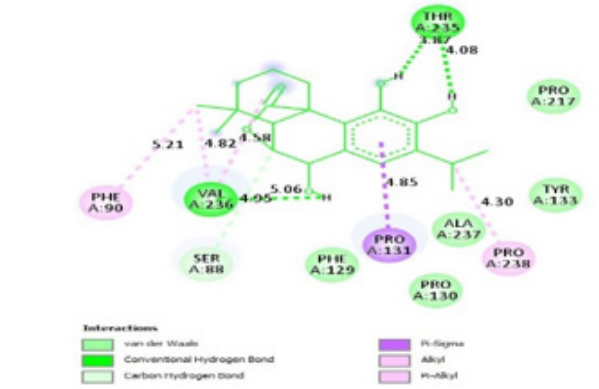
exhibited strong interactions with key targets involved in glucose metabolism. The *in silico* docking studies demonstrated that these compounds can effectively bind shown in (Table 4) to α-amylase and α-glucosidase, leading to their inhibition and potential modulation of postprandial glucose levels. Acarbose, known for its clinical use in diabetes management, showed tight binding to α-amylase, with hydrogen bonds and van der Waals interactions stabilizing its presence in the active site, thereby inhibiting the breakdown of starches into absorbable sugars. Eugenol and rosmanol, both phenolic compounds, exhibited significant binding interactions with α-amylase and α-glucosidase, especially through hydrogen bonds and hydrophobic contacts, suggesting their potential as natural inhibitors. Syringic acid and vicenin, both polyphenolic compounds, also demonstrated strong binding through hydrogen bonds, alkyl interactions, and van der Waals forces, indicating their potential as dual inhibitors of both enzymes. The hydrophobic interactions observed in all compounds are likely to play a critical role in enhancing binding specificity and stability. These findings support the therapeutic potential of these natural compounds in managing postprandial blood glucose levels and highlight the importance of these molecular interactions in drug design and development for diabetes treatment.

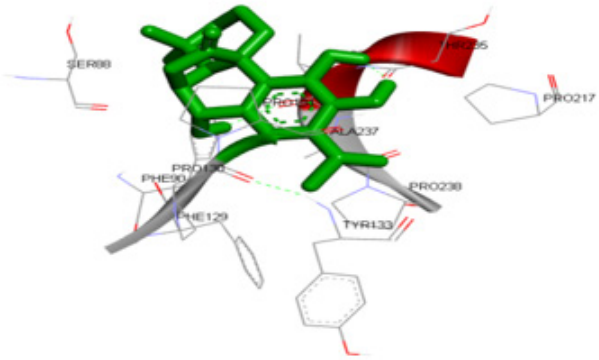




(Figure 8 a) **(Figure 8 b)**

Figure 8: (a, b) Molecular interactions of Eugenol - α- glucosidase.



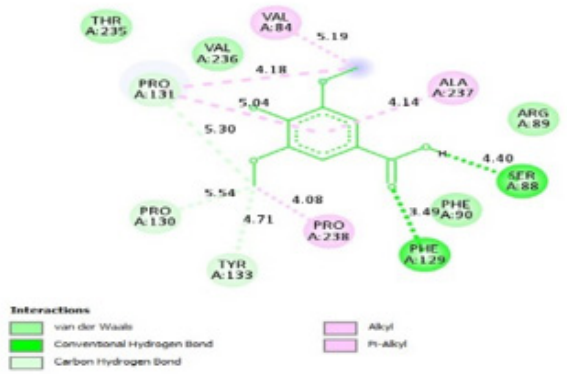


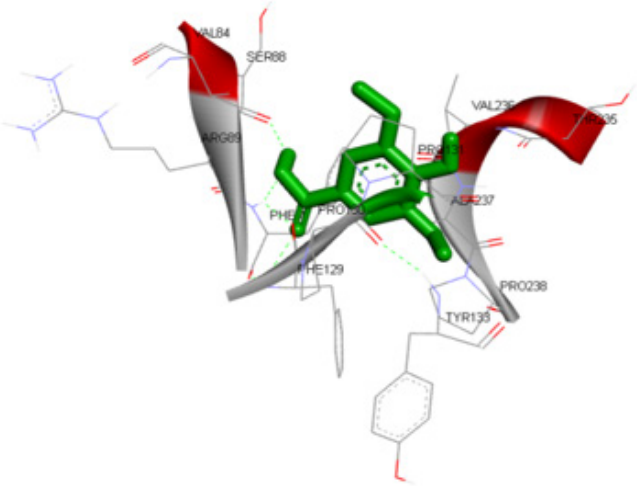
(Figure 9 a) **(Figure 9 b)**

Figure 9: (a, b) Molecular interactions Rosmanol-α-glucosidase.

Table 4: *In silico* molecular docking results.

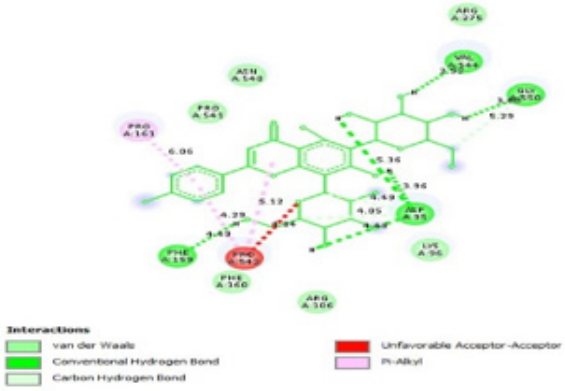
Compound	α-amylase (kcal/mol)	α-glucosidase (kcal/mol)
Acarbose	-7.1	-7
Eugenol	-5.8	-6.1
Rosmanol	-8.3	-7.4
Syringic acid	-5.8	-5.5
Vicenin	-8.3	-6.8

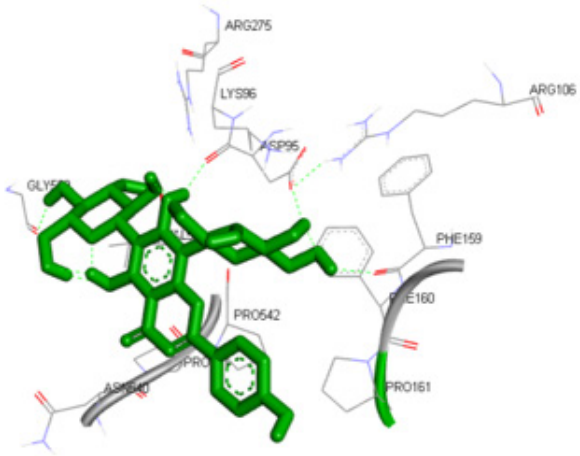




(Figure 10 a) (Figure 10 b)

Figure 10: (a, b) Molecular interactions Syringic acid- α- glucosidase.





(Figure 11 a) (Figure 11 b)

Figure 11: (a, b) Molecular interactions Vicenin-α-glucosidase.

Binding modes

In silico molecular docking results were performed to assess the binding affinities of the listed compounds towards α-amylase and α-glucosidase, indicating their potential inhibitory effects on these enzymes.

CONCLUSION

The integration of LC-MS analysis and molecular docking studies has provided valuable insights into the bioactive compounds of *Plectranthus amboinicus*, highlighting their potential as effective inhibitors of key enzymes involved in glucose metabolism, such as α-amylase and α-glucosidase. The LC-MS profiling identified over 22 phytochemicals, including eugenol, rosmanol, syringic acid and vicenin, many of which are known for their anti-diabetic properties. Molecular docking results demonstrated that these compounds, especially rosmanol and vicenin, exhibit strong binding affinities to both enzymes, suggesting their potential as dual inhibitors, with binding energies surpassing those of the established anti-diabetic drug acarbose. These findings underscore the therapeutic potential of these natural compounds in managing postprandial blood glucose levels and offer a foundation for further drug development aimed at diabetes treatment. By optimizing the interactions between these bioactive ligands and enzyme-active sites, the study contributes

to the development of more effective and sustainable plant-based therapies for metabolic disorders.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

ABBREVIATIONS

LC-MS: Liquid Chromatography-Mass Spectrometry; **PA:** *Plectranthus amboinicus*; **ASN:** Asparagine; **SER:** Serine; **ALA:** Alanine; **TYR:** Tyrosine; **VAL:** Valine; **GLN:** Glutamine; **GLN:** Glutamic Acid; **PHE:** Phenylalanine; **TRP:** Tryptophan; **LEU:** Leucine; **ILE:** Isoleucine**; PRO:** Proline; **THR:** Threonine; **HIS:** Histidine; **ARG:** Arginine; **GLY:** Glycine.

SUMMARY

Plectranthus amboinicus (*Coleus amboinicus*) is a plant with significant medicinal value, especially in managing diabetes. The plant's leaves contain bioactive compounds, including flavonoids and phenolic acids, which have demonstrated potential in lowering blood sugar levels by inhibiting key digestive enzymes like α-amylase and α-glucosidase. Liquid Chromatography-Mass Spectrometry (LC-MS) analysis revealed over 22 phytochemicals, such as eugenol, rosmarinic acid and syringic acid, which are known for their anti-diabetic properties. Molecular docking studies showed that several compounds from the plant, including rosmanol and vicenin, exhibited stronger binding affinities to α-amylase compared to the standard drug acarbose, suggesting they could be effective natural inhibitors. These interactions, mainly through hydrogen bonding and van der Waals forces, provide insights into the design of new diabetic therapies. Overall, LC-MS and molecular docking techniques highlight the therapeutic potential of *Plectranthus amboinicus* in diabetes management, offering a basis for the development of plant-based treatments for metabolic disorders.

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