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RESEARCH ARTICLE

Phytochemical profiling and antidiabetic potential of *Dactylicapnos scandens* root tuber using LC-MS, GC-MS and molecular docking

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Abstract

Dactylicapnos scandens (D. Don) Hutch represents the Papaveraceae family as climbing perennial herbs and is used by traditional healers in India, China, Nepal, Tibet and Vietnam to treat inflammation, diabetes and many other ailments. The current study investigates phytochemical composition and biological activities of root tuber of the plant. The crude extract was screened for bioactive compounds by gas chromatography mass spectroscopy (GC-MS) and liquid chromatography mass spectroscopy (LC-MS). The antidiabetic activity was determined by *in vitro* enzyme inhibition assays involving α-amylase and α-glucosidase. *In silico* molecular docking was carried out to confirm antidiabetic potential. In LC–MS analysis of the root tuber of *Dioscorea scandens*, acebutolol, hydrocortisone, disulfiram, corymbosin, vincamine, gentisic acid and andrographolide were identified. In contrast, GC–MS analysis revealed Z,Z-6,28-heptatriactontadien-2-one, 2-ethylthiolane S,S-dioxide, fumaric acid 3-methylbut-3-enyl octyl ester, succinic acid 4-methoxy-2-methylbutyl octadecyl ester, hexacosyl acetate, 2-methoxy-4-vinylphenol, 2,2-dimethyleicosane, 3-methyl-2-(2-oxopropyl)furan, oleic acid and octadecanoic acid as major components. The enzyme inhibition assay revealed lower activity than the standard drugs acarbose, but the inhibition could be considered significant. In the α-amylase inhibition assay, acarbose showed an IC_{50} value of 84.60 µg/mL, whereas the extract exhibited IC_{50} value of 95.98 µg/mL. Similarly, in the α-glucosidase assay, acarbose had the IC_{50} value of 46.38 µg/mL and root tuber extract showed activity with IC_{50} value of 66.04 µg/mL. Among the identified phytocompounds, andrographolide displayed strong binding affinities, with binding energies of −8.27 kcal/mol for human pancreatic α-amylase and −9.24 kcal/mol for human small intestinal α-glucosidase. Likewise, vincamine demonstrated notable binding energies of −7.02 kcal/mol with human pancreatic α-amylase and −8.37 kcal/mol with human small intestinal α-glucosidase. Findings suggest that *D. scandens* crude extract possesses number of antidiabetic phytochemicals. This has significant translational potential for developing antidiabetic therapies. Cytotoxic and mutagenic effect of *D. scandens* along with synergistic effects of phytoconstituents could be verified for further utilisation of the plant as a source of therapeutic.

Keywords: antidiabetic; GC-MS; hypoglycaemic; LC-MS; molecular docking

Introduction

Dactylicapnos scandens (D. Don) Hutch, commonly referred to as the yellow bleeding heart in Nagaland, India, was previously known as *Dicentra scandens*. The plant belonging to the family Papaveraceae is a climbing perennial herb bearing a tuberous rootstock (1) and is mainly distributed in Northeast India, Nepal, Tibet, Thailand and the Yunnan province of China (2). The traditional healers of Nagaland and Manipur in India use *D. scandens* for the treatment of malaria, typhoid, viral fever, diabetes, pneumonia, high blood pressure, diarrhoea, dysentery, stomach ache, etc (1). Dried powder of the root tuber of *D. scandens* is a well-known Chinese traditional medicine named "Zijinlong" used for the treatment of hypertension, inflammation and pain (2). Alkaloids like isocorydine and protopine are known to be present in *D. scandens*. In spite of being utilised in the ethnomedicinal treatment of diabetes, the plant's potential as a source of phytochemicals for diabetes treatment has not been explored.

Diabetes is classified as a metabolic disorder, characterised by hyperglycemia, which may damage kidney, heart, blood vessels and nerves, contributing to reduced lifespan and has become a serious health problem worldwide. The most common, Type-2 diabetes mellitus (T2DM) is either caused by low insulin production or when the body becomes resistant to insulin (3). According to the International Diabetes Federation (IDF), around 589 million adults aged between 20 and 79 years are living with diabetes and by the year 2050, the numbers are estimated to go up to 853 million with a 45 % increase in diabetic adults on earth (4).

Increasing evidence suggest that the pathogenesis of diabetes can be attributed to various signalling pathways, notably the insulin signalling pathway, AMP-activated protein kinase (AMPK) pathway, peroxisome proliferators-activated receptor (PPAR) regulation pathway and chromatin remodelling pathways. Moreover, glucose metabolism pathways involving α-amylase, α-glucosidase and stress related pathways mediated by protein kinase

and other oxidative pathways are also associated (5–8). A protein phosphorylation cascade is triggered by insulin for glucose uptake by tissues resulting in the migration of glucose transporter (GLUT4) to the cell surface. Impaired stimulation results in insulin resistance (6). Glucose metabolism enzymes α-amylase, α-glucosidase promote breakdown of α-linked of polysaccharides to glucose. Inhibiting these enzymes are targets for drug designing. Additionally, through PPAR pathway, ligand activated nuclear hormone receptors play an important role in lipid and glucose homeostasis. $PPAR_s$ are being targeted for drug designing, which results in stimulation of insulin sensitivity and inhibition of gluconeogenesis (9).

Although synthetic drugs are available to treat diabetes, most of them have side effects. Oral hypoglycaemic agents such as biguanides, sulfonylurea, alpha-glucosidase inhibitors, thiazolidinediones, meglitinides and insulin have unwanted effects like diarrhoea, ketoacidosis, hypothyroidism, tachycardia, weight gain, etc. (10). Plant derived medication was found to be associated with less side effects (11). The World Health Organisation (WHO) emphasises the role of medicinal plants, in terms of phyto-ingredients present in improving health and treatment of disease (12). The proper scrutiny of phytochemicals of traditionally used medicinal plants is a must to develop effective therapeutic strategies successfully (13).

Advanced methods are available to detect phytochemicals in crude samples, deduce structure and isolate them in pure form. Technology such as LC-MS, GC-MS and NMR has made it easier and less time consuming to identify and characterise phytochemicals. Secondary metabolites identified by these techniques can be utilised for *in silico* docking studies, which visualise molecular interactions towards drug discovery. Molecular docking is used to verify the fitness of a ligand to interact with receptor proteins in 3D spaces and the technique puts itself into a position of importance in drug discovery (9). Biological activity can also be determined by docking. Moreover, docking provides a rapid screening method of inhibitors and activators (14).

Human enzymes such as α-amylase and α-glucosidase play a significant role in glucose metabolism. Inhibiting α-amylase and α-glucosidase is a therapeutic strategy for managing T2DM. Pancreatic α-amylase is a key enzyme that breaks down dietary carbohydrates such as starch into simple sugars, which are further degraded by α-glucosidase, which enters the bloodstream (8). Inhibition of α-amylase and α-glucosidase enzymes can retard carbohydrate digestion. Many synthetic drugs target these enzymes as therapeutic agents for the treatment diabetes, but not without side effects (15). In the present study, metabolite profiling of the crude extract of *D. scandens* root tuber was evaluated and potential antidiabetic phytochemicals were identified. Activity was monitored through an enzyme inhibition assay and further antidiabetic activity was confirmed by molecular docking.

Materials and Methods

Collection of plant materials

Dactylicapnos scandens plant samples were collected from the agricultural field of an ethno farmer from the Phek District of Nagaland in India during the month of April 2021 (latitude is 25°70′ N and longitude is 94°35′ E), authenticated by the Department of Botany, Gauhati University, Guwahati, with accession no GUBH18640.

Preparation of plant extract

The root tubers of *D. scandens* (1000 g) were thoroughly rinsed 3–5 times with fresh water and once finally with double-distilled water to eliminate adhering dust. The root tubers were dried on sterile blotter under shade and then powdered in a mixture grinder with a yield of 450 g of dry powder (4.5:10 ratio). About 10 g of the powdered root tubers were subjected to extraction with methanol (1:10) ratio. The methanol extract was filtered using Whatman No. 1 filter paper and concentrated using a rotary evaporator at 40 °C. The crude extract was stored in sterile glass vials at 4 °C for further analysis.

α-Amylase inhibition assay

The inhibition of α-amylase was done according to given method (16). Crude extract and standards acarbose were taken in concentrations 10 µL, 20 µL, 30 µL and 40 µL. All the concentrations were taken in triplicate. To each concentration, 200 µL of α-amylase (2 units/mL), 200 µL of starch (1 %), were added and incubated for 10 min at 30 °C. The reaction was terminated by adding 0.8 mL of NaOH (2M). Following which, 20 µL of DNS (12 g sodium potassium tartrate tetrahydrate in 8.0 mL of 2 M NaOH and 20 mL of 96 mM 3,5-dinitrosalicylic acid solution) was added to the reaction solution and boiled for 10 min at 85 °C in water bath. The mixture was diluted with 2.5 mL of distilled water after cooling to room temperature. The negative control was prepared in the same way as the test samples, except that the crude extract was altered with 200 µL of buffer. The absorbance was measured at 540 nm using a UV-visible spectrophotometer. The α-amylase inhibitory activity was calculated as a percentage of inhibition using the following equation:

$$\%\ \alpha\text{-amylase inhibition} = \frac{\text{Negative control} - \text{Absorbance of sample/standard}}{\text{Negative control}} \times 100$$

The % α-amylase inhibition was plotted against the extract concentration and the IC_{50} values was calculated.

α-Glucosidase inhibition assay

The α-glucosidase inhibition test was performed according to method mentioned earlier (17). The positive control (acarbose) and crude extract were taken in concentrations ranging from 10 to 40 µL. All the concentrations were taken in triplicate. The reaction mixture was prepared by adding 100 µL of α-glucosidase (1.0 U/mL) with the replicates and incubated at 37 °C for 10 min. Later, 50 µL of *p*-nitrophenyl glucopyranoside (pNPG 3.0 mM) was added and the mixture was incubated at 37 °C for 20 min. The reaction was stopped with 2 mL of 5 % (w/v) Na_2CO_3 and cooled to room temperature. Negative control contained complete reaction mixture except that the crude extract was replaced by 50 µL of methanol. Absorbance was measured at 405 nm using a UV spectrophotometer. The α-glucosidase inhibitory activity was calculated as percentage of inhibition using the following formula:

$$\%\ \alpha\text{-glucosidase inhibition} = \frac{\text{Negative control} - \text{Absorbance of sample/standard}}{\text{Negative control}} \times 100$$

The % α-glucosidase inhibition was plotted against the extract

concentration and the IC_{50} value was calculated.

LC-MS analysis

The bioactive compounds in the methanol crude extract of *D. scandens* root tuber were analysed using an Agilent 6410B triple quadrupole LC-MS system with an ESI source. The extract was filtered with a 0.45 µm pore size sterile syringe filter prior to analysis. The column was maintained at 25 °C with an injection volume of 10 µL. The elution gradient consisted of mobile phase A (0.1 % formic acid with water) and mobile phase B (methanol) at a flow rate of 0.40 mL/min. The gradient program was fixed as follows: 0–1 min, 5 %; 1–25 min, 5 %; 25–30 min, 90 %; 30–31 min, 5 %; 31–40 min, 5 %, with a total analysis time of 40 min. Triple-quadrupole mass spectrometer (QqQ MS) in both positive and negative ionization modes was used for LC-MS.

GC-MS analysis

The methanol crude extract of *D. scandens* root was analysed using a Perkin Elmer Clarus 680 GC-MS with a Clarus 600C MS and liquid autosampler. A 1 µL sample was manually injected at a flow rate of 1 mL/min using helium as the carrier gas (99.99 %). The injector temperature was set at 280 °C, with the ion source at 180 °C. The oven temperature program started at 60 °C (1 min), ramped to 200 °C at 7 °C/min (3 min hold), then to 300 °C at 10 °C/min (5 min hold). Ionization was conducted at 70 eV in EI+ mode, with a mass scan range of 20–500 m/z at 0.2-sec intervals. Compounds were identified by comparing the obtained spectral data with the National Institute Standard and Technology Library NIST database.

Molecular docking

The compounds identified by GC-MS and LC-MS from *D. scandens* root tuber were docked into the active site of human pancreatic α-amylase and human small intestinal α-glucosidase. We considered binding energy and H-bond formation for monitoring affinity to the receptors.

Preparation of protein

The PDB structures of human pancreatic α-amylase (4W93) and human small intestinal α-glucosidase (3WY1) were retrieved from the RCSB Protein Data Bank (http://www.rcsb.org/pdb/). Using UCSF Chimera 1.17.3, water molecules, non-standard amino acids and heteroatoms were removed, while polar hydrogens and Kollman charges were added. Non-polar hydrogens were merged and pdbqt files were generated with Autodock Tools 1.5.7 (18).

Preparation of ligand

The structures of andrographolide (CID: 5318517), octadecanoic acid (CID: 5218), oleic acid (CID: 445639) and vincamine (CID: 15376) were obtained as SDF files from PubChem (https://pubchem.ncbi.nlm.nih.gov) and converted to PDB format using UCSF Chimera. QSAR studies were conducted to assess their biological activity, focusing on Lipinski's rule of five which is a set of rules used to determine the drug-likeness of small compounds. These criteria include a molecular weight of 500 g/mol or less, a Log*p* (octanol-water partition coefficient) of 5 or below, no more than 10 hydrogen bond acceptors, no more than 5 hydrogen bond donors and a topological polar surface area of 140 $Å^2$ or less. (19). ADME prediction data such as AMES toxicity, absorption (water solubility) and metabolism (CYP3A4 substrate) from pkCSM pharmacokinetics were also included. For molecular docking, the ligands were optimized, energy minimized with UCSF Chimera 1.15 and converted to pdbqt format using Autodock 1.5.7 (18).

Grid box configuration and molecular docking

Molecular docking was performed with andrographolide, octadecanoic acid, oleic acid and vincamine against α-amylase and α-glucosidase using AutoDock 4.2.6 (20). Active binding site residues of the proteins were identified through CASTp 3.0 (18) and a grid box encompassing these residues was constructed as shown in Table 1. The Lamarckian Genetic Algorithm was applied for docking, selecting conformations based on binding energies and conventional hydrogen bonds (18). Efficient binding, essential for drug-likeness, was prioritised (21).

Statistical analysis

The α-amylase and α-glucosidase inhibition assays were conducted in triplicate. Data were presented as the mean ± standard deviation of the mean. Statistical significance between the standard and the methanolic crude extract was determined using GraphPad Prism 8.0 software through one-way ANOVA, where $p < 0.05$ considered statistically significant.

Results and Discussion

Plant and herbal sources are gaining popularity among researchers and pharmaceutical companies as sources of bioactive compounds for the discovery and development of targeted novel antidiabetic therapeutics (22). Plant phytochemicals demonstrate significant antidiabetic activity by regulating glucose metabolism through mechanisms such as enhancing glucose uptake, inhibiting digestive enzymes and increasing insulin secretion (23).

Enzyme inhibition

The enzymes α-amylase and α-glucosidase play a crucial role in carbohydrate metabolism, thereby influencing blood glucose levels. The α-amylase hydrolyses the α-bonds in α-linked polysaccharides, generating large amounts of glucose. Similarly, α-glucosidase breaks down dietary carbohydrates or starch, leading to the intestinal absorption of glucose into the bloodstream. Inhibition of these enzymes can help reduce postprandial blood glucose levels in patients with hyperglycemia by delaying carbohydrate digestion and absorption (24). Strong inhibition of α-glucosidase is particularly effective in lowering elevated postprandial glucose levels (24). Their dysregulation can lead to (T2DM) hyperglycemia (25). Therefore, inhibiting these enzymes can help control the prevalence of T2DM (26). In addition, multiple studies have emphasised the importance of screening enzyme inhibitors for the development of new antidiabetic drugs (27–29). The present study reveals the inhibitory activity of *D. scandens* for α-amylase and α-glucosidase (Table 2). Previous reports indicate that *Ajuga iva* showed weak inhibition of α-

Table 1. Active binding site residues of proteins

Protein	PDB ID	Active binding site residues
α-Amylase	4W93	TRP57,TRP58,TYR61,GLN62,HIS100,TYR150,LEU161,THR162,LEU164,ARG194,ASP196,ALA197,LYS199,HIS200,GLU232,ILE234,PHE255,ASN297,HIS298,ASP299,ASN300,HIS304,GLY305,ALA306
α-Glucosidase	3WY1	TYR14,ASP59,PHE60,TYR62,HIS102,ILE143,PHE144,PHE163,GLN167,ARG197,ASP199,THR200,PHE203,THR223,LEU224,GLY225,ALA226,PRO227,GLU228,ALA229,TYR232,HIS237,LEU241,GLU268,ILE269,GLY270,ASP271,PRO274,THR294,LEU297,ASN298,MET299,HIS329,ASP330,VAL331,VAL332,ARG337,GLU374,TYR386,GLU393,PHE394,GLY396,ARG397,CYG400,ARG401

Table 2. Inhibitory effect (IC_{50}) of crude extract of *Dactylicapnos scandens* against enzyme α-amylase and α-glucosidase

Sample/Standard	IC_{50} value of α-amylase (µg/mL)	IC_{50} of α-glucosidase (µg/mL)
Acarbose	84.6 ± 1.7418	46.38 ± 1.203
DS CE	95.98 ± 1.928	66.04 ± 2.6302

DS CE = *Dactylicapnos scandens* crude extract.

amylase (IC_{50} 1586.33 µg/mL) compared to acarbose (616 µg/mL) (30), whereas *D. scandens* in the present study exhibited much stronger activity (IC_{50} 95.98 µg/mL), almost comparable to acarbose (84.60 µg/mL). For α-glucosidase, *Ajuga iva* displayed notable inhibition (IC_{50} 143.17 µg/mL) (30), even better than acarbose (195 µg/mL), but *D. scandens* showed superior potency (IC_{50} 66.04 µg/mL), closer to the standard drug (46.38 µg/mL). *Dactylicapnos scandens* demonstrates a more balanced and stronger inhibitory profile across the two enzymes, highlighting its potential in diabetes management.

LC-MS and GC-MS analysis for *Dactylicapnos scandens* of the root tuber

Screening of phytochemicals at the molecular level plays an important role in finding bioactive compounds that may lead to the development of new therapies (31). Previously methanol extract of root tuber of *D. scandens* were reported to possess diverse bioactive compounds (32). GC-MS is optimal for analysing volatile metabolites, such as organic acids, amino acids and sugars, while LC-MS primarily detects fewer volatile compounds common in secondary metabolites, including phenolics and terpenoids. *Manihot esculenta* Crantz tuberous roots were reported to contain antidiabetic bioactive molecules identified through GC-MS and LC-MS analyses, including 2-phenylpyrido[3,4-d]-1,3-oxazin-4-one, guanosine, quercetin-3-O-sophoroside and esculin (33). A total of 17 compounds were identified in the crude extract of *D. scandens*. LC-MS analysis identified acebutolol, hdrocortisone, disulfiram, corymbosin, vincamine, gentisic acid and andrographolide, based on m/z values and retention times (Table 3). Among these, andrographolide and vincamine have previously been reported for their antidiabetic activity (34, 35). GC-MS profiling, validated against the NIST library, further revealed bioactive metabolites such as Z,Z-6,28-heptatriactontadien-2-One, 2-ethylthiolane S,S-dioxide, fumaric acid 3-methylbut-3-enyl octyl ester, succinic acid 4-methoxy-2-methylbutyl octadecyl ester, hexacosyl acetate, 2-methoxy-4-vinylphenol, 2,2-dimethyleicosane, 3-methyl-2-(2-oxopropyl) furan, oleic acid and octadecanoic acid (Table 4). Notably, oleic acid and octadecanoic acid are well-documented for their antidiabetic properties (36, 37). The phytochemical analysis of *D. scandens* revealed the presence of a diverse range of bioactive compounds belonging to different classes, as mentioned in Table 5. Most of the compounds, except andrographolide, vincamine, oleic acid and octadecanoic acid, have no previous reports of antidiabetic activity (Fig. 1 and 2).

Table 3. List of compounds identified from LC-MS spectrum of *Dactylicapnos scandens*

Sl. No.	RT	Compound name	Formula	M/Z
1	2.816	Acebutolol	$C_{18}H_{28}N_2O$	336.2
2	2.897	Disulfiram	$C_{10}H_{20}N_2S_4$	174
3	15.101	Hydrocortisine	$C_{21}H_{30}O_5$	331.1
4	17.562	Vincamine	$C_{21}H_{26}N_2O_3$	294.2
5	20.953	Corymbosin	$C_{19}H1_8O_7$	738.3
6	32.55	Gentisic Acid	$C_7H_6O_4$	278.1
7	35.059	Andrographolide	$C_{20}H_{30}O_5$	474.3

Molecular docking

Molecular docking in drug designing predicts ligand-protein interactions by calculating binding affinity and visualizing key amino acid interactions (18). The chemical analysis done in the present study suggested that the plant extract is rich in bioactive compounds, which could contribute to the inhibition of α-amylase and α-glucosidase as observed in the *in vitro* enzyme inhibition experiments. To reconfirm the results, docking studies were undertaken. Previous literature has cited use of molecular docking as confirmatory test for *in vitro* enzyme inhibition assays (38). Here, the binding interaction of selected ligands identified in crude extract of *D. scandens* root tuber namely andrographolide, vincamine, octadecanoic acid and oleic acid were docked with target proteins. Human pancreatic α-amylase and small intestinal α-glucosidase were chosen as target proteins for the study as they are linked to glucose metabolism and some of the presently available drugs targets these proteins (39). The ligand enzyme interactions are expected to cause changes in the three-dimensional structure of enzymes resulting in loss of function such as inhibition, which further decreases the digestion of dietary carbohydrate and glucose intake into the blood providing antidiabetic efficacy (38).

Before performing the molecular docking studies the ligand characteristics were analysed (Table 6). Eight docking studies were conducted against these proteins, assessing binding conformation, free binding energy (ΔG kcal/mol) and hydrogen bond interactions (Table 7). The interactions between the ligands and target enzymes were found to be spontaneous, as indicated by the negative Gibbs free energy (ΔG) values as was indicated by previous studies (39, 40). Molecular docking studies showed significant binding affinities between target proteins and ligands with root mean square deviation (RMSD) as shown in Table 7. Our current investigation showed that the active site of human pancreatic α-amylase is characterized by two key amino acid residues, Asp196 and Glu232, which are essential for the enzyme's catalytic action in starch hydrolysis. The docking analysis revealed that Andrographolide identified from LC-MS exhibited a strong binding affinity (ΔG = −8.27 kcal/mol) with α-amylase, forming two hydrogen bonds with the active site residues as shown in Fig. 3. Andrographolide exhibited strong binding with the active site of human small intestine α-glucosidase also, three hydrogen bonds interacting with the residues

Table 4. List of compounds identification from GC-MS analysis of *Dactylicapnos scandens* crude extract

Sl. No.	RT	Compound name	Area %	Formula
1	5.018	Z,Z-6,28-Heptatriactontadien-2 One	7.19	$C_{37}H_{70}O$
2	12.982	2-Ethylthiolane S,S-dioxide	2.086	$C_6H_{12}O_2S$
3	13.527	Fumaric acid, 3-methylbut-3-enyl octyl ester	7.385	$C_{27}H_{48}O_4$
4	14.477	succinic acid, 4-methoxy-2-methylbutyl octadecyl ester	3.044	$C_{28}H_{54}O_5$
5	16.168	Hexacosyl acetate	1.025	$C_{28}H_{56}O_2$
6	17.889	2-Methoxy-4-vinylphenol	3.651	$C_9H_{10}O_2$
7	20.455	2,2-Dimethyleicosane	1.697	$C_{22}H_{46}$
8	24.206	3-Methyl-2-(2-oxopropyl) furan	4.246	$C_8H_{10}O_2$
9	24.331	Oleic acid	1.614	$C_{18}H_{34}O_2$
10	29.723	Octadecanoic acid	1.238	$C_{18}H_{36}O_2$

Table 5. Compound classification identified from GC-MS and LC-MS from root tuber of *Dactylicapnos scandens*

Sl. No.	Compound names	Class
1	Acebutolol	Organic acid ester
2	Disulfiram	Organic acid ester
3	Hydrocortisine	Organic acid ester
4	Vincamine	Alkaloid
5	Corymbosin	Alkaloid
6	Gentisic acid	Phenolic
7	Andrographolide	Diterpenoid
8	Z,Z-6,28-Heptatriactontadien-2 One	Aliphatic hydrocarbon
9	2-Ethylthiolane S,S-Dioxide	Organic acid ester
10	Fumaric Acid, 3-Methylbut-3-Enyl Octyl Ester	Organic acid ester
11	Succinic Acid, 4-Methoxy-2-Methylbutyl Octadecyl Ester	Organic acid ester
12	Hexacosyl Acetate	Terpenoid
13	2-Methoxy-4-Vinylphenol	phenolic
14	2,2-Dimethyleicosane	Aliphatic hydrocarbon
15	3-Methyl-2-(2-Oxopropyl) Furan	Organic acid ester
16	Oleic acid	Fatty acid
17	Octadecanoic acid	Fatty acid

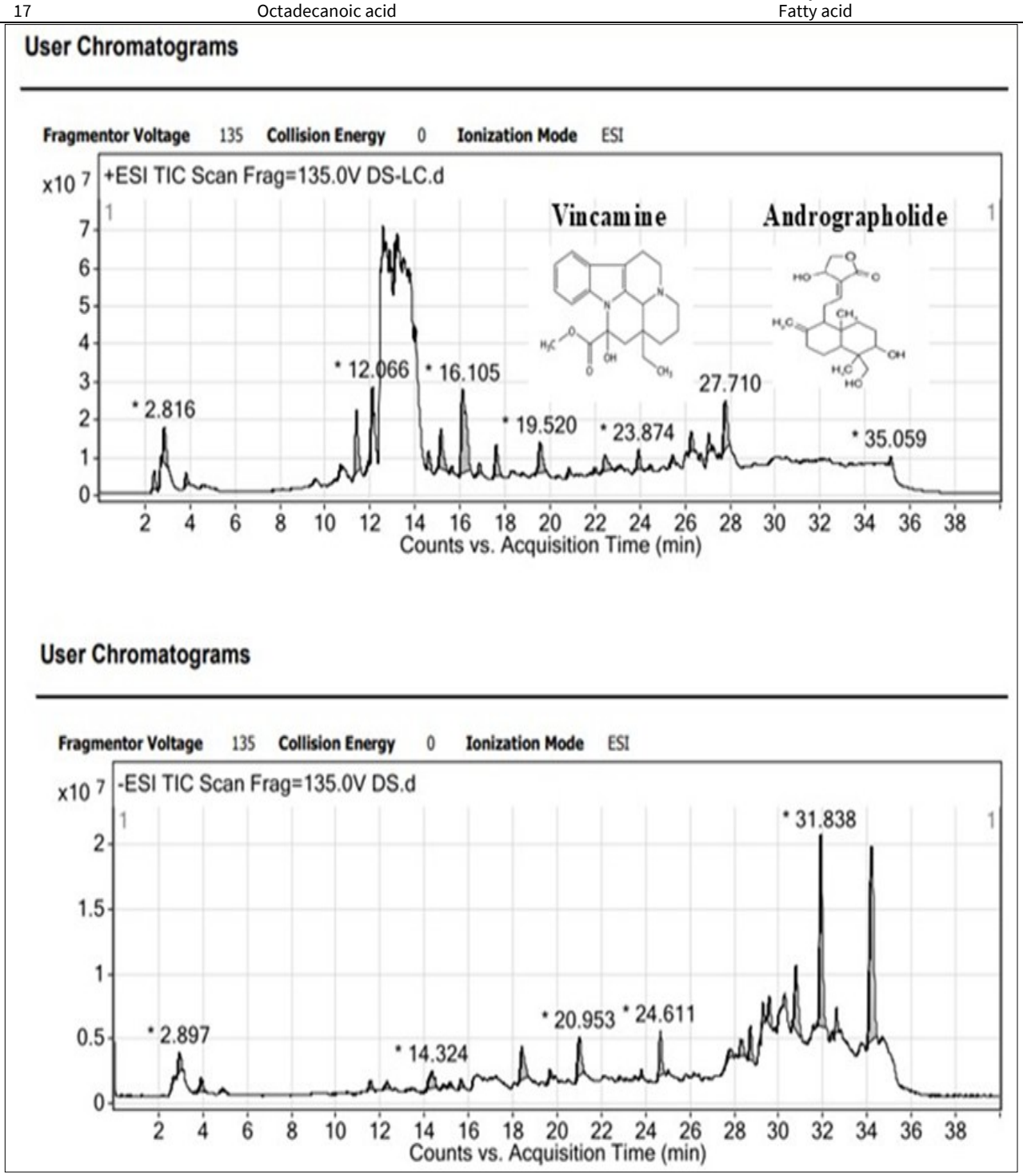

Fig. 1. The liquid chromatography-mass spectroscopy chromatogram analysis of non-volatile bioactive compounds from the crude extract of *Dactylicapnos scandens* root tuber at positive and negative ESI. Compounds were identified using MassBank Europe Database.

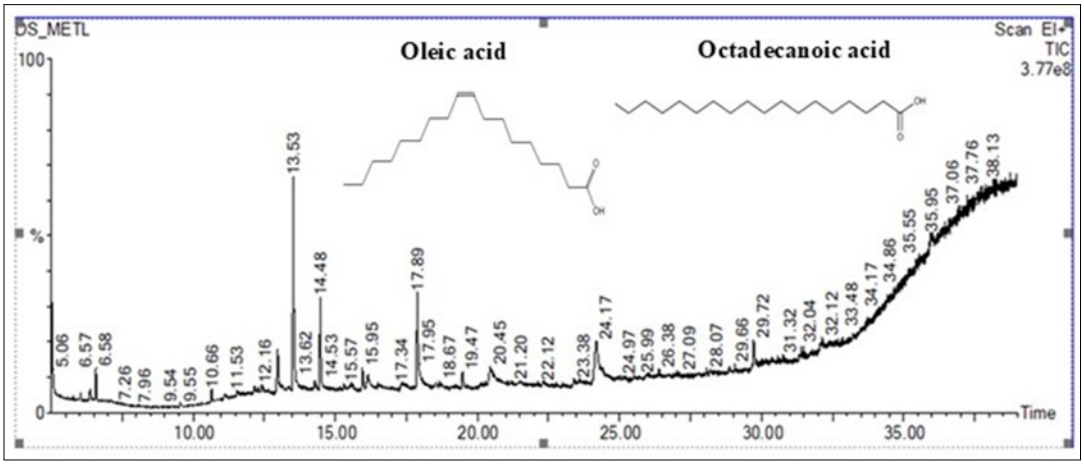

Fig. 2. The gas chromatography-mass spectroscopy analysis chromatogram of volatile bioactive compounds from crude extract of the *Dactylicapnos scandens* root tuber. Compounds were identified using the National Institute Standards and Technology Library database.

Table 6. Ligand properties analysis

Ligands	PubChem CID	Log *p*	Hydrogen bond acceptor	Hydrogen bond donor	Molecular weight	Topological polar surface area	AMES toxicity	Absorption (water solubility (log mol/L))	Metabolism (CYP3A4 substrate)
Andrographolide	5318517	2.2	5	3	350.4	87	No	-3.494	Yes
Octadecanoic acid	5281	7.4	2	1	284.5	37.3	No	-5.973	Yes
Oleic acid	445639	6.5	2	1	282.5	37.3	No	-5.924	Yes
Vincamine	15376	2.9	4	1	354.4	54.7	No	-3.643	Yes

Table 7. Docking results of protein with ligands of *Dactylicapnos scandens*

Sl no	Ligands	Proteins	Conformations	Binding energy (kcal/mol)	RMSD cluster	Numbers of hydrogen bond
1	Andrographolide	α-Amylase	1	−8.27	0.00	2
2	Octadecanoic acid		4	−4.56	0.00	2
3	Oleic acid		7	−4.20	0.00	2
4	Vincamine		10	−7.02	0.00	2
5	Andrographolide	α-Glucosidase	1	−9.24	0.00	3
6	Octadecanoic acid		2	−4.88	0.00	2
7	Oleic acid		2	−4.90	0.00	3
8	Vincamine		4	−8.37	0.00	2

Leu224, Glu393 and Lys395, showing binding energy (ΔG) of −9.24 kcal/mol (Fig. 3). Vincamine identified from LC-MS exhibited strong binding affinity with both target enzymes. It formed two hydrogen bonds with the active site residues Trp58 and Gln62 of Human pancreatic α-amylase, showing a binding energy (ΔG) of −7.02 kcal/mol. Similarly, two hydrogen bonds were interacting with the active site residues Ala375 and Gln396 of Human small intestinal α-glucosidase, with a binding energy (ΔG) of −8.37 kcal/mol (Fig. 4).

Another compound identified from GC-MS analysis, Octadecanoic acid showed weak binding affinity with both target enzymes. Two hydrogen bonds were observed to interact with the active site residues namely Tyr150 and Lys199 of human pancreatic α-amylase showing binding energy of (ΔG) of −4.56 kcal/mol. On the other hand, active site residues Leu297 and Val332 of human small intestine α-glucosidase interacted with two hydrogen bonds exhibiting a binding energy (ΔG) of −4.88 kcal/mol (Fig. 5). Oleic acid identified from GC-MS exhibited again low binding affinity with both target enzymes. it formed two hydrogen bonds with the active site residues Glu232 and Ile234 of Human pancreatic α-amylase with a binding energy (ΔG) of −4.2 kcal/mol and three hydrogen bonds with the active site residues Thr223, Tyr232 and Gly270 of human small intestinal α-glucosidase with a binding energy (ΔG) of −4.9 kcal/mol (Fig. 6).

The molecular docking results are presented in the form of a heat map in Fig. 7. A lower binding energy, or more negative free energy of binding, usually suggests better stability and binding affinity between the compound and the receptors (41). The selected ligands exhibited binding affinities of less than −6.50 kcal/mol, which are generally considered minimum for potential enzymatic activities (42). In the present study, among the four plant-derived compounds, andrographolide and vincamine (Log *p* values of 2.2 and 2.9 respectively) showed binding affinity values below -6.5 kcal/mol with both α-amylase and α-glucosidase (Table 7) suggesting their strong interaction and potential as effective enzyme inhibitors. The other two compounds octadecanoic acid and oleic acid presented binding energies above -6.5 Kcal/mol (Table 7) with Log *p* values of 7.4 and 6.5 respectively. The higher Log *p* values might pose poor absorption due to lipophilicity potentially limiting their efficacy (43). Therefore, Andrographolide and Vincamine might be considered more probable candidates for future antidiabetic drug development.

The docking study suggests that ligands have significant binding affinities as well as hydrogen bond formation with protein targets. Our *in silico* docking results reaffirm the antidiabetic potential of *D. scandens* root tuber. Phytochemicals such as andrographolide, vincamine, octadecanoic acid and oleic acid identified in the crude extract showed binding affinity towards glucose metabolism receptor proteins, α-amylase and α-glucosidase. Although andrographolide and vincamine represented highest affinity, we believe that the antidiabetic efficacy of crude extract of *D. scandens* root tubers may be due to the presence of multiple potential phytoconstituents. Further analysis would be required to establish the holistic behaviour of composite

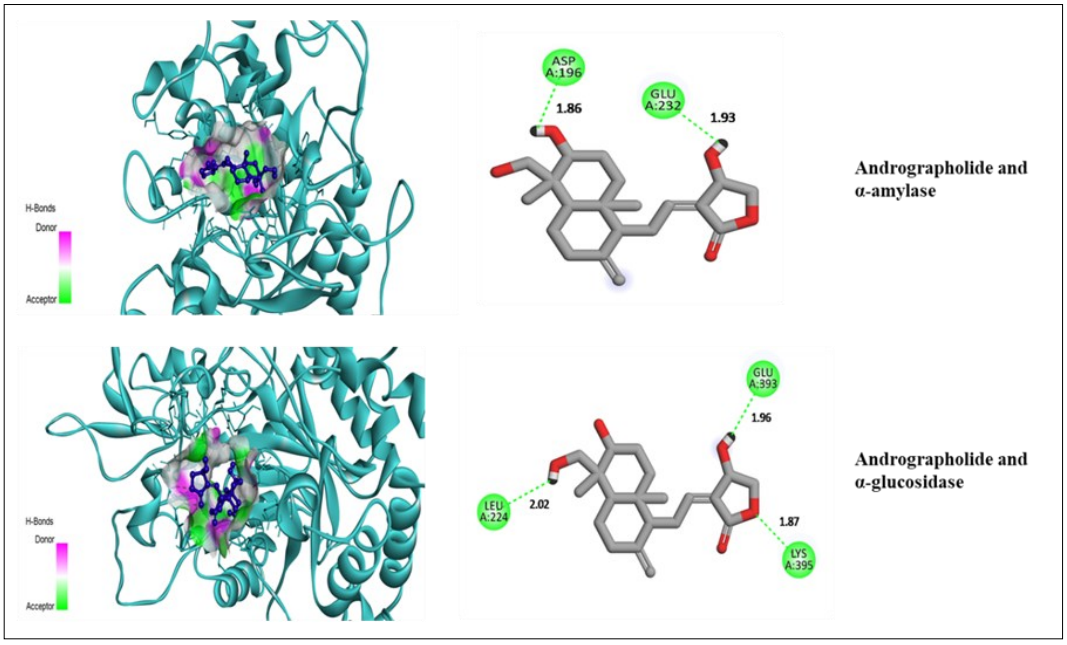

Fig. 3. Docking images 3D and 2D structure of andrographolide with α-amylase, and α-glucosidase. 2D image showing hydrogen bond numbers and distances between andrographolide and the receptors (BIOVIA Discovery Studio Visualizer).

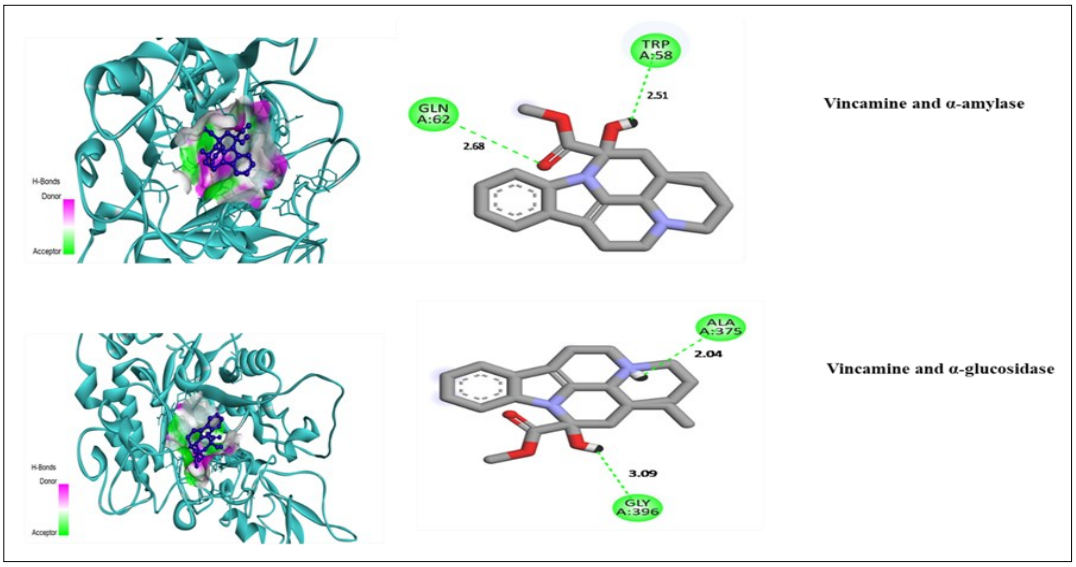

Fig.4. Docking images of vincamine with α-amylase and α-glucosidase in both 3D and 2D structures. The 2D images showing the number and distances of hydrogen bonds between vincamine and the receptors (BIOVIA Discovery Studio Visualizer).

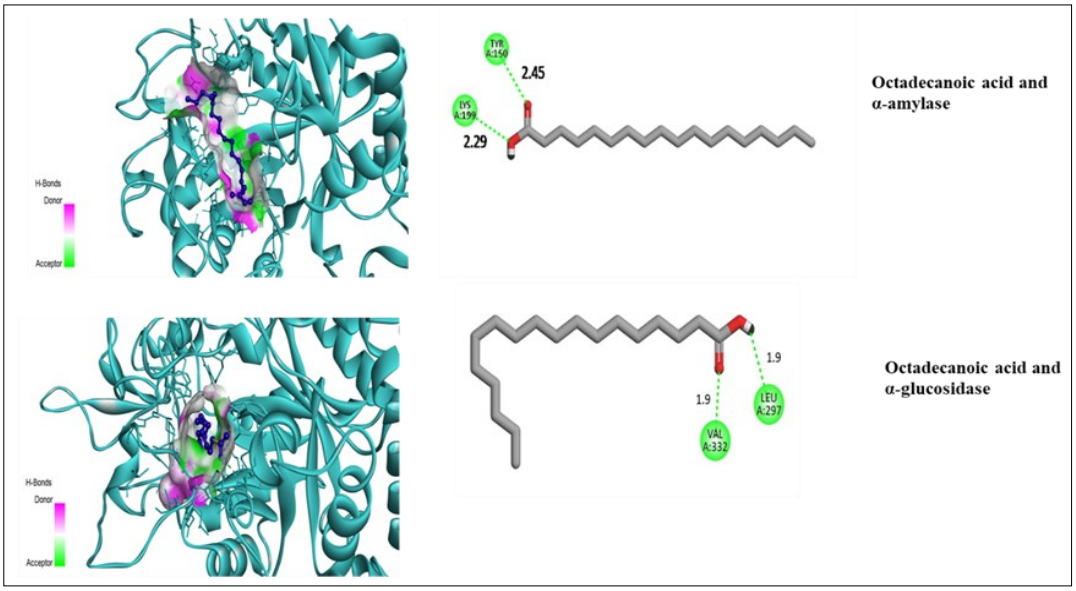

Fig. 5. 3D and 2D docking images of octadecanoic acid with α-amylase and α-glucosidase. The 2D images show the number and distances of hydrogen bonds between octadecanoic acid and the receptors (BIOVIA Discovery Studio Visualizer).

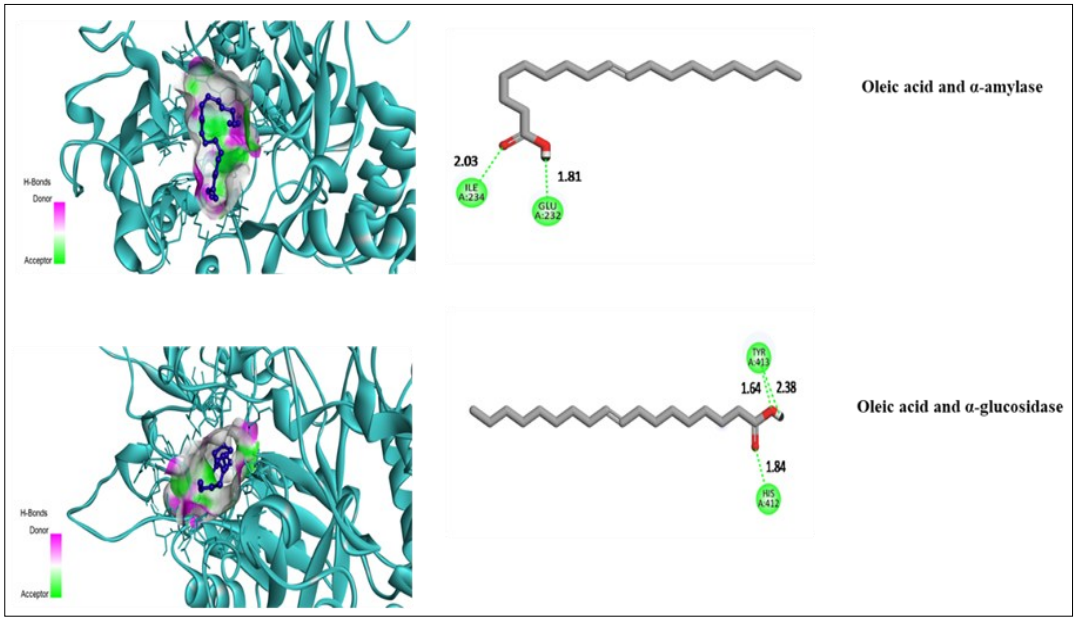

Fig. 6. Docking images show the 3D and 2D structures of oleic acid with α-amylase and α-glucosidase. The 2D images show the number and distances of hydrogen bonds between oleic acid and the receptors (BIOVIA Discovery Studio Visualizer).

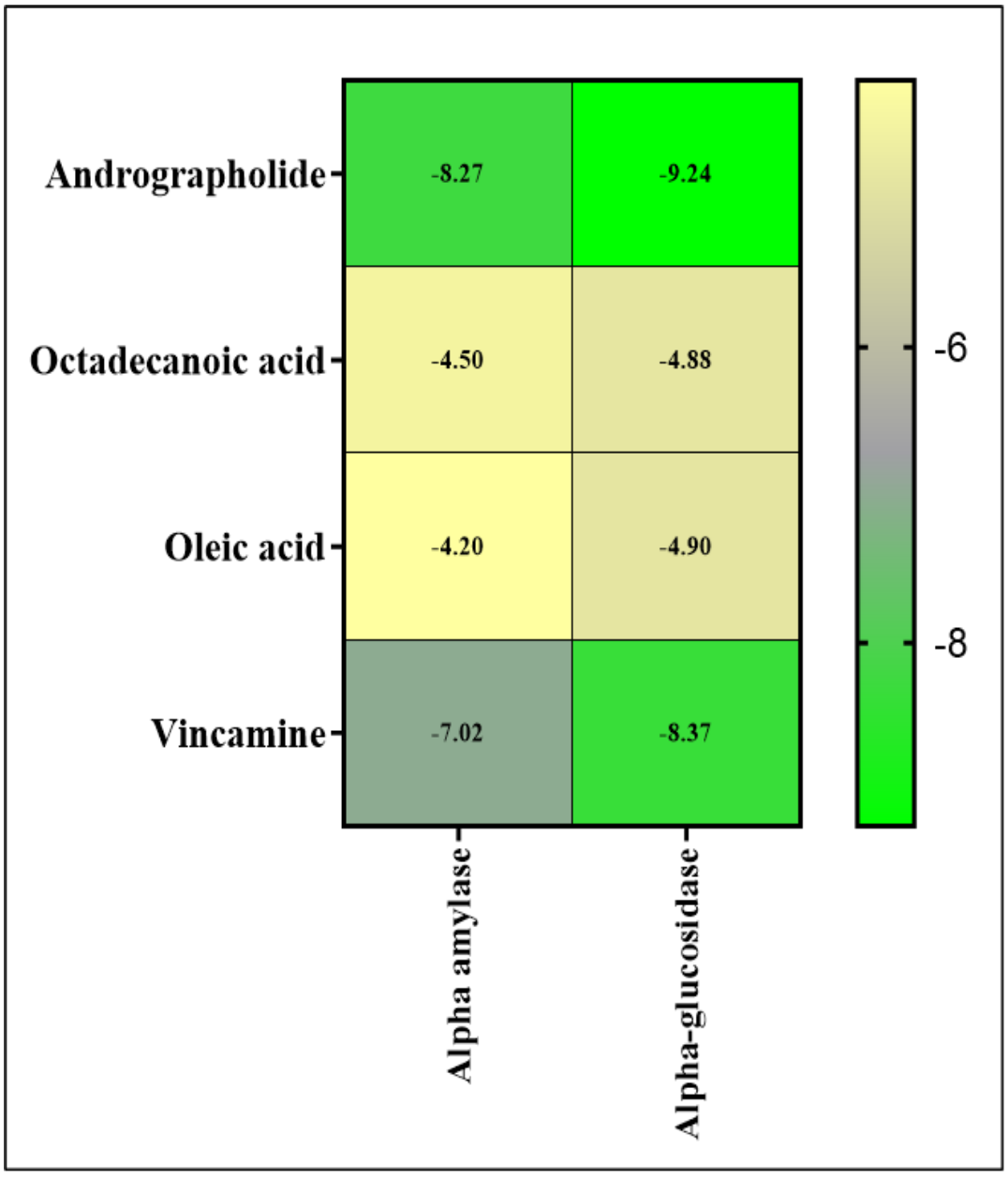

Fig. 7. Heatmap for molecular docking scores (kcal/mol) between targets and 4 antidiabetic compounds. Lower value indicates a stronger binding ability.

phytochemicals present in the root tubers of *D. scandens*.

Conclusion

Bioactive compounds from herbal sources exhibit health benefits when consumed and provide a better option compared to synthetic drugs for the treatment of chronic diseases. Addressing the complications and challenges of diabetes remains a significant concern in healthcare. This study demonstrated that the crude extract of *D. scandens* root tuber exhibited strong inhibitory activity against both α-amylase and α-glucosidase enzymes. The molecular profiling of the crude extract identified four bioactive compounds having antidiabetic activity. These compounds may serve as the active constituents of the crude extract, which potentially inhibit the α-amylase and α-glucosidase enzymes *in vitro*. Molecular docking studies reaffirmed the antidiabetic potential of these four compounds, revealing interactions with key amino acid residues located in the active sites of the target proteins. Andrographolide and Vincamine exhibited significant binding affinities. The study suggests that the root tuber extract of *D. scandens* could be beneficial in the management of diabetes and could be the source of future therapeutics. Further studies, such as cellular assays for glucose uptake, *in vivo* efficacy evaluation in diabetic models and toxicity profiling are recommended. Although the study provides evidence for the efficacy of crude extract in diabetes management, effectiveness and reliability on human must be verified scientifically before herbal formulations or drugs are designed for medical use.

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Authors' contributions

RB performed the methodology and wrote the original draft; AN carried out data curation; BD contributed to visualization; RD conducted formal analysis; MR was responsible for investigation; PB contributed to conceptualization, funding acquisition, resources, supervision and writing review and final editing. All authors read and approved the final manuscript.

Compliance with ethical standards

Conflict of interest: Authors do not have any conflict of interest to declare.

Ethical issues: None

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