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Research Article

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GC-MS Based Characterization and Bioprospecting of Novel Aromatic Compounds in Indonesian Local Golden Rice "Pulu Mandoti" as Antidiabetic and Antioxidant Agent

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ABSTRACT

Background: Diabetes mellitus and oxidative stress are major global health challenges, increasing the demand for natural compounds with therapeutic potential. Pulu Mandoti, a traditional red rice variety from Enrekang Regency, Indonesia, is recognized for its nutritional value and potential health-promoting properties due to its diverse bioactive constituents.

Aims: This study aimed to evaluate the antidiabetic and antioxidant potential of Pulu Mandoti extract using an integrated in silico approach.

Methods: Bioactive compounds in Pulu Mandoti extract were identified using Gas Chromatography–Mass Spectrometry (GC-MS). The identified compounds were subsequently subjected to molecular docking analysis against α-amylase, α-glucosidase, NADPH oxidase, and xanthine oxidoreductase to predict their antidiabetic and antioxidant activities. Drug similarity network analysis was also performed to evaluate the structural similarity of the identified compounds to established therapeutic agents.

Results: GC-MS analysis identified ten volatile compounds, with γ-sitosterol, squalene, tetradecanoic acid, hexadecanoic acid, and octadecanoic acid as the major constituents. Molecular docking demonstrated that γ-sitosterol exhibited the strongest binding affinity toward α-amylase and α-glucosidase, with binding energies of −9.1 and −8.4 kcal/mol, respectively. For antioxidant targets, compounds 2 and 1 showed the highest binding affinities toward NADPH oxidase and xanthine oxidoreductase, with binding energies of −8.7 and −8.0 kcal/mol, respectively. Drug similarity analysis further revealed that hexadecanoic acid exhibited the highest structural similarity to acarbose (0.72) and antioxidant peptide A (0.62), supporting its potential pharmacological relevance.

Conclusion: Pulu Mandoti contains several bioactive compounds with promising antidiabetic and antioxidant properties. These findings highlight the potential of this traditional red rice as a natural source of therapeutic compounds and provide a scientific basis for further experimental validation of its pharmacological activities.

INTRODUCTION

Diabetes mellitus is a major global public health problem, with the International Diabetes Federation (IDF) estimating that 537 million adults were living with diabetes in 2021. Indonesia ranks among the countries with the highest prevalence, with approximately 19.47 million cases and a national prevalence of 10.6% (International Diabetes Federation, 2021; Lin et al., 2020). Diabetes is a chronic metabolic disorder characterized by

elevated blood glucose levels, which can trigger the excessive production of reactive oxygen species and free radicals. Persistent oxidative stress contributes to tissue damage and increases the risk of complications such as nephropathy, neuropathy, retinopathy, and cognitive disorders (Bhuyan et al., 2022). Although various synthetic antidiabetic drugs are available, their use is frequently associated with adverse effects, including gastrointestinal disorders, dizziness, hypersensitivity reactions, weight gain, and hypoglycemia (Chaudhury et al., 2017). These limitations have encouraged the exploration of safer and more effective bioactive compounds from natural sources as alternative therapeutic agents (Mirmiran et al., 2014).

Rice is one of the most important staple foods worldwide and also has considerable potential as a functional food. In recent years, pigmented rice varieties, particularly red rice, have attracted attention because of their nutritional and health-promoting properties (Bhat et al., 2020). Compared with white rice, red rice contains higher levels of dietary fiber, vitamins, minerals, phenolic compounds, and anthocyanins that contribute to antioxidant and antidiabetic activities (Markus et al., 2021; Priya et al., 2019).

Previous studies demonstrated that red rice exhibits significant biological activities, including antioxidant effects and α-amylase inhibitory activity associated with antidiabetic potential (Agustin et al., 2021). In addition, several Indian red rice cultivars showed promising antihyperglycemic, antioxidant, and anti-glycation activities in both in vitro and in silico studies (Haldipur & Sridivya, 2021).

Pulu Mandoti is a local red glutinous rice variety originating from Enrekang Regency, South Sulawesi, Indonesia. This rice is known for its distinctive aroma and is traditionally cultivated in Salukanan and Kendenan villages located in the Baraka region at approximately 700 m above sea level (Amrullah et al., 2020). Previous studies reported that pigmented glutinous rice possesses strong antioxidant and antibacterial properties, particularly in darker-colored varieties (Sani et al., 2018). Red glutinous rice has also been reported to contain phenolic compounds with significant antioxidant activity (Prasmita et al., 2017).

Furthermore, Kiay et al. (2019) demonstrated the antioxidant potential of Mandoti rice from Salukanan and Kendenan, highlighting its richness in vitamins and essential minerals. However, studies investigating the antidiabetic and antioxidant potential of Pulu Mandoti through in silico approaches remain limited. Therefore, this study aimed to evaluate the potential bioactive compounds of Pulu Mandoti rice as antidiabetic and antioxidant agents using an in silico approach.

MATERIALS AND METHODS

GC-MS Analysis, Molecular Docking, and Drug Similarity Analysis of Pulu Mandoti Rice

Pulu Mandoti rice grains were cleaned to remove impurities, air-dried at room temperature, ground into a fine powder using a laboratory grinder, and sieved to obtain a homogeneous particle size. Ten grams of powdered sample were extracted by maceration in 100 mL methanol for 24–48 h at room temperature with occasional shaking. The extract was filtered through Whatman No. 1 filter paper and centrifuged at 4,000 rpm for 10 min to remove suspended particles. The resulting supernatant was concentrated using a rotary evaporator at 40 °C to obtain a crude extract. Prior to analysis, the extract was diluted with chromatographic-grade methanol, homogenized using a vortex mixer, filtered through a 0.22 µm syringe filter, and transferred into GC-MS vials. Phytochemical profiling was performed using an Agilent 7890A Gas Chromatography system coupled with a 5975C VL Mass Selective Detector (Agilent Technologies, CA, USA). Separation was achieved using a DB-5MS capillary column (30 m × 0.25 mm, film thickness 0.25 µm; J&W Scientific, USA). The oven temperature was initially maintained at 50 °C for 1 min, increased at 5 °C min^{-1} to 100 °C, and subsequently raised at 9 °C min^{-1} to 200 °C. The total run time was 30 min. Helium was used as the carrier gas at a flow rate of 0.811851 mL min^{-1}. Mass spectral data were acquired under electron ionization (EI) mode with Selected Ion Monitoring (SIM), while the ion source and quadrupole temperatures were maintained at 230 °C and 150 °C, respectively. Phytochemical compounds were identified by comparing their retention times and mass spectra with reference spectra available in the NIST 08.L and Wiley 7n.l spectral libraries.

Following compound identification, molecular docking analysis was conducted to evaluate the potential of the detected compounds as antidiabetic and antioxidant agents. The docking procedure involved several stages, including protein and ligand preparation, energy minimization, grid box determination, configuration file generation, docking simulation, and interaction analysis. Protein targets associated with antidiabetic activity included Alpha-Amylase (PDB ID: 2QV4) and Alpha-Glucosidase (PDB ID: 7KBR), while antioxidant activity was evaluated using NADPH Oxidase (PDB ID: 5O0X) and Xanthine Oxidoreductase (PDB ID: 2CKJ). Three-dimensional structures of selected compounds identified by GC-MS, together with control compounds including acarbose (antidiabetic control) and vitamin C (antioxidant control), were retrieved from

PubChem and subjected to energy minimization using Avogadro software. Hydrogen atoms were subsequently added using UCSF Chimera, and all structures were converted into pdbqt format using AutoDockTools. ollowing the preparation of the PDBQT files for both the target proteins and the selected compounds, the grid box parameters were defined (Table 1), and a configuration file (*.txt*) was generated using AutoDockTools to specify the center coordinates and dimensions of the docking search space prior to molecular docking simulations.

Docking simulations were performed using AutoDock Vina to obtain binding affinity values between ligands and target proteins. Compounds with the most negative binding affinity values were considered to possess stronger interactions and higher potential biological activity. Interaction analyses between ligands and proteins were further examined using the Protein–Ligand Interaction Profiler (PLIP), while binding site validation was performed using PrankWeb to compare amino acid residues involved in ligand binding.

In addition to molecular docking, drug similarity analysis was conducted on selected compounds exhibiting promising antidiabetic and antioxidant activities. The analysis was performed using SwissADME to evaluate physicochemical properties, lipophilicity, water solubility, pharmacokinetics, drug-likeness, and medicinal chemistry characteristics. Similarity assessment employed Gower's distance method because the dataset consisted of mixed numerical and categorical variables. A similarity threshold value of 0.4 was applied to determine the closeness of the selected compounds to known drug-like molecules. This integrated approach combining GC-MS profiling, molecular docking, and drug similarity analysis provides comprehensive insight into the bioactive potential of Pulu Mandoti rice as a source of natural antidiabetic and antioxidant compounds.

RESULTS AND DISCUSSION

The Result of GC-MS Analysis of Pulu Mandoti Rice

GC-MS analysis of Pulu Mandoti extract identified ten volatile compounds with retention times ranging from 2–22 min. Compound identification using the Wiley 7n.l library detected glycerin, cyclohexanone-oxime, guanosine, cytidine (4-amino-1-beta-d-ribofuranosyl-2 (1H)-pyrimidinone), cyclotrisiloxane, 1,3-bis (trimethylsilyl) benzene, and 3,5-dimethyl-2,6-bis (trimethylsiloxy)-pyridine. High abundance indicated greater ion stability, which depends on ion lifetime and ion energy (Harvey, 2005). Among the detected compounds, 9-octadecanoic acid and hexadecanoic acid were the dominant constituents, with relative abundances of 43.03% and 22.12%, respectively. 9-octadecanoic acid, also known as oleic acid, is a monounsaturated omega-9 fatty acid commonly found in rice bran oil. Rice bran oil contains approximately 40.8% monounsaturated fatty acids and 40.1% polyunsaturated fatty acids (Santos et al., 2005), while unsaturated fatty acids in rice bran range from 18%–23% (Vorarat et al., 2010). The complete identification results of compounds detected in the GC-MS chromatogram shown in Figure 1.

The fatty acid ionic fragments are similar to those reported by Harvey (2005). Fatty acids have negative fragment ions characterized by an odd ionic mass. Positive fragment ions are characterized by an even mass of ions (Harvey, 2005). The main target of the heating process is the transformation of unsaturated fatty acids into saturated fatty acids (Latha & Nasirullah, 2014). In this study, the separation of compounds in the column was performed at temperatures ranging from 50 °C to 200 °C. The compound detected at a retention time of 11.826 min with a relative abundance of 6.58% was identified as n-octadecanoic acid (stearic acid) based on comparisons with the Wiley 7n.l spectral library. The

Table 1. Grid box used in molecular docking analysis

Grid	Antidiabetic		Antioxidant	
	Alpha Amylase (2QV4)	Alpha Glucosidase (7KBR)	NADPH Oxidase (5O0X)	Xanthine Oxidoreductase (2CKJ)
Size x	20.0	18.0	22.0	18.0
Size x	16.0	14.0	17.0	23.0
Size x	16.0	12.0	14.0	11.0
Center x	12.875	-13.98	70.79	103.415
Center x	47.347	26.056	-3.384	107.967
Center x	26.189	-9.909	62.918	136.671
Spacing	1Å	1Å	1Å	1Å

presence of stearic acid may be associated with the thermal transformation of unsaturated fatty acids during processing, as double bonds in fatty acids are susceptible to oxidation, isomerization, and hydrogenation reactions under elevated temperatures, resulting in a reduction in the degree of unsaturation (Choe & Min, 2007; Shahidi & Zhong, 2010). These reactions can promote the formation of more stable saturated fatty acids, including stearic acid. Unlike industrial trans fatty acids, stearic acid has been reported to exert a relatively neutral effect on blood lipid profiles and cardiovascular risk, making it a more favorable saturated fatty acid in food products (Hunter et al., 2010). Nevertheless, the extent of fatty acid transformation is strongly influenced by processing conditions such as temperature, oxygen availability, heating duration, and the composition of the lipid matrix (Choe & Min, 2007). Stearic acid can substitute for trans fatty acids, which are harmful to health (Yanti *et al*., 2022).

9-Octadecanoic acid, also known as oleic acid or omega-9 fatty acid, is classified as a monounsaturated fatty acid commonly found in rice bran oil, the chemical structure shown in Figure 2. Rice bran oil contains approximately 40.8% monounsaturated fatty acids and 40.1% polyunsaturated fatty acids (Santos et al., 2005), while unsaturated fatty acids in rice bran reportedly range from 18%–23% (Vorarat et al., 2010). The fragment ion patterns of 9-octadecanoic acid detected in Pulu Mandoti extract were consistent with those reported for fatty acids by Harvey (2005), where negative fragment ions are characterized by odd ionic masses and positive ions by even masses. During GC-MS analysis, heating at 50–200 ℃ likely promoted the transformation of unsaturated fatty acids into saturated forms, resulting in the detection of n-octadecanoic acid (stearic acid). Stearic acid is considered a healthier substitute for trans fatty acids (Yanti et al., 2022). In addition, hexadecanoic acid (palmitic acid) and tetradecanoic acid (myristic acid) were identified as saturated fatty acids. Similar fatty acid profiles have also been reported in edible seeds and nut oils, where oleic acid predominates over stearic and palmitic acids (Yanti et al., 2021; Yanti et al., 2022).

A total of 4.32% of free fatty acids were found in the rice brain. The level increased to 43.08% during storage for six months at a temperature of 25 ℃. Increased free fatty acid levels during storage cause rancidity in rice brain oil. The maximum standard for free fatty acids in rice brains is 5% (Yilmaz *et al*., 2014). Observations of oil using NMR show that free fatty acids have a peak character that overlaps with that of oleic acid (Di Pietro *et al*., 2020). A high percentage of 9-octadecanoic acid and Pulu Mandoti extract has the potential to trigger rancidity. A comparison of the MS sample spectra with those of standard 9-octadecanoic acid and hexadecanoic acid is shown in figure (Figure 3a).

Rice brain contains gamma-oryzanol (Maurya & Kushawa, 2018; Vorarat *et al*., 2010; Yilmaz *et al*., 2014). This compound was a mixture of ferulic acid and sterols. According to Yilmaz *et al*. (2014), gamma-oryzanol in the rice brain was found to be 4.24 – 4.83 g/kg. Gamma-oryzanol is the strongest antioxidant in the rice brain and is more heat-resistant than tocopherol (vitamin E)

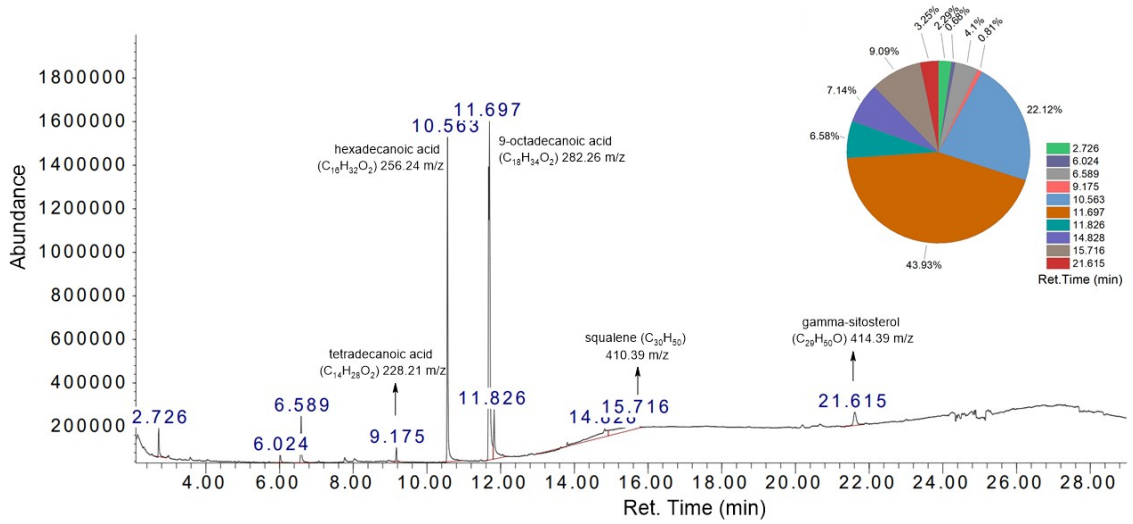

Figure 1. The result of GC-MS chromatogram from Pulu Mandoti.

(Yilmaz *et al*., 2014). The involvement of alkaline solvents during the extraction process can reduce the levels of oryzanol compounds. Rice brain contains oryzanol, tocopherol, and ferulic acid (Maurya & Kushawa, 2018). Gamma-oryzanol is a pigment found in the brain of rice. Red rice had higher gamma-oryzanol (21 mg/100 g) than white rice (19.1 mg/100 g) and purple rice (20.3 mg/100 g) (Kim *et al*., 2013). Pulu Mandoti extract contains gamma-sitosterol. Based on their chemical structures, gamma-sitosterol compounds are classified as steroids. This compound was detected at a retention time of 21.615 min. Gamma-sitosterol had an area percent of 3.21%. MS spectra of γ-sitosterol are shown in Figure 3b. Several researchers have identified the fragment ions of sterol compounds. Sterols have stable fragment ions with a mass of 145 m/z, which belongs to the ring structure. The release of side chains was detected in the presence of fragment ions at 253 m/z, 255, 257, and 259 (Münger et al., 2018). Pulu Mandoti extract contained fragment ions of 43, 107, 159, 213, 255, 329, and 414 m/z/. Gamma-sitosterol had fragments of 43, 95, 145, 213, 255, 303, 354, and 414 m/z. The 43 m/z ion belongs to the alkyl group.

Figure 3 (c) shows the fragment ions of the squalene compounds in the Pulu Mandoti extract. The fragment ion 69 m/z belongs to the compound 1,3-Pentadiene. 2,3,6-Trimethyl-1,5-heptadiene; 2,6-Dimethyl-2,6-octadiene (6Z); 2,7-Dimethyl-1,6-octadiene; and 3,3,5-Trimethyl-1,5-heptadiene are isomers with a fragment ion at 138 m/z (Moldoveanu, 2019). Fragment ions at 69 m/z and 341 m/z were negative ions (basic ions) belonging to squalene. The loss of fragment ion 69 m/z leaves a mass of 341 m/z. Another fragment ion appears at 137 m/z (Mishra *et al*., 2018). Squalene in Pulu Mandoti had fragment ions at m/z 69, 137, 191, 232, 273, 341, and 410 m/z. Pulu Mandoti contains squalene 3.25%. Squalene is a polyunsaturated hydrocarbon classified as a triterpene (Abegaz & Kinfe, 2019). The function of squalene is to prevent damage to polyunsaturated fatty acids at high temperatures. However, squalene is unstable and easily oxidized (Secmeler & Galanakis, 2019). Secondary metabolites, such as squalene, have been found in spinach oil, rice oil, olive oil, walnut oil, and Saussurea obvallata (Alonso-Salces *et al*., 2021; Gao *et al*., 2019; Kim *et al*., 2013; Mishra *et al*., 2018; Soetjipto *et al*., 2021).

Analysis of Antidiabetic and Antioxidant Activity of Pulu Mandoti Rice compounds from GC-MS

Five compounds identified by GC-MS were screened for antidiabetic potential through molecular docking against alpha-amylase and alpha-glucosidase proteins.

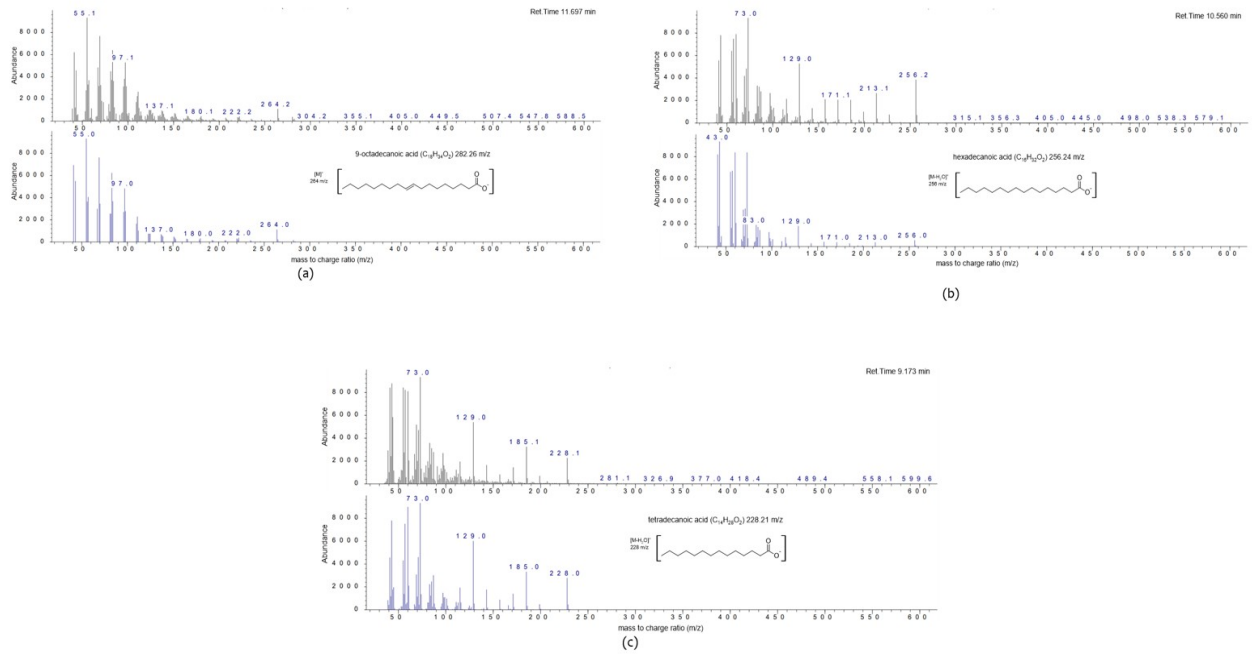

Figure 2. (a) MS spectra of 9-octadecanoic acid at 11.697 minutes (b) MS spectra of hexadecenoic acid at 10.560 minutes; (c) MS spectra tetradecanoic acid at 9.173 minutes.

Compound 1 (Gamma-sitosterol) showed the strongest interaction, with binding affinities of −9.1 kcal/mol and −8.4 kcal/mol, respectively, which were lower than acarbose as the control. In alpha-glucosidase, compounds 2, 3, and 4 also demonstrated lower binding affinities than acarbose, indicating promising antidiabetic potential.

Molecular docking analysis of five GC-MS compounds against NADPH Oxidase and Xanthine Oxidoreductase proteins showed that compounds 2 and 1 had the lowest binding affinities, with values of −8.7 kcal/mol and −8.0 kcal/mol, respectively. All compounds exhibited stronger binding affinity than vitamin C toward NADPH Oxidase, while compounds 1, 2, and 5 also showed better affinity than vitamin C against Xanthine Oxidoreductase, indicating promising antioxidant potential. Subsequent analysis involved clustering Pulu Mandoti compounds with commercial antidiabetic drugs. he complete molecular docking results are presented in Table 2.

Based on Figure 4 (a), drug network analysis of 5 compounds derived from Pulu Mandoti rice shows affinity with synthetic anti-diabetic drugs. The 3 types of synthetic drugs used in the above drug network analysis are Miglitol, Acarbose and Voglibose. The results of the analysis showed that the hexadecanoid acid compound had the highest similarity value with acarbose, namely 0.72. Based on the analysis results, acarbose is a synthetic drug that has the highest similarity index to all compounds from Pulu Mandoti rice (Tetradecanoid acid: 0.7, Octadecanoid acid: 0.66, Squalene: 0.66 and Gamma sitosterol: 0.58). Magnitol has an index of similarity with octadecanoid acid and squalene with values of 0.42 and 0.40, respectively. Voglibose has similarity with Hexadecanoid acid, Squalene and Tetradecanoid acid with values in the range of 0.40-0.43.

Based on 4 (b), drug network analysis of 5 compounds derived from Pulu Mandoti rice shows affinity with synthetic antioxidant drugs. The 3 types of synthetic drugs used in the above drug network analysis are Antioxidant petide A, Antioxidant petide A acetate and Vitamin C. The results of the analysis showed that the hexadecanoid acid compound had the highest similarity value with Antioxidant petide A namely 0.62.

The GC-MS analysis of *Pulu Mandoti* rice revealed ten volatile compounds, with five major constituents gamma-sitosterol, squalene, tetradecanoic acid, hexadecanoic acid, and octadecanoic acid selected for further in silico evaluation. The dominance of unsaturated and saturated fatty acids, particularly 9-octadecanoic acid and hexadecanoic acid, aligns with previous reports on pigmented rice varieties, where such fatty acids contribute to metabolic regulation and

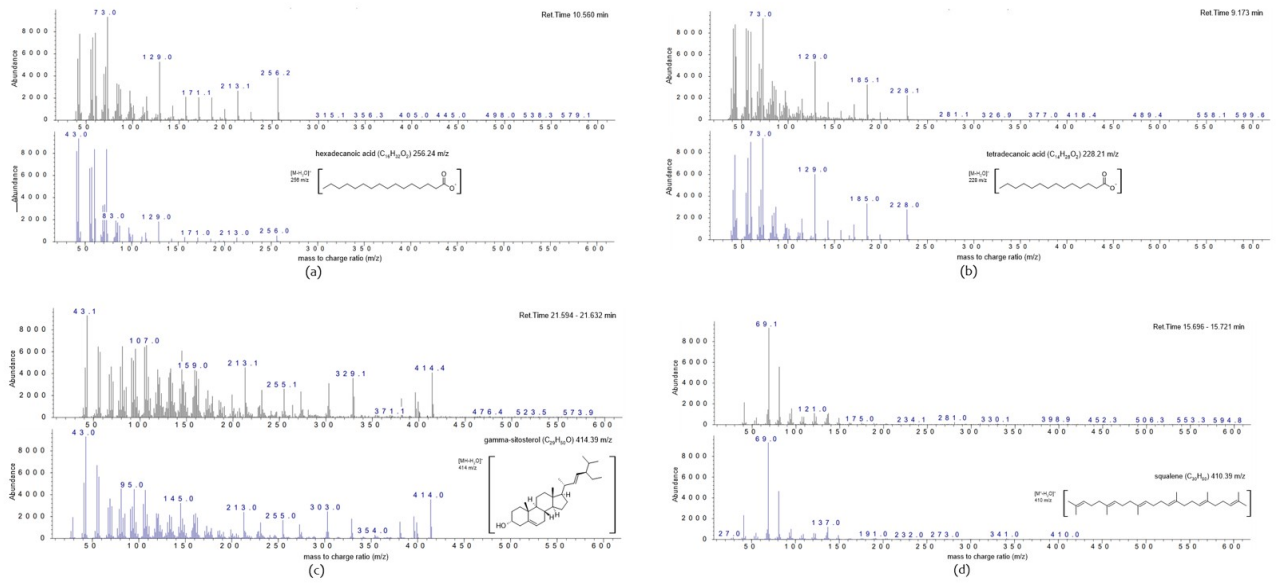

Figure 3. (a) MS spectra of hexadecenoic acid at 10.560 minutes; (b) MS spectra tetradecanoic acid at 9.173 minutes (c) MS Spectra of gamma-sitosterol at 21.632 minutes (d) MS spectra of squalene 15.696-15.721 minutes.

membrane stability. The presence of gamma-sitosterol and squalene is particularly noteworthy, as these triterpenes are known for their cholesterol-lowering and antioxidant properties. Gamma-sitosterol, a phytosterol, has been extensively studied for its ability to inhibit intestinal glucose absorption and modulate insulin signaling, while squalene serves as a precursor for steroid synthesis and protects polyunsaturated fatty acids from oxidative damage (Subba et al., 2025; Nureye et al., 2025).

Molecular docking results demonstrated that gamma-sitosterol exhibited the strongest binding affinity toward alpha-amylase and alpha-glucosidase, surpassing even the control drug acarbose. Such low binding energies indicate stable ligand-protein interactions, suggesting that gamma-sitosterol may effectively inhibit carbohydrate-hydrolyzing enzymes, thereby reducing postprandial hyperglycemia (Bhosale et al., 2024; Bababola et al., 2022). Notably, all five compounds interacted with critical catalytic residues specifically residue 59A in alpha-amylase and residue 571A in alpha-glucosidase which are predicted as active sites, reinforcing the mechanistic plausibility of enzyme inhibition. For antioxidant activity, squalene and gamma-sitosterol showed the lowest binding affinities toward NADPH oxidase and xanthine oxidoreductase, respectively, outperforming vitamin C. These target proteins are key sources of reactive oxygen species; thus, their inhibition by *Pulu Mandoti*compounds suggests a dual mechanism: direct radical scavenging and suppression of ROS-generating enzymes (Getachew et al., 2021; Surai et al., 2021).

Table 2. The result of molecular docking from GC-MS analysis for andiabetic and antioxidant

Grid	Antidiabetic		Grid	Antioxidant	
	Alpha Amylase (2QV4)	Alpha Glucosidase (7KBR)		NADPH Oxidase (5O0X)	Xanthine Oxidoreductase (2CKJ)
Compound 1	-9.1	-8.4	Compound 1	-7.8	-8.0
Compound 2	-7.2	-7.4	Compound 2	-8.7	-7.4
Compound 3	-5.4	-5.4	Compound 3	-6.1	-5.5
Compound 4	-5.1	-5.6	Compound 4	-6.6	-6.0
Compound 5	-5.1	-5.3	Compound 5	-6.7	-6.4
Acarbose	-7.7	-5.3	Vitamin C	-5.4	-6.1

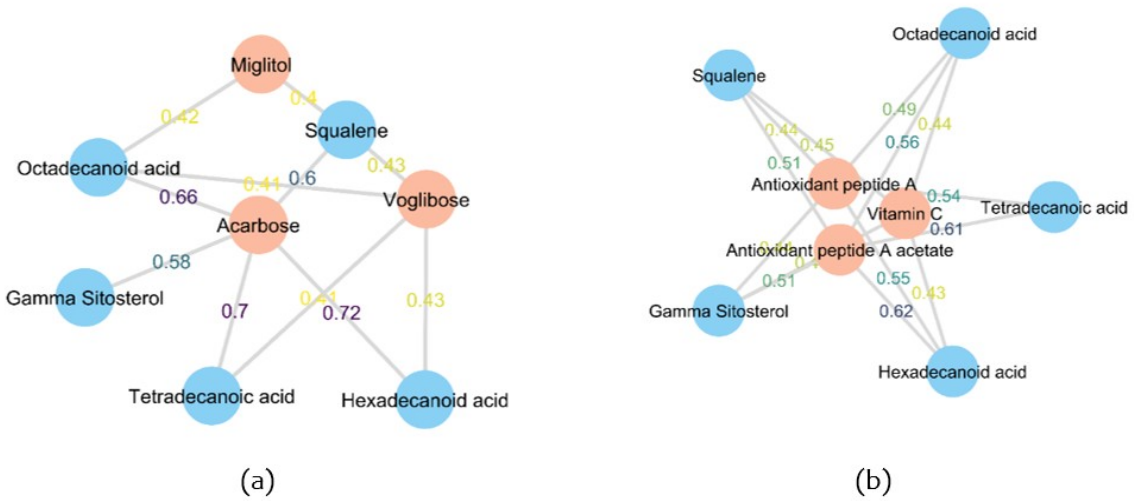

Figure 4. (a) Drug networks based on target profile cluster analysis as antidiabetic drug (b) Drug networks based on target profile cluster analysis as antioxidant drug.

The drug similarity network analysis using SwissADME and Gower's distance method provided additional translational insights. Hexadecanoic acid demonstrated the highest similarity score to acarbose among all antidiabetic compounds, followed by tetradecanoic acid and octadecanoic acid. This indicates that saturated fatty acids from *Pulu Mandoti* share physicochemical and pharmacokinetic properties with a clinically approved alpha-glucosidase inhibitor, increasing their potential as lead compounds for drug development (Savych et al., 2021).

For antioxidant applications, hexadecanoic acid again showed the highest similarity to antioxidant peptide A, suggesting that this fatty acid may mimic peptide-based radical quenching mechanisms. Despite promising in silico results, several limitations must be acknowledged: the absence of in vitro enzyme inhibition assays, lack of molecular dynamics simulations to confirm binding stability over time, and potential discrepancies between predicted and actual bioavailability (Xu et al., 2021).

CONCLUSION

In conclusion, Gamma-sitosterol showed the strongest antidiabetic potential with the lowest binding affinities toward alpha-amylase and alpha-glucosidase. Compound 2 exhibited the best antioxidant interaction with NADPH Oxidase. Hexadecanoic acid demonstrated notable similarity to acarbose and antioxidant peptide A, indicating its promising potential as a natural antidiabetic and antioxidant compound.

AUTHORS CONTRIBUTION

B.M. contributed to the conceptualization of the study, methodology development, investigation, data analysis, and preparation of the original manuscript draft. A.M. contributed through research supervision, validation of the findings, and critical review of the manuscript. S.Y. contributed to the investigation, data curation, and manuscript review. H. contributed to formal analysis and data visualization. N.H.A.S. contributed to resource provision, investigation, and manuscript review. W.P.A. contributed to research supervision, project administration, and final editing of the manuscript. All authors read and approved the final version of the manuscript.

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"The author declares that there is no conflict of interest with the parties involved in this research".

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