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Antioxidant and Antidiabetic Potential of Palmyra Treacle: In Vitro and In Silico Approaches

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Abstract

Borassus flabellifer treacle (palmyra treacle) is a traditional natural sweetener widely consumed in Sri Lanka, yet its pharmacological properties remain underexplored. This study evaluated the antioxidant and antidiabetic potential of aqueous (AE) and methanolic extracts (ME) of palmyra treacle using in vitro assays. In-silico molecular docking was additionally performed to predict the antioxidant and antidiabetic potential of well-known bioactive compounds found in palmyra treacle. Antioxidant activity was assessed by hydrogen peroxide scavenging and ferric reducing antioxidant power assays, while antidiabetic effects were investigated through glucose uptake by yeast cells and glucose adsorption capacity tests. Molecular docking examined the binding affinities and interactions of treacle-derived bioactive vitamins with key antioxidant and antidiabetic enzymes, NAD(P)H oxidase and human α-glucosidase, respectively. Both extracts exhibited notable antioxidant activity, with reducing power comparable to that of ascorbic acid. The methanolic extract showed stronger glucose uptake activity, while both extracts effectively adsorbed glucose in a dose-dependent manner. Docking results revealed thiamine as the most promising compound, demonstrating stronger binding affinities to antioxidant and antidiabetic enzyme targets than reference inhibitors. These findings highlight palmyra treacle as a natural sweetener with significant antioxidants and glucose-regulatory properties, supporting its potential for future nutraceutical and therapeutic applications.

Keywords: antidiabetic, antioxidant, aqueous extraction, methanol extraction, palmyra treacle

1. Introduction

Diabetes mellitus (DM) is a chronic condition caused by insufficient insulin production or ineffective insulin use, leading to persistent hyperglycemia and multiple organ complications [1–3]. Globally, more than 537 million individuals are living with DM, and this number is expected to increase significantly by 2045 [4–6]. In Sri Lanka, a national survey revealed that 23% of adults had diabetes, while 31% showed elevated blood sugar levels, indicating a substantial public health burden [7].

Oxidative stress plays a critical role in the development of DM. Elevated blood glucose promotes reactive oxygen species (ROS) generation through glucose auto-oxidation and protein glycation, leading to cellular and tissue damage [8–10]. This not only contributes to β-cell dysfunction but also underlies diabetic complications such as nephropathy, neuropathy, and cardiovascular disease [8,10]. Antioxidants have been shown to alleviate ROS-mediated damage, protecting pancreatic β-cells and reducing disease progression [8,11,12]. While oral hypoglycemic agents are available, their long-term use is associated with declining efficacy and adverse effects, which has increased interest in natural, plant-based alternatives that are generally considered safer and more acceptable to patients [13–15].

The palmyra palm (Borassus flabellifer), belonging to the family Arecaceae, is widely cultivated in South and Southeast Asia, including Sri Lanka [16]. Different parts of the plant, such as the flowers, fruits, seeds, and leaves, have been studied for their antioxidant and antidiabetic effects [17–25]. However, very limited evidence exists on palmyra treacle, a traditional sweetener derived from the palm sap and extensively consumed in Sri Lankan diets. Considering its widespread availability and cultural importance, evaluation of its bioactive potential is particularly relevant.

Therefore, this study was conducted to investigate the antioxidant and antidiabetic properties of aqueous and methanolic extracts of palmyra treacle through in-vitro assays. In-silico molecular docking analysis was additionally performed to predict the binding affinities and interactions of well-known bioactive compounds of palmyra treacle with key antioxidant and antidiabetic enzymes. These findings aim to provide scientific evidence for the

potential use of palmyra treacle as a functional sweetener for diabetes management.

2. Methodology

B. flabellifer treacle was collected from Palmyra development board Jaffna/Katpaham, 498 Colombo-Galle main road, Colombo.

2.1. In vitro antioxidant activity

2.1.1. Hydrogen Peroxide (H_2O_2) scavenging assay

A solution of H_2O_2 (40 mM) was prepared in phosphate buffer (pH 7.4). Both AE and ME extracts of palmyra treacle were prepared. The AE was obtained by macerating the treacle in distilled water at a 1:3 ratio, while the ME was prepared using a 1:10 ratio of treacle to methanol. Both solutions were left to stand for 48 hours, and the supernatant was collected for further analysis. To prepare the test samples, a series of two-fold dilutions was created by dissolving 1 mL of the treacle extract in 1 mL of distilled water. The concentration range of the extracts ranged from 1 mg/mL to 2×10^{-3} mg/mL [1]. 0.6 mL of the H_2O_2 solution (40 mM) was added to each of the extracts. The absorbance of H_2O_2 at 230 nm was determined after 10 minutes, with a blank solution containing only phosphate buffer (pH 7.4) without H_2O_2. The percentage of H_2O_2 scavenging by both the palmyra treacle extracts (aqueous and methanolic) and the standard (ascorbic acid) compounds was calculated using the following equation [2].

$$\%\ Scavenged\ H_2O_2 = \frac{(Ac - As)}{Ac} \times 100$$

Where Ac is the absorbance of the control (phosphate buffer and H_2O_2), and As is the absorbance in the presence of the sample (either palmyra treacle extracts or standards). All experiments were conducted in triplicate.

2.1.2. Ferric reducing antioxidant power assay

The FRAP assay was conducted to evaluate the total antioxidant power of palmyra treacle extracts (aqueous and methanolic). The assay is based on the reduction of the Fe^{3+} tripyridyltriazine complex to its ferrous (Fe^{2+}) form at low pH, which result in the formation of an intense blue color measurable at 700 nm. 1 mL of the extract at various concentrations (ranging from 1 mg/mL to 2×10^{-3} mg/mL) was mixed with 2.5 mL of 0.2 M phosphate buffer (pH 6.6) and 2.5 mL of 1% potassium ferricyanide. The mixture was incubated at 50°C for 20 minutes. After incubation, 2.5 mL of 10% trichloroacetic acid was added, and the mixture was centrifuged at 3000 rpm for 10 minutes. Then, 2.5 mL of the upper layer was mixed with 2.5 mL of distilled water and 0.5 mL of 0.1% ferric chloride solution. The absorbance was measured at 700 nm using a spectrophotometer. Increased absorbance indicated higher reducing power. All measurements were performed in triplicate, and the antioxidant capacity was expressed as ascorbic acid equivalents [3].

2.2. In vitro antidiabetic activity

2.2.1. Glucose uptake by yeast cells

The assay was performed using AE and ME of palmyra treacle. Commercial baker's yeast was washed by repeated centrifugation (3000 × g for 5 minutes) in distilled water until the supernatant became clear. A 10% (v/v) yeast suspension was then prepared in distilled water. Different concentrations of the freeze-dried palmyra treacle extracts (prepared via AE and ME methods) were added to 1 mL of glucose solution and incubated at 37°C for 10 minutes. The reaction was initiated by adding 100 µL of the yeast suspension to each tube and vortexing. The mixture was then incubated again at 37°C for 60 minutes. After incubation, the tubes were centrifuged at 2500 × g for 5 minutes, and the remaining glucose concentration in the supernatant was measured. The percentage increase in glucose uptake by yeast cells was calculated using the following formula [4]:

$$Increase\ in\ Glucose\ Uptake\ (\%) = \frac{(Abs, control - Abs, sample)}{Abs, control} \times 100$$

Where Abs, control, is the absorbance of the control reaction (containing all reagents except the extract), and Abs sample is the absorbance in the presence of the palmyra treacle extract. All the experiments were conducted in triplicate.

2.2.2. Glucose adsorption capacity test

This experiment was conducted using both AE and MEs of palmyra treacle. A 1% (w/v) solution of each freeze-dried extract was prepared by dissolving 1 g of extract in 100 mL of distilled water. From this, measured volumes were added to 25 mL of glucose at increasing concentrations (5, 10, 20, 50, and 100 mM). The mixtures were stirred thoroughly and incubated in a shaker water bath at 37°C for 6 hours. After incubation, the samples were centrifuged at 4000 × g for 20 minutes. The glucose content in the supernatant was determined using a glucose oxidase peroxidase diagnostic kit. The amount of glucose adsorbed by the extract was calculated using the following equation [5]:

$$Glucose\ Adsorbed\ (mmol/g) = \frac{(G1 - G6)}{W} \times \mathrm{V}$$

Where:

G1 – Glucose concentration of the original solution (mmol/L)

G6 - Glucose concentration after 6 hours (mmol/L)

W – Weight of the extract used (g)

V – Volume of glucose solution used (L)

2.3. Computational analysis for antioxidant activity

The antioxidant potential of well-known bioactive compounds found in Palmyra treacle, as identified from previous studies, was investigated here. This included a group of vitamins: thiamine (Vitamin B1), nicotinamide (water-soluble form of vitamin B3), pyridoxine (Vitamin B6), Ascorbic Acid (Vitamin C), and vitamin E [6], [7], [8]. These compounds were docked against FAD-dependent NAD(P)H oxidase from *Lactobacillus sanfrancisensis* (L.san-Nox2), which has been a crucial enzyme in predicting the antioxidant potential in previous in-silico studies [9], [10]. Apocynin, which is a widely studied NAD(P)H oxidase inhibitor, was used as the reference compound for this molecular docking [11].

2.4. Computational analysis for antidiabetic activity

The antidiabetic potential of the same bioactive compounds mentioned earlier was investigated through molecular docking. Here, predictions were obtained for the binding affinities of these bioactive compounds to human α-glucosidase, a key enzyme target in association with antidiabetic treatment development [12]. A second-generation human α-glucosidase inhibitor, miglitol, was used as the reference compound for this molecular docking [13].

Ligand preparation: The 3D conformer structures of the bioactive compounds, miglitol and apocynin, were retrieved from the PubChem online chemical database (https://pubchem.ncbi.nlm.nih.gov/) [14]. The chemical structures were energy minimized using Chem3D Pro 12.0 software and saved in (.mol2) file format.

Protein preparation: The X-ray diffraction PDB structures of L.san-Nox2 (PDB ID: 2CDU with resolution 1.80 Å) and human α-glucosidase (PDB ID: 5NN4 with 1.83 Å) were retrieved from RCSB online protein databank (https://www.rcsb.org/) [15]. Using BIOVIA Discovery Studio 2024 (v24.1.0.23298), all co-crystallized entities, water molecules, and chains except the chain A of both PDB structures were removed [16]. The cleaned PDB structure was energy minimized using UCSF Chimera (v1.17.1) [17].

Docking protocol for 2CDU: The molecular docking was performed using AutoDock4 software [18]. Upon adding hydrogens, merging non-polar hydrogens, adding Kollman charges, and assigning an AD4-type atomic force field, the energy-minimized PDB structure was converted to a PDBQT file. A targeted docking protocol was used based on a grid box that was prepared covering the active site amino acid residues of L.san-Nox2, such as PHE14, VAL304, HIS10, CYS42, ALA45, GLU163, TYR159, and LEU299 [19]. The docking parameters were set as default, and the number of dockings runs per ligand was set to 10. The molecular interactions of the complexes from the runs with the lowest binding energies were visualized in 3D using UCSF ChimeraX and 2D using BIOVIA Discovery Studio 2024 [20].

Docking protocol for 5NN4: A similar preparation as above was assigned for 5NN4 in the AutoDock4 software. A targeted docking protocol was used based on a grid box that was prepared covering the active site amino acid residues of human α-glucosidase, such as ASP282, ASP404, ASP518, ASP616, ASP645, ARG600, ARG672, HIS674, and GLU521 [21], [22]. The docking was performed with the same default setup, and the molecular interactions were visualized as mentioned earlier.

Statistical Analysis: All experiments were conducted in triplicate, and the results were expressed as mean standard deviation (SD). Data were analyzed to determine statistical significance using one-way analysis of variance (ANOVA), followed by Tukey's post hoc test to compare the means among different concentrations and between AE and MEs. A p-value of less than 0.05 ($p<0.05$) was considered statistically significant. All statistical analyses were performed using GraphPad Prism (version 9) and SPSS (version 27).

3. Result and Discussion

Diabetes mellitus is a major metabolic disorder with rising prevalence, particularly in Sri Lanka, where one in four adults is affected [7]. In this study, the antioxidant and antidiabetic properties of palmyra treacle extracts were evaluated using in vitro assays, and the binding affinities and interactions of well-known bioactive compounds in palmyra treacle were predicted using molecular docking. These findings provide mechanistic insights into their potential bioactivity.

3.1. In vitro antioxidant activity

The present study demonstrated the antioxidant activity of both aqueous and methanolic extracts of palmyra treacle, suggesting the presence of bioactive compounds capable of scavenging reactive oxygen species (ROS) and reducing ferric ions.

3.1.1. Hydrogen peroxide scavenging assay

As shown in Fig 1, the aqueous extract (AE) of treacle exhibited scavenging activity ranging from 21.79% to 52.09% across the tested concentration range (1 mg/mL to 2×10^{-3} mg/mL), indicating relatively weak antioxidant capacity, particularly at lower concentrations. The methanolic extract (ME) demonstrated slightly higher activity, with inhibition values ranging from 28.6% to 57.60%. In comparison, the standard Ascorbic acid exhibited substantially higher scavenging activity (49.03%-75.34%), confirming its well-established antioxidant potency. The IC_{50} values further supported this trend. The AE exhibited an IC_{50} of 0.278 ± 0.006 mg/mL, while the ME showed an IC_{50} of 0.356 ± 0.010 mg/mL. In contrast, ascorbic acid demonstrated an IC_{50} of 0.044 ± 0.021 mg/mL, indicating significantly higher antioxidant activity than both treacle extracts. These findings confirm that the crude extracts possess comparatively lower antioxidant potency

than the standard compound, although they exhibit moderate antioxidant activity. Understanding the glycemic impact of palmyra treacle is important for consumers, health practitioners, and the food industry. This information can empower consumers to make better dietary decisions and regulate their blood sugar levels, particularly beneficial for those managing diabetes. Healthcare professionals can utilize this understanding to develop dietary guidelines and recommendations for individuals with diabetes or other metabolic disorders. Additionally, the food industry can utilize this knowledge to develop healthier, low-glycemic options that align with consumers' preferences for nutritious, sustainable food choices.

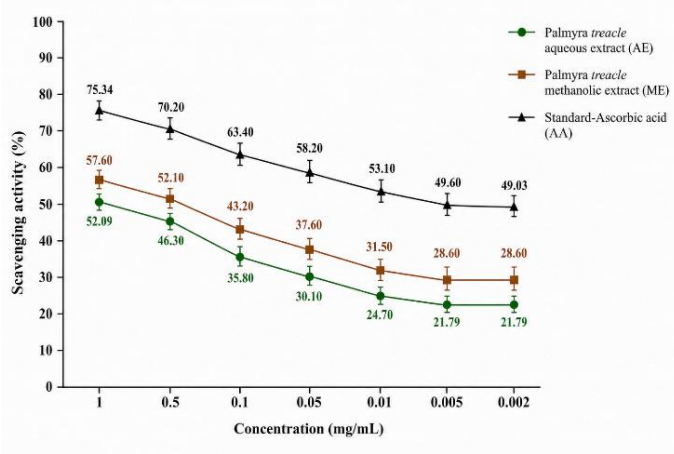

Fig 1. Hydrogen peroxide scavenging assay results for palmyra treacle's methanol and aqueous extraction.

3.1.2. Ferric reducing antioxidant power assay

Fig 2 presents the FRAP of palmyra treacle extracts. Values are presented as mean ± standard deviation (n = 3). Statistical analysis was performed using two-way analysis of variance (ANOVA) followed by Tukey's post hoc test. Differences were considered statistically significant at $p < 0.05$. The AE consistently exhibited higher absorbance than the ME across the tested concentration range, with ascorbic acid as the reference standard. This trend indicates a greater ferric ion-reducing capacity of the AE, suggesting the presence of more effective electron donors that contribute to its antioxidant potential. Both extracts demonstrated a concentration-dependent increase in absorbance; however, the overall absorbance range observed in the assay was relatively narrow (approximately 0.88 nm–1.01 nm), with the standard reaching near-saturation at lower concentrations. The antioxidant activity was interpreted based on the magnitude of absorbance increase; the AE showed a greater net change than the ME, indicating comparatively stronger reducing power. Nevertheless, both extracts exhibited lower overall activity than the saturated response observed for ascorbic acid.

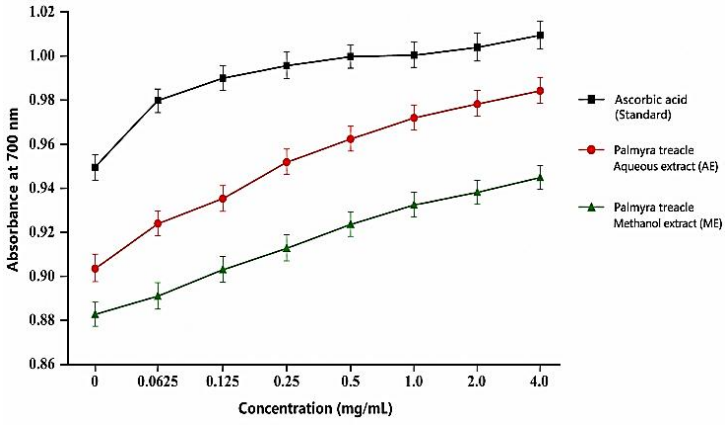

Fig 2. FRAP assay result for absorbance at 700 nm for palmyra treacle's aqueous and methanol extraction

3.1.3. Computational analysis for antioxidant activity

Table 1
Binding affinities of bioactive vitamins and miglitol to human GPx1 and their interactions.

Ligand	Binding Affinity (kcal/mol)	Inhibition Constant (Ki)	No. of H-Bonds	Amino acid residues forming H-Bonds
Apocynin	-6.17	30.10 µM	5	THR9, GLY12, THR112, SER115, LYS134
Nicotinamide	-4.94	240.33 µM	4	THR9, GLY12, ALA11, ASP282
Thiamine	-8.53	563.31 nM	*6	CSX42, ILE44, GLU163, GLY329, **ALA45**ALA45
Pyridoxine	-5.46	99.46 µM	6	THR9, THR9, THR112, THR112, GLY7, GLY12
Vitamin E	-7.93	1.55 µM	1	SER41
Ascorbic Acid	-4.76	326.05 µM	5	THR9, THR9, GLY12, ALA11, ASP282

Note. * Represents the total number of H-bonds observed from both BIOVIA Discovery Studio 2024 and UCSF ChimeraX. **Represents the 2 additional residues with which thiamine formed H-bonds according to visualization in UCSF Chimera

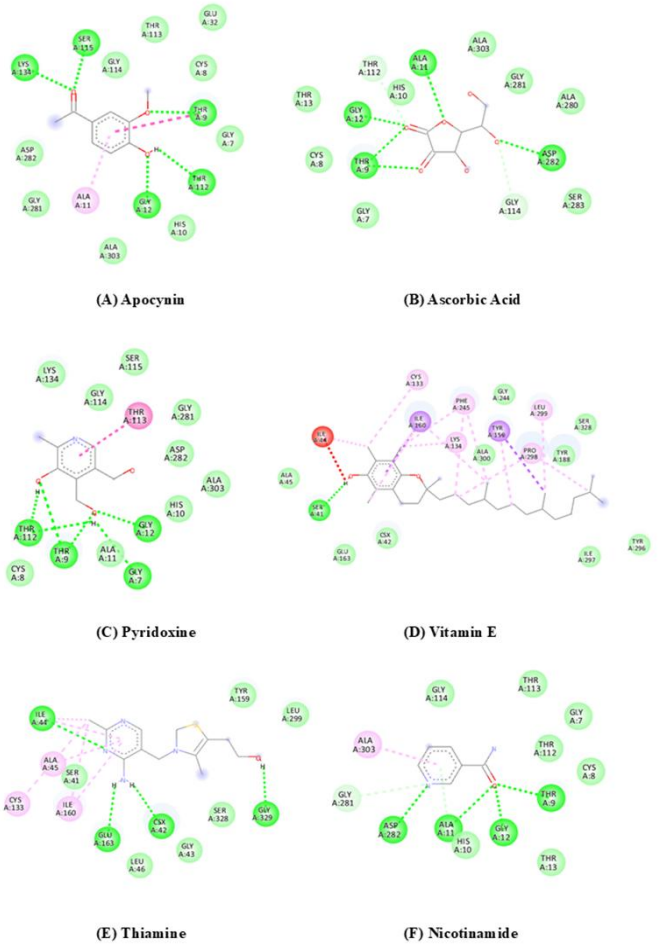

Fig 3. 2D interactions of bioactive vitamins and apocynin with L.san-Nox2

In this study, the potential of bioactive compounds in Palmyra treacle to bind the ROS-producing L.san-Nox2 enzyme, a key antioxidant target, was investigated using molecular docking. As depicted in Table 1 below, the strongest binding affinity to 2CDU was observed for thiamine with the lowest binding energy of -8.53 kcal/mol. This was with respect to the NAD(P)H oxidase inhibitor apocynin, which showed the lowest binding energy of -6.17 kcal/mol. Nicotinamide, pyridoxine, vitamin E, and ascorbic acid showed the lowest binding energies of -4.94, -5.46, -7.93, and -4.76, respectively. Thiamine also showed the lowest inhibition constant (Ki) of 563.31 nm, whereas apocynin, nicotinamide, pyridoxine, vitamin E, and ascorbic acid showed 30.10, 240.33, 99.46, 1.55, and 326.05 µM, respectively. RMSD values for all the dockings were 0.00 Å. Thiamine and pyridoxine formed the highest number of H-bonds, whereas vitamin E formed only 1 H-bond with SER41. However, the total number of H-bonds detected for thiamine was reported separately from the 2D interactions visualized in BIOVIA Discovery Studio 2024 and UCSF ChimeraX. As shown in the Figure. 3 below, there were 4 H-bonds observed for thiamine with CSX42, ILE44, GLU163, and GLY329 in the 2D interactions, whereas 3 H-bonds at distances 1.946, 2.238, and 2.227 Å were observed with residues GLY329 and ALA45, respectively, in the 3D interactions.

These findings are consistent with earlier reports on other palmyra-derived products, such as roots, fruits, and seeds, which showed significant antioxidant activity [23], [24], [25], [26], [27]. In silico results further supported this, showing that thiamine and vitamin E interacted strongly with NAD(P)H oxidase. Vitamin E protects cell membranes from lipid peroxidation [28], [29], [30], while thiamine contributes to oxidative balance as a cofactor in glucose metabolism [31]. This dual contribution may underlie the extracts' antioxidant effects.

3.2. In vitro antidiabetic activity

3.2.1. Glucose uptake by yeast cells assay

The aqueous and methanol extracts of palmyra treacle demonstrated a significant ($P < 0.05$) increase in glucose uptake in yeast cells under the tested in vitro conditions (Fig 4). The percentage increase in glucose uptake was approximately 21.1% for the AE and 17.3% for the ME, whereas the standard drug metformin exhibited a markedly higher uptake of 38.6%. These findings indicate that, although both treacle extracts enhance glucose uptake, their effects are substantially lower than that of metformin.

The comparatively greater activity observed with the aqueous extract relative to the methanol extract suggests variation in the distribution of bioactive constituents between extraction solvents. Since this assay measures glucose uptake stimulation, EC_{50} values were used for comparison. The estimated EC_{50} values were 0.461 ± 0.012 mg/mL for AE and 0.212 ± 0.008 mg/mL for ME, which are higher than that of metformin (0.083 ± 0.004 mg/mL), further confirming the lower potency of the extracts.

Overall, these results suggest that palmyra treacle extracts possess the ability to enhance glucose uptake in yeast cells in vitro. However, their activity is considerably weaker than that of the standard drug; therefore, these findings should be interpreted as preliminary evidence. Further validation using appropriate cellular and in vivo models is required before establishing any definitive antidiabetic potential.

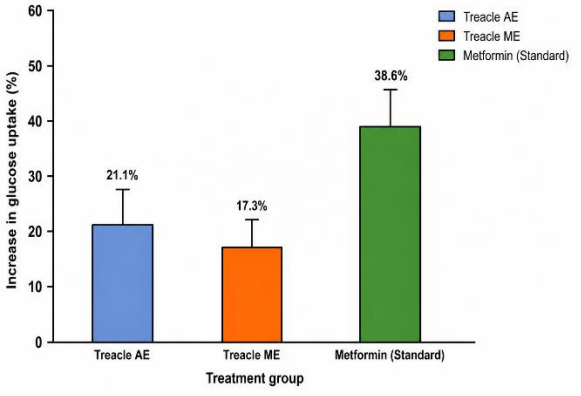

Fig 4. Increase in glucose uptake % of aqueous and methanol extract of palmyra treacle

3.2.2. Glucose adsorption capacity test

The results of the glucose adsorption capacity demonstrated the effectiveness of the AE and MEs of treacle samples in adsorbing glucose at both low and high concentrations. The result demonstrated 74.44% and 71.60% glucose absorption by ME and AE, respectively, from a 100 mM glucose solution. It was observed that the adsorption capacities of all the treacle extracts were directly proportional to the molar concentration of glucose, and higher amounts of glucose were bound with increased glucose concentration, as shown in Fig 5 below. Therefore, the glucose adsorption capacity of both extracts of palmyra treacle increased proportionately in a dose-dependent manner (Table 2). The samples were effective at adsorbing glucose at both the low (5 mM) and high (100 mM) concentrations used in the study. The results also indicated that treacle extracts can bind glucose at lower concentrations (5 mM), thereby reducing the amount of glucose available for transport across the intestinal lumen and, consequently, blunting postprandial hyperglycemia.

Table 2
Glucose adsorption capacity of the methanol and aqueous extraction of palmyra treacle.

Glucose concentration (mM)	Glucose adsorbed (mM) Methanol extract	Glucose adsorbed (mM) Aqueous extract
5	3.64 ± 0.18	3.49 ± 0.0
10	9.47 ± 0.47	8.29 ± 0.04
20	18.35 ± 0.92	14.32 ± 0.04
50	46.25 ± 2.31	42.13 ± 0.07
100	74.44 ± 3.72	71.6 ± 0.13

Values are mean ± SD of triplicate determinations.

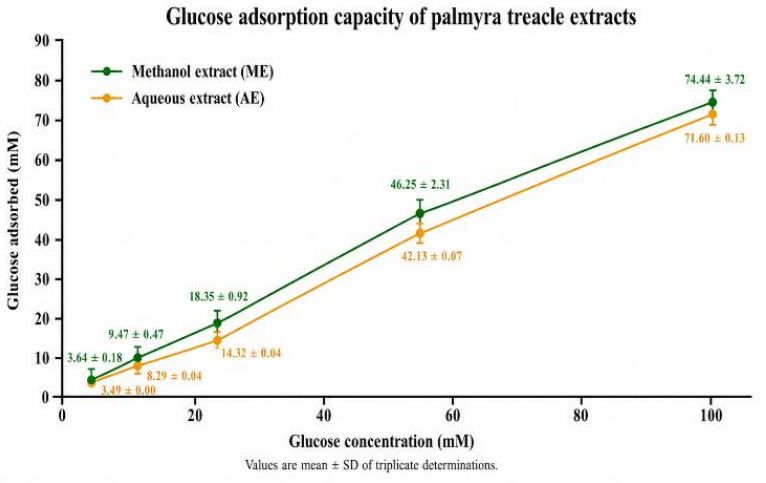

Fig 5. Glucose adsorption assay result of methanol and aqueous extract of palmyra treacle

3.2.3. Computational analysis for antidiabetic activity

In addition to the *in vitro* glucose uptake assay using yeast cells and the glucose adsorption capacity test, the present study also investigated the effect of palmyra treacle on human α-glucosidase through computational analysis, as α-glucosidase is a key enzyme involved in carbohydrate digestion.

The potential of bioactive compounds of palmyra treacle to bind to a key antidiabetic target, human α-glucosidase, was investigated. The strongest binding affinity to human α-glucosidase was observed for thiamine, with a binding energy of -9.19 kcal/mol, compared to the reference miglitol, which had a binding energy of -6.38 kcal/mol. The lowest binding energies for nicotinamide, pyridoxine, vitamin E, and ascorbic acid were -5.23, -5.26, -5.54, and -5.19 kcal/mol, respectively (Table 03). The lowest inhibition constant was observed for thiamine with a value of 184.47 nm. The inhibition constants for miglitol, nicotinamide, pyridoxine, vitamin E, and ascorbic acid were 20.99, 146.73, 139.21, 86.75, and 157.88 µM, respectively. RMSD values for all the dockings were 0.00 Å.

As shown in Fig 6 below, all the ligands except vitamin E formed H-bonds with key amino acid residues of the human α-glucosidase active site. Vitamin E formed 2 H-bonds with residues SER676 and LEU677, whereas all the other ligands formed at least one H-bond with ASP616. Miglitol formed 7 H-bonds, whereas thiamine formed only 3 H-bonds. Nicotinamide and ascorbic acid formed 4 H-bonds each, while pyridoxine formed 5 hydrogen bonds. As shown in Fig 7 below, the 3 H-bonds formed for thiamine were with residues ASP404, HIS674, and ASP616 at distances 1.978, 1.900, and 1.736 Å, respectively.

Table 3
Binding affinities of bioactive vitamins and miglitol to human α-glucosidase and their interactions.

Ligand	Binding Affinity (kcal/mol)	Inhibition Constant (Ki)	No. of H-Bonds	Amino acid residues forming H-Bonds
Miglitol	-6.38	20.99 µM	7	ASP616, ASP616, ASP282, ASP518, ASP404, HIS674, HIS674
Nicotinamide	-5.23	146.73 µM	4	ASP616, ASP645, ARG600, ARG672
Thiamine	-9.19	184.47 nM	3	ASP616, HIS674, ASP404
Pyridoxine	-5.26	139.21 µM	5	ASP616, ASP616, HIS674, ASP518, TRP481
Vitamin E	-5.54	86.75 µM	2	SER676, LEU677
Ascorbic Acid	-5.19	157.88 µM	4	ASP616, ASP616, HIS674, ARG600

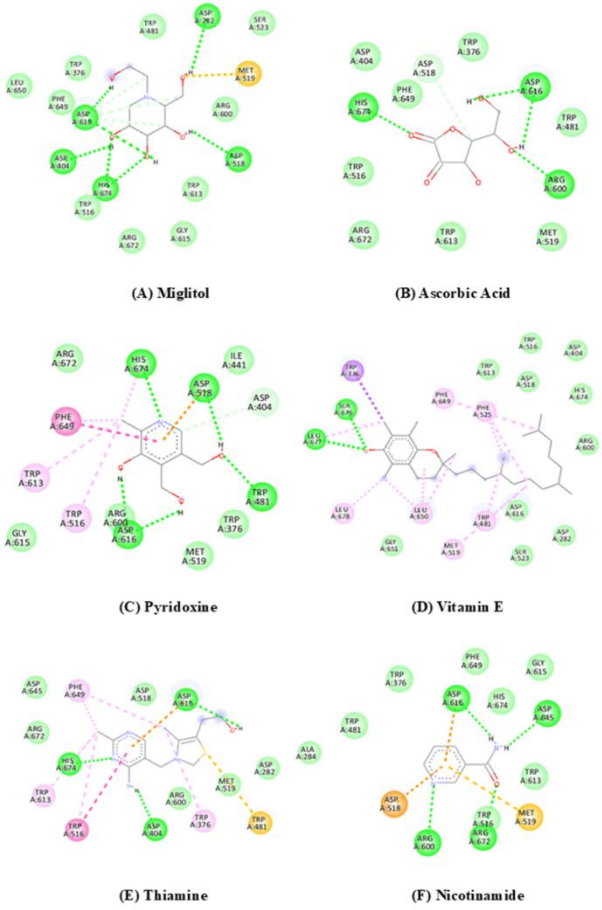

Fig 6. 2D interactions of bioactive vitamins and miglitol with human α-glucosidase

The antidiabetic potential of palmyra treacle was evident in its ability to enhance glucose uptake and adsorb glucose in vitro. These findings suggest two complementary mechanisms: stimulation of cellular glucose utilization, potentially mimicking insulin action, and the reduction of intestinal glucose absorption through glucose binding. Additionally, the molecular docking analysis highlighted the antidiabetic and antioxidant potential of palmyra treacle-derived compounds, with thiamine showing the strongest binding affinity for human α-glucosidase, surpassing the standard inhibitor miglitol. These results suggest the potential α-glucosidase inhibitory activity of treacle-derived compounds, which could lead to a reduction of carbohydrate hydrolysis and postprandial glucose levels, a mechanism comparable to other natural inhibitors [12], [13], [32]. Nicotinamide, pyridoxine, and vitamin E also exhibited moderate activity, suggesting synergistic effects of multiple bioactive compounds. The present computational findings will guide future *in vitro* investigations to experimentally validate the α-glucosidase inhibitory potential of palmyra treacle.

These findings are consistent with earlier studies on palmyra flowers, roots, and seeds, which demonstrated glucose-lowering activity in animal models [33], [34], [35], [36]. However, evidence on treacle has been scarce. The present study provides new insights by showing that treacle, a widely consumed traditional sweetener, also exhibits both antioxidant and glucose-regulatory potential. This highlights its relevance not only as a dietary product but also as a candidate for functional food and nutraceutical development.

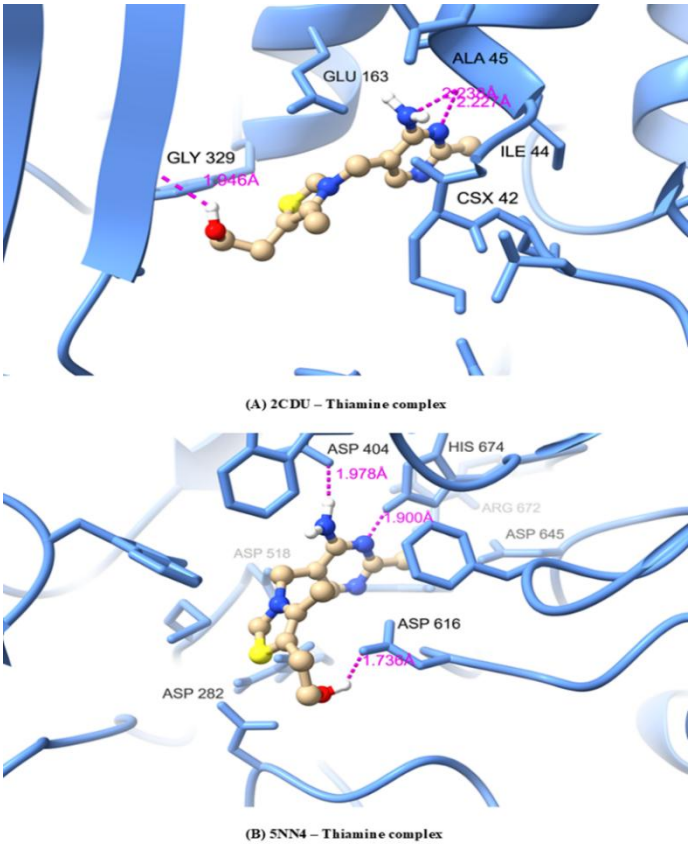

Fig 7. 3D visualization of H-bond formation of thiamine with human α-glucosidase and L.san-Nox2

4. Conclusion

The aqueous and methanolic extracts of palmyra treacle exhibited significant antioxidant and antidiabetic properties. The extracts demonstrated ferric-reducing power comparable to that of ascorbic acid, enhanced glucose uptake, and effectively adsorbed glucose, supporting their potential role in mitigating oxidative stress and hyperglycemia. Molecular docking revealed the antioxidant and antidiabetic potential of treacle-derived compounds, with thiamine emerging as a key bioactive compound with strong affinity for NAD(P)H oxidase and α-glucosidase, suggesting its dual role in antioxidant defense and glucose regulation. While the in vitro and computational methods used here provide valuable preliminary evidence, further in vivo and clinical studies are needed to validate these findings and elucidate the underlying mechanisms of action.

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Competing Interests

The authors have no competing interests to declare

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