Research Article

In Silico Evaluation of the Predicted Inhibitory Potential of p-Hydroxybenzoic Acid and Cyclohexane-1,2,3,4,5-pentol Isolated from *Hyphaene coriacea* Gaertn. Toward Human Maltase-Glucoamylase and Pancreatic α-Amylase

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Inhibition of digestive enzymes involved in carbohydrate hydrolysis is a key strategy for controlling postprandial hyperglycemia in type 2 diabetes. This study aimed to evaluate, using molecular docking, the interaction potential of p-hydroxybenzoic acid and cyclohexane-1,2,3,4,5-pentol, isolated from *Hyphaene coriacea* Gaertn., with human maltase-glucoamylase and pancreatic α-amylase. Miglitol and acarbose were used as reference compounds.

The three-dimensional structures of the ligands and target enzymes (PDB IDs: 3L4W and 1B2Y) were obtained from the PubChem and RCSB PDB databases, respectively. Molecular docking was performed using PyRx 0.8, and protein-ligand interactions were analyzed using Discovery Studio Visualizer v2020.

For maltase-glucoamylase, the predicted binding affinities were -5.9 kcal/mol for p-hydroxybenzoic acid, -6.1 kcal/mol for cyclohexane-1,2,3,4,5-pentol, and -5.8 kcal/mol for miglitol. For pancreatic α-amylase, the predicted binding affinities were -9.7 kcal/mol for acarbose, -5.2 kcal/mol for cyclohexane-1,2,3,4,5-pentol, and -5.0 kcal/mol for p-hydroxybenzoic acid. Both phytochemicals

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interacted with several active-site residues that were also involved in interactions with the reference compounds.

These results suggest that p-hydroxybenzoic acid and cyclohexane-1,2,3,4,5-pentol possess promising inhibitory potential against digestive enzymes involved in postprandial glycemic regulation and could be evaluated as natural therapeutic candidates for type 2 diabetes. Further studies are required to experimentally validate the inhibitory potential predicted.

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1. Introduction

Diabetes, characterized by chronic hyperglycemia, is a major public health problem. In 2024, approximately 589 million adults aged 20 to 79 were living with this disease worldwide, a figure projected to reach 853 million by 2050[1]. This projected increase highlights the need for new therapeutic strategies to improve glycemic control, particularly postprandial hyperglycemia.

Postprandial hyperglycemia is closely linked to the enzymatic hydrolysis of dietary carbohydrates. Pancreatic α-amylase initiates the breakdown of starch into oligosaccharides, while intestinal α-glucosidases, particularly maltase-glucoamylase, release glucose that can be absorbed by the intestinal epithelium[2][3]. Pharmacological inhibition of these digestive enzymes is an effective strategy for slowing the rate of glucose release, as evidenced by the clinical use of acarbose and miglitol, two α-glucosidase inhibitors[4][5]. Nevertheless, their clinical use can be limited by gastrointestinal adverse effects, thereby encouraging the search for new bioactive compounds, particularly those of plant origin[5][6].

Hyphaene coriacea Gaertn. is a tropical palm tree used in traditional medicine and studied for its nutritional and bioactive properties[7][8]. p-Hydroxybenzoic acid and cyclohexane-1,2,3,4,5-pentol were isolated from this species[9]. Structurally, the carboxyl and hydroxyl groups of p-hydroxybenzoic acid, as well as the multiple hydroxyl groups of cyclohexane-1,2,3,4,5-pentol, provide sites capable of hydrogen-bonding interactions that may contribute to their anchoring within the catalytic pockets of the two enzymes under consideration[10][3][11][12].

It was hypothesized that these two phytochemicals from *H. coriacea* Gaertn. may act as competitive inhibitors of human digestive enzymes. This study evaluated *in silico* the binding modes, predicted

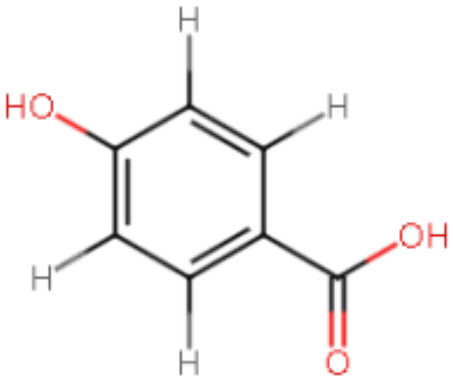
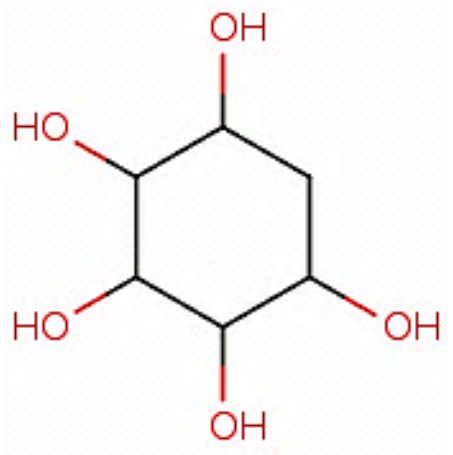
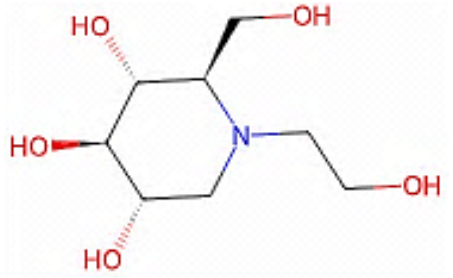
binding affinities, and interaction profiles of p-hydroxybenzoic acid and cyclohexane-1,2,3,4,5-pentol with human maltase-glucoamylase and pancreatic α-amylase, in direct comparison with the reference compounds miglitol and acarbose.

2. Materials and Methods

2.1. Selection and preparation of the ligands studied

Two phytochemicals isolated from *H. coriacea* Gaertn., p-hydroxybenzoic acid and cyclohexane-1,2,3,4,5-pentol, were studied. Miglitol and acarbose were used as reference compounds. Miglitol is an inhibitor of intestinal α-glucosidases, enzymes involved in the terminal hydrolysis of oligo- and disaccharides, whereas acarbose is a pseudo-oligosaccharide capable of inhibiting both intestinal α-glucosidases and pancreatic α-amylase[13][14].

The two-dimensional (2D) and three-dimensional (3D) structures of the ligands were downloaded from the PubChem database[15] in Structure Data File (SDF) format. The identity of each ligand was verified using its PubChem Compound Identifier (CID) and corresponding chemical structure. The 3D structures were then converted to PDB format using Open Babel[16]. The 2D structures and PubChem CIDs of the compounds are presented in Table 1.

Ligand	2D structures	PubChem CIDs
p-Hydroxybenzoic acid		135
Cyclohexane-1,2,3,4,5-pentol (without stereochemical configuration)		101715
Miglitol		441314

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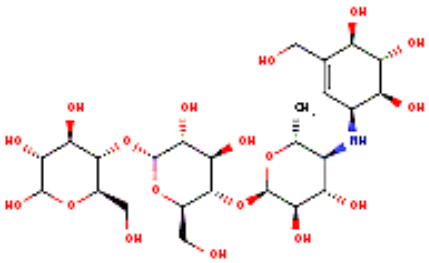
Ligand	2D structures	PubChem CIDs
Acarbose		9811704

Table 1. *Structures and PubChem identifiers of the ligands used for molecular docking*

2.2. Selection and preparation of target proteins

Human maltase-glucoamylase and human pancreatic α-amylase were selected as molecular targets based on their roles in postprandial glucose regulation.

Maltase-glucoamylase is an intestinal α-glucosidase involved in the hydrolysis of terminal α-(1→4)-glycosidic linkages in oligosaccharides. Pancreatic α-amylase is an endoglycosidase that hydrolyzes internal α-(1→4)-glycosidic linkages in starch and glycogen. These two enzymes act at complementary stages of carbohydrate digestion.

The crystallographic structure used for human maltase-glucoamylase corresponds to PDB ID 3L4W. This structure represents the N-terminal catalytic domain of human maltase-glucoamylase (ntMGAM) complexed with miglitol and was determined by X-ray diffraction at a resolution of 2.00 Å[17]. The crystallographic structure used for human pancreatic α-amylase corresponds to PDB ID 1B2Y. This structure represents human pancreatic α-amylase complexed with acarbose and was determined by X-ray diffraction at a resolution of 3.20 Å; it comprises a single protein chain (chain A) of 496 residues[10].

The target proteins were prepared using Discovery Studio Visualizer v2020[18]. Water molecules, co-crystallized ligands, and non-essential heteroatoms were removed, while necessary structural ions were retained. The prepared protein structures were saved in PDB format for subsequent docking steps.

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2.3. Identification of binding sites

Binding sites were defined based on active-site and catalytic residues of the target proteins described in the literature.

For human maltase-glucoamylase, the main active-site residues considered were Tyr299, Asp327, Ile328, Ile364, Trp406, Trp441, Asp443, Met444, Arg526, Trp539, Asp542, Phe575, and His600. Among these residues, Asp443 acts as the catalytic nucleophile, whereas Asp542 acts as the catalytic acid/base residue[17][19].

For human pancreatic α-amylase, the active-site and substrate-binding residues considered were Trp58, Trp59, Tyr62, Gln63, His101, Leu162, Thr163, Leu165, Arg195, Asp197, Ala198, Glu233, His299, Asp300, and His305[2][10]. Among these residues, Asp197, Glu233, and Asp300 constitute the catalytic residues and are located within domain A[2].

2.4. Molecular docking

Molecular docking was performed using AutoDock Vina integrated into the PyRx 0.8 software (https://pyrx.sourceforge.io/)[20][21]. The structures of the proteins and ligands were imported into the software.

Each target protein, considered as a receptor, was prepared and converted to PDBQT format using the AutoDock preparation tools integrated into PyRx 0.8. Polar hydrogen atoms were added, and Gasteiger partial charges were assigned[22]. Ligand structures were imported in SDF format and converted to PDBQT format using Open Babel[16], integrated into PyRx 0.8.

A grid-box was defined for each target to encompass the binding-site residues. The grid-box dimensions and center coordinates along the X, Y, and Z axes are presented in Table 2.

The exhaustiveness parameter was kept at the AutoDock Vina default value of 8, and the maximum number of output binding modes was set to the default value of 9. Up to nine binding modes could be generated for each protein-ligand complex. The pose retained for subsequent analysis was selected based on its predicted binding affinity, positioning within the active site, and interactions with key catalytic or substrate-binding residues. Protein-ligand interactions were analyzed using BIOVIA Discovery Studio Visualizer 2020, focusing on hydrogen bonds, hydrophobic interactions, electrostatic interactions, and non-bonded van der Waals contacts.

Targets	Size (Å)			Center (Å)		
	X	Y	Z	X	Y	Z
Maltase-glucoamylase	20.7036	24.9372	15.9528	45.3833	92.3584	34.8242
α-amylase	36.8371	25.3213	25.9322	18.9060	5.8026	47.0000

Table 2. *Grid box parameters used for molecular docking of target proteins*

3. Results

3.1. Predicted binding affinities of ligands to target proteins

Molecular docking performed with AutoDock Vina via PyRx 0.8 generated up to nine binding modes (poses) for each ligand against the two target proteins. The pose retained for each protein-ligand complex was selected based on its predicted binding affinity, positioning within the active site, and interactions with key residues. Table 3 presents the predicted binding affinities and ranks of the selected poses for the two phytochemicals and the reference compounds.

For maltase-glucoamylase, the selected poses showed predicted binding affinities of -6.1 kcal/mol for cyclohexane-1,2,3,4,5-pentol, -5.9 kcal/mol for p-hydroxybenzoic acid, and -5.8 kcal/mol for miglitol. For pancreatic α-amylase, the corresponding predicted binding affinities were -5.2 kcal/mol for cyclohexane-1,2,3,4,5-pentol and -5.0 kcal/mol for p-hydroxybenzoic acid, compared with -9.7 kcal/mol for acarbose.

Under the docking conditions used, both phytochemicals yielded more negative predicted binding affinity values for maltase-glucoamylase than for pancreatic α-amylase. Cyclohexane-1,2,3,4,5-pentol showed a predicted binding affinity of -6.1 kcal/mol for maltase-glucoamylase and -5.2 kcal/mol for pancreatic α-amylase, whereas p-hydroxybenzoic acid showed values of -5.9 and -5.0 kcal/mol, respectively.

Target protein and reference ligand	*α-amylase* *(reference: acarbose)*		*Maltase-glucoamylase* *(reference: miglitol)*	
Ligand	**Rank of the selected pose**	**Predicted affinity *(kcal/mol)***	**Rank of the selected pose**	**Predicted affinity *(kcal/mol)***
Reference molecule	1	−9.7	1	−5.8
p-Hydroxybenzoic acid	4	−5.0	2	−5.9
Cyclohexane-1,2,3,4,5-pentol	4	−5.2	1	−6.1

Table 3. *Predicted binding affinities and ranks of the selected ligand poses for the target proteins*

3.2. Analysis of the interaction modes of phytochemicals with α-amylase

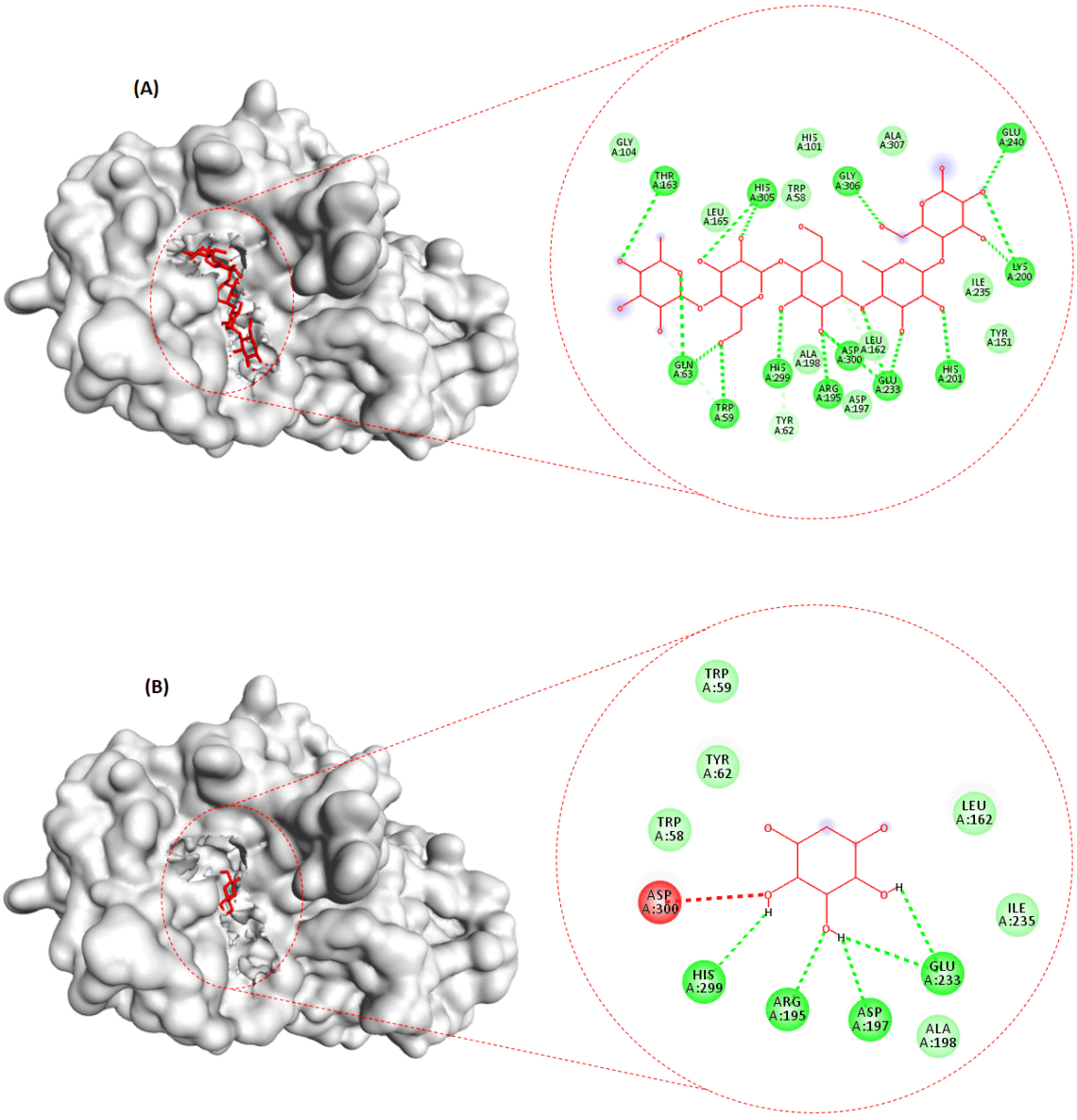
The selected poses for the ligand-α-amylase complexes were located within the enzyme active site and involved several key residues of the catalytic cavity.

The acarbose-α-amylase complex exhibited sixteen conventional hydrogen bonds involving several active-site residues, including Thr163, Gln63, Trp59, His305, His299, Arg195, Glu233, His201, Lys200, Glu240, and Gly306. Carbon-hydrogen bond interactions (C–H-O) were also observed with Glu233, Tyr62, and Trp59. Numerous van der Waals contacts extended across a large region of the active site (Figure 1A). This extensive interaction network accompanied the favorable predicted binding affinity obtained for acarbose.

Cyclohexane-1,2,3,4,5-pentol formed five conventional hydrogen bonds through its hydroxyl groups with active-site residues, including His299, Arg195, Asp197, and Glu233 (Figure 1B). An unfavorable steric contact with Asp300 was identified. Van der Waals contacts involved Trp58, Trp59, Tyr62, Leu162, Ala198, and Ile235.

p-Hydroxybenzoic acid adopted a distinct orientation within the catalytic cavity. Its hydroxyl group formed a conventional hydrogen bond with the side chain of Tyr62. Its aromatic ring formed a π-anion interaction with Asp197 and a π-alkyl interaction with Ala198 (Figure 1C). Van der Waals interactions involved Gln63, His101, Leu162, Leu165, Arg195, Glu233, Ile235, and Asp300.

Overall, both phytochemicals occupied the catalytic cavity of α-amylase and interacted with several active-site residues. Their predicted binding poses involved or were positioned near the major catalytic residues Asp197, Glu233, and Asp300, supporting their localization within the enzyme active site.



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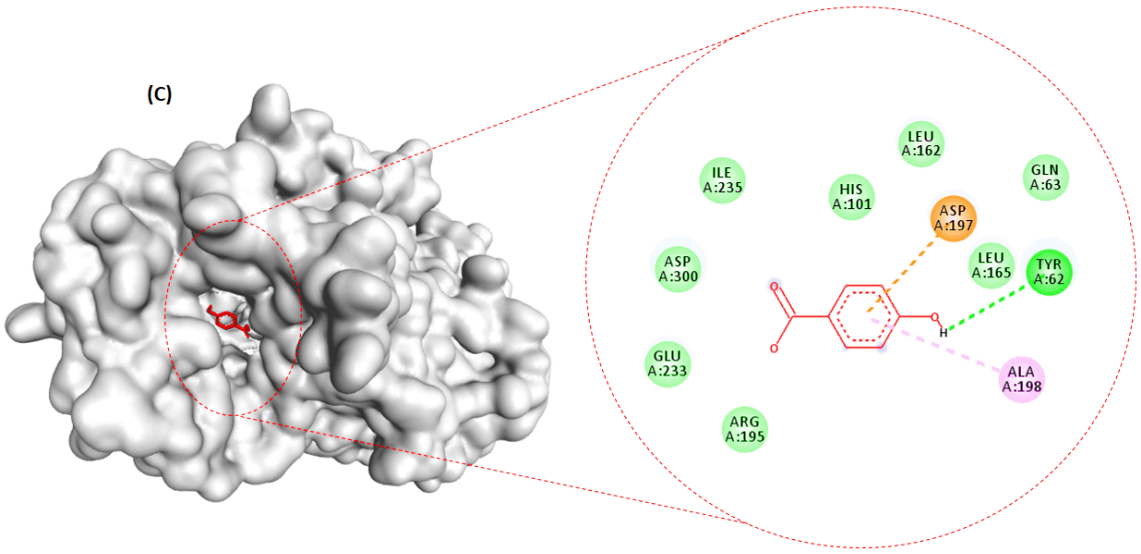

Figure 1. *3D and 2D interaction profiles of selected ligands within the active site of α-amylase: (A) acarbose; (B) cyclohexane-1,2,3,4,5-pentol; (C) p-hydroxybenzoic acid. In the 2D diagrams, hydrogen bonds are represented by green dashed lines, π−anion and π−alkyl interactions by beige and purple lines, respectively, unfavorable interactions in red, and van der Waals contacts in light green*

3.3. Analysis of the interaction modes of phytochemicals with maltase-glucoamylase

The selected poses for the ligand-maltase-glucoamylase complexes were located within the enzyme active site and involved several key residues of the catalytic pocket.

The miglitol-maltase-glucoamylase complex exhibited seven conventional hydrogen bonds involving several active-site residues, including Asp203, Asp327, Asp443, Asp542, Arg526, and His600. Carbon-hydrogen bond interactions (C–H-O) were also observed with Tyr299 and Asp542. Van der Waals contacts involved Ile328, Ile364, Trp406, Trp441, Met444, Trp539, and Phe575 (Figure 2A). Together, these interactions characterized the predicted binding pose of miglitol within the catalytic pocket.

p-Hydroxybenzoic acid exhibited predominantly π-type interactions within the catalytic cavity. Its aromatic ring formed a π-anion interaction with Asp443 and a π-alkyl interaction with Tyr299 (Figure 2B). The ligand also established van der Waals contacts with Asp327, Ile328, Trp406, Trp441, Met444, Phe450, Trp539, Asp542, Asp571, Phe575, and His600.

Cyclohexane-1,2,3,4,5-pentol formed three conventional hydrogen bonds with key active-site residues, namely Asp443, Asp542, and His600. A carbon-hydrogen bond interaction (C–H-O) with Asp443 and an unfavorable interaction involving Asp542 were also observed. Van der Waals contacts involved Asp203,

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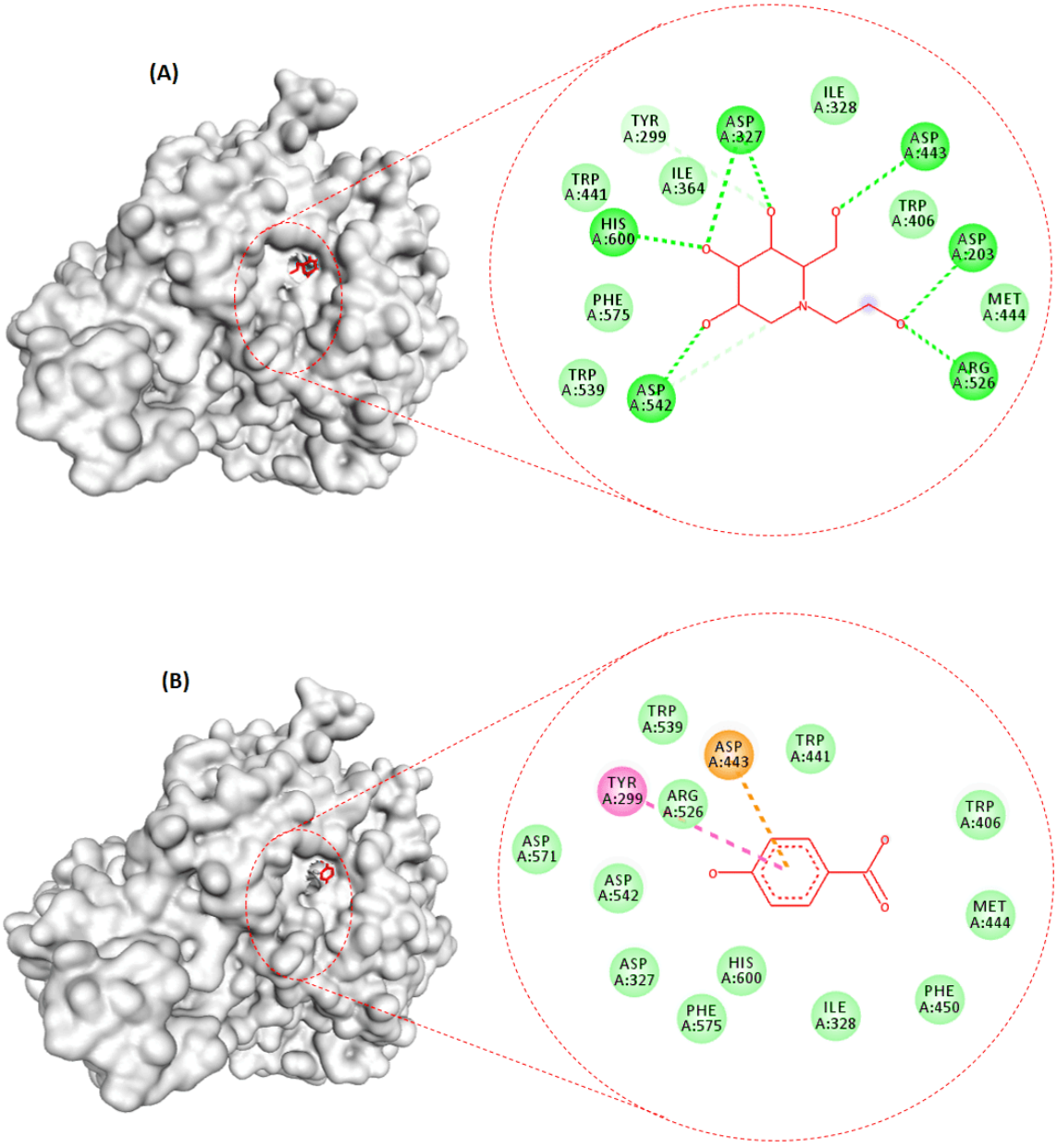
Tyr299, Asp327, Ile328, Ile364, Trp406, Trp441, Met444, Arg526, Trp539, and Phe575 (Figure 2C). These interactions accompanied the positioning of cyclohexane-1,2,3,4,5-pentol within the catalytic pocket.

Overall, both phytochemicals occupied the catalytic region of maltase-glucoamylase and shared several interacting residues with miglitol. Interactions involving the catalytic residues Asp443 and/or Asp542 supported the localization of the predicted phytochemical poses within the enzyme active site.



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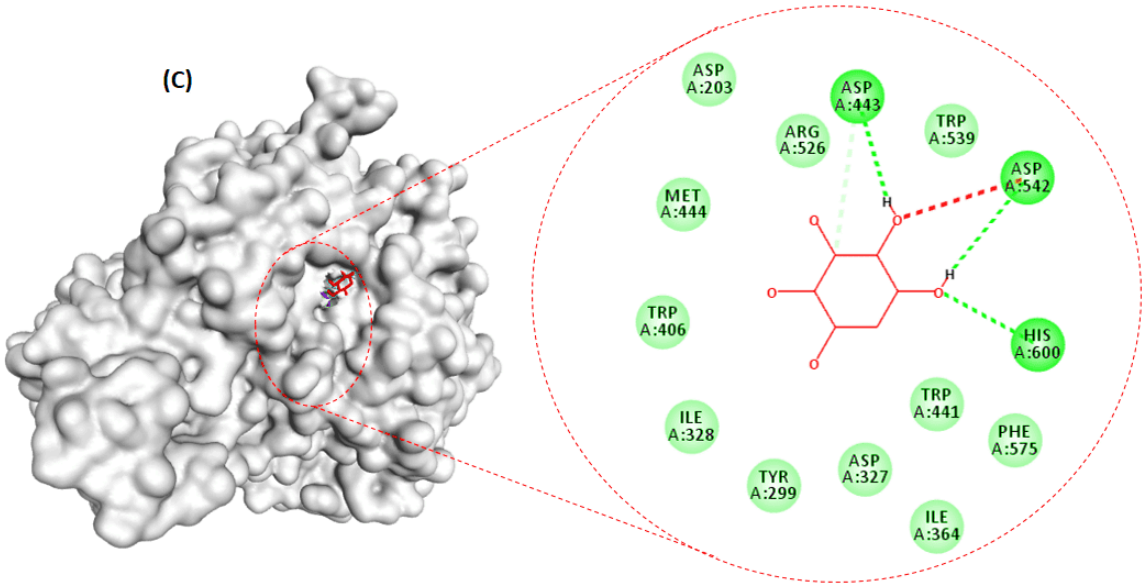

Figure 2.*3D and 2D interaction profiles of selected ligands within the active site of maltase-glucoamylase: (A) miglitol; (B) p-hydroxybenzoic acid; (C) cyclohexane-1,2,3,4,5-pentol. In the 2D diagrams, hydrogen bonds are represented by green dashed lines, π–anion and π–alkyl interactions by beige and purple lines, respectively, unfavorable interactions in red, and van der Waals contacts in light green*

4. Discussion

This study evaluated *in silico* the interaction potential of two phytochemicals isolated from *H. coriacea* Gaertn., namely p-hydroxybenzoic acid and cyclohexane-1,2,3,4,5-pentol, with two key enzymes involved in carbohydrate digestion and postprandial glycemic regulation: human maltase-glucoamylase and pancreatic α-amylase. Miglitol and acarbose were used as reference compounds for comparison of predicted binding affinities and molecular interaction modes.

Molecular docking showed that, for maltase-glucoamylase, cyclohexane-1,2,3,4,5-pentol had a predicted binding affinity of -6.1 kcal/mol, compared with -5.8 kcal/mol for miglitol, whereas its score for α-amylase was -5.2 kcal/mol. p-hydroxybenzoic acid showed a predicted binding affinity of -5.9 kcal/mol for maltase-glucoamylase. For α-amylase, both phytochemicals showed less favorable predicted binding affinity values than acarbose (-9.7 kcal/mol). The observed differences may be related, at least in part, to the structural characteristics and size of the ligands. α-Amylase possesses an extended active site comprising several carbohydrate-recognition subsites, allowing numerous contacts with oligosaccharide inhibitors such as acarbose[23][10]. The larger size and oligosaccharide-like structure of acarbose may

favor the occupation of multiple subsites within the catalytic cavity and the formation of an extensive network of interactions, consistent with its more favorable docking score.

These observations are consistent with previous reports of α-amylase and α-glucosidase inhibition by plant-derived preparations, including the study by Floris et al.[24] on *Washingtonia filifera*. Regarding cyclohexane-1,2,3,4,5-pentol, specific data remain limited. Its polyhydroxylated cyclohexane structure places it within the structural context of cyclitols and allows comparison with compounds such as D-pinitol. D-Pinitol has recently been reported to exhibit *in vitro* inhibitory activity against α-amylase and α-glucosidase, with IC_{50} values of 59.61 and 124.83 µg/mL, respectively[25]. Although these findings cannot be directly extrapolated to cyclohexane-1,2,3,4,5-pentol because of structural and stereochemical differences, they provide a useful comparison for further investigation of cyclitol-related compounds against enzymes involved in carbohydrate digestion.

The selected poses of the two phytochemicals were located within the catalytic pockets and involved several amino acid residues that also interacted with the reference compounds (Figures 1 and 2). Their positioning within the active sites is compatible with the possibility of competition with natural substrates. However, molecular docking alone is insufficient to establish a competitive inhibition mechanism, which requires confirmation by enzyme kinetic studies. Structural and kinetic studies of human α-amylase inhibitors have shown that active-site binding can be associated with experimentally demonstrated enzyme inhibition[26].

If these *in silico* findings translate into measurable enzyme inhibition under physiological conditions, p-hydroxybenzoic acid and cyclohexane-1,2,3,4,5-pentol could slow carbohydrate hydrolysis and consequently contribute to the attenuation of postprandial glucose release. However, the present docking results do not establish the magnitude of enzyme inhibition, enzyme selectivity, physiological efficacy, or gastrointestinal tolerability. The less favorable predicted binding scores of the two phytochemicals for α-amylase compared with acarbose, together with their predicted interactions within the maltase-glucoamylase active site, warrant experimental investigation to determine whether they exhibit a different balance of inhibitory activity toward the two enzymes. Such a profile could be relevant because gastrointestinal adverse effects associated with strong inhibition of carbohydrate digestion have been related to increased delivery of undigested carbohydrates to the colon and subsequent bacterial fermentation[27][28]. Whether the phytochemicals investigated here could provide a more moderate enzymatic modulation with improved gastrointestinal tolerability remains to be established experimentally.

Although molecular docking provides useful structural hypotheses regarding ligand–protein interactions, this approach relies on approximate scoring functions and does not provide experimental binding free energies or enzyme inhibition kinetics[20]. Molecular dynamics simulations could examine the dynamic behavior and persistence of the predicted protein-ligand interactions. *In vitro* enzyme inhibition assays remain essential to determine IC_{50} values and clarify the mode of inhibition toward α-amylase and maltase-glucoamylase. A network pharmacology approach could also explore interactions or synergistic effects between these phytochemicals and other secondary metabolites of *H. coriacea* Gaertn. on complementary targets involved in type 2 diabetes, such as dipeptidyl peptidase-4 (DPP-4) and protein tyrosine phosphatase 1B (PTP1B). Evaluation of absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties by combining *in silico* predictions with appropriate experimental validation would help prioritize subsequent *in vivo* investigations.

5. Conclusions

This *in silico* study indicates that p-hydroxybenzoic acid and cyclohexane-1,2,3,4,5-pentol, isolated from *H. coriacea* Gaertn., are capable of interacting with human maltase-glucoamylase and pancreatic α-amylase in molecular docking simulations. Their predicted binding poses within the catalytic sites and interactions with several key active-site residues support their potential for further investigation as modulators of these digestive enzymes. These two phytochemicals therefore warrant further experimental evaluation for their potential relevance to the control of postprandial hyperglycemia. *In vitro* enzyme inhibition studies and subsequent *in vivo* investigations are required to validate the biological significance of these *in silico* findings. Network pharmacology studies may help explore potential synergies among the secondary metabolites of *H. coriacea* Gaertn.

Statements and Declarations

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The authors reported that there is no funding associated with the work reported in this article.

Potential Competing Interests

No competing interest was reported by the authors.

Data Availability

The underlying data are available on Zenodo: NAZMOUL[29], *Molecular docking data supporting the study of Hyphaene coriacea Gaertn. phytochemicals against human maltase-glucoamylase and pancreatic α-amylase*. Zenodo. https://doi.org/10.5281/zenodo.21989937. The dataset is available under the terms of the Creative Commons Attribution 4.0 International license (CC BY 4.0).

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