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In vitro evaluation, molecular docking, and molecular dynamics studies of resorcinol derivatives against yeast α-glucosidase

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ABSTRACT Nine resorcinol derivatives were evaluated for their ability to inhibit yeast α-glucosidase using the *in vitro* method. Three molecular docking programs (Autodock Vina, Autodock4 and DockThor) were employed to determine the binding energies. The results showed that two resorcinol derivatives possessing butanoyl (1) and butyl (9) groups demonstrated good inhibitory activity against α-glucosidase, with IC_{50} values of 75.9 and 33.3 µM respectively, compared with other derivatives (2–8) and acarbose (IC_{50} = 832.8 µM). Furthermore, molecular docking indicated that compounds 1 and 9 had better binding affinities than acarbose and the native ligand. Both compounds showed similar interactions with Asp349 and Glu408, which were associated with acarbose and the native ligand. Moreover, molecular dynamics analysis indicated that compound 9 exhibited greater stability than compound 1 when complexed with α-glucosidase. Therefore, compound 9 has the potential for further studies, both *in vitro* and *in vivo*, to evaluate its toxicity, side effects and efficacy.

KEYWORDS α-glucosidase inhibitors; Inhibitors; Molecular docking; Resorcinol

1. Introduction

Diabetes mellitus (DM) has become a public health challenge in the 21st century. By 2021, this prevalent condition has affected approximately 536.6 million individuals worldwide. In the absence of effective preventive strategies, projections indicate that this number could increase to approximately 783.2 million by 2045 (Sun et al. 2022). This disease is characterized by elevated blood glucose levels, a metabolic disorder that can result in important health problems including cardiovascular diseases, hypertension, obesity, renal disorders, and vision impairment, thereby substantially contributing to the global health burden (Kshirsagar et al. 2020). Millions of individuals succumb to complications associated with this condition annually. A therapeutic approach for managing this disease in patients with diabetes reduces the degradation of dietary carbohydrates (Dowarah and Singh 2020).

α-glucosidase catalyzes the hydrolysis of long-chain dietary carbohydrates into monosaccharides within the small intestine. These monosaccharides subsequently enter the bloodstream, resulting in elevated blood glucose levels (Ghani 2015). Consequently, α-glucosidase inhibition has emerged as a vital therapeutic strategy to reduce blood glucose levels by restricting carbohydrate digestion (Dowarah and Singh 2020). α-glucosidase inhibitors primarily address elevated blood glucose levels without directly influencing insulin secretions. Therefore, these inhibitors are regarded as essential oral agents for glucose reduction and are independently utilized in cases of mild diabetes (Ghani 2015). In cases of severe diabetes, these inhibitors are administered in conjunction with insulin or other pharmacological agents (Nathan et al. 2006; Dhameja and Gupta 2019). Currently, acarbose, voglibose, and miglitol are three commercially available α-glucosidase inhibitors, but these inhibitors are associated with numerous side effects, including diarrhea, abdominal discomfort, bloating, and flatulence, as well as problems associated with their efficacy (Ghani 2015).

Up to now, many researchers have modified and evaluated the potency of some synthesized compounds bearing polyphenol derivatives against α-glucosidase, including 7-*O*-alkylated chrysin (a), 1,2,3-triazole-chalcones (b), *N*′-arylidene-4-hydroxybenzohydrazide (c), steroidal-

chalcones (d), thymol-chalcones (e), apigenin derivatives (f), tanshinone II bearing oxazole ring (g), 8-bromobaicalein (h), 3,4-dihydroxyphenylacetic acid bearing hydrazide-hydrazone derivatives (i), dihydropyridine bearing hydrazone-Schiff bases (j), and quercetin derivatives (k) (Hairani and Chavasiri 2022; Ardiansah et al. 2023; Danova et al. 2023a, 2024b; Khan et al. 2024; Kongphet et al. 2024; Liu et al. 2024a,b; Hairani and Chavasiri 2025; Zainab et al. 2025), as presented in Figure 1. Therefore, the discovery of novel drugs with minimal side effects is of utmost importance.

Furthermore, polyphenol compounds, including re-

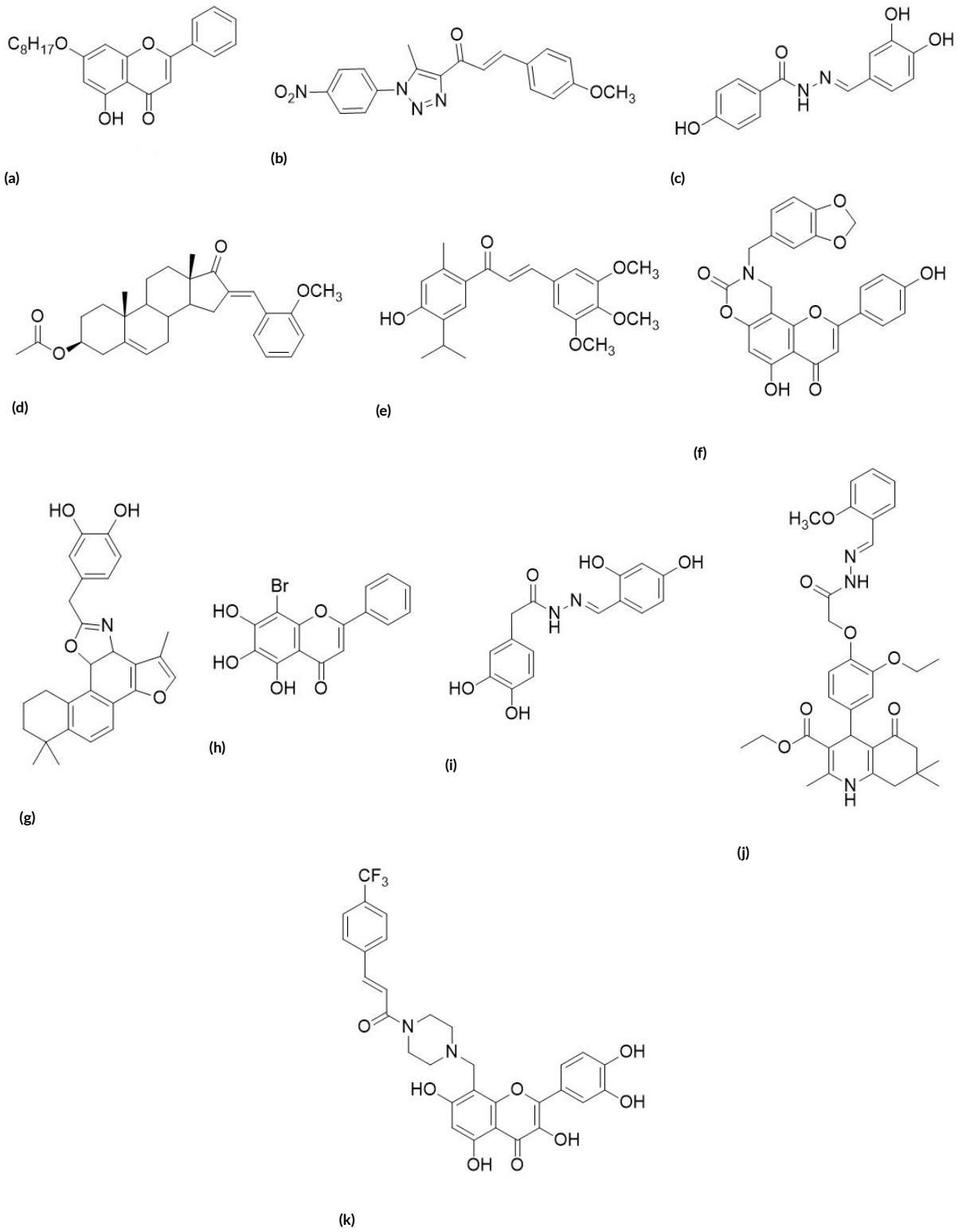


FIGURE 1 Several compounds have been synthesized as potent α-glucosidase inhibitors.

sorcinol derivatives, have been reported to inhibit α-glucosidase (Ghani 2015; Kim 2016; Hu et al. 2021; Le et al. 2022; Danova et al. 2023a; Han et al. 2023; Yuca 2024). Moreover, acyl and alkyl resorcinol derivatives inhibited tyrosinase and recombinant human aldose reductase (Ishioka and Nihei 2022; Kılınç 2022; Danova et al. 2023b). To further explore α-glucosidase inhibitors, nine 4-monoacylresorcinol derivatives that had been prepared from our previous work (Danova et al. 2023b) were tested against yeast α-glucosidase. In this study, *in vitro*, molecular docking, and molecular dynamics simulations were performed to evaluate and predict the binding interactions of 4-monoacylresorcinol derivatives with α-glucosidase.

2. Materials and Methods

2.1. Materials

α-glucosidase from *Saccharomyces cerevisiae* (EC.3.2.1.2.0), *p*-nitrophenyl-α-D-glucopyranoside (*p*-NPG), and acarbose were bought from Sigma-Aldrich and Tokyo Chemical Industry (TCI). α-glucosidase inhibition assays were performed using an ALLSHENG AMR-100 microplate reader. Compounds 1–8 had been prepared from the previous work (Danova et al. 2023b). Compound 9 was purchased from TCI (CAS No. 18979-61-8, purity >98.0%).

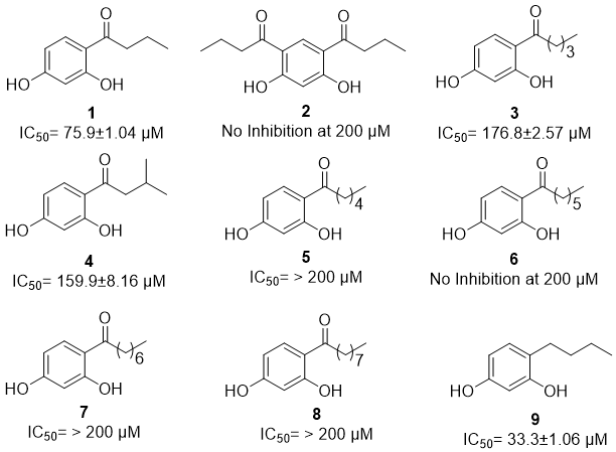


FIGURE 2 Structures of resorcinol derivatives (1–9) and inhibitory activity against yeast α-glucosidase.

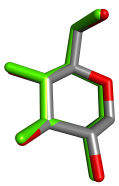


FIGURE 3 Overlapping between reference (dark gray) and redocking ligands (pure green) with RMSD 0.168 Å.

2.2. Methods

2.2.1 α-glucosidase inhibition assay

The α-glucosidase activity was executed as previously explained (Danova et al. 2024a). In this experimental procedure, 0.1 U/mL of α-glucosidase was conducted, and 1 mM *p*-NPG was prepared in a 0.1 M phosphate buffer at pH of 6.9. A 10 μL sample and 40 μL of α-glucosidase were mixed and incubated at 37 °C for 10 min. Afterwards, 50 μL of the *p*-NPG solution was added and reincubated at 37 °C for 20 min. The end of reaction was initiated by adding 100 μL of 1 M Na_2CO_3. The activity of α-glucosidase was determined at 405 nm using a microplate reader. The IC_{50} value was calculated by plotting the percentage inhibition against concentration. Acarbose served as the standard control, and the testing was conducted in triplicate.

2.2.2 Molecular docking

The molecular structures of the compounds were constructed and optimized using the Merck molecular force field (MMFF94) within ChemOffice Professional 15.0. The crystal structures of α-glucosidase from *S. cerevisiae* (PDB ID: 3A4A) were obtained from the Protein Data Bank (https://www.rcsb.org/) with native ligand (maltose). AutoDock Vina and Autodock4 tools in PyRx V.1.1 software were utilized to conduct molecular docking (Trott and Olson 2010; Dallakyan and Olson 2014) with an exhaustiveness of 32 and a mode value of nine poses for each docked ligand. DockThor is a free molecular docking program (https://dockthor.lncc.br/v2/, retrieved on April 06, 2025) (Guedes et al. 2024). The α-glucosidase-binding site was stated as a box with dimensions of 20 × 20 × 20 Å, positioned at x = 20.632, y = -7.726, and z = 23.447. The RMSD value is less than 2Å, signifying a valid docking protocol and confirming its appropriateness for the docking process. Binding interaction and visualization were achieved using the BIOVIA Discovery Studio Visualizer.

2.2.3 Molecular dynamics analysis

Compounds 1 and 9 were further studied to investigate the stability of the inhibitor-enzyme complex in aqueous condition during simulation. Molecular dynamics simulation was performed based on our previous protocol using YASARA Structure (v.21.16.17) with AMBER14 forcefield (Danova et al. 2024a).

3. Results and Discussion

3.1. Results

In this study, nine resorcinol derivatives (1–9) were assessed for their inhibitory activity against yeast α-glucosidase, followed by molecular docking to predict the interaction between the ligand and amino acid residues in the active site of α-glucosidase. As shown in Figure

2, resorcinol-containing butanoyl (1) exhibited good inhibition against α-glucosidase compared to a commercial product, acarbose (IC_{50} = 832.8 ± 46.35 µM). However, its activity dropped without inhibition when resorcinol possessed two butanoyl groups (2). Moreover, this result was not significantly different from that for the long-chain acyl group (3–8). Surprisingly, resorcinol attached to the butyl group (9) enhanced the inhibitory activity compared to compound 1. This finding suggests that the inhibitory activity of resorcinol derivatives may be influenced by the electron density and charge circulation on the aromatic ring (Shimizu et al. 2000; Dasgupta et al. 2019; Lee et al. 2021), where the acyl group prefers electron-withdrawing groups to drive electron density out of the aromatic ring, but alkyl groups prefer electron-donating groups to force electron density into aromatic ring. Thus, compounds 1 and 9 are potent inhibitors of α-glucosidase and should be developed for further studies to treat type 2 diabetes mellitus.

As shown in Figure 2, structure of compound 1 has acyl (electron-withdrawing group) and compound 9 has an alkyl (electron-donating group). However, the IC_{50} of both compounds were different. This phenomenon is very interesting. To further study, molecular docking and dynamics studies were conducted to estimate the binding interaction of both compounds to predict the complex stability of the inhibitor with protein target. Molecular docking was shown to calculate the binding energies of compounds 1–9 to α-glucosidase using three different programs (AutoDock Vina, Autodock4, and DockThor), as presented in Table 1. To verify the docking process, the ligand originally crystallized with the protein was redocked, as illustrated in Figure 3. In this study, AutoDock Vina is utilized to forecast potential docking configurations owing to its faster processing speed and ability to produce more precise binding poses, while Autodock4 has better binding affinity (Nguyen et al. 2019; Chen et al. 2023). This study also uses the DockThor program be-

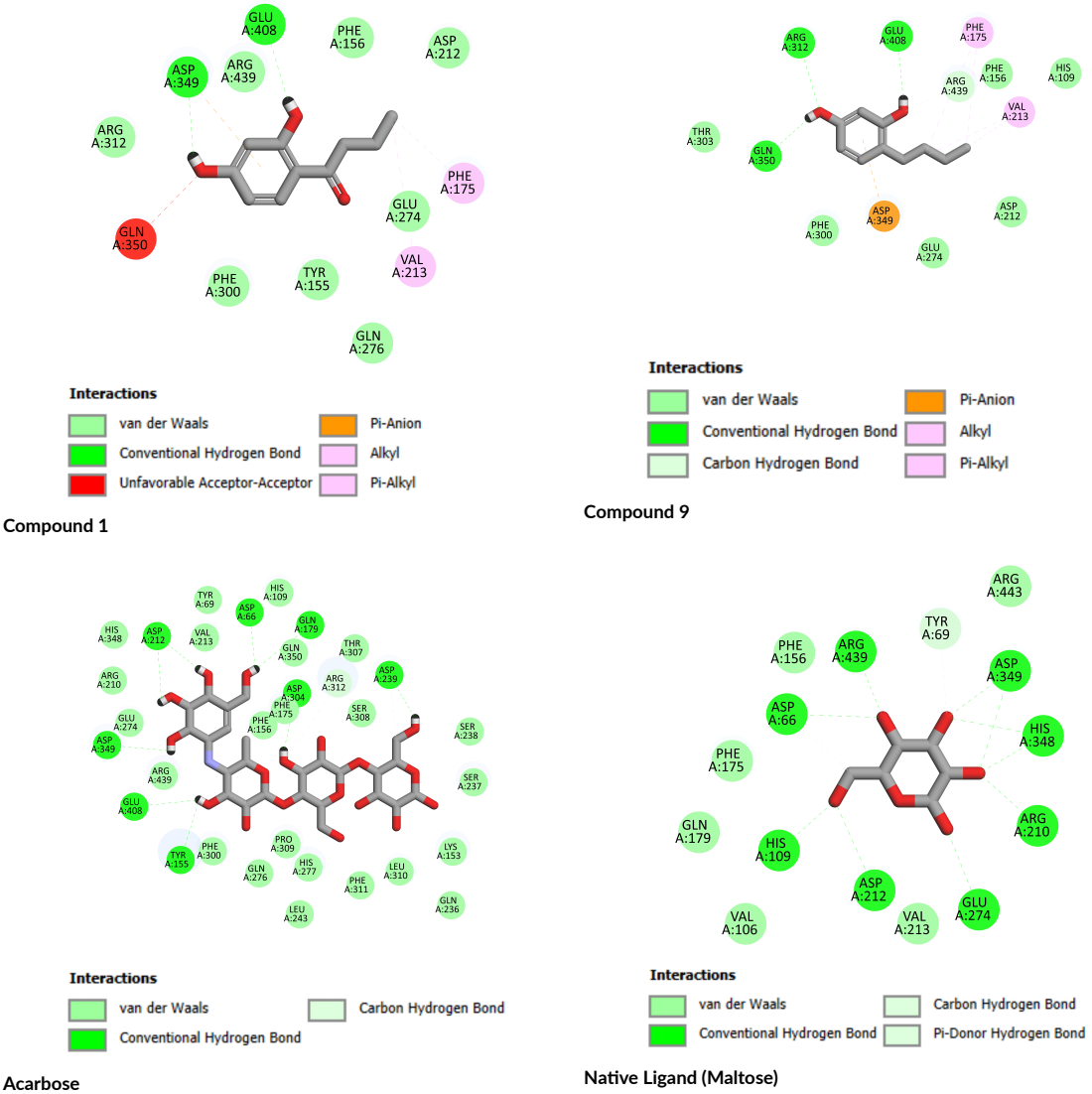


FIGURE 4 The 2D interaction plots of 1, 9, acarbose, and the native ligand in complex with α-glucosidase (PDB ID: 3A4A).

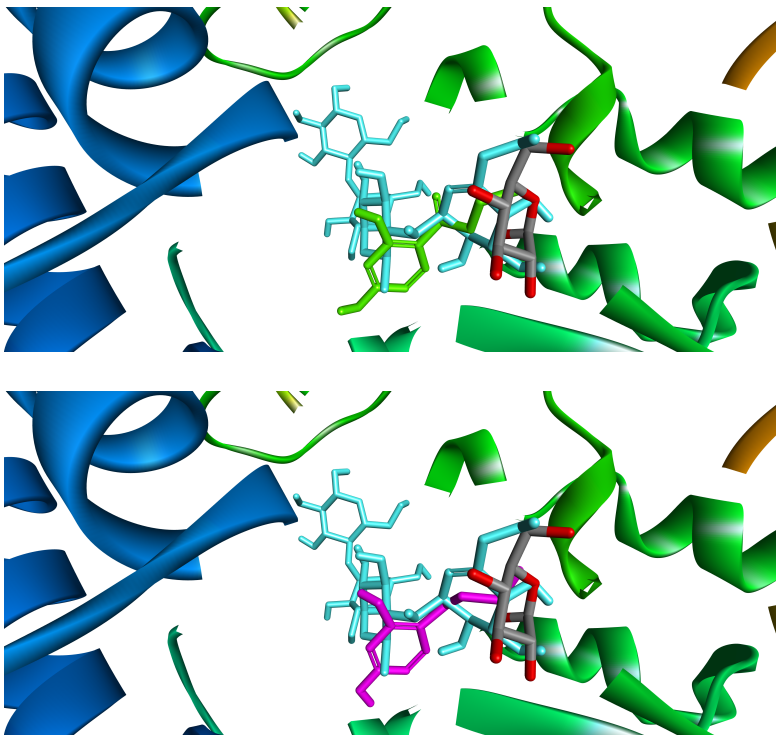
cause it has different algorithms to estimate binding energy (Guedes et al. 2024) by comparing the result with Autodock Vina and Autodock4. The molecular docking results are presented in Table 1. The binding energies of these compounds (1–9) were from -6.3 to -7.2 kcal/mol through Autodock Vina, -2.6 to -5.0 kcal/mol through Autodock4, and -6.6 to -7.5 kcal/mol through DockThor, as shown in Table 1. Moreover, two compounds with good inhibitory activity (1 and 9) exhibited strong binding affinity (-3.7 and -3.9 kcal/mol) compared with acarbose (-0.5 kcal/mol) and native ligand (-3.1 kcal/mol) using Autodock4.

Furthermore, the two-dimensional (2D) and three-dimensioanl (3D) interactions of the ligand with α-glucosidase were visualized using BIOVIA Discovery Studio Visualizer (Figure 4 and 5). Compound 1 displayed two H-bonds with Glu408 and Asp349 as well as π-anion and hydrophobic interactions with Asp349, Phe175, and Val213. Compound 9 showed π-anion and hydrophobic interactions the same as compound 1, including three H-bonds with Arg312, Gln350, Glu408. Moreover, acarbose and the native ligand mostly exhibited H-bond interactions at the orthosteric site of α-glucosidase. Compounds 1 and 9 networked with Asp349 and Glu408 that correlated with acarbose and native ligand, as shown in Figure 2.

To further our analysis, molecular dynamics were performed to analyze the stability of inhibitors in complex with protein in aqueous condition during simulation for 100 nanoseconds (ns). The findings indicate that the stability of the complex formed by compound 9 with α-glucosidase remained consistent throughout the simulation supported by the RMSD, radius of gyration, and SASA values, as depicted in Figures 6a, 6b, and 6d. Compound 1 revealed instability, as evidenced by significant fluctuations between 70 and 100 ns, in contrast to compound 9. The number of contact values was relatively comparable both compounds 1 and 9 (Figure 6c). Additionally, RMSF (root-mean-square fluctuation) computes the extent to which a ligand deviates from its average position throughout a molecular dynamics simulation (Lee et al.

TABLE 1 Binding energies (kcal/mol) of compounds 1-9, acarbose, and native ligand with 3A4A.

Cmp	Binding Energy (kcal/mol)		
	Autodock Vina	Autodock4	DockThor
1	-6.5	-3.7	-6.7
2	-6.7	-2.6	-7.5
3	-7	-3	-6.8
4	-7	-5	-6.7
5	-7.2	-3.8	-6.6
6	-7.1	-4.4	-6.8
7	-6.9	-3.3	-7.1
8	-6.4	-4	-7.5
9	-6.3	-3.9	-6.9
Acarbose®	-8.3	-0.5	-8.1
Native Ligand (maltose)	-5.7	-3.1	-6.4



(a)

(b)

FIGURE 5 The 3D visualization of 1 (green, a) and 9 (pink, b) in overlapping with acarbose (blue) and the native ligand (dark gray) in complex with α-glucosidase (PDB ID: 3A4A).

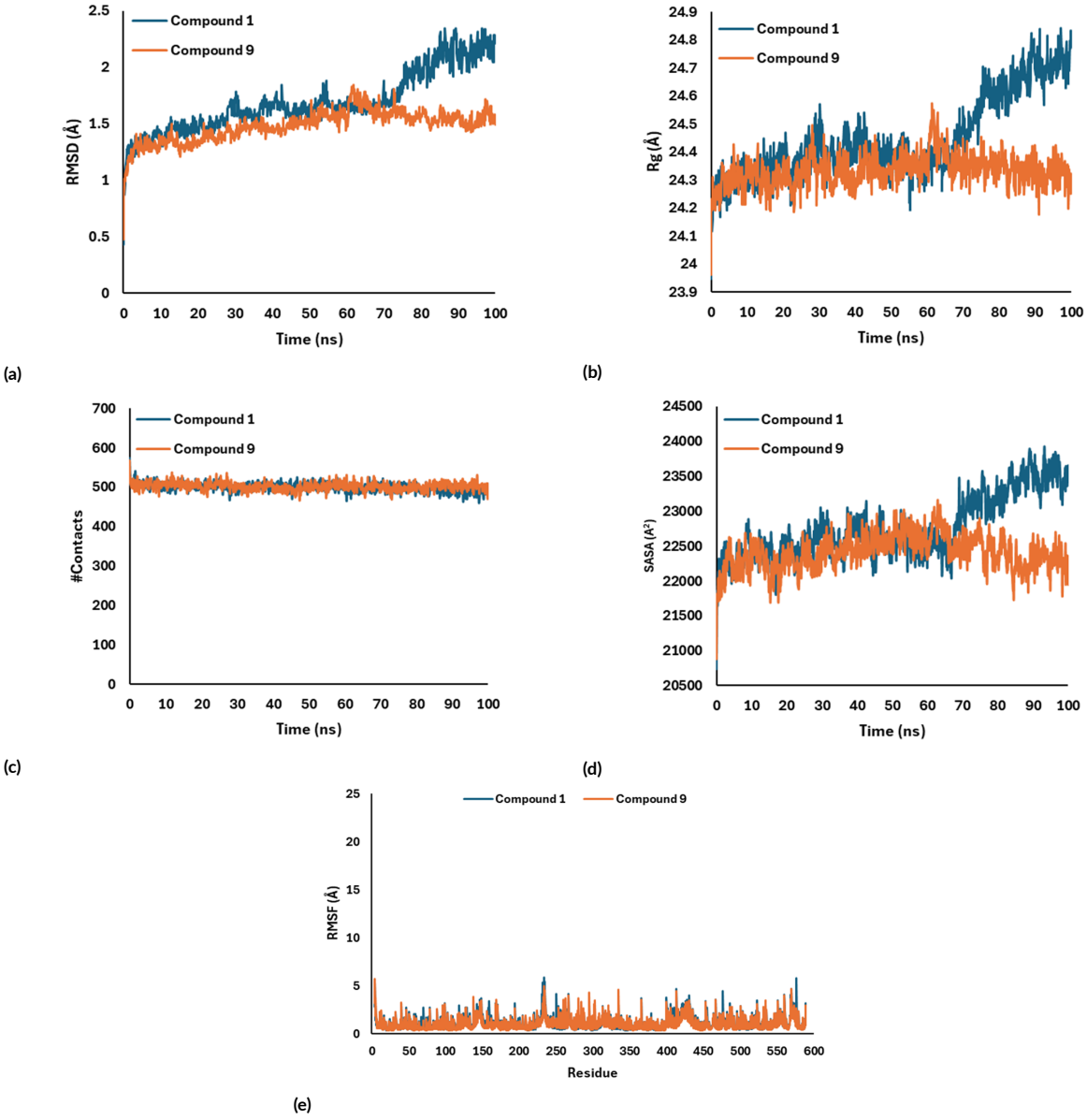


FIGURE 6 Evaluation of root-mean-square displacement (RMSD) (a), radius of gyration (Rg) (b), number of contacts (#Contacts) (c), solvent accessible surface (SASA) (d), and root-mean-square fluctuation (RMSF) (e).

2024). Compounds 1 and 9 displayed similar fluctuations in several residues during simulation, which may suggest comparable activity against α-glucosidase, as described in Figure 6e. Moreover, compound 9 was more stable than compound 1 with the average of binding values of -92.98 kJ/mol for compound 1 and -103.25 kJ/mol for compound 9. Therefore, compound 9 may have more potency for further research in the treatment of DM type 2.

4. Conclusions

In summary, nine resorcinol derivatives (1–9) were successfully investigated for their inhibitory activity against yeast α-glucosidase and their binding energies with α-glucosidase, using three molecular docking programs. The results revealed that two compounds (1 and 9) having butanoyl and butyl displayed better inhibition against α-glucosidase (IC_{50} = 75.9 and 33.3 µM) than other derivatives (2–8) and acarbose (IC_{50} = 832.8 µM). In addition, the results of molecular docking showed that compounds 1 and 9 possessed good binding affinity and similar interactions with Asp349 and Glu408, which were allied with acarbose and a native ligand. Molecular dynamics showed that compound 9 was higher stable than compound 1 in complex with α-glucosidase. Therefore, the development of compound 9 has the potential for further investigation of their efficacy using *in vitro* and *in vivo* studies.

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Authors' contributions

AD, EH, WC Design the study. AD carried out the laboratory work and wrote the original manuscript. DM, IM, FK reviewed the original manuscript. All authors read and approved the final version of the manuscript.

Competing interests

We declare that there is no conflict of interest.

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