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RESEARCH ARTICLE OPEN ACCESS

The Potential Of Bioactive Compounds Of *Moringa oleifera* Leaves as α-Glucosidase Inhibitor Reveals Antidiabetic Activity

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ABSTRACT

Type 2 diabetes mellitus is the most common type of diabetes, accounting for approximately 90% of all diabetes cases. The enzyme α-glucosidase is an important therapeutic target due to its role in breaking down carbohydrates into glucose in the small intestine. Moringa leaves (Moringa oleifera) are known to have antihyperglycemic effects through the inhibition of this enzyme, making the active compounds within them a potential natural antidiabetic agent. This study aims to evaluate the physicochemical profile, pharmacokinetics, and bioactivity of six compounds in moringa leaves (4-Undecylbenzenesulfonic acid, Apigetrin, Quercetin-3-β-D-glucoside, D-(-) -Quinic acid, Corchorifatty acid F, and 4-Hydroxybenzaldehyde) using in silico methods, with Voglibose as a control, against the α-glucosidase receptor (PDB ID: 5KZX) via the Hex 8.0.0, PyRx 0.8, and BIOVIA Discovery Studio 2019 applications. The results showed that four compounds (Apigetrin, D-(-)Quinic acid, Corchorifatty acid F, and 4-Hydroxybenzaldehyde) met Lipinski's rules and had good pharmacokinetic profiles. In terms of bioactivity, Apigetrin and D-(-)Quinic acid had Pa values >0.5, indicating potential as antidiabetic agents. Docking analysis revealed that all compounds could interact with α-glucosidase, but their binding energies were still higher than Voglibose (-1425.3 kcal/mol). Among the tested compounds, Apigetrin showed the lowest value (-334.1 kcal/mol). This study suggests that Apigetrin, D-(-)-Quinic acid, Corchorifatty acid F, and 4-Hydroxybenzaldehyde may have potential as candidates for type 2 antidiabetic drugs due to their α-glucosidase inhibitory properties. Based on the binding energy of the compounds found in moringa leaves, they bind outside the active site of the ligand.

Keywords: Type 2 Diabetes Mellitus, Moringa leaves, Molecular docking, α-Glucosidase

INTRODUCTION

Diabetes mellitus is a metabolic disorder in which a person diagnosed with diabetes experiences hyperglycemia due to insulin resistance, insulin insufficiency, or both. Due to the potential damage to vital organs, including the kidneys, eyes, and

blood vessels, this disease is considered highly dangerous (Hardianto, 2021). Although type 2 diabetes mellitus is the most common type in Indonesia, there are three subtypes to consider: type 1, type 2, and gestational diabetes, with type 2 diabetes accounting for 90–95% of all diabetes cases. The causes include obesity, unhealthy eating habits, smoking, stress, and pancreatic and hormonal disorders (Firmansya et al., n.d., 2024). According to the 2018 Basic Health Research (Riskesdas), the leading cause of death among type 2 diabetes patients in Indonesia is macrovascular complications; the prevalence of diabetes in Indonesia reaches 8.5%.

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Natural treatment alternatives, such as phytomedicine, are gaining popularity due to their minimal side effects. Moringa oleifera leaves are known to have antihyperglycemic effects through the inhibition of glucosidase enzymes, and contain bioactive compounds such as flavonoids and antioxidants that have potential in the treatment of DM (Arini Salsabila Hasibuan et al., 2023). In Fachruddin's 2024 study (Fachruddin et al., 2024), data on the phytoconstituents of moringa leaves were obtained using the LC-MS/MS method with a 70% ethanol extract yield, yielding six compounds with the highest relative abundance (molecular or ion abundance) values, namely 4 -Undecylbenzenesulfonic acid, Apigetrin, Quercetin-3 β-D-glucoside, D-(-)-Quinic acid, Corchorifatty acid F, and 4-Hydroxybenzaldehyde.

Docking has made rapid progress in the pharmaceutical sector over the past few decades. Through docking, the affinity and therapeutic efficacy of small molecules can be predicted by predicting their binding orientation to proteins. The term "in silico testing" refers to the process of conducting trials or evaluations within a digital model. The use of in silico testing has two main applications: the discovery of new drugs and the optimization of parent chemical actions. Predictions, ideas, and potential therapeutic breakthroughs can be achieved through the use of computer simulations to conduct testing (Hardjono, 2013).

MATERIAL AND METHODS

Data Mining

This study is a pre-experimental in silico study using the α-glucosidase receptor (PDB ID: 5KZX, resolution 2.00 Å) and six active compounds from moringa leaves: 4-

Undecylbenzenesulfonic acid (CID: 38222), Apigetrin (CID: 5280704), Quercetin-3 β-D-glucoside (CID: 44259136), D-(-) -Quinic acid (CID: 6508), Corchorifatty acid F (CID: 348291029), and 4-Hydroxybenzaldehyde (CID: 126), as well as Voglibose (CID: 444020) as a reference ligand. The equipment used included an Acer Aspire 5 laptop with an Intel Core i3 processor, 8 GB of RAM, and the software Hex 8.0.0, PyRx 0.8, and BIOVIA Discovery Studio 2019 Client.

Prediction of Compound Bioactivity and ADME

Bioactivity predictions were performed using the PASS Online website (https://www.way2drug.com/passonline/) and ADME analysis was performed using the SwissADME website (http://www.swissadme.ch/) by inputting SMILES codes from PubChem.

Downloading and preparation of target ligands

The ligand file was downloaded from PubChem (https://www.ncbi.nlm.nih.gov/), while the 5KZX receptor protein was obtained from RCSB PDB (https://www.rcsb.org/). The 3D structure of the ligand was constructed using PyRx and saved in PDB format, while the receptor was prepared using BIOVIA Discovery Studio with Open Babel.

Plot Ramachandran

Ramachandran plot check, by clicking on the chart in BIOVIA Discovery Studio 2019 Client and selecting the Ramachandran Plot feature, to evaluate protein structure integrity.

Molecular docking and visualization

The molecular docking process was performed using Hex 8.0.0 with default settings for Shape+Electro+DARS and specific parameters: grid dimension 0.6, solution range 180, twist range 360, distance range 40, translation step 0.8, and score threshold 0.0. The docking results were visualized in 2D and 3D using BIOVIA to identify the types of bonds and amino acid residues involved. The data were then exported to Microsoft Excel 2021.

Data analysis

Data analysis encompasses physicochemical properties (molecular weight, HBD, HBA, logP, logS), pharmacokinetics (GI absorption, BBB permeation, CYP, logKp, drug-likeness), and docking parameters (interactions, bond types, bond energy, and Ramachandran plot), all analyzed using Microsoft Excel 2021.

RESULT AND DISCUSSION

Analysis of Physicochemical, Pharmacokinetic, and Bioactivity Predictions

The nature of compound interactions with receptors can be analyzed through in silico approaches such as molecular docking, which enables the prediction of affinity and binding efficacy based on ligand-receptor binding energy (Tahir & Maryam, 2024; Wulandari, n.d.). Physicochemical evaluation using Lipinski's Rule of Five is an important indicator in assessing the suitability of compounds as oral drug candidates,

including Molecular Weight (<500 g/mol), Hydrogen Bond Acceptor (<10), Hydrogen Bond Donor (<5), Log P (High Lipophilicity) (<5), and Log S (Solubility) (Naufa et al., 2022). In this study, six compounds from moringa leaves (4-Undecylbenzenesulfonic acid, Apigetrin, Quercetin-3-β-D-glucoside, D-(-)-Quinic acid, Corchorifatty acid F, and 4-Hydroxybenzaldehyde) were tested using SwissADME. The results showed that four compounds (Apigetrin, D-(-)-Quinic acid, Corchorifatty acid F, and 4-Hydroxybenzaldehyde) met all Lipinski parameters, indicating potential as oral drugs. Quercetin-3-β-D-glucoside did not meet the criteria for (Hydrogen Bond Acceptor) HBA and (Hydrogen Bond Donor) HBD, making it too polar and difficult to penetrate cell membranes. Apigetrin and Voglibose also exceeded the HBD limit, which could hinder oral absorption.

The log P values of all compounds remain within the ideal range (0–<3), indicating good amphipathic properties for absorption. However, the log S value of 4-Undecylbenzenesulfonic acid is very low (-6.17), indicating poor water solubility, making it unsuitable for oral formulations (Muliadi et al., 2021). This issue can be addressed through structural modifications or modern formulation technologies such as nanoparticles, liposomes, and SEDDS to enhance solubility and bioavailability (Pardi et al., 2018; Wu et al., 2023). Thus, only four out of six active compounds from Moringa oleifera meet the criteria as oral drug candidates based on physicochemical parameters.

Pharmacokinetics describes the ADME (absorption, distribution, metabolism, excretion) process of a compound (Grogan & Preuss, 2025). The ADME evaluation in this study includes GI absorption, BBB permeability, CYP450, Log Kp, and Lipinski. Compounds with high GI absorption indicate good oral absorption potential, while low values indicate poor intestinal absorption and low efficacy (Dahlgren & Lennernäs, 2019). The ability to penetrate the Blood-Brain Barrier (BBB) is indicated as "no" if the compound cannot cross the blood-brain barrier, which is common in hydrophilic molecules (Sun et al., 2023; Chlebek et al., 2019). CYP450 plays a crucial role in drug metabolism; compounds that do not inhibit this enzyme ("no") tend to have a lower risk of drug interactions, while "yes" indicates a higher potential for drug interactions (Abdullah et al., 2021; Yang & Wang, 2020). Specific CYP isoforms such as CYP2C9, CYP2C19, CYP3A4, and CYP2D6 are involved in the metabolism of type 2 diabetes medications. The Log Kp (skin permeation) values for all compounds do not meet the standards; however, this is not significantly impactful, as type 2 diabetes treatment typically uses the oral route rather than the transdermal route (Hakiki et al., 2024).

To validate the pharmacological potential of the compound, an analysis was performed using PASS Online (Prediction of Activity Spectra for Substances), which predicts the biological activity of a compound based on its structural similarity to known active compounds (Pokharkar et al., 2022). The Pa (Probability to be Active) value indicates the potential activity, where Pa > 0.7 indicates high similarity to existing drugs, and Pa 0.5–0.7 indicates potential activity. However, it differs from conventional drugs, and Pa < 0.5 indicates low potential activity (Kusumawati, 2021). The results showed that Apigetrin, Quercetin-3-β-D-glucoside, and D-(-)-Quinic acid had Pa values > 0.5, indicating potential activity as type 2 antidiabetic agents. Conversely, Voglibose

has a pA of 0.384, which is lower than that of some test compounds, possibly due to its uncommon structure in the PASS database (Filimonov et al., 2014). Flavonoid or phenolic compounds in moringa leaves tend to have higher Pa values due to their similarity to known active compounds (Daina et al., 2017).

Ramachandran Plot Analysis From The Data Results Obtained

In the Ramachandran plot, there are several angles, namely the torsional phi (X-axis) (ϕ) and psi (Y-axis) (ψ) of the amino acid residue. The plot has several regions: Most Favored Regions (Quadrant I), Additional Allowed Regions (Quadrant II), Generously Allowed Regions (Quadrant III), and Disallowed Regions (Quadrant IV). The stability and quality of the model are indicated by the ratio of amino acid residues in the allowed regions to those in the disallowed regions. (Alam et al., 2020). The study states that most points are located in the allowed quadrants, indicating that the structure is in a sterically allowed conformation. There is also no significant concentration in the disallowed regions, suggesting that the structure is sufficiently stable.

Molecular Docking Analysis

Based on the docking results, each compound showed different interaction patterns with α-glucosidase. In 4-Undecylbenzene sulfonic acid, residues HIS674 and TRP376 were close to the active site (LIG1), forming Pi-Sulfur and Pi-Pi stacked interactions stabilized by hydrophobic bonds. The Apigetrin compound exhibits interactions between all residues, including hydrogen bond interactions (VAL718, ASP356, VAL357), Pi-Pi T-shaped interactions (HIS717, TYR360), Pi-Donor H-bond interactions (TYR360), and Pi-Alkyl interactions (VAL718), indicating high affinity and selectivity. In Quercetin-3 β-D-glucoside, there are hydrogen bonds (TYR360, PRO361, HIS717) and Pi-Alkyl (ARG608, VAL588) interactions, while LEU868 and HIS717 show unfavorable interactions. D-(-)-Quinic acid interacts with residues MET363, GLU866, VAL867 (hydrogen bond) and HIS717 (carbon hydrogen bond), which strengthen affinity. Corchorifatty acid F exhibits hydrogen bond interactions (GLU869), Pi-Alkyl interactions (PHE362, HIS584, PRO595), and unfavorable steric interactions (LEU865, GLU866), which may reduce affinity; however, it still shows potential as an inhibitor with structural modifications. 4-Hydroxybenzaldehyde interacts via hydrogen bonds (ASP95) and Pi-Alkyl (ALA93, PRO94), although there are unfavorable bumps at PHE159, CYS92, and PHE129. Voglibose, as a control, interacts with active site residues such as ASP616, ASP645, HIS674, ASP404, ASP518, TRP613, and TRP516 via hydrogen bonds and exhibits unfavorable bumps on some residues, indicating the need for ligand structure optimization. The absence of residue similarity between the test compound and the control suggests the possibility of allosteric binding with a different mechanism of action, yet it remains a potential α-glucosidase inhibitor. Binding outside the active site is consistent with findings that α-glucosidase has multiple types of inhibition, including allosteric. Previous studies with Metformin have mentioned the involvement of active residues such as TRP376, ASP404, ASP518, ASP616, TRP613, and HIS674, not all of which appear in the test compound interactions, possibly due to suboptimal ligand orientation. Further validation is required to confirm that interactions occur at the enzyme's active site.

Binding energy is a crucial parameter in molecular docking, reflecting the strength of interaction between the ligand and the receptor. Negative values indicate the stability of the complex (Ferreira et al., 2015). Lower binding energy indicates a stronger ligand affinity for the target protein, while high binding energy indicates a lower affinity (Aziz et al., 2016). In this study, Voglibose, used as a control, showed the lowest binding energy of -1425.3 kcal/mol, indicating the highest affinity and strong complex stability. Among the test compounds, Apigetrin had the lowest binding energy of -334.1 kcal/mol, followed by Quercetin-3 β-D-glucoside (-296.9 kcal/mol), 4-Undecylbenzene sulfonic acid (-278.0 kcal/mol), Corchorifatty acid F (-276.7 kcal/mol), D-(-)-Quinic acid (-182.6 kcal/mol), and 4-Hydroxybenzaldehyde (-169.2 kcal/mol). Although all compounds showed fairly good interaction with α-glucosidase, their binding energy values were still higher than those of Voglibose, possibly due to suboptimal ligand orientation or lack of direct binding to the main catalytic residue. Voglibose has a structure similar to that of the enzyme's natural substrate, allowing it to interact specifically with the active site and exhibit high affinity and low binding energy (Yoon et al., 2021). This is further supported by the number of hydrogen bonds, where Voglibose forms eight hydrogen bonds. In contrast, Apigetrin forms 5, indicating that the more hydrogen bonds formed, the stronger the binding affinity.

CONCLUSION

Based on the results of the study, four of the six active compounds in Moringa oleifera, namely Apigetrin, D-(-) -Quinic acid, Corchorifatty acid F, and 4-Hydroxybenzaldehyde, meet the physicochemical parameters based on Lipinski's rules. In contrast, Quercetin-3-β-D-glucoside only meets three criteria, and 4-Undecylbenzenesulfonic acid, although it meets Lipinski's rules, does not meet the Log S criteria, making it less suitable for oral formulations. Pharmacokinetically, all four compounds exhibit good ADME characteristics and have potential as drug candidates. Apigetrin and D-(-)Quinic acid also show Pa > 0.5 values in PASS Online analysis, indicating pharmacological activity as type 2 antidiabetic agents. All compounds from moringa leaves, namely 4-Undecylbenzenesulfonic acid, Apigetrin, Quercetin-3-β-D-glucoside, D-(-) -Quinic acid, Corchorifatty acid F, and 4-Hydroxybenzaldehyde, demonstrated the ability to interact with the α-glucosidase enzyme. However, their binding energy values were still higher than Voglibose as a control (-1425.3 kcal/mol), with Apigetrin having the lowest binding energy value among the tested compounds (-334.1 kcal/mol). However, all these compounds bind outside the enzyme's active site, which may affect their effectiveness in binding to the target, so further research using different conformations is needed to confirm that the six compounds in moringa leaves can indeed be considered candidates for preventing Type 2 Diabetes Mellitus.

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TABLE AND FIGURE

Table 1. Predicted Physicochemical, Pharmacokinetic, Bioactivity of *Moringa Oleifera* leaves

Physicochemical	**4 – Undecy Benzene sulfonic acid**	**Apigetrin**	**Quercetin -3 β-D-glucoside**	**D-(-)-Quinic acid**	**Corchorifat ty acid F**	**4 - Hydroxybenz aldehyde**	**Voglibose (Control)**
Molecular Weight	312,47 g/mol	432,38 g/mol	464,38 g/mol	192,17 g/mol	328,44 g/mol	122,12 g/mol	267,28 g/mol
Hydrogen Bond Aceptor	3	10	12	6	5	2	8
Hydrogen Bond Donor	1	6	8	5	4	1	8
Log P	2,81	1,98	0,94	0,22	3,06	0,99	0,88
Log S	-6,17	-2,69	-1,51	2,08	-1,86	-1,72	2,09
Pharmacokinetic							
GI absorption	High	Low	Low	Low	High	High	Low
BBB permeability	No	No	No	No	No	Yes	No
CYP1A2 inhibitor	No	No	No	No	No	No	No
CYP2C19 inhibitor	Yes	No	No	No	No	No	No
CYP2C9 inhibitor	Yes	No	No	No	No	No	No
CYP2D6 inhibitor	No	No	No	No	No	No	No
CYP3A4 inhibitor	No	No	No	No	No	No	No
Log Kp (cm/s)	-3,75	-7,65	-8,88	-9,15	-6,47	-6,09	-10,83
Lipinski	Yes	Yes	No	Yes	Yes	Yes	Yes
Bioactivity							
Pa (*Probability to be Active*)	0,238	0,681	0,661	0,540	0,269	0,130	0,384

Table 2. Interaction Between Moringa Oleifera Leaf Compounds and α-Glucosidase Receptors

Interactions	**Point interaction**	**Chemistry bond**	**Type**	**Energy binding (kcal/mol)**
4-Undecylbenzene sulfonic acid - α-Glukosidase	:LIG1:S - A:HIS674	Other	Pi-Sulfur	-278.0
	A:TRP376 - :LIG1	Hydrophobic	Pi-Pi Stacked	
Apigetrin - α-Glukosidase	:LIG1:H - A:VAL718:O	Hydrogen Bond	Conventional Hydrogen Bond	-334.1
	:LIG1:H - :LIG1:O	Hydrogen Bond	Conventional Hydrogen Bond	
	:LIG1:H - A:ASP356:O	Hydrogen Bond	Conventional Hydrogen Bond	
	:LIG1:H - A:VAL357:O	Hydrogen Bond	Conventional Hydrogen Bond	
	A:TYR360:HN - :LIG1	Hydrogen Bond	Pi-Donor Hydrogen Bond	
	A:TYR360 - :LIG1	Hydrophobic	Pi-Pi Stacked	
	A:TYR360 - :LIG1	Hydrophobic	Pi-Pi Stacked	
	A:HIS717 - :LIG1	Hydrophobic	Pi-Pi T-shaped	
	:LIG1 - A:VAL718	Hydrophobic	Pi-Alkyl	
Quercetin-3 β-D-glucoside - α-Glukosidase	:LIG1:H - :LIG1:O	Hydrogen Bond	Conventional Hydrogen Bond	-296.6
	:LIG1:H - A:TYR360:O	Hydrogen Bond	Conventional Hydrogen Bond	
	:LIG1:H - A:PRO361:O	Hydrogen Bond	Conventional Hydrogen Bond	
	:LIG1:H - A:HIS717:NE2	Hydrogen Bond	Carbon Hydrogen Bond	
	:LIG1 - A:VAL588	Hydrophobic	Pi-Alkyl	

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Interactions	Point interaction	Chemistry bond	Type	Energy binding (kcal/mol)
	:LIG1 - A:ARG608	Hydrophobic	Pi-Alkyl	
D-(-)-Quinic acid - α-Glukosidase	A:MET363:HN - :LIG1:O	Hydrogen Bond	Conventional Hydrogen Bond	-182.6
	A:GLU866:HN - :LIG1:O	Hydrogen Bond	Conventional Hydrogen Bond	
	A:VAL867:HN - :LIG1:O	Hydrogen Bond	Conventional Hydrogen Bond	
	:LIG1:H - :LIG1:O	Hydrogen Bond	Conventional Hydrogen Bond	
	A:HIS717:CE1 - :LIG1:O	Hydrogen Bond	Carbon Hydrogen Bond	
	:LIG1:H - A:HIS717:NE2	Hydrogen Bond	Carbon Hydrogen Bond	
Corchorifatty acid F - α-Glukosidase	A:GLU869:HN - :LIG1:O	Hydrogen Bond	Conventional Hydrogen Bond	-276.7
	A:GLU866:CA - :LIG1:O	Hydrogen Bond	Carbon Hydrogen Bond	
	:LIG1:C - A:PRO595	Hydrophobic	Alkyl	
	A:PHE362 - :LIG1:C	Hydrophobic	Pi-Alkyl	
	A:HIS584 - :LIG1:C	Hydrophobic	Pi-Alkyl	
4-Hydroxybenzaldehyde - α-Glukosidase	:LIG1:H - A:ASP95:OD1	Hydrogen Bond	Carbon Hydrogen Bond	-169.2
	:LIG1 - A:ALA93	Hydrophobic	Pi-Alkyl	
	:LIG1 - A:PRO94	Hydrophobic	Pi-Alkyl	
Voglibose (Kontrol) - α-Glukosidase	:UNK1:H - A:ASP616:OD1	Hydrogen Bond	Conventional Hydrogen Bond	-1425.3
	:UNK1:H - A:ASP645:OD2	Hydrogen Bond	Conventional Hydrogen Bond	
	:UNK1:H - A:HIS674:NE2	Hydrogen Bond	Carbon Hydrogen Bond	
	:UNK1:H - A:ASP404:OD1	Hydrogen Bond	Carbon Hydrogen Bond	
	:UNK1:H - A:ASP404:OD2	Hydrogen Bond	Carbon Hydrogen Bond	
	:UNK1:H - A:ASP518:OD2	Hydrogen Bond	Carbon Hydrogen Bond	
	:UNK1:H - :UNK1:O	Hydrogen Bond	Carbon Hydrogen Bond	
	:UNK1:H - A:ASP616:OD1	Hydrogen Bond	Carbon Hydrogen Bond	

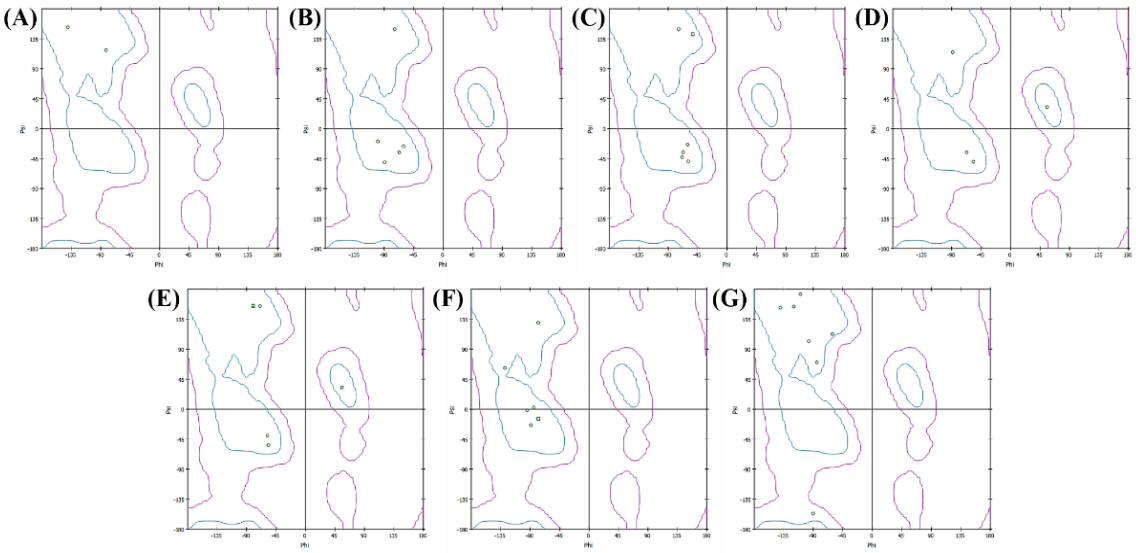

Figure 1. Ramachandran Plot Results for 4-undecylbenzene sulfonic acid (A), Apigenin (B), Quercetin-3 β-D-glucoside (C), D-(-)-Quinic acid (D), Corchorifatty F fatty acid (E), 4-Hydroxybenzaldehyde (F), Voglibose (Control) (G).

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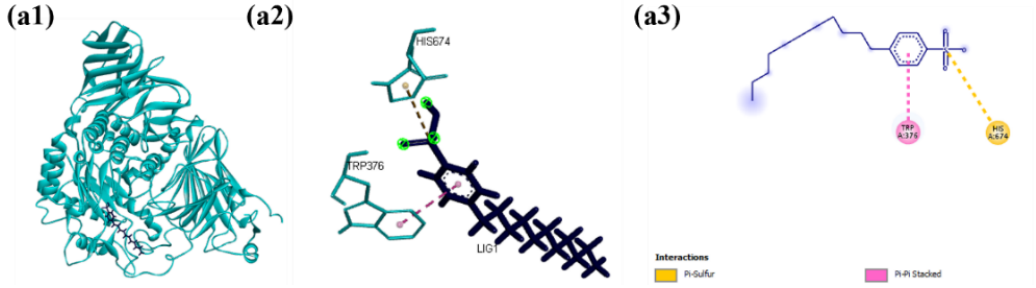
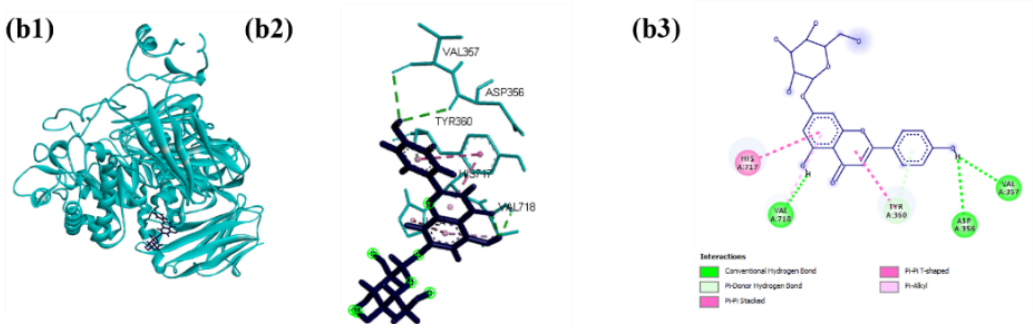
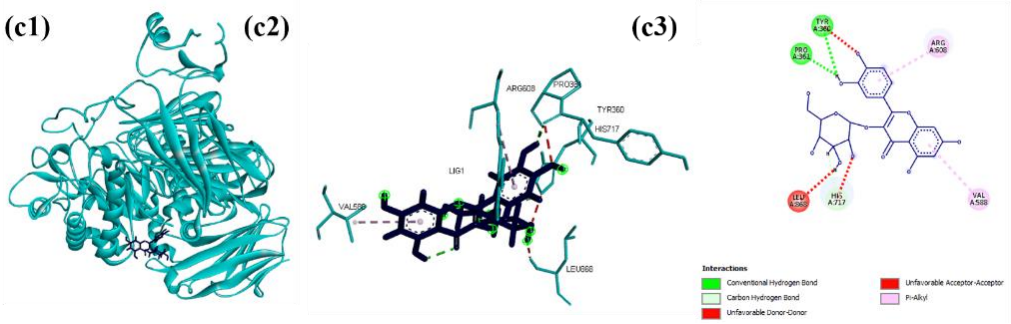
Kompleks 4-Undecylbenzene sulfonic acid - α-Glukosidase



Kompleks Apigetrin - α-Glukosidase



Kompleks Quercetin-3 β-D-glucoside - α-Glukosidase



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Kompleks D-(-)-Quinic acid - α-Glukosidase

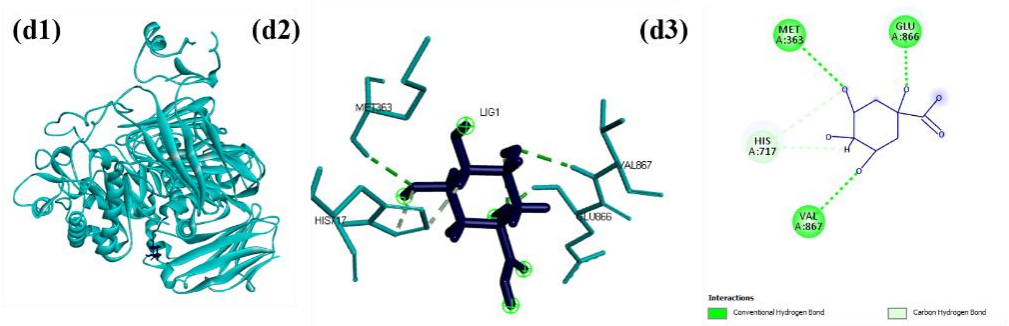
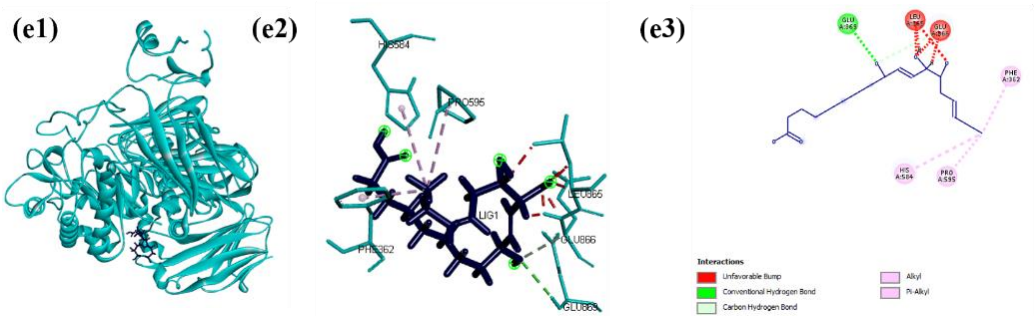
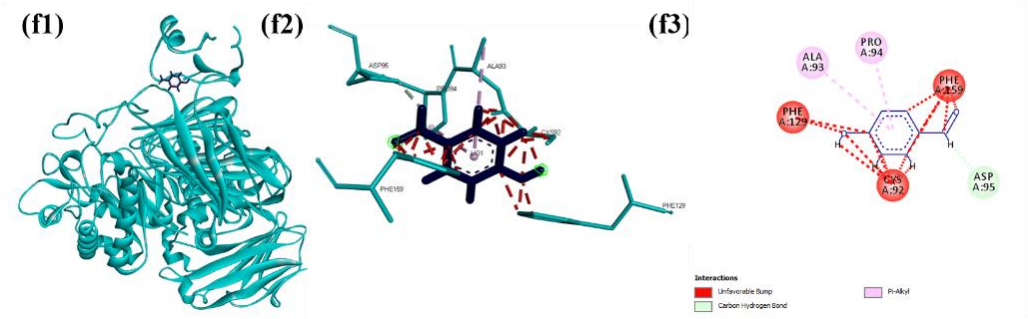


Figure 2. Molecular docking results of the interaction between the complex, 4-Undecylbenzene sulfonic acid (A), Apigetrin (B), Quercetin-3 β-D-glucoside (C), and D-(-)-Quinic acid (D). Figure 1 shows the visualization of the ligand-protein molecular complex. The 3D structures in Figures 2 and 3 show the 2D structures.

Kompleks Corchorifatty acid F - α-Glukosidase



Kompleks 4-Hydroxybenzaldehyde - α-Glukosidase



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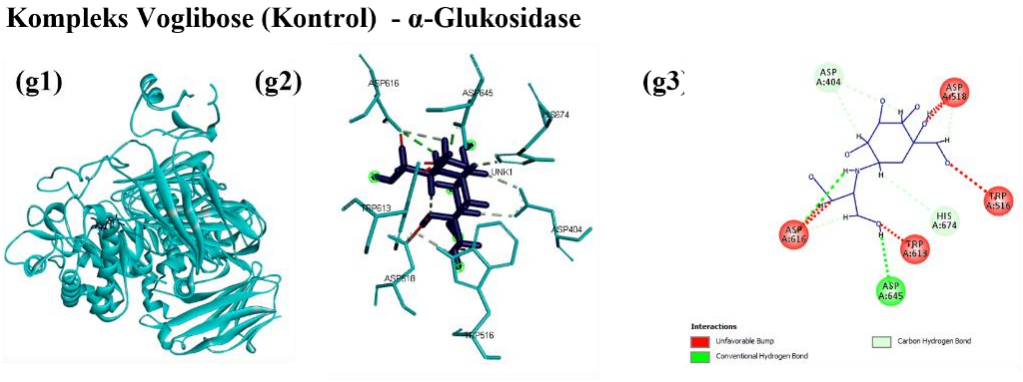

Figure 3. Molecular docking results of the interaction between the complex, Corchorifatty acid F (E), 4-Hydroxybenzaldehyde (F), and Voglibose (Control) (G). Figure 1 shows the visualization of the ligand-protein molecular complex. The 3D structures in Figures 2 and 3 show the 2D structures.