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In Silico Study of Reported Compounds from Togaku Oil Plants from Timor Island as Candidates for Plampesin X Inhibitors of *Plasmodium falciparum*

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ABSTRACT

Malaria is still a major health problem in Indonesia, especially caused by Plasmodium falciparum, so it is necessary to develop new drug candidates to overcome potential antimalarial resistance. This study aims to identify the potential of reported compounds from Togaku oil-producing plants on Timor Island as candidate inhibitors of the Plasmepsin X protein using an in-silico approach. The structure of Plasmepsin X protein (PDB ID: 7TBC) was obtained from the Protein Data Bank and prepared using YASARA Structure software. Evaluation of structural quality was performed using Ramachandran plot analysis, while active-site prediction was performed using the COACH server. Molecular docking was performed on various candidate compounds using YASARA Structure, with artemisinin as a positive control. Docking results showed that oleanane and dammarane had the highest positive binding energies, (-11.879) kcal/mol and (-8.930) kcal/mol, respectively, which were higher than the positive control, artemisinin (8.428 kcal/mol), indicating stronger binding affinity and a more stable complex. Complex interactions were dominated by hydrophobic residues, including PHE311, ILE316, ILE354, PHE355, ILE358, and PHE360, as well as by polar residues, such as SER246, GLN247, SER269, and THR460, which contributed to complex stabilization. The interaction visualization showed that the selected ligands bind to the protein's active pocket in a stable orientation. Based on these results, triterpenoid compounds, especially oleanane and dammarane, are potential candidates for Plasmepsin X inhibitors and warrant further experimental testing.

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INTRODUCTION

Malaria remains one of the significant public health problems in Indonesia. According to the 2024 country profile report by the World Health Organization, approximately 418.206 confirmed indigenous cases were recorded in 2023, with an estimated 1.1 million cases nationwide. These data indicate that malaria remains a relevant disease requiring serious attention, particularly in the development of new drug candidates [1]. In Indonesia, *Plasmodium falciparum* is the dominant species among indigenous cases, accounting for approximately 62% of cases. This species has high clinical significance because it is associated with severe malaria and an increased risk of mortality [1,2]. This condition is particularly important in East Nusa Tenggara, especially on Sumba Island and its surrounding areas, which are still categorized as regions with high malaria endemicity and remain a priority in accelerating national malaria elimination [2]. In addition, drug efficacy monitoring in Papua and East Nusa Tenggara indicates that malaria control efforts do not only depend on early diagnosis and prompt treatment, but

must also anticipate the long-term risk of the emergence of molecular markers of resistance in *P. falciparum* [3, 4].

Thus, Plasmepsin X is a relevant target to be investigated in the development of new antimalarial candidates. The selection of this target also provides novelty compared with previous studies that have more commonly used PfLDH or PfDHFR-TS, because Plasmepsin X is not only related to parasite metabolism but also to the mechanisms of parasite invasion and dissemination in the bloodstream [5, 6, 7, 8].

In the context of local biological resources, Togaku oil from Timor Island is a plant-based traditional formulation that is scientifically interesting to investigate. However, this study does not position Togaku oil as the final preparation to be directly tested, but rather as the basis for selecting its constituent plants, whose compounds have been reported in various chemical profiling studies. Several of its constituent plants have compound data based on LC-MS/MS, UPLC-MS, and GC-MS analyses. *Justicia gendarussa* has been reported to contain fatty acids and apigenin glycosides [9]. *Allium cepa* shallot contains secondary and primary metabolites, such as flavonoids, nitrogen-containing compounds, fatty acids, and volatile metabolites, which may serve as a candidate compound library [10]. *Allium sativum* garlic contains phenolic acids, flavonoids, and vitamins in various extracts. In addition, GC-MS analysis of *Cymbopogon citratus* lemongrass has consistently shown the dominance of citral, consisting of geranial and neral, along with β-myrcene, geraniol, and geranyl acetate as major components [11]. Meanwhile, *Lantana camara* has also been reported to contain compounds such as lupeol, phytol, hexadecanoic acid, and caryophyllene oxide, indicating that the plants used in this traditional formulation provide a broad chemical spectrum for computational screening [12]. Therefore, the objects of this study are the reported compounds from the constituent plants of Togaku oil, rather than a direct claim regarding the chemical composition or pharmacological efficacy of Togaku oil as a final product, because formulation processes may affect the presence and concentration of compounds in the final preparation [13].

Although several compounds from the constituent plants of Togaku oil have been reported, studies that specifically map and prioritize these compounds as candidate inhibitors of Plasmepsin X from *P. falciparum* remain limited. Previous studies have applied *in silico* approaches to compounds from the Zingiberaceae family against PfLDH, phytomolecules from *Cymbopogon citratus* against malaria-related targets, and compounds from *Carica papaya* against PfDHFR-TS [14, 15]. However, no study has specifically linked the reported compounds from the constituent plants of Togaku oil from Timor Island with Plasmepsin X as an antimalarial target. Therefore, the study entitled "In Silico Study of Reported Compounds from Togaku Oil Plants from Timor Island as Candidates for *Plampesin X* Inhibitors of *Plasmodium falciparum*" is important to conduct. This study aims to identify the reported compounds from the constituent plants of Togaku oil, evaluate their interactions with Plasmepsin X through molecular docking, analyze binding affinity and molecular interaction patterns, and prioritize the most potential compounds as antimalarial inhibitor candidates based on local natural compounds [7, 8].

RESEARCH METHODS

The target protein used in this study is Plasmepsin X from *Plasmodium falciparum* (PDB code 7TBC), obtained from the RCSB Protein Data Bank (https://www.rcsb.org/structure/7TBC). The structure of this protein was determined by X-ray diffraction at 2.76 Å resolution and is classified as a hydrolase enzyme. The structure of 7TBC is a monomeric protein consisting of 377 amino acid residues and is in complex with the inhibitor ligand WM382 [16]. Before use, the protein structure was prepared in YASARA Structure by adding hydrogen atoms, removing unnecessary water

molecules and ligands, and performing energy minimization to obtain a stable structure. The prepared structure was then saved again in (.pdb) format for use in the next analysis stage [17].

The quality of the prepared Plasmepsin X protein structure (PDB ID: 7TBC) was then evaluated using the Ramachandran Plot server (https://ramplot.in/) to assess its validity. Next, the binding pocket prediction was performed using the COACH server (https://zhanggroup.org/COACH/). The prepared 7TBC protein structure was then uploaded to the server to identify amino acid residues with potential ligand-binding sites [18].

The list of bioactive compounds used as ligands was obtained from various literature related to the secondary metabolite content of Togaku rheumatic oil plants from Tune Village, Tobu District, South Central Timor Regency, NTT. The compounds used in this study include oleanane, dammarane, terpenoids, steroids, hopane, apigenin, anthocyanins, chlorogenic acid, shogaols, gingerols, paradols, triterpenoids, farnesol, ferulic acid, zingerone, pinene, citral, myrcene, gallic acid, and hydroxybenzoic acid. In contrast, artemisinin was used as a positive control [9, 10, 11, 12]. The three-dimensional (3D) structure of each ligand was downloaded from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/) in (.sdf) format. Furthermore, the ligand structure was prepared using YASARA Structure software, which was performed via an energy minimization process to obtain a stable geometry. Before this process, a clean-all operation is performed to add hydrogen atoms to the ligand structure. The prepared ligand structure is then saved in (*.sdf) format for use in the next molecular docking stage.

Grid box validation was performed to ensure that the docking parameters accurately reproduced the ligand's position in the protein's active pocket. The validation process was carried out using the redocking method: the native ligand WM382 was separated from the Plasmepsin X protein structure (PDB ID: 7TBC), then redocked into the protein's active pocket using YASARA Structure software. The grid box determination was based on the coordinates of the native ligand in the protein's active pocket. The validation process was carried out with 999 repetitions. The validation results were assessed based on the Root Mean Square Deviation (RMSD) value between the redocked ligand position and the crystallographic ligand position. The grid box parameters were considered valid if they produced an RMSD value ≤ 2.0 Å [19].

After the grid box parameters were validated, the molecular docking process was performed between the target protein Plasmepsin X (PDB ID: 7TBC) and all test ligands using YASARA Structure software using the AMBER14 force field [20]. The docking process was performed 100 times for each ligand. The docking results were analyzed based on the binding energies calculated by YASARA Structure. Docking outcomes were ranked according to YASARA's internal scoring algorithm, in which more positive scores indicate stronger predicted ligand–protein binding within the software framework [20]. Because this scoring system differs from the conventional thermodynamic interpretation commonly used in molecular docking, where lower (more negative) binding free energy indicates more favorable and stable interactions. The YASARA scores were used primarily for comparative ligand ranking, while interaction stability was interpreted in the context of established thermodynamic principles. Analysis of the interaction between the ligand and amino acid residues in the protein's active pocket was performed using Discovery Studio Visualizer for two-dimensional interaction visualization and PyMOL for three-dimensional visualization of the complex structure.

RESULTS AND DISCUSSION

Before molecular docking analysis, a protein structure must undergo preparation to obtain a stable model suitable for molecular interaction studies. The Plasmepsin X protein structure (PDB ID: 7TBC) was prepared using YASARA Structure software by adding hydrogen atoms,

removing unnecessary water molecules and ligands, and performing energy minimization to obtain a more stable protein conformation.

After preparation, the quality of the resulting protein structure was evaluated to ensure the protein model had good geometry and was suitable for molecular docking. The quality evaluation of the Plasmepsin X protein structure was performed using Ramachandran plot analysis (Figure 1) to assess the distribution of dihedral angles (φ) and (ψ) of amino acid residues. Figure 1A shows that most residues are located in favored regions, a few in allowed regions, and no residues in disallowed regions. This indicates that the protein structure has a stable conformation. The 3D visualization in Figure 1B shows a concentrated density of residues in specific regions, indicating no significant geometric deviations. Furthermore, the distribution by residue type in Figure 1C shows a pattern consistent with each residue's characteristics, such as glycine's high flexibility and proline's conformational constraints. Overall, the analysis results indicate that the Plasmepsin X protein structure is of high quality and suitable for molecular docking.

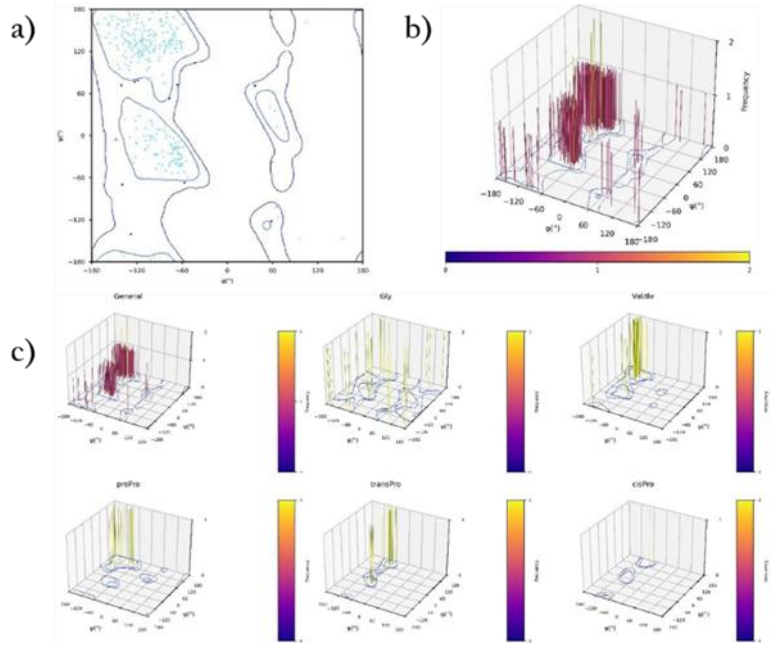

Figure 1. Evaluation of the quality of the Plasmepsin X protein structure (PDB ID: 7TBC) using Ramachandran plot analysis: (a) 2D Ramachandran plot showing the distribution of dihedral angles φ and ψ, with turquoise, blue, and red dots indicating favored, allowed, and outlier regions, respectively; (b) standard 3D Ramachandran plot; (c) 3D Ramachandran plot based on different amino acid residue categories. The vertical bars on the z-axis indicate the frequency of the torsion angle distribution.

The three-dimensional structure of the Plasmepsin X protein (PDB ID: 7TBC) bound to the native ligand WM382 is shown in **Figure 2a**. This visualization shows the location of the protein's active site, which serves as a reference in the molecular docking process. The presence of the ligand in the crystal structure helps identify important amino acid residues involved in the ligand-binding interaction. Furthermore, to confirm the protein's active site, cavity analysis was performed using the COACH server. Prediction of candidate ligand-binding sites on the target protein provides essential information regarding potential regions for ligand interaction and binding orientation [21]. The cavity analysis results (**Figure 2b**) revealed a prominent active pocket on the surface of Plasmepsin X with structural dimensions and geometry suitable for ligand accommodation. Potential binding residues within this pocket were identified as ILE72, VAL98, ALA99, GLY100, PHE173, VAL174, ALA175, LEU192, GLU193, MET194, GLU195, SER217,

ASP218, and SER227. These residues collectively form a binding environment composed of hydrophobic, polar, and charged amino acids that may facilitate ligand recognition, stabilization, and specificity through hydrophobic interactions, hydrogen bonds, van der Waals forces, and electrostatic contacts. Notably, several key residues such as VAL98, ALA99, GLY100, PHE173, GLU193, and ASP218 are likely to play important roles in ligand orientation and complex stability within the active pocket. Furthermore, the predicted cavity overlapped with the binding position of the native ligand WM382, supporting the validity of the selected docking region and indicating that the identified pocket represents a biologically relevant binding site for molecular docking analysis.

Grid box validation was then performed using the redocking method to ensure the accuracy of the docking parameters. The validation results showed an RMSD value of 0.2629 Å (**Figure 2c**), which is below the acceptable limit of ≤ 2.0 Å. The low RMSD value indicates that the ligand position obtained by redocking is very close to the crystallographic ligand position, so the grid box parameters used are considered valid and can be used for subsequent molecular docking [22].

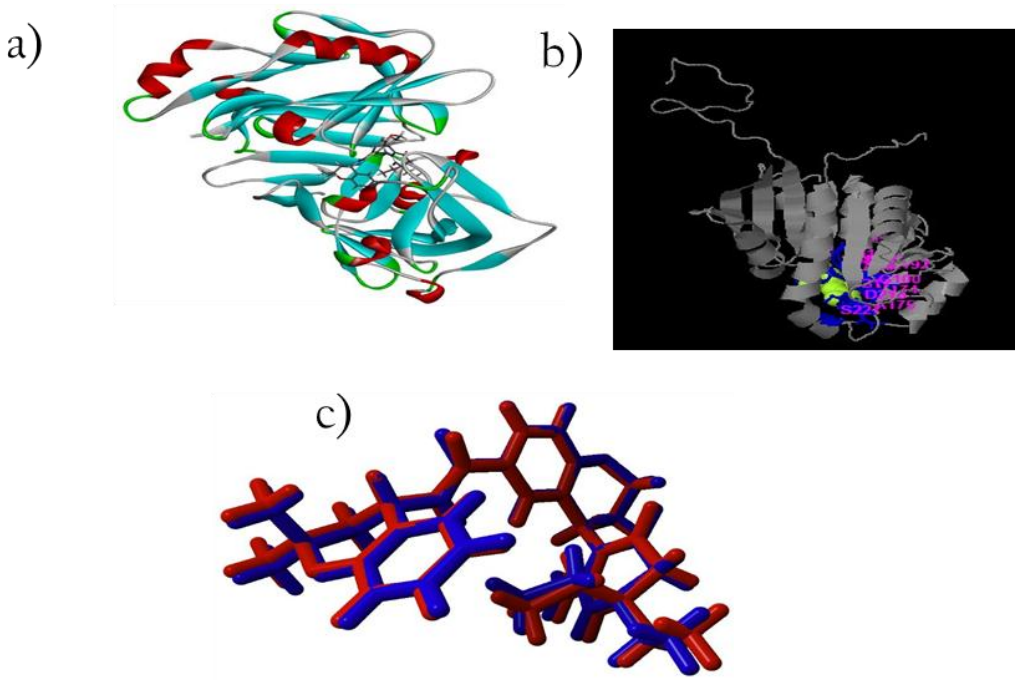

Figure 2. Protein structure visualization and binding site determination of Plasmepsin X (PDB ID: 7TBC): (a) Three-dimensional structure of the protein bound to the native ligand WM382; (b) Prediction of the binding site (cavity) using the COACH server; (c) Grid box validation using the redocking method, where the red color indicates the position of the ligand before docking and the blue color indicates the position of the ligand after docking.

Molecular docking analysis was performed to assess the ligand's ability to interact with the active site of the Plasmepsin X protein (PDB ID: 7TBC) [23]. The docking process yields binding energy values used to predict the strength and stability of the ligand-target protein interaction. Output in YASARA software: a more positive binding energy value indicates a stronger binding affinity and a more stable complex. In addition, docking results were visualized to identify the type of interaction between the ligand and amino acid residues in the protein's active pocket. The results of the molecular docking analysis, presented as binding energy values, are shown in Table 1.

Table 1. Binding energies and interacting residues of ligands docked with Plasmepsin X (PDB ID: 7TBC)

No	Name of Ligan (kcal/mol)	Bind. Energy	Contacting receptor residues
1	Artemisin (K+)	8.428	SER246, GLN247, ILE264, ASP266, PHE311, SER313,
2	Oleanane	11.879	ASP245, SER246, GLN247, ILE264, ASP266, SER269,
3	Dammarane	8.930	SER246, GLN247, ILE264, ASP266, GLY268, SER269, ILE309, PHE311, GLY312, SER313, ILE316, ILE354, PHE355, ILE358, PHE360, ILE363, MET371, TYR431, ASP457, GLY459, THR460, SER461, MET526
4	Luteone	8.533	ILE264, ASP266, GLY268, SER269, ILE309, PHE311, GLY312, SER313, ILE316, ILE354, PHE355, ILE358, PHE360, ILE363, MET371, TYR431, ASP457, GLY459, THR460, SER461
5	Steroid	8.410	GLN247, ILE264, ASP266, GLY268, SER269, ILE309, VAL310, PHE311, GLY312, ILE316, ILE354, PHE355, ILE358, PHE360, ILE363, MET371, TYR431, GLY459, THR460, PRO531
6	Hopane	8.403	SER246, GLN247, ILE264, ASP266, GLY268, SER269, PHE311, GLY312, SER313, ILE354, ILE358, TYR431, ASP457, GLY459, THR460, SER461, ILE528, VAL530, LEU539
7	Apigenin	8.324	ILE264, SER269, ASN271, TRP273, ILE309, PHE311, ILE316, ILE354, PHE355, ILE358, PHE360, ILE363, MET371, SER373, GLY459
8	Antocianin	8.301	A GLN247, A ILE264, A SER269, A ILE309, A PHE311, A SER313, A ILE316, A ILE354, A PHE355, A ILE358, A PHE360, A ILE363, A GLY459, A THR460, ASER461
9	Chlorogenic acid	8.299	ILE264, SER269, THR270, ASN271, TRP273, ILE309, PHE311, SER313, ILE316, ILE354, PHE355, ILE358, PHE360, ILE363, MET371, SER373, GLY459, THR460, SER461, TYR462, MET526
10	shogaols	7.591	LEU240, SER246, GLN247, PHE248, ILE264, PHE265, PHE311, ILE316, ILE354, PHE355, ILE358, PHE360, ILE363, PHE396, ILE398, THR458, GLY459, THR460, SER461, SER542
11	Gingerols	7.411	SER246, GLN247, PHE248, ILE264, ASP266, SER269, TRP273, ILE309, PHE311, SER313, ILE316, ILE354, PHE355, ILE358, PHE360, ILE363, THR458, GLY459, THR460, SER461, SER542
12	Paradols	7.466	SER246, GLN247, PHE248, ILE264, PHE265, ASP266, SER269, TRP273, ILE309, PHE311, ILE316, ILE354, PHE355, ILE358, PHE360, ILE363, THR458, GLY459, THR460, SER461, SER542
13	Triterpenoid	6.976	GLY268, VAL310, PHE311, GLY312, ASN347, TYR431, ILE455, ASP457, THR460, THR464, GLN527, ILE528, ASP529, VAL530, PRO531, LEU539

14	Farnesol	6.976	SER246, GLN247, PHE248, ILE264, PHE265, ASP266, PHE311, SER313, ILE316, ILE354, PHE355, ILE358, PHE360, ILE363, THR458, GLY459, THR460, SER461, SER542
15	Ferullic acid	6.744	LEU240, SER246, GLN247, PHE248, ILE264, PHE265, ILE354, ILE358, PHE396, THR458, GLY459, THR460, SER461, SER542
16	Zingerone	6.278	A SER246, A GLN247, A PHE248, A ILE264, A PHE265, A PHE311, A ILE354, A PHE355, A ILE358, A PHE360, A THR458, A GLY459, A THR460, A SER461, A SER542, A LEU543
17	Pinene	6.221	ILE264, SER269, ILE309, PHE311, ILE316, ILE354, PHE355, PHE360, ILE363, GLY459
18	Citral	6.140	A SER246, A GLN247, A PHE248, A ILE264, A PHE311, A ILE316, A ILE354, A PHE355, A ILE358, A PHE360, A ILE363, A THR458, A GLY459, A THR460, ASER461, A SER 542
19	Myrcene	5.985	LEU240, SER246, GLN247, PHE248, ILE264, PHE265, PHE396, ILE398, THR458, GLY459, THR460, SER461, SER542
20	Gallic acid	5.372	SER246, GLN247, PHE248, ILE264, PHE265, THR458, GLY459, THR460, SER461, SER542, LEU543
21	Hexadecenoic acid	5.131	SER246, GLN247, PHE248, ILE264 PHE265, THR458, THR460, SER461, SER542, LEU543

Docking results show that Oleanane and Dammarane ligands have the most positive binding energy (-11,879 and -8,930 kcal/mol), indicating high affinity to Plasmepsin X. The main interactions occur through hydrophobic and aromatic residues such as PHE311, ILE316, ILE354, PHE355, ILE358, PHE360, as well as polar residues SER246, GLN247, SER269, SER313, THR460, which play a role in stabilizing the complex through hydrogen bonds and hydrophobic interactions. Smaller and simpler ligands, such as Gallic acid, show weaker binding energy due to fewer residue contacts. These results identify Oleanane and Dammarane compounds as potential inhibitor candidates for Plasmepsin X. Visualization of ligand-protein interactions is presented in **Figure 3**.

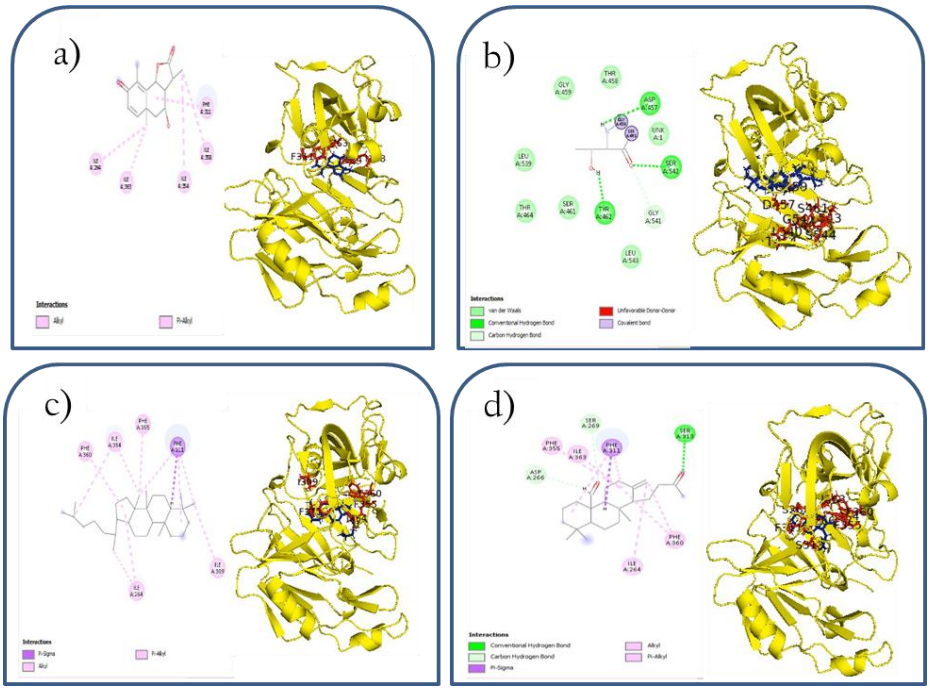

Figure 3. 2D and 3D visualization of selected Plampesin X-ligand complexes using Discovery Studio (2D) and PyMol (3D): (a) Plampesin X-artemisinin complex (positive control); (b) Plampesin X-Oleanane complex; (c) Plampesin X-Dammarane complex; and (d) Plampesin X-Luteone complex. The blue stick represents the ligand, and the red stick represents the residues interacting with the ligand while the yellow stick represents the structure of Plampesin X

In all complexes, the ligands (blue) are located within the active pocket of the protein (yellow) and interact with critical residues (red). In **Figure 3A**, the artemisinin complex, used as a positive control, shows stable interactions in the active site, dominated by hydrophobic interactions involving alkyl and π-alkyl bonds. Furthermore, in **Figure 3B**, the oleanane ligand is dominated by noncovalent interactions, including van der Waals, conventional hydrogen bonds, and carbon-hydrogen bonds, which help maintain complex stability. In addition, covalent interactions that strengthen ligand binding are identified, as are unfavorable donor-donor interactions that have the potential to reduce complex stability. In **Figure 3C**, the dammarane ligand shows a dominance of hydrophobic interactions that support complex stability in the active pocket of the protein. Meanwhile, in Figure 3D, the luteone ligand adopts a similar binding orientation, involving a combination of hydrophobic interactions and hydrogen bonds. Overall, these results indicate that all selected ligands bind stably to the active pocket of Plasmepsin X and have the potential to serve as inhibitor candidates.

CONCLUSION

Based on in silico studies, compounds reported from Togaku oil plants show potential as candidate inhibitors of *Plasmodium falciparum* Plasmepsin X. Molecular docking results indicate that oleanane and dammarane have higher binding energies than artemisinin as the positive control, suggesting stronger binding affinity and a more stable complex. The interaction of ligands with the protein's active residues is dominated by hydrophobic interactions and hydrogen bonds, which stabilize the protein-ligand complex. Visualization of 2D and 3D interactions also shows that the selected ligands bind stably to the protein's active pocket. Therefore, triterpenoid compounds, especially oleanane and dammarane, have the potential to serve as candidate inhibitors of Plasmepsin X and warrant further study through in vitro and in vivo tests.

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