



In Silico Study of Bioactive Compounds from Faloak Stem Bark (*Sterculia quadrifida* R. Br.) Against Estrogen Receptor Alpha as Potential Breast Anticancer Agents

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Abstract

Estrogen receptor alpha (ER α) is an important therapeutic target in hormone-dependent breast cancer, prompting the investigation of natural compounds with potential receptor-binding activity. This study aimed to evaluate the binding affinities and molecular interaction profiles of six bioactive compounds reported in Faloak (*Sterculia quadrifida* R. Br.) stem bark against ER α . Ligand structures were retrieved from PubChem, while the three-dimensional structure of ER α was obtained from the Protein Data Bank (PDB ID: 3ERT). Molecular docking was performed using PyRx version 0.8, and selected binding poses were analyzed using BIOVIA Discovery Studio Visualizer. The co-crystallized ligand, 4-hydroxytamoxifen, was used as the reference ligand. The docking scores of the tested compounds ranged from -7.1 to -8.6 kcal/mol, compared with -9.5 kcal/mol for 4-hydroxytamoxifen. Catechin-4-ol 3-O- α -L-rhamnopyranoside exhibited the most favorable docking score among the tested compounds and formed interactions with Glu353, Leu387, Met343, Leu525, Met421, Phe404, and Leu391. The observed hydrogen-bonding and hydrophobic interactions showed similarities to the interaction profile of the reference ligand, supporting the prioritization of this compound for further investigation. These findings identify catechin-4-ol 3-O- α -L-rhamnopyranoside as a promising computational candidate for further ER α -targeted research. However, molecular docking alone cannot establish receptor antagonistic activity or anticancer efficacy. Further molecular dynamics simulations and experimental studies are required to evaluate binding stability, biological activity, safety, and potential therapeutic relevance in breast cancer.

INTRODUCTION

Breast cancer is a malignant disease characterized by the uncontrolled proliferation of cells within breast tissue. The classification of breast cancer is generally determined by the type of breast cells undergoing malignant transformation (Feng et al., 2018). According to the latest GLOBOCAN report, breast cancer accounted for approximately 2.31 million new cases worldwide in 2022 and remains one of the leading causes of cancer-related mortality among women globally (Bray et al., 2024). Despite significant advances in diagnosis and treatment, breast cancer continues to represent a major public health challenge because of its high incidence and mortality. One of the most widely used therapeutic strategies for hormone-dependent breast cancer involves targeting estrogen signaling pathways.

Estrogen receptor alpha (ER α) is a nuclear hormone receptor that plays a crucial role in regulating cell proliferation, differentiation, and survival in breast tissue (Qi et al., 2002; Mutiah et al., 2021; Purwani et al., 2021). According to Mutia et al. (2020), overexpression or aberrant activation of ER α has been strongly associated with the development and progression

of breast cancer, making this receptor an important molecular target in anticancer drug discovery. Tamoxifen, a selective estrogen receptor modulator (SERM), has long been used as a standard endocrine therapy for ER α -positive breast cancer. Tamoxifen exerts its therapeutic effects through competitive binding to estrogen receptors and predominantly antagonizes estrogen signaling in breast tissue, thereby inhibiting estrogen-mediated tumor growth. However, despite its clinical effectiveness, tamoxifen exhibits partial agonist activity in endometrial tissue. This property has been associated with an increased risk of endometrial hyperplasia and endometrial cancer following prolonged use (Hamid et al., 2021). Consequently, the identification of novel ER α -targeting compounds with favorable efficacy and safety profiles remains an important objective in breast cancer research.

Natural products have attracted considerable attention as valuable sources of novel therapeutic agents because of their structural diversity and broad range of biological activities. Indonesia, recognized as a megadiverse country, possesses a rich variety of medicinal plants that have long been used in traditional medicine. The use of medicinal plants represents an important component of indigenous knowledge that has been passed down through generations among Indonesian communities, including those in East Nusa Tenggara (NTT). This traditional practice is supported by the diversity of medicinal plant species found in NTT, particularly on Timor Island (Matheus, 2019). Among these plants, Faloak (*Sterculia quadrifida* R. Br.) is considered a promising medicinal species with potential pharmacological applications.

Faloak (*Sterculia quadrifida* R. Br.) is an indigenous plant widely distributed in NTT, particularly on Timor Island. For generations, local communities have traditionally used Faloak stem bark to manage various diseases and health conditions. Ethnomedicinal reports indicate that Faloak bark has been used for its antimicrobial, antimalarial, hepatoprotective, and anti-inflammatory properties, as well as for enhancing stamina and managing gastrointestinal disorders and lower back pain (Siswadi et al., 2016; Tenda et al., 2017). According to Saragih and Siswadi (2019), flavonoids are predominant constituents of Faloak stem bark and exhibit strong antioxidant activity, highlighting their potential as natural antioxidant agents. Furthermore, flavonoids have been reported to exert protective effects against various diseases, including cardiovascular disorders, cancer, and other degenerative conditions (John et al., 2014; Ojha et al., 2018). Internationally, *S. quadrifida* is known as the orange-fruited kurrajong and has traditionally been used by Aboriginal communities in Australia for wound healing, mosquito-repellent applications, eye infections, and insect bites (Riwu et al., 2022).

Several studies have highlighted the medicinal potential of Faloak because of its diverse secondary metabolites and associated biological activities. In addition to its traditional uses, Faloak has demonstrated antioxidant properties that may be relevant to the investigation of degenerative diseases, including diabetes mellitus, hepatitis, and cancer (Darojati et al., 2022). The presence of these bioactive constituents makes Faloak an attractive candidate for further investigation in drug discovery and development. Meanwhile, advances in computational approaches have accelerated the early stages of drug discovery. Among these approaches, *in silico* methods have become increasingly important for predicting potential compound–target interactions and prioritizing candidate molecules for subsequent experimental investigation.

Molecular docking is a commonly employed computational technique in virtual screening and structure-based drug discovery (Ethica, 2019). It enables researchers to predict the preferred binding pose of a ligand within a receptor-binding site and estimate ligand–

receptor interactions using docking scores or predicted binding affinities (Zhang et al., 2022). More favorable docking scores, which are often represented by more negative values, may indicate stronger predicted ligand–target interactions within a given docking protocol (Naufa et al., 2022). Molecular docking can also provide information about amino acid residues involved in ligand binding, thereby facilitating the identification of potentially important molecular interactions. However, docking results represent computational predictions and do not independently establish binding stability, receptor modulation, or biological activity.

Despite growing evidence supporting the pharmacological potential of Faloak, studies investigating the interactions of its bioactive compounds with estrogen receptor alpha remain limited. Therefore, this study aimed to evaluate the predicted binding affinities and molecular interaction profiles of selected bioactive compounds from Faloak stem bark against ER α using molecular docking. The findings are expected to provide preliminary computational evidence for prioritizing Faloak-derived compounds for further investigation as potential ER α -targeting candidates in breast cancer research.

METHOD

Ligand Preparation

The ligands used in this study were selected bioactive compounds identified from the stem bark of Faloak (*S. quadrifida*), namely (+)-catechin 7-O-beta-D-xyloside, catechin-4-ol 3-O-alpha-L-rhamnopyranoside, epicatechin 5-O-beta-D-glucopyranoside-3-benzoate, icaceine, procyanidin C1, and quercetin 7-rhamnoside. Three-dimensional structures of all ligands were retrieved from the PubChem database (<https://pubchem.ncbi.nlm.nih.gov>) and downloaded in Structure Data File (.sdf) format. The selected compounds were chosen based on their reported occurrence in Faloak stem bark and their potential biological activities.

Protein Preparation

The target macromolecule employed in this study was Estrogen Receptor Alpha (ER α), a protein closely associated with the development and progression of hormone-dependent breast cancer. The crystal structure of ER α was obtained from the Protein Data Bank (PDB) under accession code 3ERT. The protein structure was downloaded in Protein Data Bank (.pdb) format. Protein preparation was conducted prior to molecular docking to ensure the accuracy of ligand–receptor interaction predictions. The preparation process included the removal of water molecules and separation of the co-crystallized native ligand from the receptor structure. The prepared protein structure was subsequently used as the docking receptor.

Molecular Docking Simulation

Molecular docking simulations were performed using PyRx version 0.8. The docking process involved the interaction between each test ligand and the prepared ER α receptor. Multiple binding conformations (poses) were generated during docking, and the most favorable pose was selected based on the lowest binding free energy (ΔG).

Binding affinity values obtained from docking simulations were used as indicators of ligand–receptor interaction strength. More negative binding energy values indicate stronger and more stable interactions between the ligand and receptor.

Interaction Analysis

The best docking poses obtained from PyRx were further analyzed using BIOVIA Discovery Studio Visualizer. Both two-dimensional (2D) and three-dimensional (3D)

interaction analyses were conducted to identify amino acid residues involved in ligand binding and to characterize the types of molecular interactions formed, including hydrogen bonds and hydrophobic interactions.

RESULTS AND DISCUSSION

Structural Characteristics of Estrogen Receptor Alpha

The Estrogen Receptor Alpha (ER α) structure used in this study consisted of a single protein chain (Chain A) and contained a co-crystallized native ligand, namely 4-hydroxytamoxifen. The presence of a native ligand is particularly important in molecular docking studies because it serves as a reference for evaluating ligand binding orientation and validating docking results. In addition, the ER α crystal structure exhibited a resolution of 1.90 Å. According to structural biology standards, protein structures with crystallographic resolutions below 2.0 Å are generally considered suitable for molecular docking studies because they provide a highly accurate representation of atomic coordinates within the active site (Sarmoko et al., 2023). Therefore, the selected ER α structure was deemed appropriate for investigating the binding behavior of Faloak-derived compounds.

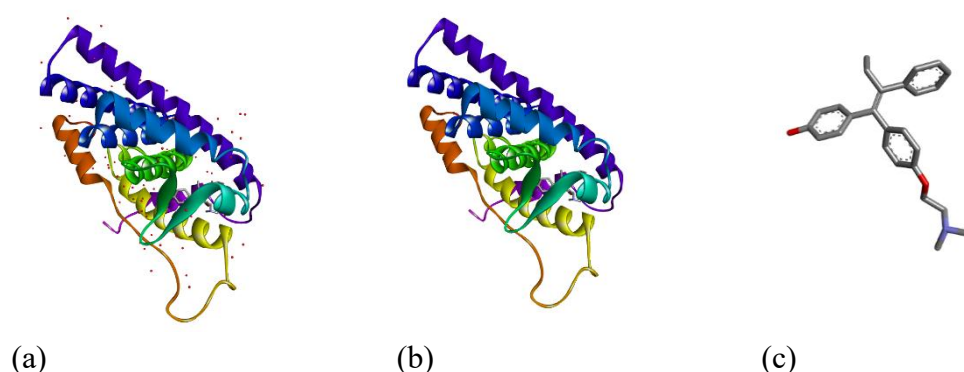


Figure 1. Three dimensional structures of the target protein and native ligand. (a) Protein structure prior to preparation; (b) protein structure after preparation; (c) native ligand 4-hydroxytamoxifen.

Molecular Docking Analysis

Molecular docking generated several binding poses representing potential interactions between the ligands and amino acid residues of the target protein. The best pose was selected based on the lowest (most negative) binding affinity value, as this indicates a more stable interaction between the ligand and the receptor. The selected pose of each ligand was subsequently analyzed using BIOVIA Discovery Studio Visualizer to evaluate the interaction profile. The analyzed parameters included binding affinity values and the types of interactions formed between the ligands and amino acid residues of the receptor. The results of the binding affinity and amino acid residue interaction analyses are presented in the following table.

Table 1. Results of molecular docking of faloak plant compounds with receptors

Ligand	Binding Energy (ΔG) (kcal/mol)	Amino Acid Interactions
4-hydroxytamoxifen	-9,5	Met421, Leu384, Leu 525, Phe 404, Met388, Leu391, Leu346, Glu353, Leu349, Leu387, Ala350, Met343.
(+)-catechin 7-O-beta-D-xyloside	-7,6	Glu353, Met343, Leu525, Leu346, Ala350, Arg394.
catechin-4-ol 3-O-alpha-L-rhamnopyranoside	-8,6	Leu387, Glu353, Met343, Leu525, Met421, Phe404, Leu391, Trp383.
epicatechin 5-O-beta-D-glucopyranoside-3-benzoate	-7,6	Met421, Met388, Leu346, Leu387, Trp383, Ala350, Leu525, Asp351.
icaceine	-7,9	Leu525, Trp383.
procyanidin C1	-8,2	Glu380, Thr460, Leu525, Tyr526, Met522, Asn519, Cys381.
quercetin 7-rhamnoside	-7,1	Leu387, Met388, Arg394, Leu384, Ala350, Leu346, Leu525, Met522, Met343, Thr347.

Receptors and ligands interact selectively based on the binding energy generated during ligand-receptor complex formation. A ligand with a lower binding energy is generally considered to have greater potential due to its stronger affinity for the target receptor. Binding energy represents the energy associated with the interaction between a ligand and its target receptor (Wulandari et al., 2023). Based on the molecular docking results, the native ligand, 4-hydroxytamoxifen, exhibited a substantially lower binding free energy than the six compounds isolated from faloak, with a value of -9.5 kcal/mol. The binding free energy values of the tested faloak compounds were as follows: (+)-catechin 7-O- β -D-xyloside (-7.6 kcal/mol), catechin-4-ol 3-O- α -L-rhamnopyranoside (-8.6 kcal/mol), epicatechin 5-O- β -D-glucopyranoside-3-benzoate (-7.6 kcal/mol), icaceine (-7.9 kcal/mol), procyanidin C1 (-8.2 kcal/mol), and quercetin 7-rhamnoside (-7.1 kcal/mol). Among these compounds, catechin-4-ol 3-O- α -L-rhamnopyranoside demonstrated the most favorable interaction with estrogen receptor alpha (ER α), as indicated by its relatively low binding free energy compared with the other five tested compounds. Furthermore, its binding free energy value was the closest to that of the native ligand. These findings suggest that bioactive compounds from faloak possess promising potential as candidates for breast cancer therapeutic agents.

Analysis of Amino Acid Residue Interactions

Visualization of docking results was performed using Discovery Studio Visualizer to investigate the molecular interactions established between each ligand and ER α . Interaction analysis provides valuable information regarding ligand stabilization within the receptor binding pocket and may contribute to the prediction of biological activity.

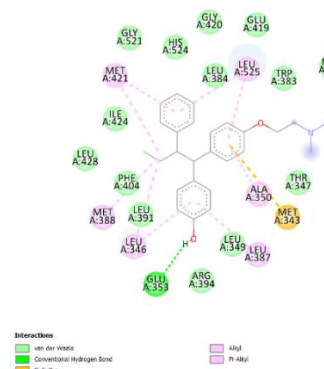
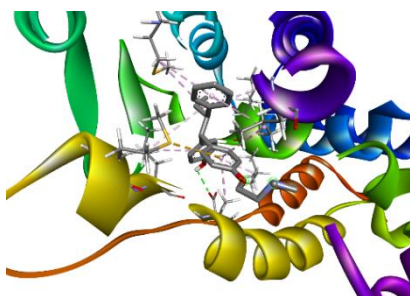


Figure 2. 4-hydroxytamoxifen best interacts with ER α

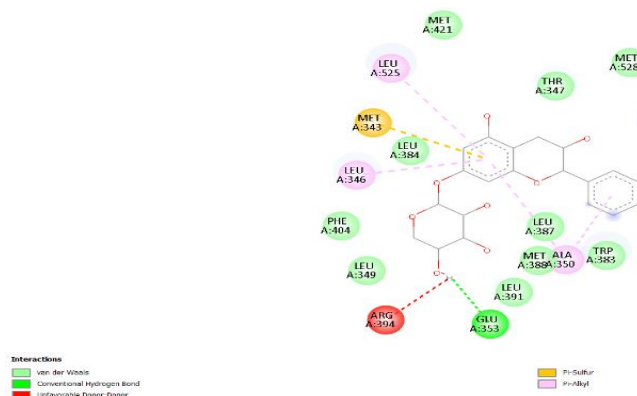
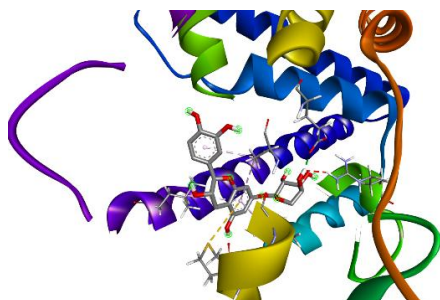


Figure 3. (+)-catechin 7-O-beta-D-xyloside best interacts with ER α

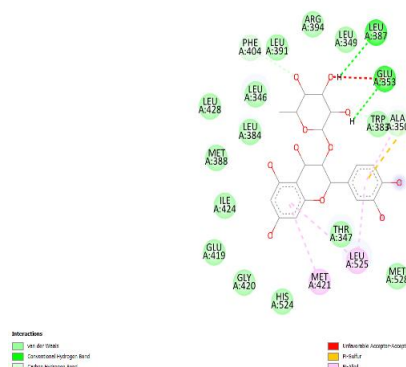
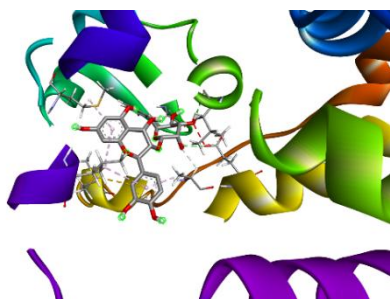


Figure 4. catechin-4-ol 3-O-alpha-L-rhamnopyranoside best interacts with ER α

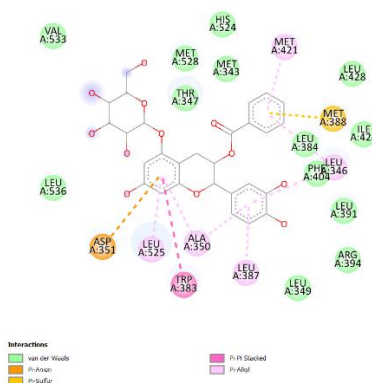
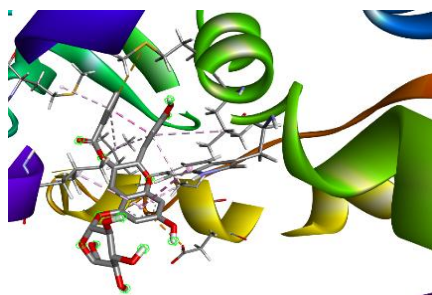


Figure 5. epicatechin 5-O-beta-D-glucopyranoside-3-benzoate best interacts with ER α

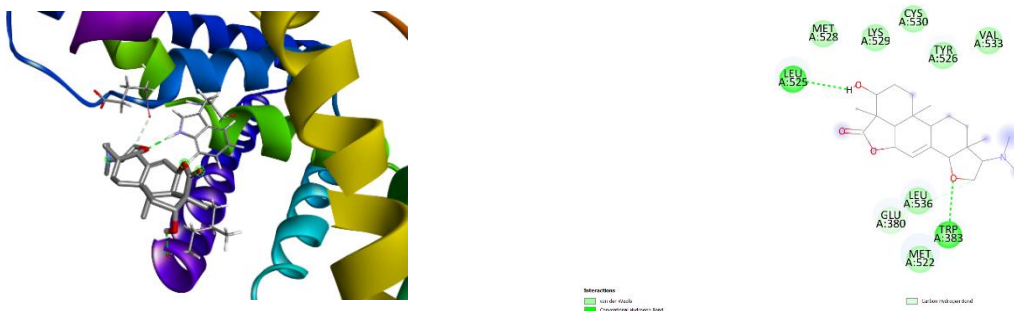


Figure 6. icaceine best interacts with ER α



Figure 7. procyanidin C1 best interacts with ER α



Figure 8. quercetin 7-rhamnoside best interacts with ER α

Visualization of amino acid residue interactions (Figures 2–8) was performed to examine the molecular docking results, particularly the interactions between estrogen receptor alpha (ER α) and the test ligands derived from faloak (*S. quadrifida*) compounds. The chemical interactions formed during molecular docking can be used as indicators of the stability of the ligand–receptor complex. Furthermore, similarities in the interaction patterns between the test ligands and the native ligand within the target receptor suggest that the active compounds may possess inhibitory activity with strong binding affinity toward the receptor (Shofi, 2021).

Based on the molecular docking results presented in the table, the interactions between the tested compounds and ER α were predominantly hydrophobic, accompanied by several hydrogen bond interactions involving specific amino acid residues. Hydrogen bonds were observed for (+)-catechin 7-*O*- β -D-xyloside and catechin-4-ol 3-*O*- α -L-rhamnopyranoside through the residue Glu353, as well as for quercetin 7-rhamnoside through Arg394. Glu353 is recognized as a key residue within the ER α binding pocket because it plays an important role in stabilizing the ligand–receptor complex through hydrogen bond formation. In addition, several compounds also interacted with Ala350, which contributes to the stability of ligand binding within the receptor active site.

Hydrophobic interactions were generally observed with residues Leu346, Leu387, Leu525, Met343, Met388, and Met421. The similarity of binding residues between the tested compounds and the native ligand, 4-hydroxytamoxifen, indicates a comparable interaction pattern within the ER α binding pocket. (+)-Catechin 7-*O*- β -D-xyloside exhibited interaction similarities with the native ligand at residues Glu353, Met343, Leu346, Ala350, and Leu525. Likewise, catechin-4-ol 3-*O*- α -L-rhamnopyranoside showed similar interactions at residues Leu387, Glu353, Met343, Leu525, Met421, Phe404, and Leu391. These similarities suggest that both compounds may possess favorable binding affinity toward ER α .

Epicatechin 5-*O*- β -D-glucopyranoside-3-benzoate interacted with residues Met421, Met388, Leu346, Leu387, Trp383, Ala350, and Leu525, most of which are hydrophobic residues located within the receptor binding pocket. In contrast, icaceine interacted only with Leu525 and Trp383, resulting in a lower number of interactions compared with the other compounds. A lower number of interactions may affect the stability of the resulting ligand–receptor complex. Unlike the other compounds, procyanidin C1 exhibited an interaction pattern involving residues outside the major ER α binding pocket, namely Glu380, Thr460, Tyr526, Met522, Asn519, and Cys381. This finding suggests that the binding position of procyanidin C1 may not be fully located within the principal binding pocket of the receptor. Meanwhile, quercetin 7-rhamnoside interacted with residues Leu387, Met388, Arg394, Leu384, Ala350, Leu346, Leu525, Met522, Met343, and Thr347. The interactions with Arg394 and Ala350 indicate the potential contribution of both polar and hydrophobic interactions to the stabilization of the ligand–receptor complex.

Comparison of Interaction Patterns with the Native Ligand

Most of the tested compounds exhibited interaction patterns similar to those of the native ligand, 4-hydroxytamoxifen, particularly at residues Glu353, Leu346, Ala350, Leu387, and Leu525. These similarities indicate that the compounds derived from *S. quadrifida* may bind within the ER α binding pocket and therefore have potential for development as breast cancer therapeutic candidates targeting estrogen receptor alpha inhibition. According to Rahmadani et al. (2024), the presence of hydrogen bond interactions with residues Glu353 or Arg394 is indicative of antagonistic activity against ER α . Hydrophobic interactions also suggest that the compounds possess the ability to penetrate biological membranes, thereby facilitating effective binding to ER α . In addition, π -sigma interactions, including π -alkyl and π -sulfur interactions, contribute to strengthening ligand binding within the receptor binding site (Ruswanto et al., 2024). Test ligands are predicted to exhibit strong binding affinity toward the target receptor when they are capable of forming hydrogen bonds and interacting with amino acid residues located in the receptor active site. The strength of these interactions can be evaluated by comparing the amino acid residue interaction patterns of the test ligands with those of the native ligand. Similarities in the amino acid residues involved in ligand–receptor interactions indicate the potential of the ligands to exert effective receptor inhibition (Iktiarani et al., 2024). Therefore, compounds derived from *S. quadrifida* may serve as promising candidates for breast cancer therapy due to their similarities in amino acid interaction profiles with the native ligand.

CONCLUSION

This study demonstrated that selected bioactive compounds from Faloak (*Sterculia quadrifida* R. Br.) stem bark exhibited favorable predicted interactions with estrogen receptor

alpha (ER α), an important molecular target in hormone-dependent breast cancer therapy. Among the investigated compounds, catechin-4-ol 3-O- α -L-rhamnopyranoside exhibited the most favorable docking score (–8.6 kcal/mol) and showed similarities in its interaction profile to the co-crystallized ligand, 4-hydroxytamoxifen. The compound interacted with several amino acid residues within the ER α binding site, including Glu353, Leu387, Met343, Leu525, Met421, Phe404, and Leu391.

Overall, the findings suggest that bioactive compounds derived from Faloak stem bark, particularly catechin-4-ol 3-O- α -L-rhamnopyranoside, represent promising computational candidates for further investigation as ER α -targeting compounds. However, molecular docking alone cannot establish receptor antagonism or anticancer efficacy. Further molecular dynamics simulations and experimental studies are required to evaluate binding stability, receptor-modulatory activity, biological efficacy, safety, and potential therapeutic relevance in breast cancer.

REFERENCES

- Bray, F., Laversanne, M., Sung, H., Ferlay, J., Siegel, R. L., Soerjomataram, I., & Jemal, A. (2024). Global cancer statistics 2022: GLOBOCAN estimates of incidence and mortality worldwide for 36 cancers in 185 countries. *CA: A Cancer Journal for Clinicians*, 74(3), 229–263. <https://doi.org/10.3322/caac.21834>
- Darojati, U. A., Murwanti, R., & Hertiani, T. (2022). *Sterculia quadrifida* R. Br.: A comprehensive review of ethnobotany, phytochemistry, pharmacology and toxicology. *JPSCR: Journal of Pharmaceutical Science and Clinical Research*, 7(1), 1. <https://doi.org/10.20961/jpscr.v7i1.52244>
- Ethica, S. N. (2019). *Pengantar bioinformatika untuk mahasiswa laboratorium medis*. Deepublish.
- Feng, Y., Spezia, M., Huang, S., Yuan, C., Zeng, Z., Zhang, L., Ji, X., Liu, W., Huang, B., Luo, W., Liu, B., Lei, Y., Du, S., Vuppapalapati, A., Luu, H. H., Haydon, R. C., He, T. C., & Ren, G. (2018). Breast cancer development and progression: Risk factors, cancer stem cells, signaling pathways, genomics, and molecular pathogenesis. *Genes & Diseases*, 5(2), 77–106. <https://doi.org/10.1016/j.gendis.2018.05.001>
- Hamid, N., Razak, R., & Najib, A. (2021). *Virtual screening pada senyawa kimia tumbuhan terap (Artocarpus elasticus) terhadap reseptor alpha estrogen*. Penerbit NEM.
- Iktiarani, A., Damayanti, S. D., & Wulandari, D. N. (2024). Prediksi mekanisme antihipertensi senyawa fitokimia daun pepaya (*Carica papaya*) melalui inhibisi endothelin converting enzyme-1 dan calcium channel secara in silico. *Jurnal Kedokteran Komunitas (Journal of Community Medicine)*, 12(1), 1–16. <https://www.way2drug.com/>
- John, B. I. J. U., Sulaiman, C. T., George, S., & Reddy, V. R. K. (2014). Total phenolics and flavonoids in selected medicinal plants from Kerala. *International Journal of Pharmacy and Pharmaceutical Sciences*, 6(1), 406–408.
- Matheus, R. (2019). *Skenario pengelolaan sumber daya lahan kering: Menuju pertanian berkelanjutan*. Deepublish.
- Mutiah, R., Firdausy, A. F., Indrawijaya, Y. Y. A., & Hibbatullah, H. (2021). In silico prediction of Heliannuol A, B, C, D, and E compounds on estrogen receptor β agonists. *Indonesian Journal of Cancer Chemoprevention*, 12(1), 37–45. <https://doi.org/10.14499/indonesianjcanchemoprev12iss1pp37-45>
- Mutiah, R., Indrawijaya, Y. Y., & Puspita, D. (2020). Study in silico compounds in 96% ethanol extract of *Chrysanthemum cinerariifolium* (Trev.) leaves towards alfa estrogen receptors. *Indonesian Journal of Cancer Chemoprevention*, 11(3), 144–153.

<https://doi.org/10.14499/indonesianjcanchemoprev11iss3pp144-153>

- Naufa, F., Mutiah, R., Yen, Y., & Indrawijaya, A. (2022). Studi in silico potensi senyawa katekin teh hijau (*Camellia sinensis*) sebagai antivirus SARS-CoV-2 terhadap spike glycoprotein (6LZG) dan main protease (5R7Y). *Journal of Food and Pharmaceutical Sciences*, 10(1), 584–596.
- Ojha, S., Raj, A., Roy, A., & Roy, S. (2018). Extraction of total phenolics, flavonoids and tannins from *Paederia foetida* L. leaves and their relation with antioxidant activity. *Pharmacognosy Journal*, 10(3), 541–547.
- Purwani, S., Nahar, J., Zulfikar, Z., Nurlelarsi, N., & Mayanti, T. (2021). Molecular docking on kokosanolid A and C for anticancer activity against human breast cancer cell MCF-7. *Jurnal Kimia Valensi*, 7(1), 52–57. <https://doi.org/10.15408/jkv.v7i1.20534>
- Qi, C., Chang, J., Zhu, Y., Yeldandi, A. V., Rao, S. M., & Zhu, Y. J. (2002). Identification of protein arginine methyltransferase 2 as a coactivator for estrogen receptor α . *Journal of Biological Chemistry*, 277(32), 28624–28630. <https://doi.org/10.1074/jbc.M201053200>
- Rahmadani, A. T. I., Lestari, W. Y., Kadir, N. A., Saputri, M., Erika, F., Usman, Salam, S. H. A. S., Herman, & Rijai, L. (2024). Sintesis, molecular docking dan aktivitas sitotoksik senyawa analog kalkon berbasis alfa tetralone terhadap sel kanker payudara MCF-7. *Jurnal Sains dan Kesehatan*, 3(1), 242–247.
- Riwu, A. G., Nugraha, J., Purwanto, D. A., & Triyono, E. A. (2022). In silico analysis of anti-dengue activity of faloak (*Sterculia quadrifida* R. Br.) stem bark compounds. *Journal of Pharmacy & Pharmacognosy Research*. https://doi.org/10.56499/jppres22.1445_10.6.1006
- Ruswanto, R., Nofianti, T., Lestari, T., Septian, A. D., Firmansyah, A. P., & Mardianingrum, R. (2024). Potential active compounds of propolis as breast anticancer candidates: In silico study. *Jordan Journal of Biological Sciences*, 17(1), 153–161. <https://doi.org/10.54319/jjbs/170115>
- Saragih, G. S., & Siswadi, S. (2019). Antioxidant activity of plant parts extracts from *Sterculia quadrifida* R. Br. *Asian Journal of Pharmaceutical and Clinical Research*, 12(7), 143–148.
- Sarmoko, Pratama, A. H., Choironi, N. A., & Fareza, M. S. (2023). Bioinformatic study of the active compound of morin in mulberry (*Morus alba*) as breast anticancer. *AIP Conference Proceedings*, 2972(1), 60–71. <https://doi.org/10.1063/5.0184914>
- Shofi, M. (2021). Analisis senyawa α -spinasterol pada biji trembesi (*Samanea saman* (Jacq.) Merr.) terhadap penghambatan 3C-like protease SARS-CoV-2 melalui uji in silico. *Jurnal Sintesis: Penelitian Sains, Terapan dan Analisisnya*, 2(2), 74–88.
- Siswadi, R. A., Pujiono, E., Saragih, G. S., & Rianawati, H. (2015). Utilization of faloak tree bark (*Sterculia quadrifida* R. Br.) as a raw material for herbal medicine on the Island of Timor. In *Proceedings of a national seminar on biodiversity of Nusa Tenggara* (pp. 43–55).
- Siswadi, S., Pujiono, E., Rianawati, H., & Saragih, G. S. (2016). Nilai ekonomi kulit batang pohon faloak (*Sterculia quadrifida* R. Br.). In *Proceeding of Mulawarman Pharmaceuticals Conferences* (Vol. 3, pp. 379–388).
- Tenda, P. E., Lenggu, M. Y., & Ngale, M. S. (2017). Antibacterial activity test of ethanol extract of faloak tree skin (*Sterculia* sp.) on *Staphylococcus aureus* bacteria. *Health Info Journal*, 15(1), 227–239.
- Wulandari, R. P., Gabriel, K., Nurdin, H. A., Diffa, H. F. P., Sabiq, S. H., Natashya, P., Pribadi, A. P. A., & Aulifa, D. L. (2023). In silico study of secondary metabolite compounds in parsley (*Petroselinum crispum*) as a drug therapy for blood cancer (myeloproliferative neoplasm [MPN]) targeting JAK-2. *Indonesian Journal of Chemical Science*, 12(2), 216–228. <http://journal.unnes.ac.id/sju/index.php/ijcs>

Zhang, B., Li, H., Yu, K., & Jin, Z. (2022). Molecular docking-based computational platform for high-throughput virtual screening. *CCF Transactions on High Performance Computing*, 4(1), 63–74. <https://doi.org/10.1007/s42514-021-00086-5>