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Molecular Docking of *Abroma augusta* Phytocompounds Against Estrogen Receptor Alpha (Er-A) for the Treatment of Menstrual Disorders

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Abstract

Menstrual disorders, including dysmenorrhea (painful menstruation), amenorrhea (absence of menstruation), and irregular menstrual cycles, significantly impact women's reproductive health and overall well-being. These conditions often arise from hormonal imbalances, inflammation, and uterine dysfunction, necessitating effective therapeutic interventions. Current treatments, such as hormonal therapies (oral contraceptives, progestin-only pills), NSAIDs, and surgical procedures (endometrial ablation, hysterectomy), provide relief but often target symptoms rather than addressing the underlying causes. Consequently, there is a growing interest in alternative plant-based therapies with gynecological benefits, with Abroma augusta emerging as a promising candidate. The objective of the study is to identify the potential phytocompounds of A. augusta and evaluate their therapeutic potential by analyzing their binding affinity with estrogen receptor alpha (ER-α) through molecular docking. By investigating the molecular interactions of these compounds, this research seeks to provide scientific validation for the traditional use of A. augusta and explore its potential as a natural therapeutic agent for menstrual disorders.

Keywords: Menstrual disorders, *Abroma augusta,* estrogen receptor alpha (ER-α), molecular docking

INTRODUCTION

Abroma augusta, commonly known as Devil's Cotton, is a medicinal plant traditionally used in Ayurvedic and homeopathic medicine to treat menstrual irregularities, dysmenorrhea, infertility, and other gynecological disorders. This plant, belonging to the Malvaceae family, is widely distributed across Asia, South and Eastern Africa, and Australia, and has been utilized for centuries by tribal communities in India and Bangladesh.

The roots, bark, leaves, and seeds of *A. augusta* are rich in bioactive phytochemicals, such as taraxerol, β-sitosterol, friedelin, α-amyrin, lupeol, and octacosanol, which exhibit anti-inflammatory, anti-diabetic, antimicrobial, and gynecological properties. Studies have shown that the root extract of *A. augusta* acts as a uterine tonic, demonstrating oxytocic effects that regulate menstrual flow and uterine contractions. Furthermore, its ethanolic and aqueous extracts have been reported to possess abortifacient and antifertility properties, making it a potential candidate for contraceptive development. In addition to its gynecological applications, *A. augusta* exhibits antioxidant, antimicrobial, and anti-inflammatory activities, further supporting its therapeutic potential. Scientific research highlights its role in regulating hormonal balance, improving reproductive health, and alleviating menstrual pain, making *A. augusta* a promising natural candidate for treating menstrual disorders. Despite its rich

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ethnopharmacological history, the molecular mechanisms underlying the therapeutic effects of *A. augusta* remain largely unexplored [1–5].

Estrogen receptor alpha (ER-α) is a critical protein that regulates estrogen signaling, endometrial function, and uterine activity, making it a key target for menstrual health interventions [6, 7]. The estrogen receptors (ERs) have two subtypes, estrogen receptors α and β (ERα and ERβ), encoded by the *ESR1* and *ESR2* genes, respectively. These receptors belong to the nuclear receptor superfamily and exert biological functions in several ways [8]. Among them, ERα is the primary mediator of estrogenic action in the normal endometrium, where its expression is significantly higher than that of ERβ [9].

ERα is predominantly expressed in the uterus and plays a crucial role in uterine cell proliferation, making it essential for maintaining menstrual cycle regularity and reproductive health [10]. Dysregulation of ERα has been associated with conditions, such as endometriosis, endometrial hyperplasia, and menstrual irregularities [11].

Phytocompounds capable of modulating ERα expression could potentially alleviate symptoms by reducing the abnormal proliferation of endometrial tissue. *A. augusta* phytocompounds exhibit estrogen-mimicking properties, allowing them to bind to ERα and influence hormonal pathways that regulate the menstrual cycle. This interaction may contribute to restoring hormonal balance in conditions, such as amenorrhea and irregular menstrual cycles.

Additionally, the modulation of ERα activity by these compounds could help reduce pain associated with dysmenorrhea by influencing uterine contractions, leading to improved menstrual flow and reduced cramping.

In this study, molecular docking techniques are employed to evaluate the binding potential of *A. augusta* phytocompounds against ER-α. By investigating the molecular interactions and pharmacological properties of these compounds, this research aims to provide scientific validation for the traditional use of *A. augusta* and explore its potential as a natural therapeutic agent for menstrual disorders.

METHODOLOGY

Retrieval of Ligands

The IMPPAT (Indian Medicinal Plants, Phytochemistry and Therapeutics) database (https://cb.imsc.res.in/imppat/) was used to look for potential ligands [12]. The canonical SMILES and the PubChem CIDs of the top 16 selected ligands were recorded from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/). The three-dimensional (3D) structures of the selected ligands were retrieved in Structure Data Format (SDF) from the PubChem database [13].

Retrieval of Protein

The 3D crystal structure of the target receptor protein, estrogen receptor alpha (E-α) with PDB (Protein Data Bank) ID of 1A52, was retrieved from the RSCB PDB databank (https://www.rcsb.org/structure/1A52). The protein was retrieved in PDB format. The resolution of the retrieved protein is 2.80 Å and the method of retrieval of the protein is X-RAY DIFFRACTION [14].

Protein Purification

During protein preparation for molecular docking, all the crystallographic water molecules were removed to prevent steric hindrance and ensure accurate protein-ligand interactions. The water molecules in the crystal structure may occupy the binding sites or form transient interactions that could interfere with the ligand binding and affect the docking results. All the other additional chains were removed from the protein structure to simplify the structure, and the A-chains were retained. The

prebound heteroatoms and the complex ligands were also deleted from the protein structure, and the polar hydrogen atoms were added to correctly define the hydrogen bonding interactions and optimize the protein's electrostatic environment, ensuring accurate docking simulations. Protein purification was carried out in BIOVIA Discovery Studio [15].

Ramachandran Plot and Secondary Structure Analysis

The purified protein structure was analyzed for secondary structure prediction using the PDBsum webserver (https://www.ebi.ac.uk/thornton-srv/databases/pdbsum/) and Ramachandran plot analysis using the PROCHECK webserver (https://saves.mbi.ucla.edu/) to assess the structural quality of the protein. The Ramachandran plot evaluates the sterically allowed regions of backbone dihedral angles (ϕ, ψ) in a protein structure, indicating energetically favorable conformations.

PHARMACOLOGICAL STUDIES

SwissADME Analysis

SwissADME (http://www.swissadme.ch/) analysis is used to evaluate the pharmacological properties of the ligands based on their physicochemical parameters [16]. The physicochemical properties that are evaluated are: lipophilicity, polarity, solubility, flexibility, size, and saturation. Then, the ligands were screened based on the LIPINSKI rule of 5, gastrointestinal (GI) absorption, and bioavailability. The toxicity parameters of the ligands were evaluated using ADMETlab 2.0 (https://admetmesh.scbdd.com/) [17, 18].

Molecular Docking

The PyRx virtual screening tool was used to evaluate the binding affinity of the phytocompounds against the estrogen receptor alpha (E-α) (PDB ID: 1A52) protein [19–21]. The PyRx software treats the protein as a macromolecule by assigning every atom an AutoDock4 type, which is required for molecular docking using AutoDock Vina. Consequently, the purified 1A52 protein was converted to pdbqt format before proceeding to docking. A total of three ligands, obtained after pharmacological screening (ADME analysis), were loaded in .sdf format. Energy minimization of the ligands was performed using the Universal Force Field, and the ligand torsions were detected. The energy-minimized ligands were then converted into pdbqt format using the OpenBabel feature in PyRx. For docking, a grid box was set with grid dimensions of X = 57.3539Å, Y = 75.9906 Å, and Z = 33.8402Å.

The ligands were docked independently against 1A52. In PyRx, nine different binding poses were generated for each ligand to identify the most favorable interaction with the target protein. The degree of binding is evaluated based on the binding affinity scores, where a lower binding affinity indicates a more favorable docking conformation. The top three selected ligands with the lowest binding affinity scores, having zero root mean square deviation (RMSD) values were visualized using BIOVIA Discovery Studio. From the docking analysis, the most effective compounds were vanillic acid, 3,4-Dihydroxybenzoic acid, and caffeic acid.

Visualization

The 2D and 3D interaction models of the three docked ligands with the best binding scores were generated and analyzed using Dassault Systèmes BIOVIA Discovery Studio Visualizer. The interaction types, non-bonded atoms, bond distances, and bond types were evaluated [15].

RESULTS

Initial Selection of Ligands

A total of 16 phytocompounds of *A. augusta* were initially retrieved from the IMPPAT database. These compounds were subjected to pharmacological screening, Lipinski's rule analysis, and SwissADME analysis. Based on these criteria, a subset of ligands was selected for further molecular docking analysis (Table 1).

Table 1. Compound name, PubChem ID, and the canonical smiles of the top 16 chosen ligands.

Compound Name	Compound CID	Canonical Smiles
Taraxerol acetate	94225	CC(=O)O[C@H]1CC[C@@]2([C@H]3CC[C@]4([C@@H]5CC(CC[C@@]5(CC=C4[C@@]3(CC[C@H]2C1(C)C)C)C)(C)C)C)C
Taraxerol	92097	C[C@]12CCC(C[C@H]1[C@@]3(CC[C@@H]4[C@]5(CC[C@@H](C([C@@H]5CC[C@]4(C3=CC2)C)(C)C)O)C)(C)C
Lupeol	259846	CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]3CC[C@@H]4[C@]5(CC[C@@H](C([C@@H]5CC[C@]4([C@@]3(CC2)C)C)(C)C)O)C)C
BETA-SITOSTEROL	222284	CC[C@H](CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)C(C)C
Betaine	247	C[N+](C)(C)CC(=O)[O–]
Choline	305	C[N+](C)(C)CCO
D-glucuronic acid	94715	[C@@H]1([C@@H]([C@H](OC([C@@H]1O)O)C(=O)O)O)O
1-Octacosanol	68406	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCO
Vanillic acid	8468	COC1=C(C=CC(=C1)C(=O)O)O
Friedelin	91472	C[C@H]1C(=O)CC[C@@H]2[C@@]1(CC[C@H]3[C@]2(CC[C@@]4([C@@]3(CC[C@@]5([C@H]4CC(CC5)(C)C)C)C)C)C)C
3,4-DIHYDROXYBENZOIC ACID	72	C1=CC(=C(C=C1C(=O)O)O)O
caffeic acid	689043	C1=CC(=C(C=C1/C=C/C(=O)O)O)O
Maslinic acid	73659	C[C@@]12CC[C@@H]3[C@@]([C@H]1CC=C4[C@]2(CC[C@@]5([C@H]4CC(CC5)(C)C)C(=O)O)C)(C[C@H]([C@@H](C3(C)C)O)O)C
STIGMASTEROL	5280794	CC[C@H](/C=C/[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C(C)C
D-galacturonic acid	439215	[C@@H]1([C@H]([C@H](OC([C@@H]1O)O)C(=O)O)O)O
1,28-Octacosanediol	54082727	C(CCCCCCCCCCCCCCO)CCCCCCCCCCCCCO

Target Protein Structure

The purified structure of the target protein, estrogen receptor alpha (ER-α), shown in Figure 1, is used as the receptor in molecular docking analysis to evaluate its potential interactions with the selected *A. augusta* phytocompounds.

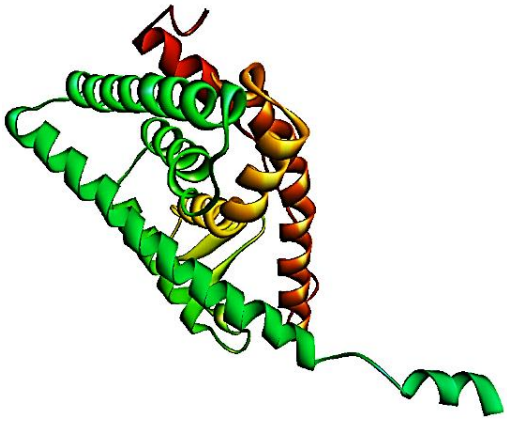

Figure 1. Purified protein structure of estrogen receptor alpha (E-α) (PDB ID: 1A52).

Protein Structure Analysis

The Ramachandran plot for the purified 1A52 protein, shown in Figure 2, was generated using PROCHECK. The most favored regions, which represent sterically permissible peptide conformations, are marked in red. Out of the 239 amino acid residues, 200 (91.3%) fall in the favored region, while 0 residues, or 0.0%, fall in the disallowed region. The remaining 8.7% are distributed

among additional allowed subregions. Out of the 239 residues, 219 are non-proline and non-glycine residues, 10 are glycine residues, 8 are proline residues, and the remaining 2 are the terminal residues (Figure 2).

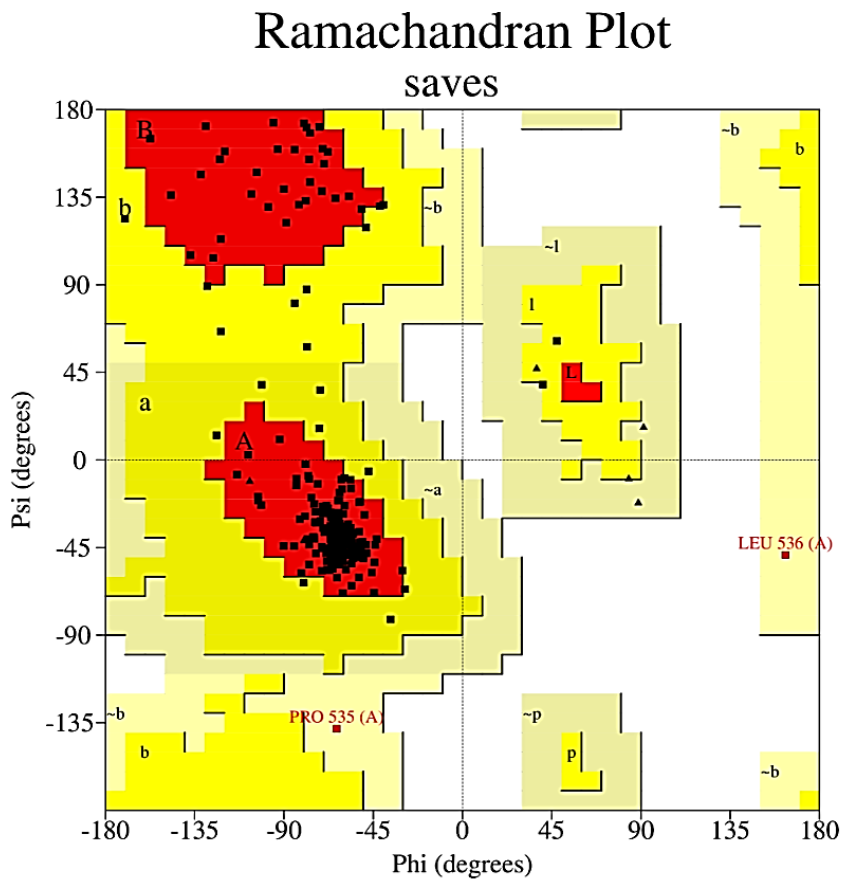

Figure 2. Ramachandran plot of 1A52 protein using PROCHECK.

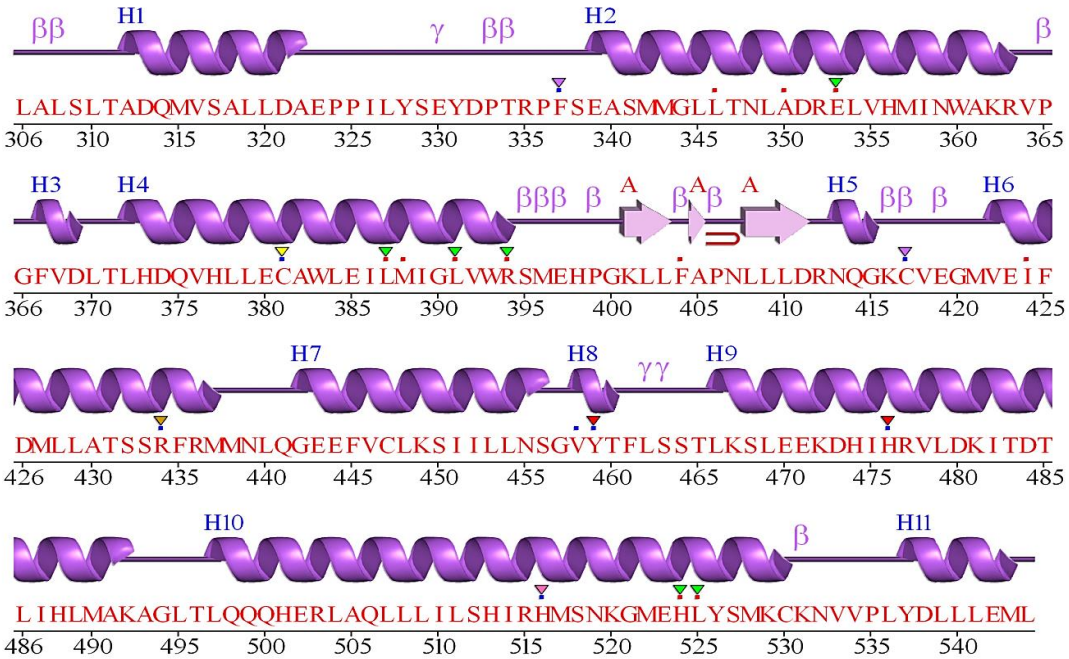

Figure 3. Secondary structure of 1A52 protein using PDBsum.

As shown in Figure 3, the secondary structure of estrogen receptor alpha (ER-α) (PDB ID: 1A52) consists predominantly of 11 α-helices (H1–H11), forming a tightly packed helical bundle crucial for ligand binding and stability. It also includes one β-sheet, two β-strands, one β-hairpin, and two β-bulges, contributing to structural integrity. The presence of 15 β-turns and three γ-turns enhances flexibility, while 22 helix–helix interactions reinforce stability within the ligand-binding domain. The annotated sequence (residues 306–540) highlights these structural features, which provide insights into the protein's overall topology and folding pattern.

Drug-Likeness Analysis

The phytocompounds were screened based on their physicochemical properties, Lipinski's Rule of Five, ADME analysis to determine their drug-like characteristics. To ensure the safety and efficacy of potential drug candidates, toxicity prediction and aggregate data were also considered. Therefore, the phytocompounds retrieved from *A. augusta* were subjected to pharmacological studies to assess their drug-likeness.

Pharmacological Data

The phytoconstituents from *A. augusta* were screened based on the physicochemical parameters listed in Table 2, and the physicochemical properties of the top ligands are summarized in Table 3.

Table 2. Parameters for physicochemical properties.

Properties		Optimal range
Lipophilicity	xLogP3	–0.7 – +5.0
Size	MW	150–500 g/moL
Polarity	TPSA	20–130
Solubility	Silicos-IT class	Soluble
Flexibility	Rotatable bonds	Not more than 9
Saturation	Sp3 hybridization	Not < 0.25

Table 3. Physicochemical properties of the ligand molecules.

Ligand	MW	Fraction Csp3	Rotatable bonds	TPSA	Lipophilicity
Vanillic acid	168.15	0.12	2	66.76	1.43
3,4-dihydroxybenzoic acid	154.12	0	1	77.76	1.15
caffeic acid	180.16	0	2	77.76	1.15

Lipinski Evaluation

Lipinski's Rule of Five assesses drug-likeness based on five key parameters, as listed in Table 4. According to this rule, a potential drug candidate should have a molecular weight between 150 and 500 Daltons, a logP (lipophilicity) value of less than 4.15, fewer than 5 hydrogen bond donors, fewer than 10 hydrogen bond acceptors, and a molar refractivity between 40 and 130 Å². The ligands were evaluated against these criteria, and the top three selected ligands met all these criteria without any violations (Table 5).

Table 4. Lipinski rule parameters.

Properties	Optimal Range
MW	150–500 Daltons
MlogP	< 4.15
H-bond donors	<5
H-bond acceptors	<10
MR	40–130 Å²

Table 5. Data for the properties of the Lipinski rule obtained using Swiss ADME.

Compound Name	Molecular Weight	M Log P	Hydrogen Donors	Hydrogen Acceptors	Molar Refractivity
Vanillic acid	168.15	0.74	2	4	41.92
Caffeic acid	180.16	0.7	3	4	47.16
3,4-dihydroxybenzoic acid	154.12	0.4	3	4	37.45

Swiss ADME Analysis

Swiss ADME (http://www.swissadme.ch/) analysis was used to evaluate the three key parameters: GI absorption, solubility, and bioavailability. High GI absorption is crucial for maximizing a drug's efficacy. Additionally, the compound should be readily soluble, as this enhances its bioavailability. Less negative solubility values are preferred. As per the results (Table 6), it is evident that all the selected ligands have high GI absorption, good solubility, and favorable bioavailability, making them promising drug candidates.

Table 6. ADME analysis.

Ligand	MW	Fraction Csp3	Rotatable Bonds	H-bond Acceptors	H-bond Donors	Silicos-IT Class	GI Absorption	Lipinski Violations	Bio Availability
Vanillic acid	168.15	0.12	2	4	2	Soluble	High	0	0.85
3,4-dihydroxy benzoic acid	154.12	0	1	4	3	Soluble	High	0	0.56
caffeic acid	180.16	0	2	4	3	Soluble	High	0	0.56

Toxicity Prediction

The following are some of the key characteristics of toxicity prediction: skin sensitivity, carcinogenicity, respiratory toxicity, AMES toxicity, rat oral acute toxicity, FDAMDD, hERG blockers, H-HT, and DILI parameters were evaluated to determine the toxicity of the top three ligands (Table 7).

Table 7. Toxicity analysis.

Ligand	hERG	H-HT	DILI	Ames	ROA	Carcinogenicity	Respiratory
Vanillic acid	0.031	0.224	0.857	0.015	0.053	0.062	0.12
3,4-dihydroxy benzoic acid	0.023	0.485	0.842	0.068	0.112	0.046	0.783
caffeic acid	0.006	0.812	0.842	0.184	0.266	0.362	0.392

- *hERG:* Human ether-a-go-go related gene, DILI: Drug-induced liver injury, ROA: Rat oral acute, H-HT: Human hepatotoxicity

Molecular Docking Analysis

The binding affinity of the top three selected ligands – vanillic acid, caffeic acid, and 3,4-Dihydroxybenzoic acid – toward estrogen receptor alpha (ER-α) was determined using PyRx and is listed in Table 8. For further analysis, the docking conformation with the lowest binding affinity and RMSD value was selected as the most favorable binding pose for each compound. Following docking, the binding affinity, RMSD upper bound (RMSD/ub), and RMSD lower bound (r/lb) were recorded. The lowest binding affinity values of the top three ligands were recorded and are considered for further analysis.

Table 8. Docking score of estrogen receptor alpha (E-α) protein with the selected ligands.

Ligand	Binding Affinity	rmsd/ub	rmsd/lb
Vanillic acid	–6	0	0
Caffeic acid	–6.4	0	0
3,4-DIHYDROXYBENZOIC ACID	–6.2	0	0

Visualization

The binding interactions of the best conformational poses of the top three selected ligands—vanillic acid, caffeic acid, and 3,4-Dihydroxybenzoic acid—with the target receptor protein, estrogen receptor alpha (ER-α), were analyzed and visualized using BIOVIA Discovery Studio (Figures 4 and 5).

The two-dimensional (2D) and 3D interaction diagrams show that vanillic acid binds to the receptor protein by forming conventional hydrogen bonds, carbon-hydrogen bonds, and hydrophobic interactions with key residues, such as MET-388, ALA-350, LEU-346, LEU-391, ARG-394, and PHE-404. Additionally, π-Alkyl interactions with PHE-404 and LEU-391 contribute to its binding stability.

Similarly, caffeic acid interacts with the receptor protein through conventional hydrogen bonds, unfavorable donor-donor interactions, and π–π T-shaped interactions involving residues, like GLU-353, THR-347, LEU-387, LEU-391, ALA-350, PHE-404, and ARG-394. Hydrogen bonding with GLU-353 and THR-347 plays a significant role in its stabilization, while π–π T-shaped interactions with PHE-404 enhance its binding.

In the case of 3,4-Dihydroxybenzoic acid, strong conventional hydrogen bonds and π-sigma interactions are observed with ASN-348, SER-341, LEU-345, and ASP-332. Hydrogen bonding with SER-341, ASN-348, and ASP-332 reinforces its binding affinity, while the π-sigma interaction with LEU-345 further stabilizes its position within the receptor site.

The visualization of these interactions highlights the importance of hydrogen bonding, hydrophobic interactions, and π-interactions in facilitating ligand binding, confirming their potential for stable interactions with the ER-α receptor.

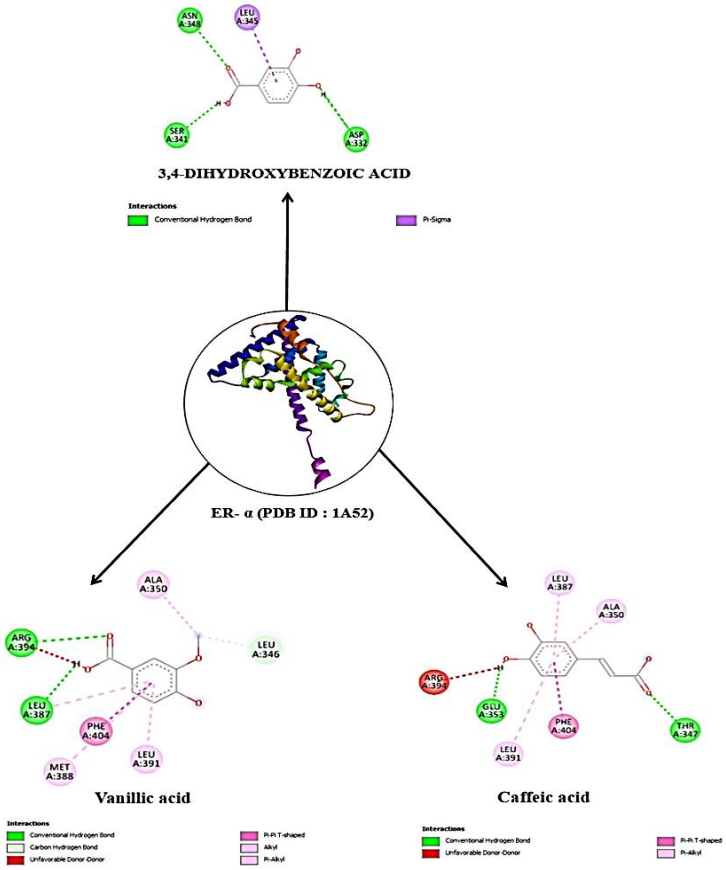

Figure 4. 2D interactions of top ligands interacting with estrogen receptor alpha (E-α).

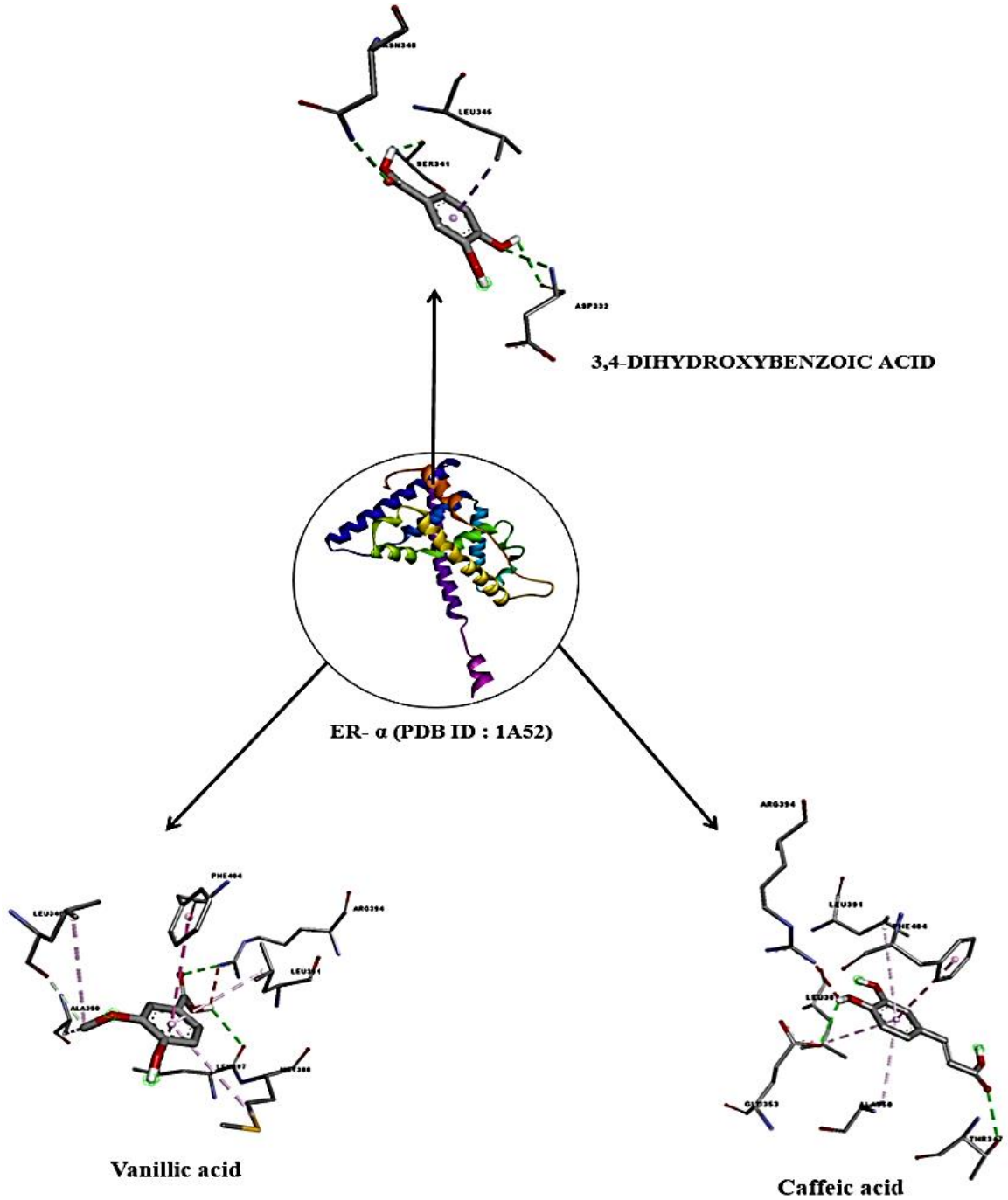

Figure 5. 3D interactions of top ligands interacting with estrogen receptor alpha (E-α).

DISCUSSION

A. augusta is a medicinal plant known for its rich phytochemical composition, which includes alkaloids, choline, betaine, beta-sitosterol, stigmasterol, and various monosaccharides and uronic acids, such as L-rhamnose, L-arabinose, D-xylose, D-mannose, D-glucose, D-galactose, D-galacturonic acid, and D-glucuronic acid. The plant has been traditionally used in tribal medicine for gynecological purposes, particularly in the treatment of menstrual disorders, menopause-related symptoms, antifertility effects, and leucorrhoea. Additionally, it has been reported to exhibit pharmacological properties, such as anti-inflammatory, anti-diabetic, and wound-healing effects. Despite its widespread ethnopharmacological use, there is still a significant lack of molecular and clinical research validating the therapeutic efficacy of *A. augusta* in gynecological treatments [1].

The present study aimed to explore the bioactive potential of *A. augusta* phytocompounds by conducting a molecular docking analysis to evaluate their interactions with estrogen receptor alpha (ER-α). Initially, 16 phytocompounds were retrieved from the IMPPAT database and subjected to pharmacological screening, Lipinski's Rule of Five analysis, and SwissADME evaluation. Following this screening process, three phytocompounds – vanillic acid, caffeic acid, and 3,4-Dihydroxybenzoic acid – were identified as the most promising candidates for docking studies with ER-α.

Molecular docking analysis revealed that all three phytocompounds demonstrated strong binding interactions with ER-α, suggesting their potential to modulate estrogenic activity. Among them, caffeic acid exhibited the lowest binding affinity, indicating a higher binding strength with the target protein. This suggests that caffeic acid could play a crucial role in influencing estrogen signaling pathways, making it a promising lead compound for further drug development. Vanillic acid and 3,4-Dihydroxybenzoic acid also displayed significant binding interactions, reinforcing the potential of *A. augusta* as a natural source for developing alternative therapeutics for menstrual health.

Caffeic acid, a naturally occurring polyphenol, has been widely studied for its anti-inflammatory, antioxidant, and hormone-modulating properties [20, 21]. Its ability to bind strongly with ER-α suggests that it may have a direct regulatory effect on estrogenic activity, which is crucial in maintaining menstrual health and managing inflammation-related menstrual disorders, such as dysmenorrhea. Similarly, vanillic acid, known for its antioxidant and anti-inflammatory effects [22], may provide additional therapeutic benefits in reducing menstrual pain and inflammation. 3,4-Dihydroxybenzoic acid, another bioactive phenolic compound, has been reported to exhibit estrogenic activity [23–25], which may contribute to its effectiveness in menstrual regulation.

The findings of this study suggest that these phytocompounds may function as natural estrogen receptor modulators, potentially offering an alternative to synthetic hormonal therapies. Since menstrual disorders are often linked to estrogen imbalances, these compounds could be explored further for their therapeutic potential in managing conditions, such as dysmenorrhea, irregular menstrual cycles, and estrogen-related gynecological disorders.

CONCLUSIONS

The molecular docking results obtained from this study indicate that *A. augusta* phytocompounds – caffeic acid, vanillic acid, and 3,4-Dihydroxybenzoic acid – exhibit significant potential in modulating estrogen receptor alpha (ER-α) activity, a crucial protein involved in menstrual regulation. The molecular docking analysis demonstrated favorable binding interactions between these phytocompounds and ER-α, indicating their possible role in influencing estrogen signaling pathways. Given that menstrual disorders often arise due to hormonal imbalances and disruptions in estrogen activity, the ability of these bioactive compounds to target ER-α highlights their therapeutic potential.

While molecular docking provides valuable preliminary insights into ligand-protein interactions, it is necessary to validate these findings through experimental studies. Further in vitro assays can assess the binding efficiency, bioavailability, and stability of these compounds in a controlled environment, while in vivo studies in animal models can offer deeper insights into their pharmacokinetics, efficacy, and potential side effects. Moreover, structure-based drug optimization techniques can be employed to enhance the affinity and specificity of these phytocompounds for ER-α, thereby improving their therapeutic efficacy.

Future research should focus on exploring the molecular mechanisms underlying the interaction of these compounds with ER-α, investigating their downstream biological effects, and evaluating their safety profiles. Additionally, the formulation of plant-based therapeutics derived from *A. augusta* could pave the way for alternative and natural treatment options for menstrual disorders, potentially reducing reliance on conventional hormone-based therapies. This study serves as a foundation for further pharmacological exploration and clinical validation of *A. augusta* phytocompounds in the context of gynecological health.

Acknowledgment

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List of Abbreviations

NSAIDs	Nonsteroidal anti-inflammatory drugs
ER-α	Estrogen Receptor Alpha
SDF	Structure Data Format
SMILES	Simplified Molecular Input Line Entry System
RCSB	Research Collaboratory for Structural Bioinformatics
PDB	Protein Data Bank
TPSA	Topological Polar Surface Area
ADME	Absorption, Distribution, Metabolism, Excretion, Toxicity
GI	Gastrointestinal Absorption
PubChem CID	PubChem Compound Identification

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