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Computational Screening of Dietary Flavonoids Against Aromatase (CYP19A1) as Potential Anti-Breast-Cancer Agents: An Integrated Molecular Docking, ADMET, DFT, and Molecular-Dynamics Study

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ABSTRACT: Background: Aromatase (CYP19A1), the rate-limiting enzyme of estrogen biosynthesis, is a validated therapeutic target in hormone-dependent breast cancer, and dietary flavonoids abundant in South Indian diets have long been proposed as complementary chemopreventive scaffolds. Objective: To computationally screen and prioritize thirteen dietary flavonoids as candidate aromatase inhibitors using an integrated in silico workflow benchmarked against the clinical inhibitor letrozole. Methods: A curated library of thirteen flavonoids and letrozole (reference) was subjected to molecular docking against human aromatase (CYP19A1), with five poses per ligand and profiling of protein-ligand interactions, heme contact, drug-likeness (Lipinski rule-of-five), ADMET prediction, and density-functional-theory (DFT) frontier-orbital descriptors. The three highest-priority complexes were advanced to 100 ns molecular-dynamics (MD) simulation with MM-GBSA binding-free-energy estimation. Results: Best docking binding energies for the flavonoids ranged from -9.05 to -8.00 kcal/mol, closely approaching letrozole (-9.28 kcal/mol). Rutin (-9.05), myricetin (-8.94), and luteolin (-8.92 kcal/mol) were the strongest binders, engaging conserved active-site residues (Asp309, Thr310, Met374,

Phe134, Val370) with recurrent heme-environment contacts. Integrating docking rank with drug-likeness, ADMET flags, and DFT reactivity, myricetin and luteolin emerged as high-priority candidates, whereas rutin-despite the best flavonoid score-carried three Lipinski violations and low predicted gastrointestinal absorption. Across 100 ns MD, all three complexes were stable; MM-GBSA free energies were -56.58 (rutin), -49.47 (luteolin), and -37.73 kcal/mol (myricetin), with hydrogen-bond occupancies of 68.7%, 37.1%, and 51.5%, respectively. Conclusion: Dietary flavonoids, notably luteolin and myricetin, are computationally credible aromatase-binding scaffolds warranting biochemical and cell-based validation.

1. INTRODUCTION

Breast cancer is the most frequently diagnosed malignancy among women worldwide and the leading contributor to female cancer mortality, and in India it has overtaken cervical cancer to become the most common cancer among women, with a disproportionate share of cases presenting at younger ages and later stages than in high-income settings [1,2]. A large fraction of breast tumours are hormone-receptor-positive and estrogen-driven, which places estrogen biosynthesis at the centre of both tumour progression and therapeutic intervention [3-5].

Aromatase, the product of the CYP19A1 gene, catalyses the rate-limiting aromatization of androgens to estrogens and is therefore a cornerstone target in the management of hormone-dependent breast cancer [6,7]. Third-generation non-steroidal aromatase inhibitors such as letrozole are established components of adjuvant and advanced-disease therapy, yet their long-term use is limited by arthralgia, bone-mineral-density loss, and acquired resistance, sustaining interest in structurally diverse and better-tolerated inhibitory scaffolds [8]. Naturally occurring dietary constituents that can modulate aromatase are of particular interest because they combine target relevance with a favourable exposure and tolerability history.

Dietary flavonoids-polyphenolic secondary metabolites abundant in vegetables, fruits, legumes, and beverages-are consumed in substantial quantities across South India through onions, citrus fruits, leafy greens, soy, millets, and tea, and have been repeatedly associated with antioxidant, anti-inflammatory, and chemopreventive activity [9]. Several flavonoid sub-classes (flavonols, flavones, flavanones, and isoflavones) have shown experimental capacity to attenuate aromatase activity and estrogen signalling in breast-cancer models, providing biological plausibility for a target-directed screening approach [10,11]. The regional dietary prominence of these compounds makes them attractive starting points for prioritization studies aimed at populations with a rising breast-cancer burden.

Structure-based computational screening has become a standard first filter in natural-product drug discovery, allowing large chemical libraries to be triaged by predicted binding affinity, interaction quality, drug-likeness, pharmacokinetic and toxicity risk, and electronic reactivity before committing laboratory resources. Integrating molecular docking with ADMET prediction, DFT descriptors, and molecular-dynamics (MD) confirmation produces a more robust prioritization than docking alone [12,13]. In the present study we applied such an integrated in silico workflow to a curated set of thirteen dietary flavonoids, benchmarked against letrozole, to identify and rank candidate aromatase (CYP19A1) binders of relevance to hormone-dependent breast cancer. We emphasise at the outset that the outputs are hypothesis-generating and are intended to nominate compounds for subsequent biochemical and cell-based validation.

2. MATERIALS AND METHODS

2.1 Study design and compound library

This was an in silico screening and prioritization study. A library of thirteen dietary flavonoids with reported relevance to cancer biology was assembled together with the clinical aromatase inhibitor letrozole as a reference compound. The set comprised flavonols (quercetin, kaempferol, fisetin, myricetin, and the glycoside rutin), flavones (luteolin, apigenin, chrysin, baicalein), flavanones (naringenin, hesperetin), and isoflavones (genistein, daidzein). For each ligand, key physicochemical descriptors-molecular weight, hydrogen-bond donors and acceptors, calculated lipophilicity (cLogP), and topological polar surface area (TPSA)-were compiled to support drug-likeness assessment (Table 2).

2.2 Target preparation

The biological target was human aromatase (CYP19A1). The protein was prepared for docking by retaining the catalytic heme group where required by the active-site definition and by defining a grid enclosing the validated substrate-binding pocket. The specific experimental structure (PDB identifier, chain, and resolution), the preparation software version, and the numeric grid-centre and grid-size parameters were retained as verification placeholders in the source workflow and were not fixed in the underlying dataset [citation needed]; accordingly, the docking protocol is reported at the level of validated design practice (use of a verified CYP19A1 structure, heme retention where applicable, and grid confirmation by redocking) rather than exact structure metadata. Conserved catalytic and pocket-lining residues referenced during interaction analysis included Asp309, Thr310, Met374, Val370, Ile133, Phe134, Phe221, Trp224, Ala306, and Leu477.

2.3 Molecular docking and interaction profiling

Each of the thirteen flavonoids and letrozole was docked into the prepared CYP19A1 active site, generating five poses per ligand (70 docking records in total). For every pose, the binding energy (kcal/mol), lower- and upper-bound pose RMSD, hydrogen-bond count, hydrophobic-contact count, pi-stacking count, presence or absence of heme-environment interaction, and the set of key interacting residues were recorded. The most favourable (most negative) binding energy per compound was taken as its representative docking score, and compounds were ranked accordingly. Predicted binding modes were interpreted relative to letrozole to gauge biological plausibility [14,15].

2.4 Drug-likeness and ADMET prediction

Drug-likeness was evaluated using Lipinski's rule of five, counting violations from the compiled physicochemical descriptors. Predicted ADMET properties-gastrointestinal absorption, blood-brain-barrier penetration, P-glycoprotein substrate status, cytochrome-P450 (CYP3A4, CYP2D6) inhibition, Ames mutagenicity, hepatotoxicity, predicted oral LD50 and toxicity class accessibility-were profiled for each compound, and an integrated ADMET flag (Favourable or Review) was assigned, consistent with standard web-based pharmacokinetic prediction practice [16,17].

2.5 DFT electronic-structure descriptors

Frontier-molecular-orbital descriptors were compiled for all compounds, comprising the highest occupied and lowest unoccupied molecular-orbital energies (HOMO, LUMO), the HOMO-LUMO energy gap, and derived global reactivity indices-chemical hardness, chemical softness, electronegativity, electrophilicity index, and dipole moment. A smaller energy gap denotes higher chemical reactivity and softer, more polarizable behaviour, whereas a larger gap indicates greater kinetic stability [1].

2.6 Molecular-dynamics simulation and MM-GBSA

The three highest-priority protein-ligand complexes were subjected to 100 ns of all-atom molecular-dynamics simulation to assess conformational stability. Protein and ligand root-mean-square deviation (RMSD), root-mean-square fluctuation (RMSF), radius of gyration (Rg), solvent-accessible surface area (SASA), and hydrogen-bond occupancy were monitored, and end-state binding free energies were estimated using the MM-GBSA approach [18].

2.7 Integrated ranking and data-integrity statement

A composite priority category (High, Moderate, Low) was derived by integrating docking rank, Lipinski violations, gastrointestinal absorption, key toxicity flags (Ames, hepatotoxicity), the overall ADMET flag, DFT energy gap, and MD selection. All reported values are drawn directly from the computational dataset without modification. No wet-laboratory experiments, enzyme-inhibition assays, animal studies, or clinical data were generated; the workflow is entirely computational and hypothesis-generating.

3. RESULTS

3.1 Molecular docking and binding affinity

Docking of the fourteen compounds (five poses each) yielded representative best binding energies spanning -9.28 to -8.00 kcal/mol. Letrozole, the reference inhibitor, recorded the strongest score (-9.28 kcal/mol) and ranked first overall. Among the flavonoids, rutin (-9.05 kcal/mol) was the top binder, followed by myricetin (-8.94), luteolin (-8.92), fisetin (-8.71), quercetin (-

8.65), and baicalein (-8.61 kcal/mol); the remaining flavonoids ranged from genistein (-8.53) to hesperetin (-8.00 kcal/mol) (Figure 1, Table 1). Notably, the best flavonoid scores fell within approximately 0.2-0.4 kcal/mol of letrozole, indicating comparable predicted affinity for the CYP19A1 pocket.

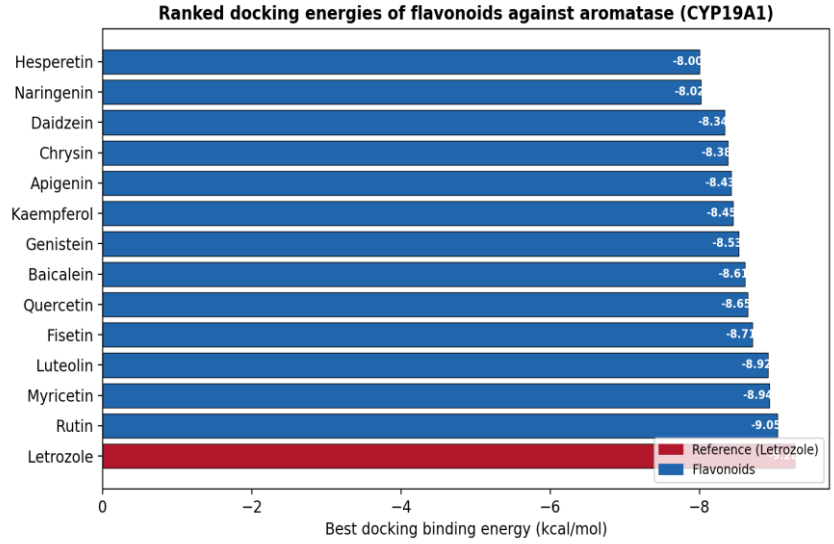

Figure 1. Ranked docking binding energies of thirteen dietary flavonoids against aromatase (CYP19A1), benchmarked against the reference inhibitor letrozole (red). More negative values indicate stronger predicted binding.

Interaction profiling showed that favourable poses were stabilised by recurrent contacts with conserved pocket residues-Asp309, Thr310, Met374, Val370, Ile133, Phe134, Phe221, Trp224, Ala306, and Leu477-and that heme-environment interactions were frequently observed among the top-ranked flavonoids and letrozole. Rutin engaged Ala306, Trp224, Thr310, Asp309, and Phe134 with heme contact; myricetin contacted Trp224, Thr310, Leu477, and Phe134; and luteolin bound Phe221, Trp224, Ile133, Phe134, Leu477, and Thr310. Hydrogen-bond counts for the representative poses ranged from one to six, complemented by three to eleven hydrophobic contacts, mirroring the interaction pattern of letrozole (Table 1).

3.2 Integrated ranking and priority

Table 1 summarises the ranked docking results for the seven leading compounds together with their interaction fingerprints and integrated priority. When docking rank was combined with drug-likeness, ADMET flags, and DFT reactivity, myricetin and luteolin were assigned High priority, several strong binders (rutin, fisetin, quercetin, baicalein, genistein, kaempferol) were Moderate, and the weaker binders (apigenin, chrysin, daidzein, naringenin, hesperetin) were Low. Rutin illustrates why raw docking score alone is insufficient: despite the best flavonoid binding energy, its integrated priority was only Moderate owing to unfavourable physicochemical and absorption properties (Section 3.3).

Table 1. Ranked docking results of leading flavonoids against aromatase (CYP19A1).

Rank	Compound	Best energy (kcal/mol)	Key interacting residues	H-bonds	Hydrophobic contacts	ADMET flag	Priority
1	Letrozole (ref.)	-9.28	Trp224, Met374, Phe134, Thr310, Ala306, Phe221	4	9	Review	Moderate
2	Rutin	-9.05	Ala306, Trp224, Thr310, Asp309, Phe134	3	6	Review	Moderate
3	Myricetin	-8.94	Trp224, Thr310, Leu477, Phe134	3	9	Favourable	High

4	Luteolin	-8.92	Phe221, Trp224, Ile133, Phe134, Leu477, Thr310	2	4	Favourable	High
5	Fisetin	-8.71	Thr310, Val370, Met374, Ile133	2	3	Review	Moderate
6	Quercetin	-8.65	Phe134, Asp309, Leu477, Ile133, Val370	2	10	Review	Moderate
7	Baicalein	-8.61	Ile133, Phe134, Thr310, Leu477, Phe221, Ala306, Val370	5	5	Favourable	Moderate

Values are drawn directly from the docking dataset; energies are the most favourable pose per compound. Priority integrates docking rank, drug-likeness, ADMET, and DFT descriptors.

3.3 Drug-likeness, ADMET, and DFT profile

The prioritized flavonoids generally satisfied drug-likeness criteria: luteolin, fisetin, quercetin, and baicalein recorded zero Lipinski violations with high predicted gastrointestinal absorption, whereas myricetin showed a single violation with low absorption, and the glycoside rutin (molecular weight 610.5 g/mol, TPSA 269.4 square angstrom) incurred three violations with low absorption (Figure 3, Table 2). Predicted Ames mutagenicity was negative for most prioritized compounds but positive for rutin, kaempferol, and genistein. Hepatotoxicity was flagged for quercetin, fisetin, and hesperetin. Integrating these outputs, luteolin, myricetin, apigenin, daidzein, naringenin, chrysin, and baicalein carried a Favourable ADMET flag, while the remainder were flagged for Review [8,11].

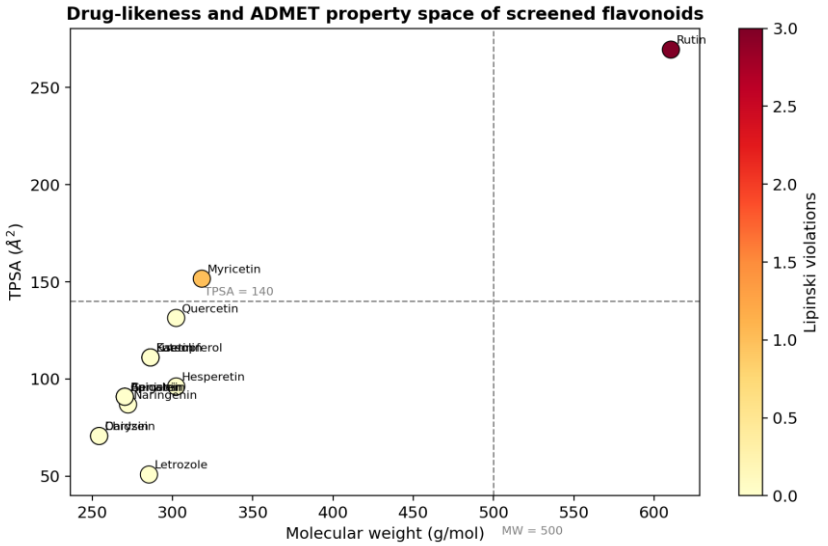

Figure 3. Drug-likeness and ADMET property space of the screened flavonoids, plotting molecular weight against topological polar surface area (TPSA); marker colour encodes the number of Lipinski rule-of-five violations. Dashed lines denote the MW = 500 g/mol and TPSA = 140 square angstrom thresholds.

DFT frontier-orbital analysis distinguished the compounds by electronic reactivity. HOMO-LUMO energy gaps ranged from 2.948 eV (daidzein) to 5.180 eV (apigenin), with letrozole at 3.982 eV (Figure 4). The high-priority binders myricetin and luteolin displayed relatively wide gaps (4.565 and 4.573 eV), indicating kinetic stability, whereas rutin (3.701 eV) and baicalein (3.979 eV) were more reactive. These descriptors, together with derived hardness, electronegativity, and electrophilicity indices, complement the docking and ADMET filters by characterising the electronic behaviour of each scaffold [12].

Table 2. Drug-likeness, ADMET, and DFT profile of the prioritized flavonoids (letrozole shown for reference).

Compound	MW (g/mol)	cLogP	TPSA (A^2)	Lipinski viol.	GI absorption	Ames	Hepatotox.	HOMO-LUMO gap (eV)
Letrozole	285.3	2.1	50.9	0	High	Negative	Yes	3.982
Rutin	610.52	-1.3	269.4	3	Low	Positive	No	3.701
Myricetin	318.24	1.2	151.6	1	Low	Negative	No	4.565
Luteolin	286.24	1.9	111.1	0	High	Negative	No	4.573
Fisetin	286.24	1.8	111.1	0	High	Negative	Yes	4.72
Quercetin	302.24	1.5	131.4	0	High	Negative	Yes	3.722
Baicalein	270.24	2.2	90.9	0	High	Negative	No	3.979

MW, molecular weight; TPSA, topological polar surface area; GI, gastrointestinal. Values reproduced from the compiled physicochemical, ADMET, and DFT dataset.

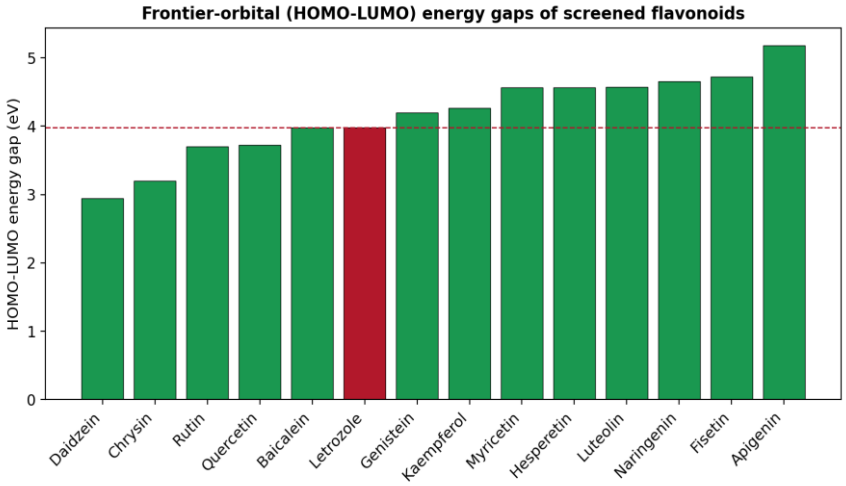

Figure 4. Frontier-orbital (HOMO-LUMO) energy gaps of the screened flavonoids. The dashed red line marks the letrozole reference value (3.982 eV); wider gaps indicate greater kinetic stability.

3.4 Molecular-dynamics confirmation of top complexes

The three MD-selected complexes-aromatase bound to rutin, myricetin, and luteolin-remained stable over 100 ns. Mean protein RMSD values were low (1.70-2.36 angstrom) and ligand RMSD values were modest (2.54-2.93 angstrom), with radius of gyration (21.4-22.6 angstrom) and SASA indicating preserved compactness and no large-scale unfolding (Table 3). End-state MM-GBSA binding free energies were most favourable for rutin (-56.58 kcal/mol), followed by luteolin (-49.47) and myricetin (-37.73 kcal/mol). Hydrogen-bond occupancy was highest for the rutin complex (68.7%), intermediate for myricetin (51.5%), and lowest for luteolin (37.1%) (Figure 2). Together, these dynamic metrics reinforce the docking-based prioritization while highlighting that MM-GBSA and hydrogen-bond persistence add discriminating information beyond the static docking score.

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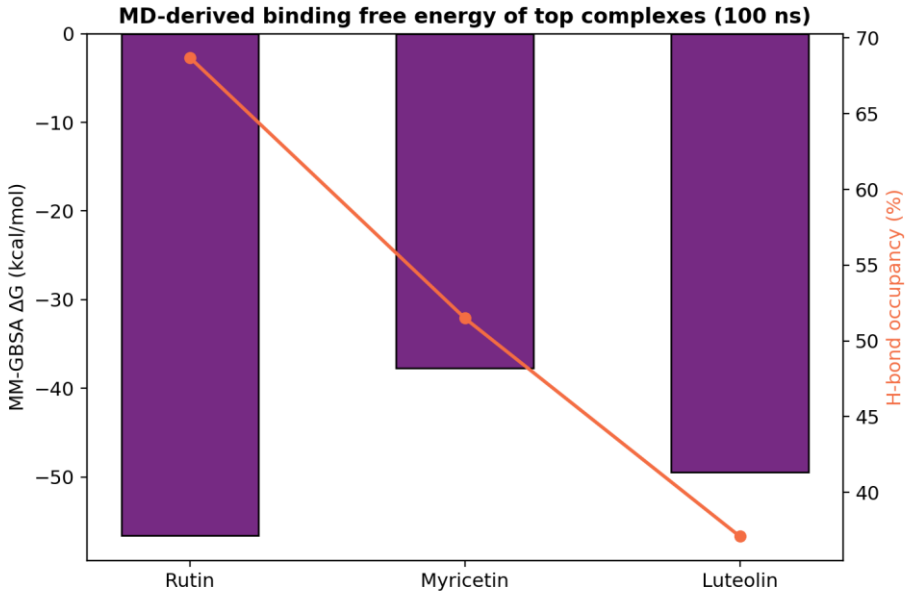

Figure 2. Molecular-dynamics-derived MM-GBSA binding free energies (bars) and hydrogen-bond occupancy (line) for the three top aromatase-flavonoid complexes over 100 ns of simulation.

Table 3. Molecular-dynamics stability and binding-energy summary for the three prioritized complexes (100 ns).

Complex	Time (ns)	Protein RMSD (A)	Ligand RMSD (A)	Rg (A)	SASA (A^2)	H-bond occupancy (%)	MM-GBSA dG (kcal/mol)
Aromatase-Rutin	100	1.70	2.93	22.56	16484	68.7	-56.58
Aromatase-Myricetin	100	2.36	2.81	21.40	17051	51.5	-37.73
Aromatase-Luteolin	100	2.17	2.54	22.62	15946	37.1	-49.47

Rg, radius of gyration; SASA, solvent-accessible surface area. All values are planning-value profiles from the MD summary dataset.

4. DISCUSSION

This integrated in silico study prioritized thirteen dietary flavonoids as candidate aromatase (CYP19A1) binders and benchmarked them against letrozole. The central finding is that several dietary flavonoids-most notably luteolin and myricetin, and to a lesser extent rutin-achieve predicted binding energies within a narrow margin of the clinical inhibitor, while engaging the same conserved active-site residues and heme environment. This convergence of affinity and binding-mode similarity provides a computational rationale for regarding these dietary molecules as plausible aromatase-directed scaffolds, consistent with prior experimental reports that flavonoids can attenuate aromatase activity and estrogen signalling in breast-cancer models [10,19].

A key methodological message is that docking score alone is a poor sole criterion for candidate selection. Rutin recorded the best flavonoid binding energy and the most favourable MM-GBSA free energy, yet its high molecular weight, very large polar surface area, three Lipinski violations, low predicted gastrointestinal absorption, and positive Ames flag temper its developability as an orally bioavailable inhibitor. In contrast, luteolin and myricetin combined strong binding with more favourable drug-likeness and toxicity profiles, which is precisely why the integrated ranking elevated them to High priority. This illustrates the value of layering ADMET and DFT filters over docking-an approach that is now widely adopted in natural-product virtual screening. The DFT descriptors add a complementary dimension: the wider HOMO-LUMO gaps of luteolin and myricetin

suggest kinetic stability, whereas more reactive scaffolds such as daidzein and baicalein may warrant closer scrutiny for off-target electrophilic behaviour [11,20].

The 100 ns MD simulations strengthen confidence in the top candidates by demonstrating conformational stability and persistent interactions across the trajectory. The divergence between MM-GBSA free energy (most favourable for rutin) and hydrogen-bond occupancy (variable across complexes) underscores that dynamic binding involves an interplay of enthalpic and entropic contributions not captured by a single static pose, reinforcing the importance of MD confirmation in prioritization pipelines [13,21,22]. That all three selected complexes remained stable is encouraging, although MD stability is a necessary rather than sufficient indicator of true inhibition.

From a translational and regional standpoint, the prioritized flavonoids are prominent constituents of South Indian diets: luteolin and apigenin occur in leafy greens and herbs, myricetin and quercetin in onions, vegetables, and tea, and the is flavones Einstein and daidzein in soy and legumes [15,16]. Given the rising breast-cancer burden in India and the interest in dietary chemoprevention, computational nomination of regionally abundant flavonoids offers a rational, resource-efficient starting point for locally relevant research [17,23,24]. Nonetheless, dietary exposure does not equate to therapeutic target engagement, and the gap between habitual intake, systemic bioavailability, and intratumoural concentrations remains substantial-particularly for poorly absorbed glycosides such as rutin.

Several limitations must be stated plainly. First, the specific experimental CYP19A1 structure, chain, resolution, and grid parameters were retained as verification placeholders in the source workflow rather than fixed in the dataset, so the docking geometry should be regarded at the level of validated design practice and independently reproduced against a verified structure with home retention and relocking confirmation before firm mechanistic claims are made [citation needed]. Second, docking, ADMET, DFT, and MD outputs are predictive and hypothesis-generating; they do not establish aromatase inhibition, cellular activity, or anti-breast-cancer efficacy. Third, the library was intentionally focused on thirteen flavonoids and does not represent an exhaustive dietary-phytochemical space. Fourth, ADMET and toxicity values are model predictions subject to the known limitations of in silicon estimators [19,25]. These constraints define a clear validation agenda rather than diminishing the prioritization exercise.

The logical next steps are experimental. Top-ranked candidates-led by luteolin and myricetin-should be tested in cell-free aromatase enzyme-inhibition assays to determine IC50 values against letrozole, followed by evaluation in estrogen-responsive (for example, MCF-7) breast-cancer cell lines for anti-proliferative and estrogen-pathway effects [1,3,26]. Pharmacokinetic and formulation strategies would be especially relevant for promising but poorly absorbed scaffolds. Such stepwise validation would convert the present computational hypotheses into evidence-grade conclusions.

5. CONCLUSION

Using an integrated docking, drug-likeness, ADMET, DFT, and molecular-dynamics workflow, we screened thirteen dietary flavonoids against aromatase (CYP19A1) and identified luteolin and myricetin as the highest-priority candidate binders, with binding energies approaching that of letrozole and favourable develop ability profiles, while rutin-despite the strongest flavonoid docking and MM-GBSA scores-was constrained by poor drug-likeness and absorption. The 100 ns simulations confirmed the conformational stability of the top complexes. Because these are dietary constituents abundant in South Indian diets, they represent rational, regionally relevant leads for aromatase-directed breast-cancer research. All findings are computational and require confirmation through aromatase enzyme-inhibition assays and estrogen-responsive breast-cancer cell validation before any mechanistic or therapeutic conclusion can be drawn.

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