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Molecular Docking, ADMET, DFT, and Molecular-Dynamics Prioritization of Common Dietary Flavonoids as Candidate Beta-Lactamase Inhibitors: An In Silico Screening Study Relevant to Antimicrobial Resistance

Prakash Ghewari[1], Uma Bhardwaj[2*], Nilufar Esanmuradova[3], Dr. Priyabrata Pattanayak[4], Dr. M. Reena Rajan[5], Cheshta Rawat[6], Siddharth Sriram[7], Dinara Oblaqulova[8]

[1] Professor of Practice, Krishna Institute of Science and Technology, Krishna Vishwa Vidyapeeth "Deemed to be University", Taluka-Karad, Dist-Satara, Pin-415 539, Maharashtra, India. prakashghewari547@gmail.com

[2] Department of Biotechnology and Department of Microbiology, Noida international University, Greater Noida, Uttar Pradesh 203201, India. vc@niu.edu.in

[3]1. Head of the Department of Physics and Chemistry, "Tashkent Institute of Irrigation and Agricultural Mechanization Engineers" National Research University, Tashkent, Uzbekistan; 2. Scientific Researcher, University of Tashkent for Applied Science; 3. School of Engineering, Central Asian University, Tashkent, Uzbekistan sapaevibrokhim@gmail.com 0009-0006-5617-0545

[4]Associate Professor, Department of Pharmaceutical Sciences, School of Pharmaceutical Sciences, Siksha 'O' Anusandhan (Deemed to be University), Bhubaneswar, Odisha, India. priyabratapattanayak@soa.ac.in, 0000-0003-4035-1182

[5]Associate Professor, Department of Microbiology, Vinayaka Mission's Kirupananda Variyar Medical College & Hospitals, Vinayaka Mission's Research Foundation (DU), Salem, Tamil Nadu, India. reenarajan83@gmail.com, 0000 0003 4121 0242

[6]School of Pharmacy and Research, Dev Bhoomi Uttarakhand University, chestarawat26@gmail.com, 0009-0003-0372-0433

[7]Centre for Research Impact & Outcome, Chitkara University Institute of Engineering and Technology, Chitkara University, Rajpura, 140401, Punjab, India. siddharth.sriram.orp@chitkara.edu.in https://orcid.org/0009-0009-8776-1390

[8]Jizzakh State Pedagogical University, Uzbekistan. Kazakova.dinara12@mail.ru, 0009-0002-0596-5672

ABSTRACT: Background: Antimicrobial resistance (AMR) is among the gravest public-health threats of the twenty-first century, and bacterial beta-lactamase enzymes are a principal driver of resistance to beta-lactam antibiotics. Dietary flavonoids, abundant in the South Indian diet, are widely explored as scaffolds for adjunctive antibacterial agents. This study applied an integrated in silico workflow to prioritize common dietary flavonoids as candidate beta-lactamase inhibitors. Methods: Thirteen dietary flavonoids and the reference inhibitor clavulanic acid were docked against a bacterial beta-lactamase, generating five poses per ligand (70 docking records). Poses were profiled for binding energy and interaction patterns. Drug-likeness and ADMET properties, density-functional-theory (DFT) electronic descriptors, and 100-ns molecular-dynamics (MD) simulations with MM-GBSA free-energy estimation for three top complexes were

integrated into a ranking scheme. Results: Best docking energies for flavonoids ranged from -7.59 to -8.74 kcal/mol, closely bracketing clavulanic acid (-8.88 kcal/mol). Epigallocatechin gallate (-8.74), myricetin (-8.63), and luteolin (-8.45 kcal/mol) were the strongest flavonoid binders. Ligands engaged conserved active-site residues including Ser70, Lys73, Ser130, Glu166, Asn170 and Lys234. Most flavonoids satisfied Lipinski rule with high predicted gastrointestinal absorption; luteolin combined favourable docking, zero Lipinski violations, high absorption, a negative AMES prediction and a low HOMO-LUMO gap (3.25 eV), earning the only High integrated priority. In MD, the luteolin complex showed the highest hydrogen-bond occupancy (72.5%), while MM-GBSA free energies ranged from -31.68 to -42.92 kcal/mol. Conclusions: Common dietary flavonoids, particularly luteolin and the strong binders epigallocatechin gallate and myricetin, emerge as hypothesis-generating candidate beta-lactamase inhibitors. These purely computational findings do not establish enzyme inhibition or reversal of resistance and require biochemical beta-lactamase assays and bacterial susceptibility testing for validation.

1. INTRODUCTION

Antimicrobial resistance (AMR) has escalated into one of the defining health-security challenges of our era. A recent systematic analysis estimated that bacterial AMR was associated with approximately 4.71 million deaths and directly responsible for about 1.14 million deaths worldwide in 2021, with the burden projected to rise further by 2050 [1,2]. Resistance emerges through diverse molecular mechanisms - enzymatic drug inactivation, target modification, reduced permeability and efflux - among which enzymatic hydrolysis of the antibiotic scaffold is especially consequential for the most widely prescribed drug class, the beta-lactams [3,4].

Beta-Lactamases hydrolyse the four-membered beta-lactam ring shared by penicillins, cephalosporins, monobactams and carbapenems, abolishing antibacterial activity [5]. Since the introduction of benzylpenicillin, successive generations of beta-lactams have been met by an expanding repertoire of beta-lactamases, now numbering several thousand variants distributed across the Ambler serine classes (A, C, D) and the metallo-enzyme class B [6,7]. Extended-spectrum beta-lactamases (ESBLs) and carbapenemases have become globally disseminated, severely narrowing therapeutic options [8]. The pharmacological countermeasure has been to pair a beta-lactam with a beta-lactamase inhibitor (BLI); classical inhibitors such as clavulanic acid, sulbactam and tazobactam have been augmented by newer diazabicyclooctane and boronic-acid inhibitors (avibactam, vaborbactam) and, most recently, combinations such as cefepime-enmetazobactam approved for multidrug-resistant Enterobacterales . Nonetheless, resistance to inhibitor combinations continues to emerge, sustaining the search for structurally novel inhibitor chemotypes [9,10].

India, and South India in particular, bears a disproportionate share of the global AMR burden, driven by high community and hospital prevalence of ESBL-producing Enterobacterales, intensive antibiotic consumption and environmental antibiotic contamination [11,12]. In this setting, safe, inexpensive and locally available chemical matter is attractive for early-stage discovery. Dietary flavonoids are polyphenolic secondary metabolites ubiquitous in the South Indian diet - onions and shallots (quercetin, kaempferol), citrus fruits (hesperetin, naringenin), tea (catechin, epigallocatechin gallate), soy and legumes (genistein, daidzein), and leafy vegetables and herbs (apigenin, luteolin). These compounds display broad antibacterial and resistance-modifying activities and have repeatedly been proposed as adjuvants against multidrug-resistant pathogens.

Computer-aided screening offers a rational, resource-efficient route to triage such natural-product libraries before committing to laboratory work. Molecular docking predicts ligand binding geometry and affinity; ADMET and drug-likeness filters flag pharmacokinetic and safety liabilities; DFT descriptors characterize electronic reactivity; and molecular-dynamics (MD) simulation with MM-GBSA free-energy estimation probes the stability and energetics of the predicted complexes [8,13]. The present study integrates these methods to screen and prioritize thirteen common dietary flavonoids against a bacterial beta-

lactamase, benchmarked against clavulanic acid, with the explicit aim of generating testable hypotheses rather than asserting biological activity.

2. MATERIALS AND METHODS

2.1 Study design and compound library

This was an in silico screening and prioritization study. The ligand set comprised thirteen dietary flavonoids spanning the major structural subclasses - flavonols (quercetin, kaempferol, fisetin, myricetin), flavones (luteolin, apigenin, chrysin), flavanones (naringenin, hesperetin), isoflavones (genistein, daidzein) and flavan-3-ols (catechin, epigallocatechin gallate) - together with clavulanic acid as a reference beta-lactamase inhibitor (14 compounds in total). Physicochemical descriptors for each compound (molecular weight 199.16-458.37 g/mol; calculated logP -1.2 to 2.4; topological polar surface area 70.7-197.4 square angstrom) are summarised in the compound library.

2.2 Target preparation and molecular docking

The macromolecular target was a bacterial beta-lactamase. Each ligand was docked into the active site, and the five top-scoring poses per ligand were retained, yielding 70 docking records. For every pose the binding energy (kcal/mol), lower- and upper-bound pose RMSD, and counts of hydrogen bonds, hydrophobic contacts and pi-stacking interactions were recorded, along with the set of contacting residues. Poses were ranked by binding energy, and the most favourable pose per compound defined its best docking score.

2.3 Drug-likeness and ADMET prediction

Drug-likeness was assessed by Lipinski rule-of-five violations. Predicted ADMET endpoints included gastrointestinal absorption, blood-brain-barrier penetration, P-glycoprotein substrate status, cytochrome-P450 (CYP3A4, CYP2D6) inhibition, AMES mutagenicity, hepatotoxicity, predicted oral LD50 and toxicity class, and synthetic accessibility. An overall ADMET flag (Favourable or Review) summarised the profile of each compound [14,15].

2.4 DFT electronic descriptors

Frontier-orbital and global reactivity descriptors were computed for each compound: HOMO and LUMO energies, the HOMO-LUMO energy gap, chemical hardness and softness, electronegativity, electrophilicity index and dipole moment. A smaller energy gap indicates greater polarizability and chemical reactivity, properties often associated with stronger charge-transfer interactions in the binding site [16].

2.5 Molecular-dynamics simulation and free-energy estimation

Three prioritized flavonoid-beta-lactamase complexes (epigallocatechin gallate, myricetin and luteolin) were carried forward to 100-ns molecular-dynamics simulations. Trajectory-derived stability metrics - mean protein and ligand RMSD, per-residue RMSF, radius of gyration (Rg), solvent-accessible surface area (SASA) and hydrogen-bond occupancy - were computed, and the effective binding free energy was estimated by the MM-GBSA end-point method [17].

2.6 Integrated ranking

Docking rank, Lipinski violations, gastrointestinal absorption, AMES and hepatotoxicity flags, the ADMET summary flag, the HOMO-LUMO gap and MD selection were combined into an integrated priority category (High, Moderate or Low) reflecting the balance between predicted potency and developability.

2.7 Data-integrity statement

All numerical values reported here derive strictly from the study workbook. This is a purely computational investigation: no wet-laboratory experiments, ethics approvals, trial registrations or external funding are associated with it. Target-structure metadata (specific enzyme class, PDB identifier, chain, resolution and grid parameters) remained placeholders in the source dataset pending verification, and the specific beta-lactamase enzyme identity should therefore be confirmed against a validated structure before follow-up work **[citation needed]**. Docking and ADMET outputs are hypothesis-generating and do not establish beta-lactamase inhibition or reversal of antimicrobial resistance.

3. RESULTS

3.1 Docking scores and ranking

Across the 70 docking records, best binding energies for the thirteen dietary flavonoids ranged from -7.59 kcal/mol (daidzein) to -8.74 kcal/mol (epigallocatechin gallate), all falling within roughly 1.3 kcal/mol of the reference inhibitor clavulanic acid (-8.88 kcal/mol). The three strongest flavonoid binders were epigallocatechin gallate (-8.74, overall rank 2), myricetin (-8.63, rank 3) and luteolin (-8.45 kcal/mol, rank 4), followed by quercetin (-8.35) and apigenin (-8.21 kcal/mol). The complete ranking is given in Table 1 and Figure 1. The narrow spread of scores indicates that several dietary flavonoids occupy the beta-lactamase active site with predicted affinities comparable to a clinically used inhibitor.

Table 1. Integrated ranking of dietary flavonoids and the reference inhibitor by best docking energy, hydrogen bonding, drug-likeness and predicted priority.

Rank	Compound	Best dG (kcal/mol)	H-bonds*	Lipinski viol.	GI absorption	Priority
1	Clavulanic acid (ref.)	-8.88	4	0	High	Moderate
2	Epigallocatechin gallate	-8.74	1	2	Low	Moderate
3	Myricetin	-8.63	3	1	Low	Moderate
4	Luteolin	-8.45	6	0	High	High
5	Quercetin	-8.35	2	0	High	Moderate
6	Apigenin	-8.21	7	0	High	Moderate
7	Kaempferol	-8.17	5	0	High	Moderate
8	Fisetin	-8.13	1	0	High	Moderate
9	Genistein	-8.06	6	0	High	Moderate
10	Chrysin	-8.02	2	0	High	Low
11	Catechin	-7.85	6	0	High	Low
12	Hesperetin	-7.69	1	0	High	Low
13	Naringenin	-7.63	4	0	High	Low
14	Daidzein	-7.59	6	0	High	Low

**Hydrogen-bond count of the best-scoring pose. dG, docking binding energy; GI, gastrointestinal.*

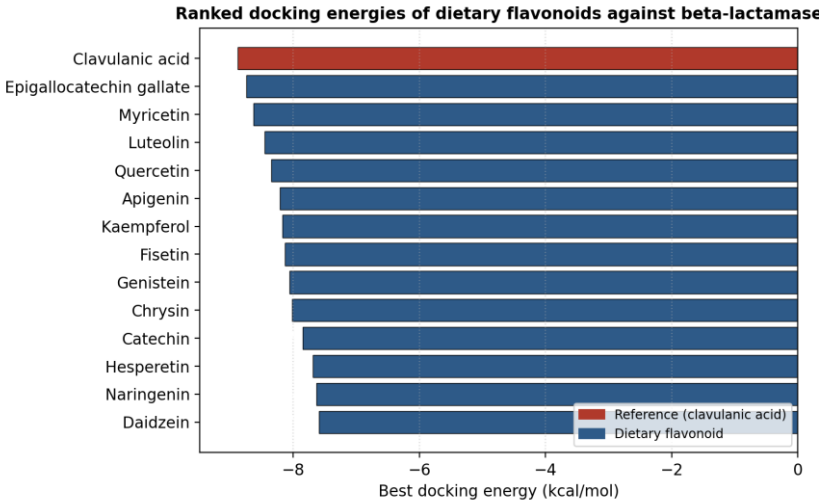

Figure 1. Ranked docking energies of common dietary flavonoids against bacterial beta-lactamase, with clavulanic acid (red) as the reference inhibitor.

3.2 Active-site interaction profile

Interaction profiling revealed a recurring set of contact residues across ligands, including Ser70, Lys73, Ser130, Asn132, Glu166, Asn170, Thr235, Gly236, Lys234 and Arg244 - residues consistent with the conserved catalytic and substrate-binding machinery of serine beta-lactamases [3,4]. Hydrogen-bond counts for best poses ranged from 1 to 7, complemented by 3-11 hydrophobic contacts and up to 2 pi-stacking interactions per pose. Among prioritized compounds, luteolin, apigenin, genistein and catechin formed particularly hydrogen-bond-rich complexes (6-7 hydrogen bonds in their best poses), while epigallocatechin gallate and myricetin achieved their high scores through extensive hydrophobic engagement of the pocket (Figure 2). The reference inhibitor clavulanic acid engaged Ser70, Lys73, Glu166 and Gly236, anchoring the same catalytic residues contacted by the leading flavonoids.

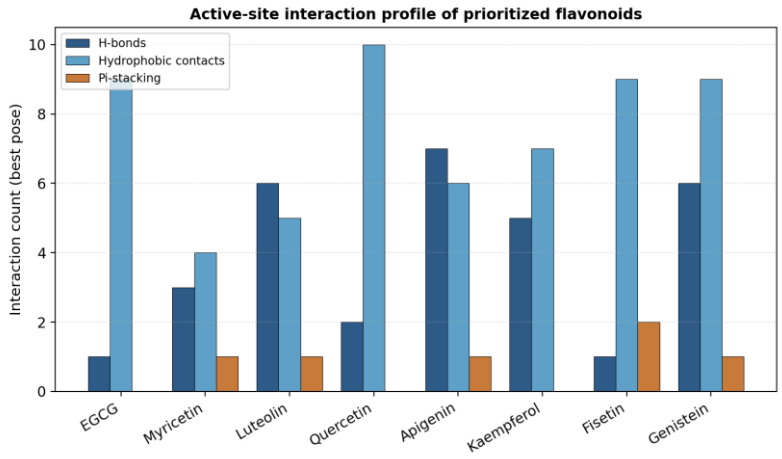

Figure 2. Active-site interaction profile (hydrogen bonds, hydrophobic contacts and pi-stacking of the best pose) for the prioritized flavonoids. EGCG, epigallocatechin gallate.

3.3 Drug-likeness and ADMET

Drug-likeness filtering favoured the smaller flavonoid aglycones. Eleven of thirteen flavonoids recorded zero Lipinski violations; only myricetin (1 violation) and epigallocatechin gallate (2 violations) breached the rule, reflecting their higher polar surface area (151.6 and 197.4 square angstrom, respectively) and hydrogen-bond-donor counts. Consistently, predicted

gastrointestinal absorption was High for all compounds except myricetin and epigallocatechin gallate, which were Low (Table 2, Figure 3). AMES mutagenicity was predicted negative for the majority, including luteolin, apigenin, quercetin, genistein, chrysin, hesperetin and daidzein, whereas kaempferol, naringenin, fisetin, myricetin and catechin returned positive AMES flags. Three compounds - luteolin, apigenin and chrysin - received an overall Favourable ADMET flag; the remainder, including the reference, were flagged for Review. Predicted oral LD50 values spanned 731-3434 mg/kg (toxicity classes 4-6), indicating generally low acute toxicity.

Table 2. Physicochemical, drug-likeness, ADMET and DFT profile of the prioritized compounds.

Compound	MW	cLogP	TPSA	GI abs.	AMES	Hepatotox.	Gap (eV)
Clavulanic acid (ref.)	199.16	-1.2	83.6	High	Neg.	Yes	3.526
Epigallocatechin gallate	458.37	1.0	197.4	Low	Neg.	No	3.706
Myricetin	318.24	1.2	151.6	Low	Pos.	No	4.143
Luteolin	286.24	1.9	111.1	High	Neg.	No	3.250
Quercetin	302.24	1.5	131.4	High	Neg.	Yes	4.393
Apigenin	270.24	2.1	90.9	High	Neg.	No	4.147
Kaempferol	286.24	1.9	111.1	High	Pos.	No	3.912

MW, molecular weight (g/mol); TPSA, topological polar surface area (square angstrom); GI abs., gastrointestinal absorption; Neg., negative; Pos., positive; Gap, HOMO-LUMO energy gap.

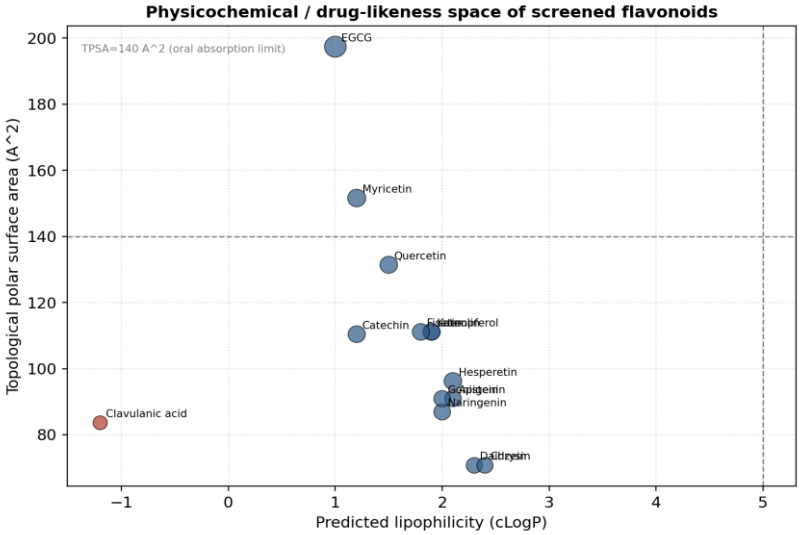

Figure 3. Physicochemical / drug-likeness space of the screened flavonoids (calculated logP versus topological polar surface area; bubble size proportional to molecular weight). Dashed lines mark common oral-absorption thresholds.

3.4 DFT electronic descriptors

HOMO-LUMO energy gaps ranged from 3.126 eV (naringenin) to 5.424 eV (hesperetin), with most flavonoids clustering between 3.1 and 4.4 eV (Figure 4). Among the top-ranked binders, luteolin displayed a notably small gap (3.250 eV), close to that of clavulanic acid (3.526 eV), indicating high polarizability and chemical reactivity that may favour charge-transfer stabilization within the active site [14]. Correspondingly, luteolin, naringenin and daidzein showed the highest electrophilicity indices (4.6-4.8 eV) and chemical softness, whereas hesperetin, with the widest gap, was the least reactive. These electronic descriptors reinforce the docking-based prioritization of luteolin.

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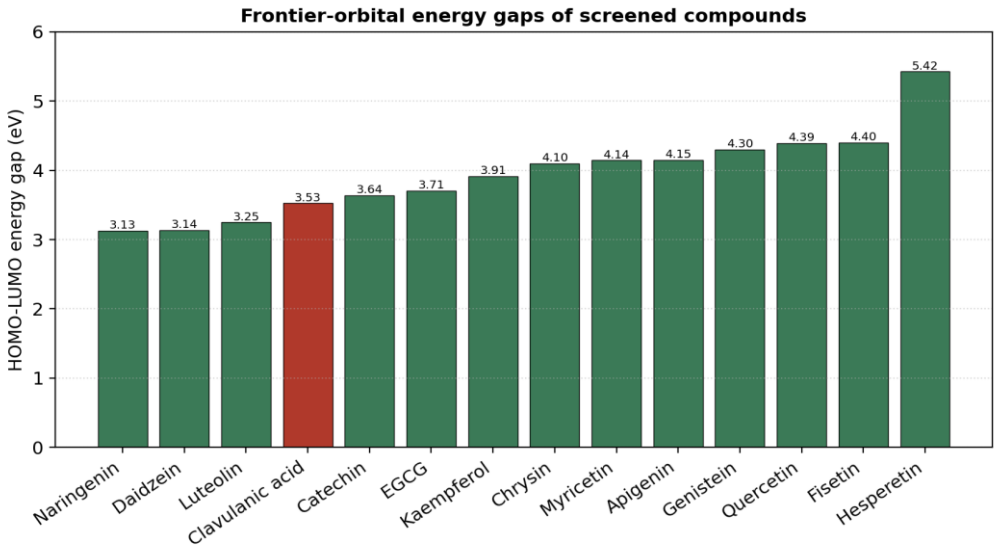

Figure 4. *Frontier-orbital (HOMO-LUMO) energy gaps of the screened compounds; the reference inhibitor is shown in red. EGCG, epigallocatechin gallate.*

3.5 Molecular-dynamics stability and free energy

The three prioritized flavonoid complexes were stable over the 100-ns simulations, with mean protein RMSD of 1.55-2.44 angstrom and radius of gyration of 18.41-20.57 angstrom, consistent with preserved global fold (Table 3). The luteolin complex exhibited the highest hydrogen-bond occupancy (72.5%), corroborating its hydrogen-bond-rich docking pose, whereas the epigallocatechin gallate and myricetin complexes showed occupancies of 59.6% and 56.9%. MM-GBSA effective binding free energies were -34.23 kcal/mol (epigallocatechin gallate), -42.92 kcal/mol (myricetin) and -31.68 kcal/mol (luteolin). These MD metrics are planning-value estimates that indicate stable-complex behaviour rather than validated affinities [12,13].

Table 3. Molecular-dynamics summary (100 ns) and MM-GBSA free-energy estimates for the three prioritized complexes.

Complex	Protein RMSD (A)	Ligand RMSD (A)	Rg (A)	H-bond occ. (%)	MM-GBSA dG
EGCG-b-lactamase	2.29	2.79	19.89	59.6	-34.23
Myricetin-b-lactamase	1.55	2.06	18.41	56.9	-42.92
Luteolin-b-lactamase	2.44	2.40	20.57	72.5	-31.68

Rg, radius of gyration; occ., occupancy; MM-GBSA dG in kcal/mol. Values are trajectory means.

Integrating all evidence, luteolin was the single compound assigned a High overall priority: it combined a strong docking score (-8.45 kcal/mol, rank 4), zero Lipinski violations, high gastrointestinal absorption, a negative AMES prediction, no predicted hepatotoxicity, a favourable overall ADMET flag, a low HOMO-LUMO gap and the highest MD hydrogen-bond occupancy. Epigallocatechin gallate and myricetin, though the strongest binders, were assigned Moderate priority because of Lipinski violations and low predicted oral absorption.

4. DISCUSSION

This integrated in silico screen indicates that several common dietary flavonoids can occupy the bacterial beta-lactamase active site with predicted binding energies approaching that of clavulanic acid, and that a subset combines this affinity with acceptable predicted drug-likeness. The convergence of orthogonal computational lines of evidence - docking geometry, interaction profiling, ADMET filtering, DFT reactivity and MD stability - strengthens confidence in the resulting prioritization beyond what any single method could provide [18].

Luteolin emerged as the most balanced candidate. Its best pose formed six hydrogen bonds with catalytic-pocket residues, it violated none of Lipinski criteria, was predicted to be well absorbed and non-mutagenic, and displayed a small HOMO-LUMO gap indicative of chemical reactivity; in simulation it maintained the highest hydrogen-bond occupancy of the three complexes. Luteolin and its close structural analogue apigenin are abundant in South Indian dietary staples such as coriander, drumstick (Moringa), celery and peppers, which supports feasibility of dietary or nutraceutical exposure. The two strongest binders, epigallocatechin gallate (the principal catechin of tea) and myricetin, illustrate a recurrent trade-off in natural-product discovery: their extensive hydroxylation drives strong predicted binding but simultaneously inflates polar surface area and hydrogen-bond-donor counts, degrading predicted oral absorption and triggering Lipinski violations [10,19,20]. Such highly polar polyphenols may nevertheless be valuable as topical, gut-restricted or chemically optimised leads.

The recurring engagement of Ser70, Lys73, Ser130, Glu166 and Asn170 across ligands is mechanistically encouraging, because these residues constitute the conserved catalytic and oxyanion-stabilising machinery of serine beta-lactamases; ligands that hydrogen-bond to this cluster could, in principle, occlude the catalytic serine and act as competitive inhibitors [21,22].

These findings should be interpreted within the wider AMR landscape. With beta-lactam/beta-lactamase-inhibitor combinations continuing to lose ground to evolving ESBLs and carbapenemases, and with newer inhibitors such as enmetazobactam only recently reaching the clinic, inexpensive and structurally diverse natural-product chemotypes are strategically valuable for the discovery pipeline [23-25]. For a high-burden, resource-constrained setting such as South India, dietary flavonoids offer an attractive starting point for locally grounded, adjuvant-focused research [18,7].

Several limitations must be emphasised. First, the study is entirely computational; docking scores, ADMET predictions, DFT descriptors and MM-GBSA free energies are approximations that do not establish enzyme inhibition or antibacterial activity. Second, and critically, the target-structure metadata in the source dataset - including the specific beta-lactamase class, PDB identifier and grid definition - were placeholders; the precise enzyme identity and the docking box must be verified against a validated crystal structure with an appropriate redocking control before any mechanistic claim is made. Third, MD was limited to three complexes and single trajectories, and MM-GBSA neglects configurational entropy and explicit active-site water, so the absolute free energies (and the counter-intuitive ordering, in which luteolin has the least negative MM-GBSA value despite the highest hydrogen-bond occupancy) should be treated as planning values only [12,26]. Fourth, flavonoid pharmacokinetics in vivo - extensive phase-II metabolism, glucuronidation and low systemic bioavailability - are not captured by static ADMET filters.

Accordingly, the top-ranked candidates require experimental confirmation: purified-enzyme beta-lactamase inhibition assays (IC50/Ki), bacterial minimum-inhibitory-concentration and checkerboard synergy testing against defined ESBL- and carbapenemase-producing clinical isolates, and, ideally, co-crystallisation or biophysical binding studies. Future computational work should extend to enzyme-class-specific structures, longer and replicated MD trajectories, and free-energy-perturbation calculations to refine the ranking [27].

5. CONCLUSION

An integrated in silico workflow combining molecular docking, interaction profiling, ADMET and drug-likeness filtering, DFT reactivity analysis and 100-ns molecular-dynamics simulation prioritized common dietary flavonoids as candidate bacterial beta-lactamase inhibitors. Epigallocatechin gallate, myricetin and luteolin were the strongest predicted binders, closely approaching the reference inhibitor clavulanic acid, while luteolin offered the best overall balance of predicted potency, drug-likeness, safety and complex stability.

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