RESEARCH PAPER

Vitex negundo Flavonoids Target Antibiotic Resistance Proteins: Molecular Docking, ADMET Profiling, and Mother Tincture Validation

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ABSTRACT

Background: Antimicrobial resistance (AMR) poses a grave global threat, responsible for approximately 1.27 million deaths in 2019. The declining antibiotic pipeline has renewed interest in plant-derived phytocompounds as adjunct antimicrobials. *Vitex negundo* (Nirgundi), widely distributed across the Indian subcontinent, contains a well-characterised set of flavonoids and phenolic acids. Its homoeopathic mother tincture has shown inhibitory activity against macrolide-resistant *Staphylococcus aureus* in prior in vitro studies, yet the molecular basis of this activity remains unexplored.

Methods: Five phytocompounds from *V. negundo* leaf tissue Casticin, Chrysophenol, Isoorientin, Luteolin, and p-Hydroxybenzoic acid were docked against three antibiotic resistance proteins (3RJK, 4ALI, 4URM) using AutoDock Vina. In silico pharmacokinetic and drug-likeness profiling was performed via SwissADME. In vitro disk diffusion data from prior experiments against resistant clinical isolates were integrated for validation.

Results: Chrysophenol produced the strongest binding affinity across all three targets, achieving −10.5 kcal/mol at the beta-lactam resistance protein 4ALI, with key hydrogen bond engagement at Lys164. Luteolin ranked second at 4ALI (−9.3 kcal/mol). Casticin, Chrysophenol, and Luteolin satisfied all Lipinski drug-likeness criteria with zero violations and high predicted gastrointestinal absorption. *V. negundo* mother tincture produced a 7 mm inhibition zone against macrolide-resistant *S. aureus*, exceeding the 6 mm ethanol control.

Conclusion: Chrysophenol and Luteolin demonstrate strong in silico binding to clinically relevant antibiotic resistance proteins alongside favorable drug-likeness profiles, providing a molecular rationale for the observed in vitro antibacterial activity of *V. negundo* mother tincture.

Keywords: Vitex negundo, Molecular Docking, Antibiotic Resistance, Drug-Likeness, ADMET, Natural Antimicrobials

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INTRODUCTION:

Antimicrobial resistance (AMR) has been ranked by the World Health Organization among the ten most pressing dangers to human health globally; data from 2019 attribute approximately 1.27 million deaths directly to infections caused by resistant organisms.[1] Gram-positive *Staphylococcus aureus* and Gram-negative *Klebsiella pneumoniae* together account for an estimated 500,000 deaths per year, placing them among the most clinically significant resistant pathogens currently encountered.[2]

The pipeline of genuinely novel antibiotic classes entering clinical use has remained sparse for three decades,[3] a reality that has redirected scientific attention toward plant-derived bioactive compounds as candidate adjuncts to existing antimicrobial treatment regimens.

Homoeopathic mother tinctures occupy a distinct position relative to highly potentised dilutions: manufactured at pharmacopoeial concentrations that retain measurable quantities of phytochemical constituents, they are appropriate candidates for

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conventional in vitro pharmacological evaluation a methodological distinction worth stating explicitly. *Vitex negundo* (Nirgundi), a shrub distributed widely across the Indian subcontinent, carries a well-characterised complement of bioactive flavonoids and phenolic acids in its leaf tissue, among them Casticin, Chrysophenol, Isoorientin, Luteolin, and p-Hydroxybenzoic acid.[4]

In traditional herbal medicine, Echinacea angustifolia has long been used as an immunostimulant and topical antiseptic, and preclinical studies suggest that its principal constituents echinacoside, verbascoside, quercetin, kaempferol, cynaropicrin, tussilagine, and anthocyanins can enhance phagocytosis, increase TNF-α release from macrophages, and modulate T-cell and B-cell-mediated immune responses.[5,10]

Two prior publications from our group documented that the mother tincture of Vitex negundo generated measurable inhibition against Staphylococcus aureus resistant to Azithromycin, Clarithromycin, and Erythromycin, exceeding the ethanol control (6 mm) with a zone of inhibition of 7 mm.[6,7] These results are consistent with the present study's validation of V. negundo mother tincture activity against macrolide-resistant S. aureus.

The mechanistic underpinning of those observations had not been examined. The present study applies computational molecular docking and ADMET profiling to the principal phytocompounds of *V. negundo* against three crystallographically characterised antibiotic resistance proteins, with the aim of providing a molecular framework for the observed in vitro activity. In vitro disk diffusion data from prior publications are integrated for validation.

2. Materials and Methods

The study design and reporting follow the REHBaR (Reporting Experiments in Homeopathy Basic Research) checklist. In vitro disk diffusion susceptibility testing was carried out at Lotus Microbiologics, Thane, Maharashtra, India, an accredited diagnostic microbiology facility. Bacterial isolates were collected during routine clinical diagnostic procedures; no patient participants were recruited and no identifying information was recorded or retained. Ethical conduct of the in vitro work conformed to applicable national guidelines for laboratory-based microbiological investigation.

2.1 Phytocompound Selection and Target Proteins

Five phytocompounds identified in *V. negundo* leaf tissue Casticin, Chrysophenol, Isoorientin, Luteolin, and p-Hydroxybenzoic acid were chosen for in silico evaluation based on their documented presence in the phytochemical profile of the plant.[4] Their chemical structures are shown in Figure 1.

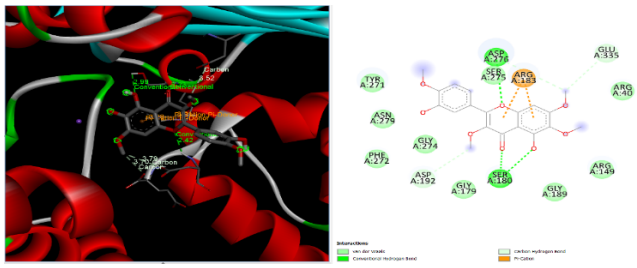
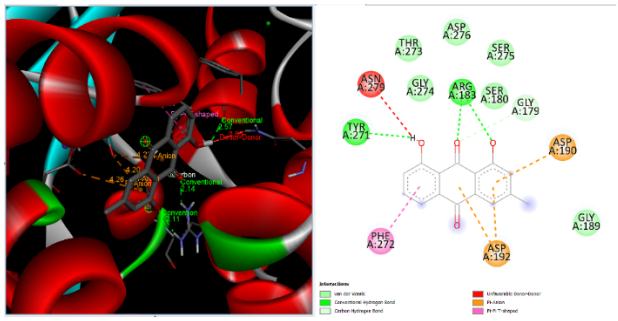


Figure 1-Two-dimensional chemical structures of the five selected *Vitex negundo* phytocompounds: (1) Casticin, (2) Chrysophenol, (3) Isoorientin, (4) Luteolin, and (5) p-Hydroxybenzoic acid.

The receptor set comprised three crystal structures deposited in the RCSB Protein Data Bank (PDB), each linked to a distinct resistance mechanism: 3RJK (macrolide resistance-associated rRNA methyltransferase), 4ALI (beta-lactam resistance protein), and 4URM (drug efflux pump). Target selection was guided by the resistance phenotypes of the two clinical isolates tested experimentally: *S. aureus* resistant to macrolides (3RJK) and *K. pneumoniae* resistant to beta-lactams and via efflux (4ALI, 4URM). The three-dimensional structures of the selected target proteins are shown in Figure 2.

Figure 2



Three-dimensional ribbon representations of the three target proteins: 3RJK (macrolide resistance-associated rRNA methyltransferase), 4ALI (beta-lactam resistance protein), and 4URM (drug efflux pump).

2.2 Molecular Docking

Two-dimensional SMILES representations for each phytocompound were obtained from PubChem and converted to three-dimensional conformations. Receptor preparation involved removal of bound water and non-structural heteroatoms, followed by MMFF94 energy minimisation. Search space grids were positioned over each protein's catalytic site, defined using coordinates of the co-crystallised ligand or conserved active-site residues. Binding free energy calculations were performed with AutoDock Vina; results are expressed as docking scores in kcal/mol. Intermolecular interaction profiles encompassing conventional hydrogen bonds, C-H bonds, pi-cation, pi-anion, pi-sigma, alkyl, and pi-

alkyl contacts were inspected and recorded using Discovery Studio Visualizer.

2.3 ADMET Profiling

In silico pharmacokinetic and drug-likeness characterisation was carried out through the SwissADME platform.[8] Canonical SMILES of the five compounds were submitted for calculation of physicochemical descriptors molecular weight (MW), hydrogen bond donors (HBD), hydrogen bond acceptors (HBA), topological polar surface area (TPSA), and rotatable bonds alongside lipophilicity (consensus LogP), water solubility (ESOL and Ali models), gastrointestinal (GI) absorption, blood–brain barrier (BBB) permeability, P-glycoprotein substrate status, cytochrome P450 (CYP) inhibition profiles (CYP1A2, CYP2C19, CYP2C9, CYP2D6, and CYP3A4), and compliance with Lipinski's rule of five, Ghose, Veber, Egan, and Muegge filters. Bioavailability and synthetic accessibility scores were also recorded.

2.4 In Vitro Antibacterial Testing

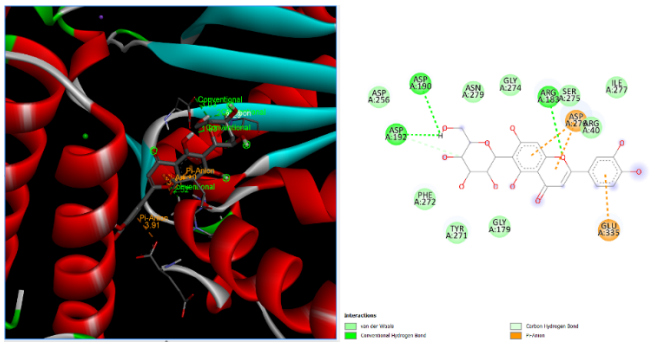
Antibacterial susceptibility was assessed by the Kirby–Bauer disk diffusion technique, carried out in full accordance with the procedures reported in our prior publications.[6,7] Briefly, *S. aureus* resistant to Azithromycin, Clarithromycin, and Erythromycin, and *K. pneumoniae* with confirmed resistance to 36 antibiotics (verified through routine sensitivity profiling) were cultured in Brain Heart Infusion broth. Five-millimetre sterile paper discs were loaded with mother tinctures of *C. officinalis*, *E. angustifolia*, and *V. negundo* (diluted to 1/10 drug strength) and positioned on inoculated agar plates incubated at 37°C. Inhibition diameters were recorded at 24 h and 48 h. Ethanol-loaded discs at the same solvent concentration served as the negative control; direct comparison with standard antibiotics was not made, as the concentration bases are not equivalent.[6] Resistance profiles were verified by routine clinical sensitivity testing before tincture evaluation commenced.

3. Results

3.1 Molecular Docking Against 3RJK

Among the five compounds docked against the 3RJK macrolide resistance-associated target, Isoorientin produced the highest binding affinity (−7.8 kcal/mol), forming conventional hydrogen bonds with ARG A:183, ASP A:190, and ASP A:192, alongside pi-anion interactions at ASP A:270 and GLU A:335. The binding interactions of all five compounds at 3RJK are illustrated in Figure 3.

Figure 3



Two-dimensional (2D) interaction diagrams and three-dimensional (3D) docked poses of Casticin (1), Chrysophenol (2), Isoorientin (3), Luteolin (4), and p-Hydroxybenzoic acid (5) at the active site of 3RJK. Colour coding: green dashed lines = conventional hydrogen bonds; orange dashed lines = pi-anion interactions; light green = carbon hydrogen bonds; red = unfavorable donor–donor interactions.

Chrysophenol and Luteolin both scored −7.4 kcal/mol. Chrysophenol engaged ARG A:183 and TYR A:271 via conventional hydrogen bonds and PHE A:272 through a pi-pi T-shaped interaction. Luteolin formed a pi-cation interaction with ARG A:183 and conventional hydrogen bonds at TYR A:271. Casticin scored −7.1 kcal/mol, interacting with SER A:180 and ASP A:276 via hydrogen bonding. p-Hydroxybenzoic acid showed the lowest affinity (−5.2 kcal/mol) through hydrogen bonds with SER A:180, ARG A:183, ASP A:192, and TYR A:271. Docking scores and key interaction residues for all compounds across all three targets are summarised in Table 1.

Table 1. Molecular docking scores (kcal/mol) and key interaction profiles of five phytocompounds from *Vitex negundo* against three antibiotic resistance-associated protein targets.

PDB Target	Compound	Dock Score (kcal/mol)	Key Interactions
3RJK	*Casticin*	−7.1	H-bond: SER A:180, ASP A:276; C-H bond: GLY A:179, SER A:275, GLU A:335; Pi-Carbon: ARG A:183
3RJK	*Chrysophenol*	−7.4	H-bond: ARG A:183, TYR A:271; C-H bond: GLY A:179; Pi-Anion: ASP A:190, ASP A:192; Pi-Pi T-shaped: PHE A:272

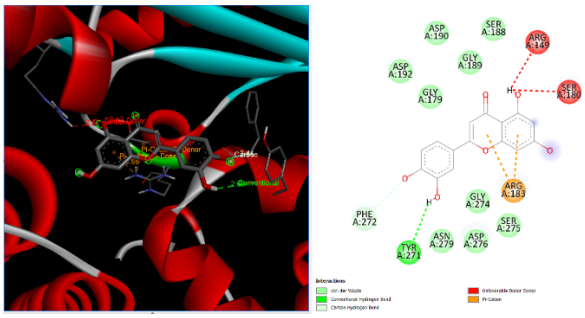
PDB Target	Compound	Dock Score (kcal/mol)	Key Interactions
3RJK	*Isoorientin*	−7.8	H-bond: ARG A:183, ASP A:190, ASP A:192; C-H bond: ASP A:276; Pi-Anion: ASP A:270, GLU A:335
3RJK	*Luteolin*	−7.4	H-bond: TYR A:271; C-H bond: PHE A:272; Pi-Cation: ARG A:183; Unfav. donor–donor: ARG A:149, SER A:180
3RJK	*p-Hydroxybenzoic acid*	−5.2	H-bond: SER A:180, ARG A:183, ASP A:192, TYR A:271; C-H bond: PHE A:272
4ALI	*Casticin*	−8.6	H-bond: ALA A:95, ILE A:20; C-H bond: ASP A:66; Pi-Cation: ARG A:40; Pi-Sigma: ILE A:94; Alkyl/Pi-Alkyl: ILE A:120, VAL A:67, ALA A:15, TCL A:1258
4ALI	*Chrysophenol*	−10.5	H-bond: LYS A:164; Pi-Sigma: ILE A:20; Alkyl/Pi-Alkyl: ALA A:190, TCL A:1258
4ALI	*Isoorientin*	−8.2	H-bond: GLY A:200, LYS A:41, ARG A:40, GLY A:13; Alkyl/Pi-Alkyl: ALA A:15, LEU A:196; Pi-Sigma: SER A:197
4ALI	*Luteolin*	−9.3	H-bond: LYS A:164, THR A:145, GLY A:191, LEU A:196; Alkyl/Pi-Alkyl: ILE A:20, ALA A:190, TCL A:1258
4ALI	*p-Hydroxybenzoic acid*	−6.3	H-bond: ILE A:193, THR A:195; Alkyl/Pi-Alkyl: ILE A:20, ALA A:190, TCL A:1258
4URM	*Casticin*	−7.0	C-H bond: GLU A:58, ASP A:81, GLY A:85; Alkyl/Pi-Alkyl: ILE A:86, ALA A:61; Pi-Anion: GLU A:58
4URM	*Chrysophenol*	−8.8	H-bond: ASP A:81, SER A:128; Amide-Pi Stacked: ASN A:54; Pi-Sigma: ILE A:86; Alkyl/Pi-Alkyl: ILE A:51, ILE A:102, ILE A:175, PRO A:87
4URM	*Isoorientin*	−7.2	H-bond: ASN A:54, ASP A:81; Pi-Sigma: ILE A:102; Alkyl/Pi-Alkyl: ILE A:86, PRO A:87
4URM	*Luteolin*	−8.0	H-bond: SER A:128, GLY A:85; Pi-Anion: GLU A:58; Pi-Sigma: ILE A:86; Amide-Pi Stacked: ASN A:54; Pi-Alkyl: PRO A:87
4URM	*p-Hydroxybenzoic acid*	−5.3	H-bond: ASN A:54, SER A:128; Pi-Sigma: ILE A:86

H-bond = Conventional Hydrogen Bond; C-H bond = Carbon Hydrogen Bond; Unfav. = Unfavorable.

3.2 Molecular Docking Against 4ALI

Docking against the 4ALI beta-lactam resistance-associated target yielded the highest overall binding affinities across the study. Chrysophenol achieved the strongest score of −10.5 kcal/mol, engaging LYS A:164 through a conventional hydrogen bond and exhibiting extensive pi-alkyl interactions with ALA A:190 and co-crystallised ligand TCL A:1258. The binding interactions at 4ALI are illustrated in Figure 4.

Figure 4

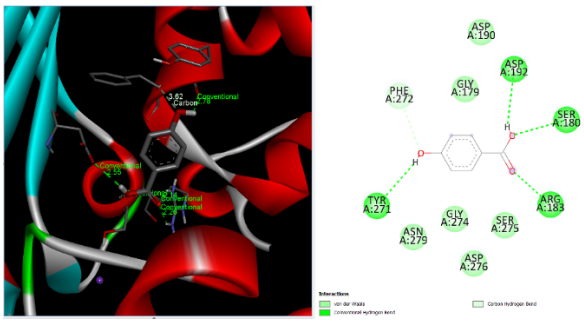


Two-dimensional (2D) interaction diagrams and three-dimensional (3D) docked poses of Casticin (6), Chrysophenol (7), Isoorientin (8), Luteolin (9), and p-Hydroxybenzoic acid (10) at the active site of 4ALI. Colour coding: green dashed lines = conventional hydrogen bonds; orange = pi-cation; pink/purple = alkyl and pi-alkyl interactions; pink = pi-sigma.

Luteolin ranked second (−9.3 kcal/mol), forming four conventional hydrogen bonds with LYS A:164, THR A:145, GLY A:191, and LEU A:196. Casticin (−8.6 kcal/mol) and Isoorientin (−8.2 kcal/mol) also demonstrated substantial binding, while p-Hydroxybenzoic acid produced a more modest score (−6.3 kcal/mol).

3.3 Molecular Docking Against 4URM

Against the 4URM efflux pump-associated target, Chrysophenol again showed the highest affinity (−8.8 kcal/mol), characterised by amide-pi stacking with ASN A:54, pi-sigma with ILE A:86, and hydrophobic interactions with ILE A:51, ILE A:102, ILE A:175, and PRO A:87. Luteolin scored −8.0 kcal/mol, Isoorientin −7.2 kcal/mol, Casticin −7.0 kcal/mol, and p-Hydroxybenzoic acid −5.3 kcal/mol. Interactions at this site were predominantly hydrophobic, involving multiple isoleucine, proline, and glycine residues. The binding interactions at 4URM are illustrated in Figure 5.



Two-dimensional (2D) interaction diagrams and three-dimensional (3D) docked poses of Casticin (11), Chrysophenol (12), Isoorientin (13), Luteolin (14), and p-Hydroxybenzoic acid (15) at the active site of 4URM. Colour coding: green dashed lines = conventional hydrogen bonds; pink = amide-pi stacked; orange = pi-anion; purple = pi-sigma; light purple = alkyl/pi-alkyl interactions.

3.4 ADMET Profiling

Key ADMET parameters for all five compounds are presented in Table 2. Casticin, Chrysophenol, and Luteolin satisfy all of Lipinski's drug-likeness criteria with zero violations, high predicted GI absorption, and moderate lipophilicity (consensus LogP 1.73–2.51). Isoorientin showed two Lipinski violations attributable to its higher molecular weight (448.38 g/mol), elevated hydrogen-bonding capacity (8 donors, 11 acceptors), and high TPSA (201.28 Å^2), consistent with reduced oral bioavailability and membrane permeability (GI absorption: Low; bioavailability score: 0.17). p-Hydroxybenzoic acid demonstrated the most favorable pharmacokinetic profile highest bioavailability score (0.85), full drug-likeness compliance, and high GI absorption but produced the weakest docking scores across all three targets. CYP450 analysis indicated that Casticin, Chrysophenol, and Luteolin are predicted inhibitors of CYP3A4; Luteolin additionally showed predicted inhibitory activity toward CYP2D6. Neither p-Hydroxybenzoic acid nor Isoorientin inhibited the tested CYP isoforms.

Figure 5

Table 2. SwissADME-predicted ADMET parameters of five phytocompounds from *Vitex negundo*.

Compound	MW (g/mol)	HBD	HBA	TPSA (Å²)	LogP	GI Absorption	Bioavail. Score	Lipinski Viol.	CYP3A4 Inhibitor
Casticin	374.34	2	8	107.59	2.51	High	0.55	0	Yes
Chrysophenol	360.31	3	8	118.59	2.01	High	0.55	0	Yes
Isoorientin	448.38	8	11	201.28	−0.34	Low	0.17	2	No
Luteolin	286.24	4	6	111.13	1.73	High	0.55	0	Yes

Compound	MW (g/mol)	HBD	HBA	TPSA (Å²)	LogP	GI Absorption	Bioavail. Score	Lipinski Viol.	CYP3A4 Inhibitor
p-Hydroxybenzoic acid	138.12	2	3	57.53	1.05	High	0.85	0	No

MW = Molecular Weight; HBD = Hydrogen Bond Donors; HBA = Hydrogen Bond Acceptors; TPSA = Topological Polar Surface Area; GI = Gastrointestinal; Bioavail. Score = Bioavailability Score; Lipinski Viol. = Number of Lipinski Rule of Five Violations. Data generated using SwissADME (http://www.swissadme.ch).

3.5 In Vitro Antibacterial Activity

Against macrolide-resistant *S. aureus* (resistant to Azithromycin, Clarithromycin, and Erythromycin), zones of inhibition were: *E. angustifolia* 9 mm, *C. officinalis* 8 mm, *V. negundo* 7 mm, and ethanol control 6 mm.[6] All three tinctures exceeded the ethanol control, confirming antibacterial activity attributable to plant-derived phytocompounds rather than the solvent vehicle.

Against pan-drug-resistant Vitex Negundo produced a zone of inhibition (7 mm) exceeding the ethanol control (6 mm), confirming antibacterial activity attributable to plant-derived phytocompounds rather than the solvent vehicle. These results are summarised in Table 3.

Table 3. Mean inhibition zones (mm) generated by homoeopathic mother tinctures against antibiotic-resistant bacteria in the Kirby–Bauer disk diffusion assay.

Remedy	Drug Strength	S. aureus (Macrolide-Resistant)
Vitex negundo (MT)	1/10	7 mm
Ethanol control	—	6 mm

MT = Mother Tincture. Zones measured after 24 hours incubation at 37°C. Data from references 6 and 7.

4. Discussion

The present study integrated molecular docking and ADMET characterisation of *V. negundo* phytocompounds with in vitro disk diffusion validation, using antibiotic resistance-associated proteins as computational targets. Chrysophenol returned the highest binding energy across all three receptors (−10.5 kcal/mol at 4ALI), accompanied by a clean ADMET profile — zero Lipinski violations, high predicted GI absorption, and a consensus LogP of 2.01. Luteolin ranked second at 4ALI (−9.3 kcal/mol); its antioxidant and direct bactericidal properties have been characterised extensively across multiple phytopharmacological investigations.[9] Casticin (−8.6 kcal/mol at 4ALI) also met pharmacokinetic acceptability criteria.

From a homoeopathic standpoint, these results carry particular weight: mother tinctures are the pharmacopoeially defined precursor to potentised preparations, retaining constituent phytochemicals at concentrations where direct pharmacological activity is measurable. *V. negundo* mother tincture produced 7 mm clearance against macrolide-resistant *S. aureus*, exceeding the ethanol control by 1 mm, validating the computational binding predictions. Establishing that key constituents bind strongly to clinically relevant resistance proteins provides a phytochemical rationale for this observed antibacterial activity. This study is exploratory; results are hypothesis-generating and do not constitute evidence of clinical efficacy.

Isoorientin scored up to −8.2 kcal/mol but carries two Lipinski violations and a TPSA of 201.28 Å^2, both of which forecast poor oral absorption. Since *V. negundo* preparations are predominantly applied topically in traditional practice, this constraint is less limiting than it would be for a candidate intended for oral use.

The ethanol control in our prior study was matched for solvent concentration rather than compared against standard antibiotics deliberate, given the non-equivalence of concentration bases.[6] *V. negundo* exceeded this control (7 mm vs. 6 mm), confirming the observed inhibition reflects genuine phytocompound activity, not a solvent artefact. Against pan-resistant *K. pneumoniae*, *V. negundo* did not surpass the ethanol control, consistent with the more complex resistance mechanisms of this organism and possible inadequate outer membrane penetration at the concentrations tested.[11]

Several limitations apply. Docking scores are computational estimates and do not confirm biological inhibition. Disk diffusion data derive from single clinical isolates, constraining generalisability across strains. Tincture batch composition was not independently verified, and the docking model cannot capture potential synergistic or antagonistic interactions among multiple constituents. Future work should prioritise minimum inhibitory concentration (MIC) determination, time-kill studies, and in vivo evaluation of lead compounds before clinical translation is considered.

5. Conclusion

V. negundo phytocompounds particularly Chrysophenol (−10.5 kcal/mol) and Luteolin (−9.3 kcal/mol) against 4ALI demonstrate strong in silico binding to antibiotic resistance proteins alongside favorable drug-likeness profiles. *V. negundo* mother tincture validates these findings with 7 mm clearance against macrolide-resistant *S. aureus*, exceeding the ethanol control. These integrated computational and experimental results provide a molecular rationale for advancing *V. negundo* phytocompounds toward further preclinical investigation as candidate antimicrobial agent against multidrug-resistant organisms. Future studies should pursue MIC determination, mechanistic pathway studies, and in vivo models to enable clinical translation.

Funding

No external funding was available.

Data Availability Statement

The docking result files and ADMET Data from this study are available from the corresponding author on reasonable request. Primary in vitro susceptibility data are reported in references 6 and 7.

Conflicts of Interest

The authors have declared no conflicts of interest.

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