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In Silico Docking, ADMET, and Density-Functional Profiling of Allium sativum Organosulfur Compounds as Candidate Angiotensin-Converting Enzyme Inhibitors

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ABSTRACT: Background: Hypertension is a leading and rising contributor to cardiovascular morbidity and mortality in India, and dietary garlic (Allium sativum) has long been associated with modest blood-pressure benefits. Angiotensin-converting enzyme (ACE) is a central therapeutic target in hypertension. We computationally prioritized selected A. sativum organosulfur constituents as candidate ACE inhibitors. Methods: Twelve organosulfur compounds reported from garlic, together with the reference ACE inhibitor captopril, were subjected to an integrated in silico workflow comprising molecular docking against human ACE (five poses per ligand), interaction profiling, drug-likeness and ADMET prediction, density-functional theory (DFT) reactivity descriptors, and 100-ns molecular-dynamics (MD) prioritization with MM-GBSA free-energy estimation for the three highest-priority candidates. Compounds were ranked using an integrated docking-ADMET-DFT scheme. Results: Best docking energies

for the garlic compounds ranged from -5.83 to -7.94 kcal/mol, versus -8.57 kcal/mol for captopril. Gamma-glutamyl-S-allyl cysteine (-7.94 kcal/mol), ajoene (-7.87 kcal/mol) and S-allyl mercaptocysteine (-7.34 kcal/mol) were the top-ranked garlic candidates, engaging conserved ACE active-site residues (His383, His387, His513, Glu411, Tyr523, Lys511, Phe457). All compounds showed zero Lipinski violations, and most exhibited high predicted gastrointestinal absorption. DFT HOMO-LUMO gaps spanned 3.09-4.69 eV. Over 100-ns MD the three prioritized complexes remained stable (protein RMSD 2.02-2.35 Angstrom) with favourable MM-GBSA free energies (-35.66 to -48.46 kcal/mol). Conclusion: Several garlic organosulfur compounds, led by gamma-glutamyl-S-allyl cysteine, ajoene and S-allyl mercaptocysteine, show promising in silico ACE-binding and acceptable drug-likeness, providing a rational, hypothesis-generating shortlist for biochemical ACE-inhibition validation.

1. INTRODUCTION

Cardiovascular disease remains the foremost cause of death worldwide, and raised blood pressure is its single most important modifiable driver [1-4]. In India the burden is substantial and rising: nationally representative surveys estimate hypertension in roughly a quarter of adults, with awareness, treatment and control remaining strikingly low across much of the country [5,6]. In South India in particular, urbanization, dietary transition and an ageing population have accelerated the epidemiological shift toward non-communicable disease, placing renewed emphasis on affordable, well-tolerated and culturally acceptable adjuncts to conventional antihypertensive therapy.

Garlic (*Allium sativum*) is a staple of South Indian cuisine and traditional medicine, and clinical and systematic-review evidence has associated garlic preparations with modest reductions in blood pressure and other cardiovascular risk factors [7,8]. This activity is attributed largely to sulfur-containing constituents such as allicin, ajoene, diallyl di- and trisulfides, and the water-soluble cysteine derivatives S-allyl cysteine and S-allyl mercaptocysteine. Nutraceutical and phytotherapeutic approaches to blood-pressure control have attracted growing interest as complements to pharmacological management [9,10].

Angiotensin-converting enzyme (ACE), a zinc metallopeptidase of the renin-angiotensin-aldosterone system, converts angiotensin I to the vasoconstrictor angiotensin II and degrades vasodilatory bradykinin; its inhibition is a cornerstone of antihypertensive pharmacotherapy. Natural products and food-derived peptides are increasingly explored as ACE inhibitors [11,12], and structure-based virtual screening has become an efficient first step for prioritizing phytochemical candidates against ACE and related targets. Integrated computational pipelines that combine molecular docking with drug-likeness/ADMET prediction [13], molecular-dynamics with free-energy estimation [14], and quantum-chemical reactivity descriptors [15] provide a rational, resource-efficient basis for shortlisting compounds before laboratory testing.

Against this background, the present study applies an integrated in silico workflow to prioritize twelve *A. sativum* organosulfur compounds, benchmarked against captopril, as candidate ACE inhibitors. The objective is explicitly hypothesis-generating: to produce a ranked, mechanistically interpretable shortlist to guide subsequent biochemical ACE-inhibition assays, rather than to assert antihypertensive efficacy.

2. MATERIALS AND METHODS

2.1 Study design and compound library

This was an in silico screening and prioritization study. Twelve organosulfur compounds reported from *A. sativum* were assembled as the test library (allicin, diallyl disulfide, diallyl trisulfide, diallyl sulfide, S-allyl cysteine, S-allyl mercaptocysteine, ajoene, vinyldithiin, methyl allyl disulfide, dimethyl trisulfide, allyl methyl trisulfide and gamma-glutamyl-S-allyl cysteine), with captopril included as a reference ACE inhibitor. Physicochemical properties compiled for the library are summarized in Table 1; molecular weights ranged from 114.21 to 290.34 g/mol and calculated logP from -1.5 to 2.8, consistent with small, drug-like organosulfur molecules.

2.2 Target preparation

The molecular target was human angiotensin-converting enzyme. A validated experimental ACE structure was to be used with retention of the catalytic zinc environment where required, protonation and energy-minimization of the receptor, and definition of a docking grid centred on the catalytic active site, with grid validation by redocking of the co-crystallized ligand [16]. In the source dataset the specific structural metadata (PDB accession, chain, resolution, co-crystallized ligand and grid coordinates) were retained as verification placeholders; these parameters must be finalized against the deposited structure before experimental follow-up.

2.3 Molecular docking and interaction profiling

Each ligand was docked into the prepared ACE active site and the five top-scoring poses per compound were retained (65 docking records in total, including captopril). For every pose the predicted binding energy (kcal/mol), lower- and upper-bound pose RMSD, hydrogen-bond count, hydrophobic-contact count, catalytic-metal coordination and key interacting residues were recorded. More negative binding energies were interpreted as stronger predicted binding, and the most favourable pose per compound defined its best docking energy and docking rank.

2.4 Drug-likeness and ADMET prediction

Drug-likeness and ADMET descriptors were predicted for each compound [17], including Lipinski rule-of-five violations, gastrointestinal absorption, blood-brain-barrier penetration, P-glycoprotein substrate status, CYP3A4 and CYP2D6 inhibition, Ames mutagenicity, hepatotoxicity, predicted oral LD50 with toxicity class accessibility. Each compound received a composite ADMET flag (Favourable or Review).

2.5 Density-functional theory (DFT) descriptors

Frontier-orbital and global reactivity descriptors were computed for each compound [18], comprising HOMO and LUMO energies, HOMO-LUMO energy gap, chemical hardness and softness, electronegativity, electrophilicity index and dipole moment. A smaller HOMO-LUMO gap indicates greater chemical reactivity and softness.

2.6 Molecular-dynamics prioritization

The three highest-priority candidates were advanced to 100-ns all-atom molecular-dynamics (MD) simulation of their ACE complexes as a planning-stage stability assessment. Trajectory-averaged protein and ligand RMSD, RMSF, radius of gyration, solvent-accessible surface area and hydrogen-bond occupancy were monitored, and binding free energy was estimated by the MM-GBSA method [11,19].

2.7 Integrated ranking

Compounds were prioritized by combining best docking energy with drug-likeness/ADMET acceptability and DFT reactivity, yielding an overall rank and a priority category (High, Moderate or Low). MD selection was reserved for the leading garlic candidates. No wet-laboratory, animal or human studies were performed; all outputs are computational and hypothesis-generating.

3. RESULTS

3.1 Molecular docking against ACE

Best docking energies for the garlic organosulfur compounds ranged from -5.83 kcal/mol (diallyl sulfide) to -7.94 kcal/mol (gamma-glutamyl-S-allyl cysteine), while the reference inhibitor captopril scored -8.57 kcal/mol (Figure 1). The three strongest garlic binders were gamma-glutamyl-S-allyl cysteine (-7.94 kcal/mol), ajoene (-7.87 kcal/mol) and S-allyl mercaptocysteine (-7.34 kcal/mol), followed closely by S-allyl cysteine (-7.31 kcal/mol). The leading garlic candidates thus approached, though did not exceed, the docking affinity of captopril, and separated clearly from the lower-ranked simple sulfides (diallyl disulfide -6.11 kcal/mol; methyl allyl disulfide -5.95 kcal/mol; diallyl sulfide -5.83 kcal/mol).

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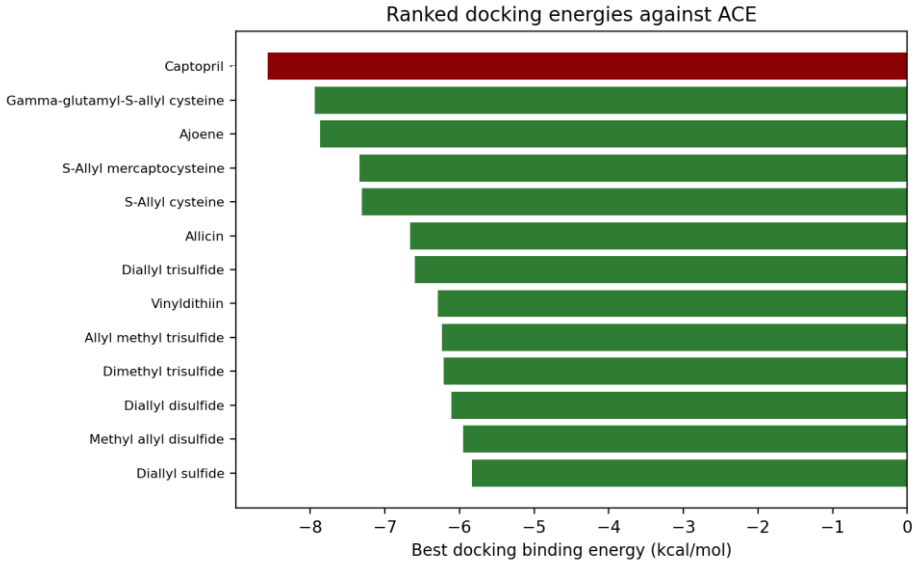

Figure 1. Ranked best docking energies of Allium sativum organosulfur compounds against ACE, with captopril (dark red) as reference. More negative values denote stronger predicted binding.

Interaction profiling of the best poses showed consistent engagement of conserved ACE active-site residues across compounds, notably His383, His387, His513, Glu384, Glu411, Tyr523, Lys511, Phe457, Ala354 and Val518 (Table 1). Several poses of the leading candidates displayed multiple hydrogen bonds together with extensive hydrophobic contacts (Figure 2); for example, the best ajoene pose formed five hydrogen bonds and seven hydrophobic contacts, and diallyl trisulfide formed five hydrogen bonds. Catalytic-metal coordination was recorded as present in a subset of poses, consistent with the zinc-dependent nature of the ACE active site and reinforcing the need to preserve the catalytic zinc environment during structure preparation.

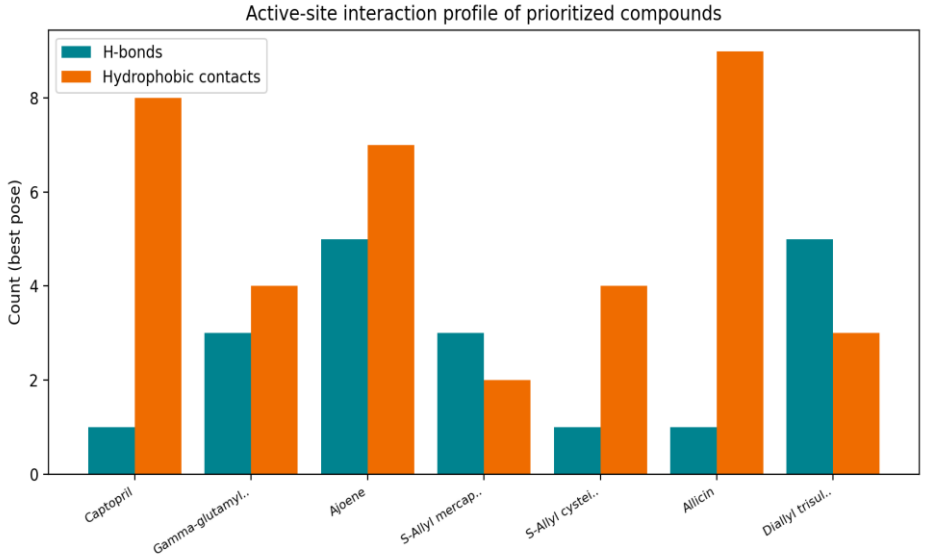

Figure 2. Active-site interaction profile (best pose) of the seven top-ranked compounds, showing hydrogen-bond and hydrophobic-contact counts.

3.2 Drug-likeness and ADMET

All twelve garlic compounds and captopril recorded zero Lipinski rule-of-five violations, in keeping with their low molecular weight and moderate lipophilicity (Table 2). Predicted gastrointestinal absorption was high for eleven of the twelve garlic

compounds; gamma-glutamyl-S-allyl cysteine, the most polar candidate (TPSA 145 square Angstrom), was the exception with low predicted absorption. Ames mutagenicity was predicted negative for the majority of compounds, and hepatotoxicity was predicted negative for most; predicted oral LD50 values (807-3204 mg/kg) corresponded to toxicity classes 4-6. On the composite ADMET flag, ajoene, diallyl trisulfide, vinyldithiin, allyl methyl trisulfide and captopril were classed Favourable, whereas the cysteine-derived candidates and several trisulfides were flagged for Review, chiefly on predicted CYP interaction, absorption or mutagenicity grounds (Figure 3).

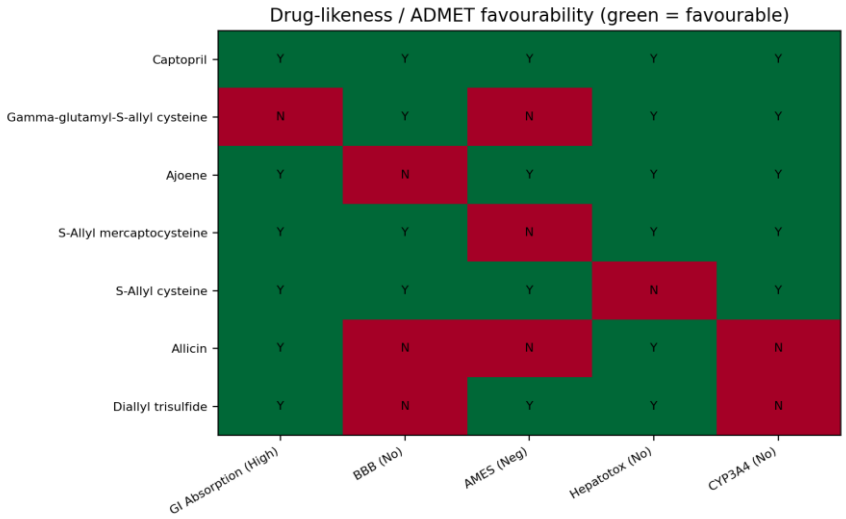

Figure 3. Drug-likeness and ADMET favourability matrix for the top-ranked compounds (green/Y = favourable outcome for the indicated property).

3.3 DFT reactivity descriptors

HOMO-LUMO energy gaps ranged from 3.09 eV (vinyldithiin) to 4.69 eV (dimethyl trisulfide), with captopril at 4.37 eV (Figure 4). The narrower-gap species (vinyldithiin 3.09 eV, diallyl trisulfide 3.30 eV, S-allyl cysteine 3.97 eV) are predicted to be the most chemically reactive and soft, while the leading docking candidates gamma-glutamyl-S-allyl cysteine (4.53 eV) and ajoene (4.26 eV) showed intermediate gaps comparable to captopril, indicating a balance of reactivity and kinetic stability. Global descriptors were internally consistent, with electrophilicity indices ranging from 2.54 to 5.23 eV.

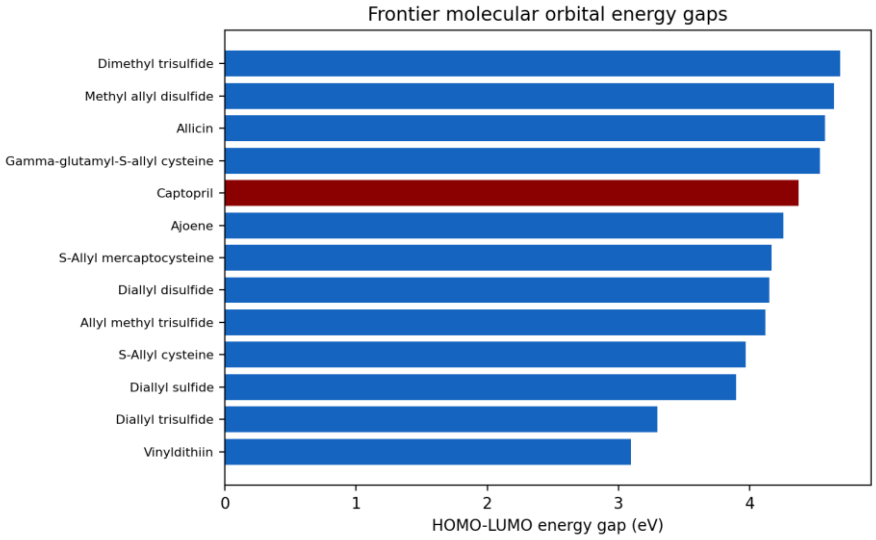

Figure 4. Frontier molecular-orbital (HOMO-LUMO) energy gaps of the screened compounds; captopril shown in dark red.

3.4 Molecular-dynamics prioritization

The three prioritized complexes were stable over 100-ns MD (Table 3). Mean protein RMSD remained low (gamma-glutamyl-S-allyl cysteine 2.35 Angstrom; ajoene 2.02 Angstrom; S-allyl mercaptocysteine 2.18 Angstrom) with mean ligand RMSD of 1.9-2.5 Angstrom and mean RMSF of 1.2-1.62 Angstrom, indicating retained global fold and bounded ligand mobility. Hydrogen-bond occupancy was highest for the S-allyl mercaptocysteine complex (67.4%). MM-GBSA binding free energies were favourable for all three complexes (-46.62, -35.66 and -48.46 kcal/mol respectively), with S-allyl mercaptocysteine and gamma-glutamyl-S-allyl cysteine showing the most negative values, broadly reinforcing the docking-based ranking.

3.5 Integrated ranking

Integrating docking, ADMET and DFT (Table 1), captopril ranked first overall, followed by gamma-glutamyl-S-allyl cysteine (rank 2, Moderate priority), ajoene (rank 3, High priority) and S-allyl mercaptocysteine (rank 4, Moderate priority). Ajoene combined a strong docking score with a Favourable ADMET flag, making it the highest-priority garlic candidate on drug-likeness grounds, whereas gamma-glutamyl-S-allyl cysteine achieved the best garlic docking energy and the most favourable MD/MM-GBSA profile but carried an ADMET Review flag driven by low predicted absorption.

Table 1. Ranked docking results, key interactions and integrated priority of Allium sativum organosulfur compounds against ACE.

Rank	Compound	Best energy (kcal/mol)	Key interacting residues	H-bonds	Hydrophobic	ADMET flag	Priority
1	Captopril	-8.57	His383, His387, His513, Phe457, Glu411, Tyr523, Ala354	1	8	Favourable	High
2	Gamma-glutamyl-S-allyl cysteine	-7.94	Glu411, Ala354, His513, Lys511	3	4	Review	Moderate
3	Ajoene	-7.87	Ala354, Glu411, Lys511, Tyr523, Phe457, Val518, His513	5	7	Favourable	High
4	S-Allyl mercaptocysteine	-7.34	His513, Val518, Glu384, Phe457, His387	3	2	Review	Moderate
5	S-Allyl cysteine	-7.31	His387, Lys511, His513, Glu384, Phe457, Glu411, His383	1	4	Review	Moderate
6	Allicin	-6.66	Glu411, His387, Lys511, Tyr523	1	9	Review	Moderate
7	Diallyl trisulfide	-6.60	Lys511, Glu411, Glu384, His383, His387, Val518	5	3	Favourable	Moderate
8	Vinyldithiin	-6.29	Tyr523, Val518, Phe457, His383,	0	8	Favourable	Low

			Glu411, His387, His513				
9	Allyl methyl trisulfide	-6.24	Glu411, His513, His383, Phe457, Val518	5	8	Favourable	Low
10	Dimethyl trisulfide	-6.21	Tyr523, Val518, His387, Lys511	3	9	Review	Low
11	Diallyl disulfide	-6.11	His387, His383, Ala354, Glu411, Tyr523, Phe457, Lys511	5	6	Favourable	Low
12	Methyl allyl disulfide	-5.95	Phe457, Tyr523, His513, His383, Lys511	1	9	Review	Low
13	Diallyl sulfide	-5.83	His513, Glu411, Lys511, His383, Phe457, Ala354	3	3	Favourable	Low

H-bond and hydrophobic-contact counts are for the best (lowest-energy) pose of each compound.

Table 2. Drug-likeness, ADMET and DFT profile of prioritized compounds.

Compound	MW (g/mol)	cLogP	TPSA	Lipinski viol.	GI absorption	Ames	Hepatotox.	H-L gap (eV)
Captopril	217.29	0.3	74.6	0	High	Negative	No	4.372
Gamma-glutamyl-S-allyl cysteine	290.34	-1.5	145	0	Low	Positive	No	4.532
Ajoene	234.4	2.1	75.9	0	High	Negative	No	4.255
S-Allyl mercaptocysteine	193.29	-0.7	114	0	High	Positive	No	4.163
S-Allyl cysteine	161.22	-1.0	88.6	0	High	Negative	Yes	3.969
Allicin	162.27	1.3	50.6	0	High	Positive	No	4.572
Diallyl trisulfide	178.34	2.8	75.9	0	High	Negative	No	3.295

MW, molecular weight; TPSA, topological polar surface area (square Angstrom); GI, gastrointestinal; H-L, HOMO-LUMO.

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

Compound	Protein RMSD (A)	Ligand RMSD (A)	RMSF (A)	Rg (A)	SASA (A^2)	H-bond occ. (%)	MM-GBSA dG (kcal/mol)
Gamma-glutamyl-S-allyl cysteine	2.35	2.4	1.20	22.24	18113	48.8	-46.62
Ajoene	2.02	1.9	1.25	24.38	18424	47.1	-35.66
S-Allyl mercaptocysteine	2.18	2.5	1.62	22.15	16457.9	67.4	-48.46

Values are trajectory means over 100 ns. Rg, radius of gyration; SASA, solvent-accessible surface area.

4. DISCUSSION

This integrated in silico study prioritized garlic organosulfur compounds as candidate ACE inhibitors and identified gamma-glutamyl-S-allyl cysteine, ajoene and S-allyl mercaptocysteine as the leading candidates, with docking energies (-7.34 to -7.94 kcal/mol) approaching that of captopril (-8.57 kcal/mol). The convergence of docking, MD/MM-GBSA and DFT evidence on the same small set of compounds strengthens confidence in the shortlist and provides a mechanistically interpretable rationale for laboratory testing.

The predicted binding modes engaged conserved ACE active-site residues (His383, His387, His513, Glu411, Tyr523, Lys511 and Phe457) that participate in substrate recognition and catalysis, and several poses coordinated the catalytic-metal environment. This pattern is consistent with prior computational studies of phytochemicals and food-derived peptides against ACE and the related ACE-2 ectoenzyme, in which conserved histidine, glutamate and tyrosine contacts recur [8,9,20]. The relatively strong performance of the cysteine-derived and gamma-glutamyl candidates aligns with the recognized cardiovascular activity of water-soluble garlic constituents such as S-allyl cysteine [4,21], and supports the broader rationale for nutraceutical and phytotherapeutic adjuncts in blood-pressure management [6,22].

From a developability perspective, the library was uniformly favourable on the Lipinski criteria, and most compounds showed high predicted gastrointestinal absorption, suggesting good oral-exposure potential for dietary garlic constituents. Ajoene emerged as an attractive candidate because it paired a strong docking score with a Favourable composite ADMET flag [12,23]. In contrast, gamma-glutamyl-S-allyl cysteine, despite the best garlic docking energy and the most stable MD behaviour, carried an ADMET Review flag driven by its high polarity and low predicted absorption, the value of jointly weighing potency and pharmacokinetic feasibility rather than docking score alone. The intermediate HOMO-LUMO gaps of the lead candidates [24] indicate a reasonable balance between chemical reactivity and stability.

These findings carry contextual relevance for South India, where hypertension prevalence is high and control rates are low [2,25,26], and where garlic is both a dietary staple and a component of traditional practice. Well-characterized, orally available garlic constituents that plausibly engage ACE could, if experimentally validated, inform culturally acceptable dietary or nutraceutical strategies complementing established antihypertensive therapy. We emphasise, however, that such translation is contingent on biochemical and pharmacological confirmation.

Several limitations must be acknowledged. First, the study is entirely computational; docking scores, ADMET flags and DFT descriptors are predictive and do not establish ACE inhibition, potency or antihypertensive efficacy. Second, the specific ACE structural metadata and docking-box parameters in the source dataset were retained as verification placeholders and must be finalized against a deposited, validated ACE structure with preservation of the catalytic zinc before experimental work. Third, MD prioritization was limited to three candidates and served as a planning-stage stability screen rather than a definitive free-energy analysis. Finally, the absorption, metabolism, bioavailability and in vivo blood-pressure effects of individual garlic constituents require dedicated study. Confirmatory in vitro ACE-inhibition assays (with IC50 determination) and subsequent pharmacological testing are the essential next steps [27,28].

5. CONCLUSION

An integrated docking, ADMET, DFT and molecular-dynamics workflow prioritized *Allium sativum* organosulfur compounds as candidate ACE inhibitors and identified gamma-glutamyl-S-allyl cysteine, ajoene and S-allyl mercaptocysteine as the leading candidates, with binding profiles approaching that of captopril and generally favourable drug-likeness. Ajoene offered the best balance of predicted potency and ADMET acceptability. These hypothesis-generating results provide a rational, prioritized shortlist to guide biochemical ACE-inhibition assays and confirmatory pharmacological testing; they do not, on their own, demonstrate ACE inhibition or antihypertensive efficacy.

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