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Molecular Docking and ADMET Profiling of *Tinospora cordifolia* Phytochemicals Against Dihydrofolate Reductase: An Integrated in Silico Docking, Drug-Likeness, DFT, and Molecular-Dynamics Prioritization Study

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ABSTRACT: Background: Dihydrofolate reductase (DHFR) is a validated target in cancer, bacterial, and protozoal chemotherapy, but classical antifolates such as methotrexate are limited by toxicity and resistance. *Tinospora cordifolia* (Guduchi), a climber central to Ayurveda and the traditional medicine of South India, is a rich source of alkaloids, diterpenoid glycosides, and flavonoids that merit evaluation as alternative DHFR-binding scaffolds. Objective: To computationally screen and prioritize twelve *T. cordifolia* phytoconstituents as DHFR inhibitors using molecular docking, drug-likeness and ADMET prediction, density functional theory (DFT), and molecular-dynamics (MD) analysis, benchmarked against methotrexate. Methods: Twelve phytochemicals and the reference inhibitor were docked into the DHFR active site (five poses each; best binding energy retained). Drug-likeness (Lipinski), ADMET descriptors, and DFT frontier-orbital parameters were computed, and three top complexes underwent 100-ns MD with MM-

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GBSA free-energy estimation, feeding a tiered priority ranking. Results: Methotrexate showed the strongest predicted binding (−9.34 kcal/mol). Among phytochemicals, cordifolioside A (−8.77 kcal/mol), cordifolioside B (−8.65 kcal/mol), berberine (−8.43 kcal/mol), and tinocordiside (−8.43 kcal/mol) ranked highest, engaging conserved residues (Ile5, Val8, Ala9, Asp27, Phe31, Lys32, Arg57, Ile94, Tyr100, Thr113). Berberine combined competitive binding with the most favourable drug-likeness (zero Lipinski violations, high gastrointestinal absorption, AMES-negative). Tinocordiside displayed the smallest HOMO–LUMO gap (3.095 eV). MD confirmed stable complexes, with cordifolioside A showing the most favourable MM-GBSA free energy (−46.98 kcal/mol) and 52.2% hydrogen-bond occupancy. Conclusion: Berberine and cordifolioside A emerge as leading *T. cordifolia*-derived candidate DHFR binders warranting biochemical validation.

1. INTRODUCTION

Dihydrofolate reductase (DHFR) catalyses the NADPH-dependent reduction of dihydrofolate to tetrahydrofolate, a cofactor indispensable for the biosynthesis of purines, thymidylate, and several amino acids. Because rapidly proliferating cells depend on continuous folate turnover, DHFR is an established target across oncology, antibacterial, antimalarial, and antiprotozoal chemotherapy [1-3]. The classical antifolate methotrexate remains a cornerstone of this class, yet its clinical utility is constrained by dose-limiting toxicity, a narrow therapeutic index, and the emergence of resistance, motivating the search for structurally novel inhibitors with improved safety [4,5].

Tinospora cordifolia (Willd.) Miers, known as Guduchi or Giloy, is a deciduous climbing shrub deeply embedded in Ayurveda and the folk medicine of South India, where it is used as a rasayana (rejuvenator) and for the management of fever, diabetes, inflammation, and immune dysfunction [6,7]. Phytochemical studies have identified more than two hundred constituents from the genus *Tinospora*, including isoquinoline and aporphine alkaloids (berberine, palmatine, jatrorrhizine, magnoflorine), diterpenoid glycosides and lactones (tinosporaside, tinocordiside, columbin), phenylpropanoid glycosides (cordifolioside A and B), phytosterols, and flavonoids such as quercetin [8,9]. Several of these scaffolds show antioxidant, immunomodulatory, antimicrobial, and anticancer activity in experimental systems [10,11].

Alkaloids and glycosides of this plant have repeatedly surfaced as promising binders in structure-based screens targeting viral, inflammatory, and oncogenic proteins [8,12]. In parallel, virtual-screening campaigns of phytochemicals against DHFR and related resistance targets have highlighted natural products such as berberine and quercetin as competitive ligands worthy of experimental follow-up [3,13]. Integrated in silico pipelines combining docking with absorption–distribution–metabolism–excretion–toxicity (ADMET) prediction, density functional theory (DFT), and molecular-dynamics (MD) simulation now allow rational prioritization of candidates before costly biochemical assays [11,14].

Despite the pharmacological prominence of *T. cordifolia*, a focused computational appraisal of its major phytoconstituents as DHFR inhibitors, integrating binding, drug-likeness, electronic-structure, and dynamic-stability evidence, has not been systematically reported. The present study therefore screens twelve *T. cordifolia* phytochemicals against DHFR, benchmarks them against methotrexate, and applies a multi-parameter prioritization to nominate leads for biochemical validation, framed within the South Indian tradition of Guduchi use while adhering strictly to the computational, hypothesis-generating nature of the data.

2. MATERIALS AND METHODS

2.1 Study design and ligand library

This was an in silico screening and prioritization study. A curated library of twelve phytochemicals reported from *T. cordifolia* was assembled: two diterpenoid glycosides (tinosporaside, tinocordiside), two phenylpropanoid glycosides (cordifolioside A and B), four isoquinoline/aporphine alkaloids (berberine, palmatine, jatrorrhizine, magnoflorine), an additional aporphine alkaloid (tembetarine), a diterpenoid lactone (columbin), a phytosterol (β-sitosterol), and the flavonol quercetin. Methotrexate served as

the reference DHFR inhibitor. Physicochemical descriptors (molecular weight, hydrogen-bond donors/acceptors, cLogP, topological polar surface area [TPSA]) were compiled for each ligand (Table 1).

2.2 Target preparation and docking

The DHFR target structure was retrieved and prepared using a validated crystal structure with defined active-site residues [placeholder: PDB ID, chain, resolution, and co-crystallized ligand to be inserted from the verified target record]. Water molecules and heteroatoms were removed, polar hydrogens and charges assigned, and a grid box centred on the folate-binding pocket [placeholder: grid centre and dimensions]. Each ligand was energy-minimized and docked, generating five poses per compound; the most favourable binding energy (kcal/mol) and its interaction profile were retained. Predicted contacts (hydrogen bonds, hydrophobic contacts, π-stacking) and key interacting residues were catalogued for each best pose.

2.3 Drug-likeness and ADMET prediction

Drug-likeness was evaluated using Lipinski's rule of five, and ADMET descriptors were predicted for gastrointestinal (GI) absorption, blood–brain-barrier penetration, P-glycoprotein substrate status, cytochrome P450 (CYP3A4, CYP2D6) inhibition, AMES mutagenicity, hepatotoxicity, predicted oral LD50 and toxicity class accessibility [15]. Each compound was assigned an overall ADMET flag (favourable versus requiring review).

2.4 DFT descriptors

Frontier-orbital energies (HOMO, LUMO) were computed and used to derive the HOMO–LUMO energy gap, chemical hardness and softness, electronegativity, electrophilicity index, and dipole moment as indicators of reactivity and charge-transfer propensity [16].

2.5 Molecular-dynamics simulation

Three prioritized protein–ligand complexes (cordifolioside A, cordifolioside B, berberine) were subjected to 100-ns MD simulations. 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 binding free energy was estimated by the MM-GBSA method [2,13].

3. RESULTS

3.1 Physicochemical profile of the ligand library

The twelve phytochemicals spanned a broad chemical space (molecular weight 302.24–522.50 g/mol; cLogP −1.0 to 8.8; TPSA 20.2–197.1 Å²). The isoquinoline alkaloids (berberine, palmatine, jatrorrhizine) were compact, moderately lipophilic cations with low TPSA, whereas the phenylpropanoid glycosides (cordifolioside A and B) were large, highly polar molecules. β-Sitosterol was a strong lipophilic outlier (cLogP 8.8), and quercetin represented a polar flavonol (Table 1).

Table 1. Physicochemical descriptors of Tinospora cordifolia phytochemicals and the reference inhibitor methotrexate.

Compound	Class	MW (g/mol)	HBD	HBA	cLogP	TPSA (Å²)
Tinosporaside	Diterpenoid glycoside	406.43	5	9	−0.4	149.8
Cordifolioside A	Phenylpropanoid glycoside	522.50	7	12	−1.0	197.1
Cordifolioside B	Phenylpropanoid glycoside	522.50	7	12	−0.9	197.1
Magnoflorine	Aporphine alkaloid	342.41	1	4	1.2	49.7
Berberine	Isoquinoline alkaloid	336.36	0	4	1.5	40.8
Palmatine	Isoquinoline alkaloid	352.41	0	4	1.8	40.8
Jatrorrhizine	Isoquinoline alkaloid	338.38	1	4	1.4	51.8
Tembetarine	Aporphine alkaloid	344.45	1	4	1.6	49.7

Tinocordiside	Diterpenoid glycoside	422.43	6	10	−0.8	170.0
Columbin	Diterpenoid lactone	358.39	0	6	2.0	78.9
β-Sitosterol	Phytosterol	414.71	1	1	8.8	20.2
Quercetin	Flavonol	302.24	5	7	1.5	131.4
Methotrexate (ref.)	Reference inhibitor	454.44	5	12	−1.9	210.5

3.2 Molecular docking against DHFR

Methotrexate exhibited the strongest predicted binding energy (−9.34 kcal/mol), consistent with its role as a high-affinity antifolate and validating the docking protocol. Among the phytochemicals, best binding energies ranged from −8.77 to −7.72 kcal/mol. Cordifolioside A (−8.77 kcal/mol) was the top-ranked natural ligand, followed by cordifolioside B (−8.65 kcal/mol), berberine (−8.43 kcal/mol), tinocordiside (−8.43 kcal/mol), jatrorrhizine (−8.26 kcal/mol), tinosporaside (−8.25 kcal/mol), and quercetin (−8.25 kcal/mol). The narrow spread of scores (within ~1.05 kcal/mol of one another) indicates that several structurally diverse scaffolds occupy the DHFR pocket with comparable predicted affinity (Figure 1, Table 2).

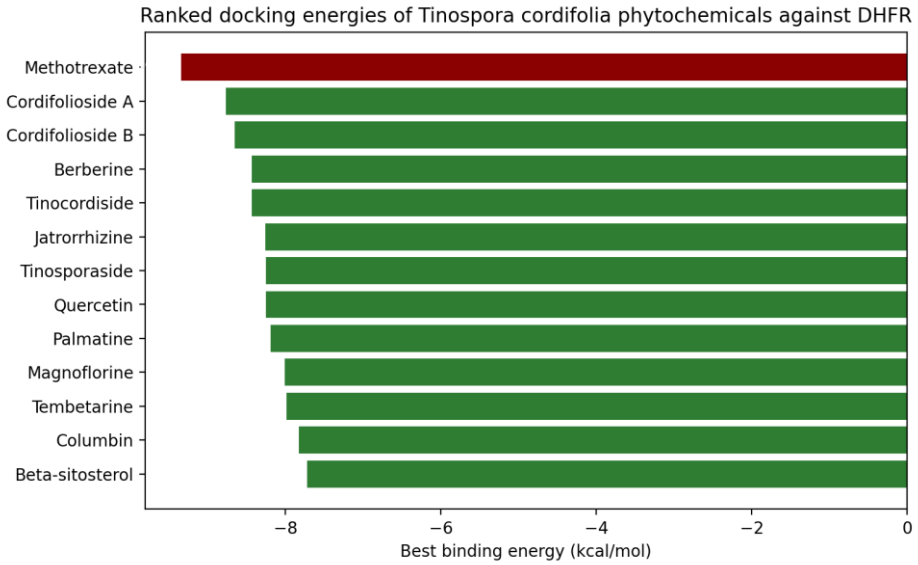

Figure 1. Ranked best docking energies of Tinospora cordifolia phytochemicals against DHFR, with methotrexate (dark red) as reference.

Interaction profiling of the best poses showed that binding was mediated by a conserved constellation of active-site residues, including Ile5, Val8, Ala9, Asp27, Phe31, Lys32, Arg57, Ile94, Tyr100, and Thr113. Cordifolioside A engaged Val8, Ile5, Ile94, Ala9, Phe31, Thr113, and Lys32 with five hydrogen bonds and seven hydrophobic contacts, while berberine formed four hydrogen bonds anchored by Tyr100, Asp27, Ile94, and Arg57. Hydrogen-bond counts, hydrophobic contacts, and π-stacking varied across the prioritized compounds, reflecting distinct binding modes among alkaloid and glycoside scaffolds (Figure 2).

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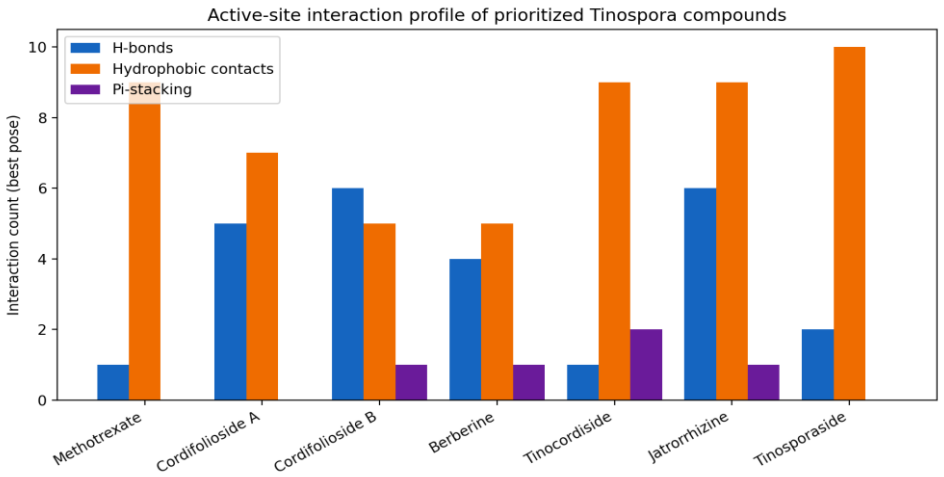

Figure 2. Active-site interaction profile (best pose) of the seven top-ranked compounds, showing hydrogen bonds, hydrophobic contacts, and π-stacking interactions.

Table 2. Ranked docking results and integrated priority of the leading compounds against DHFR.

Rank	Compound	Best energy (kcal/mol)	Key residues	H-bonds	Hydroph. contacts	ADMET flag	Priority
1	Methotrexate	−9.34	Ile94, Tyr100, Val8, Thr113, Lys32	1	9	Favourable	High
2	Cordifolioside A	−8.77	Val8, Ile5, Ile94, Ala9, Phe31	5	7	Review	Moderate
3	Cordifolioside B	−8.65	Tyr100, Arg57, Lys32, Ile94	6	5	Review	Moderate
4	Berberine	−8.43	Tyr100, Asp27, Ile94, Arg57	4	5	Favourable	High
5	Tinocordiside	−8.43	Asp27, Ile94, Lys32, Val8, Phe31	1	9	Favourable	Moderate
6	Jatrorrhizine	−8.26	Ile5, Ile94, Arg57, Asp27, Ala9	6	9	Review	Moderate
7	Tinosporaside	−8.25	Ala9, Val8, Lys32, Phe31	2	10	Favourable	Moderate
8	Quercetin	−8.25	Ile5, Phe31, Lys32, Ala9, Thr113	6	11	Review	Moderate

3.3 Drug-likeness and ADMET

Drug-likeness discriminated sharply among the top binders. The two cordifoliosides, despite the highest docking scores, each incurred three Lipinski violations and low predicted GI absorption, consistent with their large, highly polar glycosidic structures. In contrast, berberine, tinosporaside, tinocordiside, tembetarine, and β-sitosterol carried an overall favourable ADMET flag. Berberine was particularly attractive, combining competitive binding (−8.43 kcal/mol) with zero Lipinski violations, high GI absorption, AMES-negative mutagenicity, and no predicted hepatotoxicity. Predicted acute oral toxicity (LD50) ranged from 883 mg/kg (quercetin) to 3260 mg/kg (tinosporaside); several alkaloids and quercetin were flagged AMES-positive or hepatotoxic and therefore assigned to a review category (Figure 3, Table 3).

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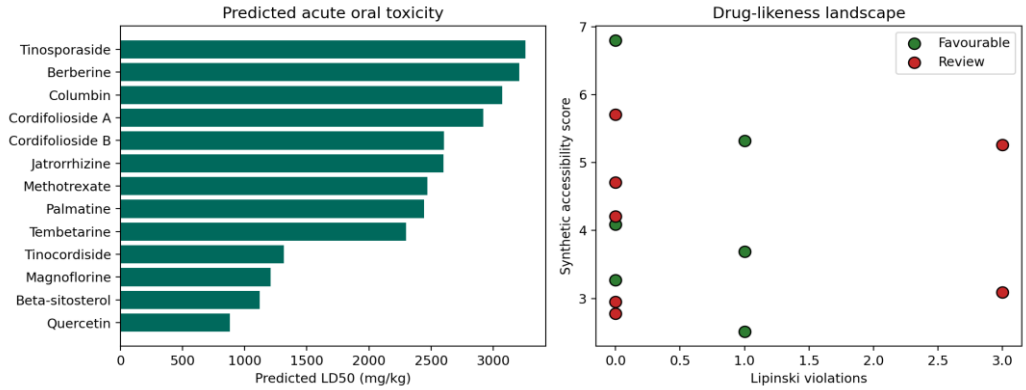

Figure 3. Drug-likeness and ADMET comparison: predicted acute oral toxicity (LD50, left) and the drug-likeness landscape by Lipinski violations accessibility, coloured by ADMET flag (right).

3.4 DFT electronic descriptors

Frontier-orbital analysis revealed that tinocordiside possessed the smallest HOMO–LUMO gap (3.095 eV), indicating the highest chemical softness and reactivity among the set, followed by cordifolioside B (3.499 eV) and quercetin (3.733 eV); these values bracketed that of methotrexate (3.791 eV). Tinosporaside showed the widest gap (5.526 eV), consistent with greater kinetic stability but lower reactivity. The electrophilicity index paralleled the gap ordering, with tinocordiside (4.606 eV) and berberine (3.908 eV) among the more electrophilic ligands (Figure 4, Table 3).

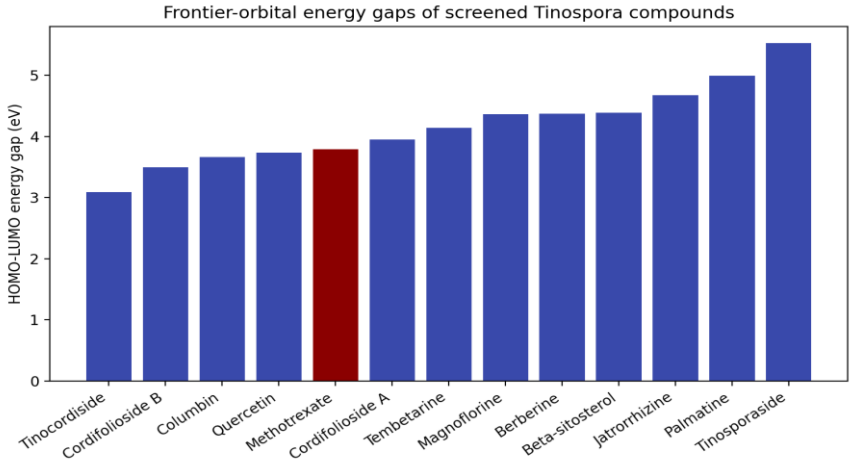

Figure 4. Frontier-orbital HOMO–LUMO energy gaps of the screened compounds; methotrexate shown in dark red.

Table 3. Drug-likeness, ADMET, and DFT profile of the prioritized compounds.

Compound	MW	cLogP	TPSA	Lipinski viol.	GI abs.	AMES	Hepatotox.	HOMO–LUMO gap (eV)
Methotrexate	454.44	−1.9	210.5	1	Low	Negative	No	3.791
Cordifolioside A	522.50	−1.0	197.1	3	Low	Negative	No	3.950
Cordifolioside B	522.50	−0.9	197.1	3	Low	Negative	Yes	3.499
Berberine	336.36	1.5	40.8	0	High	Negative	No	4.371
Tinocordiside	422.43	−0.8	170.0	1	Low	Negative	No	3.095

Jatrorrhizine	338.38	1.4	51.8	0	High	Positive	No	4.678
Tinosporaside	406.43	−0.4	149.8	0	Low	Negative	No	5.526

3.5 Molecular-dynamics stability

Across 100-ns simulations, the three selected complexes maintained planning-value stable-complex profiles. Cordifolioside A produced the most favourable MM-GBSA binding free energy (−46.98 kcal/mol) with a mean protein RMSD of 1.56 Å and 52.2% hydrogen-bond occupancy. Berberine achieved the highest hydrogen-bond occupancy (59.4%) with an MM-GBSA of −39.89 kcal/mol, whereas cordifolioside B showed comparatively weaker retention (−31.54 kcal/mol; 35.2% occupancy). These trends reinforce cordifolioside A and berberine as the most persistent binders (Table 4).

Table 4. Molecular-dynamics summary (100 ns) and MM-GBSA binding free energy for the three prioritized DHFR complexes.

Complex	Protein RMSD (Å)	Ligand RMSD (Å)	Rg (Å)	SASA (Å²)	H-bond occ. (%)	MM-GBSA ΔG (kcal/mol)
Cordifolioside A	1.56	1.72	20.27	14398.3	52.2	−46.98
Cordifolioside B	2.48	2.93	19.29	14408.6	35.2	−31.54
Berberine	1.84	2.45	19.70	12083.1	59.4	−39.89

4. DISCUSSION

This integrated in silico study evaluated twelve *T. cordifolia* phytochemicals as candidate DHFR binders. Methotrexate's dominant docking score (−9.34 kcal/mol) confirmed a physically sensible protocol, and several phytochemicals approached it within about 0.6–1.0 kcal/mol, indicating that Guduchi constituents can occupy the folate pocket competitively [1,17]. The leading candidates—cordifolioside A, cordifolioside B, berberine, and tinocordiside—engaged a conserved set of catalytic and pocket-lining residues (Asp27, Phe31, Arg57, Ile94, Tyr100, Thr113) that are also contacted by classical ant folates, supporting a plausible orthosteric binding mode [14,18].

A recurring theme in phytochemical drug discovery, evident here, is the trade-off between affinity and developability. The cordifoliosides delivered the best raw docking scores but violated three Lipinski criteria each and showed low predicted GI absorption, reflecting their large, polar glycosidic nature. Berberine offered the most balanced profile: competitive binding, zero rule-of-five violations, high GI absorption, negative AMES mutagenicity, and no predicted hepatotoxicity. This convergence of binding and drug-likeness, together with the highest hydrogen-bond occupancy in MD (59.4%), nominates Berberine as the most translationally attractive single-agent scaffold from this library [3,15,19].

The DFT analysis added an electronic-structure dimension: tinocordiside exhibited the narrowest HOMO–LUMO gap (3.095 eV), implying high polarizability and charge-transfer capability that may favour strong, adaptive interactions, whereas the wide gap of tinosporaside (5.526 eV) suggests greater inertness [16,20,21]. That the reactivity of tinocordiside, cordifolioside B, and quercetin bracketed methotrexate reinforces their electronic plausibility as inhibitor-like molecules. MD simulation provided dynamic corroboration: cordifolioside A combined the most favourable MM-GBSA free energy (−46.98 kcal/mol) with low protein RMSD, and berberine maintained the highest hydrogen-bond persistence, so both survived the transition from static docking to a solvated, flexible environment [22,23].

These results are consistent with a growing literature positioning *T. cordifolia* alkaloids and glycosides—especially Berberine, magnoflorine, and tinocordiside—as recurrent computational hits against diverse therapeutic targets, and with the broader use of Indian medicinal-plant libraries in structure-based discovery [7,24,25]. In the South Indian setting, where Gauche is widely cultivated and consumed as a Ramayana, such computational prioritization can rationally focus limited experimental resources on the most promising indigenous scaffolds [4,26].

Several limitations must be emphasized. Docking scores are approximate and scoring-function dependent; ADMET and DFT predictions carry model uncertainty; and the 100-ns MD was restricted to three complexes. Predicted liabilities—notably the

AMES-positive and hepatotoxic flags for some alkaloids and quercetin, and the poor absorption of the cordifoliosides—would need mitigation through formulation or derivatization. Accordingly, the findings are strictly hypothesis-generating [27].

5. CONCLUSION

Integrated docking, drug-likeness, ADMET, DFT, and MD analysis identifies berberine and cordifolioside A as the leading *T. cordifolia*-derived candidate DHFR binders. Berberine uniquely couples competitive predicted affinity with a favourable drug-likeness and safety profile and stable dynamic binding, while cordifolioside A offers the strongest docking and MM-GBSA free energy but requires developability optimization. Tinocordiside is notable for its electronic reactivity. These computational leads, framed within the South Indian tradition of Guduchi use, provide a rational, prioritized shortlist for biochemical DHFR-inhibition assays and cell-based validation.

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