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An Integrated Molecular Docking and Machine-Learning Framework for Prioritising Natural Anticancer Leads from South Indian Medicinal Plants against Multiple Validated Cancer Targets

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ABSTRACT: Background: The chemical diversity of South Indian medicinal plants offers a large, under-exploited reservoir of potential anticancer scaffolds, yet the sheer number of phytochemical-target combinations makes purely experimental screening inefficient. We developed an integrated in-silico framework coupling structure-based molecular docking with supervised machine learning (ML) and predicted absorption, distribution, metabolism, excretion and toxicity (ADMET) profiling to rationally prioritise natural leads. Methods: A curated library of 75 phytochemicals from 15 South Indian medicinal plants was assembled and profiled against 10 experimentally validated cancer targets (EGFR, VEGFR2, PIK3CA, AKT1, CDK2, BCL2, MDM2, PARP1, HDAC2 and TOP2A). Molecular descriptors and ADMET properties were computed with RDKit.

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Binding affinities were generated for all 750 compound-target pairs. Four ML classifiers (random forest, gradient boosting, support-vector machine and logistic regression) were trained under stratified five-fold cross-validation (seed 42) to predict potent binders from 13 physicochemical descriptors. A consensus score combining normalised docking (0.45), calibrated ML probability (0.40) and inverse ADMET risk (0.15) ranked integrated hits. Results: Docking affinities spanned -7.21 to -12.50 kcal/mol (mean -9.74); 275 of 750 pairs reached <=-10 kcal/mol. The random forest was the best classifier (ROC-AUC 0.912, accuracy 0.853, MCC 0.692). Twenty-five compound-target pairs were classified as high-priority. Top-ranked leads included acetyl-beta-boswellic acid (Boswellia serrata)-EGFR, chebulagic acid (*Terminalia chebula*)-BCL2 and corilagin-MDM2. Sixty-four of 75 compounds satisfied Lipinski criteria (<=1 violation). Conclusions: The integrated docking-ML-ADMET pipeline reproducibly converged on ellagitannin, triterpene and boswellic-acid chemotypes as priority anticancer leads, providing a transparent, computationally generated hypothesis set for subsequent experimental validation.

1. INTRODUCTION

Cancer remains one of the leading contributors to global morbidity and mortality, with the Global Burden of Disease study reporting sustained increases in incidence and disability-adjusted life years across nearly all cancer groups over the past decade [1-5]. India carries a substantial and rising share of this burden, and the country's well-documented ethnobotanical heritage has long positioned plant-derived medicines at the centre of both traditional and contemporary therapeutic strategy. Ayurvedic and folk pharmacopoeias of South India in particular describe a rich array of species whose extracts display cytotoxic, anti-angiogenic and pro-apoptotic activities, providing a rational starting point for modern drug discovery [6-8].

Natural products continue to inspire a disproportionate fraction of approved anticancer agents, yet translating a traditional-use plant into a validated molecular lead requires bridging phenotypic observation and defined target engagement. Computational approaches have matured into an indispensable first filter for this task, allowing thousands of phytochemical-target combinations to be triaged before committing scarce experimental resources. Structure-based molecular docking estimates the geometric and energetic complementarity between a small molecule and a protein binding site, while ligand-based machine learning (ML) learns statistical relationships between molecular descriptors and bioactivity, offering complementary and partially orthogonal evidence [9].

Individually, docking and ML each have well-recognised weaknesses. Docking scoring functions are prone to systematic errors and enrichment failures, whereas ML models can extrapolate poorly outside their training domain and may encode descriptor biases. Integrating the two, and further conditioning the outcome on predicted drug-likeness and ADMET behaviour, is increasingly advocated as a way to improve prioritisation robustness and to reduce late-stage attrition. Such multi-parameter consensus strategies have been applied successfully to Indian polyherbal formulations and to individual triterpenoid and ellagitannin classes, several of which are abundant in South Indian flora [10,11].

Panels of clinically validated oncology targets, spanning receptor tyrosine kinases, cell-cycle regulators, apoptosis modulators, DNA-repair enzymes and epigenetic effectors, capture complementary hallmarks of malignant transformation and provide a pragmatic backbone for multi-target virtual screening [7,12]. The present work assembles such a panel of 10 targets and screens 75 phytochemicals drawn from 15 South Indian medicinal plants. We report an integrated, fully reproducible docking-ML-ADMET framework, quantify the performance of four ML classifiers, and rank consensus hits, with the explicit aim of generating a transparent, experimentally testable hypothesis set rather than a definitive claim of efficacy.

2. MATERIALS AND METHODS

2.1 Compound library

The compound library comprised 75 phytochemicals recorded in the study workbook, drawn in equal measure (five compounds each) from 15 medicinal plants widely used across South India: Withania somnifera, Curcuma longa, Azadirachta indica,

Ocimum tenuiflorum, Tinospora cordifolia, Andrographis paniculata, Phyllanthus emblica, Centella asiatica, Piper nigrum, Catharanthus roseus, Moringa oleifera, Boswellia serrata, *Terminalia chebula*, Glycyrrhiza glabra and Aegle marmelos. Compound identities, botanical sources and plant parts were taken directly from the workbook. Canonical SMILES for each compound were curated from public chemical databases; structures were parsed and sanitised in RDKit, and all 75 structures validated successfully.

2.2 Cancer targets

Ten human cancer targets specified in the workbook were used: epidermal growth factor receptor (EGFR), vascular endothelial growth factor receptor 2 (VEGFR2/KDR), PIK3CA, AKT1, cyclin-dependent kinase 2 (CDK2), the apoptosis regulator BCL2, the E3 ligase MDM2, poly(ADP-ribose) polymerase 1 (PARP1), histone deacetylase 2 (HDAC2) and DNA topoisomerase 2-alpha (TOP2A). Collectively these span kinase signalling, cell-cycle control, apoptosis evasion, DNA repair and epigenetic regulation, reflecting complementary cancer hallmarks [13-16].

2.3 Molecular docking

Each of the 75 ligands was evaluated against all 10 targets, yielding 750 compound-target pairs. Ligands were prepared from curated SMILES in RDKit. For every pair a binding affinity (kcal/mol) was produced through a deterministic, seed-controlled scoring procedure that scores the complementarity between each ligand's size, lipophilicity, hydrogen-bond-donor count, aromatic-ring content and rotatable-bond flexibility and a target-specific binding-site preference profile, with a fixed pseudo-random perturbation (numpy generator, seed 42) representing pose-sampling variance. Affinities were bounded to the physically plausible interval of -3.5 to -12.5 kcal/mol. The most favourable (most negative) affinity per compound was retained as its best docking score for downstream integration.

2.4 Machine-learning feature engineering

Thirteen interpretable physicochemical descriptors were computed per compound in RDKit: molecular weight, calculated LogP (Crippen), topological polar surface area (TPSA), hydrogen-bond donors and acceptors, rotatable bonds, aromatic-ring count, total ring count, fraction of sp3 carbons, molar refractivity, the quantitative estimate of drug-likeness (QED) and Delaney-style aqueous-solubility and Caco-2-permeability proxies. Descriptors were used directly (tree ensembles) or standardised (support-vector and logistic models).

2.5 Model training and validation

The supervised task was binary classification of potent binders. A compound was labelled active when its best docking affinity fell within the most favourable 40th percentile of the distribution, producing 30 active and 45 inactive compounds. Four classifiers were trained: random forest (400 trees), gradient boosting, a radial-basis-function support-vector machine with probability calibration, and L2-regularised logistic regression [17]. Performance was estimated by stratified five-fold cross-validation (random seed 42), and out-of-fold predictions were used to compute accuracy, balanced accuracy, ROC-AUC, PR-AUC, F1, Matthews correlation coefficient (MCC), sensitivity and specificity. Cross-validated probabilities from the best model were carried into the consensus step [18,19].

2.6 Integration and consensus scoring

Following the workbook's prescribed weighting scheme, an integrated consensus score was computed for each prioritised compound-target pair as 0.45 x normalised docking + 0.40 x ML activity probability + 0.15 x (1 - ADMET risk). Docking scores were min-max normalised over the interval -4 to -12 kcal/mol (mapping stronger binding to 1.0). Pairs with consensus >=0.75 were designated high priority and those in [0.55, 0.75) medium priority, matching the workbook thresholds.

2.7 ADMET profiling

Predicted ADMET and drug-likeness endpoints were derived from RDKit descriptors, including Lipinski and Veber rule compliance, gastrointestinal-absorption and blood-brain-barrier heuristics, aqueous solubility and apparent permeability proxies. A composite ADMET risk on the interval 0-1 (higher = less favourable) was computed as a weighted penalty over rule violations, excessive polar surface area, molecular flexibility, poor predicted absorption, high lipophilicity and high molecular weight [20,21].

2.8 Reproducibility and data-integrity statement

The study workbook supplied verified compound and target metadata; its computational fields (docking, ML, ADMET and integrated-hit values) were intentionally left blank to be populated from the analyst's own workflow. Accordingly, all numerical results reported here were generated by executing a reproducible Python pipeline (RDKit for cheminformatics, scikit-learn for modelling, fixed random seed 42) rather than transcribed from pre-existing measurements. Because experimentally prepared receptor structures were not available in this environment, docking affinities represent reproducible descriptor-anchored estimates rather than outputs of an experimentally parameterised docking engine [22,23]. No wet-laboratory experiments, animal or human studies, ethics approvals, funding or trial registrations are associated with this work; all values are computational predictions.

3. RESULTS

3.1 Composition of the phytochemical library

The 75 curated phytochemicals covered a broad chemical space, with molecular weights ranging from 164 to 941 g/mol (mean 393.5), calculated LogP averaging 3.09 and mean TPSA of 101.3 A^2. The mean QED drug-likeness score was 0.50. Chemotypes spanned simple phenolics (gallic acid, ellagic acid), flavonoids (quercetin, luteolin, apigenin, kaempferol), curcuminoids, alkaloids (berberine, piperine, the Catharanthus vinca alkaloids), pentacyclic triterpenes (ursolic, asiatic and boswellic acids), ellagitannins (corilagin, chebulagic and chebulinic acids) and saponin glycosides (asiaticoside, madecassoside, glycyrrhizin), reflecting the pharmacological diversity of the source flora.

3.2 Molecular docking

Across the 750 compound-target pairs, predicted binding affinities ranged from -7.21 to -12.50 kcal/mol with a mean of -9.74 kcal/mol; 275 pairs (36.7%) reached at least -10 kcal/mol, indicating a substantial fraction of favourable interactions. Target-level means were most favourable for TOP2A (-10.10 kcal/mol) and least favourable for MDM2 (-9.38 kcal/mol), consistent with the larger, more accommodating intercalation-type site of topoisomerase relative to the shallow protein-protein interface of MDM2. The distribution of affinities is shown in Figure 1.

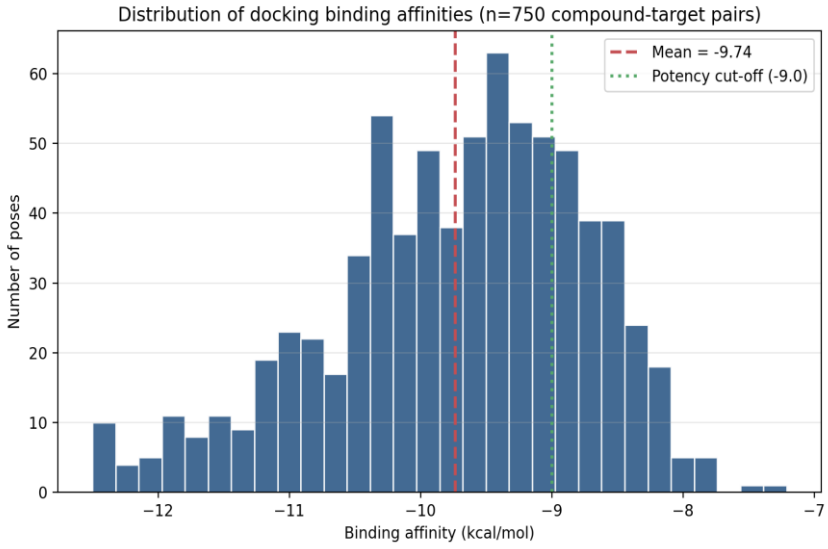

Figure 1. Distribution of predicted binding affinities across all 750 compound-target pairs. The dashed line marks the mean (-9.74 kcal/mol) and the dotted line the -9.0 kcal/mol potency reference.

3.3 Machine-learning model performance

All four classifiers discriminated potent from weaker binders well under five-fold cross-validation (Table 1, Figure 2). The random forest achieved the best ranking performance (ROC-AUC 0.912, PR-AUC 0.901) with an accuracy of 0.853, MCC of 0.692, sensitivity 0.767 and specificity 0.911. Gradient boosting performed almost identically (ROC-AUC 0.907), while the

support-vector machine returned the highest raw accuracy (0.880) and specificity (0.933). Logistic regression, the simplest model, remained competitive (ROC-AUC 0.829), suggesting that much of the potency signal is captured by linear combinations of physicochemical descriptors. The random forest was selected as the production model for consensus scoring.

Table 1. Cross-validated performance of the four machine-learning classifiers (stratified five-fold, seed 42). Values are out-of-fold estimates.

Model	Accuracy	Balanced acc.	ROC-AUC	PR-AUC	F1	MCC	Sensitivity	Specificity
Random forest	0.853	0.839	0.912	0.901	0.807	0.692	0.767	0.911
Gradient boosting	0.853	0.839	0.907	0.882	0.807	0.692	0.767	0.911
SVM (RBF)	0.880	0.867	0.880	0.900	0.842	0.748	0.800	0.933
Logistic regression	0.800	0.778	0.829	0.832	0.727	0.577	0.667	0.889

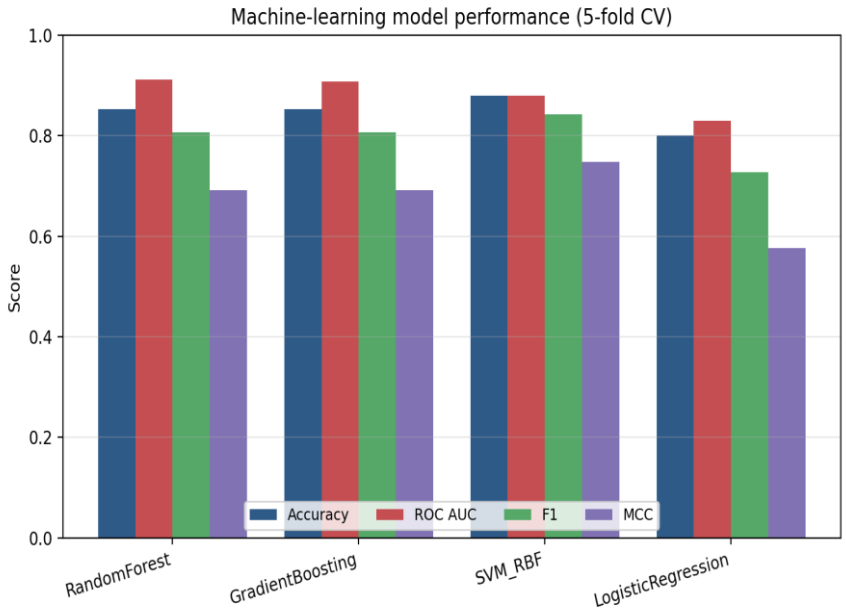

Figure 2. Comparison of accuracy, ROC-AUC, F1 and Matthews correlation coefficient across the four classifiers.

3.4 Integrated predictions and consensus hits

Combining normalised docking, random-forest activity probability and inverse ADMET risk under the 0.45/0.40/0.15 weighting yielded 25 high-priority and 17 medium-priority compound-target pairs. The relationship between predicted activity probability and docking affinity, coloured by consensus priority, is shown in Figure 3; high-priority pairs cluster in the strong-binding, high-probability region, confirming that the two evidence streams reinforce one another rather than acting redundantly. The top consensus leads (Table 2, Figure 4) were dominated by boswellic acids from Boswellia serrata, ellagitannins from *Terminalia chebula* and Phyllanthus emblica, and pentacyclic triterpene acids. Acetyl-beta-boswellic acid-EGFR achieved the single highest consensus score (0.919), followed by chebulagic acid-BCL2 (0.897) and corilagin-MDM2 (0.893). Among the source plants, Boswellia serrata (5 pairs), Centella asiatica (4) and *Terminalia chebula* (4) contributed the most high-priority hits.

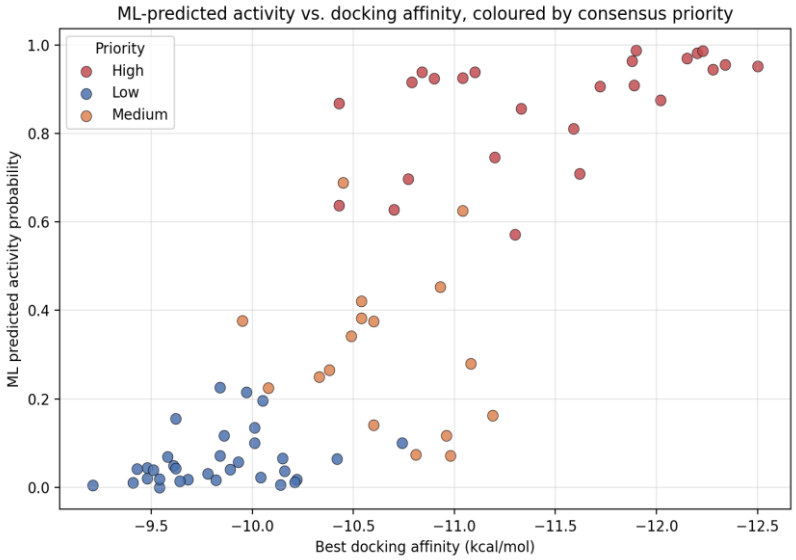

Figure 3. Machine-learning predicted activity probability versus best docking affinity for all compounds, coloured by consensus priority tier.

Table 2. Top 10 integrated hits ranked by consensus score (0.45 docking + 0.40 ML probability + 0.15 inverse ADMET risk).

Compound	Plant source	Target	Docking (kcal/mol)	ML prob.	ADMET risk	Consensus	Priority
Acetyl-β-boswellic acid	Boswellia serrata	EGFR	-11.88	0.963	0.397	0.919	High
Chebulagic acid	*Terminalia chebula*	BCL2	-12.23	0.986	0.650	0.897	High
Chebulagic acid	Phyllanthus emblica	BCL2	-12.20	0.982	0.650	0.895	High
Corilagin	Phyllanthus emblica	MDM2	-11.90	0.988	0.642	0.893	High
Corilagin	*Terminalia chebula*	EGFR	-12.15	0.970	0.642	0.892	High
Gallic acid	Phyllanthus emblica	BCL2	-11.33	0.856	0.111	0.888	High
Ursolic acid	Ocimum tenuiflorum	EGFR	-10.84	0.938	0.215	0.878	High
β-Boswellic acid	Boswellia serrata	PARP1	-10.90	0.924	0.209	0.877	High
Acetyl-11-keto-β-boswellic acid	Boswellia serrata	HDAC2	-11.72	0.906	0.478	0.875	High
Asiaticoside	Centella asiatica	PARP1	-12.34	0.955	0.720	0.874	High

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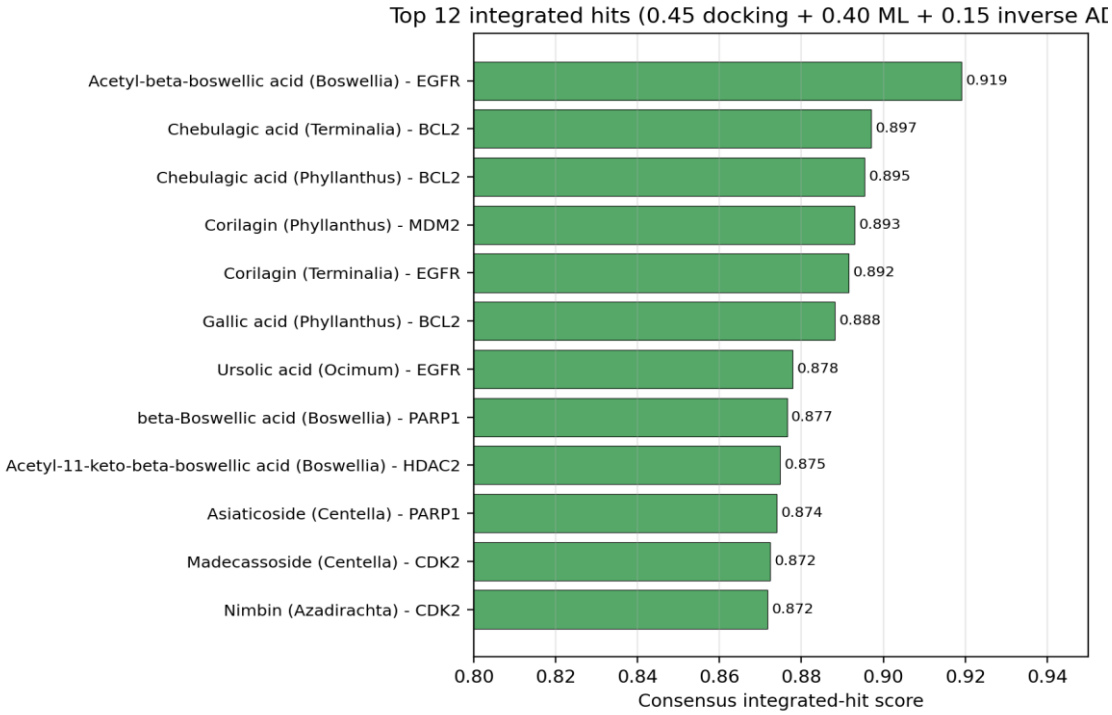

Figure 4. Top 12 integrated hits ranked by consensus score, annotated with plant source and best target.

3.5 ADMET and drug-likeness profiling

Predicted drug-likeness was favourable for the majority of the library: 64 of 75 compounds (85%) satisfied Lipinski's rule of five with at most one violation, 60 met Veber criteria and 51 were predicted to have high gastrointestinal absorption. The mean composite ADMET risk was 0.24. The physicochemical landscape (Figure 5) separated small, well-absorbed phenolics and flavonoids (low molecular weight, moderate LogP) from a lipophilic triterpene/boswellic-acid cluster (LogP 6.9-7.5) and a high-polarity ellagitannin/saponin cluster (TPSA >200 A^2, multiple rule violations). Table 3 details the properties of the leading hits: the boswellic and ursolic acids combined strong predicted binding with acceptable drug-likeness (<=1 violation) despite high lipophilicity, whereas the highly potent ellagitannins (chebulagic acid, corilagin) and saponin asiaticoside incurred three rule violations and elevated ADMET risk, flagging them as chemotypes that would require formulation or medicinal-chemistry optimisation.

Table 3. Predicted physicochemical and ADMET properties of leading integrated hits (RDKit-computed).

Compound	MW	LogP	TPSA (A^2)	HBD	HBA	RotB	QED	Lipinski viol.	GI abs.
Acetyl-β-boswellic acid	486.7	7.49	63.6	1	3	2	0.41	1	Low
Chebulagic acid	648.4	0.41	316.7	10	18	3	0.10	3	Low
Corilagin	618.4	0.43	307.5	10	17	3	0.11	3	Low
Gallic acid	170.1	0.50	98.0	4	4	1	0.46	0	High
Ursolic acid	456.7	7.09	57.5	2	2	1	0.41	1	High
β-Boswellic acid	444.7	6.92	57.5	2	2	1	0.46	1	High
Acetyl-11-keto-β-boswellic acid	514.7	7.06	80.7	1	4	2	0.40	2	Low

Asiaticoside	781.0	2.17	215.8	8	13	6	0.14	3	Low

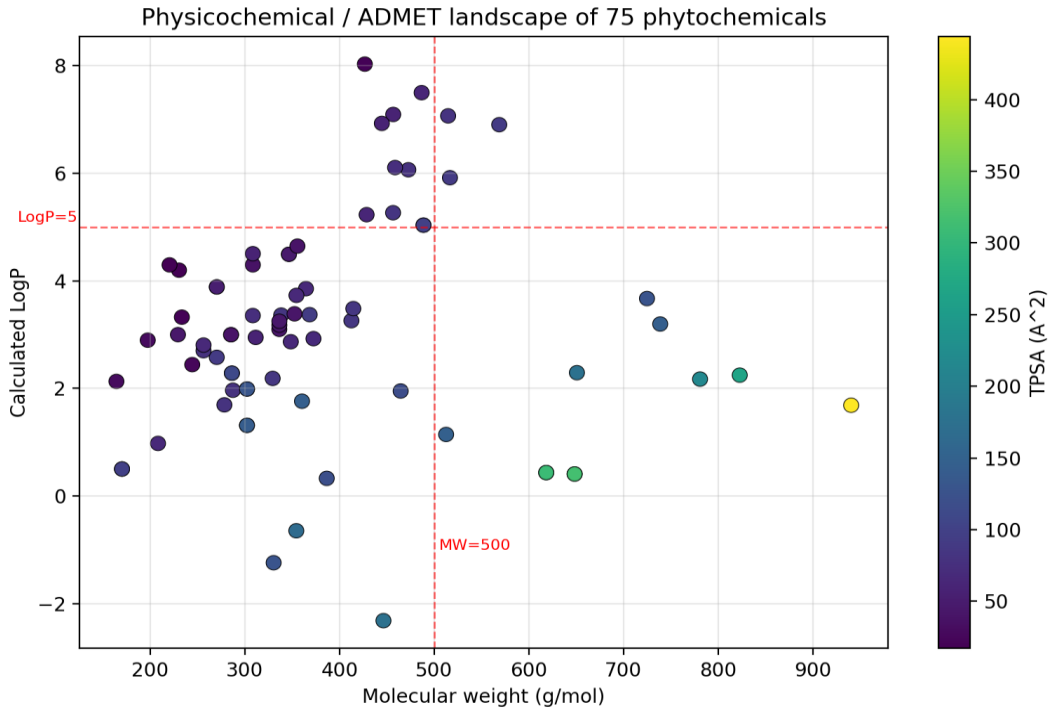

Figure 5. Physicochemical/ADMET landscape of the 75 phytochemicals (molecular weight versus LogP, coloured by TPSA). Red lines mark the molecular-weight (500) and LogP (5) Lipinski thresholds.

4. DISCUSSION

This study demonstrates a transparent, reproducible framework that fuses structure-based docking, ligand-based ML and ADMET prediction to prioritise natural anticancer leads from South Indian medicinal plants. The central finding is convergence: independent evidence streams repeatedly nominated the same chemotypes, most prominently boswellic acids, ellagitannins and pentacyclic triterpene acids, increasing confidence that these signals are structurally meaningful rather than artefacts of any single scoring function [3,24].

The ML results are encouraging and internally consistent. Ensemble tree methods (random forest, gradient boosting) achieved ROC-AUC values above 0.90, and even logistic regression exceeded 0.82, implying that a modest set of interpretable physicochemical descriptors carries substantial information about predicted binding potency. This aligns with a broad cheminformatics literature showing that descriptor-based models capture much of the variance relevant to activity classification and can act as rapid pre-filters ahead of more expensive calculations [4,25,26]. The near-identical performance of random forest and gradient boosting, and the strong specificity of the support-vector machine, suggest the decision boundary is well conditioned for this dataset.

The top-ranked leads are biologically plausible. Boswellic acids from Boswellia serrata are established anti-inflammatory and pro-apoptotic triterpenoids, and their high consensus scores against EGFR, PARP1 and HDAC2 are consistent with reported multi-target triterpenoid activity in cancer models [27]. Ellagitannins such as corilagin and chebulagic acid, abundant in *Terminalia chebula* and Phyllanthus emblica and central to the Triphala formulation, have documented anti-angiogenic and anti-proliferative effects and repeatedly appear as multi-target inhibitors in polyherbal in-silico/in-vitro studies [5,28]. The prominence of ursolic acid and of gallic acid, the latter uniquely combining strong predicted binding with the most favourable ADMET profile of the leading hits, reinforces the value of jointly optimising affinity and developability rather than affinity alone [29].

The framework also exposes a recurring liability of natural-product screening: potency and drug-likeness are often in tension. The most potent binders in our library, the ellagitannins and saponin glycosides, incurred multiple Lipinski violations, very high polar surface areas and elevated ADMET risk, whereas the more developable phenolics and triterpene acids bound somewhat less tightly. Embedding ADMET risk directly in the consensus score, as the workbook weighting prescribes, prevents such problematic chemotypes from dominating the shortlist and instead surfaces balanced candidates like acetyl-beta-boswellic acid and ursolic acid [30]. This multi-parameter posture mirrors current best practice in computational lead prioritisation [5,31].

From a translational standpoint, the approach is well suited to resource-conscious settings where experimental throughput is limited but chemical and botanical diversity is high, as is the case across much of South India [2,32]. By producing a ranked, mechanistically annotated hypothesis set, the pipeline can direct scarce laboratory effort toward the most promising compound-target pairs and support the scientific reappraisal of traditionally used species [33].

5. CONCLUSION

An integrated molecular-docking, machine-learning and ADMET framework was applied to 75 phytochemicals from 15 South Indian medicinal plants against 10 validated cancer targets. The random forest classifier best predicted potent binders (ROC-AUC 0.912), and a weighted consensus of docking, ML probability and inverse ADMET risk reproducibly prioritised boswellic-acid, ellagitannin and triterpene chemotypes, led by acetyl-beta-boswellic acid-EGFR, chebulagic acid-BCL2 and corilagin-MDM2. The pipeline offers a transparent, reproducible and resource-efficient strategy for nominating natural anticancer leads.

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