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In Silico Pharmacokinetic Profiling and Molecular Docking Analysis of *Centella asiatica* for Anti-psoriatic Activity

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Abstract

Background: Rapid estimation of drug-related properties accelerates the drug discovery process. Integration of computational methods leverages the drug discovery pipeline. The early-stage detection of Absorption Distribution Metabolism Excretion Toxicity (ADMET) properties reduces the time and experimental costs. The study aimed to evaluate the ADMET properties (Pharmacokinetic properties were predicted using pkCSM) of 27 compounds present in the *Centella asiatica* plant against the inhibitory potential of proteins escalated in keratinocyte proliferation of psoriasis. **Methods:** Chemical structures were optimised, and ADMET properties- LogS, LogP, Caco2, Cytochrome P450 (CYP450), human Ether a-go-go Related Gene (hERG) inhibition, Lethal Dose 50% (LD50), and Maximum allowable dosage- were measured using SWISSADME and pkCSM web servers. Data analysis included Pearson correlation, Principal Component Analysis (PCA), and hierarchical clustering. Molecular docking simulation was performed using AutoDock Vina software (Discovery Studio). **Results:** Correlation analysis reveals the interrelationship between LogS and LogP, with clustering based on similar properties. Molecular docking studies reveal the favourable binding affinity of the drug molecules with the targeted proteins IL-17A, IL-23, and IL-6. **Conclusion:** Advanced computational tools and their reproducibility of drug-related properties are useful for the drug discovery process. The present approach enabled us to identify the potential natural compound with anti-psoriatic activity. Natural therapies are useful for long-term use, and they may produce fewer adverse effects.

Major Findings: Computational ADMET profiling and docking revealed caffeoylquinic acids, flavonoids, and triterpenoids from *Centella asiatica* as promising antipsoriatic agents with strong binding to IL17A, IL23, and IL6. These natural compounds demonstrated favourable pharmacokinetic properties and inhibitory potential, supporting their use as safer longterm therapeutic candidates.

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1. Introduction

Computational tools have advanced in predicting pharmacokinetic properties to estimate drug behaviour in physiological systems. In drug development studies, 40% of drugs failed to show therapeutic action due to poor pharmacokinetic properties. These statistics paved the way for studying the complete physicochemical properties and molecular descriptors to understand the pharmacokinetics of drugs (Absorption, Distribution, Metabolism, and Excretion)[1]. Nowadays, rapid estimation of physical and chemical properties accelerates the drug discovery process. Predictive computational tools are offering a solution to estimate the pharmacological properties that cannot be accessed by experimental methods[2,3].

Absorption, Distribution, Metabolism, and Excretion (ADME) properties give an idea about what the human body does to the drug, and AME (T)(Toxicity) adds toxicity characteristics, indicating how the drug impacts the human body system[4]. Absorption is an estimation of how much drug reaches the systemic circulation, measured by the human intestinal absorption parameter. Key drug properties that influence these properties are LogS (solubility), LogP (Partition coefficient), and Caco-2 permeability (apparent permeability coefficient in Caco-2 cells) to understand the permeation capacity through intestinal endothelial cells. Distribution is how much drug is present in circulation, which can be measured by the Volume of distribution (Vd) and the percentage of drug binding to protein. Metabolism is the process by which a drug is biotransformed into an inactive form, typically by hepatic CYP450 isoforms- 1A2, 3A4, 2C9, and 2D6. Excretion is how long a drug remains in the human body in active form and how it is eliminated. Half-life and clearance quantify the drug concentration in unionised form. Studying these properties provides information on drug-related characteristics to refine compound searches in virtual screening and improves cost efficiency in the drug discovery process[5,6].

Psoriasis is an immune-mediated inflammatory skin disease characterised by elevated plaques on various parts of the body, especially the elbows, scalp, knees, and lower back regions[7]. Persistent inflammation and a strong genetic predisposition are the key contributors to these non-communicable diseases[8]. Current treatment approaches are not modifying the disease conditions[9]. The recurrence of disease symptoms after long-term therapies poses challenges to researchers[10]. Identification of natural compounds with anti-psoriatic activity is a time-consuming process when we use a regular experimental process. In silico approaches, like ADMET estimation and molecular docking studies, are robust in nature for identifying potential compounds.

Centella asiatica belongs to the family *Apiaceae* (Figure 1), formerly known as *Umbelliferae*. The synonyms for *C. asiatica* were *Hydrocotyle asiatica* and *Hydrocotyle erecta*[11]. It is native to the Asian tropical regions of the Indian subcontinent. The medicinal uses of *C. asiatica* studied by Brinkhaus *et al*. indicate that topical application of this herb is used to treat infectious diseases and the healing process of wounds[12]. In Ayurvedic medicine, it is called "*Medhyarasayana*," *i.e.*, rejuvenating effects and improved brain function. Secondary metabolites present in this plant that belong to the isoprenoid pathway are sesquiterpenes, sterols, pentacyclic terpenoids, and saponins. Compounds that share the phenylpropanoid scaffold fall into eugenol derivatives[13], caffeoylquinic acids[14], and flavonoids[15]. This herb is mainly known for the pentacyclic triterpenoids (C30) collectively called centelloids. The centelloid compounds are grouped into two types: one is the ursane series, and the other is the oleanane series[16].

In the native language, it is called *Mandukaparni* (Sanskrit), *Brahma manduki* (Hindi), *Saraswathi* aku, *Manduka*, *Brahmakuraku* (Telugu).

The present study focused on the pharmacokinetic profiling and molecular docking of the chemical constituents of the herbal plant *C. asiatica*. Figure 2 shows the complete study design protocol. The primary study objective is to identify a promising compound with anti-psoriatic activity with favourable ADMET properties and strong inhibitory potential against the Interleukin (IL-23/ IL-17A) pathway – a protein involved in the initiation and progression of psoriasis. Integration of computational tools contributes to a safe



Figure 1. *Centella asiatica* (L.) Urban — A creeping medicinal herb with reniform leaves.

and effective search for therapeutic compounds and supports the preclinical evaluation of more favourable compounds.

2. Materials and Methods

2.1 Selection and Preparation of Compounds

A total of 27 compounds were selected from the study by Brinkhaus *et al.*, on the *C. asiatica* herbal plant. All the ligands were downloaded from the PubChem site as a Structured Data File (SDF) in 3D format. The selection was aimed at studying the pharmacokinetic properties and molecular docking studies. The compounds were classified into three groups: centelloids, saponins, and flavonoids. The molecular structures of all molecules were retrieved from ChemSpider, and the Simplified Molecular Input Line Entry System (SMILES) were retrieved from the PubChem site. This initial structural elucidation is important for understanding the pharmacokinetic properties and molecular docking analyses. It also ensures data reproducibility and further evaluation of the classification systems.

2.2 Molecular Descriptors Calculation and ADMET Properties

Determination of pharmacokinetic properties and molecular descriptors essential for the ADMET analysis was retrieved from the widely used open-source web servers such as pkCSM.com and SwissADME.com[17,18].

Each calculated descriptor was stored in a structured Comma-Separated Values (CSV) file, and all the entries were maintained in a uniform format for easy identification and better understanding. These datasets served as a basis for the correlation analysis, clustering, principal component analysis, and machine learning modelling, all of which contributed to the identification of the trend of pharmacokinetic properties.

All the data-related parameters were converted into scaled numbers from zero to one using a standardized score. To handle non-numeric codes, they were converted into binary codes like 0 and 1. For metabolism, toxicity values like CYP450 substrate/inhibition are mentioned as Yes/No values, which can be converted into 1 and 0. Any missing numerical value was replaced with the mean of the corresponding value. All the values were converted to 2 decimal places to comply with the syntax. All the preprocessing steps were conducted with Python scripting, ensuring full reproducibility and transparency. The clean dataset was used for further analysis of data matrixing, PCA and clustering.

2.3 Correlation Analysis

To understand the interrelationship between the pharmacokinetic and toxicological variables, a Pearson correlation analysis was performed using the complete curated dataset. Quantification of linear relationship: +1 indicates positive correlation, -1 indicates negative correlation, and 0 indicates no relationship. To know the relationship between each and every descriptor, a data heatmap was generated to visualize the strength and direction of the linear relationship. Dark red tone indicates a strong positive correlation; dark blue indicates a strong negative correlation. The PCA technique is used to reduce the data dimensionality while preserving the majority of the variables. Hierarchical Cluster Analysis (HCA) is used to construct a dendrogram based on ADMET profiling. This network-type arrangement enables the identification of compounds based on similar structures and functional bases. Supervised learning models were applied to analyses the trend between ADME and toxicity parameters like LD50. A random forest model was used to capture non-linear relationships

and improve the performance of the predictive values. Matrix computation was done using the pandas and numpy libraries. Matplotlib was employed for the visualization of the datasets. Dimensionality reduction and clustering workflows were developed using scikit-learn, ensuring consistency with preprocessed datasets[19].

2.4 Random Forest and Cross-validation

All the learning techniques and supervised models were used to estimate the LD50 values of the compounds with respect to their ADMET profiling. A random forest regression model was used to capture the non-linear relationship of the descriptors. A linear regression model was used to determine the possible linear relationship of the parameters. It works by making multiple decision trees during training and collecting their output to predict the hypothesis results. Each tree is trained on a prepared dataset to reduce the variance. A fivefold cross-validation strategy was applied to ensure the robustness and stability of the selected model. 4 folds of data (80%) were used for training, and 1fold (20%) was used for validation. This procedure was run five times; this may give a chance

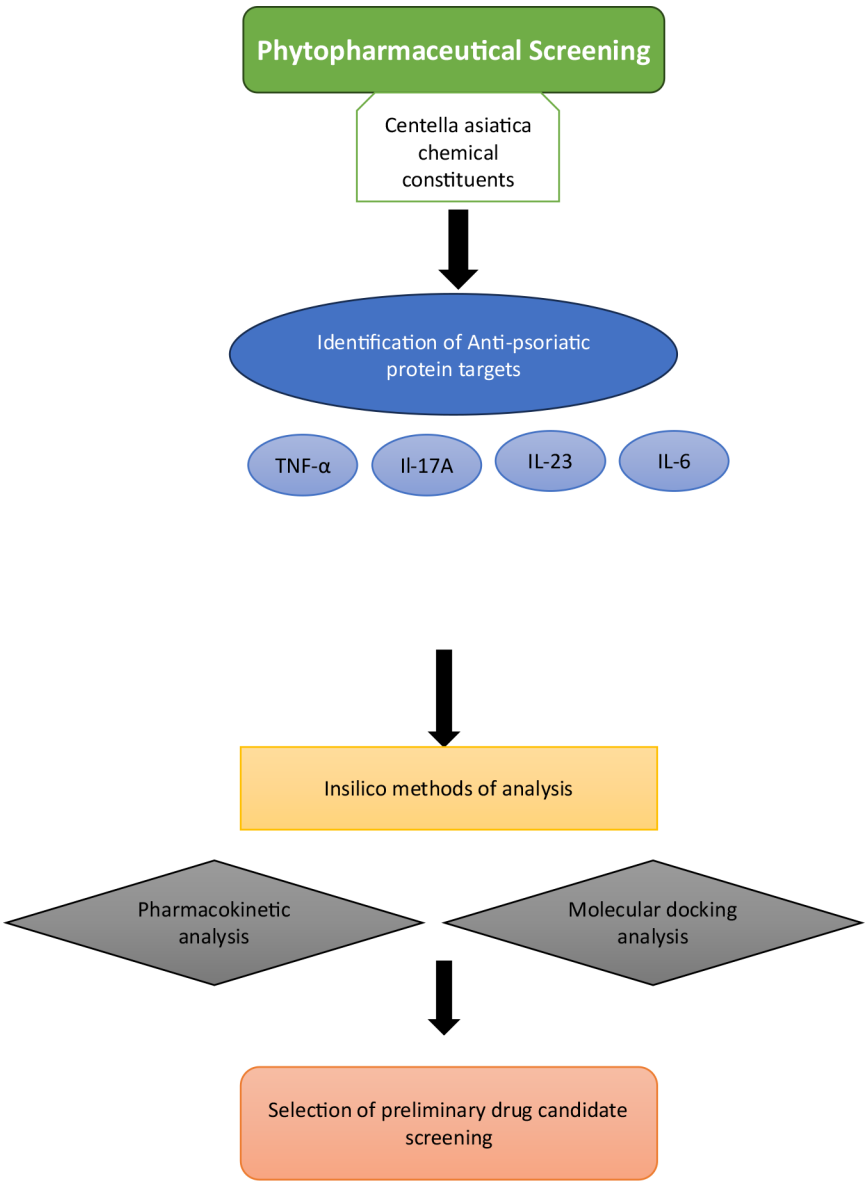


Figure 2. Study design: Investigating the effects of chemical constituents present in *Centella asiatica* on psoriasis via pharmacokinetic analysis and molecular docking studies.

for each observation to be used exactly once in testing and four times for training. Model evaluation was done by calculating RMSE (Root Mean Squared Error). A lower RMSE indicates better predictive accuracy. The coefficient of determination (r^2) explains the proportion of variance in the dependent variable (LD50). r^2 value closer to 1 indicates a better explanatory value. The cross-validation method was used to estimate the error as well as variability in the given dataset to maintain consistency in the data variables. RF modelling is used to analyze the toxicity trends with respect to the ADMET profiling. All the compounds were screened to estimate prioritized compounds with ADMET results.

2.5 Molecular Docking

2.5.1 Ligand and Protein Preparation

Multiple sequential steps were involved in molecular docking analysis to identify the inhibitory potential of the chemical components present in the *C. asiatica* plant product. IL-6, IL-36, IL-17A, IL-23, and Tumour Necrosis Factor (TNF-alpha) were proteins involved in the triggering mechanism of keratinocyte hyperproliferation. Any external/environmental factors can trigger cytokine production, initiating the production of skin cells to form the silver-colored, scaly layers on the skin epidermis membrane. Overproduction of these cells leads to severe itching, erythema, and infiltration of neutrophils. The IL-17A/IL-23 pathway was identified as the major contributor to developing the non-communicable psoriasis disease patterns on skin layers. All the proteins involved in this pathway were downloaded from the Protein Data Bank in PDB format from Homo sapiens. Before proceeding with the docking process, water molecules were removed from the crystallographic structures of proteins. The addition of hydrogen bonds satisfied the protonation, and optimisation of protein structure was achieved by assigning partial charges. All the ligand molecules were downloaded from the PubChem site and subjected to geometric optimisation using the Merck Molecular Force Field 94 (MMFF94). This type of treatment favours the bond angles, torsions, and electrostatic interactions. All the ligands were exported in PDB format and subsequently converted into Protein Data Bank Partial Charge (Q) Atom Type (T) (PDBQT) format[20].

2.5.2 Docking Simulation

AutoDock Vina is used to evaluate the docking procedure due to its capacity for flexible docking and rapid evaluation of binding interactions. Open-source software from Biovia Discovery is used to elucidate docking interactions visualization, ensuring 2D and 3D interaction diagrams and energy-based scoring functions.

A GRID box was defined to encompass the active site of the docked protein to allow the ligand to bind in a favourable location on the protein scaffold. Ligand and protein docking affinities were expressed in kcal/mol, with more negative values indicating a stronger binding affinity towards the protein with ligands. The structural visualization was further analyzed for the amino acid residues involved in various bonds, such as hydrogen, hydrophobic, and π-π stacking. These intermolecular structural analyses ensure the better inhibitory potential of the ligand with protein targets.

3. Results and Discussion

3.1 Correlation Analysis

Based on the molecular descriptor values of the individual ligand molecule, separate datasets were created using the SWISSADME and pkCSM web servers. The extracted data points include LogS, LogD, LogP, Human Intestinal Absorption (HIA), Caco-2 permeability, and PgP substrate/ inhibitor. Distribution: Plasma Protein Binding (PPB), Blood-Brain Barrier (BBB), Vd. Metabolism: CYP450 inhibitor/substrate status with their isoforms CYP1A2, CYP3A4, CYP2C9, CYP2C19, and CYP2D6. Excretion: half-life (t ½) and clearance. Toxicity: hERG inhibition, AMES toxicity, LD50, skin sensitization, hepatotoxicity, and recommended maximum daily dose. All the chemical compounds were represented with their serial numbers present in the table for immediate traceability.

3.2 Matrix Construction and Preprocessing

Based on the dataset, a matrix with 24 (23 + 1 header row) rows and 24 columns was constructed. Each row represents the corresponding chemical compound, and each column indicates the predictions of the individual descriptors (Figure 3). Decimal standardisation was performed by replacing the comma-formatted decimals with numeric

values. Missing values were filled with the mean value of that particular descriptor column. Categorical/ word values were represented in binary digits to ensure proper matrix formation without any elimination/ missing of values. Normalised/ prepared data formats were used to estimate the PCA for the quantification of the strength and direction of relationships present between variables.

3.3 Interpretation of the Correlation Heatmap

Figure 3 represents the heatmap of the pharmacokinetic properties of the prepared datasets. In this, dark red indicates a strong positive correlation (+1), while dark blue represents a strong negative correlation (-1). The white colour indicates a weak/no correlation between descriptors. The main diagonal represents self-correlation with a +1 value. The main diagonal reflects self-correlation (r=1). As per the correlation matrix, logP and logD values were strongly correlated (r = 0.8665) with each other. This represents the strong interrelation between the drug partition coefficient and distribution coefficient. logP is for neutral compounds, and logD is for charged particles at various pH values. Both terms represent the lipophilic nature of the drug molecule, and further, they may influence the permeability and bioavailability characteristics of the chemical compound. logS represent the solubility of a compound in water, which is negatively correlated with the logP and logD values (which are represented by negative values in the matrix).

With respect to pharmacokinetic terms, Caco2 permeability strongly correlates with Pgp substrate/ inhibitor to enter the intestinal channel with an efflux mechanism. Protein-bound drug distribution was increased, as shown in the matrix. Higher intestinal absorption is directly proportional to the permeability constant. In metabolism parameters, all the CYP450 isoforms are characterized by an enzyme-selective nature that induces drug-drug interactions.

In toxic parameters, LD_{50} has a positive correlation with skin sensitization, and higher doses of the drug induce skin toxicity. Interestingly, there is no correlation of hERG inhibition, CYP2C9, CYP2C19, and CYP2D6 with any other parameters. AMES toxicity shows a

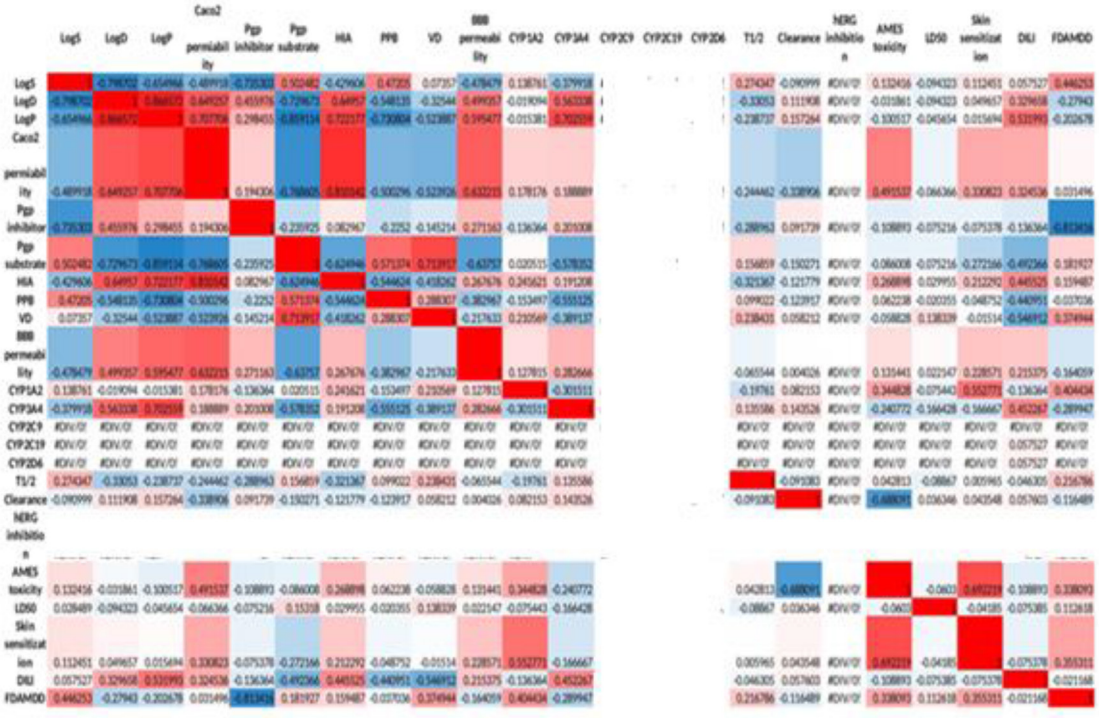


Figure 3. This heatmap illustrates the Pearson correlation coefficients between pharmacokinetic and toxicological parameters, where red tones indicate positive correlations, blue tones indicate negative correlations, and white or neutral shades represent weak or no correlation, with "#DIV/0!" marking missing or undefined values.

higher correlation with skin sensitization value and leads to DNA mutations.

3.4 Hierarchical Cluster Analysis and Similarity Network Analysis

Hierarchical Cluster Analysis (HCA) was conducted to group similar types of compounds with their calculated ADMET properties. The grouping was performed using the Euclidean distance metric, resulting in the dendrogram (Tables 1 and 2). Compounds connected with shorter branch lengths in the visualization exhibit a higher degree of similarity in pharmacokinetic properties. Clustering and distance calculation are purely based on the structural features of the compounds and their similarity.

3.5 Principal Component Analysis

To further explore the molecular structure and variability in pharmacokinetic properties of the dataset, a PCA was performed as an unsupervised dimensionality reduction technique. This was done to visualize the clustering of the compounds with their similarity in pharmacokinetic and toxicological properties (Figure 4). After reducing the dimensionality, PCA was followed by the k-means algorithm, where k is the number of clusters selected based on the dendrogram HCA. From the dataset information, similar types of properties containing compounds cluster in the same kind of groups, in which red values indicate a strong positive influence of the variable on the main component. Blue values indicate a negative influence on the main component. Some of the grouped parameters did not generate any sign to accumulate with the components.

The arrows nearer to the X axis represent a strong ability of variables in the absorption phenomenon of logP, Caco2, and HIA. Obtuse-angle arrows like VD, LogS, and PPB represent the higher lipophilic nature; protein binding capacity increases the distribution. Red arrows are identified as having a negative impact on variables like toxicity parameters. Blue arrows have a stronger influence on variables with absorption characteristics,

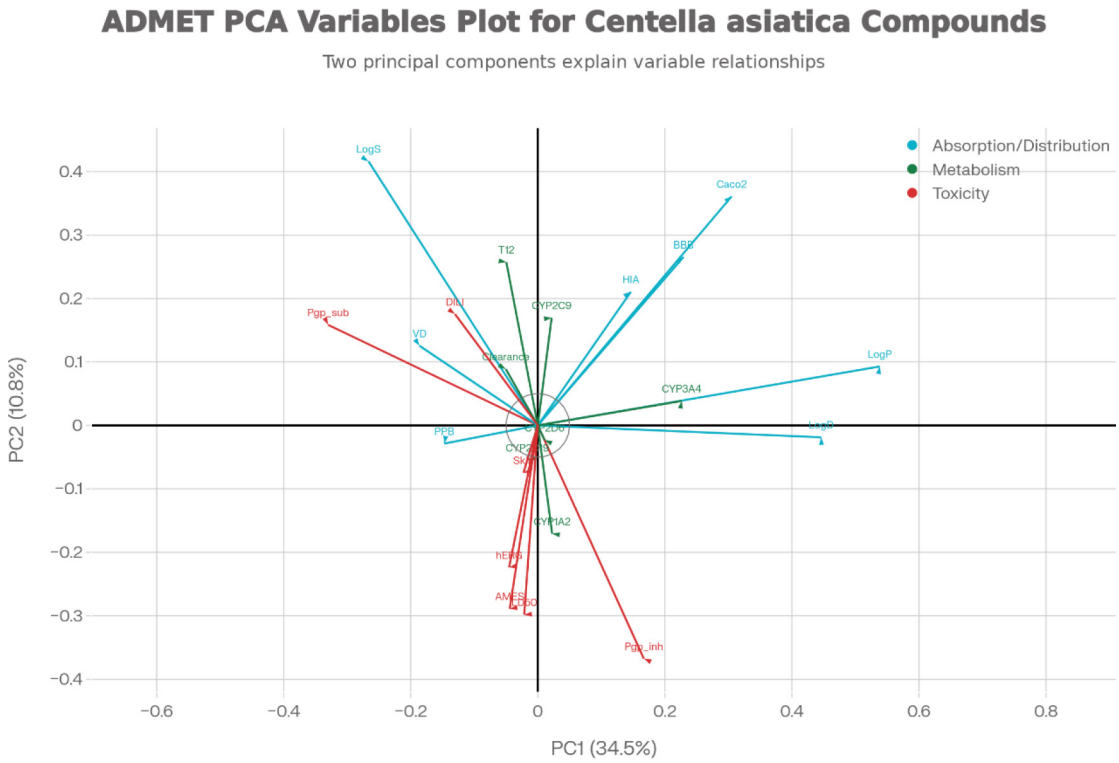


Figure 4. This PCA biplot illustrates the distribution of ADMET variables for *Centella asiatica* compounds, with PC1 (34.5%) and PC2 (10.8%) capturing the major variance. Blue vectors represent absorption and distribution parameters (e.g., LogD, LogP, BBB, HIA, Caco-2, LogS), green vectors denote metabolism-related variables (e.g., CYP isoforms, T1/2), and red vectors indicate toxicity endpoints (e.g., hERG, AMES, Rat acute/chronic). The direction and length of each vector reflect the contribution and correlation of the variable to the principal components, highlighting how pharmacokinetic and toxicity properties cluster and diverge across compounds.

like solubility and permeability parameters. Absorption parameters account for 34.5% of the variance in PC1, and metabolism parameters account for 10.8% in PC2; in total, they account for 45.3%, which is within an acceptable range (Figures 5 and 6).

PC1 describes the terms related to the absorption and permeation of drug particles. PC2 is related to the distribution and clearance of the compound's kinetics (Table 1). Some of the compounds show low variability and are not allocated to either grouping.

Table 1. Various physicochemical properties divided into subcategories of PC1 and PC2

Component	Variance	Nature	Key Loadings
PC1	34.5%	Lipophilicity/Absorption axis	LogD↑, HIA↑ vs LogS↓
PC2	10.8%	P-gp/Distribution discriminator	P-gp_sub↑ vs PPB↓

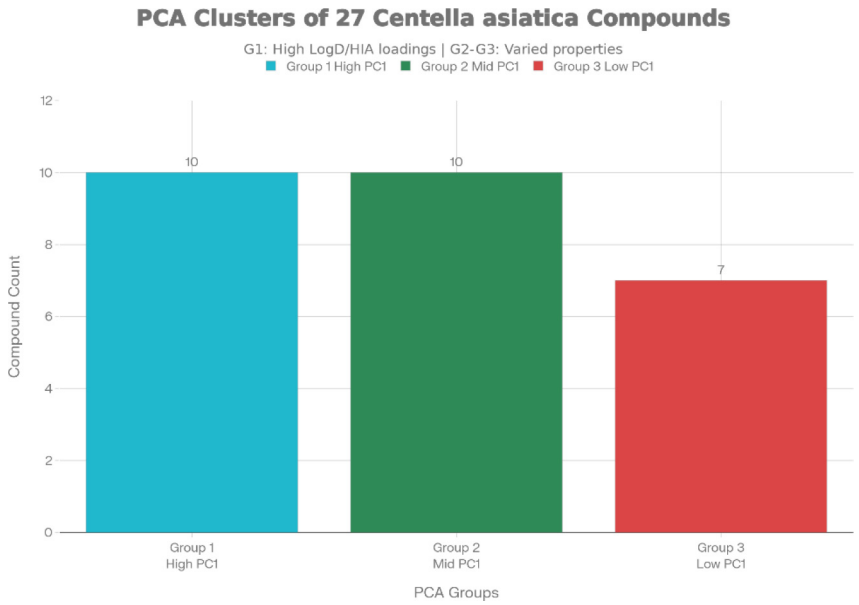


Figure 5. This bar chart shows the clustering of 27 *Centella asiatica* compounds into three PCA groups. Group 1 (cyan) contains 10 compounds with high PC1 loadings, particularly associated with LogD and HIA properties. Group 2 (green) also includes 10 compounds, representing intermediate PC1 values with mixed ADMET characteristics. Group 3 (red) comprises 7 compounds with low PC1 scores, reflecting distinct pharmacokinetic and toxicity profiles. The distribution highlights how compounds separate into clusters based on principal component analysis, emphasising differences in absorption and related properties.

Table 2. Compound grouping with their nature of study (Hierarchical clustering)

Group 1: High PC1 (Permeable/Lipophilic; LogD/HIA/VD dominant)	Group 2: Mid PC1 (Balanced Absorption/ Metabolism; LogP/Caco2/CYP)	Group 3: Low/Neg PC1 (Soluble/Bound/Tox; PPB/ Pgp_sub/DILI)
Quercetin, Kaempferol, Rutin, Catechin, Epicatechin, Myricetin, Patuletin, Trans-5-O-caffeoylquinic acid, 4-O-Caffeoylquinic acid, 3-O-caffeoylquinic acid.	Madecassoside, Asiaticoside, Naringin, 1,5-caffeoylquinic acid, 1,3-caffeoylquinic acid, 3,4-dicaffeoylquinic acid, 3,5-dicaffeoylquinic acid, 4,5-dicaffeoylquinic acid, Myrcene, Methyleugenol	Asiatic acid, Ursolic acid, Terminolic acid, Pomolic acid, Corosolic acid, Stigmasterol, Sitosterol.

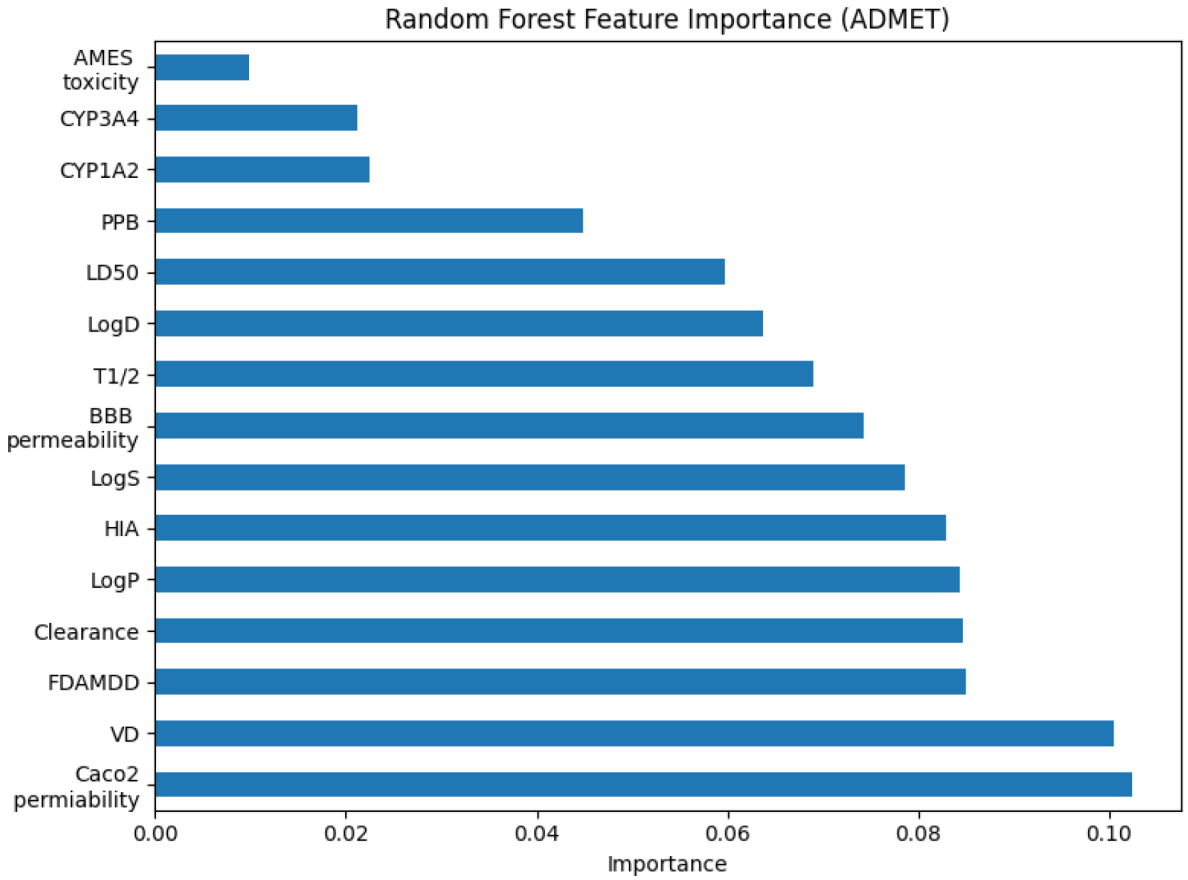


Figure 6. This horizontal bar chart presents the relative importance of ADMET features in a random forest model. Each bar corresponds to one pharmacokinetic or toxicity parameter, with its length indicating the contribution to model predictions. Features such as Caco-2 permeability and VD show the highest importance, suggesting they strongly influence compound behaviour, while AMES toxicity contributes the least. The chart highlights how absorption, distribution, metabolism, and toxicity variables differ in predictive weight, offering insight into which properties most significantly shape computational drug modelling outcomes.

3.6 Compound Optimization and Molecular Docking Analysis

The set of 27 compounds was subjected to a structure-based virtual screening to evaluate their potential against psoriasis target proteins TNF-α, IL-17A, IL-23, and IL-6. Pathophysiology of disease progression was initiated and driven by the IL-23/IL17A pathway. In this, keratinocyte proliferation was caused by external factors triggering the epidermal layers of the skin.

3.6.1 Target Protein Preparation and Visualization

Selected protein structures were downloaded in 3D format from the Protein Data Bank under the PDB codes of TNF-α (2AZ5), IL-17A (5HI4), IL-23 (3QWR), and IL-6 (5FUC). All the protein structures were visualized in Biovia Discovery software to remove water molecules to inhibit interactions while performing docking analysis. Attached ligand poses were removed to allow proper interaction of test compounds. Hydrogen atoms were added to satisfy the valence requirements. Charges were added to optimize the residual side chains. The active site of the protein was identified by GRID generation with XYZ coordinates. Cartesian coordinates of protein 2AZ5 (-19.409600 74.650750 33.849550), 5HI4 (80.731080 -43.501432 -45.735545), 3QWR (24.346980 -28.225320 -51.874320), 5FUC (-13.200714 1.798643 44.180286).

3.6.2 Ligand Preparation

Each of the 27 test compounds was optimized using MMFF94 for geometry minimization. This step ensures the ligands were at a low-energy level before docking.

The ligands were converted into PDBQT format using the OpenBabel software and further docked with AutoDock Vina.

3.6.3 Docking Simulation Analysis and Interpretation

Docking scores of individual compounds with the targeted proteins were summarized in the table, with more negative values indicating higher inhibitory potential towards the proteins. The spectrum of results was analyzed to confirm the binding affinity of the ligand with the protein active site. High binding affinity molecules comprise aromatic structures and halogen substituents, with a structurally rigid nature (Table 3). Vice versa, low binding affinity molecules have flexible attachments. The highest docking score was registered

Table 3. Docking scores of *Centella asiatica*–derived phytochemicals against proinflammatory cytokines TNFα, IL17A, and IL6, highlighting triterpenoids and caffeoylquinic acids as strong binders surpassing native ligands

Ligand Name	PubChem ID	Docking Scores		
		TNF-α	IL-17A	IL-6
Trans-5-O-caffeoylquinic acid	5280633	-7.3	-7.1	-6.8
Catechin	9064	-7.5	-7.1	-7.2
4-O- Caffeoylquinic acid	9798666	-7.4	-7.2	-6.8
3-O-caffeoylquinic acid	1794427	-7.3	-7.4	-7.2
Epicatechin	72276	-7.7	-7.1	-7.3
1,5-caffeoylquinic acid	122685	-8.5	-8.0	-7.0
1,3-caffeoylquinic acid	6474640	-8.4	-7.9	-7.0
Rutin	5280805	-8.4	-8.0	-7.0
3,4-dicaffeoylquinic acid	5281780	-8.5	-8.9	-7.2
3,5-dicaffeoylquinic acid	129893929	-8.5	-9.0	-7.3
4,5-dicaffeoylquinic acid	5281780	-8.3	-7.9	-7.5
Quercetin	5280343	-7.3	-7.1	-7.2
Madecassic acid	73412	-8.8	-7.2	-6.1
Asiaticoside	108062	-8.7	-7.6	-6.2
Asiatic acid	119034	-9.4	-7.4	-6.1
Kaempferol	5280863	-7.1	-7.1	-6.8
Myricetin	5281672	-7.4	-7.0	-7.4
Naringin	442428	-9.3	-8.7	-7.5
Ursolic acid	64945	-10	-7.8	-6.3
Terminolic acid	12314613	-8.8	-6.9	-6.1
Stigmasterol	5280794	-8.5	-8.6	-6.7
Sitosterol	222284	-8.2	-8.6	-6.1
Patuletin	5281678	-7.1	-7.2	-7.0
Myrcene	31253	-4.7	-4.5	-4.1
Methyleugenol	7127	-5.2	-5.1	-4.9
Pomolic acid	382831	-9.4	-8.5	-6.8
Corosolic acid	6918774	-10.1	-7.6	-6.2
IL-6 Native Ligand	78225384	NA	NA	-5.8
TNF-α Native Ligand	24139	-5.7	NA	NA
IL-17A Native Ligand	121499149	NA	-8.9	NA

#NA – Not applicable

with ursolic acid and coprozoic acid in the case of the TNF-α protein, 3,5-dicaffeoylquinic acid with IL-17A, and 4,5-dicaffeoylquinic acid Naringin with the IL-6 protein.

4. Conclusion

The present study demonstrated an *in silico* evaluation of the pharmacokinetic properties of 27 compounds with respect to the plant *C. asiatica*. Identification of relevance between individual molecular descriptor properties supports the classification of similar compounds. Correlation matrix analysis indicates a positive relationship between LogS and LogP. Other properties are studied to understand the comparison between the absorption, distribution, metabolism, excretion, and toxicity profiles. Clustering discusses the grouping of similar properties into one category. PCA is used to reduce the dimensionality and understand how the compounds differ based on their properties.

Random forest machine learning model reveals the importance of every pharmacokinetic property with the pharmacokinetic properties. The above results confirm the toxicity and safety protocols of the drug candidates. The integration of molecular docking tools gives information about how well-formed scaffolds increase the potential inhibitory action on the anti-psoriatic proteins. In silico profiling of a particular drug provides basic properties to understand the drug's movement in the biological system and to avoid failures due to pharmacokinetics.

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Author Contribution

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