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Original Article

Cheminformatics-Based Evaluation of Drug-Likeness in Selected Phytochemicals from *Vateria indica (Sarjarasa)*

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ABSTRACT

Background: Cheminformatics has emerged as a powerful tool in early-phase drug discovery, enabling the efficient evaluation of bioactive compounds from natural sources. *Vateria indica* (*Sarjarasa*), a medicinal plant used in traditional systems, contains a wide array of phytochemicals with various pharmacological activities. Assessing the drug-likeness of these phytochemicals can help identify promising candidates for further development. **Materials and Methods:** Phytochemical data were obtained from Computational databases. Selected compounds were analyzed using advanced software to evaluate drug-likeness based on Lipinski's Rule of Five and other key pharmacokinetic parameters. Cheminformatics techniques were employed to predict bioavailability and assess potential toxicity. **Results and Discussion:** Most of the analysed phytochemicals exhibited favourable drug-like properties, including good predicted oral bioavailability and low toxicity. However, compounds such as hopeaphenol and oleoresin turmeric violated multiple parameters of Lipinski's Rule, indicating potential limitations in oral bioavailability. These outcomes emphasize the variability among natural compounds and highlight the need for careful *in silico* screening. **Conclusion:** The study demonstrates the effectiveness of cheminformatics in evaluating drug-likeness of phytochemicals from *Vateria indica (Sarjarasa)*. While several compounds meet standard drug-likeness criteria, others require structural optimization or alternative delivery approaches. These insights support the role of *in silico* methods in accelerating natural product-based drug discovery**.**

Keywords: *Vateria indica*, Lipinski Rule of Five, Computational databases, Phytochemicals, Drug-likeness.

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INTRODUCTION

The huge tree *Vateria indica* L. is native to India. Although it is poorly inhabited, it grows in the forests and wetlands of the Midwestern Ghats. The primary habitats of this species include Maharashtra, Tamil Nadu, Kerala, and Karnataka. This tree species, which has smooth, grey bark and green and white stems, grows slowly and is found in emerging species in the canopy of low- to medium-altitude evergreen forests. and it has a white, green, and grey trunk. The plant features sweet white flowers and thick leaves. Timber is used by this species. Chamazulene, thymol, bergenin, stearic acid, palmitic acid, and other chemical components are present in different regions of the plant. It is also valued for its sticky or resinous components, which are used for their expectorant and tonic properties. Despite being a highly significant medicinal plant with numerous applications, the plant is currently in danger of being extinct. Wounds, Pharyngitis, chronic bronchitis, leprosy, eczema, rheumatism, TB, boils, and other conditions can also benefit from it. According to World Health Organization (WHO) criteria, *Vateria indica* leaves were subjected to a chemical test. The anti-inflammatory properties of *Vateria indica* leaves may have been caused by the presence of glycosides, steroids, and alkaloids (Bugade and Khan, 2023). Ethanol extract from the stem of *Vateria indica*, which has long been used for medicinal purposes, has anti-tumor properties (Sasikumar *et al.*, 2016). *Vateria indica* stem bark extract contains large amounts of phenols and flavonoids and can be used as a natural source of antioxidants and antimutagens, which may be important as therapeutic agents for the prevention or slow the progression of aging and degenerative disease-related oxidative stress (Ruma *et al.*, 2011). Anti-ulcer activity was achieved using the resin extract (Bugade and Khan, 2023).

A molecule needs to have desirable drug-like qualities such solubility, permeability, and bioavailability in order to be regarded as a promising drug candidate. For the molecule to reach the intended location in the body at therapeutic concentrations, several characteristics are essential. Lipinski's Rule of Five is frequently used to forecast drug-likeness, accounting for

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elements like molecular weight, donors and acceptors of hydrogen bonds, and the octanol-water partition coefficient (log P), whereas if the violate any of these parameters, then the drug is not considered to be active orally (Patil *et al.*, 2025). The interdisciplinary area of cheminformatics manages and analyses chemical data by fusing computer science and chemistry. It entails storing, retrieving, analysing, and visualizing data about chemical compounds-including their structures, characteristics, and activities-using computer-based tools and techniques. This area of study is especially helpful in drug discovery since it helps find new medication leads and improve drug prospects.

Most of the phytoconstituents present in *Vateria indica* possess pharmacological activities such as anti-inflammatory, anti-helminthic, anti-tumour activity, anti-ulcer, anti-oxidant and anti-mutagenic activity (Bugade and Khan, 2023). Hence, to understand which phytochemical is responsible for the respective pharmacological activities and to know the drug-likeness of the particular compound this cheminformatics paves the way for future clinical requirements.

MATERIALS AND METHODS

Databases and Softwares

IMPPAT (Indian Medicinal Plants, Phytochemistry and Therapeutics) was used to get the phytochemicals present in the drug, PubChem database helped to get the canonical smiles and Molsoft software was used to find the drug likeliness of these compounds (Kim *et al.*, 2016).

List of various Phytochemicals

The opted phytochemicals for the study include the following

Fisetinidol, Bergenin (bark), Afzelechin, (+)-Hopeaphenol (leaf), Bergenin, (+)-Hopeaphenol (root), Bergenin (leaf), Stearic acid, Palmitic acid, 1-(11Z-icosenoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphoethanolamine, Bergenin (root), Chamazulene, Thymol, alpha-Pinene, beta-Pinene, alpha-Terpineol, Oleoresin tumeric, beta-Caryophyllene, Limonene.

Compilation of Canonical SMILES of selected Phytochemicals

We proceeded to the PubChem website and entered the name of each phytochemical into the search form, and it showed several phytochemicals similar to the selected one. We then have to choose the related phytochemical to get the canonical SMILES for those compounds. When we located the compound in the results, we need to proceed with its summary page. This page's "Chemical and Physical Properties" section is where we slid down to find the "Canonical SMILES" field, which is typically found above the "Molecular Formula". Then the smiles are to be copied and pasted in the Molsoft software to proceed further. This is to be repeated for each selected phytochemicals of the drug (Patil *et al.*, 2025).

Chemical structures of selected phytochemicals

To obtain a chemical structure of the selected phytochemical, the phytochemical is to be typed in the PubChem database, which generates the similar various phytochemicals, from which the apt one is selected. This selection leads us to the compound's summary page. Under the "Contents" section, the first entry displays the 2D depiction of the chemical structure of the selected phytochemicals. Further the image was downloaded at a resolution of 500*500 pixels.

Molsoft Software to determine drug likeness score using Lipinski's rule

The Molsoft L.L.C website (www.molsoft.com) is opened, under that "Drug Likeness and molecular property prediction" is chosen. Once the page is open, the canonical SMILES of the selected phytochemical is to be copied from the PubChem database and pasted under the option called "Import" and press 'OK". It immediately gives the chemical structure of the selected phytochemical. Now click the option "Calculate Properties". It depicts the Molecular properties and drug-likeness of the selected phytochemical (Patil *et al.*, 2025).

Lipinski's Rule of Five (RO5)

Pharmacologists and medicinal chemists search for specific chemical characteristics that contribute to a drug's oral effectiveness. The "rule of five" developed by Lipinski is a rough guideline for determining whether a molecule has the necessary qualities to be used as an oral medicine. The premise behind it is that the majority of oral medications are tiny and have a tendency to favour fat (lipophilia). According to the guideline, a compound should not have the following in order to be likely to be properly absorbed when taken orally:

(1) More than five groups (such as OH or NH groups) have the ability to create hydrogen bonds with water.

(2) Over ten groups are capable of forming hydrogen bonds.

(3) A molecule is considered overly large if its weight exceeds 500 atomic units.

(4) A medication is said to be very hydrophobic (fat-loving) if its CLog P value is greater than 5, which is a measure of how fat-loving a chemical is.

By employing a chemical known as 1-octanol, the partition coefficient (P) calculates the ratio of the drug's solubility in fat-like compounds to that in water. The more hydrophobic the medication, the higher the P value. The quantity of OH or NH groups that may create hydrogen bonds with water is known as the number of hydrogen-bond donors. Although some specific atoms, such as oxygen or sulphur in particular chemical configurations, are excluded, hydrogen-bond acceptors are other

atoms in the molecule (such as some heteroatoms that are not positively charged) that can accept hydrogen bonds.

Lipinski's rule was created based on analysing the properties of over two thousand existing drugs, helping guide the development of new ones (Lipinski, 2000).

RESULTS

In drug research, the concept of drug-likeness is crucial since it indicates how similar a material is to common medications, particularly in terms of how well the body can absorb and use it. In order to better understand how easily and effectively specific plant-based molecules (phytochemicals) might become accessible in the human body, various drug-likeness metrics were computed for these substances. To calculate the drug-likeness of the phytochemicals of the drug *Vateria indica* Linn, we have assessed using the Lipinski Rule of Five, that is [Molecular Weight (MW), Hydrogen Bond Acceptors (HBA), Hydrogen Bond Donors (HBD), partition coefficient (Log P)]. The following were the acceptable ranges for these metrics, which show adequate oral bioavailability: MW<500 Daltons, RO5 violations<1, HBA≤10, HBD≤5 and Log P≤5. The results, as presented in Table 1 depicts the chemical structure of each phytochemical derived from the plant *Vateria indica* Linn, Table 2 interprets that among 19 phytochemicals, (+)-Hopeaphenol (root and leaf), Stearic acid, Palmitic acid, 1-(11Z-icosenoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphoethanolamine, Oleoresin turmeric, Chamazulene, beta-Caryophyllene were not within the normal limits in case of the above parameters especially the Molecular Weight (MW) and Calculated partition coefficients (Clog P). However, Hydrogen Bond Acceptors (HBA) and Hydrogen Bond Donors (HBD) were almost within the limits. The information about each parameter used for testing the drug-likeness of each compound were elaborated below to understand in detail.

Data Analysis: Drug-Likeness Evaluation of Selected Phytochemicals

Molecular Weight (MW)

The molecular weight of a medicine has a major impact on how well it enters the bloodstream and reaches its intended target. Since lower molecular weights can more readily cross cell membranes and are frequently appropriate for Transdermal Drug Delivery Systems (TDDS), they are typically linked to greater absorption. Drug release from dosage forms may occasionally be impacted by the molecular weight of excipients (non-active substances), as lower molecular weight excipients may cause faster drug breakdown. Drugs' molecular weights, especially those of more recent generations, are frequently studied to learn more about their pharmacokinetic characteristics and how they may affect toxicity and efficacy. Hence the phytochemical of a drug should hold the range of Lipinski Rule of Five. This rule states that compounds with a molecular weight of less than 500 Da are considered ideal for oral absorption [MW (> 500)].

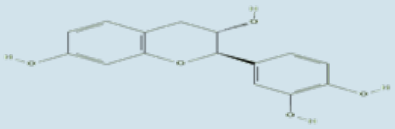
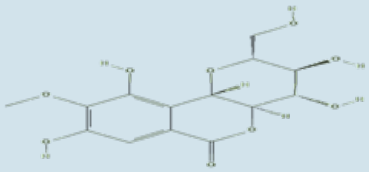
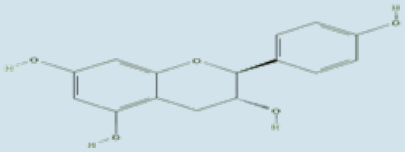
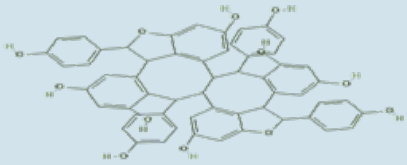
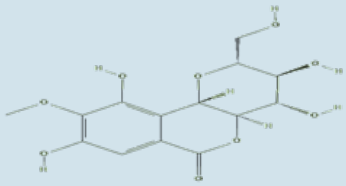
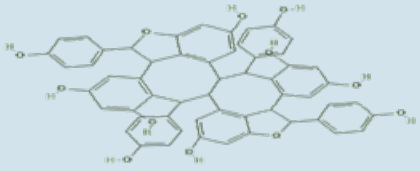
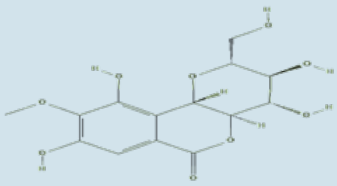
Hydrogen Bond Acceptors (HBA)

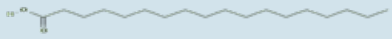
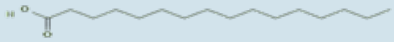
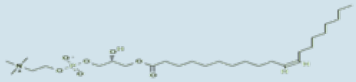
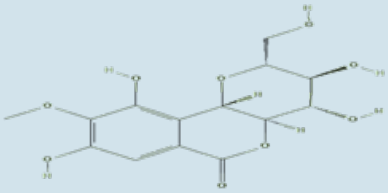
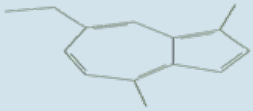
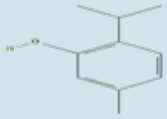
In drug design, hydrogen bond acceptors are crucial because they affect a medication's interactions with other molecules, especially those in the body, and add to the molecule's overall polarity. A drug's effectiveness, distribution, and absorption may all be impacted by these interactions. The polarity of a pharmacological molecule is influenced by hydrogen bond acceptors, such as oxygen and nitrogen atoms. A drug's ability to dissolve in water and other solvents is influenced by its polarity, which is important for the body's absorption and distribution. Water, proteins, lipids, and other compounds can all create hydrogen bonds with hydrogen bond acceptors. These interactions can influence how a drug binds to its target, affects its stability, and even its ability to cross cell membranes. The number and strength of hydrogen bond acceptors in a drug molecule can influence its bioavailability. Lipinski's rule-of-five, a well-known rule in drug design, uses the number of hydrogen bond acceptors as a predictor of oral bioavailability. Hydrogen bond acceptors can participate in key interactions with the target molecule, such as a protein or enzyme. These interactions are essential for the drug to bind to the target and exert its therapeutic effect. Alcohols, amines, ketones, ethers, carboxylic acids, esters are few examples of functional groups with Hydrogen Bond Acceptor Ability. In summary, hydrogen bond acceptors are crucial for a drug molecule's ability to interact with other molecules, affect its polarity and solubility, and ultimately influence its effectiveness in the body [HBA≤10].

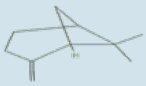
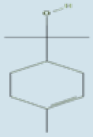
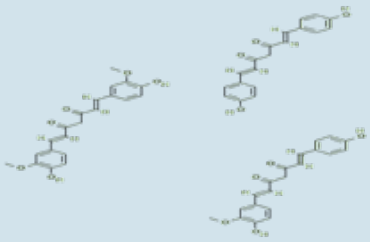
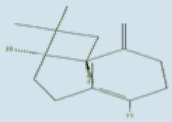
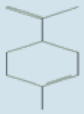
Hydrogen Bond Donors (HBD)

Molecules or portions of molecules that have the ability to give a hydrogen atom in order to create a hydrogen bond with an acceptor are known as hydrogen bond donors. Hydrogen bond donors can affect a medication's solubility, permeability, and oral bioavailability and are essential for target recognition in drug design. In order to facilitate contacts and binding, the existence of a hydrogen bond donor frequently signifies the presence of a hydrogen bond acceptor on the target. A drug's capacity to penetrate cell membranes and, consequently its bioavailability, can be influenced by the quantity and kind of hydrogen bond donors. When predicting oral bioavailability, this rule-which is frequently applied in drug design-takes the amount of hydrogen bond donors into account. In medicinal compounds, hydroxyl (OH) and amino (NH) groups, as well as acidic groups like carboxylic acids, are frequently used as hydrogen bond donors. (Kenny, 2022) states that hydrogen bonding is also essential to the stability and structure of hydrogels, which are utilized in drug delivery systems. To put it simply, knowing the characteristics and function of hydrogen bond donors is essential to creating medications that are efficient at targeting particular receptors, have

Table 1: Chemical structure of selected phytochemicals.

Sl. No.	List of Phytochemicals	Chemical Structure
1.	Fisetinidol	
2.	Bergenin (Bark)	
3.	Afzelechin	
4.	(+)-Hopeaphenol (Leaf)	
5.	Bergenin (Leaf)	
6.	(+)-Hopeaphenol (Root)	
7.	Bergenin (Root)	

Sl. No.	List of Phytochemicals	Chemical Structure
8.	Stearic acid	
9.	Palmitic acid	
10.	1-(11Z-icosenoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphoethanolamine	
11.	Bergenin	
12.	Chamazulene	
13.	Thymol	
14.	alpha-Pinene	

Sl. No.	List of Phytochemicals	Chemical Structure
15.	beta-Pinene	
16.	alpha-Terpineol	
17.	Oleoresin tumeric	
18.	beta-Caryophyllene	
19.	Limonene	

high bioavailability, and display the required pharmacological characteristics. [HBD≤5].

Calculated Partition Coefficient (Clog P)

Calculated log P, or Clog P, is a predicted indicator of a compound's lipophilicity that is frequently employed in the development of new drugs. It is computed by adding together the log P values of each molecule's constituent pieces. This computed number influences a drug's Absorption, Distribution, Metabolism, and Excretion (ADME) by forecasting how it will partition between an aqueous and lipid phase. Though it also raises questions about possible toxicity and unintended interactions with other compounds, a high Clog P value (indicating a higher preference for lipid environments) can suggest a medicine may be better absorbed across lipid membranes and have a broader distribution inside the body (Sun *et al.*, 2023). discusses using Clog P in conjunction with other parameters like molecular weight and toxicity risk to predict drug similarity and overall drug score**.** To sum up, Clog P is often considered within the context of Lipinski's Rule of 5, which suggests that oral drugs should have a log P value less than 5 for good absorption [Log P≤5].

DISCUSSION

A total of 19 phytochemicals were identified from *Vateria indica Linn* through the IMPATT database. Among these, Bergenin was found in the leaf, root, and bark, while (+)-Hopea phenol was observed in both leaf and root tissues. Accordingly, these two compounds appear in repetition in both Tables 1 and 2 due to their multi-organ distribution.

The drug-likeness of these phytoconstituents was evaluated using Lipinski's Rule of Five, a widely accepted guideline for

Table 2: Profile of Drug Likness of Phytochemicals derived from *Vateria indica Linn*.

Sl. No.	Phytochemicals	MW (<500)	Clog P (< 5)	HBA (< 10)	HBD (<5)	Number of Violations	DLS
1.	Fisetinidol	274.08	1.09	5	4	0	0.49
2.	Bergenin	328.08	-0.66	9	5	0	0.39
3.	Afzelechin	182.06	0.71	4	3	0	-0.81
4.	(+)-Hopeaphenol	906.27	9.03	12	10	4	0.26
5.	Bergenin	328.08	-0.66	9	5	0	0.39
6.	(+)-Hopeaphenol	906.27	9.03	12	10	4	0.26
7.	Bergenin	328.08	-0.66	9	5	0	0.39
8.	Stearic acid	284.27	7.65	2	1	1	-0.54
9.	Palmitic acid	256.24	6.64	2	1	1	-0.54
10.	1-(11Z-icosenoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphoethanolamine	769.56	14.64	8	3	2	-0.12
11.	Bergenin	328.08	-0.66	9	5	0	0.39
12.	Chamazulene	184.13	5.09	0	0	1	-1.32
13.	Thymol	150.1	3.43	1	1	0	-0.54
14.	alpha-Pinene	136.13	4.49	0	0	0	-1.45
15.	beta-Pinene	136.13	4.14	0	0	0	-1.39
16.	alpha-Terpineol	154.14	3.3	1	1	0	-1.05
17.	Oleoresin tumeric	1014.35	8.2	15	6	4	-0.66
18.	beta-Caryophyllene	204.19	5.35	0	0	1	-1.74
19.	Limonene	136.13	4.53	0	0	0	-1.74

predicting oral bioavailability based on key physicochemical parameters, including Molecular Weight (MW), Hydrogen Bond Donors (HBD), Hydrogen Bond Acceptors (HBA), and lipophilicity (Clog P) (Lipinski *et al*., 2001). While this rule serves as a practical and efficient screening tool in early drug discovery, it is not without exceptions. Compounds such as vitamins, antifungals, and cardiac glycosides may violate these rules due to reliance on active transport or specific delivery routes (Veber *et al*., 2002). Moreover, it may not be suitable for non-oral routes of administration such as intravenous or sublingual formulations.

In the present study, most phytochemicals complied with Lipinski's criteria. However, a few compounds demonstrated violations:

- Molecular Weight >500 Da: (+)-Hopea phenol, 1-(11Z-icosenoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphoethanolamine, and Oleoresin turmeric.
- Hydrogen Bond Acceptors (HBA) >10: (+)-Hopea phenol (leaf and root) and Oleoresin turmeric.
- Hydrogen Bond Donors (HBD) >5: (+)-Hopea phenol and Oleoresin turmeric.
- Clog P >5: (+)-Hopea phenol, Stearic acid, Palmitic acid, 1-(11Z-icosenoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphoethanolamine, Oleoresin turmeric, Chamazulene, and β-Caryophyllene.

These deviations suggest that while these phytoconstituents exhibit potential therapeutic relevance, they may require structural modifications or formulation strategies to enhance their drug-likeness profiles. Nevertheless, computational tools offer an efficient and cost-effective method for early-phase screening, minimizing the need for extensive experimental pharmacokinetic assessments (Ekins *et al*., 2007). Several of the assessed compounds satisfied all key drug-likeness parameters, supporting their potential for further development as therapeutic agents.

CONCLUSION

The present study employed computer-assisted tools to evaluate the drug-likeness properties of selected phytochemicals from *Vateria indica* Linn (*Sarjarasa*) using Lipinski's Rule of Five. Among the 19 identified compounds, most conformed to the established criteria, indicating favourable pharmacokinetic

potential. However, certain phytochemicals such as (+)-Hopea phenol and Oleoresin turmeric exhibited violations in parameters like molecular weight, hydrogen bond donors/acceptors, and lipophilicity, suggesting the need for structural refinement or specialized formulation strategies.

Despite these deviations, the use of computational prediction models provides an effective and economical approach for preliminary screening of bioactive compounds, reducing the reliance on labour-intensive experimental methods in early drug discovery. Overall, the findings suggest that several phytoconstituents from *Vateria indica* possess promising drug-like properties and warrant further investigation for their potential development as therapeutic agents.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

ABBREVIATIONS

MW: Molecular Weight; **HBA:** Hydrogen Bond Acceptors; **HBD:** Hydrogen Bond Donors; **Clog P:** Calculated partition coefficient; **DLS:** Drug-likeness; **RO5:** Lipinski's Rule of Five.

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