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Swiss ADME Prediction of Pharmacokinetics and Drug-Likeness Properties of Secondary Metabolism Present in *Buchanania lanzan*

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ABSTRACT

Modern drug development methods can be enhanced by using plants, driving a global increase in the study of traditional medicinal plants. With the progress of computer science, computational techniques like network analysis and screening have become widely used to illuminate the pharmacological mechanisms of action of these plants. By employing network pharmacology, computer-based screening, and pharmacokinetic screening, the number of active compounds among potential candidates can be enlarged, and the therapeutic plant's mode of action can be illuminated. Buchanania lanzan Spreng also known as Chironji, Charoli, or Char, is a versatile tree species in the Anacardiaceae family. This study concentrates on utilizing the Swiss ADME in silico ADME tool to characterize the pharmacological properties of secondary metabolites found in Buchanania Lanzan. The results of these studies may be utilized by researchers to carry out in vitro and in vivo experiments, thereby elucidating the pharmacological mechanisms of action of traditional medicinal herbs.

Keywords: Medicinal plant, Buchanania Lanzan, Pharmacokinetic, Swiss ADME

1. INTRODUCTION :

Buchanania lanzan Spreng, also known as chironji or char, is a member of the Anacardiaceae family. It was initially described by Francis Hamilton in 1788. The plant reaches a height of 10-15 meters and has a diameter of 1.25-1.75 centimeters. [1]The tree is perennial and flourishes in the tropical deciduous woodlands of Northern, Western, and Central India, mainly in the states of Chhattisgarh, Jharkhand, and Madhya Pradesh. [2] Buchanania lanzan is a highly nourishing plant. Traditional indigenous wisdom underscores the immense worth of nearly all parts of the plant, including the roots, leaves, fruits, seeds, and gum, for diverse medicinal applications. [3]The roots are bitter, dry, cooling, purifying, and constricting and help treat diarrhea. The leaf juice is utilized as an expectorant, a love potion, a laxative, a blood purifier, a thirst quencher, and cures digestive problems. It contains 2.64% tannins (0.35% gallo-tannins), triterpenoids, saponins, flavonoids, and reducing sugars. Chironji seeds are nourishing, flavorful, and utilized as a replacement for almonds in confectionery. The seeds, which possess a moisture content of 3.0%, are a rich source of lipids/fats (59.0%), proteins (19.0–21.6%), starches/carbohydrates (12.1%), fiber (3.8%), minerals such as calcium (279.0 mg), phosphorus (528.0 mg), iron (8.5 mg), and vitamins such as thiamine (0.69 mg), ascorbic acid/vitamin C (5.0 mg), riboflavin (0.53 mg), and niacin (1.50 mg). They also contain 34-47% fatty oil, which can be employed as a substitute for olive and almond oils. The fruits have laxative properties and are used to alleviate thirst and reduce body heat, fever, cough, and asthma. The cut bark is water-soluble and is ingested to treat intercostal pain and diarrhea. The gum, when combined with goat's milk, is an effective and curative remedy for intercostal pain, acting as a pain reliever. [4] The SwissADME platform offers insights into the absorption, distribution, metabolism, and excretion (ADME) profiles, drug-likeness, and suitability for medicinal chemistry applications of small molecules. In this study, we aimed to leverage SwissADME (http://www.swissadme.ch/index.php) to evaluate the individual ADME characteristics and interpret the results.

2. Materials and Methods:

2.1 Swiss ADME:

Created by the Swiss Institute of Bioinformatics, the Swiss ADME tool can be reached online at http://www.swissadme.ch/. This web-based platform offers a user-friendly interface for scientists to assess the ADME characteristics of specific compounds isolated from Buchanania Lanzan. The system requires users to input one molecule per line, using the SMILES format. The results for each molecule are presented in various forms, including tables, charts, and a downloadable spreadsheet.[5]

2.2 Structure and bioavailability radar:

The initial phase presents the 2D chemical structures using the conventional SMILES format. To evaluate the drug-likeness of these molecules, the bioavailability assessment leverages six physicochemical properties: lipophilicity (LIPO), size (SIZE), polarity (POLAR), insolubility (INSOLU), unsaturation (INSATU), and flexibility (FLEX). Each property adheres to defined criteria: lipophilicity should be within -0.7 to +5.0 as calculated by XLOGP3, size should have a molecular weight (MW) between 150 and 500 g/mol, polarity should exhibit a topological polar surface area (TPSA) between 20 and 130 Å², solubility should have a logarithm of solubility (log S) not exceeding 6, saturation should maintain a fraction of carbons in sp3 hybridization of at least 0.25, and flexibility should be limited to a maximum of 9 rotatable bonds. [6]

2.3 Physicochemical properties:

The compound's molecular and physicochemical characteristics, such as its molecular formula, molecular mass, heavy atom count, aromatic heavy atom count, sp3 carbon fraction, rotatable bond number, hydrogen bond acceptor and donor counts, molar refractivity, and topological polar surface area (TPSA), were calculated using Open Babel version 2.3.0. [6,7] These properties provide insights into the compound's potential drug-likeness, solubility, permeability, and metabolic stability. For instance, a high number of rotatable bonds often correlates with increased conformational flexibility, which can impact a molecule's binding affinity and selectivity. Similarly, TPSA, a measure of a molecule's polarity, can influence its ability to cross cell membranes and interact with biological targets.

2.4 Lipophilicity:

In the process of discovering and developing new drugs, lipophilicity is a crucial factor. It works alongside other fundamental physical and chemical properties in medicinal chemistry. Lipophilicity is often measured experimentally using partition coefficients (log P) or distribution coefficients (log D). Log P shows the balance of a neutral substance between water and an organic solvent that doesn't mix with water. Higher log P values signify increased lipophilicity [8] . To gauge the lipophilicity of a compound, Swiss ADME presents five freely accessible prediction models: WLOGP, XLOGP3, iLOGP, MLOGP and SILICOS-IT. XLOGP3 employs an atomic-level technique, incorporating corrective factors and a knowledge-based database. WLOGP utilizes a purely atomic-based approach using a fragmental system. [9] MLOGP is a topological technique based on a linear connection with 13 implemented molecular features.[10,11] SILICOS-IT is a composite technique that merges 27 substructures and 7 topological indicators. iLOGP is a physically grounded approach that computes the free energies of dissolution in n-octanol and water using the generalized-born and solvent-accessible surface area (GB/SA) model.[6]

2.5 Solubility:

The degree to which a compound dissolves is greatly impacted by the solvent employed, the surrounding temperature, and the pressure. The saturation point indicates the maximum solubility, the stage at which introducing additional solute doesn't lead to a higher concentration in the solution [12]. A drug is deemed highly soluble when the maximum dosage can dissolve in 250 milliliters or less of water-based solution within a pH range of 1 to 7.5. Swiss ADME utilizes two topological techniques to predict water solubility. The initial method involves the use of the ESOL model, which categorizes solubility into classes based on a logarithmic scale (Insoluble<-10, Poorly soluble<-6, Moderately soluble<-4, Soluble<-2, Very soluble<0). Both techniques deviate from the fundamental general solubility equation as they do not account for the melting point factor.[13] Nevertheless, a strong linear correlation exists between the predicted and experimental values (R^2=0.69 and 0.81, respectively). The third predictor in Swiss ADME was developed by SILICOS-IT, which similarly categorizes solubility into classes based on a logarithmic scale (Insoluble<-10, Poorly soluble<-6, Moderately soluble<-4, Soluble<-2, Very soluble<0), with the linear coefficient adjusted by molecular weight (R^2=0.75). All predicted values are presented as the decimal logarithm of molar water solubility (log S). Swiss ADME additionally provides solubility values in mol/l and mg/ml, alongside qualitative solubility classes.

2.6 Pharmacokinetics:

A graph depicting two calculated properties, ALOGP and PSA, reveals a specific region associated with favorable gastrointestinal (GI) absorption. This region, densely populated by molecules with good absorption, forms an elliptical shape and is aptly named the Egan egg. By utilizing this egg, the model's capacity to forecast passive GI absorption and brain penetration through passive diffusion is evaluated, resulting in the development of the BOILED-Egg model (Brain or Intestinal Lipid Estimate D permeation predictive model). The BOILED-Egg model offers a rapid, intuitive, efficient, and dependable method for predicting passive gastrointestinal absorption, proving invaluable in drug discovery and development [14.] The white area represents the region containing molecules with a higher rate of intestinal absorption, while the yellow area (yolk) denotes the region with the highest probability of brain penetration[6]. Cytochrome P450 (CYP) enzymes process more than 50-90% of medicinal drugs through their five primary isoforms (CYP1A2, CYP2C19, CYP3A4, CYP2C9, CYP2C19, CYP2D6, CYP2E1). P-glycoprotein (P-gp) is widely

expressed in the intestinal lining and works to expel foreign substances back into the intestinal cavity and from the capillary endothelial cells of the brain back into the capillaries [15,16] . Swiss ADME employs the support vector machine algorithm (SVM) to classify datasets containing known substrates/non-substrates or inhibitors/non-inhibitors for binary categorization. The resulting molecule will be classified as either "Yes" or "No" depending on whether it is predicted to be a substrate for both P-gp and CYP, respectively. The SVM model for the P-gp substrate was constructed using 1033 molecules for training and assessed on 415 molecules for testing, with a 10-fold cross-validation accuracy of 0.72 and an area under the curve (AUC) of 0.77. The external accuracy and AUC were 0.94, respectively. The Support Vector Machine (SVM) models for the inhibition of Cytochrome P-450 1A2, 2C19, 3A4, 2C9, 2C19, 2D6, 2E1, and molecules were developed using various training and test datasets. For the Cytochrome P-450 1A2 inhibitor molecule, the SVM model was trained on a dataset of 9145 molecules and evaluated on a dataset of 3000 molecules. The 10-fold cross-validation yielded an accuracy (ACC) of 0.83 and an area under the curve (AUC) of 0.90. The external validation resulted in an ACC of 0.84 and an AUC of 0.91. Similarly, for the Cytochrome P-450 2C19 inhibitor molecule, the SVM model was built using a training set of 9272 molecules and tested on 3000 molecules. The 10-fold cross-validation demonstrated an accuracy of 0.80 and an area under the curve of 0.86. When evaluated on an external dataset, the model achieved an accuracy of 0.80 and an area under the curve of 0.87. In the case of the Cytochrome P-450 2C9 inhibitor molecule, a support vector machine model was created using a training set of 5940 molecules and subsequently tested on a set of 2075 molecules.[17] A 10-fold cross-validation procedure yielded an accuracy of 78% and an area under the curve of 85%. External validation of the model resulted in an accuracy of 71% and an area under the curve of 81%. For the Cytochrome P-450 2D6 inhibitor molecule, a support vector machine model was developed using a training set composed of 3664 molecules and was then assessed on a set of 1068 molecules. The 10-fold cross-validation procedure revealed an accuracy of 79% and an area under the curve (AUC) of 85%. When evaluated using an external dataset, the model demonstrated an accuracy of 81% and an AUC of 87%. In the specific case of the Cytochrome P-450 3A4 inhibitor molecule, the SVM model was developed using a training set consisting of 7518 molecules and subsequently tested on a set of 2579 molecules. The 10-fold cross-validation analysis yielded an accuracy of 77% and an AUC of 85%. Furthermore, external validation resulted in an accuracy of 78% and an AUC of 80.

2.7 Medicinal chemistry:

This section intends to aid medicinal chemists in their routine drug discovery efforts. PAINS, also referred to as Pan Assay Interference Compounds or promiscuous compounds, are molecules that consistently yield strong signals in assays, irrespective of the protein targets. These compounds have exhibited activity in a broad spectrum of assays, making them appealing candidates for further investigation. Swiss ADME highlights potential problems if these chemical groups are present in the molecule being examined.[18] In a different strategy, Brenk emphasizes compounds that are smaller and less hydrophobic, departing from the rigid constraints of "Lipinski's rule of 5," to expand the possibilities for drug development. This approach involves excluding compounds containing potentially toxic, chemically reactive, or undesirable groups such as nitro groups, sulfates, phosphates, 2-halopyridines, and thiols. The Brenk model imposes restrictions on the ClogP/ClogD values, confining them to a range of 0 to 4. Furthermore, the model mandates that the number of hydrogen bond donors should be fewer than 4, while the number of hydrogen bond acceptors must be less than 7. Concerning molecular size, the model requires that compounds possess between 10 and 28 heavy atoms.[19] To be classified as medicinal, compounds must possess a simple structure, characterized by fewer than 8 rotatable bonds, fewer than 5 ring systems, and the absence of ring systems with more than 2 fused rings. [20] The concept of lead likeness aims to provide starting points with high affinity in high-throughput screening (HTS), allowing for the exploration of additional interactions during the lead optimization phase. Leads undergo chemical modifications that tend to reduce their size and increase their lipophilicity, making them less hydrophobic than drug-like molecules. Lead optimization is commonly conducted using a rule-based approach, with molecules possessing a molecular weight between 100 and 350 Da and a ClogP between 1 and 3.0 being considered superior to drug-like compounds and thus more lead-like. [21,22]

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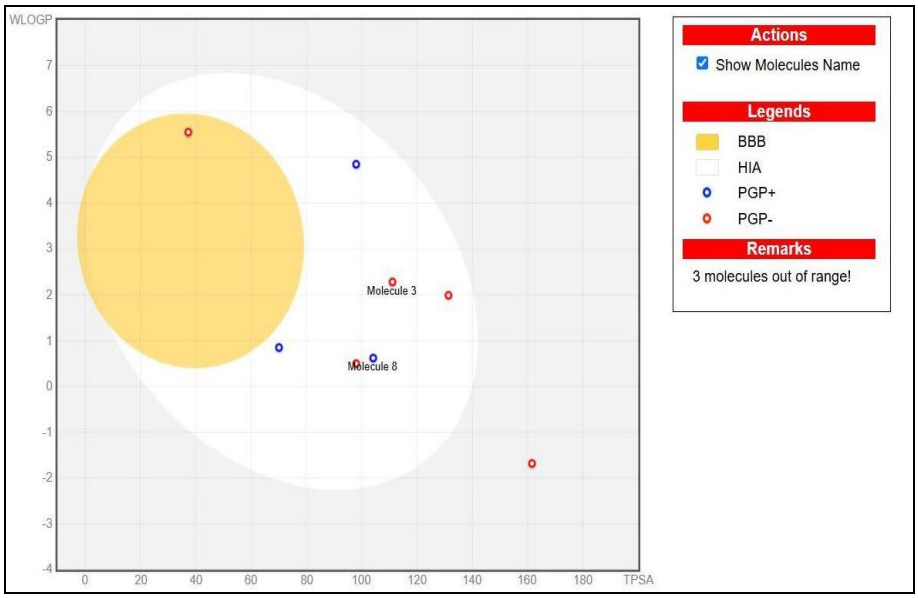

Fig1: Boiled Egg Model of the Phytoconstituents of *Buchanania Lanzan*

3.Result

Table 1 : General Characteristics of Phytoconstituents of Buchanania lanzan

Sr.no	Small Molecule	Pub Chem ID	Molecular Formula	Canonical SMILES	Molecular Weight (in g/mol)
1	Vomicine	101595	C22H24N2O4	CN1CC[C@]23[C@@H]4[C@H]5[C@@H](CC2=O)C(=CCO[C@H]5CC(=O)N4C6=C3C=CC=C6O)C1	380.4
2	Celidoniol	16057860	C29H60O	CCCCCCCCCCCCCCCCCCC[C@H](CCCCCCCCC)O	424.8
3	kaempferol	5280863	· C15H10O6	C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O	286.24
4	Glycoside	637579	C29H44O12	C[C@@H]1[C@H]([C@H]([C@H]([C@@H](O1)O[C@H]2C[C@@H]([C@@]3([C@@H]4[C@@H](CC[C@]3(C2)O)[C@@]5(CC[C@H]([C@]5(C[C@H]4O)C)C6=CC(=O)OC6)O)CO)O)O)O)O	584.7
5	Quercetin	5280343	C15H10O7	C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O	302.23
6	Triterpenoids	71597391	C29H44O5	C[C@@]12CC[C@]3(CCC(C[C@H]3C1=CC[C@H]4[C@]2(CC=C5[C@@]4(C[C@@H]([C@@H]([C@@]5(C)O)O)O)C)C)(C)C)C(=O)O	472.7
7	Saponin	22715020	C58H94O27	CC1(C2CCC3(C(C2(CCC1OC4C(C(C(CO4)OC5C(C(C(CO5)O)O)O)OC6C(C(C(C(O6)CO)O)O)O)OC7C(C(C(C(O7)CO)O)O)OC8C(C(C(C(O8)CO)O)O)O)C)CCC91C3(CC(C2(C9CC(CC2)(C)C=O)CO1)O)C)C)C	1223.3
8	Riboflavin	493570	C17H20N4O6	CC1=CC2=C(C=C1C)N(C3=NC(=O)NC(=O)C3=N2)C[C@@H]([C@@H]([C@@H](CO)O)O)O	376.4
9	Thiamine	1130	C12H17N4OS+	CC1=C(SC=[N+]1CC2=CN=C(N=C2N)C)CCO	265.36
10	Palmitic acid	985	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	256.42
11	Oleic acid	445639	C18H34O2	CCCCCCCC/C=C\CCCCCCCC(=O)O	282.5
12	stearic acid	5281	C18H36O2	CCCCCCCCCCCCCCCCCC(=O)O	284.5
13	Gallic acid	370	C7H6O5	C1=C(C=C(C(=C1O)O)O)C(=O)O	170.12
14	Beta-Amyrin	73145	C30H50O	C[C@@]12CC[C@@]3(C(=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(CC[C@@H](C5(C)C)O)C)C)[C@@H]1CC(CC2)(C)C)C	426.7

Table 2: Lipophilicity of the Phytoconstituents of Buchanania lanzan

Sr.no	Small molecule	iLOGP	XLOGP3	WLOGP	MLOGP	SILICOS-IT	Consensus Log $P^{o/w}$
1	Vomicine	2.91	-0.07	0.85	1.48	1.45	1.33
2	Celidoniol	7.30	14.03	10.53	7.27	11.23	10.07
3	kaempferol	1.70	1.90	2.28	-0.03	2.03	1.58
4	Glycoside	3.18	-1.70	-1.51	-1.11	-0.97	-0.42
5	Quercetin	1.63	1.54	1.99	-0.56	1.54	1.23
6	Triterpenoids	3.07	3.94	4.85	3.85	3.93	3.93
7	Saponin	4.37	-2.67	-4.07	-6.13	-4.09	-2.52
8	Riboflavin	1.63	-1.46	-1.68	-0.54	1.09	-0.19
9	Thiamine	-1.60	1.02	0.62	0.05	2.54	0.53
10	Palmiticacid	3.85	7.17	5.55	4.19	5.25	5.20
11	Oleic acid	4.01	7.64	6.11	4.57	5.95	5.65
12	stearic acid	4.30	8.23	6.33	4.67	6.13	5.93
13	Gallic acid	0.21	0.70	0.50	-0.16	-0.20	0.21
14	Beta-Amyrin	4.63	9.15	8.17	6.92	6.92	7.16

Table 3: Water solubility of the phytoconstituents of Buchanania lanzan

Small Molecule	ESOL				Ali				SILICOS-IT			
	LogS (ESOL)	Solubility		Class	LogS (ESOL)	Solubility		Class	LogS (ESOL)	Solubility		Class
		mg/mL	mol/L			mg/mL	mol/L			mg/mL	mol/L	
Vomicine	-2.31	1.85e+00	4.86e-03	Soluble	-0.95	4.27e+01	1.12e-01	Very Soluble	-3.31	1.88e-01	4.94e-04	Soluble
Celidoniol	-9.60	1.08e-07	2.53e-10	Poorly Soluble	-14.53	1.24e-12	2.92e-15	insoluble	-10.55	1.19e-08	2.81e-11	insoluble
kaempferol	-3.31	1.40e-01	4.90e-04	Soluble	-3.86	3.98e-02	1.39e-04	Soluble	-3.82	4.29e-02	1.50e-04	Soluble
Glycoside	-2.13	4.34e+00	7.42e-03	Soluble	-2.13	4.38e+00	7.49e-03	Soluble	0.33	1.25e+03	2.13e+00	Soluble
Quercetin	-3.16	2.11e-01	6.98e-0.4	Soluble	-3.91	3.74e-02	1.24e-04	Soluble	-3.25	1.73e-01	5.73e-04	Soluble
Triterpenoids	-5.19	3.08e-03	6.51e-06	Moderately soluble	-5.70	9.48e-04	2.01e-06	Moderately soluble	-4.32	2.27e-02	4.80e-05	Moderately soluble
Saponin	-4.82	1.86e-02	1.52e-05	Moderately soluble	-5.64	2.78e-03	2.27e-06	Moderately soluble	2.70	6.09e+05	4.98e+02	Soluble
Riboflavin	-1.31	1.85e+01	4.93e-02	Very soluble	-1.43	1.40e+01	3.72e-02	Very soluble	-2.62	9.03e-01	2.40e-03	Soluble
Thiamine	-2.32	1.28e+00	4.83e-03	Soluble	-2.80	4.24e-01	1.60e-03	Soluble	-3.30	1.32e-01	4.99e-04	Soluble
Palmitic acid	-5.02	2.43e-03	9.49e-06	Moderately soluble	-7.77	4.31e-06	1.68e-08	Poorly Soluble	-5.31	1.25e-03	4.88e-06	Moderately soluble
Oleic acid	-5.41	1.09e-03	3.85e-06	Moderately soluble	-8.26	1.54e-06	5.46e-09	Poorly Soluble	-5.39	1.14e-03	4.04e-06	Moderately soluble
stearic acid	-5.73	5.26e-04	1.85e-06	Moderately soluble	-8.87	3.80e-07	1.33e-09	Poorly Soluble	-6.11	2.19e-04	7.71e-07	Poorly Soluble
Gallic acid	-1.64	3.90e+00	2.29e-02	Very soluble	-2.34	7.86e-01	4.62e-03	Soluble	-0.04	1,55e+02	9.10e-01	Soluble
Beta-Amyrin	-8.25	2.40e-06	5.62e-09	Poorly Soluble	-9.47	1.44e-07	3.38e-10	Poorly Soluble	-7.16	2.93e-05	6.86e-08	Poorly Soluble

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Table 4: Pharmacokinetic Parameters of the Phytoconstituents of Buchanania lanzan

Moleculs	GI absorption	BBB permeant	P-Gp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	LogKp (cm/s)
Vomicine	High	No	Yes	No	No	No	Yes	No	-8.67
Celidoniol	Low	No	Yes	No	No	No	No	No	1.07
kaempferol	High	No	No	Yes	No	No	Yes	Yes	-6.70
Glycoside	Low	No	No	No	No	No	No	No	-11.07
Quercetin	High	No	No	Yes	No	No	Yes	Yes	-7.05
Triterpenoids	High	No	Yes	No	No	No	No	No	-6.39
Saponin	Low	No	Yes	No	No	No	No	No	-15.66
Riboflavin	Low	No	No	No	No	No	No	No	-9.63
Thiamine	High	No	Yes	No	No	No	No	No	-7.19
Palmitic acid	High	Yes	No	Yes	No	Yes	No	No	-2.77
Oleic acid	High	No	No	Yes	No	Yes	No	No	-2.60
stearic acid	High	No	No	Yes	No	No	No	No	-2.19
Gallic acid	High	No	No	No	No	No	No	Yes	-6.84
Beta-Amyrin	Low	No	No	No	No	No	No	No	-2.41

Table 5: Drug likeness of the Phytoconstituents of Buchanania lanzan

Molecules	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability score
Vomicine	Yes,0 Violation	Yes	Yes	Yes	Yes	0.55
Celidoniol	Yes;1 violation: MLOGP>4.15	No;3 violations: WLOGP>5.6 MR>130, #atoms>70	No;1violation: Rotors>10	No;1violation: WLOGP>5.88	No;3violations: XLOGP3>5, Heteroatoms<2, Rotors>15	0.55
kaempferol	Yes,0 Violation	Yes	Yes	Yes	Yes	0.55
Glycoside	No:3 violations: MW>500, NorO>10, NHorOH>5	No;4 violations: MW>480, WLOGP<-0.4, MR>130, #atoms>70	No;1violatio: TPSA>140	No;1violation: TPSA>131.6	No;3violations: TPSA>150, H-acc>10, H-don>5	0.17
Quercetin	Yes,0 Violation	Yes	Yes	Yes	Yes	0.55
Triterpenoids	Yes;0 violation	No;2 violations: MR>130, #atoms>70	Yes	Yes	Yes	0.56
Saponin	No;3 violations: MW>500, NorO>10, NHorOH>5	No;4 violations: MW>480, WLOGP<-0.4, MR>130, #atoms>70	No;2 violations: Rotors>10, TPSA>140	No;1 violation: TPSA>131.6	No;6 violations: MW>600, XLOGP3<-2, TPSA>150, #rings>7, H-acc>10, H-don>5	0.17
Riboflavin	Yes;0 violation	No;1 violation: WLOGP<-0.4	No;1 violation:TPSA>140	No;1violation: TPSA>131.6	No;1violation: TPSA>150	0.55
Thiamine	Yes,0 Violation	Yes	Yes	Yes	Yes	0.55
Palmitic acid	Yes;1 violation: MLOGP>4.15	Yes	No;1violation: Rotors>10	Yes	No;1violation: XLOGP3>5	0.85
Oleic acid	Yes;1 violation: MLOGP>4.15	No;1 violation: WLOGP>5.6	No;1violation: Rotors>10	No;1violation: WLOGP>5.88	No;1violation: XLOGP3>5	0.85
stearic acid	Yes;1 violation: MLOGP>4.15	No;1 violation: WLOGP>5.6	No;1violation: Rotors>10	No;1violation: WLOGP>5.88	No;2violations: XLOGP3>5, Rotors>15	0.85
Gallic acid	Yes;0 violation	No;2 violations: MR<40, #atoms<20	Yes	Yes	No;1 violation: MW<200	0.56
Beta-Amyrin	Yes;1 violation: MLOGP>4.15	No; 3 violations: WLOGP>5.6, MR>130, #atoms>70	Yes	No;1 violation: WLOGP>5.88	No;2 violations: XLOGP3>5, Heteroatoms<2	0.55

Table 6: Medicinal Chemistry Properties of Phytoconstituents of Buchanania Lanzan

Molecules	Pains	Brenk	Leadlikeness	Synthetic accessibility
Vomicine	0 alert	1 alert isolated_alkene	No;1violations: MW>350,	5.64
Celidoniol	0 alert	0 alert	No;3violations: MW>350, Rotors>7, XLOGP3>3.5	4.29
kaempferol	0 alert	0 alert	Yes	3.14
Glycoside	0 alert	1 alert: saponine_derivative	No; 1 violation: MW>350	7.13
Quercetin	1 alert catechol_A	1 alert catechol	Yes	3.23
Triterpenoids	0 alert	1 alert: isolated_alkene	No;2 violations: MW>350, XLOGP3>3.5	6.35
Saponin	0 alert	2alerts:aldehyde,saponine_derivative	No:2violations: MW>350, Rotors>7	10.00
Riboflavin	0 alert	1alert:polycyclic_aromatic_hydrocarbon_2	No;1 violation: MW>350	3.84
Thiamine	0 alert	1 alert: quaternary_nitrogen_1	Yes	2.99
Palmitic acid	0 alert	0 alert	No;2violations: Rotors>7, XLOGP3>3.5	2.31
Oleic acid	0 alert	1 alert: isolated_alkene	No;2violations: Rotors>7, XLOGP3>3.5	3.07
stearic acid	0 alert	0 alert	No;2violations: Rotors>7, XLOGP3>3.5	2.54
Gallic acid	1 alert: catechol_A	1 alert: catechol	No;1 violation: MW<250	1.22
Beta-Amyrin	0 alert	1 alert: isolated_alkene	No; 2 violations: MW>350, XLOGP3>3.5	6.04

4.Discussion

Ayurveda, one of the oldest medical systems, offers a wealth of potential therapeutic compounds derived from herbs. The increasing global popularity of herbal medicine, both in developing and developed nations, is driven by its perceived safety profile and natural origin. Computer-aided drug design, which leverages quantitative structure-activity relationships (QSAR), has emerged as a valuable tool for predicting the ADMET properties of drug candidates. Numerous software programs, such as Swiss ADME, are readily available to facilitate this process. In this study, we employed the Swiss ADME online tool to assess the ADMET characteristics of plant compounds from Buchanania lanzan. These phytoconstituents, including alkaloids like vomicine, celidoniol, kaempferol, glycoside, quercetin, triterpenoids, saponins, and various fatty acids and phenolic compounds, were evaluated for their uptake, dispersion, biotransformation, elimination, and toxicity profiles. The findings, shown in tables and figures, can be a useful resource for researchers and scientists aiming to create new, semisynthetic, or synthetic medications with various therapeutic uses.

5.Conclusion

The exponential growth of biological and chemical datasets has driven substantial advancements in drug discovery and development, enabled by computational approaches such as computer-aided drug design (CADD). Computer-based tools have revolutionized the way we discover and develop new drugs, making the process faster, cheaper, and more effective. This work presents a web-based platform, SwissADME, which offers free access for assessing the ADME profiles of phytoconstituents extracted from Buchanania lanzan. These results can lay the groundwork for future investigations into the biological and pharmacological activities of the plant. Early computational studies reveal the potential of compounds such as vomicine, celidoniol, kaempferol glycoside, quercetin, triterpenoids, and various fatty acids and phenolics as promising drug candidates for a variety of diseases. These findings necessitate further research to fully explore their therapeutic capabilities. Despite these promising results, rigorous testing is imperative to substantiate the bioactivity of these substances before their advancement to clinical trials.

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