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In silico pharmacokinetic profiling of bioactive compounds from methanolic extracts of Paederia foetida Linn.

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Abstract
The Native plant Paederia foetida, sometimes known as the skunk vine, is a member of the Rubiaceae family. A wide range of conditions can be treated with the plant, including rheumatoid arthritis and liver diseases. The goal of the current study was to utilize Swiss ADME to determine the pharmacokinetic profile of the methanolic extract from Paederia foetida leaves. Several bioactive substances were identified using GC-MS analysis, with terpenoids, fatty acid esters, and aromatic derivatives showing the largest peaks. The absorption, distribution, metabolism, and excretion (ADME) characteristics of these substances were examined in detail.Only a small percentage exhibited pharmacokinetic limitations, whereas the majority met Lipinski's rule of five and demonstrated good gastrointestinal absorption, adequate solubility, and excellent drug likeness scores.
Keywords: *Paederia foetida, pharmacokinetics, ADME Characteristics, SWISS ADME*

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I. Introduction

The perennial climbing shrub Paederia foetida, which is a member of the Rubiaceae family, is widely used in traditional medicine to treat rheumatic pain, gastritis, indigestion, stomach diseases, and to enhance liver and kidney function [1]. As the name implies, Paederia foetida is an unpleasant-smelling climber. It yields thin stems that can grow up to 30 ft (9 m) in length. The leaves are heart-shaped, opposite, and evergreen. The pungent fragrance of this herb is attributed to the sulfur compounds found in its leaves and stems [2]. In addition to having a high protein content that includes arginine, histidine, lysine, tyrosine, tryptophan, phenylalanine, cystine, methionine, and valine, leaves are also a good source of carotene and vitamin C. Additionally, the crystalline keto alcohol paederolone, a keto molecule called paederone, β- and δ-sitosterols, and two volatile alkaloids called paederine and paederenine are found in the aerial sections. Methyl mercaptan, hentriacontane, hentriacontanol, methyl mercaptan, palmitic acid, sitosterol,stigmasterol,campesterol, ursolic acid, and iridoid glycosides—paederoside, paederosidic acid, scandoside, asperuloside, and deacetyl asperuloside—have also been isolated from leaves and stems, and they contain a volatile oil with an unpleasant smell.[3,4]Many molecular structures are assessed based on a wide range of criteria during the time-consuming and resource-intensive drug discovery and development processes. This helps guide the choice of chemicals to synthesize, test, and market, ultimately identifying those with the best chance of becoming a medication that works for patients. The compounds must have low toxicity and optimal biological activity. Access to and concentration of therapeutic targets within the body are equally crucial. Pharmacokinetics, or the fate of a medicinal substance in the body, is traditionally thought of by dissecting the several actions that affect the target's access to discrete factors. Then, using specific techniques, these ADME characteristics (Absorption, Distribution, Metabolism, and Excretion) can be assessed independently. Early ADME estimation during the discovery phase has been shown to significantly lower the percentage of pharmacokinetics-related failures during the clinical phases. Computer models have been marketed as a good alternative to experimental techniques for ADME prediction, especially in the early phases when there are numerous chemical structures being studied, but few molecules are accessible.[5]

II. Materials And Methods

Swiss ADME:

The Swiss Institute of Bioinformatics ultimately produced the Swiss ADME program, which was made accessible online at www.swissadme.ch. To estimate the ADME behaviors of chemical substances derived from Paederia foetida, the Swiss ADME submission webpage was made available by Google's server. The simplified molecular input line access machine (SMILES) was used to describe each molecule in the entire list, which contained one molecule per line.[6]

Structure & Bioavailability Radar:

Using canonical SMILES, the two-dimensional chemical structure was shown in the first section. The bioavailability radar allows a first assessment of how comparable the medication is to The following six physicochemical properties of the target molecules are taken into account: The terms LIPO (lipophilicity), SIZE, POLAR (polarity), INSOLU (insolubility), INSATU (insaturation), and FLEX (flexibility) are employed in that sequence. Size: 150–500 g/mol; polarity: TPSA between 20 and 130 0A2; solubility: log S not larger than 6; saturation: fraction of carbons in the sp3 hybridization not less than 0.25; flexibility: no more than nine rotatable bonds; and lipophilicity: XLOGP3 between -0.7 and +5.0 [7].

Lipophilicity:

One physicochemical characteristic that is vital to medicinal chemistry is lipophilicity. At the molecular level, it encodes data on the network of intramolecular and intermolecular forces that influence drug interactions with the target protein and drug transport through lipid structures. Thus, lipophilicity plays a crucial role in determining the pharmacokinetics and pharmacodynamics of a pharmacological substance at the organism level [7]. In experiments, it is shown as distribution coefficients (log D) or partition coefficients (log P). A unionized solute's partition equilibrium between water and an immiscible organic solvent is depicted by log P. Higher log P values indicate higher lipophilicity[8]. Swiss ADME offers five publicly available models—XLOGP3, WLOGP, MLOGP, SILICOS-IT, and iLOGP—to assess a compound's lipophilicity character. XLOGP3 is an atomistic approach that incorporates a knowledge-based library and correction factors. WLOGP is an application of the fragmental system-based purely atomistic technique. The topological method's ancestor, MLOGP, proposed a linear relationship with 13 molecular descriptors in practice. iLOGP, a physics-based approach, relies on free energies of solvation in n-octanol and water determined by the generalized-born and solvent accessible surface area (GB/SA) model, whereas SILICOS-IT, a mongrel method, relies on 27 fragments and 7 topological descriptors[9].

Solubility:

In the pharmaceutical sector, solubility is a significant problem that is still being researched[10]. The most basic feature in pharmaceutical research is a medication's solubility, which is Necessary for numerous industrial uses such as drug solubilization, solution crystallization, liquid drug formulation, nanoparticle manufacturing, etc. Drugs with low aqueous solubility have limitations in clinical use and may potentially result in crystalluria[11]. If a drug's maximum dose power dissolves in 250 milliliters or less of aqueous liquids with a pH of 1 to 7.5, it is said to be extremely soluble. Swiss ADME expects water solubility by using topological techniques. The main approach is the ESOL version, which uses a logarithmic scale to classify solubility: extremely soluble<0, insoluble<-10, poorly soluble<-6, fairly soluble<-4, and soluble<-2. Both strategies depart somewhat from the fundamental standard solubility equation due to the omission of the melting point parameter.[12]Despite avoiding the melting point parameter, a good linear relationship was observed between the experimental and predicted values (R^2 = 0.81 and 0.69, respectively). The SILICOS-IT (Solubility) class developed the third Swiss ADME predictor: Log S Scale (insoluble <- -10, poorly soluble <-6, moderately soluble <-4, soluble <-2, very soluble <0).

Pharmacokinetics:

A graph showing the variant inside a place of fantastic qualities for gastrointestinal (GI) absorption shows two computed descriptors, ALOGP and PSA, respectively. The Egan egg is the oval area that has the highest awareness of chemicals that are nicely absorbed. For each passive GI absorption and passive diffusion brain admission to prediction, the predictive capabilities of the BOILED-Egg (brain or intestinal L Estimate D permeation predictive model) are evaluated using this egg. For drug research and discovery, the BOILED-Egg version provides a quick, spontaneous, reliable, and efficient method of estimating passive GI absorption The yellow area (yolk) denotes the space with the most potential for brain penetration, whereas the white area is the distance occupied by molecules with a higher degree of absorption through the GI tract[13] Of its five main isoforms, cytochrome p450 (CYP) isoenzymes biotransform between 50 and 90 percent of medicinal compounds (CYP1A2, CYP3A4, CYP2C9, CYP2C19, and CYP2D6).[14,15,16] For binary classification on datasets that contain known substrates and non-substrates or inhibitors and non-inhibitors, ADME uses the Swiss assist vector machine technique (SVM). Depending on whether it is expected to be a substrate for both CYP and P-gp, the resultant molecule can be classified as either "certain" or "no." The SVM model for the P-gp substrate was constructed using 1033 molecules from the training set and 415 molecules from the test set, yielding an AUC of 0.77 and a 10-fold go-validation accuracy of 0.72. AUCAUC and external accuracy are both 0.94.Several education and check sets were used to build the guiding vector system (SVM) models for the inhibition of Cytochrome P-450 1A2, 2C19, 2C9, 2D6, and 3A4 molecules. The SVM version was developed using a training set of 9145 molecules, and 3000 molecules of the medication known as a cytochrome P-450

1A2 inhibitor were employed for assessment. The region under the curve (AUC) and ten-fold cross-validation accuracy (ACC) were 0.90 and 0.83, respectively.[17]

Drug likeness:

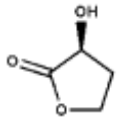
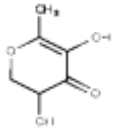
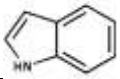
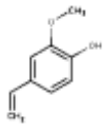
SWissADME finds compounds with drug-like qualities by removing molecules with low pharmacokinetic potential using a set of rule-based filters. The most well-known of these is Lipinski's Rule of Five (Pfizer), which states that compounds that resemble drugs often have a molecular weight of less than 500, ten hydrogen bond acceptors, no more than five hydrogen bond donors, and an MLOGP of 4.15 or below. By taking into account factors including molecular weight between 160 and 480 Da, WLOGP between -0.4 and 5.6, molar refractivity between 40 and 130, and a total atom count between 20 and 70, the Ghose filter (Amgen) further refines drug-likeness.Likewise, the Veber filter (GSK) prioritizes oral bioavailability by selecting molecules with up to twelve hydrogen bond donors and acceptors, a topological polar surface area (TPSA) of 140 Å² or fewer, and no more than 10 rotatable bonds. When assessing membrane permeability, the Egan filter (Pharmacia) accepts substances with TPSA < 131.6 and WLOGP ≤ 5.88. Together, these filters enable SwissADME to forecast drug-likeness using factors relating to physicochemistry and absorption. Furthermore, the Abbott bioavailability score forecasts the probability that a chemical will exhibit detectable permeability in Caco-2 cell assays or achieve at least 10% oral bioavailability in rats. By quickly screening chemical libraries, our scoring approach makes it possible to find interesting candidates for synthesis and additional development[18].

Medicinal chemistry:

This component's purpose is to assist medicinal chemists in their constant endeavors to create novel tablets. Regardless of the protein targets, substances referred to be PAINS (Pan test Interference Compounds, common hits, or promiscuous compounds) show robust test results. These compounds can be used as sites for further research because they exhibit activity in a variety of assays. If such moieties are present in the chemical under evaluation, Swiss ADME will provide warmth [19]. Using a unique approach, Brenk focuses on molecules that can be smaller and significantly less hydrophobic than those that meet "Lipinski's rule of five." As a result, more lead optimization chances become available [20].

III. Results:

Table 1: General Characteristics of Phytoconstituents of Paederia foetida

Sl No	Name	mol. Wt	mol. Formula	SMILES	structure
1	2-Hydroxy-gamma-butyrolactone	102	C4H6O3	C1COC(=O)[C@H]1O	
2	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	144	C6H8O4	CC1=C(C(=O)C(CO1)O)O	
3	Indole	117	C8H7N	C1=CC=C2C(=C1)C=CN2	
4	2-Methoxy-4-vinylphenol	150	C9H10O2	COC1=C(C=CC(=C1)C=C)O	

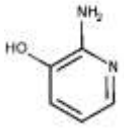
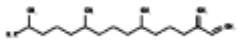
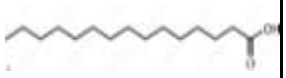
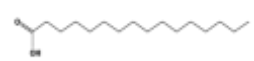
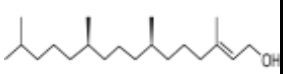
5	Cycloheptasiloxane, tetradecamethyl	518	C14H42O7Si7	C[Si]1(O[Si](O[Si](O[Si](O[Si](O[Si](O[Si](O1)(C)C)(C)C)(C)C)(C)C)(C)C)(C)C)C	
6	Cyclooctasiloxane, hexadecamethyl	592	C16H48O8Si8	C[Si]1(O[Si](O[Si](O[Si](O[Si](O[Si](O[Si](O[Si](O[Si](O1)(C)C)(C)C)(C)C)(C)C)(C)C)(C)C)(C)C)C	
7	2-Amino-3-hydroxypyridine	110	C5H6N2O	C1=CC(=C(N=C1)N)O	
8	Neophytadiene	278	C20H38	CC(C)CCCC(C)CCCC(C)CCCC(=C)C=C	
9	Pentadecanoic acid	242	C15H30O2	CCCCCCCCCCCCCCC(=O)O	
10	Hexadecanoic acid, methyl ester	270	C17H34O2	CCCCCCCCCCCCCCCC(=O)OC	
11	n-Hexadecanoic acid	256	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	
12	Tricyclo[7.1.0.0[1,3]]decane-2-carbaldehyde	164	C11H16O	C1CCC2CC23C(C3C=O)CC1	
13	Phytol	296	C20H40O	C[C@@H](CCC[C@@H](C)CCC/C(=C/CO)/C)CCCC(C)C	

Table 2: Lipophilicity of the Phytoconstituents of Paederia foetida

Sl no	Name	ILOGP	XLOGP3	WLOGP	MLOGP	SILICOS-IT	Consensus log ***P*0/*w***
1	2-Hydroxy-gamma-butyrolactone	0.67	-0.37	-0.71	-0.79	0.48	-0.14

2	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	1.19	-0.37	-0.26	-1.77	0.13	-0.22
3	Indole	1.43	2.05	2.17	1.57	2.66	1.98
4	2-Methoxy-4-vinylphenol	2.14	2.81	1.93	1.71	2.13	2.14
5	Cycloheptasiloxane, tetradecamethyl	5.28	6.95	5.03	-1.54	-7.93	1.56
6	Cyclooctasiloxane, hexadecamethyl	5.85	8.05	5.75	-1.83	-7.10	2.14
7	2-Amino-3-hydroxypyridine	0.70	0.15	0.38	-0.45	0.25	0.21
8	Neophytadiene	5.05	9.62	7.17	6.21	7.30	7.07
9	Pentadecanoic acid	3.66	6.63	5.16	3.94	4.81	4.84
10	Hexadecanoic acid, methyl ester	4.41	7.38	5.64	4.44	5.84	5.54
11	n-Hexadecanoic acid	3.85	7.17	5.55	4.29	5.25	5.20
12	Tricyclo[7.1.0.0[1,3] decane-2-carbaldehyde	2.54	2.20	3.02	2.39	3.45	2.72
13	Phytol	4.85	8.19	6.36	5.25	6.57	6.25

Table 3: Water solubility of the phytoconstituents of Paederia foetida

Name	**ESOL**				**Ali**				**SILCOS-IT**			
	Log s	**Solubility**		**Class**	**Log s**	**Solubility**		**Class**	**Log s**	**Solubility**		**Class**
		mg/mL	**mol/L**			**mg/mL**	**mol/L**			**mg/mL**	**mol/L**	
2-Hydroxy-gamma-butyrolactone	-0.24	5.88e+0.1	5.76e-0.1	Very soluble	-0.14	7.32e+0.1	7.17e-0.1	Very soluble	0.26	18.7e+0.2	1.83e+00	soluble
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl	0.50	4.55e+01	3.16e-01	Very soluble	-0.57	3.89e+01	2.70e-01	Very soluble	0.15	2.03e+02	1.41e+00	soluble
Indole	-2.60	2.96e-0.1	2.52e-03	soluble	-2.01	1.14e+00	9.77e-03	soluble	-3.23	6.90e-02	5.89e-04	soluble
2-Methoxy-4-vinylphenol	-2.81	2.31e-01	1.54e-03	soluble	-3.09	1.23e-01	8.21e-04	soluble	-2.38	6.30e-01	4.20e-03	soluble

Cycloheptasiloxane, tetradecamethyl	-7.44	1.90e-05	3.66e-08	Poorly soluble	-8.12	3.94e-06	7.59 e-09	Poorly soluble	-4.63	120e-02	2.32e-05	Moderately soluble
Cyclooctasiloxane, hexadecamethyl	-8.59	1.53e-06	2.57e-09	Poorly soluble	-9.46	2.08e-07	3.50 e-10	Poorly soluble	-4.53	1.74e-02	2.94e-05	Moderately soluble
2-Amino-3-hydroxypyridine	-1.17	7.41e+00	6.73e-02	Very soluble	-0.95	1.24e+01	1.13 e-01	Very soluble	-1.03	1.03e+01	9.38e-02	soluble
Neophytadiene	-6.77	4.74e-05	1.70e-07	Poorly soluble	-9.53	8.15e-08	2.93 e-10	Poorly soluble	-6.11	2.18e-04	7.82e-07	Poorly soluble
Pentadecanoic acid	-4.66	5.28e-03	2.18e-03	Moderately soluble	-7.21	1.48e-05	6.10 e-08	Poorly soluble	-4.91	2.98e-03	1.23e-05	Moderately soluble
Hexadecanoic acid, methyl ester	-5.18	1.80e-03	6.67e-06	Moderately soluble	-7.76	4.68e-06	1.73 e-08	Poorly soluble	-6.01	2.64e-04	9.75e-07	Poorly soluble
n-Hexadecanoic acid	-5.02	2.43e-03	9.49e-06	Moderately soluble	-7.77	4.31e-06	1.68 e-08	Poorly soluble	-5.31	1.25e-03	4.88e-06	Moderately soluble
Tricyclo[7.1.0.0[1,3]decane-2-carbaldehyde	-2.05	1.48+00	8.99e-03	soluble	-2.19	1.05e+00	6.42 e-03	soluble	-2.79	2.65e-01	1.61e-03	soluble
Phytol	-5.98	3.10e-04	1.05e-06	Moderately soluble	-8.47	9.94e-07	3.35 e-09	Poorly soluble	-5.51	9.06e-04	3.05e-06	Moderately soluble

Table 4: Pharmacokinetic Parameters of the Phytoconstituents ofPaederia foetida

Name	**GI Absorption**	**BBB Permeant**	**P-gp Substrate**	**CYP1A2 Inhibitor**	**CYP2C19 Inhibitor**	**CYP2C9 Inhibitor**	**CYP2D6 Inhibitor**	**CYP3A4 Inhibitor**	**Log Kp (cm/s)**
2-Hydroxy-gamma-butyrolactone	High	No	No	No	No	No	No	No	-7.19
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl	High	No	No	No	No	No	No	No	-7.44

Indole	High	Yes	No	Yes	No	No	No	No	-5.56
2-Methoxy-4-vinylphenol	High	Yes	No	Yes	No	No	No	No	-5.22
Cycloheptasiloxane, tetradecamethyl	High	Yes	No	No	No	No	No	No	-4.53
Cyclooctasiloxane, hexadecamethyl	High	No	No	No	No	No	No	No	-4.20
2-Amino-3-hydroxypyridine	High	No	No	No	No	No	No	No	-6.87
Neophytadiene	Low	No	Yes	No	No	Yes	No	No	-1.17
Pentadecanoic acid	High	Yes	No	Yes	No	Yes	No	No	-3.07
Hexadecanoic acid, methyl ester	High	Yes	No	Yes	No	No	No	No	-2.71
n-Hexadecanoic acid	High	Yes	No	Yes	No	Yes	No	No	-2.77
Tricyclo[7.1.0.0[1,3]]decane-2-carbaldehyde	High	Yes	No	No	No	No	No	No	-5.74
Phytol	Low	No	Yes	No	No	Yes	No	No	-2.29

Table 5: Drug likeness of the Phytoconstituents ofPaederia foetida

Name	**Lipinski**	**Ghose**	**Veber**	**Egan**	**Muegge**	**Bioavailability score**
2-Hydroxy-gamma-butyrolactone	Yes (0 violations)	No, 4 violations,MW<160,WLOGP<-0.4,MR<40,#Atoms<20	Yes	Yes	No, 2 violations, MW<200,#C<5	0.55
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl	Yes (0 violations)	No, 3 violations, MW<160,MR<40,#Atoms<20	Yes	Yes	No, 2 violations, MW<200	0.85
Indole	Yes (0 violations)	No, 3 violations, MW<160, MR<40,#Atoms<20	Yes	Yes	No, 2 violations, MW<200, Heteroatoms<2	0.55
2-Methoxy-4-vinylphenol	Yes (0 violations)	No, 1 violation, MW<160	Yes (0 violations)	Yes	No, 1 violation, MW<200	0.55
Cycloheptasiloxane, tetradecamethyl	Yes (1 violation), MW>500	No, 1 violation, MW>480	Yes	Yes	No, violation, XLOGP3>5	0.55
Cyclooctasiloxane, hexadecamethyl	Yes (1 violation), MW>500	No, 4 violations, MW>480,WLOGP>-5.6,MR>130,#Atoms>70	Yes	Yes	NO, 1 violation, XLOGP3>5	0.55
2-Amino-3-hydroxypyridine	Yes (0 violations),	No, 3 violations, MW<160,MR<40, #Atoms<20	Yes	Yes	No, 1 violation, MW<200	0.55
Neophytadiene	Yes (1 violation), MLOGP>4.5	No, 1 violation, WLOGP>5,6	No, 1 violation, Rotors>10	No, 1 violation, WLOGP>5.8	NO, 2 violatios, XLOGP3>5, Heteroatoms<2	0.55

Pentadecanoic acid	Yes (0 violations)	Yes	No, 1 violation, Rotors>10	Yes	No, 1 violation, XLOGP3 >5	0.85
Hexadecanoic acid, methyl ester	Yes (1 violation), MLOGP>4.5	No, 1 violation, WLOGP>5,6	No, 1 violation, Rotors>10	Yes	No, 1 violation	0.55
n-Hexadecanoic acid	Yes (1 violation), MLOGP>4.5	Yes	No, 1 violation, Rotors>10	Yes	No, 1 violation, XLOGP3 >5	0.85
Tricyclo[7.1.0.0[1,3]]decane-2-carbaldehyde	Yes (0 violations)	Yes	Yes	Yes	No, 2 violations, MW<200, Heteroatoms<2	0.55
Phytol	Yes (1 violation), MLOGP>4.5	No, 1 violation, WLOGP>5,6	No, 1 violation, Rotors>10	No, 1 violation, WLOGP> 5.88	No, 2 violatios, XLOGP3 >5, Heteroatoms<2	0.55

Table 6: Medicinal Chemistry Properties of Phytoconstituents of Paederia foetida

Name	**Pains**	**Brenk**	**Leadlikeness**	**Synthetic accessibility**
2-Hydroxy-gamma-butyrolactone	0 alert	0 alert	No, 1 violation, MW<250	1.85
4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl	0 alert	0 alert	No, 1 violation, MW<250	3.60
Indole	0 alert	0 alert	No, 1 violation, MW<250	1.00
2-Methoxy-4-vinylphenol	0 alert	0 alert	No, 1 violation, MW<250	1.45
Cycloheptasiloxane, tetradecamethyl	0 alert	1 alert, heavy_metal	No, 2 violations, MW>350, XLOGP3>3.5	6.58
Cyclooctasiloxane, hexadecamethyl	0 alert	1 alert, heavy_metal	No, 2 violations, MW>350, XLOGP3>3.5	6.57
2-Amino-3-hydroxypyridine	0 alert	0 alert	No, 1 violation, MW<250	1.31
Neophytadiene	0 alert	1 alert, polyene	No, 2 violations, Rotors>7, XLOGP3>3.5	4.08
Pentadecanoic acid	0 alert	0 alert	No, 3 violations, MW<250, Rotors>7, XLOGP3>3.5	2,20
Hexadecanoic acid, methyl ester	0 alert	0 alert	No, 2 violations, Rotors>7, XLOGP3>3.5	2.53
n-Hexadecanoic acid	0 alert	0 alert	No, 1 violation, Rotors>7, XLOGP3>3.5	2.31

Tricyclo[7.1.0.0[1,3]]decane-2-carbaldehyde	0 alert	1 alert, isolated alkene	No, 1 violation, MW<250	2.98
Phytol	0 alert	1 alert, isolated alkene	No, 2 violations, Rotors>7, XLOGP3>3.5	4.30

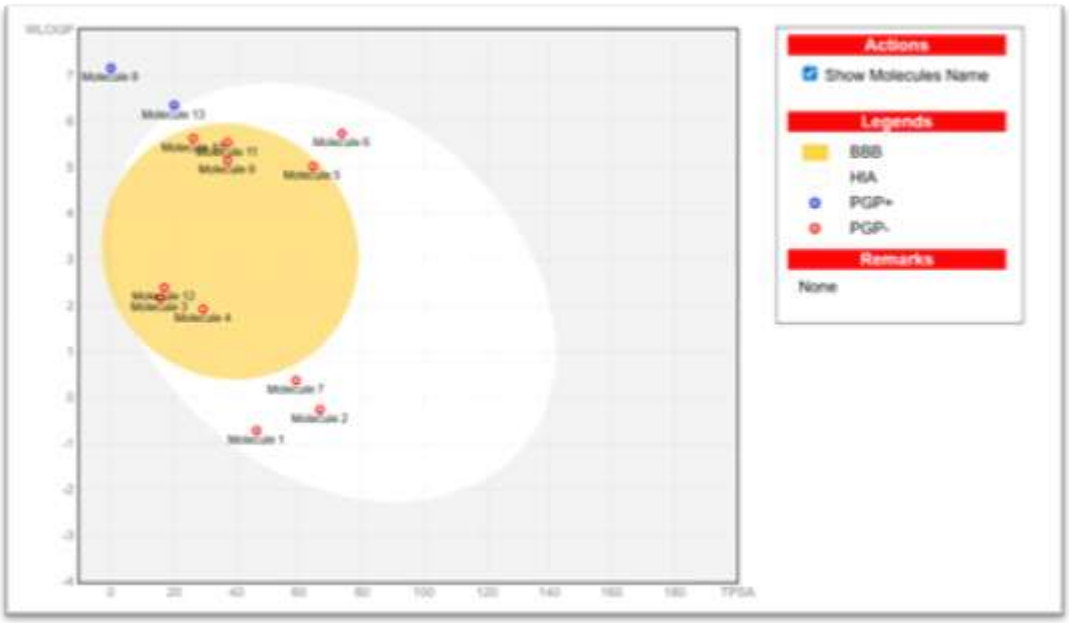


Fig 1: Boiled Egg Model of the Phytoconstituents of Paederia foetida Linn

IV. Discussion:

To assess the drug-likeness and pharmacokinetic profiles of the bioactive components found by GC-MS analysis in the methanolic extract of Paederia foetida leaves, the current study used a reliable in silico approach.Combining computational ADME prediction with phytochemical research provides a powerful strategy for ranking lead compounds for future drug development, extending beyond biological activity to assess therapeutic feasibility.A varied phytochemical profile was shown by the GC-MS analysis, with terpenoids, fatty acid esters, and aromatic derivatives predominating. Since substances like terpenoids are well known for their anti-inflammatory, analgesic, and hepatoprotective qualities, this composition is consistent with the known ethnopharmacological uses of Paederia foetida. This could account for its historical use in the treatment of rheumatoid arthritis and liver diseases. The results of the SwissADME analysis were quite encouraging. Lipinski's Rule of Five (Ro5), a crucial criterion in early-stage drug development, was successfully followed by the majority of the bioactive molecules that were discovered. If these molecules meet the following criteria (molecular weight <500 Da, XLogP<5, hydrogen bond donors <5, hydrogen bond acceptors <10), it indicates that they have the physicochemical characteristics of medications that are taken orally. This high percentage of compliance suggests that Paederia foetida extract has a great potential for creating an oral formulation that works well, which would be very beneficial for both patient compliance and business sustainability.

V. Conclusion:

This work presents a web-based tool, the freely available Swiss ADME, for assessing the ADME characteristics of phytoconstituents found in Paederia foetida. The software was used to analyze all the phytoconstituents that are available in the extract. Regarding pharmacokinetic and physicochemical characteristics, as shown in reputable tables and figures. Additionally, scientists and researchers can utilize the values as monographs to design potential synthetic and semisynthetic medications for various applications.

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