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GC - MS Profiling and *In - Silico* Pharmacokinetic Evaluation of Bioactive Compounds from *Marsilea quadrifolia* Linn.

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ABSTRACT
Water clover, or Marsilea quadrifolia Linn. (family: Marsileaceae), is an aquatic medicinal fern that has long been utilized for its neuroprotective, anti-inflammatory, antidiabetic, and antioxidant qualities. A key element of contemporary drug discovery is the in silico prediction of pharmacokinetic parameters, which allows scientists to assess a compound's Absorption, Distribution, Metabolism, and Excretion (ADME) properties before experimental validation. Drug-likeness, solubility, lipophilicity, and metabolic stability are all reliably revealed by computational platforms like SwissADME. The computational results create a theoretical foundation for additional pharmacological and toxicological research and offer initial insight into the pharmacokinetic potential of M. quadrifolia phytoconstituents.
KEYWORDS: *Marsilea quadrifolia Linn., pharmacokinetics, SwissADME, in silico analysis, drug-likeness.*

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I. INTRODUCTION

Computational pharmacology has emerged as a crucial component of drug discovery in recent years, enabling the quick screening of synthetic and phytochemical compounds for drug-like characteristics before expensive in vitro and in vivo testing [1]. A molecule's biological fate and therapeutic efficacy are determined by its pharmacokinetic profile, which includes absorption, distribution, metabolism, and excretion (ADME) [2]. In addition to saving time and money on research, in silico prediction of these characteristics aids in the identification of the most promising compounds with advantageous metabolic stability and bioavailability [3]. The aquatic fern *Marsilea quadrifolia* Linn., commonly referred to as European water clover or "Sushni" in Ayurveda, is found throughout Asia and Europe. Anxiety, inflammation, diabetes, liver problems, and diseases linked to oxidative stress have all historically been treated with it [4,5]. Numerous bioactive substances, including flavonoids (quercetin, kaempferol), alkaloids, steroids, saponins, phenolic acids (caffeic acid, ferulic acid), and triterpenoids (lupeol, oleanolic acid), have been discovered through phytochemical research [6–8]. The pharmacokinetic features of *M. quadrifolia's* phytoconstituents are still poorly understood, although a number of its pharmacological qualities have been demonstrated through experimentation. The Swiss Institute of Bioinformatics (SIB) created SwissADME, a freely available online tool that uses the chemical structure of small compounds to estimate ADME parameters, drug-likeness, and medicinal chemistry properties [9]. This tool incorporates sophisticated models such as Support Vector Machine (SVM)-based models for cytochrome P450 enzyme inhibition, Lipinski's "Rule of Five," and the BOILED-Egg model for gastrointestinal (GI) and brain permeability prediction [10,11]. Therefore, the current study employs SwissADME to estimate pharmacokinetic parameters of the main phytochemicals found in the methanolic extract of Marsilea quadrifolia in silico. In order to promote future pharmacological and therapeutic applications, this effort attempts to identify bioactive molecules with good pharmacokinetic profiles and drug-likeness.

II. MATERIALS AND METHODS

Collection of phytochemical data:

Phytoconstituents collected from the GC-MS Analysis report of the plant extract *Marsilea quadrifolia*. The selected compounds included 2-Cyclopenten-1-one, 2-hydroxy-Glycerin, 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl,Ethanamine 2-chloro-N, N-dimethyl etc. SwissADME analysis was performed using the canonical SMILES notations for each drug that were retrieved from the PubChem database.

SwissADME Platform:

The SwissADME web server (https://www.swissadme.ch) was used to perform pharmacokinetic profiling [9]. The study produced tabular data and graphical visualizations once each of the chosen compounds' SMILES strings was placed into the input box. Lipophilicity, solubility, bioavailability, pharmacokinetics, and medicinal chemistry characteristics were among the parameters that were noted.

Structure and bioavailability radar:

The first section contains the two-dimensional chemical structure with canonical SMILES to evaluate the molecules of interest's drug-likeness. The bioavailability radar took into account six distinct physicochemical characteristics, including lipophilicity (LIPO), size (SIZE), polarity (POLAR), insolubility (INSOLU), insaturation (INSATU), and flexibility (FLEX). The following standards were taken into account: Topological polar surface area (TPSA) for polarity should be between 20 and 130 0A2; solubility should have a log S of no more than 6; saturation should have a fraction of carbons in the sp hybridization of no less than 0.25; flexibility should have no more than nine rotatable bonds; and lipophilicity should have an XLOGP3 value between -0.7 and +5.0 [34].

Physicochemical Properties:

Molecular weight (MW), number of hydrogen bond donors (HBD) and acceptors (HBA), topological polar surface area (TPSA), number of rotatable bonds, and molar refractivity (MR) are among the physicochemical parameters that SwissADME forecasts. These factors affect bioavailability, permeability, and solubility [13]. TPSA values between 20 and 130 Å² and less than nine rotatable bonds are generally linked to optimal oral absorption [14].

Lipophilicity:

Drug absorption and membrane permeability are directly impacted by lipophilicity (logP), which characterizes a compound's distribution between hydrophobic (octanol) and hydrophilic (water) phases [15]. SwissADME uses five models to calculate lipophilicity.

XLOGP3:

Atomistic model based on fragment contributions and correction factors [16].

- **WLOGP**: Fragmental method using atomic contributions [17].
- **MLOGP**: Topological method derived from molecular descriptors [18].
- **SILICOS-IT**: Hybrid model integrating topological and fragmental parameters [19].
- **iLOGP**: Physics-based model that estimates logP through solvation free energies in octanol and water [20].
- The consensus **logP** represents the mean of these five values, providing a balanced estimate of lipophilicity.

Water Solubility:

A crucial component of oral medication absorption, water solubility establishes a molecule's ability to dissolve in physiological fluids [21]. SwissADME uses three models to compute solubility (logS), Based on molecular structure, the ESOL model estimates solubility and categorizes it as insoluble (<–10), poorly soluble (<–6), moderately soluble (<–4), soluble (<–2), or very soluble (<0) [22]. The Ali model improves the predictive accuracy of the ESOL equation [23]. The SILICOS-IT model modifies solubility based on topology and molecular weight [19]. A substance is deemed sufficiently soluble for oral bioavailability if logS > –4.

Pharmacokinetics:

SwissADME predicts several pharmacokinetic behaviours. The BOILED-Egg model, which plots polarity (TPSA) vs lipophilicity (WLOGP), is used to assess gastrointestinal (GI) absorption and blood–brain barrier (BBB) permeability. High GI absorption is demonstrated by molecules in the white region, whereas BBB penetration is indicated by molecules in the yellow (yolk) region [10]. P-glycoprotein (P-gp) substrate prediction influences the absorption and distribution of substances in the brain by determining whether they are effluxed out of cells [24]. Support Vector Machine (SVM) models are used to predict cytochrome P450 inhibition for the five key isoforms: **CYP1A2, CYP2C19**, **CYP2C9, CYP2D6,** and **CYP3A4** [11,25]. Drug metabolism and drug-drug interactions depend heavily on these enzymes.

Drug-Likeness Evaluation:

A compound's likelihood of becoming an orally active medication in humans is predicted by drug-likeness characteristics. SwissADME employs several filters:

- **Lipinski's Rule of Five:** MW ≤ 500 Da, logP ≤ 5, HBD ≤ 5, and HBA ≤ 10 [26].
- **Ghose filter:** MR 40–130, total atoms 20–70 [27].
- **Veber and Egan rules:** TPSA < 140 Å², rotatable bonds < 10, and logP< 5 [28].
- **Muegge rule:** Assesses drug-likeness through physicochemical and structural descriptors [29].
- **Bioavailability Score:** The likelihood that a substance will have ≥10% oral bioavailability is measured by a bioavailability score (0–1) [9].

Medicinal Chemistry Parameters:

This section evaluates a compound's suitability for lead optimization and medicinal chemistry.

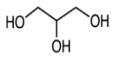
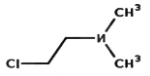
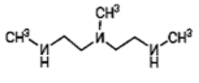
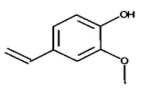
- **PAINS (Pan-Assay Interference Compounds):** Compounds that may exhibit false-positive activity in biological assays because of reactive moieties are alerted by PAINS (Pan-Assay Interference Compounds) [30].
- **Brenk filter:** Excludes substances including nitro, halopyridine, and thiol that have hazardous or unstable functional groups [31].
- **Lead-likeness:** Lead discovery optimization is appropriate for molecules with MW between 250 and 350 Da and logP between 1 and 3 [32].
- **Synthetic Accessibility (SA):** gives information about practical viability and ranges from 1 (simple synthesis) to 10 (difficult synthesis) [9].

Data Interpretation:

For the comparative study, all anticipated outcomes were combined into tables and graphs. Potential lead molecules were found to be compounds that met most ADME and drug-likeness criteria. The Lipinski and Veber recommendations were used to interpret the pharmacokinetic appropriateness of *M. quadrifolia* drugs [33].

III. RESULT:

Table 1: General Characteristics of Phytoconstituents of *Marsilea quadrifolia* through GC - MS.

Sr. No	Name of Molecule	Mol. Weight (g/mol)	Mol. Formula	SMILES	Structure
1	2-Cyclopenten-1-one,2-hydroxy	98.10	C5H6O2	O=C1CCC=C1O	
2	Glycerin	92.09	C3H8O3	OCC(CO)O	
3	4H-Pyran-4-one,2,3-dihydro-3,5-dihydroxy-6-Methyl	144.13	C6H8O4	OC1COC(=C(C1=O)O)C	
4	Ethanamine, 2-chloro-N, N-dimethyl-	107.58	C4H10ClN	ClCCN(C)C	
5	N, N', N"-Trimethyl Diitrimethylenetria-mine	173.30	C9H23N3	CN(CCN(C)C)CCN(C)C	
6	2-Methoxy-4-vinylphenol	150.17	C9H10O2	COc1cc(C=C)ccc1O	

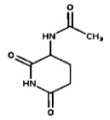
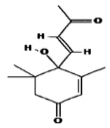
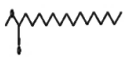
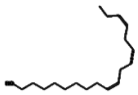
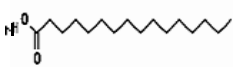
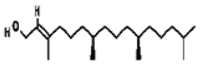
7	3-Aminopiperidine-2,6-dione, N-acetyl-	170.17	C7H10N2O3	CC(=O)NC1CCC(=O)NC1=O	
8	(S,E)-4-Hydroxy-3,5,5-trimethyl-4-(3-oxobut – 1-en-1-yl) cyclohex-2-enone	222.28	C13H18O3	CC(=O)C=CC1(O)C(=CC(=O)CC1(C)C)C	
9	Neophytadiene	278.52	C20H38	C=CC(=C)CCCC(CCCC(CCCC(C)C)C)C	
10	Hexadecanoic acid, methyl ester	270.45	C17H34O2	CCCCCCCCCCCCCCCC(=O)OC	
11	9,12,15-Octadecatrien-1-ol, (Z, Z, Z)-	264.45	C18H32O	OCCCCCCCCC=CCC=CCC=CCC	
12	n-Hexadecanoic acid	256.42	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	
13	9,12-Octadecadienoic acid, methyl ester	294.47	C19H34O2	CCCCCCC=CCC=CCCCCCCC(=O)OC	
14	9,12,15-Octadecatrienoic acid, methyl ester	292.46	C19H32O2	CCC=CCC=CCC=CCCCCCCCC(=0)OC	
15	Phytol	296.53	C20H40O	OC/C=C(/CCC[C@@H](CCC[C@@H](CCCC(C)C)C)C)\C	

Table 2: Lipophilicity of the Phytoconstituents of *Marsilea quadrifolia*

Sr. No.	Molecules Name	iLOGP	XLOGP3	WLOGP	MLOGP	SILICOS-IT	Consensus Log Po/w
1	2-Cyclopenten-1-one,2-hydroxy	1.12	0.39	0.79	-0.42	0.95	0.57
2	Glycerin	0.45	-1.76	-1.67	-1.51	-0.96	-1.09
3	4H-Pyran-4-one,2,3-dihydro-3,5-dihydroxy-6-Methyl	1.19	-0.37	-0.26	-1.77	0.13	-0.22
4	Ethanamine, 2-chloro-N,N-dimethyl-	1.84	0.32	0.79	1.16	0.48	0.92
5	N, N', N"-Trimethyl Dii trimethylenetriamine	2.83	0.34	0.04	0.73	-0.33	0.72
6	2-Methoxy-4-vinylphenol	2.14	2.81	1.93	1.71	2.13	2.14
7	3-Aminopiperidine-2,6-dione, N-acetyl-	0.66	-0.49	-1.45	-0.72	-0.01	0.40

8	(S,E)-4-Hydroxy-3,5,5-trimethyl-4-(3-oxobut – 1-en-1-yl) cyclohex-2- enone	1.91	0.50	1.81	1.05	2.63	1.58
9	Neophytadiene	5.05	9.62	7.17	6.21	7.30	7.07
10	Hexadecanoic acid, methyl ester	4.41	7.38	5.64	4.44	5.84	5.54
11	9,12,15-Octadecatrien-1-ol, (Z, Z, Z)-	4.70	6.64	5.57	4.59	6.00	5.50
12	n-Hexadecanoic acid	3.85	7.17	5.55	4.19	5.25	5.20
13	9,12-Octadecadienoic acid, methyl ester	4.97	6.82	5.97	4.70	6.36	5.76
14	9,12,15-Octadecatrienoic acid, methyl ester	4.94	6.29	5.75	4.61	6.18	5.55
15	Phytol	4.85	8.19	6.19	6.36	5.25	6.25

Table 3: Water solubility of the phytoconstituents of *Marsilea quadrifolia*

Name	ESOL				Ali				SILCOS-IT			
	Log S	Solubility		Class	Log S	Solubility		Class	LogS	Solubility		Class
		mg/mL	mol/L			mg/mL	mol/L			mg/mL	mol/L	
2-Cyclopenten-1-one,2-hydroxy	-0.69	1.98e+01	2.02e-01	Very soluble	-0.74	1.79e+01	1.82e -01	Very soluble	-0.25	5.52e+01	5.62e-01	Soluble
Glycerin	0.83	6.22e+02	6.76+00	Highly soluble	1.00	9.22e+02	1.00e+01	Highly soluble	1.08	1.11e+03	1.20e+01	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	1.14e+00	Soluble
Ethanamine, 2-chloro-N,N-dimethyl-	-0.58	2.85e+01	2.65e-01	Very soluble	0.05	1.20e+02	1.12e+00	Highly soluble	-1.35	4.81e+00	4.47e-02	Soluble
N, N', N"-Trimethyl Diitrimethylenetriamine	-0.73	3.21e+01	1.85e-01	Very soluble	-0.11	1.35e+02	7.80e-01	Very soluble	-1.44	6.29e+00	3.63e-02	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
3-Aminopiperidine-2,6-dione, N-acetyl-	-0.45	5.98e+01	3.51e-01	Very soluble	-0.62	4.05e+01	2.38e-01	Very soluble	-1.25	9.59e+00	5.64e-02	Soluble
(S,E)-4-Hydroxy-3,5,5-trimethyl-4-(3-oxobut – 1-en-1-yl) cyclohex-2-enone	-1.40	8.83e+00	3.97e-02	Very soluble	-1.21	1.36e+01	6.14e-02	Very soluble	-2.19	1.45e+00	6.53e-03	Soluble
Neophyta-diene	-6.77	4.74e-05	1.70e-07	Poorly soluble	-9.53	8.15e-08	2.93e-10	Poorly soluble	-6.11	2.18e-04	7.82e-07	Poorly soluble
Hexadeca-noic acid, methyl ester	-5.18	1.80e-03	6.67e-06	Moderately soluble	-7.76	4.68e-06	1.73e-08	Poorly soluble	-6.01	2.64e-04	9.75e-07	Poorly soluble
9,12,15-Octadecatrien-1-ol, (Z, Z, Z)-	-4.80	4.15e-03	1.57e-07	Moderately soluble	-6.87	3.60e-05	1.36e-07	Poorly soluble	-4.42	1.01e-02	3.83e-05	Moderately soluble
n-Hexadeca- noic acid	-5.02	2.43e-03	9.49e-06	Moderately soluble	-7.77	4.32e-06	1.68e-06	Poorly soluble	-5.31	1.25e-03	4.88e-06	Moderately soluble
9,12-Octadecadienoic acid, methyl ester	-4.97	3.14e-03	1.07e-05	Moderately soluble	-7.18	1.94e-05	6.60e-08	Poorly soluble	-5.37	1.25e-03	4.25e-06	Moderately soluble
9,12,15-Octadecatrienoic acid, methyl ester	-4.69	5.94e-03	2.03e-05	Moderately soluble	-6.63	6.85e-05	2.34e-07	Poorly soluble	-4.65	6.49e-03	2.22e-05	Moderately soluble
Phytol	-5.98	3.10e-04	1.05e-06	Moderately soluble	-8.47	9.94e-07	3.35e-09	Poorly soluble	-5.51	9.06e-04	3.35e-06	Moderately soluble

Table 4: Pharmacokinetics of the Phytoconstituents of *Marsilea quadrifolia*

Name	GI Absorption	BBB permeant	P-gp substrate	CYP1A inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	Log Kp (cm/s)
2-Cyclopenten-1-one,2-hydroxy	High	Yes	No	No	No	No	No	No	-6.62
Glycerin	High	No	No	No	No	No	No	No	-8.11
4H-Pyran-4-one,2,3-dihydro-3,5-dihydroxy-6-	High	No	No	No	No	No	No	No	-7.44

Methyl									
Ethanamine, 2-chloro-N, N-dimethyl-	Low	No	No	No	No	No	No	No	-6.73
N, N', N''-Trimethyl Diitrimethylene triamine	Low	No	No	No	No	No	No	No	-7.12
2-Methoxy-4-vinylphenol	High	Yes	No	No	No	No	No	No	-5.22
3-Aminopiperidine-2,6-dione, N-acetyl-	High	No	No	No	No	No	No	No	-7.69
(S,E)-4-Hydroxy-3,5,5-trimethyl-4-(3-oxobut – 1-en-1-yl) cyclohex-2-enone	High	Yes	No	No	No	No	No	No	-7.30
Neophyta-diene	Low	No	Yes	No	No	Yes	No	No	-1.17
Hexadecanoic acid, methyl ester	High	Yes	No	Yes	No	No	No	No	-2.71
9,12,15-Octadecatrien-1-ol, (Z, Z, Z)-	High	Yes	No	Yes	No	Yes	No	No	-3.20
n-Hexadeca-noic acid	High	Yes	No	Yes	No	Yes	No	No	-2.77
9,12-Octadecadienoic acid, methyl ester	High	No	No	Yes	No	Yes	No	No	-3.25
9,12,15-Octadecatrienoic acid, methyl ester	High	Yes	No	Yes	No	Yes	No	No	-3.62
Phytol	Low	No	Yes	No	No	Yes	No	No	-2.29

Table 5: Drug likeness of the Phytoconstituents of *Marsilea quadrifolia*

Name	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability Score
2-Cyclopenten-1-one,2-hydroxy	Yes; 0 violation	No; 2 violations: XLOGP3>5, Heteroatoms<2	Yes	Yes	No; 1 violation: MW<200	0.55
Glycerin	Yes 0 violation	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 violation	No; 3 violations: MW<160, MR<40, #atoms<20	Yes	Yes	No; 1 violation: MV<200	0.85
Ethanamine, 2-chloro-N, N-dimethyl-	Yes 0 violation	No; 3 violations: MW<160, MR<40, #atoms<20	Yes	Yes	No; 3 violations: MW<200, #C<5, Heteroatoms<2	0.55
N, N', N''-Trimethyl Dii trimethylene triamine	Yes 0 violation	Yes	Yes	Yes	No; 1 violation: MV<200	0.55
2-Methoxy-4-vinylphenol	Yes 0 violation	No; 1 violation: MV<160	Yes	Yes	No; 1 violation: MV<200	0.55
3-Aminopiperidine-2,6-dione, N-acetyl-	Yes 0 violation	No; 1 violation: WLOGP<-0.4	Yes	Yes	No; 1 violation: MV<200	0.55

(S, E)-4-Hydroxy-3,5,5-trimethyl-4-(3-oxobut – 1-en-1-yl) cyclohex-2-enone	Yes 0 violation	Yes	Yes	Yes	Yes	0.55
Neophyta-diene	Yes, 1 violation: MLOGP>4.15	No; 1 violation: WLOGP>5.6	No; 1 violation: Rotors>10	No, 1 violation: WLOGP>5.88	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55
Hexadeca-noic acid, methyl ester	Yes, 1 violation: MLOGP>4.15	o; 1 violation: WLOGP>5.6	No; 1 violation: Rotors>10	Yes	No 1 violations, XLOGP3>5	0.55
9,12,15-Octadecatrien-1-ol, (Z, Z, Z)-	Yes, 1 violation: MLOGP>4.15	Yes	No; 1 violation: Rotors>10	Yes	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55
n-Hexadeca-noic acid	Yes, 1 violation: MLOGP>4.15	Yes	No; 1 violation: Rotors>10	Yes	No; 1violation XLOGP3>5,	0.85
9,12-Octadecadienoic acid, methyl ester	Yes; 1 violation: MLOGP>4.15	No; 1 violation: WLOGP>5.6	No; 1 violation: Rotors>10	No; 1 violation: WLOGP>5.88	No; 1 violation: XLOGP3>5	0.55
9,12,15-Octadecatrienoic acid, methyl ester	Yes; 1 violation: MLOGP>4.15	No; 1 violation: WLOGP>5.6	No; 1 violation: Rotors>10	Yes	No; 1 violation: XLOGP3>5	0.55
Phytol	Yes; 1 violation: MLOGP>4.15	No; 1 violation: WLOGP>5.6	No; 1 violation: Rotors>10	No; 1 violation: WLOGP>5.88	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55

Table 6: Medicinal Chemistry Properties of Phytoconstituents of Marsilea quadrifolia

Name of Molecule	PAINS	Brenk	Leadlikeness	Synthetic Accessibility
2-Cyclopenten-1-one,2-hydroxy	0 alart	0 alart	No; 1 violation: MV<200	2.30
Glycerin	0 alart	0 alart	No; 1 violation: MV<250	1.31
4H-Pyran-4-one,2,3-dihydro-3,5-dihydroxy-6-Methyl	0 alart	0 alart	No; 1 violation: MV<250	3.60
Ethanamine, 2-chloro-N, N-dimethyl-	0 alart	1 alart: alkyi__halide	No; 1 violation: MV<250	1.45
N, N', N''-Trimethyl Diitrimethylenetriamine	0 alart	0 alart	No; 1 violation: MV<250	1.66
2-Methoxy-4-vinylphenol	0 alart	0 alart	No; 1 violation: MV<250	1.45
3-Aminopiperidine-2,6-dione, N-acetyl-	0 alart	1 alert: phthalimide	No; 1 violation: MV<250	1.91
(S, E)-4-Hydroxy-3,5,5-trimethyl-4-(3-oxobut – 1-en-1-yl) cyclohex-2- enone	0 alart	1 alert: michael_acceptor_1	No; 1 violation: MV<250	3.46
Neophytadiene	0 alart	1alert: polyene	No; 2 violations: Rotors>7, XLOGP3>3.5	4.08
Hexadecanoic acid, methyl ester	0 alart	0 alart	No; 2 violations: Rotors>7, XLOGP3>3.5	2.53
9,12,15-Octadecatrien-1-ol, (Z, Z, Z)-	0 alart	1 alert: isolated _alkene	No; 2 violations: Rotors>7, XLOGP3>3.5	3.22
n-Hexadecanoic acid	0 alart	0 alart	No; 2 violations: Rotors>7, XLOGP3>3.5	2.31
9,12-Octadecadienoic acid, methyl ester	0 alart	1 alert: isolated _alkene	No; 2 violations: Rotors>7, XLOGP3>3.5	3.18
9,12,15-Octadecatrienoic acid, methyl ester	0 alart	1 alert: isolated _alkene	No; 2 violations: Rotors>7, XLOGP3>3.5	3.10
Phytol	0 alart	1 alert: isolated _alkene	No; 2 violations: Rotors>7, XLOGP3>3.5	4.30

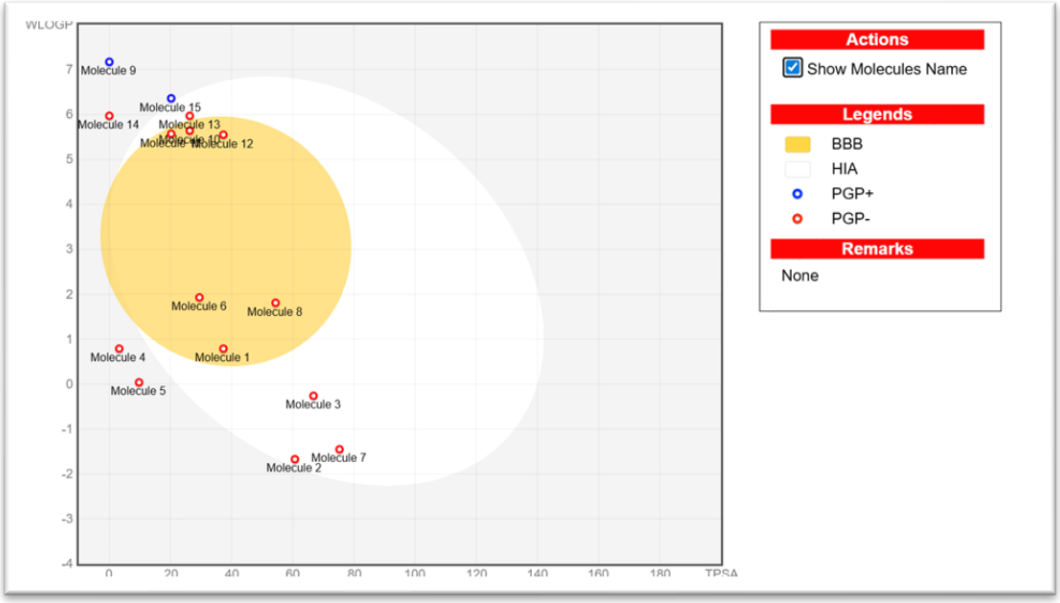


Fig 1: Boiled Egg Model of the Phytoconstituents of *Marsilea quadrifolia Linn*

IV. DISCUSSION

SwissADME's in silico pharmacokinetic analysis of *Marsilea quadrifolia's*primary phytoconstituents provides valuable initial insights into their drug-likeness and therapeutic potential. Several chemicals, especially flavonoids and triterpenoids, have desirable physicochemical features, such as excellent lipophilicity, acceptable molecular weight, and good solubility parameters, according to the ADME predictions. These characteristics facilitate effective gastrointestinal absorption and systemic bioavailability, which are important factors for medication candidates that are taken orally. Many components fall within the acceptable range for oral drug development, indicating a low probability of pharmacokinetic failure, according to models like Lipinski's Rule of Five and Veber's criterion.However, only a small number of substances demonstrated the ability to cross the blood–brain barrier. This is consistent with previous findings indicating that M. quadrifolia has both peripheral and central pharmacological effects. Furthermore, cytochrome P450 inhibition profiling revealed that certain components might interact with metabolic enzymes, underscoring the necessity of carefully assessing herb–drug interactions in subsequent studies.

Overall, the computational results uncover several bioactive compounds with potential drug-like qualities and support the traditional use of this plant. Even though they are very instructive, in silico forecasts cannot entirely take the place of laboratory-based validation. These findings must be verified by experimental pharmacokinetic investigations, metabolic stability tests, and toxicity assessments.

V. CONCLUSION

The main phytochemicals found in *Marsilea quadrifolia* through GC-MS have a good pharmacokinetic and drug-likeness potential, according to this in silico assessment. Several components, including flavonoids, phenolic acids, and triterpenoids, have appropriate physicochemical characteristics that support excellent absorption, metabolic stability, and oral bioavailability, according to SwissADME research. The fact that many compounds satisfy crucial requirements for early drug development was further verified using drug-likeness filters. These computational predictions are mainly a theoretical guide, although they offer useful preliminary information. To verify bioavailability, safety, and pharmacodynamic relevance, experimental validation using in vitro and in vivo research is still crucial.

All things considered, our study finds several interesting bioactive compounds in *M. quadrifolia*, providing a solid scientific foundation for next pharmacological studies and bolstering its conventional therapeutic uses.

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