(International Print/Online Journal)

SJIF IMPACT FACTOR: 6.829
PUBMED-National Library of Medicine ID-101739732

ISSN (Print): 2209-2870
ISSN (Online): 2209-2862

International Journal of Medical Science and Current Research (IJMSCR)
Available online at: www.ijmscr.com
Volume 9, Issue 3, Page No: 668-675
May-June 2026

IJMSCR

In Silico Evaluation Of Bioactive Compounds From Trachyspermum Ammi Through Adme And Toxicity Prediction Models

J Mithula [1*], Atul Thorat [2], KB Gudagudi [2]
[1]Institute of Applied Sciences, Parul University, Vadodara, India,
[2]School of Allied Healthcare and Sciences, JAIN (Deemed-to-be University), Bangalore, India

***Corresponding Author:**
J Mithula
Institute of Applied Sciences, Parul University, Vadodara, India

Type of Publication: Original Research Paper
Conflicts of Interest: Nil

Abstract

Trachyspermum ammi (Ajwain) is a medicinal plant widely used in traditional systems for gastrointestinal, respiratory, inflammatory, and infectious disorders Its phytochemical diversity includes thymol, carvacrol, p-cymene, γ-terpinene, flavonoids, tannins, and related bioactive constituents associated with antimicrobial, antioxidant, digestive, and respiratory benefits The present study evaluated 24 representative phytochemicals selected from the IMPPAT database using SwissADME and BOILED-Egg prediction models to assess physicochemical properties, lipophilicity, solubility, pharmacokinetics, drug-likeness, and medicinal chemistry characteristics. From 278 reported compounds, 24 were selected based on abundance, structural diversity, literature relevance, physicochemical suitability, and multi-target potential. The evaluated compounds showed molecular weights ranging from 134 to 302 Da and generally low topological polar surface area values, consistent with favorable membrane permeability. Most compounds were soluble to moderately soluble, displayed moderate lipophilicity, and showed good gastrointestinal absorption, while some also demonstrated predicted blood-brain barrier permeability. Most compounds also showed minimal interaction with P-glycoprotein and cytochrome P450 enzymes, complied with Lipinski, Veber, and Egan criteria, and exhibited no PAINS alerts with acceptable synthetic accessibility scores. Carvacrol, anethole, acetyleugenol, and 4-allylphenol emerged as the most promising compounds based on their overall pharmacokinetic and medicinal chemistry profiles. Therapeutic distribution analysis further showed that seeds had the broadest traditional application spectrum, especially in gastrointestinal and respiratory disorders. These findings support the potential of T. ammi phytochemicals as lead candidates for future phytopharmaceutical development, although molecular docking, molecular dynamics simulations, and experimental validation remain necessary.

Keywords: Trachyspermum ammi; Ajwain; SwissADME; BOILED-Egg; ADME; phytochemicals; drug-likeness; medicinal chemistry

Introduction

Trachyspermum ammi is an aromatic medicinal herb of the family Apiaceae and is widely recognized in traditional medicine for its broad therapeutic applications. Its seeds and other plant parts contain multiple phytochemicals, including thymol, carvacrol, p-cymene, γ-terpinene, flavonoids, and tannins, which are associated with antimicrobial, antioxidant, digestive, and respiratory activities. [1-6]

Natural products remain important starting points in drug discovery because structurally diverse small molecules can provide useful lead scaffolds for pharmacological development. In this context, computational screening approaches provide an efficient first-stage strategy for prioritizing phytochemicals with favorable pharmacokinetic and

drug-likeness properties before experimental validation.

The present work aimed to evaluate representative phytochemicals of T. ammi through in silico ADME and medicinal chemistry prediction models. Twenty-four representative compounds were selected from 278 reported phytochemicals in the IMPPAT resource and analyzed using SwissADME and BOILED-Egg tools to identify compounds with favorable oral bioavailability, absorption, permeability, and drug-likeness characteristics. [1-6]

Materials and Methods

Phytochemical data for T. ammi were retrieved from the IMPPAT database. IMPPAT was used as the source resource for the documented phytochemical repertoire of the plant, from which 278 compounds were initially identified. From this larger pool, 24 representative phytochemicals were selected using predefined considerations including abundance, structural diversity, literature relevance, physicochemical suitability, and multi-target potential.

The selected compounds represented multiple plant parts including aerial part, fruit, leaf, seed, stem, and whole plant, together with compounds of unspecified origin within the database record. The set included Carvacrol, Gamma-Terpinene, 3-Carene, 4-Carvomenthenol, alpha-Phellandrene, beta-Caryophyllene, (1S,2R,5S)-2-isopropyl-5-methylcyclohexyl acetate, (1R)-2-methyl-5-propan-2-ylbicyclo[3.1.0]hex-2-ene, alpha-Terpinene, Anethole, (+)-beta-Phellandrene, alpha-Pinene, Sabinene, (Z)-Non-2-enal, 4-Allylphenol, Carvacrol methyl ether, Acetyleugenol, Camphene, o-(1-Propylpentyl)phenol, cis-Sabinene hydrate, Longifolene, Humulene, Petroselinic acid, Abieta-7,13-dien-18-oic acid among others.

SwissADME was employed to assess physicochemical descriptors, lipophilicity, water solubility, pharmacokinetics, drug-likeness, medicinal chemistry alerts, and BOILED-Egg behaviour. Heatmap analysis for therapeutic distribution across plant parts was performed using Python with Pandas, Seaborn, and Matplotlib. [7,8,11,17]

Results and Discussion

The selected phytochemicals showed molecular weights between 134 and 302 Da and generally low topological polar surface area values, indicating physicochemical suitability for membrane permeation. Most compounds also exhibited moderate lipophilicity and were classified as soluble to moderately soluble across the applied solubility models.

The lipophilicity and solubility analysis showed that several compounds, including carvacrol, anethole, 4-allylphenol, acetyleugenol, sabinene, and alpha-phellandrene, were consistently predicted as soluble across multiple models. By contrast, o-(1-propylpentyl) phenol, longifolene, petroselinic acid, and abieta-7,13-dien-18-oic acid showed reduced solubility in at least one model, with petroselinic acid displaying the highest XLOGP3 value of 7.64 and poor solubility in the Ali model.

Pharmacokinetic prediction indicated high gastrointestinal absorption for carvacrol, 4-carvomenthenol, anethole, (Z)-non-2-enal, 4-allylphenol, carvacrol methyl ether, acetyleugenol, o-(1-propylpentyl) phenol, petroselinic acid, and abieta-7,13-dien-18-oic acid. Several compounds were also predicted to cross the blood-brain barrier, including carvacrol, anethole, 4-allylphenol, acetyleugenol, sabinene, alpha-pinene, camphene, and multiple monoterpenes, whereas beta-caryophyllene, longifolene, humulene, and petroselinic acid were predicted to be non-permeant.

Most compounds were not predicted to be P-glycoprotein substrates, supporting a generally favorable transport profile. Cytochrome interaction patterns were limited for many compounds, although some specific inhibitory signals were observed, such as CYP1A2 inhibition for carvacrol, anethole, 4-allylphenol, acetyleugenol, carvacrol methyl ether, o-(1-propylpentyl)phenol, and petroselinic acid, and CYP2C9 inhibition for selected compounds including 3-carene, beta-caryophyllene, alpha-pinene, camphene, cis-sabinene hydrate, humulene, petroselinic acid, and abieta-7,13-dien-18-oic acid.

Drug-likeness analysis demonstrated broad compliance with established filters including Lipinski, Veber, and Egan criteria. Medicinal chemistry assessment further identified no PAINS alerts and acceptable synthetic accessibility scores, indicating that the selected molecules generally lack major

Volume 9, Issue 3; May-June 2026; Page No 668-675

structural liabilities for early screening prioritization. [19–23].

Among the evaluated compounds, carvacrol, acetyleugenol, anethole, and related terpenoids showed the most promising overall combination of pharmacokinetic and medicinal chemistry features. The abstract specifically highlights carvacrol, anethole, acetyleugenol, and 4-allylphenol as the leading candidates emerging from the screening workflow.

Therapeutic distribution analysis indicated that seeds exhibited the broadest activity spectrum, particularly in gastrointestinal and respiratory disorders. Fruits were associated mainly with antimicrobial and digestive activities, leaves with anti-inflammatory effects, and roots with antipyretic and diuretic properties. This distribution was interpreted as consistent with the established traditional medicinal use of T. ammi.

Overall, the in silico assessment indicates that most T. ammi phytochemicals possess favorable ADME, drug-likeness, and medicinal chemistry characteristics. These findings support the value of the plant as a source of lead compounds for future phytopharmaceutical development. However, the computational predictions require further confirmation through molecular docking, molecular dynamics simulations, and experimental studie

Phytochemicals Identified from Trachyspermum ammi

Aerial Part:

Carvacrol, Gamma-Terpinene, 3-Carene, 4-Carvomenthenol, alpha-Phellandrene, beta-Caryophyllene

Fruit:

(1S,2R,5S)-2-isopropyl-5-methylcyclohexyl acetate,(1R)-2-methyl-5-propan-2 ylbicyclo[3.1.0]hex-2-ene), alpha-Terpinene, Anethole

Leaf:

(+)-beta-Phellandrene, alpha-Pinene

Seed:

13. Sabinene, (Z)-Non-2-enal, 4-Allylphenol, Carvacrol methyl ether, Acetyleugenol, Camphene, o-(1-Propylpentyl) phenol

Stem:

cis-Sabinene hydrate

Whole Plant:

Longifolene, Humulene

Unknown Plant Part:

Petroselinic acid, Abieta-7,13-dien-18-oic

Physiochemical properties

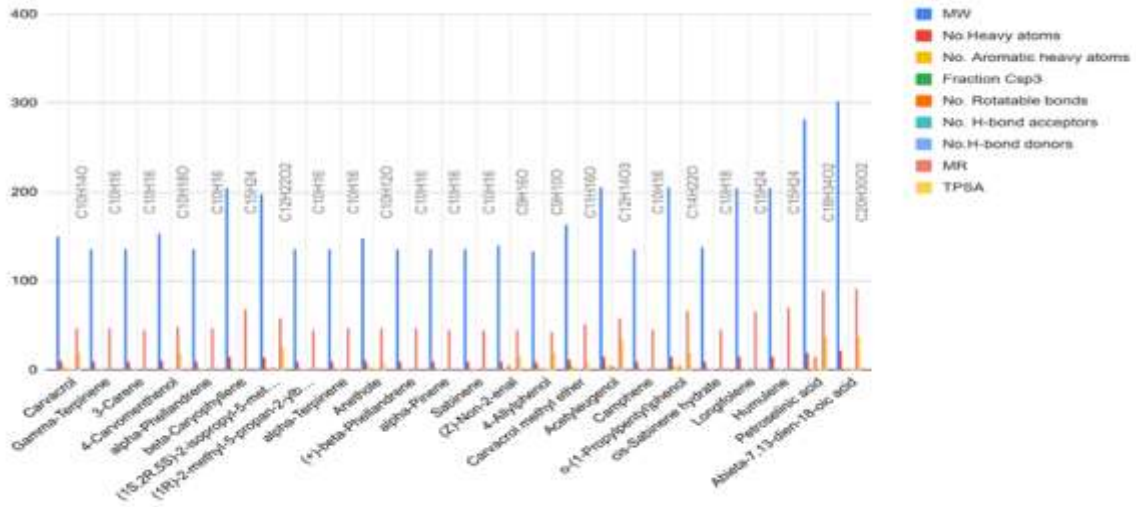

Figure 1: Physicochemical properties of Trachyspermum ammi from SWISS ADME ANALYSIS

Volume 9, Issue 3; May-June 2026; Page No 668-675

Lipophilicity and water solubility

Sl.no	Phytochemical name	XLOGP3	ESOL Class	Ali Class	Silicos-IT class
1	Carvacrol	3.49	Soluble	Soluble	Soluble
2	Gamma-Terpinene	4.5	Soluble	Moderately soluble	Soluble
3	3-Carene	4.38	Soluble	Moderately soluble	Soluble
4	4-Carvomenthenol	3.26	Soluble	Soluble	Soluble
5	alpha-Phellandrene	3.21	Soluble	Soluble	Soluble
6	beta-Caryophyllene	4.38	Soluble	Moderately soluble	Soluble
7	(1S,2R,5S)-2-isopropyl-5-methylcyclohexyl acetate	4	Soluble	Moderately soluble	Soluble
8	(1R)-2-methyl-5-propan-2-ylbicyclo[3.1.0]hex-2-ene	2.85	Soluble	Soluble	Soluble
9	alpha-Terpinene	4.25	Soluble	Soluble	Soluble
10	Anethole	3.3	Soluble	Soluble	Soluble
11	(+)-beta-Phellandrene	3.44	Soluble	Soluble	Soluble
12	alpha-Pinene	4.48	Soluble	Moderately soluble	Soluble
13	Sabinene	3.09	Soluble	Soluble	Soluble
14	(Z)-Non-2-enal	3.15	Soluble	Soluble	Soluble
15	4-Allylphenol	2.85	Soluble	Soluble	Soluble
16	Carvacrol methyl ether	3.82	Soluble	Soluble	Soluble
17	Acetyleugenol	2.3	Soluble	Soluble	Soluble
18	Camphene	4.22	Soluble	Soluble	Soluble
19	o-(1-Propylpentyl)phenol	5.44	Moderately soluble	Moderately soluble	Moderately soluble
20	cis-Sabinene hydrate	3.9	Soluble	Soluble	Soluble
21	Longifolene	5.08	Moderately soluble	Moderately soluble	Soluble
22	Humulene	4.55	Soluble	Moderately soluble	Soluble

Volume 9, Issue 3; May-June 2026; Page No 668-675

23	Petroselinic acid	7.64	Moderately soluble	Poorly soluble	Moderately soluble
24	Abieta-7,13-dien-18-oic acid	4.78	Moderately soluble	Moderately soluble	Soluble

Table 1: Lipophilicity and Water solubility of Trachyspermum ammi from SWISS ADME ANALYSIS

Pharmacokinetic properties

Molecules	GI	BBB	Pgp	C1A2	C2C19	C2C9	C2D6	C3A4	log Kp
1	H	Y	N	Y	N	N	N	N	-4.74
2	L	Y	N	N	N	N	N	N	-3.94
3	L	Y	N	N	N	Y	N	N	-4.02
4	H	Y	N	N	N	N	N	N	-4.93
5	L	Y	N	N	N	N	N	N	-4.85
6	L	N	N	N	Y	Y	N	N	-4.44
7	H	Y	N	N	N	Y	N	N	-4.67
8	L	Y	N	N	N	N	N	N	-5.11
9	L	Y	N	N	N	N	N	N	-4.11
10	H	Y	N	Y	N	N	N	N	-4.86
11	L	Y	N	N	N	N	N	N	-4.69
12	L	Y	N	N	N	Y	N	N	-3.95
13	L	Y	N	N	N	N	N	N	-4.94
14	H	Y	N	N	N	N	N	N	-4.92
15	H	Y	N	Y	N	N	N	N	-5.09
16	H	Y	N	Y	N	N	Y	N	-4.59
17	H	Y	N	Y	N	N	N	N	-5.93
18	L	Y	N	N	N	Y	N	N	-4.13
19	H	Y	N	Y	N	N	Y	N	-3.7
20	L	Y	N	N	N	Y	N	N	-4.37
21	L	N	N	N	Y	Y	N	N	-3.94
22	L	N	N	N	N	Y	N	N	-4.32
23	H	N	N	Y	N	Y	N	N	-2.6

Volume 9, Issue 3; May-June 2026; Page No 668-675

24	H	Y	N	N	Y	Y	N	N	-4.75

BOILED EGG REPRESENTATION

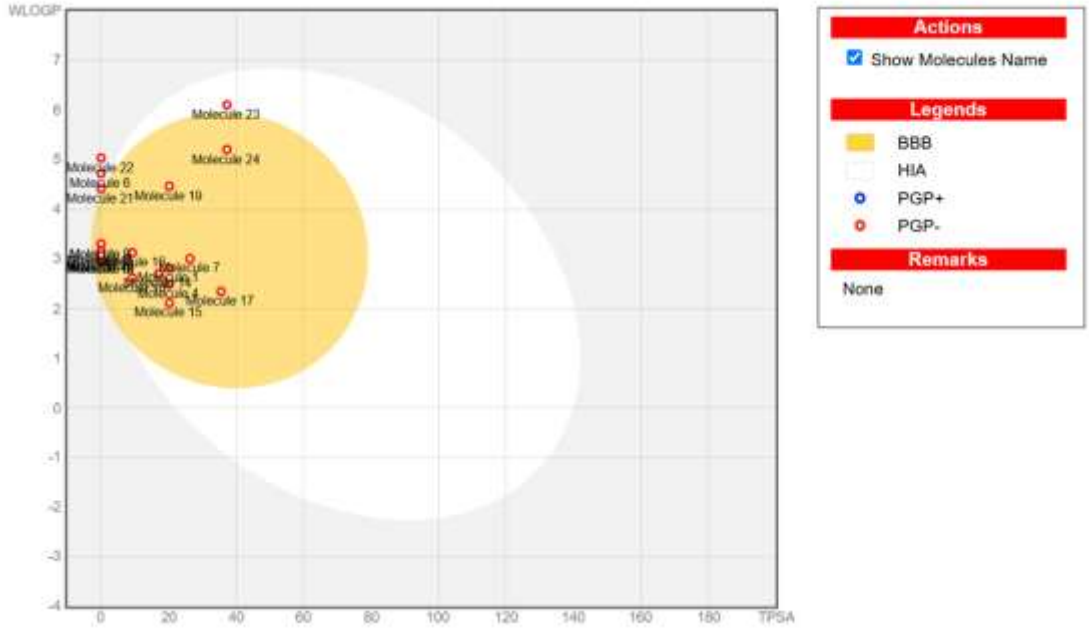

Figure 2: Druglikeness and Medicinal chemistry of Trachyspermum ammi from SWISS ADME ANALYSIS and Heat map showing the distribution of therapeutic applications across different plant parts of Trachyspermum ammi based on ethnomedicinal reports. [24]

Abbreviations

GI: H = High, L = Low, BBB: Y = Yes, N = No

Pgp: Y = Yes, N = No, C1A2 = CYP1A2 inhibitor

C2C19 = CYP2C19 inhibitor, C2C9 = CYP2C9 inhibitor

C2D6 = CYP2D6 inhibitor, C3A4 = CYP3A4 inhibitor

Predicted Druglikeness and Medicinal chemistry and Therapeutic use

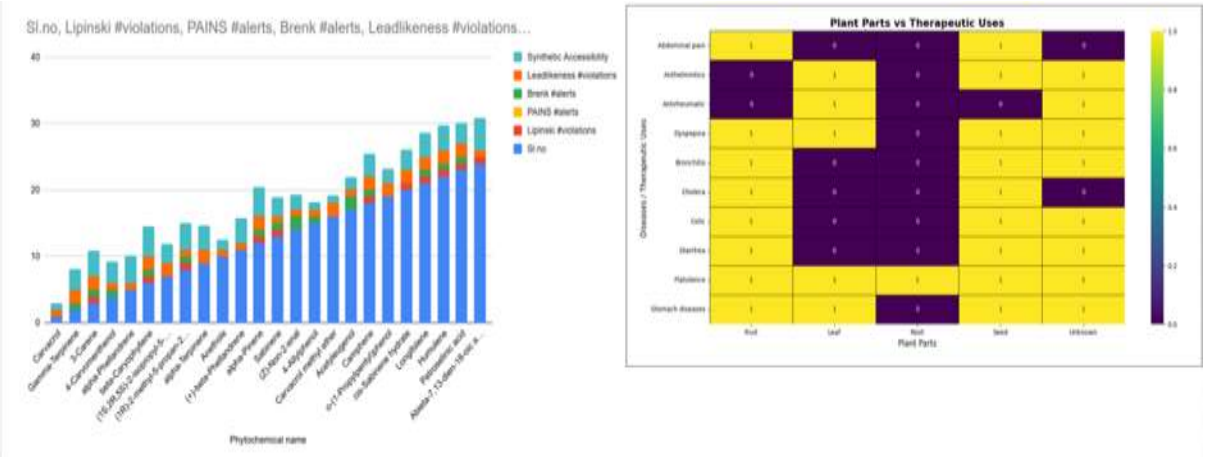

Figure 3: Druglikeness and Medicinal chemistry of Trachyspermum ammi from SWISS ADME ANALYSIS and Heat map showing the distribution of therapeutic applications across different plant parts of Trachyspermum ammi based on ethnomedicinal reports. [24]

Volume 9, Issue 3; May-June 2026; Page No 668-675

Conclusion

The present study demonstrates that representative phytochemicals from Trachyspermum ammi show favorable physicochemical, pharmacokinetic, drug-likeness, and medicinal chemistry properties in silico. Most compounds displayed acceptable membrane permeability-related descriptors, solubility, gastrointestinal absorption, and limited transporter-related liabilities, while several also showed blood-brain barrier permeability predictions. Carvacrol, anethole, acetyleugenol, and 4-allylphenol emerged as the most promising candidates for further study. The broad traditional therapeutic distribution, especially in seeds, further supports the pharmacological relevance of this plant Further validation through molecular docking, molecular dynamics simulations, and experimental assays is required before translational application.

Acknowledgement

we express my sincere gratitude to our institution and department for providing the necessary academic support and research facilities required for this study. we also acknowledge the developers and maintainers of publicly accessible databases and computational platforms, including IMPPAT, SwissADME, and ProTox-II, for providing valuable resources used during the investigation

References

1. 1.Saraswat, N., Sachan, N., & Chandra, P. (2020). A Review on Ethnobotanical, Phytochemical, Pharmacological and Traditional Aspects of Indigenous Indian Herb Trachyspermum ammi (L). Current Traditional Medicine, 6(3), 172–187. https://doi.org/10.2174/2215083805666191107115544
2. 2.Dubey, S., & Kashyap, P. (2015). Trachyspermum ammi: A Review on its Multidimensional Uses in Indian Folklore Medicines. Research Journal of Medicinal Plant, 9(8), 368–374. https://doi.org/10.3923/rjmp.2015.368.374
3. 3.Goyal, S., Chaturvedi, V., Dhingra, G., Tanwar, S., Sharma, K., & Singh, S. (2022). Trachyspermum ammi: A review on traditional and modern pharmacological aspects. Biological Sciences, 2(4), 324–337. https://doi.org/10.55006/biolsciences.2022.2401
4. 4.Bairwa, R., Sodha, R. S., & Rajawat, B. S. (2012). Trachyspermum ammi. Pharmacognosy reviews, 6(11), 56–60. https://doi.org/10.4103/0973-7847.95871
5. 5.Zarshenas, Mohammad M. & Moein, Mahmoodreza & Mohammadi-Samani, Soliman & Petramfar, Peyman. (2014). An Overview on Ajwain (Trachyspermum ammi) Pharmacological Effects; Modern and Traditional. Journal of Natural Remedies. 14. 98-105. 10.18311/jnr/2014/96.
6. 6.Siddiquie, F., Ahsan, F., Mahmood, T., Ahmad, M. A., Singh, A., & Bano, S. (2024). Unlocking the food treasures: Trachyspermum ammi–A comprehensive exploration from field to pharmacology. Food Safety and Health, 2(3), 322-343.
7. 7.Mohanraj, K., Karthikeyan, B. S., Vivek-Ananth, R. P., Chand, R. P. B., Aparna, S. R., Mangalapandi, P., & Samal, A. (2018). IMPPAT: A curated database of Indian medicinal plants, phytochemistry and therapeutics. Scientific Reports, 8: 4329. https://doi.org/10.1038/s41598-018-22631-z.
8. 8.Vivek-Ananth, R. P., Mohanraj, K., Sahoo, A. K., & Samal, A. (2023). IMPPAT 2.0: An enhanced and expanded phytochemical atlas of Indian medicinal plants. ACS Omega, 8(10), 8827–8845. https://doi.org/10.1021/acsomega.2c07019
9. 9.Beck, H., Härter, M., Haß, B., Schmeck, C., & Baerfacker, L. (2022). Small molecules and their impact in drug discovery: A perspective on the occasion of the 125th anniversary of the Bayer Chemical Research Laboratory. Drug Discovery Today, 27(6), 1560–1574. https://doi.org/10.1016/j.drudis.2022.02.015
10. 10.Wu, K., Karapetyan, E., Schloss, J., Vadgama, J., & Wu, Y. (2023). Advancements in small molecule drug design: A structural perspective. Drug discovery today, 28(10), 103730. https://doi.org/10.1016/j.drudis.2023.103730
11. 11.Daina, A., Michielin, O., & Zoete, V. (2017). SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Scientific reports, 7, 42717. https://doi.org/10.1038/srep42717

Volume 9, Issue 3; May-June 2026; Page No 668-675

12. 12.Shaikh, T. T., Adnaik, R. S., & Patil, N. B. (2025). Swiss ADME predictions of pharmacokinetics and drug-likeness properties of chemical constituents present in Embelia Ribes. Int. J. Pharm. Pharm. Res., 31, 68-76.
13. 13.O'Boyle, N. M., Banck, M., James, C. A., Morley, C., Vandermeersch, T., & Hutchison, G. R. (2011). Open Babel: An open chemical toolbox. Journal of cheminformatics, 3(1), 33.
14. 14.Yalkowsky, S. H., & Valvani, S. C. (1980). Solubility and partitioning I: Solubility of nonelectrolytes in water. Journal of Pharmaceutical Sciences, 69(5): 595–604. https://doi.org/10.1002/jps.2600690505
15. 15.Di, L., Fish, P. V., & Mano, T. (2011). Bridging solubility between drug discovery and development. Drug Discovery Today, 16(9-10): 451–457. https://doi.org/10.1016/j.drudis.2011.11.007
16. 16.Nagsen, A., Kamble, S., & Mitkar, A. A. (2023). Swiss ADME predictions of pharmacokinetics and drug-likeness properties of secondary metabolites present in Trigonella foenum-graecum. Journal of Pharmacognosy and Phytochemistry, 12(5), 341–349
17. 17.Daina, A., & Zoete, V. (2016). A BOILED-Egg To Predict Gastrointestinal Absorption and Brain Penetration of Small Molecules. ChemMedChem, 11(11), 1117–1121. https://doi.org/10.1002/cmdc.201600182
18. 18.Abhirami V., Atul Thorat. (2025). UNLOCKING NATURE'S PHARMACOLOGICAL FRAMEWORK: AN IN-SILICO EXPLORATION OF CARICA PAPAYA LINN'S THERAPEUTIC POTENTIAL. EUROPEAN JOURNAL OF BIOMEDICAL AND PHARMACEUTICAL SCIENCES, 12(11), 184–199. https://doi.org/10.5281/zenodo.17539346
19. 19.Lipinski, C. A. (2000). Drug-like properties and the causes of poor solubility and poor permeability. Journal of Pharmacological and Toxicological Methods, 44(1): 235–249. https://doi.org/10.1016/S1056-8719(00)00107-6
20. 20.Veber, D. F., Johnson, S. R., Cheng, H. Y., Smith, B. R., Ward, K. W., & Kopple, K. D. (2002). Molecular properties that influence the oral bioavailability of drug candidates. Journal of Medicinal Chemistry, 45(12): 2615-2623. https://doi.org/10.1021/jm020017n
21. 21.Martin, Y. C., & Park, B. K. (2005). Drug-likeness: screening for bioavailability in lead discovery. Nature Reviews Drug Discovery, 4(6): 467–468. https://doi.org/10.1038/nrd1754
22. 22.Baell, J. B., & Holloway, G. A. (2010). New substructure filters for the removal of Pan Assay Interference Compounds (PAINS) from screening libraries and for their exclusion in bioassays. Journal of Medicinal Chemistry, 53(7): 2719–2740. https://doi.org/10.1021/jm901137j
23. 23.Brenk, R., Schipani, A., James, D., Krasowski, A., Gilbert, I. H., Frearson, J., & Graham, P. (2008). Lessons learnt from assembling screening libraries for drug discovery for neglected diseases. ChemMedChem, 3(3): 435-444. https://doi.org/10.1002/cmdc.200700139
24. 24.are Foundation. (2024). Python programming language. https://www.python.org/
25. 25.Modareskia, M., Fattahi, M., & Mirjalili, M. H. (2022). Thymol screening, phenolic contents, antioxidant and antibacterial activities of Iranian populations of Trachyspermum ammi (L.) Sprague (Apiaceae). Scientific reports, 12(1), 15645. https://doi.org/10.1038/s41598-022-19594-7
26. 26.Daina, A., Michielin, O., & Zoete, V. (2017). SwissADME: A free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Scientific Reports, 7, 42717. https://doi.org/10.1038/srep42717
27. 27.FigureLabs AI. (2026). FigureLabs AI: Scientific illustration and figure generation platform. https://chat.figurelabs.ai/

Volume 9, Issue 3; May-June 2026; Page No 668-675