World Journal of Pharmaceutical and Life Sciences

www.wjpls.org

Impact Factor: 8.21 Coden USA: WJPLA7

PHARMACOLOGICAL ASSESSMENT OF AZELAIC ACID ISOLATED FROM DUCKWEEDS IN MALDA DISTRICT OF WEST BENGAL, INDIA

[1]Dr. Santanu Gupta, [2]Dr. Prasanta Kumar Garai, [3]Dr. Rajorshi Sen Gupta, [4]*Dr. Sudipta Kumar Sil

[1]Assistant Professor, Department of Botany, Malda College, Malda-732101, West Bengal, India.
[2]Research Scholar, Department of Botany, University of Gour Banga, Malda-732103, West Bengal, India.
[3]State Aided College Teacher (SACT), Department of Computer Science and Application, Malda College, Malda-732101, West Bengal, India.
[4]Professor, Department of Botany, University of Gour Banga, Malda-732103, West Bengal, India.

***Corresponding Author: Dr. Sudipta Kumar Sil**

Professor, Department of Botany, University of Gour Banga, Malda-732103, West Bengal, India.

DOI: https://doi.org/10.5281/zenodo.19435757

How to cite this Article: [1]Dr. Santanu Gupta, [2]Dr. Prasanta Kumar Garai, [3]Dr. Rajorshi Sen Gupta, [4]*Dr. Sudipta Kumar Sil. (2026). Pharmacological Assessment of Azelaic Acid Isolated From Duckweeds In Malda District of West Bengal, India. World Journal of Pharmaceutical and Life Sciences, 12(4), 207–210.

Article Received on 05/03/2026 Article Revised on 25/03/2026 Article Published on 04/04/2026

ABSTRACT

Plants have a large profile of useful metabolites, aquatic plants are also containing some bioactive compounds whose efficacy has to be ascertained. Duckweeds are tropical to subtropical in distribution and they occupy stagnant shallow to moderately deep waterbodies and exhibit luxuriant growth. They are nowadays considered not only fish-feed and poultry bird-feed but as a source of nutraceuticals, therefore pharmacological assessment of isolated major secondary metabolites is necessary. Duckweeds mainly *Lemna minor* L. biomass was collected from seven aquatic habitats and cultured on Gamborg's B5 basal liquid medium to harvest uniform physiologically active cells from mid-log growth phase. Preparative HPLC and subsequent LCMS profile helped to isolate and quantify some bioactive secondary metabolites, azelaic acid is one of these compounds. To assess the proposed drug likeliness of this compound, Swiss ADME and Swiss Dock platforms were used to ascertain *in-silico* pharmacological attributes of azelaic acid. Azelaic acid in aqueous methanol and 0.01% formic acid solvent phase was identified with retention time of 10.58 through LCMS chromatogram profile screened through Metlin Agilent database. Its quantitative range was found to be 2.32µg/gm of fresh fronds of lesser duckweeds. Upon assessed with Swiss ADME and Swiss Dock (Auto Dock Vina), the test compound was found to possess pharmacological applicability and might be considered as a possible ligand programmed to bind with SARS-CoV spike protein. However, immunokinetics studies has to be performedas per recommended wet laboratory testing protocols. Duckweeds contain several bioactive compounds especially azelaic acid, which exhibited its prospective candidature for considering as a potent source for drug formulations.

KEYWORDS: Duckweeds, azelaic acid, pharmacokinetics, *in-silico* drug likeliness, molecular docking.

MATERIALS AND METHODS

About 1 gram of the shade dried sample *Lemna minor* L. were taken, grinded in a mortar and pastle with 20 ml of aqueous methanol (HPLC grade FINAR) and the mixtures were kept in a conical flask for 48 hours at 20±2^{o}C. After that, the mixture were filtered using Whatman's No 1 filter paper for 4-5 times to remove the chlorophyll as much as possible. The filtrate of *Lemna minor* L. were collected and subjected to preparative HPLC (Breeze HPLC) with column 2998 Ch1 @1.2nm at flow rate 200 µl/ml and retention time 50 minutes using HPLC grade methanol as solvent along with 0.01% formic acid. The particular elute fraction from preparative HPLC of *Lemna minor* L.corresponding to retention time 18.018 min to 26.696 min for *L.minor*were selected for LC-MS analysis on the basis of trial and error experimentsusing HPLC grade methanol as solvent along with 0.01% formic acid. The instrument used Q-Exactive Plus Biopharma, Thermo ScientificData Acquisition Software: Thermo Scientific Xcalibur, Version 4.2.28.14Data Processing Software: Compound Discoverer 3.2 SP1Column details- SB-C18 RRHD 100

x 2.1 MM, 1.8 microns (Agilent Technologies). METLIN, Agilent database for were consulted identification of the compounds. For quantification of the azelaic acid "Analytical HPLC" was performed using standard solution of Azelaic acid (Sigma Aldrich) at concentration of 0.5 mg/mL. The injection volume was 10 µl/mL using HPLC grade methanol and 0.01% formic acid as solvent. Quantification was done with respect to percentage area of the peak of the corresponding substances in the standard solution and that of the selected elute fraction of lesser duckweeds.

RESULTS AND DISCUSSION

Table 1: Quantification of Azelaic acid in the aqueous methanolic extract of *Lemna minor* L.

Effective metabolites	Source plant	Retention time (LC MS)	% area of the peak of particular substance in the standard	% area of the peak of particular substance in the elute	Concentration of the substance in the plant (µg/gm of plant tissue)
Azelaic Acid	*Lemna minor* L.	10.58 min	26.470%	12.318%	2.32

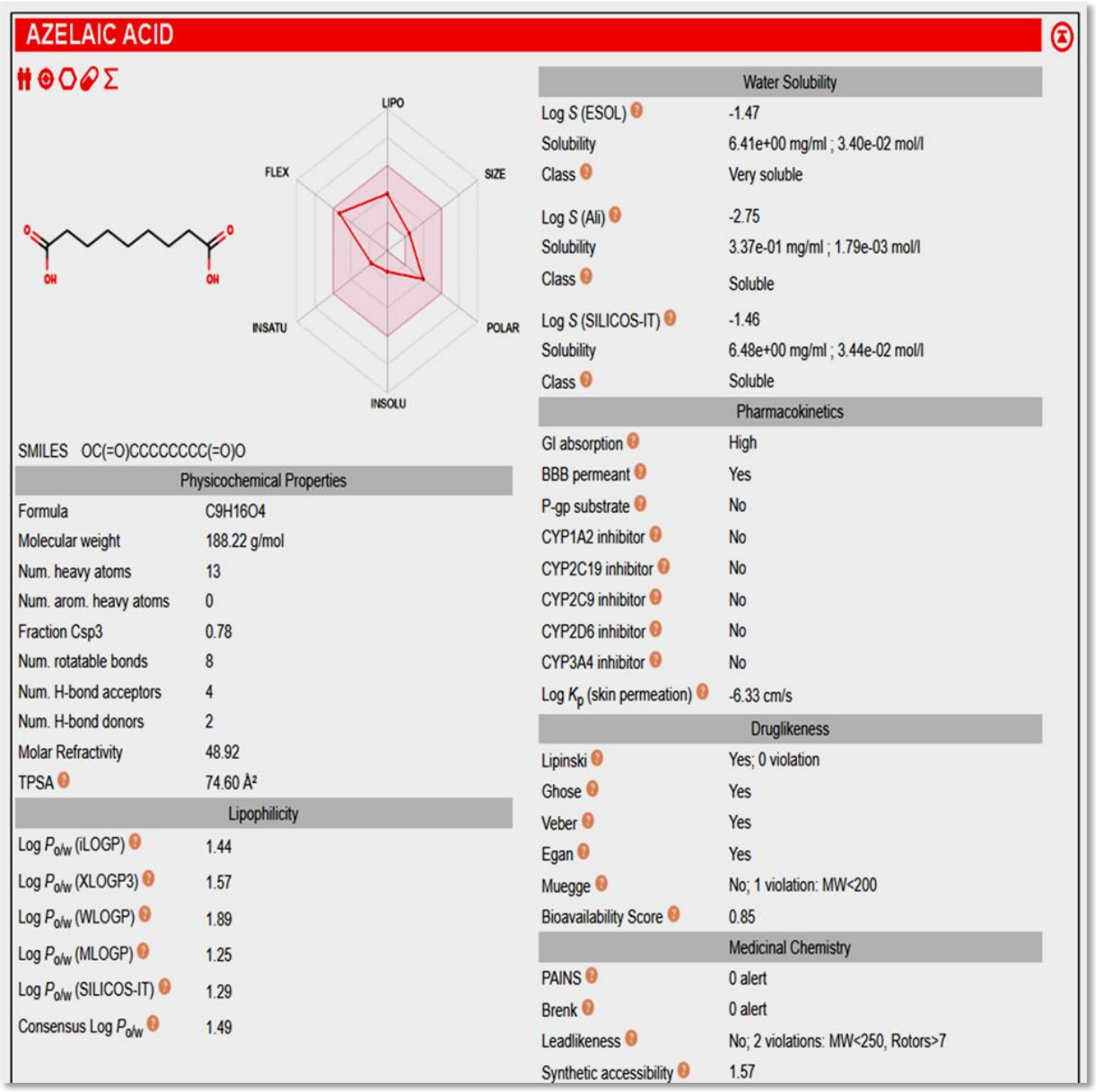

Figure 1: Result outcome window of Swiss ADME platform showing different parameters assessing the drug likeliness of azelaic acid in human physiological *in-silico* consideration.

Table 2: (below left): Affinity energy for all 19 predicted model of ligand docked on target protein, the models are represented in decreasing order of their estimated affinity energy values (as outcome shown in Swiss Dock portal).

Model	Calculated affinity (kcal/mol)
1	-3.321
2	-3.201
3	-3.122
4	-3.067
5	-3.050
6	-3.013
7	-2.969
8	-2.957
9	-2.953
10	-2.937
11	-2.928
12	-2.900
13	-2.705
14	-2.670
15	-2.613
16	-2.479
17	-2.443
18	-2.440
19	-2.406

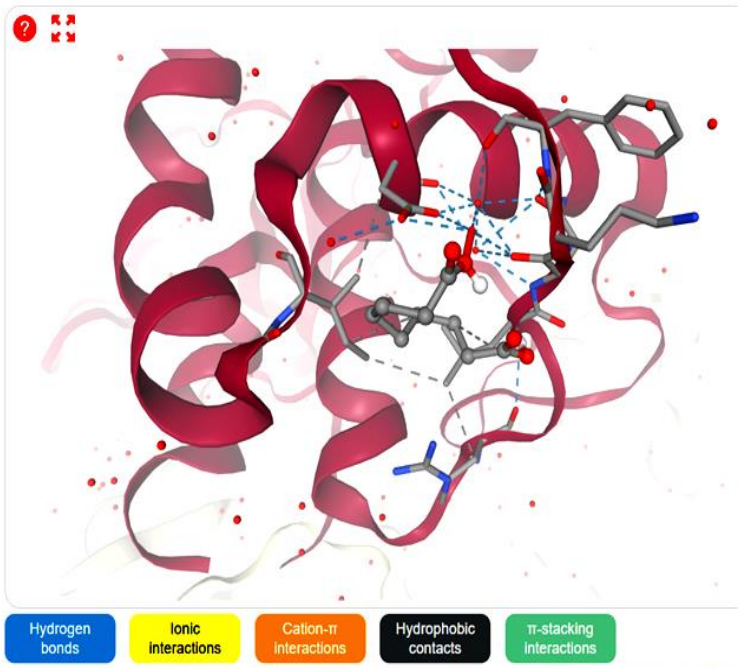

Figure 2: Molecular docking of azelaic acid on target SARS-CoV spike protein 7UUP.pdb.

The red line on the bioavailability radar chart (Fig.1) represents the molecule's properties compared to the ideal zone (the pink area). Azelaic acid sits perfectly within the pink zone for Lipophilicity, Polarity, and Solubility. This means it is highly likely to be absorbed well and can move through biological membranes effectively. The red line extends past the pink boundary. This is because Azelaic acid is a straight, 9-carbon chain with 8 rotatable bonds. In drug design, floppy molecules are sometimes less ideal because they can wrap around themselves, but for a simple acid, this is rarely a functional issue. It falls outside because it is a fully saturated hydrocarbon chain (no double bonds or rings). While many modern drugs are flat or rigid (aromatic), azelaic acid's simplicity is part of its safety profile. This is quite low. Small molecules typically permeate the skin barrier (stratum corneum) more easily than large ones Egan *et. al*., 2000). This is the polar surface area. A value around 70–80 is excellent—it's polar enough to dissolve in water-based gels but not so polar that it gets stuck outside the skin's fatty layers. Water solubility explains why it is often formulated in aqueous gels or creams. The skin penetration value of -6.33 cm/s is a standard moderate score for skin penetration. It indicates that while the molecule is small, its carboxylic acid groups (which are water-loving) slow it down slightly as it passes through the oil-loving skin barrier. This is actually beneficial for acne treatment because it allows the drug to linger in the pilosebaceous unit (the pore) where the bacteria live. This report confirms that azelaic acid is a highly efficient, non-toxic, and easily absorbed molecule. Its flaws (being too flexible or too small) are only technicalities in the context of dermatology; in practice, these traits make it a versatile and gentle treatment for sensitive skin conditions like rosacea. Azelaic Acid passes the most critical pharmaceutical filters: Lipinski's Rule of Five: Yes; 0 violations, confirming its high potential as an oral drug (Lipinski, 2001). Medicinal Chemistry: It shows 0 alerts for PAINS (molecules that give false positives in assays) or Brenk (potentially toxic groups). Synthetic Accessibility: Rated at 1.57, meaning it is very easy and inexpensive to manufacture. The ligand binding efficacy was represented by affinity matrices. Molecular docking through Auto Dock Vina platform of Swiss Dock software predicted 19 models for molecule to molecule attachment. To determine the stable bonding between the ligand and the target protein is considered to be of utmost importance. The most commonly used such parameter is the affinity energy which read as -3.321 kilocalories per mole of the ligand. This value is slightly short of the preferred range of -4.0 to -10.0 kilocalories per mole. This docking in-silico experiment was carried using a SARS-CoV spike protein7UUP.pdb, it is a **protein–ligand complex structure** from the Protein Data Bank (PDB), it is SARS-CoV-2 main protease representing a **S144A mutation** (serine at position 144 replaced with alanine). This is a variant of the viral 3C-like protease involved in viral polyprotein processing. This structure is used to study how nirmatrelvir binds to the SARS-CoV-2 main protease and how mutations like S144A could affect inhibitor binding and resistance (Bugnon*et al*., 2024) It helps in possible **drug design against COVID-19**. The molecular association between the ligand and the target is represented in Fig. 2.

CONCLUSION

The study successfully identifies and quantifies azelaic acid from the lesser duckweed, *Lemna minor* L., harvested from the Malda district of West Bengal. With a concentration of 2.32µg/gm of fresh fronds, duckweeds represent a viable natural source for this bioactive metabolite. The *in-silico* pharmacological evaluation via SwissADME confirms that azelaic acid possesses a robust drug-likeliness profile, characterized by zero violations of Lipinski's Rule of Five and high gastrointestinal absorption. Its medicinal chemistry profile is exceptionally clean, showing no alerts for PAINS or Brenk toxicities, and it features high synthetic accessibility (score of 1.57), suggesting it is an inexpensive and safe candidate for pharmaceutical development. Furthermore, molecular docking simulations using Swiss Dock demonstrate that azelaic acid can function as a ligand for the SARS-CoV spike protein (7UUP.pdb), with a stable binding affinity of -3.321 kcal/mol. While the docking energy is slightly below the preferred range, the molecule's structural simplicity, safety profile, and established efficacy in dermatology specifically its ability to linger in the pilosebaceous unit suggested its applicability.

ACKNOWLEDGEMENT

Authors thankfully acknowledge the institutional support for conducting the research.

REFERENCE

1. Azevedo, I.C., Bordalo, A.A., Duarte, P.M., Influence of River Discharge Patterns on the Hydrodynamics and Potential Contaminant Dispersion in the Douro Estuary (Portugal). Water Res., 2010; 44: 3133-3146.
2. Bugnon M, Röhrig U.F. et al., SwissDock: Major enhancements for small-molecule docking with Attracting Cavities and AutoDockVina, *Nucleic Acids Res.*, 2024; 24: 20-24.
3. Das, J., SenChowdhury, R, Sraddhya, R and Das D, Study of Phytoplankton Diversity in few water sources of Dooars area, WB through Foldsacope- an Origami Paper Microscope. International Journal of Life Sciences Research, 2019; 7(2): 373-378.
4. Dey H. S, Chakraborty S. Diversity of Non-Heterocystous Filamentous Cyanobacteria from Freshwater Bodies of Bidhannagar, North 24 Parganas, West Bengal. Asian J Biol Life Sci., 2020; 9(3): 386-90.
5. Egan W. J., Merz K. M. & Baldwin J. J. Prediction of Drug Absorption Using Multivariate Statistics. J. Med. Chem., 2000, 43: 3867–3877. https://doi.org/10.1021/jm000292e
6. Ghose A. K., Viswanadhan V. N. &Wendoloski J. J. A knowledge-based approach in designing combinatorial or medicinal chemistry libraries for drug discovery. 1. A qualitative and quantitative characterization of known drug databases. J Comb. Chem., 1999; 1: 55–68. https://pubs.acs.org/doi/10.1021/cc9800071
7. Gupta, P. Genus OscillatoriaVaucher (Cyanoprokaryota) in Maldah District, West Bengal, India. International Journal of Plant and Environment, 2017; 3(1): 53-63.
8. Lipinski C. A., Lombardo F., Dominy B. W. & Feeney P. J. Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings. Adv. Drug. Deliv. Rev., 2001; 46: 3–26. https://doi.org/10.1016/S0169-409X(00)00129-0
9. Muegge I., Heald S. L. &Brittelli D. Simple selection criteria for drug-like chemical matter. J. Med. Chem., 2001; 44: 1841–1846. https://doi.org/10.1021/jm015507e
10. Veber D. F. et al. Molecular properties that influence the oral bioavailability of drug candidates. J. Med. Chem., 2002; 45: 2615–2623. https://doi.org/10.1021/jm020017n
11. Weiniger D.SMILES, a chemical language information system. J. Chemical Information and Comp. Sci., 2001; 38(1): 31-36. http://doi.org/10.1021/ci00057a005
12. Yan, J., Liu, J.; You, X., Shi, X., Zhang, L, Simulating the Gross Primary Production and Ecosystem Respiration of Estuarine Ecosystem in North China with aquatox. Ecol. Model, 2018; 373: 1-12.