WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
Coden USA: WJPRAP Impact Factor 8.63
Volume 15, Issue 18, 64-72. Review Article ISSN 2277–7105

SWERTIAMARIN FROM *ENICOSTEMMA LITTORALE*: PHYTOCHEMISTRY, ANTIDIABETIC POTENTIAL, MOLECULAR TARGETS AND PERSPECTIVES FROM IN SILICO DRUG DISCOVERY

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Article Received on 12 August 2026,
Article Revised on 02 Sept. 2026,
Article Published on 16 Sept. 2026,
https://doi.org/10.5281/zenodo.22766708

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How to cite this Article: Rohit Saini[1*], Dr. Pramod Kumar Goyal[2] (2026). Swertiamarin From Enicostemma Littorale: Phytochemistry, Antidiabetic Potential, Molecular Targets And Perspectives From In Silico Drug Discovery. World Journal of Pharmaceutical Research, 15(18), 64–72.
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ABSTRACT

Diabetes mellitus is a complex metabolic disorder characterized by persistent hyperglycemia resulting from impaired insulin secretion, impaired insulin action, or a combination of both. The increasing prevalence of diabetes and the limitations associated with existing pharmacological therapies have stimulated considerable interest in medicinal plants and their bioactive constituents as sources of novel therapeutic agents. *Enicostemma littorale* Blume, a medicinal plant belonging to the family Gentianaceae, has traditionally been used in India for the management of diabetes, fever, inflammation, hepatic disorders and other metabolic conditions. Phytochemical investigations have demonstrated the presence of secoiridoid glycosides, flavonoids, alkaloids, phenolic compounds, saponins, steroids and other secondary metabolites. Among these constituents, swertiamarin, a secoiridoid glycoside, has emerged as an important bioactive and chemotaxonomic marker. Experimental investigations reported in the literature indicate that *E. littorale* extracts and swertiamarin possess hypoglycemic, antioxidant, hepatoprotective, hypolipidemic, anti-inflammatory and other pharmacological activities. Swertiamarin has therefore attracted attention as a potential

natural lead for antidiabetic drug discovery. In parallel, molecular docking has become an important computational approach for investigating ligand–protein interactions and prioritizing natural compounds against therapeutically relevant targets. Diabetes-related proteins such as α-glucosidase, α-amylase and dipeptidyl peptidase-4 (DPP-4) represent important molecular targets because their modulation can influence postprandial glucose regulation and incretin activity. The present review summarizes the botanical and phytochemical characteristics of *E. littorale*, with particular emphasis on swertiamarin; discusses experimental evidence supporting its antidiabetic and metabolic effects; examines the role of molecular docking in natural-product drug discovery; and highlights the significance of isolating and structurally characterizing swertiamarin before computational evaluation. The integration of pharmacognosy, phytochemical isolation, analytical characterization and structure-based computational investigation may provide a rational strategy for evaluating swertiamarin as a potential antidiabetic lead molecule.

KEYWORDS: *Enicostemma littorale*; swertiamarin; secoiridoid glycoside; diabetes mellitus; α-glucosidase; α-amylase; DPP-4; molecular docking; natural products; phytochemistry.

INTRODUCTION

Diabetes mellitus represents one of the major metabolic disorders of global public-health importance. It is characterized by chronic elevation of blood glucose resulting from inadequate insulin secretion, impaired insulin action, or both. Persistent hyperglycemia can progressively contribute to microvascular and macrovascular complications, including neuropathy, nephropathy, retinopathy and cardiovascular disease.

Current pharmacological management includes insulin, biguanides, sulfonylureas, glucagon-like peptide-1-related therapies, DPP-4 inhibitors, sodium-glucose cotransporter-2 inhibitors and other therapeutic classes. Although these agents have substantially improved diabetes management, adverse effects, variable therapeutic responses, cost and the progressive nature of metabolic disease continue to encourage the search for additional therapeutic approaches.[1]

Medicinal plants represent an important source of structurally diverse molecules with potential biological activity. Natural products have historically contributed substantially to drug discovery, and plant-derived compounds continue to provide molecular scaffolds for

pharmacological development. Computational approaches can further accelerate this process by predicting interactions between phytochemicals and disease-associated molecular targets. *Enicostemma littorale* is one such medicinal plant that has attracted attention because of its traditional antidiabetic use and experimentally reported pharmacological properties. A pharmacognostic review describes E. littorale as a perennial herb of Gentianaceae with traditional applications including regulation of blood glucose, fever, rheumatism, abdominal disorders and other conditions.

The present research concept focuses on the isolation of swertiamarin from *E. littorale* followed by structural characterization and molecular docking against diabetes-associated protein targets. The thesis identifies the central aim as isolation of swertiamarin and evaluation of its antidiabetic potential through in silico molecular docking.[2]

Botanical and Pharmacognostic Profile of *Enicostemma littorale*

Enicostemma littorale belongs to the family Gentianaceae. It is a small perennial herb distributed in India and other tropical regions. The plant is commonly associated with traditional systems of medicine and is known by vernacular names including Chota Chirayata and Mamajjaka.

The plant possesses a characteristic bitter taste, which is consistent with the presence of bitter secoiridoid constituents. Botanical descriptions included in the thesis characterize the plant as an erect perennial herb approximately 5–30 cm in height, with cylindrical glabrous stems and sessile linear to lanceolate leaves. The flowers occur in axillary clusters and are described as white with green lines.

Correct botanical authentication is particularly important in pharmacognostic and phytochemical research because differences in species identification, geographical origin, plant part and harvesting conditions may substantially influence phytochemical composition.[3]

Phytochemical Composition of *Enicostemma littorale*

Phytochemical investigations have revealed a diverse chemical profile in *E. littorale*. Reported constituents include alkaloids, flavonoids, glycosides, saponins, steroids, triterpenoids, phenolic compounds, xanthones and secoiridoid glycosides.

The isolation of several flavonoids and related compounds, including apigenin, genkwanin, isovitexin, swertisin, saponarin and glycosylated derivatives. Phenolic acids including vanillic, syringic, p-hydroxybenzoic, protocatechuic, p-coumaric and ferulic acids have also been reported.

Among the phytoconstituents, swertiamarin is particularly important. It is a secoiridoid glycoside and has been repeatedly associated with the pharmacological activity of Enicostemma species. Recent reviews describe swertiamarin as an important chemotaxonomic marker and summarize antioxidant, anti-inflammatory, antidiabetic, antihyperlipidemic, hepatoprotective and other biological activities.[4,5,6]

Swertiamarin: Chemistry and Pharmacological Significance

Swertiamarin is a naturally occurring secoiridoid glycoside found in several members of the Gentianaceae family. Its occurrence in Enicostemma species has made it particularly relevant to phytochemical standardization and pharmacological research.

The importance of swertiamarin extends beyond its presence as a phytochemical marker. Experimental literature has associated the compound with glucose-lowering, antioxidant, anti-inflammatory, hepatoprotective and lipid-modulating effects. A systematic review of swertiamarin reported evidence for antidiabetic, antioxidant, anti-inflammatory and anti-atherosclerotic effects and discussed its influence on pathways associated with metabolic and cardiovascular disease.

A separate review specifically examining molecular targets of swertiamarin concluded that it is an important candidate for understanding the molecular basis of the antidiabetic and antihyperlipidemic effects of *E. littorale*.

Thus, swertiamarin represents an appropriate candidate for investigation as an isolated phytoconstituent rather than studying only a chemically complex plant extract.[7,8,10]

Experimental Evidence for the Antidiabetic Activity of *E. littorale*

The antidiabetic activity of *E. littorale* has been investigated using different experimental models. Earlier studies reported hypoglycemic effects of aqueous extracts in chemically induced diabetic animals.

Aqueous whole-plant extract administration in alloxan-induced diabetic rats produced significant effects on blood glucose and oxidative-stress-related parameters. The thesis also describes studies in streptozotocin-induced diabetic rats in which aqueous extracts reduced food and water consumption, serum glucose and lipid parameters.

These findings are important because diabetes is not solely a disorder of blood glucose. Oxidative stress, dyslipidemia, inflammation and progressive tissue injury are closely associated with metabolic disease. Consequently, a phytoconstituent exhibiting glucose-lowering activity together with antioxidant and metabolic effects may have broader therapeutic relevance.

However, an important limitation of extract-based studies is that the observed effect cannot always be attributed to one compound. Extracts contain multiple constituents that may act independently, synergistically or antagonistically. Isolation and characterization of swertiamarin therefore provide an opportunity to investigate the contribution of a defined chemical entity.[8]

Swertiamarin and Metabolic Disease

The pharmacological importance of swertiamarin may extend beyond direct glucose reduction. Previous research summarized in the literature has reported effects on lipid metabolism, oxidative stress and inflammatory processes.

The thesis describes studies in which *E. littorale* extracts influenced cholesterol, triglycerides and oxidative-stress markers. It also reports hepatoprotective effects and restoration of antioxidant defenses in experimental models.

The systematic literature on swertiamarin similarly indicates potential effects in metabolic and cardiovascular disorders. Reported mechanisms include modulation of oxidative stress, inflammatory pathways and lipid metabolism.

Nevertheless, these findings should be interpreted as preclinical evidence. Demonstration of pharmacological activity in experimental systems does not by itself establish clinical efficacy or therapeutic safety in humans.[9]

Molecular Targets Relevant to Antidiabetic Drug Discovery

Diabetes involves multiple biological pathways, and therefore several molecular targets have been investigated for pharmacological intervention.

α-Glucosidase

α-Glucosidase is involved in the final stages of carbohydrate digestion. Inhibition of this enzyme delays carbohydrate breakdown and can reduce the rapid elevation of postprandial blood glucose.

Natural products are extensively investigated as α-glucosidase inhibitors because plant metabolites provide considerable structural diversity.

α-Amylase

α-Amylase catalyzes the hydrolysis of dietary starch into smaller carbohydrate molecules. Its inhibition can reduce the availability of absorbable glucose following carbohydrate consumption. Therefore, α-amylase is another important target for investigating natural antidiabetic compounds.

Dipeptidyl Peptidase-4

DPP-4 regulates incretin hormones and consequently influences insulin secretion and glucose homeostasis. DPP-4 inhibition has become an established therapeutic strategy in type 2 diabetes.

Recent literature specifically examining natural compounds as DPP-4 inhibitors demonstrates extensive use of molecular docking to investigate ligand–DPP-4 interactions. However, the literature also emphasizes that docking results should preferably be supported by experimental assays and complementary computational approaches.[11]

Molecular Docking in Natural-Product Drug Discovery

Molecular docking is a structure-based computational technique used to predict the orientation and interaction of a ligand within a protein-binding site. It generally involves two major processes: generation of ligand poses and ranking of these poses using a scoring function.

The thesis proposes the use of AutoDock Vina for docking and PyMOL or Discovery Studio for visualization. Protein structures are proposed to be obtained from the Protein Data Bank,

while the molecular structure of swertiamarin is proposed to be obtained from PubChem. Binding energy, hydrogen bonding and active-site interactions are among the proposed parameters for evaluation.

Docking can be particularly useful during natural-product research because it allows researchers to explore several possible targets before committing substantial resources to experimental validation. Reviews of natural products in antidiabetic drug discovery have highlighted the potential of computational methods for identifying molecular targets and prioritizing compounds for further investigation.

However, docking scores should not be interpreted as direct proof of biological activity. A more negative docking score may suggest favorable predicted interaction within the selected computational system, but it does not establish enzyme inhibition, cellular activity, pharmacokinetic suitability or clinical efficacy.

Integration of Phytochemical Isolation and Molecular Docking

A major strength of the proposed research is the integration of classical pharmacognosy with modern computational drug discovery.

The proposed workflow can be represented as: Authentication → Drying and Powdering → Extraction → Fractionation → Column Chromatography → HPTLC Monitoring → Isolation of Swertiamarin → LC-MS/UV/FTIR/NMR Characterization → Protein Selection → Ligand Preparation → Molecular Docking → Interaction Analysis → Experimental Validation

Hydroalcoholic extraction followed by chromatographic isolation, with HPTLC used for monitoring fractions. The isolated compound is proposed to be characterized by LC-MS, UV-visible spectroscopy, FTIR and NMR.

This sequence is scientifically important because computational docking should ideally be performed using a chemically characterized compound. Docking an incorrectly identified or impure compound may produce misleading conclusions.[12]

CONCLUSION

Enicostemma littorale represents an important medicinal plant with a long history of traditional use and considerable experimental evidence supporting its pharmacological potential. Its phytochemical profile includes several classes of secondary metabolites, with

swertiamarin emerging as a particularly important secoiridoid glycoside and potential chemotaxonomic marker.

Available experimental evidence supports the investigation of *E. littorale* and swertiamarin in the context of glucose regulation, oxidative stress, lipid metabolism and related metabolic abnormalities.

The proposed isolation of swertiamarin followed by LC-MS, UV, FTIR and NMR characterization and molecular docking against diabetes-related targets represents a logical progression from traditional medicinal knowledge to modern phytochemical and computational research. The thesis methodology specifically incorporates chromatographic isolation, HPTLC monitoring, spectroscopic characterization and AutoDock Vina-based molecular docking.

Nevertheless, molecular docking should be considered a hypothesis-generating rather than definitive pharmacological technique. The strongest future evidence will arise from integrating docking with molecular dynamics, enzyme inhibition assays, cellular studies, pharmacokinetics and appropriate in vivo models.

Overall, the systematic investigation of isolated swertiamarin from *E. littorale* may contribute to the identification and characterization of a plant-derived lead molecule for antidiabetic drug discovery and provide a scientific basis for further pharmacological development.

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