

Research Article

Potential Molecular Targets of α -Linolenic Acid from Green purslane (*Portulaca oleracea*) Through Swiss Target Prediction Analysis

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Abstract

α -Linolenic acid is an essential omega-3 fatty acid widely found in medicinal plants, including *Portulaca oleracea*, and is known for its diverse pharmacological activities. However, the molecular targets underlying its biological effects remain insufficiently explored. This study aimed to predict the potential molecular targets of α -linolenic acid using an in silico approach. The molecular structure of α -linolenic acid was obtained in the form of SMILES from PubChem, followed by target prediction using SwissTargetPrediction. The analysis revealed several key targets, including peroxisome proliferator-activated receptors (PPARG, PPAR α , and PPAR γ), fatty acid binding proteins (FABP4 and FABP3), free fatty acid receptor 1 (FFAR1), and cyclooxygenase-1 (PTGS1). These targets are primarily associated with lipid metabolism, glucose regulation, and inflammatory pathways. The results indicate that α -linolenic acid exhibits a multi-target mechanism of action, suggesting its potential as an antidiabetic, anti-inflammatory, and cardioprotective agent. This study provides valuable insights into the molecular basis of α -linolenic acid activity and highlights its potential for further development in pharmacological applications.

Keywords: α -Linolenic acid; *Portulaca oleracea*; In silico study; SwissTargetPrediction; Molecular target prediction

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1 Introduction

Medicinal plants have long been recognized as valuable sources of bioactive compounds with significant therapeutic potential. The increasing global interest in natural products has driven extensive research into plant-derived compounds. These compounds often exhibit diverse pharmacological activities, making them promising candidates for drug discovery [1]. Among various medicinal plants, *Portulaca oleracea* has gained considerable attention due to its rich phytochemical composition. This plant is widely distributed across tropical and subtropical regions. It is commonly consumed as a vegetable and used in traditional medicine [2]. The therapeutic potential of this plant has been documented in various ethnopharmacological studies. It is known to contain multiple classes of bioactive compounds. These include flavonoids, alkaloids, vitamins, and fatty acids. Among these compounds, fatty acids play a crucial role in maintaining physiological functions [3].

One of the most important fatty acids found in this plant is α -linolenic acid. α -Linolenic acid is an essential omega-3 fatty acid. It cannot be synthesized by the human body [4]. Therefore, it must be obtained through dietary sources. This compound has been associated with numerous health benefits. It plays a key role in reducing inflammation. It also contributes to cardiovascular health. In addition, α -linolenic acid exhibits antioxidant properties. These properties help in preventing oxidative stress-related diseases. Oxidative stress is a major factor in the development of chronic diseases [5].

Chronic diseases such as diabetes and cardiovascular disorders are increasing worldwide. These conditions are often linked to inflammation and oxidative damage. Natural compounds with anti-inflammatory and antioxidant properties are therefore of great interest [6]. α -Linolenic acid has shown promising effects in various experimental studies. However, the molecular mechanisms underlying its activity are not fully understood. Understanding these mechanisms is essential for drug development. Identifying molecular targets is a crucial step in this process. Molecular targets include proteins, enzymes, and receptors. These targets are involved in disease pathways. By interacting with these targets, bioactive compounds can exert therapeutic effects [7].

Traditional experimental approaches to identify targets are time-consuming. They are also costly and labor-intensive. Therefore, computational methods have gained popularity in recent years. In silico approaches offer a faster and more efficient alternative [8]. These methods allow researchers to predict molecular interactions. They also help in identifying potential targets. One widely used tool in this field is SwissTargetPrediction [9]. This tool predicts the most probable protein targets of small molecules. It is based on chemical similarity principles. The tool uses a combination of 2D and 3D similarity measures [10].

SwissTargetPrediction has been widely applied in drug discovery studies. It provides reliable predictions of ligand-protein interactions. The tool is user-friendly and accessible online. It supports multiple species, including humans. This makes it highly relevant for pharmacological research. The predictions generated by this tool can guide experimental validation. They can also provide insights into mechanisms of action [11]. Thus, integrating computational tools with natural product research is highly beneficial. Despite the known benefits of α -linolenic acid, its specific molecular targets remain underexplored. Particularly, studies focusing on its targets derived from *Portulaca oleracea* are limited [12]. This gap highlights the need for further investigation. Identifying these targets could enhance our understanding of its pharmacological effects. It could also support the development of novel therapeutic agents. Furthermore, such studies contribute to the validation of traditional medicinal uses [13].

The integration of bioinformatics and phytochemistry has opened new research avenues. It allows for systematic analysis of bioactive compounds. This approach is known as network pharmacology. It considers the multi-target nature of natural compounds. Unlike synthetic drugs, natural compounds often interact with multiple targets. This multi-target interaction can enhance therapeutic efficacy. It may also reduce side effects [14]. In addition, α -linolenic acid may influence various signaling pathways. These pathways include inflammatory and metabolic pathways. The modulation of these pathways is crucial for disease management. Understanding how α -linolenic acid interacts with these pathways is essential. It

can provide insights into its therapeutic potential. Moreover, it may help in identifying new drug targets [15].

The use of computational tools also supports personalized medicine. It allows for the prediction of compound-target interactions in specific populations. This can lead to more effective treatment strategies [16]. Furthermore, it reduces the need for extensive laboratory testing. This makes research more efficient and cost-effective. Given the increasing prevalence of chronic diseases, there is an urgent need for new therapies. Natural products offer a promising solution to this challenge. They are generally considered safer than synthetic drugs [17]. However, scientific validation is necessary to support their use. This includes identifying their molecular targets and mechanisms of action [18]. Therefore, this study aims to predict the potential molecular targets of α -linolenic acid. The compound is derived from *Portulaca oleracea*. The study utilizes Swiss Target Prediction as the main analytical tool. This approach provides a comprehensive understanding of the compound's activity [19]. It also highlights its potential therapeutic applications. The findings of this study are expected to contribute to drug discovery research. They may also support the development of plant-based therapies [20]. In conclusion, the exploration of α -linolenic acid targets is highly relevant. It bridges the gap between traditional medicine and modern pharmacology. The use of *in silico* tools enhances the efficiency of this process. It provides valuable insights into molecular mechanisms. Ultimately, this research contributes to the advancement of pharmaceutical sciences [21].

2 Method

This study employed an *in silico* approach to identify the potential molecular targets of α -linolenic acid derived from *Portulaca oleracea* using a computational prediction platform [22]. The research was designed as a descriptive computational study focusing on ligand-based target prediction to explore possible protein interactions associated with the selected bioactive compound.



Figure 1. Mind Maps

The workflow of this study consisted of several sequential stages, including compound identification, molecular structure retrieval, SMILES acquisition, computational target prediction, and data analysis. The selection of α -linolenic acid as the target compound was based on its known pharmacological relevance as an essential omega-3 fatty acid with anti-inflammatory and antioxidant properties. The compound was first identified and verified through the PubChem database, which is a publicly accessible repository providing comprehensive chemical information, including molecular structures, physicochemical properties, and canonical SMILES notations [22]. The search for α -linolenic acid was performed by entering the compound name into the search interface of the PubChem platform, and the correct compound entry was confirmed based on its molecular formula, molecular weight, and structural information. After identifying the appropriate compound record, the canonical SMILES (Simplified Molecular Input Line Entry System) representation of α -linolenic acid was retrieved. The SMILES format is a widely used text-based representation of chemical structures that encodes molecular connectivity and stereochemistry in a linear string, making it suitable for computational analysis and input into prediction tools. The retrieved SMILES string was carefully verified to ensure its accuracy and consistency with the known chemical structure of α -linolenic acid. This verification step is essential to avoid errors in downstream computational predictions, as incorrect structural input can lead to misleading results.

Following the acquisition of the SMILES notation, the next step involved the prediction of potential molecular targets using the SwissTargetPrediction platform. SwissTargetPrediction is an online tool designed to estimate the most probable protein targets of bioactive small molecules based on chemical similarity with known ligands. The platform integrates both two-dimensional (2D) and three-dimensional (3D) similarity measures to improve prediction accuracy. In this study, the SMILES string of α -linolenic acid obtained from PubChem was input into the SwissTargetPrediction interface. The species parameter was set to "Homo sapiens" to ensure that the predicted targets are relevant to human biological systems. This selection is critical for translational relevance, as the ultimate goal of this study is to understand the potential therapeutic effects of α -linolenic acid in humans. After entering the SMILES data and selecting the appropriate species, the prediction process was initiated by submitting the query to the server. The platform then processed the input and generated a list of predicted protein targets ranked according to their probability scores. These probability scores reflect the likelihood of interaction between the compound and the predicted targets based on similarity to known ligand-target pairs.

The output generated by SwissTargetPrediction included a list of target proteins along with associated information such as target class, gene name, and probability values. The results were carefully recorded and organized for further analysis. Only targets with significant probability values were considered for interpretation to ensure the reliability of the findings. The selection threshold was determined based on commonly accepted practices in computational pharmacology studies, where higher probability scores indicate more reliable predictions. The identified targets were then categorized based on their biological functions and involvement in specific pathways. This categorization helps to provide a clearer understanding of the potential mechanisms of action of α -linolenic acid. Furthermore, the predicted targets were analyzed in the context of their roles in disease pathways, particularly those related to inflammation, oxidative stress, and metabolic disorders. This step is important for linking the computational predictions to potential therapeutic applications.

To enhance the robustness of the analysis, the predicted targets were cross-referenced with existing literature to identify previously reported interactions and validate the plausibility of the results. This literature-based validation provides additional support for the computational findings and helps to identify novel targets that may not have been extensively studied. In addition, the study considered the multi-target nature of natural compounds, recognizing that α -linolenic acid may interact with multiple proteins simultaneously. This multi-target interaction is a key feature of phytochemicals and contributes to their broad pharmacological effects. The analysis also included the identification of major target classes, such as enzymes, receptors, and ion channels, which play critical roles in cellular signaling and physiological processes [23].

All data generated from the SwissTargetPrediction platform were compiled and tabulated to facilitate interpretation and presentation. The results were then discussed in relation to the known pharmacological properties of α -linolenic acid. The integration of computational predictions with existing biological knowledge allows for a more comprehensive understanding of the compound's activity. It also provides a basis for future experimental validation studies. The methodological approach used in this study offers several advantages, including efficiency, cost-effectiveness, and the ability to screen multiple targets simultaneously [24,25]. However, it is important to note that computational predictions are not definitive and should be validated through experimental studies.

In summary, this study utilized a systematic in silico approach involving SMILES retrieval from PubChem and target prediction using SwissTargetPrediction to identify potential molecular targets of α -linolenic acid. The methodology provides a comprehensive framework for exploring the pharmacological potential of bioactive compounds derived from *Portulaca oleracea*. This approach can be applied to other natural compounds to accelerate drug discovery and development processes.

3 Result and Discussion

The computational prediction results revealed several potential molecular targets of α -linolenic acid, highlighting its multi-target pharmacological profile.

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*
Peroxisome proliferator-activated receptor gamma	PPARG	P37231	CHEMBL235	Nuclear receptor	
Peroxisome proliferator-activated receptor delta	PPARD	Q03181	CHEMBL3979	Nuclear receptor	
Peroxisome proliferator-activated receptor alpha	PPARA	Q07869	CHEMBL239	Nuclear receptor	
Fatty acid binding protein adipocyte	FABP4	P15090	CHEMBL2083	Fatty acid binding protein family	
Fatty acid binding protein muscle	FABP3	P05413	CHEMBL3344	Fatty acid binding protein family	
Free fatty acid receptor 1	FFAR1	O14842	CHEMBL4422	Family A G protein-coupled receptor	
Cyclooxygenase-1	PTGS1	P23219	CHEMBL221	Oxidoreductase	

Figure 2. Target Prediction

The identified targets include peroxisome proliferator-activated receptors (PPARs), fatty acid binding proteins (FABPs), free fatty acid receptors, and cyclooxygenase enzymes. These targets are primarily involved in lipid metabolism, inflammation, and cellular signaling pathways, indicating that α -linolenic acid may exert its biological effects through multiple mechanisms. The presence of high-probability interactions with nuclear receptors such as PPAR γ , PPAR δ , and PPAR α suggests a strong regulatory role in gene expression related to metabolic processes. These receptors are known to function as transcription factors that modulate lipid homeostasis, glucose metabolism, and inflammatory responses. The identification of PPAR γ as a top predicted target is particularly significant, as this receptor plays a crucial role in adipogenesis and insulin sensitivity. Activation of PPAR γ has been associated with improved glucose uptake and reduced insulin resistance, which supports the potential antidiabetic effect of α -linolenic acid.

Furthermore, the prediction of PPAR δ as a potential target indicates its involvement in energy expenditure and fatty acid oxidation. PPAR δ is widely expressed in skeletal muscle and is known to enhance lipid utilization and mitochondrial activity. The interaction between α -linolenic acid and PPAR δ may

therefore contribute to improved metabolic efficiency and reduced lipid accumulation. Similarly, the identification of PPAR α highlights its role in hepatic lipid metabolism and β -oxidation processes. PPAR α activation is associated with decreased triglyceride levels and enhanced fatty acid catabolism, suggesting a cardioprotective effect of α -linolenic acid. The combined activation of PPAR isoforms indicates a coordinated regulation of metabolic pathways, which may explain the broad therapeutic potential of this compound.

In addition to nuclear receptors, the results also revealed interactions with fatty acid binding proteins, specifically FABP4 and FABP3. These proteins are involved in the intracellular transport of fatty acids and play a key role in lipid signaling and metabolism. FABP4, also known as adipocyte fatty acid binding protein, is predominantly expressed in adipose tissue and macrophages. It has been implicated in the development of metabolic syndrome, obesity, and inflammation. The interaction between α -linolenic acid and FABP4 suggests a potential modulatory effect on lipid transport and inflammatory signaling. This may contribute to the anti-inflammatory properties of α -linolenic acid by regulating lipid-mediated signaling pathways in immune cells. Similarly, FABP3, which is primarily expressed in cardiac and skeletal muscle, is involved in energy metabolism and fatty acid utilization. The binding of α -linolenic acid to FABP3 may enhance its availability for mitochondrial oxidation, thereby supporting energy production and cellular function.

Another important target identified in this study is the free fatty acid receptor 1 (FFAR1), also known as G protein-coupled receptor 40. FFAR1 is activated by medium- and long-chain fatty acids and plays a critical role in insulin secretion. The interaction between α -linolenic acid and FFAR1 suggests a mechanism by which this compound may enhance glucose-stimulated insulin secretion. This finding is consistent with previous studies that have reported the beneficial effects of omega-3 fatty acids on pancreatic β -cell function. Activation of FFAR1 leads to increased intracellular calcium levels, which in turn stimulate insulin release. Therefore, the predicted interaction with FFAR1 provides further evidence supporting the antidiabetic potential of α -linolenic acid.

Moreover, the prediction of cyclooxygenase-1 (COX-1 or PTGS1) as a target indicates the involvement of α -linolenic acid in inflammatory pathways. COX-1 is an enzyme responsible for the conversion of arachidonic acid into prostaglandins, which are key mediators of inflammation. The interaction between α -linolenic acid and COX-1 suggests a potential inhibitory effect on prostaglandin synthesis. This may result in reduced inflammation and pain, supporting the anti-inflammatory properties of the compound. Although COX-1 is constitutively expressed and involved in physiological functions such as gastric protection, modulation of its activity by α -linolenic acid may contribute to a balanced inflammatory response.

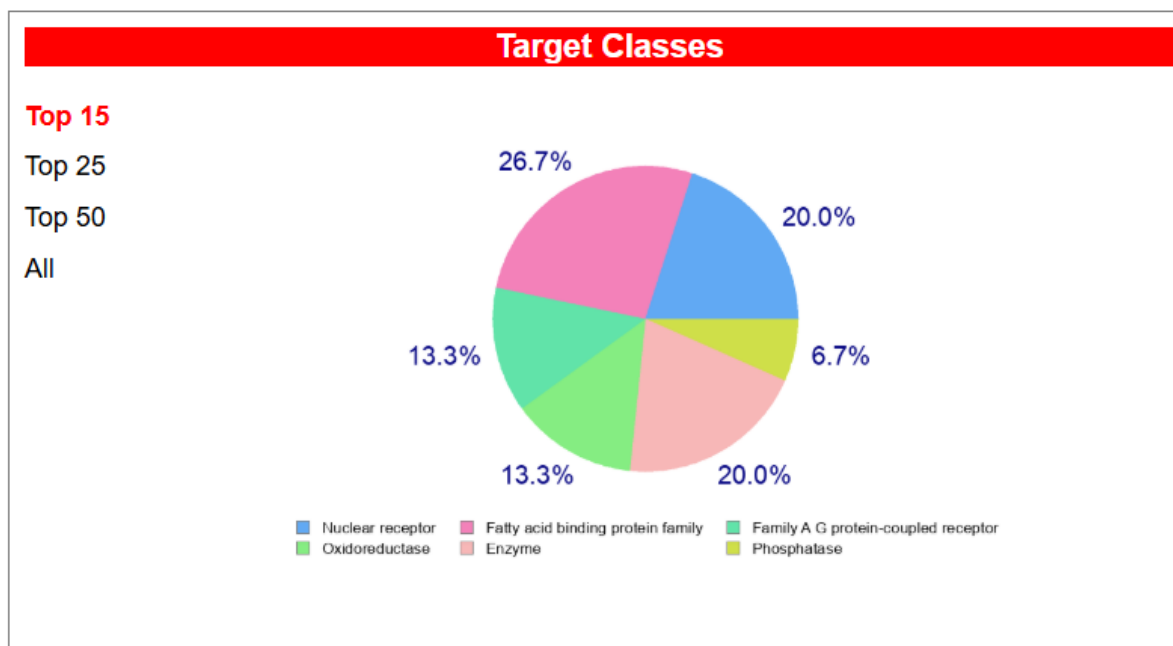


Figure 3. Target Classes

The overall pattern of predicted targets indicates that α -linolenic acid primarily interacts with proteins involved in lipid metabolism and inflammatory regulation. This is consistent with its chemical structure as a polyunsaturated fatty acid. The presence of multiple double bonds allows for flexibility and interaction with various binding sites in proteins. This structural characteristic enables α -linolenic acid to act as a ligand for different receptor types, including nuclear receptors and membrane-bound receptors. The ability to interact with multiple targets is a hallmark of natural compounds and contributes to their pleiotropic effects.

The probability scores associated with each target further support the reliability of these predictions. High probability values indicate strong similarity between α -linolenic acid and known ligands of these targets. This suggests that the predicted interactions are biologically plausible and may occur in vivo. However, it is important to note that these predictions are based on computational models and require experimental validation. Despite this limitation, the results provide valuable insights into the potential mechanisms of action of α -linolenic acid.

From a pharmacological perspective, the interaction with PPARs suggests potential applications in metabolic disorders such as diabetes, obesity, and dyslipidemia. The modulation of FABPs indicates a role in lipid transport and cellular signaling, which may be relevant in cardiovascular diseases. The activation of FFAR1 highlights its potential in enhancing insulin secretion and glucose homeostasis. Meanwhile, the interaction with COX-1 supports its use as an anti-inflammatory agent. The combination of these effects suggests that α -linolenic acid may act as a multifunctional therapeutic agent.

In addition, the multi-target nature of α -linolenic acid aligns with the concept of network pharmacology. This approach recognizes that complex diseases often involve multiple pathways and require multi-target interventions. By interacting with several key proteins, α -linolenic acid may exert synergistic effects that enhance its therapeutic efficacy. This is particularly relevant for chronic diseases, where single-target drugs may not be sufficient. The ability of α -linolenic acid to modulate multiple pathways may also reduce the risk of drug resistance and improve treatment outcomes.

Furthermore, the findings of this study support the traditional use of plant-derived compounds in medicine. The presence of α -linolenic acid in natural sources such as plant-based foods highlights the importance of diet in disease prevention and management. The identification of molecular targets provides a scientific basis for the health benefits associated with these compounds. It also opens new opportunities

for the development of functional foods and nutraceuticals.

The integration of computational tools in this study demonstrates the efficiency of in silico methods in drug discovery. By using SwissTargetPrediction, it was possible to rapidly identify potential targets without the need for extensive laboratory experiments. This approach not only saves time and resources but also provides a comprehensive overview of possible interactions. It allows researchers to prioritize targets for further investigation and design more focused experimental studies.

Table 1. Summary of Predicted Targets and Pharmacological Implications of α -Linolenic Acid

No	Target (Gene)	Target Class	Main Biological Function	Pharmacological Implication
1	PPARG	Nuclear receptor	Regulates adipogenesis and insulin sensitivity	Antidiabetic, improves insulin resistance
2	PPARD	Nuclear receptor	Enhances fatty acid oxidation and energy metabolism	Anti-obesity, improves metabolic efficiency
3	PPARA	Nuclear receptor	Controls lipid metabolism and β -oxidation	Hypolipidemic, cardioprotective
4	FABP4	Fatty acid binding protein	Intracellular lipid transport in adipocytes	Anti-inflammatory, metabolic regulation
5	FABP3	Fatty acid binding protein	Fatty acid transport in muscle and heart	Supports energy production, cardioprotective
6	FFAR1	GPCR (Family A)	Stimulates insulin secretion in pancreatic β -cells	Antidiabetic (enhances insulin release)
7	PTGS1	Oxidoreductase enzyme	Prostaglandin synthesis (inflammation pathway)	Anti-inflammatory, analgesic potential

The predicted molecular targets of α -linolenic acid demonstrate a strong association with key regulators of metabolic and inflammatory pathways. The identification of PPARG as one of the primary targets highlights its crucial role in glucose homeostasis. PPARG is a nuclear receptor that regulates adipocyte differentiation. It also plays a significant role in improving insulin sensitivity. Activation of PPARG is widely associated with antidiabetic effects. This suggests that α -linolenic acid may contribute to glucose regulation. The modulation of this receptor can enhance insulin responsiveness in peripheral tissues. Consequently, this interaction supports the potential use of α -linolenic acid in metabolic disorders. In addition to PPARG, PPARD was also identified as a significant target. PPARD is involved in fatty acid oxidation and energy metabolism. It promotes lipid utilization in skeletal muscle. This receptor enhances mitochondrial activity and energy expenditure. Therefore, the interaction between α -linolenic acid and PPARD may reduce lipid accumulation. This mechanism is particularly important in obesity management. The activation of PPARD is also linked to improved endurance and metabolic efficiency. These findings suggest that α -linolenic acid may have anti-obesity effects.

PPARA was identified as another important nuclear receptor target. PPARA plays a central role in hepatic lipid metabolism. It regulates β -oxidation of fatty acids in the liver. Activation of PPARA leads to reduced triglyceride levels. This contributes to improved lipid profiles. The interaction with PPARA indicates a cardioprotective effect. This is particularly relevant in the prevention of cardiovascular diseases. The combined targeting of PPARG, PPARD, and PPARA suggests a coordinated regulation of metabolic pathways. This multi-target interaction enhances the therapeutic potential of α -linolenic acid. In addition

to nuclear receptors, fatty acid binding proteins were also identified as key targets. FABP4 is predominantly expressed in adipose tissue. It is involved in intracellular lipid transport. FABP4 also plays a role in inflammatory signaling. Elevated levels of FABP4 are associated with metabolic syndrome. Therefore, modulation of FABP4 by α -linolenic acid may reduce inflammation. This interaction may also improve lipid metabolism. Similarly, FABP3 was identified as a target protein. FABP3 is mainly expressed in cardiac and skeletal muscle tissues. It facilitates fatty acid transport for energy production. The interaction with FABP3 suggests improved energy utilization. This may enhance cardiac function and muscle performance. These findings highlight the role of α -linolenic acid in energy metabolism.

Significant target identified in this study is FFAR1. FFAR1 is a G protein-coupled receptor activated by fatty acids. It plays an essential role in insulin secretion. Activation of FFAR1 enhances glucose-stimulated insulin release. This mechanism is crucial for maintaining glucose homeostasis. The interaction between α -linolenic acid and FFAR1 supports its antidiabetic potential. This finding is consistent with previous studies on omega-3 fatty acids. These compounds are known to improve pancreatic β -cell function. The activation of FFAR1 leads to intracellular calcium signaling. This triggers insulin exocytosis. Therefore, α -linolenic acid may enhance pancreatic function. In addition to metabolic targets, PTGS1 was also identified. PTGS1 is an enzyme involved in prostaglandin synthesis. It plays a role in inflammatory processes. The interaction with PTGS1 suggests an anti-inflammatory effect. This may reduce the production of pro-inflammatory mediators. The inhibition of prostaglandin synthesis can alleviate inflammation and pain. This mechanism supports the traditional use of plant-derived compounds in inflammatory conditions.

The predicted targets indicate that α -linolenic acid exerts its effects through multiple pathways. These pathways include lipid metabolism, glucose regulation, and inflammation. The multi-target nature of α -linolenic acid is a key advantage. It allows for a broader therapeutic impact. This is particularly important in complex diseases. Chronic diseases often involve multiple dysregulated pathways. Therefore, compounds with multi-target activity are highly valuable. The results of this study align with the concept of network pharmacology. This approach emphasizes the interaction of compounds with multiple targets. It provides a more holistic understanding of drug action. The findings also support the pharmacological potential of natural compounds derived from *Portulaca oleracea*. The presence of α -linolenic acid in this plant highlights its medicinal value. The integration of computational tools such as SwissTargetPrediction enhances the efficiency of target identification. This approach provides rapid and reliable predictions. However, experimental validation is still necessary. Future studies should focus on confirming these interactions in vitro and in vivo. Such validation will strengthen the scientific basis of these findings. In conclusion, the predicted targets of α -linolenic acid demonstrate its significant pharmacological potential. The compound shows promise as an antidiabetic, anti-inflammatory, and cardioprotective agent. These findings contribute to the advancement of natural product research. They also support the development of plant-based therapeutics.

4 Conclusion

The present study successfully identified several potential molecular targets of α -linolenic acid through an in silico approach using SwissTargetPrediction. The results demonstrate that α -linolenic acid exhibits a multi-target interaction profile, primarily involving nuclear receptors, fatty acid binding proteins, G protein-coupled receptors, and oxidoreductase enzymes. Among the identified targets, PPARG, PPAR δ , and PPAR α showed the highest probability values, indicating a strong association with lipid metabolism and glucose regulation pathways. These findings suggest that α -linolenic acid plays a significant role in modulating metabolic homeostasis.

In addition, the interaction with FABP4 and FABP3 highlights its involvement in intracellular lipid transport and energy utilization. The identification of FFAR1 further supports its potential role in enhancing insulin secretion and maintaining glucose balance. Moreover, the predicted interaction with PTGS1 indicates its possible contribution to anti-inflammatory activity through the modulation of prostaglandin synthesis.

Collectively, these results confirm that α -linolenic acid targets key proteins associated with metabolic, inflammatory, and cardiovascular processes.

5 Declarations

5.1 Acknowledgements

All authors contributed to the design, writing, and editing of the manuscript.

5.2 Author contributions

The author declares that there is no conflict of interest in this research

5.3 Conflict of Interest

The author declares that there is no conflict of interest in this research

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