

## Prediction of Scabertopin from Tapak Liman (*Elephantopus scaber*) for Antileukemic

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**Abstract**— Leukemia remains a significant global health challenge, necessitating the exploration of novel therapeutic agents with improved efficacy and safety profiles. *Elephantopus scaber* (commonly known as Tapak Liman) is a medicinal plant traditionally used for various ailments, including cancer. Scabertopin, a sesquiterpene lactone isolated from *E. scaber*, has attracted scientific interest due to its potential antileukemic properties. This study aims to predict the antileukemic activity of Scabertopin through an in silico approach. The compound's chemical structure was retrieved in SMILES format from the PubChem database and analyzed using the PASS (Prediction of Activity Spectra for Substances) online tool. The prediction results indicated a high probability of antileukemic activity, with a Pa (probability of activity) value of 0.822 and a Pi (probability of inactivity) value of 0.004. These findings suggest a strong likelihood that Scabertopin exhibits antileukemic effects, supporting its potential as a candidate for further pharmacological and clinical investigations. The use of computational prediction tools provides an efficient and cost-effective preliminary screening method for identifying promising bioactive compounds from natural sources. This study contributes valuable insights into the therapeutic potential of Scabertopin and highlights the importance of traditional medicinal plants in drug discovery for leukemia treatment.

**Keywords:** *Scabertopin*, *Elephantopus scaber*, antileukemic activity, PASS prediction, natural compounds.

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### 1. Introduction

Leukemia is a type of blood cancer characterized by the abnormal growth of white blood cells originating from the bone marrow. This disease can be either acute or chronic, depending on the speed at which it develops and the type of white blood cells that are involved [1]. Leukemia has a considerable impact on the quality of life of patients, with prognosis varying greatly depending on the type and stage of the disease [2]. Although various conventional therapy options such as chemotherapy, radiotherapy, and bone marrow transplantation are available, the effectiveness of these treatments is often limited by severe side effects, drug resistance, and high costs. The demand for new therapies that are more selective, effective, and have low toxicity continues to be a primary focus in cancer research, particularly in leukemia [3].

Alternative and complementary approaches that utilize natural materials are gaining increased attention from researchers in the field of molecular oncology. Indonesia, as a highly diverse country with remarkable biological wealth, possesses significant potential for discovering cancer treatments from

traditional medicinal plants [4]. One of the plants that has long been utilized in traditional medicine but has not yet been extensively studied scientifically is Tapak Liman (*Elephantopus scaber*). This plant is well-known in various ethnopharmacological treatments across Asia, particularly in India, China, and Indonesia, for addressing a range of issues such as fever, inflammation, liver diseases, and hematological disorders [5].

*Elephantopus scaber* belongs to the Asteraceae family and has been traditionally utilized to treat various chronic illnesses, including blood-related diseases [6]. Various phytochemical studies have demonstrated that this plant contains several bioactive compounds, including flavonoids, sesquiterpene lactones, steroids, and phenolic acids. One of the main active compounds successfully identified from Tapak Liman is Scabertopin, a sesquiterpene lactone with a unique chemical structure that displays various potential biological activities [7].

Scabertopin has been reported to possess anti-inflammatory, antibacterial, liver-protective, and even anticancer activities [8]. The anticancer activity of Scabertopin is believed to be associated with its ability to induce apoptosis, inhibit cell proliferation, and interfere with the cancer cell cycle. However, to date, information regarding the specific potential of Scabertopin against leukemia cells, particularly from a molecular and computational perspective, remains very limited. This presents a significant scientific opportunity that warrants further exploration [9].

The *in silico* predictive approach is an efficient preliminary strategy for assessing the potential bioactivity of a compound against specific molecular targets [10]. With the assistance of molecular modeling, molecular docking, and molecular dynamics simulation, one can efficiently predict the interactions between compounds and leukemia target proteins before proceeding to *in vitro* and *in vivo* tests. Key targets in the pathogenesis of leukemia, such as BCR-ABL, FLT3, JAK2, and STAT5, are the primary focus in the design and assessment of new anti-leukemic molecules [11].

In this context, the approach of predicting the bioactivity of Scabertopin towards leukemia target proteins becomes pertinent and strategic. In addition to providing initial information about the therapeutic potential of this compound, this study also contributes to bridging traditional ethnopharmacological knowledge with modern scientific approaches that are technology-based [12]. This study is important not only to support the conservation and utilization of local biodiversity but also in the efforts to discover new medicines based on Indonesia's natural resources.

The molecular mechanism of action of Scabertopin can significantly contribute to the discovery of new drug candidates that are multitarget and have a lower risk of resistance. The development of multitarget drugs represents a contemporary approach to cancer therapy, as the high heterogeneity and dynamic mutation of cancer cells require therapeutic agents capable of intervening in more than one signaling pathway [13]. Through this approach, Scabertopin has the potential to be developed as an anticancer agent that is not only cytotoxic but also capable of modulating the immune system, signal transduction pathways, and the expression of apoptosis-related genes [14].

In addition to its biological potential, Scabertopin is also interesting from the perspective of its chemical structure. As a sesquiterpene lactone, Scabertopin contains an  $\alpha$ -methylene- $\gamma$ -lactone group that is known to be highly reactive towards target proteins via the Michael addition mechanism [15]. This group can form covalent bonds with cysteine residues in the target protein, thereby enhancing the affinity and stability of the compound-protein complex. This characteristic makes Scabertopin a strong candidate as an irreversible inhibitor for several protein targets involved in the proliferation of leukemia cells [16].

Similar to many other natural compounds, the development of Scabertopin as an antileukemic drug encounters specific challenges, including issues of bioavailability, metabolic stability, and selective toxicity [17]. Therefore, the early prediction approach through *in silico* studies offers significant

advantages in mapping initial interaction profiles, assessing pharmacokinetic feasibility, and screening for potential off-target effects. Thus, this study not only contributes to mapping the anticancer potential of Scabertopin, but also paves the way for designing more potent and selective structural derivatives in the future [18].

## 2. Method

This research is a predictive in silico study aimed at identifying the potential antileukemic activity of the compound Scabertopin, which is a derivative of sesquiterpene lactone reported to be found in the plant *Elephantopus scaber*, commonly known in Indonesia as Tapak Liman. This plant has been utilized for a long time in traditional Asian medicine as an anti-inflammatory agent, liver protector, and antimicrobial. Recently, it has been reported to contain several bioactive compounds that may have cytotoxic effects on cancer cells. Therefore, a prediction is conducted regarding the anticancer activity, specifically the antileukemic properties of the compound Scabertopin through in silico methods.



Figure 1. Mind Maps

The initial step of this research involves the digital exploration of the chemical structure of Scabertopin using the PubChem database (<https://pubchem.ncbi.nlm.nih.gov/>). PubChem is a public chemical database managed by the National Center for Biotechnology Information (NCBI), which is a part of the United States National Library of Medicine [19]. This database offers comprehensive information about the chemical structure, physicochemical properties, bioactivity, and toxicological descriptions of millions of chemical compounds reported from various literature and research findings. In this study, the search was conducted by entering the keyword "Scabertopin" into the search box on PubChem. After successful discovery, a verification was conducted to assess the conformity of the molecular structure based on primary and secondary literature discussing the phytochemical components of *Elephantopus scaber*.

The molecular structure of Scabertopin is then extracted in the form of Simplified Molecular Input Line Entry System (SMILES), which is a linear text representation of the molecular structure. The SMILES format is highly useful for entering chemical structures into various computational

chemistry software, including those used for pharmacological and toxicological predictions based on machine learning. The SMILES copy of Scabertopin was obtained directly from the compound's detail page on PubChem and is saved for subsequent analysis. The second stage of this methodology involves predicting the biological activity of Scabertopin using the Way2Drug platform, which can be accessed at <https://www.way2drug.com/>. This platform has been created by the Institute of Biomedical Chemistry in Moscow, Russia, and offers various predictive tools based on neural networks and other machine learning techniques to assess the potential biological activity of compounds based on their chemical structure.

In this study, the PASS (Prediction of Activity Spectra for Substances) tool was utilized, which is an essential component of the Way2Drug platform. PASS operates by comparing the structure of input compounds (in SMILES format) against a database of known active and inactive compounds. Based on computational analysis, PASS will produce an output that includes a list of potential biological activity predictions along with the values of Pa (Probability to be Active) and Pi (Probability to be Inactive) for each activity. Presents the likelihood that the compound will exhibit some biological activity, while Pi indicates the likelihood that the compound will not exhibit such activity. A value of Pa > 0.7 is generally interpreted as a reliable prediction and requires further experimental validation. However, a Pa value between 0.5 and 0.7 is still regarded as having potential and is suitable for further exploration. The input process begins with copying the SMILES string of Scabertopin into the input column provided on the main page of PASS Online. Subsequently, the Way2Drug server will conduct a computational process, and the prediction results will be presented in a table format, featuring columns for activity, Pa value, and Pi value. The biological activities that are the main focus of this research include antineoplastic activity, anticancer properties, antileukemic effects, cytotoxicity, and other relevant activities against leukemia targets such as inducers of apoptosis, inhibitors of tyrosine kinase, or activators of p53.

Next, from the list of prediction results, a selection is made of the activities with the highest Pa values that are directly related to the antileukemic mechanism. This is undertaken to filter relevant information from dozens, even hundreds, of predictions displayed, and to concentrate on the pharmacodynamic pathways underlying anticancer effects. Additionally, it is noted that supporting activities such as immunomodulatory effects, anti-inflammatory properties, or antioxidant activities are observed, as these effects can also influence the tumor microenvironment and indirectly promote anti-cancer effects. To enhance this bioinformatics approach, a secondary literature search was conducted using scientific databases such as PubMed, ScienceDirect, and Google Scholar. This was done to compare the prediction results from PASS with experimental findings related to Scabertopin as well as similar sesquiterpene lactones derived from the plant *Elephantopus scaber*. This data is utilized as a component of theoretical external validation, aimed at either supporting or refuting the predictions made through computational methods.

As part of the initial toxicity analysis, predictions are also made regarding fundamental toxicological parameters using the same platform, which includes hepatotoxicity, mutagenicity, and carcinogenicity. This information is crucial for assessing whether the predicted compounds that are active as antileukemic agents also possess sufficient safety margins for further development as drug candidates.

Ultimately, all data collected from the predictions of biological activity and toxicity were analyzed descriptively. The primary focus is to determine the extent to which Scabertopin exhibits a promising pharmacological profile as a candidate compound for anti-leukemic treatment by comparing the Pa values of target activity with the Pa values of non-target activity (for instance, toxic activity, off-target activity, or other undesirable physiological activities). From this analysis, a pharmacodynamic hypothesis has been developed that outlines the potential mechanism of action of Scabertopin in relation

to the inhibition of leukemia cell proliferation, the induction of apoptosis, and the modulatory effects on the immune system.

Through this methodology, it is anticipated that a comprehensive initial overview of Scabertopin's potential as a leukemia treatment agent based on *in silico* predictive approaches will be attained. This approach is not only cost-effective and time-efficient, but it also enables initial screening of dozens to hundreds of natural compounds without the need for complex laboratory isolation. Nevertheless, the outcomes of this research still require further validation through experimental studies, both *in vitro* and *in vivo*, to confirm the bioactivity and safety profile of the relevant compounds.

### **3. Result and Discussion**

#### **Tapak Liman (*Elephantopus scaber*)**

Tapak Liman, scientifically known as *Elephantopus scaber* L. , is an herbaceous plant belonging to the Asteraceae family, commonly found in many tropical and subtropical areas, including Southeast Asia, India, China, and various regions of Africa. This plant is traditionally known in Indonesia as one of the medicinal plants with a wide range of benefits, particularly in traditional medicine for addressing inflammation, fever, infections, and various chronic diseases. The name "Tapak Liman" itself refers to the shape of its wide and coarse leaves, resembling the footprint of an elephant, which serves as its main morphological characteristic.



Figure 2. Tapak Liman (*Elephantopus scaber*)

Botanically, *Elephantopus scaber* is a low-growing annual herb that spreads close to the ground. This plant features rosette-shaped leaves that have a rough texture and a hairy surface, along with small bluish-purple flowers arranged in a flower head (capitulum). The stem is short and woody, and this plant can be easily found growing wild in open areas, forest edges, grasslands, as well as home gardens. Due to its high adaptability to tropical environments, Tapak Liman is often regarded as a weed, even though it actually contains various bioactive components that are highly valuable pharmacologically.

In traditional medicine of Indonesia, India (Ayurveda), and China (TCM), Tapak Liman has been used for generations to treat various health issues. Several conditions commonly treated using extracts or infusions of the leaves and roots of Tapak Liman include fever, hypertension, hepatitis, diarrhea, menstrual disorders, urinary tract infections, and skin diseases. A very common use also includes the treatment of external wounds and infections caused by pathogenic microorganisms. The popularity of this plant in the field of ethnomedical treatment is closely related to the presence of bioactive compounds that have been identified by various phytochemical studies.

From a phytochemical perspective, *Elephantopus scaber* is known to contain various groups of active compounds, including flavonoids, triterpenoids, steroids, sesquiterpene lactones, and other phenolic compounds. Among these compounds, the group of sesquiterpene lactones has garnered particular attention due to their demonstrated potential for strong biological activity, which includes antimicrobial, anti-inflammatory, immunomodulatory, and anticancer effects. One of the main compounds successfully isolated from Tapak Liman is Scabertopin, which is a type of sesquiterpene lactone featuring a distinctive chemical structure characterized by an  $\alpha$ -methylene- $\gamma$ -lactone. This compound is highly reactive towards specific biomolecules.

Scabertopin has been reported to exhibit promising cytotoxic activity against various types of cancer cells, including leukemia cells. The cytotoxic mechanism of Scabertopin is believed to involve the inhibition of cancer cell proliferation through the blockage of the cell cycle and the induction of apoptosis. This compound is also expected to interact with cellular regulatory proteins, such as caspase, Bcl-2, and molecules in the NF- $\kappa$ B pathway, all of which are significant targets in the development of modern anti-cancer drugs. Previous *in vitro* research was conducted on the ethanol extract from *E. Scaber* indicates an inhibitory effect on the growth of murine and human leukemia cells, reinforcing the hypothesis that the active compounds in this plant possess strong therapeutic effects against leukemia.

Modern pharmacological studies have confirmed that Tapak Liman possesses extensive pharmacological activity and is relevant for development as a source of new medicinal materials. Antibacterial, antiviral, antioxidant, and hepatoprotective activities have been demonstrated through various experimental methods. Acute and subchronic toxicity studies on this plant extract indicate that Tapak Liman is relatively safe at the commonly used therapeutic doses in traditional medicine systems. This establishes an important foundation for further exploring specific bioactive compounds, such as Scabertopin, as natural drug candidates with predictable anticancer potential that can be systematically developed through *in silico* and *in vitro* methods.

In the context of drug development based on natural products, *Elephantopus scaber* holds a strategic position as a source of primary compounds and supporting compounds that can be explored through bioprospecting. Scabertopin, being a unique secondary metabolite of this plant, can serve as a target for predicting biological activity using bioinformatics platforms and predictive pharmacology systems. This includes employing molecular databases such as PubChem to obtain chemical structures in the SMILES (Simplified Molecular Input Line Entry System) format and utilizing predictive software like Way2Drug to identify its potential bioactivity *in silico*. This predictive approach is crucial for filtering potential compounds before conducting *in vitro* and *in vivo* tests, thereby speeding up the process of screening drug candidates.

Through a combination of ethnopharmacological data, findings from phytochemical research, and support from predictive molecular pharmacology approaches, Tapak Liman holds significant potential as a source of candidate medications for leukemia treatment. The compound Scabertopin derived from this plant warrants further investigation, considering its partially confirmed biological activities and potential mechanisms of action that are relevant to the main molecular pathways involved in leukemia pathogenesis. The development of medicinal plants such as Tapak Liman in cancer research not only offers opportunities for innovative, locally-based, and affordable cancer therapies but also facilitates the integration of traditional knowledge and modern predictive technology within a sustainable pharmaceutical development system.

### **Scabertopin**

Scabertopin is a compound classified as a sesquiterpene lactone, which is naturally found in the plant *Elephantopus scaber* L., commonly known in Indonesia as Tapak Liman. This compound is one of the main chemical constituents that contributes to various biological activities of the plant. The chemical structure of Scabertopin is complex and characteristic of sesquiterpene lactones. It has a basic

framework of 15 carbon atoms (C<sub>15</sub>), featuring a lactone group and several double bonds, which are believed to play a role in its biological activity. In various studies, Scabertopin has been reported to possess potential pharmacological activities, including cytotoxic, anti-inflammatory, and antitumor effects. However, its specific antileukemic activity has yet to be thoroughly explained, making it an intriguing focus for further in silico exploration.

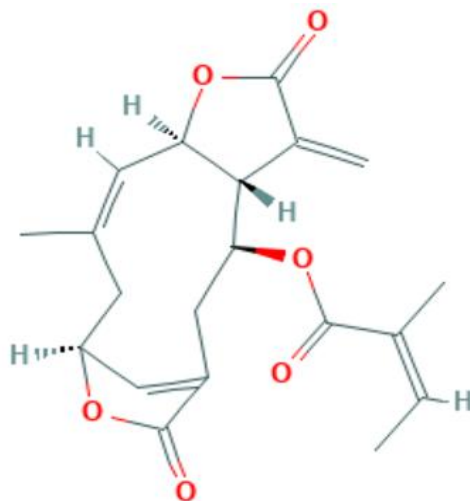


Figure 3. Chemical Structure Depiction

Previous research has indicated that sesquiterpene lactones, such as Scabertopin, can induce apoptosis in cancer cells through several mechanisms. These mechanisms include disruption of cell signaling transduction, inhibition of NF- $\kappa$ B activity, and an increase in intracellular reactive oxygen species (ROS). In the context of blood cancer such as leukemia, compounds that can trigger apoptosis with high selectivity are key candidates for development as chemotherapy agents. The electrophilic nature of the  $\alpha$ -methylene- $\gamma$ -lactone group in Scabertopin allows for interaction with the sulfhydryl groups of target proteins in cancer cells, ultimately leading to protein dysfunction and cell death. This provides a strong theoretical basis that Scabertopin has the potential to be developed as an anti-leukemia agent, both directly and as a lead compound for further structural modifications.

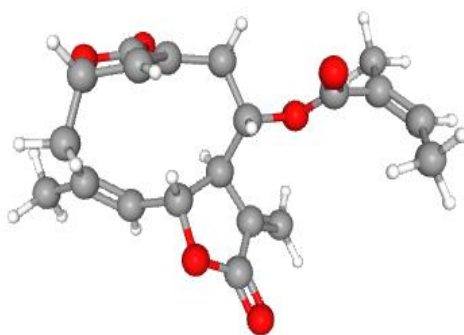


Figure 4. Interactive Chemical Structure Model

In the plant *Elephantopus scaber*, Scabertopin is typically found alongside other sesquiterpene lactones such as Elephantopin and Isoelephantopin. These three compounds often demonstrate synergistic pharmacological effects. The extraction of Scabertopin from the aerial parts of the plant is typically carried out using organic solvents such as chloroform or ethyl acetate. This is done after the processes of maceration or Soxhlet extraction, followed by purification through chromatography. However, in the context of in silico predictions, the structural data of the molecule Scabertopin can be obtained directly from databases such as PubChem, where it is available in SMILES (Simplified Molecular Input Line Entry

System) format. This format facilitates further analysis using bioactivity prediction software such as Way2Drug, PASS Online, or SwissTargetPrediction.

The potential of Scabertopin as an antileukemic agent requires further investigation using pharmacological predictive approaches, including in silico analysis to ascertain its possible molecular mechanisms of action. In a study using PASS Online, for instance, predictions can be made regarding the potential activities as an antineoplastic agent, a pro-apoptotic agent, and activities against relevant enzymes or receptors involved in the process of leukemogenesis. If a strong affinity is found towards those targets, Scabertopin should be explored further in in vitro and in vivo tests, and it may even serve as an initial candidate in the development of new drugs for leukemia.

Table 1. Computed Descriptors of Scabertopin

Parameter	Keterangan
IUPAC Name	[(3S,4R,8R,9Z,12S)-10-methyl-5-methylidene-6,14-dioxo-7,13-dioxatricyclo[10.2.1.0 <sup>4,8</sup> ]pentadeca-1(15),9-dien-3-yl] (Z)-2-methylbut-2-enoate
InChI	InChI=1S/C20H22O6/c1-5-11(3)18(21)25-16-9-13-8-14(24-20(13)23)6-10(2)7-15-17(16)12(4)19(22)26-15/h5,7-8,14H,1,6,9H2,2-4H3,(H,22,26)/b11-5-,10-7-
Molecular Formula	C <sub>20</sub> H <sub>22</sub> O <sub>6</sub>
Molecular Weight	358.385 g/mol
Canonical SMILES	C(=C)\C(=O)O[C@@H]1CC2=CC(=O)OC3C2CC[C@@H]1C(=C)C
PubChem CID	<a href="https://pubchem.ncbi.nlm.nih.gov/compound/442439">442439</a>
Compound Class	Sesquiterpene lactone ester
Source	<i>Elephantopus scaber</i> L. (Tapak Liman)

Interestingly, *Elephantopus scaber*, as a source of Scabertopin, has also been traditionally utilized to treat ailments associated with "internal heat" and blood disorders, which in traditional terminology are sometimes interpreted as forms of systemic issues, including infections and even diseases such as cancer. This provides a solid ethnopharmacological foundation indicating that this plant has indeed been used for generations in the context of treating serious illnesses, and it is highly probable that active constituents such as Scabertopin contribute to these effects. With advancements in computer technology within modern pharmacy, we can now explore the potential of these compounds further through bioinformatics and cheminformatics approaches to evaluate their pharmacological effects more rapidly, affordably, and efficiently.

Furthermore, because Scabertopin has a sesquiterpene lactone framework, this compound can also be examined from the perspective of structure-activity relationship (SAR), where the effect of functional groups on the affinity for cancer targets can be mapped out. Its known cytotoxic activity against several cancer cell lines offers hope that Scabertopin may have a similar effect on leukemia cells such as HL-60, K562, or Jurkat. In in silico research, this can be analyzed regarding its potential interactions with key enzymes such as tyrosine kinase (for example, BCR-ABL), topoisomerase, and caspase, which are involved in the apoptosis process.

#### Scabertopin from Tapak Liman (*Elephantopus scaber*) for Antileukemic

Scabertopin is one of the primary active compounds that has been successfully isolated from *Elephantopus scaber* L., an herbal plant that has long been utilized in various ethnic medicinal systems, which include Ayurveda, traditional Chinese medicine, and the traditional healing practices of Indonesia and Malaysia. Tapak Liman, recognized for its anti-inflammatory and antipyretic properties, also possesses potential as an anti-cancer agent, particularly against leukemia, due to the identification of bioactive compounds such as Scabertopin. This compound belongs to the class of sesquiterpene lactones, which are recognized for their cytotoxic activity and apoptosis-inducing effects on various

cancer cells. This occurs through the mechanism of interaction with biological targets within molecular pathways that are pertinent to the proliferation and survival of cancer cells.

Scabertopin has a complex and distinctive chemical structure, featuring conjugated lactone groups that are believed to play a crucial role in its anti-cancer activity. The lactone group can function as a mild alkylating agent, capable of binding to nucleophilic groups such as cysteine residues on target proteins within cancer cell signaling pathways. This allows Scabertopin to intervene in anti-apoptotic gene expression, accelerate DNA fragmentation events, and inhibit the cell cycle at specific phases, thereby directing leukemia cells toward programmed cell death (apoptosis).

Table 2. Prediction of Scabertopin Biological Activity

Parameter	Value	Predicted Activity
Pa (Probability "Active")	0.822	Antileukemic
Pi (Probability "Inactive")	0.004	Antileukemic

In this study, an in silico approach is utilized to assess the potential anti-leukemia activity of Scabertopin, employing the Prediction of Activity Spectra for Substances (PASS) platform, which is accessible online at <https://www.way2drug.com/>. The compounds are tested based on their SMILES structure (Simplified Molecular Input Line Entry System) obtained from the PubChem database. From the analysis results, the predicted value for antileukemic activity shows a Pa (probability of activity) of 0.822 and a Pi (probability of inactivity) of 0.004. A Pa value exceeding the general threshold of 0.5, along with a very low Pi value, indicates a strong belief that Scabertopin possesses biological activity against leukemia.

The prediction of Pa at 0.822 indicates that, in theory, there is more than an 82% chance that Scabertopin will exhibit antileukemic activity in actual experimental testing. Additionally, the value of Pi, which is only 0.004, emphasizes that the likelihood of this compound being active against leukemia is very low. The combination of these two parameters makes Scabertopin a highly promising candidate for further investigation through both in vitro and in vivo testing. Not only that, this in silico approach also offers a more efficient direction in natural product-based research, as it allows for the rational screening of compound candidates prior to advancing to more complex and costly laboratory testing phases.

Previous studies on sesquiterpene lactones from the Asteraceae family have indicated that compounds such as parthenolide, costunolide, and alantolactone can induce apoptosis in human leukemia cells through mechanisms that inhibit the NF- $\kappa$ B pathway, increase reactive oxygen species (ROS), and activate caspase-3. Scabertopin, having a pharmacophore-like structure, possesses the potential to exhibit similar pharmacodynamic effects. The presence of the  $\alpha$ -methylene- $\gamma$ -lactone system, which is also found in Scabertopin, is believed to be crucial for the binding of the compound to the target protein through a Michael addition reaction. The reactivity of that group can be utilized to inhibit the activity of important enzymes or transcription factors necessary for the proliferation of leukemia cells.

In the context of drug development, predictive information of this nature is highly valuable as it can expedite the initial identification process of candidate compounds, particularly from natural sources that are abundant in bioactive secondary metabolites. Given the growing demand for new antileukemia agents that are more selective and less toxic to normal cells, natural product-based approaches like Scabertopin present significant opportunities for further exploration. Further studies using molecular modeling, docking, molecular dynamics simulation, and biological validation will be crucial next steps in strengthening the hypothesis that Scabertopin could be developed as an alternative or adjuvant chemotherapeutic agent for leukemia.

#### 4. Conclusion

The in silico prediction of Scabertopin, a sesquiterpene lactone compound isolated from *Elephantopus scaber*, demonstrates promising antileukemic potential. Based on the computational analysis using the Way2Drug PASS platform, Scabertopin showed a high probability of biological activity (Pa = 0.822) and a

very low probability of inactivity ( $P_i = 0.004$ ) against leukemic targets. These findings suggest that Scabertopin may possess strong pharmacological relevance as a natural antileukemic agent. The results support further in vitro and in vivo investigation to validate its cytotoxic effect and molecular mechanism, potentially contributing to the development of novel plant-based leukemia therapies.

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