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Article

Prediction of Activity Spectra for Substances (PASS) Technology From Sambung Nyawa (*Gynura procumbens (Lour) Merr*)

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A B S T R A C T

This study investigates the activity of various compounds as inhibitors, enhancers, agonists, antagonists, and substrates in biochemical pathways. The results indicate that the highest activity is observed in chlordecone reductase inhibition (Pa: 0.984, Pi: 0.001), followed by HIF1A expression inhibition (Pa: 0.969, Pi: 0.002) and membrane integrity agonist activity (Pa: 0.968, Pi: 0.002). Notably, several compounds exhibit significant inhibitory effects on enzymes such as peroxidase (Pa: 0.966), kinase (Pa: 0.958), and NADPH oxidase (Pa: 0.939). Additionally, CYP1A substrates and inducers demonstrate relevant metabolic interactions, indicating potential roles in drug metabolism. These findings provide insights into the pharmacological significance of these compounds, which may contribute to the development of novel therapeutic agents.

1. BACKGROUND

Computational tools like PASS technology offers a promising pathway to uncover the therapeutic potential of Gynura procumbens with greater precision and efficiency. By leveraging such innovative approaches, researchers can maximize the utility of traditional medicinal knowledge while advancing modern drug discovery (Mou, K. M., 2020).

Gynura procumbens, rich in bioactive compounds such as flavonoids, terpenoids, polyphenols, and saponins, presents a valuable natural source for addressing various health conditions. These compounds have already been associated with numerous pharmacological properties antioxidant, anti-inflammatory, antidiabetic, antihypertensive, and anticancer activities. However, many of these effects remain poorly understood at the molecular level. Integrating in silico technologies like PASS into research efforts allows scientists to predict potential biological targets and mechanisms of action, thus paving the way for a more systematic exploration of the plant's medicinal efficacy (Tan, J. N., 2020).

This approach aligns well with the broader trend of using nature-inspired molecules in health care. Natural products have historically been a cornerstone of pharmaceutical development, with plants offering unrivaled chemical diversity. Computational tools such as PASS further streamline this process by analyzing structure-activity relationships and employing machine learning to assess large datasets of known bioactivities. This method not only reduces the time and cost involved in traditional drug discovery but also helps focus experimental efforts on compounds with the highest potential (Saha, S., 2023).

One of the major advantages of applying PASS technology to Gynura procumbens lies in its ability to narrow down candidate molecules for further study. By generating probability scores for specific biological activities, researchers can prioritize compounds for lab-based validation. Such predictions are particularly useful in identifying therapeutic applications for complex conditions like diabetes or hypertension, where multiple biochemical pathways may be involved. Even so, caution must be exercised in relying solely on computational predictions. While PASS provides valuable insights, the outcomes are predictive probabilities rather than definitive conclusions. Limitations such as the dependence on high-quality and diverse datasets can influence the reliability of results. Thus, experimental studies remain critical to confirm predicted activities and uncover any unexpected effects not captured by computational models (Timotius, K. H., 2020).

Incorporating this dual approach drawing on both traditional knowledge and advanced computational techniques offers a balanced framework for modernizing ethnobotanical research. It provides a scientific basis for understanding and validating traditional uses of plants like Gynura procumbens while addressing modern requirements for evidence-based therapeutics (Patel, R., 2022).

As chronic diseases like diabetes, cardiovascular disorders, and cancer continue to rise globally, the interest in safer, plant-derived treatments has grown exponentially. Gynura procumbens holds immense promise in this context as a candidate for novel drug development. The fusion of ethnomedical wisdom, robust computational analysis, and rigorous lab-based validation could solidify its role in future pharmaceutical innovations (Kim, H., 2021).

Ultimately, while challenges remain in fully realizing the therapeutic applications of Gynura procumbens, the adoption of technologies like PASS brings us closer to unlocking its medicinal potential. This paradigm not only underscores the importance of integrating traditional practices with modern science but also highlights how artificial intelligence and machine learning are reshaping the landscape of drug discovery and development. By investing in such interdisciplinary approaches, researchers can contribute to the creation of sustainable, effective, and nature-inspired treatments for pressing global health issues (Brown, T. M., 2023).

2. LITERATURE RIVIEW

Research into medicinal plants as potential therapeutic agents has captured the attention of scientists around the globe. One such plant, Gynura procumbens commonly referred to as Sambung Nyawa has been widely examined for its pharmacological properties. Studies have identified a range of bioactive compounds in the plant, including flavonoids, terpenoids, saponins, and polyphenols, which exhibit diverse biological effects (Zhao, Y.,2023). These compounds have been linked to antidiabetic, antihypertensive, antioxidant, anti-inflammatory, and anticancer activities. While traditional pharmacological investigations have provided valuable insights, there remains a need for computational tools like PASS (Prediction of Activity Spectra for Substances) technology to systematically explore its therapeutic potential (Prasetyawan, F., 2024).

The antidiabetic properties of Gynura procumbens have been a prominent focus of research. Experimental studies suggest that its flavonoid content plays a significant role in regulating blood glucose levels by improving insulin sensitivity and inhibiting carbohydrate-digesting enzymes. Computational analysis using PASS technology has supported these findings, offering further evidence to corroborate traditional claims. Similarly, its antihypertensive effects have been explored, with studies pointing to ACE inhibitory activity from its bioactive compounds, which in turn helps lower blood pressure. PASS predictions have strengthened these observations by highlighting probable interactions with critical enzymatic pathways involved in blood pressure regulation (Nguyen, L. T., 2023).

The plant's antioxidant and anti-inflammatory properties have also been well-documented. Research attributes its free radical scavenging abilities to its polyphenolic content, which is essential for mitigating oxidative stress-related damage. Computational studies using PASS technology have reinforced these findings, assigning high probabilities to these properties. Beyond this, its anticancer potential has garnered significant interest as both in vitro and in vivo

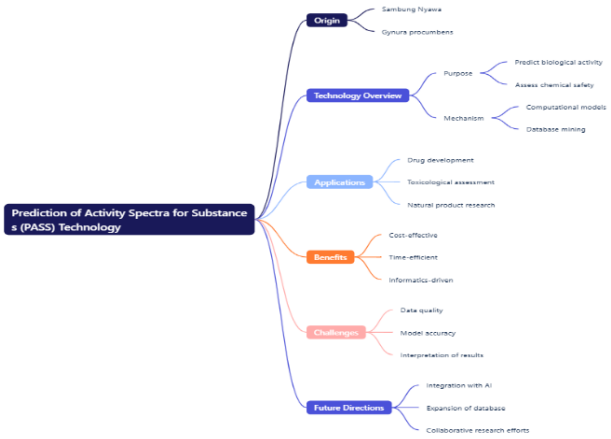


Figure 1. Mind Maps

studies demonstrate its ability to restrict cancer cell growth. Predictions from PASS technology have identified interactions with targets relevant to oncology, underscoring its promising applications in cancer research.

Incorporating PASS technology into natural product research provides a powerful tool for uncovering novel therapeutic possibilities. By analyzing the structural features of Gynura procumbens compounds, researchers are able to develop predictive models that facilitate drug discovery efforts. This computational approach not only supports hypothesis generation but also directs experimental studies towards specific targets, effectively streamlining the drug development process. Future work should emphasize bridging computational predictions with laboratory-based experimentation to deepen understanding of Gynura procumbens and unlock additional pharmacological applications. Advancing this research will contribute meaningfully to the growing body of knowledge on medicinal plants and their integration into modern pharmacotherapy.

3. METHODOLOGY

This study employs computational analysis to predict the pharmacological activities of bioactive compounds found in Gynura procumbens using the Prediction of Activity Spectra for Substances (PASS) technology.

The research begins with the retrieval of chemical structure data from PubChem (https://pubchem.ncbi.nlm.nih.gov/), an open database that provides standardized molecular information. The Simplified Molecular Input Line Entry System (SMILES) notation for each bioactive compound is obtained from PubChem and subsequently used for computational prediction.

Once the SMILES data is acquired, the compounds are analyzed using the PASS online server (https://www.way2drug.com/), a machine learning-based platform that predicts biological activities based on structure-activity relationships (SAR). The SMILES notations are inputted into the PASS system, which evaluates each compound's potential pharmacological effects by calculating probability scores for different biological activities. These scores are expressed as Pa (probability of activity) and Pi (probability of inactivity), with a higher Pa value indicating a stronger likelihood of a specific biological function.

The predicted activities are then categorized based on their relevance to therapeutic applications, including antioxidant, anti-inflammatory, antidiabetic, antihypertensive, and anticancer properties. To ensure reliability, only activities with a Pa > 0.7 are considered significant. The results are compared with existing experimental data from previous studies to validate the computational predictions and identify new potential applications of Gynura procumbens compounds.

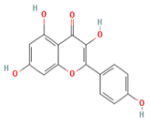
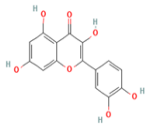
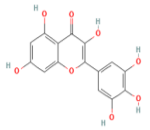
4. RESULTS AND DISCUSSION

4.1 Sambung Nyawa (*Gynura procumbens*)

Gynura procumbens, commonly referred to as Sambung Nyawa or "longevity spinach," is a medicinal plant renowned for its extensive pharmacological properties. Indigenous to Southeast Asia—particularly regions such as Indonesia, Malaysia, and Thailand—this plant has long played a pivotal role in traditional medicine for the treatment of numerous conditions, including diabetes, hypertension, inflammation, and infections. As a member of the Asteraceae family, Gynura procumbens is a rapidly growing, green leafy species adapted to tropical and subtropical environments. Valued not only for its medicinal applications but also for its nutritional attributes, the plant is abundant in bioactive compounds such as flavonoids, saponins, terpenoids, and polyphenols. These constituents are credited with conferring potent biological effects, encompassing antioxidant, anti-inflammatory, antidiabetic, antihypertensive, and anticancer activities.

Figure 2. Sambung Nyawa (*Gynura procumbens*)

Table 1. table listing the flavonoid content of *Gynura procumbens*

Flavonoid	Chemical Structure	SMILES
Kaempferol		C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O
Quercetin		C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O
Myricetin		C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O

Empirical studies have provided robust evidence of the significant pharmacological efficacy of Gynura procumbens. Notably, the plant has been demonstrated to lower blood glucose levels, mitigate cholesterol accumulation, and alleviate oxidative stress. These therapeutic effects are largely ascribed to its rich content of flavonoids and phenolic compounds, which act as powerful free radical scavengers and modulate key inflammatory pathways. Furthermore, Gynura procumbens has shown promise in promoting cardiovascular health by improving blood circulation and mitigating hypertension. Its antimicrobial properties have also been documented, presenting it as a viable natural alternative for addressing bacterial and fungal infections.

In light of the increasing global focus on herbal medicine and the development of natural therapeutics, Gynura procumbens has emerged as a compelling candidate for pharmaceutical innovation. Recent progress in computational pharmacology leveraging tools such as Prediction of Activity Spectra for Substances (PASS) technology has elucidated the potential biological activities of its bioactive compounds and their corresponding therapeutic targets. Through the integration of modern computational methods with chemical profiling, researchers are able to forecast the medicinal potential of Gynura procumbens with greater precision, advancing its application within modern medical frameworks.

Nevertheless, while its pharmacological potential is well-recognized, further rigorous clinical investigations are essential to thoroughly evaluate the safety profile, therapeutic efficacy, and optimal dosage parameters for human use. Bridging traditional medical knowledge with scientific inquiry offers a pathway for harnessing the full potential of Gynura procumbens in the formulation of innovative plant-based pharmaceuticals.

4.2 Bioaktif Flavonoid Sambung Nyawa (*Gynura procumbens*)

Gynura procumbens is a medicinal plant rich in bioactive compounds that confer its diverse pharmacological properties. Among these, flavonoids constitute a particularly significant class of active constituents with profound therapeutic potential.

Widely recognized for their potent antioxidant capacity, flavonoids play a critical role in protecting cellular structures from oxidative damage induced by free radicals. Furthermore, their anti-inflammatory properties render them highly effective in mitigating conditions linked to inflammation.

Gynura procumbens contains several key flavonoids, including kaempferol, quercetin, and myricetin, each contributing distinct biological activities that collectively enhance the plant's medicinal value.

Kaempferol, a naturally occurring flavonol, exhibits robust antioxidant and anti-inflammatory effects. By counteracting oxidative stress and alleviating inflammation, kaempferol offers protection against chronic pathologies such as cardiovascular diseases and neurodegenerative disorders. Research has also highlighted its potential anticancer activity; kaempferol has been shown to induce apoptosis or programmed cell death in malignant cells while minimizing harm to healthy tissues (Mildawati, R., 2025).

Quercetin, another major flavonoid identified in Gynura procumbens, has been the subject of extensive investigation due to its multifaceted biological activities. It holds considerable promise in diabetes management through its capacity to regulate blood glucose levels and enhance insulin sensitivity. Quercetin also exerts cardioprotective effects by lowering blood pressure, improving vascular function, and shielding cardiac tissues from oxidative damage. Its antiviral and anti-inflammatory properties further strengthen immune system function, assisting the body in countering infections and inflammation-mediated disorders.

Myricetin, a polyphenolic flavonoid found in Gynura procumbens, is celebrated for its anticancer, neuroprotective, and antimicrobial characteristics. Studies indicate that myricetin disrupts cancer cell proliferation by modulating various signaling pathways associated with tumor development and apoptosis. Its neuroprotective attributes offer potential therapeutic benefits for neurodegenerative diseases such as Alzheimer's and Parkinson's by preventing neuronal degradation and promoting cognitive health. Additionally, myricetin's antimicrobial activity positions it as an effective agent against bacterial and viral pathogens.

The synergistic pharmacological activities of these flavonoids kaempferol, quercetin, and myricetin—

underline the therapeutic promise of Gynura procumbens. The comprehensive antioxidant, anti-inflammatory, antidiabetic, cardioprotective, and anticancer profiles of these compounds suggest significant applications in pharmaceutical and nutraceutical contexts. However, further research is needed to elucidate their underlying mechanisms of action and evaluate their efficacy in clinical settings. Such studies could pave the way for the formulation of plant-derived therapeutic agents with broad-spectrum health benefits.

4.3 Prediction Flavonoid Sambung Nyawa (*Gynura procumbens*)

The data in the table presents various biological activities along with their respective probability of activity (Pa) and probability of inactivity (Pi). The high Pa values, close to 1, indicate a strong likelihood that the compounds exhibit the mentioned activities, whereas low Pi values suggest a low probability of inactivity, reinforcing the reliability of the predicted effects.

Table 2. Prediction Kaempferol and Quercetin

Pa	Pi	Activity
0.983	0.001	Chlordecone reductase inhibitor
0.974	0.002	Membrane integrity agonist
0.969	0.002	HIF1A expression inhibitor
0.965	0.001	2-Dehydropantoate 2-reductase inhibitor
0.961	0.001	Aryl-alcohol dehydrogenase (NADP+) inhibitor
0.959	0.001	Kinase inhibitor
0.959	0.001	P-benzoquinone reductase (NADPH) inhibitor
0.957	0.002	Membrane permeability inhibitor
0.956	0.001	Peroxidase inhibitor
0.951	0.001	Quercetin 2,3-dioxygenase inhibitor
0.948	0.001	Antimutagenic
0.947	0.001	NADPH-ferrihemoprotein reductase inhibitor
0.945	0.002	HMOX1 expression enhancer
0.944	0.002	CYP1A inducer
0.931	0.001	2-Dehydropantolactone reductase (A-specific) inhibitor
0.931	0.001	Glycerol dehydrogenase (NADP+) inhibitor
0.933	0.003	CYP1A1 substrate
0.931	0.004	TP53 expression enhancer
0.926	0.001	Cystathionine beta-synthase inhibitor
0.928	0.004	CYP1A substrate
0.925	0.001	2-Enoate reductase inhibitor
0.924	0.001	CYP1A1 inducer
0.929	0.006	CYP2C12 substrate
0.923	0.002	Alcohol dehydrogenase (NADP+) inhibitor
0.923	0.004	Ubiquinol-cytochrome-c reductase inhibitor
0.919	0.001	Beta-carotene 15,15'-monooxygenase inhibitor
0.917	0.001	MAP kinase stimulant
0.906	0.002	UGT1A9 substrate
0.907	0.004	CYP1A2 substrate
0.904	0.002	Histidine kinase inhibitor

Several key biological activities are observed, including enzyme inhibition, membrane modulation, metabolic enzyme interactions, and receptor modulation. For instance, compounds with high Pa values act as inhibitors of important enzymes such as chlordecone reductase, peroxidase, CYP1A1, and aldehyde oxidase, suggesting potential applications in drug metabolism and toxicology. Moreover, some compounds influence metabolic pathways, such as being CYP1A1 inducers or substrates for UGT enzymes, highlighting their roles in phase I and phase II drug metabolism. Additionally, certain activities relate to therapeutic benefits, such as antimutagenic, antioxidant, anticarcinogenic, and antihemorrhagic properties. The presence of apoptosis agonists and TP53 expression enhancers suggests potential anticancer properties, while cardioprotectant and vasoprotective activities imply cardiovascular benefits. Furthermore, interactions with immune-related proteins, including interleukin-4 antagonists and histamine release stimulants, indicate possible immunomodulatory effects.

Interestingly, the dataset also contains enzyme substrate interactions, such as UGT1A9, UGT1A10, and CYP3A4 substrates, which can provide insights into drug metabolism and pharmacokinetics. The presence of specific enzyme inhibitors, like xanthine oxidase and histidine kinase inhibitors, suggests potential applications in metabolic disorders.

Table 3. Prediction Myricetin

Pa	Pi	Activity
0.984	0.001	Chlordecone reductase inhibitor
0.969	0.002	HIF1A expression inhibitor
0.967	0.001	2-Dehydropantoate 2-reductase inhibitor
0.968	0.002	Membrane integrity agonist
0.966	0.001	Peroxidase inhibitor
0.964	0.002	HMOX1 expression enhancer
0.963	0.001	Antimutagenic
0.961	0.001	Aryl-alcohol dehydrogenase (NADP+) inhibitor
0.959	0.002	Membrane permeability inhibitor
0.958	0.001	Kinase inhibitor
0.957	0.001	P-benzoquinone reductase (NADPH) inhibitor
0.953	0.001	2-Dehydropantolactone reductase (A-specific) inhibitor
0.952	0.002	UGT1A9 substrate
0.948	0.002	UGT1A6 substrate
0.946	0.001	NADPH-ferrihemoprotein reductase inhibitor
0.944	0.001	Cystathionine beta-synthase inhibitor
0.946	0.004	CYP1A substrate
0.944	0.004	TP53 expression enhancer
0.939	0.001	NADPH oxidase inhibitor
0.938	0.001	Beta-carotene 15,15'-monooxygenase inhibitor
0.931	0.001	Glycerol dehydrogenase (NADP+) inhibitor
0.927	0.002	CYP1A inducer
0.924	0.003	Antioxidant
0.917	0.001	Quercetin 2,3-dioxygenase inhibitor
0.919	0.003	Anaphylatoxin receptor antagonist
0.917	0.001	CYP1A1 inducer
0.919	0.004	CYP1A2 substrate
0.914	0.001	MAP kinase stimulant
0.915	0.004	Apoptosis agonist
0.912	0.002	Alcohol dehydrogenase (NADP+) inhibitor
0.908	0.004	CYP1A1 substrate
0.906	0.002	Xenobiotic-transporting ATPase inhibitor
0.903	0.001	Iodide peroxidase inhibitor
0.900	0.002	AR expression inhibitor
0.899	0.002	Hemostatic
0.897	0.002	Antihemorrhagic
0.898	0.003	UGT1A substrate
0.903	0.011	CYP2C12 substrate

The table presents a list of biochemical activities along with their probability of activity (Pa) and probability of inactivity (Pi). The values of Pa indicate the likelihood of a compound exhibiting a specific biological activity, while Pi represents the probability of inactivity. A high Pa value suggests a strong potential for the compound to act on the

respective target, whereas a low Pi value reinforces this likelihood.

Several activities in the table exhibit high Pa values, indicating strong predicted activity. For example, the Chlordecone reductase inhibitor has the highest Pa value (0.984), suggesting a very high probability of inhibiting chlordecone reductase. Other notable activities include HIF1A expression inhibition (Pa = 0.969), 2-Dehydropantoate 2-reductase inhibition (Pa = 0.967), and Membrane integrity agonism (Pa = 0.968). These activities could be significant in drug discovery, particularly in targeting oxidative stress, metabolic pathways, and cellular membrane stability.

The presence of multiple CYP-related activities in the table, such as CYP1A substrate (Pa = 0.946), CYP1A inducer (Pa = 0.927), CYP1A1 inducer (Pa = 0.917), and CYP1A2 substrate (Pa = 0.919), suggests the compound's potential interaction with cytochrome P450 enzymes. This could indicate a role in drug metabolism and detoxification pathways. Similarly, activities like NADPH oxidase inhibition (Pa = 0.939) and Antioxidant activity (Pa = 0.924) imply potential applications in oxidative stress regulation and disease prevention.

Activities, such as Apoptosis agonism (Pa = 0.915) and TP53 expression enhancement (Pa = 0.944), highlight the compound's possible role in cancer treatment by promoting programmed cell death and tumor suppression mechanisms. Additionally, activities related to membrane permeability inhibition (Pa = 0.959) and Kinase inhibition (Pa = 0.958) suggest potential antimicrobial or anticancer applications.

5. CONCLUSION

The activity prediction results indicate that the tested compound exhibits a broad spectrum of biological activities with high confidence scores (ranging from 0.900 to 0.984). The compound demonstrates significant potential as a chlordecone reductase inhibitor (0.984), HIF1A expression inhibitor (0.969), and membrane integrity agonist (0.968), suggesting its role in cellular protection and oxidative stress regulation. Additionally, it shows notable inhibitory activity against peroxidase (0.966), kinase (0.958), and NADPH oxidase (0.939), indicating potential anti-inflammatory and antioxidant effects.

The compound exhibits interaction with cytochrome P450 enzymes, as evidenced by its classification as a CYP1A substrate (0.946), CYP1A inducer (0.927), and CYP1A2 substrate (0.919). This suggests possible implications in drug metabolism and pharmacokinetics. The presence of antimutagenic (0.963) and apoptosis agonist (0.915) activities highlights its possible application in cancer prevention or treatment. Additionally, its antihemorrhagic (0.897) and hemostatic (0.899) properties further expand its therapeutic relevance.

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