

Myrosmine

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summary

Myrosmine is a naturally occurring alkaloid primarily found in tobacco plants, recognized for its complex chemical properties and significant biological activities. With the chemical formula $C_9H_{10}N_2$, myrosmine exhibits a molar mass of 162.19 g·mol⁻¹ and has a melting point of 130 °C (266 °F), which indicates its stability under typical environmental conditions.[\[1\]\[2\]](#) As a plant metabolite, it plays a crucial role in tobacco's biochemical processes and has garnered attention for its potential pharmacological applications, particularly in formulations involving nicotine delivery systems.[\[2\]\[3\]](#) However, its genotoxic effects raise concerns regarding human health, particularly in the context of tobacco use and carcinogenesis.[\[4\]\[5\]](#)

The biosynthesis of myrosmine is intricately linked to glucosinolates, compounds produced by plants in the Brassicaceae family. This process involves the enzymatic activity of myrosinases, which hydrolyze glucosinolates into various bioactive compounds, including myrosmine itself.[\[6\]\[7\]](#) Such transformations are vital for the plant's defense mechanisms against herbivores and pathogens, illustrating the ecological significance of myrosmine in plant interactions with their environment.[\[6\]\[8\]](#) The regulation of its biosynthesis is influenced by a range of genetic and environmental factors, leading to variations among different plant species and their ability to produce myrosmine in response to stressors.[\[8\]\[9\]](#)

In terms of biological activities, myrosmine is noted for its dual role as both a genotoxic agent and a potential inhibitor of aromatase, which could contribute to its anti-carcinogenic properties.[\[10\]\[11\]](#) Additionally, its influence on neurotransmitter levels suggests implications for treating neurological disorders, positioning myrosmine at the intersection of toxicology and pharmacology.[\[12\]\[13\]](#) The diverse roles that myrosmine plays in plant defense, pest management, and its interactions with other phytochemicals underscore its importance in sustainable agricultural practices.[\[14\]\[15\]](#) Nevertheless, the compound's potential toxicity and persistence in the environment warrant careful scrutiny to balance its agricultural benefits with the health risks it may pose to humans and ecosystems.[\[16\]\[17\]\[18\]](#)

Chemical Properties

Myrosmine, with the chemical formula $C_9H_{10}N_2$, exhibits several notable chemical properties. It has a molar mass of 162.19 g·mol⁻¹ and appears as a white solid under standard conditions[\[1\]](#). Its melting point is recorded at 130 °C (266 °F; 403 K), indicating its stability as a solid at room temperature[\[1\]](#).

The compound is categorized as an alkaloid and is predominantly found in tobacco plants, where it plays a role as a plant metabolite[\[10\]](#). Myrosmine is recognized for its genotoxic effects and has been studied for its potential applications in pharmacology, particularly in formulations for transdermal patches and inhalation devices that contain nicotine[\[2\]](#).

The properties of myrosmine, like those of other organic compounds, are largely dependent on its functional groups. Understanding the functional groups present is crucial for predicting the reactivity and behavior of the compound in various chemical contexts[\[3\]](#). In the case of myrosmine, its structure allows it to undergo specific

biochemical transformations, which can be leveraged in synthetic routes to produce other important compounds, such as (S)-nicotine[2].

Additionally, the purity and stability of myrosmine are significant factors in its application, as high chemical purity is often required for pharmaceutical compositions[2]. The interactions between its molecular structure and the environment, including temperature and pH, can influence its efficacy as an active ingredient in medicinal formulations[19].

Biosynthesis

Overview of Myrosmine Biosynthesis

Myrosmine is derived from glucosinolates, a group of nitrogen-containing natural products predominantly found in the Brassicaceae family. The biosynthesis of myrosmine is closely associated with the enzymatic activity of myrosinases, which catalyze the hydrolysis of glucosinolates, leading to the formation of various breakdown products, including isothiocyanates, thiocyanates, and nitriles[6][7]. This process is crucial for the plant's defense mechanisms against herbivory and pathogens.

Enzymatic Pathways

The biosynthetic pathway for myrosmine begins with the synthesis of glucosinolates from primary metabolites. The pathway involves several key enzymes, notably myrosinases, which hydrolyze glucosinolates into bioactive compounds when plant tissues are damaged. This hydrolysis results in the production of myrosmine and other toxic compounds, serving as a deterrent to herbivores and pathogens[6][9].

Regulation of Biosynthesis

The regulation of myrosmine biosynthesis is complex and can vary significantly among different plant species. Factors influencing the production of glucosinolates and their subsequent hydrolysis include genetic, environmental, and developmental cues[8][9]. For example, individual Brassicaceae species may produce varying mixtures of glucosinolates, which can affect the efficacy of myrosinase activity and, consequently, the levels of myrosmine produced. Some plants may adapt to herbivory by modifying their glucosinolate profiles, thereby altering the biosynthesis of myrosmine and its related compounds[6][8].

Ecological Implications

The biosynthesis of myrosmine plays an essential role in plant ecology, particularly in the context of herbivore interactions. The production of toxic isothiocyanates, resulting from the hydrolysis of glucosinolates, can significantly deter herbivores, making myrosmine a critical component of the plant's defense strategy. However, some herbivores have developed counter-adaptations to overcome these defenses,

such as the rapid breakdown of glucosinolates into less harmful compounds, which highlights the evolutionary arms race between plants and herbivores[\[6\]\[7\]](#).

Biological Activities

Myrosmine, an alkaloid found primarily in tobacco plants, exhibits a range of biological activities that have drawn significant interest in both toxicology and pharmacology. It has been identified as a potent genotoxic agent, with studies indicating that it expresses significant genotoxic effects in human target cells, potentially influencing carcinogenic processes[\[4\]\[10\]](#). This raises concerns regarding its presence in tobacco and the implications for human health, particularly in relation to cancer development[\[5\]\[20\]](#).

In addition to its genotoxic properties, myrosmine is noted for its role as a plant metabolite and an inhibitor of aromatase, which is involved in estrogen biosynthesis. This inhibition may contribute to its potential anti-carcinogenic properties, as it could interfere with hormone-related cancers[\[10\]\[11\]](#). Furthermore, myrosmine's activities extend to modulation of neurotransmitter levels, as some research has suggested its impact on dopamine and norepinephrine levels, which are critical in the treatment of certain neurological disorders[\[12\]\[13\]](#).

The diverse biological activities of myrosmine are further complemented by its interactions with various phytochemicals in plants. These secondary metabolites, including glucosinolates, have been linked to protective effects against pests and pathogens, suggesting that compounds like myrosmine may play a role in enhancing plant defense mechanisms against herbivores and pathogens[\[21\]\[22\]\[23\]](#). As the understanding of these interactions grows, myrosmine and related compounds may reveal new avenues for therapeutic applications, especially in addressing antimicrobial resistance and developing novel anticancer strategies[\[19\]\[24\]\[25\]](#).

Applications

Sustainable Agriculture

Myrosmine, a compound derived from certain plant sources, plays a significant role in sustainable agricultural practices. It is increasingly recognized for its potential in enhancing soil health and nutrient availability. Farmers employ various management strategies, such as crop rotation and intercropping, to optimize the benefits of myrosmine in agricultural systems. These practices have been shown to positively influence the abundance and functioning of arbuscular mycorrhizal fungi (AMF) in the soil, which are crucial for nutrient cycling and plant health[\[26\]](#). For instance, the use of crop rotation can lead to increased AMF spore density and root colonization in crops like maize, subsequently improving yields in following crops such as wheat, particularly when the preceding crops are legumes like soybean or chickpea[\[26\]](#).

Pest Management

In addition to its agronomic benefits, myrosmine is being explored for its applications in pest management. The compound can contribute to developing insect-resistant crop varieties, thereby reducing the reliance on synthetic pesticides. Host plant resistance, facilitated by myrosmine, plays a crucial role in integrated pest management (IPM) strategies, making crops less susceptible to pest damage through heritable traits that confer resistance[\[14\]\[27\]](#). These traits can manifest in various forms, including antibiosis, where the pest's biology is negatively affected, and antixenosis, which discourages pest feeding through non-preference[\[14\]](#). Furthermore, modern biotechnology techniques, such as RNA interference (RNAi) and CRISPR, can be utilized to enhance plant resistance against pests by targeting specific genes related to insect susceptibility[\[14\]\[28\]](#).

Soil Health Management Systems

The application of myrosmine is also linked to the implementation of Soil Health Management Systems, which aim to improve the overall condition of agricultural soils. By incorporating myrosmine-producing cover crops into rotation systems, farmers can enhance soil organic matter, improve microbial activity, and ultimately promote healthier and more resilient cropping systems[\[15\]](#). Such practices contribute to various environmental benefits, including increased carbon sequestration and reduced soil erosion, thereby aligning with broader sustainability goals in agriculture[\[15\]](#). Cover crops, which are often rich in myrosmine, serve not only to protect the soil but also to support beneficial soil organisms, further enhancing soil fertility and plant growth[\[15\]](#).

Biotechnology Innovations

Advancements in biotechnology are also paving the way for new applications of myrosmine. Research continues to explore its potential as a natural pesticide and its effectiveness in improving the nutritional quality of crops. These innovations could lead to the development of crop varieties with enhanced resistance to pests and diseases, which is particularly beneficial for resource-poor smallholder farmers in developing nations[\[29\]\[30\]](#). The combination of myrosmine's natural properties with biotechnological tools holds promise for achieving higher agricultural productivity while minimizing environmental impacts[\[30\]](#).

Toxicology

Effects on Human Health

Myrosmine and its derivatives, such as aflatoxins, pose significant health risks to humans when ingested, inhaled, or absorbed through the skin. Aflatoxins are known for their carcinogenic, hepatotoxic, teratogenic, and mutagenic properties, leading to severe health conditions including immune deficiency and cancer over long-term exposure. Acute poisoning can result in organ failure and other serious health complications[\[16\]\[31\]](#). Moreover, the effects of mycotoxicosis from contaminated crops

can lead to severe health issues in vertebrates, emphasizing the need for careful monitoring of food safety[\[17\]](#).

Persistence in the Environment

Myrosmine-related toxins exhibit varying persistence in soil ecosystems. For example, the Bt protein is classified as moderately persistent and immobile, indicating it does not leach with groundwater and degrades rapidly under UV radiation, particularly in non-acidic conditions[\[18\]](#). This property is crucial for assessing the long-term environmental impact of myrosmine and related compounds on soil health and groundwater systems. Soil contamination from such toxins can lead to reduced plant growth, toxicity to animals, and increased health risks for humans, highlighting the importance of effective soil management practices[\[28\]](#).

Soil Ecosystem Impact

The presence of myrosmine and its derivatives can disrupt the intricate balance of soil ecosystems, which are vital for nutrient cycling and maintaining biodiversity. Soil microorganisms play essential roles in detoxifying harmful substances and contributing to soil fertility through various ecological processes[\[26\]](#)[\[15\]](#). The negative effects of soil contamination include decreased biodiversity and impaired ecosystem services, which are crucial for agricultural productivity and environmental health[\[32\]](#). Thus, addressing the toxicological implications of myrosmine is critical for both human health and the sustainability of soil ecosystems.

Research

Myrosmine and Agricultural Sustainability

Recent studies have explored the potential of myrosmine in enhancing agricultural sustainability through its role in soil health and pest management. For instance, crop rotation practices that incorporate myrosmine-producing plants, such as those from the Brassica family, have been shown to influence the abundance and functioning of arbuscular mycorrhizal fungi (AMF) in the soil. This relationship is crucial, as increased AMF activity can enhance root colonization and nutrient uptake in crops like maize and wheat, ultimately contributing to higher yields[\[26\]](#). However, caution is advised, as rotating with non-mycorrhizal crops may reduce AMF abundance and the associated symbiotic benefits due to the production of antimicrobial compounds like isothiocyanates[\[26\]](#).

Phytochemical Contributions to Plant Defense

Myrosmine, along with other phytochemicals, plays a significant role in plant defense mechanisms. The metabolic changes associated with myrosmine biosynthesis can lead to the production of direct inhibitors or repellents of insect herbivores. Such changes may also enhance the physical strength of plant cell walls through lignifi-

cation, thus providing additional defense against pest attacks[14]. The integration of beneficial soil microorganisms into crop management may offer a sustainable alternative to chemical pesticides, enhancing plant productivity while inducing systemic resistance against herbivores[14].

Hormonal Interactions

The interaction of myrosmine with plant hormones, such as jasmonic acid and salicylic acid, highlights its importance in coordinating plant responses to biotic stressors. These phytohormones are integral to the signaling pathways activated during plant-microbe and plant-insect interactions, ultimately influencing plant resilience and productivity[14][33]. The modulation of these signaling pathways by myrosmine can lead to enhanced plant defenses and improved interactions with beneficial microbes, further emphasizing its potential in sustainable agricultural practices[21].

Future Research Directions

Further investigation into myrosmine's multifaceted role in agriculture is warranted. Future studies could focus on understanding the complexities of myrosmine interactions within diverse cropping systems, particularly in relation to soil health, plant defense mechanisms, and the ecological impacts of varying crop rotations[26][14]. Establishing a comprehensive framework that integrates these factors could significantly enhance our understanding of myrosmine's potential benefits in sustainable agricultural production.

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