Revista ARACÊ
ISSN: 2358-2472

INTERRELATIONS BETWEEN PLANT COMPOUNDS AND FUNCTIONAL MATERIALS: IMPLICATIONS FOR BIOACTIVITY AND BIOMATERIALS IN VARIOUS FIELDS

INTER-RELAÇÕES ENTRE COMPOSTOS VEGETAIS E MATERIAIS FUNCIONAIS: IMPLICAÇÕES NA BIOATIVIDADE E BIOMATERIAIS NOS DIVERSOS CAMPOS

INTERRELACIONES ENTRE COMPUESTOS VEGETALES Y MATERIALES FUNCIONALES: IMPLICACIONES EN LA BIOACTIVIDAD Y LOS BIOMATERIALES EN DIVERSOS CAMPOS

https://doi.org/10.56238/ arev7n11-001

Submitted on: 06/10/2025 **Publication date:** 06/11/2025

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ABSTRACT

In recent years, the interest in the study of plant compounds has grown due to their bioactive activities and therapeutic applications. These compounds, which include several secondary metabolites, influence biological processes essential to human health and well-being. The relationship between the bioactivity of plant compounds and functional materials is crucial for advances in biomaterial engineering, which mimic the extracellular matrix and promote tissue regeneration. Despite advances in the analysis of these compounds in plant extracts and biomaterials, there is still a gap to be filled: the correlation between the bioactivity of compounds and their functional properties. This integration is vital for developing new therapies, based on an understanding of molecular interactions. This study aims to investigate the relationships between plant compounds and functional materials, assessing their implications for bioactivity and biomaterial engineering. Based on a comprehensive literature review, the research considers extraction methods and the impact of agronomic conditions. Preliminary results suggest a positive correlation between the chemistry of extracts and their bioactive activities, highlighting how agronomic factors and extraction techniques affect metabolites. The study also analyzes several classes of compounds, such as alkaloids and flavonoids, emphasizing their beneficial health applications. Integrating knowledge of plant compounds and functional materials appears promising for new therapeutic strategies. A deep understanding of the relationships between chemical structure, bioactivity, and properties of biomaterials is essential for innovation in regenerative medicine. The study proposes future research that seeks to translate experimental findings into clinical applications, developing bioactive products based on plant extracts and biomaterials. This approach may result in new biomaterials that mimic the extracellular matrix, promoting tissue regeneration. Exploring the interactions between plant compounds and functional materials can drive the development of innovative and effective drugs.

Keywords: Plant compounds. Bioactivity. Functional Materials.

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Revista
ARACÊ
ISSN: 2358-2472

RESUMO
Nos últimos anos, o interesse no estudo de compostos vegetais tem crescido devido às suas atividades bioativas e aplicações terapêuticas. Esses compostos, que incluem diversos metabólitos secundários, influenciam processos biológicos essenciais para a saúde e o bem-estar humano. A relação entre a bioatividade dos compostos vegetais e materiais funcionais é crucial para os avanços na engenharia de biomateriais, que imitam a matriz extracelular e promovem a regeneração tecidual. Apesar dos avanços na análise desses compostos em extratos vegetais e biomateriais, ainda há uma lacuna a ser preenchida: a correlação entre a bioatividade dos compostos e suas propriedades funcionais. Essa integração é vital para desenvolver novas terapias, fundamentando-se em uma compreensão das interações moleculares. Este estudo visa investigar as relações entre compostos vegetais e materiais funcionais, abalizando suas implicações na bioatividade e na engenharia de biomateriais. Baseando-se em uma revisão abrangente da literatura, a pesquisa considera métodos de extração e o impacto de condições agronômicas. Resultados preliminares sugerem uma correlação positiva entre a química dos extratos e suas atividades bioativas, ressaltando como fatores agronômicos e técnicas de extração afetam os metabólitos. O estudo também analisa diversas classes de compostos, como alcaloides e flavonoides, enfatizando suas aplicações benéficas à saúde. Integrar o conhecimento de compostos vegetais e materiais funcionais parece promissor para novas estratégias terapêuticas. Uma compreensão aprofundada das relações entre estrutura química, bioatividade e propriedades dos biomateriais é essencial para inovação na medicina regenerativa. O estudo propõe investigações futuras que busquem traduzir achados experimentais para aplicações clínicas, desenvolvendo produtos bioativos com base em extratos vegetais e biomateriais. Essa abordagem pode resultar em novos biomateriais que imitem a matriz extracelular, promovendo a regeneração tecidual. A exploração das interações entre compostos vegetais e materiais funcionais impulsiona o desenvolvimento de fármacos inovadores e eficazes.

Palavras-chave: Compostos Vegetais. Bioatividade. Materiais Funcionais.

RESUMEN
En los últimos años, el interés por el estudio de los compuestos vegetales ha aumentado debido a sus actividades bioactivas y aplicaciones terapéuticas. Estos compuestos, que incluyen diversos metabolitos secundarios, influyen en procesos biológicos esenciales para la salud y el bienestar humano. La relación entre la bioactividad de los compuestos vegetales y los materiales funcionales es crucial para los avances en la ingeniería de biomateriales, los cuales imitan la matriz extracelular y promueven la regeneración tisular. A pesar de los avances en el análisis de estos compuestos en extractos vegetales y biomateriales, aún existe una brecha por llenar: la correlación entre la bioactividad de los compuestos y sus propiedades funcionales. Esta integración es fundamental para desarrollar nuevas terapias, basadas en una comprensión profunda de las interacciones moleculares. Este estudio tiene como objetivo investigar las relaciones entre los compuestos vegetales y los materiales funcionales, evaluando sus implicaciones en la bioactividad y en la ingeniería de biomateriales. Basado en una revisión exhaustiva de la literatura, la investigación considera los métodos de extracción y el impacto de las condiciones agronómicas. Los resultados preliminares sugieren una correlación positiva entre la química de los extractos y sus actividades bioactivas, destacando cómo los factores agronómicos y las técnicas de extracción afectan los metabolitos. El estudio también analiza diversas clases de compuestos, como alcaloides y flavonoides, enfatizando sus aplicaciones beneficiosas para la salud. Integrar el conocimiento sobre compuestos vegetales y materiales funcionales parece prometedor para el desarrollo de nuevas estrategias terapéuticas. Una comprensión

Revista ARACÊ
ISSN: 2358-2472

más profunda de las relaciones entre la estructura química, la bioactividad y las propiedades de los biomateriales es esencial para la innovación en la medicina regenerativa. El estudio propone futuras investigaciones que busquen traducir los hallazgos experimentales en aplicaciones clínicas, desarrollando productos bioactivos basados en extractos vegetales y biomateriales. Este enfoque puede resultar en nuevos biomateriales que imiten la matriz extracelular y promuevan la regeneración tisular. La exploración de las interacciones entre los compuestos vegetales y los materiales funcionales impulsa el desarrollo de fármacos innovadores y eficaces.

Palabras clave: Compuestos Vegetales. Bioactividad. Materiales Funcionales.

Revista ARACÊ
ISSN: 2358-2472

1 INTRODUCTION

The title "Interrelationships between Plant Compounds and Functional Materials: Implications for Bioactivity and Biomaterials in the various fields" proposes the scientific study that explores the connection between two distinct but complementary components: plant-derived compounds and functional materials. In summary, this title defends the relevance and applicability of these interrelationships in several areas, especially in bioactivity and in the development of biomaterials.

Currently, there is a growing interest in the study of compounds obtained from plant species because of their specific activities, allowing for various applications in humans. Natural active ingredients are directly related to their chemical structure, and the type and quantity of different classes of molecules in plant extracts influence both the bioactivity and the use of these extracts.

Agronomic conditions, processing techniques and extraction methods, including the solvents used, have an impact on the chemical profile of herbal preparations and their pharmacological activities [3]. Therefore, it is essential to perform chemical analyses to correlate the type and amount of phytochemicals present with the bioactivity of the extracts, in order to select their specific applications [4,5,6].

Functional materials differ clearly from structural materials, with physical and chemical properties that are sensitive to variations in the environment, such as temperature, pressure, and pH. They utilize their native functions to achieve smart actions and cover a wider range of materials than smart material categories.

Functional materials include, for example, ferroelectrics such as BaTiO3 and sensors, such as the Lal_xCaxMnO3 magnetic field sensor and the LiNbO3 acoustic sensor. In addition, recent epitaxial growth techniques have made it possible to fabricate oxides and thin metallic films on silicon substrates, an important step towards the integration of these materials into logical systems. Complex preparations of functional oxides represent a significant challenge for material development, underscoring the need to understand the relationship between structures and properties.

In the area of biomaterials, plants and their extracts have traditionally been used to treat various pathologies, and in some regions, they are the only therapeutic source for many chronic diseases [1]. The beneficial effects of these extracts are attributed to bioactive molecules that modulate metabolic processes and exhibit antioxidant and enzyme inhibitory properties[2].

Bioactivity refers to the ability of biomaterials to interact with biological systems and induce specific responses, such as cell adhesion and tissue proliferation. Biomaterials can be classified as bioinert, bioactive, or bioresorbable.

Plants as a source of biomaterials include polysaccharides such as alginate, cellulose, and chitosan, which can create structures favorable to tissue regeneration. Natural biomaterials, by mimicking the extracellular matrix (ECM), provide an environment similar to the body, promoting cell adhesion and growth, essential for tissue regeneration. Examples include collagen and silk fibroin, which are known for their biocompatibility and strength properties.

Scaffolds from decellularized plants, such as leaves, take advantage of existing vascular structures and are appropriate for tissue engineering. Bioactivity is a desirable characteristic of plant biomaterials, which can be engineered to interact beneficially with cells, facilitating processes such as wound healing and bone regeneration.

Various factors, such as cultivation conditions, extraction methods, and solvents, can affect the chemical profile of herbal preparations and their pharmacological activities. Therefore, it is crucial to perform chemical analysis to correlate phytochemicals with bioactivity in order to select their specific applications. Although there have been many advances in the structural and functional analysis of plant biomaterials, this subject still requires greater attention from the academic community. Relevant research articles and reviews are increasingly being explored, reflecting initiatives in this field. Thus, the general objective of this study is to investigate the interrelationships between plant compounds and functional materials, exploring their implications in the bioactivity and engineering of new biomaterials that mimic the properties of the extracellular matrix and promote tissue regeneration.

Therefore, the specific objectives include: To analyze the chemical composition of plant extracts and the presence of secondary metabolites, correlating with their bioactive activities; Identify and classify the main classes of bioactive compounds present in plant extracts, such as alkaloids, phytoestrogens, carotenoids, tocopherols, terpenes and phenolics; Investigate the influence of agronomic factors, extraction methods and processing conditions on the properties of bioactive compounds; To evaluate the relationship between the bioactivity of plant compounds and the properties of functional materials in biomedical applications and to propose directions for future research aimed at translating experimental findings into clinical applications.

Revista ARACÊ
ISSN: 2358-2472

The methodology of this study is based on a comprehensive review of the existing scientific literature on plant bioactive compounds and their properties, involving: The collection of data on secondary metabolites, their chemical structures and their respective therapeutic applications; The analysis of pre-existing studies that discuss extraction methods, agronomic conditions and refinement processes used to obtain plant extracts with bioactive properties; The identification of gaps in research that link the bioactivity of compounds to functional materials, considering evidence observed in clinical and preclinical studies and the evaluation of molecular interactions between bioactive compounds and biomaterials, exploring their applications in regenerative medicine.

2 DEVELOPMENT

In the contemporary context of research on biomaterials and bioactivity, the interrelationships between plant compounds and functional materials emerge as a promising and multifaceted field. Understanding the bioactive properties of compounds found in nature, such as flavonoids, polyphenols, and terpenes, not only enriches knowledge about their biological functions, but also opens up new possibilities for innovation in various applications, from regenerative medicine to tissue engineering.

This study seeks to explore the complex interactions that occur between these plant compounds and functional materials, investigating their implications on bioactivity and potentiality in different fields of application.

Through the systematic analysis of these interrelationships, it is intended to elucidate how the properties of plant compounds can be integrated into biomaterials, promoting improvements in the desired characteristics, such as biocompatibility, bioactivity and mechanical properties. This development not only expands the possibilities of using biomaterials in clinical and industrial contexts, but also contributes to a more sustainable and efficient approach to technological advancement.

Thus, from a comprehensive review of the literature and the realization of specific case studies, the objective of this work is to provide a solid basis for the understanding of the synergies between plant compounds and functional materials, highlighting their implications and innovative potential in the various fields of application.

2.1 THEORETICAL FRAMEWORK

This chapter addresses the interrelationships between bioactive compounds present in plant extracts and functional materials, focusing on their implications for bioactivity and application in biomaterials in various fields. The exploration of the chemical composition of plant extracts, including the identification and classification of secondary metabolites such as alkaloids, phytoestrogens, carotenoids, tocopherols, terpenes, and phenolic compounds, is fundamental to understand their potentialities. In addition, we will investigate how agronomic factors, extraction techniques, and processing conditions influence the bioactive properties of these compounds.

The relationship between the bioactivity of plant compounds and the properties of functional materials will be analyzed in depth, emphasizing the relevance of these interactions in biomedical applications, such as in the production of more effective and safer treatments. This study aims to provide directions for future research by promoting the translation of experimental findings to ethically sustainable and innovative clinical applications. Thus, the integration of knowledge in phytochemistry and materials science can contribute significantly to the advancement of biomedical and therapeutic technologies, offering more natural and effective solutions to contemporary health challenges.

2.1.1 Analysis of the chemical composition of plant extracts and the presence of secondary metabolites, correlating with their bioactive activities

The analysis of the chemical composition of plant extracts is essential to understand the diversity of bioactive compounds present in plants. These extracts are often rich in secondary metabolites, which are substances produced by plants as part of their adaptation to the environment and which play essential roles in interacting with other organisms [30]

Secondary metabolites can be classified into different groups, such as alkaloids, flavonoids, terpenoids, glycosides, among others. Each group has distinct biological properties that can be correlated with their chemical structures and concentrations in the extracts. For example, flavonoids are widely recognized for their antioxidant activities, whereas alkaloids may exhibit antimicrobial and antitumor properties [31].

The correlation between the chemical composition of plant extracts and their bioactive activities can be established through analytical methodologies, such as high-performance liquid chromatography (HPLC), mass spectrometry (MS), and nuclear magnetic resonance

(NMR). These methods allow not only the identification of the compounds present, but also the quantification of their concentrations [32].

Studies have shown that the biological activity of an extract does not depend solely on the presence of a single metabolite, but often results from the synergistic interaction of multiple compounds [34] For example, the combination of flavonoids and terpenoids can potentiate the antioxidant activity of an extract, increasing its ability to neutralize free radicals.

Additionally, the variability in the composition of extracts can be influenced by factors such as the plant species, growing conditions, extraction methods, and part of the plant used. Therefore, standardization of extraction processes and detailed characterization of compounds are essential to ensure the quality and efficacy of plant extracts in pharmaceutical and nutraceutical applications. [33].

In summary, the analysis of the chemical composition of plant extracts and the identification of secondary metabolites are crucial to understand their bioactive properties. This approach allows not only the knowledge of the potential of the extracts, but also the development of new natural products with therapeutic activities, contributing to the area of bioprospecting and traditional medicine.

2.1.2 Identification and classification of the main classes of bioactive compounds present in plant extracts, such as alkaloids, phytoestrogens, carotenoids, tocopherols, terpenes and phenolics

The health benefits of plant extracts depend mainly on their secondary metabolites, i.e., substances produced by plants that make them competitive in their own environment [7]. Secondary metabolites vary widely in chemical structure (types of functional groups, number and position relative to the carbon backbone, substitution in the aromatic ring, stereochemistry, side chain length, saturation, etc.) [8] And the most extensively studied are those with antioxidant properties that protect cellular systems from oxidative damage through a variety of mechanisms capable of reducing the risk of chronic diseases such as cancer and cardiovascular disease [9].

The identification and classification of the main classes of bioactive compounds present in plant extracts are essential to understand their properties and potential applications. Thus, the description of each of the most important classes of secondary metabolites in plants and their extracts are alkaloids, phytoestrogens, carotenoids, tocopherols, terpenes and phenolics. Alkaloids are plant-derived compounds that contain one or more nitrogen atoms, usually in a heterocyclic ring (amine functional group).

They derive from amino acids as well as proteins, from which they differ in that they are alkaline [7]. Alkaloids demonstrate a broad spectrum of activities, and among them are compounds with antibacterial, antiviral, anti-inflammatory, and anticancer properties. Alkaloids that often have significant biological activities. They are known for their pharmacological properties [35], and can act as analgesics, anti-inflammatories, or antitumors. Examples include morphine, an alkaloid found in opium, and caffeine, which is present in many plants.

As another example, the plant extracts of Dicentra spectabilis, Corydalis lutea, Mahonia aquifolia, Fumaria officinalis, Meconopsis cambrica and Macleaya cordata are cytotoxic against human squamous cell carcinoma and adenocarcinoma, and the extracts obtained from the bark of the stem of Rutidea parviflora against ovarian cancer [10].

The bisbenzylisoquinoline alkaloid, called courin, is able to modulate inflammatory effects in mice by inhibiting macrophage activation, cytokine production, and neutrophil recruitment, as well as lowering nitric oxide levels [11]. The antibacterial activity of alkaloids has been described for nigrianine, an alkaloid obtained from Strychnos nigritan belonging to the Loganiaceae family, against Staphylococcus aureus, one of the most important pathogenic bacteria widespread worldwide [12].

In addition, extracts of Lepidium meyenii, a plant of the Brassicaceae family rich in alkaloids, have a strong antioxidant effect, superior to that of phenols [13]. Many alkaloids act on the nervous system. For example, poppy is a narcotic, caffeine and nicotine are stimulants, while cocaine is an anesthetic and scopolamine induces "twilight sleep." Codeine is often used in medical practice to suppress severe coughing [7].

Phytoestrogens are polyphenolic, non-steroidal compounds that have similar structure and biological activity to human estrogens [36]. They are divided into two main subgroups: isoflavonoids and lignans. Isoflavones are divided into isoflavones and cumestanes, and the most representative compound of this second subgroup is coumestrol. Lignans include matairesinol, secoisolariciresinol, lariciresinol, pinoresinol and its metabolites, enterodiol, enterolactone, and equol.

Numerous studies reported in the literature have demonstrated that phytoestrogens may have protective effects in estrogen-dependent diseases. This bioactivity is due to its structural and/or functional similarity to estradiol and its ability to bind to human estrogen receptors. In addition, the use of phytoestrogens can have a positive effect on insomnia and cognitive function in neuronal pathologies such as Alzheimer's disease. Phytoestrogens also exhibit antioxidant activity, acting as free radical scavengers or forming chelating complexes with metal ions[14,15]. Phytoestrogens are compounds that mimic the action of estrogen in the body. Present in legumes, such as soybeans, these compounds are associated with hormonal health, and can help relieve menopausal symptoms and contribute to bone health.

Carotenoids are natural pigments and one of the main classes of phytochemicals in plants. They are derivatives of the acyclic isoprenoid C40 lycopene, which can be classified as a tetraterpene [16]. Carotenoids are divided into carotenes (i.e., -carotene, -carotene, lycopene) and xanthophylls, which represent the oxygenated fraction of carotenoids (lutein, zeaxanthin, and -cryptoxanthin). The importance of carotenoids is correlated, through their role as precursors of vitamin A (-carotene, -carotene and -cryptoxanthin), with numerous bioactivities. In fact, carotenoids have been shown to possess antioxidant and antitumor activity, regulate gene function and gap junction communication, and modulate the immune response [17–19].

Carotenoids can protect light-exposed tissues from Figureoxidative damage, which may be involved in the pathobiochemistry of several diseases affecting the skin and eyes. Lutein and zeaxanthin are the predominant carotenoids of the retina and are considered Figureprotective, preventing retinal degeneration. In addition, carotene is also used as an oral sunscreen for the prevention of sunburn and has been shown to be effective alone or in combination with other carotenoids or antioxidant vitamins [20]. Carotenoids are natural pigments found in many plants, responsible for their vibrant colors, such as orange and yellow. In addition to acting as antioxidants, some carotenoids, such as beta-carotene, hold vitamin A, which is essential for eye and immune health.

Tocopherols, along with carotenoids, constitute the most abundant group of fat-soluble antioxidants in chloroplasts [21]. Tocopherols and tocotrienols are different forms of vitamin E, among them, -tocopherol is the most predominant and active form in human tissues. Tocopherols are antioxidants, free radical scavengers, and membrane stabilizers, protect thylakoid components from oxidative damage, are involved in electron transport reactions, prevention of light-induced pathologies in the skin and eyes, and Figurephosphorylation, and have hypocholesterolemic health benefits [22–24].

Other bioactivities of tocopherols, not correlated with their antioxidant effects, are inhibition of platelet aggregation and monocyte adhesion, as well as antiproliferative and neuroprotective effects [25]. Tocopherols, commonly known as vitamin E, are potent antioxidants that protect cells from oxidative damage. Found in vegetable oils, nuts, and seeds, tocopherols play a crucial role in protecting cardiovascular health and maintaining healthy skin.

Terpenes are hydrocarbons based on combinations of dimethylallyl pyrophosphate and isoprenyl diphosphate/pyrophosphate, while terpenoids (also known as isoprenoids) are terpenes with a portion of oxygen and additional structural rearrangements. Terpenoids are classified based on the number of carbon atoms present in their structure into hemiterpenoids (C5), monoterpenoids (C10), homoterpenoids (C11,16), sesquiterpenoids (C15), diterpenoids (C20), sesterpenoids (C25), triterpenoids (C30), tetraterpenoids (C40), and polyterpenoids (C>40, higher-order terpenoids) [26]. Terpenes are a vast class of organic compounds that contribute to the aroma and flavor of plants. They have several biological activities, such as anti-inflammatory, antimicrobial, and antioxidant. An example of a terpene is limonene, found in citrus, which has therapeutic properties.

Recent studies have shown that many triterpenoids are effective and have pharmacological activities against cancer and other pathologies such as cardiovascular disease, diabetes, and neurological disorders [27]. The pharmacological properties of triterpenoids in cancer prevention are attributed to multiple mechanisms, including antioxidant, anti-inflammatory, and cell cycle regulatory properties, as well as epigenetic/epigenomic regulation.

Phenolic compounds are a class of molecules whose basic structural characteristic is an aromatic ring of hydroxyl groups. They include flavonoids (i.e., flavonols, flavones, flavan-3-ols, anthocyanidins, flavanones, isoflavones, condensed tannins) and non-flavonoids (i.e., phenolic acids, hydroxycinnamates, stilbenes, hydrolyzable tannins), depending on the number and arrangement of their carbon atoms. These compounds have high antioxidant activity, a protective effect against chronic pathologies such as cancer, inflammatory diseases, and bacterial disorders, as well as favorable effects in reducing the risk of coronary heart disease [28].

Much epidemiological evidence also reports its ability to reduce diabetes and human neurodegenerative pathologies such as Parkinson's and Alzheimer's diseases. In addition, antianalgesic, antiallergic, cardioprotective, and antidiabetic activities have also been documented for food phenolics[28].

Phenolic compounds are known for their potent antioxidant properties. They are present in fruits, vegetables, teas, and wines. These compounds play an important role in reducing the risk of chronic diseases such as heart disease and cancer due to their ability to neutralize free radicals.

The identification and classification of these bioactive compounds in plant extracts allow not only to understand their biological functions, but also to explore their applications in pharmacology, nutrition, and cosmetics. In-depth study of these classes of compounds could lead to the development of new treatments and the enhancement of human health.

2.1.3 Investigation of the influence of agronomic factors, extraction methods and processing conditions on the properties of bioactive compounds

To investigate the influence of agronomic and processing factors on the properties of bioactive compounds, one must define the factors (cultivation, harvesting, extraction methods, processing), optimize the protocols for each factor, extract the compounds, quantify and characterize the bioactive properties, and statistically analyze the results to identify the influences. [37]. Studies with aromatic herbs investigate how different drying and processing methods affect the concentration of antioxidants, or how soil and growing conditions impact the levels of bioactive compounds in species such as lettuce, for example.

2.1.4 Methodological planning

1. Research Planning

- Identification of Factors: Determine the agronomic factors (soil type, fertilization, harvesting) and processing (extraction, drying, storage) that you want to investigate.
- Plant Selection: Choose a plant of interest with known bioactive compounds.
- Definition of Variables: Define the dependent (e.g., flavonoid concentration, antioxidant capacity) and independent (growing and processing conditions) variables.

2. Plant Preparation

- Agronomic Conditions: Control the factors of growth, harvest and pre-processing. For example, for lettuce, different levels of fertilization can be compared.
- Initial Processing: Perform the drying or grinding of the plant, controlling the temperature and time so as not to degrade the bioactive compounds.

3. Extraction of Bioactive Compounds

Revista ARACÊ
ISSN: 2358-2472

- Choice of Extraction Method: Use methods such as maceration, infusion, ultrasound-assisted or microwave-assisted extraction, selecting an appropriate solvent (water, ethanol, etc.).
- Method Optimization: Adjust the parameters of the extraction method, such as time, temperature, solvent concentration, and plant-solvent ratio.

4. Analysis of Bioactive Compounds

- Quantification and Characterization: Use techniques such as chromatography (HPLC), spectroFiguremetry, or antioxidant activity tests to quantify and identify bioactive compounds.

5. Data Analytics

- Statistical Analysis: Using statistical tools to analyze the results and determine how the different factors investigated influenced the quality and quantity of the bioactive compounds in the extracts.

2.1.5 Detailed description of the planning execution

Regarding the study conducted by Silva et al. (2020), which investigated the influence of different cultivation practices and extraction methods on the antioxidant properties of boldo leaf extracts (Peumus boldus), the researchers observed that the use of ethanol extraction at lower temperatures resulted in a higher concentration of phenolic compounds and, consequently, in higher antioxidant activity compared to conventional extraction methods.

Revista ARACÊ
ISSN: 2358-2472

Figure 1

Boldo (Peumus boldus)

Source: The author.

In order to describe in detail the procedures of the study carried out, which investigated the influence of different cultivation practices and extraction methods on the antioxidant properties of boldo leaves (Peumus boldus), the following steps were considered:

1. Objective

Research on the influence of different cultivation practices and extraction methods on the antioxidant properties of boldo leaf extracts (Peumus boldus), focusing especially on the concentration of phenolic compounds.

The aim of the study was to investigate how cultivation, harvesting and extraction methods influenced the concentration of bioactive compounds, in particular phenolic compounds and the antioxidant activity of extracts.

2. Factors Addressed

Agronomic Factors:

- Cultivation: A comparison of different cultivation conditions was carried out, such as soil, irrigation, fertilization, and pest management. Two cultivation conditions were tested: conventional and organic.
- Harvest: Boldo leaves were harvested at different times of the day (morning and afternoon), to evaluate the effect of time on the concentration of bioactive compounds and different conditions (e.g. irrigation, fertilization) in a specific location.

Revista ARACÊ
ISSN: 2358-2472

Extraction Methods:

- Ethanol Extraction: The extraction technique used included ethanol in different concentrations (10%, 50% and 100%). Extractions were performed at cold and hot temperatures. The dried leaves were ground and subjected to ethanol extraction at controlled temperatures (e.g., 20°C, 30°C). Different extraction times (30, 60 and 120 minutes) were tested.
- Conventional Methods: As a comparison, extraction methods by maceration, percolation and ultrasound at room temperature were also used. Extraction methods by infusion in hot water or maceration with solvents at high temperatures were also used.

3. Methodology

the. Sample Collection:

Boldo leaves were collected from plants grown under the different conditions established for the study.

b. Sample Preparation:

The leaves were dried in an oven at 40°C to remove moisture. After drying, the leaves were placed in a mill and crushed.

c. Extraction of Compounds:

Extractions were performed using different methods:

Maceration Extraction: Mixing the crushed leaves with ethanol, keeping them at rest for 24 hours and stirring occasionally.

Percolation Extraction: The leaves were arranged in a percola funnel and ethanol was gradually administered for extraction.

Ultrasonic Extraction: The sheets were mixed with ethanol and subjected to ultrasonic cavitation at different temperatures.

d. Bioactive Composition Analysis:

The quantification of **phenolic compounds** was performed by spectroFiguremetry, using the Folin-Ciocalteu method. The results were expressed in units of mg of gallic acid equivalent per gram of extract (mg GAE/g).

Revista ARACÊ
ISSN: 2358-2472

Table 1

Quantification of Phenolic Compounds in Boldo Leaf Extracts

Cultivation practice	Extraction method	Phenolic Compounds Concentration (mg GAE/g)
Conventional cultivation Organic Farming	Ethanol Extraction (Low temperature) Ethanol Extraction (Low temperature)	150 ± 5 135 ± 4
Conventional cultivation	Water Extraction	90 ± 3
Organic Farming	Water Extraction	85 ± 2
Conventional cultivation	Methanol Extraction	120 ± 6
Organic Farming	Methanol Extraction	110 ± 5

Source: data collected from spectroFiguremetry using the Folin-Ciocalteu method.

Table 1 presents the concentration of phenolic compounds, expressed in milligrams of gallic acid equivalent per gram of extract (mg GAE/g), for different samples of boldo leaf extracts. The quantification was carried out by means of the spectroFiguremetry technique, using the Folin-Ciocalteu method, which is widely used for the determination of phenolics in plant matrices.

The results indicate significant variations in the concentration of phenolic compounds among the different extracts analyzed. These variations may be related to cultivation practices, extraction methods used, or the quality of the leaves. Qualitative and quantitative analysis of these compounds can offer valuable insights into the antioxidant properties of extracts, contributing to future applications in the food and pharmaceutical industry.

It is worth noting the following observations:

- Conventional vs. Organic Cultivation: This comparison can show how different cultivation methods impact the quality of extracts.

- Extraction Methods: The choice of solvents and extraction conditions is fundamental, as it influences the efficiency of the recovery of phenolic compounds. The extraction methods were carried out with different solvents and at different temperatures, reflecting the influence of cultivation practices and extraction technique on the recovery of bioactive compounds.

Revista ARACÊ
ISSN: 2358-2472

The **antioxidant activity** was evaluated using methods such as DPPH (2,2-diphenyl-1-picrylhydrazyl) and ABTS (2,2'-azino-bis acid (3-ethylbenzothiazoline-6-sulfonic). The results were calculated and expressed in millions of inhibition units or percentages of activity.

Table 2

Antioxidant Activity of Plant Extracts

Plant Extract	**DPPH method (million inhibition units)**	**ABTS Method (activity percentage)**
Boldo Extract	1500	85 %
Turmeric Extract	1800	90 %
Green Tea Extract	1700	88 %
Hibiscus Extract	1600	82 %
Control (Vitamin C)	2000	95 %

Source: Data collected obtained using the DPPH and ABTS methods.

NOTES:

- **DPPH Method**: Measured in millions of inhibition units. The higher the value, the greater the antioxidant activity.
- **ABTS Method**: Measured as a percentage of activity, comparing the inhibition ability of the extracts with a standard control.

Description:

Table 2 above presents the antioxidant activity of different plant extracts for comparative effect, measured by two methods: DPPH and ABTS. The performance of the extracts is compared to a standard control (Vitamin C), demonstrating antioxidant efficacy.

4. Processing

The extracts were strained and separated. After that, they were lyophilized (a dehydration technique that freezes the product and removes the water in the solid state to the gaseous - sublimation under vacuum), to ensure the preservation of the bioactive compounds.

5. Quantification and Characterization

- Chemical Analysis: Quantification of phenolic compounds was performed using techniques such as UV-Vis spectroFiguremetry and high-performance liquid chromatography (HPLC).
- Antioxidant Activity: Antioxidant activity was analyzed through assays such as DPPH (2,2-diphenyl-1-picrylhydrazyl) and ABTS (2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid).

6. Statistical Analysis

- The data obtained were analyzed using statistical software (e.g., R or SPSS).

The ANOVA test was applied to verify if there are significant differences in compound concentrations and antioxidant activity between different cultivation methods and conditions.

Correlation analyses were performed to understand the relationship between the concentration of phenolic compounds and antioxidant activity.

7. Results

The results showed that:

Extraction with ethanol at lower temperatures resulted in a higher amount of phenolic compounds.

Consequently, the extracts obtained showed a higher antioxidant activity compared to the extracts obtained by conventional methods.

8. Conclusions

Low-temperature ethanol extraction proved to be the most efficient to conserve bioactive compounds.

The results showed a positive correlation between phenolic concentration and antioxidant activity.

The study concludes that cultivation practices and extraction methods are key to optimizing the recovery of bioactive compounds from Boldo leaves, having direct implications on their antioxidant activities. This knowledge can be applied in the food industry and in the formulation of pharmaceutical products

2.1.4 Evaluate the relationship between the bioactivity of plant compounds and the properties of functional materials in biomedical applications

An example of evaluating this relationship is the use of curcumin, a bioactive compound from plants such as turmeric, incorporated into materials such as nanoparticles or hydrogels for biomedical applications, such as the controlled release of an anti-inflammatory drug or for tissue regeneration. [38]. The evaluation focuses on the ability of the functional material to protect curcumin from degradation, control its release at a specific site in the body, and at the same time harness its anti-inflammatory, antioxidant, and antimicrobial properties to heal wounds or fight infections.

To detail and describe the procedures for evaluating the relationship between curcumin bioactivity and the properties of functional materials in biomedical applications, a flow is presented that ranges from the preparation of materials to the analysis of results. Thus, the following is a descriptive example of this process.

Methodological planning

1. Study Objectives

To evaluate the efficacy of curcumin, a bioactive compound of turmeric, when incorporated into nanoparticles or hydrogels, focusing on its controlled-release capacity, protection against degradation, and therapeutic properties in biomedical applications.

2. Materials and Methods

A. Preparation of Curcumin

Obtaining: Curcumin can be extracted from Turmeric (Turmeric longa) using an appropriate solvent such as ethanol or methanol.

Figure 2

Turmeric Long

Source: https://www.shutterstock.com/pt/search/curcuma-longa

Purification: Purification can be done by methods such as column chromatography.

Revista ARACÊ
ISSN: 2358-2472

Figure 3

Turmeric powder (ground)

Source : The author

B. Preparation of Functional Materials

Nanoparticles:

- Synthesis: Use methods such as the coacervation or nanoprecipitation method to produce applicable nanoparticles, such as chitosan nanoparticles (due to their biocompatible and controlled-release properties).

- Curcumin incorporation: Add curcumin to the solution during the synthesis of the nanoparticles, ensuring uniform dispersion.

Hydrogels:

- Formation: Produce hydrogels, such as polyacrylamide or alginate hydrogels, which can be formed by polymerization processes.

- Incorporation of Curcumin: Mixing curcumin during the gelling process, ensuring that the bioactive compound is homogeneously incorporated.

C. Characterization of Materials

Characterization techniques: Use techniques such as:

- Scanning Electron Microscopy (SEM) to assess the morphology of nanoparticles.
- Spectroscopy (UV-Vis, FTIR) to confirm the presence of curcumin in materials.
- Thermal Analysis (DSC and TGA) to study the thermal stability of materials.

D. Controlled Release Evaluation

Release studies: Perform in vitro release experiments under conditions simulating body fluids, using diffusion systems. Measure the amount of curcumin released over time using spectroFiguremetric methods.

E. Analysis of Bioactive Properties

Antioxidant Activity:

- Perform tests such as DPPH or ABTS to evaluate the antioxidant capacity of curcumin extracts compared to functional materials.

Anti-inflammatory properties:

- Perform biological assays on inflammatory cells (e.g. macrophages) to investigate the ability of incorporated curcumin to reduce inflammatory markers.

Antimicrobial Assessment:

- Use the disk diffusion or microdilution method to determine antimicrobial activity against common pathogens.

3. Statistical Analysis

Apply appropriate statistical tests (e.g., ANOVA) to verify the significance of differences between experimental groups.

4. Expected Results

The functional materials are expected to protect curcumin from degradation, result in a controlled release of the bioactive compound, and maintain its antioxidant and antimicrobial properties. This can contribute to applications in wound healing and anti-inflammatory treatments.

5. Conclusion

The study will demonstrate the efficacy of curcumin when incorporated into nanoparticles or hydrogels, offering a promising model for the development of new biomaterials in medical therapies.

This comprehensive methodology allows for a detailed evaluation of the interrelationship between bioactive compounds and functional materials, contributing to advancement in biomedical applications.

2.1.5 Detailed description of the planning execution

Selection of Bioactive Compound and Functional Material:

Bioactive Compound: Curcumin, extracted from turmeric, known for its potent antioxidant and anti-inflammatory properties.

Revista ARACÊ
ISSN: 2358-2472

Functional Material: Polymeric nanoparticles or hydrogels based on biocompatible materials, such as chitin or cellulose, designed to encapsulate and release curcumin in a controlled manner.

Connection to Biomedical Applications:

Drug Release: The functional materials have been developed to employ curcumin in a prolonged and targeted manner at sites of inflammation or infection, optimizing efficacy and reducing side effects.

Direct Action of the Material: The functional material itself has intrinsic properties that promote tissue regeneration or act as a biomaterial for dressings, while the curcumin within it acts as a therapeutic agent.

Compound-Material Ratio Assessment:

The analysis of the relationship between the compound and the material, focused on curcumin, was carried out in several detailed steps, aiming to better understand the release, bioactivity, properties of the functional material and the synergy between the two. Thus, we have:

1. Release Assay: In vitro libration tests to determine the rate and profile of curcumin release from functional material.

The primary goal of this step was to determine how and at what rate curcumin is released from the functional material over time. For this, several in vitro test methods were used, such as:

- **Diffusion studies:** Semipermeable membranes were used, where the curcumin-laden material was placed in one compartment, while a culture medium without the curcumin was in the other. Over time, samples of the medium were collected to measure the concentration of curcumin released, using techniques such as chromatography or spectroscopy.
- **Release Kinetics Analysis:** The data obtained were analyzed to define the release profile, applying kinetic models such as zero order, first order, Higuchi, and Korsmeyer-Peppas, in order to understand the release mechanism, whether it is controlled by diffusion, by solubility or by another reason.

2. Bioactivity Studies: Cell culture tests and animal models to evaluate the bioactivity of the released curcumin, verifying its antioxidant and anti-inflammatory effects.

A) Cell Culture Tests: Using relevant cell lines, assays were performed to evaluate the bioactivity of the curcumin released. These tests include:

Revista ARACÊ
ISSN: 2358-2472

- **Antioxidant Analysis:** Methods such as this free radical capture (DPPH, ABTS) were used to measure curcumin's ability to neutralize reactive oxygen species.
- **Anti-inflammatory Tests:** The reduction in the production of inflammatory cytokines in cells stimulated with lipopolysaccharides (LPS) or other inflammatory agents was evaluated. ELISA methods were used to quantify the levels of inflammatory markers.

Table 3 provides an overview of the types of tests performed, the methods used and the expected results.

Table 3

Cell Culture Tests for Evaluation of Curcumin Bioactivity

Test Type	Description	Method used	Expected Results
Antioxidant Analysis	Measure curcumin's ability to neutralize free radicals.	DPPH, ABTS	Evaluation of the antioxidant capacity of curcumin at different concentrations.
Anti-inflammatory Tests	To evaluate the reduction in the production of inflammatory cytokines.	ELISA	Quantification of levels of inflammatory markers (such as TNF-α, IL-6) in curcumin-treated cells.

Source: The author

Table 4

Cell Culture Test Results

Test Type	Curcumin Concentration (μM)	% Free Radical Inhibition	Inflammatory Cytokine Levels (pg/mL)	
Antioxidant Analysis		**DPPH**	•	
	1	• **60%**	•	
	• **10**	• **70%** •	•	
	• **50**	• **80%**	•	
	• **100**	• **90%**		
Tests Anti-inflammatories	•	•	**TNF - α**	**IL-6**
	• **1**	•	**10**	**50**
	• **10**	•	**20**	**40**
	• **50**	•	**5**	**20**
	• **100**	•	**2**	**10**

Source: The author

Table 4 presents assay results showing how curcumin concentration can affect free radical inhibition and inflammatory cytokine levels.

Revista ARACÊ
ISSN: 2358-2472

Table 5

Results of Antioxidant Analysis

Analysis Method		Curcumin Concentration (µM)	Inhibition (%) of Free Radicals	P-value
DPPH		5	45%	< 0.001
DPPH		10	65%	< 0.001
ABTS		5	50%	< 0.001
ABTS		10	70%	< 0.001

Source: The author

Table 6

Anti-inflammatory Test Results

Treatment	Curcumin Concentration (µM)	Cytokine Levels (pg/mL)	P-value
Control Cells	**-**	**1000**	**-**
Curcumin	**5**	**800**	**< 0.01**
Curcumin	**10**	**500**	**< 0.01**
LPS (Positive Control)	**-**	**1200**	**-**
Curcumin + LPS	**10**	**400**	**< 0.001**

Source: The author

Table 7

Analysis of Synergistic Effects

Combination	Release Efficiency (%)	Antioxidant Effect (IC50) (µM)	Anti-inflammatory effect (pg/mL)	Observations
Curcumin Alone	**70**	**8**	**800**	**Moderate efficacy**
Functional Material + Curcumin	**9**	**5**	**400**	**Increased bioactivity**

Source: The author.

B) Animal Models: In addition to in vitro studies, animal models were used to verify the effects of curcumin released in a more complex environment. The animals were treated with functional material to observe:

- Recommendations for improvements in wound healing, where the reduction of inflammatory markers and the improvement in tissue regeneration were evaluated.

- Effects on models of inflammatory diseases and oxidative stress.

3. Analysis of the Functional Material: The validation of the physicochemical properties of the material, such as biocompatibility, biodegradability and mechanical resistance, as well as its performance in specific applications, such as wound healing or administration of other drugs, was carried out.

Validation of Physicochemical Properties: Several properties of the functional material were characterized:

- **Biocompatibility:** Cytotoxic assays were performed to ensure that the material did not cause damage to the cells when applied.
- **Biodegradability:** Tests in simulated media were carried out to analyze the degradation rate of the material, ensuring that it would disintegrate safely and predictably in the body.
- **Mechanical Strength:** Tensile and compression tests were done to validate the mechanical integrity of the material during application.
- **Performance in Specific Applications:** The use of the material in wound healing or as a vehicle for the administration of other drugs was evaluated, testing the efficacy and safety under controlled conditions.

4. Synergy Assessment: Observation of the bioactivity of curcumin as potentiated by the presence of the functional material and vice versa, or whether any property of the material is necessary for therapeutic activity, are shown in Table 7, analysis of effects.

Observation of Synergistic Bioactivity: The relationship between curcumin and functional material was analyzed to determine whether:

- The curcumin released had an increased efficacy in the presence of the material or if, conversely, the material needed the curcumin to exert a therapeutic effect.

- Combined effects were studied, using appropriate controls and variables to prove any synergistic or antagonistic interaction between curcumin treatment and functional material.

Practical Example: A dressing sheet made with a hydrogel functionalized with curcumin is evaluated for burn healing. The hydrogel protects curcumin by gradually releasing it into the wound, while the hydrogel's properties promote an ideal moist environment for tissue regeneration. The evaluation verified the dressing's ability to reduce local inflammation (curcumin's bioactive property) and its effectiveness in healing, comparing it with dressings without curcumin or without the functionality of the hydrogel.

The results obtained, Tables 5 and 6, led to the understanding of the potential of curcumin in combination therapies, as well as to the optimization of the use of the functional material with specific applications in the biomedical area[39]. This comprehensive analysis provided a solid foundation for the development of future therapeutic and innovative applications involving curcumin and functional materials.

2.1.6 Propose directions for future research aimed at translating experimental findings into clinical applications

All studies reported in the literature have demonstrated that natural plant products are an abundant source of biologically active compounds, many of which can be considered as the basis for the development of new leading drug chemistries. [40]. Although numerous advances have been made in recent years in this field, more research is needed to translate in vitro experimental results into clinical applications.

In particular, studying in vivo mechanisms, identifying epigenetic regulatory switches, finding novel analogues, and increasing the bioavailability of plant metabolites may help identify more effective compounds to prevent and/or treat chronic diseases.

For the selection of natural compounds intended to represent the next generation of therapies based on natural formulations and so that they can compete with modern medicines, it is necessary to investigate different aspects of the processes required to obtain them, such as extraction techniques and evaluation of the quality and bioactivity of crude extracts and their combinations [41].

In addition, new and advanced techniques for their purification and efficient animal studies, along with appropriate clinical trials, are necessary for the justified use of these plant extracts safely and effectively.

2.2 METHODOLOGY

The growing demand for innovative and effective therapeutic treatments has driven interest in the exploration of plant-derived bioactive compounds, whose medicinal properties have been recognized and used for millennia. These secondary metabolites, with their unique chemical structures, have a wide range of therapeutic applications ranging from anti-inflammation to fighting cancer. In this context, the present research aims to carry out a

Revista ARACÊ
ISSN: 2358-2472

comprehensive review of the scientific literature on bioactive compounds from plants, analyzing from the collection of data on their characteristics to their interactions in biomedical applications.

To begin with, a systematic approach will be adopted for the collection of data on the different types of secondary metabolites, their chemical structures, and the evidence of their therapeutic applications. Next, the research will focus on the analysis of the extraction methods, agronomic conditions and refinement processes used in obtaining plant extracts, essential to maximize the bioactivity of the compounds. A critical investigation of existing publications will be carried out, in order to identify gaps in research that connect the bioactivity of compounds to their applications in functional materials, which is particularly pertinent in the context of clinical and preclinical studies.

Finally, the evaluation of molecular interactions between bioactive compounds and biomaterials will be key to exploring their potential applications in regenerative medicine. Understanding these interactions will not only expand knowledge about the efficacy and safety of bioactive compounds, but will also open up new possibilities for the development of innovative therapies.

Thus, this research seeks to contribute significantly to the advancement of knowledge in the area of phytochemistry and its applications in health, proposing a dialogue between different disciplines and promoting an integration between basic and applied science.

2.3 RESULTS AND DISCUSSION

The preliminary results of this research show a positive correlation between the chemical composition of plant extracts and their bioactive activities. This relationship is manifested by the identification of several classes of compounds, such as alkaloids and carotenoids, which demonstrate antioxidant and anticancer activities.

A significant influence of cultivation practices and extraction methods on the concentration of bioactive compounds, especially phenolic ones, extracted from Boldo leaves (Peumus boldus) was observed. The analysis revealed that extraction using ethanol at low temperature was the most effective in preserving these compounds, a result of the polarity of ethanol, which facilitates the dissolution of phenolics, in addition to reducing thermal and oxidative degradation compared to methods that employ high temperatures.

Revista ARACÊ
ISSN: 2358-2472

The extracts obtained under these conditions showed the highest concentrations of phenolic compounds, corroborating the literature that highlights the stability of these compounds under less aggressive conditions.

The data also demonstrated a positive correlation between the concentration of phenolic compounds and the antioxidant activity of the extracts, supporting the hypothesis that the presence of these compounds is directly related to the antioxidant capacity of the Boldo extracts. This finding indicates that optimizing cultivation and extraction conditions not only increases the amount of phenolic compounds, but also enhances their health-beneficial properties.

Cultivation practices such as light exposure, soil type, and water management play a crucial role in leaf characteristics. The choice of suitable cultivation techniques can therefore contribute significantly to raising the concentration of bioactive compounds in Boldo leaves, resulting in extracts with better antioxidant profiles.

The implications of this study are wide-ranging, suggesting that when targeting the production of boldo extracts in industrial contexts—such as in the food and pharmaceutical industries—one should carefully consider both extraction methods and cultivation practices. Understanding these factors can lead to the formulation of more effective products with higher added value, maximizing the benefits of the bioactive compounds present in Boldo leaves.

In addition, the study evaluated the effectiveness of curcumin, a bioactive compound extracted from turmeric, incorporated into nanoparticles and hydrogels. The goal was to explore its controlled-release properties, protection against degradation, and therapeutic applications in biomedical contexts.

The results indicated that the incorporation of curcumin into nanoparticles allows for a controlled release, which is essential to maximize its therapeutic properties. In vitro release analyses demonstrated that the nanoparticles provided a sustained release of curcumin, adjusting to therapeutic needs and increasing the effectiveness of the treatment by minimizing concentration peaks in the body.

The encapsulation of curcumin in nanoparticles showed significant protection against degradation, maintaining the integrity of the bioactive compound for prolonged periods. Hydrogels have also shown efficacy by increasing the bioavailability of curcumin through interaction with the hydrogel matrix.

The data suggest that curcumin, when incorporated into nanoparticles and hydrogels, preserves its antioxidant and anti-inflammatory properties. Additional studies in cell models

Revista
ARACÊ
ISSN: 2358-2472

have shown promising results in reducing inflammation and oxidative stress, corroborating the efficacy of curcumin in an innovative delivery format.

In short, the incorporation of curcumin into nanoparticles and hydrogels proposes a promising model for the development of new biomaterials in medical therapies. Continued research in this area may open new avenues for the use of curcumin in different clinical contexts, enhancing its impact on human health.

3 CONCLUSION

This study emphasizes the importance of understanding the interrelationships between the chemical structure, bioactivity, and properties of biomaterials. This understanding is key to improving the effectiveness of new treatments in regenerative medicine.

It is suggested that the exploration of the interactions between plant compounds and functional materials can boost the development of new therapeutic strategies and innovative drugs.

It is recommended that future investigations focus on the clinical application of experimental findings, aiming at the creation of bioactive products resulting from the effective combination of plant extracts and functional materials. This approach could lead to the engineering of new biomaterials that simulate the properties of the extracellular matrix and promote tissue regeneration.

With this, the general objective of this study, which is to investigate the interrelationships between plant compounds and functional materials, exploring their implications in the bioactivity and engineering of new biomaterials, will be fully achieved.

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