

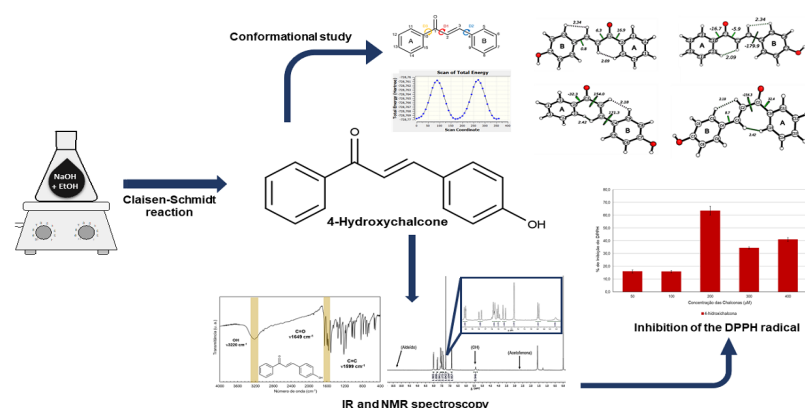
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Synthesis, Characterization, Antioxidant Activity and Conformational Study of 4-Hydroxychalcone

André Luis Kerek , Thiago de Castro Rozada , and Barbara Celânia Fiorin* 

The objective of this work was to develop a synthesis, characterization, and conformational study of 4-hydroxychalcone. The chalcone was obtained using Claisen-Schmidt reaction. The product was characterized by FTIR and NMR spectroscopy. The latter technique was extremely important to verify the presence of the vinyl double bond formed in the reaction and to determine its *trans* configuration. The antioxidant activity of 4-hydroxychalcone showed a satisfactory result when compared to antioxidants already reported in the literature, with 63.4% inhibition of the DPPH radical. Also, theoretical calculations were performed to determine conformational preference. The *s-cis* (b) (52.0%) and the *s-cis* (a) (35.0%) conformers showed less energy when compared to *s-trans* conformers, due to the higher stabilizing effect of electron delocalization involving the π orbitals resulting from the higher planarity of *s-cis* conformers. However, the *s-cis* (a) conformer showed greater stabilization energy (510.37 kcal mol⁻¹) in relation to the *s-cis* (b) conformer (505.32 kcal mol⁻¹), this fact might be explained by the hydroxyl group interaction with the aromatic ring B, as observed by the NBO calculations.

Graphical abstract



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1. Introduction

Chalcones, with a general structure 1,3-diphenyl-2 propen-1-one [1] are α,β -unsaturated ketones that are found in the main plant structures, such as roots, leaves and flowers, being a natural precursors of flavonoids. There are different methods to obtain chalcones via synthetic routes with the purpose to produce compounds with interesting pharmacological properties [2]. The most common method is

Claisen-Schmidt condensation with acid or basic catalysis [2, 3]. After synthesized, the products are characterized by Fourier transformed infrared (FTIR) and nuclear magnetic resonance (NMR) spectroscopy. Also, analysis to verify possible pharmacological activity, such as antioxidant, antibacterial, antifungal, anticancer, among others are performed [4]. The conformational behavior of chalcones is

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A Study of Antioxidant Properties and a Pharmacokinetic Investigation of Chalcones and Pyrazolines

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Antioxidant compounds are widely studied in the literature because they minimize oxidative damage in biological processes. In this context, chalcones and pyrazolines are considered prototype compounds for this purpose. This study describes the synthesis and characterization of seven compounds, including chalcones and pyrazolines, which were evaluated for their antioxidant power and pharmacokinetic properties. Compound **2b**, a pyrazoline with a para-substituted hydroxyl group, exhibited greater antioxidant activity compared to the other compounds in the study, thus showing good potential for future applications in biological activities.

Graphical abstract



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1. Introduction

Currently, numerous studies are focused on seeking the discovery of new pharmacologically relevant compounds for the treatment of existing diseases and potential new illnesses, as exemplified by the case of SARS-CoV-2. In this scenario, certain classes of compounds have increasingly attracted the attention of researchers, such as chalcones and hybrids of this class with the pyrazole group, resulting in pyrazolines [1].

Pyrazolines are characterized by five-membered rings composed of three carbon atoms and two adjacent nitrogen atoms, along with an endocyclic double bond [2]. These

possess various bioactive properties, including but not limited to antioxidant [3], anti-inflammatory [4], antiviral [5], antimicrobial [6, 7], antibacterial [8, 9], antitumor [10-13], and antituberculosis effects, particularly concerning conditions like rheumatoid arthritis and polyarthritis [14].

The biological activities of pyrazolines are of significant interest in pharmacokinetics, a central field in the development of new drugs, which analyzes the distribution of medications in the body from their initial absorption to metabolism and excretion processes. Consequently, through

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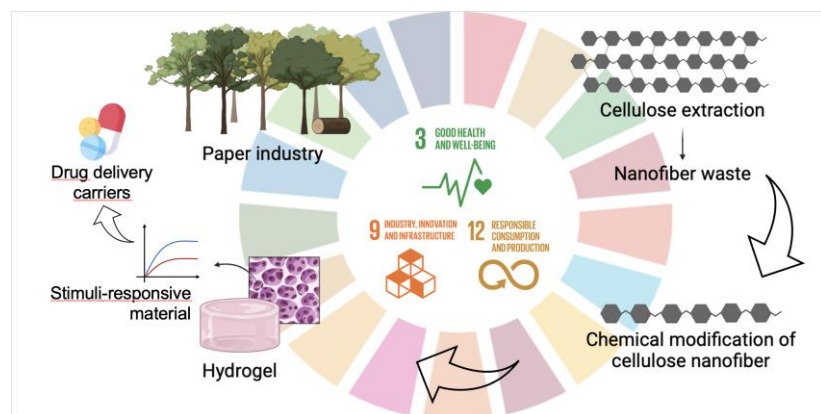
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Chemically Cross-linked Hydrogels Based on Cellulose Nanofibril for Oral Drug Delivery

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Nanocellulose-based hydrogels have emerged as promising platforms for drug delivery in the gastrointestinal environment due to their biocompatible and biodegradable properties, aligning with the 3, 9, and 12 Sustainable Development Goals (SDG). In this study, we investigated the modification of cellulose nanofibrils (CNF) with glycidyl methacrylate and the subsequent synthesis of chemical hydrogels containing *N,N'*-dimethylacrylamide (DMA), and sodium acrylate (NaAc). The structural and morphological characterization of the hydrogels was carried out using techniques such as FTIR (Fourier-transform infrared spectroscopy), ¹H NMR (proton Nuclear magnetic resonance), and SEM (scanning electron microscopy). The fluid absorption capacity and swelling kinetics were evaluated, as well as the contribution of swelling mechanisms to these processes. Among the formulations developed, H2 (50 mg of CNF, 50 mg of DMA, 50 mg of NaAc) was demonstrated to be responsive to changes in pH and ionic strength, which can potentially generate a material capable of acting as a carrier for controlled drug release systems in the gastrointestinal environment. This study suggests that modified CNF hydrogels have potential applications as a controlled release device in the gastrointestinal environment and contribute to achieving the SDG, offering a strategy to improve therapeutic efficacy, reduce side effects, and promote responsible consumption and production practices.

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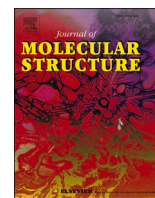
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1. Introduction

The search for effective and sustainable drug delivery systems is a crucial challenge in the biomedical field,

especially when considering the use of materials from natural and non-toxic origins. In this context, studies using hydrogels

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Exploring the antioxidant potential of hydroxychalcones: A comprehensive investigation integrating theoretical and experimental analyses

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ABSTRACT

Chalcones belong to a class of compounds that hold significant interest in medicinal chemistry due to documented instances of diverse biological activities in the literature. Moreover, their structural framework allows the incorporation of various functional groups, potentially enhancing specific biological activities. This study seeks to elucidate the synthesis of hydroxychalcones and explores their antioxidant properties. To this end, the antioxidant efficacy of the synthesized chalcones was assessed utilizing the DPPH radical inhibition assay. Additionally, electrochemical tests were conducted to estimate and establish correlations between the antioxidant effects. Concurrently, a conformational analysis of the compounds was conducted via theoretical calculations. Next, the conformer demonstrating the highest population percentage for each chalcone was scrutinized for its impact on modulating energy levels in Frontier Molecular Orbitals (FMO). Finally, utilizing these theoretical insights, chemical properties were computed and correlated with experimental data.

1. Introduction

Antioxidants can be enzymatic or non-enzymatic, with the latter also found in natural or synthetic forms. Their primary function is to reduce damage caused by free radicals, ROS (reactive oxygen species) and RNS (reactive nitrogen species) to biomolecules [1,2]. Free radicals are molecules characterized by an unpaired electron and are known for initiating chain reactions, which lead to cell oxidative damage. ROS and RNS are also capable of causing this damage to biomolecules, such as proteins, lipids or nucleic acids [3–6].

However, the importance of free radicals and reactive species in biological processes is also known. For example, free radicals are involved in the intracellular destruction of bacteria by phagocytes and ROS appear crucial in the regulation of several normal cellular functions [6,7].

Despite playing an important biological role, excessive production of ROS, RNS and free radicals, whether stemming from normal biochemical reactions or increased exposure to the xenobiotics, leads to oxidative stress [2,6,8]. This condition is linked to the aging process [9,10] and

various diseases, such as cancer [11,12], inflammation [4,13,14], diabetes [15,16], Alzheimer's [3,12,17], cardiovascular diseases [14], and Parkinson's [17,18], among others.

Taking that into account, to avoid damage caused by oxidative stress, it is extremely important to have antioxidants in sufficient quantity to neutralize the effects of free radicals and ROS and RNS. While the human organism possesses endogenous antioxidants that act to protect cells and organs against oxidative damage, their levels may prove insufficient, thus requiring the use of exogenous antioxidants, obtained from the individuals' diet and/or supplementation [19,20].

Antioxidants act through different mechanisms of action, such as free radical scavenging, decomposing hydrogen peroxide or hydroperoxides, and chelating metal ions. Antioxidants can also be classified as primary, those that actively inhibit oxidation reactions, as well as secondary, which act indirectly in oxidation reactions [4,21].

There are several classes of natural product compounds that present antioxidant properties, among them we can mention the flavonoid family, whose main characteristic is the presence of polyphenolics in its structure [2,22]. The capability of these compounds to scavenge free

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