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In silico study of potential anti-inflammatory and gastroprotective markers of *Jacaranda decurrens* species

Estudo *in silico* de potenciais marcadores anti-inflamatórios e gastroprotetores da espécie *Jacaranda decurrens*

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Abstract
Brazil boasts the most extraordinary biodiversity in the world, with six distinct biomes spanning its vast territory, including the Cerrado. The species *Jacaranda decurrens,* commonly known as “carobinha” or “caroba”, is used for the treatment of certain illnesses, including gastrointestinal problems and inflammatory conditions. This study is an *in silico* prediction of the bioactivity of plant-derived compounds. Initially, twenty-five molecules from this species were analyzed, and sixteen were selected based on the highest scores in the computational analyses. The pharmacodynamic characteristics of the structures were elucidated using the PASS prediction servers from the Way 2 Drug platform and Swiss Target Prediction, while the pharmacokinetic characteristics were assessed using SwissADME. Toxicity analysis was performed using the Pred-hERG tool for cardiotoxicity evaluation and ProTox-II, allowing the exclusion of molecules with some degree of toxicity. After these analyses, two structures were highlighted: the compounds quinic acid and kaempferol, which proved to be highly compatible molecular targets for our study, as well as being very safe in their toxicological prediction, presenting the highest LD50 values among the studied components and no toxicity found in the other analyses. Additionally, they were shown to be drug-like, characterized by possessing physicochemical properties that make them suitable for therapeutic use. Thus, the bioactive compounds found in the plant, especially Kaempferol and Quinic Acid, proved to be promising in preliminary studies regarding their therapeutic potential, standing out for their significant biological activities and low toxicity. Therefore, the findings of this study provide a solid basis for future investigations, both *in vitro* and *in vivo* , using isolated molecules from the studied phytotherapeutic to test and prove the anti-inflammatory and gastroprotective actions.
Keywords: Bioactivity, Carobinha, Biological markers, Medicinal Plants.

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Resumo

O Brasil ostenta a mais extraordinária biodiversidade do mundo, com seis biomas distintos abrangendo seu vasto território, incluindo o Cerrado. A espécie *Jacaranda decurrens*, comumente conhecida como “carobinha” ou “caroba”, é usada para o tratamento de certas doenças, incluindo problemas gastrointestinais e condições inflamatórias. Este estudo é uma predição in silico da bioatividade de compostos derivados de plantas. Inicialmente, vinte e cinco moléculas desta espécie foram analisadas, e dezesseis foram selecionadas com base nas maiores pontuações nas análises computacionais. As características farmacodinâmicas das estruturas foram elucidadas usando os servidores de predição PASS da plataforma Way 2 Drug e Swiss Target Prediction, enquanto as características farmacocinéticas foram avaliadas usando SwissADME. A análise de toxicidade foi realizada usando a ferramenta Pred-hERG para avaliação de cardiotoxicidade e ProTox-II, permitindo a exclusão de moléculas com algum grau de toxicidade. Após essas análises, duas estruturas foram destacadas: os compostos ácido quínico e kaempferol, que se mostraram alvos moleculares altamente compatíveis para o nosso estudo, além de serem muito seguros em sua predição toxicológica, apresentando os maiores valores de DL50 entre os componentes estudados e nenhuma toxicidade encontrada nas demais análises. Além disso, demonstraram ser do tipo drug-like, caracterizados por possuírem propriedades físico-químicas que os tornam adequados para uso terapêutico. Assim, os compostos bioativos encontrados na planta, especialmente kaempferol e ácido quínico, mostraram-se promissores em estudos preliminares quanto ao seu potencial terapêutico, destacando-se por suas atividades biológicas significativas e baixa toxicidade. Portanto, os achados deste estudo fornecem uma base sólida para futuras investigações, tanto *in vitro* quanto *in vivo*, utilizando moléculas isoladas do fitoterápico estudado para testar e comprovar as ações anti-inflamatória e gastroprotetora.

Palavras-chave: Bioatividade, Carobinha, Marcadores biológicos, Plantas medicinais.

INTRODUCTION

Natural sources were society's first therapeutic resources for dealing with illnesses and health problems among its inhabitants. Thus, studies and attempts to continue and expand the use of plants and their therapeutic properties have been passed down from generation to generation, extending far beyond preserving family and historical traditions. [1] Medicinal plants are therefore used as a mechanism for expanding resources and advancing the search for diversifying the pharmacological and therapeutic matrix, in the face of problems such as the increase in antimicrobial resistance and the adverse effects of existing drugs, due to their high chemical complexity and great pharmacological potential [2].

In Brazil, this traditional knowledge has been recognized through national public health initiatives. The National Policy on Medicinal Plants and Herbal Medicines (PNPMF), established in 2006, was designed to promote safe, rational, and sustainable access to medicinal plants and phytotherapeutics [3]. In light of this, this public health policy also aims to encourage family farming, generate employment, and develop the entire process, from biodiversity conservation through the industrial process to delivery and commercialization at distribution centers.

Furthermore, the PNPMF and the subsequent creation of the medicinal plants and phytotherapeutic program in 2008, converge towards the regulation and transformation of cultural and ancient knowledge into traditional remedies, but with scientifically proven efficacy, bringing the

viability of combining popular practice with the possibilities of treating patients of the Unified Health System (SUS) and the private network[1-3].

Within this context, the species *Jacaranda decurrens,* endemic to the Brazilian Cerrado biome,stands out. Know locally as “carobinha”, “caroba” and “caroba-fazer campo”[4]. This member of the *Bignoniaceae* family is traditionally used in everyday life to treat infectious processes, gastrointestinal, gynecological, and inflammatory diseases, as well as liver and ulcerative disorders[5]. Therefore, due to the uses mentioned above and the prospective studies, “carobinha” proved to be an interesting object of study for the work that aims to identify anti-inflammatory and gastroprotective markers in *Jacaranda decurrens.*

To explore this potential, *in silico* tools were employed that utilized computational simulations to perform efficient initial screenings and assess the viability of molecules based on their structure, which contributed to the prediction of pharmacological activities and the development of new candidate compounds to be tested in *in vitro* and *in vivo* models.

Accordingly, the present study aimed to perform a computational simulation to investigate potential molecules with anti-inflammatory and gastroprotective properties present in the phytotherapeutic *Jacaranda decurrens* , through predictions of biological activities, identification of pharmacophoric similarities and characterization of bioactive compounds present in this medicinal plant, using molecular modeling tools.

METHODS

This computational study aimed to perform an *in silico* screening of the compounds present in the essential oil of the plant species *Jacaranda decurrens* . The selection of phytochemical compounds was based on a systematic literature review conducted across the ScienceDirect (https://www.sciencedirect.com/) and PubMed (https://pubmed.ncbi.nlm.nih.gov/) databases, using descriptors such as “Jacaranda decurrens ” and “*Chemical Compounds* ”. Only full-text articles published in the last five years were considered. Therefore, of the 28 articles initially identified, 5 were aligned with the research objectives, resulting in the selection of 24 components for further study and analysis of their biological functions. The following compounds were selected for their relevance to the study’s objectives: 2-alpha-hydroxyoleanolic acid, arjunolic acid, caffeic acid, caffeoyl acid, carobic acid, gallic acid, maslinic acid, oleanolic acid, quinic acid, ursolic acid, beta-sistosterol, carobine, kaempferol, kaempferol-3-O-rhamnopyranoside, kaempferol-3-O-rutinoside, lapachol, luteolin, luteolin-7-O-glucoside, quercitin, quercitin-3-O-glucoside, quercitin-pentoside-hexoside, quercitin-hexoside, rutin, and hydroquinone[7-10.]

Several methods and tools were employed to investigate the primary components of Jacaranda decurrens, with the goal of conducting biochemical and functional analyses of the relevant

structures, thereby enabling us to demonstrate the effects of each compound studied on the human organism. This research method will provide a deeper understanding of the therapeutic effects of the molecules, thus assisting in the identification and selection of promising prototypes for new drugs.

Chemical compounds were identified using CANONICAL SMILES codes obtained via PubChem (https://pubchem.ncbi.nlm.nih.gov/). The pharmacodynamic characteristics of the structures were clarified using the PASS prediction[11] [https://www.way2drug.com/ passonline/], Swiss Target Prediction[12] [http://www.swisstargetprediction.ch] servers and the pharmacokinetic characteristics by using SwissADME[13] [http://www.swissadme.ch]. Way 2 Drug , in particular, integrates Pass Prediction servers, which indicate the probabilities of interaction with receptors and associated diseases, filtering molecules with a probability higher than 0.7 (*Pa* > 0.7).

During the study, some molecules were excluded for presenting two or more violations of Lipinski 's Rule of 5 , a practical tool used to assess whether the physicochemical properties of a compound with pharmacological activity are suitable for oral administration [14] . This information was acquired from the Swiss Target software. Thus, the molecular behavior was mapped, and the pharmacological and pharmacokinetic properties of the molecules were identified, revealing which molecules exhibit drug-like behavior, a phenomenon known as "*Druglikeness"*.

In addition to molecular analyses regarding druglikeness behavior, following Lipinski's rules, gastrointestinal absorption properties, permeability across the blood-brain barrier, and the number of inhibited cytochromes P450 were also analyzed. Furthermore, toxicity analysis was performed using the Pred-hERG tool to assess cardiotoxicity and ProTox-II, which allowed the exclusion of more molecules configured with some degree of toxicity to the organism.

RESULTS AND DISCUSSION

Regarding the first descriptions of the use of plants for therapeutic purposes in our country, it was in 1587, with the *Tratado Descritivo do Brasil* , written by Gabriel Soares de Souza, that they were made, containing the description of the products used by indigenous peoples and an account of the arrival of European doctors, making clearer the need to use plants in treatment at that time, "the trees and herbs of virtue"[1].

As a result, it is clear that, from the beginning, Brazilian biodiversity has been the subject of numerous citations highlighting its importance to the local, national, and even global community in terms of health, and has also been portrayed in literary works. "Whoever has a swollen head, bring it here, and I will cure it; with gameleira milk, jatobá resin"[15]. In the book *Urubuquaquá, no Pinhém* , João Guimarães Rosa made one of his most open citations about medicinal plants and also used other works to talk about phytotherapeutics from the backlands, such as in "Sagarana e Grande

Sertão Veredas". The author of the third modernist phase mentioned approximately 964 species, utilizing his knowledge as a diplomat and physician to portray some medicinal effects in a literary manner, without revealing the therapeutic effects, believing that he was protecting regions such as the cerrado. This reveals Brazil's strong relationship with phytotherapeutics in various historical periods[16-17].

In this sense, in 2009 the National List of Medicinal Plants (ReniSUS) was created with 71 species of phytotherapeutic medicinal plants used, forming a list of priority species for research and development, with the aim of directing and increasing the study of native species, and encouraging the production of medicines and scientific productions on this subject[18]. The species *Jacaranda decurrens* is not on the ReniSUS list, showing that the study is promising to add a new species with positive variables for the possible development of a drug, as well as showing new possibilities of species with phytotherapeutic interest for the country and the world. Thus, the National Health Plan (PNS) 2020-2023 aims to increase to 25% the number of municipalities that make the current 12 herbal medicines from the National List of Essential Medicines (RENAME) available in primary health care[16-17], revealing that the country is increasingly interested in disseminating traditional knowledge, popular culture, herbal medicines and medicinal plants as a therapeutic option for all users of the Unified Health System (SUS).

Based on this information framework, *Jacaranda decurrens* is the subject of studies as a whole, from the roots to the leaves, with a focus on its therapeutic properties. Accordingly, regarding the different compounds of the bignoniaceae, we have certain satisfactory and promising results to support and guide this present work. Thus, a study with the leaves of *Jacaranda decurrens* was carried out and its dry extract passed through a chromatographic column that fractionated the sample into 3 parts with methanol. As part of the process, it was noted that two fractions had non-enzymatic oxidative activity linked to the presence of ursolic and oleanolic acids (triptenes) and the third fraction has a higher percentage of glycosylated flavonoids with antioxidant potential by inhibiting the oxidative process of lipoproteins, in addition to inhibiting the production of nitric oxide and tumor necrosis factor[19].

In this perspective, an *in vivo* study with Wistar rats treated with the plant extract of the bark of the root or stem of *Jacaranda decurrens and subjected to the* carrageenan - induced paw edema test, with subsequent analysis of the thickness of the edema and activity of the myeloperoxidase enzyme, showed that the extract of *J. decurrens* presents anti-inflammatory activity. Regarding the root of Bignoniaceae, an in vivo study with Wistar rats subjected to an acute toxicity test revealed that the plant extract in 0.7 L of ethanol/water does not exhibit signs of toxicity up to 2000 mg/kg. Another *in vivo* acute toxicity study carried out with Wistar rats showed that Jacaranda decurrens does not present mortality and signs of toxicity up to the dose of 5000 mg/kg, based on the analysis

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from the macerated extract of the leaf of *J. decurrens* that was initially placed in the solution of 0.8 L of ethanol/water with a yield of 12% and having as test dose 2 and 5 g/kg[21].

Regarding the inflammatory process, there is a clear need to expand studies on less toxic and more selective anti-inflammatory drugs, since the inflammatory response is part of the pathophysiology of several diseases. In this context, the search for new molecular targets that act on the most diverse stages of the process is necessary and important to diversify the medications available to society, since many of those available generate intolerance and systemic toxicity, including gastric toxicity[22].

According to the Brazilian Society of Coloproctology (SBCP), diseases that cause inflammation in the intestine affect approximately five million people worldwide and have no cure. Corroborating the data cited, we have that in Brazil there was a 15% increase in the registration of these pathologies[23]. As such, searching for the chemical compounds and molecular targets of *Jacaranda decurrens* to identify a relationship with its gastroprotective and anti-inflammatory effects is of utmost importance for the continuity of drug discoveries aimed at reducing the harmful effects of general inflammation in the body and its local incidence in the gastric tract.

Moreover, the execution of this project allowed us to investigate the correlation between the structure and activity of chemical compounds reported in the literature on the species *Jacaranda decurrens*. Our objective was to elucidate already known biological action mechanisms and identify possible new mechanisms, using *in silico models* to justify the expected activities of the molecules Kampferol and Quinic Acid. Initially, 25 compounds were selected for study. However, due to toxicological predictions and unsuitability for oral administration, only 10 compounds remained for analysis.

Molecules such as Kaempferol-3-O-rutinoside and Rutin were excluded for presenting two or more violations of Lipinski 's Rule of 5, which evaluates the viability of compounds for oral administration, as shown in Table 1. This rule considers parameters such as molecular weight, number of hydrogen bond donors and acceptors, and octanol -water partition coefficient (log P), being essential to predict the absorption and permeability of compounds[24].

Table 1. Components of *Jacaranda decurrens* according to Lipinski ’s Rule of 5 .

Molecules	Lipinski 's rule of thumb 5
Luteolin	Drug -like; 0 violations
Kaempferol	Drug -like; 0 violations
Arjunolic Acid	Drug -like; 0 violations
Gallic Acid	Drug -like; 0 violations
Caffeic Acid	Drug -like; 0 violations

Quinic Acid	Drug -like; 0 violations
Kaempferol-3-O-Rhamnopyranoside	Drug -like; 1 violation: NHorOH >5
Ursolic Acid	Drug -like; 1 violation: MLOGP>4.15
Caffeoyl Acid	Drug -like; 0 violations
Kaempferol-3-O-Rutinoside	3 violations: MW>500, NorO >10, NHorOH >5
Routine	3 violations: MW>500, NorO >10, NHorOH >5
Quercetin -3-O-Glycoside	2 violations: NorO >10, NHorOH >5
Luteolin-7-O-Glycoside	2 violations: NorO >10, NHorOH >5
Luteolin-7-O-Glycoside	2 violations: NorO >10, NHorOH >6
Lapachol	Drug -like; 0 violations
Hydroquinone	Drug -like; 0 violations
Quercetin	Drug -like; 0 violations
Oleanolic Acid	Drug -like; 1 violation: MLOGP>4.15
Maslinic Acid	Drug -like; 1 violation: MLOGP>4.15
2 Alpha Hydroxyoleanolic Acid	Drug -like; 0 violations

Source: Prepared by the authors based on Karami, 2022.

Lapachol and beta- sitosterol were ruled out because of their high probability of being cardiac blockers, as indicated by the Pred-HERG prediction in Table 2. This predictive model is crucial for assessing the risk of chemicals causing cardiac arrhythmias, a significant limiting factor in new drug discovery[25-26]. In addition, oleanolic acid and maslinic acid were ruled out because of their high probabilities of toxicity, as indicated by the toxicology prediction report.

Table 2. Prediction of toxicity of *Jacaranda decurrens* components according to the Pred-HERG tool.

Name	Binary Prediction	Reliability	Weighted Consensus	Multiclass Prediction	Reliability
Quercetin	Non-blocking	93.82	Non-blocking	Weak blocker	34.3
Luteolin	Non-blocking	84.43	Non-blocking	Moderate blocker	34.3
Kaempferol	Non-blocking	81.29	Non-blocking	Weak blocker	33.3
Arjunolic Acid	Non-blocking	95.39	Non-blocking	Weak blocker	37.1
Gallic Acid	Non-blocking	99.99	Non-blocking	Weak blocker	40.19
Caffeic Acid	Non-blocking	99.64	Non-blocking	Non-blocking	33.0

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Lapachol	Blocker	69.73	Non-blocking	Weak blocker	32.03
Quinic Acid	Non-blocking	99.72	Non-blocking	Non-blocking	51.1
Kaempferol-3-O-Rhamnopyranoside	Non-blocking	89.54	Non-blocking	Weak blocker	45533
Ursolic Acid	Non-blocking	94.85	Non-blocking	Weak blocker	39.6
Oleanolic Acid	Non-blocking	98.47	Non-blocking	Weak blocker	35.2
Maslinic Acid	Non-blocking	91.17	Non-blocking	Non-blocking	33.2
Caffeoyl Acid	Non-blocking	98.73	Non-blocking	Weak blocker	36.52
2 Alpha Hydroxyoleanolic Acid	Non-blocking	87.63	Non-blocking	Non-blocking	39.6
Beta- Sitosterol	Blocker	60.8	Blocker	Moderate blocker	36.37
Hydroquinone	Non-blocking	99.96	Non-blocking	Non-blocking	46.59

Source: Prepared by the authors based on Braga, 2015.

The potential toxicity of these compounds was assessed in Table 3 using the ProTox-II tool, which considers multiple toxicological parameters, including hepatotoxicity, genotoxicity and reproductive toxicity. The ProTox-II server is a machine learning model-based tool that predicts the toxicity of chemicals based on their molecular structures, providing a comprehensive and accurate assessment of toxicological risk[27–29].

Table 3. Selected compounds from *Jacaranda decurrens according to the* ProTox II tool

Compounds	**Activity**	**Probability**
Kaempferol	**Activity**	**Probability**
Aryl Hydrocarbon Receiver (Ahr)	Active	1.0
Aromatase	Active	0.96
Estrogen Receptor Alpha (Er)	Active	1.0
Estrogen Receptor Ligand Binding Domain (Er- Lbd)	Active	0.95
Mitochondrial Membrane Potential (Mmp)	Active	1.0
Phosphoprotein (Tumor Suppressor) P53	Active	1.0
Quinic Acid	**Activity**	**Probability**
No Active Toxicological Activity		

Source: Prepared by the authors based on Banerjee, 2018.

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Hydroquinone and Quercetin showed extremely low LD50 (Median Lethal Dose) values, indicating high toxicity, as shown in Table 4. The LD50 represents the amount of a chemical substance that, when administered in a single oral dose, causes the death of 50% of the exposed animals within a period of observation. Low LD50 values are indicative of high acute toxicity, making these compounds unsuitable for safe therapeutic use[30]. Subsequently, an individual study was carried out to identify molecules with greater compatibility for targets of gastroprotective and anti-inflammatory biological function.

Table 4. Components of *Jacaranda decurrens* according to their Median Lethal Dose (LD50)

Molecules	LD50 Expected
Luteolin	3919mg/kg
Kaempferol	3919mg/kg
Arjunolic acid	2000mg/kg
Gallic acid	2000mg/kg
Caffeic acid	2980mg/kg
Quinic Acid	9800mg/kg
Kaempferol-3-O-rhamnopyranoside	5000mg/kg
ursolic acid	1000mg/kg
Caffeoyl acid	3800mg/kg
Lapachol	680mg/kg
Beta- sitosterol	890mg/kg
Hydroquinone	225mg/kg
Quercetin	159mg/kg
Oleanolic acid	2000mg/kg
Maslinic acid	2000mg/kg
2 alpha acid hydroxyoleanolic	3400mg/kg

Source: Prepared by the authors based on Friedman, 1985.

This study involved the detailed analysis of each remaining compound, considering their pharmacokinetic and pharmacodynamic properties, as well as their molecular interactions with specific biological targets. Through this approach, it was possible to select the most promising

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compounds for future preclinical and clinical investigations, aiming at the development of new drug prototypes.

Arjunolic acid has demonstrated significant potential to protect the intestinal epithelial barrier and improve Crohn 's disease-like colitis . This compound restored the composition of the intestinal microbiota and inhibited Toll-like receptor 4 (TLR4) signaling, resulting in reduced production of inflammatory cytokines such as IL-1β, IL-6, and TNF-α[31]. Gallic acid increased the expression of Nrf2 and HO-1, suggesting that activation of this signaling pathway is crucial for gastric protection. Furthermore, there was a decrease in the expression of pro-apoptotic proteins (Bax and Caspase-3) and an increase in the expression of anti-apoptotic proteins (Bcl-2). Gallic acid treatment also resulted in a reduction of gastric juice acidity and an increase in gastric mucus production, contributing to the protection of the gastric mucosa, especially against ulcers[32]. Caffeic acid is known for its high antioxidant and anti-inflammatory potential. Studies have shown that caffeic acid can modify lipopolysaccharides, which are primarily involved in inflammatory responses[33]. Ursolic acid has also been shown to have significant anti-inflammatory properties. Studies indicate that it can inhibit the production of inflammatory mediators, such as pro-inflammatory cytokines, and the NF-κB pathway, which is linked to inflammatory processes[34]. No significant studies on the biological activities of interest for caffeoylquinic acid were found.

In this context, a "*drug -like*" molecule is characterized by having physicochemical properties that make it suitable for therapeutic use, including chemical stability, solubility, bioavailability and a favorable distribution profile in the human body[35], a factor that was also preponderant in the choice of the molecules for analysis and was measured in Table 5. After excluding unsuitable compounds, the biological studies of the remaining compounds identified two main candidates with high compatibility for targets related to gastroprotective and anti-inflammatory biological functions: quinic acid and kaempferol-3-O-rhamnopyranoside.

Table 5. Components of *Jacaranda decurrens* according to drug -like assessment.

Molecules	GI absorption	Permeability in the BBB	CYP1A2 Inhibitor	CYP2C19 Inhibitor	CYP2C9 Inhibitor	CYP2D6 Inhibitor	CYP3A4 Inhibitor
Quercetin	High	No	Yes	No	No	Yes	Yes
Luteolin	High	No	Yes	No	No	Yes	Yes
Kaempferol	High	No	Yes	No	No	Yes	Yes
Arjunolic Acid	High	No	No	No	No	No	No
Gallic Acid	High	No	No	No	No	No	Yes
Caffeic Acid	High	No	No	No	No	No	No
Lapachol	High	Yes	Yes	Yes	No	No	No

Quinic Acid	High	Yes	Yes	Yes	No	No	No
Kaempferol-3-O-Rhamnopyranoside	Low	No	No	No	No	No	No
Ursolic Acid	Low	No	No	No	No	No	No
Oleanolic Acid	Low	No	No	No	No	No	No
Maslinic Acid	High	No	No	No	No	No	No
Caffeoyl Acid	High	No	No	No	No	No	No
2 Alpha Hydroxyoleanolic Acid	High	Yes	No	No	No	No	No
Beta- Sitosterol	Low	No	No	No	No	No	No
Hydroquinone	High	Yes	No	No	No	No	Yes
Kaempferol-3-O-Rutinoside	Low	No	No	No	No	No	No
Routine	Low	No	No	No	No	No	No
Quercetin -3-O-Glycoside	Low	No	No	No	No	No	No
Luteolin-7-O-Glycoside	Low	No	No	No	No	No	No
Luteolin-7-O-Glycoside	Low	No	No	No	No	No	No

Source: Prepared by the authors based on Clauss and Abbehausen, 2021.

Quinic acid proved to be a highly compatible molecular target for our study, as it is very safe in its toxicological prediction, presenting the highest LD_{50} values among the components studied, and no toxicity was observed in the other analyses. However, this component exhibits permeability at the blood-brain barrier and contains cytochromes that enhance its metabolism, such as CYP1A2 and CYP2C19. The results indicated that quinic acid has significant anti-inflammatory activity, helping to reduce inflammation in the colon of rats. This compound demonstrated gastroprotective properties, alleviating the symptoms of ulcerative colitis and inhibiting the production of inflammatory mediators, such as cytokines and prostaglandins, which are responsible for the inflammatory response in the body.

Quinic acid acts by inhibiting the production of inflammatory mediators, such as pro-inflammatory cytokines (e.g., TNF-α, IL-1β, and IL-6). These cytokines are responsible for amplifying the inflammatory response and, when inhibited, inflammation is reduced. In addition, quinic acid protects cells against inflammatory damage, promoting cellular integrity and helping in the recovery of damaged tissues.

Kaempferol (KAE), together with its subtype kaempferol-3-O-rhamnopyranoside, was also identified as a target compatible with our research. This compound presented a high LD50 value

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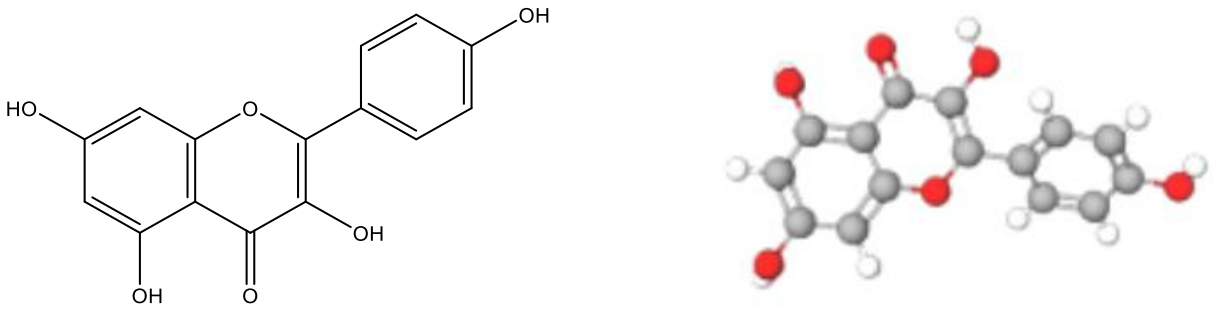
(5000 mg/kg), indicating low toxicity. Furthermore, it is not metabolized by the aforementioned cytochromes and does not cross the blood-brain barrier, despite having a lower absorption capacity via the gastrointestinal route.

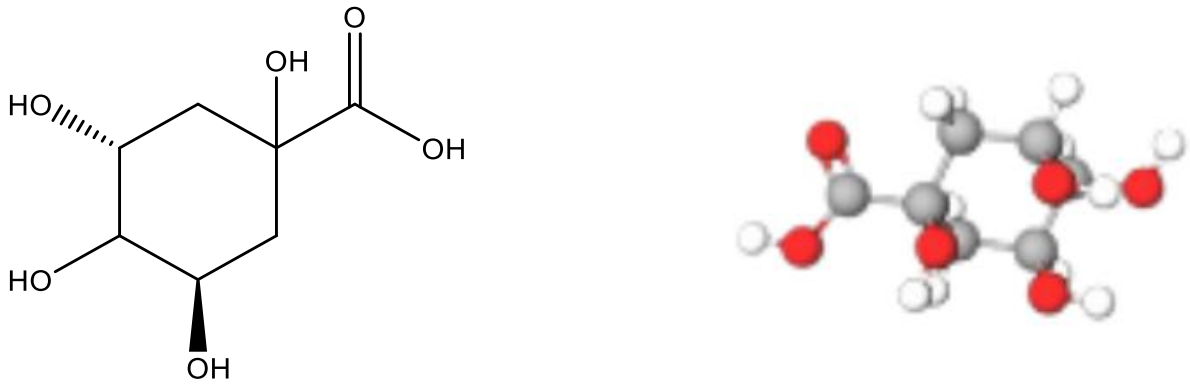
The gastroprotective activity of KAE can be attributed to the preservation of gastric mucosal glycoprotein levels, inhibition of neutrophil accumulation and myeloperoxidase (MPO) activity, adjustment of pro-inflammatory cytokine levels and improvement of nitric oxide production. The compound showed effects comparable to omeprazole, a proton pump inhibitor widely used to treat gastric ulcers, presenting itself as a promising treatment alternative with fewer side effects compared to current clinical drugs[36]. Thus, the most promising compounds are depicted in their molecular forms in figures 1 and 2.

Figure 1. 2D and 3D representation of the kaempferol molecule.



Source: Prepared by the authors with the help of Molview, 2014

Figure 2. 2D and 3D representation of the quinic acid molecule.



Source: Prepared by the authors with the help of Molview, 2014

CONCLUSION

The development of this research allowed us to explore the relationship between the structure and activity of the chemical compounds documented in the literature on the species *Jacaranda decurrens* . As a result, the bioactive compounds found in the plant, particularly Kaempferol and Quinic Acid, have shown promise in preliminary studies regarding their therapeutic potential, standing out for their significant biological activities and low toxicity. Therefore, the findings of this study provide a solid basis for future investigations, both *in vitro* and *in vivo* models, using molecules isolated from the studied phytotherapeutic to test and prove the anti-inflammatory and gastroprotective actions. Consequently, these investigations may deepen the understanding of the molecular mechanisms underlying the observed therapeutic properties, contributing to the scientific validation and potential inclusion of this species in the National List of Medicinal Plants (ReniSUS).

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