

**ANTICANCER ACTIVITY OF AMINOCHALCONES. SCIENTIFIC And
TECHNOLOGICAL PROSPECTING**

**ATIVIDADE ANTICANCER DE AMINOCHALCONAS. PROSPECÇÃO
CIENTÍFICA E TECNOLÓGICA**

**ACTIVIDAD ANTICANCERÍGENA DE AMINOCHALCONAS. PROSPECTIVA
CIENTÍFICA Y TECNOLÓGICA**



<https://doi.org/10.56238/sevened2026.020-021>

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ABSTRACT

Chalcones are a group of polyphenolic compounds derived from plants that exhibit a wide variety of biological activities, notably their cytotoxic capacity. The aim of the present study is to describe available articles regarding the cytotoxic characteristics of aminochalcones, and analyzed patent deposits this theme. The research was conducted by searching for the terms "Aminochalcones" AND/OR "cancer" "Biological action" AND/OR "Technological prospecting" in the Medical Subject Headings (MeSH) database as equated terms referring to the toxicological properties of aminochalcones. Patentaries bases using INPI, EPO, USPTO e WIPO was used to research inovation and Tecnology. Out of the 2,179 articles, only 10 were selected, with 2015 being the year of highest scientific productivity. Regarding patents, China ranks first, so out of the 112 patents observed, only 7 stand out due to their methodological relevance and innovations. The majority of researchers do not request patent deposits for the toxicological activity containing the study's technology. Patents, in summary, create favorable environments for the scientific and technological development of a country. Based on the data obtained, it is inferred that the quantity of publications regarding the anticancer properties of chalcones has increased over time; however, such compounds still have limited investigations, despite holding potential anticancer properties.

Keywords: Chalcones. Cytotoxicity. *In vitro*. Anticancer.

RESUMO

As chalconas são um grupo de compostos polifenólicos derivados de plantas que possuem uma ampla variedade de atividades biológicas, destacando-se sua capacidade citotóxica. O

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objetivo do presente estudo é descrever sobre artigos disponíveis a respeito das características citotóxicas de aminochalconas e análise dos depósitos de patente nesta temática. A pesquisa foi realizada por meio da busca dos termos: “Aminochalcones” AND/OR “cancer” “Biological action” AND/OR “Technological prospecting” usando o Medical Subject Headings (MeSH) como termos equacionados referentes às propriedades toxicológicas das aminochalconas. As bases patentárias INPI, EPO, USPTO e WIPO foram usadas para pesquisa de tecnologia e inovação. Dos 2.179 artigos, apenas 10 foram selecionados, sendo 2015 o ano de maior produtividade científica. Quanto às patentes, a China ficou em primeiro lugar como depositária, de forma que das 112 patentes avaliadas, apenas 7 se destacaram pela relevância metodológica e inovações. Com base nos dados obtidos, infere-se que a quantidade de publicações acerca das propriedades anticâncer das chalconas aumentou ao longo do tempo, todavia, tais compostos ainda apresentam investigações limitadas, mesmo detendo potencial propriedade anticancerígena.

Palavras-chave: Chalconas. Citotoxicidade. *In vitro*. Anticâncer.

RESUMEN

Las chalconas son un grupo de compuestos polifenólicos derivados de plantas que presentan una amplia variedad de actividades biológicas, destacándose su capacidad citotóxica. El objetivo del presente estudio es describir los artículos disponibles acerca de las características citotóxicas de las aminochalconas y analizar los depósitos de patentes en esta temática. La investigación se realizó mediante la búsqueda de los términos: “Aminochalcones” AND/OR “cancer” “Biological action” AND/OR “Technological prospecting”, utilizando los Medical Subject Headings (MeSH) como términos estandarizados relacionados con las propiedades toxicológicas de las aminochalconas. Las bases de datos de patentes INPI, EPO, USPTO y WIPO fueron utilizadas para la prospección tecnológica y de innovación. De los 2.179 artículos identificados, solo 10 fueron seleccionados, siendo 2015 el año de mayor productividad científica. En cuanto a las patentes, China ocupó el primer lugar como principal solicitante, de modo que, de las 112 patentes evaluadas, solo 7 se destacaron por su relevancia metodológica e innovaciones. Con base en los datos obtenidos, se infiere que la cantidad de publicaciones sobre las propiedades anticancerígenas de las chalconas ha aumentado con el tiempo; sin embargo, estos compuestos aún presentan investigaciones limitadas, a pesar de su potencial propiedad anticancerígena.

Palabras clave: Chalconas. Citotoxicidad. *In vitro*. Anticancerígeno.

1 INTRODUCTION

The World Health Organization (WHO) reported that 65-80% of the population in developing countries depended on medicinal plants as the only form of access to basic health care (OKPUZOR et al., 2021). Nature is characterized as the best source of medicines, where most modern pharmaceuticals are derived or inspired by medicinal plants (FANG et al., 2021)

Plants containing chalcones have long been used in clinical practice and continue to expand rapidly around the world. The first chalconic structures were isolated from plant species in 1910, being present in the families Asteraceae, Moraceae, Fabaceae and Aristolochiaceae (IWASHINA T, 2000).

Chalcones are a group of polyphenolic compounds that have a wide variety of biological activities, and were discovered by Alexander Borodin in 1869, who isolated it from the Chinese licorice, Glycyrrhizainflate. Subsequently, chalcones were recognized by numerous researchers for their clinical applications that led to other synthetic and natural chalcones such as Butein, Boesenbergine A, and Lophirona B (RANI et al., 2019; DAN; DAI, 20206; JASIM, 2021). The literature describes aminochalcones as promising agents with antitumor (KALMOUCH et al., 2020), antimicrobial (EL-MESSERY et al., 2018), antioxidant (MPHAHLELE; AGBO; CHOONG, 2021), antiproliferative (LU et al., 2020), cytotoxic (DIMMOCK et al., 2003) and antiparasitic (DE BRITO et al., 2022).

The cytotoxic activity of aminochalcones, a group of mattresses, has been an area of interest due to the possibility of an increased electrophilic attack on cellular proteins through covalent bonds. Covalent inhibitors are an emerging area of drug discovery, and aminochalcones have the potential to serve as clues for the development of inhibitors that target specific cellular proteins (MPHAHLELE; AGBO; CHOONG, 2021; ZHOU; PARADIES, 2021).

The most studied aminochalcone contains an NH₂-substitution at position 4 on ring A. The amino group on ring A increases the magnitude of the positive charge on the olefin carbon atom adjacent to ring B (PARK D Y et al., 2018; LEE S Y, CHEON C H, 2018). This has been proposed to increase the electrophilic attack of these compounds on cancer cells (CHELGHOUM M et al., 2012).

In this sense, the present study aimed to describe the available articles regarding the cytotoxic characteristics of aminochalcones.

2 METHODOLOGY

This is a scientific and technological prospecting study, where the following terms were chosen from the Medical Subject Headings (MeSH) database: "Aminochalcones" AND/OR "cancer" "Biological action" AND/OR "Technological prospecting" as terms equated referring to the toxicological properties of aminochalcones.

Non-original studies, duplicates, reviews, articles not available in full, as well as research whose theme did not address the toxicological and anticancer properties of aminochalcones were excluded.

To carry out the scientific study and technological prospecting, a search was made in the PubMed, Science Direct and Web of Science databases. For the search for technologies and innovations, a search was made in the INPI, EPO, USPTO and WIPO databases.

3 RESULTS

The scan of the databases revealed a total of 2,179 articles, however, the articles presented information only about chalcones in isolation. Thus, only 10 articles were selected (Table 1)

Table 1

Main information found in the scientific articles

Author/Year	Type of study	Objective	Considerations and results
Xia et al (2000)	In Vitro (Cell Culture)	Identify the design, synthesis and biological evaluation of 2'-amino chalcone	Discovery of a new class of 2'-amino chalcones as potential antitumor agents in cell lines of: Human squamous cell carcinoma of the nasopharynx (KB); human squamous cell carcinoma of the nasopharynx expressing PGP (KB-VIN); osteosarcoma (Hos); human melanoma (SKMEL-2); human ileocecal carcinoma (HCT-8); human breast cancer (MCF-7), human lung adenocarcinoma (A-549) and human ovarian cancer (1A9).
Dimmock et al (2003)	In Vitro (Cell Culture)	To evaluate the cytotoxic activity of 4'-aminochalcones	The cell lines were: human Molt 4/C8 T lymphocytes and EMFs, as well as P388 and L1210 murine leukemia cells. It was observed that aminochalcone presented a selective toxicity to tumor strains.
Abuo-rahma et al (2012)	In Vivo (Rats)	To evaluate the anti-inflammatory effects of chalcone-releasing hybrids of the amino group in the presence of ulcers.	Significant anti-inflammatory activity using carrageenan-induced adult male albino rat paw edema method compared to indomethacin.
Prasad; Rani; Rao (2013)	In vitro	To evaluate the antioxidant activity of a series of 4'-aminochalcones replaced.	Antioxidant activity of chalcones 9 and 10 composed of 3,4,5-trimethoxyphenyl and 4-dimethylaminophenyl as B-ring moieties of chalcones, respectively, exhibited maximum activity in various antioxidant assays, which may be due to free radical scavenging activity.

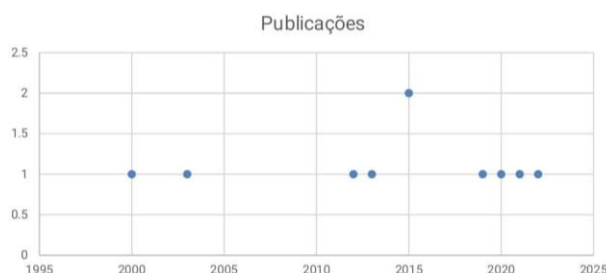
Ruanwas; Chantrapromma; Fun (2015)	In Vitro	To evaluate the synthesis, characterization, antioxidant and antibacterial activities of 2-Aminochalcones	Compound 1 ((2E)-1-(2-aminophenyl)-3-phenyl-2-propen-1-one), which does not have a substituent group in the B ring, showed the highest antioxidant activity with 18.71% inhibition of free radical production.
Radhakrishnan et al (2015)	<i>In Vitro</i> (Cell Culture)	To evaluate the synthesis and biological evaluation of hydroxy-substituted aminochalcone for antityrosinase activity in B16 cells	Compounds inhibited melanin production and tyrosinase activity in B16 cells.
Novilla et al (2019)	In Vitro (Cell Culture)	To evaluate the anticancer activity and selectivity of seven chalcone derivatives against the K562 and HL-60 leukemia cell lines.	The study revealed that the number and position of methoxy groups in chalcone derivatives influenced selectivity for leukemia cells.
Lu et al (2020)	In Vitro (Cell Culture)	To investigate fourteen effective chalcone derivatives with anticancer activity.	Some of the compounds showed moderate to good activity against three human tumor cells (human gastric carcinoma cells - MGC-803, human cervical cancer - HCT-116 and human breast cancer - MCF-7) and compound 13e ((E)-4-chloro-N-(4-(3-oxo-3-(3,4,5-trimethoxyphenyl)prop-1-en-1-yl) phenyl) butanamide) exhibited the best antiproliferative activity against such cells.
Oyenehin et al (2021)	In Vitro (Cell Culture) and in Silico (MCF-7 Breast Cancer)	To investigate Aminochalcone derivatives as antiproliferative agents against MCF-7 Breast Cancer Cell Lines	All molecules were free of cytotoxicity, as well as the standard drug, 5-Fu (fluorouracil).
De Brito et al., (2022)	In Vitro (Cell Culture) and in Silico	Perform a structural and spectroscopic analysis and antiproliferative activity of chalcone derivative (E)-1-(4-aminophenyl)-3-(benzo[b]thiofen-2-yl)prop2-en-1-one	Regarding activity against <i>T. cruzi</i> , the compound exhibited more activity in the trypomastigote forms than in the epimastigote forms, with lower toxicity in the LLC-MK2 host cells. In addition, it had a more potent inhibitory effect than benznidazole.

Source: The authors.

When observing the number of articles per year, it was shown that in 2015 there was a higher productivity (Figure 1).

Figure 1

Distribution of the quantity of articles



Source: The authors.

Table 2

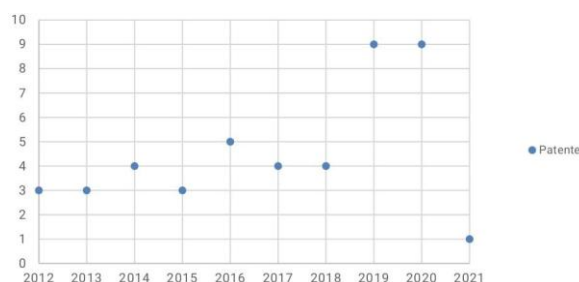
Patents of the research technology in the abstract field, in the INPI, EPO, USPTO and WIPO databases

Keyword	INPI	EPO	USPTO	WIPO
<i>Amino chalcone</i>	0	5	16	122
<i>Amino chalcone/aminochalcone</i>	0	0	0	0

Source: The authors.

Figure 2

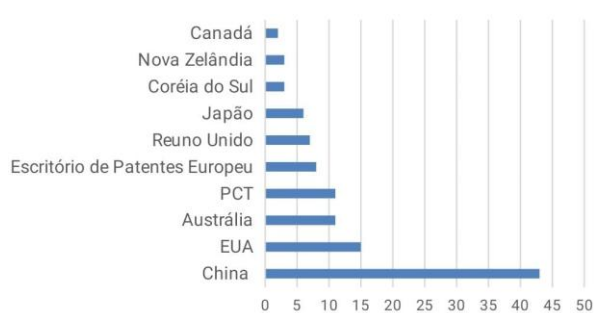
Distribution of the number of patents per year



Source: The authors.

Figure 3

Distribution of patents by countries and patent production institutions



Source: The authors.

Table 3

Main innovations proposed by the patents filed

Patent Number/ Owner	Title	Innovation
201811030086/ Awasthi Satish Kumar	Novel hybrid 1,2,4,5-tetraoxane and analogs as antimalarial drugs	Incorporation of amino chalcones into tetraoxanes for the production of hybrid drugs, in order to increase their solubility in protic solvents. Sodium triacetoxyborohydride efficiently used as a reducing agent in the synthesis of novel tetraoxane-chalcone hybrid analogues.
201811030086/ Awasthi Satish Kumar	Novel hybrid 1,2,4,5-tetraoxane and analogs as antimalarial drugs	It refers to the novel hybrid antimalarial analogues 1,2,4,5 - tetraoxane - amino chalcones and the method of preparation. Hybrid analogues were synthesized by an economic synthesis method
0328669/ Hayashi Akio	Chalcone derivative compounds	Chalcone-derived compounds represented by the general formula (I) or (II), where R1 and R2 each represent a halogen atom, a hydroxy group, an amino group, a dimethylamine group, a nitro group, a cyan group, a phenyl group, an acetyl group, an alkyl group containing 1 to 18 carbon atoms, or an alkoxy group containing 1 to 22 carbon atoms, N1 and N2 each represent an integer from 0 to 21, and m1 and m2 each represent an integer from 0 to 5.
1020200142470 Lee EungSeok	Novel 1-tetralone chalcone-based compound, and composition for preventing or treating inflammatory diseases and containing same as active ingredient	The present invention refers to a new compound based on 1-tetralone chalcone and a composition for the prevention or treatment of inflammatory diseases and containing it as an active ingredient. A compound derived from 6-amino-1-tetralone chalcone according to the present invention is represented by the chemical formula 1. In chemical formula 1, R is selected from halogen, trifluoroalkyl C1-C4 and trifluoroalkoxy C1-C4. According to the present invention, a composition can be provided to prevent, relieve or treat inflammatory diseases.
108863930/ Gao WenChao	Synthetic method of 3-sulfo-2,3-dihydroquinoline-4(1H)-ketone compounds	It describes a synthetic method of 3-sulfo-2,3-dihydroquinoline-4(1H)-ketone compounds and pertains to organic synthesis. Taking amino chalcone as raw material and having diethyl boron ether trifluoride as catalyst, an electrophilic sulfur reagent is used to induce amino chalcone to perform the intramolecular reaction of electrophilic cyclization.
1506157/ Nielsen Simon Feldbaek	Amino-chalcones functional	The invention provides novel derivatives of functional amino chalcones and their analogues. The use of compounds, or compositions that comprise them as pharmaceutically active agents, in particular against bacterial and parasitic infections, is also disclosed. The invention also refers to a method for detecting

inhibitory effects against, for example, bacteria, parasites, fungi, and helminths.

109232621/ Shaojinjun	Preparationmethod substituted fluoroboratefluorescentnearinfrareddye	for	amino aza-	The invention corresponds to an organic photoelectric functional material and specifically describes a method of preparation of a BODIPY aza based near-infrared fluorescent dye and application of the near-infrared fluorescent dye for Hg ²⁺ detection, cell imaging and biomarker. The material is a near-infrared micromolecular dye based on BODIPY aza, and the wavelength of near-infrared absorption and emission is adjusted by the change of the Ar group. The material can be used as fluorescent material in the near infrared and has good application prospects in ion detection, cell imaging, and biomarker.
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Source: The authors.

4 DISCUSSION

In vivo tests, aminochalcones showed activity for the treatment of gastric and duodenal ulcers, bronchial asthma, poisoning by food and medications, and skin diseases such as eczema and urticaria, as well as relief of rheumatic pain and other types of pain and healing effect on ulcers, as well as anti-inflammatory activity. (ABUO-RAHMA et al., 2012).

In vitro studies have demonstrated improved antiproliferative activity of chalcones with amino substituted groups (XIA Yi et al., 2000) corroborating with the studies of Radhakrishnan et al. (2015) who demonstrated that methoxylated chalcones with a 3'-amino group had submicromolar mean inhibitory concentration values against murine melanoma B16 cells and Novilla et al. (2019) in evaluating the anticancer selectivity of chalcone derivatives in K562 and HL-60 leukemia cell lines.

Research proposes that the presence of the amino function increases the reactivity of chalcones as Michael acceptors. The electron-removing effect of the protonated ammonium function would increase the electrophilicity of the β carbon at the ninth bond, thus increasing its reactivity as a Michael acceptor, when evaluated the cytotoxic activity of 4'-aminochalcones (DIMMOCK J. R. et al., 2003)

Studies conducted in vitro and in silico, Oyenehin et al. (2021) showed that some aminochalcone derivatives were obtained through the functional density theory; some of the optimized molecules were also anchored to the active site of a human serine/threonine-protein kinase receptor, 3FC2, to obtain their binding affinities.

De Brito et al. (2022) in *In vitro* and *In Silico* research evidenced antiproliferative activity in LLC-MK2 host cells. Aminochalcone showed cytotoxicity at the concentrations tested, and was described by the authors as a potent candidate for the development of a new option for the treatment of Chagas disease.

According to studies conducted by Ruanwas et al. (2015), in a DPPH assay on aminochalcones, proved their ability to scavenge free radicals. The mentioned activity was satisfactory and comparable to that of ascorbic acid, a reference compound known for its high antioxidant properties when evaluated in 4'aminochalcones substituted in studies carried out by Prasad et al, 2013.

To carry out an analysis on the most appropriate prospection, a good number of patents must be observed, the fact that aminochalcones have a relatively low value of patents may be related to their relatively recent innovation and discovery as an anticancer agent¹¹ (LU, C. F. et al, 2020)

When comparing the number of articles published with the data in Table 1, in relation to the number of patent documents published, it can be observed that most of the research related to aminochalcones is published in the form of articles and researchers do not request patent applications. Table 2 presents all the keywords searched in their respective patent search databases.

Initially, the results observed in the global database (WIPO) were analyzed, in which the largest number of patents was obtained, a number of 112 patents, through the platform it was only possible to observe the patents distributed in the 2012-2021 time interval by eight countries, a cooperative (PCT-Treaty of Patent Cooperatives) and a European patent office.

The distribution among the countries showed a concentration of patents located in China, with a total of 43 patents, followed by the USA with 15 of the productions and in third is Australia and the Patent Cooperation Treaty (PCT) with 11 publications of each.

The present research showed that it is necessary to reflect on the role of patents in technological development, both in increasing the market potential and in research in general.

The largest producers of the most relevant patents, observed by the WIPO database, stand out, with a total of five major producers, highlighting Emmerling Michael e Spangenberg German who have filed a total of 10 patents each.

Patents, in short, create favorable environments for the scientific and technological development of a country, hence the importance of prospecting studies.

5 CONCLUSION

Based on the data obtained, it is inferred that the number of publications on the anticancer properties of aminochalcones has increased over time, however, these compounds still have limited investigations and the number of in vitro studies exceeds the in vivo results. The position of the substitutions in the amino group in chalcones influences the selectivity in cancer cell lines. China and the US are the champions in patent filings when it comes to production efficiency. The use of aminochalcones as an antitumor potential depends on designs that seek to unravel their properties, minimize unwanted interactions, and carry out further experiments to prove their pharmacological effects and possible future use in clinical studies.

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