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Anthraquinone derivatives pdf

Anthraquinone derivatives examples. Anthraquinone derivatives. Anthraquinone. Types of derivatives pdf.

Anthraquinones are a class of natural and synthetic compounds with diverse applications and have been utilized for centuries for medical purposes. These compounds exhibit various pharmacological actions such as antioxidant, anti-inflammatory, and anticancer properties, making them valuable tool compounds for biochemical and pharmacological studies. The quinone moiety in anthraquinones raises safety concerns, leading to critical reassessment of their use as laxatives. This review article provides an overview of the chemistry, biology, and toxicology of anthraquinones, focusing on their potential as drugs and therapeutic agents. Given article text here ROS can cause various diseases including neurodegenerative disorders, cancer, liver diseases and cardiovascular disease etc. The mechanism of these diseases are ROS mediated. For example in Alzheimer's disease ,the long lasting generation of ROS by amyloid beta peptides causes damage to the brain. Elevated levels of ROS can also damage DNA, transform normal cells into cancerous ones and promote tumor growth. Excessive amount of ROS leads to fibrosis, liver inflammation and hepatocellular carcinoma. Endothelial cells and vascular smooth muscle cells are targets for ROS. High levels of ROS can damage vascular cells, cause proliferation and migration of vascular muscle cells leading to vascular remodeling. Therapeutic strategy involves maintaining the balance of ROS by targeting ROS producing system. Antioxidants such as enzymes like superoxide dismutase and catalase and nonenzymatic antioxidants like polyphenols are studied for their ability to reduce oxidative damage. Natural anthraquinones with antioxidant properties have been found in various plants, they can directly degrade ROS and interact with signaling pathways to reduce oxidative stress. The anthraquinone compounds, renowned for their antioxidant properties, have been extensively reviewed. The primary focus of this work is depicted in Figure 2. Free radicals are ubiquitous in all molecules with unpaired electrons [25]. As aerobic organisms, humans inevitably generate free radicals [26]. Mitochondrial enzymes, NADPH oxidase, nitric oxide synthase, and xanthine oxidase are significant endogenous sources [27-30]. External factors like environmental pollutants, radiation, smoking, and drugs can also contribute to ROS formation [31]. ROS products include hydroxyl radicals, superoxide anions, nitric oxide, and peroxy radicals in radical forms [32], as well as hydrogen peroxide, singlet oxygen, hypochlorous acid, and peroxytrite in nonradical forms [33-34]. ROS have both beneficial and detrimental effects on biological systems [31]. The delicate balance between these two effects is achieved through redox regulation [35]. Oxidative stress arises from the imbalance between antioxidant defenses and intracellular accumulation of ROS [36], which can contribute to life-threatening diseases like Alzheimer's disease, liver injury, and cancer. Consequently, counteracting harmful effects generated by ROS is crucial, achievable through antioxidant use [37]. Metals play a vital role in ROS formation and elimination [38-39]. Metal ions with redox activity, such as iron and copper, are cofactors for various enzymes but can also produce ROS and cause harm [40]. For instance, Fe2+ catalyzes the Haber-Weiss reaction to generate more harmful hydroxyl radicals from superoxide anions [41]. Cu2+ directly causes ROS production and reduces glutathione levels at high concentrations [43]. Zinc is an essential nutrient for maintaining life forms. Zn2+ primarily protects proteins and enzymes from oxidation or inhibits the formation of hydroxyl radicals by hydrogen peroxide through the Fenton reaction [44]. Hydroxyl radicals are the most destructive species in free radical pathology, inducing oxidative damage in almost all cell molecules [45]. A detailed illustration of ROS formation is shown in Figure S1. Living cells contain both low molecular weight antioxidants and enzymes shield cells from damage caused by rogue free radicals, both preventing and repairing harm. These powerful agents can be broadly categorized into two types: preventive antioxidants that neutralize free radicals at the initiation stage, and chain-breaking antioxidants that capture and prevent further propagation of free radical chains. Studies have shown that phenolic compounds possess three primary antioxidant mechanisms: hydrogen atom transfer, single-electron transfer followed by proton transfer, and sequential proton loss and electron transfer. The effectiveness of these mechanisms can be influenced by factors such as bond dissociation enthalpy, ionization potential, and proton affinity potential. Furthermore, the choice of solvent can also impact the preferred reaction pathway, with hydrogen atom transfer often favored in non-aqueous solvents and sequential proton loss and electron transfer in aqueous solutions. A density functional theory approach has been applied to accurately predict the antioxidant activity of various polyphenol extracts and elucidate their structure-activity relationships. By utilizing the density functional theory calculation with the B3LYP hybrid functional and the 6-311++G** basis set, the study revealed that compound 2 demonstrated the lowest HOMO-LUMO energy gap value (Table S1 in Supplementary Materials), indicating its increased propensity to donate electrons and exhibit superior antioxidant activity compared to compounds 2a, 2b, and others. This was attributed to the presence of more electron-donating phenoxy groups in compound 2. Theoretical studies by Jeremic et al. [59] and Markovic et al. [62] employed various methods to investigate the antioxidant capacities of different anthraquinone compounds. The results showed that compounds with hydroxy groups on the ortho position exhibited higher reactivity, while those with three or two hydroxy groups displayed moderate and low antioxidant capacities, respectively. Isin [60] utilized a conductor-like polarizable continuum model to study the free radical scavenging activities of four hydroxyanthraquinones. The order of hydrogen supply capacity was found to be compounds 11 > 12 > 14 > 13, with BDE values indicating that compounds with ortho-hydroxy groups had lower values compared to those with carboxyl groups. Theoretical studies also identified the most active sites for different compounds: 1-OH and 8-OH for compounds 2 and 5, and 3-OH for compounds 1 and 6 [61]. Markovic et al. [62] analyzed the BDE values of all hydroxyl positions in compound 1 to clarify the role of 3-OH in antioxidant properties. The study also evaluated the antioxidant activity of compound 10 theoretically by its BDE and IP values (Table S3 in Supplementary Materials). The results indicated that the free radical scavenging characteristics were well explained by HAT, with a lower IP value for aqueous solution suggesting the SET-PT mechanism was reasonable. In summary, anthraquinone compounds can scavenge various radicals, including •OH, DPPH•, and O2•–, and inhibit lipid peroxide to exert their antioxidant effects. Phenolic Compounds Exhibiting Antioxidant Properties Plant phenols, particularly compounds 1, 2, and 3, have been found to play a protective role in protecting against DNA and mesenchymal stem cell damage induced by •OH. These compounds exhibit antioxidant effects through HAT (hydroxylation at the α-position) and SET-PT (ethylation at the γ-position) mechanisms, which involve the partial oxidation of phenolic hydroxyl groups into stable semiquinone forms. The stability of these semiquinone forms is crucial in determining the protective or antioxidant effect of plant phenols. Studies have shown that compound 1 and 15 can significantly eliminate DPPH• radicals, with a dose-dependent scavenging ability at concentrations of 0.5–100 μM. Compound 10 has also been found to possess high radical scavenging effects, with an IC50 value of 3.491 μg/mL. The number and site of the OH groups in these compounds appear to be primary factors affecting their antioxidant abilities. For instance, the ortho-hydroxyl group in compound 10 reacts with free radicals to form a more stable conjugated semiquinone radical, thereby interrupting the free radical chain reaction and exhibiting stronger antioxidant properties. Compound 5 has also been found to exhibit scavenging effects on DPPH• radicals, although with an IC50 value of 26.56 μg/mL. A comparative study involving compounds 10 and 11 revealed that compound 10 had the greatest scavenging activity, followed by compound 11. The general mechanism for scavenging •OH radicals involves a radical adduct formation process, where a radical adduct with phenol is formed, followed by the elimination of water molecules. Alternatively, scavenging of DPPH• can occur through the abstraction of hydrogen atoms from antioxidants or the transfer of electrons from phenoxide anions to DPPH•. In addition, the lipid peroxidation reaction, which involves the initiation of free radical formation in cells and tissues, has been found to be inhibited by anthraquinone compounds. The order of inhibitory activities was reported to be anthrone compound > 2 > 3> 1 > anthraquinone. However, other reports suggest that these anthraquinone compounds exhibit good antioxidant properties against lipid peroxidation. The research explores the potential benefits of anthraquinone compounds in various biological processes, including oxidative stress reduction, cytotoxicity prevention, and inflammatory inhibition. The studies found that certain compounds could effectively combat cellular damage caused by cisplatin, hydrogen peroxide, or lipopolysaccharide. For instance, Compound 1 was shown to restore GSH and TAC levels, as well as enhance antioxidant enzyme activity in human embryonic kidney cells. Similarly, Compound 2 prevented cytotoxicity in PC12 cells by reducing NO release and ROS accumulation, while Compound 3 increased the viability of HUVECs by downregulating MDA and LDH and upregulating NOS and GSH-PX. Additionally, studies have demonstrated that metal complexes often exhibit enhanced antioxidant activity compared to individual ligands. The combination of traditional Chinese medicine active ingredients with metal ions can produce synergistic effects. Our research found that metal complexes exhibited higher antioxidant activities than the ligand alone. Furthermore, various reports investigated the antioxidant properties of metal complexes of Compound 1, including Cu(II), Fe(II), Zn(II), Mg(II), and Mn(II). The results showed that all these metal complexes displayed higher antioxidant activities than the original ligand. The coordination of the 9-carbonyl group and 1-phenolic hydroxyl group in Compound 1 forms a stable hexacoordinated ring structure with metal ions, enabling the transfer of the active center from the hydroxyl group to the metal ion. The electron donor sites, including C=O and phenolic hydroxyl groups, can be coordinated with metals, leading to the splitting of merged orbitals into different energy levels. Given article text here After absorbing electromagnetic wave energy, electrons can move from low-energy d orbitals to high-energy d* orbitals, producing absorption bands in the visible region. Anthraquinone compounds contain metal chelation sites due to their large π-conjugated system and strong coordination of oxygen atoms. This makes them effective ligands for metal ions to form complexes [50,73]. Studying anthraquinone's structural modifications can improve its antioxidant activity. The type of substituent affects the scavenging ability, mainly by stabilizing free radicals [91]. Comparing compounds 17a and 18, which have different parent structures but the same substituent group, showed that compound 18 had higher antioxidant capacity than compound 17a. This was likely due to the lower electronegativity of sulfur atoms compared to oxygen atoms, resulting in stronger reducing capacity and increased antioxidant activity [92]. Compounds 17a-e share a similar structure with varying R groups, and their antioxidant activities were found to be related to chain length. When phenyl substitution was introduced, the conjugation system between the phenyl group and parent structure increased antioxidant activities due to enhanced n-conjugation [92]. However, compound 17c exhibited lower inhibition due to steric hindrance caused by ortho-substitution [92]. Anthraquinones exhibit a wide range of biological activities and can treat various diseases such as Alzheimer's disease, inflammation, cancer, liver injury, diabetes, gastrointestinal disorders, ulcers, radiation injury, and burns [93-95]. They have strong abilities to scavenge free radicals and prevent oxidative damage to tissues [96]. Although the relationship between antioxidant mechanism and activity in vivo is not fully understood, bioactivity and pharmacokinetic studies provide valuable information. The enhancement of antioxidant enzyme activity may relate to anthraquinones' redox activity or ability to bind specific proteins. Oxidative stress plays a crucial role in Alzheimer's disease development and progression [97]. It disrupts calcium homeostasis and leads to apoptosis, contributing significantly to the pathogenesis of Alzheimer's disease [98]. Clinical studies have reported strong evidence for oxidative stress involvement in Alzheimer's disease. Compound 1 showed inhibition of Aβ42 fibrillogenesis and Aβ-induced toxicity [99]. Chen et al. found that compound 1 has neuroprotective effects by reducing ERK1/2 phosphorylation, decreasing ROS, and protecting mitochondrial function. Tao et al. discovered that compound 2 may have a role in cognitive deficits in a scopolamine-induced amnesia animal model, while increasing SOD, GPX, and acetylcholine but decreasing MDA and acetylcholinesterase activity. This suggests compound 2 might have a neuroprotective effect on Alzheimer's disease by inhibiting acetylcholinesterase and regulating oxidative stress. Zhao et al. found that compound 5 reduced neuronal damage in a mouse middle cerebral artery occlusion model by reducing nitric oxide production and enhancing SOD and manganese-dependent SOD activity. Zhang et al. discovered that compound 5 alleviated hippocampal neuronal injury, decreased MDA levels, and increased SOD and GPX activity in lead-exposed neonatal mice. The study also reported that oxidative stress is associated with carcinogenesis by causing DNA degradation, increasing free radicals, and reducing nuclear factor erythroid 2-related factor 2 signaling. Compound 1, when combined with cisplatin, inhibited the growth of human ovarian and gallbladder carcinoma cells in vivo, possibly through downregulating MRP1 expression. Wang et al. found that compound 1 induced necroptosis by activating JNK signaling pathway and inhibiting glycolysis by downregulating GLUT1 expression. The study also highlighted the role of oxidative stress in liver inflammation, fibrosis, and hepatocellular carcinoma. The antioxidant activities of certain compounds have been connected to the inhibition of contractile effects and the enhancement of diastolic effects related to up-regulation of free radicals, hydrogen peroxidation, and cGMP. Inflammatory responses produce a large amount of reactive oxygen species (ROS) and are associated with various diseases. The NF-κB transcription factor family plays a central role in mediating the inflammatory process and participating in immune responses. Studies have shown that ROS or metals can affect nuclear NF-κB transcription factors, leading to the activation of NF-κB and the subsequent regulation of inflammatory cytokines. Given article text here Rhubarb Decoction Metabolism and Bioavailability The metabolites of rhubarb decoction were identified in rat urine, bile, and plasma. Compounds 1-5 may be metabolized into sulfonated forms. Compound 2 was transformed to glucoside derivatives through hydroxylation, hydrogenation, and glucuronidation. Oxidation increased anthraquinone bioavailability. The order of anthraquinone bioavailability was: compound 3 > compound 1 > compound 5 > compound 2. This may result from compounds 2 and 5 being oxidized to compound 3. Sulfonated forms may decrease oral bioavailability. Anthraquinones are not only phenols but also p-quinones. Oxidation of phenols generates quinones, which undergo enzyme-catalyzed reduction reactions producing semiquinone or hydroquinone. The redox cycle leads to oxidative stress. After oral administration, anthraquinones are absorbed into the blood, combined with glucuronic acid, and transported to various tissues. They undergo oxidation, methylation, esterification, and glycosylation. Anthraquinones have biological activity but low solubility and rapid elimination rate limit their use. Side effects include genotoxicity, nephrotoxicity, and hepatotoxicity. Improving bioavailability through structure modification or drug dosage form changes is necessary for safe and effective clinical applications. Three structural characteristics of anthraquinone compounds are closely linked to their antioxidant activity: the benzene ring and carbonyl group, the number and position of hydroxyl groups, and the position and number of other substituents. The benzene ring is hydrophobic, while the phenolic hydroxyl group is hydrophilic. Anthraquinone compounds can be roughly divided into two types: emodin type and alizarin type. Emodin-type compounds have distributed hydroxyl groups on both sides of the benzene ring, whereas alizarin-type compounds have distributed hydroxyl groups on one side. The antioxidant activity of anthraquinones is mainly related to phenolic hydroxyl groups. There are three main mechanisms: HAT, SET-PT, and SPLET. Experimental results support these mechanisms. The structural characteristics that affect antioxidant activity include the position and number of phenoxy groups, the position of ortho-substitutions, and the carbonyl group on the parent structure. For example, when the carbonyl group is ortho-positioned to the hydroxyl group or the methoxy group is meta-positioned, they act as antioxidant inhibitors and cytotoxic activities. These compounds may have potential therapeutic applications. Structurally diverse metabolites from Ophiorrhiza japonica Bl. and their antioxidant activities in vitro and PPARα agonistic activities in silico were investigated. The results suggest that these compounds may be useful for the development of new drugs. Rubiadin, a promising natural anthraquinone, has been identified as a potential lead compound for drug discovery and development. Its chemistry, biosynthesis, physicochemical, and biological properties make it an attractive candidate for further study. 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Research has shown that antioxidants can help prevent or treat conditions such as Alzheimer's disease, Parkinson's disease, and certain types of cancer. **Natural and Synthetic Antioxidants** Studies have identified both natural and synthetic compounds with antioxidant properties. Natural antioxidants include polyphenols, which have been shown to improve cognitive function by reducing amyloid beta peptide burden in mice. Other natural compounds, such as chromones, coumarins, and flavonoids, have also demonstrated antioxidant activity. Metal ions and Oxidative Stress** The presence of metal ions can lead to oxidative stress, which contributes to the development of various diseases. 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