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*Review*

# Characteristics, Isolation Methods, and Biological Properties of Aucubin

**Kartini Kartini *, Michelle Abigail Irawan, Finna Setiawan and Nikmatul Ikhrom Eka Jayani**

Department of Pharmaceutical Biology, Faculty of Pharmacy, University of Surabaya, Surabaya 60293, Indonesia; michelle.abigail99@gmail.com (M.A.I.); finna@staff.ubaya.ac.id (F.S.); nikmatul.ikhrom@staff.ubaya.ac.id (N.I.E.J.)
* Correspondence: kartini@staff.ubaya.ac.id; Tel.: +62-31-298-1110

**Abstract:** Aucubin is an iridoid glycoside widely spread in the families *Cornaceae*, *Garryaceae*, *Orobanchaceae*, *Globulariaceae*, *Eucommiaceae*, *Scrophulariaceae*, *Plantaginaceae*, and *Rubiaceae*. This review is intended to provide data on the physicochemical characteristics, isolation methods, and biological activities of aucubin and its producing plants. Aucubin is unstable and can be deglycosylated into its aglycone, aucubigenin. Various chromatographic methods (column chromatography, vacuum liquid chromatography, medium pressure liquid chromatography, and high-performance liquid chromatography) have been used together to isolate aucubin, mainly with the stationary phase C-18 and the mobile phase water–methanol solution made in gradients. In vitro and in vivo studies reveal that aucubin has a wide range of activities, including anti-inflammatory, antioxidant, anxiolytic and antidepressant, antidiabetic, antifibrotic, antimicrobial, anticancer, antihyperlipidemic, gastroprotective, cardioprotective, hepatoprotective, retinoprotective, neuroprotective, osteoprotective, and renoprotective. Even though aucubin has been extensively investigated, further research in humans is urgently needed primarily to substantiate the clinical evidence. Moreover, extensive studies on its drug delivery systems will help maximize efficacy and minimize side effects.

**Keywords:** aucubin; biological properties; iridoid; isolation; physicochemical properties



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## 1. Introduction

For clinical and pharmaceutical practices, plants can be used in the form of crude drugs, extracts, extract fractions, and isolates. An isolate is a single compound separated from other compounds in a plant and thus has a distinguishable chemical structure. In medicine, isolates can be administered at doses accurate enough to ensure consistency in their efficacy and safety of use. In addition, isolates may act as lead compounds in developing and discovering new drugs. Active plant compounds are generally secondary metabolites, i.e., organic compounds that do not play a direct role in plant growth but as a defense against the environment, including animals and humans. Some examples of secondary metabolites are terpenoids, essential oils, alkaloids, coumarins, phenolics, and flavonoids [1]. Iridoids belong to the terpenoid group and contain a six-membered ring structure with oxygen atoms fused to a cyclopentane ring. In nature, iridoids commonly exist in the form of a glycoside. There are four major groups of iridoids: simple iridoids, iridoid glycosides, secoiridoids, and bis-iridoids [2,3].

Aucubin is a type of iridoid found in several plant families, particularly *Scrophulariaceae*, *Plantaginaceae*, and *Rubiaceae*, as their chemotaxonomic marker. Aucubin is generally present in plants' leaves, fruits, and stems, but its presence in root wastes has also been reported [4]. Different kinds of biological activity testing, both in vitro using various cell types and in vivo using test animals in varying conditions, have been documented. These studies discovered the potential of aucubin as an anti-inflammatory, antioxidant, anxiolytic and antidepressant, antidiabetic, antifibrotic, antimicrobial, anticancer, antihyperlipidemic, gastroprotective, cardioprotective, and retinoprotective agent [5]. Moreover, numerous

isolation and purification techniques have been conducted to separate aucubin from other groups of compounds and iridoid compounds. This review article provides a detailed description of the physicochemical characteristics, producing plants, isolation methods, and biological activities of aucubin. This study is a literature review that collects data and information from well-published books, the Internet, and journals. The literature search was carried out without being limited by year and it was performed using search engines on PubMed and Google Scholar as well as manual searching of other databases. The comprehensive data presented here can be used for further development of aucubin.

## 2. Physicochemical Characteristics

Aucubin (Figure 1) is an iridoid compound. Based on etymology, the term iridoid means that it is obtained from the volatile monoterpenes iridodial and iridomyrmecin, which compose the defensive secretion of Australian ants from the genus Iridomyrmex. According to its biosynthetic origin, the classical name iridoid refers to natural monoterpenoids, i.e., secondary plant metabolites characterized by a cyclopenta[c]pyranoid skeleton, also called iridane (cis-2-oxabicyclo [4.3.0]-nonane). Iridoids are frequently detected in plants as glycosides and very few as non-glycosidic compounds. Iridoids are liquid or solid compounds that are most stable at normal temperatures and have a crystalline or amorphous structure with high melting points. Most iridoids have a bitter taste. Polar iridoid glycosides are dissolve well in water and alcohols (methanol, ethanol, n-butanol). In contrast, the relative solubility of aglycones in these media is slightly poorer but increases with the number of hydroxyl groups.

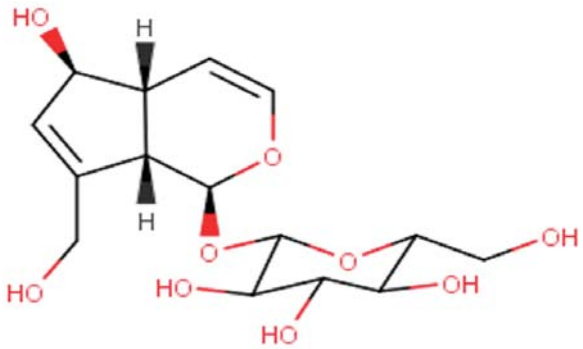


**Figure 1.** Chemical structure of aucubin.

Aucubin has a molecular weight of 346.33 g/mol, a melting point of 181 °C, water solubility of 3.56 × $10^{-5}$ mg/L at 20 °C, and a logP value of −3.49 [6–8]. Aucubin is a glycoside whose aglycone (i.e., aucubigenin) binds to the glucose group using an O-glycosidic bond. Phytochemical screening of aucubin in a plant can be performed with the Trim–Hill color test, and the process is as follows: First, the plant material is cut into small sizes and put into a test tube containing 5 mL of 1% HCl. After 3–6 h, 0.1 mL of the extract was collected and put into another tube containing 1 mL of Trim–Hill reagent (i.e., a mixture of 10 mL of acetic acid, 1 mL of 0.2% $CuSO_4 \cdot 5H_2O$ in water, and 0.5 mL of concentrated HCl). Then, the tube is heated using fire for a short time, and the solution turns blue in the presence of aucubin [9]. Ultraviolet absorption spectra can detect some properties and reactions of aucubin. Generally, aucubin neither reacts with $FeCl_3$, as evidenced by the absence of color change, nor reduces Fehling's solution. However, this substance reduces the Tollens' $AgNO_3$ reagent slowly at cool temperatures and in a few seconds when heated to 100 °C.

The UV spectrum of aucubin in MeOH has $\lambda_{max}$ of 204 nm, and the IR spectrum (KBr) gives $\upsilon_{max}$ between 3629 and 1666 $cm^{-1}$, indicative of O-H and C=C, respectively. Meanwhile, the LC-ESIMS spectrum of aucubin presents m/z of 368 $[M + Na]^+$ calculated for $C_{21}H_{32}O_{13}$. The $^1H$ NMR spectrum (300 MHz, DMSO-$d_6$) shows δ 4.98 (1H, d, H-1),

6.27 (1H, d, *J* = 5.8, H-3), 4.81 (1H, d, *J* = 4.3, H-4), 2.92 (1H, m, H-5), 4.70 (1H, m, *J* = 7.6, H-6), 5.62 (1H, brs, H-7), 2.92 (1H, m, H-9), 3.94 (1H, d, H-10a), 4.14 (1H, d, H-10b), 4.48 (1H, d, *J* = 7.8, H-1′), 3.12 (1H, d, H-2′), 3.41 (1H, H-3′), 2.98 (1H, dd, H-4′), 3.35 (1H, m, H-5′), 3.64 (1H, d, H-6′a), and 3.90 (1H, H-6′b), and the $^{13}$C NMR spectrum (75 MHz, DMSO-$d_6$) shows δ 97.5 (C-1), 141 (C-3), 105.9 (C-4), 46.1 (C-5), 82.0 (C-6), 130.7 (C-7), 147.9 (C-8), 47.9 (C-9), 61.0 (C-10), 100.6 (C-1′), 75.1 (C-2′), 78.8 (C-3′), 71.6 (C-4′), 78.5 (C-5′), and 62.6 (C-6′) [10].

An X-ray diffraction (XRD) analysis of aucubin (iridoid glycoside) and its aglycone form (aucubigenin) can be used to derive information on physicochemical properties, including the orthorhombic crystal of aucubin with the space group $P2_12_12_1$, cyclopentane and pyran ring adopting an envelope conformation, and the Glc group in the $^4C_1$ conformation. Moreover, aucubigenin's crystals are monoclinic, with space group $P2_1$ and the envelope conformation of cyclopentane and pyran rings [11].

Iridoids are known to be very sensitive to treatment with acidic reagents, which hydrolyze glycosidic bonds and decompose the structure of aglycones, resulting in blue-colored products. Aucubin degradation is pH-specific and occurs in highly acidic environments. The half-life is 5.02, 5.78, and 14.84 h at a pH of 1.2, 1.6, and 2.0, respectively, but can extend to more than several days at pH levels above 3.0. Moreover, aucubin is stable in plasma for at least 6 h at 37 °C [12].

Aucubin only exhibits biological activities when the glycoside is converted into its aglycone form through deglycosylation, either in vivo or in vitro. Although the exact structure of the hydrolyzed iridoid product remains undetermined, it can be assumed that the monoterpene ring is cleaved. The glucose part of the structure needs to be hydrolyzed because aucubin is more easily transported into the cell membrane in its aglycone than in glycoside form [13].

## 3. Aucubin-Producing Plants

Aucubin is the most widespread iridoid glycoside in plants. It is commonly included in the iridoids group, which currently contains almost one thousand compounds. Bourquelot and Harissey first isolated this compound in 1905 from the leaves of *Aucuba japonica* of the family *Cornaceae*. Furthermore, aucubin has also been separated from other plant families, such as *Cornaceae*, *Garryaceae*, *Orobanchaceae*, *Globulariaceae*, *Eucommiaceae*, *Scrophulariaceae*, *Plantaginaceae*, and *Rubiaceae* [14]. Plants documented as containing aucubin are presented in Table 1. *Plantaginaceae* is particularly rich in aucubin; therefore, the compound is used as a chemotaxonomic marker for this plant family. In terms of distribution, aucubin is found in all parts of plants: flowers, seeds, fruits, leaves, stems, and roots.

**Table 1.** Aucubin-producing plant species.

| Family | Species | Part of Plant | Reference |
|---|---|---|---|
| *Cornaceae* | *Aucuba japonica* | Leaves | [14] |
| *Eucommiaceae* | *Eucommia ulmoides* | Seeds, fruits | [15–17] |
| *Buddlejaceae* | *Buddleja globosa* | Leaves | [18] |
| | *Buddleja asiatica* | Aerial flowering parts | [19] |
| *Lamiaceae* | *Vitex agnus-castus* | Flowers, leaves, twigs | [20] |
| *Lentibulariaceae* | *Utricularia australis* | N/A | [21] |
| *Orobanchaceae* | *Bellardia trixago* | Aerial parts | [22] |
| | *Castilleja tenuiflora* | Aerial parts | [23] |
| | *Centranthera grandiflora* | Roots, stems, leaves, flowers | [24] |
| | *Melampyrum arvense* | Aerial parts | [25] |
| | *Parentucellia viscosa* | Whole plants | [26] |
| | *Rehmannia glutinosa* | Roots, leaves | [27] |

**Table 1.** *Cont.*

| Family | Species | Part of Plant | Reference |
|---|---|---|---|
| *Plantaginaceae* | *Aragoa cundinamarcensis* | Aerial parts | [28] |
| | *Campylanthus salsaloides* | Aerial parts | [29] |
| | *Campylanthus glaber* | Aerial parts | [29] |
| | *Globularia alypum* | Leaves, flowers, woody stems, underground parts | [30] |
| | *Globularia dumulosa* | Aerial parts | [31] |
| | *Globularia cordifolia* | Roots, rhizomes | [30,32] |
| | *Globularia meridionalis* | Leaves, flowers, woody stems, underground parts | [30] |
| | *Globularia punctata* | Leaves, flowers, woody stems, underground parts | [30] |
| | *Linaria alpina* | Aerial parts | [33] |
| | *Paederota lutea* | Whole plants | [34] |
| | *Plantago lanceolata* | Aerial parts | [35] |
| | *Plantago lagopus* | Aerial parts | [36] |
| | *Plantago major* | Aerial parts | [37] |
| | *Plantago myosuros* | Whole plants | [38] |
| | *Veronica beccabunga* | Leaves | [39] |
| | *Veronica hookeri* | N/A | [40] |
| | *Veronica pectinata* | Aerial parts | [41] |
| | *Veronica pinguifolia* | N/A | [40] |
| *Scrophulariaceae* | *Scrophularia nodosa* | Leaves, flowers, stems, roots | [42] |
| | *Sutera dissecta* | Aerial parts | [43] |
| | *Verbascum lasianthum* | Flowers, roots | [10,44] |
| | *Verbascum macrurum* | Aerial parts | [45] |
| | *Verbascum mucronatum* | Flowers | [46] |

N/A: not mentioned in the source document.

## 4. Isolation of Aucubin

Currently, pure aucubin is needed for varying purposes, including standardization of raw materials and traditional medicinal products, synthesis of other iridoid glycosides [47,48], product development, and pharmacological, pharmacodynamic, and pharmacokinetic studies. Scholars have been using different separation and purification methods because aucubin is located in a different matrix of compounds in each plant or plant part. The reported yields also vary from 0.004% to 1.7%.

The isolation process generally starts with air-drying and grinding the harvested plant material into powder to increase the surface area for optimal extraction. However, some researchers chose to use fresh materials to maximize compound stability, e.g., the isolation of aucubin from *Campylanthus glaber* and *Plantago myosuros* [29,38]. This was conducted to avoid enzymatic degradation. In previous studies, it has also been proven that aucubin is easily changed due to temperature, weak base, and oxidation. Therefore, it is relatively stable if extracted and separated quickly and stored hermetically [49]. A universal solvent such as ethanol or methanol, which can dissolve various compounds with a wide range of polarities, is used in extraction from plant tissues because aucubin co-occurs with iridoids and other active compounds. For instance, aucubin was successfully isolated from the flowers of *Verbascum mucronatum* with three other iridoid glucosides (ajugol, lasianthoside I, and catalpol), two saponins (ilwensisaponin A, ilwensisaponin C), and one phenylethanoid glycoside (verbascoside) [46]. To increase yields, Yang et al. used the ionic liquid 1-Butyl-3-methylimidazolium bromide (BmimBr) to extract aucubin from *Eucommia ulmoides* [17].

After digestion at 40–45 °C, the powdered material is macerated at room temperature. Maceration is the most widely used extraction method for aucubin and may be repeated two to four times to maximize yields. Another documented method is extraction by boiling and subsequent cold maceration. Unconventional methods such as ultrasound-assisted extraction (UAE) and supercritical fluid extraction (SFE) have also been also applied to extract aucubin from *E. ulmoides* [17,50]. The ethanol- or methanol-derived extract is then concentrated or dried to produce a crude extract.

The first step for separating aucubin from other compounds is partitioning the crude extract into two immiscible liquids: ether–water, chloroform–water, dichloroethane–water, or petroleum ether–water. This is mainly to separate aucubin from chlorophyll and other lipophilic compounds. Afterward, the $H_2O$ phase is evaporated or lyophilized. Then the aqueous phase containing aucubin is further separated using open-column chromatography (CC), vacuum liquid chromatography (VLC), or medium-pressure liquid chromatography (MPLC). Finally, the chromatography is performed with a reverse system using the stationary phase C-18 and the mobile phase water–methanol solution made in gradients. Because aucubin is a glycoside of high polarity, it has a high affinity for the mobile than the stationary phase in the reverse system, meaning that aucubin is eluted into the mobile phase and thus separated easily. In previous research, chromatography with stationary phase polyamide and gradient mobile phase methanol–water was also used to extract aucubin from *Verbascum lasianthum*, *Veronica pectinate*, and *Plantago lagopus* [10,36,41]. In 2018, Yang et al. used adsorption by macroporous resins to isolate this compound from the fruits of *Eucommia ulmoides*. Aucubin was adsorbed onto HPD850 resins and then desorbed by eluting the column in a gradient manner using 10–80% ethanol [17]. Based on these works, the chemical structure of the isolated aucubin can be determined using UV spectrophotometry, mass spectrometry, infrared spectrometry, $^1$H NMR, $^{13}$C NMR, or optical rotation. Table 2 summarizes the isolation methods of aucubin from various plant species. The general steps in the isolation process of aucubin was proposed and it is presented in Figure 2.

**Table 2.** Aucubin isolation methods from different plant species.

| No | Plant and Plant Part | Extraction Method and Solvent | Isolation Method | Yield (%) | Ref. |
|---|---|---|---|---|---|
| 1 | *Eucommia ulmoides*; seeds | Smashing tissue extraction using methanol | The crude extract was defatted using petroleum ether; then, column chromatography of the residue was conducted using Si gel as stationary phase and petroleum ether-EtOAc (50:1 to 1:10) as the mobile phase, followed by another column chromatography using Sephadex LH-20 as the stationary phase and petroleum ether-EtOAc (1:8) as the mobile phase. | 0.28 | [16] |
| 2 | *Plantago major*; aerial parts | Maceration using methanol | The crude extract was partitioned using dichloroethane-$H_2O$; the water-soluble part was then cleaned using charcoal, followed by CC using stationary phase C-18 and different mobile phases: $H_2O$, $H_2O$-MeOH (95:5, 70:30, 50:50), MeOH, MeOH-$Me_2CO$ (1:1), and MeOH-$Cl(CH_2)_2Cl$ (1:1). Then, the MeOH-$Cl(CH_2)_2Cl$ (1:1) fraction was purified with Si gel. | 0.055 | [37] |
| 3 | *Campylanthus salsaloides*; dried and fresh aerial parts | Boiling in ethanol for 5 min, followed by 6 d of maceration | The crude extract was partitioned in $Et_2O$-$H_2O$; the aqueous phase was then evaporated and treated with charcoal, followed by reversed-phase CC (C-size Lobar®) using mobile phase $H_2O$-MeOH (1:0 to 2:1). | 0.15 (dried aerial parts), 0.32 (fresh aerial parts) | [29] |

**Table 2.** *Cont.*

| No | Plant and Plant Part | Extraction Method and Solvent | Isolation Method | Yield (%) | Ref. |
|---|---|---|---|---|---|
| 4 | *Globularia dumulosa*; aerial parts | Digestion using methanol at 45 °C | The crude extract was partitioned in $H_2O$-$CHCl_3$; then, the water fraction was lyophilized, followed by VLC with stationary phase C-18 and different mobile phases: $H_2O$, $H_2O$-MeOH (5–80% MeOH in $H_2O$), and MeOH. The subsequent VLC used Si gel as the stationary phase and $CHCl_3$-MeOH-$H_2O$ (90:10:1 to 50:50:5) as the mobile phase, followed by MPLC using stationary phase C-18 and mobile phase MeOH in water (0–40%). | 0.079 | [31] |
| 5 | *Aragoa cundinamarcensis*; aerial parts | Boiling in EtOH, followed by maceration for 3 d | The crude extract was partitioned in $Et_2O$-$H_2O$; the aqueous phase was then cleaned using activated carbon in MeOH, followed by CC using stationary phase C-18 and mobile phase $H_2O$-MeOH (1:0 to 2:1). | 1.7 | [28] |
| 6 | *Verbascum lasianthum*; roots | Digestion using methanol at 40 °C | The crude extract was partitioned in $CHCl_3$-$H_2O$; the aqueous phase was then lyophilized, followed by CC using polyamide as the stationary phase and $H_2O$ and an $H_2O$-MeOH mixture as the mobile phase. Then, VLC was conducted using C-18 as the stationary phase and $H_2O$-MeOH as the mobile phase (0–100%, gradient). | 0.06 | [10] |
| 7 | *Verbascum mucronatum*; flowers | Digestion using methanol at 40 °C | The crude extract was partitioned in $CHCl_3$-$H_2O$, followed by CC using polyamide as the stationary phase and $H_2O$ and an $H_2O$-MeOH mixture as the mobile phase. Then, VLC using stationary phase C-18 and gradient mobile phase $H_2O$-MeOH (0–100%) was conducted. | 0.02 | [46] |
| 8 | *Plantago myosuros*; whole plants, frozen | Maceration using ethanol | The crude extract was partitioned using $Et_2O$-$H_2O$; the aqueous phase was then cleaned using activated carbon in MeOH, followed by CC using stationary phase Lobar $RP_{18}$ and mobile phase $H_2O$-MeOH (25:1 to 1:1). | 0.04 | [38] |
| 9 | *Eucommia ulmoides*; fruits | UAE using 0.5 mol/L ([Bmim]Br) ionic liquid | The ionic liquid extract was placed onto a glass column containing HPD850 resins; then, the column was washed using deionized water and eluted (desorption) using 10–80% EtOH. This process ended with the vacuum distillation of the eluent, 40–80% ethanol. | N/A | [17] |

**Table 2.** *Cont.*

| No | Plant and Plant Part | Extraction Method and Solvent | Isolation Method | Yield (%) | Ref. |
|---|---|---|---|---|---|
| 10 | *Globularia cordifolia*; roots and rhizomes | Digestion using methanol at 45 °C | The crude extract was partitioned using $H_2O$-$CHCl_3$; then, the aqueous phase was lyophilized, followed by VLC using LiChroprep C-18 as the stationary phase and $H_2O$ and a mixture of $H_2O$-MeOH (10–90% MeOH) as the mobile phase. The subsequent MPLC was performed using C-18 as the stationary phase and MeOH in $H_2O$ (0–50%, MeOH) as the mobile phase, followed by CC using stationary phase Si gel and mobile phase $CH_2Cl_2$-MeOH-$H_2O$ (70:30:3). | 0.004 | [32] |
| 11 | *Bellardia trixago*; aerial parts | Remaceration using methanol | The crude extract was partitioned using water–petroleum ether, followed by chloroform and n-butanol. The butanol fraction was then column-chromatographed using stationary phase Si gel and mobile phase $CHCl_3$-MeOH-$H_2O$ (80:20:1, 80:20:2, to 50:50:5). Fraction D underwent MPLC using 15–25% MeOH as the mobile phase. | 0.06 | [51] |
| 12 | *Veronica pectinata* L. Var. *glandulosa;* aerial parts | Digestion using MeOH at 40 °C | The crude extract was partitioned using water-$CHCl_3$. The water fraction was then lyophilized, followed by CC using stationary phase polyamide and mobile phase $H_2O$-MeOH, made in gradients by increasing the MeOH concentration to produce five fractions. Fraction A was then chromatographed using stationary phase Si gel and mobile phase $CHCl_3$:MeOH:$H_2O$ (90:10:1 to 60:40:4), followed by MPLC using stationary phase RP-18 and gradient mobile phase MeOH (20–50%). | 0.027 | [41] |
| 13 | *Paederota lutea*; whole plants | Brought to a boil using EtOH, followed by 7 d of maceration | The crude extract was partitioned using $H_2O$-$Et_2O$. The water fraction was then chromatographed using stationary phase RP-18 and mobile phase $H_2O$-MeOH (25:1 to 1:1). | 0.349 | [34] |
| 14 | *Vitex agnus-castus*; flowers, leaves, and twigs | Digestion using MeOH at 45 °C | The crude extract was partitioned using $H_2O$-$CHCl_3$, followed by n-BuOH. The n-BuOH fraction was then column-chromatographed using stationary phase Si gel and mobile phase $CHCl_3$ (by increasing MeOH gradually). Further separation and purification were conducted by CC using Si gel as the stationary phase and EtOAc:MeOH:$H_2O$ (100:5:2 to 100:17:13) and $CHCl_3$:MeOH:$H_2O$ (90:10:1 to 60:40:4) as mobile phases, CC using stationary phase Sephadex LH-20 and mobile phase MeOH, and CC using stationary phase RP-18 and mobile phase MeOH in $H_2O$ (made in gradients). | 0.006 | [20] |

**Table 2.** *Cont.*

| No | Plant and Plant Part | Extraction Method and Solvent | Isolation Method | Yield (%) | Ref. |
|---|---|---|---|---|---|
| 15 | *Verbascum lasianthum*; flowers | Digestion using MeOH at 40 °C | The crude extract was partitioned using $H_2O$-$CHCl_3$. The water phase was lyophilized and then processed with VLC using polyamide as the stationary phase and $H_2O$ as the mobile phase (with increasing MeOH concentrations), VLC using stationary phase C-18 and mobile phase $H_2O$-MeOH (0–100% MeOH). Further separation was conducted by CC using Si gel as the stationary phase and $CHCl_3$, $CHCl_3$:MeOH (95:5), and $CHCl_3$:MeOH:$H_2O$ (70:30:3) as mobile phases, and VLC with C-18 as the stationary phase and $H_2O$ and gradient MeOH-$H_2O$ (0–20% MeOH) as mobile phases. | 0.028 | [44] |
| 16 | *Castilleja tenuiflora*; aerial parts | Maceration using ethanol | The crude extract was partitioned using $H_2O$-$Et_2O$. The $H_2O$ phase was then concentrated, dissolved in MeOH, and cleaned using activated carbon. Further separation was carried out using CC (stationary phase Si gel and mobile phase hexane-$CH_2Cl_2$-AcOEt-MeOH with increasing polarity) and MPLC (C-18 as the stationary phase, $H_2O$:MeOH (10:0 to 1:1) as the mobile phase). | 0.46 | [23] |
| 17 | *Plantago lagopus*; aerial parts | Digestion using MeOH at 40 °C | The crude extract was partitioned using water–petroleum ether. The $H_2O$ phase was column-chromatographed (polyamide as the stationary phase, 0–100% MeOH as the mobile phase). The water fraction was then extracted using n-butanol, followed by MPLC and CC (Si gel as the stationary phase; $CHCL_3$:MeOH at 100:0, 95:5, 90:10, 85:15, 80:20; and 75:25 as the mobile phase). | N/A | [36] |
| 18 | *Parentucellia viscosa*; whole plants | Remaceration using 96% EtOH | The crude extract was column-chromatographed using Si gel as the stationary phase and n-butanol saturated with water and $CHCl_3$/MeOH at various ratios as the mobile phase. | 0.16 | [26] |
| 19 | *Veronica beccabunga*; leaves | Brought to boil using EtOH | The crude extract was partitioned using $Et_2O$-$H_2O$; then, the $H_2O$ phase was dried and dissolved in 10% acetic acid. The aliquots were then column-chromatographed with stationary phase RP-18 and mobile phase $H_2O$-MeOH (1:0 to 1:1). | 0.25 | [39] |
| 20 | *Veronica hookeri* and *Veronica pinguifolia*; N/A | Maceration using MeOH | The crude extract was partitioned using $Et_2O$-$H_2O$; then, the $H_2O$ phase was dried and column-chromatographed with stationary phase RP-18 and mobile phase $H_2O$-MeOH (25:1 to 1:1). | 0.18 (*V. hookeri*), 0.08 (*V. pinguifolia*) | [40] |

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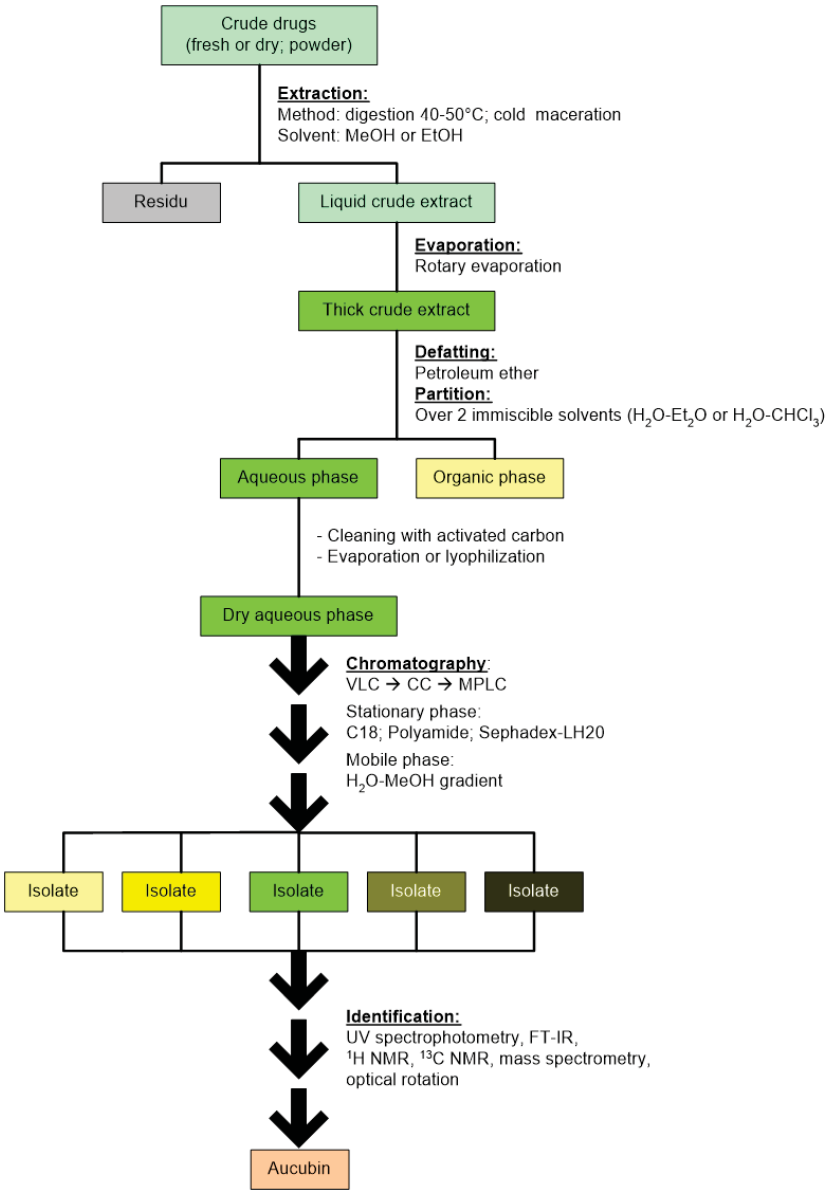


**Figure 2.** The general steps in the isolation process of aucubin.

## 5. Biological Properties

The biological activities of aucubin (Figure 3) have been extensively identified, both in vitro and in vivo. In in vivo testing, aucubin is administered via the intraperitoneal (i.p.) injection route more often than orally (p.o.). Pharmacokinetic testing proves the bioavailability of aucubin to be higher with the former (76.8%) than the latter route (19.8%). This may result from the unstable nature of aucubin in the acidic gastric juice, poor absorption onto the gastrointestinal tract due to low lipophilicity, and possible first-pass effects in the liver [12]. In in vitro assays, aucubin is tested on various animal and human cell cultures, either with or without prior induction. The biological activities of aucubin are generally dose- or concentration-dependent.

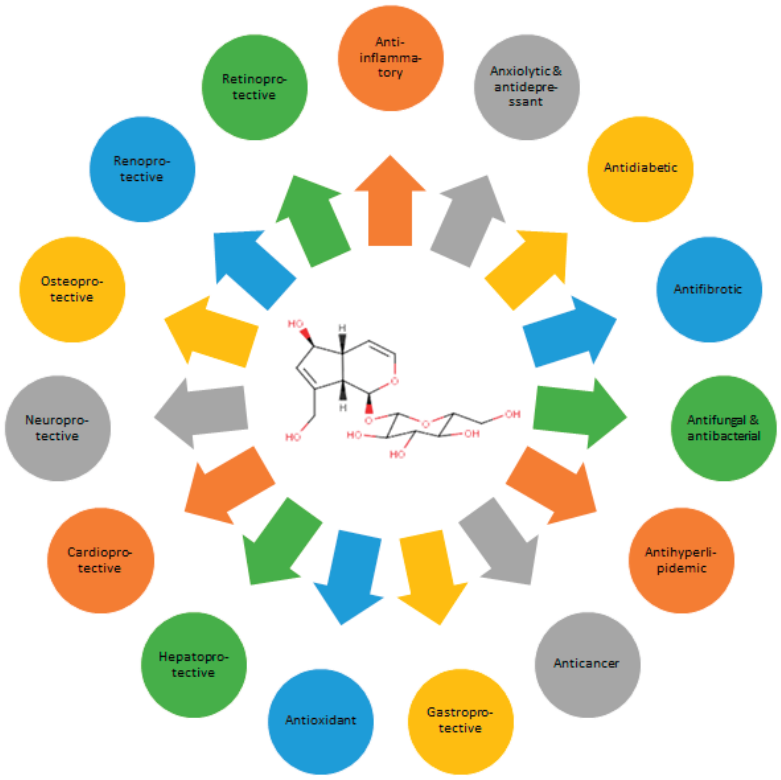


**Figure 3.** Spectra of the biological activities of aucubin.

### *5.1. Anti-Inflammatory Activities*

Inflammation is the body's response to cell and tissue damage caused by various stimuli, which can be mechanical stimulants (abrasion, impact, distortion), chemical stimulants (inflammatory cytokines, chemotherapy), infections by pathogenic organisms (bacteria or viruses), etc. [52]. When tissues are exposed to and damaged by stimulants, phospholipids in the cell membrane are converted to arachidonic acid by phospholipase and then to inflammatory mediators called prostaglandins by cyclooxygenase (COX-1, COX-2) and leukotrienes by lipoxygenase (LOX). One of the signaling pathways involved in forming inflammatory cytokines (e.g., COX-2, IL-1β, IL-8, IL-10, and TNF-α) is the NF-κB pathway. Previous studies on the anti-inflammatory properties of aucubin are summarized in Table 3.

Table 3 shows that the in vitro anti-inflammatory testing of aucubin involves various types of cell lines and stimulations by different chemicals, such as LPS, IL-1β, and TNF-α. This aims to increase the release of inflammatory mediators to make the anti-inflammatory effect easily observable. In vitro testing on 3T3-L1 adipocytes with TNF-α-induced inflammation proved that aucubin could suppress the secretion of proinflammatory cytokines (MCP-1, PAI-1, and IL-6) by inhibiting the degradation of IκBα and the translocation of the p65 subunit, thus inactivating NF-κB [53]. In murine chondrocytes, aucubin inhibited the phosphorylation of IKKα/β, IκBα, and p65 (IL-1β) and p65 translocation from the cytosol to the nucleus. Both inhibitory responses prevented the expression of inflammatory mediators (MMP, iNOS, COX-2, NO, etc.) [54]. Meanwhile, in THP-1 macrophages stimulated using LPS, aucubin could impede the production of TNF-α, IL-6, IL-1β, and IFN-γ [55].

Aucubin also has the potential as an anti-inflammatory in certain pathological conditions, including diabetes, gastric mucosal lesions, and epilepsy. In vivo administration of aucubin to hyperglycemic mice decreased p-IκBα expression, accumulated p65 nuclei in the NF-κB pathway, and inhibited the expression of inflammatory cytokines (IL-1β, IL-8, IL-10, and TNF-α) [56]. In a different study, intragastrical administration of aucubin to mice with gastric mucosal lesions reduced the IL-6 and TNF-α levels in the gastric mucosa by

blocking the activation of NF-κB [57]. In mice with pilocarpine-induced epilepsy, aucubin lowered proinflammatory cytokine levels (IL-1β, HMGB1, and TNF-α) [58].

Furthermore, aucubin is a promising anti-inflammatory in neurons. It inhibits the release of HMGB1 in $H_2O_2$-stimulated neurons by reducing oxidative stress, thus decreasing HMGB1-TLR4 binding, NF-κB activation and, consequently, inflammatory cytokine levels. A similar effect was also observed after the intraperitoneal administration of aucubin to male and pregnant mice with traumatic brain injury [59]. Moreover, aucubin also has anti-inflammatory potential in the eyes. In the corneal cells of humans and male rats that had their left exorbital lacrimal gland removed, aucubin inhibited the inflammatory response induced by proinflammatory cytokines by inhibiting NF-κB signals, e.g., suppressing the mRNA expression of IL-1β, IL-8, and TNF-α [60].

**Table 3.** Anti-inflammatory activities of aucubin.

| No | Compound | In Vitro/In Vivo | Cell or Animal Model | Concentration/Dose | Administration Route | Ref. |
|---|---|---|---|---|---|---|
| 1 | Aucubin | In vitro | 3T3-L1 adipocytes, stimulated using 10 ng/mL TNF-α | 1, 3, 10, 30 μM | N/A | [53] |
| 2 | Aucubin | In vitro | Murine chondrocytes, stimulated using 10 ng/mL IL-1β | 1, 10, 20, 50 μM | N/A | [54] |
| 3 | Aucubin | In vitro | THP-1 macrophages, stimulated using LPS 5 μg/mL | 10, 25, 50, 100, 300 μg/mL | N/A | [55] |
| 4 | Aucubin | In vivo | Normal C57BL/6 male mice, diabetes was induced using a high-fat diet and streptozotocin | 20, 40, 80 mg/kg BW | p.o. | [56] |
| 5 | Aucubin | In vivo | Male Kunming mice; gastric mucosal injury was induced using 70% ethanol | 20, 40, 80 mg/kg BW | i.g. | [57] |
| 6 | Aucubin | In vivo | Mouse model of epileptic ICR with pilocarpine at 320 mg/kg BW | 50, 100 mg/kg BW | i.p. | [58] |
| 7 | Aucubin | In vivo | Male BALB/c mice; induced using cisplatin | 1, 5, 5 mg/kg BW | p.o.<br>i.p. | [61] |
| 8 | Aucubin | In vitro | Neuron cells, stimulated using $H_2O_2$ | 50, 100, 200 μg/mL | N/A | [59] |
| 9 | Aucubin | In vivo | Male and pregnant C57BL/6 mice with traumatic brain injury | 20, 40 mg/kg BW | i.p. | [59] |
| 10 | Aucubin | In vitro | 3T3-L1 cells, stimulated using apoC-III | 35, 70, 140, 280 μg/mL | N/A | [62] |
| 11 | Aucubin | In vivo | C57/BL6 mice, administered tyloxapol with/without aucubin using intraperitoneal injection | 10, 20, 40 mg/kg BW | i.p. | [62] |
| 12 | Aucubin | In vitro | Neonatal rat cardiomyocytes, stimulated using 10 μg/mL LPS | 5,15, 45 μM | N/A | [63] |
| 13 | Aucubin | In vivo | C57BL/6 mice, stimulated using LPS at 6 mg/kg BW | 20, 80 mg/kg BW | Gavage | [63] |
| 14 | Aucubin | In vitro | Human corneal cells, subjected to desiccation stress | 0,1, 1, 7, 15 μg/mL | N/A | [60] |
| 15 | Aucubin | In vivo | Male rats that had their left exorbital lacrimal gland removed (mouse model of dry eye disease) | 75 mg/kg BW | p.o. | [60] |
| 16 | Aucubin | In vitro | Human hepatocyte HL7702 (LO2), overexpression of TLR-4 | 2, 4, 8, 16, 32, 64, 128, 256 μM | N/A | [64] |
| 17 | Aucubin | In vivo | Sprague–Dawley rats with IRL condition | 1, 5, 10 mg/kg BW | i.p. | [64] |
| 18 | Aucubin | In vitro | RAW264.7 cells and macrophage-like THP-1 cells | 50, 100 μM | N/A | [65] |
| 19 | Aucubin | In vivo | Wild-type (WT) male C57BL/6 J mice and Nrf2 knockout mice, induced using LPS | 10, 20 mg/kg BW | i.p. | [65] |

N/A: not applicable in the in vitro study; p.o.: per oral; i.g.: intragastric; i.p.: intraperitoneal.

Aucubin should also be considered for its anti-inflammatory effects in acute kidney failure. This compound suppressed the activation of signaling pathways involved in inflammation and apoptosis, such as NF-κB, STAT3, Akt, ERK1/2, and FOXO3a, after being orally and intraperitoneally administered to mice with cisplatin-induced kidney injury [61]. Aucubin also prevented the elevation of MMP-9, MCP-1, apoC-III, ICAM-1, VCAM-1, TNF-α, IL-1β, and IL-6 levels after stimulation by apoC-III in 3T3-L1 cells and in mice with tyloxapol-induced nonalcoholic fatty liver disease (NAFLD) [62]. In HL7702 (LO2) hepatocytes and Sprague–Dawley mice, aucubin regulated the HMGB1/TLR-4/NF-κB signaling pathway to reduce the expression of proinflammatory cytokines: TNF-α and IL-1β. Based on these results, aucubin displayed the potential as an anti-inflammatory agent in chronic liver diseases [64]. In addition to kidney failure and liver disease, this compound also shows anti-inflammatory activities in the heart. In neonatal rat cardiomyocytes (NRCMs), this compound prevented the activation of NLRP3 inflammasomes (NLRP3, ASC, pro-caspase-1) and, subsequently, reduced the expression of proinflammatory cytokines (C-caspase and IL-1β). A similar effect was observed in C57BL/6 mice administered aucubin using a gavage for 7 d [63]. The anti-inflammatory potential of aucubin in acute lung injury is supported by Qiu et al., who proved the compound's ability to inhibit proinflammatory cytokines (IL-6, IL -18, TNF-α, IL-1β, COX2, and iNOS) and NF-κB expression in RAW264.7 and THP-1 cells, wild-type (WT) male C57BL/6 J mice, and Nrf2 knockout mice [65].

### *5.2. Antioxidant*

Antioxidants are compounds that can prevent or slow down cell damage due to oxidative stress. Aucubin has demonstrated antioxidant activities in several disorders, including diabetic nephropathy, traumatic brain injury, cardiovascular disorders, liver disease, osteoarthritis, and infertility. The antioxidant activity test results of aucubin and its aglycones are summarized in Table 4.

Oxidative stress occurs when the antioxidant defense cannot balance the excess production of reactive oxygen species (ROS). This condition also refers to disruptions to the cellular redox balance. Reactive oxygen and nitrogen species originating from intracellular redox metabolism are superoxide anion radicals ($O_2^{\bullet -}$), hydroxyl ($OH^{\bullet}$), alkoxyl and peroxyl radicals ($ROO^{\bullet}$), nitric oxide ($NO^{\bullet}$), peroxynitrite ($ONOO^-$), hydrogen peroxide ($H_2O_2$), and hypochlorite (HOCl) [66]. Damage to cells, tissues, and organ systems resulting from oxidative stress is associated with a number of serious diseases, such as cancers, cataracts, neurodegenerative diseases, and even the aging process [67]. Aucubin's potential to prevent or treat numerous diseases owing to its antioxidant properties has been confirmed using various test models.

**Table 4.** Antioxidant activities of aucubin and aucubigenin.

| No | Compound | In Vitro/In Vivo | Cell or Animal Model | Concentration/Dose | Administration Route | Ref. |
|---|---|---|---|---|---|---|
| 1 | Aucubin and aucubigenin | In vitro | LX-2 cells (human hepatic stellate cell lines), induced using TGF-β1 | Aucubin: 1, 10, 100, 200, 400, 800 μM Aucubigenin: 100 μM | N/A | [68] |
| 2 | Aucubin | In vitro | MC3T3-E1 (murine osteoblastic cell lines), induced using Ti particles | 0.1, 1, 10 μM | N/A | [69] |
| 3 | Aucubin | In vivo | Wild-type (WT) C57BL/6 and Nrf2 knockout mice, induced using LPS | 10, 20 mg/kg BW | i.p. | [65] |
| 4 | Aucubin | In vivo | C57BL/6 mice, diabetes was induced using a high-fat diet and streptozotocin | 20, 40, 80 mg/kg BW | p.o. | [56] |

**Table 4.** *Cont.*

| No | Compound | In Vitro/In Vivo | Cell or Animal Model | Concentration/Dose | Administration Route | Ref. |
|---|---|---|---|---|---|---|
| 5 | Aucubin | In vivo | Kunming mice, gastric mucosal lesions were induced using 70% ethanol | 20, 40, 80 mg/kg BW | i.g. | [57] |
| 6 | Aucubin | In vitro | Neuron cells, stimulated using 100 μM $H_2O_2$ | 50, 100, 200 μg/mL | N/A | [59] |
| 7 | Aucubin | In vivo | C57BL/6 mice, traumatic brain injury was induced using lentivirus at 4 μL | 20, 40 mg/kg BW | i.p. | [59] |
| 8 | Aucubin | In vitro | 3T3-L1 cells, stimulated using apolipoprotein C-III at 100 μg/mL | 35, 70, 140, 280 μg/mL | N/A | [62] |
| 9 | Aucubin | In vivo | C57BL/6 mice, stimulated using tyloxapol at 300 mg/kg BW | 10, 20, 40 mg/kg BW | i.p. | [62] |
| 10 | Aucubin | In vitro | Sertoli cells (primary cells and the cell line TM4), induced using 0.5 μM triptolide | 5, 10, 20 μM | N/A | [70] |
| 11 | Aucubin | In vivo | Mice, induced using triptolide at 120 μg/kg BW | 5, 10, 20 mg/kg BW | i.p. | [70] |
| 12 | Aucubin | In vitro | H9c2 cells, exposed to hypoxia | 10, 50 μM | N/A | [71] |
| 13 | Aucubin | In vivo | C57BL/6 mice by inducing myocardial infarction | 10 mg/kg BW | i.p. | [71] |
| 14 | Aucubin | In vitro | MG63 cells (human osteoblast-like cells), stimulated using dexamethasone or $H_2O_2$ | 1, 2.5, 5 μM | N/A | [72] |
| 15 | Aucubin | In vivo | C57BL/6 mice, stimulated using dexamethasone at 30 mg/kg BW | 5, 15, 45 mg/kg BW | i.g. | [72] |
| 16 | Aucubin | In vivo | Sprague–Dawley rats with liver ischemia–reperfusion injury | 1, 5, 10 mg/kg BW | i.p. | [64] |
| 17 | Aucubin | In vitro | Neonatal rat cardiomyocytes, stimulated using LPS at 10 μg/mL | 5, 15, 45 μM | N/A | [63] |
| 18 | Aucubin | In vivo | C57BL/6 mice, stimulated using LPS at 6 mg/kg BW | 20, 80 mg/kg BW | Gavage | [63] |
| 19 | Aucubin | In vitro | Mouse chondrocytes, induced using IL-1β | 10, 20, 50 μM | N/A | [73] |

N/A: not applicable in the in vitro study; p.o.: per oral; i.g.: intragastric; i.p.: intraperitoneal.

ROS, MDA, LDH, SOD, and GPx are cells' most significant markers of oxidative stress [69]. In LX-2 cells (human hepatic stellate cell lines) stimulated using TGF-β1, aucubin and aucubigenin reduced intracellular ROS production and the mRNA expression of NOX4. Excessive ROS contributes to activating liver stellate cells (HSCs) and liver fibrosis, while NOX4 is an NADPH oxidase influencing the activation of ROS and HSCs [68]. Meanwhile, in murine osteoblastic cell cultures (MC3T3-E1) induced using Ti particles, aucubin lowered ROS, MDA, and LDH levels and increased SOD and GPx activity in cells [69]. In mouse models of diabetic nephropathy—where STZ and a high-fat diet were used to induce hyperglycemia—aucubin reduced MDA levels in kidney tissue and increased the activity of antioxidant enzymes, such as SOD, catalase, and GSH/T-GSH [56]. Lowered MDA levels and elevated SOD activities and GSH levels after the administration of aucubin were also identified in mice with induced gastric mucosal lesions [57]. In H9c2 cell cultures exposed to hypoxia and C57/BL6 mice with induced myocardial infarction, aucubin successfully reduced the NADPH oxidase subunit, P67, gp91; increased SOD and thioredoxin (Trx)

levels; and lowered ROS production [71]. In rat liver homogenates with simulated IRI (liver ischemia–reperfusion injury), aucubin pretreatment significantly reduced MDA and ROS levels and elevated SOD levels, suggesting good antioxidant activity in the liver IRI model [64]. In neonatal rat cardiomyocytes (NRCMs) and C57BL/6 mice, aucubin inhibited LPS-induced oxidative stress by lowering ROS and thioredoxin interaction protein (TXNIP) levels [63]. In IL-1β-stimulated mouse chondrocytes, aucubin substantially suppressed ROS production, which is one of its mechanisms of action in treating osteoarthritis [73].

In wild-type and Nrf-2 knockout mice (i.e., model mice for studying endothelial dysfunction, oxidative stress, and microvascular attenuation), aucubin ameliorated oxidative stress by decreasing MDA and $O_2^{\bullet -}$ activities and increased Nrf2-targeted signals, such as heme oxygenase-1 (HO-1) and quinone oxidoreductase-1 (NQO-1) [65]. Nrf2 is a transcription factor that can increase the transcription of numerous antioxidants and detoxification enzymes. These protective genes can quickly neutralize ROS. In neuronal cells stimulated using $H_2O_2$ on mice with traumatic brain injury, aucubin increased the translocation of cytoplasmic Nrf2 to the nucleus and the expression of antioxidant enzymes (NQO-1, HO-1, Bcl2, SOD, GSH, and GSH-Px), inhibited intercellular ROS, balanced the expression of Bcl2 and Bax, and suppressed caspase-3 activation [59]. To test the antioxidant effect on nonalcoholic fatty liver disease (NAFLD), aucubin was tested on 3T3-L1 cells stimulated using apoC-III on mice with tyloxapol-induced NAFLD. In this work, aucubin demonstrated antioxidant activities, as evident from its ability to activate Nrf2, HO-1, and PPARα and PPARγ (translocation into the nucleus), increased the phosphorylation of ACC, AMPKα, and AKT, and elevated SOD levels [62].

Oxidative stress also plays an essential part in male infertility, as it triggers apoptosis of Sertoli cells and destroys the integrity of the blood–testis barrier, thus causing testicular injury and, ultimately, spermatogenic dysfunction when exposed to pollutants or drugs. The antioxidant effect of aucubin on testicular injury was demonstrated in Sertoli cell cultures and adult male mice with triptolide-induced apoptosis. It was also confirmed that aucubin could inhibit apoptosis in the PERK/CHOP and JNK-dependent pathways by triggering Nrf2 translocation, which increased the accumulation of nucleus Nrf2 and started the expression of antioxidant enzymes in the testes and Sertoli cells [70].

Aucubin scavenges ROS directly and reduces intracellular ROS production. Aucubin also upregulates SIRT1/SIRT3, increasing FOXO3a translocation to produce antioxidant enzymes such as Mn-SOD and catalase. Generally, this effect can be detected from the low levels of malondialdehyde (MDA), which is a product of unsaturated lipid peroxidation due to ROS. In addition, aucubin can increase the translocation of Nrf2 from the cytoplasm to the nucleus. Under normal conditions, Nrf2 binds to Keap1 in the cytoplasm and triggers the translocation of the Nrf2 dimer to the nucleus, where it binds to the antioxidant response element (ARE) and induces the expression of antioxidant enzymes and protein derivatives (e.g., HO-1, NADPH, NQO-1, GPx, GST, and SOD). Aucubin regulates and balances the Bcl2-to-Bax ratio by elevating Bcl2 levels and lowering Bax levels. Bax is a proapoptotic protein, whereas Bcl2 is a protein that binds to proapoptotic proteins such as Bax.

Overall, it can be concluded that aucubin has the potential to alleviate oxidative stress in cases of liver fibrosis and nonalcoholic fatty liver disease, diabetic nephropathy, gastric mucosal lesions, myocardial infarction, liver ischemia–reperfusion injury, traumatic brain injury, osteoarthritis, and male infertility.

### *5.3. Anxiolytic and Antidepressant*

Depression is a common mental health disorder, etiology and pathophysiology of which are rarely understood. There are many theories regarding the causes and mechanisms of depression, including the lack of function of the brain's monoaminergic transmitters such as norepinephrine, 5-HT, dopamine, or their combination. Depression can be caused by decreased GABA concentrations in the cortical portions of the brain and cerebrospinal fluid [74–76].

Administering aucubin orally to mice at 20 and 40 mg/kg BW for 7 d proved effective in reducing anxiety. Furthermore, when administered at 10, 20, and 40 mg/kg BW, it also produced an antidepressant effect equivalent to fluoxetine [16]. The anxiolytic and antidepressant properties of aucubin are believed to result from its ability to lower glutamate levels, increase GABA levels, and inhibit monoamine oxidase A (MAO-A) and catechol-O-methyltransferase (COMT), which normally act as catalysts for the catabolism of catecholamine neurotransmitters, including dopamine, serotonin, noradrenaline, and adrenaline. However, further research is still needed to determine the real mechanism.

### *5.4. Antidiabetic*

Diabetes mellitus (DM) is a chronic metabolic disease characterized by high glucose in the blood. While type 1 DM occurs due to impaired insulin synthesis and secretion (pancreatic β-cell damage), type 2 DM is caused by impaired sensitivity of the tissues (receptors) where insulin works [77]. When left unmanaged, DM can lead to various complications, such as chronic kidney disorders, retinal damage, and cardiovascular disorders.

Long-term intraperitoneal injection of aucubin can help control blood glucose levels in diabetic rats and diabetic encephalopathic rats and reduce damage to neuron cells [78]. This compound also alleviates inflammation, renal fibrosis, albuminuria, and enlargement of the glomerular extracellular matrix caused by DM by inhibiting NF-κB activation and inducing the SIRT1/SIRT3-FOXO3a signaling pathway [56]. Examining the antiglycation activity in vitro at concentrations of 0.22 mmol/L and in vivo at 10 and 25 mg/kg revealed that aucubin suppressed the formation of advanced glycation end products (AGEs). This inhibitory effect on the formation of AGEs is dose-dependent [79]. AGEs are a causative factor for, among others, chronic kidney disease and atherosclerosis. AGEs form slowly in aging, but this process is accelerated under diabetic conditions and tissue oxidation.

### *5.5. Antifibrotic*

Fibrosis is a process in which fibroblasts synthesize collagen and other matrix aggregates to form scar tissue, which can disrupt organ functions because scar tissue cannot perform the role of actual parenchyma tissue [80]. Aucubin displayed a protective effect against bleomycin-induced pulmonary fibrosis in mice [81]. It reduced the mRNA expression of TGF-β1, leading to the decreased expression of TGF-β1, which regulates proliferation, extracellular matrix deposition, and the conversion of fibroblasts into myofibroblasts. In other words, aucubin inhibited the proliferation and differentiation of fibroblasts into myofibroblasts. This effect was further confirmed by the decreased levels of α-SMA, which is a key marker of myofibroblasts. In the lungs, aucubin impedes infiltration of inflammatory cells and neutrophils and reduces lactate dehydrogenase (LDH) activity. LDH is an enzyme that acts as a catalyst for converting pyruvate to lactate under anaerobic conditions [77]. The presence of lactate can activate extracellular TGF-β [82]. In addition, aucubin also reduces oxidative stress that can otherwise trigger inflammation, as characterized by low levels of MDA—i.e., a product of unsaturated lipid peroxidation by ROS [77].

### *5.6. Antifungal and Antibacterial*

*Candida albicans* is a flora naturally found in the human body, especially in the mouth and teeth, throat, skin, and mucous membranes of the gastrointestinal and genitourinary tract [80,83]. *Candida* can become an opportunistic pathogen if other local normal flora and tissue health conditions that prevent the development of candidiasis decrease or an environmental imbalance occurs, such as a change in pH and nutrition. In addition, *C. albicans* can form biofilms—i.e., complex structures made up of communities of cells (e.g., hyphae, pseudohyphae, and yeast cells) attached to host tissues or surfaces, such as medical devices—as a protective mechanism for these organisms, thus complicating treatment and increasing the degree of virulence [84]. Administered at 61–244 μg/mL, aucubin exhibited an inhibitory effect on total growth, biofilm formation, metabolic activity,

and cell surface hydrophobicity of *C. albicans*. Meanwhile, at 244 μg/mL, it could develop a fungicidal effect. The mechanisms involved in the antifungal activity of aucubin are still not clearly understood but are assumed to be by the inhibition of the cell surface hydrophobicity (CSH) pathway [85].

Apart from being antifungal, aucubin also shows potential as an antibacterial. This compound showed antibacterial activity on various Gram positive (*Staphylococcus epidermidis*, *S. aureus*, *Enterococcus faecalis*, and *Bacillus subtilis*) and Gram negative (*Proteus vulgaris*, *Enterobacter aerogenes*, *Klebsiella pneumoniae*, *Proteus mirabilis*, and *Citrobacter diversus*) bacteria, with MIC values from 8–128 μg/mL [86]. Moreover, aucubin extracted from *Eucommia ulmoides* leaves using the cellulase method could obviously inhibit *Escherichia coli* and *Staphylococcus aureus*, with MIC values of 9.664 and 4.832 mg/mL, respectively. However, aucubin presented weak inhibitory effect on *Streptococcus pneumonia* and *MG-hemolytic streptococcus* [87].

### *5.7. Antihyperlipidemic*

Hyperlipidemia refers to a condition of elevated levels of blood lipids, such as cholesterol, triglycerides, cholesterol esters, phospholipids, and/or plasma lipoproteins, including very-low-density lipoproteins and low-density lipoproteins, and decreased levels of high-density lipoproteins. Hyperlipidemia can cause numerous medical complications, including atherosclerosis, coronary artery disease, myocardial infarction, and ischemic stroke [88]. In 3T3-L1 cells stimulated using apoC-III on C57/BL6 mice with tyloxapol-induced NAFLD, aucubin hampered the development of hyperlipidemia by influencing the regulation of ApoC-III, which controls total cholesterol, triglyceride, LDL, and VLDL levels, and by activating AMPK, Nrf2, PPARα, and PPARγ pathways, leading to the activation of fatty acid oxidation [62].

### *5.8. Anticancer*

One of the targets used in cancer immunotherapy is STAT3, which is involved in cell proliferation, survival, differentiation, and angiogenesis. Under normal conditions, activation (phosphorylation) of STAT3 can release transcriptional signals from cytokine and the growth factor receptors on the plasma membrane into the nucleus [89]. However, with cancer, STAT3 becomes hyperactive and can increase cancer cells' proliferation and survival, making it the target of cancer immunotherapy. In the cytotoxic test on human myeloid leukemia cells (KBM-5, THP-1, K562), it was found that hydrolyzed aucubin (H-aucubin) had a significant cytotoxic effect on K562 cells. In contrast, aucubin did not show any cytotoxic effects on all three cells. The cytotoxic effect of H-aucubin occurred because this compound suppressed STAT3 activation by inhibiting the protein tyrosine kinase JAK2 and c-Src, which are upstream proteins of STAT3. Aucubin's role in suppressing STAT3 activation was also reported by Potočnjak et al. [61]. Furthermore, aucubin inhibited the phosphorylation and expression of the BCR-ABL protein in human myeloid leukemia cells, where BCR-ABL encoded tyrosine kinases—i.e., an enzyme playing an essential role in many cell functions, e.g., signaling and cell growth [90].

### *5.9. Gastroprotective*

Gastric ulcers are lesions in the inner curvature of the stomach caused by *Helicobacter pylori* bacteria, use of drugs, stress, hypersecretion of HCl, etc. [80]. Administering aucubin orally at 20, 40, and 80 mg/kg BW for 3 d produced a gastroprotective effect in mice with ethanol-induced gastric mucosal lesions. The mechanism involved is the inhibition of NF-κB activation, which determines the production of proinflammatory cytokines such as TNF-α and IL-6. Aucubin increases levels of epidermal growth factor (EGF) and vascular endothelial growth factor (VEGF) to protect against ethanol-induced injuries and accelerate the healing of gastric mucosal erosion and elevates COX-1 levels, promoting prostaglandin biosynthesis that maintains gastric mucosal integrity and starting wound healing [57].

### *5.10. Hepatoprotective*

The hepatoprotective activity of aucubin has been demonstrated in mice with hepatic reperfusion–ischemic injury. Administering aucubin at a dose of 5 mg/kg BW relieved liver injury through an anti-inflammatory mechanism, i.e., inhibiting the HMGB1/TLR-4/NF-κB pathway that plays a role in producing inflammatory cytokines (TNF-α, IL-1β, and HMGB1), and through an antioxidant mechanism. The latter includes elevating SOD levels, increasing mitochondrial activity, inhibiting ROS production, and reducing apoptosis through the increased expression of PGC-1α and UCP2, which can hinder ROS, and the reduced expression of caspase-3 as the cause of apoptosis [64].

Aucubin can also alleviate nonalcoholic fatty liver disease (NAFLD) caused by obesity [62] through several mechanisms: inhibiting the release of proinflammatory cytokines (TNF-α, IL-1β, IL-6) and increasing the phosphorylation of ACC, AMPKα, and AKT that stimulate more production of antioxidant enzymes. Nrf2 activation can also inhibit lipogenesis and trigger fatty acid oxidation by inhibiting the ACC1/ACC2 enzymes (catalysts for converting acetyl-CoA to malonyl-CoA), thus reducing malonyl-CoA and elevating the levels of fatty acids entering the mitochondria to be oxidized. Moreover, AMPK triggers the expression of the tricarboxylic acid cycle and increases PGC-1α expression and SOD levels.

In addition to the two conditions above, aucubin and aucubigenin also have a protective effect on hepatic fibrosis. These two compounds inhibit HSC activation by suppressing α-SMA expression, prevent over-expression of extracellular matrix (Col I, Col III) that can be deposited in interstitial cells and cause fibrosis, and decrease intracellular ROS production by reducing the mRNA expression of NOX4. NOX4 is an NADPH oxidase that determines the generation of ROS and activation of hepatic stellate cells [68].

### *5.11. Cardioprotective*

In cardiac dysfunction caused by lipopolysaccharide induction, administering aucubin at 20 and 40 mg/kg BW produced a protective effect. Here, aucubin suppresses the transcription of inflammatory cytokines by inhibiting the NLRP3 inflammasomes, thereby reducing proinflammatory cytokine expression. This compound also ameliorates oxidative stress by lowering MDA, TXNIP levels, and ROS generation [63]. Furthermore, it affects the nNOS/NO pathway, alleviating oxidative stress and inhibiting ASK1/JNK signaling. With oxidative stress being reduced, the consumption of thioredoxin also decreases (Trx), causing ASK1 to form an inactive complex with Trx and prevent apoptosis in myocardial infarction [71]. In addition, aucubin also regulates Bcl2 protein expression and reduces caspase-3 activation, causing the inhibition of apoptosis. The role of aucubin in nNOS regulation was also demonstrated by other studies, where the results showed aucubin suppressing oxidative stress during cardiac remodeling and inhibiting cardiac hypertrophy due to excess pressure, hypertrophy, fibrosis, and inflammation. The cardioprotective mechanism includes the increased expression of nNOS, i.e., by regulating ion channels and thus modulating abnormal $Ca^{2+}$ homeostasis, and mitochondrial function. nNOS expression can increase in conditions of ischemia–reperfusion injuries, infarctions, hypertrophies, and heart failures [91].

### *5.12. Neuroprotective*

In research on traumatic brain injury, aucubin was reported to produce a neuroprotective effect when administered at 20 and 40 mg/kg BW as a result of its antioxidant activities (increasing Nrf2 translocation into the nucleus, activating antioxidant enzymes, suppressing ROS generation, and reducing cell apoptosis) and anti-inflammatory activities (suppressing HMGB1-mediated inflammation) [59]. In addition, aucubin at a concentration of 0.1 to 1 mM protected cells from apoptosis induced using $H_2O_2$ and facilitated neurite extension and axon regeneration in the peripheral nervous system [92]. The neuroprotective activity was also demonstrated by the ability of aucubin to prevent diabetic encephalopathy by reducing oxidative stress and inhibiting neuronal apoptosis [78].

### *5.13. Osteoprotective*

Aucubin has an anti-osteoporotic effect, as it increases the expression of cytokines by differentiating osteoblasts (such as collagen I, osteocalcin, osteopontin, and osterix) in bone tissue [72]. Osteocalcin and osteopontin influence the osteoclast activity responsible for bone development and regeneration, and osterix activates osteocalcin in mature osteoblasts and regulates the final stages of bone formation. In addition, aucubin has been reported to increase the expression of antioxidative factors Nrf2 (SOD-1, HO-1, catalase), suppress ROS production, reduce Bax and cleaved caspase-3 expression, increase Bcl2 expression, and reduce the rate of apoptosis. Its osteoprotective effect is generated through anti-inflammatory and antioxidant activities. The anti-inflammatory activities include the inhibition of IKKα/β and IKBα phosphorylation and p65 subunit translocation, reducing the expression of inflammatory mediators (MMP, iNOS, COX-2, NO) and inflammatory cytokines. Meanwhile, the antioxidant activities are the inhibition of IL-1β-induced apoptosis of chondrocytes by increasing Bax expression, reducing Bcl2 expression, and suppressing ROS generation [54,73].

### *5.14. Renoprotective*

Cisplatin is an anticancer compound with various side effects, including nephrotoxicity. The activity of aucubin against cisplatin-induced acute kidney injuries has been tested; the results showed that administering aucubin orally and intraperitoneally at 1.5 and 5 mg/kg BW could reduce tissue changes in the kidney. The renoprotective mechanisms involve suppressing the expression of p65 NF-κB in proximal tubular cells and TNF-α expression in the kidney, suppressing STAT3 activation that can lead to dose-dependent apoptosis, increasing the expression of antioxidant genes such as HO-1, and reducing the lipid peroxidation product 4-HNE based on the dose administered. Aucubin also suppresses the increased expression of FOXO3a, thus preventing cisplatin-induced renal cell apoptosis [61].

The renoprotective effect of aucubin can also be seen from its ability to relieve albuminuria and contain the expansion of the glomerular extracellular matrix, renal fibrosis, and inflammation caused by diabetes [56]. Aucubin inhibits the expression of p-IκBα and inflammatory cytokines (IL-1β, IL-8, IL-10, and TNF-α) and p65 nucleus accumulation. Furthermore, it upregulates SIRT1/SIRT3, causes deacetylation, increases FOXO3a translocation, and intensifies the activity of the Nrf2 signaling pathway. FOXO3a transcription produces Mn-SOD and CAT, and Nrf2 transcription generates NQO1 and HO-1; all four compounds can inhibit ROS and provide antioxidant effects.

### *5.15. Retinoprotective*

Because of its anti-inflammatory and antioxidant activities, the retinoprotective effect of aucubin is expected. The mechanism involved is the inhibition of the NF-κB signal, which can suppress the mRNA expression of IL-1β, IL-8, and TNF-α and regulate the expression of the Bcl2 protein group (as a regulator of apoptosis), thus inhibiting apoptosis [60]. In another work, administering oral aucubin at a dose of 15 mg/kg BW prevented retinal degeneration induced using N-methyl-N-nitrosourea in mice. This effect is believed to result from the inhibition of oxidative damage and apoptosis of DNA, as shown by the decrease in 8-OHdG generally formed due to the generation of excess ROS [79].

## 6. Safety and Toxicity

Various studies have successfully demonstrated the biological activity of aucubin. Unfortunately, toxicity tests on aucubin have not been widely carried out. On the other hand, safety is one of the mandatory requirements for a compound to be used as a medicine. However, Chang et al. reported the results of the toxicity test on mice [93]. A series of aucubin doses (100, 300, 600, and 900 mg/kg BW) were administered i.p. in mice to measure its lethal dose. None of the test animals died after 24 h, but the activity of serum GOT and alkaline phosphatase decreased slightly at doses of 300 to 900 mg/kg BW, and triglyceride

levels increased slightly. To determine the acute toxicity, three dose levels of aucubin (20, 40, and 80 mg/kg BW on mice) were administered intraperitoneally. There was no change in the enzyme activity (alkaline phosphatase, GOT, GPT) and the levels of triglycerides, glucose, urea nitrogen, and total protein in the test groups compared to the control group. Therefore, it can be concluded that aucubin is a compound with low toxicity and its lethal dose is estimated to be above 0.9 g [93,94]. Further toxicity tests, especially sub-chronic and chronic toxicity tests, are needed to determine the safety of aucubin in long-term use.

## 7. Conclusions

Aucubin is an iridoid glycoside widely distributed in the families *Cornaceae*, *Garryaceae*, *Orobanchaceae*, *Globulariaceae*, *Eucommiaceae*, *Scrophulariaceae*, *Plantaginaceae*, and *Rubiaceae*. Various isolation methods have been tested and developed, considering that pure aucubin plays an essential role in standardizing raw materials and traditional medicinal products, synthesizing other iridoid glycosides, product development, and pharmacological, pharmacodynamic, and pharmacokinetic studies. Aucubin shows promise for a variety of therapeutic and biomedical applications because of its biological activities as an anti-inflammatory, antioxidant, anxiolytic and antidepressant, antidiabetic, antifibrotic, antifungal and antimicrobial, anticancer, antihyperlipidemic, gastroprotective, cardioprotective, hepatoprotective, retinoprotective, neuroprotective, osteoprotective, and renoprotective agent. Further research in human application is urgently needed to substantiate the clinical evidence of aucubin. Sub-chronic and chronic toxicity tests are indispensable in determining the safety of aucubin in long-term use. In addition, research related to drug delivery systems must be conducted considering the unstable nature of aucubin.

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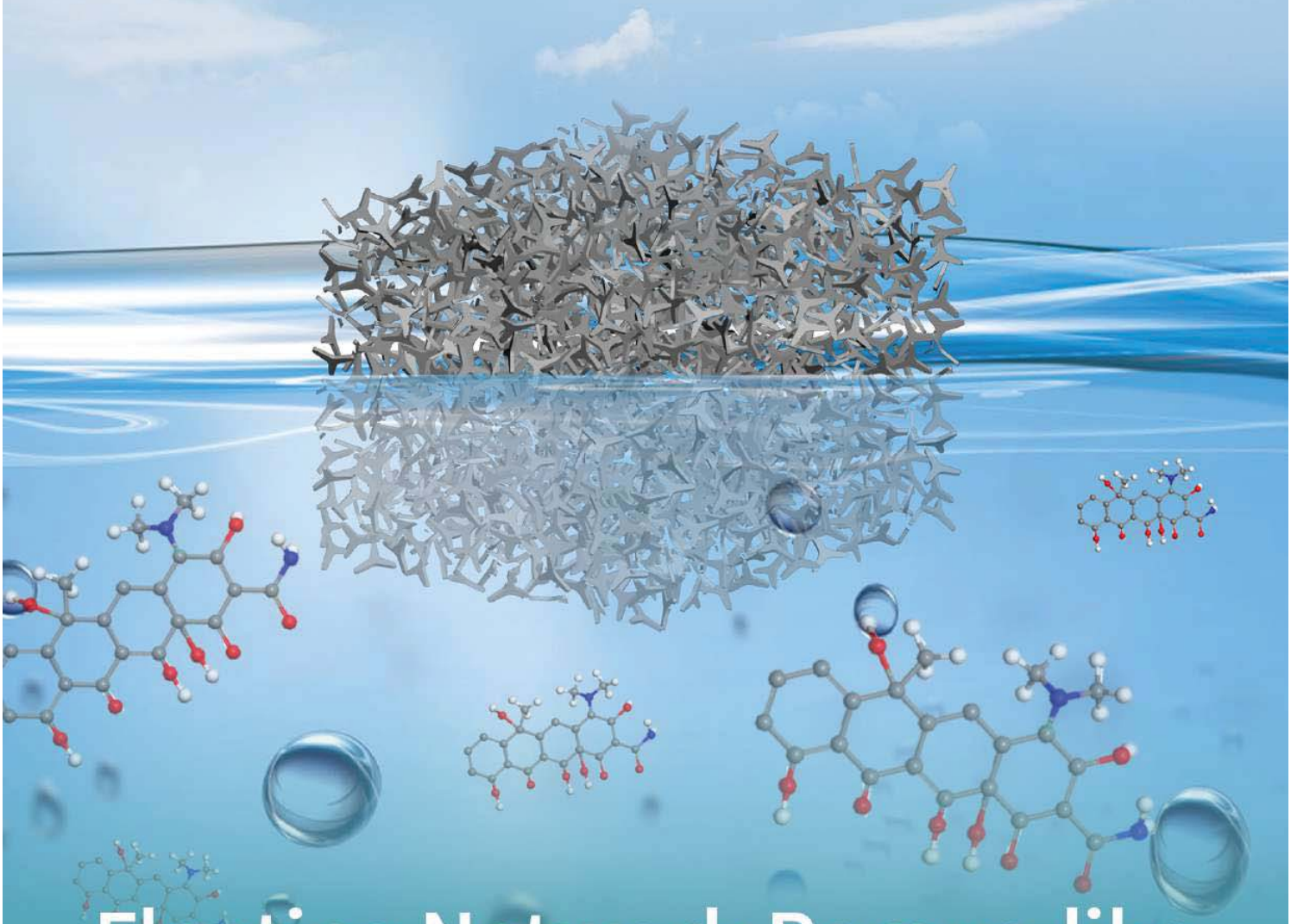

# Floating Network Porous-like Sponge Monolithic Structure g-$C_3N_4$ Photocatalyst

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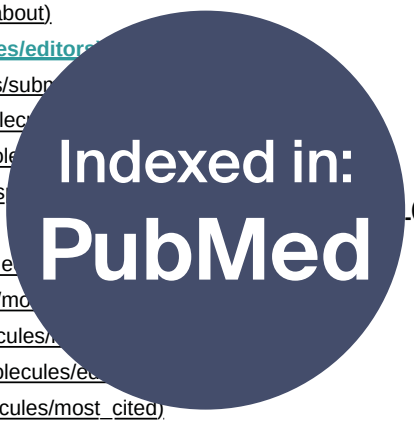


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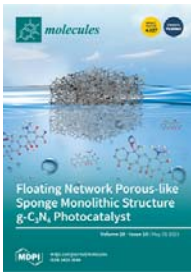


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by **Taghreed Alsufyani**, **Najwa Al-Otaibi**, **Noura J. Alotaibi**, **Nour Houda M'sakni** and **Eman M. Alghamdi**

*Molecules* **2023**, *28*(10), 4255; **https://doi.org/10.3390/molecules28104255 (https://doi.org/10.3390/molecules28104255)** - 22 May 2023

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**Abstract** Bacterial secondary metabolites are a valuable source of various molecules that have antibacterial and anticancer activity. In this study, ten endosymbiotic bacteria of aphids, aphid predators and ants were isolated. Bacterial strains were identified according to the 16S rRNA gene. Ethyl acetate fractions **[...] Read more.**

(This article belongs to the Special Issue **Characterization, Properties and Applications of Natural Products-2nd Edition ( /journal/molecules/special_issues/4Q5ICQ47SQ )**)

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Open Access Article 14 pages, 2812 KiB (/1420-3049/28/10/4254/pdf?version=1684817568)

**The First Phytochemical Investigation of *Artemisia divaricate*: Sesquiterpenes and Their Anti-Inflammatory Activity (/1420-3049/28/10/4254)**

by **Siqi Yan**, **Changqiang Ke**, **Zheling Feng**, **Chunping Tang** and **Yang Ye**

*Molecules* **2023**, *28*(10), 4254; **https://doi.org/10.3390/molecules28104254 (https://doi.org/10.3390/molecules28104254)** - 22 May 2023

**Cited by 4 (/1420-3049/28/10/4254#metrics)** | Viewed by 1750

**Abstract** *Artemisia divaricate* belongs to the *Artemisia* genus of the family of Compositae, a sort of perennial herb endemic in most regions of China. For the first time, a phytochemical investigation was carried out on the whole plant of *Artemisia divaricate*, resulting in **[...] Read more.**

(This article belongs to the Special Issue **Chemicals of Natural Origin and Their Biological Activities ( /journal/molecules/special_issues/S8R51C95XS )**)

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Open Access Article 18 pages, 5032 KiB (/1420-3049/28/10/4253/pdf?version=1684811289)

**Structural Quantification of the Surface-Confined Metal-Organic Precursors Simulated with the Lattice Monte Carlo Method (/1420-3049/28/10/4253)**

by **Jakub Lisiecki** and **Paweł Szabelski**

*Molecules* **2023**, *28*(10), 4253; **https://doi.org/10.3390/molecules28104253 (https://doi.org/10.3390/molecules28104253)** - 22 May 2023

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**Abstract** The diversity of surface-confined metal-organic precursor structures, which recently have been observed experimentally, poses a question of how the individual properties of a molecular building block determine those of the resulting superstructure. To answer this question, we use the Monte Carlo simulation technique **[...] Read more.**

(This article belongs to the Special Issue **Exclusive Feature Papers in Physical Chemistry ( /journal/molecules/special_issues/FP_physchem )**)

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Open Access Review 38 pages, 13790 KiB (/1420-3049/28/10/4252/pdf?version=1684815851)

**Recent Progress in the Rational Design of Biothiol-Responsive Fluorescent Probes (/1420-3049/28/10/4252)**

by **Wenzhi Xie**, **Jinyu Jiang**, **Dunji Shu**, **Yanjun Zhang**, **Sheng Yang** and **Kai Zhang**

*Molecules* **2023**, *28*(10), 4252; **https://doi.org/10.3390/molecules28104252 (https://doi.org/10.3390/molecules28104252)** - 22 May 2023
**Cited by 19 (/1420-3049/28/10/4252#metrics)** | Viewed by 3689

**Abstract** Biothiols such as cysteine, homocysteine, and glutathione play significant roles in important biological activities, and their abnormal concentrations have been found to be closely associated with certain diseases, making their detection a critical task. To this end, fluorescent probes have become increasingly popular **[...] Read more.**

(This article belongs to the Special Issue **Functionalized Inorganic and Organic Materials: Applications in Sensing, Diagnosis and Pharmaceutics ( /journal/molecules/special_issues/PB3R92930J )**)

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Open Access Article 11 pages, 2368 KiB (/1420-3049/28/10/4251/pdf?version=1684820480)

**Synthesis of *meta*-Aminophenol Derivatives via Cu-Catalyzed [1,3]-Rearrangement—Oxa-Michael Addition Cascade Reactions (/1420-3049/28/10/4251)**

by **Itaru Nakamura**, **Mai Tachibana**, **Riku Konta**, **Hiroki Tashiro** and **Masahiro Terada**

*Molecules* **2023**, *28*(10), 4251; **https://doi.org/10.3390/molecules28104251 (https://doi.org/10.3390/molecules28104251)** - 22 May 2023

**Cited by 2 (/1420-3049/28/10/4251#metrics)** | Viewed by 2400

**Abstract** Cu-catalyzed reactions of *N*-alkoxy-2-methylanilines and alcohols in the presence of catalytic amounts of IPrCuBr and $AgSbF_6$ afforded the corresponding *meta*-aminophenol derivatives in good to high yields. These reactions proceed via a [1,3]-rearrangement, in which the alkoxy group migrates from the **[...] Read more.**

(This article belongs to the Special Issue **Advances on the Application of N-O Bond Compounds ( /journal/molecules/special_issues/60DF1XCDNT )**)

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Open Access Article 13 pages, 3901 KiB (/1420-3049/28/10/4250/pdf?version=1684828237)

**The Fate of the Chlorophyll Derivatives in Olives Preserved and/or Packaged in Presence of Exogenous Copper (/1420-3049/28/10/4250)**

by **Fausta Natella**, **Gianni Pastore**, **Altero Aguzzi**, **Paolo Gabrielli**, **Nicoletta Nardo** and **Roberto Ambra**

*Molecules* **2023**, *28*(10), 4250; **https://doi.org/10.3390/molecules28104250 (https://doi.org/10.3390/molecules28104250)** - 22 May 2023

**Cited by 3 (/1420-3049/28/10/4250#metrics)** | Viewed by 1574

**Abstract** Chlorophyll pigments are thought to be responsible for the highly appreciated green color of unfermented Castelvetrano-style table olives, but no studies have considered the effects of a controlled addition of copper during storage or packaging at the industrial level. For this purpose, chlorophyll **[...] Read more.**

(This article belongs to the Special Issue **Feature Papers in Food Chemistry—2nd Edition ( /journal/molecules/special_issues/4PYC394G23 )**)

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Open Access Review 36 pages, 13691 KiB (/1420-3049/28/10/4249/pdf?version=1684835649)

**Radical Decarboxylative Carbon–Nitrogen Bond Formation (/1420-3049/28/10/4249)**

by **Xiangting Li**, **Xiaobin Yuan**, **Jiahao Hu**, **Yajun Li** and **Hongli Bao**

*Molecules* **2023**, *28*(10), 4249; **https://doi.org/10.3390/molecules28104249 (https://doi.org/10.3390/molecules28104249)** - 22 May 2023

**Cited by 12 (/1420-3049/28/10/4249#metrics)** | Viewed by 4269

**Abstract** The carbon–nitrogen bond is one of the most prevalent chemical bonds in natural and artificial molecules, as many naturally existing organic molecules, pharmaceuticals, agrochemicals, and functional materials contain at least one nitrogen atom. Radical decarboxylative carbon–nitrogen bond formation from readily available carboxylic acids **[...] Read more.**

(This article belongs to the Section **Organic Chemistry (/journal/molecules/sections/organic_chemistry)**)

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Open Access Article 15 pages, 2442 KiB (/1420-3049/28/10/4248/pdf?version=1684808737)

Detection of Hazelnut and Almond Adulteration in Olive Oil: An Approach by qPCR (/1420-3049/28/10/4248)

by **So** **amos-Gómez**, **María D. Busto** and **Natividad Ortega**

*Molecules* **2023**, *28*(10), 4248; https://doi.org/10.3390/molecules28104248 (https://doi.org/10.3390/molecules28104248) - 22 May 2023

**Abstract** Virgin olive oil (VOO), characterized by its unique aroma, flavor, and health benefits, is subject to adulteration with the addition of oils obtained from other edible species. The consumption of adulterated olive oil with nut species, such as hazelnut or almond, leads to **[...] Read more.**
(This article belongs to the Special Issue **Virgin Olive Oil: Processing, Byproducts, Quality Control, and Nutraceutical Profile ( /journal/molecules/special_issues/virgin_olive_oil_processing )**)

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Open Access Article 19 pages, 2022 KiB **(/1420-3049/28/10/4247/pdf?version=1684816610)**

**Effect of Heating Temperature of High-Quality Arbequina, Picual, Manzanilla and Cornicabra Olive Oils on Changes in Nutritional Indices of Lipid, Tocopherol Content and Triacylglycerol Polymerization Process (/1420-3049/28/10/4247)**

by **Dominik Kmiecik**, **Monika Fedko**, **Justyna Małecka**, **Aleksander Siger** and **Przemysław Łukasz Kowalczewski**
*Molecules* **2023**, *28*(10), 4247; **https://doi.org/10.3390/molecules28104247 (https://doi.org/10.3390/molecules28104247)** - 22 May 2023
**Cited by 8 (/1420-3049/28/10/4247#metrics)** | Viewed by 3351

**Abstract** The aim of the study was to determine the stability and heat resistance of extra premium olive oil. The study material consisted of six extra virgin olive oils (EVOO) obtained from Spain. Four samples were single-strain olive oils: Arbequina, Picual, Manzanilla, and Cornicabra. **[...] Read more.**
(This article belongs to the Special Issue **Virgin Olive Oil: Processing, Byproducts, Quality Control, and Nutraceutical Profile ( /journal/molecules/special_issues/virgin_olive_oil_processing )**)

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Open Access Review 37 pages, 8426 KiB **(/1420-3049/28/10/4246/pdf?version=1684822945)**

**A Review of Research Progress on the Performance of Intelligent Polymer Gel (/1420-3049/28/10/4246)**

by **Shuangchun Yang**, **Zhenye Liu**, **Yi Pan**, **Jian Guan**, **Peng Yang** and **Muratbekova Asel**
*Molecules* **2023**, *28*(10), 4246; **https://doi.org/10.3390/molecules28104246 (https://doi.org/10.3390/molecules28104246)** - 22 May 2023
**Cited by 8 (/1420-3049/28/10/4246#metrics)** | Viewed by 2501

**Abstract** Intelligent polymer gel, as a popular polymer material, has been attracting much attention for its application. An intelligent polymer gel will make corresponding changes to adapt to the environment after receiving stimuli; therefore, an intelligent polymer gel can play its role in many **[...] Read more.**
(This article belongs to the Special Issue **Smart Polymeric Micro/Nanomaterials ( /journal/molecules/special_issues/smart_polymeric_materials )**)

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Open Access Article 17 pages, 6818 KiB (/1420-3049/28/10/4245/pdf?version=1684761369)

**Efficient Conversion of Lignin to Aromatics via Catalytic Fast Pyrolysis over Niobium-Doped HZSM-5 (/1420-3049/28/10/4245)**

by **Zhen Li**, **Huihui Zhang**, **Deshi Yang**, **Zhipeng Hu**, **Fengqiang Wang** and **Zhijun Zhang**

*Molecules* **2023**, *28*(10), 4245; **https://doi.org/10.3390/molecules28104245 (https://doi.org/10.3390/molecules28104245)** - 22 May 2023
**Cited by 7 (/1420-3049/28/10/4245#metrics)** | Viewed by 2270

**Abstract** A niobium-doped HZSM-5 (H[Nb]ZSM-5) was prepared by a hydrothermal synthesis method. The morphology, phase structure, composition, pore structure, and acid content of the catalyst were characterized using a series of analysis techniques such as scanning electron microscope (SEM), energy-dispersive X-ray (EDX), X-ray diffraction **[...] Read more.**

(This article belongs to the Collection **Recycling of Biomass Resources: Biofuels and Biochemicals ( /journal/molecules/topical_collections/biomass_biochemicals )**)

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Open Access Article 17 pages, 3953 KiB (/1420-3049/28/10/4244/pdf?version=1684760197)

**_p_-Synephrine Indicates Internal Maturity of _Citrus grandis_ (L.) Osbeck cv. Mato Peiyu—Reclaiming Functional Constituents from Nonedible Parts (/1420-3049/28/10/4244)**

by **Li-Yun Lin**, **Chiung Chi Peng**, **Yi-Ping Huang**, **Kuan-Chou Chen** and **Robert Y. Peng**

*Molecules* **2023**, *28*(10), 4244; **https://doi.org/10.3390/molecules28104244 (https://doi.org/10.3390/molecules28104244)** - 22 May 2023

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**Abstract** The processing of *Citrus grandis* Osbeck cv. Mato Peiyu (CGMP) fruits generates a considerable amount of waste, mainly the flavedo, albedo, and segment membrane; the generated waste yields severe environmental and economic challenges. In this study, we tried to reclaim some functional chemicals **[...] Read more.**

(This article belongs to the Special Issue **Biosynthesis and Metabolism of Bioactive Components in Fruits and Vegetables ( /journal/molecules/special_issues/76L8MG7075 )**)

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Open Access Review 20 pages, 1464 KiB (/1420-3049/28/10/4243/pdf?version=1684760109)

**Application of Rosmarinic Acid with Its Derivatives in the Treatment of Microbial Pathogens (/1420-3049/28/10/4243)**

by **Ourdia-Nouara Kernou**, **Zahra Azzouz**, **Khodir Madani** and **Patricia Rijo**

*Molecules* **2023**, *28*(10), 4243; **https://doi.org/10.3390/molecules28104243 (https://doi.org/10.3390/molecules28104243)** - 22 May 2023

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**Abstract** The emergence of the antimicrobial resistance phenomena on and the harmful consequences of the use of antibiotics motivate the necessity of innovative antimicrobial therapies, while natural substances are considered a promising alternative. Rosmarin is an original plant compound listed among the hydroxycinnamic acids. **[...] Read more.**

(This article belongs to the Special Issue **Drug Development Inspired by Natural Products II ( /journal/molecules/special_issues/9809W0LY93 )**)

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Open Access Article 10 pages, 3287 KiB (/1420-3049/28/10/4242/pdf?version=1684761854)

**Cocrystallization of Progesterone with Nitrogen Heterocyclic Compounds: Synthesis, Characterization, Calculation and Property Evaluation (/1420-3049/28/10/4242)**

by **Juan Xu**, **Wei Gao**, **Qi Zhang** and **Lifeng Ning**

*Molecules* **2023**, *28*(10), 4242; **https://doi.org/10.3390/molecules28104242 (https://doi.org/10.3390/molecules28104242)** - 22 May 2023

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**Abstract** Progesterone injection is oily because of its poor solubility. It is necessary to develop new dosage forms or delivery methods for Progesterone. Six cocrystals of Progesterone with nitrogen heterocyclic compounds (2,6-diaminopyridine, isonicotinamide, 4-aminopyridine, aminopyrazine, picolinamide and pyrazinamide) have been designed and prepared by **[...] Read more.**

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Open Access Article 15 pages, 4902 KiB (/1420-3049/28/10/4241/pdf?version=1684754281)

## Leocarpinolide B Attenuates Collagen Type II-Induced Arthritis by Inhibiting DNA Binding Activity of NF-κB (/1420-3049/28/10/4241)

by **Ke-Gang Linghu**, **Guan-Ding Zhao**, **Dai-Yan Zhang**, **Shi-Hang Xiong**, **Guo-Ping Wu**, **Li-Yu Shen**, **Wen-Qing Cui**, **Tian Zhang**, **Yuan-Jia Hu**, **Bing Guo**, **Xiang-Chun Shen** and **Hua Yu**

*Molecules* **2023**, *28*(10), 4241; **https://doi.org/10.3390/molecules28104241 (https://doi.org/10.3390/molecules28104241)** - 22 May 2023
**Cited by 4 (/1420-3049/28/10/4241#metrics)** | Viewed by 2555

**Abstract** Rheumatoid arthritis (RA) is a chronic autoimmune disease triggered by a cascading inflammatory response. Sigesbeckia Herba (SH) has long been utilized as a traditional remedy to alleviate symptoms associated with rheumatism. Our previous study found that leocarpinolide B (LB), a sesquiterpene lactone isolated **[...] Read more.**

(This article belongs to the Special Issue **Novel Therapeutic Targets and Potential Drugs for Inflammatory Disease ( /journal/molecules/special_issues/Therapeutic_Targets_Inflammatory )**)

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Open Access Article 25 pages, 3767 KiB (/1420-3049/28/10/4240/pdf?version=1684760629)

## Novel Thiazolylketenyl Quinazolinones as Potential Anti-MRSA Agents and Allosteric Modulator for PBP2a (/1420-3049/28/10/4240)

by **Jie Dai**, **Narsaiah Battini**, **Zhonglin Zang**, **Yan Luo** and **Chenghe Zhou**

*Molecules* **2023**, *28*(10), 4240; **https://doi.org/10.3390/molecules28104240 (https://doi.org/10.3390/molecules28104240)** - 22 May 2023
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**Abstract** Bacterial infections caused by methicillin-resistant *Staphylococcus aureus* have seriously threatened public health. There is an urgent need to propose an existing regimen to overcome multidrug resistance of MRSA. A unique class of novel anti-MRSA thiazolylketenyl quinazolinones (TQs) and their analogs were developed. Some synthesized **[...] Read more.**

(This article belongs to the Special Issue **Biological Activity of Natural and Synthetic Compounds 2.0 ( /journal/molecules/special_issues/8SE89QXNJA )**)

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Open Access Review 23 pages, 441 KiB (/1420-3049/28/10/4239/pdf?version=1685027970)

**The Genus *Capsicum*: A Review of Bioactive Properties of Its Polyphenolic and Capsaicinoid Composition (/1420-3049/28/10/4239)**

by **Rodrigo Alonso-Villegas**, **Rosa María González-Amaro**, **Claudia Yuritzi Figueroa-Hernández** and **Ingrid Mayanin Rodríguez-Buenfil**
*Molecules* **2023**, *28*(10), 4239; **https://doi.org/10.3390/molecules28104239 (https://doi.org/10.3390/molecules28104239)** - 22 May 2023
**Cited by 21 (/1420-3049/28/10/4239#metrics)** | Viewed by 5067

**Abstract** Chili is one of the world's most widely used horticultural products. Many dishes around the world are prepared using this fruit. The chili belongs to the genus *Capsicum* and is part of the *Solanaceae* family. This fruit has essential biomolecules such as carbohydrates, **[...] Read more.**
(This article belongs to the Special Issue **Biological Activity of Phenolics and Polyphenols in Nature Products ( /journal/molecules/special_issues/200064T4W9 )**)

Open Access Article 12 pages, 2364 KiB (/1420-3049/28/10/4238/pdf?version=1684751520)

**Exploring *Echinops polyceras* Boiss. from Jordan: Essential Oil Composition, COX, Protein Denaturation Inhibitory Power and Antimicrobial Activity of the Alcoholic Extract (/1420-3049/28/10/4238)**

by **Hazem S. Hasan**, **Ashok K. Shakya**, **Hala I. Al-Jaber**, **Hana E. Abu-Sal** and **Lina M. Barhoumi**
*Molecules* **2023**, *28*(10), 4238; **https://doi.org/10.3390/molecules28104238 (https://doi.org/10.3390/molecules28104238)** - 22 May 2023
**Cited by 4 (/1420-3049/28/10/4238#metrics)** | Viewed by 2127

**Abstract** In this article, we present the first detailed analysis of the hydro-distilled essential oil (HDEO) of the inflorescence heads of *Echinops polyceras* Boiss. (Asteraceae) from the flora of Jordan, offering observations at different growth (pre-flowering, full-flowering and post-flowering) stages. Additionally, we investigated the **[...] Read more.**

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Open Access Article 16 pages, 3676 KiB (/1420-3049/28/10/4237/pdf?version=1684751672)

**Photosensitive Dye as an Ideal Peroxymonosulfate Activator for Efficient Self-Degradation: A Novel Idea of Using Waste to Treat Waste (/1420-3049/28/10/4237)**

by **Zhiyao Zhang**, **Zhaolin Li**, **Xue Bai**, **Juan Shi**, **Min Hu**, **Jin Chai**, **Keqian Li** and **Pengkang Jin**
*Molecules* **2023**, *28*(10), 4237; **https://doi.org/10.3390/molecules28104237 (https://doi.org/10.3390/molecules28104237)** - 22 May 2023
**Cited by 2 (/1420-3049/28/10/4237#metrics)** | Viewed by 1822

**Abstract** Commonly used peroxydisulfate (PS) or peroxymonosulfate (PMS) activation methods have been limited in their practical application due to certain drawbacks, such as high cost, high energy consumption and secondary pollution. In this study, a catalyst-free alizarin green (AG) self-activating PMS catalytic system was **[...] Read more.**
(This article belongs to the Special Issue **Energy-Relevant Advanced Materials ( /journal/molecules/special_issues/VZU37XDZ48 )**)

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Open Access Article 10 pages, 1532 KiB (/1420-3049/28/10/4236/pdf?version=1684978697)

**A Quick Method to Synthesize Extrachromosomal Circular DNA In Vitro (/1420-3049/28/10/4236)**

by **Sh Zuo**, **Xueguang Li**, **Yide Yang**, **Junhua Zhou** and **Quanyuan He**
*Molecules* **2023**, *28*(10), 4236; **https://doi.org/10.3390/molecules28104236 (https://doi.org/10.3390/molecules28104236)** - 22 May 2023

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**Abstract** Extrachromosomal circular DNA (eccDNA) is a special class of circular DNA in eukaryotes. Recent studies have suggested that eccDNA is the product of genomic instability and has important biological functions to regulate many downstream biological processes. While NGS (Next-Generation Sequencing)-based eccDNA sequencing has **[...] Read more.**

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Open Access Article 14 pages, 1399 KiB (/1420-3049/28/10/4235/pdf?version=1684803618)

## Highly-Selective Analytical Strategy for 90 Pesticides and Metabolites Residues in Fish and Shrimp Samples (/1420-3049/28/10/4235)

by **Yage Guo**, **Jun Xie**, **Fengshou Dong**, **Xiaohu Wu**, **Xinglu Pan**, **Xingang Liu**, **Yongquan Zheng**, **Jie Zhang** and **Jun Xu**

*Molecules* **2023**, *28*(10), 4235; https://doi.org/10.3390/molecules28104235 (https://doi.org/10.3390/molecules28104235) - 22 May 2023

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**Abstract** The analysis of pesticide residues in aquatic products is challenging due to low residue levels and the complex matrix interference. In this study, we developed a simple, fast method for the trace analysis of 90 pesticides and metabolites in aquatic products. The analytes **[...] Read more.**

(This article belongs to the Section **Analytical Chemistry (/journal/molecules/sections/Analytical_Chemistry)**)

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Open Access Article 20 pages, 2070 KiB (/1420-3049/28/10/4234/pdf?version=1684743049)

## Synthesis, Pharmacological Evaluation, and Molecular Modeling of Lappaconitine–1,5-Benzodiazepine Hybrids (/1420-3049/28/10/4234)

by **Kirill P. Cheremnykh**, **Arkadiy O. Bryzgalov**, **Dmitry S. Baev**, **Sergey A. Borisov**, **Yulia S. Sotnikova**, **Victor A. Savelyev**, **Tatyana G. Tolstikova**, **Shamansur S. Sagdullaev** and **Elvira E. Shults**

*Molecules* **2023**, *28*(10), 4234; https://doi.org/10.3390/molecules28104234 (https://doi.org/10.3390/molecules28104234) - 22 May 2023

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**Abstract** Diterpenoid alkaloids, originating from the amination of natural tetracyclic diterpenes, have long interested scientists due to their medicinal uses and infamous toxicity which has limited the clinical application of the native compound. Alkaloid lappaconitine extracted from various *Aconitum* and *Delphinium* species has displayed **[...] Read more.**

(This article belongs to the Section **Medicinal Chemistry (/journal/molecules/sections/medicinal_chemistry)**)

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Open Access Review 29 pages, 7216 KiB (/1420-3049/28/10/4233/pdf?version=1684978091)

## Added Complexity!—Mechanistic Aspects of Heterobimetallic Complexes for Application in Homogeneous Catalysis (/1420-3049/28/10/4233)

by **Zeno Fickenscher** and **Evamarie Hey-Hawkins**

*Molecules* **2023**, *28*(10), 4233; https://doi.org/10.3390/molecules28104233 (https://doi.org/10.3390/molecules28104233) - 22 May 2023

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**Abstract** Inspired by multimetallic assemblies and their role in enzyme catalysis, chemists have developed a plethora of heterobimetallic complexes for application in homogeneous catalysis. Starting with small heterobimetallic complexes with σ-donating and π-accepting ligands, such as N-heterocyclic carbene and carbonyl ligands, more and more **[...] Read more.**

(This article belongs to the Topic **Catalytic Applications of Transition Metals (/topics/Catalytic_Metals)**)

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Open Access Review 14 pages, 2079 KiB (/1420-3049/28/10/4232/pdf?version=1684741784)

**Honey Quality Control: Review of Methodologies for Determining Entomological Origin (/1420-3049/28/10/4232)**

by **Saeed Mohamadzade Namin**, **Sampat Ghosh** and **Chuleui Jung**

*Molecules* **2023**, *28*(10), 4232; **https://doi.org/10.3390/molecules28104232 (https://doi.org/10.3390/molecules28104232)** - 22 May 2023

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**Abstract** Honey is a widely consumed natural product, and its entomological origin can significantly influence its market value. Therefore, traceability of the entomological origin of honey should also be considered in honey quality control protocols. Although several methods exist, such as physicochemical characterization and **[...] Read more.**

(This article belongs to the Special Issue **The Chemistry of Honey and Other Bee Products: Novel Applications and Quality ( /journal/molecules/special_issues/honey_chemistry )**)

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Open Access Article 17 pages, 3396 KiB (/1420-3049/28/10/4231/pdf?version=1684739264)

**Dextran Methacrylate Reactions with Hydroxyl Radicals and Hydrated Electrons in Water: A Kinetic Study Using Pulse Radiolysis (/1420-3049/28/10/4231)**

by **Kamil J. Szafulera**, **Radosław A. Wach** and **Piotr Ulański**

*Molecules* **2023**, *28*(10), 4231; **https://doi.org/10.3390/molecules28104231 (https://doi.org/10.3390/molecules28104231)** - 22 May 2023

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**Abstract** Dextran methacrylate (Dex-MA) is a biodegradable polysaccharide derivative that can be cross-linked by ionizing radiation. It is therefore considered a potential replacement for synthetic hydrophilic polymers in current radiation technologies used for synthesizing hydrophilic cross-linked polymer structures such as hydrogels, mainly for medical **[...] Read more.**

(This article belongs to the Special Issue **Polysaccharide-Based Biopolymer: Recent Development and Applications ( /journal/molecules/special_issues/ABPCJCSOR8 )**)

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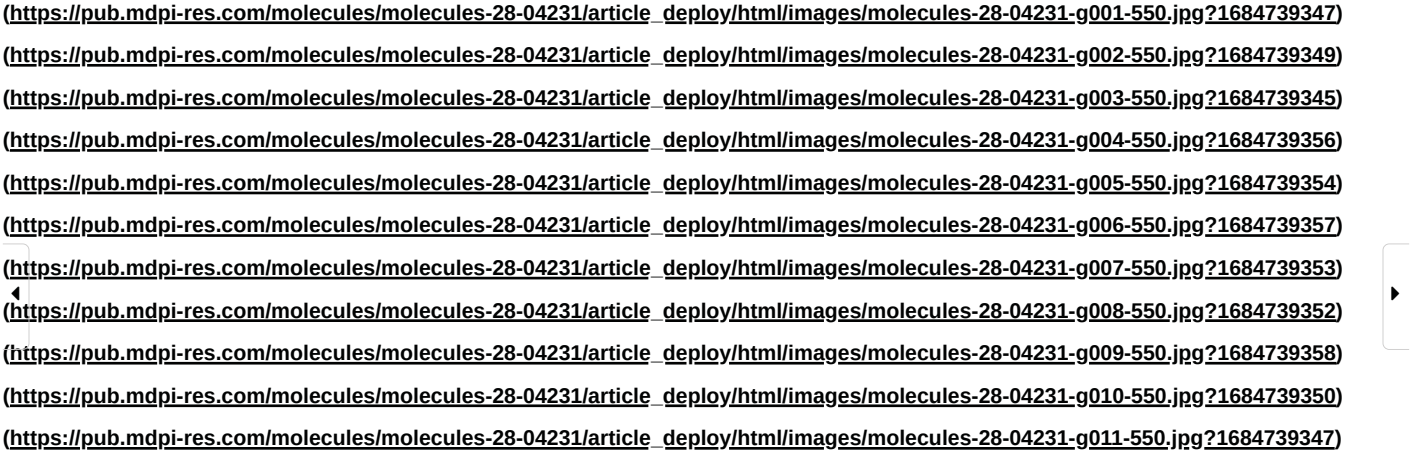

Open Access Article 25 pages, 5133 KiB (/1420-3049/28/10/4230/pdf?version=1684741702)

## The Impact of Fermentation Temperature and Cap Management on Selected Volatile Compounds and Temporal Sensory Characteristics of Grenache Wines from the Central Coast of California (/1420-3049/28/10/4230)

by **Emily S. Stoffel**, **Taylor M. Robertson**, **Anibal A. Catania** and **L. Federico Casassa**

*Molecules* **2023**, *28*(10), 4230; **https://doi.org/10.3390/molecules28104230 (https://doi.org/10.3390/molecules28104230)** - 22 May 2023

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**Abstract** Grenache wines from the Central Coast of California were subjected to different alcoholic fermentation temperature regimes (Cold, Cold/Hot, Hot) and cap management protocols, namely, punch down (PD), or no punch down (No PD), to determine the effect of these practices on the color, **[...] Read more.**

(This article belongs to the Topic **Advances in Analysis of Flavors and Fragrances: Chemistry, Properties and Applications in Food Quality Improvement (/topics/K95102U32T)**)

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Open Access Review 15 pages, 2466 KiB (/1420-3049/28/10/4229/pdf?version=1684737558)

## The History of *Desulfovibrio gigas* Aldehyde Oxidoreductase—A Personal View (/1420-3049/28/10/4229)

by **José J. G. Moura**

*Molecules* **2023**, *28*(10), 4229; **https://doi.org/10.3390/molecules28104229 (https://doi.org/10.3390/molecules28104229)** - 22 May 2023

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**Abstract** A story going back almost 40 years is presented in this manuscript. This is a different and more challenging way of reporting my research and I hope it will be useful to and target a wide-ranging audience. When preparing the manuscript and collecting **[...] Read more.**

(This article belongs to the Special Issue **Molybdenum and Tungsten Enzymes—State of the Art in Research ( /journal/molecules/special_issues/9YY8Q0OE7H )**)

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Open Access Article 16 pages, 3986 KiB (/1420-3049/28/10/4228/pdf?version=1684736002)

**Optimization and Validation of a Method to Determine Enolones and Vanillin Derivatives in Wines—Occurrence in Spanish Red Wines and Mistelles (/1420-3049/28/10/4228)**

by **Mónica Bueno**, **Julián Zapata**, **Laura Culleré**, **Ernesto Franco-Luesma**, **Arancha de-la-Fuente-Blanco** and **Vicente Ferreira**
*Molecules* **2023**, *28*(10), 4228; **https://doi.org/10.3390/molecules28104228 (https://doi.org/10.3390/molecules28104228)** - 22 May 2023
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**Abstract** Understanding the chemical nature of wine aroma demands accurate quantitative determinations of different odor-active compounds. Quantitative determinations of enolones (maltol, furaneol, homofuraneol, and sotolon) and vanillin derivatives (vanillin, methyl vanillate, ethyl vanillate, and acetovanillone) at low concentrations are complicated due to their high **[...] Read more.**
(This article belongs to the Special Issue **Analytical Methods for Characterization and Isolation of Natural Products ( /journal/molecules/special_issues/natural_products_isolation )**)

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Open Access Article 17 pages, 2035 KiB (/1420-3049/28/10/4227/pdf?version=1684730416)

**Proteomic Signature of Extracellular Vesicles Associated with Colorectal Cancer (/1420-3049/28/10/4227)**

by **Natalia Soloveva**, **Svetlana Novikova**, **Tatiana Farafonova**, **Olga Tikhonova** and **Victor Zgoda**
*Molecules* **2023**, *28*(10), 4227; **https://doi.org/10.3390/molecules28104227 (https://doi.org/10.3390/molecules28104227)** - 22 May 2023
**Cited by 7 (/1420-3049/28/10/4227#metrics)** | Viewed by 3064

**Abstract** The proteins of extracellular vesicles (EVs) provide proteomic signatures that reflect molecular features of EV-producing cells, including cancer cells. Detection of cancer cell EV proteins is of great interest due to the development of novel predictive diagnostic approaches. Using targeted mass spectrometry with **[...] Read more.**
(This article belongs to the Special Issue **Mass Spectrometry in Biomarkers Discovery ( /journal/molecules/special_issues/7YN28U2559 )**)

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Open Access Article 17 pages, 8429 KiB (/1420-3049/28/10/4226/pdf?version=1684729563)

**Mössbauer and Structure-Magnetic Properties Analysis of $A_yB_{1-y}C_xFe_{2-x}O_4$ (C=Ho,Gd,Al) Ferrite Nanoparticles Optimized by Doping (/1420-3049/28/10/4226)**

by **Qing Lin**, **Fang Yang**, **Qian Zhang**, **Kaimin Su**, **Huiren Xu**, **Yun He** and **Jinpei Lin**
*Molecules* **2023**, *28*(10), 4226; **https://doi.org/10.3390/molecules28104226 (https://doi.org/10.3390/molecules28104226)** - 22 May 2023
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**Abstract** $A_yB_{1-y}C_xFe_{2-x}O_4$ (C=Ho,Gd,Al) ferrite powders have been synthesized by the sol-gel combustion route. The X-ray diffraction of the $CoHo_xFe_{2-x}O_4$ ($x$ = 0~0.08) results indicated **[...] Read more.**
(This article belongs to the Special Issue **Magnetic Nanomaterials: Modern Trends and Prospects ( /journal/molecules/special_issues/magnetic_nanomaterials_prospects )**)

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Open Access Article 15 pages, 4924 KiB (/1420-3049/28/10/4225/pdf?version=1684726621)

**Investigation of Fenebrutinib Metabolism and Bioactivation Using $MS^3$ Methodology in Ion Trap LC/MS (/1420-3049/28/10/4225)**

by **Aishah M. Alsibaee**, **Haya I. Aljohar**, **Mohamed W. Attwa**, **Ali S. Abdelhameed** and **Adnan A. Kadi**

*Molecules* **2023**, *28*(10), 4225; **https://doi.org/10.3390/molecules28104225 (https://doi.org/10.3390/molecules28104225)** - 22 May 2023

**Cited by 2 (/1420-3049/28/10/4225#metrics)** | Viewed by 2274

**Abstract** Fenebrutinib is an orally available Bruton tyrosine kinase inhibitor. It is currently in multiple phase III clinical trials for the management of B-cell tumors and autoimmune disorders. Elementary in-silico studies were first performed to predict susceptible sites of metabolism and structural alerts for **[...] Read more.**

(This article belongs to the Special Issue **New Advances in Drug Metabolism and Pharmacokinetics ( /journal/molecules/special_issues/BG1VMW0T04 )**)

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Open Access Article 14 pages, 2645 KiB (/1420-3049/28/10/4224/pdf?version=1684725475)

**A MD Simulation Prediction for Regulation of *N*-Terminal Modification on Binding of CD47 to CD172a in a Force-Dependent Manner (/1420-3049/28/10/4224)**

by **Yang Zhao**, **Liping Fang**, **Pei Guo**, **Ying Fang** and **Jianhua Wu**

*Molecules* **2023**, *28*(10), 4224; **https://doi.org/10.3390/molecules28104224 (https://doi.org/10.3390/molecules28104224)** - 22 May 2023

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**Abstract** Cancer cells can evade immune surveillance through binding of its transmembrane receptor CD47 to CD172a on myeloid cells. CD47 is recognized as a promising immune checkpoint for cancer immunotherapy inhibiting macrophage phagocytosis. *N*-terminal post-translated modification (PTM) via glutaminyl cyclase is a landmark **[...] Read more.**

(This article belongs to the Special Issue **Advances in Molecular Modeling in Chemistry ( /journal/molecules/special_issues/W83C91Y936 )**)

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Open Access Article 18 pages, 5828 KiB **(/1420-3049/28/10/4223/pdf?version=1684720261)**

**Dental Bleaching with Phthalocyanine Photosensitizers: Effects on Dentin Color and Collagen Content (/1420-3049/28/10/4223)**

by **Zhouyan Wu**, **Guodong Wang**, **Zhiming Li**, **Zhengquan Li**, **Dandan Huang**, **Mingdong Huang** and **Minkui Lin**

*Molecules* **2023**, *28*(10), 4223; **https://doi.org/10.3390/molecules28104223 (https://doi.org/10.3390/molecules28104223)** - 22 May 2023

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**Abstract** With the increasing demand for tooth bleaching in esthetic dentistry, its safety has been the focus of a comprehensive body of literature. In this context, the aim of the present study was to evaluate the application effects of pentalysine β-carbonylphthalocyanine zinc ($ZnPc(Lys)_5$ **[...] Read more.**

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Open Access Article 12 pages, 2236 KiB **(/1420-3049/28/10/4222/pdf?version=1684666865)**

**Nonadiabatic Derivative Couplings Calculated Using Information of Potential Energy Surfaces without Wavefunctions: Ab Initio and Machine Learning Implementations (/1420-3049/28/10/4222)**

by **Wen-Kai Chen**, **Sheng-Rui Wang**, **Xiang-Yang Liu**, **Wei-Hai Fang** and **Ganglong Cui**

*Molecules* **2023**, *28*(10), 4222; **https://doi.org/10.3390/molecules28104222 (https://doi.org/10.3390/molecules28104222)** - 21 May 2023

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**Abstract** In this work, we implemented an approximate algorithm for calculating nonadiabatic coupling matrix elements (NACMEs) of a polyatomic system with ab initio methods and machine learning (ML) models. Utilizing this algorithm, one can calculate NACMEs using only the information of potential energy surfaces **[...] Read more.**

(This article belongs to the Special Issue **Advanced Research in Machine Learning in Chemistry ( /journal/molecules/special_issues/machine_learning_computational_chemistry )**)

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Open Access Article 14 pages, 2286 KiB **(/1420-3049/28/10/4221/pdf?version=1684661799)**

**Development and Validation of Green and High-Throughput Microwell Spectrophotometric Assay for the Determination of Selective Serotonin Reuptake Inhibitors in Their Pharmaceutical Dosage Forms (/1420-3049/28/10/4221)**

by **Ibrahim A. Darwish** and **Nourah Z. Alzoman**

*Molecules* **2023**, *28*(10), 4221; **https://doi.org/10.3390/molecules28104221 (https://doi.org/10.3390/molecules28104221)** - 21 May 2023

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**Abstract** This study describes the development and validation of a new green and high-throughput microwell spectrophotometric assay (MW-SPA)

for the determination of three selective serotonin reuptake inhibitors (SSRIs) in their pharmaceutical dosage forms. These SSRIs are fluoxetine, fluvoxamine, and paroxetine, the most prescribed drugs **[...] Read more.**
(This article belongs to the Special Issue **Advances in Pharmaceutical Analytical Technologies ( /journal/molecules/special_issues/RZ0127PIB )**)

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**Design, Synthesis, and Antiproliferative Activity of Benzopyran-4-One-Isoxazole Hybrid Compounds (/1420-3049/28/10/4220)**

by **Shilpi Gupta**, **Shang Eun Park**, **Saghar Mozaffari**, **Bishoy El-Aarag**, **Keykavous Parang** and **Rakesh Kumar Tiwari**
*Molecules* **2023**, *28*(10), 4220; **https://doi.org/10.3390/molecules28104220 (https://doi.org/10.3390/molecules28104220)** - 21 May 2023
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**Abstract** The biological significance of benzopyran-4-ones as cytotoxic agents against multi-drug resistant cancer cell lines and isoxazoles as anti-inflammatory agents in cellular assays prompted us to design and synthesize their hybrid compounds and explore their antiproliferative activity against a panel of six cancer cell **[...] Read more.**
(This article belongs to the Special Issue **Discovery of Small Molecules for Cancer Therapy: Current Challenges, Recent Trends, and Future Perspectives ( /journal/molecules/special_issues/5F0819P2A9 )**)

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Open Access Article 22 pages, 5524 KiB **(/1420-3049/28/10/4219/pdf?version=1684822143)**

**Dynamic and Static Nature of XH-⁎-π and YX-⁎-π (X = F, Cl, Br, and I; Y = X and F) in the Distorted π-System of Corannulene Elucidated with QTAIM Dual Functional Analysis (/1420-3049/28/10/4219)**

by **Satoko Hayashi**, **Takahiro Kato**, **Yuji Sugibayashi** and **Waro Nakanishi**
*Molecules* **2023**, *28*(10), 4219; **https://doi.org/10.3390/molecules28104219 (https://doi.org/10.3390/molecules28104219)** - 21 May 2023
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**Abstract** The dynamic and static nature of the XH-⁎-π and YX-⁎-π (X = F, Cl, Br, and I; Y = X and F) interactions in the distorted π-system of corannulene (π($C_{20}H_{10}$)) is elucidated with a QTAIM dual functional analysis (QTAIM-DFA), **[...] Read more.**
(This article belongs to the Special Issue **Research on Nanostructured Materials 2.0 ( /journal/molecules/special_issues/NanostructureMaterials2 )**)

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Open Access Article 14 pages, 2561 KiB (/1420-3049/28/10/4218/pdf?version=1684656330)

**Fluorine-Functionalized Polyphosphazene Immunoadjuvant: Synthesis, Solution Behavior and In Vivo Potency (/1420-3049/28/10/4218)**

by **Harichandra D. Tagad**, **Alexander Marin**, **Ruixue Wang**, **Abdul S. Yunus**, **Thomas R. Fuerst** and **Alexander K. Andrianov**
*Molecules* **2023**, *28*(10), 4218; **https://doi.org/10.3390/molecules28104218 (https://doi.org/10.3390/molecules28104218)** - 21 May 2023
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**Abstract** The inclusion of fluorine motifs in drugs and drug delivery systems is an established tool for modulating their biological potency. Fluorination can improve drug specificity or boost the vehicle's ability to cross cellular membranes. However, the approach has yet to be applied to **[...] Read more.**
(This article belongs to the Special Issue **Featured Papers in Medicinal Chemistry II ( /journal/molecules/special_issues/Featured_Papers_Medicinal_ChemistryII )**)

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Open Access Article 16 pages, 10536 KiB (/1420-3049/28/10/4217/pdf?version=1684654212)

**Docosahexaenoic Acid Promotes Cd Excretion by Restoring the Abundance of *Parabacteroides* in Cd-Exposed Mice (/1420-3049/28/10/4217)**

by **Jianzhen Liao**, **Siyuan Bi**, **Zhijia Fang**, **Qi Deng**, **Yinyan Chen**, **Lijun Sun**, **Yongqing Jiang**, **Linru Huang** and **Ravi Gooneratne**
*Molecules* **2023**, *28*(10), 4217; **https://doi.org/10.3390/molecules28104217 (https://doi.org/10.3390/molecules28104217)** - 21 May 2023
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**Abstract** As a common harmful pollutant, cadmium (Cd) can easily enter the human body through the food chain, posing a major threat to human health. Gut microbiota play a key role in Cd absorption. Docosahexaenoic acid (DHA) is thought to have a potential role **[...] Read more.**
(This article belongs to the Special Issue **Heavy Metals and Metalloids in Environmental, Food and Nutrients Samples ( /journal/molecules/special_issues/heavy_metals_metalloids_environ_food_nutrients )**)

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Open Access Review 30 pages, 11482 KiB (/1420-3049/28/10/4216/pdf?version=1684896267)

**Perspectives on the Lindman Hypothesis and Cellulose Interactions (/1420-3049/28/10/4216)**

by **Magnus Norgren**, **Carolina Costa**, **Luís Alves**, **Alireza Eivazi**, **Christina Dahlström**, **Ida Svanedal**, **Håkan Edlund** and **Bruno Medronho**
*Molecules* **2023**, *28*(10), 4216; **https://doi.org/10.3390/molecules28104216 (https://doi.org/10.3390/molecules28104216)** - 21 May 2023
**Cited by 16 (/1420-3049/28/10/4216#metrics)** | Viewed by 3428

**Abstract** In the history of cellulose chemistry, hydrogen bonding has been the predominant explanation when discussing intermolecular interactions between cellulose polymers. This is the general consensus in scholarly textbooks and in many research articles, and it applies to several other biomacromolecules' interactions as well. **[...] Read more.**
(This article belongs to the Special Issue **Colloids and Polymers: An Issue in Honor of Professor Björn Lindman ( /journal/molecules/special_issues/colloid_polym )**)

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Open Access Article 15 pages, 4717 KiB (/1420-3049/28/10/4215/pdf?version=1684575843)

**Thiocarbonyl Derivatives of Natural Chlorins: Synthesis Using Lawesson's Reagent and a Study of Their Properties (/1420-3049/28/10/4215)**

by **Viktor Pogorilyy**, **Petr Ostroverkhov**, **Valeria Efimova**, **Ekaterina Plotnikova**, **Olga Bezborodova**, **Ekaterina Diachkova**, **Yuriy Vasil'ev**, **Andrei Pankratov** and **Mikhail Grin**

*Molecules* **2023**, *28*(10), 4215; **https://doi.org/10.3390/molecules28104215 (https://doi.org/10.3390/molecules28104215)** - 20 May 2023

**Cited by 2 (/1420-3049/28/10/4215#metrics)** | Viewed by 2624

**Abstract** The development of sulfur-containing pharmaceutical compounds is important in the advancement of medicinal chemistry. Photosensitizers (PS) that acquire new properties upon incorporation of sulfur-containing groups or individual sulfur atoms into their structure are not neglected, either. In this work, a synthesis of sulfur-containing **[...] Read more.**

(This article belongs to the Special Issue **Macrocyclic Compounds: Derivatives and Applications ( /journal/molecules/special_issues/Macrocyclic_Compounds_Derivatives )**)

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Open Access Article 12 pages, 17559 KiB (/1420-3049/28/10/4214/pdf?version=1684575793)

**Synthesis of $Eu^{3+}$-Doped $NaGd_9Si_6O_{26}$ Sub-Microcrystals from a $NaGdF_4$@$SiO_2$ Structure (/1420-3049/28/10/4214)**

by **Tianyun Du**, **Xiaojie Xue** and **Xiuxun Han**

*Molecules* **2023**, *28*(10), 4214; **https://doi.org/10.3390/molecules28104214 (https://doi.org/10.3390/molecules28104214)** - 20 May 2023

**Cited by 2 (/1420-3049/28/10/4214#metrics)** | Viewed by 1728

**Abstract** Rare earth silicate phosphors of high quantum efficiency with a stable performance are promising materials in the fields of display and illumination. The grain sizes of products synthesized via the conventional solid-state reaction method are usually too large to satisfy the requirements of **[...] Read more.**

(This article belongs to the Special Issue **2D Nanomaterials and Composites for Energy and Environmental Sustainability ( /journal/molecules/special_issues/AFDY903CVU )**)

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Open Access Article 18 pages, 3436 KiB (/1420-3049/28/10/4213/pdf?version=1684575648)

**An Automated Continuous Synthesis and Isolation for the Scalable Production of Aryl Sulfonyl Chlorides (/1420-3049/28/10/4213)**

by **Matthew Glace**, **Cameron Armstrong**, **Nathan Puryear**, **Colin Bailey**, **Roudabeh Sadat Moazeni-Pourasil**, **Drew Scott**, **Sherif Abdelwahed** and **Thomas. D. Roper**

*Molecules* **2023**, *28*(10), 4213; **https://doi.org/10.3390/molecules28104213 (https://doi.org/10.3390/molecules28104213)** - 20 May 2023

**Cited by 3 (/1420-3049/28/10/4213#metrics)** | Viewed by 2366

**Abstract** In this work, a continuous system to produce multi-hundred-gram quantities of aryl sulfonyl chlorides is described. The scheme employs multiple continuous stirred-tank reactors (CSTRs) and a continuous filtration system and incorporates an automated process control scheme. The experimental process outlined is intended to **[...] Read more.**

(This article belongs to the Special Issue **Importance of Flow Chemistry: Active Pharmaceutical Production ( /journal/molecules/special_issues/DUO3VDF9J2 )**)

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Open Access Communication 10 pages, 2057 KiB (/1420-3049/28/10/4212/pdf?version=1684575377)

**(1→3)-α-D-Glucooligosaccharides Increase the Killing Capacity of NK Cells against Selected Human Colon Cancer Cells (/1420-3049/28/10/4212)**

by **Marta Kinga Lemieszek**, **Paulina Adamczyk**, **Iwona Komaniecka**, **Wojciech Rzeski**, **Michał Tomczyk** and **Adrian Wiater**

*Molecules* **2023**, *28*(10), 4212; **https://doi.org/10.3390/molecules28104212 (https://doi.org/10.3390/molecules28104212)** - 20 May 2023

**Cited by 2 (/1420-3049/28/10/4212#metrics)** | Viewed by 1850

**Abstract** Despite the progress of medicine, colorectal cancer has occupied one of the highest positions in the rankings of cancer morbidity and mortality for many years. Thus, alternative methods of its treatment are sought. One of the newer therapeutic strategies is immunotherapy based on **[...] Read more.**

(This article belongs to the Special Issue **Bioactive Natural Products for Prevention and Treatment of Cancer, Cardiovascular and Neurodegenerative Diseases, and Aging ( /journal/molecules/special_issues/308C4QW85W )**)

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Open Access Article 28 pages, 8306 KiB (/1420-3049/28/10/4211/pdf?version=1684738788)

**Development and Characterization of Novel Selective, Non-Basic Dopamine $D_2$ Receptor Antagonists for the Treatment of Schizophrenia (/1420-3049/28/10/4211)**

by **Piotr Stępnicki**, **Sylwia Wośko**, **Agata Bartyzel**, **Agata Zięba**, **Damian Bartuzi**, **Klaudia Szałaj**, **Tomasz M. Wróbel**, **Emilia Fornal**, **Jens [illegible]son**, **Ewa Kędzierska**, **Ewa Poleszak**, **Marián Castro** and **Agnieszka A. Kaczor**

*Molecules* **2023**, *28*(10), 4211; **https://doi.org/10.3390/molecules28104211 (https://doi.org/10.3390/molecules28104211)** - 20 May 2023

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**Abstract** The dopamine $D_2$ receptor, which belongs to the family of G protein-coupled receptors (GPCR), is an important and well-validated drug target in the field of medicinal chemistry due to its wide distribution, particularly in the central nervous system, and involvement in the **[...] Read more.**

(This article belongs to the Special Issue **Progress in the Treatment of CNS Disorders: From In Silico to In Vivo ( /journal/molecules/special_issues/68AW420UZA )**)

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Open Access Article 13 pages, 2621 KiB **(/1420-3049/28/10/4210/pdf?version=1684573486)**

**Metal Complexes of Omadine (*N*-Hydroxypyridine-2-thione): Differences of Antioxidant and Pro-Oxidant Behavior in Light and Dark Conditions with Possible Toxicity Implications (/1420-3049/28/10/4210)**

by **Olga Yu. Selyutina**, **Viktor A. Timoshnikov**, **Nikolay E. Polyakov** and **George J. Kontoghiorghes**

*Molecules* **2023**, *28*(10), 4210; **https://doi.org/10.3390/molecules28104210 (https://doi.org/10.3390/molecules28104210)** - 20 May 2023

**Cited by 3 (/1420-3049/28/10/4210#metrics)** | Viewed by 1626

**Abstract** Omadine or *N*-hydroxypyridine-2-thione and its metal complexes are widely used in medicine and show bactericidal, fungicidal, anticancer, and photochemical activity. The redox activity of omadine complexes with iron, copper, and zinc on lipid peroxidation under light and dark conditions has been investigated. **[...] Read more.**

(This article belongs to the Section **Inorganic Chemistry (/journal/molecules/sections/Inorganic_Chemistry)**)

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Open Access Review 47 pages, 33285 KiB **(/1420-3049/28/10/4209/pdf?version=1684836063)**

**Synthetic Routes to Approved Drugs Containing a Spirocycle (/1420-3049/28/10/4209)**

by **Nazar Moshnenko**, **Alexander Kazantsev**, **Evgeny Chupakhin**, **Olga Bakulina** and **Dmitry Dar'in**

*Molecules* **2023**, *28*(10), 4209; **https://doi.org/10.3390/molecules28104209 (https://doi.org/10.3390/molecules28104209)** - 20 May 2023

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**Abstract** The use of spirocycles in drug discovery and medicinal chemistry has been booming in the last two decades. This has clearly translated into the landscape of approved drugs. Among two dozen clinically used medicines containing a spirocycle, 50% have been approved in the **[...] Read more.**

(This article belongs to the Special Issue **Spirocycles in Medicinal Chemistry ( /journal/molecules/special_issues/74AWZ43257 )**)

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Open Access Review 24 pages, 2417 KiB (/1420-3049/28/10/4208/pdf?version=1684733336)

**Application of Electrochemical Oxidation for Water and Wastewater Treatment: An Overview (/1420-3049/28/10/4208)**

by **Mohammad Saleh Najafinejad**, **Simeone Chianese**, **Angelo Fenti**, **Pasquale Iovino** and **Dino Musmarra**

*Molecules* **2023**, *28*(10), 4208; **https://doi.org/10.3390/molecules28104208 (https://doi.org/10.3390/molecules28104208)** - 20 May 2023



**Abstract** In recent years, the discharge of various emerging pollutants, chemicals, and dyes in water and wastewater has represented one of the prominent human problems. Since water pollution is directly related to human health, highly resistant and emerging compounds in aquatic environments will pose **[...] Read more.**

(This article belongs to the Special Issue **Chemical Technologies for Environmental Analysis and Pollution Removal ( /journal/molecules/special_issues/5929373EX5 )**)

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Open Access Article 19 pages, 2958 KiB (/1420-3049/28/10/4207/pdf?version=1684829329)

**Comparative Study on Assisted Solvent Extraction Techniques for the Extraction of Biologically Active Compounds from *Sideritis raeseri* and *Sideritis scardica* (/1420-3049/28/10/4207)**

by **Marika Mróz**, **Edyta Malinowska-Pańczyk**, **Agnieszka Bartoszek** and **Barbara Kusznierewicz**
*Molecules* **2023**, *28*(10), 4207; **https://doi.org/10.3390/molecules28104207 (https://doi.org/10.3390/molecules28104207)** - 20 May 2023
**Cited by 11 (/1420-3049/28/10/4207#metrics)** | Viewed by 2627

**Abstract** The plants in the *Sideritis* genus are postulated to exhibit several important medicinal properties due to their unique chemical composition. To isolate the targeted phytochemical compounds, the selection of a suitable extraction method is of primary importance. In this work, a comparative study **[...] Read more.**
(This article belongs to the Special Issue **Extraction and Application of Nutrients and Functional Compounds from Food ( /journal/molecules/special_issues/M6W378LN4F )**)

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Open Access Article 13 pages, 2367 KiB (/1420-3049/28/10/4206/pdf?version=1684569505)

***Rosmarinus officinalis* L. Essential Oils Impact on the Microbiological and Oxidative Stability of Sarshir (Kaymak) (/1420-3049/28/10/4206)**

by **Seyed Mohammad Bagher Hashemi**, **Aliakbar Gholamhosseinpour** and **Francisco J. Barba**
*Molecules* **2023**, *28*(10), 4206; **https://doi.org/10.3390/molecules28104206 (https://doi.org/10.3390/molecules28104206)** - 20 May 2023
**Cited by 4 (/1420-3049/28/10/4206#metrics)** | Viewed by 2131

**Abstract** This study investigated the effect of *Rosmarinus officinalis* L. essential oil, REO (one, two and three percent) on the microbiological and oxidative stability of Sarshir during 20 days of refrigerated storage (4 °C). Initially, the chemical composition (gas chromatography/mass spectrometry, GC/MS), antimicrobial (paper **[...] Read more.**

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Open Access Review 21 pages, 837 KiB (/1420-3049/28/10/4205/pdf?version=1684565147)

**Valorization of Fibrous Plant-Based Food Waste as Biosorbents for Remediation of Heavy Metals from Wastewater—A Review (/1420-3049/28/10/4205)**

by **Ahasanul Karim**, **Zarifeh Raji**, **Antoine Karam** and **Seddik Khalloufi**
*Molecules* **2023**, *28*(10), 4205; **https://doi.org/10.3390/molecules28104205 (https://doi.org/10.3390/molecules28104205)** - 20 May 2023
**Cited by 17 (/1420-3049/28/10/4205#metrics)** | Viewed by 3213

**Abstract** Mobilization of heavy metals in the environment has been a matter of concern for several decades due to their toxicity for humans, environments, and other living organisms. In recent years, use of inexpensive and abundantly available biosorbents generated from fibrous plant-based food-waste materials **[...] Read more.**
(This article belongs to the Special Issue **Polysaccharide-Based Biopolymer: Recent Development and Applications ( /journal/molecules/special_issues/ABPCJCSOR8 )**)

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**Triggering RNA Interference by Photoreduction under Red Light Irradiation (/1420-3049/28/10/4204)**

by **Jennifer Rühle**, **Insa Klemt** and **Andriy Mokhir**

*Molecules* **2023**, *28*(10), 4204; **https://doi.org/10.3390/molecules28104204 (https://doi.org/10.3390/molecules28104204)** - 20 May 2023

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**Abstract** RNA interference (RNAi) using small interfering RNAs (siRNAs) is a powerful tool to target any protein of interest and is becoming more suitable for in vivo applications due to recent developments in RNA delivery systems. To exploit RNAi for cancer treatment, it is **[...] Read more.**

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Open Access Article 16 pages, 4729 KiB (/1420-3049/28/10/4203/pdf?version=1684559735)

**Biosynthesis and Characterization of Silver Nanoparticles Using *Tribulus terrestris* Seeds: Revealed Promising Antidiabetic Potentials (/1420-3049/28/10/4203)**

by **Abdur Rahman**, **Gauhar Rehman**, **Nasrullah Shah**, **Muhammad Hamayun**, **Sajid Ali**, **Abid Ali**, **Said karim Shah**, **Waliullah Khan**, **Muhammad Ishaq Ali Shah** and **Abdulwahed Fahad Alrefaei**

*Molecules* **2023**, *28*(10), 4203; **https://doi.org/10.3390/molecules28104203 (https://doi.org/10.3390/molecules28104203)** - 20 May 2023

**Cited by 13 (/1420-3049/28/10/4203#metrics)** | Viewed by 3031

**Abstract** Green synthesis is the most effective and environmentally friendly way to produce nanoparticles. The present research aimed at the biosynthesizing of silver nanoparticles (AgNPs) using *Tribulus terrestris* seed extract as the reducing and stabilizing agent and investigating their anti-diabetic properties. Fourier transformation infrared **[...] Read more.**

(This article belongs to the Special Issue **New Trends in the Design of Metal Nanoparticles and Their Medical Applications ( /journal/molecules/special_issues/7AT2BMIMY6 )**)

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Open Access Article 10 pages, 2886 KiB (/1420-3049/28/10/4202/pdf?version=1684512648)

**Lipidomic Characterization of Oocytes at Single-Cell Level Using Nanoflow Chromatography-Trapped Ion Mobility Spectrometry-Mass Spectrometry (/1420-3049/28/10/4202)**

by **Pujia Zhu**, **Guowei Bu**, **Ruifeng Hu**, **Xianqin Ruan**, **Rongrong Fu**, **Zhourui Zhang**, **Qiongqiong Wan**, **Xin Liu**, **Yiliang Miao** and **Suming Chen**

*Molecules* **2023**, *28*(10), 4202; **https://doi.org/10.3390/molecules28104202 (https://doi.org/10.3390/molecules28104202)** - 19 May 2023

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**Abstr**ass spectrometry (MS)-based lipidomic has become a powerful tool for studying lipids in biological systems. However, lipidome analysis at the single-cell level remains a challenge. Here, we report a highly sensitive lipidomic workflow based on nanoflow liquid chromatography and trapped ion mobility spectrometry **[...] Read more.**

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(This article belongs to the Special Issue **Imaging and Spatial Lipidomic Analysis ( /journal/molecules/special_issues/ImaSpa_Lipidomic )**)

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Open Access Article 13 pages, 2386 KiB (/1420-3049/28/10/4201/pdf?version=1684725104)

**Assessment of the Prediction Power of Forced Ageing Methodology on Lager Beer Aldehyde Evolution during Maritime Transportation (/1420-3049/28/10/4201)**

by **Dayana Aguiar**, **Ana C. Pereira** and **José C. Marques**

*Molecules* **2023**, *28*(10), 4201; **https://doi.org/10.3390/molecules28104201 (https://doi.org/10.3390/molecules28104201)** - 19 May 2023

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**Abstract** The globalisation of the beer market forces brewers to have methodologies that rapidly evaluate the evolution of beer flavour stability. Commonly used forced ageing methods have limitations since temperature and transportation conditions (temperature, vibrations, long-distance travel, and other factors) impact beer quality. This **[...] Read more.**

(This article belongs to the Special Issue **Characterization and Instrumental Analysis of Aroma-Active Compounds in Fermented Food and Beverage ( /journal/molecules/special_issues/R566ULZ93D )**)

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Open Access Article 13 pages, 7926 KiB (/1420-3049/28/10/4200/pdf?version=1684505544)

**Nanocomposites Based on Spin-Crossover Nanoparticles and Silica-Coated Gold Nanorods: A Nonlinear Optical Study (/1420-3049/28/10/4200)**

by **Eleni Zygouri**, **Aristeidis Stathis**, **Stelios Couris** and **Vassilis Tangoulis**

*Molecules* **2023**, *28*(10), 4200; **https://doi.org/10.3390/molecules28104200 (https://doi.org/10.3390/molecules28104200)** - 19 May 2023

**Cited by 2 (/1420-3049/28/10/4200#metrics)** | Viewed by 1654

**Abstract** A nanocomposite based on silica-coated AuNRs with the aminated silica-covered spin-crossover nanoparticles (SCO NPs) of the 1D iron(II) coordination polymer with the formula $[Fe(Htrz)_2(trz)](BF_4)$ is presented. For the synthesis of the SCO NPs, the reverse micelle method was used, **[...] Read more.**

(This article belongs to the Special Issue **Inorganic Young Investigators' Contributions Collection ( /journal/molecules/special_issues/Inorganic_Young_Investigator )**)

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Open Access Article 25 pages, 11579 KiB (/1420-3049/28/10/4199/pdf?version=1685092072)

**Trisubstituted 1,3,5-Triazines as Histamine $H_4$ Receptor Antagonists with Promising Activity In Vivo (/1420-3049/28/10/4199)**

by **Agnieszka Olejarz-Maciej**, **Szczepan Mogilski**, **Tadeusz Karcz**, **Tobias Werner**, **Katarzyna Kamińska**, **Jarosław Kupczyk**, **Ewelina Honkisz-Orzechowska**, **Gniewomir Latacz**, **Holger Stark**, **Katarzyna Kieć-Kononowicz** and **Dorota Łażewska**

*Molecules* **2023**, *28*(10), 4199; **https://doi.org/10.3390/molecules28104199 (https://doi.org/10.3390/molecules28104199)** - 19 May 2023

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**Abstract** Pain is a very unpleasant experience that makes life extremely uncomfortable. The histamine $H_4$ receptor ($H_4R$) is a promising target for the treatment of inflammatory and immune diseases, as well as pain. $H_4R$ ligands have demonstrated analgesic effects **[...] Read more.**
(This article belongs to the Special Issue **Progress in the Treatment of CNS Disorders: From In Silico to In Vivo ( /journal/molecules/special_issues/68AW420UZA )**)

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Open Access Review 24 pages, 5314 KiB **(/1420-3049/28/10/4198/pdf?version=1684505771)**

**The Reducing Agents in Sonochemical Reactions without Any Additives (/1420-3049/28/10/4198)**

by **Kyuichi Yasui**

*Molecules* **2023**, *28*(10), 4198; **https://doi.org/10.3390/molecules28104198 (https://doi.org/10.3390/molecules28104198)** - 19 May 2023
**Cited by 8 (/1420-3049/28/10/4198#metrics)** | Viewed by 2064

**Abstract** It has been experimentally reported that not only oxidation reactions but also reduction reactions occur in aqueous solutions under ultrasound without any additives. According to the numerical simulations of chemical reactions inside an air or argon bubble in water without any additives under **[...] Read more.**
(This article belongs to the Section **Ultrasound Chemistry (/journal/molecules/sections/ultrasound_chemistry)**)

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Open Access Article 12 pages, 1486 KiB **(/1420-3049/28/10/4197/pdf?version=1684506330)**

**Enhancement of Inhibitory Activity by Combining Allosteric Inhibitors Putatively Binding to Different Allosteric Sites on Cathepsin K (/1420-3049/28/10/4197)**

by **Shun Sato**, **Kana Yamamoto**, **Moeno Ito**, **Katsutoshi Nishino**, **Takanao Otsuka**, **Kazuhiro Irie** and **Masaya Nagao**

*Molecules* **2023**, *28*(10), 4197; **https://doi.org/10.3390/molecules28104197 (https://doi.org/10.3390/molecules28104197)** - 19 May 2023
**Cited by 1 (/1420-3049/28/10/4197#metrics)** | Viewed by 1881

**Abstr** ackground: Cathepsin K, which is involved in bone resorption, is a good target for treating osteoporosis, but no clinically approved medicine has been developed. Recently, allosteric inhibitors with high specificity and few side effects have been attracting attention for use in new

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medicines. **[...] Read more.**
(This article belongs to the Special Issue **Naturally Inspired Molecules as Inhibitors in Drug Discovery ( /journal/molecules/special_issues/YMQYPOYE84 )**)

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Open Access Article 20 pages, 6353 KiB (/1420-3049/28/10/4196/pdf?version=1684502569)

**Columnar Liquid Crystals of Copper(I) Complexes with Ionic Conductivity and Solid State Emission (/1420-3049/28/10/4196)**

by **Viorel Cîrcu**, **Constantin P. Ganea**, **Mihail Secu**, **Doina Manaila-Maximean**, **George Cătălin Marinescu**, **Roua Gabriela Popescu** and **Iuliana Pasuk**

*Molecules* **2023**, *28*(10), 4196; **https://doi.org/10.3390/molecules28104196 (https://doi.org/10.3390/molecules28104196)** - 19 May 2023
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**Abstract** Two neutral copper(I) halide complexes ([Cu(BTU)$_2$X], *X* = Cl, Br) were prepared by the reduction of the corresponding copper(II) halides (chloride or bromide) with a benzoylthiourea (BTU, *N*-(3,4-diheptyloxybenzoyl)-*N'*-(4-heptadecafluorooctylphenyl)thiourea) ligand in ethanol. The two copper(I) complexes show a very **[...] Read more.**
(This article belongs to the Special Issue **Liquid Crystals II ( /journal/molecules/special_issues/2W4480X2AX )**)

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Open Access Article 13 pages, 4032 KiB (/1420-3049/28/10/4195/pdf?version=1684501740)

**Removal of *p*-Nitrophenol by Adsorption with 2-Phenylimidazole-Modified ZIF-8 (/1420-3049/28/10/4195)**

by **Yu Zhao**, **Peiqing Yuan**, **Xinru Xu** and **Jingyi Yang**

*Molecules* **2023**, *28*(10), 4195; **https://doi.org/10.3390/molecules28104195 (https://doi.org/10.3390/molecules28104195)** - 19 May 2023
**Cited by 12 (/1420-3049/28/10/4195#metrics)** | Viewed by 2435

**Abstract** Petrochemical wastewater contains *p*-nitrophenol, a highly toxic, bioaccumulative and persistent pollutant that can harm ecosystems and environmental sustainability. In this study, ZIF-8-PhIm was prepared for *p*-nitrophenol removal from petrochemical wastewater using solvent-assisted ligand exchange (SALE) with 2-phenylimidazole(2-PhIm). The ZIF-8-PhIm's composition and **[...] Read more.**
(This article belongs to the Section **Materials Chemistry (/journal/molecules/sections/materials_chemistry)**)

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Open Access Article 14 pages, 1765 KiB (/1420-3049/28/10/4194/pdf?version=1684495171)

**Changing on the Concentrations of Neonicotinoids in Rice and Drinking Water through Heat Treatment Process (/1420-3049/28/10/4194)**

by **Ziyang Wei**, **Bo Zhang**, **Xu Li**, **Yanxia Gao**, **Yuan He**, **Jingchuan Xue** and **Tao Zhang**

*Molecules* **2023**, *28*(10), 4194; **https://doi.org/10.3390/molecules28104194 (https://doi.org/10.3390/molecules28104194)** - 19 May 2023

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**Abstract** Neonicotinoids (NEOs) have become the most widely used insecticides in the world since the mid-1990s. According to Chinese dietary habits, rice and water are usually heated before being consumed, but the information about the alteration through the heat treatment process is very limited. **[...] Read more.**

(This article belongs to the Section **Green Chemistry (/journal/molecules/sections/green-chemistry)**)

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Open Access Article 16 pages, 7092 KiB (/1420-3049/28/10/4193/pdf?version=1684808896)

**Effect of Indole-2-carboxylic Acid on the Self-Corrosion and Discharge Activity of Aluminum Alloy Anode in Alkaline Al–Air Battery (/1420-3049/28/10/4193)**

by **Lei Guo**, **Yue Huang**, **Alessandra Gilda Ritacca**, **Kai Wang**, **Ida Ritacco**, **Yan Tan**, **Yujie Qiang**, **Nabil Al-Zaqri**, **Wei Shi** and **Xingwen Zheng**

*Molecules* **2023**, *28*(10), 4193; **https://doi.org/10.3390/molecules28104193 (https://doi.org/10.3390/molecules28104193)** - 19 May 2023

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**Abstract** Al–air battery has been regarded as a promising new energy source. However, the self-corrosion of aluminum anode leads to a loss of battery capacity and a decrease in battery longevity, limiting its commercial applications. Herein, indole-2-carboxylic acid (ICA) has been added to 4 **[...] Read more.**

(This article belongs to the Special Issue **Battery Chemistry: Recent Advances and Future Opportunities ( /journal/molecules/special_issues/S26MD67L5R )**)

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Open Access Review 50 pages, 3389 KiB (/1420-3049/28/10/4192/pdf?version=1695714712)

**Medicinal Plants of the Flora of Kazakhstan Used in the Treatment of Skin Diseases (/1420-3049/28/10/4192)**

by **Gulzat Berganayeva**, **Bates Kudaibergenova**, **Yuliya Litvinenko**, **Irada Nazarova**, **Sandugash Sydykbayeva**, **Gulzira Vassilina**, **Nazerke Izdik** and **Moldyr Dyusebaeva**

*Molecules* **2023**, *28*(10), 4192; **https://doi.org/10.3390/molecules28104192 (https://doi.org/10.3390/molecules28104192)** - 19 May 2023

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**Abstract** The skin shows the physiological condition of the body's organs and systems that prevent infections and physical damage. Throughout the

ages, in folk medicine, phytotherapy was considered a primary form of treatment in all countries, including Kazakhstan, due to the abundance and availability [...] Read more.

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Open Access Article 27 pages, 5696 KiB (/1420-3049/28/10/4191/pdf?version=1684742052)

**Exploring the Role of Anionic Lipid Nanodomains in the Membrane Disruption and Protein Folding of Human Islet Amyloid Polypeptide Oligomers on Lipid Membrane Surfaces Using Multiscale Molecular Dynamics Simulations (/1420-3049/28/10/4191)**

by **Ngoc Nguyen**, **Amber Lewis**, **Thuong Pham**, **Donald Sikazwe** and **Kwan H. Cheng**

*Molecules* **2023**, *28*(10), 4191; **https://doi.org/10.3390/molecules28104191 (https://doi.org/10.3390/molecules28104191)** - 19 May 2023

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**Abstract** The aggregation of human Islet Amyloid Polypeptide (hIAPP) on cell membranes is linked to amyloid diseases. However, the physio-chemical mechanisms of how these hIAPP aggregates trigger membrane damage are unclear. Using coarse-grained and all-atom molecular dynamics simulations, we investigated the role of lipid **[...] Read more.**

(This article belongs to the Special Issue **Exclusive Feature Papers in Physical Chemistry ( /journal/molecules/special_issues/FP_physchem )**)

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Open Access Article 26 pages, 6806 KiB (/1420-3049/28/10/4190/pdf?version=1684488038)

**Xanthophyll-Rich Extract of *Phaeodactylum tricornutum* Bohlin as New Photoprotective Cosmeceutical Agent: Safety and Efficacy Assessment on In Vitro Reconstructed Human Epidermis Model (/1420-3049/28/10/4190)**

by **Antonella Smeriglio**, **Joseph Lionti**, **Mariarosaria Ingegneri**, **Bruno Burlando**, **Laura Cornara**, **Federica Grillo**, **Luca Mastracci** and **Domenico Trombetta**

*Molecules* **2023**, *28*(10), 4190; **https://doi.org/10.3390/molecules28104190 (https://doi.org/10.3390/molecules28104190)** - 19 May 2023

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**Abstract** The nutritional and health properties of algae make them perfect functional ingredients for nutraceutical and cosmeceutical applications. In this study, the *Phaeodactylum tricornutum* Bohlin (Phaeodactylaceae), a pleiomorphic diatom commonly found in marine ecosystems, was investigated. The in vitro culture conditions used favoured the **[...] Read more.**

(This article belongs to the Special Issue **Synthesis, Extraction and Biological Evaluations of Natural Products ( /journal/molecules/special_issues/Biological_Natural_Products )**)

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Open Access Review 35 pages, 2112 KiB (/1420-3049/28/10/4189/pdf?version=1684487930)

## Encapsulation of Polyphenolic Compounds Based on Hemicelluloses to Enhance Treatment of Inflammatory Bowel Diseases and Colorectal Cancer (/1420-3049/28/10/4189)

by **Miłosz Caban** and **Urszula Lewandowska**

*Molecules* **2023**, *28*(10), 4189; **https://doi.org/10.3390/molecules28104189 (https://doi.org/10.3390/molecules28104189)** - 19 May 2023

**Cited by 9 (/1420-3049/28/10/4189#metrics)** | Viewed by 3931

**Abstract** Inflammatory bowel diseases (IBD) and colorectal cancer (CRC) are difficult to cure, and available treatment is associated with troubling side effects. In addition, current therapies have limited efficacy and are characterized by high costs, and a large segment of the IBD and CRC **[...] Read more.**

(This article belongs to the Special Issue **New Technologies for Encapsulation of Small Molecules and Plant Extracts II ( /journal/molecules/special_issues/9TB663L5LT )**)

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Open Access Article 14 pages, 4476 KiB (/1420-3049/28/10/4188/pdf?version=1685005044)

## Levocetirizine-Loaded Electrospun Fibers from Water-Soluble Polymers: Encapsulation and Drug Release (/1420-3049/28/10/4188)

by **Lan Yi**, **Lu Cui**, **Linrui Cheng**, **János Móczó** and **Béla Pukánszky**

*Molecules* **2023**, *28*(10), 4188; **https://doi.org/10.3390/molecules28104188 (https://doi.org/10.3390/molecules28104188)** - 19 May 2023

**Cited by 4 (/1420-3049/28/10/4188#metrics)** | Viewed by 1641

**Abstract** Electrospun fibers containing levocetirizine, a BCS III drug, were prepared from three water-soluble polymers, hydroxypropyl methylcellulose (HPMC), polyvinylpyrrolidone (PVP) and polyvinyl alcohol (PVA). Fiber-spinning technology was optimized for each polymer separately. The polymers contained 10 wt% of the active component. An amorphous drug **[...] Read more.**

(This article belongs to the Special Issue **Nanofibers and Nanotextured Materials: Their Multipurpose Applications ( /journal/molecules/special_issues/695C799B8L )**)

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Open Access Review 12 pages, 528 KiB (/1420-3049/28/10/4187/pdf?version=1684478320)

**Coriander (*Coriandrum sativum*) Polyphenols and Their Nutraceutical Value against Obesity and Metabolic Syndrome (/1420-3049/28/10/4187)**

by **Samir Scandar**, **Claudia Zadra** and **Maria Carla Marcotullio**

*Molecules* **2023**, *28*(10), 4187; **https://doi.org/10.3390/molecules28104187 (https://doi.org/10.3390/molecules28104187)** - 19 May 2023

**Cited by 25 (/1420-3049/28/10/4187#metrics)** | Viewed by 6853

**Abstract** Coriander is a widely used plant for its medicinal and biological properties. Both coriander essential oil and extracts are interesting sources of bioactive compounds and are widely used as spices in culinary practice due to their exclusive aroma and flavour. We focus our **[...] Read more.**

(This article belongs to the Special Issue **Biological Activity of Phenolics and Polyphenols in Nature Products ( /journal/molecules/special_issues/200064T4W9 )**)

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Open Access Article 17 pages, 1026 KiB (/1420-3049/28/10/4186/pdf?version=1684478950)

**Phytochemical and Biological Investigation of an Indigenous Plant of Bangladesh, *Gynura procumbens* (Lour.) Merr.: Drug Discovery from Nature (/1420-3049/28/10/4186)**

by **Md. Abu Jobaer**, **Sania Ashrafi**, **Monira Ahsan**, **Choudhury Mahmood Hasan**, **Mohammad Abdur Rashid**, **Sheikh Nazrul Islam** and **Mohammad Mehedi Masud**

*Molecules* **2023**, *28*(10), 4186; **https://doi.org/10.3390/molecules28104186 (https://doi.org/10.3390/molecules28104186)** - 19 May 2023

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**Abstract** *Gynura procumbens* (Lour.) Merr. (Family: Asteraceae) is a tropical Asian medicinal plant found in Thailand, China, Malaysia, Indonesia, and Vietnam. It has long been utilized to treat a variety of health concerns in numerous countries around the world, such as renal discomfort, constipation, **[...] Read more.**

(This article belongs to the Special Issue **Repositioning Natural Products in Drug Discovery ( /journal/molecules/special_issues/repositioning )**)

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Open Access Article 17 pages, 5437 KiB (/1420-3049/28/10/4185/pdf?version=1684477786)

**Sustainable Phenylalanine-Derived SAILs for Solubilization of Polycyclic Aromatic Hydrocarbons (/1420-3049/28/10/4185)**

by **Illia V. Kapitanov**, **Surya M. Sudheer**, **Toshikee Yadav**, **Kallol K. Ghosh**, **Nicholas Gathergood**, **Vijai K. Gupta** and **Yevgen Karpichev**

*Molecules* **2023**, *28*(10), 4185; **https://doi.org/10.3390/molecules28104185 (https://doi.org/10.3390/molecules28104185)** - 19 May 2023

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**Abstract** The solubilization capacity of a series of sustainable phenylalanine-derived surface-active ionic liquids (SAILs) was evaluated towards polycyclic aromatic hydrocarbons—naphthalene, anthracene and pyrene. The key physico-chemical parameters of the studied systems (critical micelle concentration, spectral properties, solubilization parameters) were determined, analyzed and compared with **[...] Read more.**

(This article belongs to the Special Issue **Recent Advances in Ionic Liquids and Their Applications ( /journal/molecules/special_issues/5H257MHJ2K )**)

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Open Access Article 20 pages, 4623 KiB (/1420-3049/28/10/4184/pdf?version=1684475517)

**Chemical Profile, Antibacterial, Antibiofilm, and Antiviral Activities of *Pulicaria crispa* Most Potent Fraction: An In Vitro and In Silico Study (/1420-3049/28/10/4184)**

by **Fatma Abo-Elghiet**, **Areej Rushdi**, **Mona H. Ibrahim**, **Sara H. Mahmoud**, **Mohamed A. Rabeh**, **Saad Ali Alshehri** and **Nagwan Galal El Menofy**

*Molecules* **2023**, *28*(10), 4184; **https://doi.org/10.3390/molecules28104184 (https://doi.org/10.3390/molecules28104184)** - 19 May 2023

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**Abstract** Infectious diseases caused by viruses and bacteria are a major public health concern worldwide, with the emergence of antibiotic resistance, biofilm-forming bacteria, viral epidemics, and the lack of effective antibacterial and antiviral agents exacerbating the problem. In an effort to search for new **[...] Read more.**

(This article belongs to the Special Issue **Antimicrobial Activity of Natural Extracts ( /journal/molecules/special_issues/Antimicrobial_Activity_of_Natural_Extracts )**)

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Open Access Review 26 pages, 5073 KiB (/1420-3049/28/10/4183/pdf?version=1684480350)

**Combating Antimicrobial Resistance in the Post-Genomic Era: Rapid Antibiotic Discovery (/1420-3049/28/10/4183)**

by **Yuehan Yang**, **Mara Grace C. Kessler**, **Maria Raquel Marchán-Rivadeneira** and **Yong Han**

*Molecules* **2023**, *28*(10), 4183; **https://doi.org/10.3390/molecules28104183 (https://doi.org/10.3390/molecules28104183)** - 19 May 2023

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**Abstract** Constantly evolving drug-resistant “superbugs” have caused an urgent demand for novel antimicrobial agents. Natural products and their analogs have been a prolific source of antimicrobial agents, even though a high rediscovery rate and less targeted research has made the field challenging in the **[...] Read more.**

(This article belongs to the Special Issue **Medicinal Value of Natural Bioactive Compounds and Plant Extracts ( /journal/molecules/special_issues/S16ILBF53Q )**)

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Open Access Article 14 pages, 8036 KiB (/1420-3049/28/10/4182/pdf?version=1684475297)

**Synthesis of Transition-Metal-Doped Nanocatalysts with Antibacterial Capabilities Using a Complementary Green Method (/1420-3049/28/10/4182)**

by **Anshul Singh**, **Ranjana Choudhary Ahirwar**, **Kavindra Borgaonkar**, **Neeta Gupta**, **Muhammad Ahsan**, **Jyoti Rathore**, **P. Das**, **S. Ganguly** and **Reena Rawat**

*Molecules* **2023**, *28*(10), 4182; **https://doi.org/10.3390/molecules28104182 (https://doi.org/10.3390/molecules28104182)** - 19 May 2023

**Cited by 7 (/1420-3049/28/10/4182#metrics)** | Viewed by 1963

**Abstract** A facile single-step wet chemical synthesis of a transition-metal-doped molybdate derivative was achieved via an *Ocimum tenuiflorum* extract-mediated green approach. The Synthesized nanomaterials of doped molybdate were characterized by optical and other spectroscopic techniques, which confirmed the size of nanocrystalline (~27.3 nm). The **[...] Read more.**

(This article belongs to the Special Issue **Metal Nanoparticles for a New Generation of Antibacterial Agents ( /journal/molecules/special_issues/CM09MS9L3I )**)

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Open Access Article 14 pages, 1448 KiB (/1420-3049/28/10/4181/pdf?version=1684470190)

**Characterization of the Nonpolar and Polar Extractable Components of Glanded Cottonseed for Its Valorization (/1420-3049/28/10/4181)**

by **Zhongqi He**, **Sunghyun Nam**, **Shasha Liu** and **Qi Zhao**

*Molecules* **2023**, *28*(10), 4181; **https://doi.org/10.3390/molecules28104181 (https://doi.org/10.3390/molecules28104181)** - 19 May 2023

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**Abstract** Cottonseed is the second major product of cotton (*Gossypium* spp.) crops after fiber. Thus, the characterization and valorization of cottonseed are important parts of cotton utilization research. In this work, the nonpolar and polar fractions of glanded (Gd) cottonseed were sequentially extracted **[...] Read more.**

(This article belongs to the Section **Natural Products Chemistry (/journal/molecules/sections/natural_products_chemistry)**)

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Open Access Article 26 pages, 3734 KiB (/1420-3049/28/10/4180/pdf?version=1684476979)

**Synthesis and Molecular Docking Studies of Alkoxy- and Imidazole-Substituted Xanthones as α-Amylase and α-Glucosidase Inhibitors (/1420-3049/28/10/4180)**

by **Dolores G. Aguila-Muñoz**, **Gabriel Vázquez-Lira**, **Erika Sarmiento-Tlale**, **María C. Cruz-López**, **Fabiola E. Jiménez-Montejo**, **Víctor E. López y López**, **Carlos H. Escalante**, **Dulce Andrade-Pavón**, **Omar Gómez-García**, **Joaquín Tamariz** and **Aarón Mendieta-Moctezuma**

*Molecules* **2023**, *28*(10), 4180; **https://doi.org/10.3390/molecules28104180 (https://doi.org/10.3390/molecules28104180)** - 18 May 2023

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**Abstr**urrent antidiabetic drugs have severe side effects, which may be minimized by new selective molecules that strongly inhibit α-glucosidase and weakly inhibit α-amylase. We have synthesized novel alkoxy-substituted xanthones and imidazole-substituted xanthones and have evaluated them for their in silico and in vitro **[...] Read more.**

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Open Access Article 18 pages, 6871 KiB **(/1420-3049/28/10/4179/pdf?version=1684505762)**

**Ultrasonication-Tailored Graphene Oxide of Varying Sizes in Multiple-Equilibrium-Route-Enhanced Adsorption for Aqueous Removal of Acridine Orange (/1420-3049/28/10/4179)**

by **Zhaoyang Han**, **Ling Sun**, **Yingying Chu**, **Jing Wang**, **Chenyu Wei**, **Yifang Liu**, **Qianlei Jiang**, **Changbao Han**, **Hui Yan** and **Xuemei Song**
*Molecules* **2023**, *28*(10), 4179; **https://doi.org/10.3390/molecules28104179 (https://doi.org/10.3390/molecules28104179)** - 18 May 2023
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**Abstract** Graphene oxide (GO) has shown remarkable performance in the multiple-equilibrium-route adsorption (MER) process, which is characterized by further activation of GO through an in-situ reduction process based on single-equilibrium-route adsorption (SER), generating new adsorption sites and achieving an adsorption capacity increase. However, the **[...] Read more.**
(This article belongs to the Special Issue **Wastewater Treatment: Functional Materials and Advanced Technology ( /journal/molecules/special_issues/wastewater_treatment_materials_technology )**)

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Open Access Article 13 pages, 22374 KiB **(/1420-3049/28/10/4178/pdf?version=1684463126)**

**Opening a Band Gap in Biphenylene Monolayer via Strain: A First-Principles Study (/1420-3049/28/10/4178)**

by **Yinlong Hou**, **Kai Ren**, **Yu Wei**, **Dan Yang**, **Zhen Cui** and **Ke Wang**
*Molecules* **2023**, *28*(10), 4178; **https://doi.org/10.3390/molecules28104178 (https://doi.org/10.3390/molecules28104178)** - 18 May 2023
**Cited by 10 (/1420-3049/28/10/4178#metrics)** | Viewed by 2414

**Abstract** A biphenylene network is a novel 2D allotropy of carbon with periodic 4-6-8 rings, which was synthesized successfully in 2021. In recent years, although the mechanical properties and thermal transport received a lot of research attention, how to open the Dirac cone in **[...] Read more.**

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Open Access Article 11 pages, 2732 KiB **(/1420-3049/28/10/4177/pdf?version=1684419768)**

**Surfactant Additives Containing Hydrophobic Fluorocarbon Chains and Hydrophilic Sulfonate Anion for Highly Reversible Zn Anode**

(/1420-3049/28/10/4177)

by **Jinxian Huang**, **Zhao Fu**, **Chuan-Fu Sun** and **Wenzhuo Deng**

*Molecules* **2023**, *28*(10), 4177; **https://doi.org/10.3390/molecules28104177 (https://doi.org/10.3390/molecules28104177)** - 18 May 2023

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**Abstract** Aqueous zinc-ion batteries (AZIBs) show enormous potential as a large-scale energy storage technique. However, the growth of Zn dendrites and serious side reactions occurring at the Zn anode hinder the practical application of AZIBs. For the first time, we reported a fluorine-containing surfactant, **[...] Read more.**

(This article belongs to the Special Issue **Multifunctional Metal Oxides: Synthesis and Applications ( /journal/molecules/special_issues/55446M089U )**)

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Open Access Article 22 pages, 2786 KiB **(/1420-3049/28/10/4176/pdf?version=1684482420)**

**Influence of Different Rootstocks on Fruit Quality and Primary and Secondary Metabolites Content of Blood Oranges Cultivars (/1420-3049/28/10/4176)**

by **María Ángeles Forner-Giner**, **Manuel Ballesta-de los Santos**, **Pablo Melgarejo**, **Juan José Martínez-Nicolás**, **Dámaris Núñez-Gómez**, **Alberto Continella** and **Pilar Legua**

*Molecules* **2023**, *28*(10), 4176; **https://doi.org/10.3390/molecules28104176 (https://doi.org/10.3390/molecules28104176)** - 18 May 2023

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**Abstract** Blood oranges have high concentrations of bioactive compounds that are beneficial to health. In Europe, the cultivation of blood oranges is increasing due to their excellent nutritional properties. In *Citrus* crops, rootstocks play an important role in juice and can increase the content **[...] Read more.**

(This article belongs to the Special Issue **Analyses and Applications of Phenolic Compounds in Food ( /journal/molecules/special_issues/Food_Phenolic )**)

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Open Access Article 27 pages, 7335 KiB **(/1420-3049/28/10/4175/pdf?version=1685004073)**

***In Silico* Drug Design of Anti-Breast Cancer Agents (/1420-3049/28/10/4175)**

by **Kalirajan Rajagopal**, **Anandarajagopal Kalusalingam**, **Anubhav Raj Bharathidasan**, **Aadarsh Sivaprakash**, **Krutheesh Shanmugam**, **Monall Sundaramoorthy** and **Gowramma Byran**

*Molecules* **2023**, *28*(10), 4175; **https://doi.org/10.3390/molecules28104175 (https://doi.org/10.3390/molecules28104175)** - 18 May 2023

**Cited by 7 (/1420-3049/28/10/4175#metrics)** | Viewed by 4954

**Abstract** Cancer is a condition marked by abnormal cell proliferation that has the potential to invade or indicate other health issues. Human beings are affected by more than 100 different types of cancer. Some cancer promotes rapid cell proliferation, whereas others cause cells to **[...] Read more.**

(This article belongs to the Special Issue **Artificial Intelligence and Data Science in the Drug Discovery ( /journal/molecules/special_issues/1TS23B5O8J )**)

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Open Access Article 16 pages, 4129 KiB (/1420-3049/28/10/4174/pdf?version=1684466329)

**Fully Room Temperature Reprogrammable, Recyclable, and Photomobile Soft Actuators from Physically Cross-Linked Main-Chain Azobenzene Liquid Crystalline Polymers (/1420-3049/28/10/4174)**

by **Shengkui Ma**, **Lei Wang**, **Yan Zhou** and **Huiqi Zhang**

*Molecules* **2023**, *28*(10), 4174; **https://doi.org/10.3390/molecules28104174 (https://doi.org/10.3390/molecules28104174)** - 18 May 2023

**Cited by 6 (/1420-3049/28/10/4174#metrics)** | Viewed by 1849

**Abstract** Fully room temperature three-dimensional (3D) shape-reprogrammable, recyclable, and photomobile azobenzene (azo) polymer actuators hold much promise in many photoactuating applications, but their development is challenging. Herein, we report on the efficient synthesis of a series of main-chain azo liquid crystalline polymers (LCPs) with **[...] Read more.**

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Open Access Correction 2 pages, 1217 KiB (/1420-3049/28/10/4173/pdf?version=1684412855)

**Correction: Mansoor et al. Effect of Currently Available Nanoparticle Synthesis Routes on Their Biocompatibility with Fibroblast Cell Lines. *Molecules* 2022, *27*, 6972 (/1420-3049/28/10/4173)**

by **Afsheen Mansoor**, **Zohaib Khurshid**, **Emaan Mansoor**, **Muhammad Talal Khan**, **Jithendra Ratnayake** and **Asif Jamal**

*Molecules* **2023**, *28*(10), 4173; **https://doi.org/10.3390/molecules28104173 (https://doi.org/10.3390/molecules28104173)** - 18 May 2023

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**Abstract** The authors wish to make the following correction to this paper [...] **Full article (/1420-3049/28/10/4173)**

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Open Access Review 17 pages, 4781 KiB (/1420-3049/28/10/4172/pdf?version=1684415454)

**High Hydrostatic Pressure in the Modulation of Enzymatic and Organocatalysis and Life under Pressure: A Review (/1420-3049/28/10/4172)**

by **Hana Scepankova**, **Diogo Galante**, **Edelman Espinoza-Suaréz**, **Carlos A. Pinto**, **Letícia M. Estevinho** and **Jorge Saraiva**

*Molecules* **2023**, *28*(10), 4172; **https://doi.org/10.3390/molecules28104172 (https://doi.org/10.3390/molecules28104172)** - 18 May 2023

**Cited by 7 (/1420-3049/28/10/4172#metrics)** | Viewed by 2861

**Abstract** The interest in high hydrostatic pressure (HHP) is mostly focused on the inactivation of deleterious enzymes, considering the quality-related issues associated with enzymes in foods. However, more recently, HHP has been increasingly studied for several biotechnological applications, including the possibility of carrying out **[...] Read more.**

(This article belongs to the Special Issue **Exclusive Review Papers in Green Chemistry ( /journal/molecules/special_issues/exclusive_reviewpaper )**)

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Open Access Article 14 pages, 4305 KiB (/1420-3049/28/10/4171/pdf?version=1684411394)

**Anticancer Effect of Cold Atmospheric Plasma in Syngeneic Mouse Models of Melanoma and Colon Cancer (/1420-3049/28/10/4171)**

by **Joon-Min Jung**, **Hae-Kyeong Yoon**, **Su-Yeon Kim**, **Mi-Ra Yun**, **Gyeong-Hoon Kim**, **Woo-Jin Lee**, **Mi-Woo Lee**, **Sung-Eun Chang** and **Chong-Hyun Won**

*Molecules* **2023**, *28*(10), 4171; **https://doi.org/10.3390/molecules28104171 (https://doi.org/10.3390/molecules28104171)** - 18 May 2023

**Cited by 7 (/1420-3049/28/10/4171#metrics)** | Viewed by 2282

**Abstract** Cold atmospheric plasma (CAP) may have applications in treating various types of malignant tumors. This study assessed the anticancer effects of CAP using melanoma and colon cancer cell lines. CAP treatment significantly reduced the in vitro viability of melanoma and colon cancer cell **[...] Read more.**

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Open Access Article 14 pages, 3215 KiB (/1420-3049/28/10/4170/pdf?version=1684406397)

**Screening of Tyrosinase, Xanthine Oxidase, and α-Glucosidase Inhibitors from Polygoni Cuspidati Rhizoma et Radix by Ultrafiltration and HPLC Analysis (/1420-3049/28/10/4170)**

by **Jing Chen**, **Qi Huang**, **Zhuobin He**, **Guoying Tan**, **Yuansheng Zou**, **Juying Xie** and **Zhengming Qian**

*Molecules* **2023**, *28*(10), 4170; **https://doi.org/10.3390/molecules28104170 (https://doi.org/10.3390/molecules28104170)** - 18 May 2023

**Cited by 9 (/1420-3049/28/10/4170#metrics)** | Viewed by 2071

**Abstract** Polygoni Cuspidati Rhizoma et Radix (PCR), the rhizome and root of *Polygonum cuspidatum* Sieb. et Zucc., has been used as an herbal medicine for a long time. In this study, the ultrafiltration combined with high performance liquid chromatography (UF-HPLC) method was developed to **[...] Read more.**

(This article belongs to the Special Issue **Discovery of Enzyme Inhibitors from Natural Products II ( /journal/molecules/special_issues/JU5S6FVETE )**)

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Open Access Review 26 pages, 3909 KiB (/1420-3049/28/10/4169/pdf?version=1684742306)

**The Power of Field-Flow Fractionation in Characterization of Nanoparticles in Drug Delivery (/1420-3049/28/10/4169)**

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by **Juan Bian**, **Nemal Gobalasingham**, **Anatolii Purchel** and **Jessica Lin**
*Molecules* **2023**, *28*(10), 4169; **https://doi.org/10.3390/molecules28104169 (https://doi.org/10.3390/molecules28104169)** - 18 May 2023
**Cited by 16 (/1420-3049/28/10/4169#metrics)** | Viewed by 5637

**Abstract** Asymmetric-flow field-flow fractionation (AF4) is a gentle, flexible, and powerful separation technique that is widely utilized for fractionating nanometer-sized analytes, which extend to many emerging nanocarriers for drug delivery, including lipid-, virus-, and polymer-based nanoparticles. To ascertain quality attributes and suitability of these **[...] Read more.**
(This article belongs to the Special Issue **Recent Trends of Functional Nanomaterials for Biomedical and Healthcare Applications ( /journal/molecules/special_issues/3J36W4I3X7 )**)

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Open Access Article 11 pages, 3490 KiB **(/1420-3049/28/10/4168/pdf?version=1684405536)**

**Poly(styrene sulfonic acid)-Grafted Carbon Black Synthesized by Surface-Initiated Atom Transfer Radical Polymerization (/1420-3049/28/10/4168)**

by **Artavazd Kirakosyan**, **Donghyun Lee**, **Yoonseong Choi**, **Namgee Jung** and **Jihoon Choi**
*Molecules* **2023**, *28*(10), 4168; **https://doi.org/10.3390/molecules28104168 (https://doi.org/10.3390/molecules28104168)** - 18 May 2023
**Cited by 9 (/1420-3049/28/10/4168#metrics)** | Viewed by 2564

**Abstract** Owing to their excellent electrical conductivity and robust mechanical properties, carbon-based nanocomposites are being used in a wide range of applications and devices, such as electromagnetic wave interference shielding, electronic devices, and fuel cells. While several approaches have been developed for synthesizing carbon **[...] Read more.**
(This article belongs to the Special Issue **Advanced Functional Polymer Nanocomposites ( /journal/molecules/special_issues/af_polymer_nanocomposites )**)

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Open Access Article 13 pages, 2550 KiB **(/1420-3049/28/10/4167/pdf?version=1684404677)**

**Purification, Structural Analysis and Cardio-Protective Activity of Polysaccharides from Radix Astragali (/1420-3049/28/10/4167)**

by **Shilei Wang**, **Yuan Peng**, **Yixin Zhuang**, **Nan Wang**, **Jianchang Jin** and **Zhajun Zhan**
*Molecules* **2023**, *28*(10), 4167; **https://doi.org/10.3390/molecules28104167 (https://doi.org/10.3390/molecules28104167)** - 18 May 2023
**Cited by 8 (/1420-3049/28/10/4167#metrics)** | Viewed by 2262

**Abstract** Two polysaccharides, named APS2-I and APS3-I, were purified from the water extract of Radix Astragali. The average molecular weight of APS2-I was 1.96 × $10^6$ Da and composed of Man, Rha, GlcA, GalA, Glc, Gal, Xyl, and Ara in a molar ratio **[...] Read more.**

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Open Access Article 13 pages, 3015 KiB (/1420-3049/28/10/4166/pdf?version=1684407451)

**A Highly Selective and Sensitive Sequential Recognition Probe $Zn^{2+}$ and $H_2PO_4^-$ Based on Chiral Thiourea Schiff Base (/1420-3049/28/10/4166)**

by **Shan Yang**, **Yichuan Huang**, **Aidang Lu**, **Ziwen Wang** and **Hongyan Li**
*Molecules* **2023**, *28*(10), 4166; **https://doi.org/10.3390/molecules28104166 (https://doi.org/10.3390/molecules28104166)** - 18 May 2023
**Cited by 9 (/1420-3049/28/10/4166#metrics)** | Viewed by 2042

**Abstract** A series of novel chiral thiourea fluorescent probes **$HL_1$**–**$HL_6$** were designed and synthesized from (1*R*,2*R*)-1,2-diphenylethylenediamine, phenyl isothiocyanate, and different substituted salicylic aldehydes. All of the compounds were confirmed by $^1$H NMR, $^{13}$C NMR, **[...] Read more.**
(This article belongs to the Special Issue **Design and Synthesis of Novel Fluorescent Molecules ( /journal/molecules/special_issues/58BZ4UEFSE )**)

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Open Access Article 21 pages, 2925 KiB (/1420-3049/28/10/4165/pdf?version=1684404078)

**Rovibrational Spectroscopy of Trans and Cis Conformers of 2-Furfural from High-Resolution Fourier Transform and QCL Infrared Measurements (/1420-3049/28/10/4165)**

by **Sathapana Chawananon**, **Pierre Asselin**, **Jordan A. Claus**, **Manuel Goubet**, **Anthony Roucou**, **Robert Georges**, **Joanna Sobczuk**, **Colwyn Bracquart**, **Olivier Pirali** and **Arnaud Cuisset**
*Molecules* **2023**, *28*(10), 4165; **https://doi.org/10.3390/molecules28104165 (https://doi.org/10.3390/molecules28104165)** - 18 May 2023
**Cited by 1 (/1420-3049/28/10/4165#metrics)** | Viewed by 2118

**Abstract** The ortho-isomer 2-furfural (2-FF), which is a primary atmospheric pollutant produced from biomass combustion, is also involved in oxidation processes leading to the formation of secondary organic aerosols. Its contribution to radiative forcing remains poorly understood. Thus, monitoring 2-FF directly in the atmosphere **[...] Read more.**
(This article belongs to the Special Issue **The Interplay between Spectroscopy and Quantum Chemistry for Environment: From Atmospheric Monitoring to Climate Changes ( /journal/molecules/special_issues/interplay_spectroscopy_quantum_chemistry )**)

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Open Access Article 18 pages, 28012 KiB (/1420-3049/28/10/4164/pdf?version=1684404897)

**The S...esis of Glycerol Carbonate from Glycerol and Carbon Dioxide over Supported CuO-Based Nanoparticle Catalyst (/1420-...49/28/10/4164)**

by **Jassim Mohamed Hamed Al-Kurdhani** and **Huajun Wang**

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*Molecules* **2023**, *28*(10), 4164; **https://doi.org/10.3390/molecules28104164 (https://doi.org/10.3390/molecules28104164)** - 18 May 2023
**Cited by 7 (/1420-3049/28/10/4164#metrics)** | Viewed by 2893

**Abstract** A series of supported CuO-based nanoparticle catalysts were prepared by the impregnation method and used for the synthesis of glycerol carbonate from glycerol and $CO_2$ in the presence of 2-cyanopyridine as a dehydrant and DMF as a solvent. The effects of supports **[...] Read more.**

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Open Access Article 15 pages, 1576 KiB **(/1420-3049/28/10/4163/pdf?version=1684401612)**

**Design, Synthesis and Various Bioactivity of Acylhydrazone-Containing Matrine Analogues (/1420-3049/28/10/4163)**

by **Wanjun Ni**, **Hongjian Song**, **Lizhong Wang**, **Yuxiu Liu** and **Qingmin Wang**
*Molecules* **2023**, *28*(10), 4163; **https://doi.org/10.3390/molecules28104163 (https://doi.org/10.3390/molecules28104163)** - 18 May 2023
**Cited by 8 (/1420-3049/28/10/4163#metrics)** | Viewed by 2277

**Abstract** Compounds with acylhydrazone fragments contain amide and imine groups that can act as electron donors and acceptors, so they are easier to bind to biological targets and thus generally exhibit significant biological activity. In this work, acylhydrazone fragments were introduced to the C-14 **[...] Read more.**
(This article belongs to the Special Issue **Emerging Trends in Pesticides Discovery Based on Natural Products ( /journal/molecules/special_issues/8206O3Y6L9 )**)

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Open Access Feature Paper Article 10 pages, 479 KiB **(/1420-3049/28/10/4162/pdf?version=1690192486)**

**Cannabinoid and Opioid Receptor Affinity and Modulation of Cancer-Related Signaling Pathways of Machaeriols and Machaeridiols from *Machaerium* Pers. (/1420-3049/28/10/4162)**

by **Ilias Muhammad**, **Mohammad A. Ibrahim**, **Mallika Kumarihamy**, **Janet A. Lambert**, **Jin Zhang**, **Marwa H. Mohammad**, **Shabana I. Khan**, **David S. Pasco** and **Premalatha Balachandran**
*Molecules* **2023**, *28*(10), 4162; **https://doi.org/10.3390/molecules28104162 (https://doi.org/10.3390/molecules28104162)** - 18 May 2023
**Cited by 3 (/1420-3049/28/10/4162#metrics)** | Viewed by 2652

**Abstract** Machaeriols and machaeridiols are unique hexahydrodibenzopyran-type aralkyl phytocannabinoids isolated from *Machaerium* Pers. Earlier studies of machaeriol A (**1**) and B (**2**) did not show any affinity for cannabinoid receptor 1 (CB1 or CNR1), although they are structural analogs of **[...] Read more.**
(This article belongs to the Special Issue **Plant Bioactive Compounds: Extraction, Identification and Biological Activities ( /journal/molecules/special_issues/plant_bioact_compd )**)

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Open Access Article 24 pages, 5513 KiB (/1420-3049/28/10/4161/pdf?version=1684397921)

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**Tetrasubstituted Pyrrole Derivative Mimetics of Protein–Protein Interaction Hot-Spot Residues: A Promising Class of Anticancer Agents Targeting Melanoma Cells (/1420-3049/28/10/4161)**

by **Marco Persico**, **Paola Galatello**, **Maria Grazia Ferraro**, **Carlo Irace**, **Marialuisa Piccolo**, **Avazbek Abduvakhidov**, **Oleh Tkachuk**, **Maria Luisa d'Aulisio Garigliota**, **Pietro Campiglia**, **Patrizia Iannece**, **Michela Varra**, **Anna Ramunno** and **Caterina Fattorusso**

*Molecules* **2023**, *28*(10), 4161; **https://doi.org/10.3390/molecules28104161 (https://doi.org/10.3390/molecules28104161)** - 18 May 2023

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**Abstract** A new series of tetrasubstituted pyrrole derivatives (TSPs) was synthesized based on a previously developed hypothesis on their ability to mimic hydrophobic protein motifs. The resulting new TSPs were endowed with a significant toxicity against human epithelial melanoma A375 cells, showing $IC_{50}$ **[...] Read more.**

(This article belongs to the Special Issue **Featured Papers in Medicinal Chemistry II ( /journal/molecules/special_issues/Featured_Papers_Medicinal_ChemistryII )**)

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Open Access Review 30 pages, 6703 KiB (/1420-3049/28/10/4160/pdf?version=1684395684)

**Molecular Design of Porous Organic Polymer-Derived Carbonaceous Electrocatalysts for Pinpointing Active Sites in Oxygen Reduction Reaction (/1420-3049/28/10/4160)**

by **Xiaofeng Mou**, **Xiaoyu Xin**, **Yanli Dong**, **Bin Zhao**, **Runze Gao**, **Tianao Liu**, **Na Li**, **Huimin Liu** and **Zhichang Xiao**

*Molecules* **2023**, *28*(10), 4160; **https://doi.org/10.3390/molecules28104160 (https://doi.org/10.3390/molecules28104160)** - 18 May 2023

**Cited by 6 (/1420-3049/28/10/4160#metrics)** | Viewed by 2543

**Abstract** The widespread application of fuel cells is hampered by the sluggish kinetics of the oxygen reduction reaction (ORR), which traditionally necessitates the use of high-cost platinum group metal catalysts. The indispensability of these metal catalysts stems from their ability to overcome kinetic barriers, **[...] Read more.**

(This article belongs to the Special Issue **Potential Applications of Functional Porous Organic Frameworks ( /journal/molecules/special_issues/organic_frameworks )**)

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Open Access Article 17 pages, 2038 KiB (/1420-3049/28/10/4159/pdf?version=1684395916)

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**Nature of Luminescence and Pharmacological Activity of Sulfaguanidine (/1420-3049/28/10/4159)**

by **Olga Tchaikovskaya**, **Elena Bocharnikova**, **Olga Bazyl**, **Vlada Chaidonova**, **George Mayer** and **Paul Avramov**

*Molecules* **2023**, *28*(10), 4159; **https://doi.org/10.3390/molecules28104159 (https://doi.org/10.3390/molecules28104159)** - 18 May 2023

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**Abstract** Sulfonamides are one of the oldest groups of veterinary chemotherapeutic agents. Physico-chemical properties, the concentration and the nature of the environment are the factors responsible for the distribution of sulfonamides in the living organism. Although these drug compounds have been in use for **[...] Read more.**

(This article belongs to the Special Issue **Recent Advances in Spectroscopy of Molecular Ensembles and Low-Dimensional Phases ( /journal/molecules/special_issues/0167TZWXXV )**)

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Open Access Article 13 pages, 1630 KiB **(/1420-3049/28/10/4158/pdf?version=1684390752)**

**Determination of Multiple Neurotransmitters through LC-MS/MS to Confirm the Therapeutic Effects of *Althaea rosea* Flower on TTX-Intoxicated Rats (/1420-3049/28/10/4158)**

by **Yichen Wang**, **Renjin Zheng**, **Pingping Wu**, **Youjia Wu**, **Lingyi Huang** and **Liying Huang**

*Molecules* **2023**, *28*(10), 4158; **https://doi.org/10.3390/molecules28104158 (https://doi.org/10.3390/molecules28104158)** - 18 May 2023

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**Abstract** Tetrodotoxin (TTX) inhibits neurotransmission in animals, and there is no specific antidote. In clinical practice in China, *Althaea rosea* (*A. rosea* flower) extract has been used to treat TTX poisoning. In this work, the efficacy of the ethyl acetate fraction extract of **[...] Read more.**

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Open Access Article 15 pages, 1848 KiB **(/1420-3049/28/10/4157/pdf?version=1684391875)**

**Antitumor Effect of Bleomycin Nanoaerosol in Murine Carcinoma Model (/1420-3049/28/10/4157)**

by **Saida S. Karshieva**, **Gulalek Babayeva**, **Vadim S. Pokrovsky**, **Yuri M. Shlyapnikov**, **Elena A. Shlyapnikova**, **Anna E. Bugrova**, **Alexey S. Kononikhin**, **Evgeny N. Nikolaev** and **Igor L. Kanev**

*Molecules* **2023**, *28*(10), 4157; **https://doi.org/10.3390/molecules28104157 (https://doi.org/10.3390/molecules28104157)** - 18 May 2023

**Cited by 3 (/1420-3049/28/10/4157#metrics)** | Viewed by 2556

**Abstract** Bleomycin, which is widely used as an antitumor agent, possesses serious adverse effects such as pulmonary toxicity. Local nanoaerosol deposition for lung cancer treatment is a promising alternative to drug delivery to lung lesions. The aim of this work is to test the **[...] Read more.**

(This article belongs to the Special Issue **Nano-Based Drug Delivery and Diagnostics: Innovation and Applications ( /journal/molecules/special_issues/A4YN348WTG )**)

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Open Access Article 14 pages, 6717 KiB **(/1420-3049/28/10/4156/pdf?version=1684380029)**

**Comparative Virucidal Activities of Essential Oils and Alcohol-Based Solutions against Enveloped Virus Surrogates: In Vitro and In Silico Analysis (/1420-3049/28/10/4156)**

by **Valentina Parra-Acevedo**, **Raquel E. Ocazionez**, **Elena E. Stashenko**, **Lina Silva-Trujillo** and **Paola Rondón-Villarreal**

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*Molecules* **2023**, *28*(10), 4156; **https://doi.org/10.3390/molecules28104156 (https://doi.org/10.3390/molecules28104156)** - 18 May 2023
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**Abstract** The large-scale use of alcohol (OH)-based disinfectants to control pathogenic viruses is of great concern because of their side effects on humans and harmful impact on the environment. There is an urgent need to develop safe and environmentally friendly disinfectants. Essential oils (EOs) **[...] Read more.**
(This article belongs to the Topic **Biological Activity of Plant Extracts (/topics/plant_extracts)**)

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Open Access Article 17 pages, 5166 KiB **(/1420-3049/28/10/4155/pdf?version=1684337955)**

**One-Step Synthesis of $Ag_2O/Fe_3O_4$ Magnetic Photocatalyst for Efficient Organic Pollutant Removal via Wide-Spectral-Response Photocatalysis–Fenton Coupling (/1420-3049/28/10/4155)**

by **Chuanfu Shan**, **Ziqian Su**, **Ziyi Liu**, **Ruizheng Xu**, **Jianfeng Wen**, **Guanghui Hu**, **Tao Tang**, **Zhijie Fang**, **Li Jiang** and **Ming Li**
*Molecules* **2023**, *28*(10), 4155; **https://doi.org/10.3390/molecules28104155 (https://doi.org/10.3390/molecules28104155)** - 17 May 2023
**Cited by 7 (/1420-3049/28/10/4155#metrics)** | Viewed by 2401

**Abstract** Photocatalysis holds great promise for addressing water pollution caused by organic dyes, and the development of $Ag_2O/Fe_3O_4$ aims to overcome the challenges of slow degradation efficiency and difficult recovery of photocatalysts. In this study, we present a novel, **[...] Read more.**
(This article belongs to the Special Issue **Photocatalytic Materials and Photocatalytic Reactions ( /journal/molecules/special_issues/87U2U4T532 )**)

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Open Access Review 23 pages, 923 KiB **(/1420-3049/28/10/4154/pdf?version=1684373518)**

**Characteristics, Isolation Methods, and Biological Properties of Aucubin (/1420-3049/28/10/4154)**

by **Kartini Kartini**, **Michelle Abigail Irawan**, **Finna Setiawan** and **Nikmatul Ikhrom Eka Jayani**
*Molecules* **2023**, *28*(10), 4154; **https://doi.org/10.3390/molecules28104154 (https://doi.org/10.3390/molecules28104154)** - 17 May 2023
**Cited by 10 (/1420-3049/28/10/4154#metrics)** | Viewed by 3769

**Abstract** Aucubin is an iridoid glycoside widely spread in the families *Cornaceae*, *Garryaceae*, *Orobanchaceae*, *Globulariaceae*, *Eucommiaceae*, *Scrophulariaceae*, *Plantaginaceae*, and *Rubiaceae*. This review is intended to provide data on the physicochemical characteristics, isolation methods, and biological activities **[...] Read more.**
(This article belongs to the Special Issue **Isolation, Identification and Application of Biologically Active Natural Products ( /journal/molecules/special_issues/biologically_natural_products )**)

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Open Access Review 36 pages, 11109 KiB **(/1420-3049/28/10/4153/pdf?version=1684397093)**

**Green Synthesis of Aromatic Nitrogen-Containing Heterocycles by Catalytic and Non-Traditional Activation Methods (/1420-3049/28/10/4153)**

by **R. [illegible]adett Vlocskó**, **Guoshu Xie** and **Béla Török**
*Molecules* **2023**, *28*(10), 4153; **https://doi.org/10.3390/molecules28104153 (https://doi.org/10.3390/molecules28104153)** - 17 May 2023
**Cited by 14 (/1420-3049/28/10/4153#metrics)** | Viewed by 4104

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**Abstract** Recent advances in the environmentally benign synthesis of aromatic N-heterocycles are reviewed, focusing primarily on the application of catalytic methods and non-traditional activation. This account features two main parts: the preparation of single ring N-heterocycles, and their condensed analogs. Both groups include compounds **[...] Read more.**

(This article belongs to the Special Issue **Recent Developments in the Synthesis and Functionalization of Nitrogen Heterocycles (/journal/molecules/special_issues/Synthesis_Nitrogen_Heterocycles)**)

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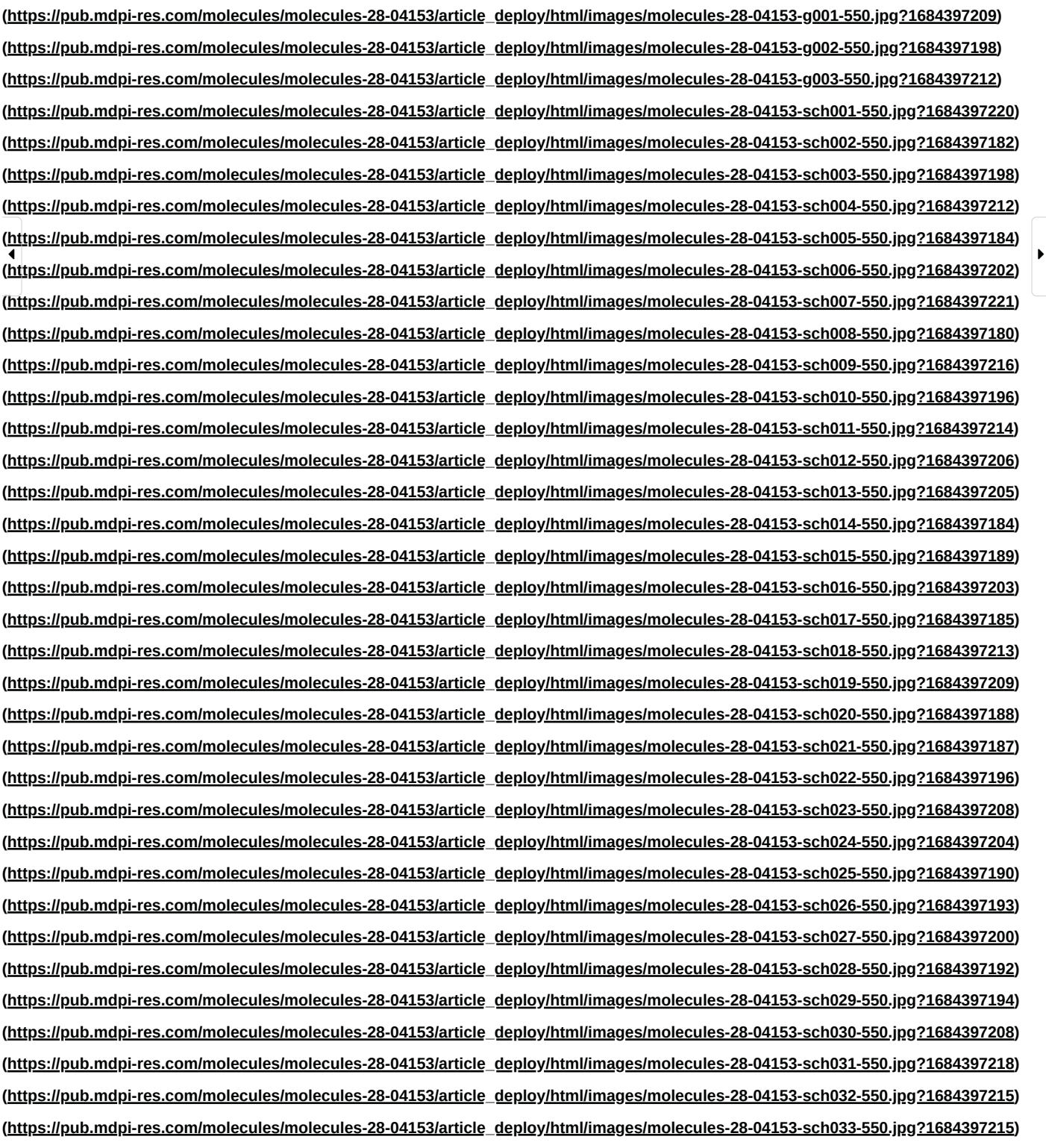

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Open Access Article 13 pages, 4056 KiB **(/1420-3049/28/10/4152/pdf?version=1684333689)**

**A Quantitative Approach to Determine Hydrophobe Content of Associating Polyacrylamide Using a Fluorescent Probe (/1420-3049/28/10/4152)**

by **Ziyang Su**, **Yu Zhang**, **Weidong Liu**, **Ruijing Han**, **Xuezhi Zhao**, **Xiaohuo Shi**, **Xingyu Lu**, **Yan Zhang** and **Yujun Feng**

*Molecules* **2023**, *28*(10), 4152; **https://doi.org/10.3390/molecules28104152 (https://doi.org/10.3390/molecules28104152)** - 17 May 2023

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**Abstract** Hydrophobically associating polymers have found widespread applications in many domains due to their unique rheological behavior, which

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is primarily dictated by the hydrophobe content. However, the low fraction of hydrophobic monomers in polymers makes this parameter's precise and straightforward measurement difficult. Herein, a **[...] Read more.**

(This article belongs to the Section **Macromolecular Chemistry (/journal/molecules/sections/macromolecular_chemistry)**)

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Open Access Review 45 pages, 12047 KiB (/1420-3049/28/10/4151/pdf?version=1684392328)

**Electromagnetic Radiation Effects on MgO-Based Magnetic Tunnel Junctions: A Review (/1420-3049/28/10/4151)**

by **Dereje Seifu**, **Qing Peng**, **Kit Sze**, **Jie Hou**, **Fei Gao** and **Yucheng Lan**

*Molecules* **2023**, *28*(10), 4151; **https://doi.org/10.3390/molecules28104151 (https://doi.org/10.3390/molecules28104151)** - 17 May 2023

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**Abstract** Magnetic tunnel junctions (MTJs) have been widely utilized in sensitive sensors, magnetic memory, and logic gates due to their tunneling magnetoresistance. Moreover, these MTJ devices have promising potential for renewable energy generation and storage. Compared with Si-based devices, MTJs are more tolerant to **[...] Read more.**

(This article belongs to the Special Issue **Synthesis, Characterization, and Applications of Nanomaterials for Energy Conversion and Storage (/journal/molecules/special_issues/energetic_nanomaterials)**)

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Open Access Article 26 pages, 1741 KiB (/1420-3049/28/10/4150/pdf?version=1684372324)

**Critical Evaluation of Two Qualitative Analytical Approaches for Multiclass Determination of Veterinary Drugs in Bovine Muscle Using**

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**UHPLC-Q-Orbitrap: The Wind of Change in Brazilian Monitoring (/1420-3049/28/10/4150)**

by **Ramon Alves de Oliveira Paula**, **Carina de Souza Gondim**, **Eduardo Morgado Schmidt**, **Maria Helena Glicério Marcelina Diniz**, **Mary Ane Gonçalves Lana** and **Leandro Soares de Oliveira**

*Molecules* **2023**, *28*(10), 4150; **https://doi.org/10.3390/molecules28104150 (https://doi.org/10.3390/molecules28104150)** - 17 May 2023

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**Abstract** Food safety is recognized as a main requirement for consumers, food industries, and official laboratories. Here, we present the optimization and screening qualitative validation of two multianalyte methods in bovine muscle tissues by ultra-high-performance liquid chromatography coupled to high-resolution mass spectrometry with an **[...] Read more.**

(This article belongs to the Special Issue **Analytical Methods in the Field of Foods Analysis ( /journal/molecules/special_issues/analyt_food_analy )**)

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Open Access Article 23 pages, 3061 KiB **(/1420-3049/28/10/4149/pdf?version=1684397386)**

**Ligand−Structure Effects on *N*−Heterocyclic Carbene Rhenium Photo− and Electrocatalysts of $CO_2$ Reduction (/1420-3049/28/10/4149)**

by **Lauren Kearney**, **Michael P. Brandon**, **Andrew Coleman**, **Ann M. Chippindale**, **František Hartl**, **Ralte Lalrempuia**, **Martin Pižl** and **Mary T. Pryce**

*Molecules* **2023**, *28*(10), 4149; **https://doi.org/10.3390/molecules28104149 (https://doi.org/10.3390/molecules28104149)** - 17 May 2023

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**Abstract** Three novel rhenium *N*−heterocyclic carbene complexes, [Re]−NHC−1−3 ([Re] = *fac*−$Re(CO)_3Br$), were synthesized and characterized using a range of spectroscopic techniques. Photophysical, electrochemical and spectroelectrochemical studies were carried out to probe the properties of these organometallic compounds. Re−NHC−1 and Re−NHC−2 **[...] Read more.**

(This article belongs to the Special Issue **Molecules in 2023 ( /journal/molecules/special_issues/49X1JIB4SS )**)

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Open Access Article 15 pages, 4234 KiB **(/1420-3049/28/10/4148/pdf?version=1684481068)**

**Interaction of Graphene Oxide Nanoparticles with Human Mesenchymal Stem Cells Visualized in the Cell-IQ System (/1420-3049/28/10/4148)**

by **Sergey Lazarev**, **Sofya Uzhviyuk**, **Mikhail Rayev**, **Valeria Timganova**, **Maria Bochkova**, **Olga Khaziakhmatova**, **Vladimir Malashchenko**, **Larisa Litvinova** and **Svetlana Zamorina**

*Molecules* **2023**, *28*(10), 4148; **https://doi.org/10.3390/molecules28104148 (https://doi.org/10.3390/molecules28104148)** - 17 May 2023

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**Abstract** Graphene oxide is a promising nanomaterial with many potential applications. However, before it can be widely used in areas such as drug delivery and medical diagnostics, its influence on various cell populations in the human body must be studied to ensure its safety. **[...] Read more.**

(This article belongs to the Special Issue **2D Materials for Biomedical Applications ( /journal/molecules/special_issues/2D_materials_biomedical )**)

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Open Access Article 14 pages, 12728 KiB (/1420-3049/28/10/4147/pdf?version=1684320163)

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**Synthesis of Chitosan Oligosaccharide-Loaded Glycyrrhetinic Acid Functionalized Mesoporous Silica Nanoparticles and In Vitro Verification of the Treatment of APAP-Induced Liver Injury (/1420-3049/28/10/4147)**

by **Xinghua Guo**, **Chengcheng Zhang**, **Yan Bai**, **Qishi Che**, **Hua Cao**, **Jiao Guo** and **Zhengquan Su**

*Molecules* **2023**, *28*(10), 4147; **https://doi.org/10.3390/molecules28104147 (https://doi.org/10.3390/molecules28104147)** - 17 May 2023

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**Abstract** Objective: the study was to find a suitable treatment for acute drug-induced liver injury. The use of nanocarriers can improve the therapeutic effect of natural drugs by targeting hepatocytes and higher loads. Methods: firstly, uniformly dispersed three-dimensional dendritic mesoporous silica nanospheres (MSNs) were **[...] Read more.**

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Open Access Article 15 pages, 3420 KiB (/1420-3049/28/10/4146/pdf?version=1684320603)

**Targeted Drug Administration onto Cancer Cells Using Hyaluronic Acid–Quercetin-Conjugated Silver Nanoparticles (/1420-3049/28/10/4146)**

by **Rasha H. Al-Serwi**, **Mohamed A. Eladl**, **Mohamed El-Sherbiny**, **Mohamed A. Saleh**, **Gamal Othman**, **Sultan M. Alshahrani**, **Rasha Alnefaie**, **Afnan M. Jan**, **Sulaiman M. Alnasser**, **Aishah E. Albalawi**, **Jamal Moideen Muthu Mohamed** and **Farid Menaa**

*Molecules* **2023**, *28*(10), 4146; **https://doi.org/10.3390/molecules28104146 (https://doi.org/10.3390/molecules28104146)** - 17 May 2023

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**Abstract** Quercetin (QtN) displays low systemic bioavailability caused by poor water solubility and instability. Consequently, it exerts limited anticancer action in vivo. One solution to increase the anticancer efficacy of QtN is the use of appropriate functionalized nanocarriers that preferentially target and deliver the **[...] Read more.**

(This article belongs to the Special Issue **Nanomaterials for Advanced Biomedical Applications ( /journal/molecules/special_issues/nanomaterials_for_advanced_biomedical_applications )**)

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Open Access Article 22 pages, 3815 KiB (/1420-3049/28/10/4145/pdf?version=1684316624)

**Unravelling Novel Phytochemicals and Anticholinesterase Activity in Irish *Cladonia portentosa* (/1420-3049/28/10/4145)**

by **Shipra Nagar**, **Maria Pigott**, **Wirginia Kukula-Koch** and **Helen Sheridan**

*Molecules* **2023**, *28*(10), 4145; **https://doi.org/10.3390/molecules28104145 (https://doi.org/10.3390/molecules28104145)** - 17 May 2023

**Cited by 5 (/1420-3049/28/10/4145#metrics)** | Viewed by 2123

**Abstract** Acetylcholinesterase inhibitors remain the mainstay of symptomatic treatment for Alzheimer's disease. The natural world is rich in acetylcholinesterase inhibitory molecules, and research efforts to identify novel leads is ongoing. *Cladonia portentosa*, commonly known as reindeer lichen, is an abundant lichen species found **[...] Read more.**

(This belongs to the Special Issue **Bioactive Compounds from Natural Sources II ( /journal/molecules/special_issues/Bioactive_NSII )**)

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Open Access Feature Paper Article 12 pages, 1081 KiB (/1420-3049/28/10/4144/pdf?version=1684316030)

**Antibacterial and Analgesic Properties of Beta-Caryophyllene in a Murine Urinary Tract Infection Model (/1420-3049/28/10/4144)**

by **Kayle Dickson**, **Cassidy Scott**, **Hannah White**, **Juan Zhou**, **Melanie Kelly** and **Christian Lehmann**

*Molecules* **2023**, *28*(10), 4144; **https://doi.org/10.3390/molecules28104144 (https://doi.org/10.3390/molecules28104144)** - 17 May 2023

**Cited by 9 (/1420-3049/28/10/4144#metrics)** | Viewed by 3259

**Abstract** Beta-caryophyllene has demonstrated anti-inflammatory effects in a variety of conditions, including interstitial cystitis. These effects are mediated primarily via the activation of the cannabinoid type 2 receptor. Additional antibacterial properties have recently been suggested, leading to our investigation of the effects of beta-caryophyllene **[...] Read more.**

(This article belongs to the Special Issue **Bioactive Molecules Targeting Inflammation Processes in Related Diseases ( /journal/molecules/special_issues/Bioactive_Inflammation_Diseases )**)

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Open Access Feature Paper Article 21 pages, 2627 KiB (/1420-3049/28/10/4143/pdf?version=1684319058)

**Tethered Indoxyl-Glucuronides for Enzymatically Triggered Cross-Linking (/1420-3049/28/10/4143)**

by **Juno Son**, **Zhiyuan Wu**, **Jinghuai Dou**, **Hikaru Fujita**, **Phuong-Lien Doan Cao**, **Qihui Liu** and **Jonathan S. Lindsey**

*Molecules* **2023**, *28*(10), 4143; **https://doi.org/10.3390/molecules28104143 (https://doi.org/10.3390/molecules28104143)** - 17 May 2023

**Cited by 2 (/1420-3049/28/10/4143#metrics)** | Viewed by 2053

**Abstract** Indoxyl-glucuronides, upon treatment with β-glucuronidase under physiological conditions, are well known to afford the corresponding indigoid dye via oxidative dimerization. Here, seven indoxyl-glucuronide target compounds have been prepared along with 22 intermediates. Of the target compounds, four contain a conjugatable handle (azido-PEG, hydroxy-PEG, **[...] Read more.**

(This article belongs to the Section **Organic Chemistry (/journal/molecules/sections/organic_chemistry)**)

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Open Access Article 15 pages, 10832 KiB (/1420-3049/28/10/4142/pdf?version=1684393232)

**A Planar Disk Electrode Chip Based on MWCNT/CS/$Pb^{2+}$ Ionophore IV Nanomaterial Membrane for Trace Level $Pb^{2+}$ Detection (/1420-3049/28/10/4142)**

by **Yu Huang**, **Cong Wang**, **Wei Qu**, **Yirou Yan**, **Ping Wang** and **Chengjun Qiu**

*Molecules* **2023**, *28*(10), 4142; **https://doi.org/10.3390/molecules28104142 (https://doi.org/10.3390/molecules28104142)** - 17 May 2023

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**Abstract** Unlike conventional lead ion ($Pb^{2+}$) detecting methods, electrochemical methods have the attractive advantages of rapid response, good portability and high sensitivity. In this paper, a planar disk electrode modified by multiwalled carbon nanotube (MWCNTs)/chitosan (CS)/lead ($Pb^{2+}$) ionophore **[...] Read more.**

(This article belongs to the Special Issue **Recent Progress in Nanomaterials in Electrochemistry ( /journal/molecules/special_issues/98SB919GAB )**)

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Open Access Article 25 pages, 7510 KiB **(/1420-3049/28/10/4141/pdf?version=1684313340)**

**Novel Route to Cationic Palladium(II)–Cyclopentadienyl Complexes Containing Phosphine Ligands and Their Catalytic Activities (/1420-3049/28/10/4141)**

by **Dmitry S. Suslov**, **Mikhail V. Bykov**, **Marina V. Pakhomova**, **Timur S. Orlov**, **Zorikto D. Abramov**, **Anastasia V. Suchkova**, **Igor A. Ushakov**, **Pavel A. Abramov** and **Alexander S. Novikov**

*Molecules* **2023**, *28*(10), 4141; **https://doi.org/10.3390/molecules28104141 (https://doi.org/10.3390/molecules28104141)** - 17 May 2023

**Cited by 3 (/1420-3049/28/10/4141#metrics)** | Viewed by 2218

**Abstract** The Pd(II) complexes $[Pd(Cp)(L)_n]_m[BF_4]_m$ were synthesized via the reaction of cationic acetylacetonate complexes with cyclopentadiene in the presence of $BF_3{\cdot}OEt_2$ ($n$ = 2, $m$ = 1: L = $PPh_3$ (**1 [...] Read more.**

(This article belongs to the Special Issue **Feature Papers in Applied Chemistry 2.0 ( /journal/molecules/special_issues/UO552KTZN6 )**)

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Open Access Article 12 pages, 4354 KiB **(/1420-3049/28/10/4140/pdf?version=1684310767)**

**Dispersive Micro-Solid Phase Extraction Using a Graphene Oxide Nanosheet with Neocuproine and Batocuproine for the Preconcentration of Traces of Metal Ions in Food Samples (/1420-3049/28/10/4140)**

by **Barbara Feist**

*Molecules* **2023**, *28*(10), 4140; **https://doi.org/10.3390/molecules28104140 (https://doi.org/10.3390/molecules28104140)** - 17 May 2023

**Cited by 6 (/1420-3049/28/10/4140#metrics)** | Viewed by 1589

**Abstract** A dispersive micro-solid phase extraction (Dμ-SPE) method for the preconcentration of trace metal ions (Pb, Cd, Cr, Mn, Fe, Co, Ni, Cu, Zn) on graphene oxide with the complexing reagents neocuproine or batocuproine is presented here. Metal ions form cationic complexes with neocuproine **[...] Read more.**

(This article belongs to the Special Issue **Nanomaterials Applied to Analytical Chemistry ( /journal/molecules/special_issues/Nanomaterials_Sample_Preparation )**)

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Open Access Article 20 pages, 8651 KiB (/1420-3049/28/10/4139/pdf?version=1684312055)

**Fabrication and Characterization of Ag-Graphene Nanocomposites and Investigation of Their Cytotoxic, Antifungal and Photocatalytic Potential (/1420-3049/28/10/4139)**

by **Sidra Batool Malik**, **Asma Gul**, **Javed Iqbal Saggu**, **Banzeer Ahsan Abbasi**, **Beenish Azad**, **Javed Iqbal**, **Mohsin Kazi**, **Wadie Chalgham** and **Seyed Arshia Mirjafari Firoozabadi**

*Molecules* **2023**, *28*(10), 4139; **https://doi.org/10.3390/molecules28104139 (https://doi.org/10.3390/molecules28104139)** - 17 May 2023

**Cited by 7 (/1420-3049/28/10/4139#metrics)** | Viewed by 2553

**Abstract** In the present study, we aimed to synthesize $(Ag)_{1-x}(GNPs)_x$ nanocomposites in variable ratios (25% GNPs–Ag, 50% GNPs–Ag, and 75% GNPs–Ag) via an ex situ approach to investigate the incremental effects of GNPs (graphene nanoparticles) on AgNPs (silver nanoparticles). The prepared **[...] Read more.**

(This article belongs to the Special Issue **Synthesis and Application of Nanoparticles and Nanocomposites ( /journal/molecules/special_issues/3FY2580B6V )**)

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Open Access Editorial 3 pages, 158 KiB (/1420-3049/28/10/4138/pdf?version=1684307432)

**Editorial: Nanomedicine-Based Drug Delivery Systems: Recent Developments and Future Prospects (/1420-3049/28/10/4138)**

by **Faiyaz Shakeel**

*Molecules* **2023**, *28*(10), 4138; **https://doi.org/10.3390/molecules28104138 (https://doi.org/10.3390/molecules28104138)** - 17 May 2023

**Cited by 7 (/1420-3049/28/10/4138#metrics)** | Viewed by 1828

**Abstract** Since the discovery of nanomedicine-based drug delivery carriers such as nanoparticles, liposomes, and self-nanoemulsifying drug delivery systems (SNEDDS), enormous progress has been achieved in the field of innovative active biomolecule drug delivery systems [...] **Full article (/1420-3049/28/10/4138)**

(This article belongs to the Special Issue **Nanomedicine Based Drug Delivery Systems: Recent Developments and Future Prospects ( /journal/molecules/special_issues/Nanomedicine_Drug )**)

Open Access Article 18 pages, 3049 KiB (/1420-3049/28/10/4137/pdf?version=1684307273)

**Dragon's Blood Sap Microencapsulation within Whey Protein Concentrate and Zein Using Electrospraying Assisted by Pressurized Gas Technology (/1420-3049/28/10/4137)**

by **Juan David Escobar-García**, **Cristina Prieto**, **Maria Pardo-Figuerez** and **Jose M. Lagaron**

*Molecules* **2023**, *28*(10), 4137; **https://doi.org/10.3390/molecules28104137 (https://doi.org/10.3390/molecules28104137)** - 17 May 2023

**Cited by 3 (/1420-3049/28/10/4137#metrics)** | Viewed by 1795

**Abstract** Dragon's blood sap (DBS) obtained from the bark of Croton lechleri (Müll, Arg.) is a complex herbal remedy of pharmacological interest due to its high content in polyphenols, specifically proanthocyanidins. In this paper, electrospraying assisted by pressurized gas (EAPG) was first compared with **[...] Read more.**

(This article belongs to the Special Issue **New Technologies for Encapsulation of Small Molecules and Plant Extracts II ( /journal/molecules/special_issues/9TB663L5LT )**)

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Open Access Article 14 pages, 3164 KiB (/1420-3049/28/10/4136/pdf?version=1684307009)

**Construction of N-Doped Carbon-Modified Ni/$SiO_2$ Catalyst Promoting Cinnamaldehyde Selective Hydrogenation (/1420-3049/28/10/4136)**

by **Yongwang Ren**, **Huizhong Xu**, **Beibei Han** and **Jing Xu**

*Molecules* **2023**, *28*(10), 4136; **https://doi.org/10.3390/molecules28104136 (https://doi.org/10.3390/molecules28104136)** - 17 May 2023

**Cited by 5 (/1420-3049/28/10/4136#metrics)** | Viewed by 1789

**Abstract** At present, the selective hydrogenation of α, β-unsaturated aldehydes remains a challenge due to competition between unsaturated functional groups (C=C and C=O). In this study, N-doped carbon deposited on silica-supported nickel Mott–Schottky type catalysts (Ni/$SiO_2$@$N_x$C) was prepared for the **[...] Read more.**

(This article belongs to the Special Issue **Molecular Catalysts for $CO_2$ Reduction ( /journal/molecules/special_issues/carbondioxide_reduction )**)

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Open Access Article 16 pages, 631 KiB (/1420-3049/28/10/4135/pdf?version=1684301170)

**Chemical Composition and Antimicrobial Properties of Honey Bee Venom (/1420-3049/28/10/4135)**

by **Valery Isidorov**, **Adam Zalewski**, **Grzegorz Zambrowski** and **Izabela Swiecicka**

*Molecules* **2023**, *28*(10), 4135; **https://doi.org/10.3390/molecules28104135 (https://doi.org/10.3390/molecules28104135)** - 17 May 2023

**Cited by 14 (/1420-3049/28/10/4135#metrics)** | Viewed by 3621

**Abstract** Due to its great medical and pharmaceutical importance, honey bee venom is considered to be well characterized both chemically and in terms of biomedical activity. However, this study shows that our knowledge of the composition and antimicrobial properties of *Apis mellifera* venom is **[...] Read more.**

(This article belongs to the Special Issue **Bioactive Compounds from Natural Sources III ( /journal/molecules/special_issues/811KP6LQI6 )**)

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Open Access Article 15 pages, 10086 KiB (/1420-3049/28/10/4134/pdf?version=1684324392)

**In Situ Filling of the Oxygen Vacancies with Dual Heteroatoms in $Co_3O_4$ for Efficient Overall Water Splitting (/1420-3049/28/10/4134)**

by **Wei Duan**, **Shixing Han**, **Zhonghai Fang**, **Zhaohui Xiao** and **Shiwei Lin**

*Molecules* **2023**, *28*(10), 4134; **https://doi.org/10.3390/molecules28104134 (https://doi.org/10.3390/molecules28104134)** - 16 May 2023

**Cited by 14 (/1420-3049/28/10/4134#metrics)** | Viewed by 2563

**Abstract** Electrocatalytic water splitting is a crucial area in sustainable energy development, and the development of highly efficient bifunctional catalysts that exhibit activity toward both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) is of paramount importance. $Co_3O_4$ is a **[...] Read more.**

(This article belongs to the Collection **Green Energy and Environmental Materials ( /journal/molecules/topical_collections/5020AHCL0X )**)

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Open Access Article 14 pages, 1705 KiB (/1420-3049/28/10/4133/pdf?version=1684989152)

**Wheat Oxylipins in Response to Aphids, $CO_2$ and Nitrogen Regimes (/1420-3049/28/10/4133)**

by **Mari Merce Cascant-Vilaplana**, **Eduardo Viteritti**, **Víctor Sadras**, **Sonia Medina**, **María Puerto Sánchez-Iglesias**, **Camille Oger**, **Jean-Marie Galano**, **Thierry Durand**, **José Antonio Gabaldón**, **Julian Taylor**, **Federico Ferreres**, **Manuel Sergi** and **Angel Gil-Izquierdo**
*Molecules* **2023**, *28*(10), 4133; **https://doi.org/10.3390/molecules28104133 (https://doi.org/10.3390/molecules28104133)** - 16 May 2023
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**Abstract** Wheat is critical for food security, and is challenged by biotic stresses, chiefly aphids and the viruses they transmit. The objective of this study was to determine whether aphids feeding on wheat could trigger a defensive plant reaction to oxidative stress that involved **[...] Read more.**
(This article belongs to the Special Issue **Molecules in 2023 ( /journal/molecules/special_issues/49X1JIB4SS )**)

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Open Access Article 19 pages, 1898 KiB (/1420-3049/28/10/4132/pdf?version=1684334288)

**Synthesis, Structure and Biological Activity of Indole–Imidazole Complexes with $ZnCl_2$: Can Coordination Enhance the Functionality of Bioactive Ligands? (/1420-3049/28/10/4132)**

by **Karolina Babijczuk**, **Beata Warżajtis**, **Justyna Starzyk**, **Lucyna Mrówczyńska**, **Beata Jasiewicz** and **Urszula Rychlewska**
*Molecules* **2023**, *28*(10), 4132; **https://doi.org/10.3390/molecules28104132 (https://doi.org/10.3390/molecules28104132)** - 16 May 2023
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**Abstract** The ability of the indole–imidazole hybrid ligands to coordinate with the Zn(II) ion and the resulting structures of this new class of coordination compounds were analyzed in order to determine their structural properties and biological functionalities. For this purpose, six novel Zn(II) complexes, **[...] Read more.**
(This article belongs to the Special Issue **Applications of Metal Complexes ( /journal/molecules/special_issues/application_metal_complexes )**)

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Open Access Article 15 pages, 5524 KiB (/1420-3049/28/10/4131/pdf?version=1684286307)

**The Study of Alanine Transaminase Activity in Tissues of Silkworm (*Bombyx mori*) via Direct Analysis in Real-Time (DART) Mass Spectrometry (/1420-3049/28/10/4131)**

by **Guohua Wu**, **Lei Jiang**, **Jianjun Guo**, **Wushuang Li**, **Lin Ma**, **Bozhi Tang** and **Charles C. Liu**
*Molecules* **2023**, *28*(10), 4131; **https://doi.org/10.3390/molecules28104131 (https://doi.org/10.3390/molecules28104131)** - 16 May 2023
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**Abstract** Alanine transaminase (ALT) is an important amino acid-metabolizing enzyme in silkworm *Bombyx mori* L., and is mainly involved in transferring glutamate to alanine (serving as an essential precursor in silk protein synthesis) through transamination. Therefore, it is generally believed that silk protein synthesis **[...] Read more.**
(This article belongs to the Section **Analytical Chemistry (/journal/molecules/sections/Analytical_Chemistry)**)

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Open Access Review 24 pages, 772 KiB (/1420-3049/28/10/4130/pdf?version=1684244985)

**Could Selenium Supplementation Prevent COVID-19? A Comprehensive Review of Available Studies (/1420-3049/28/10/4130)**

by **Roberto Ambra**, **Sahara Melloni** and **Eugenia Venneria**

*Molecules* **2023**, *28*(10), 4130; **https://doi.org/10.3390/molecules28104130 (https://doi.org/10.3390/molecules28104130)** - 16 May 2023

**Cited by 6 (/1420-3049/28/10/4130#metrics)** | Viewed by 3645

**Abstract** The purpose of this review is to systematically examine the scientific evidence investigating selenium's relationship with COVID-19, aiming to support, or refute, the growing hypothesis that supplementation could prevent COVID-19 etiopathogenesis. In fact, immediately after the beginning of the COVID-19 pandemic, several speculative **[...] Read more.**

(This article belongs to the Special Issue **Functional Foods and Dietary Bioactives in Human Health ( /journal/molecules/special_issues/96HQAG4JV5 )**)

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Open Access Article 21 pages, 7193 KiB (/1420-3049/28/10/4129/pdf?version=1684292921)

**Adsorption of Brilliant Green Dye onto a Mercerized Biosorbent: Kinetic, Thermodynamic, and Molecular Docking Studies (/1420-3049/28/10/4129)**

by **Andra-Cristina Enache**, **Corneliu Cojocaru**, **Petrisor Samoila**, **Victor Ciornea**, **Roxana Apolzan**, **Georgeta Predeanu** and **Valeria Harabagiu**

*Molecules* **2023**, *28*(10), 4129; **https://doi.org/10.3390/molecules28104129 (https://doi.org/10.3390/molecules28104129)** - 16 May 2023

**Cited by 21 (/1420-3049/28/10/4129#metrics)** | Viewed by 3288

**Abstract** This study reports the valorization of pistachio shell agricultural waste, aiming to develop an eco-friendly and cost-effective biosorbent for cationic brilliant green (BG) dye adsorption from aqueous media. Pistachio shells were mercerized in an alkaline environment, resulting in the treated adsorbent ($PS_{NaOH}$ **[...] Read more.**

(This article belongs to the Special Issue **Exclusive Feature Papers in Physical Chemistry ( /journal/molecules/special_issues/FP_physchem )**)

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Open Access Article 16 pages, 19371 KiB (/1420-3049/28/10/4128/pdf?version=1684302048)

**The In Situ Preparation of Ni–Zn Ferrite Intercalated Expanded Graphite via Thermal Treatment for Improved Radar Attenuation Property (/1420-3049/28/10/4128)**

by **Ning Xiang**, **Zunning Zhou**, **Xiaoxia Ma**, **Huichao Zhang**, **Xiangyuan Xu**, **Yongpeng Chen** and **Zerong Guo**

*Molecules* **2023**, *28*(10), 4128; **https://doi.org/10.3390/molecules28104128 (https://doi.org/10.3390/molecules28104128)** - 16 May 2023

**Cited by 4 (/1420-3049/28/10/4128#metrics)** | Viewed by 1698

**Abstract** The composites of expanded graphite (EG) and magnetic particles have good electromagnetic wave attenuation properties in the centimeter band, which is valuable in the field of radar wave interference. In this paper, a novel preparation method of Ni–Zn ferrite intercalated EG (NZF/EG) is **[...] Read more.**

(This article belongs to the Special Issue **Functional Hybrid Materials: Design, Synthesis, and Applications ( /journal/molecules/special_issues/functional_hybridmaterials )**)

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Open Access Article 16 pages, 2327 KiB (/1420-3049/28/10/4127/pdf?version=1684375100)

**Ultrasound-Assisted Fermentation to Remove Cadmium from Rice and Its Application (/1420-3049/28/10/4127)**

by **Xiaotong Yang**, **Jie Yin**, **Yahui Guo**, **Hang Yu**, **Shaofeng Yuan**, **He Qian**, **Weirong Yao** and **Jiangfeng Song**
*Molecules* **2023**, *28*(10), 4127; **https://doi.org/10.3390/molecules28104127 (https://doi.org/10.3390/molecules28104127)** - 16 May 2023
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**Abstract** Rice, which is a major part of the daily diet, is becoming more and more contaminated by cadmium (Cd). This study combined low-intensity ultrasonic waves with the *Lactobacillus plantarum* fermentation method and optimized this technique by a single-factor and response surface experiment, aiming **[...] Read more.**

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Open Access Communication 10 pages, 1541 KiB (/1420-3049/28/10/4126/pdf?version=1684289818)

**Ultrahigh Carrier Mobility in Two-Dimensional IV–VI Semiconductors for Photocatalytic Water Splitting (/1420-3049/28/10/4126)**

by **Zhaoming Huang**, **Kai Ren**, **Ruxin Zheng**, **Liangmo Wang** and **Li Wang**
*Molecules* **2023**, *28*(10), 4126; **https://doi.org/10.3390/molecules28104126 (https://doi.org/10.3390/molecules28104126)** - 16 May 2023
**Cited by 6 (/1420-3049/28/10/4126#metrics)** | Viewed by 1852

**Abstract** Two-dimensional materials have been developed as novel photovoltaic and photocatalytic devices because of their excellent properties. In this work, four δ-IV–VI monolayers, GeS, GeSe, SiS and SiSe, are investigated as semiconductors with desirable bandgaps using the first-principles method. These δ-IV–VI monolayers exhibit exceptional **[...] Read more.**
(This article belongs to the Special Issue **Functional Photocatalysts: Material Design, Synthesis and Applications ( /journal/molecules/special_issues/G1ORMYGKA1 )**)

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Open Access Editorial 5 pages, 218 KiB (/1420-3049/28/10/4125/pdf?version=1684240479)

**Contribution of Enzyme Catalysis to the Achievement of the United Nations' Sustainable Development Goals (/1420-3049/28/10/4125)**

by **Dirk Holtmann**, **Frank Hollmann** and **Britte Bouchaut**
*Molecules* **2023**, *28*(10), 4125; **https://doi.org/10.3390/molecules28104125 (https://doi.org/10.3390/molecules28104125)** - 16 May 2023
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**Abstract** In September 2015, the United Nations General Assembly established the 2030 Agenda for Sustainable Development, which includes 17

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Sustainable Development Goals (SDGs) [...] **Full article (/1420-3049/28/10/4125)**
(This article belongs to the Special Issue **Contribution of Enzyme Catalysis to the Achievement of the UN Sustainable Development Goals ( /journal/molecules/special_issues/Enzyme_Catalysis_SDGs )**)

Open Access Article 11 pages, 2285 KiB **(/1420-3049/28/10/4124/pdf?version=1684242593)**

**Highly Flexible Poly(1,12-dodecylene 5,5′-isopropylidene-bis(ethyl 2-furoate)): A Promising Biobased Polyester Derived from a Renewable Cost-Effective Bisfuranic Precursor and a Long-Chain Aliphatic Spacer (/1420-3049/28/10/4124)**

by **Sami Zaidi**, **Abdelkader Bougarech**, **Majdi Abid**, **Souhir Abid**, **Armando J. D. Silvestre** and **Andreia F. Sousa**
*Molecules* **2023**, *28*(10), 4124; **https://doi.org/10.3390/molecules28104124 (https://doi.org/10.3390/molecules28104124)** - 16 May 2023
**Cited by 4 (/1420-3049/28/10/4124#metrics)** | Viewed by 1870

**Abstract** The continuous search for novel biobased polymers with high-performance properties has highlighted the role of monofuranic-based polyesters as some of the most promising for future plastic industry but has neglected the huge potential for the polymers' innovation, relatively low cost, and synthesis easiness **[...] Read more.**
(This article belongs to the Special Issue **Synthesis, Properties and Applications of Biobased Polymers ( /journal/molecules/special_issues/Biobased_Polymers_Synthesis )**)

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Open Access Article 28 pages, 7856 KiB **(/1420-3049/28/10/4123/pdf?version=1684233207)**

**Identification of Some Glutamic Acid Derivatives with Biological Potential by Computational Methods (/1420-3049/28/10/4123)**

by **Octavia-Laura Moldovan**, **Alexandra Sandulea**, **Ioana-Andreea Lungu**, **Șerban Andrei Gâz** and **Aura Rusu**
*Molecules* **2023**, *28*(10), 4123; **https://doi.org/10.3390/molecules28104123 (https://doi.org/10.3390/molecules28104123)** - 16 May 2023
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**Abstract** Glutamic acid is a non-essential amino acid involved in multiple metabolic pathways. Of high importance is its relationship with glutamine, an essential fuel for cancer cell development. Compounds that can modify glutamine or glutamic acid behaviour in cancer cells have resulted in attractive **[...] Read more.**
(This article belongs to the Special Issue **Computational Drug Discovery: Methods and Applications ( /journal/molecules/special_issues/3Q6OV9M879 )**)

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Open Access Review 30 pages, 6500 KiB **(/1420-3049/28/10/4122/pdf?version=1684230943)**

**Nanoparticle-Based Radioconjugates for Targeted Imaging and Therapy of Prostate Cancer (/1420-3049/28/10/4122)**

by **Anna Lankoff**, **Malwina Czerwińska** and **Marcin Kruszewski**
*Molecules* **2023**, *28*(10), 4122; **https://doi.org/10.3390/molecules28104122 (https://doi.org/10.3390/molecules28104122)** - 16 May 2023
**Cited by 4 (/1420-3049/28/10/4122#metrics)** | Viewed by 3005

**Abstract** Prostate cancer is the second most frequent malignancy in men worldwide and the fifth leading cause of death by cancer. Although most patients initially benefit from therapy, many of them will progress to metastatic castration-resistant prostate cancer, which still remains incurable. The significant **[...] Read more.**
(This article belongs to the Special Issue **Targeted Radionuclide Diagnosis and Therapy of Prostate Cancer—From Basic Research to Clinical Perspectives ( /journal/molecules/special_issues/Radionuclide_Diagnosis )**)

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Open Access Article 17 pages, 2402 KiB (/1420-3049/28/10/4121/pdf?version=1684230587)

**Optimization of Phytochemical-Rich *Citrus maxima* Albedo Extract Using Response Surface Methodology (/1420-3049/28/10/4121)**

by **Woorawee Inthachat**, **Piya Temviriyanukul**, **Nattira On-Nom**, **Panyaporn Kanoongon**, **Sirinapa Thangsiri**, **Chaowanee Chupeerach** and **Uthaiwan Suttisansanee**

*Molecules* **2023**, *28*(10), 4121; **https://doi.org/10.3390/molecules28104121 (https://doi.org/10.3390/molecules28104121)** - 16 May 2023

**Cited by 9 (/1420-3049/28/10/4121#metrics)** | Viewed by 3200

**Abstract** In the present study, response surface methodology (RSM) and Box–Behnken design (BBD) were employed to optimize the conditions for the extraction of *C. maxima* albedo from agricultural waste, to obtain notable phytochemicals. Ethanol concentration, extraction temperature, and extraction time were included as key **[...] Read more.**

(This article belongs to the Special Issue **Sustainable Bioactive and Functional Molecules from Agri-Food Waste: A Tour to Applications ( /journal/molecules/special_issues/Bioactive_Agrifood )**)

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Open Access Article 17 pages, 9255 KiB (/1420-3049/28/10/4120/pdf?version=1684231582)

**Influence of a Composite Polylysine-Polydopamine-Quaternary Ammonium Salt Coating on Titanium on Its Ostogenic and Antibacterial Performance (/1420-3049/28/10/4120)**

by **Lei Xing**, **Hongyang Song**, **Jinjian Wei**, **Xue Wang**, **Yaozhen Yang**, **Pengbo Zhe**, **Mingming Luan** and **Jing Xu**

*Molecules* **2023**, *28*(10), 4120; **https://doi.org/10.3390/molecules28104120 (https://doi.org/10.3390/molecules28104120)** - 16 May 2023

**Cited by 3 (/1420-3049/28/10/4120#metrics)** | Viewed by 1995

**Abstract** Thin oxide layers form easily on the surfaces of titanium (Ti) components, with thicknesses of <100 nm. These layers have excellent corrosion resistance and good biocompatibility. Ti is susceptible to bacterial development on its surface when used as an implant material, which reduces **[...] Read more.**

(This article belongs to the Special Issue **Design of Molecularly Interfaced Nanostructures for Biological, Environmental and Food Applications ( /journal/molecules/special_issues/molecularly_nanostructures )**)

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Open Access Article 13 pages, 1070 KiB (/1420-3049/28/10/4119/pdf?version=1684230383)

**Effect of Instant Controlled Pressure Drop (DIC) on Polyphenols, Flavonoids and Antioxidant Capacity of Green Lentils (*Lens culinaris*) (/1420-3049/28/10/4119)**

by **Mario Adrian Tienda-Vazquez**, **Rocío Daniela Soto-Castro**, **Oscar Carrasco-Morales**, **Carmen Téllez-Pérez**, **Roberto Parra-Saldívar**, **Maritza Alonzo-Macías** and **Anaberta Cardador-Martínez**

*Molecules* **2023**, *28*(10), 4119; **https://doi.org/10.3390/molecules28104119 (https://doi.org/10.3390/molecules28104119)** - 16 May 2023

**Cited by 1 (/1420-3049/28/10/4119#metrics)** | Viewed by 2042

**Abstract** Instant controlled pressure drop (DIC) is one of the emerging technologies in food processing; it can be used for drying, freezing and the extraction of bioactive molecules without damaging their properties. Legumes, such as lentils, are one of the most consumed foods in **[...] Read more.**

(This article belongs to the Special Issue **Bioactive Substances from Food ( /journal/molecules/special_issues/31362V7N21 )**)

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Open Access Article 17 pages, 4165 KiB (/1420-3049/28/10/4118/pdf?version=1684229828)

**Metallacarborane Synthons for Molecular Construction—Oligofunctionalization of Cobalt Bis(1,2-dicarbollide) on Boron and Carbon Atoms with Extendable Ligands (/1420-3049/28/10/4118)**

by **Krzysztof Śmiałkowski**, **Carla Sardo** and **Zbigniew J. Leśnikowski**

*Molecules* **2023**, *28*(10), 4118; **https://doi.org/10.3390/molecules28104118 (https://doi.org/10.3390/molecules28104118)** - 16 May 2023

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**Abstract** The exploitation of metallacarboranes' potential in various fields of research and practical applications requires the availability of convenient and versatile methods for their functionalization with various functional moieties and/or linkers of different types and lengths. Herein, we report a study on cobalt bis(1,2-dicarbollide) **[...] Read more.**

(This article belongs to the Special Issue **New Developments in Boron Chemistry: From Oxidoborates to Hydrido(hetero)borane Derivatives – in Celebration of Professor John D. Kennedy's 80th Birthday ( /journal/molecules/special_issues/040620O9G4 )**)

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Open Access Article 17 pages, 5358 KiB (/1420-3049/28/10/4117/pdf?version=1684230192)

**Salvianolic Acid B Inhibits Ferroptosis and Apoptosis during Myocardial Ischemia/Reperfusion Injury via Decreasing the Ubiquitin-Proteasome Degradation of GPX4 and the ROS-JNK/MAPK Pathways (/1420-3049/28/10/4117)**

by **Xiaojin Xu**, **Chenhan Mao**, **Chengbo Zhang**, **Meng Zhang**, **Jianbin Gong** and **Xindong Wang**

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*Molecules* **2023**, *28*(10), 4117; **https://doi.org/10.3390/molecules28104117 (https://doi.org/10.3390/molecules28104117)** - 16 May 2023
**Cited by 22 (/1420-3049/28/10/4117#metrics)** | Viewed by 2994

**Abstract** Myocardial ischemia/reperfusion injury (MIRI) is related to ferroptosis and apoptosis elicited by reactive oxygen species (ROS). In this research, we investigated the protective effect of salvianolic acid B (SAB) as a natural antioxidant on ferroptosis and apoptosis in the MIRI process, and discussed **[...] Read more.**
(This article belongs to the Topic **Antioxidant Activity of Natural Products (/topics/Antioxidant_Activity_of_Natural_Products)**)

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Open Access Article 20 pages, 6622 KiB **(/1420-3049/28/10/4116/pdf?version=1684220873)**

**Determination of Phosphodiesterase Type-5 Inhibitors (PDE-5) in Dietary Supplements (/1420-3049/28/10/4116)**

by **Oana Ramona Cătălina Gheorghiu**, **Anne Marie Ciobanu**, **Claudia Maria Guțu**, **Carmen Lidia Chițescu**, **Giorgiana Valentina Costea**, **Daniela Mădălina Anghel**, **Ana Maria Vlasceanu** and **Daniela Luiza Baconi**
*Molecules* **2023**, *28*(10), 4116; **https://doi.org/10.3390/molecules28104116 (https://doi.org/10.3390/molecules28104116)** - 16 May 2023
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**Abstract** This study proposed a high-performance thin-layer chromatography (HPTLC) screening method to detect phosphodiesterase 5 (PDE-5) inhibitors as possible adulterant agents in various dietary supplements. Chromatographic analysis was performed on silica gel 60F254 plates using a mixture of ethyl acetate:toluene:methanol:ammonia in a volume ratio **[...] Read more.**
(This article belongs to the Special Issue **Forensic Analysis in Chemistry ( /journal/molecules/special_issues/8JY39P9672 )**)

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Open Access Article 12 pages, 5504 KiB **(/1420-3049/28/10/4115/pdf?version=1684220029)**

**Phosphates Induced H-Type or J-Type Aggregation of Cationic Porphyrins with Varied Side Chains (/1420-3049/28/10/4115)**

by **Zhiliang Li**, **Charles J. Zeman IV**, **Silvano Valandro**, **Jose Paolo O. Bantang** and **Kirk S. Schanze**
*Molecules* **2023**, *28*(10), 4115; **https://doi.org/10.3390/molecules28104115 (https://doi.org/10.3390/molecules28104115)** - 16 May 2023
**Cited by 4 (/1420-3049/28/10/4115#metrics)** | Viewed by 2530

**Abstract** Non-covalent interactions have been extensively used to fabricate nanoscale architectures in supramolecular chemistry. However, the biomimetic self-assembly of diverse nanostructures in aqueous solution with reversibility induced by different important biomolecules remains a challenge. Here, we report the synthesis and aqueous self-assembly of two **[...] Read more.**
(This article belongs to the Special Issue **Chemical Insights in Photofunctional Organic Compounds—a Themed Issue Dedicated to Professor Vaidhyanathan Ramamurthy ( /journal/molecules/special_issues/33LL88487B )**)

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Open Access Article 11 pages, 4644 KiB (/1420-3049/28/10/4114/pdf?version=1684214131)

**Application of Alkali Lignin and Spruce Sawdust for the Effective Removal of Reactive Dyes from Model Wastewater (/1420-3049/28/10/4114)**

by **Kateřina Hájková**, **Michaela Filipi**, **Roman Fojtík** and **Ali Dorieh**

*Molecules* **2023**, *28*(10), 4114; **https://doi.org/10.3390/molecules28104114 (https://doi.org/10.3390/molecules28104114)** - 16 May 2023

**Cited by 2 (/1420-3049/28/10/4114#metrics)** | Viewed by 2000

**Abstract** Today, the emphasis is on environmentally friendly materials. Alkali lignin and spruce sawdust are suitable natural alternatives for removing dyes from wastewater. The main reason for using alkaline lignin as a sorbent is the recovery of waste black liquor from the paper industry. **[...] Read more.**

(This article belongs to the Special Issue **Sustainable Development and Application of Renewable Chemicals from Biomass and Waste II ( /journal/molecules/special_issues/KW126S22XJ )**)

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Open Access Article 14 pages, 2969 KiB (/1420-3049/28/10/4113/pdf?version=1684215003)

**Molecular Design of Luminescent Complexes of Eu(III): What Can We Learn from the Ligands (/1420-3049/28/10/4113)**

by **Julia Romanova**, **Rumen Lyapchev**, **Mihail Kolarski**, **Martin Tsvetkov**, **Denitsa Elenkova**, **Bernd Morgenstern** and **Joana Zaharieva**

*Molecules* **2023**, *28*(10), 4113; **https://doi.org/10.3390/molecules28104113 (https://doi.org/10.3390/molecules28104113)** - 16 May 2023

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**Abstract** The luminescent metal-organic complexes of rare earth metals are advanced materials with wide application potential in chemistry, biology, and medicine. The luminescence of these materials is due to a rare photophysical phenomenon called antenna effect, in which the excited ligand transmits its energy **[...] Read more.**

(This article belongs to the Section **Organometallic Chemistry (/journal/molecules/sections/organometallic_chemistry)**)

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Open Access Article 15 pages, 3473 KiB (/1420-3049/28/10/4112/pdf?version=1684214340)

**Novel Biotinylated Cu(II)-Phenanthroline Complexes: 2D and 3D Cytotoxic Activity and Mechanistic Insight (/1420-3049/28/10/4112)**

by **Stephen Barrett**, **Michele De Franco**, **Chiara Donati**, **Cristina Marzano**, **Valentina Gandin** and **Diego Montagner**

*Molecules* **2023**, *28*(10), 4112; **https://doi.org/10.3390/molecules28104112 (https://doi.org/10.3390/molecules28104112)** - 16 May 2023

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**Abstract** The interest in the use of copper as a metal scaffold for the development of novel chemotherapeutics has considerably grown in recent years. This is mainly due to the relatively lower toxicity of copper complexes with respect to platinum drugs (i.e., cisplatin), the **[...] Read more.**

(This article belongs to the Special Issue **Metal-Based Drugs: Past, Present and Future ( /journal/molecules/special_issues/MB_Drugs )**)

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Open Access Article 13 pages, 2987 KiB (/1420-3049/28/10/4111/pdf?version=1684210769)

## Exploration of the Transglycosylation Activity of Barley Limit Dextrinase for Production of Novel Glycoconjugates (/1420-3049/28/10/4111)

by **Malene Bech Vester-Christensen**, **Jesper Holck**, **Martin Rejzek**, **Léa Perrin**, **Morten Tovborg**, **Birte Svensson**, **Robert A. Field** and **Marie Sofie Møller**

*Molecules* **2023**, *28*(10), 4111; **https://doi.org/10.3390/molecules28104111 (https://doi.org/10.3390/molecules28104111)** - 16 May 2023

**Cited by 3 (/1420-3049/28/10/4111#metrics)** | Viewed by 2204

**Abstract** A few α-glucan debranching enzymes (DBEs) of the large glycoside hydrolase family 13 (GH13), also known as the α-amylase family, have been shown to catalyze transglycosylation as well as hydrolysis. However, little is known about their acceptor and donor preferences. Here, a DBE **[...] Read more.**

(This article belongs to the Special Issue **Advances in Amylases ( /journal/molecules/special_issues/G7C8D1F97U )**)

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Open Access Article 19 pages, 3899 KiB (/1420-3049/28/10/4110/pdf?version=1684204570)

## Reduced Chitosan as a Strategy for Removing Copper Ions from Water (/1420-3049/28/10/4110)

by **Pedro M. C. Matias**, **Joana F. M. Sousa**, **Eva F. Bernardino**, **João P. Vareda**, **Luisa Durães**, **Paulo E. Abreu**, **Jorge M. C. Marques**, **Dina Murtinho** and **Artur J. M. Valente**

*Molecules* **2023**, *28*(10), 4110; **https://doi.org/10.3390/molecules28104110 (https://doi.org/10.3390/molecules28104110)** - 16 May 2023

**Cited by 12 (/1420-3049/28/10/4110#metrics)** | Viewed by 2253

**Abstract** Toxic heavy metals are priority pollutants in wastewater, commonly present in dangerous concentrations in many places across the globe. Although in trace quantities copper is a heavy metal essential to human life, in excess it causes various diseases, whereby its removal from wastewater **[...] Read more.**

(This article belongs to the Special Issue **Innovative Adsorbents for Pollutant Removal: An Overview of Current Research ( /journal/molecules/special_issues/Adsorbents_Pollutant_Removal )**)

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Open Access Article 14 pages, 2532 KiB (/1420-3049/28/10/4109/pdf?version=1684161830)

## Nematicidal Coumarins from *Cnidium monnieri* Fruits and *Angelica dahurica* Roots and Their Physiological Effect on Pine Wood Nematode (*Bursaphelenchus xylophilus*) (/1420-3049/28/10/4109)

by **Jiale Feng**, **Chenglei Qin**, **Xiaohong Liu**, **Ronggui Li**, **Chao Wang**, **Chunhan Li**, **Guicai Du** and **Qunqun Guo**

*Molecules* **2023**, *28*(10), 4109; https://doi.org/10.3390/molecules28104109 (https://doi.org/10.3390/molecules28104109) - 15 May 2023



**Abstract** Pine wood nematode (PWN), *Bursaphelenchus xylophilus*, is a major pathogen of pine wilt disease (PWD), which is a devastating disease affecting pine trees. Eco-friendly plant-derived nematicides against PWN have been considered as promising alternatives to control PWD. In this study, the ethyl **[...] Read more.**

(This article belongs to the Section **Natural Products Chemistry (/journal/molecules/sections/natural_products_chemistry)**)

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Open Access Article 17 pages, 4006 KiB (/1420-3049/28/10/4108/pdf?version=1684222580)

## Binding and Dynamics Demonstrate the Destabilization of Ligand Binding for the S688Y Mutation in the NMDA Receptor GluN1 Subunit (/1420-3049/28/10/4108)

by **Jake Zheng Chen**, **William Bret Church**, **Karine Bastard**, **Anthony P. Duff** and **Thomas Balle**

*Molecules* **2023**, *28*(10), 4108; https://doi.org/10.3390/molecules28104108 (https://doi.org/10.3390/molecules28104108) - 15 May 2023



**Abstract** Encephalopathies are brain dysfunctions that lead to cognitive, sensory, and motor development impairments. Recently, the identification of several mutations within the *N*-methyl-D-aspartate receptor (NMDAR) have been identified as significant in the etiology of this group of conditions. However, a complete understanding of **[...] Read more.**

(This article belongs to the Special Issue **Role of Computer Aided Drug Design in Drug Development ( /journal/molecules/special_issues/Computer_Aided_Drug_Development_medicinal_emistry )**)

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Open Access Article 16 pages, 4674 KiB (/1420-3049/28/10/4107/pdf?version=1684161465)

## Chitosan, Chitosan/IgG-Loaded, and N-Trimethyl Chitosan Chloride Nanoparticles as Potential Adjuvant and Carrier-Delivery Systems (/1420-3049/28/10/4107)

by **Aldo Y. Tenorio-Barajas**, **María de la L. Olvera**, **Gabriel Romero-Paredes**, **Victor Altuzar**, **Efraín Garrido-Guerrero** and **Claudia Mendoza-Barrera**

*Molecules* **2023**, *28*(10), 4107; https://doi.org/10.3390/molecules28104107 (https://doi.org/10.3390/molecules28104107) - 15 May 2023



**Abstract** This work proposes a feasible, reproducible, and low-cost modified method to manufacture chitosan, chitosan/IgG-protein-loaded, and trimethylated chitosan nanoparticles, using microfluidics combined with the microemulsion technique, which differs from the traditional batch process of chitosan-based nanoparticles. The synthesis process consists of generating microreactors of **[...] Read more.**

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Open Access Communication 10 pages, 2409 KiB (/1420-3049/28/10/4106/pdf?version=1684161352)

**Ameliorating Phosphonic-Based Nonflammable Electrolytes Towards Safe and Stable Lithium Metal Batteries (/1420-3049/28/10/4106)**

by **Sha Fu**, **Xuanzhi Xie**, **Xiaoyi Huangyang**, **Longxi Yang**, **Xianxiang Zeng**, **Qiang Ma**, **Xiongwei Wu**, **Mingtao Xiao** and **Yuping Wu**
*Molecules* **2023**, *28*(10), 4106; **https://doi.org/10.3390/molecules28104106 (https://doi.org/10.3390/molecules28104106)** - 15 May 2023
**Cited by 2 (/1420-3049/28/10/4106#metrics)** | Viewed by 2030

**Abstract** High-energy-density lithium metal batteries with high safety and stability are urgently needed. Designing the novel nonflammable electrolytes possessing superior interface compatibility and stability is critical to achieve the stable cycling of battery. Herein, the functional additive dimethyl allyl-phosphate and fluoroethylene carbonate were introduced **[...] Read more.**

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Open Access Article 16 pages, 7286 KiB (/1420-3049/28/10/4105/pdf?version=1684157938)

**Antibacterial Effect of Shrimp By-Products Hydrolysate on Specific Spoilage Organisms of Squid (/1420-3049/28/10/4105)**

by **Luo Gu**, **Qiuyu Zhu**, **Xiaoyu Zou** and **Ru Song**
*Molecules* **2023**, *28*(10), 4105; **https://doi.org/10.3390/molecules28104105 (https://doi.org/10.3390/molecules28104105)** - 15 May 2023
**Cited by 4 (/1420-3049/28/10/4105#metrics)** | Viewed by 2121

**Abstract** In order to further develop and utilize shrimp processing by-products, in this study, a novel antibacterial hydrolysate of shrimp by-products by pepsin hydrolysis (SPH) was prepared. The antibacterial effect of SPH on specific spoilage organisms of squid after end storage at room temperature **[...] Read more.**
(This article belongs to the Special Issue **Novel Antimicrobial Bioactive Molecules for Sustainable Development and Health Care ( /journal/molecules/special_issues/4O52H9J252 )**)

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Open Access Article 17 pages, 2953 KiB (/1420-3049/28/10/4104/pdf?version=1684157552)

**The Mechanism of Peach Gum Polysaccharide Preventing UVB-Induced Skin Photoaging by Regulating Matrix Metalloproteinanse and Oxidative Factors (/1420-3049/28/10/4104)**

by **Min Yang**, **Liang Tao**, **Zilin Wang**, **Lingfei Li**, **Junyi Luo**, **Kuannu Pai**, **Weitong Li**, **Cunchao Zhao**, **Jun Sheng** and **Yang Tian**
*Molecules* **2023**, *28*(10), 4104; **https://doi.org/10.3390/molecules28104104 (https://doi.org/10.3390/molecules28104104)** - 15 May 2023
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**Abstr** Exposure to ultraviolet light can cause oxidative damage and accelerate skin aging and is one of the main causes of skin aging. Peach gum polysaccharide (PG) is a natural edible plant component that has many biological activities, such as regulating blood glucose and **[...] Read more.**
(This article belongs to the Special Issue **Research and Application of Plant Sourced Polysaccharides ( /journal/molecules/**

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Open Access Article 14 pages, 2076 KiB (/1420-3049/28/10/4103/pdf?version=1684155607)

**Improving Crystallization and Stability of Perovskite Solar Cells Using a Low-Temperature Treated A-Site Cation Solution in the Sequential Deposition (/1420-3049/28/10/4103)**

by **Tinghao Li**, **Qiu Xiong**, **Chongzhu Hu**, **Can Wang**, **Ni Zhang**, **Shui-Yang Lien** and **Peng Gao**

*Molecules* **2023**, *28*(10), 4103; https://doi.org/10.3390/molecules28104103 (https://doi.org/10.3390/molecules28104103) - 15 May 2023

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**Abstract** The two-step sequential deposition is a commonly used method by researchers for fabricating perovskite solar cells (PSCs) due to its reproducibility and tolerant preparation conditions. However, the less-than-favorable diffusive processes in the preparation process often result in subpar crystalline quality in the perovskite **[...] Read more.**

(This article belongs to the Special Issue **Materials for Emerging Electrochemical Devices ( /journal/molecules/special_issues/emerging_electrochemical_devices )**)

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Open Access Article 10 pages, 2046 KiB (/1420-3049/28/10/4102/pdf?version=1684209057)

**Synthesis and Characterization of New-Type Soluble β-Substituted Zinc Phthalocyanine Derivative of Clofoctol (/1420-3049/28/10/4102)**

by **Sabrine Dridi**, **Jamel Eddine Khiari**, **Gabriele Magna**, **Manuela Stefanelli**, **Larisa Lvova**, **Federica Mandoj**, **Khaoula Khezami**, **Mahmut Durmuş**, **Corrado Di Natale** and **Roberto Paolesse**

*Molecules* **2023**, *28*(10), 4102; https://doi.org/10.3390/molecules28104102 (https://doi.org/10.3390/molecules28104102) - 15 May 2023

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**Abstract** In this work, we have described the synthesis and characterization of novel zinc (II) phthalocyanine bearing four 2-(2,4-dichloro-benzyl)-4-(1,1,3,3-tetramethyl-butyl)-phenoxy substituents on the peripheral positions. The compound was characterized by elemental analysis and different spectroscopic techniques, such as FT-IR, $^{1}$H NMR, MALDI-TOF, and UV-Vis. **[...] Read more.**

(This article belongs to the Special Issue **Porphyrin-Based Compounds: Synthesis and Application ( /journal/molecules/special_issues/Porphyrin_Based_Compounds )**)

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Open Access Article 12 pages, 615 KiB (/1420-3049/28/10/4101/pdf?version=1684156205)

**Investigation of Polyphenolic Compounds in Different Varieties of Black Chokeberry *Aronia melanocarpa* (/1420-3049/28/10/4101)**

by **Makar A. Gerasimov**, **Irina B. Perova**, **Konstantin I. Eller**, **Michail Y. Akimov**, **Anna M. Sukhanova**, **Galina M. Rodionova** and **Galina V. Ramenskaya**

*Molecules* **2023**, *28*(10), 4101; https://doi.org/10.3390/molecules28104101 (https://doi.org/10.3390/molecules28104101) - 15 May 2023

Cited by 13 (/1420-3049/28/10/4101#metrics) | Viewed by 2232

**Abstract** The purpose of this work was to study the qualitative and quantitative composition of the main groups of biologically active substances in the fresh fruits of five different varieties of black chokeberry (*Aronia melanocarpa* (Michx.) Elliot), carried out within the framework of **[...] Read more.**

(This article belongs to the Special Issue **Feature Papers in Food Chemistry—2nd Edition ( /journal/molecules/special_issues/4PYC394G23 )**)

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Open Access Article 14 pages, 4694 KiB (/1420-3049/28/10/4100/pdf?version=1684145775)

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**Bioinformatic Analysis of Key Regulatory Genes in Adult Asthma and Prediction of Potential Drug Candidates (/1420-3049/28/10/4100)**

by **Shaojun Chen**, **Jiahao Lv**, **Yiyuan Luo**, **Hongjiang Chen**, **Shuwei Ma** and **Lihua Zhang**

*Molecules* **2023**, *28*(10), 4100; **https://doi.org/10.3390/molecules28104100 (https://doi.org/10.3390/molecules28104100)** - 15 May 2023

**Cited by 6 (/1420-3049/28/10/4100#metrics)** | Viewed by 2235

**Abstract** Asthma is a common chronic disease that is characterized by respiratory symptoms including cough, wheeze, shortness of breath, and chest tightness. The underlying mechanisms of this disease are not fully elucidated, so more research is needed to identify better therapeutic compounds and biomarkers **[...] Read more.**

(This article belongs to the Special Issue **Computational Studies on the Development and Characterization of Pharmaceutical Materials ( /journal/molecules/special_issues/Pharm_materials )**)

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Open Access Article 18 pages, 3743 KiB (/1420-3049/28/10/4099/pdf?version=1684145563)

**Preparation and In Vitro and In Vivo Evaluation of Rectal In Situ Gel of Meloxicam Hydroxypropyl-β-cyclodextrin Inclusion Complex (/1420-3049/28/10/4099)**

by **Xiaomeng Lei**, **Guansheng Zhang**, **Tao Yang**, **Yuhuan Wu**, **Ying Peng**, **Tiantian Wang**, **Dongxun Li**, **Qian Liu**, **Canjian Wang** and **Guosong Zhang**

*Molecules* **2023**, *28*(10), 4099; **https://doi.org/10.3390/molecules28104099 (https://doi.org/10.3390/molecules28104099)** - 15 May 2023

**Cited by 5 (/1420-3049/28/10/4099#metrics)** | Viewed by 2054

**Abstract** Meloxicam (MLX) is one of the most effective NSAIDs, but its poor water solubility and low bioavailability limit its clinical application. In this study, we designed a thermosensitive in situ gel of the hydroxypropyl-β-cyclodextrin inclusion complex (MLX/HP-β-CD-ISG) for rectal delivery to improve bioavailability. **[...] Read more.**

(This article belongs to the Special Issue **Design and Synthesis of Novel Anti-Inflammatory Agents ( /journal/molecules/special_issues/inflammatory_agents_diseases )**)

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**Okara-Enriched Gluten-Free Bread: Nutritional, Antioxidant and Sensory Properties (/1420-3049/28/10/4098)**

by **Mi[illegible]B. Pešić**, **Milica M. Pešić**, **Jelena Bezbradica**, **Anđela B. Stanojević**, **Petra Ivković**, **Danijel D. Milinčić**, **Mirjana Demin**, **Aleksandar Ž. Kostić**, **Biljana Dojčinović** and **Sladjana P. Stanojević**

*Molecules* **2023**, *28*(10), 4098; **https://doi.org/10.3390/molecules28104098 (https://doi.org/10.3390/molecules28104098)** - 15 May 2023

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Abstract The aim of this study was to produce an eco-innovative gluten-free bread with a pleasant taste and a unique formulation that includes the highest quality grains and pseudocereals (buckwheat; rice; and millet); and okara; a by-product of soy milk production. The mixture of [...] Read more.

(This article belongs to the Special Issue Food Processing and Its Impact on Phenolic and Other Bioactive Constituents in Food – Second Edition ( /journal/molecules/special_issues/food_phenol_second_ed ))

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Open Access Review 16 pages, 1969 KiB (/1420-3049/28/10/4097/pdf?version=1684154858)

## Recent Advances of Diketopyrrolopyrrole Derivatives in Cancer Therapy and Imaging Applications (/1420-3049/28/10/4097)

by **Lingyun Wang**, **Bihong Lai**, **Xueguang Ran**, **Hao Tang** and **Derong Cao**

*Molecules* **2023**, *28*(10), 4097; https://doi.org/10.3390/molecules28104097 (https://doi.org/10.3390/molecules28104097) - 15 May 2023

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Abstract Cancer is threatening the survival of human beings all over the world. Phototherapy (including photothermal therapy (PTT) and photodynamic therapy (PDT)) and bioimaging are important tools for imaging–mediated cancer theranostics. Diketopyrrolopyrrole (DPP) dyes have received more attention due to their high thermal and [...] Read more.

(This article belongs to the Special Issue Fluorescent Probes for Imaging and Diagnostics ( /journal/molecules/special_issues/fluorescent_image_diag ))

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Open Access Article 18 pages, 4241 KiB (/1420-3049/28/10/4096/pdf?version=1684145366)

## Characterization of Thymoquinone-Sulfobutylether-β-Cyclodextrin Inclusion Complex for Anticancer Applications (/1420-3049/28/10/4096)

by **Eltayeb E. M. Eid**, **Amer A. Almaiman**, **Salah Abdalrazak Alshehade**, **Wardah Alsalemi**, **Sareh Kamran**, **FakhrEldin O. Suliman** and **Mohammed Abdullah Alshawsh**

*Molecules* **2023**, *28*(10), 4096; https://doi.org/10.3390/molecules28104096 (https://doi.org/10.3390/molecules28104096) - 15 May 2023

Cited by 12 (/1420-3049/28/10/4096#metrics) | Viewed by 3101

Abstract Thymoquinone (TQ) is a quinone derived from the black seed *Nigella sativa* and has been extensively studied in pharmaceutical and nutraceutical research due to its therapeutic potential and pharmacological properties. Although the chemopreventive and potential anticancer effects of TQ have been reported, its [...] Read more.

(This article belongs to the Special Issue Design, Synthesis, and Evaluation of Anticancer Drugs ( /journal/molecules/special_issues/ZWQ3G0J0HH ))

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Open Access Review 33 pages, 4322 KiB (/1420-3049/28/10/4095/pdf?version=1684378462)

**Tropylium Ion, an Intriguing Moiety in Organic Chemistry (/1420-3049/28/10/4095)**

by **Fatima Tuz Zahra**, **Aamer Saeed**, **Khansa Mumtaz** and **Fernando Albericio**

*Molecules* **2023**, *28*(10), 4095; **https://doi.org/10.3390/molecules28104095 (https://doi.org/10.3390/molecules28104095)** - 15 May 2023

**Cited by 7 (/1420-3049/28/10/4095#metrics)** | Viewed by 7257

**Abstract** The tropylium ion is a non-benzenoid aromatic species that works as a catalyst. This chemical entity brings about a large number of organic transformations, such as hydroboration reactions, ring contraction, the trapping of enolates, oxidative functionalization, metathesis, insertion, acetalization, and trans-acetalization reactions. The **[...] Read more.**

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Open Access Review 30 pages, 491 KiB (/1420-3049/28/10/4094/pdf?version=1684237221)

**Ethnobotany, Biological Activities and Phytochemical Compounds of Some Species of the Genus *Eryngium* (Apiaceae), from the Central-Western Region of Mexico (/1420-3049/28/10/4094)**

by **Jeanette G. Cárdenas-Valdovinos**, **Ignacio García-Ruiz**, **María V. Angoa-Pérez** and **Hortencia G. Mena-Violante**

*Molecules* **2023**, *28*(10), 4094; **https://doi.org/10.3390/molecules28104094 (https://doi.org/10.3390/molecules28104094)** - 15 May 2023

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**Abstract** There are approximately 250 species of *Eryngium* L. distributed throughout the world, with North America and South America being centers of diversity on this continent. In the central-western region of Mexico there may be around 28 species of this genus. Some *Eryngium* species **[...] Read more.**

(This article belongs to the Section **Natural Products Chemistry (/journal/molecules/sections/natural_products_chemistry)**)

Open Access Article 15 pages, 10187 KiB (/1420-3049/28/10/4093/pdf?version=1684140932)

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**Preparation of $PO_4^{3-}$-Intercalated Calcium–Aluminum Hydrotalcites via Coprecipitation Method and Its Flame-Retardant Effect on Bamboo Scrimber (/1420-3049/28/10/4093)**

by **Ying Ran**, **Ailian Hu**, **Fei Yang**, **Chungui Du**, **Jiawei Zhu**, **Yuran Shao**, **Yuting Wang** and **Qichao Bao**

*Molecules* **2023**, *28*(10), 4093; **https://doi.org/10.3390/molecules28104093 (https://doi.org/10.3390/molecules28104093)** - 15 May 2023

**Cited by 7 (/1420-3049/28/10/4093#metrics)** | Viewed by 1796

**Abstract** To improve the flame retardancy of bamboo scrimber, flame-retardant CaAl-$PO_4$-LDHs were synthesized via the coprecipitation method using $PO_4^{3-}$ as the anion of an intercalated calcium–aluminum hydrotalcite in this work. The fine CaAl-$PO_4$-LDHs were characterized via X-ray diffraction **[...] Read more.**

(This article belongs to the Special Issue **Flame-Resistant Materials ( /journal/molecules/special_issues/0136A0C4CC )**)

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Open Access Article 16 pages, 4860 KiB **(/1420-3049/28/10/4092/pdf?version=1684220918)**

**Biocytin-Labeling in Whole-Cell Recording: Electrophysiological and Morphological Properties of Pyramidal Neurons in CYLD-Deficient Mice (/1420-3049/28/10/4092)**

by **Shuyi Tan**, **Xiuping Mo**, **Huihui Qin**, **Binbin Dong**, **Jiankui Zhou**, **Cheng Long** and **Li Yang**

*Molecules* **2023**, *28*(10), 4092; **https://doi.org/10.3390/molecules28104092 (https://doi.org/10.3390/molecules28104092)** - 15 May 2023

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**Abstract** Biocytin, a chemical compound that is an amide formed from the vitamin biotin and the amino acid L-lysine, has been used as a histological dye to stain nerve cells. Electrophysiological activity and morphology are two key characteristics of neurons, but revealing both the **[...] Read more.**

(This article belongs to the Special Issue **Functional Proteomics in Cell Biology and Beyond ( /journal/molecules/special_issues/R8NJ105493 )**)

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Open Access Article 12 pages, 5815 KiB **(/1420-3049/28/10/4091/pdf?version=1684132651)**

**Co-Crystallization between Aliphatic Polyesters through Co-Inclusion Complexation with Small Molecule (/1420-3049/28/10/4091)**

by **Jia-Yao Chen**, **Xue-Wen Zhang**, **Tian-Yu Wu** and **Hai-Mu Ye**

*Molecules* **2023**, *28*(10), 4091; **https://doi.org/10.3390/molecules28104091 (https://doi.org/10.3390/molecules28104091)** - 15 May 2023

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**Abstract** Crystalline/crystalline blends of polymer have shown advantages in the preparation of new polymeric materials. However, the regulation of co-crystallization in a blend is still full of challenges due to the preferential self-crystallization driven by thermodynamics. Here, an inclusion complex approach is proposed to **[...] Read more.**

(This article belongs to the Special Issue **Exclusive Feature Papers in Macromolecular Chemistry ( /journal/molecules/special_issues/macro_EFP )**)

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Open Access Review 13 pages, 289 KiB (/1420-3049/28/10/4090/pdf?version=1684205873)

**The Antibiotics Degradation and Its Mechanisms during the Livestock Manure Anaerobic Digestion (/1420-3049/28/10/4090)**

by **Muhammad Zubair**, **Zhaojun Li**, **Rongsheng Zhu**, **Jiancai Wang**, **Xinghua Liu** and **Xiayan Liu**

*Molecules* **2023**, *28*(10), 4090; **https://doi.org/10.3390/molecules28104090 (https://doi.org/10.3390/molecules28104090)** - 15 May 2023

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**Abstract** Antibiotics are administered to livestock at subtherapeutic levels to promote growth, and their degradation in manure is slow. High antibiotic concentrations can inhibit bacterial activity. Livestock excretes antibiotics via feces and urine, leading to their accumulation in manure. This can result in the **[...] Read more.**

(This article belongs to the Section **Natural Products Chemistry (/journal/molecules/sections/natural_products_chemistry)**)

Open Access Article 14 pages, 2964 KiB (/1420-3049/28/10/4089/pdf?version=1684130827)

**Effects of Taraxerol on Oxidative and Inflammatory Mediators in Isoproterenol-Induced Cardiotoxicity in an Animal Model (/1420-3049/28/10/4089)**

by **Alhussain H. Aodah**, **Sushma Devi**, **Faisal K. Alkholifi**, **Hasan S. Yusufoglu**, **Ahmed I. Foudah** and **Aftab Alam**

*Molecules* **2023**, *28*(10), 4089; **https://doi.org/10.3390/molecules28104089 (https://doi.org/10.3390/molecules28104089)** - 15 May 2023

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**Abstract** Myocardial infarction (MI) continues to be an important issue in healthcare systems worldwide, leading to high rates of morbidity and mortality. Despite ongoing efforts towards the development of preventive measures and treatments, addressing the challenges posed by MI remains difficult both in developed **[...] Read more.**

(This article belongs to the Topic **Research in Pharmacological Therapies (/topics/99X64ZT450)**)

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Open Access Article 15 pages, 2541 KiB (/1420-3049/28/10/4088/pdf?version=1684125703)

**Physicochemical Properties, Thermal Stability, and Pyrolysis Behavior of Antioxidative Lignin from Water Chestnut Shell Obtained with Ternary Deep Eutectic Solvents (/1420-3049/28/10/4088)**

by **Feng Li**, **Wenzhi Lv**, **Dena Huang**, **Chenglu Zeng** and **Runping Wang**

*Molecules* **2023**, *28*(10), 4088; **https://doi.org/10.3390/molecules28104088 (https://doi.org/10.3390/molecules28104088)** - 15 May 2023

**Cited by 12 (/1420-3049/28/10/4088#metrics)** | Viewed by 2274

**Abstract** The molecular weight of lignin extracted from lignocellulosic biomass is an important factor in determining its valorization in industrial processes. Herein, this work aims to explore the extraction of high molecular weight and bioactive lignin from water chestnut shells under mild conditions. Five **[...] Read more.**

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Open Access Article 11 pages, 1110 KiB (/1420-3049/28/10/4087/pdf?version=1684061086)

**Synthesis of New Polyheterocyclic Pyrrolo[3,4-*b*]pyridin-5-ones via an Ugi-Zhu/Cascade/Click Strategy (/1420-3049/28/10/4087)**

by **Roberto E. Blanco-Carapia**, **Enrique A. Aguilar-Rangel**, **Mónica A. Rincón-Guevara**, **Alejandro Islas-Jácome** and **Eduardo González-Zamora**

*Molecules* **2023**, *28*(10), 4087; **https://doi.org/10.3390/molecules28104087 (https://doi.org/10.3390/molecules28104087)** - 14 May 2023

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**Abstract** A diversity-oriented synthesis (DOS) of two new polyheterocyclic compounds was performed via an Ugi-Zhu/cascade (*N*-acylation/*aza* Diels-Alder cycloaddition/decarboxylation/dehydration)/click strategy, both step-by-step to optimize all involved experimental stages, and in one pot manner to evaluate the scope and sustainability of this polyheterocyclic-focused **[...] Read more.**

(This article belongs to the Collection **Heterocyclic Compounds ( /journal/molecules/topical_collections/heterocyclic-compounds )**)

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Open Access Article 18 pages, 5178 KiB (/1420-3049/28/10/4086/pdf?version=1684053247)

**Photochemistry and Photophysics of Cholesta-5,7,9(11)-trien-3β-ol in Ethanol (/1420-3049/28/10/4086)**

by **Jack Saltiel**, **Sumesh B. Krishnan**, **Shipra Gupta**, **Anjan Chakraborty**, **Edwin F. Hilinski** and **Xinsong Lin**

*Molecules* **2023**, *28*(10), 4086; **https://doi.org/10.3390/molecules28104086 (https://doi.org/10.3390/molecules28104086)** - 14 May 2023

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**Abstract** Cholesta-5,7,9(11)-trien-3β-ol (9,11-dehydroprovitamin $D_3$, CTL) is used as a fluorescent probe to track the presence and migration of cholesterol in vivo. We recently described the photochemistry and photophysics of CTL in degassed and air-saturated tetrahydrofuran (THF) solution, an aprotic solvent. The zwitterionic **[...] Read more.**

(This article belongs to the Special Issue **Chemical Insights in Photofunctional Organic Compounds—a Themed Issue Dedicated to Professor Vaidhyanathan Ramamurthy ( /journal/molecules/special_issues/33LL88487B )**)

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Open Access Review 20 pages, 2547 KiB (/1420-3049/28/10/4085/pdf?version=1684053039)

**Biological Action of Singlet Molecular Oxygen from the Standpoint of Cell Signaling, Injury and Death (/1420-3049/28/10/4085)**

by **Junichi Fujii**, **Yuya Soma** and **Yumi Matsuda**

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*Molecules* **2023**, *28*(10), 4085; **https://doi.org/10.3390/molecules28104085 (https://doi.org/10.3390/molecules28104085)** - 14 May 2023
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**Abstract** Energy transfer to ground state triplet molecular oxygen results in the generation of singlet molecular oxygen ($^1O_2$), which has potent oxidizing ability. Irradiation of light, notably ultraviolet A, to a photosensitizing molecule results in the generation of $^1O_2$ **[...] Read more.**
(This article belongs to the Section **Medicinal Chemistry (/journal/molecules/sections/medicinal_chemistry)**)

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Open Access Article 14 pages, 1848 KiB **(/1420-3049/28/10/4084/pdf?version=1684050082)**

**Phenolic Acids Rescue Iron-Induced Damage in Murine Pancreatic Cells and Tissues (/1420-3049/28/10/4084)**

by **Tugba Kose**, **Paul A. Sharp** and **Gladys O. Latunde-Dada**
*Molecules* **2023**, *28*(10), 4084; **https://doi.org/10.3390/molecules28104084 (https://doi.org/10.3390/molecules28104084)** - 14 May 2023
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**Abstract** Iron is an essential element involved in a variety of physiological functions. However, excess iron catalyzes the generation of reactive oxygen species (ROS) via the Fenton reaction. Oxidative stress, caused by an increase in intracellular ROS production, can be a contributory factor to **[...] Read more.**
(This article belongs to the Special Issue **New Anticancer Agents Based on Natural Products ( /journal/molecules/special_issues/Natural_Products_Anticancer )**)

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Open Access Article 13 pages, 2889 KiB **(/1420-3049/28/10/4083/pdf?version=1684049764)**

**Flexible and Wearable Strain–Temperature Sensors Based on Chitosan/Ink Sponges (/1420-3049/28/10/4083)**

by **Xiaoying Lin**, **Feng Wu**, **Yunqing He** and **Mingxian Liu**
*Molecules* **2023**, *28*(10), 4083; **https://doi.org/10.3390/molecules28104083 (https://doi.org/10.3390/molecules28104083)** - 14 May 2023
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**Abstract** A simple and economic strategy to construct a chitosan-ink carbon nanoparticle sponge sensor was proposed by freeze-drying of chitosan and Chinese ink mixture solution. The microstructure and physical properties of the composite sponges with different ratios are characterized. The interfacial compatibility of chitosan **[...] Read more.**
(This article belongs to the Special Issue **Chitosan, Chitosan Derivatives and Their Applications ( /journal/molecules/special_issues/chitosan_chemistry )**)

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Open Access Article 12 pages, 3095 KiB **(/1420-3049/28/10/4082/pdf?version=1684312682)**

**Visible Light-Mediated Organoboron-Catalyzed Metal-Free Synthesis of Silanols from Silanes (/1420-3049/28/10/4082)**

by **Jinbo Yang**, **Xiangxue Cao**, **Lanfeng Wei**, **Jianshu Zhang**, **Jinli Zhang**, **Ping Liu**, **Liang Xu** and **Pengfei Li**
*Molecules* **2023**, *28*(10), 4082; **https://doi.org/10.3390/molecules28104082 (https://doi.org/10.3390/molecules28104082)** - 13 May 2023
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**Abstract** Herein, a four-coordinated organoboron compound, aminoquinoline diarylboron (AQDAB), is utilized as the photocatalyst in the oxidation of silane to silanol. This strategy effectively oxidizes Si–H bonds, affording Si–O bonds. Generally, the corresponding silanols can be obtained in moderate to good yields at room **[...] Read more.**

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Open Access Review 20 pages, 5050 KiB **(/1420-3049/28/10/4081/pdf?version=1683972705)**

**The Recycling of Spent Lithium-Ion Batteries: Crucial Flotation for the Separation of Cathode and Anode Materials (/1420-3049/28/10/4081)**

by **Xuesong Ma**, **Peng Ge**, **Lisha Wang**, **Wei Sun**, **Yongjie Bu**, **Miaomiao Sun** and **Yue Yang**

*Molecules* **2023**, *28*(10), 4081; **https://doi.org/10.3390/molecules28104081 (https://doi.org/10.3390/molecules28104081)** - 13 May 2023

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**Abstract** The recycling of spent lithium-ion batteries (LIBs) has attracted great attention, mainly because of its significant impact on resource recycling and environmental protection. Currently, the processes involved in recovering valuable metals from spent LIBs have shown remarkable progress, but little attention has been **[...] Read more.**

(This article belongs to the Special Issue **Lithium-Ion Batteries: Recent Advances and Future Opportunities in Chemistry ( /journal/molecules/special_issues/5MQP9SCKK1 )**)

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**Application of Polyphenols and Flavonoids in Oncological Therapy (/1420-3049/28/10/4080)**

by **Szymon Roszkowski**

*Molecules* **2023**, *28*(10), 4080; **https://doi.org/10.3390/molecules28104080 (https://doi.org/10.3390/molecules28104080)** - 13 May 2023

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**Abstract** The use of naturally derived drugs in anti-cancer therapies has grown exponentially in recent years. Among natural compounds, polyphenols have shown potential therapeutic applications in treatment due to their protective functions in plants, their use as food additives, and their excellent antioxidant properties, **[...] Read more.**

(This article belongs to the Special Issue **Research on Polyphenolic Compounds from Nature Products: Extraction, Analysis and Biological Properties ( /journal/molecules/special_issues/8EAT703NS1 )**)

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Open Access Article 15 pages, 3148 KiB **(/1420-3049/28/10/4079/pdf?version=1683972701)**

**Evaluation of the Biological Properties of an Optimized Extract of *Polygonum cuspidatum* Using Ultrasonic-Assisted Extraction (/1420-3049/28/10/4079)**

by **Gabriela Fletes-Vargas**, **Rogelio Rodríguez-Rodríguez**, **Neith Pacheco**, **Alejandro Pérez-Larios** and **Hugo Espinosa-Andrews**

*Molecules* **2023**, *28*(10), 4079; **https://doi.org/10.3390/molecules28104079 (https://doi.org/10.3390/molecules28104079)** - 13 May 2023

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**Abstract** Phytochemicals are natural compounds found in plants that have potential health benefits such as antioxidants, anti-inflammatory and anti-cancer properties, and immune reinforcement. *Polygonum cuspidatum* Sieb. et Zucc. is a source rich in resveratrol, traditionally consumed as an infusion. In this study, *P. cuspidatum* root **[...] Read more.**

(This article belongs to the Special Issue **Natural Bioactive Compounds and Human Health ( /journal/molecules/special_issues/Natural_Bioactive_Health )**)

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Open Access Review 16 pages, 2806 KiB (/1420-3049/28/10/4078/pdf?version=1683972285)

**Modification and Solubility Enhancement of Rice Protein and Its Application in Food Processing: A Review (/1420-3049/28/10/4078)**

by **Jingjing Yang**, **Dan Meng**, **Zijian Wu**, **Jinyu Chen** and **Lu Xue**

*Molecules* **2023**, *28*(10), 4078; **https://doi.org/10.3390/molecules28104078 (https://doi.org/10.3390/molecules28104078)** - 13 May 2023

**Cited by 15 (/1420-3049/28/10/4078#metrics)** | Viewed by 4293

**Abstract** Rice protein is a high-quality plant-based protein source that is gluten-free, with high biological value and low allergenicity. However, the low solubility of rice protein not only affects its functional properties such as emulsification, gelling, and water-holding capacity but also greatly limits its **[...] Read more.**

(This article belongs to the Special Issue **Study on Physicochemical Properties of Food Protein ( /journal/molecules/special_issues/food_protein_properties )**)

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Open Access Article 16 pages, 2336 KiB (/1420-3049/28/10/4077/pdf?version=1683972046)

**Photoactive Yellow Protein Adsorption at Hydrated Polyethyleneimine and Poly-L-Glutamic Acid Interfaces (/1420-3049/28/10/4077)**

by **Szilvia Krekic**, **Mark Mero**, **Michel Kuhl**, **Kannan Balasubramanian**, **András Dér** and **Zsuzsanna Heiner**

*Molecules* **2023**, *28*(10), 4077; **https://doi.org/10.3390/molecules28104077 (https://doi.org/10.3390/molecules28104077)** - 13 May 2023

**Cited by 2 (/1420-3049/28/10/4077#metrics)** | Viewed by 1728

**Abstract** Chiral and achiral vibrational sum-frequency generation (VSFG) spectroscopy was performed in the 1400–1700 and 2800–3800 $cm^{-1}$ range to study the interfacial structure of photoactive yellow protein (PYP) adsorbed on polyethyleneimine (PEI) and poly-L-glutamic acid (PGA) surfaces. Nanometer-thick polyelectrolyte layers served **[...] Read more.**

(This article belongs to the Topic **Modelling and Characterization of Soft and Supersoft Materials (/topics/KLEA635KH5)**)

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Open Access Article 23 pages, 10953 KiB (/1420-3049/28/10/4076/pdf?version=1683969810)

**Fluoride Adsorption from Aqueous Solution by Modified Zeolite—Kinetic and Isotherm Studies (/1420-3049/28/10/4076)**

by **Thouraya Turki**, **Abdelkader Hamdouni** and **Alexandru Enesca**

*Molecules* **2023**, *28*(10), 4076; **https://doi.org/10.3390/molecules28104076 (https://doi.org/10.3390/molecules28104076)** - 13 May 2023

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**Abstract** Fluorine is a very common element in the Earth's crust and is present in the air, food, and in natural waters. It never meets in the free state in nature due to its high reactivity, and it comes in the form of fluorides. **[...] Read more.**

(This article belongs to the Special Issue **Zeolites and Porous Materials for Catalysis, Energy Transition and Adsorption Processes ( /journal/molecules/special_issues/18DGWEM7OO )**)

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Open Access Article 14 pages, 1818 KiB (/1420-3049/28/10/4075/pdf?version=1683969579)

**Differentiation of Medicinal Plants According to Solvents, Processing, Origin, and Season by Means of Multivariate Analysis of Spectroscopic and Liquid Chromatography Data (/1420-3049/28/10/4075)**

by **Lenka Burdejova**, **Blanka Tobolkova**, **Martin Polovka** and **Jarmila Neugebauerova**

*Molecules* **2023**, *28*(10), 4075; **https://doi.org/10.3390/molecules28104075 (https://doi.org/10.3390/molecules28104075)** - 13 May 2023

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**Abstract** Effects of processing and extraction solvents on antioxidant properties and other characteristics were evaluated for ten medicinal plant species originating from two different localities and two production years. A combination of spectroscopic and liquid chromatography techniques possessed data for multivariate statistics. Water, 50% **[...] Read more.**

(This article belongs to the Special Issue **Application of Spectroscopy and Chemometrics for Authentication of Foods and Drugs (Volume II) (/journal/molecules/special_issues/1F67AC56Q1 )**)

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Open Access Article 19 pages, 2990 KiB (/1420-3049/28/10/4074/pdf?version=1683968168)

**Characterization of Some Stilbenoids Extracted from Two Cultivars of Lambrusco—*Vitis vinifera* Species: An Opportunity to Valorize Pruning Canes for a More Sustainable Viticulture (/1420-3049/28/10/4074)**

by **Veronica D'Eusanio**, **Francesco Genua**, **Andrea Marchetti**, **Lorenzo Morelli** and **Lorenzo Tassi**

*Molecules* **2023**, *28*(10), 4074; **https://doi.org/10.3390/molecules28104074 (https://doi.org/10.3390/molecules28104074)** - 13 May 2023

**Cited by 1 (/1420-3049/28/10/4074#metrics)** | Viewed by 1528

**Abstract** Pruning canes from grape vines are valuable byproducts that contain resveratrol and other health-boosting stilbenoids. This study aimed to assess the effect of roasting temperature on the stilbenoid content of vine canes by comparing two *Vitis vinifera* cultivars, Lambrusco Ancellotta and

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Salamino. Samples **[...] Read more.**
(This article belongs to the Special Issue **Bioactive Compounds in Food Bioscience and Pharmacology ( /journal/molecules/special_issues/bioactive_food_pharmacology )**)

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Open Access Article 20 pages, 4426 KiB **(/1420-3049/28/10/4073/pdf?version=1683968871)**

**The Chemical Space of Marine Antibacterials: Diphenyl Ethers, Benzophenones, Xanthones, and Anthraquinones (/1420-3049/28/10/4073)**

by **José X. Soares**, **Inês Afonso**, **Adaleta Omerbasic**, **Daniela R. P. Loureiro**, **Madalena M. M. Pinto** and **Carlos M. M. Afonso**
*Molecules* **2023**, *28*(10), 4073; **https://doi.org/10.3390/molecules28104073 (https://doi.org/10.3390/molecules28104073)** - 13 May 2023
**Cited by 3 (/1420-3049/28/10/4073#metrics)** | Viewed by 2449

**Abstract** The emergence of multiresistant bacteria and the shortage of antibacterials in the drug pipeline creates the need to search for novel agents. Evolution drives the optimization of the structure of marine natural products to act as antibacterial agents. Polyketides are a vast and **[...] Read more.**
(This article belongs to the Section **Medicinal Chemistry (/journal/molecules/sections/medicinal_chemistry)**)

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Open Access Article 18 pages, 5492 KiB **(/1420-3049/28/10/4072/pdf?version=1683965425)**

**The Synergistic Effect of Triazine and Phosphaphenanthrene Units on the Physico-Chemical Behavior of Polyimides (/1420-3049/28/10/4072)**

by **Irina Butnaru** and **Mariana-Dana Damaceanu**
*Molecules* **2023**, *28*(10), 4072; **https://doi.org/10.3390/molecules28104072 (https://doi.org/10.3390/molecules28104072)** - 13 May 2023
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**Abstract** With the aim to develop polymers with appealing, multifunctional characteristics, a series of polyimides were designed by anchoring 9,10-dihydro-9-oxa-10-phosphaphenanthrene 10-oxide (DOPO) units on the main polymer chains containing 1,3,5-triazine and several flexible moieties, such as ether, hexafluoroisopropylidene, or isopropylidene. A detailed study was **[...] Read more.**
(This article belongs to the Special Issue **Exclusive Feature Papers in Macromolecular Chemistry ( /journal/molecules/special_issues/macro_EFP )**)

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Open Access Article 14 pages, 4247 KiB (/1420-3049/28/10/4071/pdf?version=1683962335)

## Novel Carbonaceous Adsorbents Prepared from Glycerin Waste and Dopamine for Gas Separation (/1420-3049/28/10/4071)

by **Mary Batista**, **Renato Carvalho**, **Moisés L. Pinto** and **João Pires**

*Molecules* **2023**, *28*(10), 4071; https://doi.org/10.3390/molecules28104071 (https://doi.org/10.3390/molecules28104071) - 13 May 2023
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**Abstract** Glycerin, a low-valued waste from biodiesel production, and dopamine were used as precursors for adsorbent materials. The study is centered on the preparation and application of microporous activated carbon as adsorbent materials in the separation of ethane/ethylene and of gases that are natural **[...] Read more.**

(This article belongs to the Collection **Porous Materials ( /journal/molecules/topical_collections/TC_Porous_Materials )**)

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Open Access Article 10 pages, 2370 KiB (/1420-3049/28/10/4070/pdf?version=1683958293)

## Aggregation of Amyloidogenic Peptide Uperin—Molecular Dynamics Simulations (/1420-3049/28/10/4070)

by **Elena Ermakova**, **Olga Makshakova**, **Rauf Kurbanov**, **Ilya Ibraev**, **Yuriy Zuev** and **Igor Sedov**

*Molecules* **2023**, *28*(10), 4070; https://doi.org/10.3390/molecules28104070 (https://doi.org/10.3390/molecules28104070) - 13 May 2023
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**Abstract** Uperin 3.5 is a remarkable natural peptide obtained from the skin of toadlets comprised of 17 amino acids which exhibits both antimicrobial and amyloidogenic properties. Molecular dynamics simulations were performed to study the β-aggregation process of uperin 3.5 as well as two of **[...] Read more.**

(This article belongs to the Special Issue **Protein Folding, towards the Comprehensive Understanding from Various Aspects ( /journal/molecules/special_issues/Protein_Folding_Aspects )**)

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Open Access Feature Paper Article 13 pages, 4281 KiB (/1420-3049/28/10/4069/pdf?version=1684203939)

## Magnetic $CoFe_2O_4$ and $NiFe_2O_4$ Induced Self-Assembled Graphene Nanoribbon Framework with Excellent Properties for Li-Ion Battery (/1420-3049/28/10/4069)

by **Xiyu Zhao**, **Chunyang He**, **Qiujv Bai**, **Xiangwen Miao**, **Cheng Cao** and **Tianli Wu**

*Molecules* **2023**, *28*(10), 4069; https://doi.org/10.3390/molecules28104069 (https://doi.org/10.3390/molecules28104069) - 12 May 2023
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**Abstract** A magnetically induced self-assembled graphene nanoribbons (GNRs) method is reported to synthesize $MFe_2O_4$/GNRs (M = Co,Ni). It is found that $MFe_2O_4$ compounds not only locate on the surface of GNRs but anchor on the interlayers of **[...] Read more.**

(This article belongs to the Special Issue **Nanomaterials for Energy Storage and Conversion ( /journal/molecules/special_issues/36O2867K2Q )**)

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Open Access Review 20 pages, 6871 KiB (/1420-3049/28/10/4068/pdf?version=1683902793)

**Photocatalysis in Water-Soluble Supramolecular Metal Organic Complex (/1420-3049/28/10/4068)**

by **Dongfeng Hong**, **Linlin Shi**, **Xianghui Liu**, **Huiyuan Ya** and **Xin Han**

*Molecules* **2023**, *28*(10), 4068; **https://doi.org/10.3390/molecules28104068 (https://doi.org/10.3390/molecules28104068)** - 12 May 2023

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**Abstract** As an emerging subset of organic complexes, metal complexes have garnered considerable attention owing to their outstanding structures, properties, and applications. In this content, metal-organic cages (MOCs) with defined shapes and sizes provide internal spaces to isolate water for guest molecules, which can **[...] Read more.**

(This article belongs to the Special Issue **Featured Reviews in Applied Chemistry 2.0 ( /journal/molecules/special_issues/5C45W1PE4B )**)

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Open Access Article 13 pages, 3021 KiB (/1420-3049/28/10/4067/pdf?version=1683971001)

**Synthesis of Aminoalkyl Sclareolide Derivatives and Antifungal Activity Studies (/1420-3049/28/10/4067)**

by **Ziyi Li**, **Hua Gao**, **Haibo Mei**, **Guangwei Wu**, **Vadim A. Soloshonok** and **Jianlin Han**

*Molecules* **2023**, *28*(10), 4067; **https://doi.org/10.3390/molecules28104067 (https://doi.org/10.3390/molecules28104067)** - 12 May 2023

**Cited by 3 (/1420-3049/28/10/4067#metrics)** | Viewed by 1895

**Abstract** Sclareolide was developed as an efficient *C*-nucleophilic reagent for an asymmetric Mannich addition reaction with a series of *N*-*tert*-butylsulfinyl aldimines. The Mannich reaction was carried out under mild conditions, affording the corresponding aminoalkyl sclareolide derivatives with up to 98% **[...] Read more.**

(This article belongs to the Special Issue **Natural Product Chemistry in China-2nd Edition ( /journal/molecules/special_issues/Natural_Product_Chemistry_in_China_2nd_Edition )**)

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Open Access Article 18 pages, 4611 KiB (/1420-3049/28/10/4066/pdf?version=1684145864)

**Novel Adsorbent Material from *Plinia cauliflora* for Removal of Cationic Dye from Aqueous Solution (/1420-3049/28/10/4066)**

by **Nat[illegible]Nara Janner**, **Luana Vaz Tholozan**, **Guilherme Kurz Maron**, **Neftali Lenin Villarreal Carreno**, **Alaor Valério Filho** and **Gabri[illegible]lveira da Rosa**

*Molecules* **2023**, *28*(10), 4066; **https://doi.org/10.3390/molecules28104066 (https://doi.org/10.3390/molecules28104066)** - 12 May 2023

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**Abstract** The food industry is responsible for the generation of large amounts of organic residues, which can lead to negative environmental and economic impacts when incorrectly disposed of. The jaboticaba peel is an example of organic waste, widely used in industry due to its **[...] Read more.**

(This article belongs to the Special Issue **Biomass Materials in Materials Chemistry: Preparation and Characterization ( /journal/molecules/special_issues/biomass_materials_preparation_characterization )**)

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Open Access Article 15 pages, 4060 KiB (/1420-3049/28/10/4065/pdf?version=1683901139)

## Synthesis and Application of a New Polymer with Imprinted Ions for the Preconcentration of Uranium in Natural Water Samples and Determination by Digital Imaging (/1420-3049/28/10/4065)

by **Caio S. A. Felix**, **Adriano V. B. Chagas**, **Rafael F. de Jesus**, **Willams T. Barbosa**, **Josiane D. V. Barbosa**, **Sergio L. C. Ferreira** and **Víctor Cerdà**

*Molecules* **2023**, *28*(10), 4065; **https://doi.org/10.3390/molecules28104065 (https://doi.org/10.3390/molecules28104065)** - 12 May 2023

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**Abstract** This work proposes the synthesis of a new polymer with imprinted ions (IIP) for the pre-concentration of uranium in natural waters using digital imaging as a detection technique. The polymer was synthesized using 2-(5-bromo-2-pyridylazo)-5-diethylaminophenol (Br-PADAP) for complex formation, ethylene glycol dimethacrylate (EGDMA) as **[...] Read more.**

(This article belongs to the Special Issue **Advanced Analytical Techniques in Environmental Chemistry ( /journal/molecules/special_issues/greenanalysis_enviromental )**)

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Open Access Article 18 pages, 6663 KiB (/1420-3049/28/10/4064/pdf?version=1683899068)

## UPLC-QE-Orbitrap-Based Cell Metabolomics and Network Pharmacology to Reveal the Mechanism of N-Benzylhexadecanamide Isolated from Maca (*Lepidium meyenii* Walp.) against Testicular Dysfunction (/1420-3049/28/10/4064)

by **Kai-Yue Zhang**, **Chun-Nan Li**, **Nan-Xi Zhang**, **Xiao-Chen Gao**, **Jia-Ming Shen**, **Duan-Duan Cheng**, **Yue-Long Wang**, **Hui Zhang**, **Jing-Wei Lv** and **Jia-Ming Sun**

*Molecules* **2023**, *28*(10), 4064; **https://doi.org/10.3390/molecules28104064 (https://doi.org/10.3390/molecules28104064)** - 12 May 2023

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**Abstract** Testicular dysfunction (TDF) is characterized by testosterone deficiency and is caused by oxidative stress injury in Leydig cells. A natural fatty amide named N-benzylhexadecanamide (NBH), derived from cruciferous maca, has been shown to promote testosterone production. Our study aims to reveal the anti-TDF **[...] Read more.**

(This article belongs to the Special Issue **Advances in Natural Products and Their Biological Activities ( /journal/molecules/special_issues/natural_products_2022 )**)

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Open Access Review 33 pages, 8143 KiB (/1420-3049/28/10/4063/pdf?version=1684135414)

**Multiple Bioimaging Applications Based on the Excellent Properties of Nanodiamond: A Review (/1420-3049/28/10/4063)**

by **Xinyue Wang**, **Dandan Sang**, **Liangrui Zou**, **Shunhao Ge**, **Yu Yao**, **Jianchao Fan** and **Qinglin Wang**
*Molecules* **2023**, *28*(10), 4063; **https://doi.org/10.3390/molecules28104063 (https://doi.org/10.3390/molecules28104063)** - 12 May 2023
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**Abstract** Nanodiamonds (NDs) are emerging as a promising candidate for multimodal bioimaging on account of their optical and spectroscopic properties. NDs are extensively utilized for bioimaging probes due to their defects and admixtures in their crystal lattice. There are many optically active defects presented **[...] Read more.**
(This article belongs to the Topic **Advances on the Application of Nanomaterials and 2D Materials for Sensors, Solar Cells, Microelectronics, and Optoelectronics (/topics/application_materials)**)
(This article belongs to the Section **Materials Chemistry (/journal/molecules/sections/materials_chemistry)**)

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Open Access Article 20 pages, 2251 KiB (/1420-3049/28/10/4062/pdf?version=1683896261)

**Chemical Composition and In Vitro Antioxidant Activity of *Salvia aratocensis* (Lamiaceae) Essential Oils and Extracts (/1420-3049/28/10/4062)**

by **Juan C. Henríquez**, **Laura V. Duarte**, **Lady J. Sierra**, **José L. Fernández-Alonso**, **Jairo R. Martínez** and **Elena E. Stashenko**
*Molecules* **2023**, *28*(10), 4062; **https://doi.org/10.3390/molecules28104062 (https://doi.org/10.3390/molecules28104062)** - 12 May 2023
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**Abstract** *Salvia aratocensis* (Lamiaceae) is an endemic shrub from the Chicamocha River Canyon in Santander (Colombia). Its essential oil (EO) was distilled from the aerial parts of the plant via steam distillation and microwave-assisted hydrodistillation and analyzed using GC/MS and GC/FID. Hydroethanolic extracts were isolated **[...] Read more.**
(This article belongs to the Section **Natural Products Chemistry (/journal/molecules/sections/natural_products_chemistry)**)

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Open Access Article 15 pages, 1139 KiB (/1420-3049/28/10/4061/pdf?version=1684809285)

**Comparison of Identification and Quantification of Polyphenolic Compounds in Skins and Seeds of Four Grape Varieties (/1420-3049/28/10/4061)**

by **Zlatina Chengolova**, **Yavor Ivanov** and **Tzonka Godjevargova**

*Molecules* **2023**, *28*(10), 4061; **https://doi.org/10.3390/molecules28104061 (https://doi.org/10.3390/molecules28104061)** - 12 May 2023

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**Abstract** The aim of this study was to identify and quantify polyphenolic compounds in skin extracts from four Bulgarian grape varieties and compare them to those of seed extracts. The values of total phenolic contents, flavonoids, anthocyanins, procyanidins and an ascorbic acid in grape **[...] Read more.**

(This article belongs to the Special Issue **Bioactive Compounds from Plants: Extraction and Characterization ( /journal/molecules/special_issues/G06U065H1V )**)

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**Transition Metal Sensing with Nitrogenated Holey Graphene: A First-Principles Investigation (/1420-3049/28/10/4060)**

by **Uroosa Sohail**, **Faizan Ullah**, **Nur Hazimah Binti Zainal Arfan**, **Malai Haniti Sheikh Abdul Hamid**, **Tariq Mahmood**, **Nadeem S. Sheikh** and **Khurshid Ayub**

*Molecules* **2023**, *28*(10), 4060; **https://doi.org/10.3390/molecules28104060 (https://doi.org/10.3390/molecules28104060)** - 12 May 2023

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**Abstract** The toxicity of transition metals, including copper(II), manganese(II), iron(II), zinc(II), hexavalent chromium, and cobalt(II), at elevated concentrations presents a significant threat to living organisms. Thus, the development of efficient sensors capable of detecting these metals is of utmost importance. This study explores the **[...] Read more.**

(This article belongs to the Special Issue **Computational Studies of Novel Function Materials ( /journal/molecules/special_issues/Y9PL52RVZC )**)

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Open Access Article 15 pages, 2313 KiB (/1420-3049/28/10/4059/pdf?version=1683890660)

**Novel Approach to the Construction of Fused Indolizine Scaffolds: Synthesis of Rosettacin and the Aromathecin Family of Compounds (/1420-3049/28/10/4059)**

by **Shohta Mizuno**, **Takashi Nishiyama**, **Mai Endo**, **Koharu Sakoguchi**, **Takaki Yoshiura**, **Hana Bessho**, **Toshio Motoyashiki**, **Noriyuki Hatae** and **Tominari Choshi**

*Molecules* **2023**, *28*(10), 4059; **https://doi.org/10.3390/molecules28104059 (https://doi.org/10.3390/molecules28104059)** - 12 May 2023

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**Abstract** Camptothecin-like compounds are actively employed as anticancer drugs in clinical treatments. The aromathecin family of compounds, which contains the same indazolidine core structure as the camptothecin family of compounds, is also expected to display promising anticancer activity. Therefore, the development of a suitable **[...] Read more.**

(This article belongs to the Special Issue **Recent Advances in Indole Derivatives in Medicinal and Synthetic Organic Chemistry ( /journal/molecules/special_issues/in_Indole_Derivatives )**)

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Open Access Article 15 pages, 1685 KiB (/1420-3049/28/10/4058/pdf?version=1683890257)

**Microbial Diversity and Bioactive Compounds in Dried *Lycium barbarum* Fruits (Goji): A Comparative Study (/1420-3049/28/10/4058)**

by **Katarzyna Rajkowska**, **Anna Otlewska**, **Natalia Broncel** and **Alina Kunicka-Styczyńska**

*Molecules* **2023**, *28*(10), 4058; **https://doi.org/10.3390/molecules28104058 (https://doi.org/10.3390/molecules28104058)** - 12 May 2023

**Cited by 5 (/1420-3049/28/10/4058#metrics)** | Viewed by 1833

**Abstract** This study compares the microbial diversity and content of bioactive compounds in dried goji berries available on the Polish market to those of the most highly valued goji berries from the Ningxia region in China. The content of phenols, flavonoids, and carotenoids were **[...] Read more.**

(This article belongs to the Special Issue **Recent Insights on the Molecular Basis Food Quality and Security Analysis ( /journal/molecules/special_issues/SFR3L916X4 )**)

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Open Access Article 12 pages, 4096 KiB (/1420-3049/28/10/4057/pdf?version=1683890638)

**Light Control-Induced Oxygen Vacancy Generation and In Situ Surface Heterojunction Reconstruction for Boosting $CO_2$ Reduction (/1420-3049/28/10/4057)**

by **Zhimin Yuan**, **Xianglin Zhu**, **Qichao Gao** and **Zaiyong Jiang**

*Molecules* **2023**, *28*(10), 4057; **https://doi.org/10.3390/molecules28104057 (https://doi.org/10.3390/molecules28104057)** - 12 May 2023

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**Abstract** The weak adsorption of $CO_2$ and the fast recombination of photogenerated charges harshly restrain the photocatalytic $CO_2$ reduction efficiency. The simultaneous catalyst design with strong $CO_2$ capture ability and fast charge separation efficiency is challenging. Herein, taking advantage of the **[...] Read more.**

(This article belongs to the Special Issue **Photocatalysis in the Control of Environmental Pollution ( /journal/molecules/special_issues/966F958032 )**)

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Open Access Article 16 pages, 2934 KiB (/1420-3049/28/10/4056/pdf?version=1683897932)

**New Random Aromatic/Aliphatic Copolymers of 2,5-Furandicarboxylic and Camphoric Acids with Tunable Mechanical Properties and Exceptional Gas Barrier Capability for Sustainable Mono-Layered Food Packaging (/1420-3049/28/10/4056)**

by **Giulia Guidotti**, **Michelina Soccio**, **Massimo Gazzano**, **Valentina Siracusa** and **Nadia Lotti**

*Molecules* **2023**, *28*(10), 4056; **https://doi.org/10.3390/molecules28104056 (https://doi.org/10.3390/molecules28104056)** - 12 May 2023

**Cited by 5 (/1420-3049/28/10/4056#metrics)** | Viewed by 1879

**Abstract** High molecular weight, fully biobased random copolymers of 2,5-furandicarboxylic acid (2,5-FDCA) containing different amounts of (1R, 3S)-(+)-Camphoric Acid (CA) have been successfully synthesized by two-stage melt polycondensation and compression molding in the form of films. The s sized copolyesters have been first subjected to **[...] Read more.**

(This article belongs to the Special Issue **Synthesis, Properties and Applications of Biobased Polymers ( /journal/molecules/special_issues/Biobased_Polymers_Synthesis )**)

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Open Access Review 29 pages, 4884 KiB (/1420-3049/28/10/4055/pdf?version=1683884570)

**Advances on the Amaryllidacea Alkaloids Collected in South Africa, Andean South America and the Mediterranean Basin (/1420-3049/28/10/4055)**

by **Antonio Evidente**

*Molecules* **2023**, *28*(10), 4055; **https://doi.org/10.3390/molecules28104055 (https://doi.org/10.3390/molecules28104055)** - 12 May 2023

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**Abstract** The alkaloids are one of the most represented family of natural occurring biological active compounds. Amaryllidaceae are also very well known for their beautiful flower and are thus used as ornamental plants in historic and public gardens. The Amaryllidacea alkaloids constitute an important **[...] Read more.**

(This article belongs to the Section **Natural Products Chemistry (/journal/molecules/sections/natural_products_chemistry)**)

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Open Access Article 18 pages, 7057 KiB (/1420-3049/28/10/4054/pdf?version=1684126784)

**Antihyperglycemic Properties of Extracts and Isolated Compounds from Australian *Acacia saligna* on 3T3-L1 Adipocytes (/1420-3049/28/10/4054)**

by **Anjar P. Asmara**, **Anchalee Prasansuklab**, **Anchalee Chiabchalard**, **Hui Chen** and **Alison T. Ung**

*Molecules* **2023**, *28*(10), 4054; **https://doi.org/10.3390/molecules28104054 (https://doi.org/10.3390/molecules28104054)** - 12 May 2023

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**Abstract** Our early work indicated that methanolic extracts from the flowers, leaves, bark, and isolated compounds of *Acacia saligna* exhibited significant antioxidant activities in vitro. The overproduction of reactive oxygen species (ROS) in the mitochondria (mt-ROS) interfered with glucose uptake, metabolism, and its AMPK-dependent **[...] Read more.**

(This article belongs to the Special Issue **Key Role of Natural Bioactive Compounds in Health and Diseases ( /journal/molecules/special_issues/283K1Y9DX7 )**)

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Open Access Article 14 pages, 657 KiB (/1420-3049/28/10/4053/pdf?version=1683876566)

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**Chitosan Modulates Volatile Organic Compound Emission from the Biocontrol Fungus *Pochonia chlamydosporia* (/1420-3049/28/10/4053)**

by **Jorge Mestre-Tomás**, **David Esgueva-Vilà**, **Alba Fuster-Alonso**, **Federico Lopez-Moya** and **Luis V. Lopez-Llorca**

*Molecules* **2023**, *28*(10), 4053; **https://doi.org/10.3390/molecules28104053 (https://doi.org/10.3390/molecules28104053)** - 12 May 2023

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**Abstract** Fungal volatile organic compounds (VOCs) are responsible for fungal odor and play a key role in biological processes and ecological interactions. VOCs represent a promising area of research to find natural metabolites for human exploitation. *Pochonia chlamydosporia* is a chitosan-resistant nematophagous fungus used **[...] Read more.**

(This article belongs to the Special Issue **Chitosan, Chitosan Derivatives and Their Applications ( /journal/molecules/special_issues/chitosan_chemistry )**)

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Open Access Article 15 pages, 1486 KiB **(/1420-3049/28/10/4052/pdf?version=1683878693)**

**Carbene-Catalyzed Atroposelective Annulation for Quick Access to Axially Chiral Thiazine Derivatives (/1420-3049/28/10/4052)**

by **Xiaoqun Yang**, **Tingting Li**, **Jinli Chen**, **Yixian Huang**, **Tingwei Shen**, **Shiguang Li**, **Zhichao Jin** and **Shi-Chao Ren**

*Molecules* **2023**, *28*(10), 4052; **https://doi.org/10.3390/molecules28104052 (https://doi.org/10.3390/molecules28104052)** - 12 May 2023

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**Abstract** An *N*-heterocyclic carbene (NHC)-catalyzed atroposelective annulation reaction is disclosed for quick and efficient access to thiazine derivatives. A series of axially chiral thiazine derivatives bearing various substituents and substitution patterns were produced in moderate to high yields with moderate to excellent optical **[...] Read more.**

(This article belongs to the Special Issue **Synthesis and Application of Atropisomeric Molecules ( /journal/molecules/special_issues/5ICJWD0Q46 )**)

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Open Access Article 16 pages, 2776 KiB **(/1420-3049/28/10/4051/pdf?version=1683874897)**

**Synthesis and Antiproliferative Insights of Lipophilic Ru(II)-Hydroxy Stearic Acid Hybrid Species (/1420-3049/28/10/4051)**

by **Giacomo Drius**, **Silvia Bordoni**, **Carla Boga**, **Magda Monari**, **Jessica Fiori**, **Erika Esposito**, **Chiara Zalambani**, **Luca Pincigher**, **Giovanna Farruggia**, **Natalia Calonghi** and **Gabriele Micheletti**

*Molecules* **2023**, *28*(10), 4051; **https://doi.org/10.3390/molecules28104051 (https://doi.org/10.3390/molecules28104051)** - 12 May 2023

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**Abstract** Metallodrugs represent a combination of multifunctionalities that are present concomitantly and can act differently on diverse biotargets. Their efficacy is often related to the lipophilic features exhibited both by long carbo-chains and the phosphine ligands. Three Ru(II) complexes containing hydroxy stearic acids (HSAs) **[...] Read more.**

(This article belongs to the Special Issue **Synthesis and Applications in Catalysis or as Anticancer and Antimicrobial Agents of Unique Organometallic Compounds ( /journal/molecules/special_issues/W8UMC87201 )**)

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Open Access Review 27 pages, 2110 KiB **(/1420-3049/28/10/4050/pdf?version=1683873423)**

**Collision Cross Section Prediction Based on Machine Learning (/1420-3049/28/10/4050)**

by **Xiaohang Li**, **Hongda Wang**, **Meiting Jiang**, **Mengxiang Ding**, **Xiaoyan Xu**, **Bei Xu**, **Yadan Zou**, **Yuetong Yu** and **Wenzhi Yang**

*Molecules* **2023**, *28*(10), 4050; **https://doi.org/10.3390/molecules28104050 (https://doi.org/10.3390/molecules28104050)** - 12 May 2023

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**Abstract** Ion mobility-mass spectrometry (IM-MS) is a powerful separation technique providing an additional dimension of separation to support the enhanced separation and characterization of complex components from the tissue metabolome and medicinal herbs. The integration of machine learning (ML) with IM-MS can overcome the **[...] Read more.**

(This article belongs to the Special Issue **LC-MS in Bioactive Molecules Study ( /journal/molecules/special_issues/LC_MS_Bio_Molecules )**)

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Open Access Article 19 pages, 2420 KiB **(/1420-3049/28/10/4049/pdf?version=1683872191)**

**Development of Green and High Throughput Microplate Reader-Assisted Universal Microwell Spectrophotometric Assay for Direct Determination of Tyrosine Kinase Inhibitors in Their Pharmaceutical Formulations Irrespective the Diversity of Their Chemical Structures (/1420-3049/28/10/4049)**

by **Ibrahim A. Darwish** and **Nourah Z. Alzoman**

*Molecules* **2023**, *28*(10), 4049; **https://doi.org/10.3390/molecules28104049 (https://doi.org/10.3390/molecules28104049)** - 12 May 2023

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**Abstract** This study discusses the development and validation of a universal microwell spectrophotometric assay for TKIs, regardless of the diversity in their chemical structures. The assay depends on directly measuring the native ultraviolet light (UV) absorption of TKIs. The assay was carried out using **[...] Read more.**

(This article belongs to the Section **Analytical Chemistry (/journal/molecules/sections/Analytical_Chemistry)**)

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Open Access Article 20 pages, 3233 KiB **(/1420-3049/28/10/4048/pdf?version=1683866660)**

**Exploitation of Sugarcane Bagasse and Environmentally Sustainable Production, Purification, Characterization, and Application of Lovastatin by *Aspergillus terreus* AUMC 15760 under Solid-State Conditions (/1420-3049/28/10/4048)**

by **Ahmed M. A. A. Ramadan**, **Reda M. Shehata**, **Hussein H. EL-Sheikh**, **Fuad Ameen**, **Steven L. Stephenson**, **Sabry A. H. Zidan** and **Osama A. M. Al-Bedak**

*Molecules* **2023**, *28*(10), 4048; **https://doi.org/10.3390/molecules28104048 (https://doi.org/10.3390/molecules28104048)** - 12 May 2023

**Cited by 6 (/1420-3049/28/10/4048#metrics)** | Viewed by 3946

**Abstract** Using the internal transcribed spacer (ITS) region for identification, three strains of *Aspergillus terreus* were identified and designated AUMC 15760, AUMC 15762, and AUMC 15763 for the Assiut University Mycological Centre culture collection. The ability of the three strains to manufacture lovastatin in **[...] Read more.**

(This article belongs to the Special Issue **Discovery of Bioactive Ingredients from Natural Products, 4th Edition ( /journal/molecules/special_issues/F905JORND2 )**)

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Open Access Review 17 pages, 1106 KiB **(/1420-3049/28/10/4047/pdf?version=1683870735)**

**Machine Learning Generation of Dynamic Protein Conformational Ensembles (/1420-3049/28/10/4047)**

by **Li-E Zheng**, **Shrishti Barethiya**, **Erik Nordquist** and **Jianhan Chen**

*Molecules* **2023**, *28*(10), 4047; **https://doi.org/10.3390/molecules28104047 (https://doi.org/10.3390/molecules28104047)** - 12 May 2023

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**Abstract** Machine learning has achieved remarkable success across a broad range of scientific and engineering disciplines, particularly its use for

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predicting native protein structures from sequence information alone. However, biomolecules are inherently dynamic, and there is a pressing need for accurate predictions of dynamic **[...] Read more.**

(This article belongs to the Section **Computational and Theoretical Chemistry (/journal/molecules/sections/computational_theoretical_chemistry)**)

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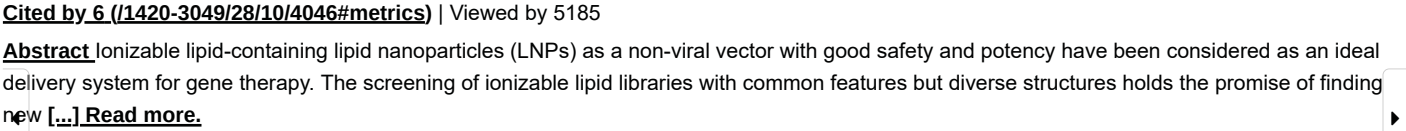

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**Ionizable Lipids with Triazole Moiety from Click Reaction for LNP-Based mRNA Delivery (/1420-3049/28/10/4046)**

by **Yixiang Wang**, **Xiao Si**, **Yi Feng**, **Dan Feng**, **Xiaoyu Xu** and **Yan Zhang**

*Molecules* **2023**, *28*(10), 4046; **https://doi.org/10.3390/molecules28104046 (https://doi.org/10.3390/molecules28104046)** - 12 May 2023

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**Abstract** Ionizable lipid-containing lipid nanoparticles (LNPs) as a non-viral vector with good safety and potency have been considered as an ideal delivery system for gene therapy. The screening of ionizable lipid libraries with common features but diverse structures holds the promise of finding new **[...] Read more.**

(This article belongs to the Section **Chemical Biology (/journal/molecules/sections/Chemical_Biology)**)

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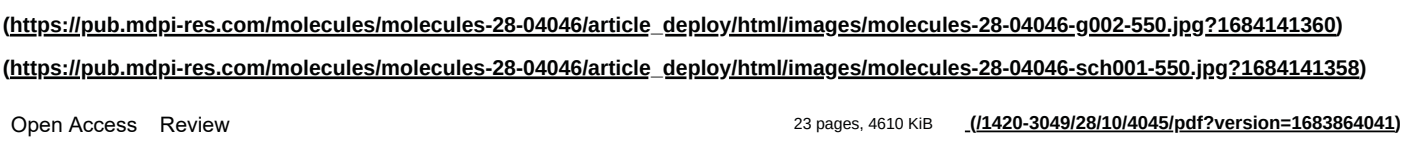

Open Access Review 23 pages, 4610 KiB **(/1420-3049/28/10/4045/pdf?version=1683864041)**

**Repositioned Natural Compounds and Nanoformulations: A Promising Combination to Counteract Cell Damage and Inflammation in Respiratory Viral Infections (/1420-3049/28/10/4045)**

by **Alessia Mariano**, **Irene Bigioni**, **Magda Marchetti**, **Anna Scotto d'Abusco** and **Fabiana Superti**

*Molecules* **2023**, *28*(10), 4045; **https://doi.org/10.3390/molecules28104045 (https://doi.org/10.3390/molecules28104045)** - 12 May 2023

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**Abstract** Respiratory viral diseases are among the most important causes of disability, morbidity, and death worldwide. Due to the limited efficacy or side effects of many current therapies and the increase in antiviral-resistant viral strains, the need to find new compounds to counteract these **[...] Read more.**

(This article belongs to the Special Issue **Advances on Nanomedicine and Nanoparticle-Based Drug Delivery ( /journal/molecules/special_issues/drug_delivery_nano )**)

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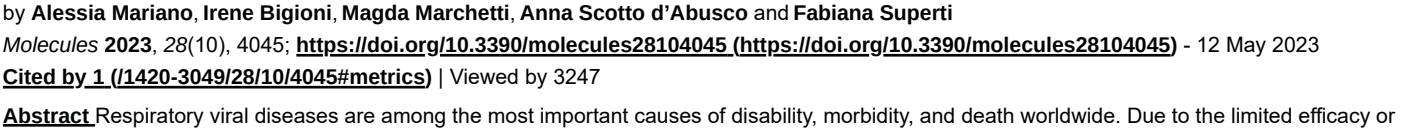

Open Access Article 24 pages, 7385 KiB **(/1420-3049/28/10/4044/pdf?version=1683861977)**

**Pharmacophore-Based Virtual Screening and In-Silico Explorations of Biomolecules (Curcumin Derivatives) of *Curcuma longa* as Potential Lead Inhibitors of ERBB and VEGFR-2 for the Treatment of Colorectal Cancer (/1420-3049/28/10/4044)**

by **Syeda Abida Ejaz**, **Mubashir Aziz**, **Mohamed Fawzy Ramadan**, **Ammara Fayyaz** and **Muhammad Sajjad Bilal**

*Molecules* **2023**, *28*(10), 4044; **https://doi.org/10.3390/molecules28104044 (https://doi.org/10.3390/molecules28104044)** - 12 May 2023

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**Abstract** The newly FDA-approved drug, Axitinib, is an effective therapy against RTKs, but it possesses severe adverse effects like hypertension, stomatitis, and dose-dependent toxicity. In order to ameliorate Axitinib's downsides, the current study is expedited to search for energetically stable and optimized pharmacophore features **[...] Read more.**

(This article belongs to the Special Issue **Computational Drug Discovery: Methods and Applications ( /journal/molecules/special_issues/3Q6OV9M879 )**)

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Open Access Article 13 pages, 2049 KiB (/1420-3049/28/10/4043/pdf?version=1684388953)

**Selecting Nanobodies Specific for the Epidermal Growth Factor from a Synthetic Nanobody Library (/1420-3049/28/10/4043)**

by **Yunier Serrano-Rivero**, **Julieta Salazar-Uribe**, **Marcela Rubio-Carrasquilla**, **Frank Camacho-Casanova**, **Oliberto Sánchez-Ramos**, **Alaín González-Pose** and **Ernesto Moreno**

*Molecules* **2023**, *28*(10), 4043; **https://doi.org/10.3390/molecules28104043 (https://doi.org/10.3390/molecules28104043)** - 12 May 2023
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**Abstract** The epidermal growth factor (EGF) is one of the most critical ligands of the EGF receptor (EGFR), a well-known oncogene frequently overexpressed in cancerous cells and an important therapeutic target in cancer. The EGF is the target of a therapeutic vaccine aimed at **[...] Read more.**

(This article belongs to the Special Issue **Converging Nanochemistry: From Disease Prevention to Diagnosis and Treatment ( /journal/molecules/special_issues/nano_bioengineering )**)

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Open Access Article 19 pages, 3960 KiB (/1420-3049/28/10/4042/pdf?version=1683854515)

***Lactiplantibacillus plantarum* NKK20 Alleviates High-Fat-Diet-Induced Nonalcoholic Fatty Liver Disease in Mice through Regulating Bile Acid Anabolism (/1420-3049/28/10/4042)**

by **Chang Sun**, **Chenguang Qiu**, **Yanyan Zhang**, **Man Yan**, **Jiajun Tan**, **Jiayuan He**, **Dakai Yang**, **Dongxu Wang** and **Liang Wu**

*Molecules* **2023**, *28*(10), 4042; **https://doi.org/10.3390/molecules28104042 (https://doi.org/10.3390/molecules28104042)** - 12 May 2023
**Cited by 8 (/1420-3049/28/10/4042#metrics)** | Viewed by 2463

**Abstract** Nonalcoholic fatty liver disease (NAFLD) is the most prevalent chronic disease in modern society. It is characterized by an accumulation of lipids in the liver and an excessive inflammatory response. Clinical trials have provided evidence that probiotics may prevent the onset and relapse **[...] Read more.**

(This article belongs to the Special Issue **Discovery of New Functional Foods with Bioactive Compounds ( /journal/molecules/special_issues/56GLM8IAT9 )**)

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Open Access Article 24 pages, 11023 KiB (/1420-3049/28/10/4041/pdf?version=1683818861)

**HPLC Analysis and Molecular Docking Study of *Myoporum serratum* Seeds Extract with Its Bioactivity against Pathogenic Microorganisms and Cancer Cell Lines (/1420-3049/28/10/4041)**

by **Abdullah Mashraqi**, **Yosra Modafer**, **Mohamed A. Al Abboud**, **Hanaa M. Salama** and **Emad Abada**

*Molecules* **2023**, *28*(10), 4041; **https://doi.org/10.3390/molecules28104041 (https://doi.org/10.3390/molecules28104041)** - 11 May 2023

**Cited by 6 (/1420-3049/28/10/4041#metrics)** | Viewed by 2972

**Abstract** Natural constituents have been utilized to avoid humanity from various diseases, such as microbial infection and cancer, over several decades due to bioactive compounds. *Myoporum serratum* seeds extract (MSSE) was formulated via HPLC for flavonoid and phenolic analysis. Moreover, antimicrobial via well diffusion **[...] Read more.**

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Open Access Editorial 12 pages, 317 KiB (/1420-3049/28/10/4040/pdf?version=1683819792)

**Electrochemistry of Thin Films and Nanostructured Materials (/1420-3049/28/10/4040)**

by **Grzegorz Dariusz Sulka**

*Molecules* **2023**, *28*(10), 4040; **https://doi.org/10.3390/molecules28104040 (https://doi.org/10.3390/molecules28104040)** - 11 May 2023

**Cited by 13 (/1420-3049/28/10/4040#metrics)** | Viewed by 4244

**Abstract** In the last few decades, the development and use of thin films and nanostructured materials to enhance physical and chemical properties of materials has been common practice in the field of materials science and engineering. The progress which has recently been made in **[...] Read more.**

(This article belongs to the Special Issue **Electrochemistry of Thin Films and Nanostructured Materials ( /journal/molecules/special_issues/Electrochemistry_Nanostructured_Materials )**)

Open Access Article 15 pages, 1526 KiB (/1420-3049/28/10/4039/pdf?version=1683814823)

**Oligosaccharide Ligands of Galectin-4 and Its Subunits: Multivalency Scores Highly (/1420-3049/28/10/4039)**

by **Kristýna Slámová**, **Jakub Červený**, **Zuzana Mészáros**, **Tereza Friede**, **David Vrbata**, **Vladimír Křen** and **Pavla Bojarová**

*Molecules* **2023**, *28*(10), 4039; **https://doi.org/10.3390/molecules28104039 (https://doi.org/10.3390/molecules28104039)** - 11 May 2023

**Cited by 6 (/1420-3049/28/10/4039#metrics)** | Viewed by 2459

**Abstract** Galectins are carbohydrate-binding lectins that modulate the proliferation, apoptosis, adhesion, or migration of cells by cross-linking glycans on cell membranes or extracellular matrix components. Galectin-4 (Gal-4) is a tandem-repeat-type galectin expressed mainly in the epithelial cells of the gastrointestinal tract. It consists of **[...] Read more.**

(This article belongs to the Special Issue **Synthesis and Biological Applications of Glycoconjugates III ( /journal/molecules/special_issues/synthesis_applications_glycoconjugates )**)

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Open Access Article 18 pages, 3540 KiB (/1420-3049/28/10/4038/pdf?version=1683814077)

**Tailoring of Mesoporous Silica-Based Materials for Enhanced Water Pollutants Removal (/1420-3049/28/10/4038)**

by **Daniela Flores**, **C. Marisa R. Almeida**, **Carlos R. Gomes**, **Salete S. Balula** and **Carlos M. Granadeiro**

*Molecules* **2023**, *28*(10), 4038; **https://doi.org/10.3390/molecules28104038 (https://doi.org/10.3390/molecules28104038)** - 11 May 2023

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**Abstract** The adsorptive performance of mesoporous silica-based materials towards inorganic (metal ions) and organic (dyes) water pollutants was investigated. Mesoporous silica materials with different particle size, surface area and pore volume were prepared and tailored with different functional groups. These materials were then characterised **[...] Read more.**

(This article belongs to the Special Issue **Mesoporous Silica-Based Materials for Sustainable Technologies ( /journal/molecules/special_issues/Mesoporous_Silica_Sustainable )**)

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Open Access Article 15 pages, 7862 KiB (/1420-3049/28/10/4037/pdf?version=1683813436)

**Distribution of Bipartite and Tripartite Entanglement within a Spin-1/2 Heisenberg Star in a Magnetic Field (/1420-3049/28/10/4037)**

by **Katarína Karlóvá** and **Jozef Strečka**

*Molecules* **2023**, *28*(10), 4037; **https://doi.org/10.3390/molecules28104037 (https://doi.org/10.3390/molecules28104037)** - 11 May 2023

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**Abstract** The spatial distribution of entanglement within a spin-1/2 Heisenberg star composed from a single central spin and three peripheral spins is examined in the presence of an external magnetic field using the Kambe projection method, which allows an exact calculation of the bipartite **[...] Read more.**

(This article belongs to the Special Issue **Molecular Magnetism: Modern Trends and Future Perspectives ( /journal/molecules/special_issues/Molecular_Magnet )**)

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Open Access Article 16 pages, 5277 KiB (/1420-3049/28/10/4036/pdf?version=1683813070)

**Efficient Treatment of Oily Sludge via Fast Microwave-Assisted Pyrolysis, Followed by Thermal Plasma Vitrification (/1420-3049/28/10/4036)**

by **Qinglong Xie**, **Zhen Chen**, **Yuqiang Zhou**, **Tongbo Pan**, **Ying Duan**, **Shangzhi Yu**, **Xiaojiang Liang**, **Zhenyu Wu**, **Weirong Ji** and **Yong Nie**

*Molecules* **2023**, *28*(10), 4036; **https://doi.org/10.3390/molecules28104036 (https://doi.org/10.3390/molecules28104036)** - 11 May 2023

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**Abstract** Oily sludge, as a critical hazardous waste, requires appropriate treatment for resource recovery and harmfulness reduction. Here, fast microwave-assisted pyrolysis (MAP) of oily sludge was conducted for oil removal and fuel production. The results indicated the priority of the fast MAP compared with **[...] Read more.**

(This article belongs to the Special Issue **The Application of Microwave-Assisted Technology in Chemical Reaction ( /journal/molecules/special_issues/94AQZ82MO3 )**)

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Open Access Article 14 pages, 8638 KiB (/1420-3049/28/10/4035/pdf?version=1683810625)

## Hybrid Nanocomposites of Tenoxicam: Layered Double Hydroxides (LDHs) vs. Hydroxyapatite (HAP) Inorganic Carriers (/1420-3049/28/10/4035)

by **Lauretta Maggi**, **Valeria Friuli**, **Giovanna Bruni**, **Alessia Rinaldi** and **Marcella Bini**

*Molecules* **2023**, *28*(10), 4035; https://doi.org/10.3390/molecules28104035 (https://doi.org/10.3390/molecules28104035) - 11 May 2023

Cited by 4 (/1420-3049/28/10/4035#metrics) | Viewed by 1829

**Abstract** The search for effective systems to facilitate the release of poorly bioavailable drugs is a forefront topic for the pharmaceutical market. Materials constituted by inorganic matrices and drugs represent one of the latest research strategies in the development of new drug alternatives. Our **[...] Read more.**

(This article belongs to the Special Issue **Exclusive Feature Papers in Physical Chemistry ( /journal/molecules/special_issues/FP_physchem )**)

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Open Access Article 21 pages, 18709 KiB (/1420-3049/28/10/4034/pdf?version=1683809967)

## Rosmarinic Acid-Grafted Dextran/Gelatin Hydrogel as a Wound Dressing with Improved Properties: Strong Tissue Adhesion, Antibacterial, Antioxidant and Anti-Inflammatory (/1420-3049/28/10/4034)

by **Yi Yin**, **Qianqian Xu**, **Xin Wei**, **Qianyun Ma**, **Dongsheng Li** and **Juanjuan Zhao**

*Molecules* **2023**, *28*(10), 4034; https://doi.org/10.3390/molecules28104034 (https://doi.org/10.3390/molecules28104034) - 11 May 2023

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**Abstract** Designing a strong tissue adhesive and multifunctional hydrogel dressing for various skin injuries is still a significant challenge. Based on the bioactive activities of rosmarinic acid (RA) and its catechol structure being similar to dopamine, RA-grafted dextran/gelatin hydrogel (ODex−AG−RA) was designed and systemically **[...] Read more.**

(This article belongs to the Special Issue **Bioactive Material for Wound Healing, Tissue Engineering and Regenerative Medicine ( /journal/molecules/special_issues/Y9SAR92L83 )**)

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Open Access Article 12 pages, 1861 KiB (/1420-3049/28/10/4033/pdf?version=1683807627)

**Extended-Synaptotagmin 1 Enhances Liver Cancer Progression Mediated by the Unconventional Secretion of Cytosolic Proteins (/1420-3049/28/10/4033)**

by **Kohji Yamada**, **Yoshito Hannya**, **Tsunekazu Oikawa**, **Ayano Yoshida**, **Kuniko Katagiri**, **Saishu Yoshida**, **Rei Koizumi**, **Naoko Tago**, **Yuya Shimoyama**, **Akira Kawamura**, **Yuta Mochimaru**, **Ken Eto** and **Kiyotsugu Yoshida**

*Molecules* **2023**, *28*(10), 4033; **https://doi.org/10.3390/molecules28104033 (https://doi.org/10.3390/molecules28104033)** - 11 May 2023

**Cited by 4 (/1420-3049/28/10/4033#metrics)** | Viewed by 2586

**Abstract** Extended-synaptotagmin 1 (E-Syt1) is an endoplasmic reticulum membrane protein that is involved in cellular lipid transport. Our previous study identified E-Syt1 as a key factor for the unconventional protein secretion of cytoplasmic proteins in liver cancer, such as protein kinase C delta (PKCδ); **[...] Read more.**

(This article belongs to the Special Issue **Targeting of Signaling Pathways for Cancer Therapy, 2nd Edition ( /journal/molecules/special_issues/signaling_pathways_cancer_therapy_2 )**)

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Open Access Review 25 pages, 2583 KiB (/1420-3049/28/10/4032/pdf?version=1683810318)

**The Potential of Algae in the Nutricosmetic Sector (/1420-3049/28/10/4032)**

by **Irene Dini**

*Molecules* **2023**, *28*(10), 4032; **https://doi.org/10.3390/molecules28104032 (https://doi.org/10.3390/molecules28104032)** - 11 May 2023

**Cited by 18 (/1420-3049/28/10/4032#metrics)** | Viewed by 5013

**Abstract** Seaweeds or algae are marine autotrophic organisms. They produce nutrients (e.g., proteins, carbohydrates, etc.) essential for the survival of living organisms as they participate in biochemical processes and non-nutritive molecules (such as dietary fibers and secondary metabolites), which can improve their physiological functions. **[...] Read more.**

(This article belongs to the Special Issue **Nutricosmetics: A New Area of Cosmetic Product ( /journal/molecules/special_issues/Nutricosmetics )**)

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Open Access Article 13 pages, 1634 KiB (/1420-3049/28/10/4031/pdf?version=1683815401)

**Synthesis of Glycopolymer Micelles for Antibiotic Delivery (/1420-3049/28/10/4031)**

by **Xuan Chen**, **Bin Wu**, **Harini A. Perera** and **Mingdi Yan**

*Molecules* **2023**, *28*(10), 4031; **https://doi.org/10.3390/molecules28104031 (https://doi.org/10.3390/molecules28104031)** - 11 May 2023

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**Abstract** In this work, we designed biodegradable glycopolymers consisting of a carbohydrate conjugated to a biodegradable polymer, poly(lactic acid) (PLA), through a poly(ethylene glycol) (PEG) linker. The glycopolymers were synthesized by coupling alkyne end-functionalized PEG-PLA with azide-derivatized mannose, trehalose, or maltoheptaose via the click **[...] Read more.**

(This article belongs to the Special Issue **New Insights in Antimicrobial Nanomaterials ( /journal/molecules/special_issues/antimicrobial_nanomaterial )**)

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Open Access Article 20 pages, 5142 KiB (/1420-3049/28/10/4030/pdf?version=1683803968)

## The Photodynamic Anticancer and Antibacterial Activity Properties of a Series of *meso*-Tetraarylchlorin Dyes and Their Sn(IV) Complexes (/1420-3049/28/10/4030)

by **Rodah Soy**, **Balaji Babu**, **John Mack** and **Tebello Nyokong**

*Molecules* **2023**, *28*(10), 4030; https://doi.org/10.3390/molecules28104030 (https://doi.org/10.3390/molecules28104030) - 11 May 2023
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**Abstract** A series of tetraarylchlorins with 3-methoxy-, 4-hydroxy- and 3-methoxy-4-hydroxyphenyl *meso*-aryl rings (**1**-**3**-Chl) and their Sn(IV) complexes (**1**-**3**-SnChl) were synthesized and characterized so that their potential utility as photosensitizer dyes for use in photodynamic therapy **[...] Read more.**

(This article belongs to the Special Issue **Dye Chemistry—In Memory of Prof. Michael R. Detty ( /journal/molecules/special_issues/Dye_Chemistry )**)

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## Improved Synthesis of Deoxyadenosine Triphosphate by *Saccharomyces cerevisiae* Using an Efficient ATP Regeneration System: Optimization of Response Surface Analysis (/1420-3049/28/10/4029)

by **Jian Xiong**, **Hanghang Xu**, **Qi Wang** and **Wenyuan Sun**

*Molecules* **2023**, *28*(10), 4029; https://doi.org/10.3390/molecules28104029 (https://doi.org/10.3390/molecules28104029) - 11 May 2023
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**Abstract** Deoxyadenosine triphosphate (dATP) is an important biochemical molecule. In this paper, the synthesis of dATP from deoxyadenosine monophosphate (dAMP), catalyzed by *Saccharomyces cerevisiae,* was studied. By adding chemical effectors, an efficient ATP regeneration and coupling system was constructed to achieve efficient synthesis of **[...] Read more.**

(This article belongs to the Topic **Advances in Chemistry and Chemical Engineering (/topics/RICCCE22)**)

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Open Access Article 28 pages, 5564 KiB (/1420-3049/28/10/4028/pdf?version=1684309631)

## Combining the Classification and Pharmacophore Approaches to Understand Homogeneous Olfactory Perceptions at Peripheral Level: Focus on Two Aroma Mixtures (/1420-3049/28/10/4028)

by **Marylène Rugard**, **Karine Audouze** and **Anne Tromelin**

*Molecules* **2023**, *28*(10), 4028; https://doi.org/10.3390/molecules28104028 (https://doi.org/10.3390/molecules28104028) - 11 May 2023
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**Abstract** The mechanisms involved in the homogeneous perception of odorant mixtures remain largely unknown. With the aim of enhancing knowledge about blending and masking mixture perceptions, we focused on structure-odor relationships by combining the classification and pharmacophore approaches. We built a dataset of about **[...] Read more.**

(This article belongs to the Section **Flavours and Fragrances (/journal/molecules/sections/flavours_and_fragrances)**)

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Open Access Review 13 pages, 2188 KiB (/1420-3049/28/10/4027/pdf?version=1683811748)

**Hard-Carbon Negative Electrodes from Biomasses for Sodium-Ion Batteries (/1420-3049/28/10/4027)**

by **Bin Lu**, **Chengjun Lin**, **Haiji Xiong**, **Chi Zhang**, **Lin Fang**, **Jiazhou Sun**, **Ziheng Hu**, **Yalong Wu**, **Xiaohong Fan**, **Guifang Li**, **Jile Fu**, **Dingrong Deng** and **Qihui Wu**

*Molecules* **2023**, *28*(10), 4027; **https://doi.org/10.3390/molecules28104027 (https://doi.org/10.3390/molecules28104027)** - 11 May 2023

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**Abstract** With the development of high-performance electrode materials, sodium-ion batteries have been extensively studied and could potentially be applied in various fields to replace the lithium-ion cells, owing to the low cost and natural abundance. As the key anode materials of sodium-ion batteries, hard **[...] Read more.**

(This article belongs to the Special Issue **Advances in Carbon-Based Materials for Lithium Ion Batteries ( /journal/molecules/special_issues/LV22N9349L )**)

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Open Access Article 18 pages, 2560 KiB (/1420-3049/28/10/4026/pdf?version=1683875928)

**Nanoparticle-Imprinted Silica Gel for the Size-Selective Capture of Silver Ultrafine Nanoparticles from Water (/1420-3049/28/10/4026)**

by **Piersandro Pallavicini**, **Luca Preti**, **Maria L. Protopapa**, **Daniela Carbone**, **Laura Capodieci**, **Yuri A. Diaz Fernandez**, **Chiara Milanese**, **Angelo Taglietti** and **Lavinia Doveri**

*Molecules* **2023**, *28*(10), 4026; **https://doi.org/10.3390/molecules28104026 (https://doi.org/10.3390/molecules28104026)** - 11 May 2023

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**Abstract** A synthetic approach has been developed to prepare silica gel monoliths that embed well separated silver or gold spherical nanoparticles (NP), with diameters of 8, 18 and 115 nm. $Fe^{3+}$, $O_2$/cysteine and $HNO_3$ were all successfully used to **[...] Read more.**

(This article belongs to the Special Issue **Materials Chemistry in Italy ( /journal/molecules/special_issues/materials_chemistry_Italy )**)

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Open Access Article 11 pages, 2614 KiB (/1420-3049/28/10/4025/pdf?version=1683800587)

***N*-Heterocyclic Carbene Copper (I) Complexes Incorporating Pyrene Chromophore: Synthesis, Crystal Structure, and Luminescent Properties (/1420-3049/28/10/4025)**

by **Yaping Cheng**, **Geoffrey Gontard**, **Abderrahim Khatyr**, **Michael Knorr** and **Hani Amouri**

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*Molecules* **2023**, *28*(10), 4025; **https://doi.org/10.3390/molecules28104025 (https://doi.org/10.3390/molecules28104025)** - 11 May 2023
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**Abstract** Luminescent *N*-heterocyclic carbene chloride copper (I) complexes incorporating pyrene chromophore (1-Pyrenyl-NHC-R)-Cu-Cl, (**3**, **4**) have been prepared and fully characterized. Two complexes were prepared with R = methyl (**3**) and R = naphthyl groups (**4**) at **[...] Read more.**
(This article belongs to the Section **Inorganic Chemistry (/journal/molecules/sections/Inorganic_Chemistry)**)

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Open Access Review 21 pages, 872 KiB **(/1420-3049/28/10/4024/pdf?version=1683799231)**

**Antioxidant Activity in Extracts from *Zingiberaceae* Family: Cardamom, Turmeric, and Ginger (/1420-3049/28/10/4024)**

by **Pura Ballester**, **Begoña Cerdá**, **Raúl Arcusa**, **Ana María García-Muñoz**, **Javier Marhuenda** and **Pilar Zafrilla**
*Molecules* **2023**, *28*(10), 4024; **https://doi.org/10.3390/molecules28104024 (https://doi.org/10.3390/molecules28104024)** - 11 May 2023
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**Abstract** An increase in life expectancy leads to a greater impact of chronic non-communicable diseases. This is even more remarkable in elder populations, to whom these become main determinants of health status, affecting mental and physical health, quality of life, and autonomy. Disease appearance **[...] Read more.**
(This article belongs to the Special Issue **Antioxidant Activity of Natural Products ( /journal/molecules/special_issues/antioxidant_activity_of_natural_products )**)

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**Semi-Synthesis of Different Pyranoflavonoid Backbones and the Neurogenic Potential (/1420-3049/28/10/4023)**

by **Corinna Urmann**, **Lara Bieler**, **Michael Hackl**, **Olivia Chia-Leeson**, **Sebastien Couillard-Despres** and **Herbert Riepl**
*Molecules* **2023**, *28*(10), 4023; **https://doi.org/10.3390/molecules28104023 (https://doi.org/10.3390/molecules28104023)** - 11 May 2023
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**Abstract** Flavonoids and chalcones are known for their manifold biological activities, of which many affect the central nervous system. Pyranochalcones were recently shown to have a great neurogenic potential, which is partly due to a specific structural motif-the pyran ring. Accordingly, we questioned if **[...] Read more.**
(This article belongs to the Section **Natural Products Chemistry (/journal/molecules/sections/natural_products_chemistry)**)

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Open Access Article 20 pages, 5543 KiB **(/1420-3049/28/10/4022/pdf?version=1683794144)**

**Preclinical Evaluation of a PSMA-Targeting Homodimer with an Optimized Linker for Imaging of Prostate Cancer (/1420-3049/28/10/4022)**

by **Erika Murce**, **Savanne Beekman**, **Evelien Spaan**, **Maryana Handula**, **Debra Stuurman**, **Corrina de Ridder** and **Yann Seimbille**
*Molecules* **2023**, *28*(10), 4022; **https://doi.org/10.3390/molecules28104022 (https://doi.org/10.3390/molecules28104022)** - 11 May 2023
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**Abstract** Prostate-specific membrane antigen (PSMA) targeting radiopharmaceuticals have been successfully used for diagnosis and therapy of prostate cancer. Optimization of the available agents is desirable to improve tumor uptake and reduce side effects to non-target organs. This can be achieved, for instance, via linker **[...] Read more.**
(This article belongs to the Special Issue **Novel Targeted Radiopharmaceuticals for Diagnosis and Therapy ( /journal/molecules/special_issues/therapy_molecules )**)

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Open Access Article 15 pages, 3951 KiB (/1420-3049/28/10/4021/pdf?version=1683793106)

## A New Self-Healing Degradable Copolymer Based on Polylactide and Poly(p-dioxanone) (/1420-3049/28/10/4021)

by **Laifa Tong**, **Mi Zhou**, **Yulong Chen**, **Kai Lu**, **Zhaohua Zhang**, **Yuesong Mu** and **Zejian He**

*Molecules* **2023**, *28*(10), 4021; **https://doi.org/10.3390/molecules28104021 (https://doi.org/10.3390/molecules28104021)** - 11 May 2023

**Cited by 7 (/1420-3049/28/10/4021#metrics)** | Viewed by 2046

**Abstract** In this paper, the copolymerization of poly (p-dioxanone) (PPDO) and polylactide (PLA) was carried out via a Diels–Alder reaction to obtain a new biodegradable copolymer with self-healing abilities. By altering the molecular weights of PPDO and PLA precursors, a series of copolymers (DA2300, **[...] Read more.**

(This article belongs to the Section **Macromolecular Chemistry (/journal/molecules/sections/macromolecular_chemistry)**)

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Open Access Article 16 pages, 3449 KiB (/1420-3049/28/10/4020/pdf?version=1683792140)

## Inhibition Studies on Human and Mycobacterial Carbonic Anhydrases with *N*-((4-Sulfamoylphenyl)carbamothioyl) Amides (/1420-3049/28/10/4020)

by **Morteza Abdoli**, **Alessandro Bonardi**, **Niccolò Paoletti**, **Ashok Aspatwar**, **Seppo Parkkila**, **Paola Gratteri**, **Claudiu T. Supuran** and **Raivis Žalubovskis**

*Molecules* **2023**, *28*(10), 4020; **https://doi.org/10.3390/molecules28104020 (https://doi.org/10.3390/molecules28104020)** - 11 May 2023

**Cited by 8 (/1420-3049/28/10/4020#metrics)** | Viewed by 2107

**Abstract** A library of structurally diverse *N*-((4-sulfamoylphenyl)carbamothioyl) amides was synthesized by selective acylation of easily accessible 4-thioureidobenzenesulfonamide with various aliphatic, benzylic, vinylic and aromatic acyl chlorides under mild conditions. Inhibition of three α-class cytosolic human (h) carbonic anhydrases (CAs) (EC 4.2.1.1); that is, **[...] Read more.**

(This article belongs to the Special Issue **Metalloenzyme Modulators and Enzyme Mimics: Synthesis and Applications ( /journal/molecules/special_issues/Metalloenzyme_Enzyme_Mimics )**)

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Open Access Article 15 pages, 1137 KiB (/1420-3049/28/10/4019/pdf?version=1683788983)

## Phytochemical Analysis and Evaluation of the Antioxidant, Antiproliferative, Antibacterial, and Antibiofilm Effects of *Globularia alypum* (L.) Leaves (/1420-3049/28/10/4019)

by **Sahar Nouir**, **Amal Dbeibia**, **Rim Bouhajeb**, **Houda Haddad**, **Amani Khélifa**, **Lotfi Achour**, **Mariem Ghardallou** and **Amira Zaïri**

*Molecules* **2023**, *28*(10), 4019; **https://doi.org/10.3390/molecules28104019 (https://doi.org/10.3390/molecules28104019)** - 11 May 2023

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**Abstract** *Globularia alypum* L. (GA) is a Mediterranean plant of the *Globulariaceae* family which is widely used in traditional Tunisian medicine. The main goal of this study was to evaluate the phytochemical composition, antioxidant, antibacterial, and antibiofilm activities, and the antiproliferative potential of different **[...] Read more.**

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Open Access Article 17 pages, 3259 KiB (/1420-3049/28/10/4018/pdf?version=1683786582)

***Tremella fuciformis* Polysaccharide Induces Apoptosis of B16 Melanoma Cells via Promoting the M1 Polarization of Macrophages (/1420-3049/28/10/4018)**

by **Lingna Xie**, **Guangrong Liu**, **Zebin Huang**, **Zhenyuan Zhu**, **Kaiye Yang**, **Yiheng Liang**, **Yani Xu**, **Lanyue Zhang** and **Zhiyun Du**

*Molecules* **2023**, *28*(10), 4018; **https://doi.org/10.3390/molecules28104018 (https://doi.org/10.3390/molecules28104018)** - 11 May 2023

**Cited by 8 (/1420-3049/28/10/4018#metrics)** | Viewed by 3453

**Abstract** Anti-tumor activity of *Tremella fuciformis* polysaccharides (TFPS) has been widely reported, but its mechanism remains poorly understood. In this study, we established an in vitro co-culture system (B16 melanoma cells and RAW 264.7 macrophage-like cells) to explore the potential anti-tumor mechanism of TFPS. **[...] Read more.**

(This article belongs to the Section **Natural Products Chemistry (/journal/molecules/sections/natural_products_chemistry)**)

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Open Access Review 18 pages, 3576 KiB (/1420-3049/28/10/4017/pdf?version=1683786483)

**The Development of Tungsten Biochemistry—A Personal Recollection (/1420-3049/28/10/4017)**

by **Wilfred R. Hagen**

*Molecules* **2023**, *28*(10), 4017; **https://doi.org/10.3390/molecules28104017 (https://doi.org/10.3390/molecules28104017)** - 11 May 2023

**Cited by 2 (/1420-3049/28/10/4017#metrics)** | Viewed by 2209

**Abstract** The development of tungsten biochemistry is sketched from the viewpoint of personal participation. Following its identification as a bio-element, a catalogue of genes, enzymes, and reactions was built up. EPR spectroscopic monitoring of redox states was, and remains, a prominent tool in attempts **[...] Read more.**

(This article belongs to the Special Issue **Molybdenum and Tungsten Enzymes—State of the Art in Research ( /journal/molecules/special_issues/9YY8Q0OE7H )**)

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Open Access Review 20 pages, 3926 KiB (/1420-3049/28/10/4016/pdf?version=1683784387)

**Updates on Plant-Based Protein Products as an Alternative to Animal Protein: Technology, Properties, and Their Health Benefits (/1420-3049/28/10/4016)**

by **Xiao Xiao**, **Peng-Ren Zou**, **Fei Hu**, **Wen Zhu** and **Zhao-Jun Wei**

*Molecules* **2023**, *28*(10), 4016; **https://doi.org/10.3390/molecules28104016 (https://doi.org/10.3390/molecules28104016)** - 11 May 2023

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**Abstract** Plant-based protein products, represented by “plant meat”, are gaining more and more popularity as an alternative to animal proteins. In the present review, we aimed to update the current status of research and industrial growth of plant-based protein products, including plant-based meat, plant- **[...] Read more.**

(This article belongs to the Special Issue **The Processing and Function of Natural Compounds and Nutraceuticals from Foods ( /journal/molecules/special_issues/Nutraceuticals_from_Foods )**)

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Open Access Review 21 pages, 6263 KiB (/1420-3049/28/10/4015/pdf?version=1683783460)

**Analogy of the Reactions of Aromatic and Aliphatic π-Electrophiles with Nucleophiles (/1420-3049/28/10/4015)**

by **Michał Barbasiewicz**, **Michał Fedoryński**, **Rafał Loska** and **Mieczysław Mąkosza**

*Molecules* **2023**, *28*(10), 4015; **https://doi.org/10.3390/molecules28104015 (https://doi.org/10.3390/molecules28104015)** - 11 May 2023

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**Abstract** The aim of this essay is to disclose the similarity of a great variety of reactions that proceed between nucleophiles and π-electrophiles—both aromatic and aliphatic. These reactions proceed via initial reversible addition, followed by a variety of transformations that are common for the **[...] Read more.**

(This article belongs to the Special Issue **Feature Papers in Organic Chemistry (Volume II) ( /journal/molecules/special_issues/S39J77T6FS )**)

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Open Access Review 29 pages, 8431 KiB (/1420-3049/28/10/4014/pdf?version=1683730316)

**PROTACs: Emerging Targeted Protein Degradation Approaches for Advanced Druggable Strategies (/1420-3049/28/10/4014)**

by **Nuwayo Ishimwe Sincere**, **Krishnan Anand**, **Sumel Ashique**, **Jing Yang** and **Chongge You**

*Molecules* **2023**, *28*(10), 4014; **https://doi.org/10.3390/molecules28104014 (https://doi.org/10.3390/molecules28104014)** - 10 May 2023

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**Abstract** A potential therapeutic strategy to treat conditions brought on by the aberrant production of a disease-causing protein is emerging for targeted protein breakdown using the PROTACs technology. Few medications now in use are tiny, component-based and utilize occupancy-driven pharmacology (MOA), which inhibits protein **[...] Read more.**

(This article belongs to the Section **Medicinal Chemistry (/journal/molecules/sections/medicinal_chemistry)**)

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Open Access Article 21 pages, 5936 KiB (/1420-3049/28/10/4013/pdf?version=1683726694)

**Conformational Distributions of Phenyl β-D-Glucopyranoside and Gastrodin in Solution by Vibrational Optical Activity and Theoretical Calculations (/1420-3049/28/10/4013)**

by **Mutasem Alshalalfeh**, **Ningjie Sun**, **Amanda Hanashiro Moraes**, **Alexandra Paola Aponte Utani** and **Yunjie Xu**

*Molecules* **2023**, *28*(10), 4013; **https://doi.org/10.3390/molecules28104013 (https://doi.org/10.3390/molecules28104013)** - 10 May 2023

**Cited by 2 (/1420-3049/28/10/4013#metrics)** | Viewed by 2128

**Abstract** The conformational landscapes of two highly flexible monosaccharide derivatives, namely phenyl β-D-glucopyranoside (ph-β-glu) and 4-(hydroxymethyl)phenyl β-D-glucopyranoside, also commonly known as gastrodin, were explored using a combined experimental and theoretical approach. For the infrared, Raman, and the associated vibrational optical activity (VOA), i.e., vibrational **[...] Read more.**

(This article belongs to the Special Issue **Theoretical and Computational and Experimental Advances on Molecular Optical Properties ( /journal/molecules/special_issues/mole_optic )**)

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Open Access Review 34 pages, 21979 KiB (/1420-3049/28/10/4012/pdf?version=1683722661)

**Analysis of Chlorophylls/Chlorophyllins in Food Products Using HPLC and HPLC-MS Methods (/1420-3049/28/10/4012)**

by **Badal Kumar Mandal** and **Yong-Chien Ling**

*Molecules* **2023**, *28*(10), 4012; **https://doi.org/10.3390/molecules28104012 (https://doi.org/10.3390/molecules28104012)** - 10 May 2023

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**Abstract** Of the different quality parameters of any food commodity or beverage, color is the most important, attractive and choice-affecting sensory factor to consumers and customers. Nowadays, food industries are interested in making the appearance of their food products attractive and interesting in order **[...] Read more.**

(This article belongs to the Special Issue **Application of Liquid Chromatography in Food and Natural Products Extracts Analysis ( /journal/molecules/special_issues/Liquid_Chromatography_Application )**)

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Open Access Article 12 pages, 920 KiB (/1420-3049/28/10/4011/pdf?version=1683871889)

**Impact of the Addition of Fruits of Kamchatka Berries (*L. caerulea* var. *kamtschatica*) and Haskap (*L. caerulea* var. *emphyllocalyx*) on the Physicochemical Properties, Polyphenolic Content, Antioxidant Activity and Sensory Evaluation Craft Wheat Beers (/1420-3049/28/10/4011)**

by **Justyna Belcar**, **Ireneusz Kapusta**, **Tomasz R. Sekutowski** and **Józef Gorzelany**

*Molecules* **2023**, *28*(10), 4011; **https://doi.org/10.3390/molecules28104011 (https://doi.org/10.3390/molecules28104011)** - 10 May 2023

**Cited by 4 (/1420-3049/28/10/4011#metrics)** | Viewed by 2334

**Abstract** Kamchatka berry (*Lonicera caerulea* var. *kamtschatica*) and haskap (*Lonicera caerulea* var. *emphyllocalyx*) fruit are important sources of bioactive compounds, mainly polyphenols, but also macro- and microelements. Physico-chemical analysis showed that wheat beers with added fruit were characterised by an **[...] Read more.**

(This article belongs to the Special Issue **Nutrition and Sensory Analysis of Food ( /journal/molecules/special_issues/6U3U3LPS01 )**)

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Open Access Article 20 pages, 3870 KiB (/1420-3049/28/10/4010/pdf?version=1683716040)

**Semisynthesis, Biological Evaluation and Molecular Docking Studies of Barbatic Acid Derivatives as Novel Diuretic Candidates (/1420-3049/28/10/4010)**

by **Xiang Yu**, **Yi Sui**, **Yinkai Xi**, **Yan Zhang**, **Guoyong Luo**, **Yi Long** and **Wude Yang**

*Molecules* **2023**, *28*(10), 4010; **https://doi.org/10.3390/molecules28104010 (https://doi.org/10.3390/molecules28104010)** - 10 May 2023

**Cited by 2 (/1420-3049/28/10/4010#metrics)** | Viewed by 1963

**Abstract** Barbatic acid, a compound isolated from lichen, has demonstrated a variety of biological activities. In this study, a series of esters based on barbatic acid (**6a**–**q′**) were designed, synthesized, and evaluated for their diuretic and litholytic activity at a **[...] Read more.**

(This article belongs to the Special Issue **Discovery of Bioactive Ingredients from Natural Products, 4th Edition ( /journal/molecules/special_issues/F905JORND2 )**)

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Open Access Review 28 pages, 4887 KiB (/1420-3049/28/10/4009/pdf?version=1683713233)

**Anticancer Activity of Chalcones and Its Derivatives: Review and In Silico Studies (/1420-3049/28/10/4009)**

by **Fernando Ferreira Leite**, **Natália Ferreira de Sousa**, **Bruno Hanrry Melo de Oliveira**, **Gabrielly Diniz Duarte**, **Maria Denise Leite Ferreira**, **Marcus Tullius Scotti**, **José Maria Barbosa Filho**, **Luís Cezar Rodrigues**, **Ricardo Olímpio de Moura**, **Francisco Jaime Bezerra Mendonça-Junior** and **Luciana Scotti**

*Molecules* **2023**, *28*(10), 4009; **https://doi.org/10.3390/molecules28104009 (https://doi.org/10.3390/molecules28104009)** - 10 May 2023
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**Abstract** Chalcones are direct precursors in the biosynthesis of flavonoids. They have an α,β-unsaturated carbonyl system which gives them broad biological properties. Among the biological properties exerted by chalcones, their ability to suppress tumors stands out, in addition to their low toxicity. In this **[...] Read more.**

(This article belongs to the Special Issue **Natural Products in Anticancer Activity ( /journal/molecules/special_issues/1I099R5R4V )**)

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Open Access Article 23 pages, 2338 KiB (/1420-3049/28/10/4008/pdf?version=1683712722)

**Assessment of the Use of Common Juniper (*Juniperus communis* L.) Foliage following the Cascade Principle (/1420-3049/28/10/4008)**

by **Irene Mediavilla**, **Raquel Bados**, **Lillian Barros**, **Virginie Xavier**, **Tiane C. Finimundy**, **Tania C. S. P. Pires**, **Sandrina A. Heleno**, **Ricardo C. Calhelha**, **Joana S. Amaral**, **Andrea Maria Rizzo**, **David Casini**, **Giacomo Lombardi**, **David Chiaramonti**, **Miguel Cámara**, **Ana Suárez**, **Tomás Ardid** and **Luis Saúl Esteban**

*Molecules* **2023**, *28*(10), 4008; **https://doi.org/10.3390/molecules28104008 (https://doi.org/10.3390/molecules28104008)** - 10 May 2023
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**Abstract** *Juniperus communis* L. is a species commonly grown in regions of the Northern Hemisphere, and is a good candidate to be cultivated in marginal lands. Plants coming from a pruning performed in a natural population located in Spain were used to assess the **[...] Read more.**

(This article belongs to the Special Issue **Research on Chemical Composition and Activity of Natural Products ( /journal/molecules/special_issues/WI249VOQY2 )**)

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Open Access Review 17 pages, 3882 KiB (/1420-3049/28/10/4007/pdf?version=1683711785)

**Layered-Oxide Cathode Materials for Fast-Charging Lithium-Ion Batteries: A Review (/1420-3049/28/10/4007)**

by **Xin Meng**, **Jiale Wang** and **Le Li**

*Molecules* **2023**, *28*(10), 4007; **https://doi.org/10.3390/molecules28104007 (https://doi.org/10.3390/molecules28104007)** - 10 May 2023

**Cited by 10 (/1420-3049/28/10/4007#metrics)** | Viewed by 6678

**Abstract** Layered oxides are considered prospective state-of-the-art cathode materials for fast-charging lithium-ion batteries (LIBs) owning to their economic effectiveness, high energy density, and environmentally friendly nature. Nonetheless, layered oxides experience thermal runaway, capacity decay, and voltage decay during fast charging. This article summarizes various **[...] Read more.**

(This article belongs to the Special Issue **Battery Chemistry: Recent Advances and Future Opportunities ( /journal/molecules/special_issues/S26MD67L5R )**)

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Open Access Article 25 pages, 2020 KiB (/1420-3049/28/10/4006/pdf?version=1683765125)

**Exploring Routes to Enhance the Calculation of Free Energy Differences via Non-Equilibrium Work SQM/MM Switching Simulations Using Hybrid Charge Intermediates between MM and SQM Levels of Theory or Non-Linear Switching Schemes (/1420-3049/28/10/4006)**

by **Andreas Schöller**, **H. Lee Woodcock** and **Stefan Boresch**

*Molecules* **2023**, *28*(10), 4006; **https://doi.org/10.3390/molecules28104006 (https://doi.org/10.3390/molecules28104006)** - 10 May 2023

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**Abstract** Non-equilibrium work switching simulations and Jarzynski's equation are a reliable method for computing free energy differences, $\Delta A^{\mathrm{low}\to\mathrm{high}}$, between two levels of theory, such as a pure molecular mechanical (MM) and a quantum mechanical/molecular mechanical (QM/MM) description of a **[...] Read more.**

(This article belongs to the Special Issue **Advances in Computational and Theoretical Chemistry ( /journal/molecules/special_issues/JE8L4W9822 )**)

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Open Access Review 26 pages, 1557 KiB (/1420-3049/28/10/4005/pdf?version=1683708200)

**Enrichment of Cookies with Fruits and Their By-Products: Chemical Composition, Antioxidant Properties, and Sensory Changes (/1420-3049/28/10/4005)**

by **Anna Krajewska** and **Dariusz Dziki**

*Molecules* **2023**, *28*(10), 4005; **https://doi.org/10.3390/molecules28104005 (https://doi.org/10.3390/molecules28104005)** - 10 May 2023

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**Abstract** Cookies made from wheat have become increasingly popular as a snack due to their various advantages, such as their convenience as a ready-to-eat and easily storable food item, wide availability in different types, and affordability. Especially in recent years, there has been a **[...] Read more.**

(This article belongs to the Special Issue **Natural Bioactive Compounds from Edible and Inedible Parts of Plants ( /journal/molecules/special_issues/Q54QV1T006 )**)

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Open Access Article 18 pages, 1055 KiB (/1420-3049/28/10/4004/pdf?version=1683707242)

## Edible Halophytes with Functional Properties: In Vitro Protein Digestibility and Bioaccessibility and Intestinal Absorption of Minerals and Trace Elements from Australian Indigenous Halophytes (/1420-3049/28/10/4004)

by **Sukirtha Srivarathan**, **Rama Addepalli**, **Oladipupo Qudus Adiamo**, **Gethmini Kavindya Kodagoda**, **Anh Dao Thi Phan**, **Olivia Renee Louise Wright**, **Yasmina Sultanbawa**, **Simone Osborne** and **Michael Erich Netzel**

*Molecules* **2023**, *28*(10), 4004; https://doi.org/10.3390/molecules28104004 (https://doi.org/10.3390/molecules28104004) - 10 May 2023

Cited by 3 (/1420-3049/28/10/4004#metrics) | Viewed by 2289

**Abstract** Halophytes are considered emerging functional foods as they are high in protein, minerals, and trace elements, although studies investigating halophyte digestibility, bioaccessibility, and intestinal absorption are limited. Therefore, this study investigated the in vitro protein digestibility, bioaccessibility and intestinal absorption of minerals and **[...] Read more.**

(This article belongs to the Special Issue **Advances in Functional Foods ( /journal/molecules/special_issues/adv_func_food )**)

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Open Access Article 14 pages, 3986 KiB (/1420-3049/28/10/4003/pdf?version=1683709774)

## Tuning the Site-to-Site Interaction of Heteronuclear Diatom Catalysts MoTM/$C_2N$ (TM = 3d Transition Metal) for Electrochemical Ammonia Synthesis (/1420-3049/28/10/4003)

by **Xiaoli Yang**, **Ping An**, **Ruiying Wang** and **Jianfeng Jia**

*Molecules* **2023**, *28*(10), 4003; https://doi.org/10.3390/molecules28104003 (https://doi.org/10.3390/molecules28104003) - 10 May 2023

Cited by 3 (/1420-3049/28/10/4003#metrics) | Viewed by 1965

**Abstract** Ammonia ($NH_3$) synthesis is one of the most important catalytic reactions in energy and chemical fertilizer production, which is of great significance to the sustainable development of society and the economy. The electrochemical nitrogen reduction reaction (eNRR), especially when driven by **[...] Read more.**

(This article belongs to the Section **Physical Chemistry (/journal/molecules/sections/Phys_Chem)**)

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Open Access Article 31 pages, 4515 KiB (/1420-3049/28/10/4002/pdf?version=1683792294)

## Formulation and Characterization of Mucoadhesive Polymeric Films Containing Extracts of Taraxaci Folium and Matricariae Flos (/1420-3049/28/10/4002)

by **Oana Mihaela Neagu**, **Timea Ghitea**, **Eleonora Marian**, **Laurian Vlase**, **Ana-Maria Vlase**, **Gabriela Ciavoi**, **Pálma Fehér**, **Annamária Pallag**, **Ildikó Bácskay**, **Dániel Nemes**, **Laura Grațiela Vicaș**, **Alin Teușdea** and **Tünde Jurca**

*Molecules* **2023**, *28*(10), 4002; https://doi.org/10.3390/molecules28104002 (https://doi.org/10.3390/molecules28104002) - 10 May 2023

Cited by (/1420-3049/28/10/4002#metrics) | Viewed by 2526

**Abstract** Taraxaci folium and Matricariae flos plant extracts contain a wide range of bioactive compounds with antioxidant and anti-inflammatory effects. The aim of the study was to evaluate the phytochemical and antioxidant profile of the two plant extracts to obtain a mucoadhesive polymeric

film [...] **Read more.**
(This article belongs to the Special Issue **Chemical Analysis of Bioactive Compounds ( /journal/molecules/special_issues/chem_analysis_bio_comp )**)

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Open Access Article 20 pages, 5837 KiB **(/1420-3049/28/10/4001/pdf?version=1683706627)**

**The Structural Combination of SIL and MODAG Scaffolds Fails to Enhance Binding to α-Synuclein but Reveals Promising Affinity to Amyloid β (/1420-3049/28/10/4001)**

by **Adriana Di Nanni**, **Ran Sing Saw**, **Gregory D. Bowden**, **Natasha S. R. Bidesi**, **Kaare Bjerregaard-Andersen**, **Špela Korat**, **Matthias M. Herth**, **Bernd J. Pichler**, **Kristina Herfert** and **Andreas Maurer**
*Molecules* **2023**, *28*(10), 4001; **https://doi.org/10.3390/molecules28104001 (https://doi.org/10.3390/molecules28104001)** - 10 May 2023
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**Abstract** A technique to image α-synuclein (αSYN) fibrils in vivo is an unmet scientific and clinical need that would represent a transformative tool in the understanding, diagnosis, and treatment of various neurodegenerative diseases. Several classes of compounds have shown promising results as potential PET **[...] Read more.**
(This article belongs to the Section **Medicinal Chemistry (/journal/molecules/sections/medicinal_chemistry)**)

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Open Access Editorial 3 pages, 169 KiB **(/1420-3049/28/10/4000/pdf?version=1683700360)**

**Applications of Catalytic Nanomaterials in Energy and Environment (/1420-3049/28/10/4000)**

by **Hongda Li**, **Shuai Jian** and **Mohammed Baalousha**
*Molecules* **2023**, *28*(10), 4000; **https://doi.org/10.3390/molecules28104000 (https://doi.org/10.3390/molecules28104000)** - 10 May 2023
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**Abstract** Nanotechnology is a crucial technology for the development of science and technology [...] **Full article (/1420-3049/28/10/4000)**
(This article belongs to the Special Issue **Catalytic Nanomaterials: Energy and Environment ( /journal/molecules/special_issues/Photocatalytic_Nanomaterials )**)

Open Access Article 11 pages, 7640 KiB **(/1420-3049/28/10/3999/pdf?version=1683698346)**

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**Magnetic and Electronic Properties of Sr Doped Infinite-Layer $NdNiO_2$ Supercell: A Screened Hybrid Density Functional Study (/1420-3049/28/10/3999)**

by **Yawen Hua**, **Meidie Wu**, **Qin Qin**, **Siqi Jiang**, **Linlin Chen** and **Yiliang Liu**

*Molecules* **2023**, *28*(10), 3999; **https://doi.org/10.3390/molecules28103999 (https://doi.org/10.3390/molecules28103999)** - 10 May 2023

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**Abstract** To understand the influence of doping Sr atoms on the structural, magnetic, and electronic properties of the infinite-layer $NdSrNiO_2$, we carried out the screened hybrid density functional study on the $Nd_{9-n}Sr_nNi_9O_{18}$ (*n* **[...] Read more.**

(This article belongs to the Special Issue **Computational Studies of Novel Function Materials ( /journal/molecules/special_issues/Y9PL52RVZC )**)

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Open Access Article 12 pages, 3363 KiB **(/1420-3049/28/10/3998/pdf?version=1683697511)**

**Superior Heavy Metal Ion Adsorption Capacity in Aqueous Solution by High-Density Thiol-Functionalized Reduced Graphene Oxides (/1420-3049/28/10/3998)**

by **Ho-Geun Kim**, **Jong-Seong Bae**, **Injoo Hwang**, **Sung-Hoon Kim** and **Ki-Wan Jeon**

*Molecules* **2023**, *28*(10), 3998; **https://doi.org/10.3390/molecules28103998 (https://doi.org/10.3390/molecules28103998)** - 10 May 2023

**Cited by 5 (/1420-3049/28/10/3998#metrics)** | Viewed by 2478

**Abstract** The preparation of mercapto-reduced graphene oxides (***m*-RGOs**) via a solvothermal reaction using $P_4S_{10}$ as a thionating agent has demonstrated their potential as an absorbent for scavenging heavy metal ions, particularly $Pb^{2+}$, from aqueous solutions due **[...] Read more.**

(This article belongs to the Special Issue **Carbon Nanomaterials Synthesis and Application for Electronic Materials ( /journal/molecules/special_issues/Carbon_Nanomaterials_Electronic )**)

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Open Access Article 13 pages, 4486 KiB **(/1420-3049/28/10/3997/pdf?version=1683695925)**

**Amelioration of Obesity-Related Disorders in High-Fat Diet-Fed Mice following Fecal Microbiota Transplantation from Inulin-Dosed Mice (/1420-3049/28/10/3997)**

by **Yinli Huang**, **Na Ying**, **Qihui Zhao**, **Junli Chen**, **Sin-Yeang Teow**, **Wei Dong**, **Minjie Lin**, **Lingling Jiang** and **Hong Zheng**

*Molecules* **2023**, *28*(10), 3997; **https://doi.org/10.3390/molecules28103997 (https://doi.org/10.3390/molecules28103997)** - 10 May 2023

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**Abstract** The role of inulin in alleviating obesity-related disorders has been documented; yet, its underlying mechanisms still need to be further investigated. This study attempted to elucidate the causative link between the gut microbiota and the beneficial effect of inulin on obesity-related disorders via **[...] Read more.**

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Open Access Review 43 pages, 1899 KiB **(/1420-3049/28/10/3996/pdf?version=1683683125)**

**Food Polyphenols and Type II Diabetes Mellitus: Pharmacology and Mechanisms (/1420-3049/28/10/3996)**

by **Rabia Naz**, **Fatima Saqib**, **Samir Awadallah**, **Muqeet Wahid**, **Muhammad Farhaj Latif**, **Iram Iqbal** and **Mohammad S. Mubarak**

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*Molecules* **2023**, *28*(10), 3996; **https://doi.org/10.3390/molecules28103996 (https://doi.org/10.3390/molecules28103996)** - 10 May 2023
**Cited by 52 (/1420-3049/28/10/3996#metrics)** | Viewed by 12467

**Abstract** Type II diabetes mellitus and its related complications are growing public health problems. Many natural products present in our diet, including polyphenols, can be used in treating and managing type II diabetes mellitus and different diseases, owing to their numerous biological properties. Anthocyanins, **[...] Read more.**

(This article belongs to the Special Issue **Novel Natural Compounds in Treatment of Diabetes ( /journal/molecules/special_issues/Natural_Compounds_Diabetes )**)

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Open Access Article 19 pages, 3185 KiB **(/1420-3049/28/10/3995/pdf?version=1683681870)**

## Microwave-Assisted Synthesis of Aminophosphonic Derivatives and Their Antifungal Evaluation against *Lomentospora prolificans* (/1420-3049/28/10/3995)

by **Zuleyma Martínez-Campos**, **Mariana Elizondo-Zertuche**, **Emanuel Hernández-Núñez**, **Eugenio Hernández-Fernández**, **Efrén Robledo-Leal** and **Susana T. López-Cortina**

*Molecules* **2023**, *28*(10), 3995; **https://doi.org/10.3390/molecules28103995 (https://doi.org/10.3390/molecules28103995)** - 10 May 2023
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**Abstract** *Lomentospora prolificans* is a pathogenic and multidrug-resistant fungus that can infect both immunocompetent and immunocompromised patients, with mortality rates up to 87%. The World Health Organization (WHO) included this fungal species in its first list of 19 priority fungal pathogens, which focused on **[...] Read more.**

(This article belongs to the Special Issue **From a Molecule to a Drug: Chemical Features Enhancing Pharmacological Potential II ( /journal/molecules/special_issues/mol_drug_II )**)

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Open Access Article 16 pages, 840 KiB **(/1420-3049/28/10/3994/pdf?version=1683702000)**

## Evaluation of Selected Medicinal, Timber and Ornamental Legume Species' Seed Oils as Sources of Bioactive Lipophilic Compounds (/1420-3049/28/10/3994)

by **Anna Grygier**, **Suryakant Chakradhari**, **Katarzyna Ratusz**, **Magdalena Rudzińska**, **Khageshwar Singh Patel**, **Danija Lazdiņa**, **Dalija Segliņa** and **Paweł Górnaś**

*Molecules* **2023**, *28*(10), 3994; **https://doi.org/10.3390/molecules28103994 (https://doi.org/10.3390/molecules28103994)** - 9 May 2023
**Cited by 3 (/1420-3049/28/10/3994#metrics)** | Viewed by 2577

**Abstract** Bioactive lipophilic compounds were investigated in 14 leguminous tree species of timber, agroforestry, medicinal or ornamental use but little industrial significance to elucidate their potential in food additive and supplement production. The tree species investigated were: *Acacia auriculiformis*, *Acacia concinna*, *Albizia* **[...] Read more.**

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Open Access Review 54 pages, 19096 KiB **(/1420-3049/28/10/3993/pdf?version=1683639764)**

## The Potential of *Ginkgo biloba* as a Source of Biologically Active Compounds—A Review of the Recent Literature and Patents (/1420-3049/28/10/3993)

by **Patrycja Biernacka**, **Iwona Adamska** and **Katarzyna Felisiak**

*Molecules* **2023**, *28*(10), 3993; **https://doi.org/10.3390/molecules28103993 (https://doi.org/10.3390/molecules28103993)** - 9 May 2023
**Cited by 39 (/1420-3049/28/10/3993#metrics)** | Viewed by 13408

**Abstract** *Ginkgo biloba* is a relict tree species showing high resistance to adverse biotic and abiotic environmental factors. Its fruits and leaves have high medicinal value due to the presence of flavonoids, terpene trilactones and phenolic compounds. However, ginkgo seeds contain toxic and

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allergenic **[...] Read more.**
(This article belongs to the Special Issue **Natural Bioactive Compounds from Edible and Inedible Parts of Plants ( /journal/molecules/special_issues/Q54QV1T006 )**)

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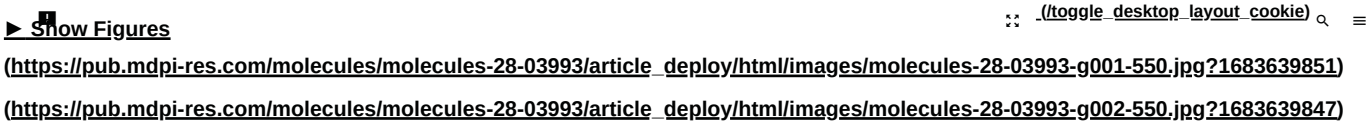

Open Access Feature Paper Review 29 pages, 12364 KiB **(/1420-3049/28/10/3992/pdf?version=1683699793)**

## Visualization of Phototherapy Evolution by Optical Imaging (/1420-3049/28/10/3992)

by **Zhiheng Li**, **Zheng Li** and **Jie Wang**
*Molecules* **2023**, *28*(10), 3992; **https://doi.org/10.3390/molecules28103992 (https://doi.org/10.3390/molecules28103992)** - 9 May 2023
**Cited by 4 (/1420-3049/28/10/3992#metrics)** | Viewed by 2919

**Abstract** Phototherapy, including photodynamic therapy (PDT) and photothermal therapy (PTT), is a non-invasive and effective approach used for cancer treatment, in which phototherapeutic agents are irradiated with an appropriate light source to produce cytotoxic reactive oxygen species (ROS) or heat to ablate cancer cells. **[...] Read more.**
(This article belongs to the Special Issue **Fluorescent Probes: From Structure Design to Property Tuning and Versatile Application ( /journal/molecules/special_issues/K6G0ZONS07 )**)

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## Structural Modeling of Nanobodies: A Benchmark of State-of-the-Art Artificial Intelligence Programs (/1420-3049/28/10/3991)

by **Mario S. Valdés-Tresanco**, **Mario E. Valdés-Tresanco**, **Daiver E. Jiménez-Gutiérrez** and **Ernesto Moreno**
*Molecules* **2023**, *28*(10), 3991; **https://doi.org/10.3390/molecules28103991 (https://doi.org/10.3390/molecules28103991)** - 9 May 2023
**Cited by 11 (/1420-3049/28/10/3991#metrics)** | Viewed by 3918

**Abstract** The number of applications for nanobodies is steadily expanding, positioning these molecules as fast-growing biologic products in the biotechnology market. Several of their applications require protein engineering, which in turn would greatly benefit from having a reliable structural model of the nanobody of **[...] Read more.**
(This article belongs to the Special Issue **Converging Nanochemistry: From Disease Prevention to Diagnosis and Treatment ( /journal/molecules/special_issues/nano_bioengineering )**)

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Open Access Article 15 pages, 2765 KiB (/1420-3049/28/10/3990/pdf?version=1683683297)

## Identification of *Daphne genkwa* and Its Vinegar-Processed Products by Ultraperformance Liquid Chromatography–Quadrupole Time-of-Flight Mass Spectrometry and Chemometrics (/1420-3049/28/10/3990)

by **Hongying Mi**, **Ping Zhang**, **Lingwen Yao**, **Huiyuan Gao**, **Feng Wei**, **Tulin Lu** and **Shuangcheng Ma**

*Molecules* **2023**, *28*(10), 3990; https://doi.org/10.3390/molecules28103990 (https://doi.org/10.3390/molecules28103990) - 9 May 2023

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**Abstract** Crude herbs of *Daphne genkwa* (CHDG) are often used in traditional Chinese medicine to treat scabies baldness, carbuncles, and chilblain owing to their significant purgation and curative effects. The most common technique for processing DG involves the use of vinegar to reduce the **[...] Read more.**

(This article belongs to the Section **Analytical Chemistry (/journal/molecules/sections/Analytical_Chemistry)**)

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Open Access Article 13 pages, 4358 KiB (/1420-3049/28/10/3989/pdf?version=1683637755)

## Rational Design of Monolithic g-$C_3N_4$ with Floating Network Porous-like Sponge Monolithic Structure for Boosting Photocatalytic Degradation of Tetracycline under Simulated and Natural Sunlight Illumination (/1420-3049/28/10/3989)

by **Delu Cao**, **Xueying Wang**, **Hefan Zhang**, **Daiqiong Yang**, **Ze Yin**, **Zhuo Liu**, **Changyu Lu** and **Feng Guo**

*Molecules* **2023**, *28*(10), 3989; https://doi.org/10.3390/molecules28103989 (https://doi.org/10.3390/molecules28103989) - 9 May 2023

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**Abstract** In order to solve the problems of powder g-$C_3N_4$ catalysts being difficult to recycle and prone to secondary pollution, floating network porous-like sponge monolithic structure g-$C_3N_4$ (FSCN) was prepared with a one-step thermal condensation method using melamine **[...] Read more.**

(This article belongs to the Section **Green Chemistry (/journal/molecules/sections/green-chemistry)**)

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Open Access Article 12 pages, 2022 KiB (/1420-3049/28/10/3988/pdf?version=1683628096)

## Determination of Minerals in Soft and Hard Cheese Varieties by ICP-OES: A Comparison of Digestion Methods (/1420-3049/28/10/3988)

by **Gaurav K. Deshwal**, **Laura G. Gómez-Mascaraque**, **Mark Fenelon** and **Thom Huppertz**

*Molecules* **2023**, *28*(10), 3988; https://doi.org/10.3390/molecules28103988 (https://doi.org/10.3390/molecules28103988) - 9 May 2023

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**Abstract** For sample preparation prior to mineral analysis, microwave digestion (~2 h) is quicker and requires lower acid volume as compared to dry (6–8 h) and wet digestion (4–5 h). However, microwave digestion had not yet been compared systematically with dry and wet digestion **[...] Read more.**

(This article belongs to the Special Issue **Nutrition and Sensory Analysis of Food ( /journal/molecules/special_issues/6U3U3LPS01 )**)

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Open Access Review 24 pages, 2822 KiB (/1420-3049/28/10/3987/pdf?version=1683630095)

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**Chemical Constitution, Pharmacological Effects and the Underlying Mechanism of Atractylenolides: A Review (/1420-3049/28/10/3987)**

by **Zhiyi Xie**, **Minqiu Lin**, **Xinglishang He**, **Yingjie Dong**, **Yigong Chen**, **Bo Li**, **Suhong Chen** and **Guiyuan Lv**

*Molecules* **2023**, *28*(10), 3987; **https://doi.org/10.3390/molecules28103987 (https://doi.org/10.3390/molecules28103987)** - 9 May 2023

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**Abstract** Atractylenolides, comprising atractylenolide I, II, and III, represent the principal bioactive constituents of *Atractylodes macrocephala*, a traditional Chinese medicine. These compounds exhibit a diverse array of pharmacological properties, including anti-inflammatory, anti-cancer, and organ-protective effects, underscoring their potential for future research and development. **[...] Read more.**

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Open Access Article 13 pages, 1645 KiB (/1420-3049/28/10/3986/pdf?version=1684906238)

**Chemical Characterization and Cytotoxic and Antioxidant Activity Evaluation of the Ethanol Extract from the Bulbs of *Pancratium maritimun* Collected in Sicily (/1420-3049/28/10/3986)**

by **Adele Cicio**, **Stefania Sut**, **Stefano Dall'Acqua**, **Maurizio Bruno**, **Claudio Luparello**, **Rosa Serio** and **Maria Grazia Zizzo**

*Molecules* **2023**, *28*(10), 3986; **https://doi.org/10.3390/molecules28103986 (https://doi.org/10.3390/molecules28103986)** - 9 May 2023

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**Abstract** *P. maritimum* L., belonging to the Amaryllidaceae family, is a species that grows on beaches and coastal sand dunes mainly on both sides of the Mediterranean Sea and Black Sea, the Middle East, and up to the Caucasus region. It has been largely **[...] Read more.**

(This article belongs to the Special Issue **Bioactive Compounds and Antioxidant Activity of Extracts from Different Natural Plants ( /journal/molecules/special_issues/antioxid_extra )**)

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Open Access Article 14 pages, 2363 KiB (/1420-3049/28/10/3985/pdf?version=1683626712)

**CH vs. HC—Promiscuous Metal Sponges in Antimicrobial Peptides and Metallophores (/1420-3049/28/10/3985)**

by **Kinga Garstka**, **Valentyn Dzyhovskyi**, **Joanna Wątły**, **Kamila Stokowa-Sołtys**, **Jolanta Świątek-Kozłowska**, **Henryk Kozłowski**, **Miquel Barceló-Oliver**, **Denise Bellotti** and **Magdalena Rowińska-Żyrek**

*Molecules* **2023**, *28*(10), 3985; **https://doi.org/10.3390/molecules28103985 (https://doi.org/10.3390/molecules28103985)** - 9 May 2023

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**Abstract** Histidine and cysteine residues, with their imidazole and thiol moieties that deprotonate at approximately physiological pH values, are primary binding sites for Zn(II), Ni(II) and Fe(II) ions and are thus ubiquitous both in peptidic metallophores and in antimicrobial peptides that may use nutritional **[...] Read more.**

(This article belongs to the Special Issue **Bioactive Peptides and Their Metal Complexes as Novel Antimicrobial Agents ( /journal/molecules/special_issues/bio_pepti_antimi )**)

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## Selenium Organic Content Prediction in Jengkol (*Archidendron pauciflorum*) and Its Molecular Interaction with Cardioprotection Receptors PPAR-γ, NF-κB, and PI3K (/1420-3049/28/10/3984)

by **Ayu Shalihat**, **Ronny Lesmana**, **Aliya Nur Hasanah** and **Mutakin Mutakin**

*Molecules* **2023**, *28*(10), 3984; https://doi.org/10.3390/molecules28103984 (https://doi.org/10.3390/molecules28103984) - 9 May 2023
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**Abstract** Selenium (Se) is a trace mineral found in plants with a distinct sulfuric odor that is cardioprotective and reported to have low toxicity. West Java, Indonesia, has a variety of plants with a distinct odor that are consumed raw, such as jengkol ( **[...] Read more.**
(This article belongs to the Special Issue **Bioactive Compounds in Food: Characterization and Role in Human Health ( /journal/molecules/special_issues/Z84TN6ONSM )**)

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## Ru-Controlled Thymine Tautomerization Frozen by a $k^1$(O)-, $k^2$(N,O)-Metallacycle: An Experimental and Theoretical Approach (/1420-3049/28/10/3983)

by **Silvia Bordoni**, **Riccardo Tarroni**, **Magda Monari**, **Stefano Cerini**, **Fabio Battaglia**, **Gabriele Micheletti**, **Carla Boga** and **Giacomo Drius**

*Molecules* **2023**, *28*(10), 3983; https://doi.org/10.3390/molecules28103983 (https://doi.org/10.3390/molecules28103983) - 9 May 2023
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**Abstract** The reaction of *mer*-$(Ru(H)_2(CO)(PPh_3)_3)$ (**1**) with one equivalent of thymine acetic acid (THAcH) unexpectedly produces the macrocyclic dimer $k^1$(O), $k^2$(N,O)-$(Ru(CO)(PPh_3)_2THAc)_2$ (**4**) and, concomitantly, **[...] Read more.**
(This article belongs to the Special Issue **Synthesis and Modification of Nitrogen Heterocyclic Compounds ( /journal/molecules/special_issues/X80O60664K )**)

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Open Access Review 17 pages, 2149 KiB (/1420-3049/28/10/3982/pdf?version=1683622124)

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**Advances in the Application of Bi-Based Compounds in Photocatalytic Reduction of $CO_2$ (/1420-3049/28/10/3982)**

by **Cheng Zuo**, **Qian Su** and **Zaiyong Jiang**

*Molecules* **2023**, *28*(10), 3982; **https://doi.org/10.3390/molecules28103982 (https://doi.org/10.3390/molecules28103982)** - 9 May 2023

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**Abstract** Bi-based semiconductor materials have special layered structure and appropriate band gap, which endow them with excellent visible light response ability and stable photochemical characteristics. As a new type of environment-friendly photocatalyst, they have received extensive attention in the fields of environmental remediation and **[...] Read more.**

(This article belongs to the Special Issue **Photocatalysis for Energy Transformation Reactions and Wastewater Treatment ( /journal/molecules/special_issues/24F024S7OS )**)

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Open Access Article 13 pages, 1246 KiB **(/1420-3049/28/10/3981/pdf?version=1683618763)**

**Fatty Acid-Rich Extract from *Holothuria atra* for Hyperuricemia via Expressions Modulation of GLUT9a and GLUT9b in Rat Model (/1420-3049/28/10/3981)**

by **Ikhsan Ikhsan**, **Rinaldi Idroes**, **Azharuddin Azharuddin**, **Rosnani Nasution**, **Rika Yusnaini** and **Muhammad Iqhrammullah**

*Molecules* **2023**, *28*(10), 3981; **https://doi.org/10.3390/molecules28103981 (https://doi.org/10.3390/molecules28103981)** - 9 May 2023

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**Abstract** An edible sea cucumber *Holothuria atra* has been hypothesized to have medicinal benefits against hyperuricemia owing to its bioactive compounds, including mono- and poly-unsaturated fatty acids. Herein, we aimed to investigate the fatty acids-rich extract produced from *H. atra* to treat hyperuricemic rats **[...] Read more.**

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**Phytochemical Characterization and Antimicrobial Activity of Several *Allium* Extracts (/1420-3049/28/10/3980)**

by **Ioana Andreea Barbu**, **Alexandra Ciorîță**, **Rahela Carpa**, **Augustin Catalin Moț**, **Anca Butiuc-Keul** and **Marcel Pârvu**

*Molecules* **2023**, *28*(10), 3980; **https://doi.org/10.3390/molecules28103980 (https://doi.org/10.3390/molecules28103980)** - 9 May 2023

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**Abstract** Microbial infections affect both the human population and animals. The appearance of more and more microbial strains resistant to classical treatments led to the need to develop new treatments. *Allium* plants are known for their antimicrobial properties due to their high content of **[...] Read more.**

(This article belongs to the Special Issue **Plant Bioactive Compounds: Extraction, Identification and Biological Activities ( /journal/molecules/special_issues/plant_bioact_compd )**)

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Open Access Article 11 pages, 1001 KiB **(/1420-3049/28/10/3979/pdf?version=1683614039)**

**Evaluation of Different Processes Impact on Flavor of Camellia Seed Oil Using HS-SPME-GC/MS (/1420-3049/28/10/3979)**

by **Ziming Li**, **Xiangyu Zhou**, **Hongai Li**, **Wenhua Zhou**, **Yuheng Tan**, **Yuxin Zhang**, **Jiarong She**, **Jun Lu** and **Ninghua Yu**

*Molecules* **2023**, *28*(10), 3979; **https://doi.org/10.3390/molecules28103979 (https://doi.org/10.3390/molecules28103979)** - 9 May 2023

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**Abstract** In this study, the flavor compounds of Camellia seed oils obtained by four processes were characterized by headspace solid phase microextraction/gas chromatography/mass spectrometry (HS-SPME/GC/MS). A variety of about 76 volatile flavor compounds were identified from all the oil samples. Of the four processing **[...] Read more.**

(This article belongs to the Special Issue **Preparation and Evaluation of Functional Components of Economic Crops and Their Multipurpose**

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Open Access Review 22 pages, 1340 KiB (/1420-3049/28/10/3978/pdf?version=1683613701)

**Aryl Hydrocarbon Receptor as an Anticancer Target: An Overview of Ten Years Odyssey (/1420-3049/28/10/3978)**

by **Hamza Hanieh**, **Mohammad Bani Ismail**, **Manal A. Alfwuaires**, **Hairul-Islam M. Ibrahim** and **Mahdi Farhan**

*Molecules* **2023**, *28*(10), 3978; **https://doi.org/10.3390/molecules28103978 (https://doi.org/10.3390/molecules28103978)** - 9 May 2023

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**Abstract** Aryl hydrocarbon receptor (AhR), a ligand-activated transcription factor belonging to the basic helix–loop–helix (bHLH)/per-Arnt-sim (PAS) superfamily, is traditionally known to mediate xenobiotic metabolism. It is activated by structurally diverse agonistic ligands and regulates complicated transcriptional processes through its canonical and non-canonical pathways in **[...] Read more.**

(This article belongs to the Special Issue **Molecular Targets and Mechanisms of Action of Anti-cancer Agents ( /journal/molecules/special_issues/Inhibitors_AntiCancer )**)

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Open Access Article 15 pages, 8073 KiB (/1420-3049/28/10/3972/pdf?version=1683605238)

**The Distinctive Permutated Domain Structure of Periplasmic α-Amylase (MalS) from Glycoside Hydrolase Family 13 Subfamily 19 (/1420-3049/28/10/3972)**

by **Yan An**, **Phuong Lan Tran**, **Min-Jee Yoo**, **Hyung-Nam Song**, **Kwang-Hyun Park**, **Tae-Jip Kim**, **Jong-Tae Park** and **Eui-Jeon Woo**

*Molecules* **2023**, *28*(10), 3972; **https://doi.org/10.3390/molecules28103972 (https://doi.org/10.3390/molecules28103972)** - 9 May 2023

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**Abstract** Periplasmic α-amylase MalS (EC. 3.2.1.1), which belongs to glycoside hydrolase (GH) family 13 subfamily 19, is an integral component of the maltose utilization pathway in *Escherichia coli* K12 and used among Ecnterobacteriaceae for the effective utilization of maltodextrin. We present the crystal structure **[...] Read more.**

(This article belongs to the Special Issue **Advances in Amylases ( /journal/molecules/special_issues/G7C8D1F97U )**)

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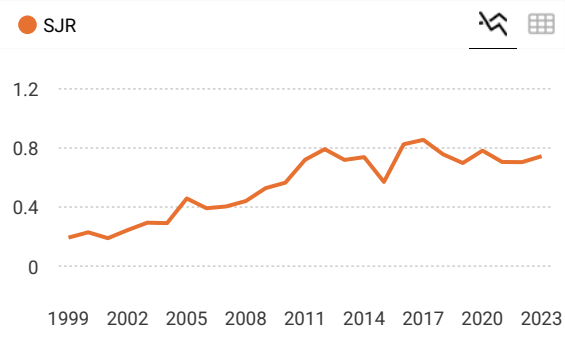
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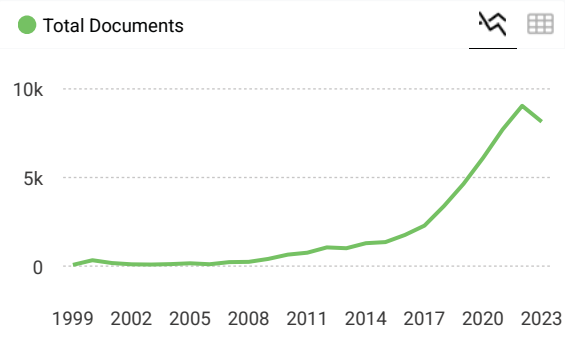
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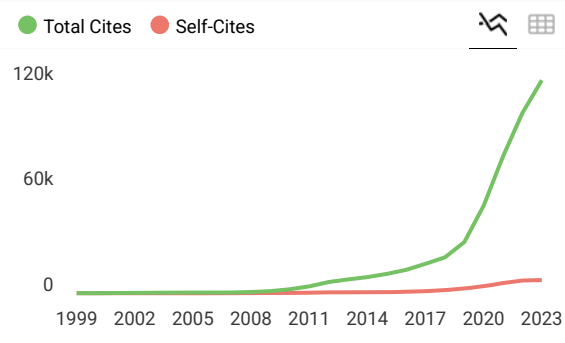
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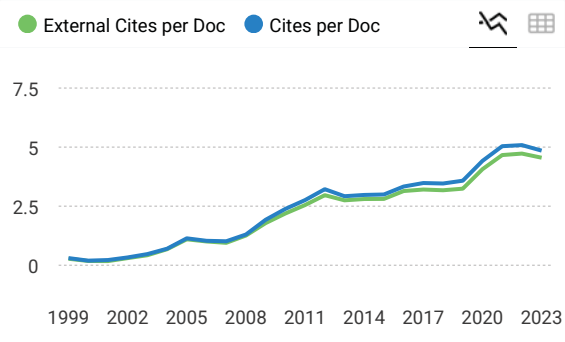
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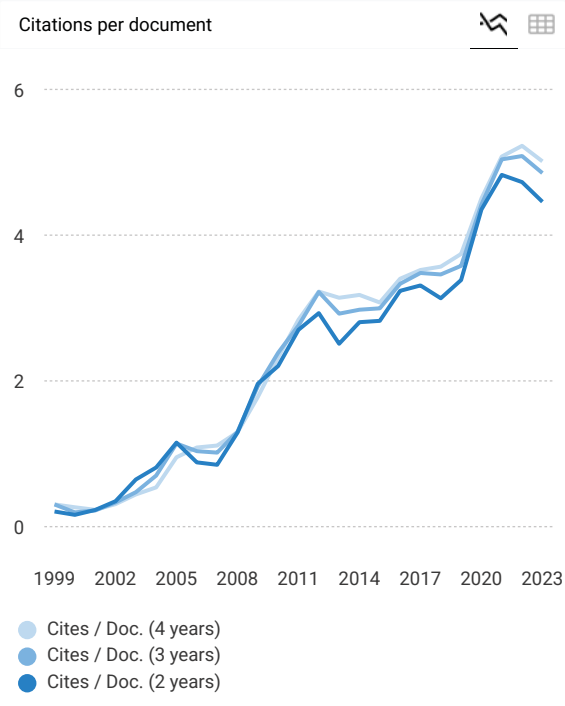
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1999 2002 2005 2008 2011 2014 2017 2020 2023
Cites / Doc. (4 years)
Cites / Doc. (3 years)
Cites / Doc. (2 years)


% International Collaboration
40
20
0
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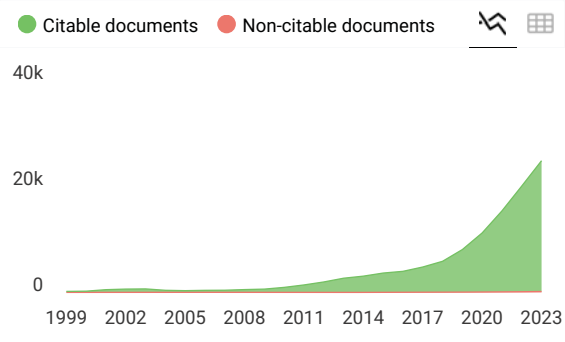
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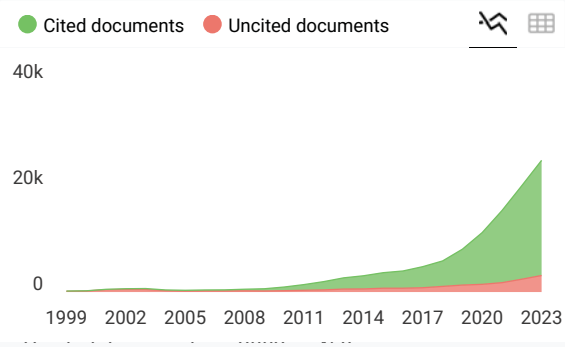
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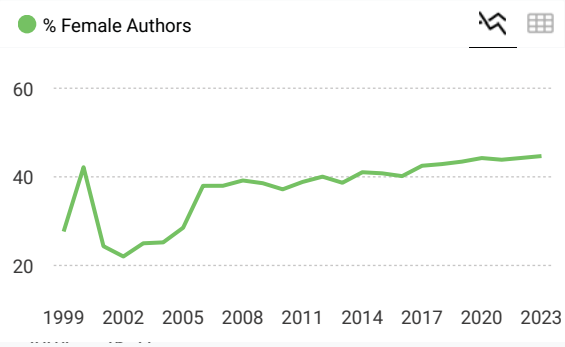
% Female Authors
60
40
20
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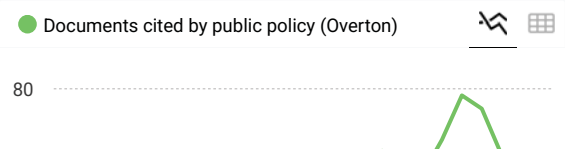
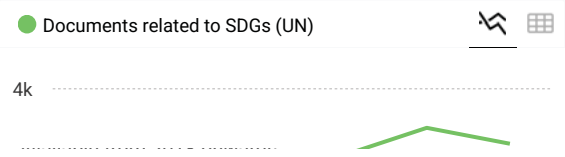

Documents cited by public policy (Overton)
80


Documents related to SDGs (UN)
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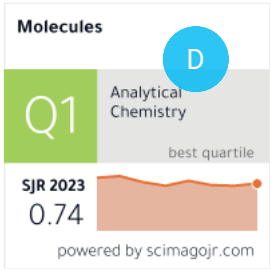
on

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M **Mervat Hamdy** 3 months ago

I would be grateful if you could let me know the impact factor of the journal for the year 2023.

reply

SCImago Team

**Melanie Ortiz** 3 months ago

Dear Mervat, thank you very much for your comment. SCImago Journal and Country Rank uses Scopus data, our impact indicator is the SJR (Check it above). We suggest you consult the Journal Citation Report for other indicators (like Impact Factor) with a Web of Science data source. Best Regards, SCImago Team

R **roderick bhig** 7 months ago

dear editor,

good evening. will you accept my article the title is "trends in electrochemistry". please send me the template.

many thanks

dick bhig

reply

SCImago Team

**Melanie Ortiz** 6 months ago

Dear Roderick,
Thank you for contacting us.
We suggest you visit the journal's homepage (See submission/author guidelines) or contact the journal's editorial staff , so they could inform you more deeply.
Best Regards, SCImago Team

M **Melva Silitonga** 2 years ago

Dear Sir or Madam, I want to publish in this journal, send me this journal template please

reply

SCImago Team

**Melanie Ortiz** 2 years ago

Dear Melva,
Thank you for contacting us.
We suggest you visit the journal's homepage (See submission/author guidelines) or contact the journal's editorial staff , so they could inform you more deeply.
Best Regards, SCImago Team

A **Andrey Kistanov** 2 years ago

Highly DISrecommend MDPI journal "Molecules" and its Special Issue "2D Materials: Synthesis and Energy Applications". Very unprofessional review process. Incredible disrespect of Editor to authors.

reply

H **heyam Saad Ali** 4 years ago

Dear sir,
I would be grateful if you let me know if the coverage of this journal is included in this year 2021 in Scopus?

reply

SCImago Team

**Melanie Ortiz** 4 years ago

Dear Heyam,
Thank you very much for your comment.
All the metadata have been provided by Scopus /Elsevier in their last update sent to SCImago, including the Coverage's period data. The SJR for 2019 was released on 11 June 2020. We suggest you consult the Scopus database directly to see the current index status as SJR is a static image of Scopus, which is changing every day.
Best Regards, SCImago Team

A **Aliaa Ali El Shamy** 4 years ago

Dear editor
Would you please inform me about the publication fees in Molecules, thanks in advance.

reply

M **Mohammad Alhilal** 4 years ago

APC=2000 CHF (Swiss Francs)

SCImago Team

**Melanie Ortiz** 4 years ago

Dear Aliaa,
thank you for contacting us.
Unfortunately, we cannot help you with your request, we suggest you visit the journal's homepage or contact the journal's editorial staff , so they could inform you more deeply.
Best Regards, SCImago Team

R **Rodriguez-Mora** 5 years ago

Dear Editor,
Is molecules Q1 or Q2? in the main list appear like Q2 but then homepage like Q1.

reply

A **Adil** 5 years ago

Is molecules journal Q1 or Q2, please?

SCImago Team

**Melanie Ortiz** 5 years ago

Dear Adil, thank you for contacting us. For every journal, the annual value of the SJR is integrated into the distribution of SJR values of all the thematic categories to which the journal belongs. There are more than 300 thematic categories. The position of each journal is different in any category and depends on the performance of the category, in general, and the journal, in particular. See the Quartile's data for all the categories just above. Best Regards, SCImago Team

SCImago Team

**Melanie Ortiz** 5 years ago

Dear Rodríguez-Mora,
thank you for contacting us.
We are sorry to tell you that we are not the journal's editor. SCImago Journal & Country Rank is not a journal. SJR is a portal with scientometric indicators of journals indexed in Elsevier/Scopus.
In the case of SCImago, for every journal, the annual value of the SJR is integrated into the distribution of SJR values of all the thematic categories to which the journal belongs.

There are more than 300 thematic categories. The position of each journal is different in any category and depends on the performance of the category, in general, and the journal, in particular . See the Quartiles'data just above.

Best Regards, SCImago Team

D

**Dr. Mejdi Snoussi** 5 years ago

Please how can provide a list of qi and Q2 journals in Microbiology and essential oil characterization

reply

SCImago Team

**Melanie Ortiz** 5 years ago

Dear Mejdi, thank you very much for your comment. If you need bibliographic information or full text, we suggest you to do a research by subjetc area/category here: https://www.scimagojr.com/journalrank.php

Best Regards, SCImago Team

K

**khulud** 5 years ago

Dear Editor,
what is SJR for journal in 2010 ? Thank you

reply

SCImago Team

**Melanie Ortiz** 5 years ago

Dear user,

as it appears in SJR website, the SJR for this journal in 2010 is 0.565. Best Regards, SCImago Team

S

**Seham Abdel-Shafi** 6 years ago

Dear Editor,
Is the Molecules Q1 or Q2

reply

M

**Maximus M Taek** 6 years ago

Dear Editor,
Do this journal receive original article from the field of ethnomedicinal research? Thank you

reply

SCImago Team

**Elena Corera** 6 years ago

Dear Maximus,

thank you very much for your comment. Unfortunately, we cannot help you with your request, we suggest you contact journal's editorial staff so they could inform you more deeply. You can find contact information in SJR website https://www.scimagojr.com

Anyway, if there is any user who has already published in the journal, maybe could help us with your request.

Best Regards,
SCImago Team

H

**heyam saad ali** 7 years ago

Dear sir,
i would be grateful if you let me know the impact factor of the journal for the year 2018

reply

SCImago Team

**Elena Corera** 7 years ago

Dear Heyam, the 2018 articles have not been published yet, therefore, there is no citation flow available for those articles either. The 2018 indicators will be available in 2019. Best Regards, SCImago Team

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Email
(will not be published)

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The users of Scimago Journal & Country Rank have the possibility to dialogue through comments linked to a specific journal. The purpose is to have a forum in which general doubts about the processes of publication in the journal, experiences and other issues derived from the publication of papers are resolved. For topics on particular articles, maintain the dialogue through the usual channels with your editor.

# Source details

## Molecules

*Open Access*

Years currently covered by Scopus: from 1996 to 2025

Publisher: Multidisciplinary Digital Publishing Institute (MDPI)

E-ISSN: 1420-3049

Subject area: Chemistry: Chemistry (miscellaneous) | Chemistry: Organic Chemistry | Pharmacology, Toxicology and Pharmaceutics: Pharmaceutical Science | Chemistry: Physical and Theoretical Chemistry | Chemistry: Analytical Chemistry | View all

Source type: Journal

CiteScore 2023
7.4

SJR 2023
0.744

SNIP 2023
1.064

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CiteScore | CiteScore rank & trend | Scopus content coverage

### CiteScore 2023

$$7.4 = \frac{228{,}683 \text{ Citations } 2020 - 2023}{30{,}773 \text{ Documents } 2020 - 2023}$$

Calculated on 05 May, 2024

### CiteScoreTracker 2024

$$8.5 = \frac{261{,}750 \text{ Citations to date}}{30{,}709 \text{ Documents to date}}$$

Last updated on 05 March, 2025 • Updated monthly

### CiteScore rank 2023

| Category | Rank | Percentile |
|---|---|---|
| Chemistry<br>Chemistry (miscellaneous) | #19/111 | 83rd |
| Chemistry<br>Organic Chemistry | #39/211 | 81st |
| Pharmacology, | | |

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