CAS SciFinder

Task History

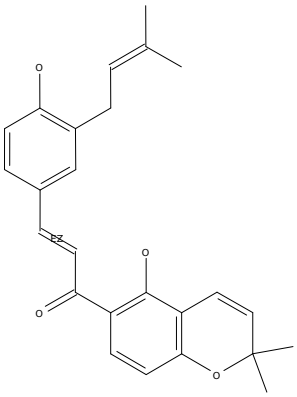
Initiating Search

July 8, 2024, 7:25 PM

Substances:

Filtered By:

Stereochemistry: **Double Bond Geometry As Drawn**



Structure Match: **As Drawn**

Search Tasks

Task	Search Type	View
Returned Substance Results + Filters (1)	**Substances**	View Results
Exported: Retrieved Related Reference Results (13)	**References**	View Results

CAS SciFinder

References (13)

View in CAS SciFinder

1

Phytoconstituents, antioxidant, and cholinesterase inhibitory activities of the leaves and stem extracts of Artocarpus sericicarpus

35 Substances • 0 Reactions • 0 Citations

By: Suciati, Suciati; Laili, Erlinda Rhohmatul; Haula, Hamizah; Tumewu, Lidya; Nuengchamnong, Nitra; Suphrom, Nungruthai; Widyawaruyanti, Aty

Pharmacia (Sofia, Bulgaria) (2024), 71(1), 1-8 | Language: English, Database: CAplus

The study aimed to investigate the antioxidant and cholinesterase inhibitory activities of the leaves and stems of Artocarpus serici carpus and to analyze the phenolic compounds in the extracts The modified Ellmans method was used to determine the choline sterase inhibitory activities against acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) enzymes. The antiox idant properties were evaluated using DPPH and ABTS methods. The total phenolic content (T PC) was measured by spectro metric assay, and compound identification was carried out by LC-MS/MS anal. The results showed that the leaf and stem extracts of A. serici carpus exerted significant inhibitory effects against AChE and BChE, as well as antioxidant activities. The stem ethanolic extract exhibited the highest potency against AChE and BChE with IC50 values of 5.81 and 11.46 μg/m L, resp. The leaf and stem ethanolic extracts gave higher antioxidant activities and TPC compared to the water-based extracts The LC-MS/MS anal. indicated the presence of phenolic compounds, such as flavones, flavonols, flavanones, prenylated chalcones, and xanthones in the extracts

Keywords: Artocarpus chlorogenic acid isoquercetin artoninJ artonin B AChE BChE LCMSMS

Substances (35) | Reactions (0) | Citing (0)

2

Revisiting Licorice as a functional food in the management of neurological disorders: Bench to trend

10 Substances • 0 Reactions • 5 Citations

By: Sharma, Ruchi; Singla, Rajeev K.; Banerjee, Subhadip; Sharma, Rohit

Neuroscience & Biobehavioral Reviews (2023), 155, 105452 | Language: English, Database: CAplus and MEDLINE

A review. Traditional and scientific evidence attribute numerous bioacti vities of Licorice (Glycyr rhiza glabra Linn.) in aging-related disorders. In this state-of-art review, an extensive search in several databases was conducted to collect all relevant literature and comprehensively analyze Licorice's pharmacol. attributes, neuroprotective properties, safety, and its mechanistic role in treating various neurol. conditions. Network pharmacol. was employed for the first time exploring the mechan istic role of Licorice in neurol. disorders. Its neuroprotective role is attributed to phytocons tituents, including liquiritin, glycyrrhizic acid, liquirit igenin, glabridin, 18ss-glycyrrhetinic acid, quercetin, isoliquir itigenin, paratocarpin B, glycyglabrone, and hispaglabridin B, as evident from in vitro and in vivo studies. Network pharmacol. anal. reveals that these compounds protect against long-term depression, aging-associated diseases, Alzheimer's disease, and other addictions through inter actions with cholin ergic, dopamin ergic, and seroto nergic proteins, validated in animal studies only. Future clin. trials are warranted as Licorice administration has a limiting factor of mild hypert ension and hypokalemia. Hopefully, scientific updates on Licorice will propagate a paradigm shift in medicine, research propag ation, and development of the central nervous system phytoph armaceuticals.

Keywords: review Glycyrrhiza neurol disorder aging related disease; Licorice; Network pharmac ology; Neurodegeneration; Neurol ogical disease; Oxidative stress; Pathways

Substances (10) | Reactions (0) | Citing (5)

3

Computational prediction of phytochemical inhibitors against the cap-binding domain of Rift Valley fever virus

9 Substances • 0 Reactions • 0 Citations

By: Muralitharan, Ishwarya; Sahoo, Ajaya Kumar; Augusthian, Priya Dharshini; Samal, Areejit
Molecular Diversity, | Language: English, Database: CAplus and MEDLINE

Rift Valley fever is a zoonotic disease that can spread through livestock and mosquitoes, and its symptoms include retinitis, photop hobia, hemorrhagic fever and neurol. effects. The World Health Organi zation has identified Rift Valley fever as one of the viral infections that has potential to cause a future epidemic. Hence, efforts are urgently needed toward development of therapeutics and vaccine against this infectious disease. Notably, the causative virus namely, the Rift Valley fever virus (RVFV), utilizes the cap-snatching mechanism for viral transcr iption, rendering its cap-binding domain (CBD) as an effective antiviral target. To date, there are no published studies towards identification of potential small mol. inhibitors for the C BD of RVFV. Here, we employ a virtual screening workflow comprising of mol. docking and mol. dynamics (MD) simulation, to identify 5 potential phytochem. inhibitors of the CBD of RVFV. These 5 phytochem. inhibitors can be sourced from Indian medicinal plants, Ferula assa- foetida, Glycyrrhiza glabra and Leucas cephalotes, used in traditional medicine. In sum, the 5 phytochem. inhibitors of the C BD of RVFV identified by this purely computational study are promising drug lead mols. which can be considered for detailed exptl. validation against R VFV infection.

Keywords: phytochem retinitis antiviral agent rift valley fever virus; Cap-binding domain; Molecular docking; Molecular dynamics; Phytochemical inhibitors; Rift Valley fever virus; Virtual screening

Substances (9) Reactions (0) Citing (0)

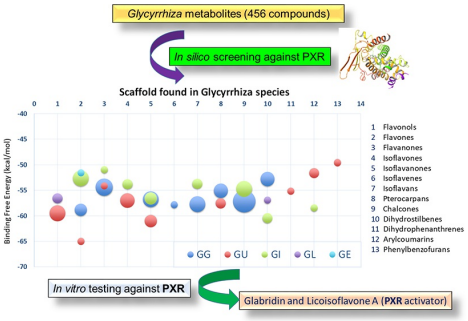
4

Computational Tools to Expedite the Identification of Potential PXR Modulators in Complex Natural Product Mixtures: A Case Study with Five Closely Related Licorice Species

94 Substances • 0 Reactions • 0 Citations

By: Alhusban, Manal; Pandey, Pankaj ; Ahn, Jongmin ; Avula, Bharathi; Haider, Saqlain ; Avonto, Cristina ; Ali, Zulfiqar ; Khan, Shabana I.; Ferreira, Daneel ; Khan, Ikhlas A.; et al

ACS Omega (2022), 7(30), 26824-26843 | Language: English, Database: CAplus and MEDLINE



The genus Glycyrrhiza, comprising approx. 36 spp., possesses complex structural diversity and is documented to possess a wide spectrum of biol. activities. Understanding and finding the mechanisms of efficacy or safety for a plant- based therapy is very challe nging, yet it is crucial and necessary to understand the polypha rmacol. of traditional medicines. Licorice extract was shown to modulate the xenobiotic receptors, which might manifest as a potential route for natural product-induced drug interactions. However, different mechanisms could be involved in this phenomenon. Since the induced herb-drug interaction of licorice supple ments via Pregnane X receptor (P XR) is understudied, we ventured out to analyze the potential modulators of P XR in complex mixtures such as whole extracts by applying computational mining tools. A total of 518 structures from five species of Glycyr rhiza: 183 (G. glabra), 180 (G. uralensis), 100 (G. inflata), 33 (G. echinata), and 22 (G. lepidota) were collected and post- processed to yield 387 unique compounds Visual inspection of top candidates with favorable ligand-PXR interactions and the highest docking scores were identified. The in vitro testing revealed that glabridin (G G-14) is the most potent PXR activator among the tested compounds, followed by licoisoflavone A, licoisoflavanone, and glycycoumarin. A 200 ns mol. dynamics study with glabridin confirmed the stability of the glabridin-PXR complex, highlighting the importance of computational methods for rapid derepli cation of potential xenobiotic modulators in a complex mixture instead of undertaking time-consuming classical biol. testing of all compounds in a given botanical.

Keywords: computational identification PXR modulator Glycyrrhiza natural product mixture

Substances (94) | Reactions (0) | Citing (0)

5

Bio-chemical characterization and in silico computational experimental properties of Trianthema triquetra Rottler & Willd.: A desert medicinal plant for industrial products

24 Substances • 0 Reactions • 1 Citation

By: Khurshid, Umair; Ahmad, Saeed; Saleem, Hammad; Aziz, Marya; Wazir, Muhammad Asif; Sarfraz, Muhammad; Anwar, Sirajudheen; Ansari, Siddique Akber; Ahmed, Sarfaraz; Mollica, Adriano; et al
Industrial Crops and Products (2022), 177, 114474 | Language: English, Database: CAplus

This research work prospects the phytochem. and biol. properties of different polarity solvent (methanol, ethyl-acetate, n-hexane, and n-butanol) extracts of Trianthema triquetra Rottler & Willd. The assessment of chem. profile was done by ascert aining total bioactive contents and UHPLC-MS anal. Similarly, biol. profile was analyzed via determi nation of antiox idant (DPPH, ABTS, FRAP, CUP RAC, phosphomolybdenum and metal chelation) and key enzyme inhibition (acetylc holinesterase, butyrylcholinesterase, α-amylase, α-glucosidase, and tyrosinase) potential. Principal component anal. (P CA) was also conducted to highlight the correl ation amongst bioactive contents and tested bioassays. The highest proportion of total phenolic (59.85 mg GAE/g extract) and flavonoid (19.85 mg RE/g extract) contents were exhibited by methanol extract which might be correlated with its higher antiox idant capacity. Similarly, UHPLC-MS phytochem. profiling of the methanol extract unveiled the identif ication of 26 secondary metabo lites belonging to phenolic, flavonoids, glucoside, coumarin, alkaloid, and fatty acid deriva tives The ethyl-acetate fraction exhibited the highest inhibition against BChE, α-amylase and α-glucosidase, while the n-butanol and n-hexane extracts were found to be the active against AChE and tyrosinase enzymes and the mol. docking studies explained the possible mechanism of enzyme inhibi tion. Results of antioxidant assays were further confirmed by P CA anal., which shows highly effective associ ation amid total bioactive contents and antioxidant assays.

Keywords: Trianthema medicinal plant acetylcholinesterase tyrosinase

Substances (24) Reactions (0) Citing (1)

6

New insights into binding of natural chalcones to Bcl-2, Bcl-xL and Mcl-1 anti-apoptotic proteins

62 Substances • 0 Reactions • 0 Citations

By: Cirin, Dejan; Krstonosic, Veljko
Journal of Molecular Structure (2021), 1241, 130700 | Language: English, Database: CAplus

Knowledge about mechanisms responsible for induction of tumor cell apoptosis is important for the develo pment of anticancer drugs. Mounting evidence suggests that the inhibition of anti-apoptotic proteins of Bcl-2 family is important part of antitumor activity of natural chalcones. In order to gain insights into their binding affinity and binding mechanism, the MM-GBSA binding energies were determined for 63 natural chalcones to Bcl-2, Bcl-xL and Mcl-1, by employing multiple crystal structures of each anti-apoptotic protein. It was noticed that the chalcones have high affinity to the B H3-binding groove. The driving forces behind the binding and the anchor points on the proteins were determined for the top-ranked chalcones, whereas the 300-ns Mol. Dynamics (MD) simulations provided more insights into the binding in the most stable complexes. The importance of ring A, ring B and the side chains of the chalcones for the interactions with the hydrop hobic cavities of anti-apoptotic proteins was noticed. Although the natural compounds showed mainly favorable pharmacokinetic properties, some limitations in binding to the proteins, compared to the synthetic ligands, were noticed. This pointed out towards possible future directions of chem. modifications of the most potent natural compounds It is envisioned that the results of this study could be useful for the selection of lead antitumor natural compounds as well as for the design of new synthetic BH3-mimetics.

Keywords: natural chalcone binding antiapoptotic protein inhibition antitumor activity

Substances (62) Reactions (0) Citing (0)

7

Screening of hepatoprotective compounds from licorice against carbon tetrachloride and acetaminophen induced HepG2 cells injury

171 Substances • 0 Reactions • 37 Citations

By: Kuang, Yi; Lin, Yan; Li, Kai; Song, Wei; Ji, Shuai; Qiao, Xue; Zhang, Qingying; Ye, Min

Phytomedicine (2017), 34, 59-66 | Language: English, Database: CAplus and MEDLINE

Licorice and its constituents, especially licorice flavonoids have been reported to possess signif icant hepatoprotective activities. However, previous studies mainly focus on the extract and major compounds, and few reports are available on other licorice compounds This work aims to evaluate the in vitro hepatoprotective activities of licorice compounds and screen active compounds, and to establish the structure-activity relationship. A compound library consisting of 180 compounds from three medicinal licorice species, Glycyrrhiza uralensis, G. glabra and G. inflata was establ ished. HepG2 cells were incubated with the compounds, together with the treatment of 0.35% CCl_4 for 6h and 14m M APAP for 24h, resp. A total of 62 compounds at 10μ M showed protective effects against CCl_4 to improve cell viability from 52.5% to >60%, and compounds 5 (licofl avone A), 104 (3,4-didehydroglabridin), 107 (isoliquiritigenin), 108 (3,4,3',4'-tetrahydroxychalcone), and 111 (licoch alcone B) showed the most potent activities, improving cell viability to >80%. And 64 compounds showed protective effects against APAP to improve cell viability from 52.0% to >60%, and compounds 47 (derrone), 76 (xambioona), 77 ((2S)-abyssinone I), 107 (isoliquiritigenin), 118 (licoagrochalcone A), and 144 (2'-O-demethybidwillol B) showed the most potent activi ties, improving cell viability to >80%. Prelim inary structure-activity anal. indicated that free phenolics compounds especially chalcones showed relatively stronger protective activities than other types of compounds Compounds 5, 76, 104, 107, 111, 118 and 144 possess potent activities against both CCl_4 and APAP, and 5, 76 and 118 were reported for the first time. They could be the major active compounds of licorice for the treatment of liver injury.

Keywords: Glycyrrhiza xambioona carbon tetrach loride acetami nophen hepatoprotection licorice cell injury; Acetami nophen; CCl(4); Hepatoprotective; Licorice; Liver injury

Substances (171) | Reactions (0) | Citing (37)

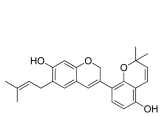
8

Glycybridins A-K, bioactive phenolic compounds from Glycyrrhiza glabra

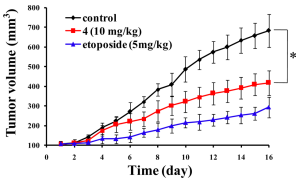
69 Substances • 0 Reactions • 68 Citations

By: Li, Kai; Ji, Shuai; Song, Wei; Kuang, Yi; Lin, Yan; Tang, Shunan; Cui, Zexu; Qiao, Xue; Yu, Siwang; Ye, Min

Journal of Natural Products (2017), 80(2), 334-346 | Language: English, Database: CAplus and MEDLINE



glycybridin D (4)



In an attempt to discover bioactive agents from the herbal medicine Glycyrrhiza glabra (widely known as licorice), 11 new phenolic compounds, glycybridins A-K (1-11), along with 47 known phenolics (12-58) were isolated. Their structures were elucidated on the basis of extensive NMR and MS analyses as well as exptl. and computed E CD data. According to the clin. therap eutic effects of licorice, enzyme or cell-based bioactivity screenings of 1-58 were conducted. A number of compounds signifi cantly activate Nrf2, inhibit tyrosinase or PTP1B, inhibit LPS-induced NO production and NF-κB transcription, and inhibit the proliferation of human cancer cells (HepG2, SW480, A549, MCF7). Glycybridin D (4) showed moderate cytotoxic activities against the four cancer cell lines, with IC_{50} values ranging from 4.6 to 6.6 μ M. Further studies indicated that 4 (10 mg/kg, i.p.) decreased tumor mass by 39.7% on an A549 human lung carcinoma xenograft mice model, but showed little toxicity.

Keywords: glycybridin bioactive phenolic compound Glycyr rhiza

Substances (69) | Reactions (0) | Citing (68)

9

Prenylated chalcones from Desmodium renifolium

11 Substances • 0 Reactions • 17 Citations

By: Li, Yan-Ping; Yang, Yu-Chun; Li, Yin-Ke; Jiang, Zhi-Yong; Huang, Xiang-Zhong; Wang, Wei-Guang; Gao, Xue-Mei; Hu, Qiu-Fen

Phytochemistry Letters (2014), 9, 41-45 | Language: English, Database: CAplus

Three new prenylated chalcones, renifolins A-C (1-3), together with seven known ones (4- 10), were isolated from whole Desmodium renifolium plants. All of their structures were determined by spectroscopic methods including 1D and 2D NMR. Compounds 1 and 2 are the first naturally occurring chalcones possessing a 4-methylfuran-2(5*H*)-one unit. All of the isolates were evaluated for cytotoxicity using five tumor cell lines. Compounds 3- 8, and 10 exhibited moderate cytotoxicity against certain cell lines with IC$_{50}$ values from 4.2 to 8.8 μM.

Keywords: Desmodium chalcone renifolin cytotoxicity

Substances (11) | Reactions (0) | Citing (17)

10

Studies of traditional folk medicines in Xinjiang Uighur autonomous. II. Research for chemical constituents of Xinjiang licorice

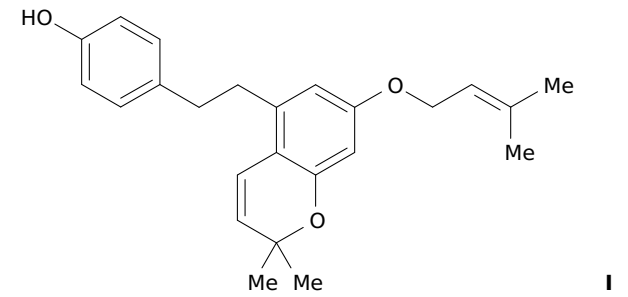
10 Substances • 0 Reactions • 9 Citations

By: Iwasaki, Noriaki; Baba, Masaki; Aishan, Halisha; Okada, Yoshihito; Okuyama, Toru

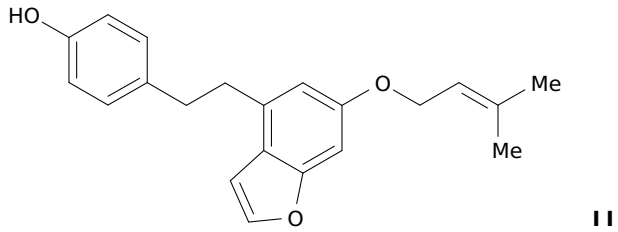
Heterocycles (2009), 78(6), 1581-1587 | Language: English, Database: CAplus

A new chromene, 5-[2-(4-hydroxyphenyl)ethyl]-2,2-dimethyl-7-[(3-methyl-2-butenyl)oxy]chromene, named xinjiastilbene A (**I**), a new benzofuran, 4-[2-(4-hydroxyphenyl)ethyl]-6-[(3-methyl-2-butenyl)oxy]benzofuran, named xinjiastilbene B (**II**), and a chalcone, 4'-hydroxy-2-methoxy-4-prenyloxy-chalcone, named xinjiachalcone A (**III**), were isolated from licorice of Xinjiang origin (botanically assigned to Glycyrrhiza inflata Batalin), together with seven known phenolic compounds The structure was elucidated on the basis of spectrometric evidence.

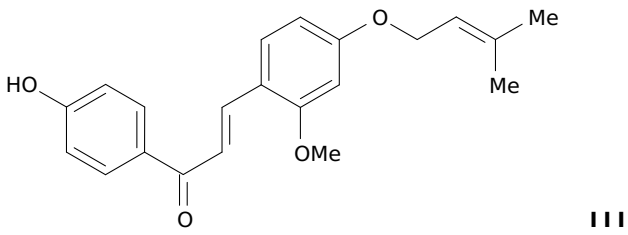
Keywords: Glycyrrhiza phenolics



I



II



III

Substances (10) | Reactions (0) | Citing (9)

11

Anti-oxidant Constituents of the Roots and Stolons of Licorice (Glycyrrhiza glabra)

14 Substances • 1 Reaction • 183 Citations

By: Chin, Young-Won; Jung, Hyun-Ah; Liu, Yue; Su, Bao-Ning; Castoro, John A.; Keller, William J.; Pereira, Michael A.; Kinghorn, A. Douglas

Journal of Agricultural and Food Chemistry (2007), 55(12), 4691-4697 | Language: English, Database: CAplus and MEDLINE

As part of a search for new cancer chemopreventive agents, a new chalcone derivative (1), a novel group of neolignan lipid esters (2), and seven known phenolic compounds (formono netin, glabridin, hemileiocarpin, hispaglabridin B, isoliquiritigenin, 4'-O-methylglabridin, and paratocarpin B) (3-9) were isolated from the roots and stolons of licorice (Glycyrrhiza glabra). The structures of compound 1 and the individual components of isolate 2 were elucidated using various spectroscopic and chem. methods. All isolates were tested in an authentic peroxynitrite antioxidant assay. Of these compounds, hispaglabridin B, isoliquiritigenin, and paratocarpin B were found to be the most potent antioxidant agents. Furthermore, isoliquiritigenin was demonstrated to prevent the incidence of 1,2-dimethylhydrazine-induced colon and lung tumors in mice when administered at a dose of 300 mg/kg.

Keywords: licorice Glycyrrhiza antioxidant antitumor

Substances (14) | Reaction (1) | Citing (183)

12

"Phenolic constituents of Glycyrrhiza species". An isoprenylated flavanone from Glycyrrhiza glabra and rec-assay of licorice phenols

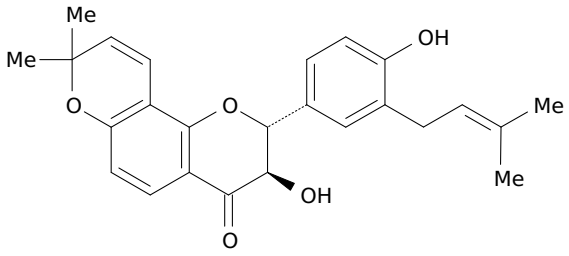
105 Substances • 0 Reactions • 38 Citations

By: Fukai, Toshio; Cai, Bao-Sheng; Maruno, Kanako; Miyakawa, Yukiko; Konishi, Masataka; Nomura, Taro

Phytochemistry (1998), 49(7), 2005-2013 | Language: English, Database: CAplus

A new prenylated 3-hydroxypyranoflavanone, kanzonol Z (**I**), was isolated from cultivated licorice, Glycyrrhiza glabra, and the structure elucidated from spectral evidence. The stereochem. structure of kanzonol Y previously isolated from the licorice has been shown to be (αR)-3,5'-diprenyl-α,2',4,4'-tetrahydroxydihydrochalcone by Mosher's method. In a prescreening test for bioactive compounds amongst licorice phenols using a recombinationless mutant of Bacillus subtilis M45, seven compounds showed induction activities of DNA damage.

Keywords: isoprenylated flavanone licorice phenol; phenolic constituent Glycyrrhiza DNA damage; kanzonol Z Glycyrrhiza structure



I

Substances (105) | Reactions (0) | Citing (38)

13

Constituents of the Moraceae plants. 22. Paratocarpins A-E, five new isoprenoid-substituted chalcones from Paratocarpus venenosa zoll

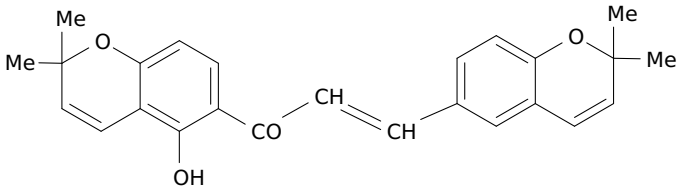
7 Substances • 0 Reactions • 15 Citations

By: Hano, Yoshio; Itoh, Naoyuki; Hanaoka, Akio; Itoh, Yoshimitsu; Nomura, Taro

Heterocycles (1995), 41(1), 191-8 | Language: English, Database: CAplus

Five new isoprenoid-substituted chalcones, paratocarpins A (**I**), B, C, D, and E were isolated from the Indonesian moraceous plant, P. (=Artocarpus) venenosa. The structures of the paratocarpins were determination on the basis of spectroscopic data.

Keywords: paratocarpin isolation Paratocarpus



I

Substances (7) Reactions (0) Citing (15)