CAS SciFinder

Task History

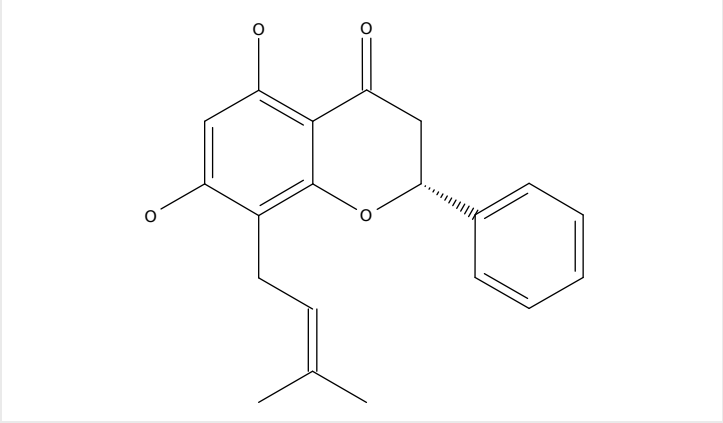
Initiating Search

July 8, 2024, 7:07 PM

Substances:

Filtered By:

Stereochemistry: **Absolute Stereo Match, Absolute Stereo Mirror Image**



Structure Match: **As Drawn**

Search Tasks

Task	Search Type	View
Returned Substance Results + Filters (2)	**Substances**	View Results
Exported: Retrieved Related Reference Results (143)	**References**	View Results

CAS SciFinder

References (4)

View in CAS SciFinder

1

Discovery of Isojacareubin as a covalent inhibitor of SARS-CoV-2 main protease using structural and experimental approaches

3 Substances • 0 Reactions • 4 Citations

By: Khan, Abbas ; Heng, Wang; Imran, Kashif; Zhu, Guanghao; Ji, Jun; Zhang, Yani; Guan, Xiaoqing; Ge, Guangbo; Wei, Dong-Qing

Journal of Medical Virology (2023), 95(2), e28542 | Language: English, Database: CAplus and MEDLINE

The ongoing pandemic with the emergence of immune evasion potential and, particularly, the current omicron subvariants intens ified the situation further. Although vaccines are available, the immune evasion capabi lities of the recent variants demand further efficient therapeutic choices to control the severe acute respir atory syndrome corona virus 2 (SARS-CoV-2) pandemic. Hence, consid ering the necessity of the small mol. inhibitor, we target the main protease (3 CLpro), which is an appealing target for the develo pment of antiviral drugs against SARS-CoV-2. High-throughput mol. in silico screening of South African natural compounds database reported Isojacareubin and Glabranin as the potential inhibitors for the main protease. The calculated docking scores were reported to be -8.47 and -8.03 kcal/mol, resp. Moreover, the structural dynamic assessment reported that Isojaca reubin in complex with 3CLpro exhibit a more stable dynamic behavior than Glabranin. Inhibition assay indicated that Isojaca reubin could inhibit SARS-CoV-2 3CLpro in a time- and dose- dependent manner, with half maximal inhibitory concent ration values of 16.00 ± 1.35μM (60 min incubation). Next, the covalent binding sites of Isojaca reubin on SARS-CoV-2 3CLpro was identified by biomass spectrometry, which reported that Isojaca reubin can covalently bind to thiols or Cysteine through Michael addition To evaluate the inactivation potency of Isojacareubin, the inactivation kinetics was further investigated. The inactivation kinetic curves were plotted according to various concentrations with gradient-ascending incubation times. The KI value of Isojaca reubin was determined as 30.71μM, whereas the Kinact value was calculated as 0.054 min- 1. These results suggest that Isojaca reubin is a covalent inhibitor of SARS-CoV-2 3CLpro.

Keywords: SARS CoV2 3CLpro isojacareubin glabranin antiviral drug discovery; 3 CLpro; IC50; SARS-CoV-2; drugs screening; inacti vation kinetics; simulation

Substances (3) | Reactions (0) | Citing (4)

2

The potential of Clerodendrum paniculatum leaves fraction as a 3-chymotrypsin-like (3CL) protease inhibitor of SARS-CoV-2

37 Substances • 0 Reactions • 1 Citation

By: Arba, Muhammad; Arfan, Arfan; Yamin, Yamin; Zubair, Muhammad Sulaiman

Indonesian Journal of Chemistry (2023), 23(3), 770-781 | Language: English, Database: CAplus

We described the biol. activity of the Clerodendrum paniculatum leaf fraction against the SARS-CoV-2 3-Chymotrypsin-like 3CL protease at the mol. level. This study applied LC-MS/MS to identify bioactive compounds from fractions, computa tional studies, and fluorescence resonance energy transfer (FRET) assays to ascertain their inhibitory activity. LC-MS/MS anal. of the three samples revealed that sample 1 contained 18 compound peaks. In samples 2 and 3, there were 23 and 25 compounds with different mol. weights, resp. Docking's study identified that the alkaloids (komarovicine and roemerine) have lower binding energies than other metabolites and standard compounds, with values of - 33.47 and -32.63 kJ/mol, resp. Roemerine demonstrated excellent stability based on dynamic simulation results and confirmed its affinity for 3CL protease predicted by the MM-PBSA approach of -89.44 k J/mol. The FRET method for testing 3CL protease activity revealed that sample 2 had an enzyme inhibitory activity of 94.3%, which was close to that of GC376 (98.19%). Meanwhile, samples 1 and 3 yielded satisf actory inhibition activity by 89.64% and 85.24%, resp. The antiviral activity of C. paniculatum leaves was discovered for the first time by inhibiting the 3 CL protease SARS-CoV-2, providing an excellent opportunity for its develo pment as an anti-SARS-CoV-2.

Keywords: Clerodendrum leaf komarovicine 3CL protease inhibitor anticoronaviral SARSCoV2

Substances (37) | Reactions (0) | Citing (1)

3

Compounds and methods for treating viral infections or thrombosis

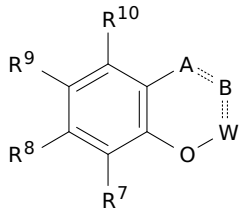
250 Substances • 0 Reactions • 0 Citations

Assignee: Beth Israel Deaconess Medical Center, Inc.

World Intellectual Property Organization, WO2022104153 A2 2022-05-19 | Language: English, Database: CAplus

The present application provides a compound of Formula (**I**), or a pharmaceutically acceptable salt thereof. Pharmac eutical compos itions containing the compound of Formula **I**, and methods of using the compound of Formula **I** for treating viral infections and inhibiting thrombosis are also provided. Disclosed area method of modulating activity of a main protease of a virus selected from S ARS-CoV, SARS-CoV-2, and MERS-CoV in a cell, a method of treating or preventing corona virus infection, a method of inhibiting protein disulfide isomerase (PDI) in a cell, and a method of inhibiting thrombosis in a subject using the compound **I**.

Keywords: flavonoid anticoronavirus protease inhibitor SARS COVID19 MERS; thrombosis antithrombotic flavone



I

PatentPak available

Substances (250) | Reactions (0) | Citing (0)

4

Ayurveda drug formulation containing 6-gingesulfonic acid for SARS-CoV-2

70 Substances • 0 Reactions • 0 Citations

Assignee: Unknown
India, IN202111010632 A 2021-05-28 | Language: English, Database: CAplus

The invention relates to an Ayurveda drug, which can be considered as Janapadodhwamsa, vata-kafaz Sannipata jwara, Aupsargik vyadhi and Dhatupaka awastha, in the mol. docking study the binding energy and inhibition of 6-gingesulfonic acid from Zingiber officinale are greater than hydroxychloroquine and quinine, target prediction of selected phytocons tituents are done on target of S ARS-CoV-2, humoral immunity and antiviral, every selected phytocons tituents are work on min. of the target.

Keywords: gingesulfonic acid ayurveda drug formul ation SARS CoV

PatentPak available

Substances (70) | Reactions (0) | Citing (0)