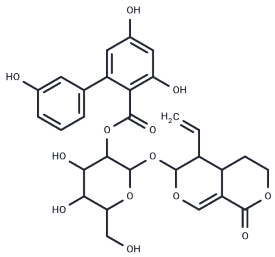
Data Sheet (Cat.No.T5497)

TargetMol

AMAROGENTIN

Chemical Properties



CAS No. : 21018-84-8

Formula: C29H30O13

Molecular Weight: 586.54

Storage: Keep away from direct sunlight
Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Amarogentin is mainly extracted from Swertia and Gentiana roots. It plays cemopreventive/therapeutic role during liver carcinogenesis through modulation of cell cycle and apoptosis
Targets(IC50)	Apoptosis,AMPK
In vivo	Amarogentin, a bitter secoiridoid glycoside from S. chirayita, shows varied activity in several patho-physiological conditions, predominantly in leishmaniasis and carcinogenesis.?Experimental analysis has revealed that Amarogentin downregulates the cyclooxygenase-2 (COX-2) activity and helps to curtail skin carcinogenesis in mouse models;?however, there exists no account on selective inhibition of the inducible cyclooxygenase (COX) isoform by Amarogentin[1].marogentin inhibits the growth of SNU-16 human gastric cancer cells (IC50 = 12.4 μM after 48 hours) and increases apoptosis when used at a concentration of 50 μM. Amarogentin (10-50 mg/kg, s.c.) dose-dependently reduces tumor growth in a SNU-16 nude mouse xenograft model[2].
Kinase Assay	The computer-aided drug discovery methods were used to unravel the COX-2 inhibitory mechanism of Amarogentin and to check its selectivity for the inducible isoform over the constitutive one.?The generated theoretical models of both isoforms were subjected to molecular docking analysis with Amarogentin and twenty-one other Food and Drug Authority (FDA) approved lead molecules.?The post-docking binding energy profile of Amarogentin was comparable to the binding energy profiles of the FDA approved selective COX-2 inhibitors.?Subsequent molecular dynamics simulation analysis delineated the difference in the stability of both complexes, with Amarogentin-COX-2 complex being more stable after 40ns simulation.?The total binding free energy calculated by MMGBSA for the Amarogentin-COX-2 complex was -52.35 KCal/mol against a binding free energy of -8.57 KCal/mol for Amarogentin-COX-1 complex, suggesting a possible selective inhibition of the COX-2 protein by the natural inhibitor.?Amarogentin achieves this potential selectivity by small, yet significant, structural differences inherent to the binding cavities of the two isoforms.?Hypothetically, it might block the entry of the natural substrates in the hydrophobic binding channel of the COX-2, inhibiting the cyclooxygenation step[1].

Solubility Information

Solubility	DMSO: 250 mg/mL (426.23 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 1 mg/mL (1.7 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.7049 mL	8.5246 mL	17.0491 mL
5 mM	0.341 mL	1.7049 mL	3.4098 mL
10 mM	0.1705 mL	0.8525 mL	1.7049 mL
50 mM	0.0341 mL	0.1705 mL	0.341 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Shantanu S , Khushboo B , Durai S , et al. The Bitter Barricading of Prostaglandin Biosynthesis Pathway: Understanding the Molecular Mechanism of Selective Cyclooxygenase-2 Inhibition by Amarogentin, a Secoiridoid Glycoside from Swertia chirayita[J]. PLoS ONE, 2014, 9(3):e90637-.

Zhang H, Liang B, Sang X, et al.Discovery of Potential Inhibitors of SARS-CoV-2 Main Protease by a Transfer Learning Method.Viruses.2023, 15(4): 891.

Zhao, J.G., Zhang, L., Xiang, X.-j., et al. Amarogentin secoiridoid inhibits in vivo cancer cell growth in xenograft mice model and induces apoptosis in human gastric cancer cells (SNU-16) through G2/M cell cycle arrest and PI3K/Akt signalling pathway. J. BUON. 21(3), 609-617 (2016).