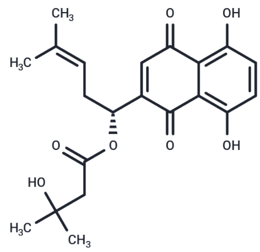
Data Sheet (Cat.No.TN1440)

TargetMol

Beta-Hydroxyisovalerylshikonin

Chemical Properties



CAS No. :	7415-78-3
Formula:	C21H24O7
Molecular Weight:	388.41
Storage:	Keep away from moisture,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	Beta-Hydroxyisovalerylshikonin is an inhibitor of protein-tyrosine kinases such as v-Src and EGFR, and has been shown to induce apoptosis in several human tumor cell lines. Beta-Hydroxyisovalerylshikonin significantly decreased viability of HCT116 cells (IC50 values = 30.9 μg/mL).
Targets(IC50)	EGFR,AMPK,Fatty Acid Synthase,Prostaglandin Receptor,Src,Tyrosine Kinases
In vitro	By using different chromatographic techniques and appropriate spectroscopic methods, the seven naphthoquinones were described: deoxyshikonin (1), isobutyrylshikonin (2), α±-methylbutyrylshikonin (3), acetylshikonin (4), Beta-Hydroxyisovalerylshikonin(5), 5,8-O-dimethyl isobutyrylshikonin (6) and 5,8-O-dimethyl deoxyshikonin (7). Among the tested compounds, 3 and 4 exhibited the highest antibacterial activities toward all tested bacterial species (MIC50 and MIC90 for gram positive bacteria: 6.40 μg/mL-12.79 μg/mL and 6.82 μg/mL-13.60 μg/mL, respectively; for gram negative bacteria: 4.27 μg/mL-8.53 μg/mL and 4.77 μg/mL-9.54 μg/mL, respectively). Also, naphthoquinones 3 and 4 exhibited strong cytotoxic activity against MDA-MB-231 cells (IC50 values 86.0 μg/mL and 80.2 μg/mL, respectively), while compounds 1 , 3 , 4 and 5 significantly decreased viability of HCT116 cells (IC50 values of 97.8 μg/mL, 15.2 μg/mL, 24.6 μg/mL and 30.9 μg/mL, respectively)[1]

Solubility Information

Solubility	DMSO: 10 mg/mL (25.75 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 (2.57 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	2.5746 mL	12.873 mL	25.746 mL
5 mM	0.5149 mL	2.5746 mL	5.1492 mL
10 mM	0.2575 mL	1.2873 mL	2.5746 mL
50 mM	0.0515 mL	0.2575 mL	0.5149 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

Vukic MD, et al. Antibacterial and cytotoxic activities of naphthoquinone pigments from Onosma visianii Clem. EXCLI J. 2017 Feb 16;16:73-88.

Hashimoto S, et al. Beta-hydroxyisovalerylshikonin is a novel and potent inhibitor of protein tyrosine kinases. Jpn J Cancer Res. 2002 Aug;93(8):944-51.

Chen X , et al. β-Hydroxyisovalerylshikonin inhibits IL-1β-induced chondrocyte inflammation via Nrf2 and retards osteoarthritis in mice. Food Funct. 2020 Nov 18;11(11):10219-10230.

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