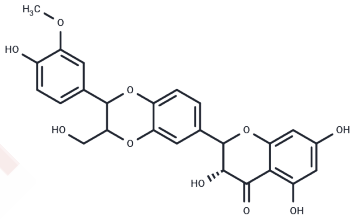
Data Sheet (Cat.No.T3797)

TargetMol

Isosilybin

Chemical Properties



CAS No. : 72581-71-6

Formula: C25H22O10

Molecular Weight: 482.44

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	Isosilybin (Isosilibinin) and Silybin might be suitable candidates to design potent PXR antagonists to prevent drug-drug interactions via CYP3A4 in cancer patients.
Targets(IC50)	Cytochromes P450
In vitro	The reporter gene assay demonstrates that the milk thistle constituents silybin and isosilybin inhibit the PXR-mediated induction of CYP3A4, with isosilybin being a more potent inhibitor. Concentrations of 89, 133, and 200 μM of isosilybin decrease CYP3A4 induction by 64, 82, and 88%, respectively, and achieve an IC50 of 74 μM[1]. Additionally, the diastereoisomers isosilybin B and isosilybin A, derived from silymarin, exhibit anti-prostate cancer (PCA) activity through cell cycle arrest and apoptosis induction in human prostate cancer cells LNCaP and 22Rv1[2]. Isosilybin B enhances phosphorylation of Akt and Mdm2, leading to androgen receptor degradation, which is reversed by PI3K inhibitor pretreatment. This process facilitates the formation of a complex that promotes phosphorylation-dependent ubiquitination and subsequent degradation of the androgen receptor[3]. Isosilybin A significantly activates PPARγ at a 30 μM concentration, leading to a concentration-dependent transactivation of a PPARγ-dependent luciferase reporter. In silico docking studies indicate isosilybin A interacts with the receptor's ligand-binding domain through an additional hydrogen bond not found with inactive silymarin constituents[4].
Cell Research	LNCaP cells and 22Rv1 cells are plated and treated at 40–50% confluency with different doses of isosilybin B and isosilybin A (10–90 μM in medium) dissolved originally in Dimethyl sulfoxide (DMSO) for the desired time periods (24–48 h) in serum condition. An equal amount of DMSO (vehicle) is present in each treatment, including control; DMSO concentration did not exceed 0.1% (v/v) in any treatment. At the end of desired treatments, total cell number is determined by counting each sample in duplicate using a hemocytometer under an inverted microscope. Cell viability is determined using trypan blue exclusion method[2].

Solubility Information

Solubility	DMSO: 125 mg/mL (259.1 mM),Sonication is recommended. Chloroform, Dichloromethane, Ethyl Acetate: Soluble, (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 3.3 mg/mL (6.84 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	2.0728 mL	10.364 mL	20.728 mL
5 mM	0.4146 mL	2.0728 mL	4.1456 mL
10 mM	0.2073 mL	1.0364 mL	2.0728 mL
50 mM	0.0415 mL	0.2073 mL	0.4146 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

Mooiman KD, et al. Milk thistle's active components silybin and isosilybin: novel inhibitors of PXR-mediated CYP3A4 induction. Drug Metab Dispos. 2013 Aug;41(8):1494-504.

Deep G, et al. Isosilybin B and isosilybin A inhibit growth, induce G1 arrest and cause apoptosis in human prostate cancer LNCaP and 22Rv1 cells. Carcinogenesis. 2007 Jul;28(7):1533-42.

Deep G, et al. Isosilybin B causes androgen receptor degradation in human prostate carcinoma cells via PI3K-Akt-Mdm2-mediated pathway. Oncogene. 2008 Jun 26;27(28):31986-98.

Pferschy-Wenzig EM, et al. Identification of isosilybin a from milk thistle seeds as an agonist of peroxisome proliferator-activated receptor gamma. J Nat Prod. 2014 Apr 25;77(4):842-7.