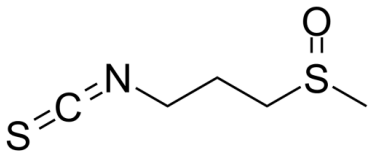
Data Sheet

Product Name:	Iberin
Cat. No.:	CS-6348
CAS No.:	505-44-2
Molecular Formula:	C5H9NOS2
Molecular Weight:	163.26
Target:	Apoptosis; Bacterial; Endogenous Metabolite
Pathway:	Anti-infection; Apoptosis; Metabolic Enzyme/Protease
Solubility:	DMSO : ≥ 310 mg/mL (1898.81 mM); Ethanol : 10 mg/mL (61.25 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Iberin, a sulfoxide analogue of sulforaphane, is a naturally occurring member of isothiocyanate family. It inhibits cell survival with an **IC $_{50}$** of 2.3 μM in HL60 cell. IC50 & Target: IC50: 2.3 μM (HL60 cell)[1] **In Vitro:** Iberin inhibits the growth of neuroblastoma cells in a dose- and time-dependent manner. The iberin-induced cell cycle arrest in neuroblastoma cells is associated with inhibition of expression of cyclin-dependent kinase Cdk2, Cdk4, and Cdk6 proteins. There is an increase in apoptotic cell death in iberin treated cells as compared with control cells. The iberin-induced apoptosis is found to be associated with activation of caspase-9, caspase-3, and PARP[2]. Iberin inhibits growth of human glioblastoma cells in cell proliferation assays, enhances cytotoxicity, and induces apoptosis by activation of caspase-3 and caspase-9[3]. **In Vivo:** Iberin is tested in an in vivo foreign-body infection mouse model, and the results show no significantly difference in bacterial clearance between treated and nontreated miced[4]. Iberin increases tissue levels of the phase II detoxification enzymes quinone reductase and glutathione S-transferase in a variety of rat tissues[5].

PROTOCOL (Extracted from published papers and Only for reference)

Cell Assay: [2]Cells are plated at a density of 1×10^5 cells/well in microtiter plates and treated with different concentrations of iberin (1, 2.5, 10 and 25 μM). Then 20 μL of 5 mg/mL MTT in PBS, is added to each well and allowed to incubate for a further 4 h. After 4 h of incubation, 100 μL of DMSO is added to each well to dissolve the formazan crystals. Absorbance values at 550 nm are measured with a microplate reader[2]. **Animal Administration:** [4][5]Rats: Groups of five rats are dosed by oral intubation with the test compounds, as solutions in soybean oil, each day for 5 days. This doses used are 4.0 mg/kg/day for AITC, 5.9 mg/kg/day for iberverin, 6.5 mg/kg/day for iberin, 6.4 mg/kg/day for erucin, 7.1 mg/kg/day for sulforaphane, and 7.2 mg/kg/day for cheirolin. The volume of solution administered is 2 mL/kg in all cases. Ten control rats are dosed with soybean oil alone[5].

Mice: Iberin is diluted in 96% ethanol to a concentration of 32 mg/mL followed by a 40x dilution in 0.9% NaCl. The mice are injected with 0.2 mL of the final solution, corresponding to 8 μg/g of body weight. The placebo group is injected with a 2.4% ethanol solution (96% ethanol–0.9% NaCl) corresponding to the amount of ethanol that the iberin-treated group received. Mice are treated every 12 h from day 2 preinsertion to day 2 postinsertion, and treatment is continued until 12 h before the mice are euthanized[4].

References:

[1]. Jakubikova J, et al. Isothiocyanates induce cell cycle arrest, apoptosis and mitochondrial potential depolarization in HL-60 and multidrug-resistant cell lines. Anticancer Res. 2005 Sep-Oct;25(5):3375-86.

[2]. Jadhav U, et al. Iberin induces cell cycle arrest and apoptosis in human neuroblastoma cells.

[3]. Jadhav U, et al. Dietary isothiocyanate iberin inhibits growth and induces apoptosis in human glioblastoma cells. J Pharmacol Sci. 2007 Feb;103(2):247-51.

[4]. Jakobsen TH, et al. Food as a source for quorum sensing inhibitors: iberin from horseradish revealed as a quorumsensing inhibitor of Pseudomonas aeruginosa. Appl Environ Microbiol. 2012 Apr;78(7):2410-21.

[5]. Munday R, et al. Induction of phase II detoxification enzymes in rats by plant-derived isothiocyanates: comparison of allyl isothiocyanate with sulforaphane and related compounds. J Agric Food Chem. 2004 Apr 7;52(7):1867-71.

CAIndexNames:

Propane, 1-isothiocyanato-3-(methylsulfinyl)-

SMILES:

O=S(CCCN=C=S)C

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