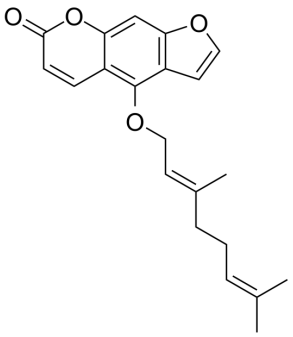
Bergamottin



Cat. No.: HY-N2194

CAS No.: 7380-40-7

Molecular Formula: $C_{21}H_{22}O_4$

Molecular Weight: 338.4

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

Storage: 4°C, protect from light

* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)

SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (147.75 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.9551 mL	14.7754 mL	29.5508 mL
	5 mM	0.5910 mL	2.9551 mL	5.9102 mL
	10 mM	0.2955 mL	1.4775 mL	2.9551 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (7.39 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (7.39 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Bergamottin is a potent and competitive CYP1A1 inhibitor with a K_i of 10.703 nM.

IC_{50} & Target

CYP1A1 10.703 nM (Ki)	CYP1A1 0.192 μM (IC_{50})	CYP1A2 5.077 μM (IC_{50})	CYP2B2 4.535 μM (IC_{50})
CYP2B1 9.495 μM (IC_{50})			

In Vitro

Bergamottin is a competitive inhibitor of CYP1A1. Bergamottin inhibits CYP1A1, CYP1A2, CYP2B1, and CYP2B2 with IC_{50}s of 0.192±0.029 μM, 5.077±0.31 μM, 9.495±0.979 μM, 4.535±0.092 μM, respectively[1]. Bergamottin has potent antiproliferative effects on the A549 cells. Bergamottin shows both concentration-dependent as well as time-dependent growth inhibitory effects against these cells. Bergamottin also inhibits the clonogenic activity of the A549 cancer cells by reducing the number

	of cancer colony forming cells. A reduction in clonogenicity also follows the concentration dependence on Bergamottin[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	The anticancer efficacy of Bergamottin under in vivo conditions using female BALB/c nude mice (a total of 20 mice are used) is determined. Tumors are induced in the mice by injecting non-small cell lung cancer A549 cells (1×10^6 cells/mouse). After tumor formation, the mice are sacrificed and tumors are removed and their weights and volumes are calculated. The results show that 25, 50 and 100 mg/kg Bergamottin injection reduce the tumor weight from 1.61 g in the PBS-treated group (control) to 1.21, 0.42 and 0.15 g, respectively. Tumor weight in the nude mice is reduced much more significantly in the highest-concentration Bergamottin group (100 mg/kg body weight) compared with the vehicle group ($P<0.05$). Likewise, 25, 50 and 100 mg/kg Bergamottin injection reduces the tumor volume from 2.2 cm^3 in the PBS-treated group (control) to 1.71, 1.1 and 0.51 cm3, respectively. The periodic measurement of the tumor xenograft volume indicates that the tumor volume in the nude mice is reduced considerably in the highest-concentration Bergamottin group (100 mg/kg body weight) compared with the vehicle group ($P<0.05$)[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Kinase Assay [1]	CYP1A1 Supersomes and different concentrations of 7-ethoxyresorufin (ER) are used to determine CYP1A1 enzymatic kinetics. A typical Michaelis-Menten curve is found. The final reaction mixture contains: 1 pmol CYP1A1, 0.5 mM NADPH, different ER concentrations and 0, 4, 8 and 16 nM of Bergamottin (BG). The reaction is started with the addition of NADPH. Kinetic constants are obtained by a nonlinear regression analysis of experimental data fitted to Michaelis-Menten equation with competitive-type inhibition. Kinetic analysis is also shown by using the Lineweaver-Burk, Dixon and replot of the slopes of the Dixon plot[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Cell Assay [2]	Inhibition of cell proliferation by Bergamottin is measured by the MTT assay. Briefly, the human lung adenocarcinoma cancer A549 cells are plated in 96-well culture plates (1×10^5 cells/well). After 24 h of incubation, the cells are treated with Bergamottin (0, 5, 10, 25, 50, 75 and 100 μM) for 24 and 48 h, MTT solution (10 mg/mL) is then added to each well. After a 4-h incubation, the formazan precipitate is dissolved in 100 μL DMSO, and then the absorbance is measured in an automated microplated reader at 570 nm. The cell viability ratio is calculated. Cytotoxicity is expressed as the concentration of Bergamottin needed to inhibit cell growth by 50% (IC_{50} value)[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Animal Administration [2]	Mice[2] Female BALB/c nude mice (six weeks old) (a total of 20 are obtained) are maintained with water and food ad libitum in a pathogen-free environment with a 12 h light and 12 h dark cycle in an animal care facility. Human non□small cell lung carcinoma A549 cells (2×10^6 cells/mouse) are injected into the right axilla of the nude mice (5 mice/group) to create tumors in the mice. Subsequent to tumor development, the mice are divided into 4 groups and treated with Bergamottin injected intraperitoneally. The control group in the study is treated with an equal amount of PBS while the other three groups are treated with 25, 50 and 100 mg/kg of Bergamottin. Afterwards, the mice are sacrificed after 18 days, and the tumor weight and volume of each mouse are evaluated. Tumor length and width are measured using a Vernier caliper and the tumor volume (TV) is calculated[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Antiviral Res. 2022 Jun 19;204:105365.
- Int J Mol Sci. 2022 Oct 19;23(20):12565.

- Viruses. 2023 Jun 13, 15(6), 1367.
- Immunol Res. 2021 Oct 11.

See more customer validations on www.MedChemExpress.com

REFERENCES

[1]. Olguín-Reyes S, et al. Bergamottin is a competitive inhibitor of CYP1A1 and is antimutagenic in the Ames test. Food Chem Toxicol. 2012 Sep;50(9):3094-9.

[2]. Wu HJ, et al. Bergamottin isolated from Citrus bergamia exerts in vitro and in vivo antitumor activity in lung adenocarcinoma through the induction of apoptosis, cell cycle arrest, mitochondrial membrane potential loss and inhibition of cell migration and invasion. Oncol Rep. 2016 Jul;36(1):324-32.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA