Bergaptol

Cat. No.: HY-76316

CAS No.: 486-60-2

Molecular Formula: $C_{11}H_6O_4$

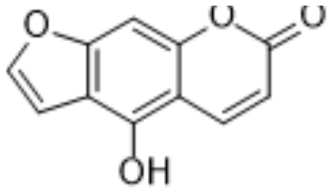
Molecular Weight: 202.16

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 50 mg/mL (247.33 mM)

H_2O : < 0.1 mg/mL (ultrasonic) (insoluble)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	4.9466 mL	24.7329 mL	49.4658 mL
5 mM	0.9893 mL	4.9466 mL	9.8932 mL
10 mM	0.4947 mL	2.4733 mL	4.9466 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: 2.5 mg/mL (12.37 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

Bergaptol is an inhibitor of debenzylation of the CYP3A4 enzyme with an IC_{50} of 24.92 μM. Recent studies have shown that it has anti-proliferative and anti-cancer properties[1].

IC_{50} & Target

CYP3

In Vitro

Bergaptol (0-800 ppm) shows free radical scavenging activity, tested by ABTS and DPPH methods[1].

Bergaptol (50 μg/mL, 24 h) inhibits LPS-induced production of NO, IL-6, and TNF-α in RAW264.7 cells[3].

Bergaptol (50 μg/mL, 24 h) inhibits LPS-induced MAPK phosphorylation and nuclear factor-kappa B (NF-κB) activation in RAW264.7 cells[3].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Western Blot Analysis[3]

Cell Line:	LPS-induced RAW264.7 cells
Concentration:	50 μg/mL
Incubation Time:	24 h
Result:	Inhibited JNK phosphorylation and NF-κB activation. Inhibited NF-κB P65 translocation from the cytosol to nucleus.

In Vivo

Bergaptol (10-40 mg/kg, i.p., once a day for two weeks) improves the cognitive impairment in LPS-treated mice[4].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	LPS (40 μg/kg, i.c.v.)-treated mice[4]
Dosage:	10-40 mg/kg
Administration:	i.p., once a day for two week
Result:	Reduced LPS-induced fixation and cleavage of neuronal nuclei in the CA1 region of the hippocampus (H&E staining). Increasead the dendritic spine density of mice. Inhibited LPS-induced neuroinflammation.

REFERENCES

[1]. Shen CY, et al. Bergaptol from blossoms of Citrus aurantium L. var. amara Engl inhibits LPS-induced inflammatory responses and ox-LDL-induced lipid deposition. Food Funct. 2020 Jun 24;11(6):4915-4926.

[2]. Wu J, et al. Bergaptol Alleviates LPS-Induced Neuroinflammation, Neurological Damage and Cognitive Impairment via Regulating the JAK2/STAT3/p65 Pathway. J Inflamm Res. 2022 Nov 9;15:6199-6211.

[3]. Basavaraj Girennavar et al. Radical scavenging and cytochrome P450 3A4 inhibitory activity of bergaptol and geranylcoumarin from grapefruit. Bioorganic & Medicinal Chemistry.June 2007, Pages 3684-3691

[4]. Yucheng Zhao et al. Cloning, Functional Characterization, and Catalytic Mechanism of a Bergaptol O-Methyltransferase from Peucedanum praeruptorum Dunn. Front Plant Sci, 2016, 7: 722.

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