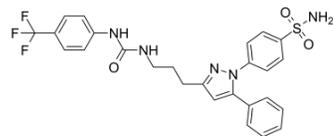


PTUPB

Cat. No.:	HY-122591		
CAS No.:	1287761-01-6		
Molecular Formula:	C ₂₆ H ₂₄ F ₃ N ₅ O ₃ S		
Molecular Weight:	543.56		
Target:	COX		
Pathway:	Immunology/Inflammation		
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	6 months
		-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (183.97 mM; Need ultrasonic)

	Solvent Concentration	Mass		
		1 mg	5 mg	10 mg
Preparing Stock Solutions	1 mM	1.8397 mL	9.1986 mL	18.3972 mL
	5 mM	0.3679 mL	1.8397 mL	3.6794 mL
	10 mM	0.1840 mL	0.9199 mL	1.8397 mL

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

In Vivo

- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
Solubility: ≥ 2.08 mg/mL (3.83 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
Solubility: ≥ 2.08 mg/mL (3.83 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil
Solubility: ≥ 2.08 mg/mL (3.83 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PTUPB is a potent and dual sEH and COX-2 enzymes inhibitor with IC₅₀ of 0.9 nM and 1.26 μM, respectively^[1].

IC₅₀ & Target

COX-1 1.26 μM (IC ₅₀)	COX-1 100 μM (IC ₅₀)	sEH 0.9 nM (IC ₅₀)
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In Vitro

PTUPB (1-10 μM; 24 hours) shows an inhibitory activity against human 5-LOX, exhibits a 83% and 44% inhibition at 10 μM and 1 μM, respectively^[1].

PTUPB (10-20 μM ; 72 hours) has minimal inhibitory effects on cell proliferation in multiple cancer cell lines, including human melanoma cell and a transformed endothelial cell, whereas it potently inhibits HUVEC proliferation after 3 days of application^[1].

PTUPB (10-20 μM ; 72 hours) induces cell cycle arrest at the G0/1 phase at different various. The percentage of cell number of PTUPB are 65.15%, 66.87%, and 65.91% at 10 μM , 15 μM , and 20 μM , respectively^[1].

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

Cell Viability Assay^[1]

Cell Line:	Multiple cancer cell lines: PC-3 cells, Met-1, H-1, A375, and transformed endothelial cell line (bEnd.3)
Concentration:	10 μM , 15 μM , and 20 μM
Incubation Time:	72 hours
Result:	Inhibited HUVEC proliferation after 3 days.

Cell Cycle Analysis^[1]

Cell Line:	HUVECs
Concentration:	10 μM , 15 μM , and 20 μM
Incubation Time:	72 hours
Result:	Induced cell cycle arrest at the G0/1 phase.

In Vivo

PTUPB (subcutaneous injection; 30 mg/kg; 4 weeks) inhibits LLC tumor growth by 70-83% and exhibits with no overt toxicity, such as any weight loss when it is compared with the control group. After a period of treatment, the peak plasma concentration of PTUPB is high^[1].

PTUPB (subcutaneous injection; 5 mg/kg; once daily; 12 weeks) ameliorates high-fat diet-induced non-alcoholic fatty liver disease via inhibiting NLRP3 inflammasome activation. It reduces body weight, liver weight, liver triglyceride and cholesterol content. It also decreases the expression of lipolytic/lipogenic and lipid uptake related genes^[2].

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

Animal Model:	C57BL/6 mice with LLC cells ^[1]
Dosage:	30 mg/kg; 4 weeks
Administration:	Subcutaneous injection via Alzet osmotic minipumps; once daily; 4 weeks
Result:	Inhibited LLC tumor growth and metastasis.

Animal Model:	High-fat diet (HFD)-induced obese adult male C57BL/6 mice ^[2]
Dosage:	5 mg/kg; 12 weeks
Administration:	Subcutaneous injection; once daily; 12 weeks
Result:	Arrested fibrotic progression and ameliorated high-fat diet-induced non-alcoholic fatty liver disease.

REFERENCES

[1]. Sun CC, et al. PTUPB ameliorates high-fat diet-induced non-alcoholic fatty liver disease via inhibiting NLRP3 inflammasome activation in mice. *Biochem Biophys Res Commun.* 2020 Mar 19;523(4):1020-1026.

[2]. Zhang G, et al. Dual inhibition of cyclooxygenase-2 and soluble epoxide hydrolase synergistically suppresses primary tumor growth and metastasis. *Proc Natl Acad Sci U S A.* 2014 Jul 29;111(30):11127-32.

[3]. Hwang SH, et al. Synthesis and structure-activity relationship studies of urea-containing pyrazoles as dual inhibitors of cyclooxygenase-2 and soluble epoxide hydrolase. *J Med Chem.* 2011 Apr 28;54(8):3037-50.

Caution: Product has not been fully validated for medical applications. For research use only.

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