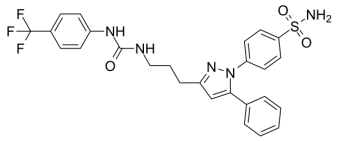
PTUPB

Cat. No.:	HY-122591
CAS No.:	1287761-01-6
Molecular Formula:	$C_{26}H_{24}F_3N_5O_3S$
Molecular Weight:	543.56
Target:	COX
Pathway:	Immunology/Inflammation
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 : 100 mg/mL (183.97 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	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

1. 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
2. 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
3. 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 IC_{50} of 0.9 nM and 1.26 μM, respectively[1].

IC_{50} & Target

COX-2	COX-1	sEH
1.26 μM (IC_{50})	100 μM (IC_{50})	0.9 nM (IC_{50})

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 obeseadult 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.

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