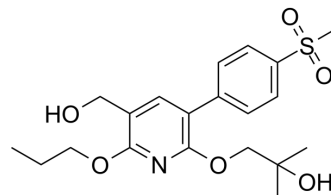


COX-2-IN-6

Cat. No.:	HY-115866
CAS No.:	2756347-91-6
Molecular Formula:	C ₂₀ H ₂₇ NO ₆ S
Molecular Weight:	409.5
Target:	COX
Pathway:	Immunology/Inflammation
Storage:	4°C, sealed storage, away from moisture and light * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (244.20 mM; Need ultrasonic)

Concentration	Solvent	Mass		
		1 mg	5 mg	10 mg
Preparing Stock Solutions	1 mM	2.4420 mL	12.2100 mL	24.4200 mL
	5 mM	0.4884 mL	2.4420 mL	4.8840 mL
	10 mM	0.2442 mL	1.2210 mL	2.4420 mL

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

BIOLOGICAL ACTIVITY

Description

COX-2-IN-6 (compound 10) is an orally active, gut-restricted and selective cyclooxygenase-2 (COX-2) inhibitor for colorectal Chemoprevention of cancer. COX-2-IN-6 selectively targets COX-2 with an IC₅₀ of 0.84 μM and a Ki of 69 nM. COX-2-IN-6 also inhibits COX-2-driven PGE₂ synthesis with an IC₅₀ of 0.60 μM^[1].

IC₅₀ & Target

COX-2

In Vitro

COX-2-IN-6 (compound 10) inhibits human COX-2/COX-1 enzymes, and COX-2/COX-1-driven PGE₂ synthesis in HEK293 cells with IC₅₀s of 0.84 μM, >50 μM, 0.60 μM, and >50 μM, respectively^[1].
COX-2-IN-6 shows liver microsomal and hepatocyte stability in vitro of human or mouse. And the T_{1/2} values are 3.1 min for human hepatocyte and 3.0 min for mouse hepatocyte^[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

COX-2-IN-6 (compound 10) (30-300 mg/kg; po; single dose) inhibits adenoma progression and enhances survival extension in an APCmin/+ mouse model^[1].
COX-2-IN-6 (10 mg/kg; po; single dose) displays high colonic exposures (>4300 ng/g) and a low systemic exposure (<6 ng/mL) with a distribution ratio of C/P >1200 at 4 h^[1].

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

Animal Model:	APCmin/+ mouse model ^[1]
Dosage:	30 mg/kg, 100 mg/kg, 300 mg/kg
Administration:	PO; daily in chow diet
Result:	Significantly decreased [18F]-FDG uptake and polyp area.

REFERENCES

[1]. Zhang Z, et al. Gut-Restricted Selective Cyclooxygenase-2 (COX-2) Inhibitors for Chemoprevention of Colorectal Cancer. J Med Chem. 2021 Aug 12;64(15):11570-11596.

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

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