Phenacetin

Cat. No.: HY-B0476

CAS No.: 62-44-2

Molecular Formula: $C_{10}H_{13}NO_2$

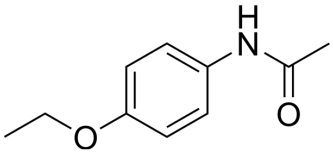
Molecular Weight: 179.22

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 (557.97 mM)

H_2O : 0.67 mg/mL (3.74 mM; Need ultrasonic)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	5.5797 mL	27.8987 mL	55.7973 mL
5 mM	1.1159 mL	5.5797 mL	11.1595 mL
10 mM	0.5580 mL	2.7899 mL	5.5797 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 (13.95 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (13.95 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (13.95 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Phenacetin (Acetophenetidin) is a non-opioid analgesic/antipyretic agent. Phenacetin is a selective COX-3 inhibitor. Phenacetin is used as probe of cytochrome P450 enzymes CYP1A2 in human liver microsomes and in rats[1][2][3].

IC_{50} & Target

COX-3

102 μM (IC_{50})

In Vitro	Phenacetin shows inhibitory activity for COX-3 with an IC_{50} value of 102 μM in insect cells [1]. Phenacetin is a substrate widely used as an in vitro and in vivo probe to measure the activity of CYP1A2, because the metabolism of phenacetin to acetaminophen is thought to be a selective CYP1A2-mediated reaction[2][3]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Phenacetin exhibits elimination half-life (rat 2.06 h) and C_{max} (6,728.3 μg/L) following oral administration (rat 20 mg/kg)[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male Sprague-Dawley rats (180-200 g)[2]
Dosage:	20 mg/kg
Administration:	Oral administration (Pharmacokinetic Analysis)
Result:	$T_{1/2}$ (2.06 hours), C_{max} (6,728.3 μg/L).

REFERENCES

[1]. Chandrasekharan NV, et al. COX-3, a cyclooxygenase-1 variant inhibited by acetaminophen and other analgesic/antipyretic drugs: cloning, structure, and expression. Proc Natl Acad Sci U S A. 2002 Oct 15;99(21):13926-31.

[2]. Xiao-Meng He, et al. Effects of long-term smoking on the activity and mRNA expression of CYP isozymes in rats. J Thorac Dis. 2015 Oct; 7(10): 1725–1731.

[3]. Na Gao, et al. Inhibition of Baicalin on Metabolism of Phenacetin, a Probe of CYP1A2, in Human Liver Microsomes and in Rats. PLoS One. 2014; 9(2): e89752.

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