Ticlopidine

Cat. No.: HY-100386

CAS No.: 55142-85-3

Molecular Formula: $C_{14}H_{14}ClNS$

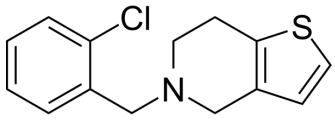
Molecular Weight: 263.79

Target: Cytochrome P450

Pathway: Metabolic Enzyme/Protease

Storage: 4°C, protect from light

* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (379.09 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Concentration / Solvent / Mass	1 mg	5 mg	10 mg
	1 mM	3.7909 mL	18.9545 mL	37.9089 mL
	5 mM	0.7582 mL	3.7909 mL	7.5818 mL
	10 mM	0.3791 mL	1.8954 mL	3.7909 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (9.48 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (9.48 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Ticlopidine (PCR 5332), an antithrombotic proagent, acts as an allosteric, noncompetitive inhibitor of CD39 with the IC50 of 81.7 μM. Ticlopidine blocks several NTPDase isoenzymes with IC50s of 170 μM and 149 μM for NTPDase2 and NTPDase3, respectively. Ticlopidine is an inhibitor of CYP2C19 human liver cytochrome. Ticlopidine inhibits CYP2C9 and CYP3A4 with IC50s of 26.0 and 32.3 μM, respectively.

IC_{50} & Target	CYP2	CYP3

In Vitro

Ticlopidine exhibits activity against human CD39 with apparent $K_{i,app}$ values of 14 μM[1].
Ticlopidine inhibits recombinant human CD39 expressed in COS-7-cells with the K_i value of 127±12 μM[1].
Growth rate is affected during the first days of culture, Ticlopidine (30 and 150 μM) reducing its effect in the following days[4].

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

Cell Proliferation Assay[4]

Cell Line:	Human endothelial cells
Concentration:	30 and 150 μM
Incubation Time:	2, 6; 10 days
Result:	Treated cells grow slower if compared with controls and this effect correlates with the concentration of Ticlopidine in the culture medium.

In Vivo

Oral administration of Losartan with 10 mg/kg Ticlopidine significantly increases the AUC (by 65.0%), suggesting that Ticlopidine can effectively inhibit the metabolism of losartan in the intestine and/or liver[3].

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

Animal Model:	Male Sprague-Dawley rats (7-8 weeks old, weighing 270-300 g)[3]
Dosage:	4 or 10 mg/kg
Administration:	Orally administered 30 min before oral administration of losartan.
Result:	The AUC and C_{max} of Losartan after oral administration with Losartan and 10 mg/kg Ticlopidine were significantly greater (by 65.0% and 49.4%, respectively) than those of control rats.

REFERENCES

[1]. Laura Schäkel, et al. 2-Substituted thienotetrahydropyridine derivatives: Allosteric ectonucleotidase inhibitors. Arch Pharm (Weinheim). 2021 Dec;354(12):e2100300.

[2]. I.KRASLOVA1, et al. Ticlopidine-Induced Cholestatic Inflammatory Hepatitis: New Insights into Pathogenetic Mechanisms of Drug-Related Hepatotoxicity.

[3]. Si-hyung Yang, et al. Effects of ticlopidine on pharmacokinetics of losartan and its main metabolite EXP-3174 in rats. Acta Pharmacol Sin. 2011 Jul;32(7):967-72.

[4]. F Piovella, et al. The effect of Ticlopidine on human endothelial cells in culture. Thromb Res. 1984 Feb 1;33(3):323-32.

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