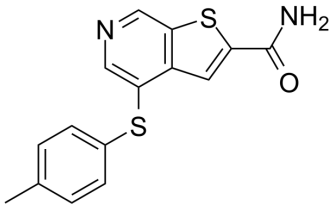
A-205804

Cat. No.:	HY-100226
CAS No.:	251992-66-2
Molecular Formula:	$C_{15}H_{12}N_2OS_2$
Molecular Weight:	300.4
Target:	Integrin
Pathway:	Cytoskeleton
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 (332.89 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.3289 mL	16.6445 mL	33.2889 mL
	5 mM	0.6658 mL	3.3289 mL	6.6578 mL
	10 mM	0.3329 mL	1.6644 mL	3.3289 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: ≥ 2.08 mg/mL (6.92 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (6.92 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

A-205804 is an orally bioavailable, potent and selective lead inhibitor of E-selectin and ICAM-1 expression, with an IC_{50} of 20 nM and 25 nM for E-selectin and ICAM-1, respectively. A-205804 can be used in the research of chronic inflammatory diseases [1].

IC_{50} & Target

IC50: 20 nM (E-selectin), 25 nM (ICAM-1)[1]

In Vitro

A-205804 exhibits Cellular Toxicities for HUVEC with an IC_{50} of 152 μM[1].
A-205804 is an effective inhibitor of cell-cell adhesion in an in vitro flow experiment, demonstrating relevance in a model physiological system[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

A-205804 (5 mg/kg; p.o.) shows a half-life of 1 hour for rat[1].

A-205804 (10 mg/kg; p.o.; 3 times per week; for 2 weeks) attenuates the E-selectin expression on the endothelial vascular niche cells in mice[2].

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

Animal Model:	C57BL/6 mice[2]
Dosage:	10 mg/kg
Administration:	Oral administration, 3 times per week, for 2 weeks
Result:	Efficiently decreased the expression of E-selectin on the endothelial vascular niche cells

Animal Model:	Rat[1]
Dosage:	5 mg/kg (Pharmacokinetic Analysis)
Administration:	Oral administration
Result:	$t_{1/2}$ = 1 hour

REFERENCES

[1]. Stewart AO, et al. Discovery of inhibitors of cell adhesion molecule expression in human endothelial cells. 1. Selective inhibition of ICAM-1 and E-selectin expression. J Med Chem. 2001 Mar 15;44(6):988-1002.

[2]. Morita K, et al. RUNX transcription factors potentially control E-selectin expression in the bone marrow vascular niche in mice. Blood Adv. 2018 Mar 13;2(5):509-515.

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