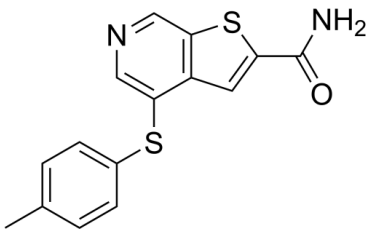
Data Sheet

Product Name:	A-205804
Cat. No.:	CS-0018356
CAS No.:	251992-66-2
Molecular Formula:	$C_{15}H_{12}N_2OS_2$
Molecular Weight:	300.40
Target:	Integrin
Pathway:	Cytoskeleton
Solubility:	DMSO : 100 mg/mL (332.89 mM; ultrasonic and warming and heat to 60°C)



BIOLOGICAL ACTIVITY:

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]. IC50 & 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].

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].

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.

CAIndexNames:

Thieno[2,3-c]pyridine-2-carboxamide, 4-[(4-methylphenyl)thio]-

SMILES:

O=C(C(S1)=CC2=C1C=NC=C2SC3=CC=C(C)C=C3)N

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

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