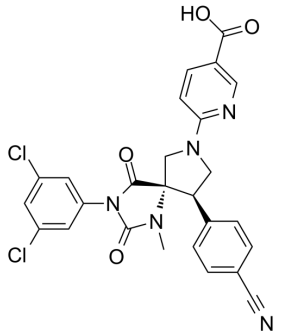
BMS-688521

Cat. No.:	HY-10596
CAS No.:	893397-44-9
Molecular Formula:	$C_{26}H_{19}Cl_2N_5O_4$
Molecular Weight:	536.37
Target:	Integrin
Pathway:	Cytoskeleton
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (186.44 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	1.8644 mL	9.3219 mL	18.6438 mL
	5 mM	0.3729 mL	1.8644 mL	3.7288 mL
	10 mM	0.1864 mL	0.9322 mL	1.8644 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: 5 mg/mL (9.32 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 5 mg/mL (9.32 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BMS-688521 is a highly potent, orally active inhibitor of the LFA-1/ICAM interaction, with an IC_{50} of 2.5 nM in the adhesion assay and an IC_{50} of 60 nM in the MLR assay. BMS-688521 is efficacious in a mouse allergic eosinophilic lung inflammation model[1].

In Vitro

BMS-688521 in a mouse specific adhesion assay employed mouse splenocytes and a mouse ICAM-1 expression cell line, b.END3. BMS-688521 has an IC_{50} of 78 nM, representing an approximately 30-fold decrease in activity relative to the human T-cell/HUVEC assay data ($ICIC_{50}$=2.5 nM)[1].

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

In Vivo

BMS-688521 (1-10 mg/kg; p.o.; BID for a three-day) is efficacious in a mouse allergic eosinophilic lung inflammation model[1]. BMS-688521 (5 mg/kg; p.o.) treatment shows the C_{max}, T_{max}, AUC, F values are 0.32 μM, 1.0 μM, 1.5 μM h, and 50%,

respectively[1].

BMS-688521 (1 mg/kg; i.v.) treatment shows the $T_{1/2}$, MRT, CL and Vss values are 1.6 hours, 1.7 hours, 50 mL/mim/kg, and 5.1 L/kg, respectively in BALB/c mice[1].

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Animal Model:	BALB/c female mice, 6-8 week of age (OVA Lung Inflammation in Mice)[1]
Dosage:	1, 3, and 10 mg/kg
Administration:	p.o.; BID for a three-day
Result:	Significant inhibition of eosinophil accumulation was seen at a dose of 1 mg/kg BID, with dose-dependent inhibition at 3 mg/kg and 10 mg/kg.

REFERENCES

[1]. Watterson SH, et al. Small molecule antagonist of leukocyte function associated antigen-1 (LFA-1): structure-activity relationships leading to the identification of 6-((5S,9R)-9-(4-cyanophenyl)-3-(3,5-dichlorophenyl)-1-methyl-2,4-dioxo-1,3,7-triazaspiro[4.4]nonan-7-yl)nicotinic acid (BMS-688521). J Med Chem. 2010 May 13;53(9):3814-30.

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