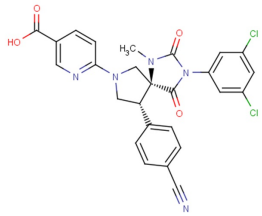
Data Sheet (Cat.No.T14676)

TargetMol
A DRUG SCREENING EXPERT

BMS-688521

Chemical Properties



CAS No.:	893397-44-9
Formula:	C26H19Cl2N5O4
Molecular Weight:	536.37
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	BMS-688521 is efficacious in a mouse allergic eosinophilic lung inflammation model and it is a highly potent, orally active inhibitor of the LFA-1/ICAM interaction. With an IC50 of 2.5 nM in the adhesion assay and an IC50 of 60 nM in the MLR assay .
Targets(IC_{50})	Others: None
In vitro	BMS-688521 has an IC50 of 78 nM, representing an approximately 30-fold decrease in activity relative to the human T-cell/HUVEC assay data (ICIC50=2.5 nM). BMS-688521 in a mouse specific adhesion assay employed mouse splenocytes and a mouse ICAM-1 expression cell line, b.END3[1].
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 (1 mg/kg; i.v.) treatment shows the T1/2, 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]. BMS-688521 (5 mg/kg; p.o.) treatment shows the Cmax, Tmax, AUC, F values are 0.32 μM, 1.0 μM, 1.5 μM h, and 50%, respectively[1].

Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.864 mL	9.322 mL	18.644 mL
5 mM	0.373 mL	1.864 mL	3.729 mL
10 mM	0.186 mL	0.932 mL	1.864 mL
50 mM	0.037 mL	0.186 mL	0.373 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

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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Tel:781-999-4286 E-mail:info@targetmol.com Address:36 Washington Street,Wellesley Hills,MA 02481