

Product Name: BMS 688521

Catalog No.: 4970

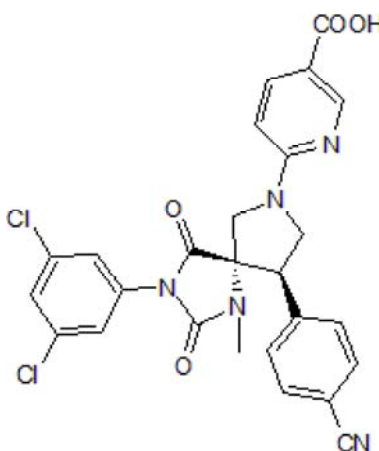
Batch No.: 1

CAS Number: 893397-44-9

IUPAC Name: 6-[(5*S*,9*R*)-9-(4-Cyanophenyl)-3-(3,5-dichlorophenyl)-1-methyl-2,4-dioxo-1,3,7-triazaspiro[4,4]non-7-yl]-3-pyridinecarboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₁₉Cl₂N₅O₄.H₂O
Batch Molecular Weight: 554.39
Physical Appearance: Off White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.35 (Dichloromethane:Methanol [95:5])
HPLC: Shows 98.1% purity
Chiral HPLC: Shows 99.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = +90 (Concentration = 1, Solvent = Methanol)
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.33	3.82	12.63
Found	56.26	3.79	12.49

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Description:

Potent inhibitor of the LFA-1/ICAM-1 interaction (IC₅₀ values are 2.5 and 78 nM in HUVEC adhesion and mouse specific adhesion assays respectively). Inhibits eosinophil accumulation in the lungs in a mouse allergic eosinophilic lung inflammation model.

Physical and Chemical Properties:

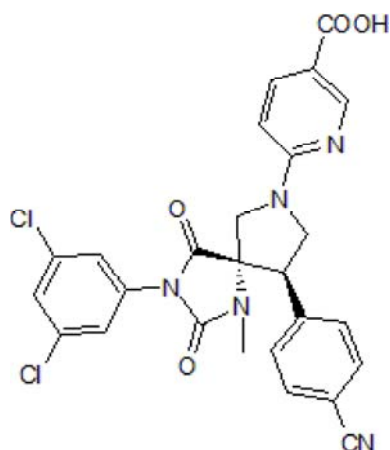
Batch Molecular Formula: C₂₆H₁₉Cl₂N₅O₄.H₂O

Batch Molecular Weight: 554.39

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Watterson *et al* (2010) Small molecule antagonist of leukocyte function associated antigen-1 (LFA-1): structure-activity relationships leading to the identification of 6-((5*S*,9*R*)-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.* **53** 3814. PMID: 20405922.

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