# **Product data sheet**



MedKoo Cat#: 524484				
Name: BMS-509744				
CAS#: 439575-02-7				
Chemical Formula: C <sub>32</sub> H <sub>41</sub> N <sub>5</sub> O <sub>4</sub> S <sub>2</sub>				
Exact Mass: 623.26				
Molecular Weight: 623.83				
Product supplied as: Powder			$\geq$	
Purity (by HPLC):	$\geq 98\%$		-	
Shipping conditions	pping conditions Ambient temperature			
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.			
	In solvent: -80°C 3 months; -20°C 2 weeks.			



## 1. Product description:

BMS-509744 is a potent interleukin-2 inducible T cell kinase (ITK) inhibitor (IC50 = 19 nM). It displays 200-fold selectivity over Tec family kinases and 55-fold selectivity over other kinases tested. BMS-509744 reduces HIV infection of primary CD4+ T cells and attenuates the establishment of HIV infection in vitro. BMS-509744 also reduces T cell proliferation and IL-2 production in vitro.

## 2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

## 3. Solubility data

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Solvent	Max Conc. mg/mL	Max Conc. mM			
DMSO	26.55	42.56			

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.60 mL	8.02 mL	16.03 mL
5 mM	0.32 mL	1.60 mL	3.21 mL
10 mM	0.16 mL	0.80 mL	1.60 mL
50 mM	0.03 mL	0.16 mL	0.32 mL

## 5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

## 6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Liu Y, Wang X, Deng L, Ping L, Shi Y, Zheng W, Lin N, Wang X, Tu M, Xie Y, Liu W, Ying Z, Zhang C, Pan Z, Wang X, Ding N, Song Y, Zhu J. ITK inhibition induced in vitro and in vivo anti-tumor activity through downregulating TCR signaling pathway in malignant T cell lymphoma. Cancer Cell Int. 2019 Feb 14;19:32. doi: 10.1186/s12935-019-0754-9. PMID: 30814910; PMCID: PMC6376795.

In vivo study

1. Otake S, Otsubaki T, Uesato N, Ueda Y, Murayama T, Hayashi M. Topical Application of BMS-509744, a Selective Inhibitor of Interleukin-2-Inducible T Cell Kinase, Ameliorates Imiquimod-Induced Skin Inflammation in Mice. Biol Pharm Bull. 2021 Apr 1;44(4):528-534. doi: 10.1248/bpb.b20-00850. Epub 2021 Jan 20. PMID: 33473072.

2. Lin TA, McIntyre KW, Das J, Liu C, O'Day KD, Penhallow B, Hung CY, Whitney GS, Shuster DJ, Yang X, Townsend R, Postelnek J, Spergel SH, Lin J, Moquin RV, Furch JA, Kamath AV, Zhang H, Marathe PH, Perez-Villar JJ, Doweyko A, Killar L, Dodd JH, Barrish JC, Wityak J, Kanner SB. Selective Itk inhibitors block T-cell activation and murine lung inflammation. Biochemistry. 2004 Aug 31;43(34):11056-62. doi: 10.1021/bi049428r. PMID: 15323564.

## 7. Bioactivity

Biological target:

## **Product data sheet**



BMS-509744 is a potent, selective and ATP competitive Itk inhibitor with an IC50 of 19 nM.

### In vitro activity

Consistent with these results, treatment with the ITK inhibitor BMS-509744 also efficiently inhibited invasion and migration in malignant T cells in a dose- and time-dependent manner (Fig. 3c, d; Additional file 1: Figure S2B).

Reference: Cancer Cell Int. 2019; 19: 32. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6376795/

#### In vivo activity

Topical application of BMS-509744 to the IMQ-treated skin markedly reduced psoriasis-like skin lesions, such as redness, erythema, scaling, and thickening on day 5. Daily administration of IMQ on the left ear increased the ear thickness in a time-dependent manner (Fig. 1C), and topical application of BMS-509744 significantly reduced the increase in ear thickness on day 5 in IMQ-treated mice.

Reference: Biol Pharm Bull. 2021 Apr 1;44(4):528-534. https://pubmed.ncbi.nlm.nih.gov/33473072/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.