

Certificate of Analysis

www.tocris.com

Product Name: BMS 509744

Catalog No.: 5009

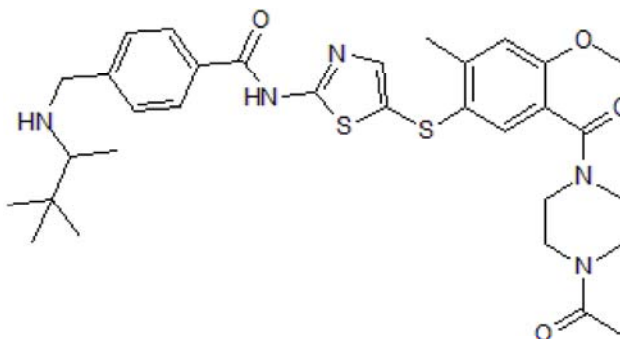
Batch No.: 2

CAS Number: 439575-02-7

IUPAC Name: *N*-[5-[[[5-[(4-Acetyl-1-piperazinyl)carbonyl]-4-methoxy-2-methylphenyl]thio]-2-thiazolyl]-4-[[[(1,2,2-trimethylpropyl)amino]methyl]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₂H₄₁N₅O₄S₂
Batch Molecular Weight: 623.83
Physical Appearance: White solid
Solubility: 1eq. HCl to 100 mM
DMSO to 50 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Chloroform:Methanol [9:1])
HPLC: Shows 98.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.61	6.62	11.23
Found	61.54	6.57	11.2

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel: +1 612 379 2956

Product Name: BMS 509744

Catalog No.: 5009

Batch No.: 2

CAS Number: 439575-02-7

IUPAC Name: N-[5-[[5-[(4-Acetyl-1-piperazinyl)carbonyl]-4-methoxy-2-methylphenyl]thio]-2-thiazolyl]-4-[[[(1,2,2-trimethylpropyl)amino]methyl]benzamide

Description:

Potent and selective interleukin-2 inducible T cell kinase (ITK) inhibitor (IC₅₀ = 19 nM). Displays 200-fold selectivity over Tec family kinases and 55-fold selectivity over other kinases tested. Reduces HIV infection of primary CD4⁺ T cells and attenuates the establishment of HIV infection in vitro. Reduces T cell proliferation and IL-2 production in vitro. Reduces lung inflammation in a mouse model of ovalbumin-induced allergy/asthma.

Physical and Chemical Properties:

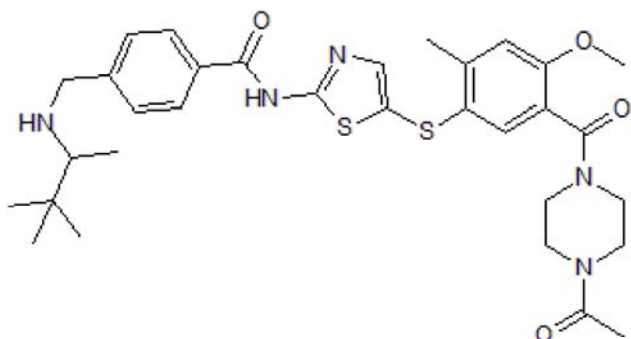
Batch Molecular Formula: C₃₂H₄₁N₅O₄S₂

Batch Molecular Weight: 623.83

Physical Appearance: White solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

1eq. HCl to 100 mM

DMSO to 50 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:

Kutach et al (2010) Crystal structures of IL-2-inducible T cell kinase complexed with inhibitors: insights into rational drug design and activity regulation. *Chem Biol Drug Des.* **76** 154. PMID: 20545945.

Readinger et al (2008) Selective targeting of ITK blocks multiple steps of HIV replication. *Proc.Natl.Acad.Sci.U.S.A.* **105** 6684. PMID: 18443296.

Das et al (2006) Discovery and SAR of 2-amino-5-(thioaryl)thiazoles as potent and selective Itk inhibitors. *Bioorg.Med.Chem.Lett.* **16** 3706. PMID: 16682193.

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel:+1 612 379 2956