

Product Name: SP 100030

Catalog No.: 5309

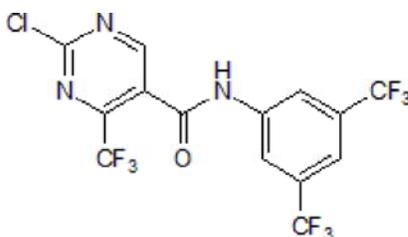
Batch No.: 1

CAS Number: 154563-54-9

IUPAC Name: *N*-[3,5-Bis(trifluoromethyl)phenyl]-2-chloro-4-(trifluoromethyl)-5-pyrimidinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₄H₅ClF₉N₃O
Batch Molecular Weight: 437.65
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Ethyl acetate:Petroleum ether [4:1])
HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	38.42	1.15	9.6
Found	38.5	1.12	9.64

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

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Description:

Potent dual inhibitor of NF-κB and AP-1 transcriptional activity (IC₅₀ = 50 nM). Blocks production of IL-2, IL-8 and TNF-α from Jurkat T cells. Inhibits cytokine production selectively in T cells; exhibits minimal inhibition of cytokine production in other cell types. Decreases arthritic severity in a mouse model of collagen-induced arthritis. Also ameliorates muscle wasting in a rat model of cancer cachexia.

Physical and Chemical Properties:

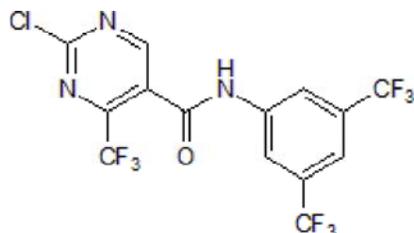
Batch Molecular Formula: C₁₄H₅ClF₉N₃O

Batch Molecular Weight: 437.65

Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Moore-Carrasco et al (2007) The AP-1/NF-κB double inhibitor SP100030 can revert muscle wasting during experimental cancer cachexia. *Int.J.Oncol.* **30** 1239. PMID: 17390027.

Gerlag et al (2000) The effect of a T cell-specific NF-κB inhibitor on *in vitro* cytokine production and collagen-induced arthritis. *J.Immunol.* **165** 1652. PMID: 10903776.

Sullivan et al (1998) 2-Chloro-4-(trifluoromethyl)pyrimidine-5-N-(3',5'- bis(trifluoromethyl)phenyl)-carboxamide: a potent inhibitor of NF-κB- and AP-1-mediated gene expression identified using solution-phase combinatorial ch. *J.Med.Chem.* **41** 413. PMID: 9484492.

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