

Certificate of Analysis

Product Name: NG 25

Catalog No.: 5429

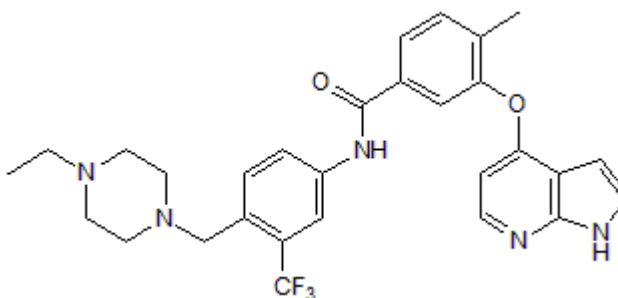
Batch No.: 1

CAS Number: 1315355-93-1

IUPAC Name: *N*-[4-[(4-Ethyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]-4-methyl-3-(1*H*-pyrrolo[2,3-*b*]pyridin-4-yloxy)benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₉ H ₃₀ F ₃ N ₅ O ₂
Batch Molecular Weight:	537.58
Physical Appearance:	White solid
Solubility:	DMSO to 20 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

TLC:	R _f = 0.24 (Chloroform:Methanol [9:1])
HPLC:	Shows 99.1% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	64.79	5.62	13.03
Found	64.48	5.58	13.08

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

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Description:

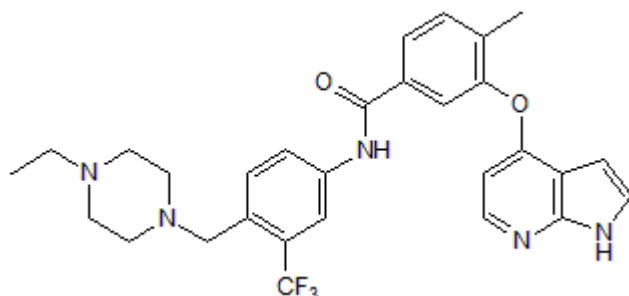
TGF- β -activated kinase (TAK1) inhibitor (IC₅₀ = 149 nM). Also inhibits LYN, MAP4K2 and Abl kinase activity (IC₅₀ values are 12.9, 21.7 and 75.2 nM, respectively). Suppresses CpG A and CpG B-stimulated secretion of IFN- α and TLR7/8 agonist CL097-stimulated secretion of IFN- β in Gen 2.2 leukemia cells in vitro.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₉H₃₀F₃N₅O₂
 Batch Molecular Weight: 537.58
 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

- Pauls et al** (2012) Essential role for IKK β in production of type 1 interferons by plasmacytoid dendritic cells. *J.Biol.Chem.* **287** 19216. PMID: 22511786.
- Dzamko et al** (2012) The I κ B kinase family phosphorylates the Parkinson's disease kinase LRRK2 at Ser935 and Ser910 during Toll-like receptor signaling. *PLoS ONE* **7** e39132. PMID: 22723946.
- Tan et al** (2015) Discovery of type II inhibitors of TGF β -activated kinase 1 (TAK1) and mitogen-activated protein kinase kinase kinase 2 (MAP4K2). *J.Med.Chem.* **58** 183. PMID: 25075558.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 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.

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