

Certificate of Analysis

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Product Name: CU-T12-9

Catalog No.: 5414

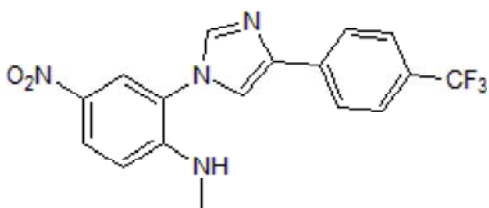
Batch No.: 1

CAS Number: 1821387-73-8

IUPAC Name: *N*-Methyl-4-nitro-2-(4-(4-trifluoromethyl)phenyl)-1*H*-imidazol-1-yl)aniline

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₃F₃N₄O₂
Batch Molecular Weight: 362.31
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
ethanol to 20 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.56 (Chloroform:Methanol [95:5])
HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.36	3.62	15.46
Found	56.47	3.59	15.44

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

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Description:

Potent TLR1/2 agonist (EC₅₀ = 52.9 nM). Activates the NF-κB pathway and upregulates proinflammatory cytokines in vitro. Also enhances TLR1 and TLR2 dimerization.

Physical and Chemical Properties:

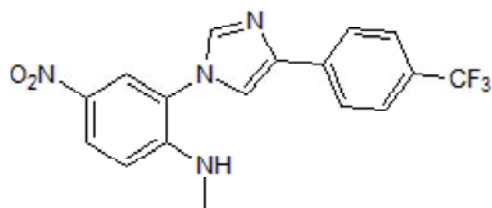
Batch Molecular Formula: C₁₇H₁₃F₃N₄O₂

Batch Molecular Weight: 362.31

Physical Appearance: Yellow solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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.

Licensing Information:

Sold under license from the University of Colorado

References:

Cheng et al (2015) Specific activation of the TLR1-TLR2 heterodimer by small-molecule agonists *Sci.Adv.* **1** e1400139. PMID: 26101787.

Cheng et al (2013) Discovery of small molecule inhibitors of the TLR1-TLR2 complex. *Angew.Chem.Int.Ed.Engl.* **51** 12246. PMID: 22969053.

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