

Certificate of Analysis

Print Date: Oct 21st 2024

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Product Name: A 33 Catalog No.: 6313 Batch No.: 2

CAS Number: 915082-52-9

IUPAC Name: 2-[4-[[2-(5-Chloro-2-thienyl)-5-ethyl-6-methyl-pyrimidin-4-yl]amino]phenyl]acetic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₁₈ClN₃O₂S.1¹/₄H₂O

Batch Molecular Weight: 410.4

Physical Appearance: Off White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 55.61 5.03 10.24 Found 54.74 4.65 10.09



Product Information

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IUPAC Name: 2-[4-[[2-(5-Chloro-2-thienyl)-5-ethyl-6-methyl-pyrimidin-4-yl]amino]phenyl]acetic acid

Description:

A 33 is a potent and selective PDE4B inhibitor (IC $_{50}$ = 15 nM); exhibits >100-fold selectivity for PDE4B over 4D. Regulates cAMP in inflammatory cells. Inhibits LPS-induced TNF- α production and neutrophil accumulation in mouse lungs. Reduces microglial and neutrophil activation, and improves behavioral deficits in a traumatic brain injury model in vivo. Also exhibits antidepressant-like effects. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₉H₁₈CIN₃O₂S.1¹/₄H₂O

Batch Molecular Weight: 410.4 Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Wilson et al (2017) Therapeutic benefits of phosphodiesterase 4B inhibition after traumatic brain injury. PLoS One 12 e0178013. PMID: 28542295.

Zhang *et al* (2017) Comparison of the pharmacological profiles of selective PDE4B and PDE4D inhibitors in the central nervous system. Sci.Rep. **7** 40115. PMID: 28054669.

Naganuma et al (2009) Discovery of selective PDE4B inhibitors. Bioorg.Med.Chem.Lett. 19 3174. PMID: 19447034.