

Product Name: A 33

Catalog No.: 6313

Batch No.: 1

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

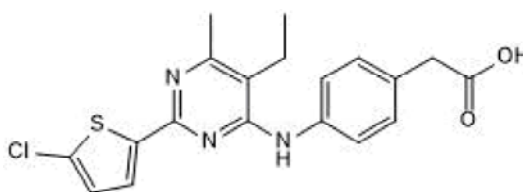
Batch Molecular Weight: 387.88

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.42 (Dichloromethane:Methanol [95:5])

HPLC: Shows 99.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.83	4.68	10.83
Found	58.76	4.67	10.74

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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

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Description:

Potent and selective PDE4B inhibitor (IC₅₀ = 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:

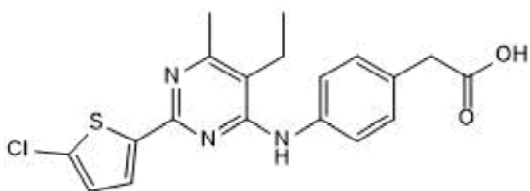
Batch Molecular Formula: C₁₉H₁₈ClN₃O₂S

Batch Molecular Weight: 387.88

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. 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:

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.

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North America

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Tel:+1 612 379 2956