

Certificate of Analysis

Product Name: SM 324405

Catalog No.: 5445

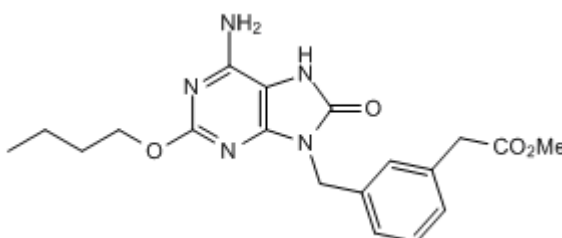
Batch No.: 1

CAS Number: 677773-91-0

IUPAC Name: Methyl 3-[(6-amino-2-butoxy-7,8-dihydro-8-oxo-9H-purin-9-yl)methyl]benzeneacetate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₂₃N₅O₄
Batch Molecular Weight: 385.42
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Dichloromethane:Methanol [95:5])
HPLC: Shows 98.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.21	6.02	18.17
Found	58.9	5.94	18.01

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

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Description:

Potent TLR7 agonist (EC₅₀ = 50 nM). Exhibits selectivity for TLR7 over TLR8. Induces IFN- α and - γ expression in human PBMCs and mouse splenocytes, and inhibits IL-5 production in human PBMCs in vitro. Rapidly metabolized to acid metabolite (t_{1/2} = 2.6 min in human plasma).

Physical and Chemical Properties:

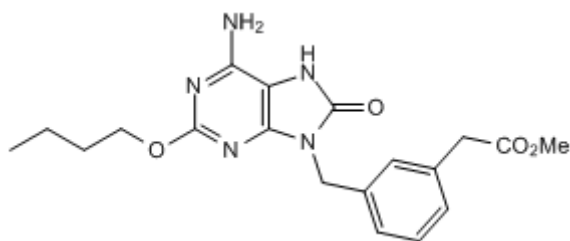
Batch Molecular Formula: C₁₉H₂₃N₅O₄

Batch Molecular Weight: 385.42

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°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:

Biffen *et al* (2012) Biological characterization of a novel class of toll-like receptor 7 agonists designed to have reduced systemic activity. *Br.J.Pharmacol.* **166** 573. PMID: 22122192.

Kurimoto *et al* (2010) Synthesis and biological evaluation of 8-oxoadenine derivatives as toll-like receptor 7 agonists introducing the antedrug concept. *J.Med.Chem.* **53** 2964. PMID: 20232824.

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