

Certificate of Analysis

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Product Name: Ro 51

Catalog No.: 4391

Batch No.: 2

CAS Number: 1050670-85-3

IUPAC Name: 2-[[4-Amino-5-[5-iodo-4-methoxy-2-(1-methylethyl)phenoxy]-2,4-pyrimidinyl]amino]-1,3-propanediol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₂₃IN₄O₄·½H₂O

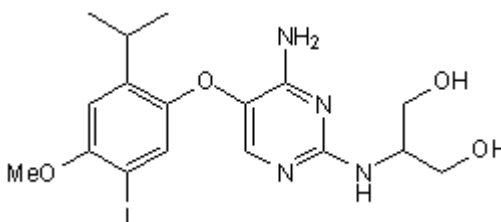
Batch Molecular Weight: 483.3

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	42.25	5.01	11.59
Found	42.12	4.71	11.69

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

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Description:

Potent, dual P2X₃ and P2X_{2/3} antagonist (IC₅₀ values are 2 and 5 nM for rP2X₃ and hP2X_{2/3} respectively). Selective for P2X₃ and P2X_{2/3} over other P2X receptors (IC₅₀ values are > 10 μM for P2X₁, P2X₂, P2X₄, P2X₅, and P2X₇). Cell permeable.

Physical and Chemical Properties:

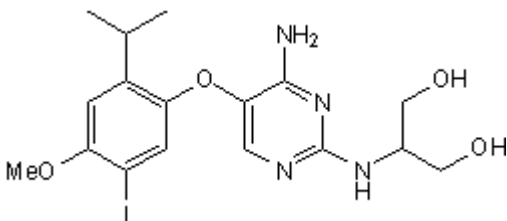
Batch Molecular Formula: C₁₇H₂₃IN₄O₄·½H₂O

Batch Molecular Weight: 483.3

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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:

Jahangir et al (2009) Identification and SAR of novel diaminopyrimidines. Part 2: The discovery of RO-51, a potent and selective, dual P2X₃/P2X_{2/3} antagonist for the treatment of pain. *Bioorg.Med.Chem.Lett.* **19** 1632. PMID: 19231178.

Syed and Kennedy (2012) Pharmacology of P2X receptors *WIREs.Membr.Transp.Signal.* **1** 16.

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