Print Date: Jun 26th 2012

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: $C_{17}H_{23}IN_4O_4 \cdot \frac{1}{2}H_2O$

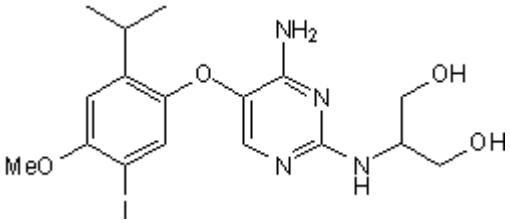
Batch Molecular Weight: 483.3

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

^{1}H 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

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Description:

Potent, dual $P2X_3$ and $P2X_{2/3}$ antagonist (IC_{50} values are 2 and 5 nM for $rP2X_3$ and $hP2X_{2/3}$ respectively). Selective for $P2X_3$ and $P2X_{2/3}$ over other P2X receptors (IC_{50} values are > 10 µM for $P2X_1$, $P2X_2$, $P2X_4$, $P2X_5$, and $P2X_7$). Cell permeable.

Physical and Chemical Properties:

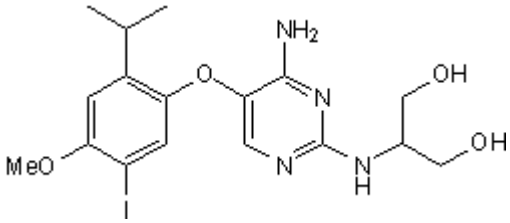
Batch Molecular Formula: $C_{17}H_{23}IN_4O_4.½H_2O$

Batch Molecular Weight: 483.3

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

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 $P2X_3/P2X_{2/3}$ 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.