



Certificate of Analysis

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Product Name: RO-3 Catalog No.: 3052 Batch No.: 3

CAS Number: 1026582-88-6

IUPAC Name: 5-[[4,5-Dimethoxy-2-(methylethyl)phenyl]methyl]-2,4-pyrimidinediamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{22}N_4O_2$ Batch Molecular Weight: 302.37

Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: R_f = 0.22 (Dichloromethane:Methanol:Ammonia soln. [99:9:1])

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 63.55 7.33 18.53 Found 63.65 7.35 18.55



Product Information

Print Date: Jan 13th 2022

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IUPAC Name: 5-[[4,5-Dimethoxy-2-(methylethyl)phenyl]methyl]-2,4-pyrimidinediamine

Description:

RO-3 is a selective homomeric P2X $_3$ and heteromeric P2X $_{2/3}$ receptor antagonist (pIC $_{50}$ values are 7.0 and 5.9 respectively) that exhibits no activity at P2X $_1$, P2X $_2$, P2X $_4$, P2X $_5$ and P2X $_7$ receptors (IC $_{50}$ > 10 μ M). Attenuates nociceptive sensitivity in animal models of pain. Orally active and brain penetrant.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{16}H_{22}N_4O_2$ Batch Molecular Weight: 302.37 Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at RT

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:

Donnelly-Roberts *et al* (2008) Painful purinergic receptors. J.Pharmacol.Exp.Ther. **324** 409. PMID: 18042830. **Ford** *et al* (2006) Purinoceptors as therapeutic targets for lower urinary tract dysfunction. Br.J.Pharmacol. **147** S132. PMID: 16465177.

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

Gever et al (2006) Pharmacology of P2X channels. Eur.J.Physiol. 452 513.