

Certificate of Analysis

Product Name: A 839977

Catalog No.: 4232

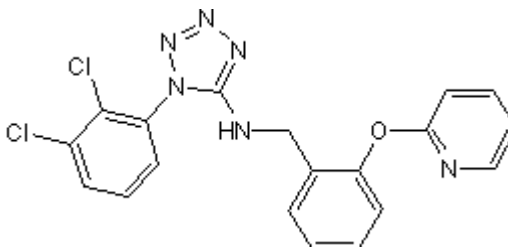
Batch No.: 2

CAS Number: 870061-27-1

IUPAC Name: 1-(2,3-Dichlorophenyl)-N-[[2-(2-pyridinyloxy)phenyl]methyl]-1*H*-tetrazol-5-amine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₁₄Cl₂N₆O
Batch Molecular Weight: 413.26
Physical Appearance: White solid
Solubility: DMSO to 100 mM
ethanol to 5 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.28 (Ethyl acetate:Petroleum ether [4:1])
HPLC: Shows >99.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 55.22 | 3.41 | 20.34 |
| Found | 54.97 | 3.44 | 20.26 |

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

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Description:

Potent P2X₇ antagonist; blocks BzATP-evoked calcium influx at recombinant human, rat and mouse P2X₇ receptors (IC₅₀ values are 20, 42 and 150 nM respectively). Displays antinociceptive effects in rat and mice models of inflammatory pain. CNS penetrant.

Physical and Chemical Properties:

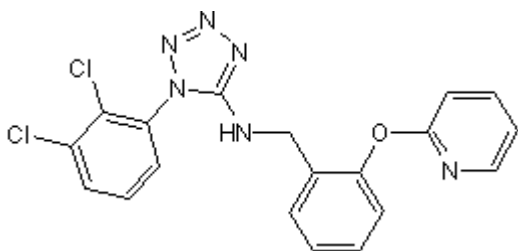
Batch Molecular Formula: C₁₉H₁₄Cl₂N₆O

Batch Molecular Weight: 413.26

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Honore *et al* (2009) The antihyperalgesic activity of a selective P2X₇ receptor antagonist, A-839977, is lost in IL-1αβ knockout mice. *Behav.Brain.Res.* **204** 77. PMID: 19464323.

Friedle *et al* (2010) Recent patents on novel P2X₇ receptor antagonists and their potential for reducing central nervous system inflammation. *Recent Pat.CNS Drug Discov.* **5** 35. PMID: 19705995.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 5 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.

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