



Certificate of Analysis

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Product Name: A 438079 hydrochloride Catalog No.: 2972 Batch No.: 6

CAS Number: 899431-18-6

IUPAC Name: 3-[[5-(2,3-Dichlorophenyl)-1*H*-tetrazol-1-yl]methyl]pyridine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

C₁₃H₉Cl₂N₅.HCl.1¹/₄H₂O **Batch Molecular Formula:**

Batch Molecular Weight: 365.13 **Physical Appearance:** White solid

DMSO to 100 mM Solubility: Storage: Desiccate at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure Consistent with structure Mass Spectrum:

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 42.76 3.45 19.18 Found 42.46 3.29 19.12

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

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Product Information

Print Date: Mar 11th 2022

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IUPAC Name: 3-[[5-(2,3-Dichlorophenyl)-1*H*-tetrazol-1-yl]methyl]pyridine hydrochloride

Description:

A 438079 hydrochloride is a competitive P2X₇ receptor antagonist (pIC $_{50}$ = 6.9 for the inhibition of Ca $^{2+}$ influx in the human recombinant P2X₇ cell line). Devoid of activity at other P2 receptors (IC $_{50}$ > 10 μ M). Possesses antinociceptive activity in models of neuropathic pain in vivo. Inhibits methamphetamine-induced microglial migration and phagocytosis in vitro.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₃H₉Cl₂N₅.HCl.11/4H₂O

Batch Molecular Weight: 365.13 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Desiccate 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).

Catalog No.: 2972

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:

Fernandes *et al* (2016) Methamphetamine alters microglial immune function through P2X₇R signaling. J.Neuroinflammation. *13* 91. PMID: 27117066.

Donnelly-Roberts and Jarvis (2007) Discovery of P2X₇ receptor-selective antagonists offers new insights into P2X₇ receptor function and indicates a role in chronic pain states. Br.J.Pharmacol. **151** 571. PMID: 17471177.

McGaraughty et al (2007) P2X₇-related modulation of pathological nociception in rats. Neuroscience 146 1817. PMID: 17478048.