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Print Date: Jul 14th 2023

Batch No.: 4

Certificate of Analysis

www.tocris.com

Catalog No.: 4716

Product Name: A 967079

CAS Number:1170613-55-4IUPAC Name:(1E,3E)-1-(4-Fluorophenyl)-2-methyl-1-pentene-3-one oxime

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C₁₂H₁₄FNO 207.24 White solid DMSO to 100 mM ethanol to 100 mM Store at +4°C

Storage: **Batch Molecular Structure:**

OH

2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

Shows 99.8% purity Consistent with structure Consistent with structure

	Carbon H	ydrogen N	litrogen
Theoretical	69.55	6.81	6.76
Found	69.7	6.84	6.81

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

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A 967079 Product Name:

CAS Number: 1170613-55-4 **IUPAC Name:**

(1E,3E)-1-(4-Fluorophenyl)-2-methyl-1-pentene-3-one oxime

Description:

A 967079 (also known as A-079) is a selective TRPA1 channel blocker (IC_{50} values are 67 and 289 nM at human and rat TRPA1 receptors respectively) that displays 1000-fold selectivity for TRPA1 over other TRP channels, and is >150-fold selective over 75 other ion channels, enzymes and G-protein-coupled receptors. A 967079 exhibits analgesic effects in a rat osteoarthritic pain model.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₂H₁₄FNO Batch Molecular Weight: 207.24 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Chen et al (2011) Selective blockade of TRPA1 channel attenuates pathological pain without altering noxious cold sensation or body temperature regulation. Pain 152 1165. PMID: 21402443.

McGaraughty et al (2010) TRPA1 modulation of spontaneous and mechanically evoked firing of spinal neurons in uninjured, osteoarthritic, and inflamed rats. Mol.Pain 6 14. PMID: 20205719.

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