

Certificate of Analysis

Print Date: Jan 14th 2016

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Product Name: ICA 069673 Catalog No.: 4305 Batch No.: 2

CAS Number: 582323-16-8

IUPAC Name: N-(2-Chloro-5-pyrimidinyl)-3,4-difluorobenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{11}H_6CIF_2N_3O$

Batch Molecular Weight: 269.63 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

ethanol to 25 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.36$ (Ethyl acetate:Petroleum ether [2:3])

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 49 2.24 15.58 Found 49.02 2.38 15.56



Product Information

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IUPAC Name: N-(2-Chloro-5-pyrimidinyl)-3,4-difluorobenzamide

Description:

Selective $K_V7.2/K_V7.3$ (KCNQ2/3) channel opener (EC₅₀ = 0.69 μM). Exhibits 20-fold selectivity for $K_V 7.2/K_V 7.3$ over K_V7.3/K_V7.5, with no measurable activity over a panel of cardiac ion channels. Hyperpolarizes resting membrane potential and inhibits spontaneous action potentials in guinea pig detrusor muscle (DSM) isolated cells. Orally active in animal models of epilepsy.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₁H₆CIF₂N₃O

Batch Molecular Weight: 269.63 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM ethanol to 25 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:

Amato et al (2011) N-pyridyl and pyrimidine benzamides as KCNQ2/Q3 potassium channel openers for the treatment of epilepsy. ACS Med.Chem.Lett. 2 481. PMID: 24900334.

Provence et al (2015) The novel K_v7.2/K_v7.3 channel opener ICA-069673 reveals subtype-specific functional roles in quinea pig detrusor smooth muscle excitability and contractility. J.Pharmacol.Exp.Ther. 354 290. PMID: 26087697.