

Certificate of Analysis

Print Date: Jan 15th 2016

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Product Name: VU 0240551 Catalog No.: 3888 Batch No.: 1

CAS Number: 893990-34-6

IUPAC Name: N-(4-Methyl-2-thiazolyl)-2-[(6-phenyl-3-pyridazinyl)thio]acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{14}N_4OS_2$

Batch Molecular Weight: 342.43 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

ethanol to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

Microanalysis:

HPLC: Shows 99.5% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Theoretical 56.12 4.12 16.36 Found 56.11 4.19 16.37

Carbon Hydrogen Nitrogen



Product Information

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IUPAC Name: N-(4-Methyl-2-thiazolyl)-2-[(6-phenyl-3-pyridazinyl)thio]acetamide

Description:

Inhibitor of the neuronal K-CI cotransporter, KCC2 (IC $_{50}$ = 560 nM for K+ uptake assay in KCC2-overexpressing cells). Exhibits selectivity over the Na-K-2CI cotransporter, NKCCI. Also inhibits hERG and L-type Ca $^{2+}$ channels.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₆H₁₄N₄OS₂ Batch Molecular Weight: 342.43 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°C

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:

Delpire et al (2009) Small-molecule screen identifies inhibitors of the neuronal K-Cl cotransporter KCC2. Proc.Natl.Acad.Sci.USA 106 5383. PMID: 19279215.

Delpire et al (2012) Further optimization of the K-Cl cotransporter KCC2 antagonist ML077: development of a highly selective and more potent *in vitro* probe. Bioorg.Med.Chem.Lett. **22** 4532. PMID: 22727639.

Deisz et al (2014) Effects of VU0240551, a novel KCC2 antagonist, and DIDS on chloride homeostasis of neocortical neurons from rats and humans. Neuroscience **277** 831. PMID: 25086309.