Certificate of Analysis

Product Name: **VU 0463271** **Catalog No.: 4719** **Batch No.: 1**

CAS Number: 1391737-01-1

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{18}N_4OS_2.¼H_2O$

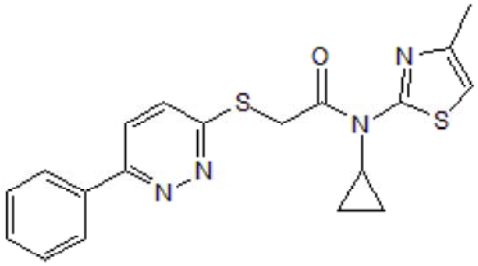
Batch Molecular Weight: 387

Physical Appearance: Yellow solid

Solubility: DMSO to 50 mM
ethanol to 10 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.6 (Ethyl acetate:Petroleum ether [7:3])

HPLC: Shows 98.2% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.97	4.82	14.48
Found	58.71	4.73	14.53

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Description:

Potent and selective inhibitor of the neuronal K-Cl cotransporter, KCC2 (IC_{50} = 61 nM); displays >100-fold selectivity versus the Na-K-2Cl cotransporter 1 (NKCC1) and no activity against a panel of 68 GPCRs, ion channels and transporters.

Physical and Chemical Properties:

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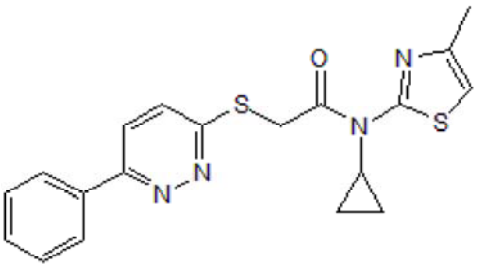
Batch Molecular Weight: 387

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 50 mM
ethanol to 10 mM with gentle warming

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:

Sivakumaran *et al* (2015) Selective inhibition of KCC2 leads to hyperexcitability and epileptiform discharges in hippocampal slices and *in vivo*. J.Neurosci. ***35*** 8291. PMID: 26019342.

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.