

Certificate of Analysis

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Product Name: Zoniporide dihydrochloride

Catalog No.: 2727

Batch No.: 2

CAS Number: 241799-10-0

IUPAC Name: [1-(Quinolin-5-yl)-5-cyclopropyl-1*H*-pyrazole-4-carbonyl]guanidine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₆N₆O.2HCl

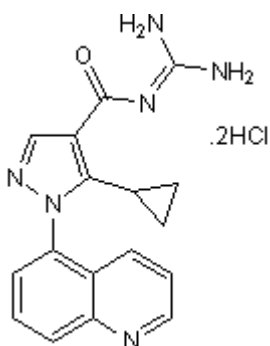
Batch Molecular Weight: 393.27

Physical Appearance: Off-white solid

Solubility: water to 10 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.92	4.61	21.37
Found	52.22	4.95	20.95

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

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Description:

Sodium-hydrogen exchanger isoform 1 (NHE1) inhibitor that displays selectivity over other NHE isoforms (K_i values are 14, 2200 and 220000 nM for human NHE1, human NHE2 and rat NHE3 respectively). Inhibits NHE1 dependent $^{22}\text{Na}^+$ uptake in vitro ($\text{IC}_{50} = 14$ nM) and provides cardioprotection from myocardial ischemic injury in vivo ($\text{EC}_{50} = 0.25$ nM). Also inhibits MMP2/9 activity and invasion in breast cancer cells.

Physical and Chemical Properties:

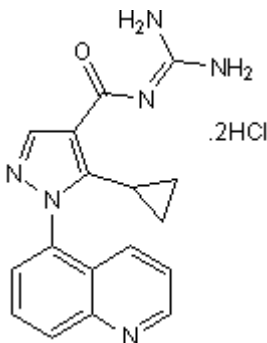
Batch Molecular Formula: $\text{C}_{17}\text{H}_{16}\text{N}_6\text{O} \cdot 2\text{HCl}$

Batch Molecular Weight: 393.27

Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Knight et al (2001) A novel sodium-hydrogen exchanger isoform-1 inhibitor, zoniporide, reduces ischemic myocardial injury in vitro and in vivo. *J.Pharmacol.Exp.Ther.* **297** 254. PMID: 11259552.

Marala et al (2002) Zoniporide: a potent and highly selective inhibitor of human Na^+/H^+ exchanger-1. *Eur.J.Pharmacol.* **451** 37. PMID: 12223226.

Clements-Jewery et al (2004) Cardioprotective efficacy of zoniporide, a potent and selective inhibitor of Na^+/H^+ exchanger isoform-1, in an experimental model of cardiopulmonary bypass. *Br.J.Pharmacol.* **142** 57. PMID: 15037516.

Storage: Store at -20°C

Solubility & Usage Info:

water to 10 mM
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 $45\text{-}60^\circ\text{C}$ 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.

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