

Product Name: BIX NHE1 inhibitor

Catalog No.: 5512

Batch No.: 1

CAS Number: 1422252-46-7

IUPAC Name: 4-(1-Acetyl-4-piperidiny)-N-(aminoiminomethyl)-3-(trifluoromethyl)benzamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₉F₃N₄O₂.HCl

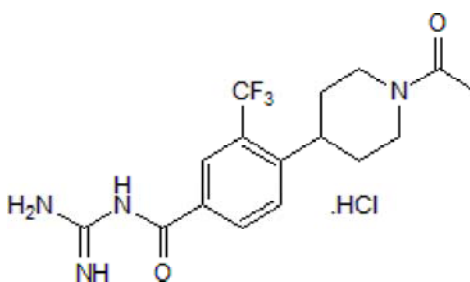
Batch Molecular Weight: 392.8

Physical Appearance: White solid

Solubility: DMSO to 50 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.25 (Chloroform:Methanol [9:1])

HPLC: Shows 99.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	48.92	5.13	14.26
Found	48.98	5.15	14.18

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

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Description:

Potent and selective NHE1 inhibitor ($IC_{50} = 31$ nM). Selective for NHE1 over NHE2 and NHE3. Prevents ischemic damage in an ischemia reperfusion injury isolated rat heart model ex vivo. Prevents phenylephrine-induced cardiomyocyte hypertrophy in vitro, and attenuates cardiac hypertrophy and left ventricular dysfunction postinfarction in rats. Orally bioavailable.

Physical and Chemical Properties:

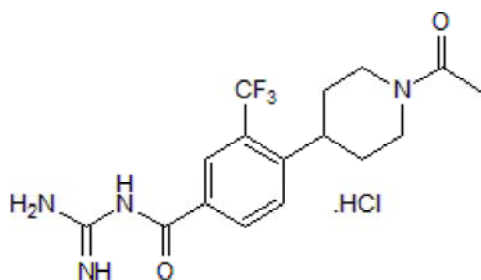
Batch Molecular Formula: $C_{16}H_{19}F_3N_4O_2.HCl$

Batch Molecular Weight: 392.8

Physical Appearance: White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



References:

Kilić *et al* (2014) Early and transient sodium-hydrogen exchanger isoform 1 inhibition attenuates subsequent cardiac hypertrophy and heart failure following coronary artery ligation. *J.Pharmacol.Exp.Ther.* **351** 492. PMID: 25216745.

Huber *et al* (2012) Identification of a potent sodium hydrogen exchanger isoform 1 (NHE1) inhibitor with a suitable profile for chronic dosing and demonstrated cardioprotective effects in a preclinical model of myocardial infarction in the rat. *J.Med.Chem.* **55** 7114. PMID: 22803959.

Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 50 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.

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