

**Product Name:** CaCCinh-A01

**Catalog No.:** 4877

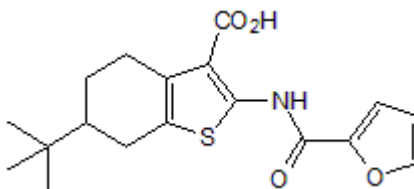
**Batch No.:** 3

CAS Number: 407587-33-1

IUPAC Name: 6-(1,1-Dimethylethyl)-2-[(2-furanylcarbonyl)amino]-4,5,6,7-tetrahydrobenzo[b]thiophene-3-carboxylic acid

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>18</sub>H<sub>21</sub>NO<sub>4</sub>S·¼H<sub>2</sub>O  
**Batch Molecular Weight:** 351.93  
**Physical Appearance:** Off White solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 10 mM with gentle warming  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows >99.7% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	61.43	6.16	3.98
Found	61.08	6.07	4.04

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

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**Description:**

Calcium-activated chloride channel (CaCC) inhibitor ( $IC_{50} \sim 10 \mu M$ ). Inhibits CaCC currents in human bronchial and intestinal cells. Also inhibits TMEM16A channels ( $IC_{50} = 2.1 \mu M$ , in TMEM16A-expressing FRT cells).

**Physical and Chemical Properties:**

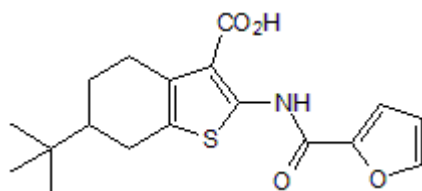
Batch Molecular Formula:  $C_{18}H_{21}NO_4 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 351.93

Physical Appearance: Off White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**References:**

**Namkung et al** (2011) TMEM16A inhibitors reveal TMEM16A as a minor component of calcium-activated chloride channel conductance in airway and intestinal epithelial cells. *J.Biol.Chem.* **286** 2365. PMID: 21084298.

**De La Fuente et al** (2008) Small-molecule screen identifies inhibitors of a human intestinal calcium-activated chloride channel. *Mol.Pharmacol.* **73** 758. PMID: 18083779.

**Storage:** Store at  $-20^{\circ}C$

**Solubility & Usage Info:**

DMSO to 100 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  $45-60^{\circ}C$  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  $-20^{\circ}C$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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