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: \( \text{C}_{18}\text{H}_{21}\text{NO}_4\text{S} \cdot \frac{1}{4}\text{H}_2\text{O} \)
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:

![Molecular Structure](image)

2. ANALYTICAL DATA

HPLC: Shows >99.7% purity
\(^1\text{H NMR:}\) Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>61.43</td>
<td>6.16</td>
<td>3.98</td>
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<tr>
<td>Found</td>
<td>61.08</td>
<td>6.07</td>
<td>4.04</td>
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</tbody>
</table>

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$_{50}$ ~ 10 μM). Inhibits CaCC currents in human bronchial and intestinal cells. Also inhibits TMEM16A channels (IC$_{50}$ = 2.1 μM, in TMEM16A-expressing FRT cells).

Physical and Chemical Properties:
Batch Molecular Formula: C$_{18}$H$_{21}$NO$_5$S.½H$_2$O
Batch Molecular Weight: 351.93
Physical Appearance: Off White solid
Minimum Purity: >99%

Storage: Store at -20°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°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: