1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{14}\text{H}_{21}\text{N}_3\text{O}.2\text{HCl}.\frac{1}{2}\text{H}_2\text{O} \)

Batch Molecular Weight: 329.27

Physical Appearance: White solid

Solubility: phosphate buffered saline to 100 mM
water to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.8% purity

\(^1\text{H NMR:} \) Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: \([\alpha]_D = +3 \) (Concentration = 1.0, Solvent = Methanol)

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>51.07</td>
<td>7.35</td>
<td>12.76</td>
</tr>
<tr>
<td>Found</td>
<td>51.4</td>
<td>7.51</td>
<td>12.45</td>
</tr>
</tbody>
</table>
Product Name: Y-27632 dihydrochloride
Catalog No.: 1254        Batch No.: 37
CAS Number: 129830-38-2
IUPAC Name: trans-4-[(1R)-1-Aminoethyl]-N-4-pyridinylcyclohexanecarboxamide dihydrochloride

Description:
Selective p160ROCK inhibitor (K values are 0.14, 26, 25 and > 250 μM for p160ROCK, PKC, PKA and MLCK respectively). Also inhibits PRK2 (IC50 = 600 nM). Smooth muscle relaxant and orally active in vivo. Increases survival rate of human embryonic stem (hES) cells and iPSC-BMECs undergoing cryopreservation. Also optimizes naïve human pluripotent stem cell growth and viability following naïve cell derivation from primed ESCs and iPSCs using naïve human stem cell medium (NHSM).

Physical and Chemical Properties:
Batch Molecular Formula: C14H21N3O2.HCl.½H2O
Batch Molecular Weight: 329.27
Physical Appearance: White solid
Minimum Purity: >98%

Storage: Desiccate at RT
Solubility & Usage Info:
- phosphate buffered saline to 100 mM
- water 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 45-60°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: