1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{20}\text{H}_{19}\text{N}_3\text{O}_2\cdot\frac{1}{4}\text{H}_2\text{O} \)

Batch Molecular Weight: 337.88

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM, ethanol to 25 mM

Storage: Store at RT

2. ANALYTICAL DATA

TLC: \( R_f = 0.45 \) (Chloroform:Methanol [9:1])

HPLC: Shows 99.4% purity

Chiral HPLC: Shows 100% purity

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

Mass Spectrum: Consistent with structure

Optical Rotation: \([\alpha]_D = +85.8 \) (Concentration = 0.68, 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>71.09</td>
<td>5.82</td>
<td>12.44</td>
</tr>
<tr>
<td>Found</td>
<td>71.38</td>
<td>5.71</td>
<td>12.54</td>
</tr>
</tbody>
</table>
Product Name: AS 1892802
Catalog No.: 4927
Batch No.: 1

CAS Number: 928320-12-1
IUPAC Name: N-{(1S)-2-Hydroxy-1-phenylethyl}-N'-[4-(4-pyridinyl)phenyl]-urea

Description:
Potent, ATP-competitive ROCK inhibitor (IC_{50} values are 52, 57 and 122 nM for human ROCK2, rat ROCK2 and human ROCK1 respectively by ELISA); also inhibits PKA and PRKX (IC_{50} values are 200 and 325 nM respectively). Exhibits analgesic effects in rat models of inflammatory (AIA) and noninflammatory (MIA) arthritic pain. Orally bioavailable.

Physical and Chemical Properties:
Batch Molecular Formula: C_{20}H_{16}N_{2}O_{7}·\frac{1}{4}H_{2}O
Batch Molecular Weight: 337.88
Physical Appearance: Off-white solid
Minimum Purity: >99%

Storage: Store at RT

Solubility & Usage Info:
DMSO to 100 mM
ethanol to 25 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:

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