**Product Name:** Y 39983 dihydrochloride  
**Catalog No.:** 3846  
**Batch No.:** 1  
**CAS Number:** 203911-26-6  
**IUPAC Name:** 4-[(1R)-1-Aminoethyl]-N-1H-pyrrolo[2,3-b]pyridin-4-ylbenzamide dihydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** \( \text{C}_{16}\text{H}_{16}\text{N}_4\text{O}.2\text{HCl}.1\frac{3}{4}\text{H}_2\text{O} \)
- **Batch Molecular Weight:** 384.77
- **Physical Appearance:** Off-white solid
- **Solubility:**  
  - Water to 100 mM
  - DMSO to 100 mM
  - Ethanol to 5 mM
- **Storage:** Desiccate at RT

### 2. ANALYTICAL DATA

- **HPLC:** Shows 99.4% purity
- **\(^1\text{H} NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Optical Rotation:** \([\alpha]_D = +5.4\) (Concentration = 1, Solvent = Methanol)
- **Microanalysis:**  
<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
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<tbody>
<tr>
<td>Carbon</td>
<td>49.94</td>
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<tr>
<td>Hydrogen</td>
<td>5.63</td>
<td>5.52</td>
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<tr>
<td>Nitrogen</td>
<td>14.56</td>
<td>14.46</td>
</tr>
</tbody>
</table>

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

bio-technet.com  
info@bio-technet.com  
techsupport@bio-technet.com  
North America  
Tel: (800) 343 7475

China  
info.cn@bio-technet.com  
Tel: +86 (21) 52380373

Europe Middle East Africa  
Tel: +44 (0)1235 529449

Rest of World  
www.tocris.com/distributors  
Tel:+1 612 379 2956
Product Name: Y 39983 dihydrochloride
Catalog No.: 3846
Batch No.: 1

CAS Number: 203911-26-6
IUPAC Name: 4-[(1R)-1-Aminoethyl]-N-H-pyrrolo[2,3-b]pyridin-4-ylbenzamide dihydrochloride

Description:
Selective Rho-kinase inhibitor (IC_{50} values are 0.0036, 0.42 and 0.81 μM for ROCK, PKC and CaMKII respectively). Promotes neurite regeneration in vitro and induces axonal regeneration in vivo. Derived from Y-27632 (Cat. No. 1254).

Physical and Chemical Properties:
Batch Molecular Formula: C_{10}H_{16}N_{4}O\cdot2HCl\cdot0.8H_{2}O
Batch Molecular Weight: 384.77
Physical Appearance: Off-white solid
Minimum Purity: >98%

Storage: Desiccate at RT

Solubility & Usage Info:
- water to 100 mM
- DMSO to 100 mM
- ethanol to 5 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: