1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( C_{25}H_{25}ClN_2O_4S \)

Batch Molecular Weight: 485

Physical Appearance: White solid

Solubility:
- DMSO to 100 mM
- Ethanol to 100 mM

Storage: Store at +4°C

2. ANALYTICAL DATA

TLC: \( R_f = 0.4 \) (Dichloromethane:Methanol [9:1])

HPLC: Shows 98% purity

\(^1\)H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: \([\alpha]_D = +195\) (Concentration = 1.01, Solvent = Chloroform)

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>61.91</td>
<td>62.14</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.20</td>
<td>5.22</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>5.77</td>
<td>5.85</td>
</tr>
</tbody>
</table>

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

**Product Name:** GLPG 0974
**Catalog No.:** 5621  **Batch No.:** 2

**CAS Number:** 1391076-61-1  
**IUPAC Name:** 4-(((2R)-1-(Benzo[b]thien-3-ylcarbonyl)-2-methyl-2-azetidinyl)carbonyl)[(3-chlorophenyl)methyl]amino]butanoic acid

**Description:**

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C₂₅H₂₅ClN₂O₂S
- **Batch Molecular Weight:** 485
- **Physical Appearance:** White solid
- **Minimum Purity:** >98%
- **Batch Molecular Structure:**

![Molecular Structure](image)

**Storage:** Store at +4°C

**Solubility & Usage Info:**
- DMSO to 100 mM
- Ethanol 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:**