1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{25}\text{H}_{35}\text{N}_3\text{O}_2\cdot 2\text{HCl}\cdot \text{H}_2\text{O} \)

Batch Molecular Weight: 500.51

Physical Appearance: White solid

Solubility:
- Water to 50 mM
- DMSO to 50 mM
- Ethanol to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.4% purity

Chiral HPLC: Shows 100% purity

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

Mass Spectrum: Consistent with structure

Optical Rotation: \([\alpha]_D = -5.7 \) (Concentration = 1, Solvent = Ethanol)

Microanalysis:

<table>
<thead>
<tr>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>59.99</td>
<td>7.85</td>
</tr>
<tr>
<td>Found</td>
<td>60.01</td>
<td>8</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
**Product Name:** PF 429242  
**Catalog No.:** 3354  
**Batch No.:** 3

**CAS Number:** 947303-87-9  
**IUPAC Name:** 4-[(Diethylamino)methyl]-N-[2-(2-methoxyphenyl)ethyl]-N-(3R)-3-pyrrolidinylbenzamide

**Description:**
Reversible, competitive inhibitor of sterol regulatory element-binding protein (SREBP) site 1 protease (IC_{50} = 0.175 \mu M). Selective for site 1 protease against a panel of serine proteases. Inhibits rate of cholesterol synthesis in CHO cells (IC_{50} = 0.53 \mu M). Also displays antiviral activity. Cell permeable.

**Physical and Chemical Properties:**
**Batch Molecular Formula:** C_{25}H_{35}N_{3}O_{2}.2HCl.H_{2}O  
**Batch Molecular Weight:** 500.51  
**Physical Appearance:** White solid  
**Minimum Purity:** >97%

**Storage:** Desiccate at RT

**Solubility & Usage Info:**
- water to 50 mM
- DMSO to 50 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.

**Licensing Information:**
Sold for research purposes under agreement from Pfizer Inc.

**References:**
- **Olmstead (2012)** Human subtilase SKI-1/S1P is a master regulator of the HCV lifecycle and a potential host cell target for developing indirect-acting antiviral agents. PLoS.Pathog. 8 e1002468. PMID: 22241994.  