1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** C_{31}H_{39}FN_{4}O_{7}
- **Batch Molecular Weight:** 598.66
- **Physical Appearance:** White solid
- **Solubility:** DMSO to 100 mM
- **Storage:** Store at -20°C

Batch Molecular Structure:

![Molecular Structure](image)

2. ANALYTICAL DATA

- **HPLC:** Shows 98.6% purity
- **¹H NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Optical Rotation:** [α]_D = +40.8 (Concentration = 0.5, Solvent = Chloroform)
- **Microanalysis:**
  
<table>
<thead>
<tr>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>62.19</td>
<td>6.57</td>
</tr>
<tr>
<td>Found</td>
<td>62.21</td>
<td>6.64</td>
</tr>
</tbody>
</table>
Product Name: Rupintrivir  
Catalog No.: 6414  
Batch No.: 1

CAS Number: 223537-30-2

IUPAC Name: Ethyl (2E,4S)-4-[(2R,5S)-2-[(4-fluorophenyl)methyl]-6-methyl-5-[[5-methyl-3-isoxazolyl]carbonyl]amino]-1,4-dioxoheptyl]amino]-5-[(3S)-2-oxo-3-pyrrolidinyl]-2-pentenoate

Description:
Potent and selective irreversible human rhinovirus (HRV) 3C protease inhibitor (EC₅₀ = 5 nM). Exhibits no significant inhibition against a variety of serine and cysteine proteases. Inhibits replication of a panel of 48 different HRV serotypes in H1-HeLA and MRC-5 cell protection assays.

Physical and Chemical Properties:
Batch Molecular Formula: C₃₁H₃₉FN₄O₇
Batch Molecular Weight: 598.66
Physical Appearance: White solid

Minimum Purity: >98%

Storage: Store at -20°C

Solubility & Usage Info:
DMSO 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: