Product Name: Zileuton  
CAS Number: 111406-87-2  
IUPAC Name: \(N\)\{(1-Benzоз\[b\]thien-2-ylethyl)\}\(N\)\-hydroxyurea

1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** \(C_{11}H_{12}N_{2}O_{2}S\)
- **Batch Molecular Weight:** 236.29
- **Physical Appearance:** white solid
- **Solubility:** DMSO to 100 mM
- **Storage:** Store at +4°C
- **Batch Molecular Structure:**

```
\[ \text{Structure Image} \]
```

2. ANALYTICAL DATA

- **HPLC:** Shows >99.9% purity
- **\(^1\)H NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Microanalysis:**

```
<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>55.92</td>
<td>55.86</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.12</td>
<td>5.07</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>11.85</td>
<td>11.89</td>
</tr>
</tbody>
</table>
```

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: Zileuton  
CAS Number: 111406-87-2  
IUPAC Name: \(N\)-(1-Benzob[\(b\]thien-2-yl)ethyl\)-\(N\)-hydroxyurea

**Description:**
Orally active 5-lipoxygenase (5-LOX) inhibitor that inhibits LTB\(_4\) synthesis (IC\(_{50}\) values are 0.56, 2.3 and 2.6 \(\mu\)M in dog, rat and human blood respectively). Inhibits antigen-induced contraction of tracheal strips in vitro (IC\(_{50}\) = 6 \(\mu\)M) and exhibits antiasthmatic activity in vivo. Also weakly inhibits CYP1A2 (\(K_i = 66 - 98\) \(\mu\)M).

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** \(C_{11}H_{12}N_2O_2S\)
- **Batch Molecular Weight:** 236.29
- **Physical Appearance:** white solid
- **Minimum Purity:** >99%
- **Batch Molecular Structure:**

![](image)

**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.

**References:**