Product Name: Ambrisentan
Catalog No.: 5828
Batch No.: 1
CAS Number: 177036-94-1
IUPAC Name: (αS)-α-[4,6-Dimethyl-2-pyrimidinyl]oxy]-β-methoxy-β-phenylbenzenepropanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

- Batch Molecular Formula: C_{22}H_{22}N_{2}O_{4}
- Batch Molecular Weight: 378.42
- Physical Appearance: White solid
- Solubility: DMSO to 38 mM, ethanol to 38 mM
- Storage: Store at +4°C
- Batch Molecular Structure:

![Molecular Structure](image)

2. ANALYTICAL DATA

- HPLC: Shows 99.7% purity
- ¹H NMR: Consistent with structure
- Mass Spectrum: Consistent with structure
- Optical Rotation: [α]D = +171.4 (Concentration = 0.5, Solvent = Methanol)
- Microanalysis:
  
<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>69.83</td>
<td>69.71</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.86</td>
<td>5.92</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>7.4</td>
<td>7.2</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: Ambrisentan

CAS Number: 177036-94-1

IUPAC Name: \((\alpha^S)-\alpha-\{[4,6-Dimethyl-2-pyrimidinyl]oxy\}-\beta\text{-methoxy-}\beta\text{-phenylbenzenepropanoic acid}\)

**Description:**
Selective endothelin receptor \(\text{ET}_A\) antagonist. Displays approximately 200-fold selectivity for \(\text{ET}_A\) over \(\text{ET}_B\) (\(K_i\) values are 1 nM and 195 nM for respectively). Prevents endothelin-induced sudden death in rats.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** \(\text{C}_{22}\text{H}_{22}\text{N}_{2}\text{O}_{4}\)
- **Batch Molecular Weight:** 378.42
- **Physical Appearance:** White solid

**Minimum Purity:** >99%

**Storage:** Store at +4°C

**Solubility & Usage Info:**
- DMSO to 38 mM
- Ethanol to 38 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:**