Product Name: A 127722
Catalog No.: 5730
Batch No.: 1

CAS Number: 195704-72-4
IUPAC Name: \(\text{rel-} (2R, 3R, 4S)-4\{-1, 3\text{-Benzodioxol-5-yl}\}-1\{-[2\{-\text{dibutylamino}-2\text{-oxoethyl}\}\]-2\{-\text{4-methoxyphenyl}\}\}-3\text{-pyrrolidinecarboxylic acid}\)

1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** \(\text{C}_{29}\text{H}_{38}\text{N}_{2}\text{O}_{6}\)
**Batch Molecular Weight:** 510.62
**Physical Appearance:** Off White solid
**Solubility:** DMSO to 100 mM
**Storage:** Store at -20°C

2. ANALYTICAL DATA

**HPLC:** Shows 98% purity
**\(^1\text{H NMR:}\)** Consistent with structure
**Mass Spectrum:** Consistent with structure
**Microanalysis:**

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
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<tbody>
<tr>
<td>Carbon</td>
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<tr>
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<tr>
<td>Nitrogen</td>
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</tr>
</tbody>
</table>

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

Product Name: A 127722
Catalog No.: 5730

CAS Number: 195704-72-4
IUPAC Name: \textit{rel}(2R,3R,4S)-4-(1,3-Benzodioxol-5-yl)-1-[2-(dibutylamino)-2-oxoethyl]-2-(4-methoxyphenyl)-3-pyrrolidinecarboxylic acid

Description:
A 127722 is a highly potent and selective ET\textsubscript{A} endothelin receptor antagonist (IC\textsubscript{50} values are 0.11 nM and 98 nM for human ET\textsubscript{A} and ET\textsubscript{B} receptors, respectively). Attenuates hypoxia-induced pulmonary hypertension in rats. Orally bioavailable.

Physical and Chemical Properties:
- Batch Molecular Formula: C\textsubscript{29}H\textsubscript{38}N\textsubscript{2}O\textsubscript{6}
- Batch Molecular Weight: 510.62
- Physical Appearance: Off White solid
- Minimum Purity: \textgeq 98%

Storage: Store at -20°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: