

Product Name: A 127722

Catalog No.: 5730

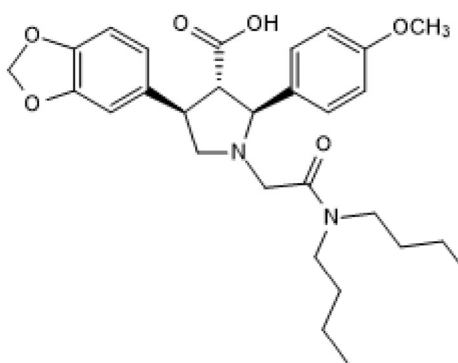
Batch No.: 1

CAS Number: 195704-72-4

IUPAC Name: *rel*-(2*R*,3*R*,4*S*)-4-(1,3-Benzodioxol-5-yl)-1-[2-(dibutylamino)-2-oxoethyl]-2-(4-methoxyphenyl)-3-pyrrolidinecarboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₉ H ₃₈ N ₂ O ₆
Batch Molecular Weight:	510.62
Physical Appearance:	Off White solid
Solubility:	DMSO to 100 mM ethanol to 100 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



(and enantiomer)

2. ANALYTICAL DATA

HPLC:	Shows 98% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	68.21	7.5	5.49
Found	68.25	7.54	5.5

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

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CAS Number:	195704-72-4			
IUPAC Name:	<i>rel</i> -(2 <i>R</i> ,3 <i>R</i> ,4 <i>S</i>)-4-(1,3-Benzodioxol-5-yl)-1-[2-(dibutylamino)-2-oxoethyl]-2-(4-methoxyphenyl)-3-pyrrolidinecarboxylic acid			

Description:

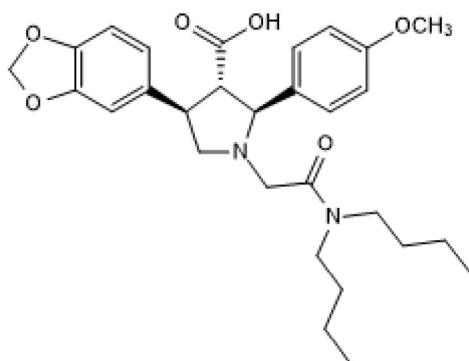
A 127722 is a highly potent and selective ET_A endothelin receptor antagonist (IC₅₀ values are 0.11 nM and 98 nM for human ET_A and ET_B receptors, respectively). Attenuates hypoxia-induced pulmonary hypertension in rats. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₉H₃₈N₂O₆
 Batch Molecular Weight: 510.62
 Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



(and enantiomer)

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:

Chen et al (1997) The orally active nonpeptide endothelin A-receptor antagonist A-127722 prevents and reverses hypoxia-induced pulmonary hypertension and pulmonary vascular remodeling in Sprague-Dawley rats. *J.Cardiovasc.Pharmacol* **29** 713. PMID: 9234651.

Oppenoth et al (1996) Pharmacological characterization of A-127722: an orally active and highly potent ET_A-selective receptor antagonist. *J.Pharmacol.Exp.Ther.* **276** 473. PMID: 8632312.

Winn et al (1996) 2,4-Diarylpyrrolidine-3-carboxylic acids--potent ET_A selective endothelin receptor antagonists. 1. Discovery of A-127722. *J.Med.Chem.* **39** 1039. PMID: 8676339.

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