TOCRIS
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Print Date: Jan 15th 2016

Certificate of Analysis

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Product Name: **FR 139317** **Catalog No.: 1210** **Batch No.: 1**

CAS Number: 142375-60-8

IUPAC Name: *N*-[*N*-[*N*-[(Hexahydro-1*H*-azepin-1-yl)carbonyl]-L-leucyl]-1-methyl-D-tryptophyl]-3-(2-pyridinyl)-D-alanine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{33}H_{44}N_6O_5 \cdot \frac{1}{2}H_2O$

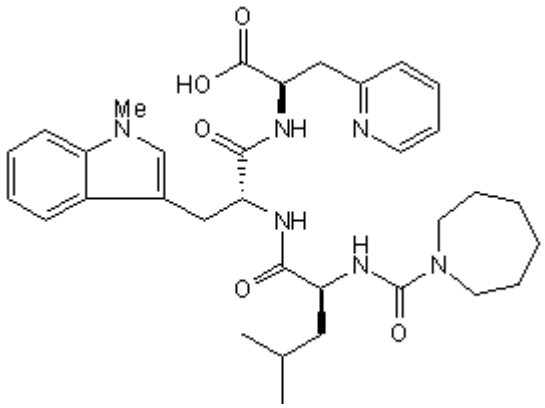
Batch Molecular Weight: 613.76

Physical Appearance: White solid

Solubility: 1eq. HCl to 100 mM
DMSO to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.65 (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])

Melting Point: Between 113 - 120°C

HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	
Theoretical	64.6	7.39	13.7	0 0 0
Found	64.55	7.35	13.63	0 0 0

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

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Description:

A highly potent and selective ET_A endothelin receptor antagonist (K_i values are 1 nM and 7.3 µM at ET_A and ET_B subtypes respectively). Active in vivo.

Physical and Chemical Properties:

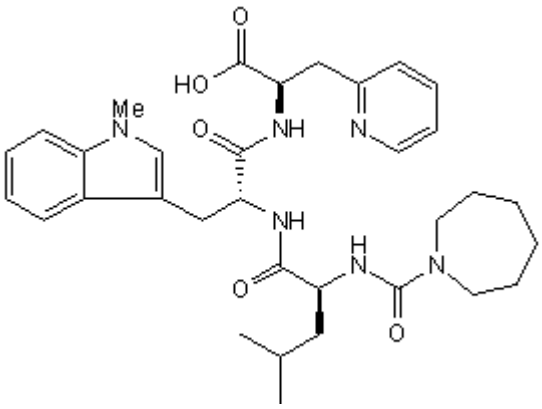
Batch Molecular Formula: $C_{33}H_{44}N_6O_5.½H_2O$

Batch Molecular Weight: 613.76

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

1eq. HCl to 100 mM
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:

Aramori *et al* (1993) Subtype selectivity of a novel endothelin antagonist, FR139317, for the two endothelin receptors in transfected Chinese hamster ovary cells. Mol.Pharmacol. ***43*** 127. PMID: 8429819.

Sogabe *et al* (1993) Pharmacological profile of FR139317, a novel, potent endothelin ET_A receptor antagonist. J.Pharmacol.Exp.Ther. ***264*** 1040. PMID: 8450448.

Rubanyi and Polokoff (1994) Endothelins: molecular biology, biochemistry, pharmacology, physiology, and pathophysiology. Pharmacol.Rev. ***46*** 325. PMID: 7831383.

Palacios *et al* (2002) Role of endothelin ET_A- and ET_B-receptors in haemodynamic compensation following haemorrhage in anaesthetized rats. Br.J.Pharmacol. ***135*** 876. PMID: 11861314.