

# Certificate of Analysis

**Product Name:** Bosentan

**Catalog No.:** 6232

**Batch No.:** 1

CAS Number: 147536-97-8

IUPAC Name: 4-(1,1-Dimethylethyl)-N-[6-(2-hydroxyethoxy)-5-(2-methoxyphenoxy)[2,2'-bipyrimidin]-4-yl]benzenesulfonamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>27</sub>H<sub>29</sub>N<sub>5</sub>O<sub>6</sub>S.H<sub>2</sub>O

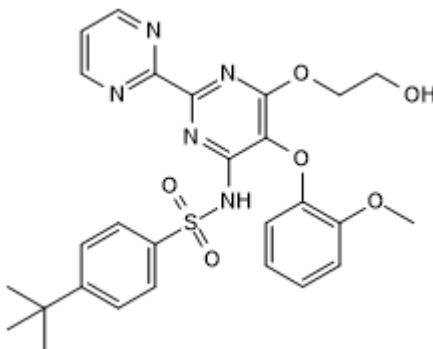
**Batch Molecular Weight:** 569.63

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM  
ethanol to 50 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 99.2% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

Carbon Hydrogen Nitrogen

Theoretical 56.93 5.49 12.29

Found 56.91 5.47 12.34

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

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**Description:**

High affinity dual ET<sub>A</sub> and ET<sub>B</sub> receptor antagonist (K<sub>i</sub> values are 4.7 and 95 nM for ET<sub>A</sub> and ET<sub>B</sub>, respectively). Inhibits ET-1 induced contraction of isolated rat aorta and sarafotoxin S6C-induced contraction of rat trachea in vitro. Orally bioavailable.

**Physical and Chemical Properties:**

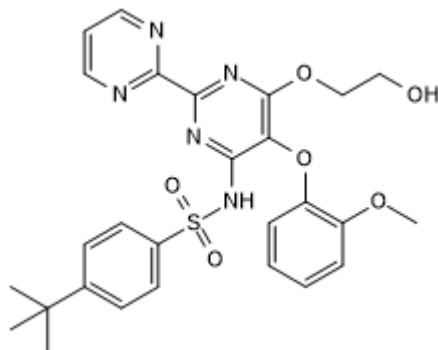
Batch Molecular Formula: C<sub>27</sub>H<sub>29</sub>N<sub>5</sub>O<sub>6</sub>S.H<sub>2</sub>O

Batch Molecular Weight: 569.63

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM  
ethanol to 50 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:**

**Clozel et al** (1994) Pharmacological characterization of bosentan, a new potent orally active nonpeptide endothelin receptor antagonist. *J.Pharmacol.Exp.Ther.* **270** 228. PMID: 8035319.

**Gardiner et al** (1994) Effects of bosentan (Ro 47-0203), an ET<sub>A</sub>-, ET<sub>B</sub>-receptor antagonist, on regional haemodynamic responses to endothelins in conscious rats. *Br.J.Pharmacol.* **112** 823. PMID: 7921608.

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