

**Product Name:** IRL-2500

**Catalog No.:** 1838

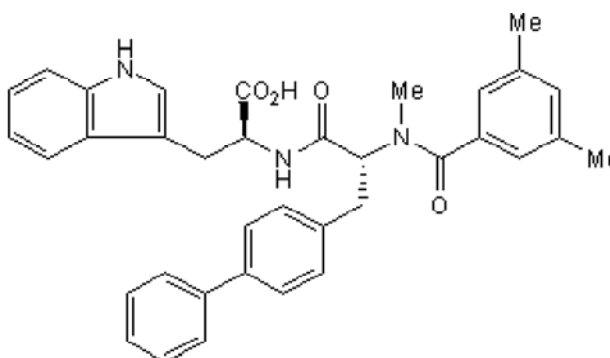
**Batch No.:** 2

CAS Number: 169545-27-1

IUPAC Name: *N*-3-[1,1'-Biphenyl]-4-yl-*N*-(3,5-dimethylbenzoyl)-*N*-methyl-*D*-alanyl-*L*-tryptophan

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>36</sub>H<sub>35</sub>N<sub>3</sub>O<sub>4</sub>·¼H<sub>2</sub>O  
**Batch Molecular Weight:** 578.19  
**Physical Appearance:** White crystalline solid  
**Solubility:** 1eq. NaOH to 75 mM with gentle warming  
**Storage:** Desiccate at RT  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.85 (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])  
**Melting Point:** Between 83 - 88°C(dec)  
**HPLC:** Shows >99.9% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**<sup>13</sup>C NMR:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = +3 (Concentration = 1, Solvent = Ethanol)  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	74.78	6.19	7.27
Found	74.77	6.15	7.26

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

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**Description:**

Potent endothelin receptor antagonist; shows some selectivity for ET<sub>B</sub> receptors (IC<sub>50</sub> values are 1.3 and 94 nM for ET<sub>B</sub> and ET<sub>A</sub> receptors respectively). Inhibits ET<sub>B</sub> receptor-mediated blood pressure increase and renal vascular resistance in rats in vivo.

**Physical and Chemical Properties:**

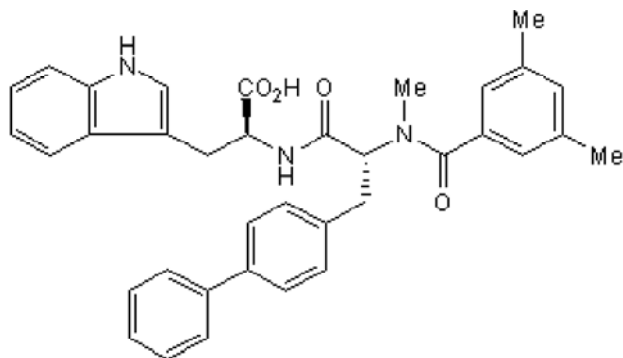
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Batch Molecular Weight: 578.19

Physical Appearance: White crystalline solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Desiccate at RT

**Solubility & Usage Info:**

1eq. NaOH to 75 mM with gentle warming

**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:**

**Leung et al** (2002) Use of A-192621 and IRL-2500 to unmask the mesenteric and renal vasodilator role of endothelin ET<sub>B</sub> receptors. *J.Cardiovasc.Pharmacol.* **39** 533. PMID: 11904527.

**Balwierczak et al** (1995) Characterization of a potent and selective endothelin-B receptor antagonist, IRL 2500. *J.Cardiovasc.Pharmacol.* **26** S393. PMID: 8587424.

**Webb et al** (1995) Effects of the ET<sub>B</sub>-selective antagonist IRL 2500 in conscious spontaneously hypertensive and Wistar-Kyoto rats. *J.Cardiovasc.Pharmacol.* **26** S389. PMID: 8587423.

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