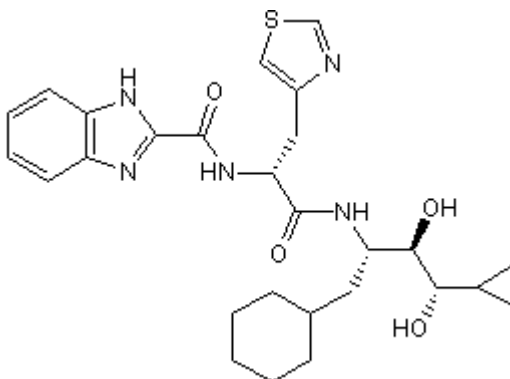


**Product Name:** Ro 0437626 **Catalog No.:** 2188 **Batch No.:** 2  
**CAS Number:** 134362-79-1  
**IUPAC Name:** *N*-[(1*R*)-2-[[[(1*S*,2*R*,3*S*)-1-(Cyclohexylmethyl)-3-cyclopropyl-2,3-dihydroxypropyl]amino]-2-oxo-1-(4-thiazolylmethyl)ethyl]-1*H*-benzimidazole-2-carboxamide

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>27</sub>H<sub>35</sub>N<sub>5</sub>O<sub>4</sub>S  
**Batch Molecular Weight:** 525.66  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.26 (Dichloromethane:Methanol [95:5])  
**HPLC:** Shows >99.4% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	61.69	6.71	13.32
Found	61.59	6.73	13.2

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**Product Name:** Ro 0437626

**Catalog No.:** 2188

**Batch No.:** 2

CAS Number: 134362-79-1

IUPAC Name: *N*-[*(1R)*-2-[[*(1S,2R,3S)*-1-(Cyclohexylmethyl)-3-cyclopropyl-2,3-dihydroxypropyl]amino]-2-oxo-1-(4-thiazolylmethyl)ethyl]-1*H*-benzimidazole-2-carboxamide

**Description:**

Selective P2X<sub>1</sub> purinergic receptor antagonist (IC<sub>50</sub> = 3 μM) that displays > 30-fold selectivity over P2X<sub>2</sub>, P2X<sub>3</sub> and P2X<sub>2/3</sub> receptors (IC<sub>50</sub> > 100 μM).

**Physical and Chemical Properties:**

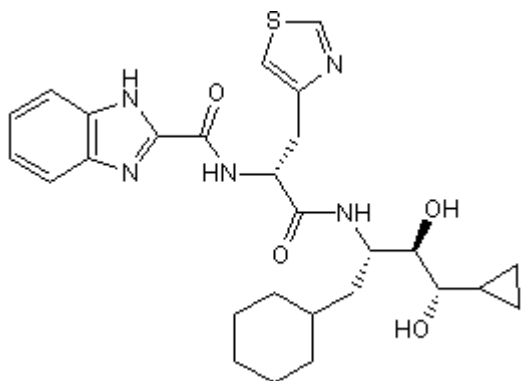
Batch Molecular Formula: C<sub>27</sub>H<sub>35</sub>N<sub>5</sub>O<sub>4</sub>S

Batch Molecular Weight: 525.66

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**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:**

**King et al** (2004) Investigation of the effects of P2 purinoceptor ligands on the micturition reflex in female urethane-anaesthetized rats. *Br.J.Pharmacol.* **142** 519. PMID: 15148261.

**Jaime-Figueroa et al** (2005) Discovery and synthesis of a novel and selective drug-like P2X<sub>1</sub> antagonist. *Bioorg.Med.Chem.Lett.* **15** 3292. PMID: 15927468.

**Ford et al** (2006) Purinoceptors as therapeutic targets for lower urinary tract dysfunction. *Br.J.Pharmacol.* **147** S132. PMID: 16465177.

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