

# **Certificate of Analysis**

# www.tocris.com

## Product Name: AR-C 118925XX

## Catalog No.: 4890 Batch No.: 8

CAS Number: IUPAC Name: 216657-60-2

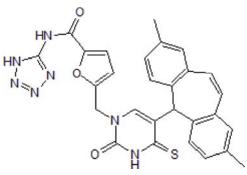
5-[[5-(2,8-Dimethyl-5*H*-dibenzo[*a,d*]cyclohepten-5-yl)-3,4-dihydro-2-oxo-4-thioxo-1(2*H*)-pyrimidinyl]methyl] -*N*-2*H*-tetrazol-5-yl-2-furancarboxamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage:

**Batch Molecular Structure:** 

C<sub>28</sub>H<sub>23</sub>N<sub>7</sub>O<sub>3</sub>S.¾H<sub>2</sub>O 551.1 Yellow solid DMSO to 100 mM Store at -20°C



## 2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis: Shows 99.2% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 61.02 4.48 17.79 Found 60.93 4.4 17.82

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



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**IUPAC Name:** 

5-[[5-(2,8-Dimethyl-5*H*-dibenzo[*a*,*d*]cyclohepten-5-yl)-3,4-dihydro-2-oxo-4-thioxo-1(2*H*)-pyrimidinyl]methyl] -*N*-2*H*-tetrazol-5-yl-2-furancarboxamide

#### **Description:**

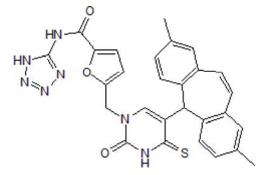
AR-C 118925XX is a potent, selective, competitive and reversible P2Y<sub>2</sub> receptor antagonist (pA<sub>2</sub> = 8.43). Inactive against a panel of 37 other receptors at a concentration of 10  $\mu$ M. AR-C 118925XX inhibits ATP- $\gamma$ S-induced mucin secretion in bronchial epithelial cells (IC<sub>50</sub> = 1  $\mu$ M). Inhibits P2Y<sub>2</sub> receptor-induced β-arrestin translocation in vitro (pA<sub>2</sub> = 37.2-51.3 nM).

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>28</sub>H<sub>23</sub>N<sub>7</sub>O<sub>3</sub>S.<sup>3</sup>/<sub>4</sub>H<sub>2</sub>O Batch Molecular Weight: 551.1 Physical Appearance: Yellow solid

#### Minimum Purity: ≥97%

#### **Batch Molecular Structure:**



#### Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Catalog No.: 4890

#### Solubility & Usage Info:

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:

**Muoboghare** *et al* (2019) Characterisation of P2Y<sub>2</sub> receptors in human vascular endothelial cells using AR-C118925XX, a competitive and selective P2Y<sub>2</sub> antagonist. Br.J.Pharmacol. **176** 2894. PMID: 31116875.

**Rafehi** *et al* (2017) Synthesis, characterization, and in vitro evaluation of the selective P2Y<sub>2</sub> receptor antagonist AR-C118925. Purinergic.Signal. **13** 89. PMID: 27766552.

**Kemp** *et al* (2004) Nucleotide-mediated mucin secretion from differentiated human bronchial epithelial cells. Am.J.Respir.Cell Mol.Biol. *31* 446. PMID: 15231488.

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