

**Certificate of Analysis** 

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Print Date: Jan 16th 2016

Product Name: S 18886 Catalog No.: 5568 Batch No.: 1

CAS Number: 165538-40-9

IUPAC Name: (6R)-6-[[(4-Chlorophenyl)sulfonyl]amino]-5,6,7,8-tetrahydro-2-methyl-1-naphthalenepropanoic acid

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C<sub>20</sub>H<sub>22</sub>CINO<sub>4</sub>S

**Batch Molecular Weight:** 407.91 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

ethanol to 20 mM with gentle warming

Storage: Store at -20°C

**Batch Molecular Structure:** 

# 2. ANALYTICAL DATA

HPLC: Shows 98.3% purity
Chiral HPLC: Shows 99.2% purity

1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

**Optical Rotation:**  $[\alpha]_D = +29$  (Concentration = 1, Solvent = DMSO)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 58.89 5.44 3.43 Found 58.9 5.41 3.33



# **Product Information**

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## **Description:**

Potent thromboxane  $A_2$  (TP) inhibitor ( $IC_{50}$  = 16.4 nM). Inhibits U 46619 (Cat. No. 1932) induced human platelet aggregation and contraction of isolated rabbit saphenous vein in vitro. Also inhibits U 46619 induced increase in tracheal pressure in guinea pigs. Orally available.

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

Batch Molecular Formula: C<sub>20</sub>H<sub>22</sub>CINO<sub>4</sub>S Batch Molecular Weight: 407.91 Physical Appearance: White solid

Minimum Purity: >98%

## **Batch Molecular Structure:**

Storage: Store at -20°C

# Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 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:

Cimetière et al (1998) Synthesis and biological evaluation of new tetrahydronaphthalene derivatives as thromboxane receptor antagonists. Bioorg.Med.Chem.Lett. 8 1375. PMID: 9871769.

**Wang** *et al* (2014) Potent, long-acting cyclopentane-1,3-Dione thromboxane (A<sub>2</sub>)-receptor antagonists. ACS Med.Chem.Lett. *5* 1015. PMID: 25221659.