

# **Certificate of Analysis**

Print Date: Jan 15<sup>th</sup> 2016

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Product Name: RWJ 50271 Catalog No.: 4227 Batch No.: 1

CAS Number: 162112-37-0

IUPAC Name: N-(3-Hydroxypropyl)-5-methyl-1-[-4-[3-(trifluoromethyl)phenyl)]-2-thiazolyl]-1H-pyrazole-4-carboxamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{18}H_{17}F_3N_4O_2S$ 

Batch Molecular Weight: 410.41

Physical Appearance: White solid

Solubility: DMSO to 100 mM

ethanol to 10 mM

Storage: Store at RT

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.5$  (Dichloromethane:Methanol [9:1])

**HPLC:** Shows 99.7% purity

<sup>1</sup>H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 52.68 4.18 13.65 Found 52.7 4.14 13.6



## **Product Information**

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### **Description:**

Selective inhibitor of LFA-1 (lymphocyte function-associated antigen-1) adhesion to soluble intercellular adhesion molecule (sICAM) (IC<sub>50</sub> =  $5 \mu M$  in HL60 cells).

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

Batch Molecular Formula: C<sub>18</sub>H<sub>17</sub>F<sub>3</sub>N<sub>4</sub>O<sub>2</sub>S

Batch Molecular Weight: 410.41 Physical Appearance: White solid

## **Minimum Purity: >99%**

## **Batch Molecular Structure:**

Storage: Store at RT

#### Solubility & Usage Info:

DMSO to 100 mM ethanol to 10 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:

Sanfilippo et al (1995) Novel thiazole based heterocycles as inhibitors of LFA-1/ICAM-1 mediated cell adhesion. J.Med.Chem. 38 1057. PMID: 7707308.

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