

# **Certificate of Analysis**

Print Date: Aug 24th 2021

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Product Name: KF 38789 Catalog No.: 2748 Batch No.: 2

CAS Number: 257292-29-8

IUPAC Name: 3-[7-(2,4-Dimethoxyphenyl)-2,3,6,7-tetrahydro-1,4-thiazepin-5-yl]-4-hydroxy-6-methyl-2*H*-pyran-2-one

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

 $\textbf{Batch Molecular Formula:} \qquad \qquad C_{19}H_{21}NO_5S$ 

Batch Molecular Weight: 375.44

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM

Storage: Desiccate at +4°C

**Batch Molecular Structure:** 

# 2. ANALYTICAL DATA

**HPLC:** Shows 97.4% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 60.78 5.64 3.73 Found 60.54 5.77 3.73

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



# **Product Information**

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### **Description:**

KF 38789 is a selective inhibitor of P-selectin-mediated cell adhesion ( $IC_{50}$  = 1.97  $\mu$ M) that displays no effects on L-selectin-and E-selectin-mediated adhesion. KF 38789 blocks P-selectin-mediated binding in vitro and leukocyte accumulation in vivo.

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

Batch Molecular Formula: C<sub>19</sub>H<sub>21</sub>NO<sub>5</sub>S Batch Molecular Weight: 375.44 Physical Appearance: Off-white solid

Minimum Purity: ≥97%

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

Storage: Desiccate at +4°C

#### 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:

**Kaila** *et al* (2007) Synthesis and biological evaluation of quinoline salicylic acids as P-selectin antagonists. J.Med.Chem. *50* 21. PMID: 17201408.

**Ohta** *et al* (2001) Inhibition of P-selectin specific cell adhesion by a low molecular weight, non-carbohydrate compound, KF38779. Inflamm.Res. *50* 544. PMID: 11766994.

**Haggerty** *et al* (2000) Dissecting cellular processes using small molecules: identification of colchicine-like, taxol-like and other small moleculaes that perturb mitosis. Chem.Biol. **7** 275. PMID: 10780927.

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