

Certificate of Analysis

Print Date: May 4th 2022

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Product Name: WEB 2086 Catalog No.: 2339 Batch No.: 2

CAS Number: 105219-56-5

IUPAC Name: 4-[3-[4](2-Chlorophenyl)-9-methyl-6*H*-thieno[3,2-*f*][1,2,4]triazolo[4,3-*a*]diazepin-2-yl]-1-oxopropyl]morpholine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₂N₅O₂SCI

Batch Molecular Weight: 455.96 **Physical Appearance:** Beige solid

Solubility: DMSO to 100 mM

ethanol to 100 mM with gentle warming

Storage: Desiccate at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.55$ (Dichloromethane:Methanol [9:1])

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 57.95 4.86 15.36 Found 58.01 4.88 15.34



Product Information

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Description:

WEB 2086 is a potent, selective platelet-activating factor (PAF) receptor antagonist ($K_i = 16.3 \text{ nM}$). Displays anti-inflammatory, antiangiogenic and anticancer activity. Inhibits growth and proliferation of MCF-7 breast cancer cells.

Physical and Chemical Properties:

Batch Molecular Formula: C22H22N5O2SCI

Batch Molecular Weight: 455.96 Physical Appearance: Beige solid

Minimum Purity: ≥99%

Batch Molecular Structure:

Storage: Desiccate at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 100 mM with gentle warming

When purched as a 1mg unit, this product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Cellai *et al* (2006) Growth inhibition and differentiation of human breast cancer cells by the PAFR antagonist WEB-2086. Br.J.Cancer *94* 1637. PMID: 16721373.

Sariahmetoglu *et al* (1998) Effects of WEB 2086 on the protective role of preconditioning against arrhythmias in rats. Pharmacol.Res. **38** 173. PMID: 9782066.

Dent et al (1989) Characterization of PAF receptors on human neutrophils using the specific antagonist, WEB 2086. FEBS Lett. 244 365. PMID: 2537761.

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