



Certificate of Analysis

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Product Name: J 113863 Catalog No.: 2595 Batch No.: 4

CAS Number: 202796-41-6

IUPAC Name: 1,4-cis-1-(1-Cycloocten-1-ylmethyl)-4-[[(2,7-dichloro-9*H*-xanthen-9-yl)carbonyl]amino]-1-ethylpiperidinium iodide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{30}H_{37}Cl_2lN_2O_2.\frac{1}{4}H_2O$

Batch Molecular Weight: 659.94

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM

ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:

(and enantiomer)

2. ANALYTICAL DATA

HPLC: Shows 98.2% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.6 5.73 4.24 Found 54.2 5.74 4.32

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



Product Information

Print Date: Aug 13th 2020

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Description:

Potent chemokine receptor 1 (CCR1) antagonist (IC_{50} values are 0.9 and 5.8 nM for human and mouse CCR1 receptors respectively). Also displays high selectivity for human but not mouse CCR3 receptors (IC_{50} values are 0.58 and 460 nM respectively). Improves paw inflammation, joint damage and dramatically reduces cell infiltration into joints in collageninduced arthritis in mice. Isomer also available.

Physical and Chemical Properties:

Batch Molecular Formula: C₃₀H₃₇Cl₂IN₂O₂.½H₂O

Batch Molecular Weight: 659.94 Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:

(and enantiomer)

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM ethanol to 50 mM

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:

Amat *et al* (2006) Pharmacological blockade of CCR1 ameliorates murine arthritis and alters cytokine networks in vivo. Br.J.Pharmacol. *149* 666. PMID: 17016504.

Naya et al (2001) Design, synthesis, and discovery of a novel CCR1 antagonist. J.Med.Chem. 44 1429. PMID: 11311066.

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