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-9H-xanthen-9-yl)carbonyl]amino]-1-ethylpiperidinium iodide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{30}H_{37}Cl_{2}I_{N_{2}}O_{2}.\frac{1}{2}H_{2}O

Batch Molecular Weight: 659.94

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM, ethanol to 50 mM

Storage: Store at +4°C

2. ANALYTICAL DATA

HPLC: Shows 98.2% purity

\textsuperscript{1}H 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
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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 collagen-induced arthritis in mice. Isomer also available.

Physical and Chemical Properties:
Batch Molecular Formula: C$_{36}$H$_{37}$Cl$_2$IN$_2$O$_2$·½H$_2$O
Batch Molecular Weight: 659.94
Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:
DMSO to 100 mM
ethanol to 50 mM

When purchased 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: