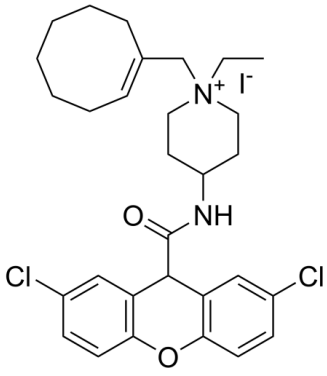
Data Sheet

Product Name:	J-113863
Cat. No.:	CS-0027742
CAS No.:	353791-85-2
Molecular Formula:	$C_{30}H_{37}Cl_2IN_2O_2$
Molecular Weight:	655.44
Target:	CCR
Pathway:	GPCR/G Protein; Immunology/Inflammation
Solubility:	DMSO : 50 mg/mL (ultrasonic)



BIOLOGICAL ACTIVITY:

J-113863 is a potent and selective **CCR1** antagonist with **IC_{50}** values of 0.9 nM and 5.8 nM for human and mouse **CCR1** receptors, respectively. J-113863 is also a potent antagonist of the human **CCR3** (**IC_{50}** of 0.58 nM) , but a weak antagonist of the mouse **CCR3** (**IC_{50}** of 460 nM). J-113863 is inactive against CCR2, CCR4 and CCR5, as well as the LTB4 or TNF-α receptors. Anti-inflammatory effect[1][2][3]. ***In Vitro:***Modified Vaccinia virus Ankara (MVA) but not MVA and vaccinia virus (VACV) infected MH-S cells increase the expression of the CXCR2 acting chemokine CXCL2. MH-S cells constitutively produce CCL2 and CCR1 acting chemokines CCL3, CCL5 and CCL9. Consequently, supernatants of mock treated and virus infected MH-S cells induce chemotaxis of murine promyelocyte MPRO cells and human monocytic THP-1 cells at the same level. However, supernatants of MVA infected MH-S cells significantly increase chemotaxis of the CCR2 deficient human monocytic cell line U-937. Chemotaxis of all above cell types is inhibited by J-113863[1]. ***In Vivo:***J-113863 (3-10 mg/kg; intraperitoneal injection; once daily; for 11 days; DBA-1 male mice) treatment improves paw inflammation and joint damage, and dramatically decreases cell infiltration into joints in arthritic mice[2].

References:

[1]. Lehmann MH, et al. Modified Vaccinia virus Ankara but not vaccinia virus induces chemokine expression in cells of the monocyte/macrophage lineage. Virol J. 2015 Feb 12;12:21.

[2]. Amat M, et al. Pharmacological blockade of CCR1 ameliorates murine arthritis and alters cytokine networks in vivo. Br J Pharmacol. 2006 Nov;149(6):666-75.

[3]. Naya A, et al. Design, synthesis, and discovery of a novel CCR1 antagonist. J Med Chem. 2001 Apr 26;44(9):1429-35.

CAIndexNames:

Piperidinium, 1-(1-cycloocten-1-ylmethyl)-4-[[(2,7-dichloro-9H-xanthen-9-yl)carbonyl]amino]-1-ethyl-, iodide (1:1)

SMILES:

CC[N+]1(C/C2=C/CCCCCC2)CCC(NC(C3C4=C(OC5=C3C=C(Cl)C=C5)C=CC(Cl)=C4)=O)CC1.[I-]

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 610-426-3128 Fax: 888-484-5008 E-mail: sales@ChemScene.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA