TOCRIS
a bio-techne brand

Print Date: Jan 15th 2016

Certificate of Analysis

www.tocris.com

Product Name: **JNJ 27141491** **Catalog No.: 5176** **Batch No.: 1**

CAS Number: 871313-59-6

IUPAC Name: 3-[(1*S*)-1-(3,4-Difluorophenyl)propyl]-2,3-dihydro-5-(5-isoxazolyl)-2-thioxo-1*H*-imidazole-4-carboxylic acid methyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{15}F_2N_3O_3S$

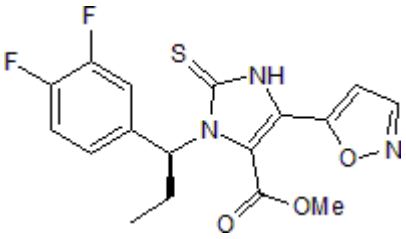
Batch Molecular Weight: 379.38

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.31 (Ethyl acetate:Petroleum ether [3:7])

HPLC: Shows 99.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -178.5 (Concentration = 1, Solvent = Chloroform)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.82	3.99	11.08
Found	54	4.01	10.83

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

Product Name: **JNJ 27141491** **Catalog No.: 5176** **Batch No.: 1**

CAS Number: 871313-59-6

IUPAC Name: 3-[(1*S*)-1-(3,4-Difluorophenyl)propyl]-2,3-dihydro-5-(5-isoxazolyl)-2-thioxo-1*H*-imidazole-4-carboxylic acid methyl ester

Description:

Potent, noncompetitive human CCR2 antagonist; inhibits MCP-1-induced Ca^{2+} mobilization in hCCR2-CHO cells (IC_{50} = 13 nM). Exhibits selectivity for CCR2 over CCR1, CCR3-8 and CXCR1-3. Delays onset and reduces neurological signs in an experimental autoimmune encephalomyelitis model of multiple sclerosis in hCCR2 knock-in mice. Orally active.

Physical and Chemical Properties:

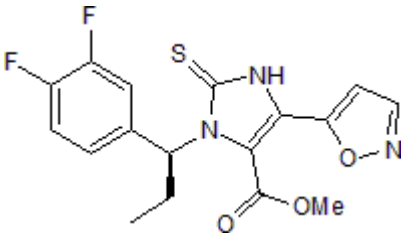
Batch Molecular Formula: $C_{17}H_{15}F_2N_3O_3S$

Batch Molecular Weight: 379.38

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Buntinx *et al* (2008) Pharmacological profile of JNJ-27141491 [(*S*)-3-[3,4-difluorophenyl)-propyl]-5-isoxazol-5-yl-2-thioxo-2,3-dihydro-1*H*-imidazole-4-carboxyl acid methyl ester], as a noncompetitive and orally active antagonist of the human chemokine receptor CCR2. J.Pharmacol.Exp.Ther. ***327*** 1. PMID: 18599682.