TOCRIS
a bio-techne brand

Print Date: Jun 26th 2019

Certificate of Analysis

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Product Name: **Reparixin L-lysine salt** **Catalog No.: 6957** **Batch No.: 1**

CAS Number: 266359-93-7

IUPAC Name: (α*R*)-α-Methyl-4-(2-methylpropyl)-*N*-(methylsulfonyl)benzeneacetamide L-Lysine salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{14}H_{21}NO_3S.C_6H_{14}N_2O_2.H_2O$

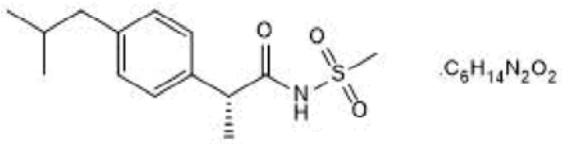
Batch Molecular Weight: 447.6

Physical Appearance: White solid

Solubility: DMSO to 50 mM
water to 5 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -21.1 (Concentration = 1.15, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.67	8.33	9.39
Found	53.41	8.18	9.15

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Description:

Potent and noncompetitive CXCR1 and CXCR2 allosteric antagonist (IC_{50} = 1 nM for inhibition of CXCL8-induced human polymorphonuclear cell migration). Also inhibits migration of rodent neutrophils induced by CXCL1, CXCL2, CXCL8 and CINC-1. Inhibits vascular permeability and neutrophil recruitment in in vivo models of mild and severe ischemia/reperfusion injury. Also selectively depletes cancer stem cells in human breast cancer cell lines and xenograft models.

Physical and Chemical Properties:

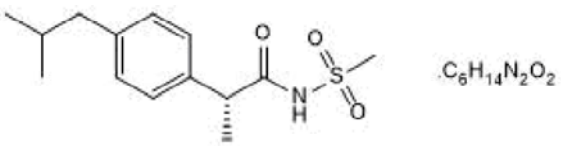
Batch Molecular Formula: $C_{14}H_{21}NO_3S.C_6H_{14}N_2O_2.H_2O$

Batch Molecular Weight: 447.6

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 mM
water to 5 mM with gentle warming

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:

Ginestier *et al* (2010) CXCR1 blockade selectively targets human breast cancer stem cells *in vitro* and in xenografts. J.Clin.Invest. ***120*** 485. PMID: 20051626.

Bertini *et al* (2004) Noncompetitive allosteric inhibitors of the inflammatory chemokine receptors CXCR1 and CXCR2: prevention of reperfusion injury. Proc.Natl.Acad.Sci.U.S.A. ***101*** 11791. PMID: 15282370.

Souza *et al* (2004) Repertaxin, a novel inhibitor of rat CXCR2 function, inhibits inflammatory responses that follow intestinal ischaemia and reperfusion injury. Br.J.Pharmacol. ***143*** 132. PMID: 15302676.