

Certificate of Analysis

Print Date: Jan 13th 2016

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Product Name: PD 166793 Catalog No.: 2520 Batch No.: 2

CAS Number: 199850-67-4

IUPAC Name: N-[(4'-Bromo[1,1'-biphenyl]-4-yl)sulfonyl]-L-valine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₈BrNO₄S

Batch Molecular Weight: 412.3

Physical Appearance: White crystalline solid Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.15$ (Ethyl acetate)

HPLC: Shows 99.8% purity

Chiral HPLC: Shows 100% purity

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

Optical Rotation: $[\alpha]_D = +49.3$ (Concentration = 2, Solvent = Methanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 49.52 4.4 3.4 Found 49.42 4.39 3.46



Product Information

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Description:

Broad spectrum MMP inhibitor. Displays high affinity for MMP-2, -3 and -13 (IC_{50} values are 4, 7 and 8 nM respectively) and exhibits > 750-fold selectivity over MMP-1, -7 and -9. Attenuates left ventricular remodelling and dysfunction in rat model of heart failure.

Physical and Chemical Properties:

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Batch Molecular Weight: 412.3

Physical Appearance: White crystalline solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Desiccate 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:

O'Brien et al (2000) Structure-activity relationships and pharmacokinetic analysis for a series of potent, systemically available Biphenylsulfonamide matrix metalloproteinase inhibitors. J.Med.Chem. **43** 156. PMID: 10649971.

Peterson *et al* (2001) Matrix metalloproteinase inhibition attenuates left ventricular remodeling and dysfunction in a rat model of progressive heart failure. Circulation *103* 2303. PMID: 11342481.

Chancey et al (2002) Effects of matrix metalloproteinase inhibition on ventricular remodeling due to volume overload. Circulation 105 1983. PMID: 11997287.