

Print Date: Mar 7th 2019

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Product Name: JNJ 0966 Catalog No.: 6439 Batch No.: 1

Certificate of Analysis

CAS Number: 315705-75-0

IUPAC Name: N-[2-[(2-Methoxyphenyl)amino]-4'-methyl[4,5'-bithiazol]-2'-yl]acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_{16}H_{16}N_4O_2S_2$ **Batch Molecular Formula:**

Batch Molecular Weight: 360.45 **Physical Appearance:** Beige solid

DMSO to 50 mM Solubility: Store at -20°C Storage:

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.7% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 53.31 4.47 15.54 Found 53.39 4.5 15.4

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use



Product Information

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IUPAC Name: N-[2-[(2-Methoxyphenyl)amino]-4'-methyl[4,5'-bithiazol]-2'-yl]acetamide

Description:

Pro-MMP9 activation inhibitor (IC $_{50}$ = 440 nM). Inhibits the conversion of pro-MMP9 to active MMP9, without directly affecting MMP9 enzymatic activity. Exhibits selectivity for pro-MMP9 over pro-MMP1, 2 and 3. Inhibits cell invasion in in vitro assays. Reduces motor impairment in a mouse EAE model. Brain penetrant.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₆H₁₆N₄O₂S₂

Batch Molecular Weight: 360.45 Physical Appearance: Beige solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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:

Scannevin *et al* (2017) Discovery of a highly selective chemical inhibitor of matrix metalloproteinase-9 (MMP-9) that allosterically inhibits zymogen activation. J.Biol.Chem. **292** 17963. PMID: 28860188.