



Certificate of Analysis

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Product Name: TAK 715 Catalog No.: 4254 Batch No.: 1

CAS Number: 303162-79-0

IUPAC Name: N-[4-[2-Ethyl-4-(3-methylphenyl)-5-thiazolyl]-2-pyridinyl]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{21}N_3OS$

Batch Molecular Weight: 399.51 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.5$ (Ethyl acetate:Petroleum ether [1:2])

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 72.15 5.3 10.52 Found 72.13 5.29 10.53



Product Information

Print Date: Dec 14th 2011

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Description:

Inhibitor of p38 MAPK (IC $_{50}$ = 7.1 nM for p38 MAPK α). Also inhibits Wnt-3a-stimulated β -catenin signaling. Inhibits 22 kinases by more than 80%, including CK1 δ / ϵ . Anti-inflammatory and anti-rheumatoid arthritis agent. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{24}H_{21}N_3OS$

Batch Molecular Weight: 399.51 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Useage Info:

DMSO to 100 mM ethanol 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:

Miwatashi *et al* (2005) Novel inhibitor of p38 MAP kinase as an anti-TNF- α drug: discovery of *N*-[4-{2-ethyl-4-(3-methylphenyl)-1,3-thiazol-5-yl]-2-pyridyl]benzamide (TAK-715) as a potent and orally active anti-rheumatoid arthritis agent. J.Med.Chem. **48** 5966. PMID: 16162000.

Verkaar *et al* (2011) Inhibition of Wnt/β-catenin signaling by p38 MAP kinase inhibitors is explained by cross-reactivity with casein kinase Iδ/ε. Chem.Biol. *18* 485. PMID: 21513885.

