

Certificate of Analysis

Print Date: Jan 14th 2016

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Product Name: JW 67 Catalog No.: 4651 Batch No.: 1

CAS Number: 442644-28-2

IUPAC Name: Trispiro[3*H*-indole-3,2'-[1,3]dioxane-2",3"'-[3*H*]indole]-2,2"'(1*H*,1"'H)-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

 $\begin{array}{lll} \textbf{Batch Molecular Formula:} & \textbf{C_{21}H}_{18}\textbf{N_2O}_6\\ \\ \textbf{Batch Molecular Weight:} & 394.38\\ \\ \textbf{Physical Appearance:} & \text{Beige solid} \\ \end{array}$

Solubility: DMSO to 100 mM Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 97.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 63.95 4.6 7.1 Found 63.7 4.81 6.91



Product Information

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Description:

Inhibitor of canonical Wnt pathway signaling (IC $_{50}$ = 1.17 μ M); targets the β -catenin destruction complex (GSK-3 β /AXIN/APC) to induce β -catenin degradation. Selective for the canonical Wnt pathway over the Sonic hedgehog (Shh) and NF- κ B pathways. Blocks G $_1$ /S cell cycle progression in colorectal cancer (CRC) cell lines (GI $_{50}$ = 7.8 μ M).

Physical and Chemical Properties:

Batch Molecular Formula: C₂₁H₁₈N₂O₆ Batch Molecular Weight: 394.38 Physical Appearance: Beige solid

Minimum Purity: >97%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO 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:

Waaler et al (2011) Novel synthetic antagonists of canonical Wnt signaling inhibit colorectal cancer cell growth. Cancer Res. 71 197. PMID: 21199802.

Shultz *et al* (2012) [1,2,4]triazol-3-ylsulfanylmethyl)-3-phenyl-[1,2,4]oxadiazoles: antagonists of the Wnt pathway that inhibit tankyrases 1 and 2 via novel adenosine pocket binding. J.Med.Chem. *55* 1127. PMID: 22260203.

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