Certificate of Analysis

Print Date: May 11th 2023

IWP 2 **Product Name:**

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Catalog No.: 3533 Batch No.: 6

CAS Number: **IUPAC Name:**

TOCRIS

686770-61-6

N-(6-Methyl-2-benzothiazolyl)-2-[(3,4,6,7-tetrahydro-4-oxo-3-phenylthieno[3,2-d]pyrimidin-2-yl)thio]-acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: **Batch Molecular Structure:**

 $C_{22}H_{18}N_4O_2S_3.1/_4H_2O_2$ 471.1 Off White solid DMSO to 5 mM with gentle warming Store at +4°C



2. ANALYTICAL DATA

TLC: HPLC: ¹H NMR: Mass Spectrum: **Microanalysis:**

R_f = 0.83 (Dichloromethane:Methanol [95:5]) Shows 98.1% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 56.09 3.96 11.89

3.81

11.8

55.8

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Product Name: IWP 2

CAS Number: 686770-61-6 IUPAC Name: *N*-(6-Methyl-2

N-(6-Methyl-2-benzothiazolyl)-2-[(3,4,6,7-tetrahydro-4-oxo-3-phenylthieno[3,2-d]pyrimidin-2-yl)thio]-acetamide

Description:

IWP 2 is a potent inhibitor of Wnt processing and secretion (IC₅₀ = 27nM). IWP 2 inactivates PORCN, a membrane-bound O-acyltransferase (MBOAT), and selectively inhibits palmitoylation of Wnt. Blocks Wnt-dependent phosphorylation of Lrp6 receptor and Dvl2, and β -catenin accumulation. IWP 2 suppresses self-renewal in R1 embryonic stem cells and promotes cardiomyocyte differentiation from hPSCs. The compound has also been used in protocols to reprogram human somatic cells to chemically-induced PSCs.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{22}H_{18}N_4O_2S_3$.¹/₄ H_2O Batch Molecular Weight: 471.1 Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO 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 $45-60^{\circ}C$ water bath).

Catalog No.: 3533

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:

Guan et al (2022) Chemical reprogramming of human somatic cells to pluripotent stem cells. Nature 605 325. PMID: 35418683.

Noor et al (2019) 3D printing of personalized thick and perfusable cardiac patches and hearts. Adv Sci (Weinh) 6 1900344. PMID: 31179230.

Hoang *et al* (2018) Generation of spatial-patterned early-developing cardiac organoids using human pluripotent stem cells. Nat.Protoc. **13** 723. PMID: 29543795.

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