

Product Name: IWP 12

Catalog No.: 5279

Batch No.: 1

CAS Number: 688353-45-9

IUPAC Name: *N*-(6-Methyl-2-benzothiazolyl)-2-[(3,4,6,7-tetrahydro-3,6-dimethyl-4-oxothieno[3,2-*d*]pyrimidin-2-yl)thio]acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₈N₄O₂S₃·¼H₂O

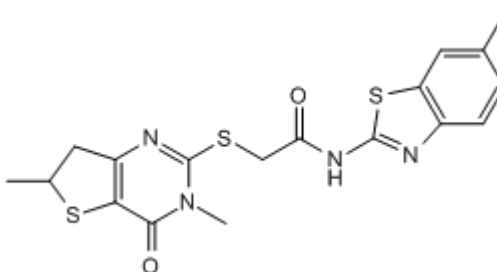
Batch Molecular Weight: 423.06

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.45 (Acetone:Chloroform [20:80])

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.1	4.41	13.24
Found	50.96	4.26	13.16

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

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Description:

Potent inhibitor of Porcupine (PORCN), a membrane-bound O-acyltransferase (MBOAT) (IC₅₀ = 15 nM). Inhibits Wnt/β-catenin and Wnt/planar cell polarity (PCP) signaling pathways. Blocks zebrafish tailfin regeneration in vivo.

Physical and Chemical Properties:

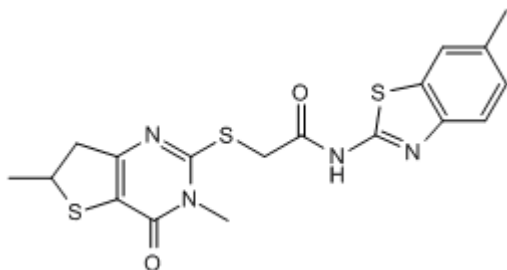
Batch Molecular Formula: C₁₈H₁₈N₄O₂S₃·½H₂O

Batch Molecular Weight: 423.06

Physical Appearance: White solid

Minimum Purity: >98%

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:

Dodge et al (2012) Diverse chemical scaffolds support direct inhibition of the membrane-bound O-acyltransferase porcupine. *J.Biol.Chem.* **287** 23246. PMID: 22593577.

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