

Certificate of Analysis

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Product Name: LDN 27219

Catalog No.: 4602

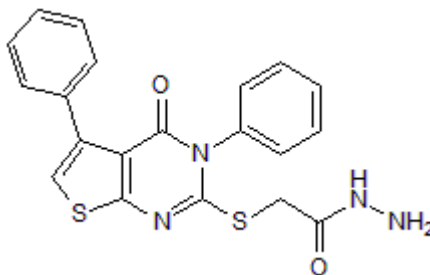
Batch No.: 1

CAS Number: 312946-37-5

IUPAC Name: 2-[(3,4-Dihydro-4-oxo-3,5-diphenylthieno[2,3-d]pyrimidin-2-yl)thio]acetic acid hydrazide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₁₆N₄O₂S₂
Batch Molecular Weight: 408.5
Physical Appearance: White solid
Solubility: DMSO to 100 mM
ethanol to 5 mM with gentle warming
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.8	3.95	13.72
Found	58.75	3.92	13.75

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

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Description:

Transglutaminase 2 (TG2) inhibitor (IC₅₀ = 0.25 μM). Binds at GTPase site; reversible.

Physical and Chemical Properties:

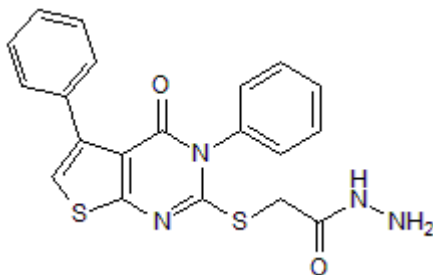
Batch Molecular Formula: C₂₀H₁₆N₄O₂S₂

Batch Molecular Weight: 408.5

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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°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:

Duval et al (2005) Structure-activity relationship study of novel tissue transglutaminase inhibitors. *Bioorg.Med.Chem.Lett.* **15** 1885. PMID: 15780627.

Case and Stein (2007) Kinetic analysis of the interaction of tissue transglutaminase with a nonpeptidic slow-binding inhibitor. *Biochemistry* **46** 1106. PMID: 17240993.

Prime et al (2012) Discovery and structure-activity relationship of potent and selective covalent inhibitors of transglutaminase 2 for Huntington's disease. *J.Med.Chem.* **55** 1021. PMID: 22224594.

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