

Product Name: SHIN 1

Catalog No.: 6998

Batch No.: 1

CAS Number: 2146095-85-2

IUPAC Name: 6-Amino-1,4-dihydro-4-[5-(hydroxymethyl)[1,1'-biphenyl]-3-yl]-3-methyl-4-(1-methylethyl)pyrano[2,3-c]pyrazole-5-carbonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₄N₄O₂·½H₂O

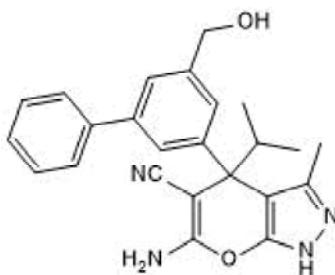
Batch Molecular Weight: 409.49

Physical Appearance: Off-white solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	70.4	6.15	13.68
Found	70.49	5.97	13.79

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

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Description:

Potent serine hydroxymethyltransferase (SHMT) inhibitor (IC₅₀ values are 5 and 13 nM at SHMT1 and SHMT2, respectively). Inhibits growth of HCT-116 cells in vitro (IC₅₀ = 870 nM). Unstable in liver microsome assays.

Physical and Chemical Properties:

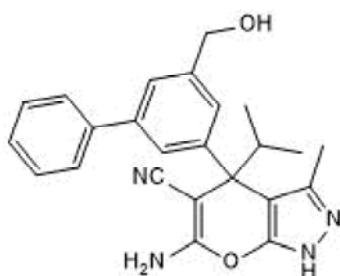
Batch Molecular Formula: C₂₄H₂₄N₄O₂·½H₂O

Batch Molecular Weight: 409.49

Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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.

Licensing Information:

Sold under license from Princeton University.

References:

Ducker *et al* (2017) Human SHMT inhibitors reveal defective glycine import as a targetable metabolic vulnerability of diffuse large B-cell lymphoma. *Proc.Natl.Acad.Sci.U.S.A.* **114** 11404. PMID: 29073064.

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