

Name: SHIN2 Cat#: EX-A5815

Chemical Structure:



Chemical	6-amino-4-(3-(hydroxymethyl)-5-(5-hydroxypent-1-yn-1-yl)phenyl)-4-
Name	isopropyl-3-methyl-1,4-dihydropyrano[2,3-c]pyrazole-5-carbonitrile

Molecular Weight	406.48	Ctorogo	2 years 4°C powder 3 years -20°C powder
Formula	C23H26N4O3	Storage	6 months -80°C in solvent Away from light
CAS No.	2204289-53-0	Synonyms	(Rac)-SHIN2

Solubility (25°C) *	In vitro	DMSO	DMSO : 100 mg/mL (246.03 mM; Need ultrasonic)
		Ethanol	N/A
		Water	N/A
	In vivo (should be freshly prepared each time)	In Vivo 1. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (6.15mM); Clear solution	



Product Data Sheet

2. 10% DMSO >> 40% PEG300 >> 5%
Tween-80 >> 45% saline
Solubility: \geq 2.5 mg/mL (6.15 mM); Clear
solution
3. 10% DMSO >> 90% (20% SBE-β-CD
in saline)
Solubility: \geq 2.5 mg/mL (6.15 mM); Clear
solution

* <1 mg/ml means slightly soluble or insoluble.

* Please note that Selleck tests the solubility of all compounds in-house, and the actual solubility may differ slightly from published values. This is normal and is due to slight batch-to-batch variations.

Preparing Stock Solutions:

Mass	1 mg	5 mg	10 mg
Volume Concentration			
1 mM	2.4601 mL	12.3007 mL	24.6015 mL
5 mM	0.4920 mL	2.4601 mL	4.9203 mL
10 mM	0.2460 mL	1.2301 mL	2.4601 mL

DMSO :

*The above data is based on the product molecular weight 406.48.

Biological Activities:

Description	SHIN2 is a novel SHMT inhibitor, increasing survival in NOTCH1-driven mouse primary T-ALL in vivo.
IC₅₀ & Target	Serine hydroxymethyltransferase (SHMT)

References	[1]. García-Cañaveras, Juan C et al. "SHMT inhibition is effective and
	synergizes with methotrexate in T-cell acute lymphoblastic leukemia."
	<u>Leukemia vol. 35,2 (2021): 377-388.</u>
	[2]. Mootha Vamsi, et al. Method of treating and preventing viral
	infection comprising inhibitors of folate or one-carbon metabolism
	pathways such as serine hydroxymethyltransferase inhibitors: World
	Intellectual Property Organization, WO2022120195[P]. 2022-06-09.