Product Data Sheet

Product Name: KHK-IN-1 (ketohexokinase inhibitor)
Cat. No.: GC30367

Chemical Properties

Cas. No.	1303469-70-6		
SMILES	CSC(C=CC=C1)=C1NC2=NC(N3CCNCC3)=NC4=C2N=CN=C4NCC5CC5		
Formula	$C_{21}H_{26}N_8S$	M.Wt	422.55
Solubility	Soluble in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure			

Protocol

Cell experiment [1]:

Cell lines	NCI-N87 cells
Preparation Method	NCI-N87 cells were cultured in RPMI1640 medium supplemented with 10% fetal bovine serum (FBS) and 1% of penicillin/streptomycin at 37℃ in the presence of 5% CO_2. Cells were plated onto a 96-well plate at a density of 1×10^4 cells/ml for 24h, and were treated with different concentrations of KHK-IN-1 hydrochloride (0, 1, 2, 3, 4, 5, and 6μM). After 4 days, cell viability was analyzed.
Reaction Conditions	0, 1, 2, 3, 4, 5, and 6μM; 4 days

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Applications	KHK-IN-1 hydrochloride treatment significantly reduced the cell viability of NCI-N87 cells in a dose-dependent manner.

Animal experiment [1]:

Animal models	Balb/c nude mice
Preparation Method	Female Balb/c nude mice (5-week-old) were maintained under specific-pathogen-free (SPF) conditions. Five mice were held in each individually ventilated cage on a 12h/12h light/dark cycle with food and water ad libitum. The living status of mice was checked every day, and all the experiments were conducted after mice were housed for 7 days. 1.5×10^6 NCI-N87 cells were injected subcutaneously into Balb/c nude mice. When the tumor masses grew to approximate $50mm^3$, 100μl KHK-IN-1 hydrochloride (50μM) was peritumorally injected every day. The treatment duration was 14 days. The sizes of the tumor masses and the body weights of mice were measured every day.
Dosage form	50μM (100μl); once a day for 14 days; peritumoral injection
Applications	KHK-IN-1 hydrochloride treatment inhibited tumor growth in the NCI-N87-xenograft mouse models, without affecting the body weight.

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References:
[1] Ma G, Liu S, Cai F, et al. Ketohexokinase-A deficiency attenuates the proliferation via reducing β-catenin in gastric cancer cells[J]. Experimental Cell Research, 2024, 438(1): 114038.

Background

KHK-IN-1 (ketohexokinase inhibitor) is a selective and cell membrane-permeable ketohexokinase (KHK) inhibitor with an IC_{50} value of 12nM [1]. KHK-IN-1 hydrochloride inhibits the activity of KHK by docking within the ATP-binding pocket of KHK, with a good solubility[2]. KHK-IN-1 hydrochloride has been widely used to inhibit the *C. auris* strain 0390 and prevent the formation of biofilms[3].

In vitro, KHK-IN-1 hydrochloride treatment for 4 days significantly inhibited the proliferation of NCI-N87 and HGC-27 cells, with IC_{50} values of 3.66μM and 2.31μM, respectively[4].

In vivo, KHK-IN-1 hydrochloride treatment via daily peritumoral injection of 100μl (50μM) for 14 days significantly inhibited tumor growth in the NCI-N87-xenograft mouse models, without affecting the body weight of the mice[4].

References:
[1] Maryanoff B E, O'Neill J C, McComsey D F, et al. Pyrimidinopyrimidine inhibitors of ketohexokinase: exploring the ring C2 group that interacts with Asp-27B in the ligand binding pocket[J]. Bioorganic & medicinal chemistry letters, 2012, 22(16): 5326-5329.

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[2] Maryanoff B E, O'Neill J C, McComsey D F, et al. Inhibitors of ketohexokinase: discovery of pyrimidinopyrimidines with specific substitution that complements the ATP-binding site[J]. ACS medicinal chemistry letters, 2011, 2(7): 538-543.
[3] Ajetunmobi O H, Wall G, Vidal Bonifacio B, et al. High-throughput screening of the repurposing hub library to identify drugs with novel inhibitory activity against Candida albicans and Candida auris biofilms[J]. Journal of Fungi, 2023, 9(9): 879.
[4] Ma G, Liu S, Cai F, et al. Ketohexokinase-A deficiency attenuates the proliferation via reducing β-catenin in gastric cancer cells[J]. Experimental Cell Research, 2024, 438(1): 114038.

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