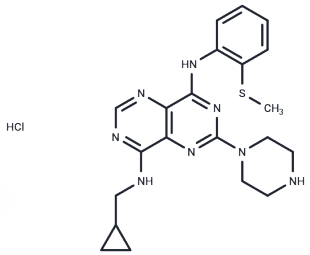
Data Sheet (Cat.No.T15659)

TargetMol

KHK-IN-1 hydrochloride

Chemical Properties



CAS No. : 1303470-48-5

Formula: C21H27ClN8S

Molecular Weight: 459.01

Storage: Keep away from moisture
Store at -20°C
Actual storage temperature shall be subject to the COA.

Biological Description

Description	KHK-IN-1 hydrochloride is a selective, cell-permeable, and efficient hexokinase (KHK) inhibitor, useful for studying diabetes and obesity.
Targets(IC50)	Others
In vitro	Methods: HepG2 cells were treated with KHK-IN-1 hydrochloride (0-10 μM) and the level of KHK product F1P in cell lysates was measured using LC-MS quantification of F1P Results: KHK-IN-1 hydrochloride inhibited the production of F1P in HepG2 cell lysates with an IC50 value of 400 nM.[1]
In vivo	Methods: Rats were treated with KHK-IN-1 hydrochloride (10 mg/kg, oral) for pharmacokinetic studies. Results: KHK-IN-1 hydrochloride showed reasonable oral bioavailability in rats (F = 34%; oral t1/2 = 4 h); high distribution volume (Vdss = 32 L/kg) and high clearance (CL = 160 mL/min/kg); its plasma Cmax was only 0.16 μM.[2]

Solubility Information

Solubility	DMSO: 20 mg/mL (43.57 mM),Sonication is recommended. H2O: 10 mg/mL (21.79 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (4.36 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.1786 mL	10.893 mL	21.786 mL
5 mM	0.4357 mL	2.1786 mL	4.3572 mL
10 mM	0.2179 mL	1.0893 mL	2.1786 mL
50 mM	0.0436 mL	0.2179 mL	0.4357 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Maryanoff BE, et al. Pyrimidinopyrimidine inhibitors of ketohexokinase: exploring the ring C2 group that interacts with Asp-27B in the ligand binding pocket. Bioorg Med Chem Lett. 2012 Aug 15;22(16):5326-9.
Maryanoff BE, et al. Inhibitors of Ketohexokinase: Discovery of Pyrimidinopyrimidines with Specific Substitution that Complements the ATP-Binding Site. ACS Med Chem Lett. 2011 Apr 18;2(7):538-43.