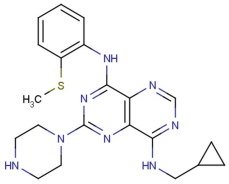
Data Sheet (Cat.No.T15660)

TargetMol
A DRUG SCREENING EXPERT

KHK-IN-1

Chemical Properties



CAS No.:	1303469-70-6
Formula:	C21H26N8S
Molecular Weight:	422.55
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	KHK-IN-1 is a potent inhibitor of ketohexokinase (KHK) (IC50: 12 nM). In the ATP-binding region of KHK, KHK-IN-1 interacts with Asp-27B.
Targets(IC_{50})	Others: None

Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.367 mL	11.833 mL	23.666 mL
5 mM	0.473 mL	2.367 mL	4.733 mL
10 mM	0.237 mL	1.183 mL	2.367 mL
50 mM	0.047 mL	0.237 mL	0.473 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. 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.
2. 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.

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