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Lieferung & Zahlungsart

siehe unsere Liefer- und Versandbedingungen

Zuschläge

- Mindermengenzuschlag
- Trockeneiszuschlag
- Gefahrgutzuschlag
- Expressversand

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KHK-IN-1 hydrochloride

Cat. No.: HY-12841A

CAS No.: 1303470-48-5

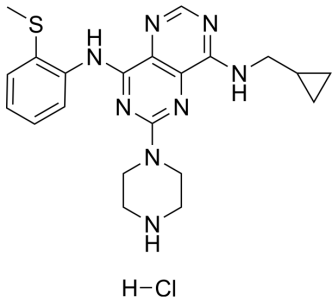
Molecular Formula: $C_{21}H_{27}ClN_8S$

Molecular Weight: 459.01

Target: Ketohexokinase

Pathway: Metabolic Enzyme/Protease

Storage: -20°C, sealed storage, away from moisture
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 25 mg/mL (54.47 mM; Need ultrasonic)
H_2O : 14.29 mg/mL (31.13 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions

Concentration \ Solvent \ Mass	1 mg	5 mg	10 mg
1 mM	2.1786 mL	10.8930 mL	21.7860 mL
5 mM	0.4357 mL	2.1786 mL	4.3572 mL
10 mM	0.2179 mL	1.0893 mL	2.1786 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (4.53 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (4.53 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

KHK-IN-1 hydrochloride (compound 8) is a selective and cell membrane permeable ketohexokinase (KHK) inhibitor (IC_{50}=12 nM; F=34%). KHK-IN-1 hydrochloride inhibits the production of F1P in HepG2 cell lysates (IC>sub>50=400 nM). KHK-IN-1 hydrochloride has potential for the study of diabetes and obesity[1].

IC_{50} & Target

IC50=12 nM (KHK)[1].

In Vitro

KHK-IN-1 hydrochloride stable in human and rat liver microsome preparations (88 and 72% remaining at 10 min) and do not significantly inhibit cytochrome P450s from human liver microsomes (1A2, 2C19, 2D6, 2C9, and 3A4)[1].
KHK-IN-1 hydrochloride (0-10 μM; incubate 30 min, then add to 15 mM fructose and incubate for another 3 h) inhibits production of F1P in HepG2 cell lysates with an IC_{50} value of 400 nM[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[1]

Cell Line:	HepG2 cells
Concentration:	0-10 μM
Incubation Time:	Incubate 30 min, then add to 15 mM fructose and incubate for another 3 h
Result:	Exhibited inhibition of F1P production in HepG2 cell lysates (IC_{50}=400 nM).

In Vivo

KHK-IN-1 hydrochloride (10 mg/kg; p.o.; single) shows oral bioavailability of 34% in rats[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male Sprague-Dawley rats (~250 g)[1].
Dosage:	10 mg/kg
Administration:	Oral gavage; single
Result:	Exhibited reasonable oral bioavailability in rats (F=34%; oral $t_{1/2}$=4 h), but had a high volume of distribution (Vd_{ss}= 32 L/kg) and a high rate of clearance (CL=160 mL/min/kg).

REFERENCES

[1]. 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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