## LY3522348

 Cat. No.:
 HY-149987 

 CAS No.:
 2568608-48-8 

 Molecular Formula:
  $C_{18}H_{22}F_3N_7O$  

 Molecular Weight:
 409.41 

Target: Ketohexokinase

Pathway: Metabolic Enzyme/Protease

Storage: Powder -20°C 3 years

 $\begin{tabular}{ll} $4^{\circ}C$ & 2 years \\ In solvent & -80^{\circ}C$ & 6 months \\ \end{tabular}$ 

-20°C 1 month

## **SOLVENT & SOLUBILITY**

In Vitro

DMSO: 100 mg/mL (244.25 mM; Need ultrasonic)

	Solvent Mass Concentration	1 mg	5 mg	10 mg
Preparing Stock Solutions	1 mM	2.4425 mL	12.2127 mL	24.4254 mL
	5 mM	0.4885 mL	2.4425 mL	4.8851 mL
	10 mM	0.2443 mL	1.2213 mL	2.4425 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: 2.5 mg/mL (6.11 mM); Clear solution; Need ultrasonic
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE- $\beta$ -CD in saline) Solubility: 2.5 mg/mL (6.11 mM); Clear solution; Need ultrasonic
- Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (6.11 mM); Clear solution; Need ultrasonic

## **BIOLOGICAL ACTIVITY**

Description

KHK-IN-3 (Example 1) is a ketohexokinase (KHK) inhibitor. KHK-IN-3 can be used in the study of kidney disease, nonalcoholic steatohepatitis (NASH), diabetes and heart failure. KHK is a rate-limiting enzyme and fructokinase involved in fructose metabolism. KHK catalyzes the phosphorylation of fructose to fructose-1-phosphate (FIP) at the expense of ATP. The lack of feedback inhibition of fructose metabolism triggers the accumulation of downstream intermediates such as lipogenesis, gluconeogenesis, and oxidative phosphorylation<sup>[1]</sup>.

[1]. Coates David Andrew, et a	l. Preparation of the disubstitute	d pyrazole compound and their medical applications. United States, US2020	0392118 A1. 2020-12-17.
	Caution: Product has not	peen fully validated for medical applications. For research use only.	
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