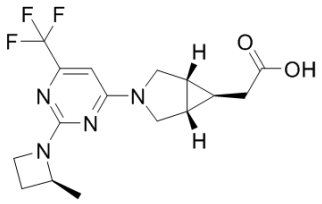
Ketohexokinase inhibitor 1

Cat. No.:	HY-U00461
CAS No.:	2102501-84-6
Molecular Formula:	$C_{16}H_{19}F_3N_4O_2$
Molecular Weight:	356.34
Target:	Others
Pathway:	Others
Storage:	4°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 : 100 mg/mL (280.63 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.8063 mL	14.0315 mL	28.0631 mL
	5 mM	0.5613 mL	2.8063 mL	5.6126 mL
	10 mM	0.2806 mL	1.4032 mL	2.8063 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 (5.84 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (5.84 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.84 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Ketohexokinase inhibitor 1 is an inhibitor of ketohexokinase (KHK), with IC_{50}s of 8.4 nM and 66 nM for KHK-C and KHK-A, respectively, extracted from patent US 20170183328 A1, example 4.

IC_{50} & Target

IC50: 8.4 nM (KHK-C), 66 nM (KHK-A)[1]

In Vitro

Ketohexokinase inhibitor 1 (Example 4) is an inhibitor of ketohexokinase (KHK), with IC_{50}s of 8.4 nM and 66 nM for KHK-C and KHK-A, sepctively[1].

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

PROTOCOL

Kinase Assay [1]

A 384-well format on a assay plate is used in the assay and monitored by UV-vis spectroscopy in continuous mode at room temperature (rt). Compounds (Ketohexokinase inhibitor 1) are prepared in DMSO as 4 mM stocks, diluted using an 11-point half-log scheme on a Biomek FX, and incubated at rt for 30 minutes with the reaction mixture containing 50 mM HEPES, pH 7.4, 140 mM KCl, 3.5 mM $MgCl_2$, 0.8 mM fructose, 2 mM TCEP, 0.8 mM PEP, 0.7 mM NADH, 0.01% Triton X-100, 30 U/mL pyruvate kinase-lactate dehydrogenase, and 10 nM purified KHK-C. The compound concentration in each well ranged from 1 nM to 100 μM. The reaction is initiated with the addition of 0.2 mM ATP. The absorbance is measured for 30 minutes on a SpectraMax reader after ATP is added. The concentrations provided are based on the final mixture volume of 40 μL[1].

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

REFERENCES

[1]. SUBSTITUTED 3-AZABICYCLO[3.1.0]HEXANES AS KETOHEXOKINASE INHIBITORS. US 20170183328 A1

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