Product Data Sheet

Product Name: Ketohexokinase inhibitor 1
Cat. No.: GC31400

Chemical Properties

Cas. No.	2102501-84-6		
SMILES	O=C(C[C@H]1[C@@]2(CN(C[C@]12[H])C3=NC(N4[C@H](CC4)C)=NC(C(F)(F)F)=C3)[H])O		
Formula	$C_{16}H_{19}F_3N_4O_2$	M.Wt	356.34
Solubility	DMS : ≥ 125 mg/mL (350.79 mM)	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	Ketohexokinase inhibitor 1		

Protocol

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Kinase experiment:

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 MgCl2, 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].

References:

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

Background

Ketohexokinase inhibitor 1 is an inhibitor of ketohexokinase (KHK), with IC50s of 8.4 nM and 66 nM for KHK-C and KHK-A, respectively, extracted from patent US 20170183328 A1, example 4.

Ketohexokinase inhibitor 1 (Example 4) is an inhibitor of ketohexokinase (KHK), with IC50s of 8.4 nM and 66 nM for KHK-C and KHK-A, sepctively[1].

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

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