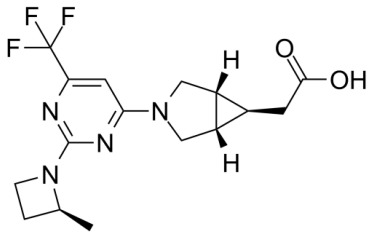
Data Sheet

Product Name:	Ketohexokinase inhibitor 1
Cat. No.:	CS-0039434
CAS No.:	2102501-84-6
Molecular Formula:	C16H19F3N4O2
Molecular Weight:	356.34
Target:	Others
Pathway:	Others
Solubility:	DMS : ≥ 125 mg/mL (350.79 mM)



BIOLOGICAL ACTIVITY:

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. IC50 & 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].

PROTOCOL (Extracted from published papers and Only for reference)

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].

References:

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

CAIndexNames:

2-((1R,5S,6R)-3-(2-((S)-2-methylazetidin-1-yl)-6-(trifluoromethyl)pyrimidin-4-yl)-3-azabicyclo[3.1.0]hexan-6-yl)acetic acid

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

Caution: Product has not been fully validated for medical applications. For research use only.

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