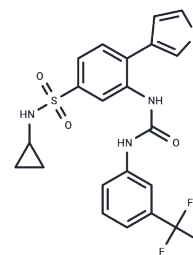


AGI-6780

## Chemical Properties

CAS No. : 1432660-47-3  
 Formula: C<sub>21</sub>H<sub>18</sub>F<sub>3</sub>N<sub>3</sub>O<sub>3</sub>S<sub>2</sub>  
 Molecular Weight: 481.51  
 Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year  
*Actual storage temperature shall be subject to the COA.*



## Biological Description

Description	AGI-6780 is a potent and selective inhibitor of IDH2 R140Q mutant.
Targets(IC50)	Dehydrogenase, Isocitrate Dehydrogenase (IDH)
In vivo	AGI-6780 reverses differentiation blockage induced by IDH2/R140Q in TF-1 cells and induces rapid differentiation in primary samples from patients with IDH2/R140Q AML. It effectively reduces the levels of (R)-2-hydroxyglutarate (2-HG) in cell lines overexpressing ectopic IDH2/R140Q, with an EC <sub>50</sub> of 20 nM, demonstrating excellent selectivity compared to other dehydrogenases.
Kinase Assay	AGI-6780 is prepared as 10 mM stock in DMSO and diluted to 50X final concentration in DMSO, for a 50 µL reaction mixture. IDH enzyme activity converting alpha-ketoglutarate to 2-hydroxyglutarate is measured using a NADPH depletion assay. In the assay the remaining cofactor is measured at the end of the reaction with the addition of a catalytic excess of diaphorase and resazurin, to generate a fluorescent signal in proportion to the amount of NADPH remaining. IDH enzyme activity in the direction of isocitrate to alpha-ketoglutarate conversion is measured by direct coupling of the NADPH production to conversion of resazurin to resorufin by diaphorase. In both cases, resorufin is measured fluorometrically at Ex544 Em590[1].
Cell Research	AGI-6780 is dissolved in DMSO and stored, and then diluted with appropriate media before use[1]. Cells are sorted from fresh or frozen bone marrow aspirates and blood samples after labelling with PE-CD34, APC-CD38, PE-CD14, FITC-CD3 (clone HIT3a) and PECy7-CD19 (clone SJ25C1) antibodies using a MoFlow cell sorter. Unfractionated nucleated blood or bone marrow cells are plated in Methocult H4434 methylcellulose medium at 104 cells/dish, in duplicate dishes per condition. AGI-6780 (5 mM) is directly added to the medium. Dishes are incubated in a humidified incubator at 37°C and colonies containing at least 30 cells are counted after 13 days[1].

## Solubility Information

Solubility	DMSO: 125 mg/mL (259.6 mM), Sonication is recommended. H <sub>2</sub> O: < 1 mg/mL (insoluble or slightly soluble), Ethanol: 89 mg/mL (184.84 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
------------	--

## A DRUG SCREENING EXPERT

In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 3.3 mg/mL (6.85 mM), Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>
---------------------	---

### Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.0768 mL	10.384 mL	20.768 mL
5 mM	0.4154 mL	2.0768 mL	4.1536 mL
10 mM	0.2077 mL	1.0384 mL	2.0768 mL
50 mM	0.0415 mL	0.2077 mL	0.4154 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

### Reference

Wang F, et al. Science. 2013, 340(6132), 622-666.

Chen J, Yang J, Wei Q, et al. Identification of a selective inhibitor of IDH2/R140Q enzyme that induces cellular differentiation in leukemia cells. Cell Communication and Signaling. 2020, 18(1): 1-12

Chen J, Yang J, Wei Q, et al. Cell Communication and Signaling. 2020, 18(1): 1-12.

Tan Q, Zhang X, Li S, et al. DMT1 differentially regulates mitochondrial complex activities to reduce glutathione loss and mitigate ferroptosis. Free Radical Biology and Medicine. 2023

Chen J, Yang J, Wei Q, et al. Identification of a selective inhibitor of IDH2/R140Q enzyme that induces cellular differentiation in leukemia cells[J]. Cell Communication and Signaling. 2020, 18: 1-12.

Yang J, Chen J, Chang J, et al. IDH2/R140Q mutation confers cytokine-independent proliferation of TF-1 cells by activating constitutive STAT3/5 phosphorylation. Cell Communication and Signaling. 2024, 22(1): 116.

Chen J, Yang J, Wei Q, et al. Identification of a selective inhibitor of IDH2/R140Q enzyme that induces cellular differentiation in leukemia cells[J]. Cell Communication and Signaling . 2020, 18: 1-12.

**Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins**

This product is for Research Use Only · Not for Human or Veterinary or Therapeutic Use

Tel: 781-999-4286 E\_mail: info@targetmol.com Address: 34 Washington Street, Wellesley Hills, MA 02481