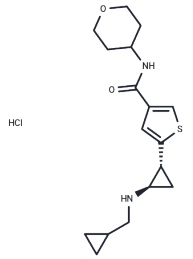
Data Sheet (Cat.No.T39252)

TAK-418

Chemical Properties



CAS No. :	1818252-53-7
Formula:	C17H25ClN2O2S
Molecular Weight:	356.91
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	TAK-418 is a selective and orally active inhibitor of LSD1/KDM1A enzyme with an IC50 of 2.9 nM. TAK-418 unlocks abnormal epigenetic mechanisms and improves autism symptoms in models of neurodevelopmental disorders.
Targets(IC50)	Histone Demethylase
In vivo	TAK-418 (1 mg/kg; oral; once daily for 14 days) improves certain autism spectrum disorder (ASD)-like behaviors in rodents that model neurodevelopmental disorders.[1] TAK-418 increases H3K4me1/2/3 and H3K9me2 levels of the Ucp2 gene and induces Ucp2 mRNA expression in primary cultured rat neurons. TAK-418 also increases H3K4me1/2/3 of the Bdnf gene. TAK-418 avoids steric interference of GFI1B in the binding pocket by generating a tightly formylated adduct form of coenzyme flavin adenine dinucleotide (FAD). TAK-418 exhibits favorable pharmacokinetic profiles in rodents and inhibits LSD1 enzymatic activity in the brain without causing hematological toxicity in rodents.[1] A single administration of 1 or 3 mg/kg of TAK-418 increases H3K4me2 levels of the Ucp2 gene in the mouse brain.[1] TAK-418 can improve neurological problems at cellular, molecular, gene expression, functional, and functional levels in the KS mouse model (Kmt2d+/βGeo mice).[2]

Solubility Information

Solubility	DMSO: 49.5 mg/mL (138.69 mM),Sonication and heating to 60°C are recommended. H2O: 15 mg/mL (42.03 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 5 mg/mL (14.01 mM),Sonication is recommended. *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.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.8018 mL	14.0091 mL	28.0183 mL
5 mM	0.5604 mL	2.8018 mL	5.6037 mL
10 mM	0.2802 mL	1.4009 mL	2.8018 mL
50 mM	0.056 mL	0.2802 mL	0.5604 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

Baba R, et al. LSD1 enzyme inhibitor TAK-418 unlocks aberrant epigenetic machinery and improves autism symptoms in neurodevelopmental disorder models. Sci Adv. 2021;7(11):eaba1187.
Zhang L, et al. Inhibition of KDM1A activity restores adult neurogenesis and improves hippocampal memory in a mouse model of Kabuki syndrome. Mol Ther Methods Clin Dev. 2021;20:779-791.