

AZ505 ditrifluoroacetate

Chemical Properties

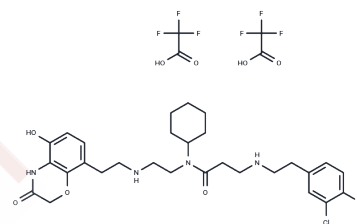
CAS No. : 1035227-44-1

Formula: C₃₃H₄₀Cl₂F₆N₄O₈

Molecular Weight: 805.59

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	AZ505 ditrifluoroacetate is an effective and selective SMYD2 inhibitor (IC ₅₀ : 0.12 μM).
Targets(IC ₅₀)	Histone Methyltransferase
In vitro	AZ505 ditrifluoroacetate is highly selective and active at submicromolar concentrations in vitro, with an IC ₅₀ of 0.12 μM for SMYD2, over 600-fold lower than its IC ₅₀ for other histone methyltransferases such as SMYD3 (IC ₅₀ >83.3 μM) and DOT1L (IC ₅₀ >83.3 μM) [1]. It has been nominated for ITC binding study (K _d : 0.5 μM), in contrast to the calculated K _d of 3.7 μM for the p53 substrate peptide. The binding of AZ505 ditrifluoroacetate to SMYD2 is primarily driven by entropy, suggesting hydrophobic interactions with minimal specific hydrogen bonds [2].

Solubility Information

Solubility	DMSO: 125 mg/mL (155.17 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: 3.3 mg/mL (4.1 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	1.2413 mL	6.2066 mL	12.4133 mL
5 mM	0.2483 mL	1.2413 mL	2.4827 mL
10 mM	0.1241 mL	0.6207 mL	1.2413 mL
50 mM	0.0248 mL	0.1241 mL	0.2483 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

Komatsu S, et al. Overexpression of SMYD2 contributes to malignant outcome in gastric cancer. *Br J Cancer*. 2015 Jan 20;112(2):357-64.

Li X, Wang Y, Zhang Y, et al. Overexpression of MCAM induced by SMYD2-H3K36me2 in breast cancer stem cell properties. *Breast Cancer*. 2022: 1-15

Ferguson AD, et al. Structural basis of substrate methylation and inhibition of SMYD2. *Structure*. 2011 Sep 7;19(9):1262-73.

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