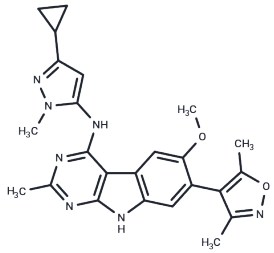
Data Sheet (Cat.No.T10773)

TargetMol

CF53

Chemical Properties



CAS No. : 1808160-52-2

Formula: C24H25N7O2

Molecular Weight: 443.5

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	CF53 is a highly potent, selective, and orally active inhibitor of BET protein, with a Ki of <1 nM, Kd of 2.2 nM, and an IC50 of 2 nM for BRD4 BD1. CF53 binds to both the BD1 and BD2 domains of BRD2, BRD3, BRD4, and BRDT BET proteins with high affinities, being very selective over non-BET bromodomain-containing proteins. CF53 exhibits potent anti-tumor activity both in vitro and in vivo.
Targets(IC50)	Epigenetic Reader Domain,Histone Acetyltransferase,CDK
In vitro	CF53 exhibits high binding affinities to the BD1 and BD2 domains of BRD2, BRD3, BRD4, and BRDT within the BET protein family, with dissociation constants (Kds) as follows: 1.1 nM for BRD2 BD1, 0.6 nM for BRD2 BD2, 0.52 nM for BRD3 BD1, 0.49 nM for BRD3 BD2, 0.8 nM for BRD4 BD2, 2 nM for BRDT BD1, and 2.1 nM for BRDT BD2. Additionally, it displays Kds of 47 nM, 570 nM, and 110 nM for CREBBP, CECR2, and EP300, respectively. In terms of biological activity, CF53 shows IC50 values of 7 nM and 85 nM against MOLM-13 acute leukemia and MDA-MB-231 breast cancer cell lines, respectively[1].
In vivo	CF53, administered orally at doses of 25 and 50 mg/kg, demonstrates strong anti-tumor efficacy in both the MDA-MB-231 xenograft tumor model and the RS4;11 model in mice [1].

Solubility Information

Solubility	DMSO: 99 mg/mL (223.22 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: 2 mg/mL (4.51 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	2.2548 mL	11.274 mL	22.5479 mL
5 mM	0.451 mL	2.2548 mL	4.5096 mL
10 mM	0.2255 mL	1.1274 mL	2.2548 mL
50 mM	0.0451 mL	0.2255 mL	0.451 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

Zhao Y, et al. Structure-Based Discovery of CF53 as a Potent and Orally Bioavailable Bromodomain and Extra-Terminal (BET) Bromodomain Inhibitor. J Med Chem. 2018 Jul 26;61(14):6110-6120.