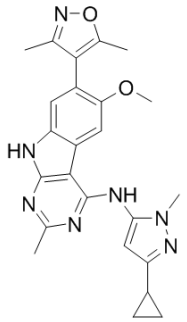
CF53

Cat. No.:	HY-112610
CAS No.:	1808160-52-2
Molecular Formula:	$C_{24}H_{25}N_7O_2$
Molecular Weight:	443.5
Target:	Epigenetic Reader Domain; Histone Acetyltransferase
Pathway:	Epigenetics
Storage:	-20°C, stored under nitrogen * In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 110 mg/mL (248.03 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.2548 mL	11.2740 mL	22.5479 mL
5 mM	0.4510 mL	2.2548 mL	4.5096 mL
10 mM	0.2255 mL	1.1274 mL	2.2548 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 1.83 mg/mL (4.13 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.83 mg/mL (4.13 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

CF53 is a highly potent, selective and orally active inhibitor of BET protein, with a K_i of <1 nM, K_d of 2.2 nM and an IC_{50} 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, very selective over non-BET bromodomain-containing proteins. CF53 shows potent anti-tumor activity both in vitro and in vivo[1].

IC_{50} & Target

BRD4 (BD1) <1 nM (Ki)	BRD4 (BD1) 2 nM (IC_{50})	BRD4 (BD1) 2.2 nM (Kd)	BRD4 (BD2) 0.8 nM (Kd)
BRD2 (BD2) 0.6 nM (Kd)	BRD2 (BD1) 1.1 nM (Kd)	BRD3 (BD2) 0.49 nM (Kd)	BRD3 (BD1) 0.52 nM (Kd)
BRDT (BD2)	BRDT (BD1)	CREBBP	EP300

	1 nM (Kd)	2 nM (Kd)	47 nM (Kd)	110 nM (Kd)
	CECR2 570 nM (Kd)			
In Vitro	CF53 (Compound 28) binds to both the BD1 and BD2 domains of BRD2, BRD3, BRD4, and BRDT BET proteins with high affinities, K_ds are 1.1 nM (BRD2 BD1), 0.6 nM (BRD2 BD2), 0.52 nM (BRD3 BD1), 0.49 nM (BRD3 BD2), 0.8 nM (BRD4 BD2), 2 nM (BRDT BD1), 2.1 nM (BRDT BD2), 47 nM (CREBBP), 570 nM (CECR2), 110 nM (EP300), respectively[1]. CF53 exhibits IC_{50}s of 7, 85 nM against MOLM-13 acute leukemia and MDA-MB-231 breast cancer cell lines, respectively[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.			
In Vivo	CF53 (25, 50 mg/kg, p.o.) exhibits potent anti-tumor activity both in MDA-MB-231 xenograft tumor model and in RS4;11 model in mice[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.			

REFERENCES

[1]. 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.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA