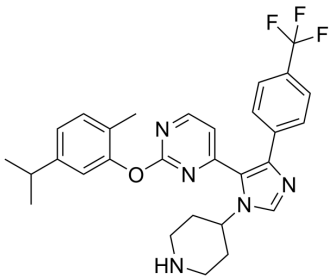
iBRD4-BD1

Cat. No.:	HY-151594
CAS No.:	2839318-17-9
Molecular Formula:	$C_{29}H_{30}F_3N_5O$
Molecular Weight:	521.58
Target:	Epigenetic Reader Domain
Pathway:	Epigenetics
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (191.73 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9173 mL	9.5863 mL	19.1725 mL
	5 mM	0.3835 mL	1.9173 mL	3.8345 mL
	10 mM	0.1917 mL	0.9586 mL	1.9173 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: 2.5 mg/mL (4.79 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (4.79 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (4.79 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

iBRD4-BD1 is selective BRD4 bromodomain inhibitor. iBRD4-BD1 has inhibition activity for BRD4 bromodomain with an IC_{50} value of 12 nM. iBRD4-BD1 can be used for the research of inflammation and oncology[1].

In Vitro

iBRD4-BD1 has affinity and selectivity for the BET-family BRD4-BD1 with an IC_{50} value of 12 nM[1].
iBRD4-BD1 has affinity and selectivity for the BET-family BRD4-BD2, BRD3-BD1, BRD3-BD2, BRD2-BD1 and BRD2-BD2 with IC $_{50}$ values of 16 μM, 1.0 μM , 75 μM , 280 nM and 7.1 μM, respectively[1].
iBRD4-BD1 (0-50 μM; 72 h) has cytotoxicity with an EC_{50} value of 2.3 μM in MM.1S cells[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Western Blot Analysis[1]	
Cell Line:	MM.1S cells
Concentration:	0-300 pM
Incubation Time:	1 h
Result:	Prevented the denaturation of BRD4 in a dose-dependent manner and showed stabilization of BRD4 at concentrations above 3 nM.

Cell Cytotoxicity Assay[1]	
Cell Line:	MM.1S cells
Concentration:	0-50 μM
Incubation Time:	72 h
Result:	Showed cytotoxicity with an EC_{50} value of 2.3 μM in MM.1S cells.

REFERENCES

[1]. Anand Divakaran, et al. Development of an N-Terminal BRD4 Bromodomain-Targeted Degrader. ACS Med Chem Lett. 2022 Sep 29;13(10):1621-1627.

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