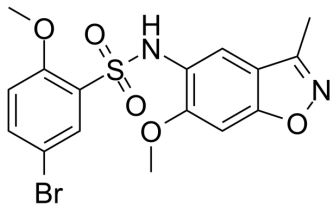
Y06036

Cat. No.:	HY-111502
CAS No.:	1832671-96-1
Molecular Formula:	$C_{16}H_{15}BrN_2O_5S$
Molecular Weight:	427.27
Target:	Epigenetic Reader Domain
Pathway:	Epigenetics
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 130 mg/mL (304.26 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.3404 mL	11.7022 mL	23.4044 mL
5 mM	0.4681 mL	2.3404 mL	4.6809 mL
10 mM	0.2340 mL	1.1702 mL	2.3404 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: ≥ 2.17 mg/mL (5.08 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.17 mg/mL (5.08 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Y06036 is a potent and selective BET inhibitor, which binds to the BRD4(1) bromodomain with K_d value of 82 nM[1]. Antitumor activity[1].

IC_{50} & Target

BRD4(1)
82 nM (Kd)

In Vitro

Y06036 (0.001-100 nM, 96 hours for LNCaP, C4-2B, and 22Rv1 cells; 144 hours for VCaP cells) exhibits low micromolar or nanomolar potencies (IC_{50}: 0.29-2.6 μM) in the four androgen receptor (AR)-positive prostate cancer cell lines LNCaP, C4-2B, 22Rv1, and VCaP. Treatment of 22Rv1 cells with Y06036 (1, 2, 4, 8, and 16 μM, 48 hours) results in significant down-regulation of both full-length (AR-fl) and AR variants levels[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[1]

Cell Line:	LNCaP, C4-2B, 22Rv1, and VCaP prostate cancer cells
Concentration:	0.001-100 μM
Incubation Time:	96 hours for LNCaP, C4-2B, and 22Rv1; 144 hours for VCaP
Result:	Inhibited LNCaP, C4-2B, 22Rv1, and VCaP cells with IC_{50}s of 1.06, 2.62, 1.50, 0.63 μM, respectively.

Western Blot Analysis[1]

Cell Line:	22Rv1 cells
Concentration:	1,2,4,8, and 16 μM
Incubation Time:	48 hours
Result:	Resulted in significant down-regulation of both AR-fl and AR variants levels

In Vivo

Y06036 (50 mg/kg, i.p. injection, 5 times per week, 25 days) demonstrates therapeutic effects in a C4-2B CRPC xenograft tumor model in mice. Y06036 is well tolerated in the treated mice, based on the weight of the animal body and their general behavior[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Four-week-old male mice (strain: C.B-17/IcrHsd-Prkdc^{scid} for C4-2B) with C4-2B mouse xenograft model[1]
Dosage:	50 mg/kg, 100 μL
Administration:	Intraperitoneal (i.p.) injection, 5 times per week, 25 days
Result:	Exhibited strong antitumor activities during the 25-day treatment period, with a tumor growth inhibition (TGI) of 70%.

REFERENCES

[1]. Zhang M, et al. Structure-Based Discovery and Optimization of Benzo[d]isoxazole Derivatives as Potent and Selective BET Inhibitors for Potential Treatment of Castration-Resistant Prostate Cancer (CRPC). J Med Chem. 2018 Apr 12;61(7):3037-3058.

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