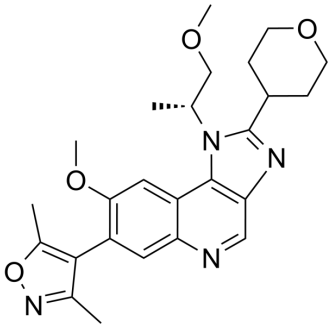
I-BET282

Cat. No.:	HY-19760		
CAS No.:	1422554-34-4		
Molecular Formula:	$C_{25}H_{30}N_4O_4$		
Molecular Weight:	450.53		
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 : 100 mg/mL (221.96 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.2196 mL	11.0980 mL	22.1961 mL
	5 mM	0.4439 mL	2.2196 mL	4.4392 mL
	10 mM	0.2220 mL	1.1098 mL	2.2196 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 (5.55 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.55 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.55 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

I-BET282 is a pan-inhibitor of all eight BET bromodomains, and selectivity over other representative bromodomain-containing proteins. I-BET282 shows pIC_{50}s ranging 6.4-7.7 for BRD2 (BD1/BD2), BRD2 (BD1/BD), BRD3 (BD1/BD), and BRD4 (BD1/BD)[1].

In Vitro

I-BET282 has a weak inhibition of the hERG potassium ion channel (pIC_{50} 4.4-5.1 in a variety of assay formats). I-BET282 shows a low potential to inhibit CYP proteins in vitro, with no evidence of time-dependent inhibition of 2D6 or 3A4[1].

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

In Vivo

I-BET282 (Male CD1 Mice; 3 mg/kg-p.o.; 1 mg/kg-i.v.) treatment shows the Cl_b, LBF, Vss, $t_{1/2}$ (i.v.), and F values of 23

mL/min/kg, 19%, 1.9 L/kg, and 51%, respectively. I-BET282 (Male Wistar Han Rats; 1 mg/kg; p.o.) treatment shows the AUC_{0-t}, C_{max} and T_{max} values of 467 ng h/mL, 125 ng/mL, and 1 hour, respectively[1].

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

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