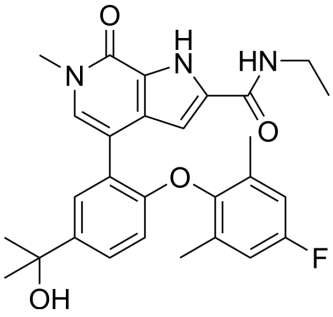
ABBV-744

Cat. No.:	HY-112090
CAS No.:	2138861-99-9
Molecular Formula:	$C_{28}H_{30}FN_3O_4$
Molecular Weight:	491.55
Target:	Epigenetic Reader Domain; HIV
Pathway:	Epigenetics; Anti-infection
Storage:	4°C, stored under nitrogen * In solvent : -80°C, 1 years; -20°C, 6 months (stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (203.44 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.0344 mL	10.1719 mL	20.3438 mL
	5 mM	0.4069 mL	2.0344 mL	4.0688 mL
	10 mM	0.2034 mL	1.0172 mL	2.0344 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 (5.09 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.09 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.09 mM); Clear solution
4. Add each solvent one by one: 50% PEG300 >> 50% saline
   Solubility: 2.5 mg/mL (5.09 mM); Suspended solution; Need ultrasonic
5. Add each solvent one by one: 5% DMSO >> 40% PEG300 >> 5% Tween-80 >> 50% saline
   Solubility: ≥ 2 mg/mL (4.07 mM); Clear solution
6. Add each solvent one by one: 5% DMSO >> 95% (20% SBE-β-CD in saline)
   Solubility: ≥ 2 mg/mL (4.07 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ABBV-744 is a first-in-class, orally active and selective inhibitor of the BDII domain of BET family proteins with IC_{50} values ranging from 4 to 18 nM for BRD2, BRD3, BRD4 and BRDT. ABBV-744 is primarily metabolized by CYP3A4 with agent-like

	properties enable the investigation of its antitumor efficacy and tolerability[1].

IC_{50} & Target

BRD2 (BD2) 8 nM (IC_{50})	BRD3 (BD2) 13 nM (IC_{50})	BRDT (BD2) 18 nM (IC_{50})	BRD4 (BD2) 4 nM (IC_{50})
BRD4 (BD2) 3 nM (Kd)			

In Vitro

ABBV-744 (90 nM; 0~24 h; LNCaP cells) downregulates the expression of KLK2 and MYC genes[1].
?ABBV-744 (90 nM; 0~72 h; LNCaP cells) induces cell cycle arrest in G1 followed by senescence[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Western Blot Analysis[1]

Cell Line:	LNCaP cells
Concentration:	90 nM
Incubation Time:	0~24 hours
Result:	Downregulated the expression of KLK2 and MYC genes.

Cell Cycle Analysis[1]

Cell Line:	LNCaP cells
Concentration:	90 nM
Incubation Time:	0~72 hours
Result:	Induced cell cycle arrest in G1 followed by senescence.

In Vivo

ABBV-744 (4.7 mg/kg; oral gavage; 28 days) causes a delay in tumor growth and displays equivalent or better antitumor activity compared with ABBV-075[1].
?ABBV-744 (30 mg/kg; 14 days) is able to produce significant antitumor activity. ABBV-744 (30 mg/kg) triggers a reduction in platelets of only 20 %[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Mice
Dosage:	4.7 mg/kg (Pharmacokinetic Analysis)
Administration:	Oral gavage; 28 days
Result:	Caused a delay in tumor growth and displayed equivalent or better antitumor activity compared with ABBV-075.

Animal Model:	Sprague-Dawley rats
Dosage:	30 mg/kg (Pharmacokinetic Analysis)
Administration:	14 days
Result:	Produced significant antitumor activity.

CUSTOMER VALIDATION

- Cell. 2021 Apr 15;184(8):2167-2182.e22.
- Science. 2020 Apr 24;368(6489):387-394.
- Analysis & Sensing. 22 June 2022.

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REFERENCES

[1]. Faivre EJ, et al. Selective inhibition of the BD2 bromodomain of BET proteins in prostate cancer. Nature. 2020;578(7794):306-310.

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