BET BD2-IN-1

®

MedChemExpress

Cat. No.:	HY-155680	
CAS No.:	2677039-24-4	
Molecular Formula:	$C_{_{30}}H_{_{30}}N_{_{4}}O_{_{2}}$	
Molecular Weight:	478.58	$\sim \alpha \beta$
Target:	Epigenetic Reader Domain	
Pathway:	Epigenetics	N H
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.	~

BIOLOGICAL ACTIVITY

Description	BET BD2-IN-1 (compound 45) is a potent and selective inhibitor of BET BD2 (IC ₅₀ =1.6 nM). BET BD2-IN-1 inhibits the differentiation of Th17 cells by decreasing the activation of STAT3 and NF-κB. BET BD2-IN-1 is used in psoriasis and inflammatory bowel disease (IBD) research ^[1] .			
IC ₅₀ & Target	BRD2 BD1 570 nM (IC ₅₀) BRD4 BD1 524 nM (IC ₅₀)	BRD2 BD2 5.9 nM (IC ₅₀) BRD4 BD2 1.6 nM (IC ₅₀)	BRD3 BD1 465 nM (IC ₅₀) BRDT BD1 527 nM (IC ₅₀)	BRD3 BD2 6.0 mM (IC ₅₀)
In Vitro	inhibits has exce BD1 ^[1] . BET BD2 BD2 in ir stabiliza MCE has confirme method	P-IN-1 (500 i Th17 cell di ellent select P-IN-1 (4 nM ntact cells a tion effect not indepe ed the accu s. They are erentiation	ifferentiation ivity for BL) binds to B and has on BRD4 B endently tracy of the for referen	Don and D2 over BRD4 D2 ^[1] .

Product Data Sheet

	Time:							
	Result:	Showed the strongest inhibitory activity and reduced differentiation from 19.0 to 7.81%.						
	Cell Migration As	say ^[1]						
	Cell Line:	HEK 293 T cells						
	Concentration:	4, 20, 100, 500, 2500, 10000 nM						
	Incubation Time:	30 min						
	Result:	Stabilized BRD4 BD2 at 50.4 °C.						
	daily for seven d protein expression NF-κB in mouse seffectively ameli pathological char mouse model ^[1] . BET BD2-IN-1 (20 daily for seven d decreases the dis (DAI) score in des (DSS) induced IB Pharmacokinetic	ays) inhibits the on of p-STAT3 and p- skin tissues, orates the inges in the psoriasis 0 mg/kg for i.v; once ays) significantly sease activity index xtran sulfate sodium D mouse model ^[1] . c Analysis of BET	parameter	AUC(0⊠t) (ng•h/mL)	C0 (ng/mL)	T1/2 (h)	CL (mL/kg/min)	Vdss (L/kg)
272 ± 7.2	2	79 ± 78	1.5 ± 0.1	60 ± 2.0	6.6±0.8			
AUC(0⊠t) (ng•h/mL)	Cma	x (ng/mL)	T1/2 (h)	Tmax (h)	F (%)			
		Result: Cell Migration As Cell Line: Concentration: Incubation Time: Result: BET BD2-IN-1 (20) daily for seven d protein expression NF-kB in mouse effectively ameli pathological chai mouse model ^[1] . BET BD2-IN-1 (20) daily for seven d potein expression NF-kB in mouse effectively ameli pathological chai mouse model ^[1] . BET BD2-IN-1 (20) daily for seven d decreases the die (DAI) score in dee (DSS) induced IB Pharmacokinetic BD2-IN-1 in Spra Model ^[1] .	Time:Result:Showed the strongest inhibitory activity and reduced differentiation from 19.0 to 7.81%.Cell Migration Assar[1]Cell Line:HEK 293 T cellsConcentration:4,20,100,500, 2500,10000 nMIncubation Time:30 minResult:Stabilized BRD4 BD2 at 50.4 °C.BET BD2-IN-1 (20 mg/kg for i.v; once daily for seven days) inhibits the protein expression of p-STAT3 and p- NF-kB in mouse skin tissues, effectively ameliorates the pathological charges in the psoriasis mouse model ^[11] .BET BD2-IN-1 (20 mg/kg for i.v; once daily for seven days) significantly decreases the disease activity index (DAI) score in dextran sulfate sodium (DSS) induced IBD mouse model ^[13] . Pharmacokinetic Analysis of BET BD2-IN-1 in Sprague Dawley Rats Model ^[1] .272 ± 22279 ± 78	Time: Result: Showed the strongest inhibitory activity and reduced differentiation from 19.0 to 7.81%. Cell Migration Assay ^[1] Cell Migration (4, 20, 100, 500, 2500, 10000 nM) Incubation 30 min Time: HEK 293 T cells Concentration: 4, 20, 100, 500, 2500, 10000 nM Incubation 30 min Time: Stabilized BRD4 BET BD2-IN-1 (20 mg/kg for i.v; once daily for seven days) inhibits the protein expression of p-STAT3 and p-NF-x8 in mouse skin tissues, effectively ameliorates the pathological changes in the psoriasis mouse model ^[1] . parameter daily for seven days) significantly decreases the disease activity index (DAI) score in dextran sulfate sodium (DSS) induced IBD mouse model ^[1] . Pharmacokinetic Analysis of BET BD2-IN-1 in Sprayue Dawley Rats Model ^[1] . parameter daily for seven days) significantly decreases the disease activity index (DAI) score in dextran sulfate sodium (DSS) induced IBD mouse model ^[1] . Pharmacokinetic Analysis of BET BD2-IN-1 in Sprayue Dawley Rats Model ^[1] . 272 ± 7.2 279 ± 78 1.5 ± 0.1	Time:Result:Showed the strongest inhibitory activity and reduced differentiation from 19.0 to 7.81%.Cell Migration Assay [1]Cell Line:HEK 293 T cells Concentration:Concentration:4,20,100,500, 2500,10000 nMIncubation Time:30 min Time:Result:Stabilized BRD4 BD2 at 50.4 °C.BET BD2-IN-1 (20 mg/kg for i.v; once daily for seven days) inhibits the protein expression of p-STAT3 and p- NF-KB in mouse skin tissues, effectively ameliorates the pathological changes in the psoriasis mouse model[1].BET BD2-IN-1 (20 mg/kg for i.v; once daily for seven days) significantly decreases the disease activity index (DAI) score in dextran sulfate sodium (DSS) induced IBD mouse model[1]. Pharmacokinetic Analysis of BET BD2-IN-1 in Sprague Dawley Rats Model[1]parameterAUC(08t) (ngh/mL)272 ± 72279 ± 781.5 ± 0.160 ± 2.0	Time:Result:Showed the strongest inhibitory activity and reduced differentiation from 19.0 to 7.81%.Cell Migration Assay [1]Cell Line:HEK 293 T cells Concentration: 4,20, 100, 500, 2500, 10000 nMIncubation Time:30 min Time: BD2 at 50.4 *C.BET BD2-IN-1 (20 mg/kg for i.v; once dially for seven days) inhibits the protein expression of p-STAT3 and p- NFi-kB in mouse skin tissues, effectively ameliorates the pathological changes in the psoriasis mouse model ^[1] . BET BD2-IN-1 (20 mg/kg for i.v; once daily for seven days) significantly decreases the disease activity index (DAI) score in dextran sulfate sodium (DSS) induced IBD mouse model ^[1] . Pharmacokinetic Analysis of BET BD2-IN-1 in Sprayue Dawley Rats Model ^[1] AUC(08t)C0 (ng/mL)272 ± 72279 ± 781.5 ± 0.160 ± 2.06.6 ± 0.8	Time:Result:Showed the strongest inhibitory activity and reduced differentiation from 19.0 to 7.81%.Cell Migration Assay (1)Cell Line:HEK 293 T cells Concentration: 4,20,100,500, 2500,1000 nMConcentration: Time:4,20,100,500, 2500,1000 nMIncubation Time: Result:30 min Time: BET BD2-1N-1 (20 mg/kg for iv; once daily for seven days) inhibits the profiein expression of p-STAT3 and p- NF-xB in mouse skin tissues, effectively ameliorates the pathological changes in the psoriasis mouse model ¹¹ . BET BD2-1N-1 (20 mg/kg for i.v; once daily for seven days) inhibits the profiein expression of p-STAT3 and p- NF-xB in mouse skin tissues, effectively ameliorates the pathological changes in the psoriasis mouse model ¹¹ . Pharmacokinetic Analysis of BET BD2-1N-1 in Spraysure Dawley Rats Model ^{[11} AUC(08t) parameterC0 (ng/mL)T1/2 (h)2722 T2279 ± 7815±0.10±2.06.6±0.8	Time:Image:Result:Showed the strongest inhibitory activity and reduced differentiation from 19.0 to 7.81%.Cell Migration Assay I ¹ Cell Line:MEK 293 T cellsConcentratio:4.20, 100, 500, 2500, 1000 nMIncubation30 minTime:\$tabilized BRD4 BD2 at 50.4 *C.BET BD2-IN-1 (2) mg/kg for i.v; once daily for seven days) inhibits the protein expression of p-STAT3 and p- NF-kB in mouse skin tissues, effectively ameliorates the pathological changes in the psoriasis mouse model ^[11] .BET BD2-IN-1 (2) org/kg for i.v; once daily for seven days) significantly decreases the disease activity index (DA) score in dextra sulfate sodium (DSS) induced IBD mouse model ^[12] .PT22 1279 T 7315 ± 0160 ± 206 ± 2026.5 ± 802

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

Animal Model:	Imiquimod (HY-B0180)-induced Psoriasis mouse model ^[1]
Dosage:	10 and 20 mg/kg
Administration:	Intravenous injection (i.v.) ; Once daily for seven days
Result:	Significantly alleviated the Imiquimod-induced skin lesions in a dose-dependent manner. Obviously reduced the enlarged spleen.
	Significantly decreased the expression of p-STAT3 and p-NF-κB in mouse skin tissues.
Animal Model:	DSS (HY-116282C)-induced IBD mouse model ^[1]
Dosage:	10 and 20 mg/kg
Administration:	Intravenous injection (i.v.) ; Once daily for seven days
	Intravenous injection (i.v.) ; Once daily for seven days Effectively prevented colon shortening.
Administration:	

REFERENCES

[1]. Wang Z, et al. Discovery of a Bromodomain and Extra Terminal Domain (BET) Inhibitor with the Selectivity for the Second Bromodomain (BD2) and the Capacity for the Treatment of Inflammatory Diseases. J Med Chem. 2023 Aug 10;66(15):10824-10848.

Caution: Product has not been fully validated for medical applications. For research use only.

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