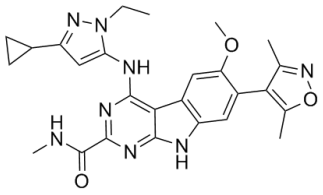
HJB97

Cat. No.:	HY-112429
CAS No.:	2093391-24-1
Molecular Formula:	$C_{26}H_{28}N_8O_3$
Molecular Weight:	500.55
Target:	Epigenetic Reader Domain
Pathway:	Epigenetics
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 30 mg/mL (**59.93 mM;** Need ultrasonic)
H_2O : < 0.1 mg/mL (insoluble)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9978 mL	9.9890 mL	19.9780 mL
	5 mM	0.3996 mL	1.9978 mL	3.9956 mL
	10 mM	0.1998 mL	0.9989 mL	1.9978 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 (4.99 mM); Clear solution
2. Add each solvent one by one: **10% DMSO >> 90% corn oil**
   Solubility: ≥ 2.5 mg/mL (4.99 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

HJB97 is a high-affinity **BET** inhibitor with **K_i**s of 0.9 nM (**BRD2 BD1**), 0.27 nM (**BRD2 BD2**), 0.18 nM (**BRD3 BD1**), 0.21 nM (**BRD3 BD2**), 0.5 nM (**BRD4 BD1**), 1.0 nM (**BRD4 BD2**), respectively. HJB97 is employed for the design of potential **PROTAC BET** degrader and has antitumor activity[1].

IC_{50} & Target

BRD2 BD1 0.9±0.2 nM (Ki)	BRD2 BD2 0.27±0.09 nM (Ki)	BRD3 BD1 0.18±0.01 nM (Ki)	BRD3 BD2 0.21±0.03 nM (Ki)
BRD4 BD1	BRD4 BD2	BRD2 BD1	BRD2 BD2

	0.5±0.2 nM (Ki)	1.0±0.1 nM (Ki)	3.1±0.7 nM (IC_{50})	3.9±0.5 nM (IC_{50})
	BRD3 BD1 6.6±0.2 nM (IC_{50})	BRD3 BD2 1.9±0.4 nM (IC_{50})	BRD4 BD1 7.0±0.6 nM (IC_{50})	BRD4 BD2 7.0±0.1 nM (IC_{50})

In Vitro

HJB97 is a highly potent and efficacious bomodomain and extra terminal (BET) inhibitor with IC_{50}s of 3.1 nM (BRD2 BD1), 3.9 nM (BRD2 BD2), 6.6 nM (BRD3 BD1), 1.9 nM (BRD3 BD2), 7.0 nM (BRD4 BD1), 7.0 nM (BRD4 BD2)[1].

HJB97 (10-1000 nM, 4 days) potently inhibits cell growth in RS4;11 and MOLM-13 acute leukemia cell lines with IC_{50}s of 24.1 nM and 25.6 nM[1].

HJB97 can effectively down-regulate the level of c-Myc at concentrations of 300-1000 nM in the RS4;11 cell line (treated for 24 h)[1].

Cell Viability Assay[1]

Cell Line:	The human acute leukemia RS4;11 cell line; The human acute leukemia MOLM-13 cell line
Concentration:	10-1000 nM
Incubation Time:	4 days
Result:	Achieved IC_{50}s value of 24.1±5.3 nM and 25.6±1.9 nM in inhibition of the RS4;11 cell and MOLM-13 cell growth.

Western Blot Analysis[1]

Cell Line:	RS4;11 cells
Concentration:	30, 100, 300, 1000 nM
Incubation Time:	24 h
Result:	Down-regulated the level of c-Myc but at concentrations of 300-1000 nM in the RS4;11 cell line.

REFERENCES

[1]. Zhou B, et al. Discovery of a Small-Molecule Degrader of Bromodomain and Extra-Terminal (BET) Proteins with Picomolar Cellular Potencies and Capable of Achieving Tumor Regression. J Med Chem. 2018 Jan 25;61(2):462-481.

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