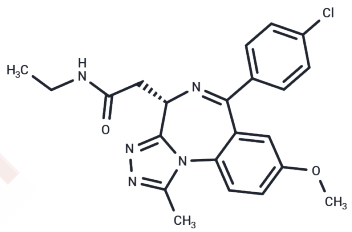
Data Sheet (Cat.No.T1906)

TargetMol

Molibresib

Chemical Properties



CAS No. : 1260907-17-2

Formula: C22H22ClN5O2

Molecular Weight: 423.9

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Molibresib (GSK525762) is an inhibitor of BET proteins (IC50: about 35 nM).
Targets(IC50)	Epigenetic Reader Domain
In vitro	At day 2 of differentiation, I-BET-762 treatment altered cytokine production in CD4+ T cells, up-regulating the expression of some anti-inflammatory gene products and down-regulating the expression of some pro-inflammatory cytokines.I-BET-762 inhibited the binding of bromodomain and additional terminal domain proteins and BRD2/3/4 to the tandem bromodomain of the BET (Kd: 50.5-61.3 nM). In FRET analysis, displacement of the BET tandem bromodomain a tetraacetylated H4 peptide (IC50: 32.5-42.5 nM).
In vivo	At day 2 of differentiation, I-BET-762 treatment altered cytokine production in CD4+ T cells, up-regulating the expression of some anti-inflammatory gene products and down-regulating the expression of some pro-inflammatory cytokines.I-BET-762 inhibited the binding of bromodomain and additional terminal domain proteins and BRD2/3/4 to the tandem bromodomain of the BET (Kd: 50.5-61.3 nM). In FRET analysis, displacement of the BET tandem bromodomain a tetraacetylated H4 peptide (IC50: 32.5-42.5 nM).
Kinase Assay	Fluorescence resonance energy transfer (FRET) titrations: Fluorescence resonance energy transfer (FRET) titrations. I-BET is titrated against BRD2 (200 nM), BRD3 (100 nM) and BRD4 (50 nM) in 50 mM HEPES pH7.5, 50 mM NaCl, 0.5 mM CHAPS in the presence of tetra-acetylated Histone H4 peptide (200 nM). After equilibrating for 1 hour, the bromodomain protein : peptide interaction is detected using FRET following the addition of 2 nM Europium cryptate labelled streptavidin and 10 nM XL-665-labelled anti-6His antibody in assay buffer containing 0.05% (v/v) BSA and 400 mM KF. Plates are read using an Envision Plate reader (excitation 320 nm, emission 615 nm and 665 nm).
Cell Research	CD4+ T cells are isolated from lymph nodes and spleens of 10- to 12-wk old mice and activated with plate bound anti-CD3 and anti-CD28 antibodies in the presence of indicated cytokines. I-BET-762 compounds is included during the 60–72 h of initial activation. Over the course of 5 d of T-cell culture and expansion, the compounds is diluted 12-fold relative to the starting concentrations.(Only for Reference)

Solubility Information

Solubility	Ethanol: 39 mg/mL (92 mM),Sonication is recommended. H2O: < 1 mg/mL (insoluble or slightly soluble), DMSO: 250 mg/mL (589.76 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Saline: < 10 mg/mL (23.59 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+40% PEG300+5% Tween 80+45% Saline: 10 mg/mL (23.59 mM),Solution. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.359 mL	11.7952 mL	23.5905 mL
5 mM	0.4718 mL	2.359 mL	4.7181 mL
10 mM	0.2359 mL	1.1795 mL	2.359 mL
50 mM	0.0472 mL	0.2359 mL	0.4718 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Nicodeme E, et al. Nature, 2010, 468(7327), 1119-1123.
Bandukwala HS, et al. PNAS, 2012, 109(36), 14532-14537.