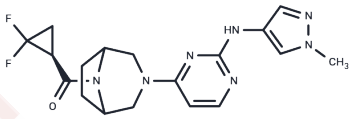
Data Sheet (Cat.No.TQ0010)

TargetMol

Brepocitinib

Chemical Properties



CAS No. : 1883299-62-4

Formula: C18H21F2N7O

Molecular Weight: 389.4

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	Brepocitinib (PF-06700841) is a potent dual JAK1/TYK2 inhibitor with IC50 values of 17 nM and 23 nM, respectively, and also inhibits JAK2 and JAK3 with IC50 values of 77 nM and 6.49 μM.
Targets(IC50)	JAK,Tyrosine Kinases
In vitro	PF-06700841 inhibits TYK2/JAK2 mediated IL-12/pSTAT4 and IL-23/pSTAT3 (human whole blood IC50s: 65/120 nM). PF-06700841 inhibits the JAK1/JAK3 driven γ-common chain cytokines, represented by IL-15/pStat5 and IL-21/pSTAT3 with reasonable potency (IC50s: 238/204 nM). PF-06700841 also has good potency against IL6/pStat1 in the CD3+ cellular subset (IC50: 81 nM), but lower inhibition of IL6/pSTAT3, again in the CD3+ cellular subset (IC50: 641 nM). PF-06700841 inhibits EPO/pSTAT5 (JAK2 homodimer) in HWB spiked with CD34+ progenitor cells (IC50: 577 nM). IL10/pSTAT3 (TYK2/JAK1) and IL27/pSTAT3 (JAK1/JAK2/TYK2) are also inhibited by PF-06700841 (IC50s: 305 nM/86 nM).
In vivo	PF-06700841 (3-30 mg/kg; p.o; for 7 consecutive days; female Lewis rats) treatment significantly reduces paw volume increase in a dose-dependent manner. The plasma concentrations in animals dosed with PF-06700841 at peak (30 min) and trough (24 h) time intervals post final dose respectively are as follows: 3 mg/kg, 3.54 μM, 0.0221 μM; 10 mg/kg, 10.95 μM, 0.06 μM; and 30 mg/kg, 23.89 μM, 0.06 μM.

Solubility Information

Solubility	Ethanol: 75 mg/mL (192.6 mM),Sonication is recommended. DMSO: 150 mg/mL (385.21 mM),Sonication is recommended. H2O: Insoluble, (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.5681 mL	12.8403 mL	25.6805 mL
5 mM	0.5136 mL	2.5681 mL	5.1361 mL
10 mM	0.2568 mL	1.284 mL	2.5681 mL
50 mM	0.0514 mL	0.2568 mL	0.5136 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

Fensome A, et al. Dual Inhibition of TYK2 and JAK1 for the Treatment of Autoimmune Diseases: Discovery of ((S) -2,2-Difluorocyclopropyl)((1 R,5 S)-3-(2-((1-methyl-1 H-pyrazol-4-yl)amino)pyrimidin-4-yl)-3,8-diazabicyclo[3.2.1] octan-8-yl)methanone (PF-06700841). J Med Chem. 2018 Oct 11;61(19):8597-8612.