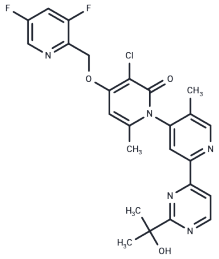
Data Sheet (Cat.No.T39126)

TargetMol

Zunsemetinib

Chemical Properties



CAS No. : 1640282-42-3

Formula: C25H22ClF2N5O3

Molecular Weight: 513.92

Storage: Store at low temperature
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	Zunsemetinib (ATI-450) is an orally active and selective inhibitor of the p38α mitogen-activated protein kinase-activated protein kinase 2 (MK2) pathway.Zunsemetinib is used to study spondyloarthritis and rheumatoid arthritis.
Targets(IC50)	MAPK
In vitro	Zunsemetinib selectively blocks p38α MAPK activation of the proinflammatory kinase MK2 while sparing p38α activation of other effectors such as PRAK and ATF2, and inhibits in vitro osteoclast formation induced by RANKL.[1] Zunsemetinib (1 and 10 μM; 1h) decreases IL-1β expression by promoting IL-1β mRNA degradation and has no effect on NLRP3 expression.[1] Zunsemetinib (0.4 nM~1 μM; 16h; PBMC cells) reduces IL-1β secretion and promotes IL-1β mRNA instability.[1]
In vivo	Zunsemetinib (1,000 ppm; p.o.; 8-week-old WT female mice) blocks LPS-induced TNF-α expression persisted for up to 4 weeks after dosing.[1] Zunsemetinib (10 and 20 mg/kg; p.o.) prevents osteopenia in NOM IDc mice through inhibition of osteoclastogenesis and increases bone density.[1]

Solubility Information

Solubility	DMSO: 80 mg/mL (155.67 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween-80+45% Saline: 3.3 mg/mL (6.42 mM),Sonication is recommended. *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	1.9458 mL	9.7291 mL	19.4583 mL
5 mM	0.3892 mL	1.9458 mL	3.8917 mL
10 mM	0.1946 mL	0.9729 mL	1.9458 mL
50 mM	0.0389 mL	0.1946 mL	0.3892 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

Zunsemetinib (ATI-450) – Investigational oral MK2 pathway inhibitor
Aclaris Therapeutics Announces ATI-450 (MK2 pathway Inhibitor) publication in Journal of Experimental Medicine
Wang C, et al. Selective inhibition of the p38α MAPK-MK2 axis inhibits inflammatory cues including inflammasome priming signals. J Exp Med. 2018;215(5):1315-1325.