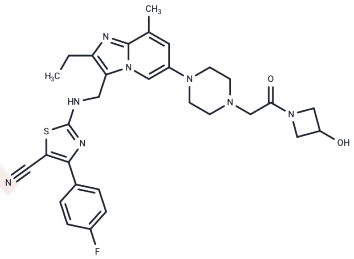
Data Sheet (Cat.No.T4041)

TargetMol

Ziritaxestat

Chemical Properties



CAS No. : 1628260-79-6

Formula: C30H33FN8O2S

Molecular Weight: 588.7

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	Ziritaxestat (GLPG1690), an autotaxin inhibitor, currently being evaluated in an exploratory phase 2 study in idiopathic pulmonary fibrosis patients.
Targets(IC50)	PDE
Kinase Assay	Glutaminase Inhibition: Cell Free Assay: Assay plates are prepared containing 2 μL test compound in DMSO/well. The enzyme is diluted to 1 unit (liver) or 0.8 unit (kidney)/100 μL in glutaminase assay buffer, and 100 μL diluted enzyme is added to each well of the assay plate by Multidrop. The contents are mixed by shaking at full speed for 1 min on TiterMix 100. The plates are preincubated at room temperature (RT) for 20 min to allow binding of test compounds to glutaminase, and 50 μL glutamine solution (7 mM in assay buffer) is added to each well by Multidrop. The contents are shaken at full speed for 30 sec on TiterMix 100, and the plates are then incubated at RT for 60 min (liver) or 90 min (kidney). To stop the reactions, 20 μL HCl (0.3 N) is added to each well by Multidrop and mixed immediately by shaking for 30 sec on TiterMix 100. For quantification, glutamate (formed by glutaminase-catalyzed hydrolysis of glutamine) is oxidized to 2-oxoglutarate by a second enzyme, glutamate dehydrogenase (GDH), with the concomitant production of the reduced form of nicotinamide adenine dinucleotide (NADH). Reduction of nitro blue tetrazolium (NBT) in the assay solution by NADH, catalyzed by phenazine methosulphate (PMS), results in the formation of a blue-purple formazan. The absorption of formazan at 540 nm is linearly proportional to the concentration of glutamate up to 200 μM. NBT/GDH reagent (50 μL) is added to each well by Multidrop and mixed by shaking for 30 sec on TiterMix 100, and the plates are incubated at RT for 20 min to allow color formation by the GDH reaction. Glutamate concentration is determined from formazan concentration as determined by reading OD540 nm on a SpectraMax 340.

Solubility Information

Solubility	H2O: < 0.1 mg/mL (insoluble), DMSO: 50 mg/mL (84.93 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.6987 mL	8.4933 mL	16.9866 mL
5 mM	0.3397 mL	1.6987 mL	3.3973 mL
10 mM	0.1699 mL	0.8493 mL	1.6987 mL
50 mM	0.034 mL	0.1699 mL	0.3397 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.

Reference

Desroy N., et al. Discovery of 2-[[2-Ethyl-6-[4-[2-(3-hydroxyazetidin-1-yl)-2-oxoethyl]piperazin-1-yl]-8-methylimidazo[1,2-a]pyridin-3-yl]methylamino]-4-(4-fluorophenyl)thiazole-5-carbonitrile (GLPG1690), a First-in-Class Autotaxin Inhibitor Undergoing Clinicalal Evaluation for the Treatment of Idiopathic PulmoN/Ary Fibrosis. J Med Chem. 2017 May 11;60(9):3580-3590.

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Chen J, Guan Z, Dong N, et al. A novel LC-MS/MS method for the determination of ziritaxestat in rat plasma and its pharmacokinetic study. Biomedical Chromatography. 2020: e4863.

Balupuri A., et al. Design, synthesis, docking and biological evaluation of 4-phenyl-thiazole derivatives as autotaxin (ATX) inhibitors. Bioorg Med Chem Lett. 2017 Jul 16. pii: S0960-894X(17)30718-7.

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Hu Y, Li L, Tian Y, et al.Design, synthesis and evaluation of novel UDCA-aminopyrimidine hybrids as ATX inhibitors for the treatment of hepatic and pulmonary fibrosis.European Journal of Medicinal Chemistry.2023: 116029.

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