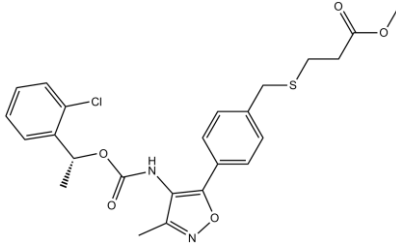


Product Data Sheet

Chemical Properties

Product Name:	Ki16198	
Cas No.:	355025-13-7	
M.Wt:	488.98	
Formula:	C ₂₄ H ₂₅ ClN ₂ O ₅ S	
Chemical Name:	methyl 3-[[4-[4-[1-(2-chlorophenyl)ethoxycarbonylamino]-3-methyl-1,2-oxazol-5-yl]phenyl]methylsulfanyl]propanoate	
Canonical SMILES:	CC1=NOC(=C1NC(=O)OC(C)C2=CC=CC=C2Cl)C3=CC=C(C=C3)CSCCC(=O)OC	
Solubility:	≥24.45mg/mL in DMSO	
Storage:	Store at -20°C	
General tips:	For obtaining a higher solubility , please warm the tube at 37° C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20° C for several months.	
Shopping Condition:	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request	

Biological Activity

Targets : GPCR/G protein

Pathways: LPA Receptor

Description:

Ki16198 is the methyl ester of Ki16425. Ki16198, a LPA antagonist, inhibits LPA1- and LPA3-induced inositol phosphate production with the Ki of 0.34 μM and 0.93 μM, respectively, shows weaker inhibition for LPA2, no activity at LPA4, LPA5, LPA6[1].

Lysophosphatidic acid (LPA) is an extracellular signaling lipid involved in regulating cell proliferation, survival, and motility of normal and cancer cells[2].

In vitro: In YAPC-PD cancer cell line, Ki16198 substantially inhibited LPA1- and LPA3-mediated

responses with low potency to LPA2 and no activity to LPA4, LPA5 and LPA6. Treatment with Ki16198 (10 μ M) effectively inhibited migration and invasion responses to LPA in YAPC-PD cancer cell line. Incubation of Ki16198 (10 μ M) inhibited the LPA-induced expression of proMMP-9 protein and mRNA in YAPC-PD cells [1]. Administration of Ki16198 (1 μ M) inhibited the proliferation of lpa1 Δ -1 and lpa1 Δ +1 cells by about 70% [2].

In vivo: In YAPC-PD pancreatic cancer cell-inoculated nude xenograft mouse model, Oral administration of Ki16198 (2 mg/kg) significantly inhibited tumor weight and remarkably attenuated invasion and metastasis to lung, liver, and brain and decreased the total metastatic node weight in the peritoneal cavity and ascites formation by 50% [1]. Oral administration of Ki16198 (60 mg/kg) significantly inhibited lactate-induced limb lesions in rats [3].

Reference:

[1]. Komachi M, Sato K, Tobo M, et al. Orally active lysophosphatidic acid receptor antagonist attenuates pancreatic cancer invasion and metastasis in vivo[J]. *Cancer science*, 2012, 103(6): 1099-1104.

[2]. Shano S, Hatanaka K, Ninose S, et al. A lysophosphatidic acid receptor lacking the PDZ-binding domain is constitutively active and stimulates cell proliferation[J]. *Biochimica et Biophysica Acta (BBA)-Molecular Cell Research*, 2008, 1783(5): 748-759.

[3]. Kimura T, Mogi C, Sato K, et al. p2y5/LPA6 attenuates LPA1-mediated VE-cadherin translocation and cell-cell dissociation through G12/13 protein-Src-Rap1[J]. *Cardiovascular research*, 2011: cvr154.

Protocol

Cell experiment:

Cell lines	YAPC-PD cells
Preparation method	The solubility of this compound in DMSO is > 24.5 mg/mL. General tips for obtaining a higher concentration: Please warm the tube at 37 °C for 10 minutes and/or shake it in the ultrasonic bath for a while. Stock solution can be stored below - 20 °C for several months.
Reacting conditions	
Applications	In YAPC-PD cells, Ki16198 inhibited LPA-mediated migration and invasion. Moreover, Ki16198 inhibited LPA-induced expression of proMMP-9 protein and mRNA.

Animal experiment [3]:

Animal models	Mice bearing YAPC-PD xenografts
Dosage form	2 mg/kg; p.o.

Applications	In mice bearing YAPC-PD xenografts, Ki16198 (2 mg/kg) substantially decreased the total metastatic node weight in the peritoneal cavity, as well as ascites formation by 50%.
Other notes	Please test the solubility of all compounds indoor, and the actual solubility may slightly differ with the theoretical value. This is caused by an experimental system error and it is normal.

Reference:

[1]. Komachi M, Sato K, Tobo M, et al. Orally active lysophosphatidic acid receptor antagonist attenuates pancreatic cancer invasion and metastasis in vivo[J]. Cancer science, 2012, 103(6): 1099-1104.

Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most ApexBio products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Shortterm storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.

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