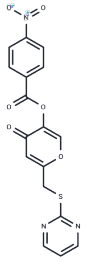
Data Sheet (Cat.No.T4390)

TargetMol

ML221

Chemical Properties



CAS No. : 877636-42-5

Formula: C17H11N3O6S

Molecular Weight: 385.35

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	ML221 is a potent apelin /APJ functional antagonist, inhibiting apelin-13-mediated activation of APJ, with IC50s of 0.70 μM in the cAMP assay, and 1.75 μM in the β-arrestin assay, and EC80 of 10 nM in both assays.
Targets(IC50)	Apelin receptor,Arrestin
In vitro	ML221 is a potent apelin/APJ functional antagonist, inhibiting apelin-13-mediated activation of APJ, with IC50s of 0.70 μM in the cAMP assay, and 1.75 μM in the β-arrestin assay, and EC80 of 10 nM in both assays. ML221 is >37-fold selective over the closely related angiotensin II type 1 (AT1) receptor (IC50, >79 μM) in cells. ML221 displays limited cross reactivity against a range of GPCRs except the κ-opioid and benzodiazepinone receptors (<50/<70%I at 10 μM)
Cell Research	ML221 is dissolved in DMSO. Cells (angiotensin II receptor-like 1 (AGTRL-1) cell line) are seeded at 1000 cell/well (1536 plate) in 4 μL and grown overnight (16-18 h) at 37°C, 5% CO2, 100% humidity, then 60 nL of either DMSO control or 2 mM stock test compounds (ML221, etc.) in DMSO are transferred to each well, followed by 2 μL of 30 nM Apelin-13 to negative control and test compound wells, and 2 μL of assay media (F12 nutrient mix HAMs supplemented with 10% hi-FBS, 1× penicillin/streptomycin) to positive control wells. This yields a final concentration of test compound (ML221, etc.) of 20 μM and 1% final DMSO. Assay is incubated for 90 min at room temperature, and then developed with 3 μL of detection reagent for 60 min and luminescence read on a ViewLux. They are for reference only.

Solubility Information

Solubility	DMSO: 6.25 mg/mL (16.22 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: 1.09 mg/mL (2.83 mM),Suspension. 10% DMSO+90% Saline: < 1.09 mg/mL (2.83 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. *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	2.595 mL	12.9752 mL	25.9504 mL
5 mM	0.519 mL	2.595 mL	5.1901 mL
10 mM	0.2595 mL	1.2975 mL	2.595 mL
50 mM	0.0519 mL	0.2595 mL	0.519 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

Maloney PR, etal. Discovery of 4-oxo-6-((pyrimidin-2-ylthio)methyl)-4H-pyran-3-yl 4-nitrobenzoate (ML221) as a functional antagonist of the apelin (APJ) receptor. Bioorg Med Chem Lett. 2012 Nov 1;22(21):6656-60.
Xiong M, Chen H, Fan Y, et al.Tubular Elabela-APJ axis attenuates ischemia-reperfusion induced acute kidney injury and the following AKI-CKD transition by protecting renal microcirculation.Theranostics.2023, 13(10): 3387.
Ye L, Huang Y, Liu X, et al.Apelin/APJ system protects placental trophoblasts from hypoxia-induced oxidative stress through activating PI3K/Akt signaling pathway in preeclampsia.Free Radical Biology and Medicine.2023