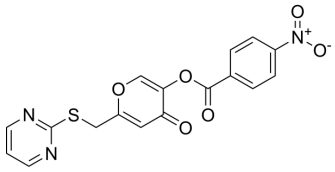
ML221

Cat. No.:	HY-103254
CAS No.:	877636-42-5
Molecular Formula:	$C_{17}H_{11}N_3O_6S$
Molecular Weight:	385.35
Target:	Arrestin; Apelin Receptor (APJ)
Pathway:	GPCR/G Protein
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 31 mg/mL (80.45 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.5950 mL	12.9752 mL	25.9504 mL
	5 mM	0.5190 mL	2.5950 mL	5.1901 mL
	10 mM	0.2595 mL	1.2975 mL	2.5950 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2 mg/mL (5.19 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ML221 is a potent apelin (APJ) functional antagonist, inhibiting apelin-13-mediated activation of APJ, with IC_{50}s of 0.70 μM in the cAMP assay, and 1.75 μM in the β-arrestin assay, and EC_{80} of 10 nM in both assays.

IC_{50} & Target

IC50: 1.75 μM (APJ, cell-based)[1]

In Vitro

ML221 is a potent apelin/APJ functional antagonist, inhibiting apelin-13-mediated activation of APJ, with IC_{50}s of 0.70 μM in the cAMP assay, and 1.75 μM in the β-arrestin assay, and EC_{80} of 10 nM in both assays. ML221 is >37-fold selective over the closely related angiotensin II type 1 (AT1) receptor (IC_{50}, >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)[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Cell Assay [1]

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% CO_2, 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 μ L 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[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Eur J Pharmacol. 2021, 174149.
- Neuropharmacology. 2022 Aug 27;109235.
- Stem Cells Int. 2022 Mar 21;2022:3742678.
- Oxid Med Cell Longev. 2021 Jan 27.
- Research Square Preprint. 2020 Jul.

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REFERENCES

[1]. Maloney PR, et al. 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.

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