ML241 hydrochloride

Cat. No.: HY-19797A

CAS No.: 2070015-13-1

Molecular Formula: $C_{23}H_{25}ClN_4O$

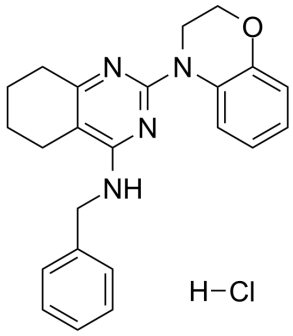
Molecular Weight: 408.92

Target: p97

Pathway: Cell Cycle/DNA Damage

Storage: 4°C, sealed storage, away from moisture

* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 34 mg/mL (83.15 mM)

H_2O : < 0.1 mg/mL (ultrasonic;warming;heat to 60°C) (insoluble)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Concentration \ Solvent \ Mass	1 mg	5 mg	10 mg
1 mM	2.4455 mL	12.2273 mL	24.4547 mL
5 mM	0.4891 mL	2.4455 mL	4.8909 mL
10 mM	0.2445 mL	1.2227 mL	2.4455 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (6.11 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.11 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.11 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ML241 hydrochloride is a potent p97 inhibitor, inhibiting p97 ATPase with IC_{50} value of 100 nM.

IC_{50} & Target

IC50: 100 nM (p97)[1]

In Vitro

ML241 hydrochloride is a potent p97 inhibitor, inhibiting p97 ATPase with IC_{50} values of 100 nM. ML241 inhibits p97 competitively with respect to ATP with a K_i values of 0.35 μM. ML241 (20 μM) shows no obvious inhibition of the appr 170 kinases tested. ML241 stabilizes Ub^{G76V}-GFP with IC_{50} of 3.5 μM[1]. ML241 is cytotoxic to HCT15 and SW403 cells, with GI_{50}s

of 53 and 33 μM after treatment for 24 h, and 13 and 12 μM after treatment for 72 h, respectively[2].

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

PROTOCOL

Cell Assay [2]

HeLa cells stably expressing ODD-luciferase are seeded onto a 96-well white solid bottom plate (5000 cells/well) and cells are grown for 16 h. Cells are treated with DMEM containing MG132 (4 μM) for 1h and washed with 100 μL PBS twice. DMEM containing 2.5% FBS, cycloheximide (50 μg/mL) and ML241 are added into the well. Four 96-well plates are prepared and one of the plates is taken out from incubator at each time point (70, 90, 120, or 150 min). Luciferin (50 μL of 1 mg/mL in PBS) is added into each well containing 50 μL of medium and incubated at room temperature with shaking at 500 rpm for 5 min. Luminescence intensity is determined with 0.1 ms integration time on the Synergy HT Microplate Reader[2].

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

REFERENCES

[1]. Chou TF, et al. Structure-activity relationship study reveals ML240 and ML241 as potent and selective inhibitors of p97 ATPase. ChemMedChem. 2013 Feb;8(2):297-312.

[2]. Chou TF, et al. Selective, reversible inhibitors of the AAA ATPase p97. Probe Reports from the NIH Molecular Libraries Program. April 14, 2011.

Caution: Product has not been fully validated for medical applications. For research use only.

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