ZZW-115 hydrochloride

Cat. No.: HY-111838A

CAS No.: 10122-45-9

Molecular Formula: $C_{24}H_{34}Cl_3F_3N_4S$

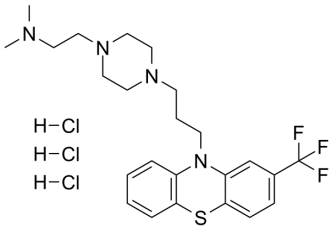
Molecular Weight: 573.97

Target: Apoptosis

Pathway: Apoptosis

Storage: 4°C, stored under nitrogen

* In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 83.33 mg/mL (145.18 mM; Need ultrasonic)

H_2O : 60 mg/mL (104.54 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.7423 mL	8.7113 mL	17.4225 mL
5 mM	0.3485 mL	1.7423 mL	3.4845 mL
10 mM	0.1742 mL	0.8711 mL	1.7423 mL

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

In Vivo

1. Add each solvent one by one: PBS
   Solubility: 50 mg/mL (87.11 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 6.25 mg/mL (10.89 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 6.25 mg/mL (10.89 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ZZW-115 hydrochloride is a potent NUPR1 inhibitor, with a K_d of 2.1 μM. ZZW-115 hydrochloride induces tumor cell death by necroptosis and apoptosis. Anticancer activity[1][2].

In Vitro

ZZW-115 hydrochloride (0.1-33 μM; 72 hours) is efficient in killing cancer cells, with an IC_{50} in the range of 0.84 μM (ANOR) to 4.93 μM (HN14)[1].

ZZW-115 hydrochloride (0-100 μM; 24-72 hours) is efficient to kill these tumor cells with an IC_{50} in the range of 0.42 μM (Hep2G cells) to 7.75 μM (SaOS-2 cells)[1].

ZZW-115 hydrochloride induces pancreatic cell death by necrosis and apoptosis. ZZW-115 hydrochloride treatment induces

a decrease in ATP production and induces a ROS overproduction[1].
LDH release is significantly higher in ZZW-115 hydrochloride-treated cells (MiaPaCa-2, 02-063, LIPC, Foie8b, and HN14 cells) than in control cells in a concentration-dependent manner. Similarly, caspase 3/7 activity is also greater in ZZW-115 hydrochloride-treated cells. These experiments demonstrated that ZZW-115 hydrochloride exerted both pronecrotic and proapoptotic effects[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[1]

Cell Line:	ANOR cells, MiaPaCa-2, 02-063, 01008, LIPC, 02136, HN01,01046, AOIPC, Foie8b, HN14 cells
Concentration:	0.1- 33 μM
Incubation Time:	72 hours
Result:	Was efficient in killing cancer cells, with an IC_{50} in the range of 0.84 μM (ANOR) to 4.93 μM (HN14).

Cell Proliferation Assay[1]

Cell Line:	U87, A375, U2OS, SaOS-2, HT29, SK-CO-1, LS174T, H1299 and H358, HepG2, PC3, THP-1, Daudi, Jurkat and MDA-MB-231 cells
Concentration:	0-100 μM
Incubation Time:	24 or 72 hours
Result:	Was efficient to kill these tumor cells with an IC_{50} in the range of 0.42 μM (Hep2G cells) to 7.75 μM (SaOS-2 cells).

In Vivo

ZZW-115 hydrochloride (0.5-5 mg/kg; injection; daily for 30 days) inhibits the growth of pancreatic xenografted tumors[1].
ZZW-115 hydrochloride (5 mg/kg for 30 days; immunocompetent C57BL/6 mice were orthotopically implanted with Panc02 cells) treatment shows the tumor size is almost unmeasurable in some cases[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	NMRI-Foxn1nu/Foxn1nu mice (nude mice) xenografted with MiaPaCa-2 cells [1]
Dosage:	5, 2.5, 1.0, or 0.5 mg/kg
Administration:	Injection; daily for 30 days
Result:	When the mice were injected with 5 mg/kg ZZW-115 hydrochloride, the tumors stopped growing a few days after treatment and their size decreased progressively, almost disappearing at the end of the treatment.

CUSTOMER VALIDATION

- BMC Med. 2022 Oct 19;20(1):365.

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REFERENCES

[1]. Santofimia-Castaño P, et al. Ligand-based design identifies a potent NUPR1 inhibitor exerting anticancer activity via necroptosis. J Clin Invest. 2019;129(6):2500-2513. Published 2019 Mar 28.

[2]. Santofimia-Castaño P, et al. Targeting the Stress-Induced Protein NUPR1 to Treat Pancreatic Adenocarcinoma. Cells. 2019;8(11):1453. Published 2019 Nov 17.

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