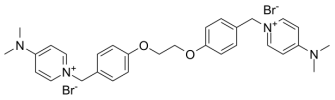
EB-3D

Cat. No.:	HY-115463
CAS No.:	1839150-63-8
Molecular Formula:	$C_{30}H_{36}Br_2N_4O_2$
Molecular Weight:	644.44
Target:	Apoptosis; AMPK
Pathway:	Apoptosis; Epigenetics; PI3K/Akt/mTOR
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 : 50 mg/mL (77.59 mM; Need ultrasonic)

H_2O : ≥ 9.09 mg/mL (14.11 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.5517 mL	7.7587 mL	15.5173 mL
5 mM	0.3103 mL	1.5517 mL	3.1035 mL
10 mM	0.1552 mL	0.7759 mL	1.5517 mL

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

BIOLOGICAL ACTIVITY

Description

EB-3D is a potent and selective choline kinase α (ChoKα) inhibitor, with an IC_{50} of 1 μM for ChoKα1. EB-3D exerts effects on ChoKα expression, AMPK activation, apoptosis, endoplasmic reticulum stress and lipid metabolism. EB-3D exhibits a potent antiproliferative activity in a panel of T-leukemia cell lines. Anti-cancer activity[1][2][3].

IC_{50} & Target

IC50: 1 μM; Kd: 0.7 μM[3]

In Vitro

EB-3D displays (0-100 μM; 72 hours) excellent antiproliferative activity against a wide cohort of T-leukemic cell lines, with GI GI_{50}s 13 values in the nanomolar range[1].

EB-3D (1.25-5μM; 24 hours) induced apoptosis in leukemia cell lines[1].

EB-3D (0.5-1 μM; 24 hours) induces a G0/G1 arrest that lead to apoptosis[1].

EB-3D (0.3 μM; 48 hours) shows a first spike of activation of AMPKα after 30 minutes and a later increase in the phosphorylation of T172[1].

EB-3D (1-40 μM; 48 hours) inhibits cell growth in HepG2 cells with a GI_{50} of 14.55 μM[2].

EB-3D induces deregulation of the AMPK-mTOR pathway and apoptosis in leukemia T-cells[1].

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

Cell Proliferation Assay[1]

Cell Line:	JURKAT, CCRF-CEM, HSB-2, MOLT-16, DNA-41, LOUCY, PEER, ALL-SIL cells
Concentration:	0.001, 0.01, 0.1, 1, 10, 100 μM
Incubation Time:	72 hours
Result:	Inhibited JURKAT, CCRF-CEM, HSB-2, MOLT-16, DNA-41, LOUCY, PEER, and ALL-SIL cells growth with GI_{50}s of 136.2, 478.8, 17.7, 0.9, 60.6, 200, 265, and 132 nM, respectively.

Apoptosis Analysis[1]

Cell Line:	Jurkat, CCRF-CEM and HSB-2 cells
Concentration:	1.25, 2.5, 5 μM
Incubation Time:	24 hours
Result:	Induced apoptosis in leukemia cell lines.

Cell Cycle Analysis[1]

Cell Line:	Jurkat, CCRF-CEM and HSB-2 cells
Concentration:	0.5, 1 μM
Incubation Time:	24 hours
Result:	Induces cell cycle arrest in G0/G1 phase.

Western Blot Analysis[1]

Cell Line:	Jurkat cells
Concentration:	0.3 μM
Incubation Time:	48 hours
Result:	Showed a first spike of activation of AMPKα after 30 minutes of treatment and a later increase in the phosphorylation of T172. The increase in S79 phosphorylation of its main target ACC (acetyl-coenzyme A (CoA) carboxylase), followed the same pattern. This rapid activation of AMPK, in turn induced a consequent reduction in mTOR phosphorylation that is visible already at 30' and that becomes amplified at longer time probably due to the interruption of feedback loops that are characteristic of mTOR connecting pathways.

In Vivo

EB-3D (1 mg/kg; i.p.; every other day) impairs mammary tumor growth in syngeneic orthotopic E0771-C57BL/6 mouse model [4].

EB-3D (2.5 mg/kg; every other day for 4 weeks) shows a reduction of the number of spontaneous lung macro- and micrometastasis[4].

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

Animal Model:	E0771-C57BL/6 mice[4]
Dosage:	I.p.; every other day for 4 weeks
Administration:	2.5 mg/kg

Result:	A reduction of the number of spontaneous lung macro- and micrometastasis.

CUSTOMER VALIDATION

- J Lipid Res. 2022 Apr 18;100213.

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REFERENCES

[1]. Mariotto E, et al. EB-3D a novel choline kinase inhibitor induces deregulation of the AMPK-mTOR pathway and apoptosis in leukemia T-cells. Biochem Pharmacol. 2018 Sep;155:213-223.

[2]. Sola-Leyva A, et al. Choline kinase inhibitors EB-3D and EB-3P interferes with lipid homeostasis in HepG2 cells. Sci Rep. 2019 Mar 25;9(1):5109.

[3]. Schiaffino-Ortega S, et al. Design, synthesis, crystallization and biological evaluation of new symmetrical biscationic compounds as selective inhibitors of human Choline Kinase α1 (ChoKα1).

[4]. Mariotto E, et al. Choline Kinase Alpha Inhibition by EB-3D Triggers Cellular Senescence, Reduces Tumor Growth and Metastatic Dissemination in Breast Cancer. Cancers (Basel). 2018;10(10):391. Published 2018 Oct 22.

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