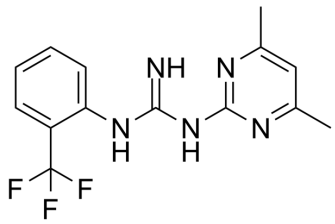
ZINC69391

Cat. No.:	HY-102078
CAS No.:	303094-67-9
Molecular Formula:	$C_{14}H_{14}F_3N_5$
Molecular Weight:	309.29
Target:	Ras; Apoptosis
Pathway:	GPCR/G Protein; MAPK/ERK Pathway; Apoptosis
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 25 mg/mL (80.83 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.2332 mL	16.1661 mL	32.3321 mL
	5 mM	0.6466 mL	3.2332 mL	6.4664 mL
	10 mM	0.3233 mL	1.6166 mL	3.2332 mL

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

BIOLOGICAL ACTIVITY

Description

ZINC69391, a specific Rac1 inhibitor, interferes with Rac1-GEF interaction by masking Trp56 residue on Rac1 surface. ZINC69391 interferes with the interaction of Rac1 with Dock180 and reduces Rac1-GTP levels. ZINC69391 induces apoptosis, and shows antiproliferative and antimetastatic effects[1][2][3].

In Vitro

ZINC69391 inhibits growth of U937, HL-60, KG1A and Jurkat cells with IC_{50}s ranging from 41 to 54 μM[1].
ZINC69391 (50-100 μM; 24 hours) augments the enzymatic activity of caspase 3 in a concentration dependent manner[1].
ZINC69391 (0-125 μM; 72h) reduces cell proliferation of human glioma cells[2].
ZINC69391 (50-100 μM; 48 hours) triggers cell cycle arrest[2].
ZINC69391 (50 μM; 24 hours) triggers apoptosis on human acute leukemic cells[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Proliferation Assay[2]

Cell Line:	U-87 MG, LN229 cells
Concentration:	0-125μM

Incubation Time:	72 hours
Result:	Reduced cell proliferation in a concentration-dependent manner.

Cell Cycle Analysis[2]

Cell Line:	LN229 cells
Concentration:	50, 100 μM
Incubation Time:	48 hours
Result:	Resulted in a significant increased percentage of cells in the sub-G0/G1 phase in a concentration dependent manner.

Apoptosis Analysis[1]

Cell Line:	HL-60, U937 and KG1A cell lines
Concentration:	50 μM
Incubation Time:	24 hours
Result:	Led to a significant increase in apoptotic cells.

In Vivo

ZINC69391 (25 mg/kg; i.p; daily for 21 days) impairs metastatic lung colonization in a syngeneic animal model[3].

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Animal Model:	Specific pathogen-free female BALB/c inbred mice (bearing F3II cells)[3]
Dosage:	25 mg/kg body weight
Administration:	I.p; daily for 21 days
Result:	Significantly reduced by about 60% the formation of total metastatic lung colonies.

CUSTOMER VALIDATION

- Cell Rep. 2023 Aug 12;42(8):112969.

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REFERENCES

[1]. Cabrera M, et al. Pharmacological Rac1 inhibitors with selective apoptotic activity in human acute leukemic cell lines. Oncotarget. 2017;8(58):98509-98523. Published 2017 Oct 4.

[2]. Cardama GA, et al. Proapoptotic and antiinvasive activity of Rac1 small molecule inhibitors on malignant glioma cells. Onco Targets Ther. 2014;7:2021-2033. Published 2014 Oct 30.

[3]. Cardama GA, et al. Preclinical development of novel Rac1-GEF signaling inhibitors using a rational design approach in highly aggressive breast cancer cell lines. Anticancer Agents Med Chem. 2014;14(6):840-851.

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

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