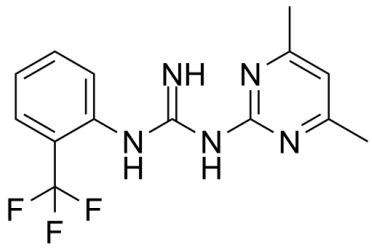
Data Sheet

Product Name:	ZINC69391
Cat. No.:	CS-0022957
CAS No.:	303094-67-9
Molecular Formula:	$C_{14}H_{14}F_3N_5$
Molecular Weight:	309.29
Target:	Apoptosis; Ras
Pathway:	Apoptosis; GPCR/G Protein
Solubility:	10 mM in DMSO



BIOLOGICAL ACTIVITY:

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

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.

CAIndexNames:

Guanidine, N-(4,6-dimethyl-2-pyrimidinyl)-N'-[2-(trifluoromethyl)phenyl]-

SMILES:

N=C(NC1=CC=CC=C1C(F)(F)F)NC2=NC(C)=CC(C)=N2

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

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